SUPPORTING INFORMATION

Competition Between the Donor and Acceptor Hydrogen Bonds of the Threads in the Formation of [2]Rotaxane by Clipping Reaction

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CONTENTS

1. Supramolecular Cluster for diamide 8c and 9c

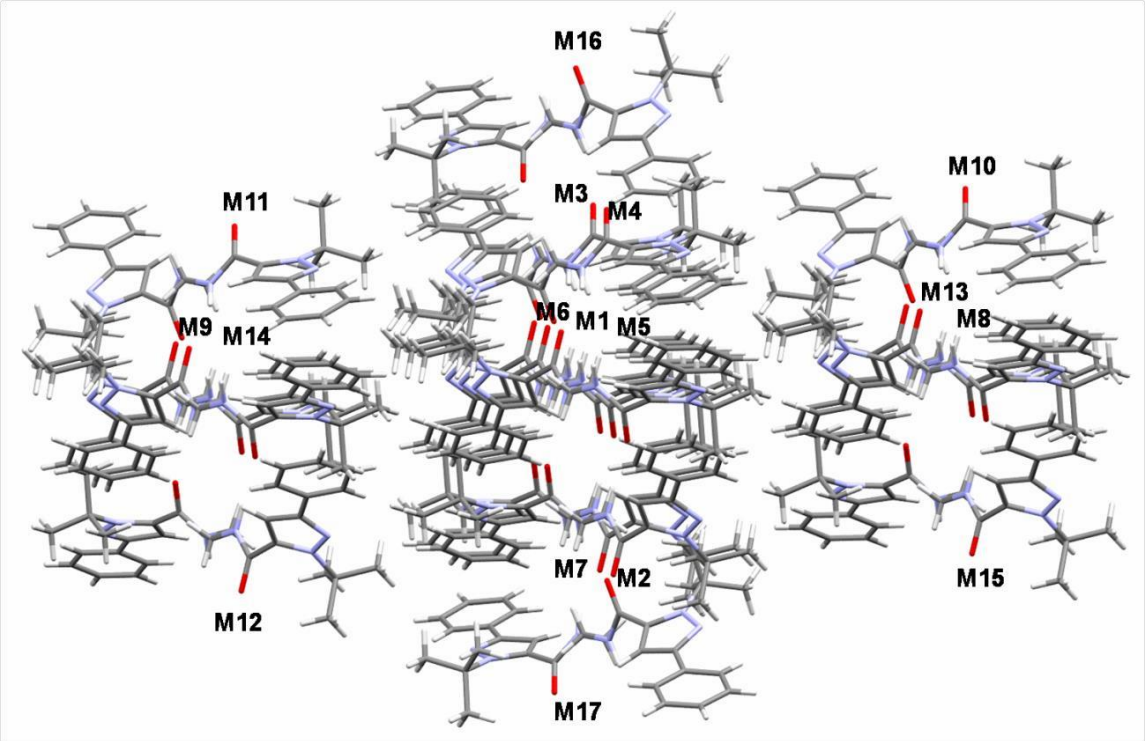


Figure S1 Supramolecula Cluster os *1',5'*-isomer **8c**. (NCM 16) ·

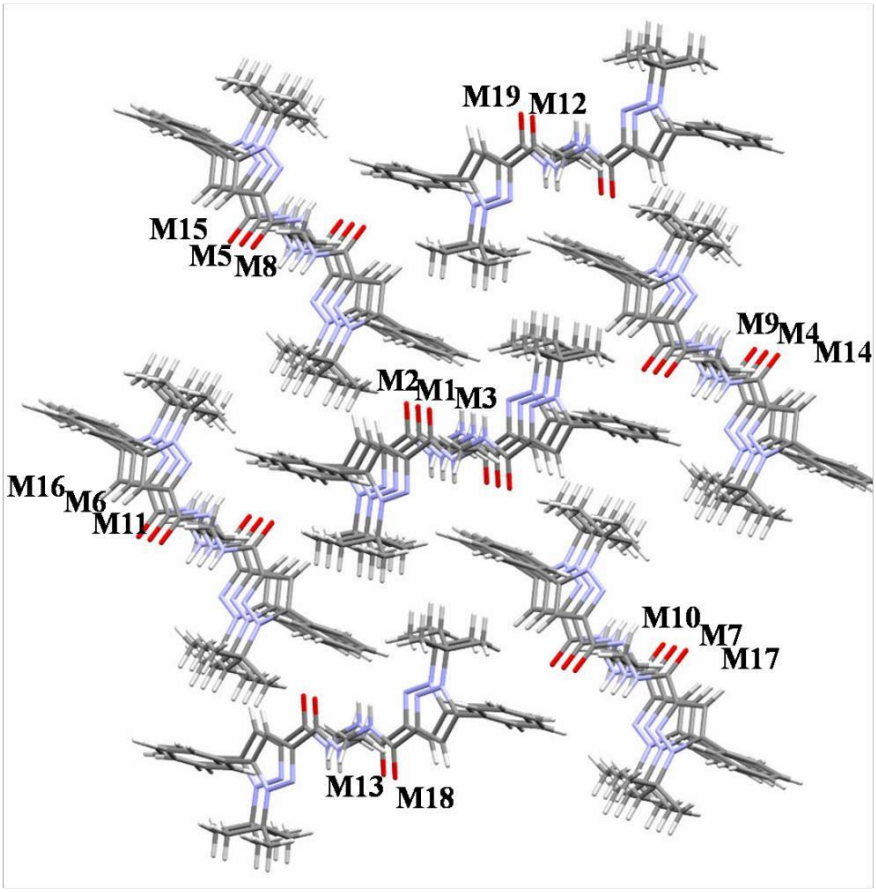


Figure S2 Supramolecular Cluster of *1',3'*-isomer **9c**. (MCN 18).

Table S1. Energy of the dimers present in the clusters of compounds **8c** and **9c**, with and BSSE correction.

Dimer	**8c**	**9c**
	$G_{M1\cdots MN}$ [a]	$G_{M1\cdots MN}$ [a]
M1···M2	-31.76	-20.31
M1···M3	-21.76	-20.31
M1···M4	-21.76	-8.09
M1···M5	-9.53	-8.08
M1···M6	-9.53	-8.06
M1···M7	-4.29	-8.06
M1···M8	-3.18	-7.61
M1···M9	-3.18	-7.61
M1···M10	-3.04	-7.59
M1···M11	-3.04	-7.59
M1···M12	-2.16	-2.49
M1···M13	-2.13	-2.49
M1···M14	-2.13	-1.76
M1···M15	-1.63	-1.76
M1···M16	-0.89	-1.74
M1···M17	-0.89	-1.74
M1···M18	-	-0.52
M1···M19	-	-0.52
$G_{cluster}$	-120.89	-116.34

[a] The Cluster was determined using software TOPOS Pro®. Energy was obtained from equation $G_{M1\cdots Mn} = (G_{M1\cdots Mn} - G_{M1} + G_{Mn})$, the energies (kcal·mol^{-1}) were determined using density functional theory (DFT) at the ωB97X-D/cc-pVDZ level of theory, with BSSE correction.

2. Data of Symmetry code

Table S2. Data of Symmetry code

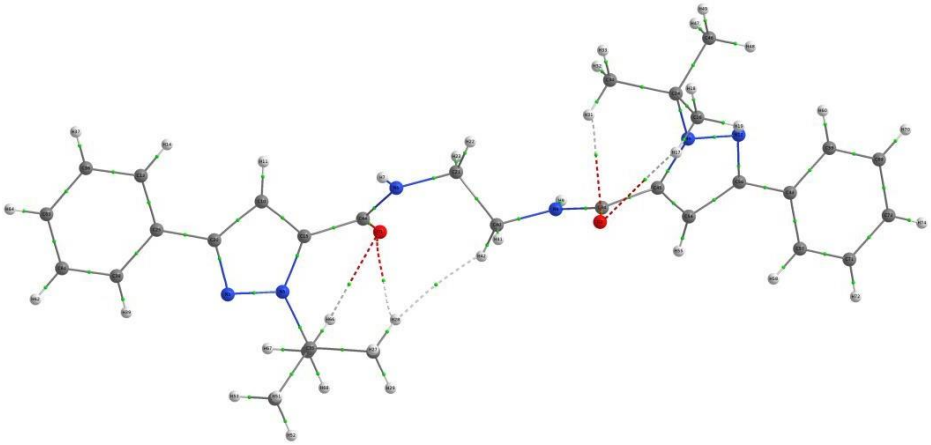
Dimer	**8c**	**9c**
M1	x,y,z	x,y,z
M2	1-x,-y,1-z	-1+x,y,z
M3	-1/2+x,1/2-y,z	1+x,y,z
M4	1/2+x,1/2-y,z	1+x,1/2-y,1/2+z
M5	1+x,y,z	-1+x,1/2-y,-1/2+z
M6	-1+x,y,z	-1+x,1.5-y,-1/2+z
M7	-x,-y,1-z	1+x,1.5-y,1/2+z
M8	1+x,y,-1+z	x,1/2-y,-1/2+z
M9	-1+x,y,1+z	x,1/2-y,1/2+z
M10	1/2+x,1/2-y,-1+z	x,1.5-y,1/2+z
M11	-1/2+x,1/2-y,1+z	x,1.5-y,-1/2+z
M12	-x,-y,2-z	2+x,-1+y,z
M13	x,y,-1+z	-2+x,1+y,z
M14	x,y,1+z	2+x,1/2-y,1/2+z
M15	1-x,-y,-z	-2+x,1/2-y,-1/2+z
M16	1/2-x, 1/2+y,1-z	-2+x,1.5-y,-1/2+z
M17	1/2-x, -1/2+y,1-z	2+x,1.5-y,1/2+z
M18	-	-1+x,1+y,z
M19	-	1+x,-1+y,z

3. QTAIM DATA

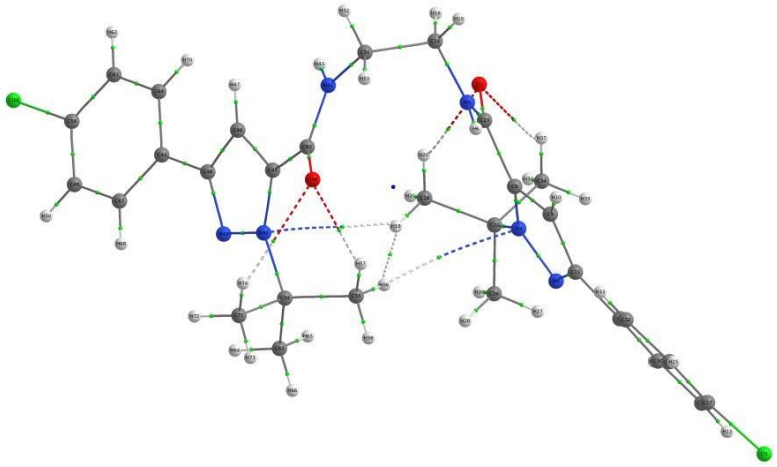
Table S3. The ρ_{int} (from QTAIM)[a] for M1 for compound **8c**, **8e** and **9c**

Compound	Interaction	ρ_{int} (a.u.)	ε	K	V	G	H[b]
8c	H···H	0,004137	0,86477	-0,000943	-0,002319	0,003261	0,000942
	CH···O	0,008091	0,140544	-0,000683	-0,00559	0,006272	0,000682
	CH···O	0,011758	0,096129	-0,000464	-0,008565	0,009029	0,000464
	CH···O	0,01312	0,951453	-0,001449	-0,009068	0,010517	0,001449
	CH···O	0,013736	0,725149	-0,001676	-0,0095	0,011176	0,001676
8e	H···H	0,003253	0,688689	-0,001002	-0,001531	0,002533	0,001002
	H···H	0,003253	0,688563	-0,001002	-0,001531	0,002533	0,001002
	CH···π	0,013684	0,628516	-0,001835	-0,008224	0,010059	0,001835
	CH···π	0,013684	0,628565	-0,001835	-0,008224	0,010059	0,001835
9c	H···H	0.003253	0.688689	-0.001002	-0.001531	0.002533	0.001002
	H···H	0.003253	0.688563	-0.001002	-0.001531	0.002533	0.001002
	CH···π	0.013684	0.628516	-0.001835	-0.008224	0.010059	0.001835
	CH···π	0.013684	0.628565	-0.001835	-0.008224	0.010059	0.001835

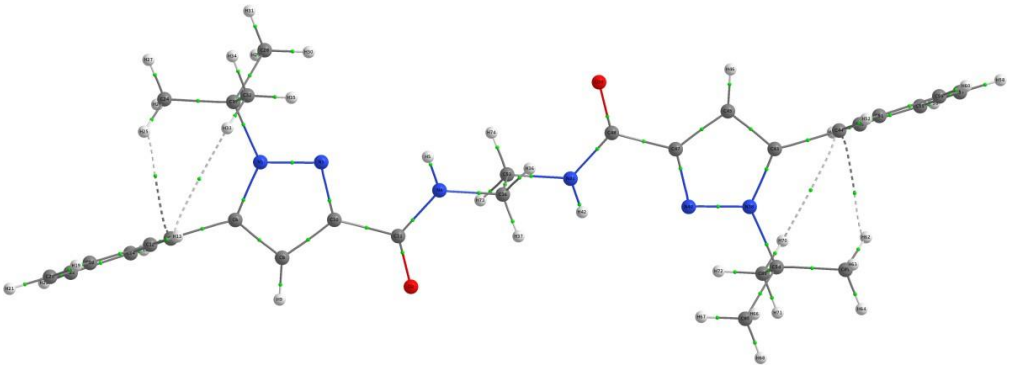
[a] Quantum Theory of Atoms in Molecules;. [b] *H*=G+V.



8c



8e



9c

Figure S3. View of all BCPs intramolecular connecting atoms in compound **8c**, **8e** and **9c**.

Table S4. The ρ_{int} (from QTAIM)[a] and atom interaction energy (G_{AI})[b] for dimer M1···M2 compound **8c**

Dimer	Interaction	ρ_{int} (a.u.)	G_{AI} (X···Y)[b]	ε	K	V	G	H[c]
M1···M2	H···H	0.001842	-0.65	1.1501400	-0.000616	-0.000766	0.001381	0.000615
	H···H	0.001842	-0.65	1.1516290	-0.000616	-0.000766	0.001381	0.000615
	π···π	0.001939	-0.69	0.3934430	-0.000213	-0.000825	0.001039	0.000214
	π···π	0.001939	-0.69	0.3933650	-0.000213	-0.000825	0.001039	0.000214
	H···H	0.002251	-0.80	0.6625010	-0.000672	-0.000898	0.00157	0.000672
	H···H	0.002251	-0.80	0.6624960	-0.000672	-0.000898	0.00157	0.000672
	CH···π	0.002884	-1.02	1.2623780	-0.000602	-0.001303	0.001905	0.000602
	CH···π	0.002884	-1.02	1.2606510	-0.000602	-0.001303	0.001905	0.000602
	CH···N	0.003655	-1.29	1.8737470	-0.000642	-0.002244	0.002886	0.000642
	CH···N	0.003655	-1.29	1.8755620	-0.000642	-0.002244	0.002886	0.000642
	π···π	0.004766	-1.69	0.8385970	-0.00037	-0.002084	0.002454	0.00037
	π···π	0.004766	-1.69	0.8388790	-0.00037	-0.002084	0.002454	0.00037
	π···π	0.006184	-2.19	1.0793410	-0.000575	-0.002533	0.003108	0.000575
	π···π	0.006184	-2.19	1.0793410	-0.000575	-0.002533	0.003108	0.000575
	NH···O	0.021389	-7.56	0.0428830	-0.002248	-0.016909	0.019158	0.002249
	NH···O	0.021390	-7.56	0.0428790	-0.002248	-0.01691	0.019158	0.002248
		0.089821	-31.76					

[a] Quantum Theory of Atoms in Molecules; [b] Interaction Energy (G_{AI}(X···Y) in kcal·mol^{-1}. [c] *H*=G+V.

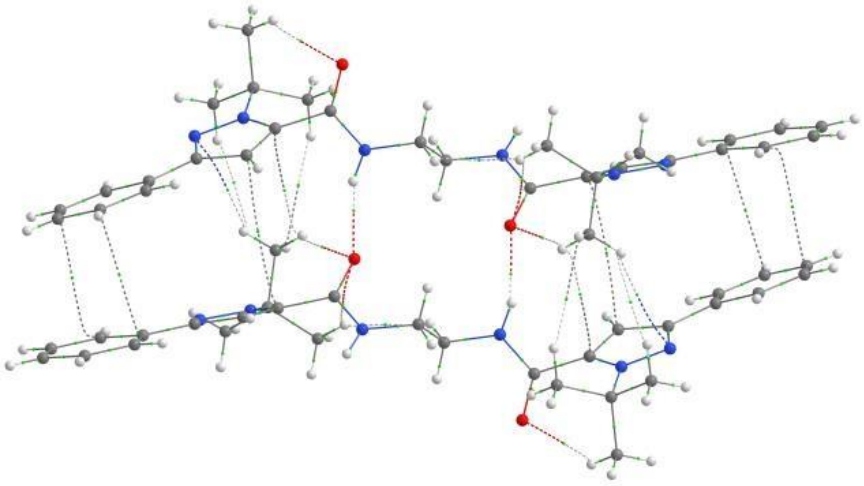


Figure S4. View of all BCPs connecting atoms in compound **8c** dimer M1···M2.

Table S5. The ρ_{int} (from QTAIM)[a] and atom interaction energy (G_{AI})[b] for dimers M1···M2 and M1···M3, compound **9c.**

Dimer	Interaction	ρ_{int} (a.u.)	G_{AI} (X···Y)[b]	ε	K	V	G	H[c]
	H···H	0.000527	-0.27	1,059064	-0,000149	-0,000171	0,000320	0,000149
	H···H	0.000527	-0.27	1,059230	-0,000149	-0,000171	0,000320	0,000149
	H···H	0.001933	-0.99	1,470751	-0,000636	-0,000775	0,001412	0,000637
M1···M2	H···H	0.001933	-0.99	1,470212	-0,000636	-0,000775	0,001412	0,000637
M1···M3	CH···N	0.003154	-1.62	0,649756	-0,000667	-0,001604	0,002271	0,000667
	CH···N	0.003154	-1.62	0,650081	-0,000667	-0,001604	0,002271	0,000667
	CH···N	0.004303	-2.21	1,471154	-0,000521	-0,002772	0,003294	0,000522
	CH···N	0.004303	-2.21	1,470985	-0,000521	-0,002772	0,003294	0,000522
	π_{hole}···π	0.004647	-2.38	2,690644	-0,000520	-0,002391	0,002912	0,000521
	π_{hole}···π	0.004648	-2.38	2,684677	-0,000520	-0,002392	0,002912	0,000520
	CH···π	0.005241	-2.69	0,131289	-0,000914	-0,002414	0,003328	0,000914
	CH···π	0.005241	-2.69	0,131431	-0,000914	-0,002414	0,003329	0,000915
Total		0.039611	-20.31					

[a] Quantum Theory of Atoms in Molecules; [b] Interaction Energy (G_{AI}(X···Y) in kcal.mol^{-1}. [c] *H*=G+V.

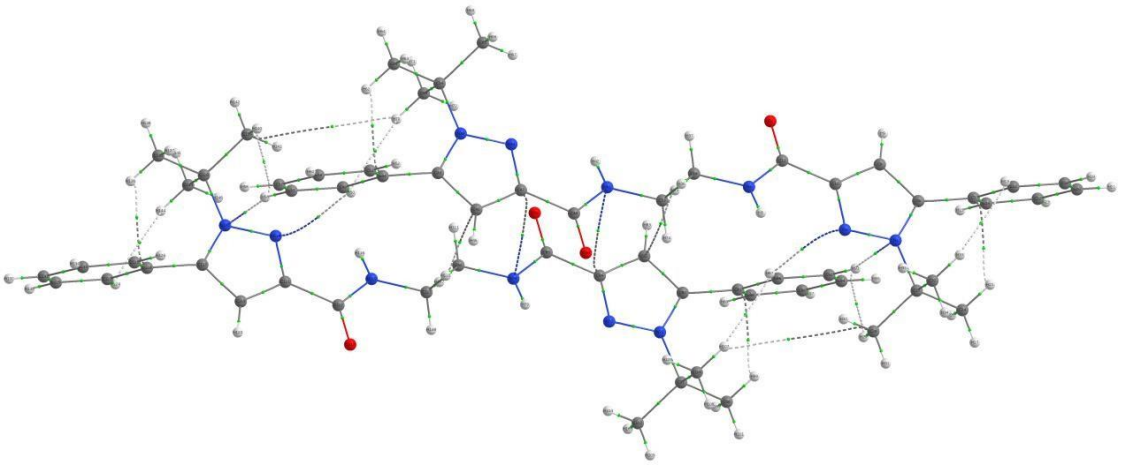


Figure S5 View of all BCPs connecting atoms in compound **9c**, dimers M1···M2/M1···M3.

Table S6. The ρ_{int} (from QTAIM)[a] and atom interaction energy (G_{AI})[b] for M1 compound **10e**.

Dimer	Interaction	ρ_{int} (a.u.)	GAI (X···Y)[b]	**ε**	**K**	**V**	**G**	**H**[c]
	H···H	0.001747	-0.50	0.374563	-0.000457	-0.000779	0.001237	0.000458
	H···H	0.001747	-0.50	0.374556	-0.000457	-0.000779	0.001237	0.000458
	H···H	0.00231	-0.66	0.172171	-0.00052	-0.001082	0.001602	0.00052
	H···H	0.002311	-0.66	0.172167	-0.00052	-0.001082	0.001602	0.00052
	LP···π	0.003608	-1.03	1.724326	-0.000631	-0.001733	0.002365	0.000632
	LP···π	0.003608	-1.03	1.724577	-0.000631	-0.001733	0.002365	0.000632
	H···H	0.003758	-1.07	0.457246	-0.000945	-0.001729	0.002674	0.000945
	H···H	0.003758	-1.07	0.457185	-0.000945	-0.001729	0.002674	0.000945
	CH···π	0.004052	-1.16	1.115506	-0.000701	-0.001712	0.002413	0.000701
	CH···π	0.004052	-1.16	1.114974	-0.000701	-0.001712	0.002413	0.000701
	CH···O	0.004241	-1.21	0.537987	-0.000914	-0.002293	0.003208	0.000915
	CH···O	0.004241	-1.21	0.538017	-0.000914	-0.002294	0.003208	0.000914
	CH···N	0.00556	-1.59	0.116791	-0.000942	-0.002605	0.003547	0.000942
M1	CH···N	0.00556	-1.59	0.116829	-0.000942	-0.002605	0.003547	0.000942
	π···π	0.005668	-1.62	0.50615	-0.001073	-0.00229	0.003363	0.001073
	π···π	0.005668	-1.62	0.505946	-0.001073	-0.00229	0.003363	0.001073
	LP···π	0.005728	-1.63	0.447718	-0.001099	-0.003028	0.004126	0.001098
	LP···π	0.005728	-1.63	0.447963	-0.001099	-0.003028	0.004127	0.001099
	CH···O	0.005902	-1.68	0.156475	-0.001092	-0.003104	0.004197	0.001093
	CH···O	0.005902	-1.68	0.156474	-0.001092	-0.003104	0.004197	0.001093
	CH···O	0.007067	-2.02	0.018825	-0.001215	-0.003882	0.005097	0.001215
	CH···O	0.007067	-2.02	0.018835	-0.001215	-0.003882	0.005098	0.001216
	NH···π	0.007232	-2.06	0.927983	-0.001287	-0.003468	0.004755	0.001287
	NH···π	0.007232	-2.06	0.92788	-0.001287	-0.003469	0.004756	0.001287
	NH···O	0.019672	-5.61	0.087888	-0.003153	-0.015459	0.018612	0.003153
	NH···O	0.019672	-5.61	0.087879	-0.003153	-0.015459	0.018612	0.003153
	Total	0.153091	-43.69					

[a] Quantum Theory of Atoms in Molecules; [b] Interaction Energy (G_{AI}(X···Y) in kcal·mol^{-1}. [c] *H*=G+V.

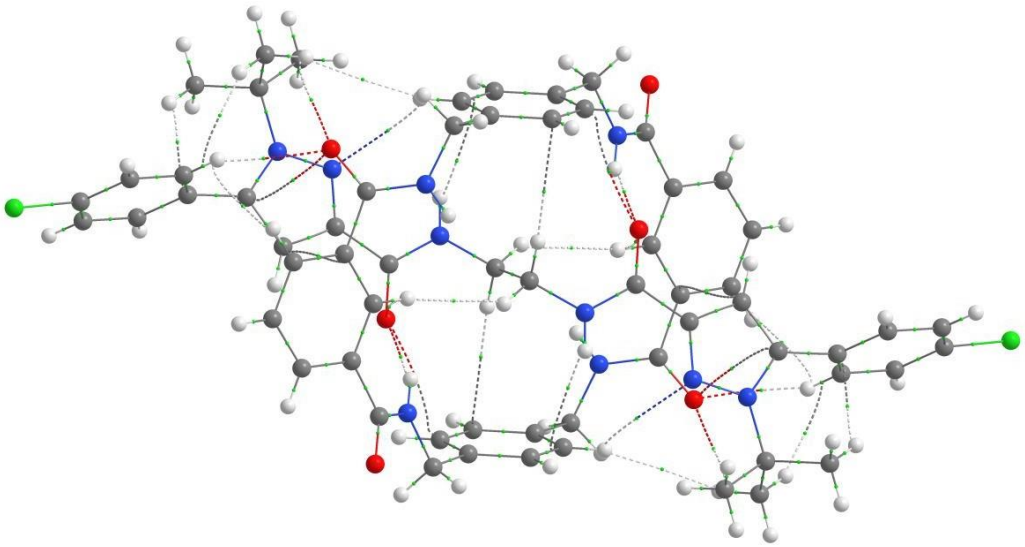


Figure S6. View of all BCPs connecting atoms in compound **10e**.

4. The ^{1}H NMR dilution and dilution curves

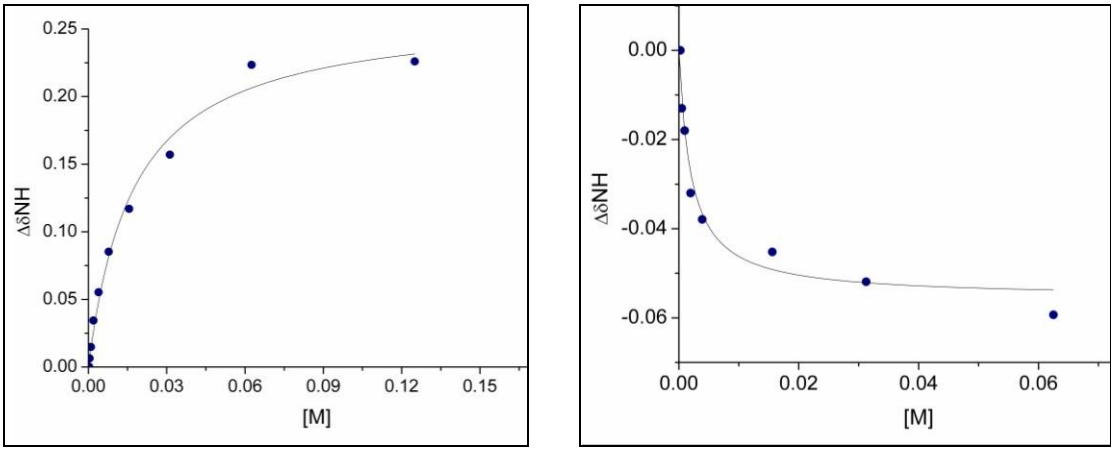


Figure S7: Diamide ^{1}H NMR chemical shift of at 25°C as function of concentration (M) in $CDCl_3$ **(a) 8e** (*1',5'*-isomer) and (b) **9e** (*1',3'*-isomer).

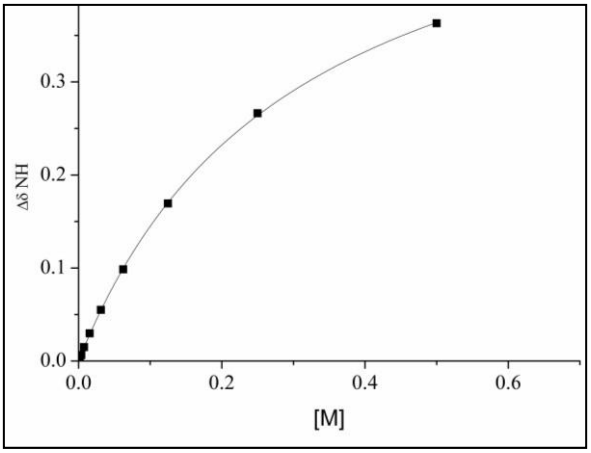


Figure S8. ^{1}H NMR chemical shift of at 25°C as function of concentration (M) in $CDCl_3$ *N*-benzylbenzamide.

4.1 ^{1}H NMR dilution hetero-assembly of compound 8c, 8e, 9c and 9e.

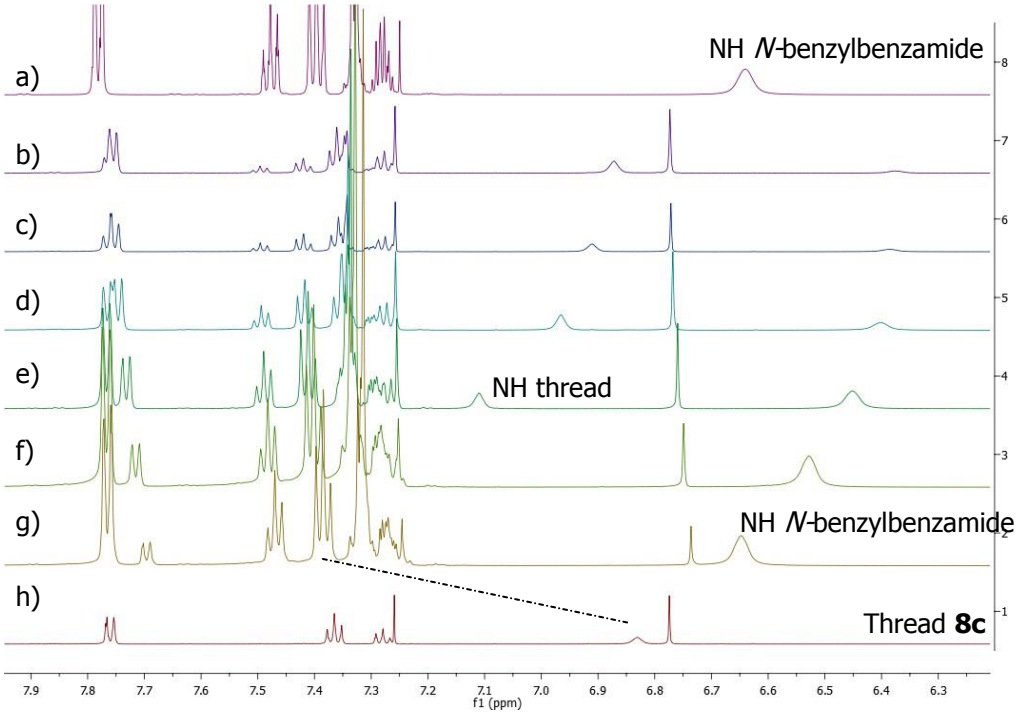


Figure S9. Thread **8c** (0.032 M) and *N*-benzylbenzamide ^{1}H NMR chemical shift of at 25°C as function of concentration (M) in $CDCl_3$: a) *N*-benzylbenzamide 0.25 M pure; mixture of thread **8c** (0.032M) and b) 0.0078 M *N*-benzylbenzamide; c) 0.0152 M *N*-benzylbenzamide; d) 0.03125 M *N*-benzylbenzamide; e) 0.0625 M *N*-benzylbenzamide; f) 0.125 M *N*-benzylbenzamide; g) 0.25 M *N*-benzylbenzamide; h) thread **8c** 0.0156 M pure.

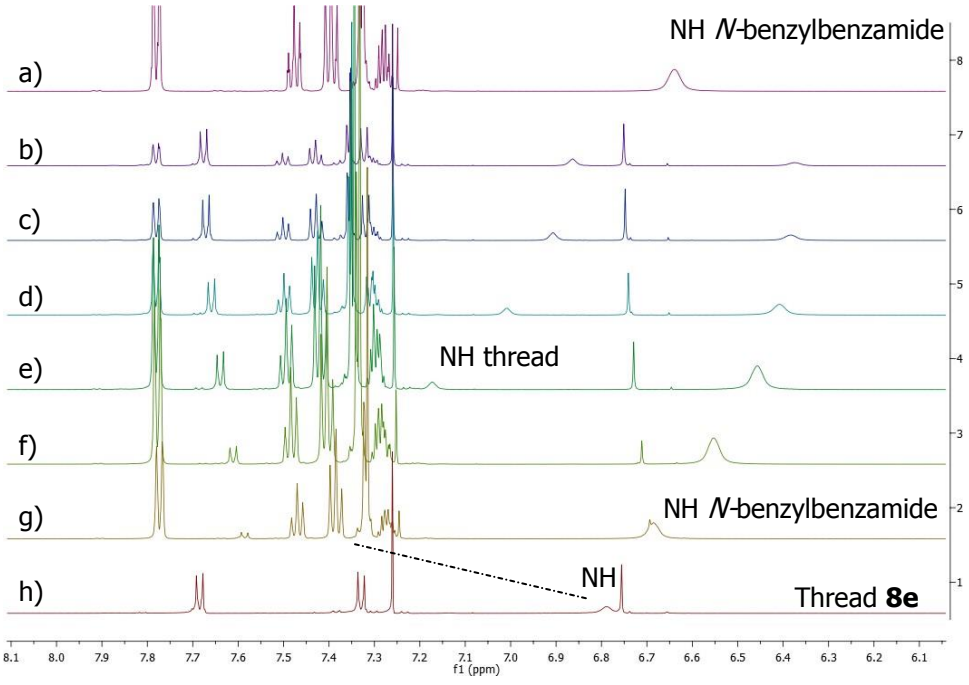


Figure S10. Thread **8e** (0.0156 M) and *N*-benzylbenzamide ^{1}H NMR chemical shift of at 25°C as function of concentration (M) in $CDCl_3$: a) *N*-benzylbenzamide 0.25 M pure; mixture of thread **8e** (0.0156M) and b) 0.0078 M *N*-benzylbenzamide; c) 0.0152 M *N*-benzylbenzamide;

d) 0.03125 M *N*-benzylbenzamide; e) 0.0625 M *N*-benzylbenzamide; f) 0.125 M *N*-benzylbenzamide; g) 0.25 M *N*-benzylbenzamide; h) Thread **8e** 0.0156 M pure.

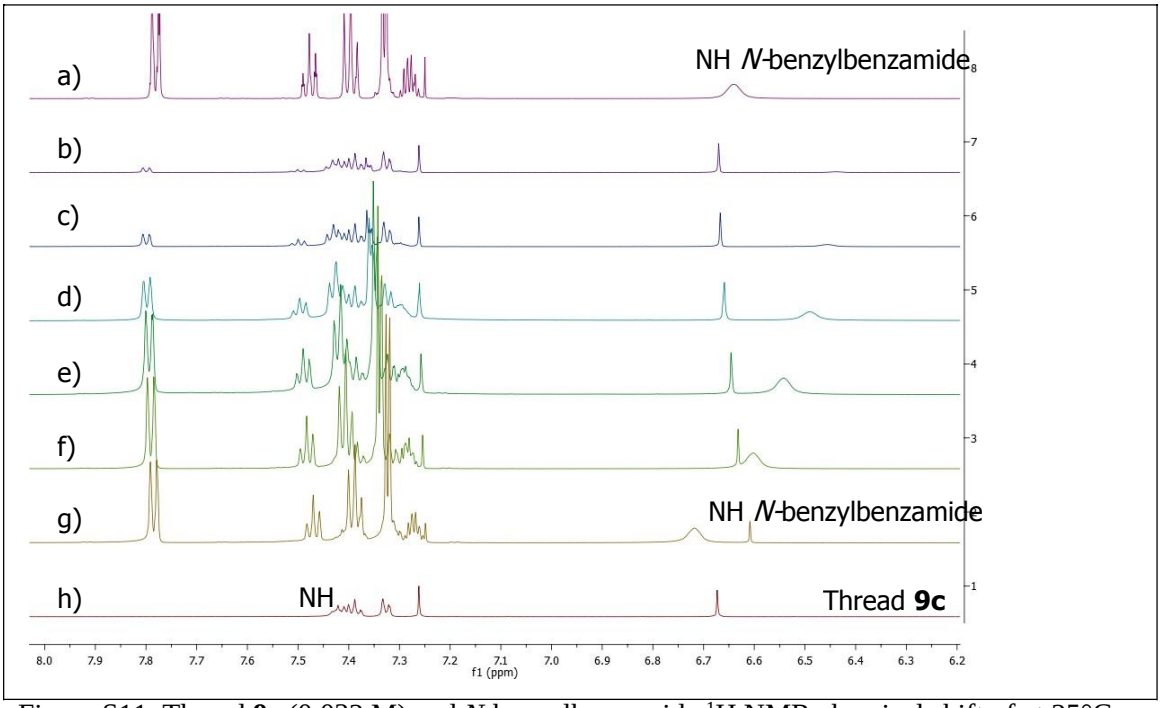


Figure S11. Thread **9c** (0.032 M) and *N*-benzylbenzamide ^{1}H NMR chemical shift of at 25°C as function of concentration (M) in $CDCl_3$: a) *N*-benzylbenzamide 0.25 M pure; mixture of thread **9c** (0.032M) and b) 0.0078 M *N*-benzylbenzamide; c) 0.0152 M *N*-benzylbenzamide; d) 0.03125 M *N*-benzylbenzamide; e) 0.0625 M *N*-benzylbenzamide; f) 0.125 M *N*-benzylbenzamide; g) 0.25 M *N*-benzylbenzamide; h) thread **9c** 0.0156 M pure.

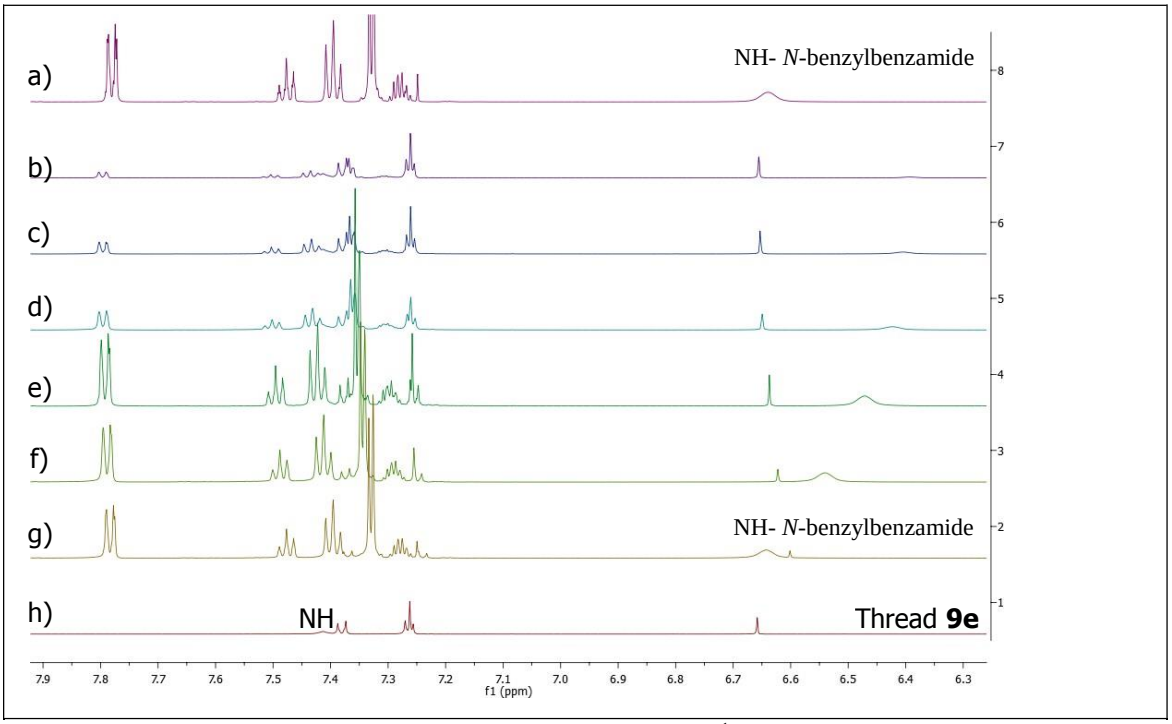


Figure S12. Thread **9e** (0.0156 M) and *N*-benzylbenzamide ^{1}H NMR chemical shift of at 25°C as function of concentration (M) in $CDCl_3$: a) *N*-benzylbenzamide 0.25 M pure; mixture of thread **9e** (0.0156M) and b) 0.0078 M *N*-benzylbenzamide; c) 0.0152 M *N*-benzylbenzamide; d)

0.03125 M *N*-benzylbenzamide; e) 0.0625 M *N*-benzylbenzamide; f) 0.125 M *N*-benzylbenzamide; g) 0.25 M *N*-benzylbenzamide; h) Thread **9e** 0.0156 M pure.

5. ^{1}H and ^{13}C NMR spectra, Mass spectra, IR and Thermogravimetric analysis

5.1. ^{1}H and ^{13}C NMR spectra.

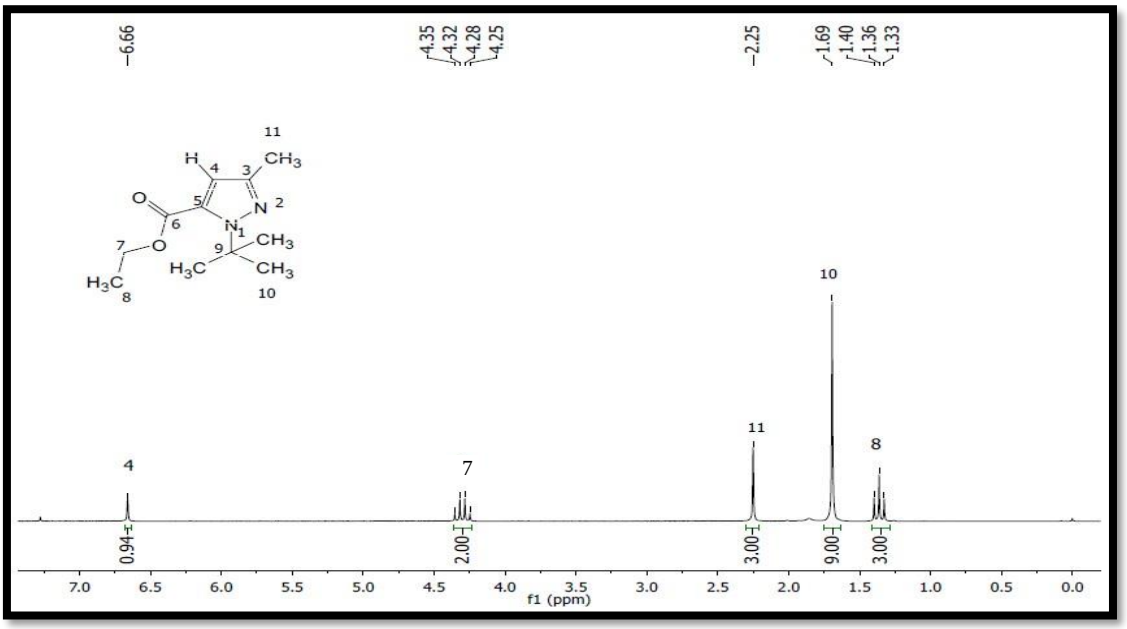


Figure S13: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **3a**.

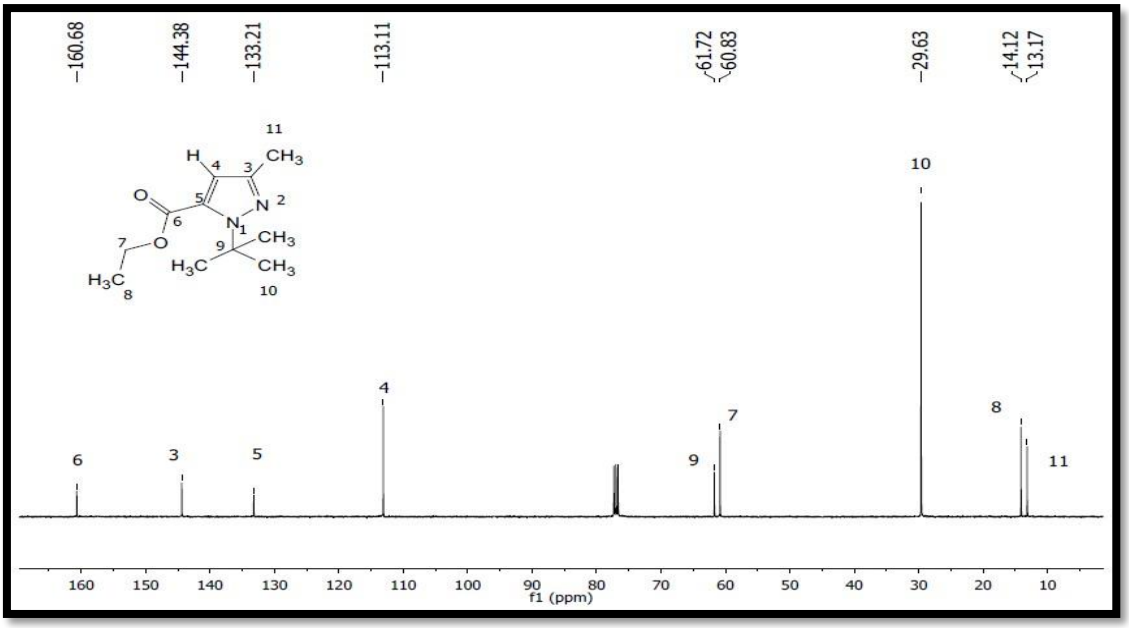


Figure S14: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **3a**.

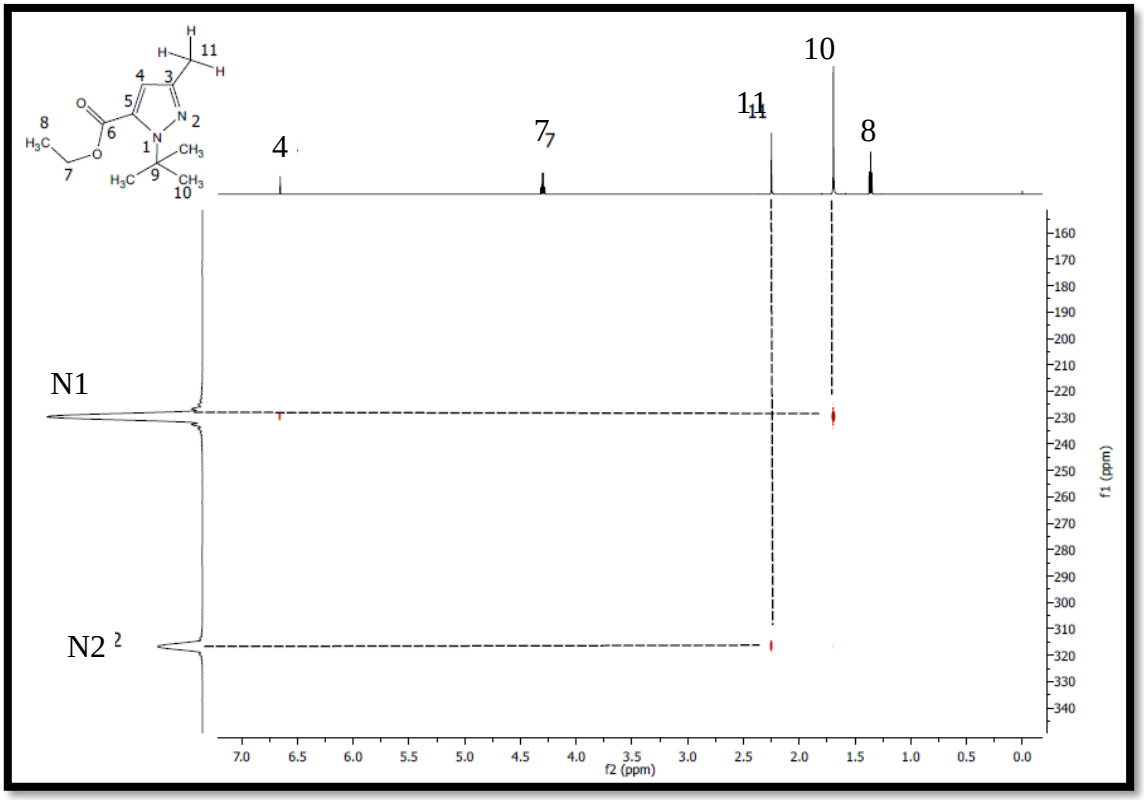


Figure S15. ^{15}N-^{1}H HMBC (600 MHz, $CDCl_3$) spectrum of **3a.**

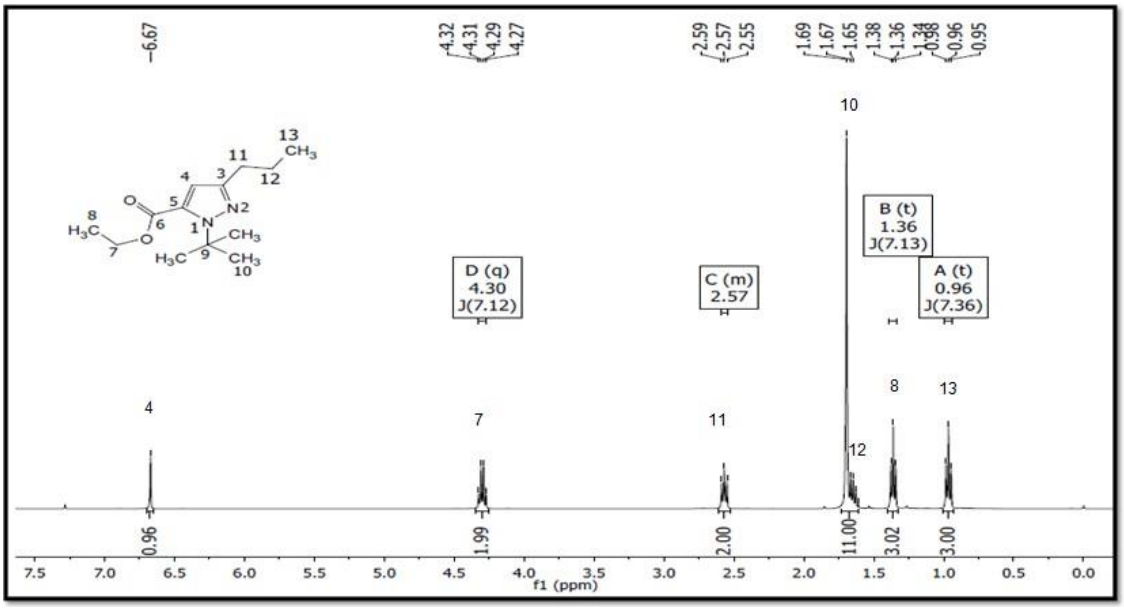


Figure S16: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **3b.**

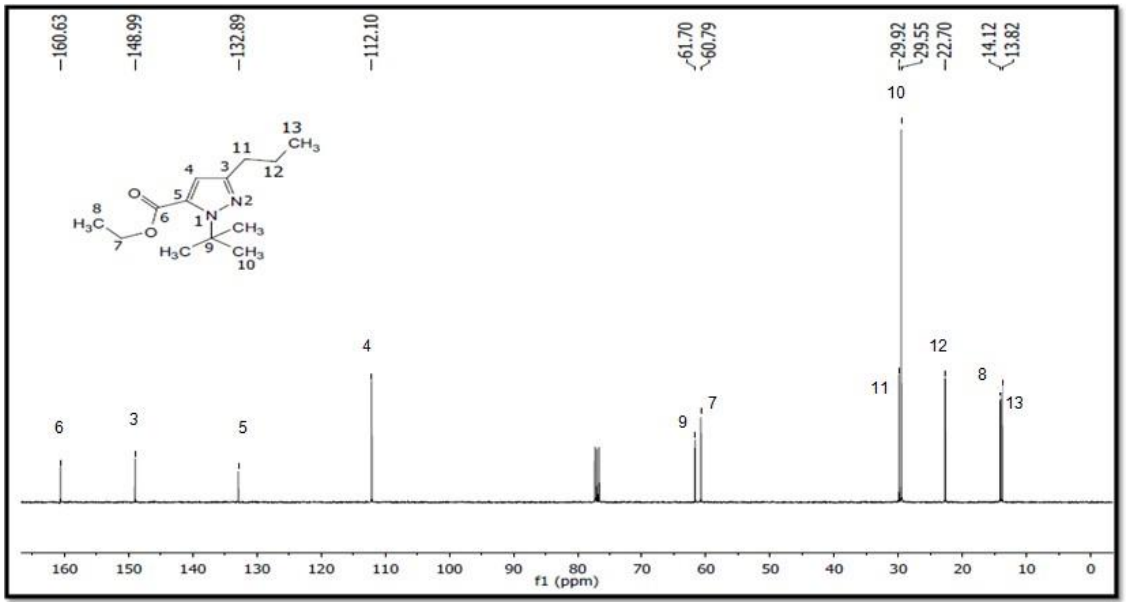


Figure S17: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **3b**.

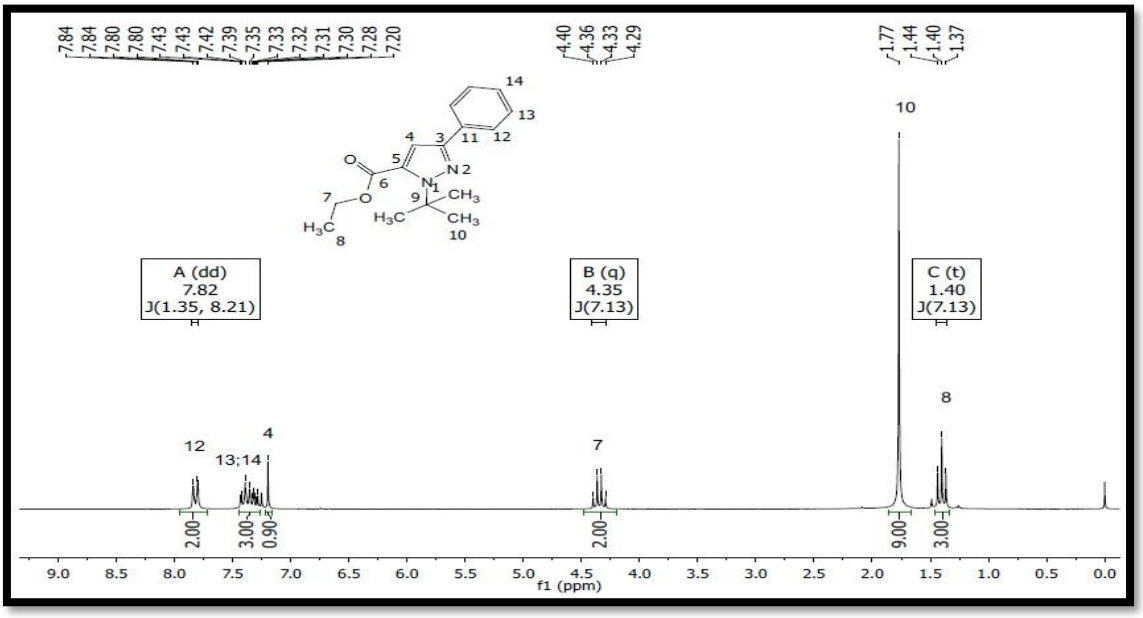


Figure S18: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **3c**.

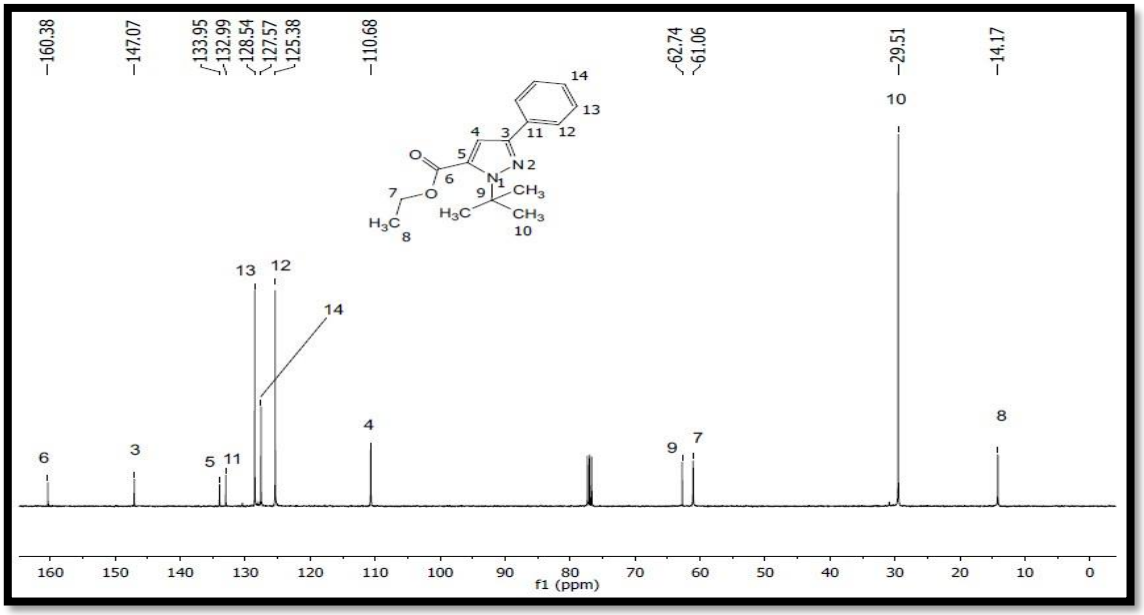


Figure S19: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **3c**.

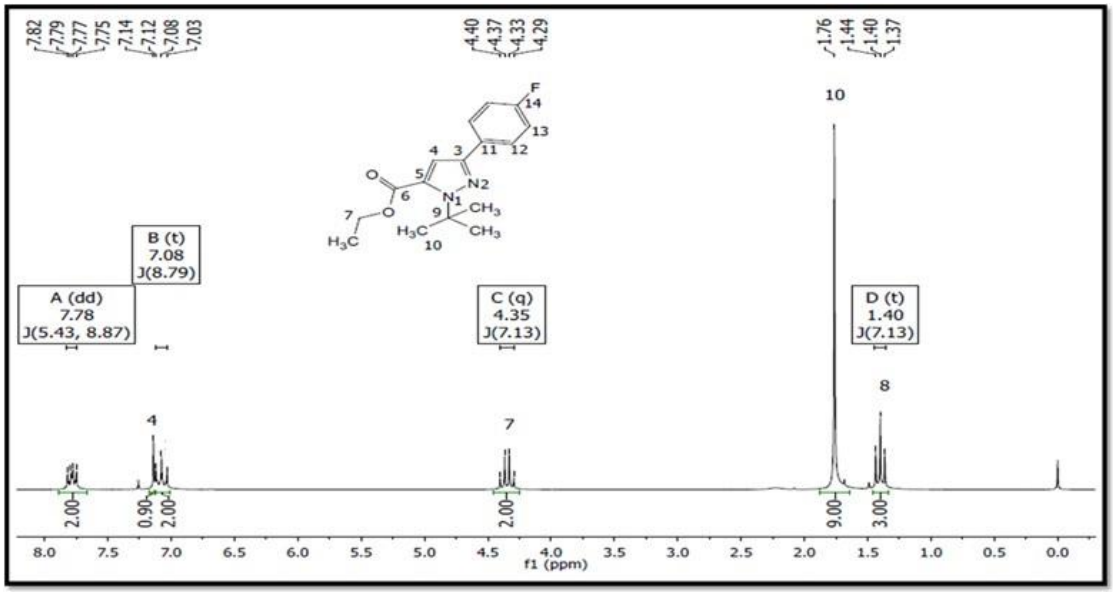


Figure S20: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **3d**.

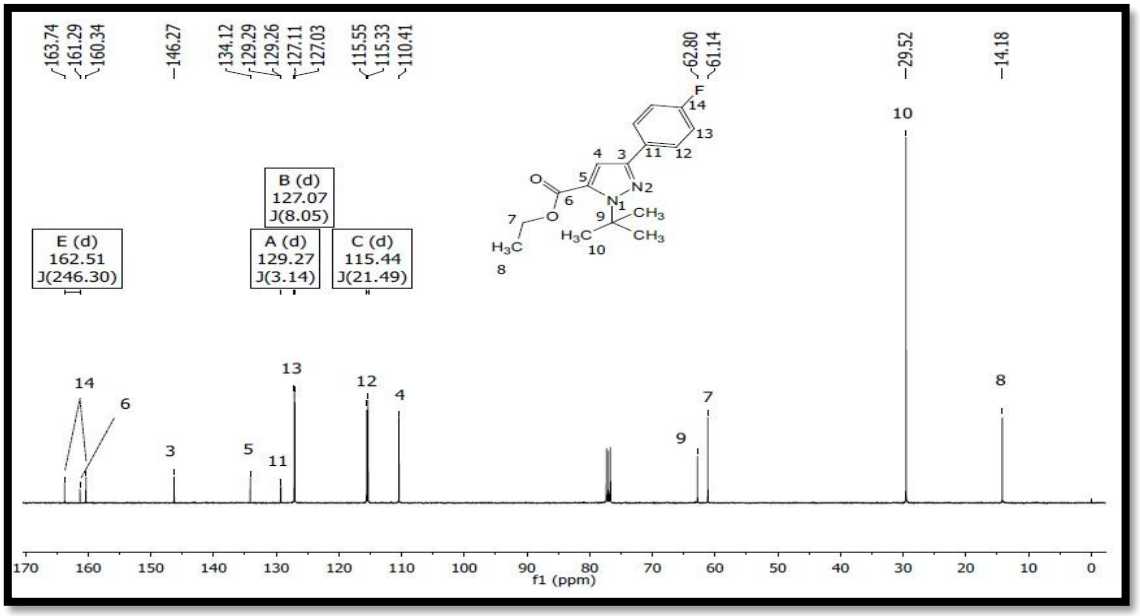


Figure S21: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **3d**.

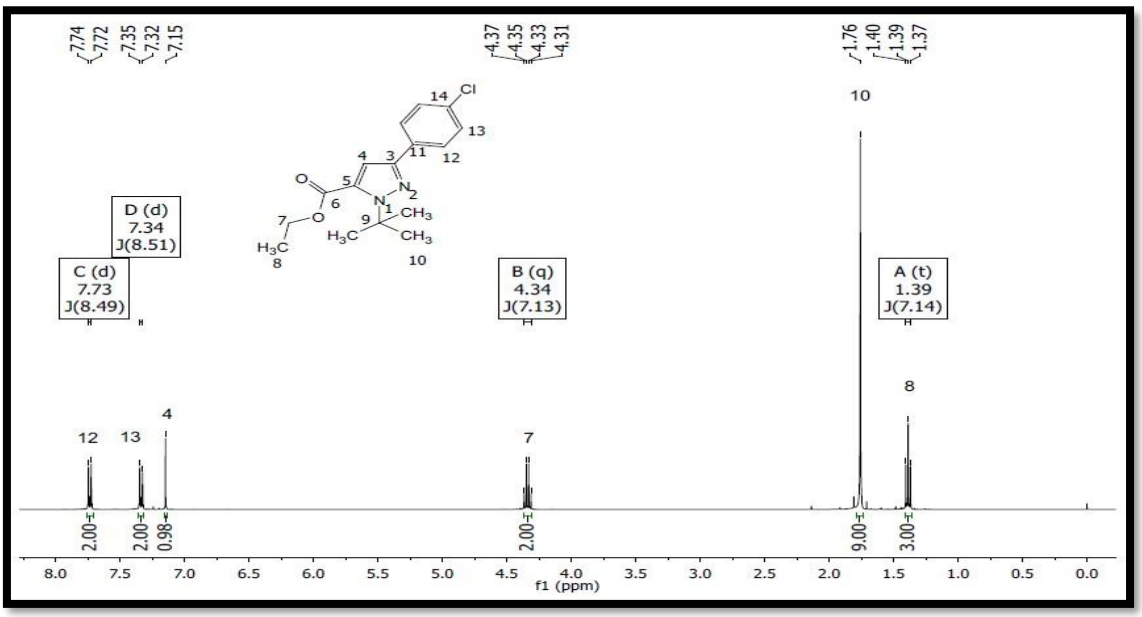


Figure S22: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **3e**.

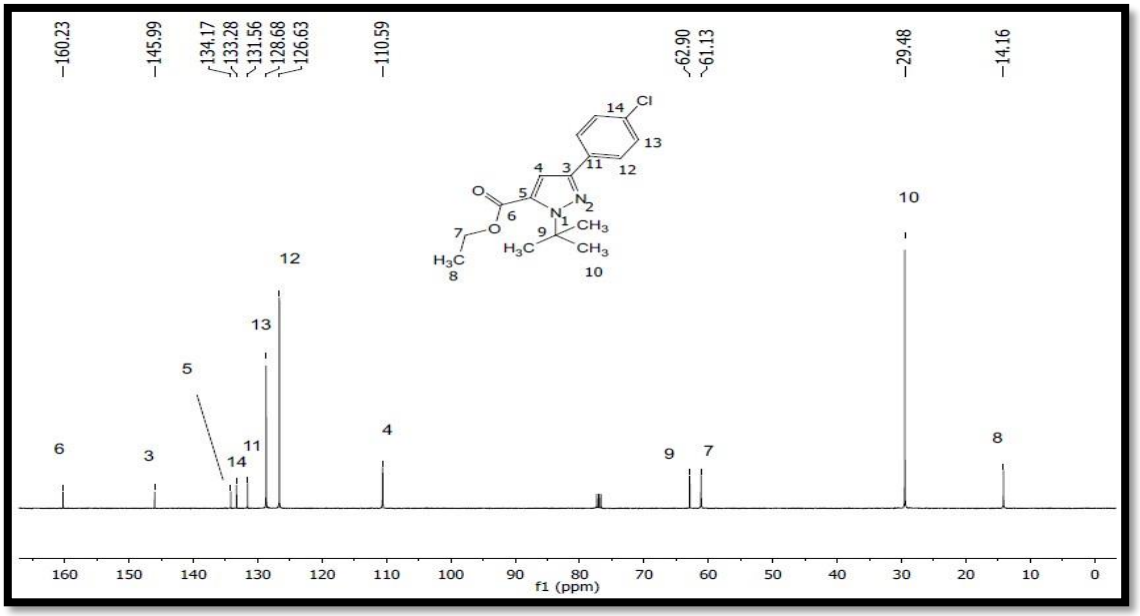


Figure S23: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **3e**.

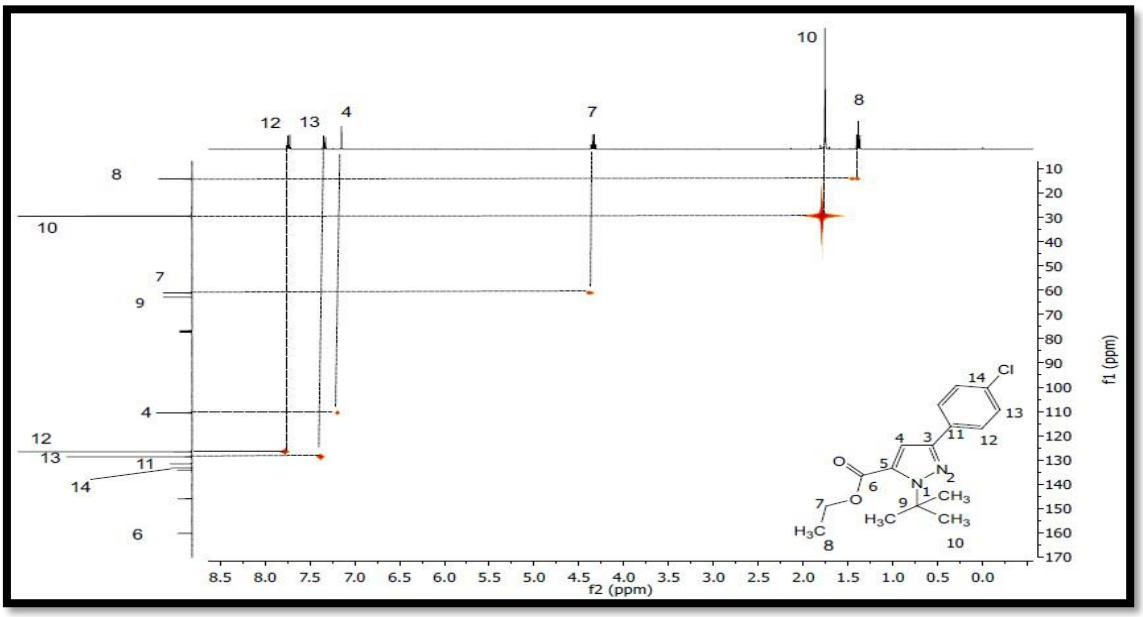


Figure S24: HMQC NMR (600 MHz. $CDCl_3$) spectrum of **3**e.

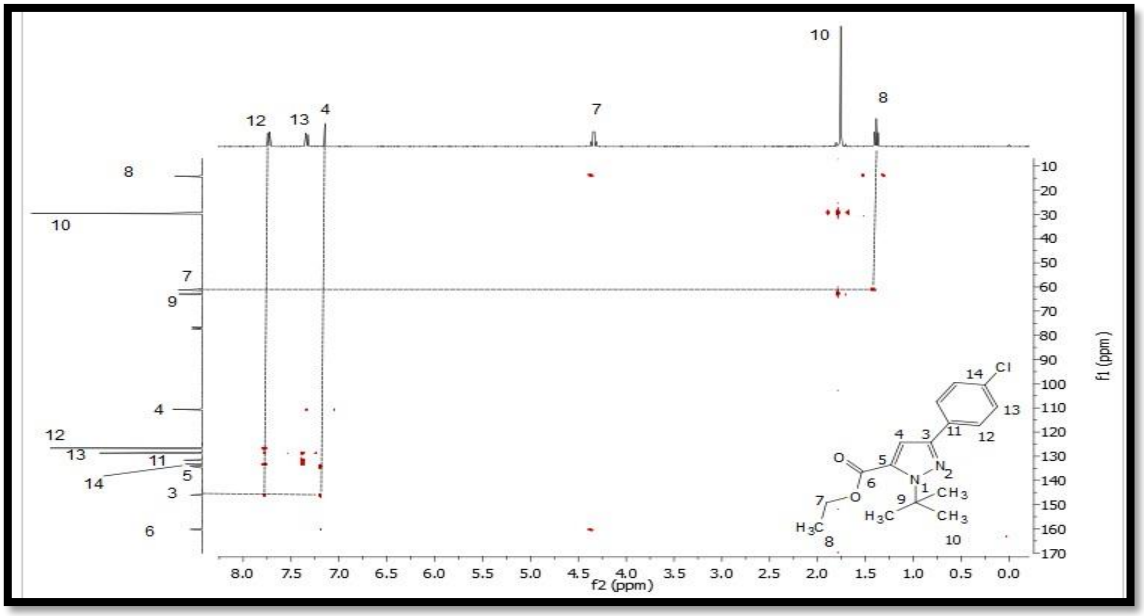


Figure S25: HMBC NMR (600 MHz. $CDCl_3$) spectrum of **3e**.

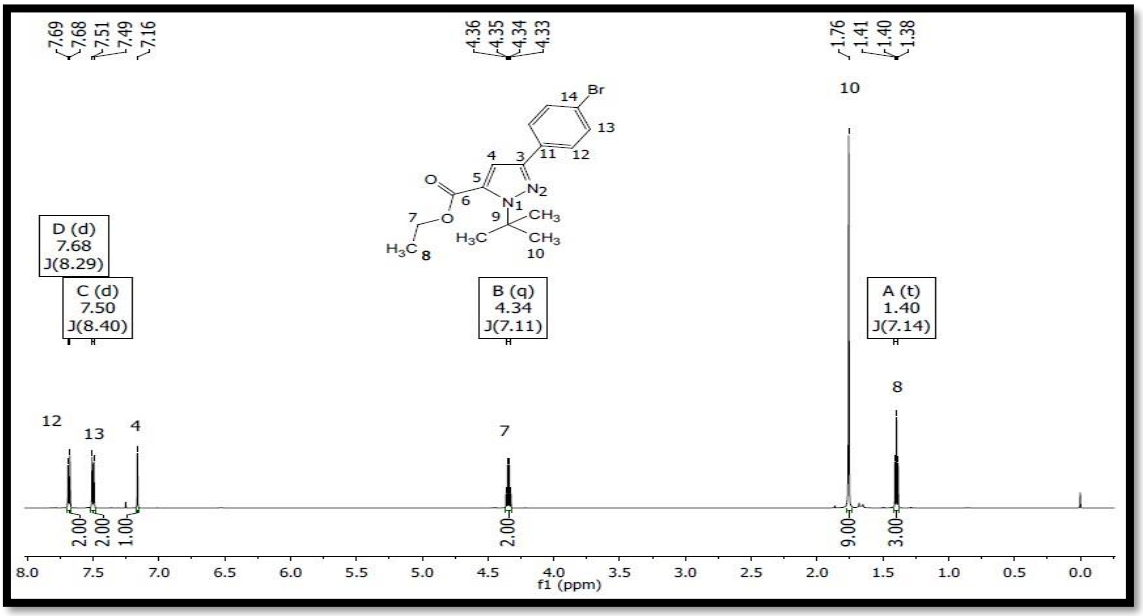


Figure S26: ^1H NMR (200 MHz. $CDCl_3$) spectrum of **3f**.

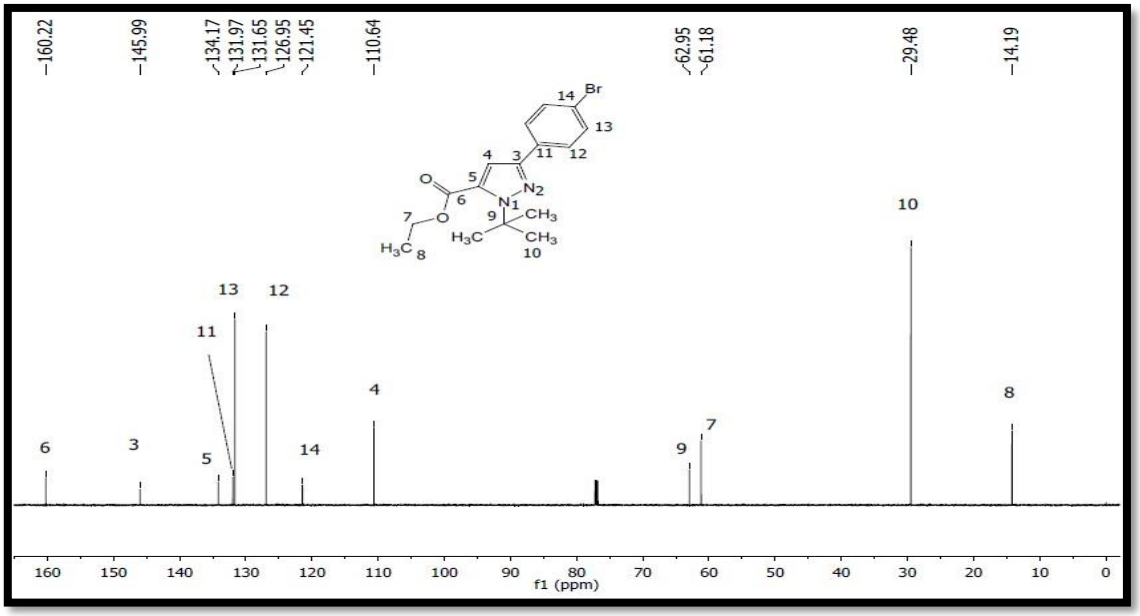


Figure S27: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **3f**.

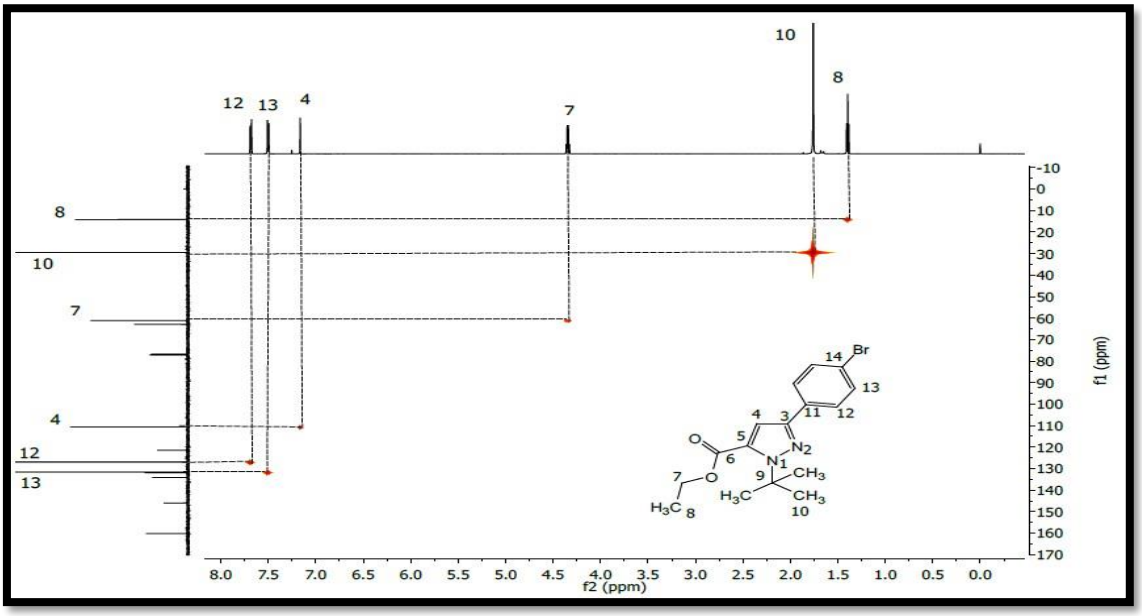


Figure S28: HMQC NMR (600 MHz. $CDCl_3$) spectrum of **3f**.

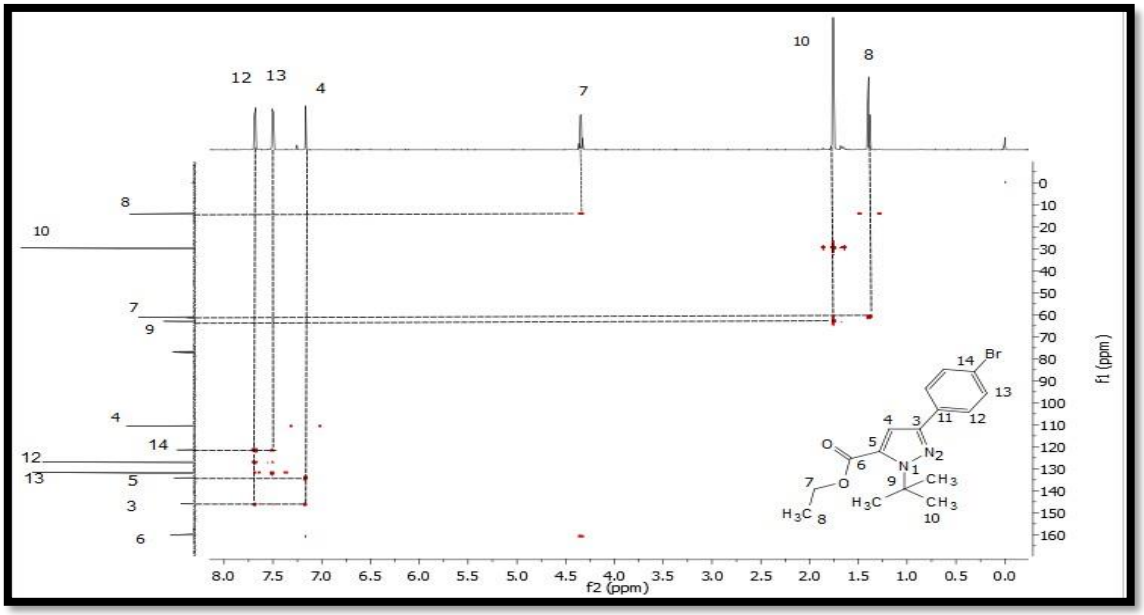


Figure S29: HMBC NMR (600 MHz. $CDCl_3$) spectrum of **3f**.

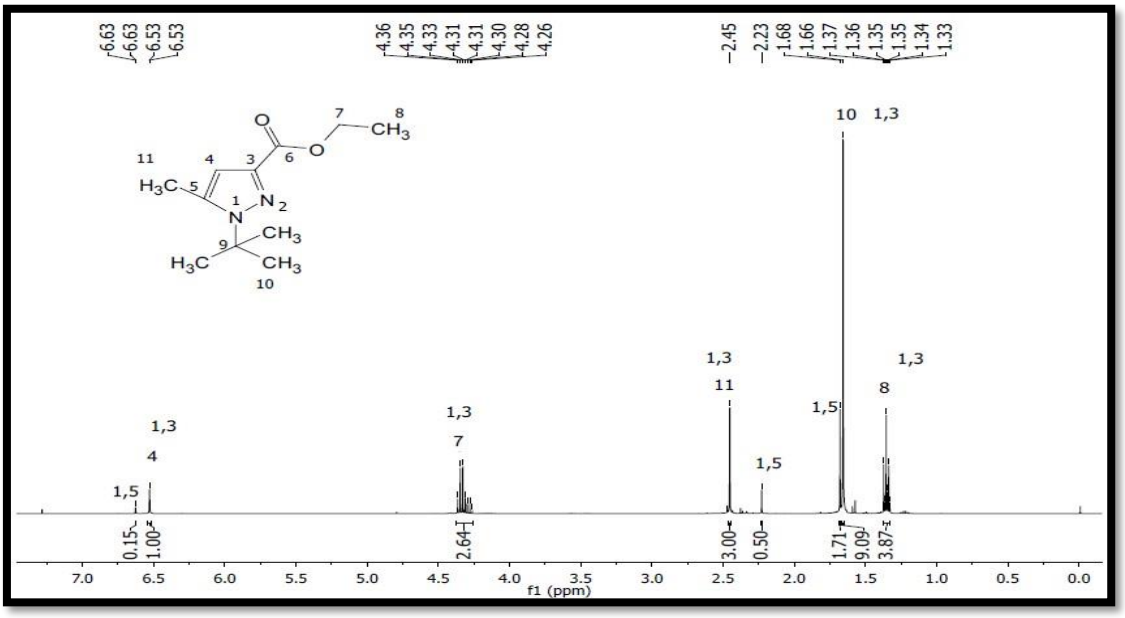


Figure S30: ^{1}H NMR (400 MHz. $CDCl_3$) spectrum of **3**a and **4a.**

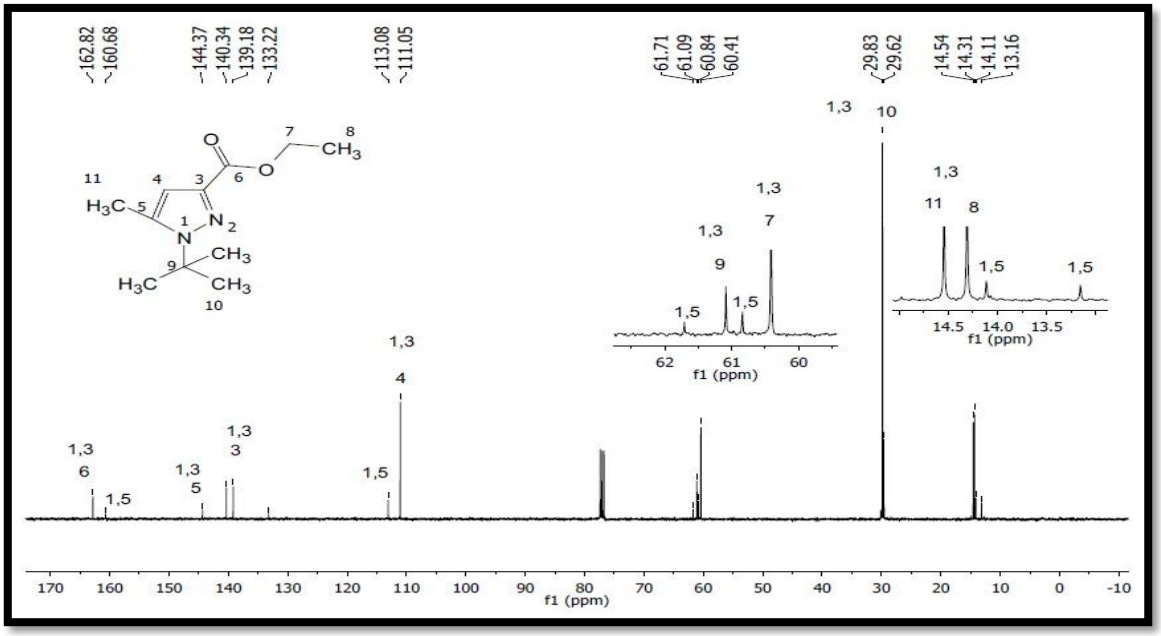


Figure S31: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **3**a and **4a**.

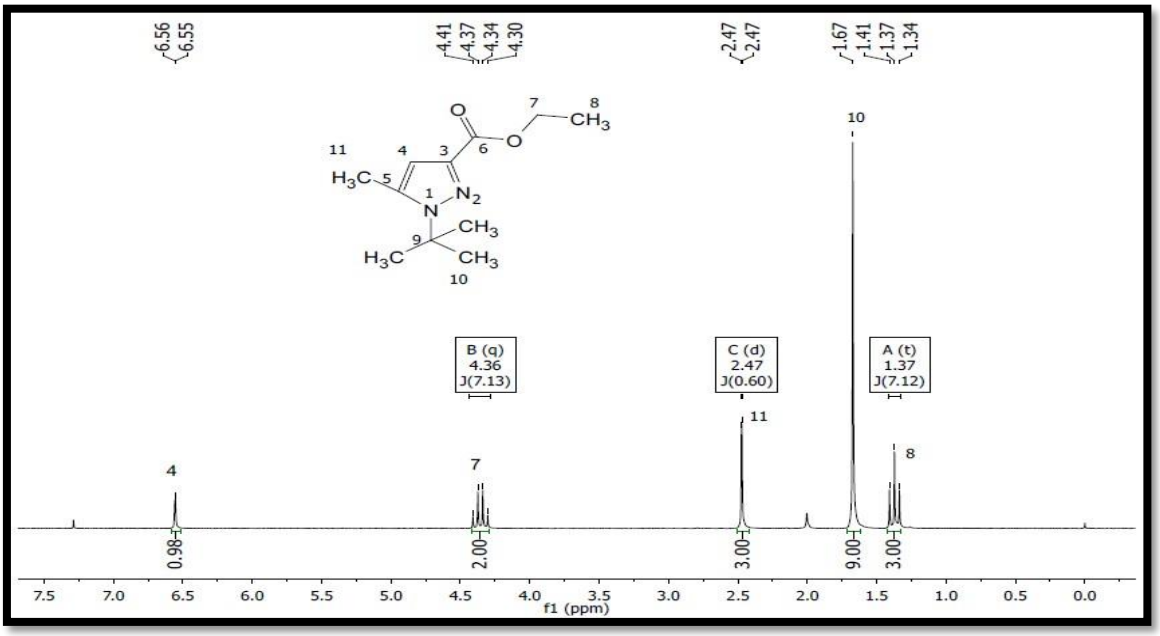


Figure S32: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **4a**.

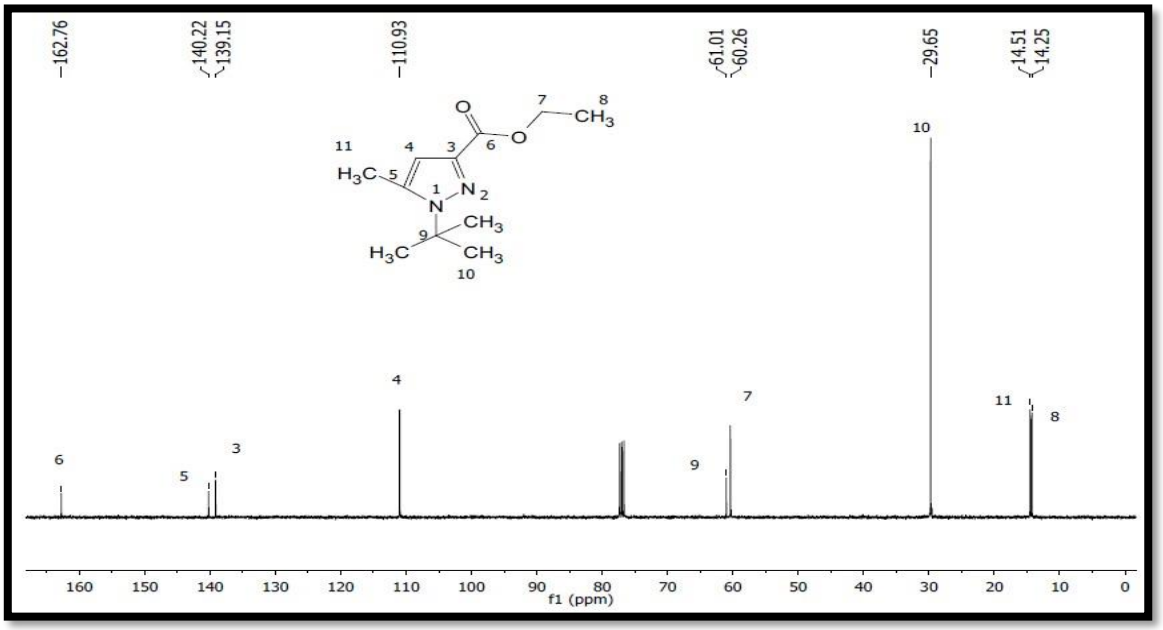


Figure S33: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **4**a.

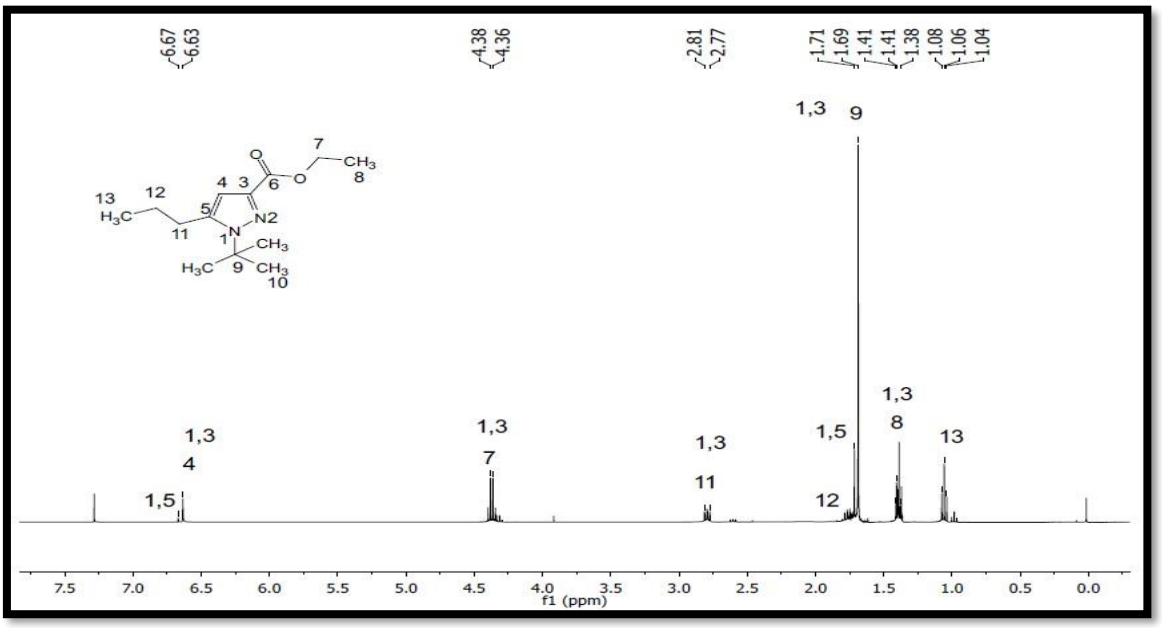


Figure S34: ^{1}H NMR (400 MHz. $CDCl_3$) spectrum of **3b** and **4b.**

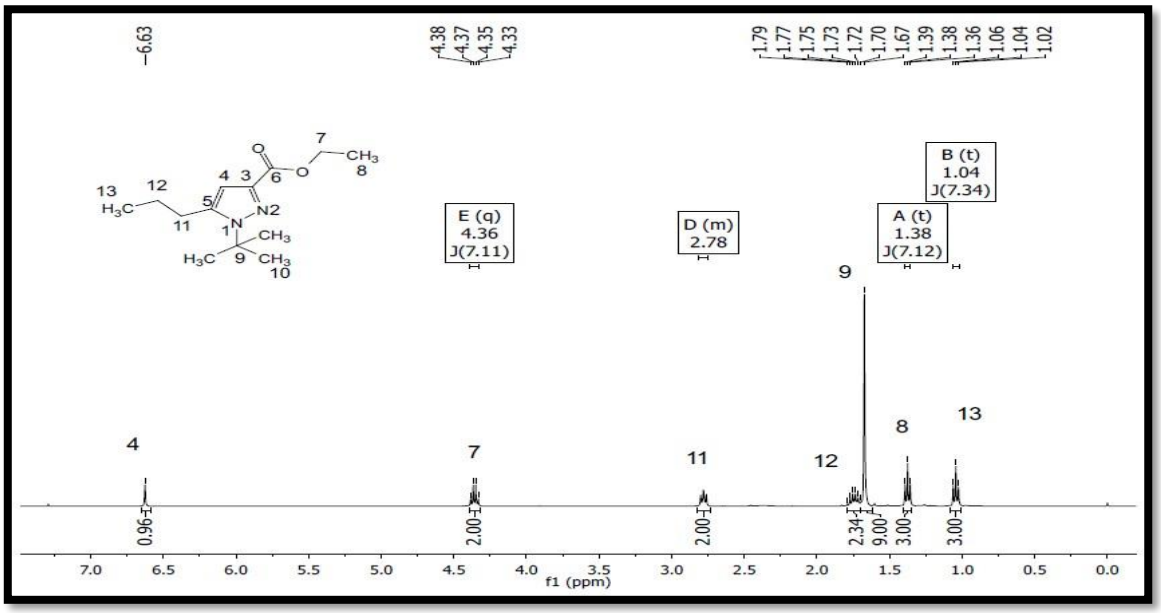


Figure S35: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **4b.**

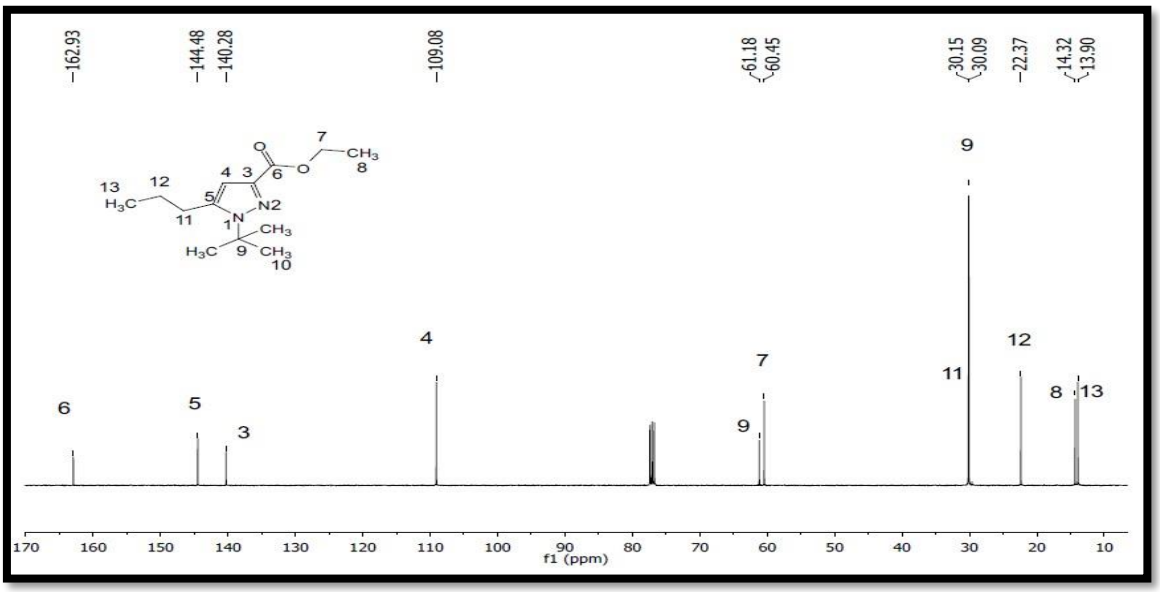


Figure S36: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **4b**.

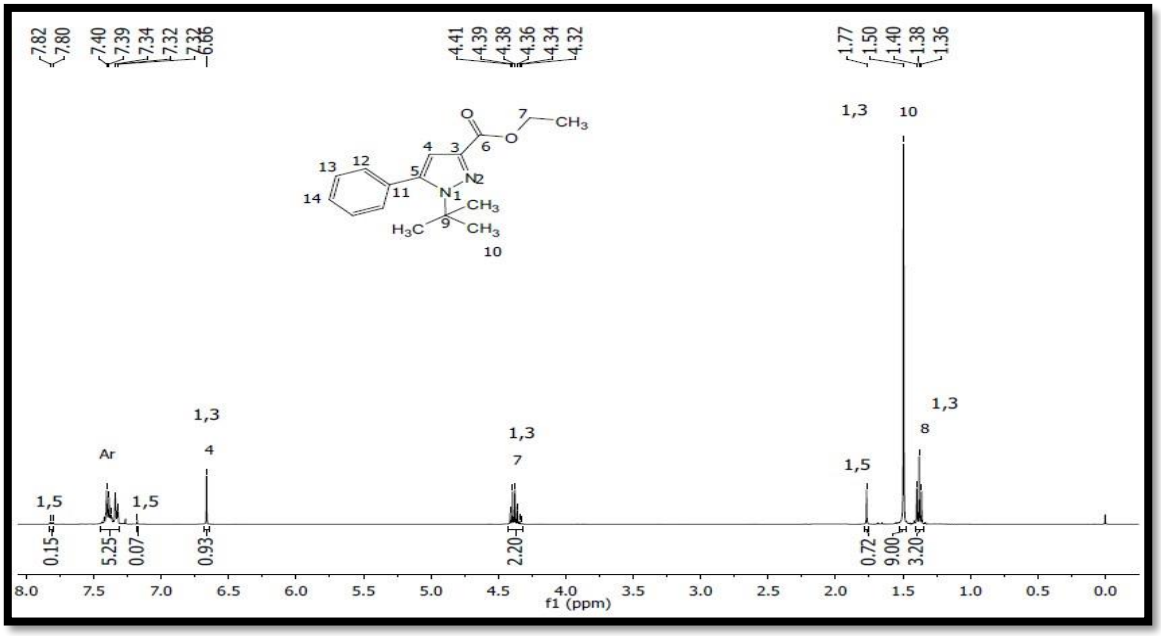


Figure S37: ^{1}H NMR (400 MHz. $CDCl_3$) spectrum of **3c** and **4c.**

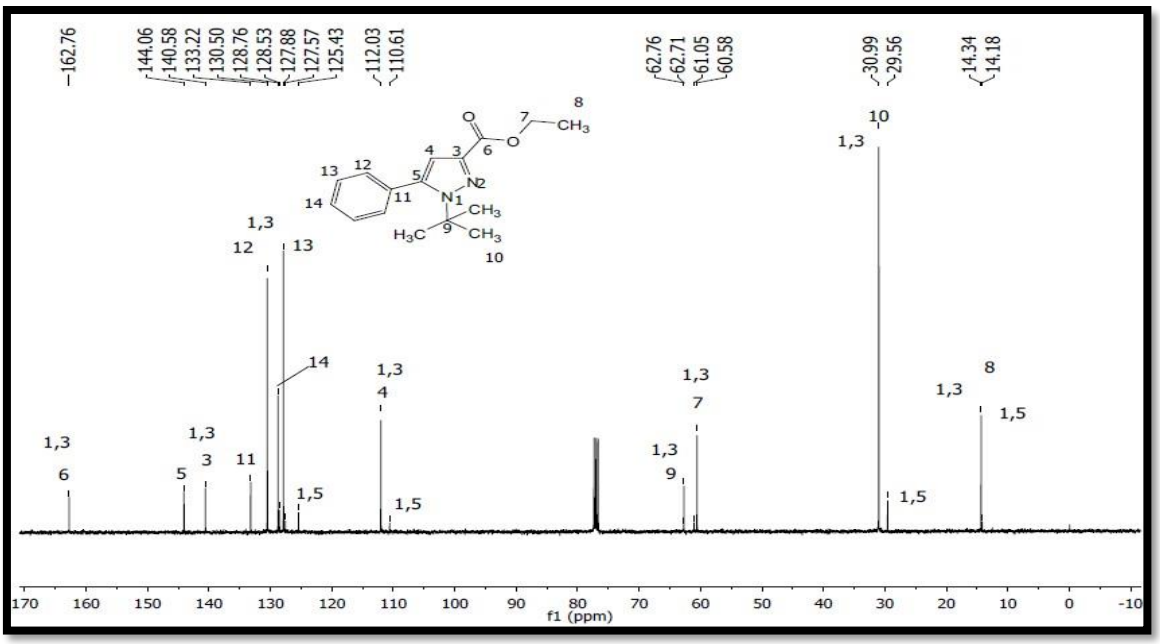


Figure S38: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **3**c and **4c.**

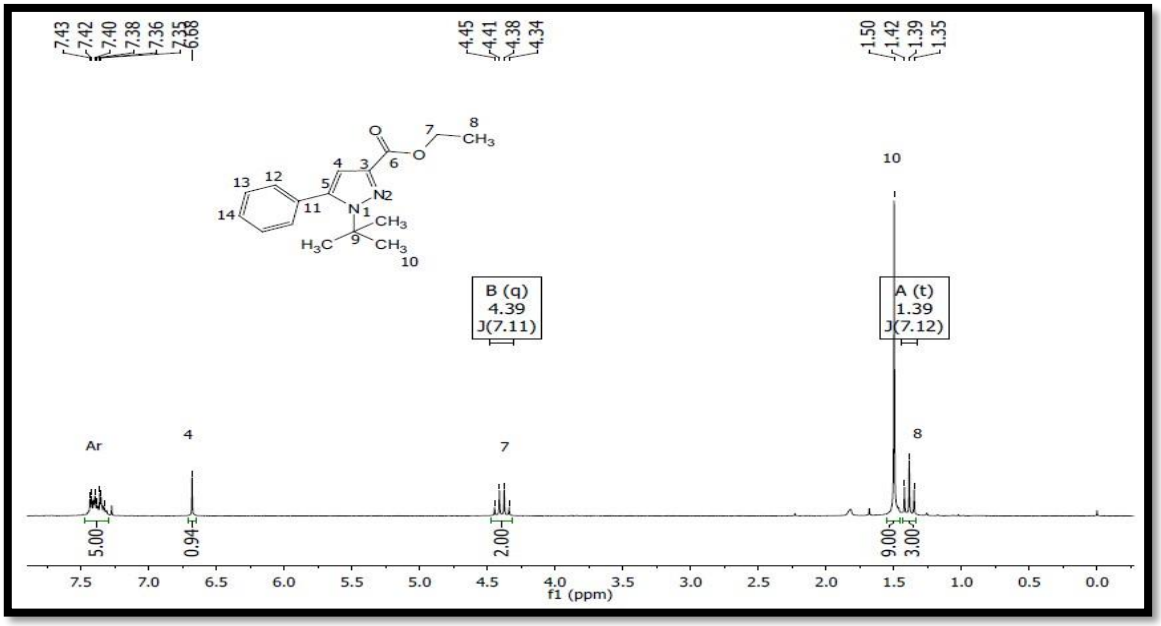


Figure S39: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **4c.**

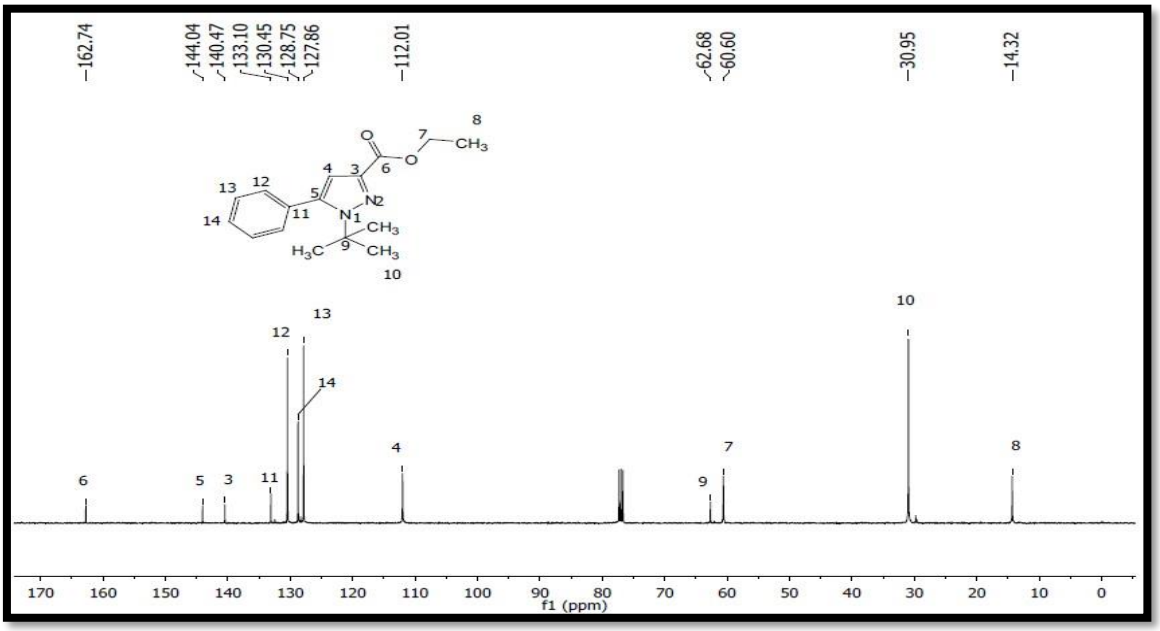


Figure S40: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **4c.**

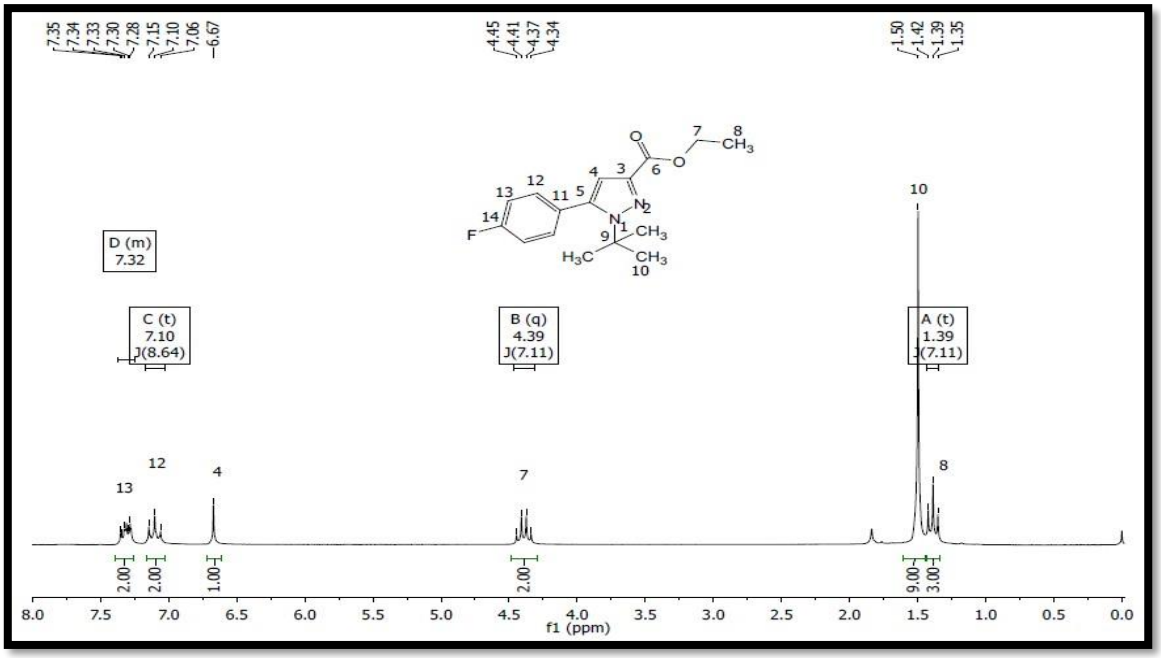


Figure S41: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **4d.**

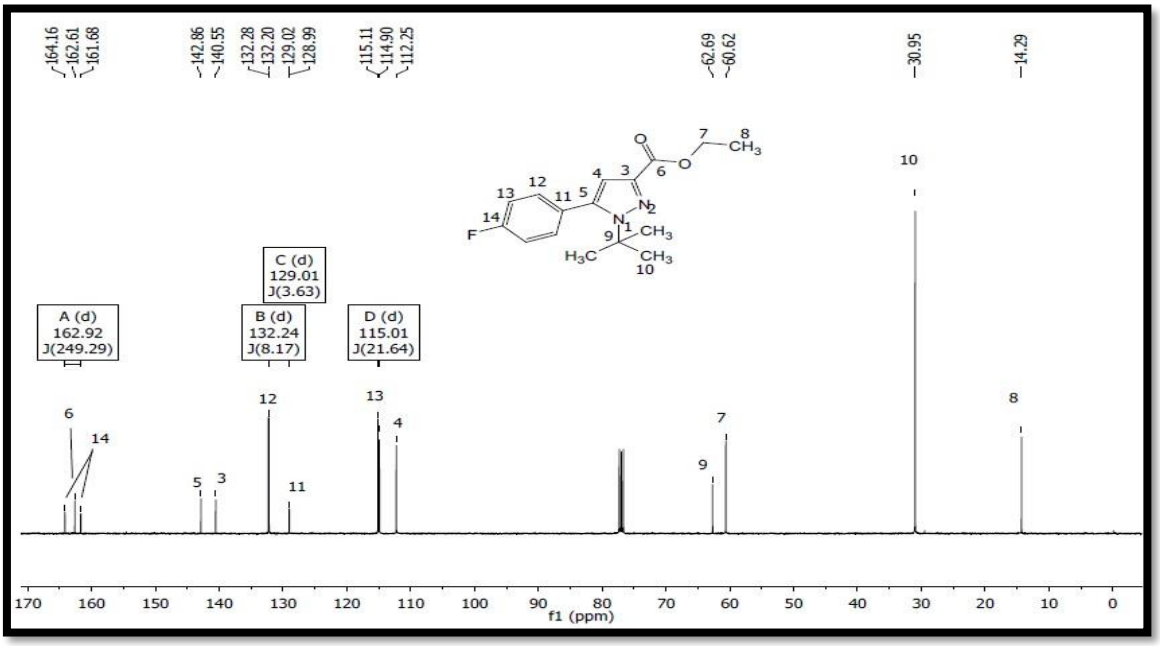


Figure S42: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **4d.**

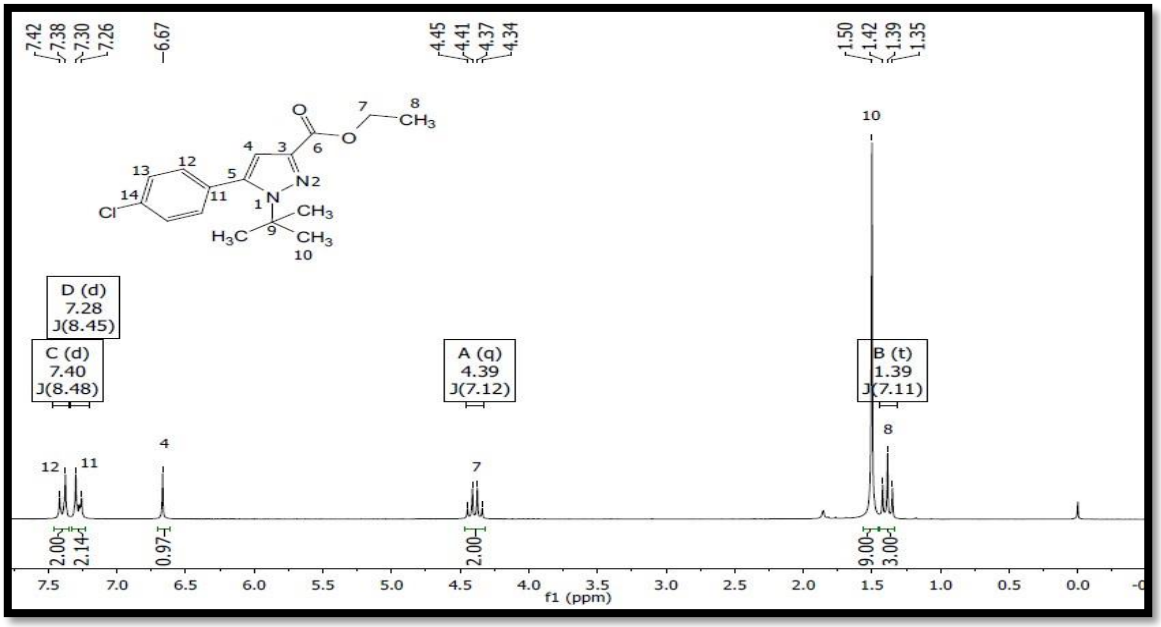


Figure S43: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **4e.**

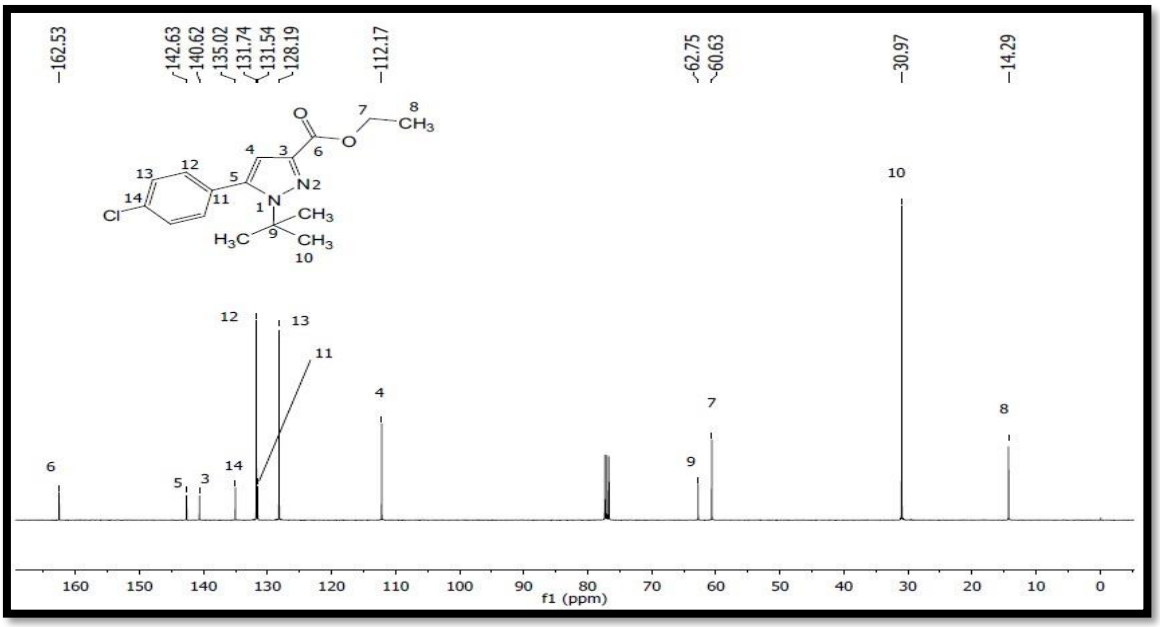


Figure S44: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **4e.**

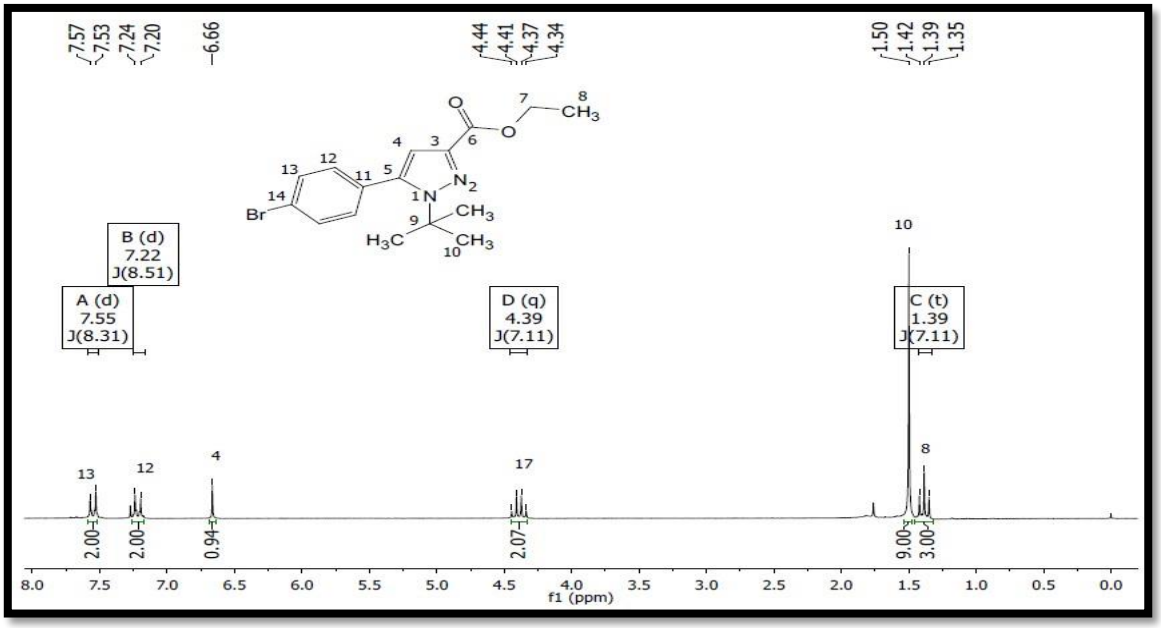


Figure S45: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **4f.**

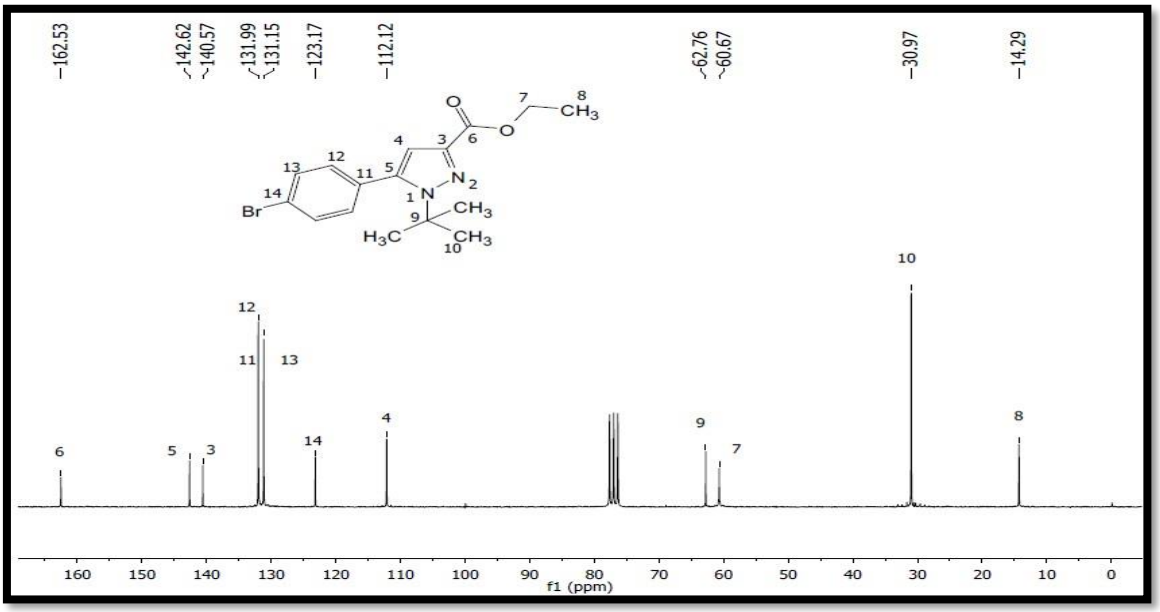


Figure S46: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **4f.**

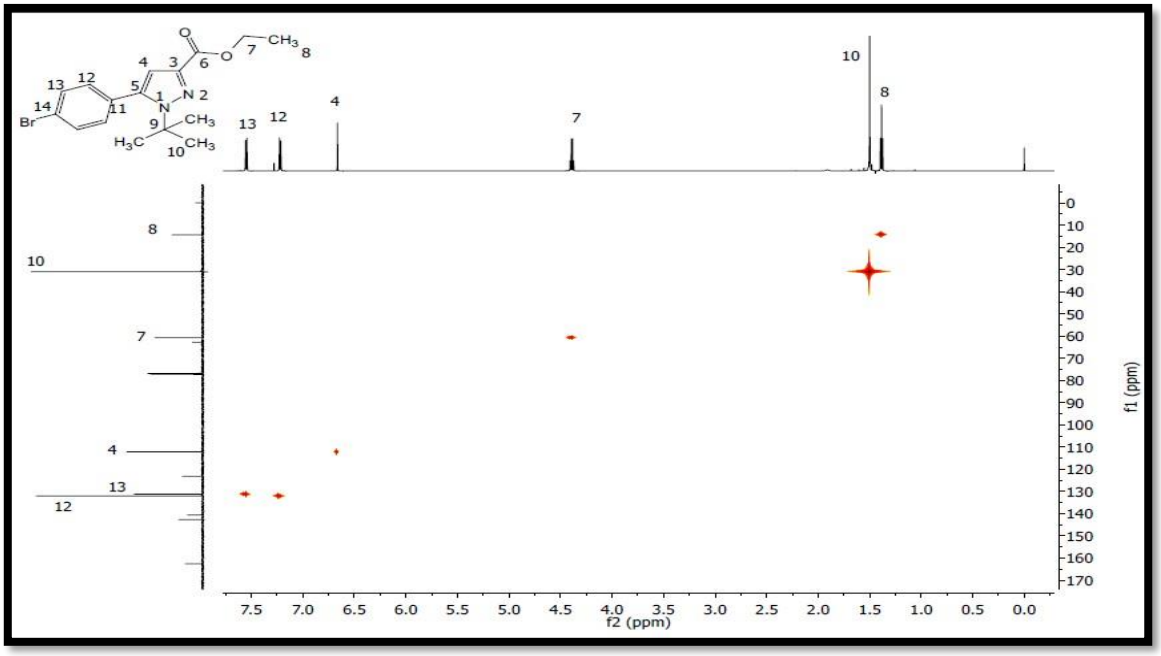


Figure S47: HMQC NMR (600 MHz. $CDCl_3$) spectrum of **4f**.

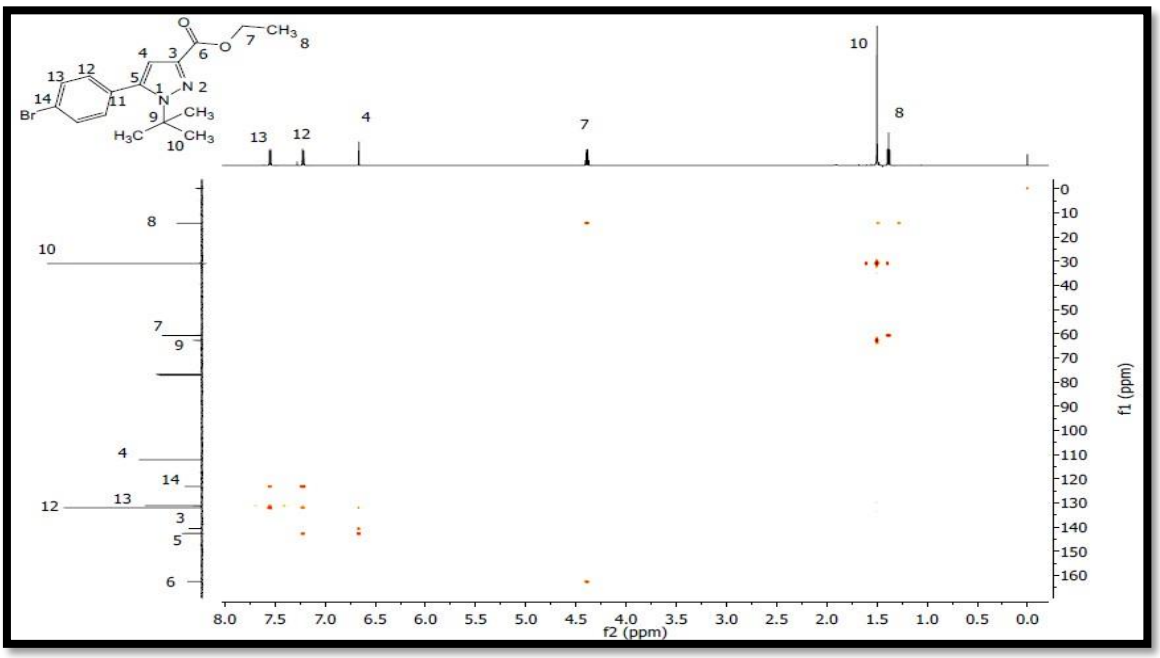


Figure S48: HMBC NMR (600 MHz. $CDCl_3$) spectrum of **4f**.

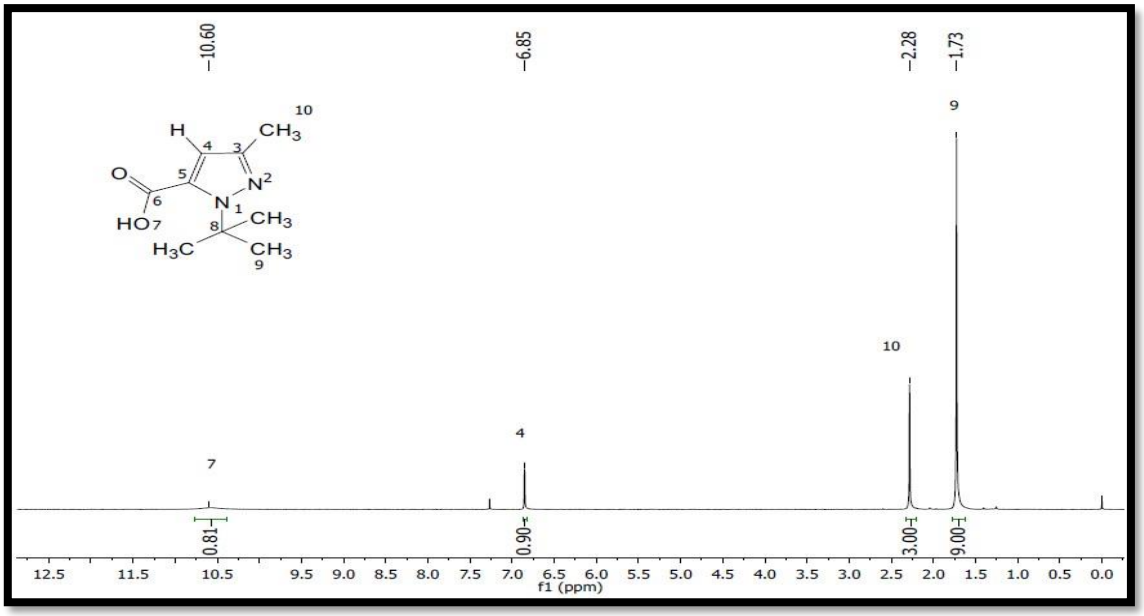


Figure S49: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **5a.**

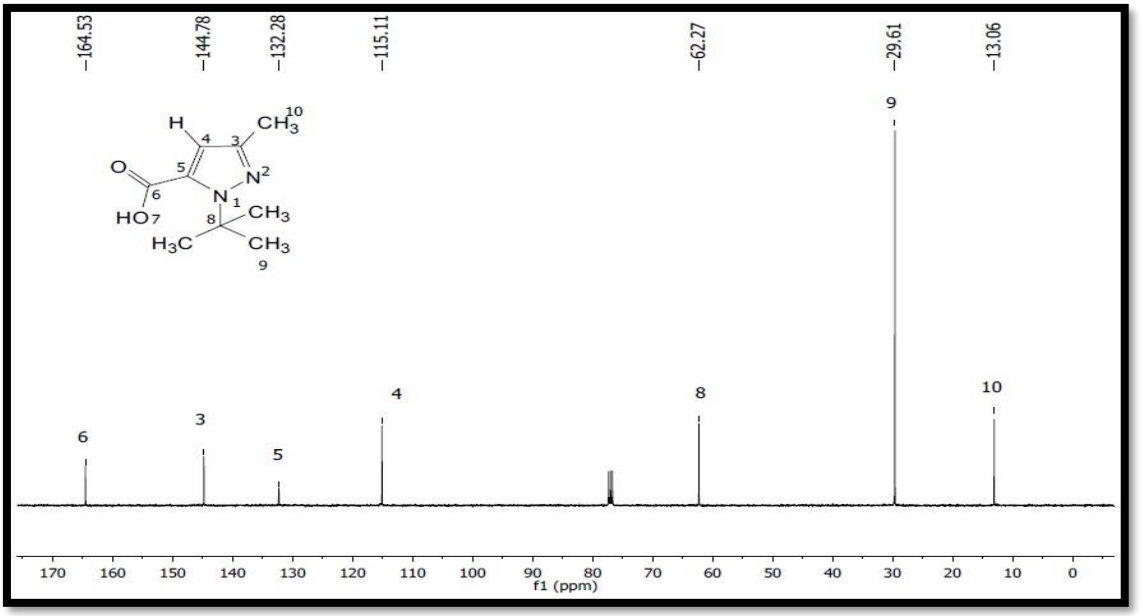


Figure S50: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **5a**.

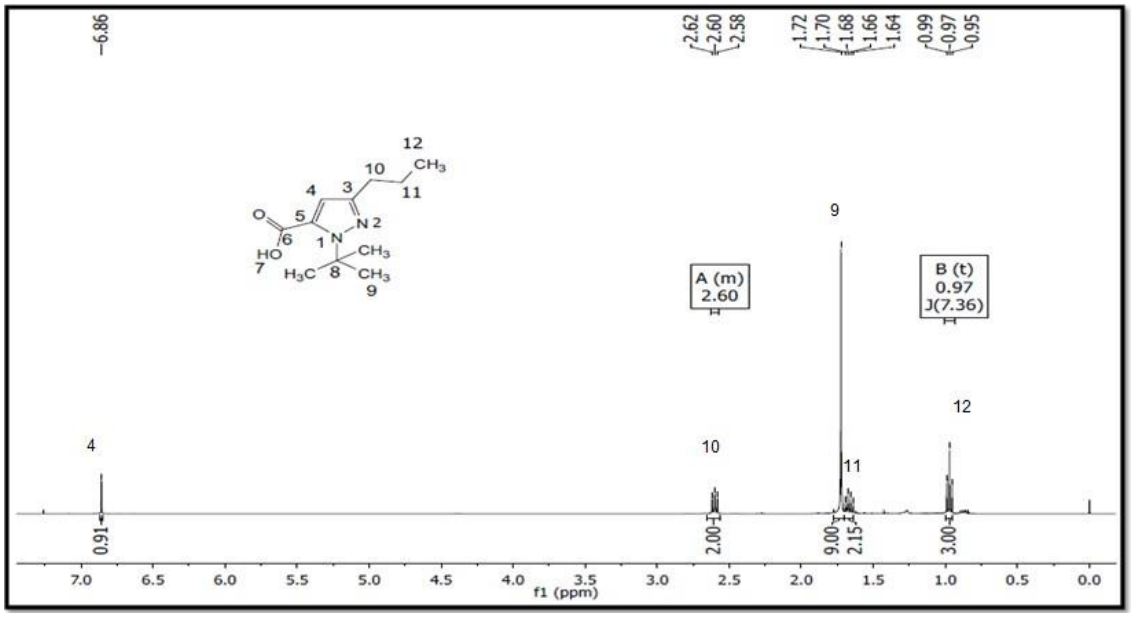


Figure S51: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **5b.**

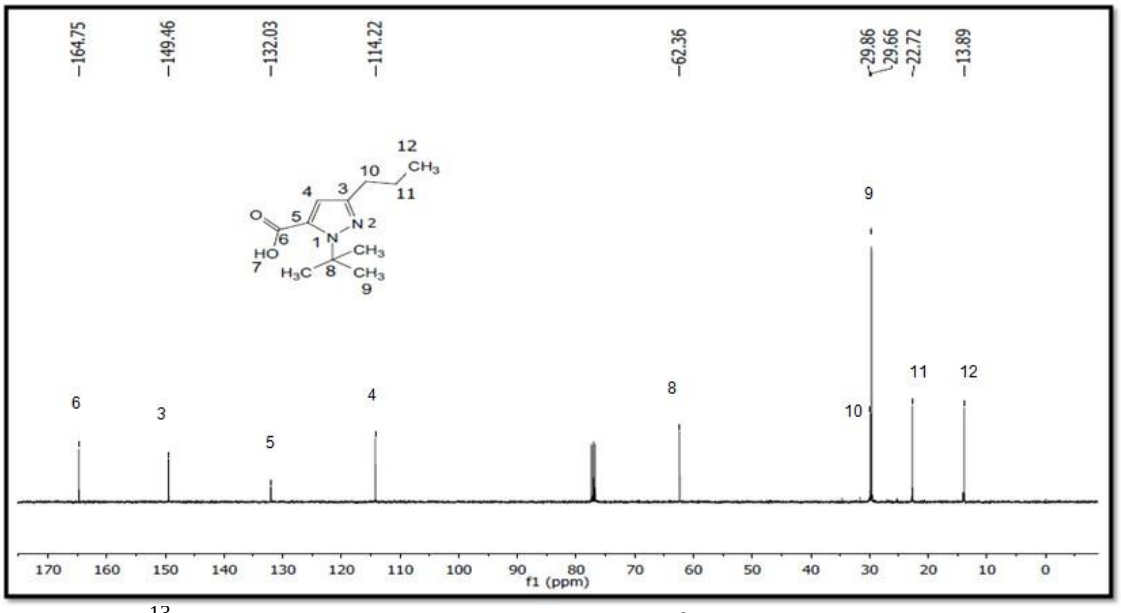


Figure S52: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **5b.**

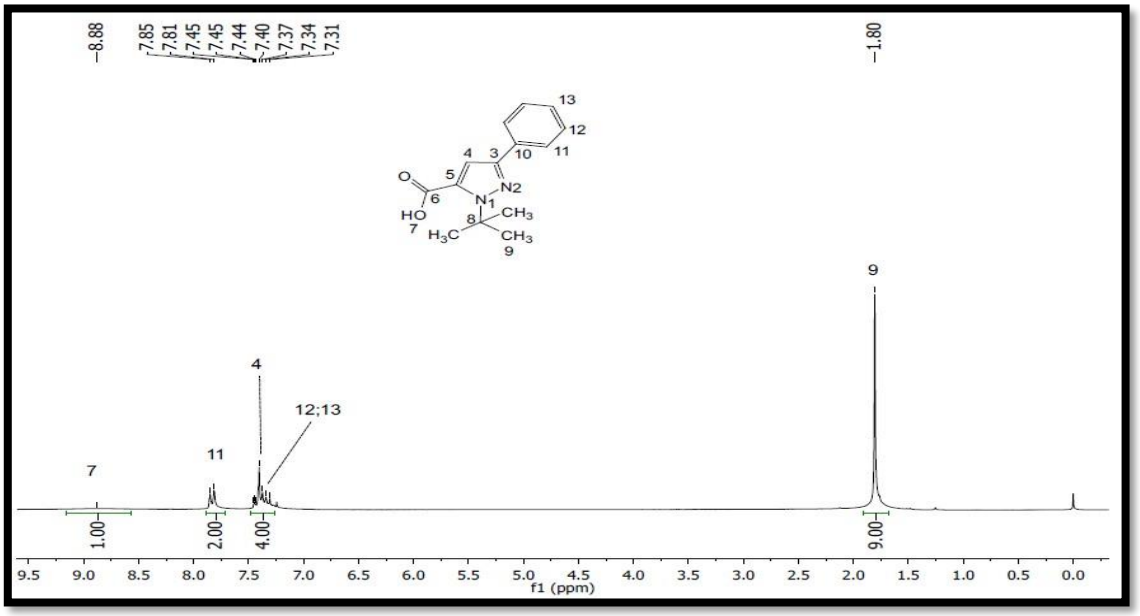


Figure S53: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **5c.**

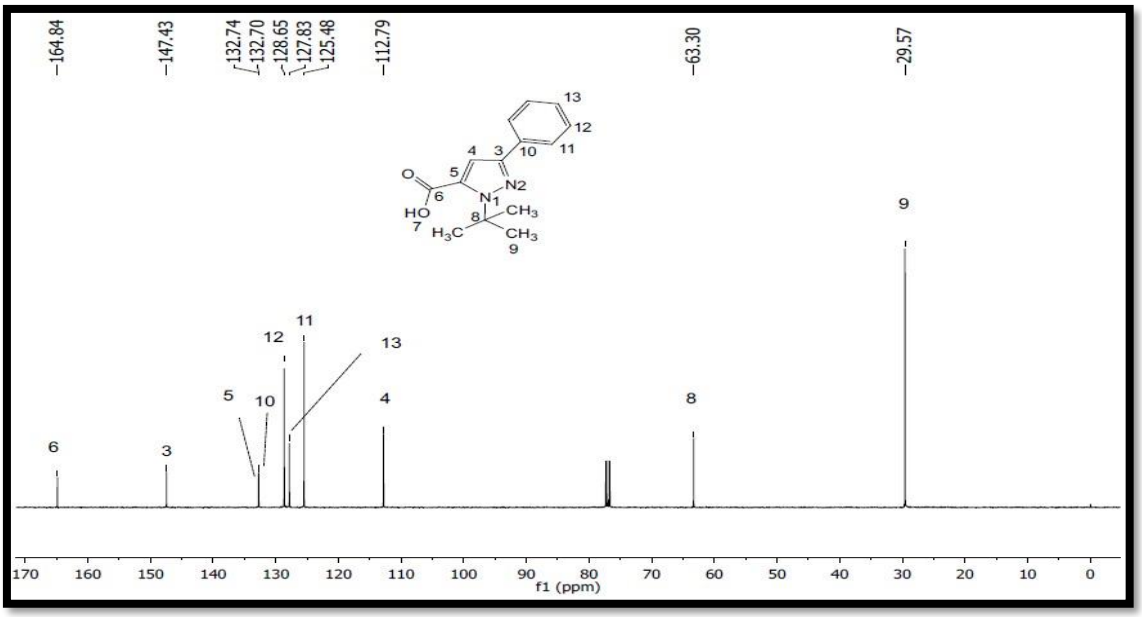


Figure S54: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **5c**.

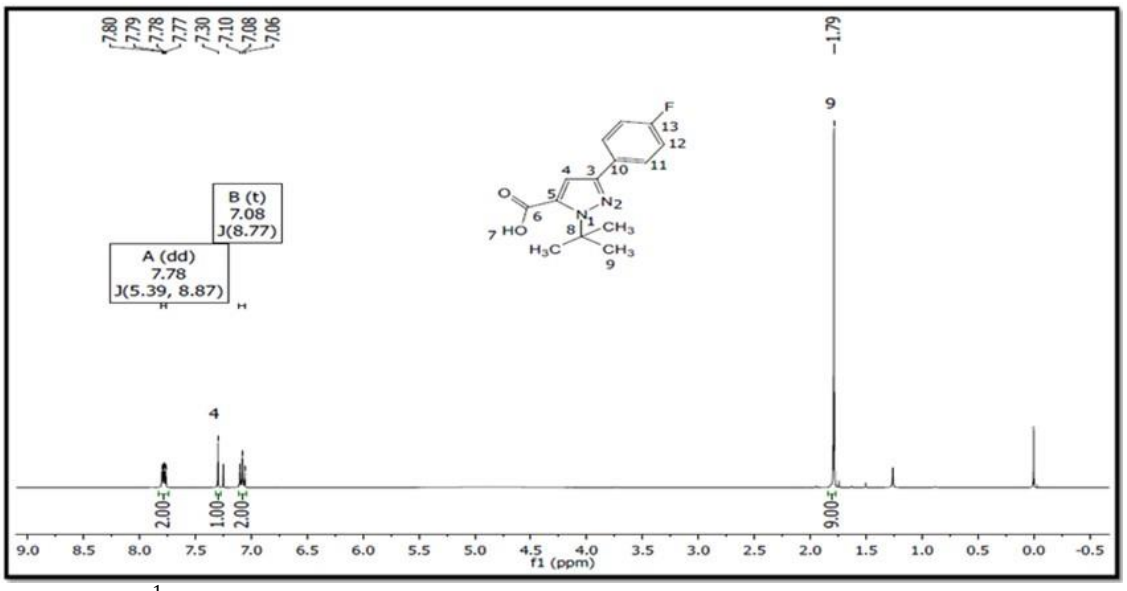


Figure S55: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **5d**.

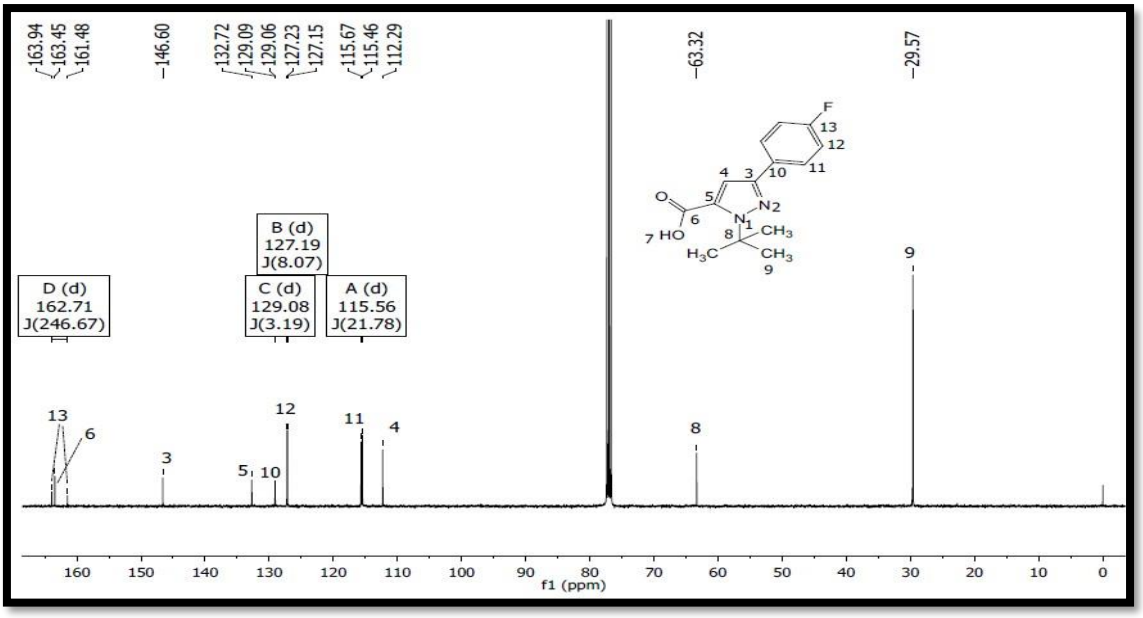


Figure S56: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **5d**.

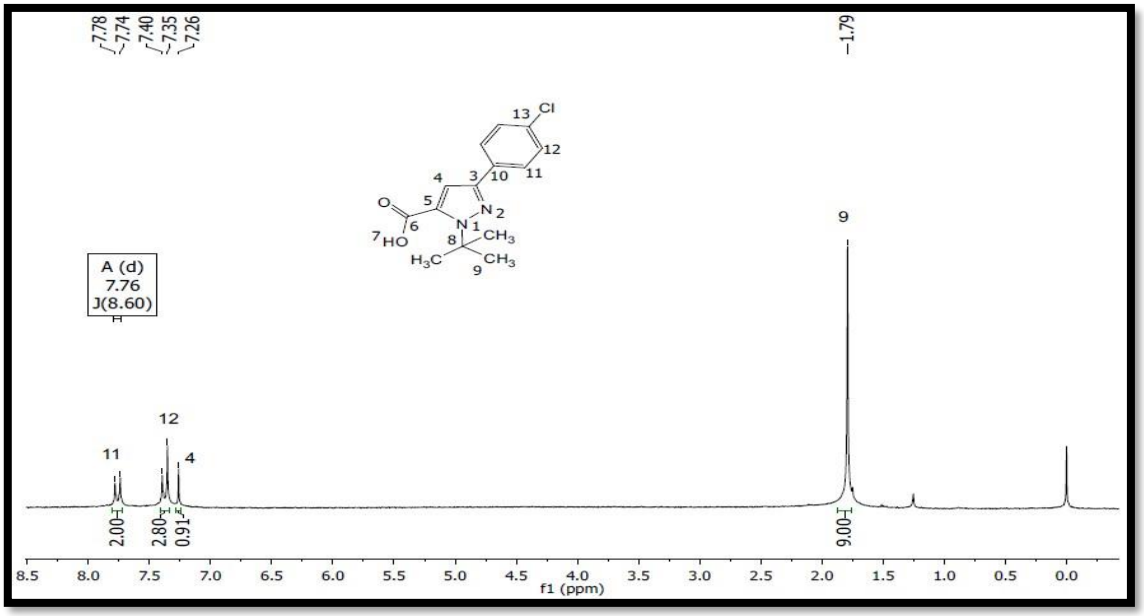


Figure S57: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **5e**.

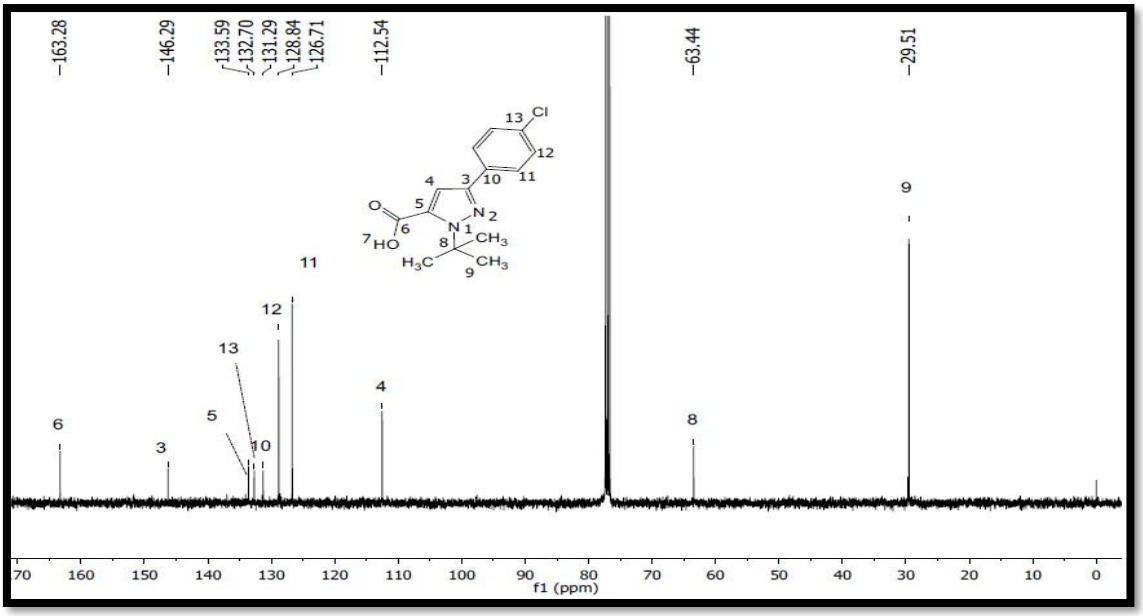


Figure S58: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **5e**.

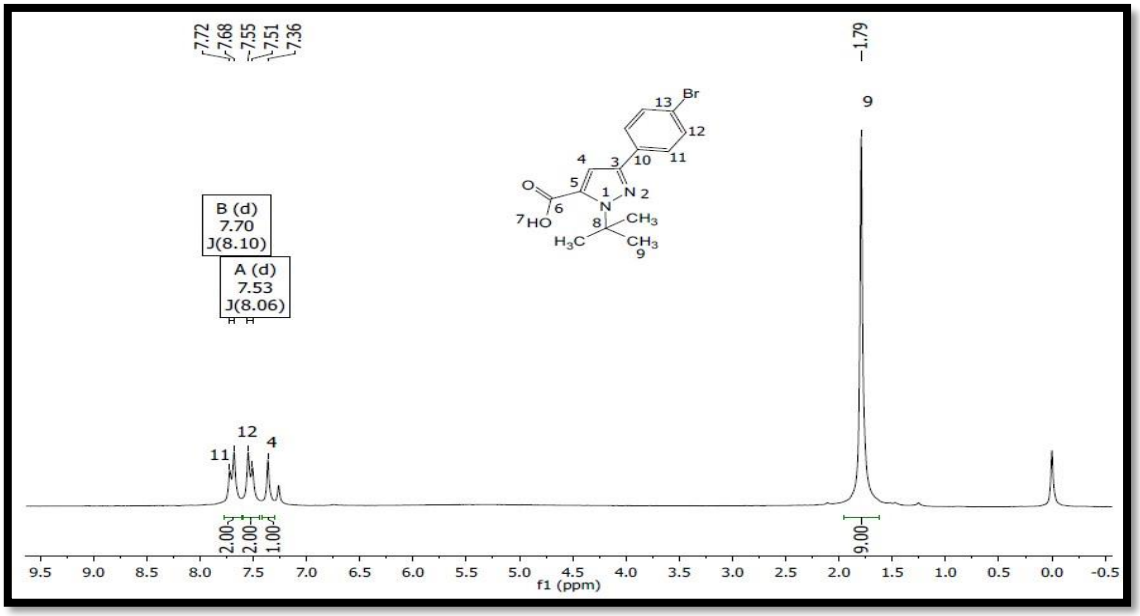


Figure S59: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **5f.**

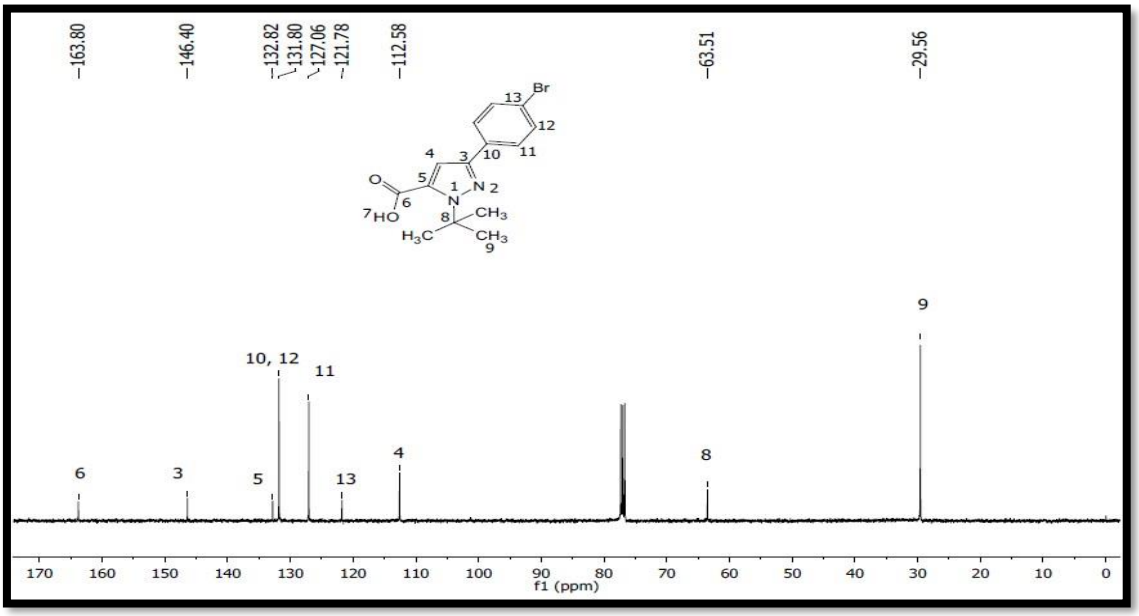


Figure S60: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **5f**.

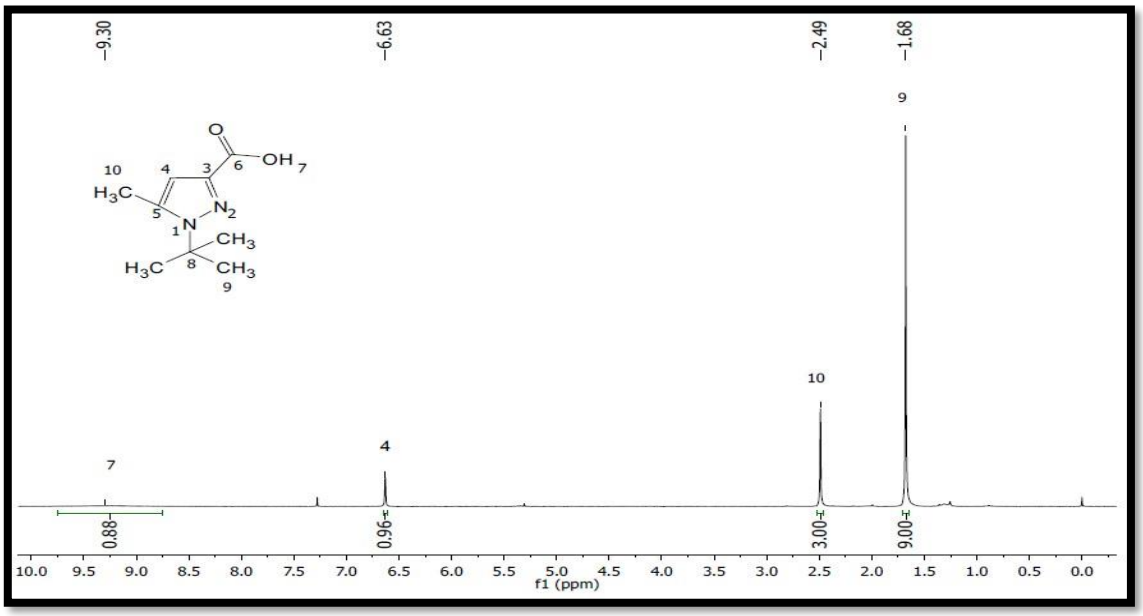


Figure S61: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **6a**

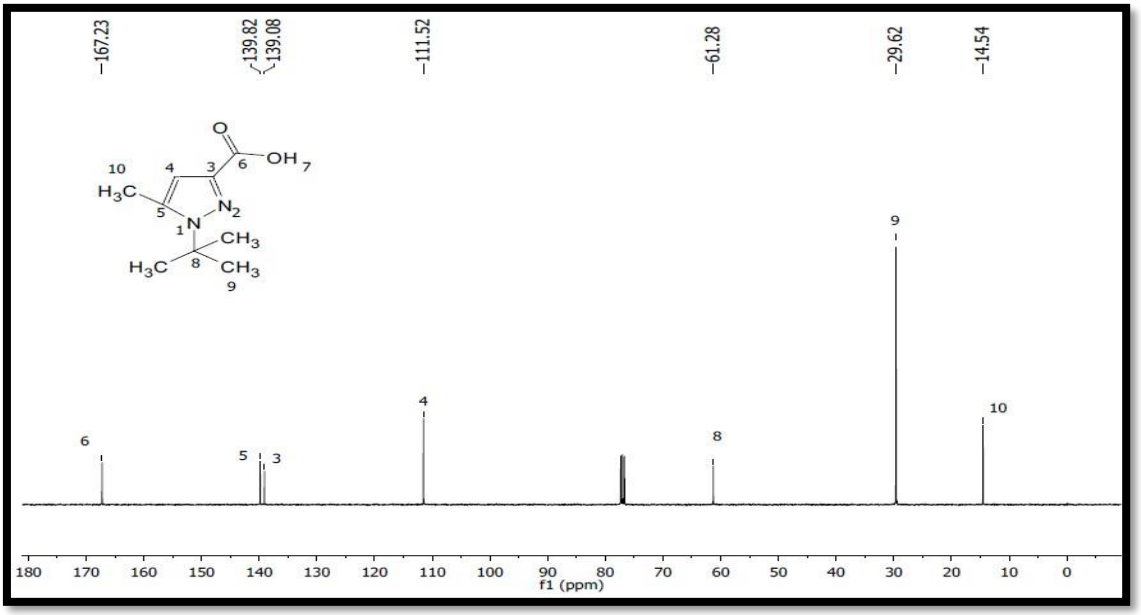


Figure S62: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **6a**.

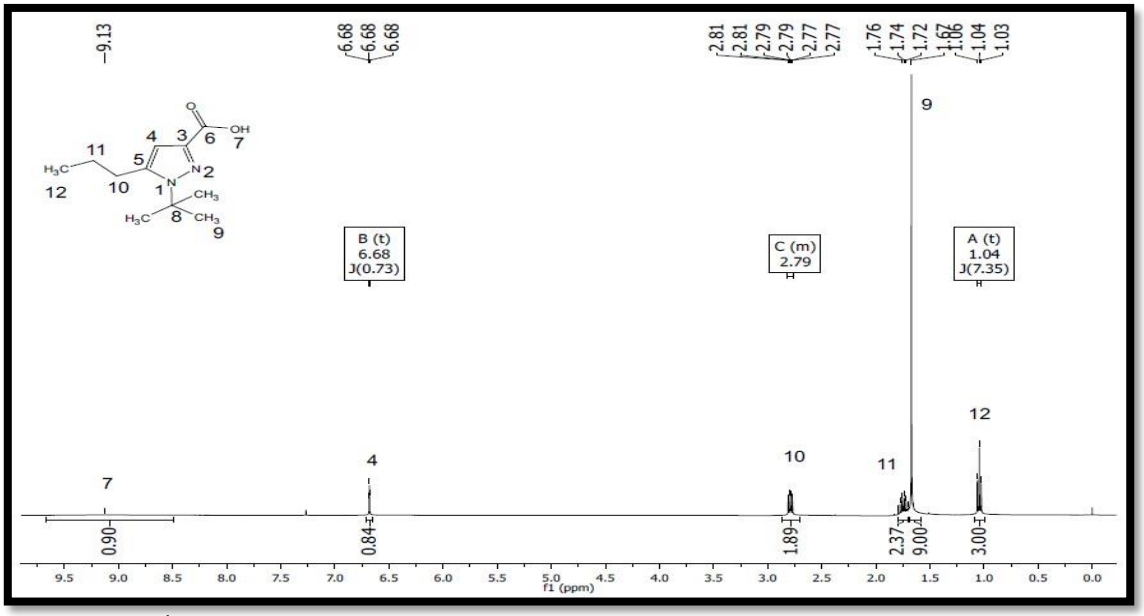


Figure S63: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **6b.**

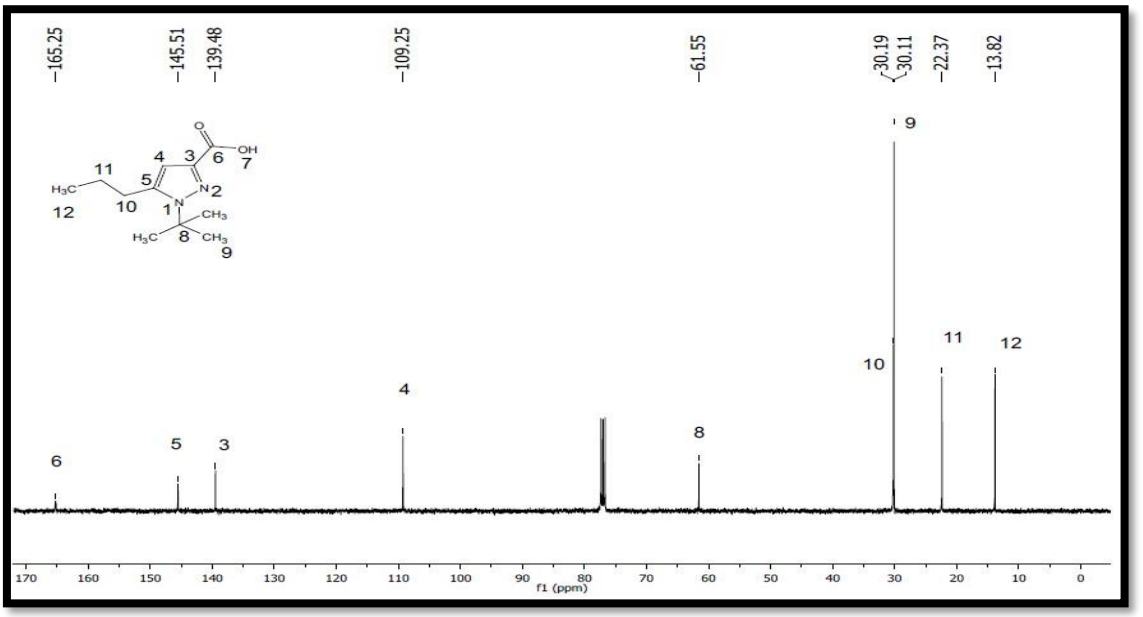


Figure S64: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **6b**.

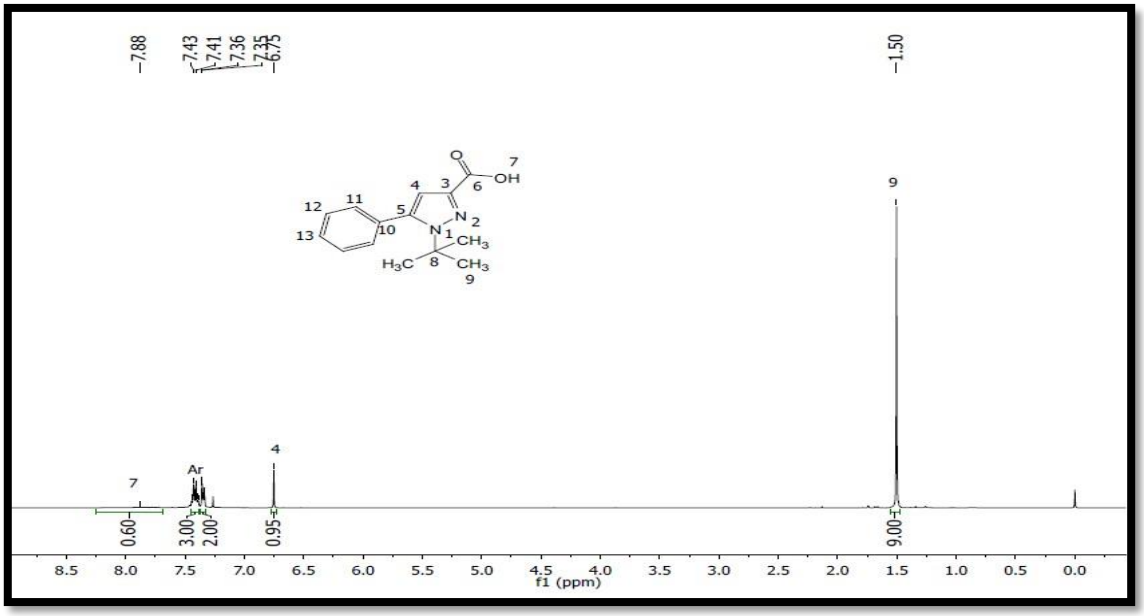


Figure S65: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **6c.**

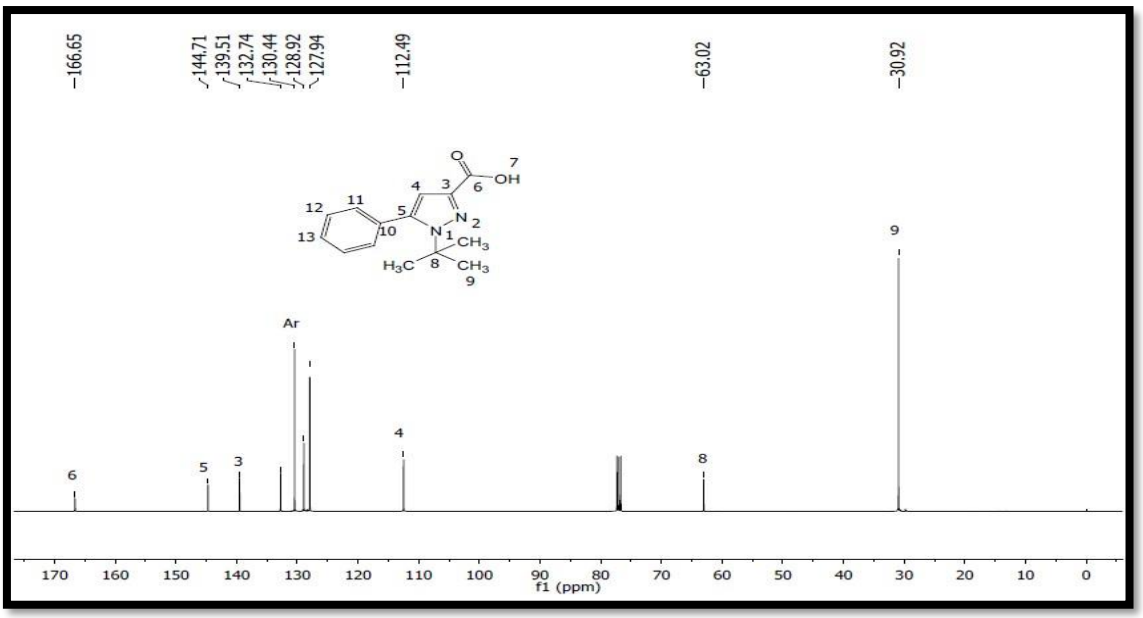


Figure S66: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **6c**.

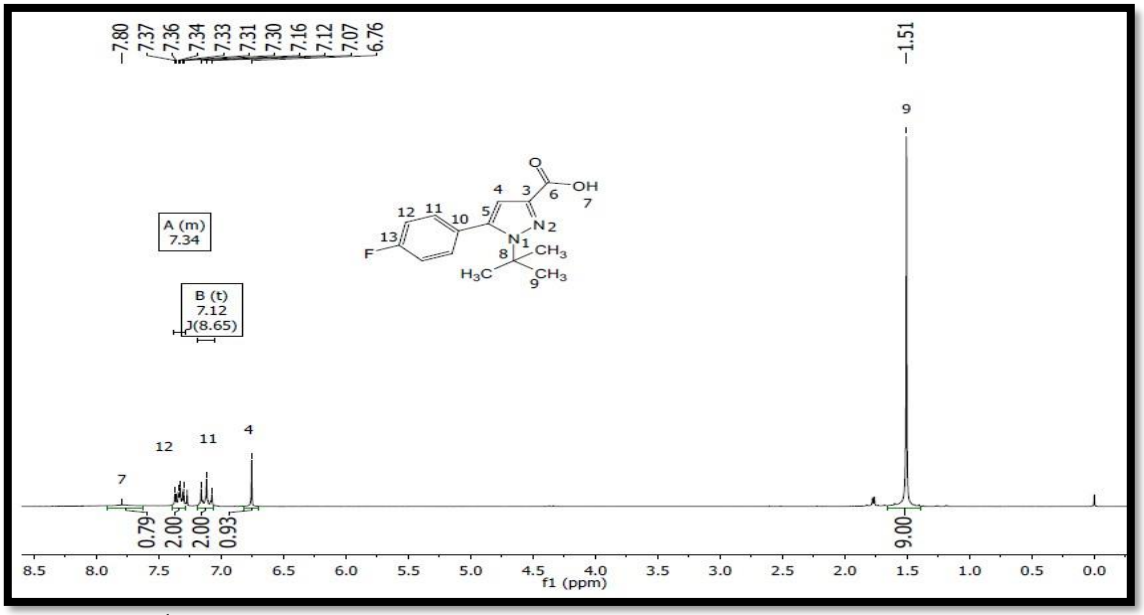


Figure S67: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **6d.**

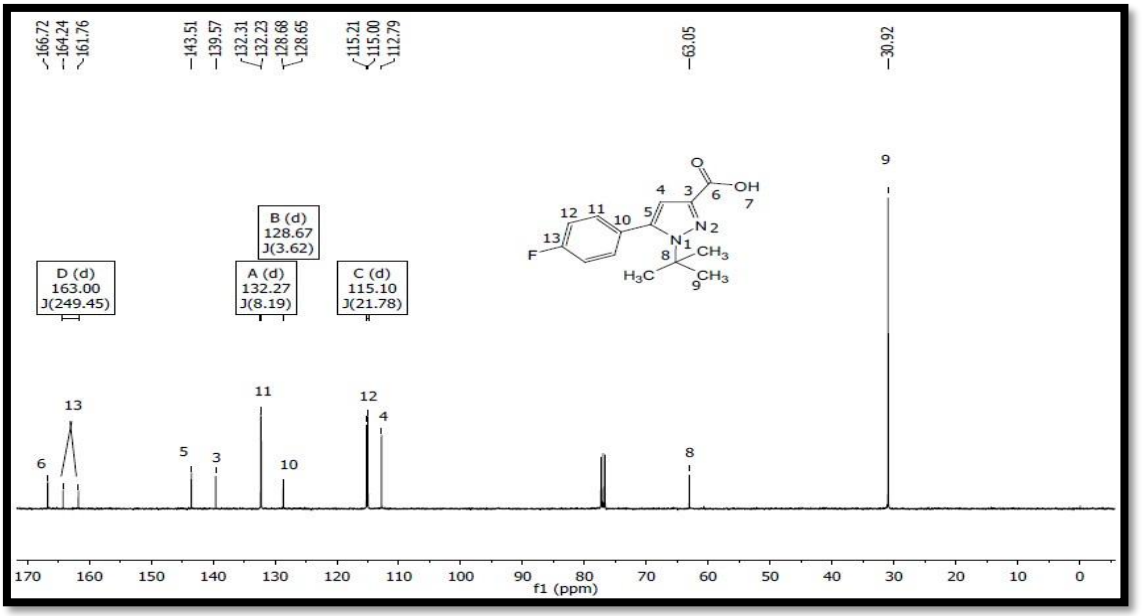


Figure S68: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **6d**.

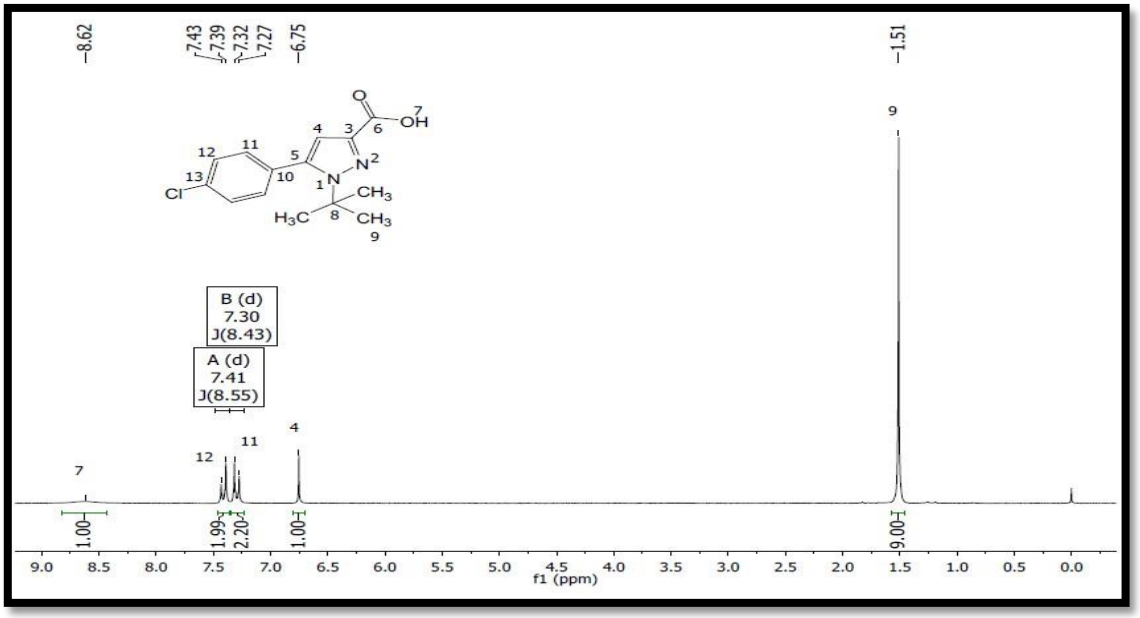


Figure S69: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **6e.**

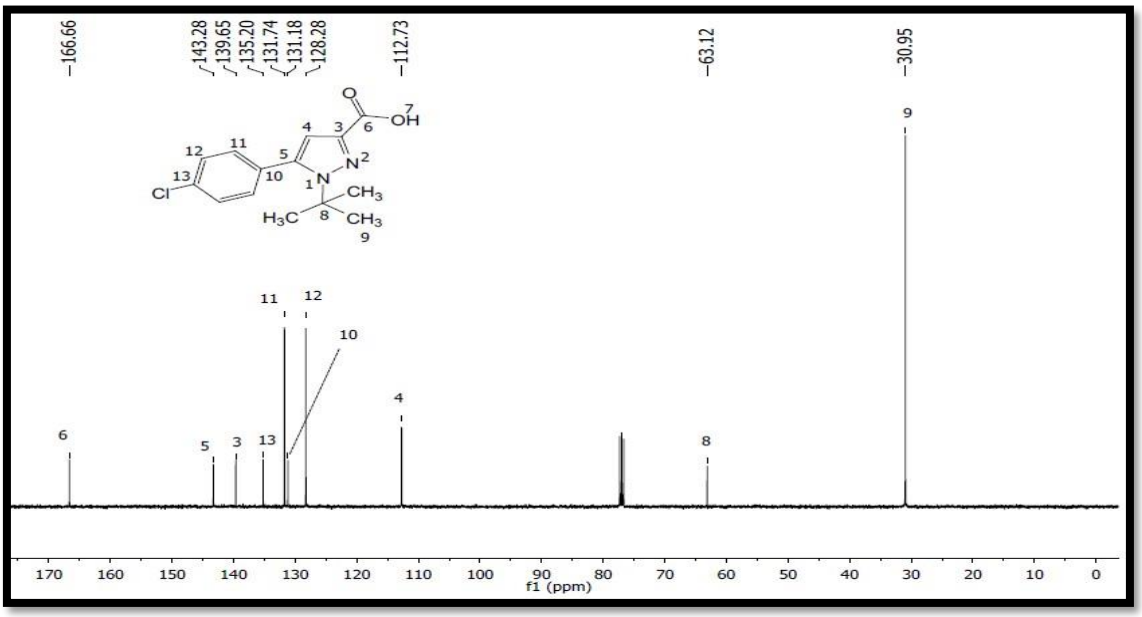


Figure S70: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **6e**.

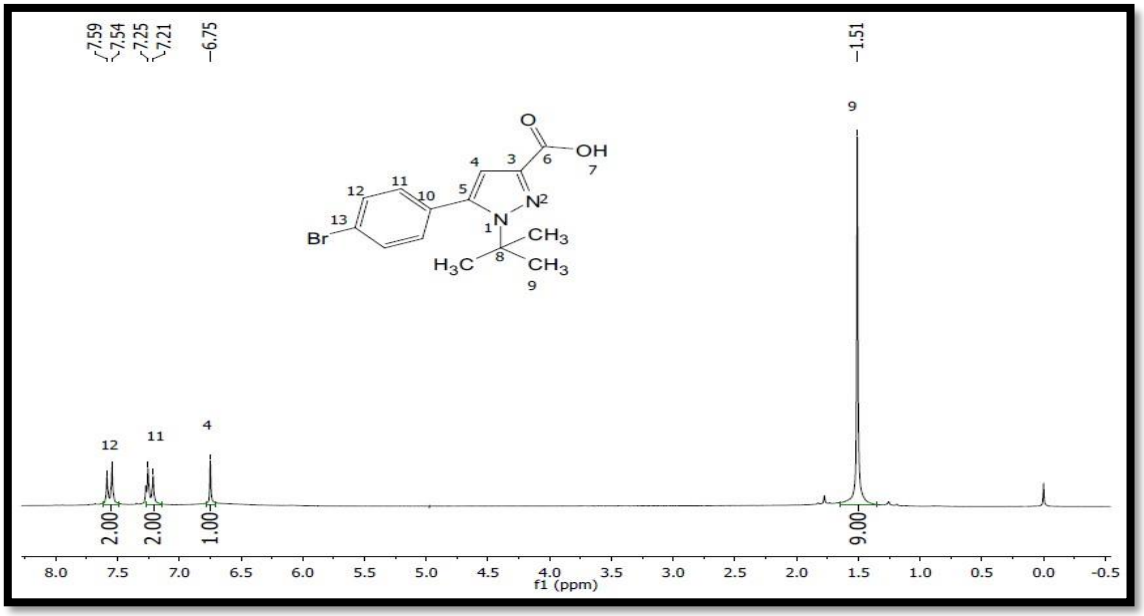


Figure S71: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **6f.**

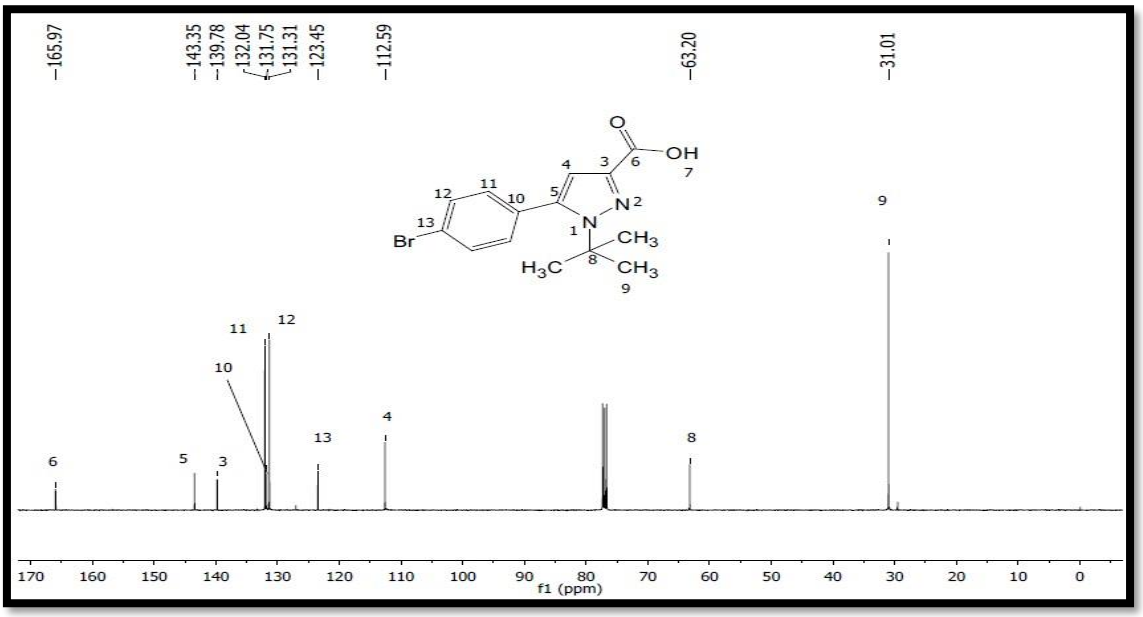


Figure S72: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **6f**.

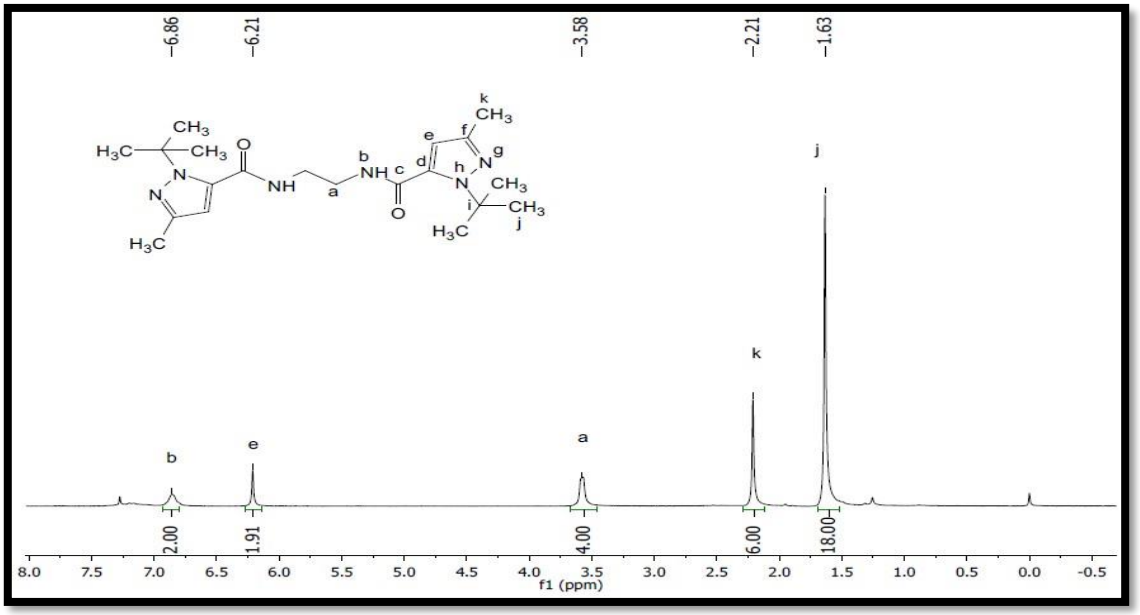


Figure S73: ^{1}H NMR (200 MHz, $CDCl_3$) spectrum of **8a**.

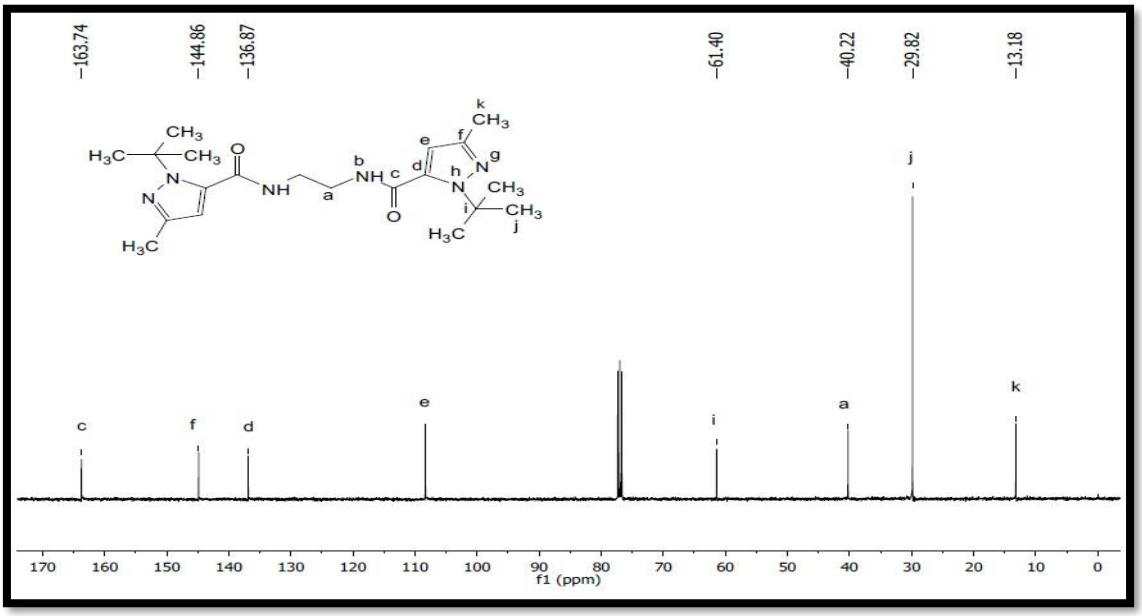


Figure S74: ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **8a**.

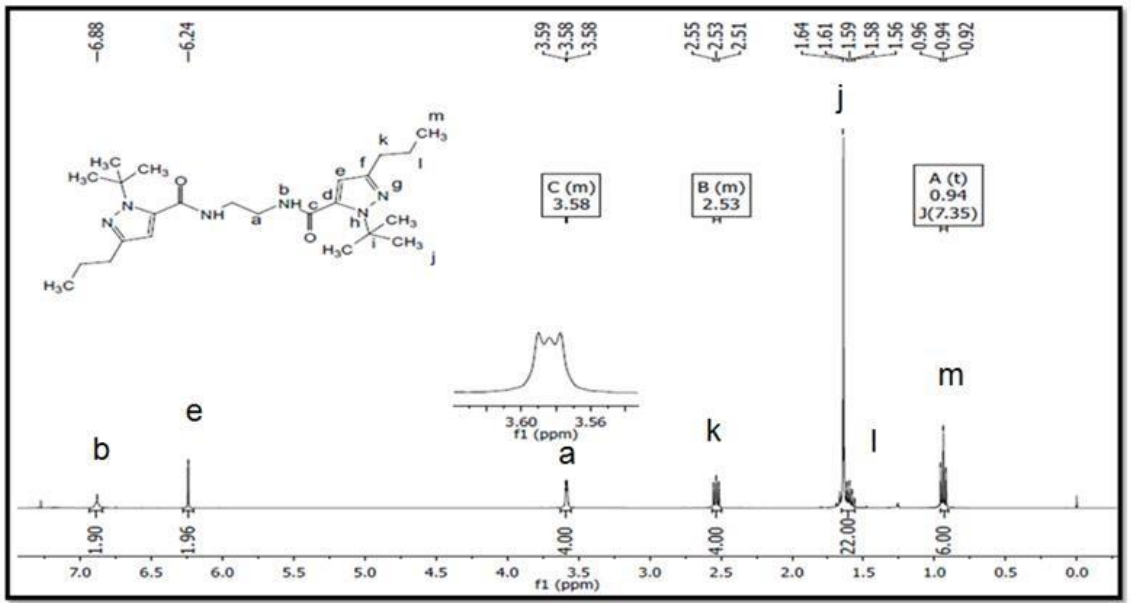


Figure S75: ^{1}H NMR (200 MHz, $CDCl_3$) spectrum of **8b**.

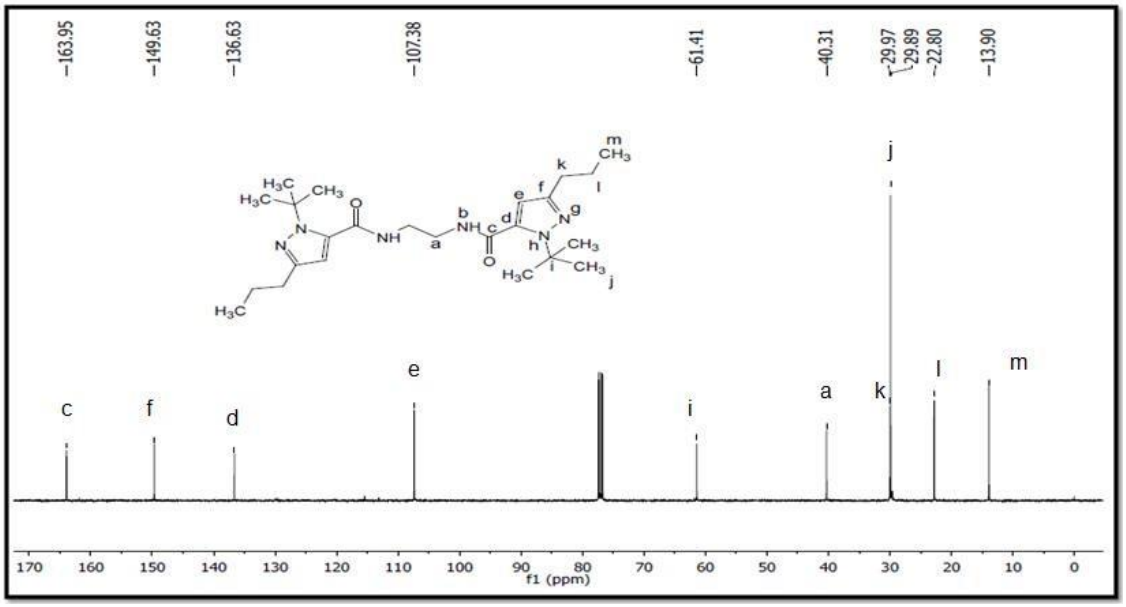


Figure S76: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **8b**.

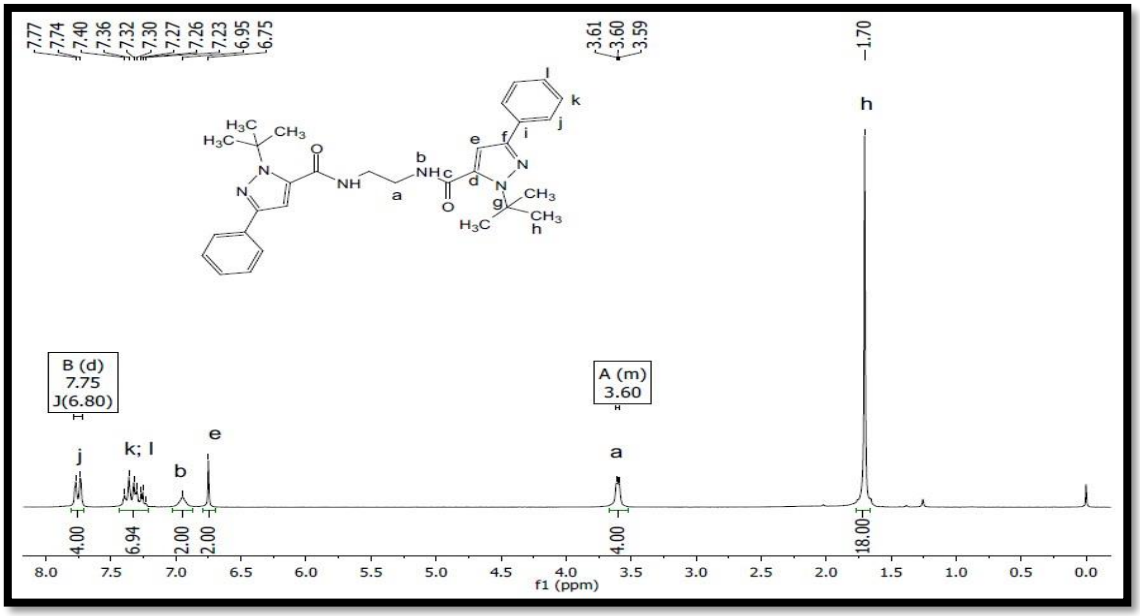


Figure S77: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **8c**.

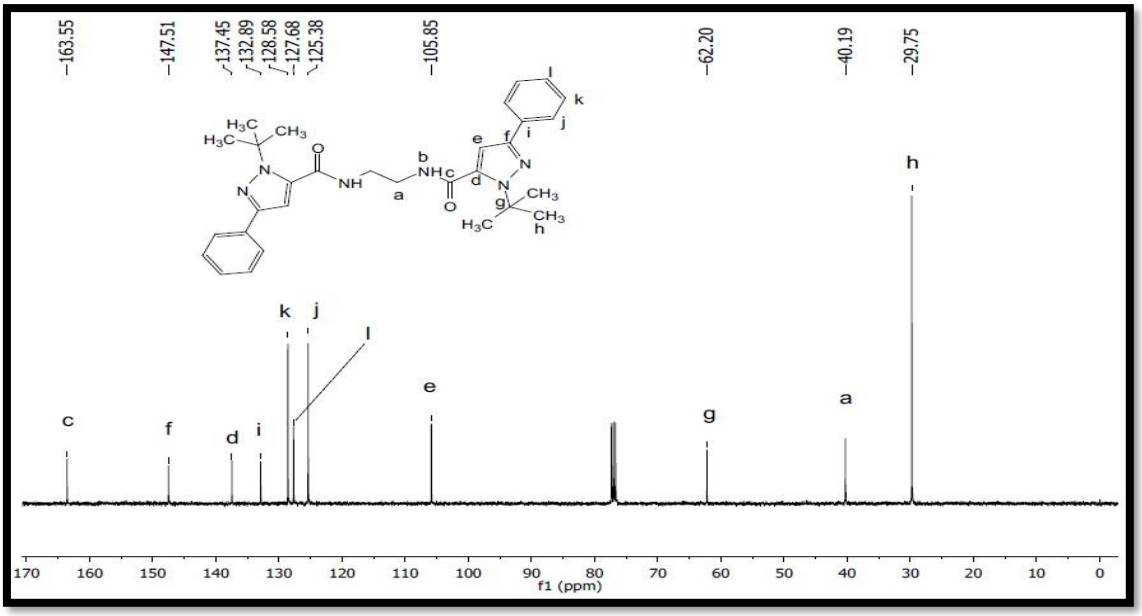


Figure S78: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **8c**.

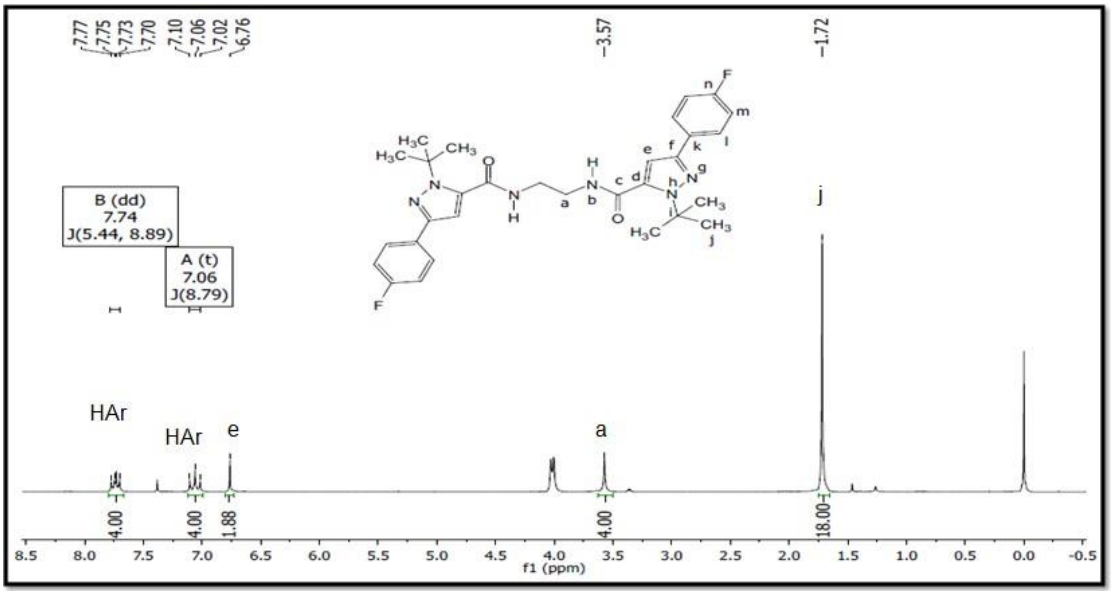


Figure S79: ^{1}H NMR (400 MHz. $CDCl_3$: MeOD (9:1)) spectrum of **8d**.

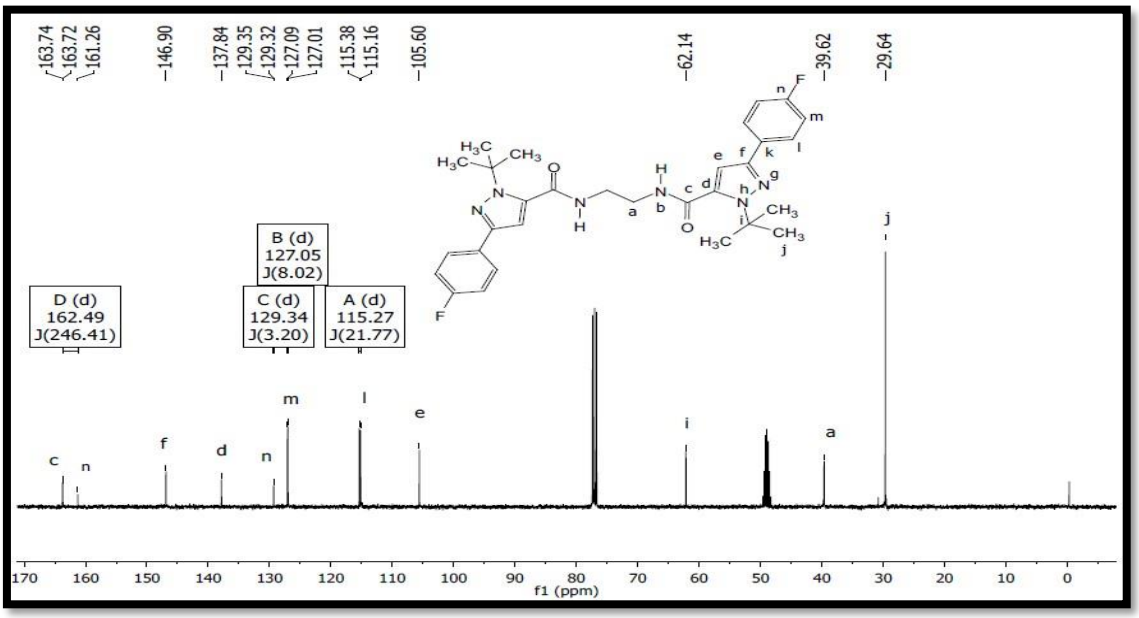


Figure S80: ^{13}C NMR (100 MHz. $CDCl_3$: MeOD (9:1)) spectrum of **8d**.

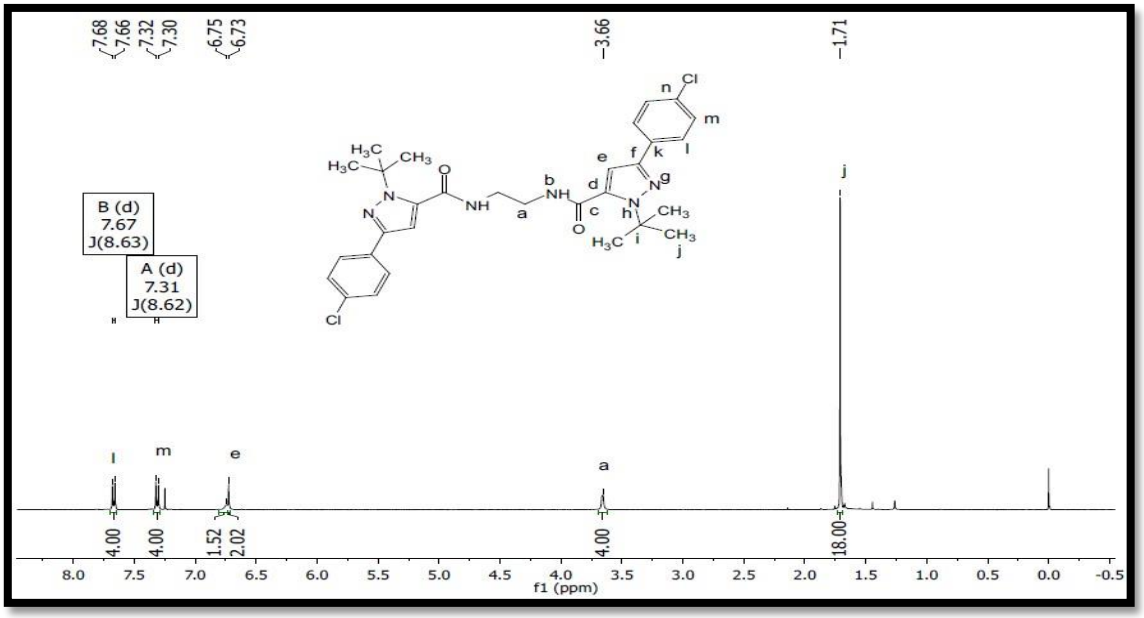


Figure S81: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **8e.**

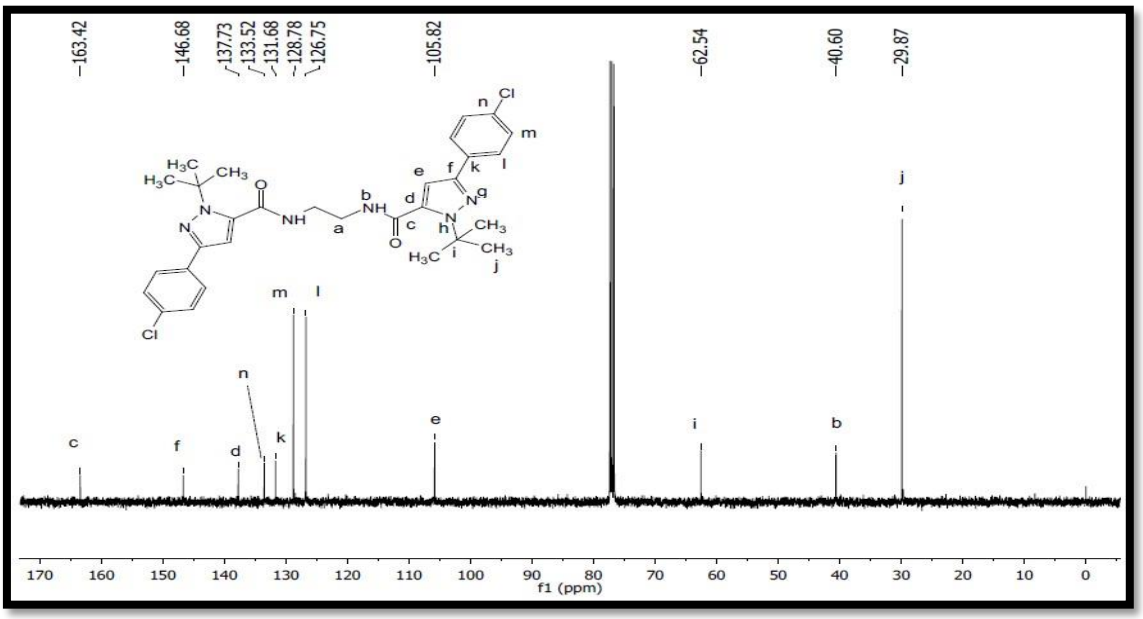


Figure S82: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **8e.**

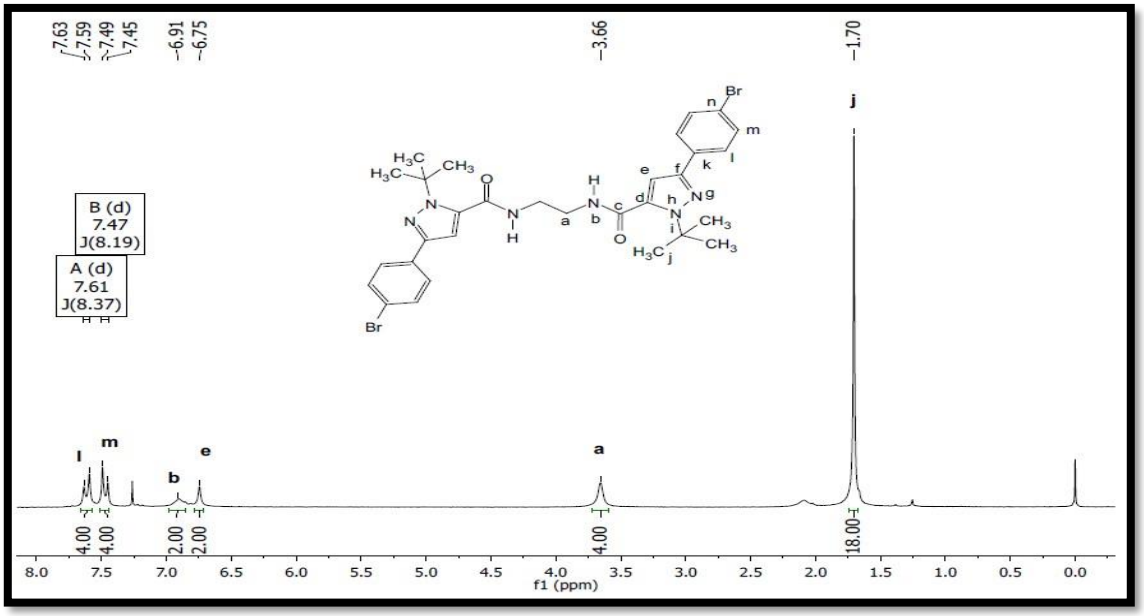


Figure S83: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **8f.**

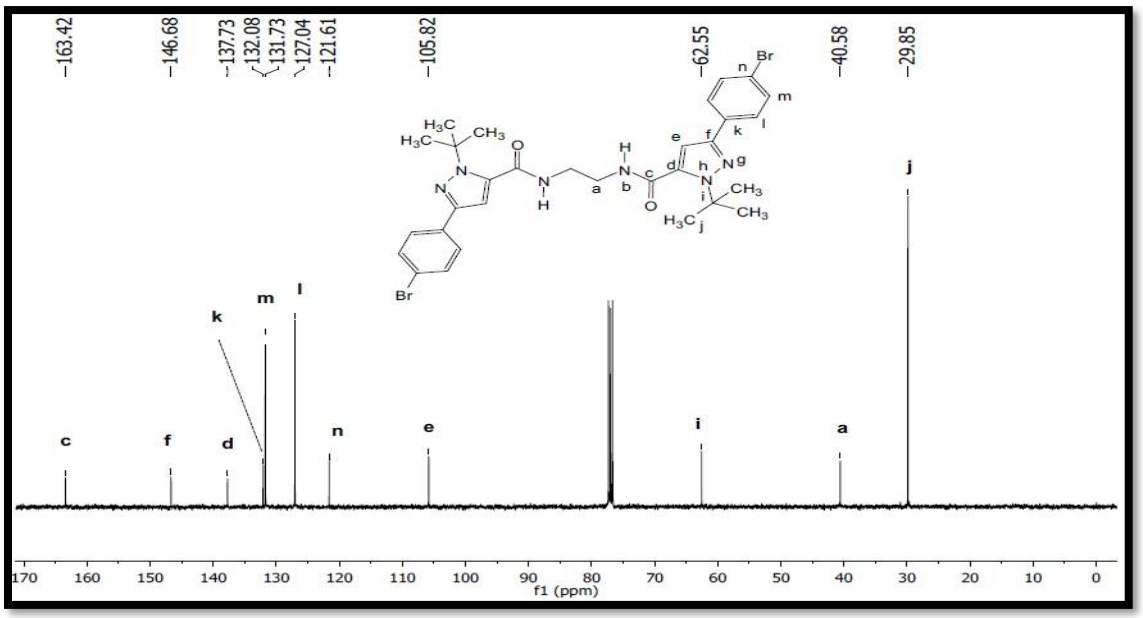


Figure S84: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **8f.**

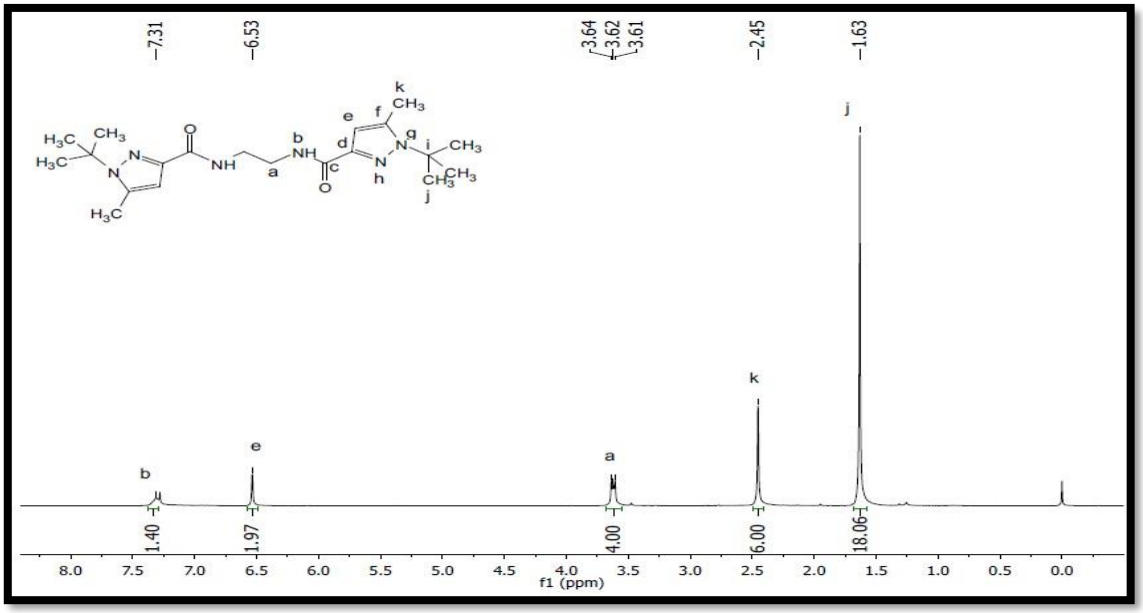


Figure S85: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **9a.**

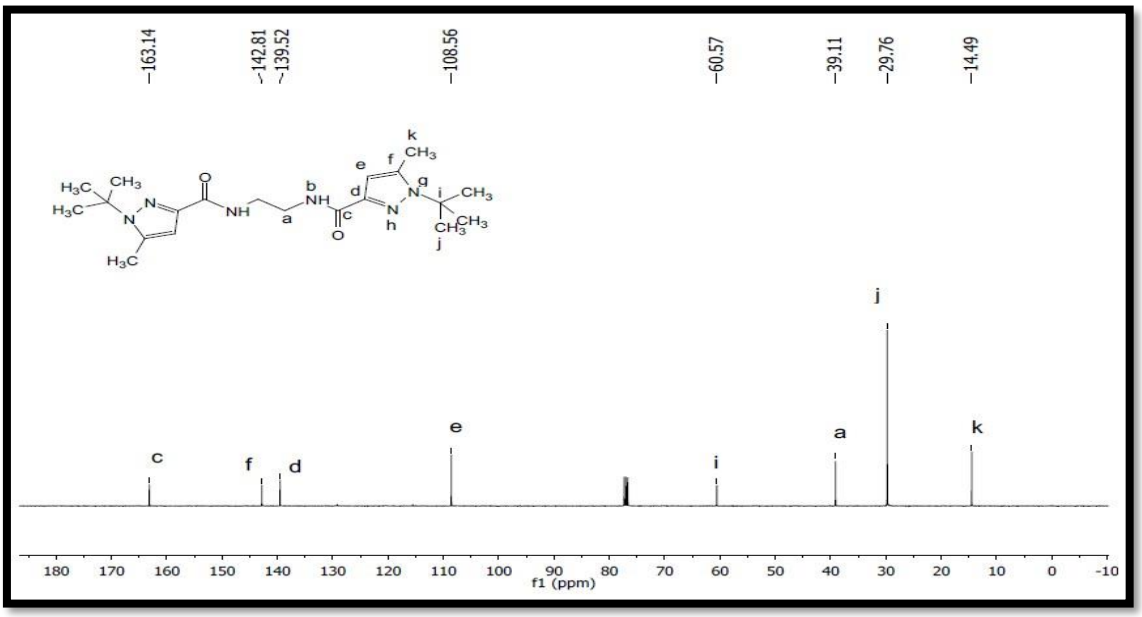


Figure S86: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **9a**.

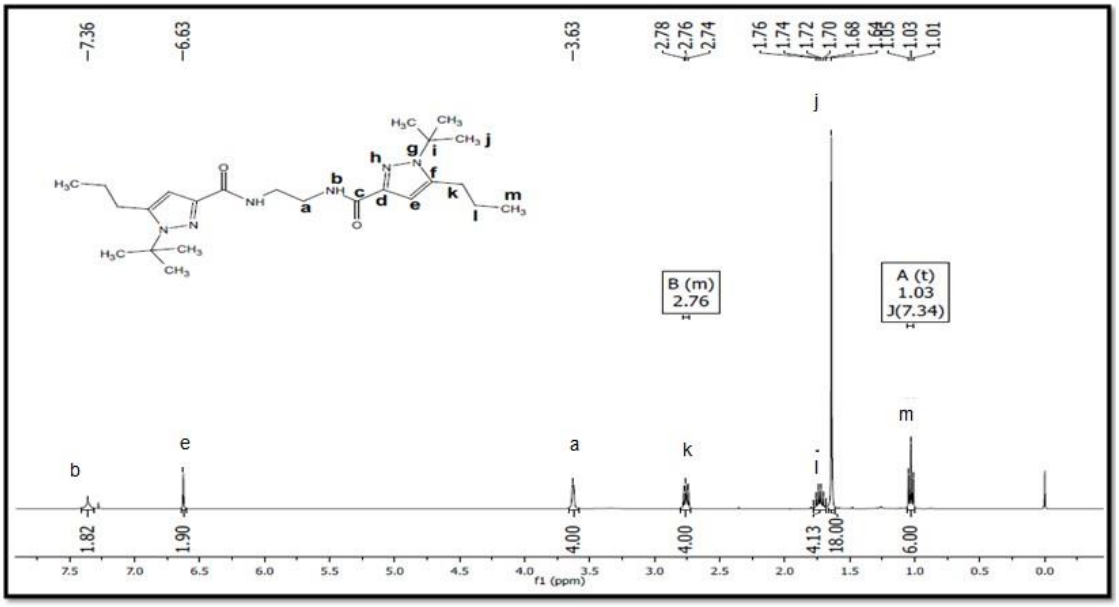


Figure S87: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **9b.**

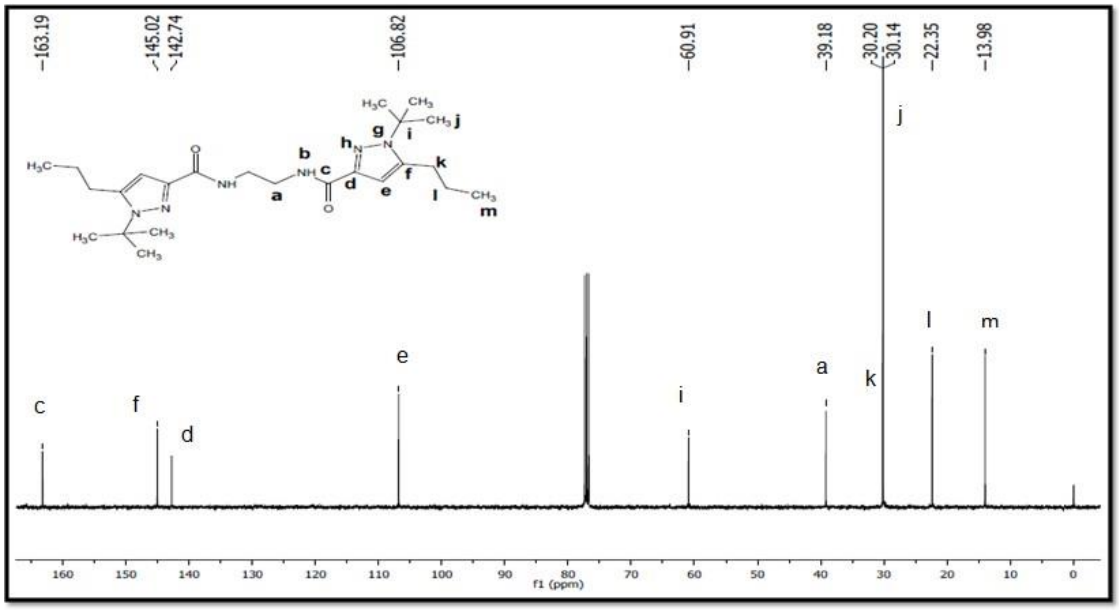


Figure S88: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **9b**.

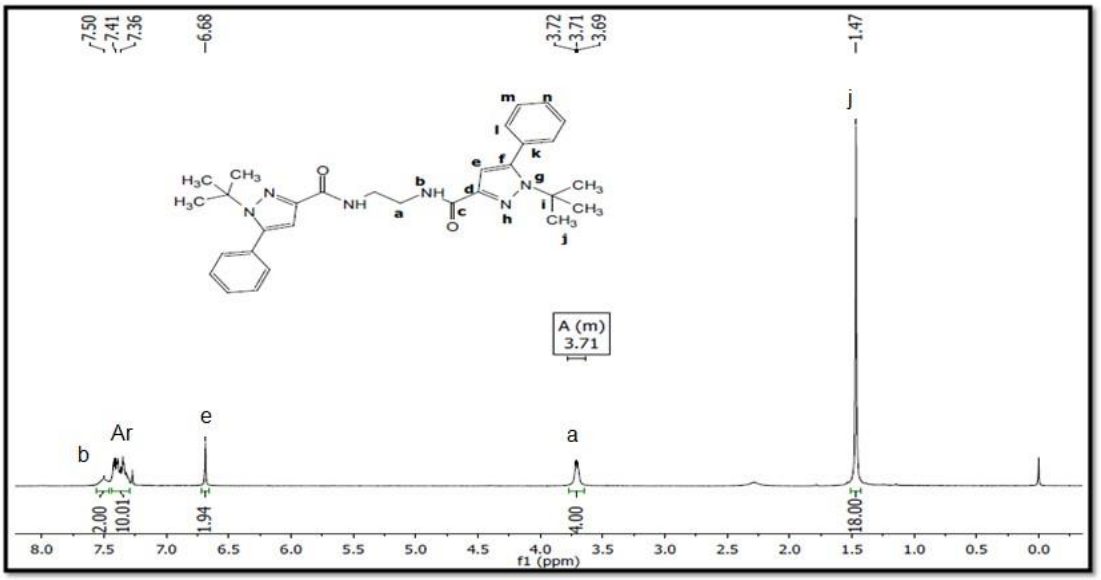


Figure S89: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **9c.**

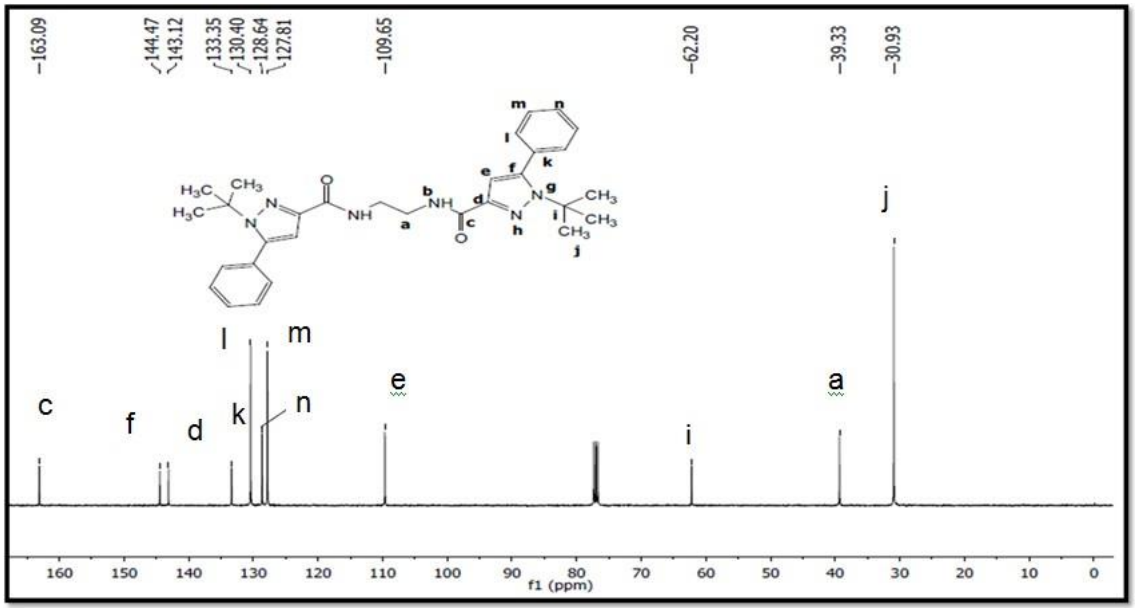


Figure S90: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **9c**.

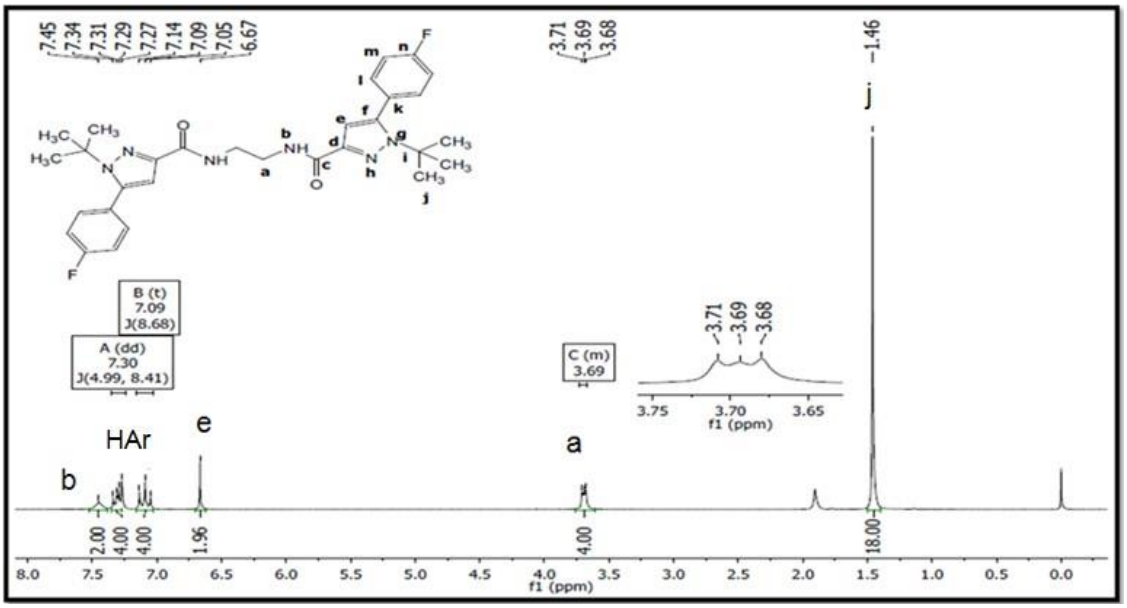


Figure S91: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **9d**.

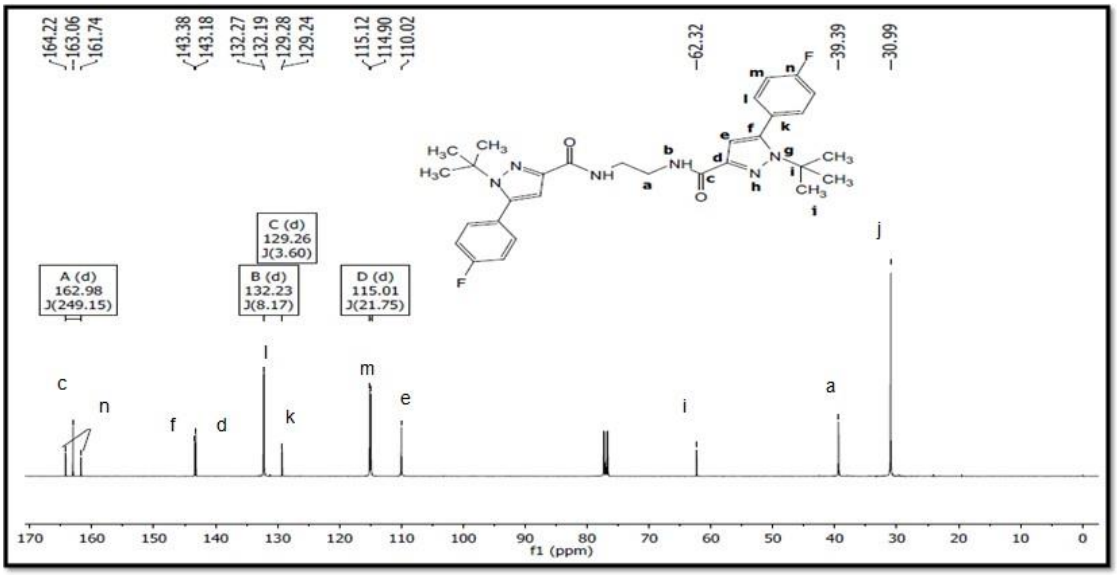


Figure S92: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **9d**.

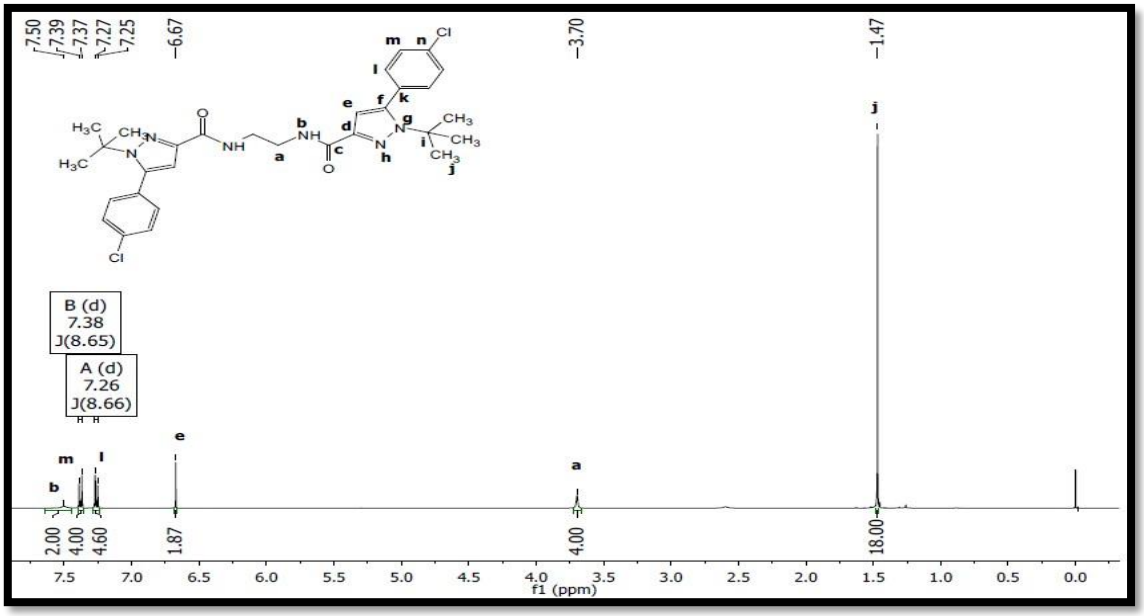


Figure S93: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **9e**.

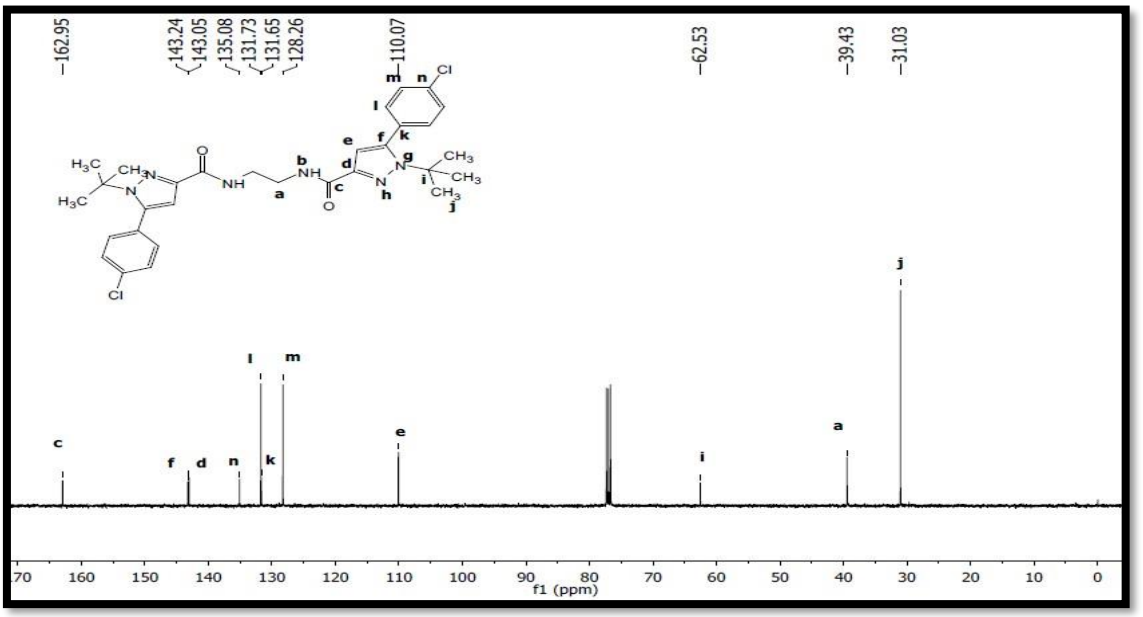


Figure S94: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **9e**.

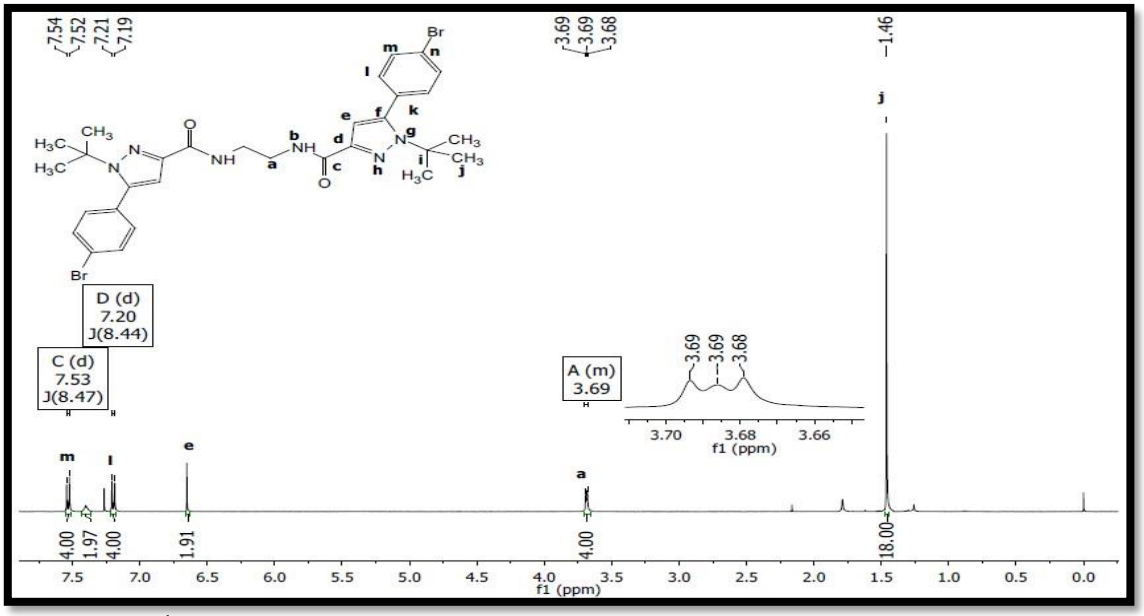


Figure S95: ^{1}H NMR (200 MHz. $CDCl_3$) spectrum of **9f**.

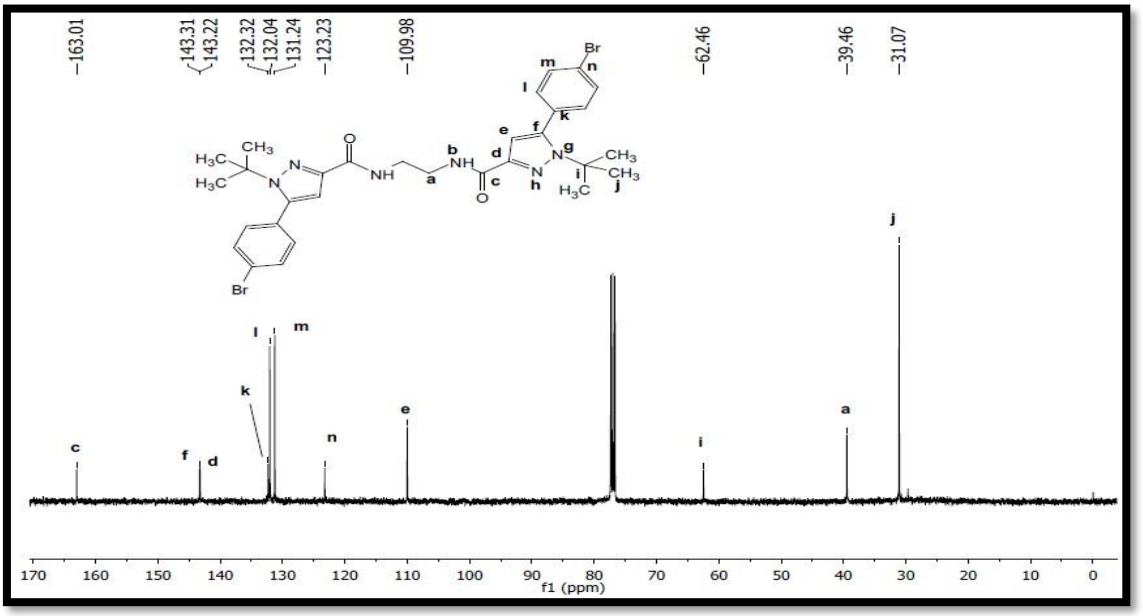


Figure S96: ^{13}C NMR (100 MHz. $CDCl_3$) spectrum of **9f**.

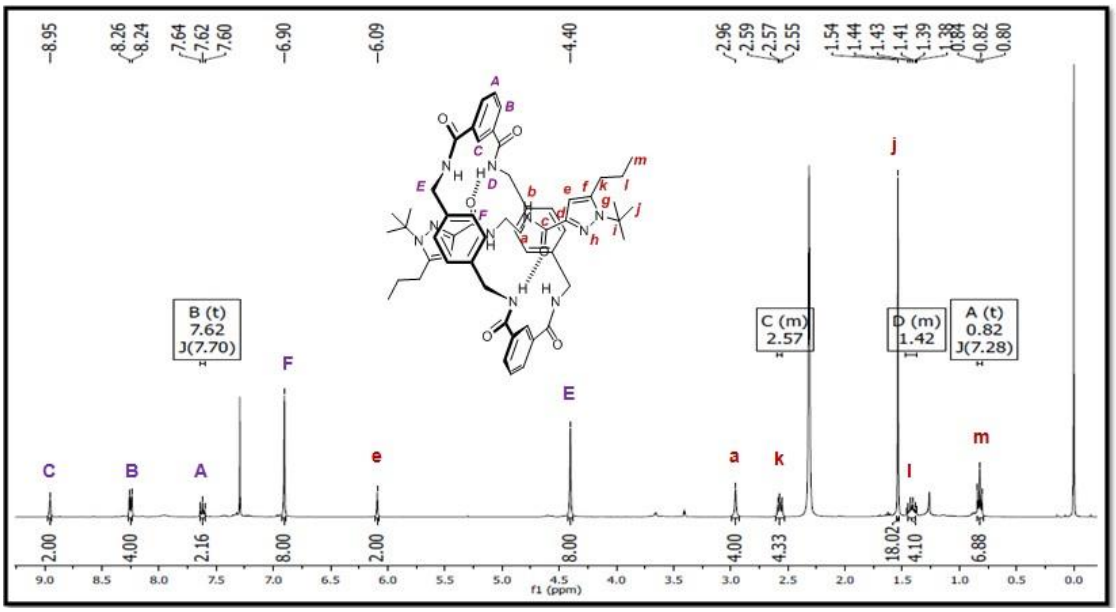


Figure S97: ^{1}H NMR (400 MHz. $CDCl_3$:MeOD (9:1)) spectrum of **10b**.

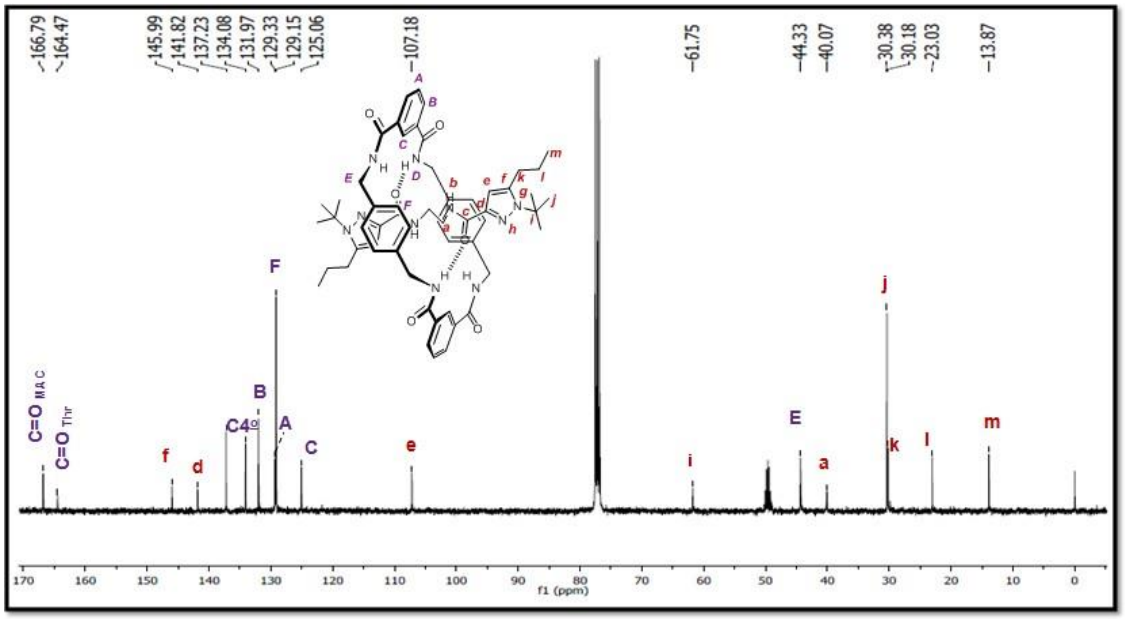


Figure S98: ^{13}C NMR (100 MHz. $CDCl_3$:MeOD (9:1).) spectrum of **10b**.

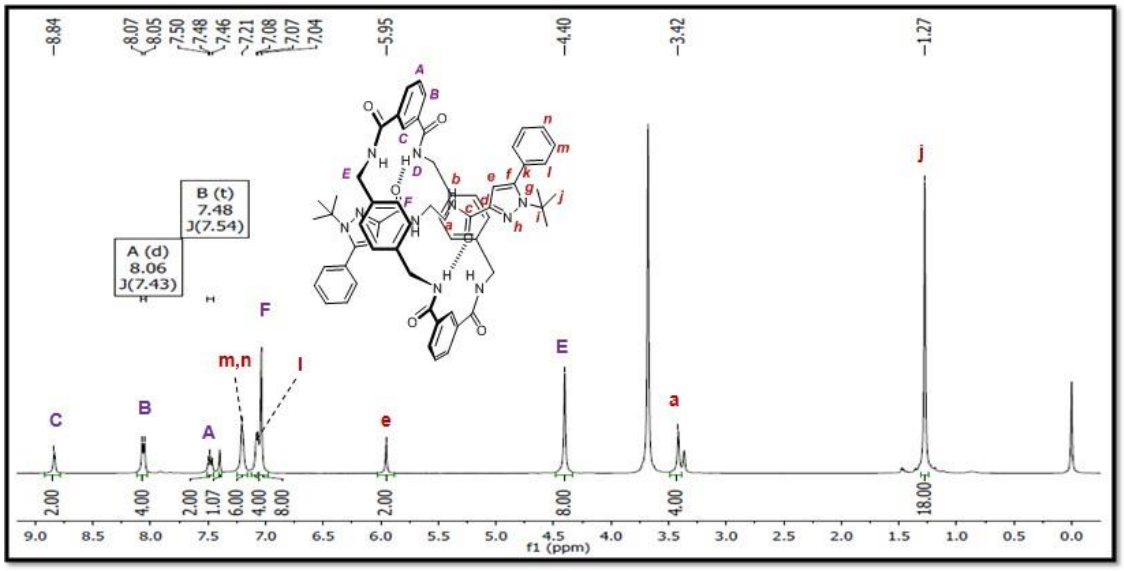


Figure S99: ^{1}H NMR (400 MHz. $CDCl_3$:MeOD (9:1)) spectrum of **10c**.

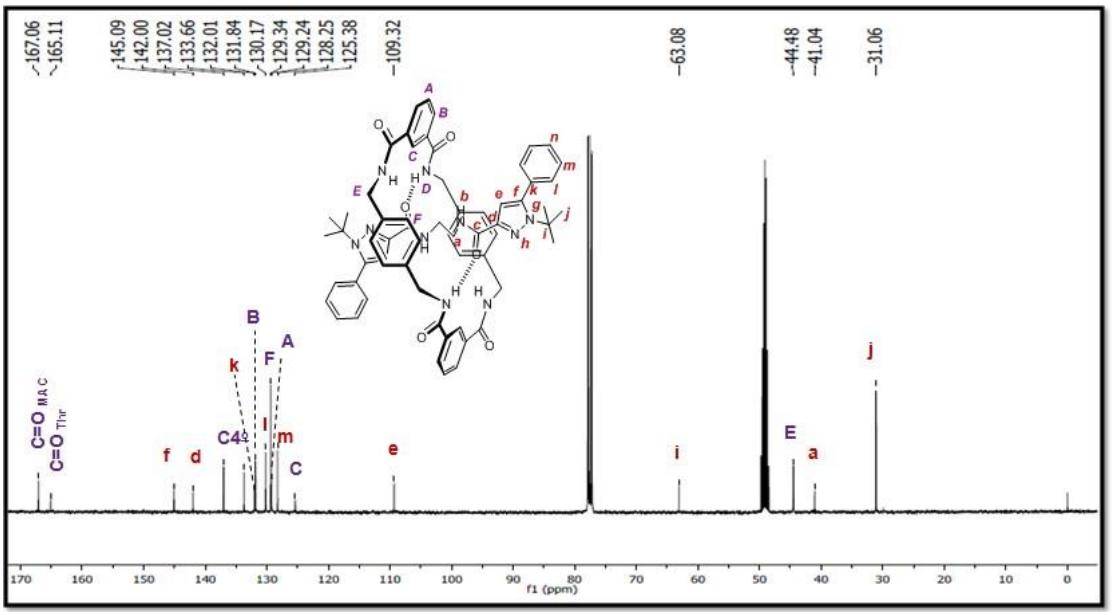


Figure S100: ^{13}C NMR (100 MHz. $CDCl_3$:MeOD (9:1).) spectrum of **10c**.

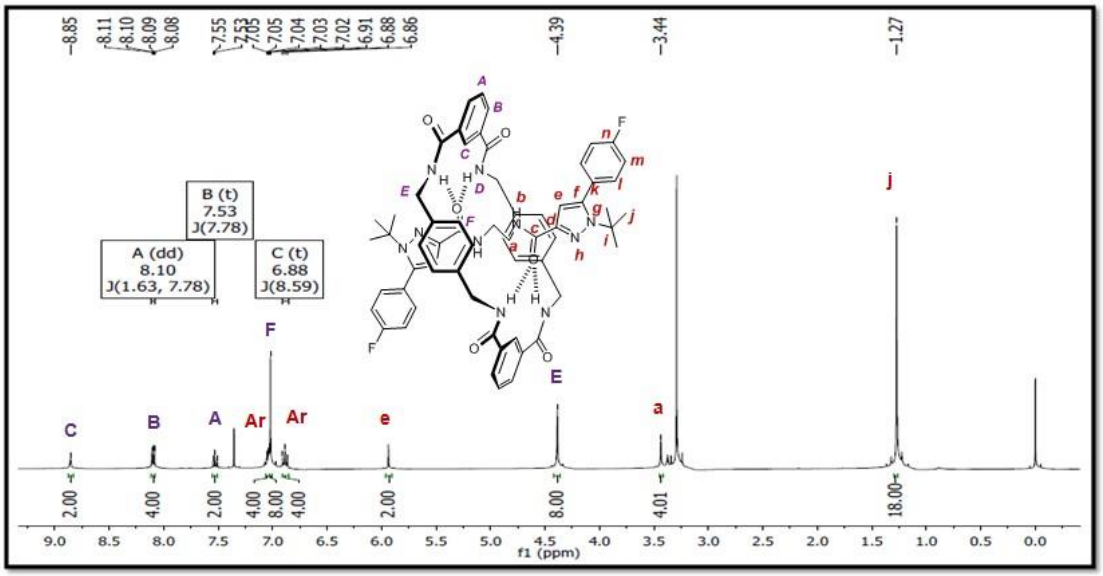


Figure S101: ^{1}H NMR (400 MHz. $CDCl_3$:MeOD (9:1)) spectrum of **10d**.

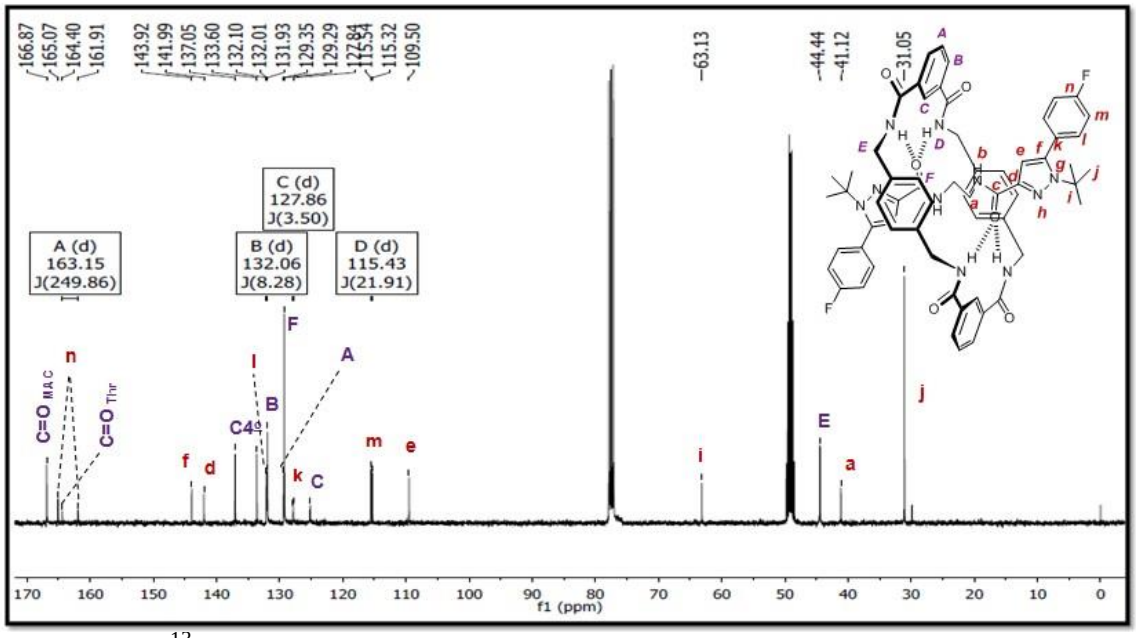


Figure S102: ^{13}C NMR (100 MHz. $CDCl_3$:MeOD (9:1).) spectrum of **10d**.

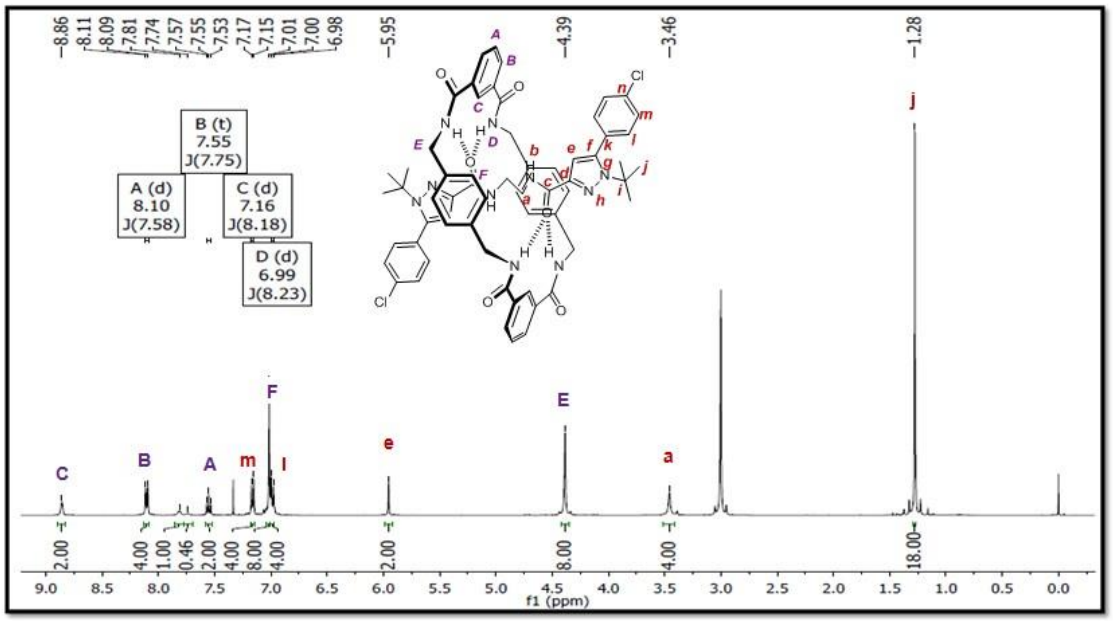


Figure S103: ^{1}H NMR (400 MHz. $CDCl_3$:MeOD (9:1)) spectrum of **10e**.

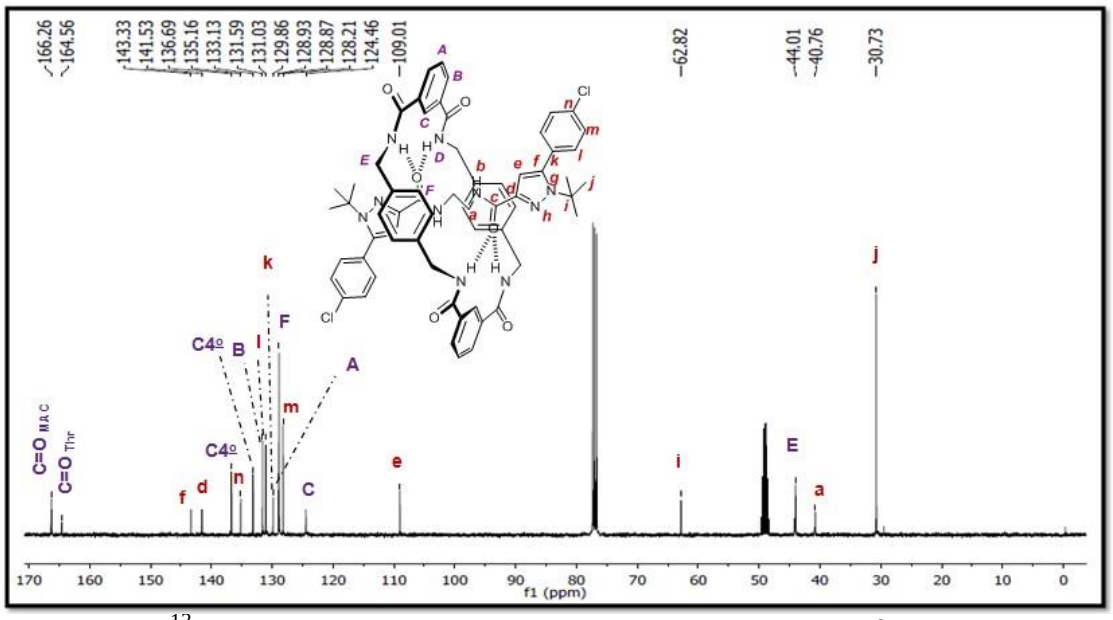


Figure S104: ^{13}C NMR (100 MHz. $CDCl_3$:MeOD (9:1).) spectrum of **10e**.

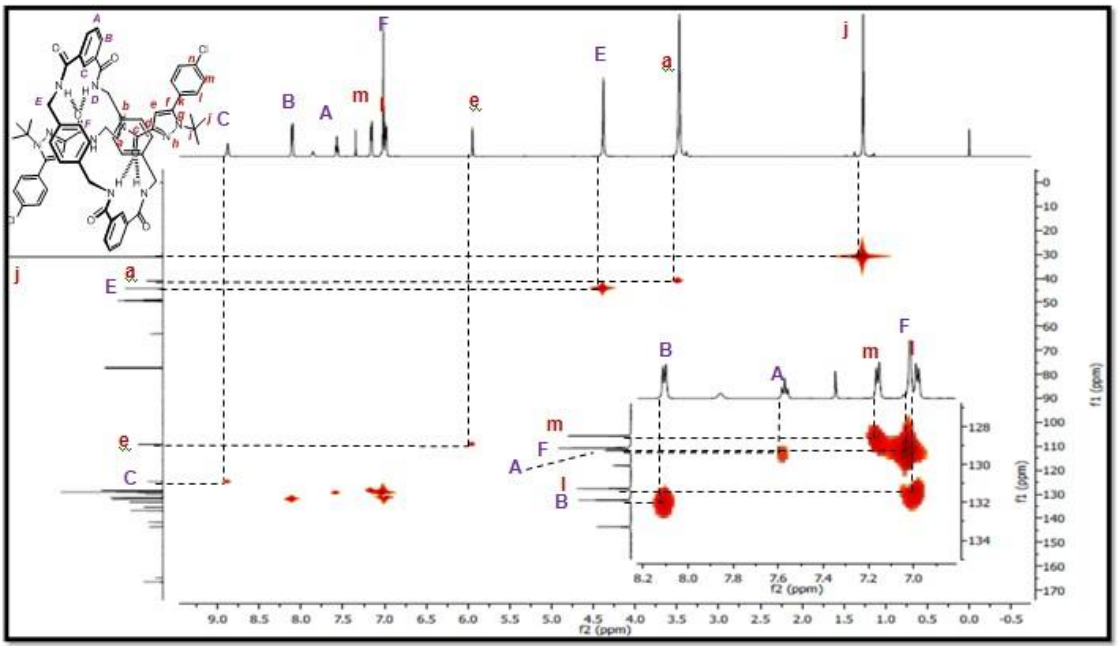


Figure S105: HMQC NMR (600 MHz. $CDCl_3$:MeOD (9:1)) spectrum of **10e**.

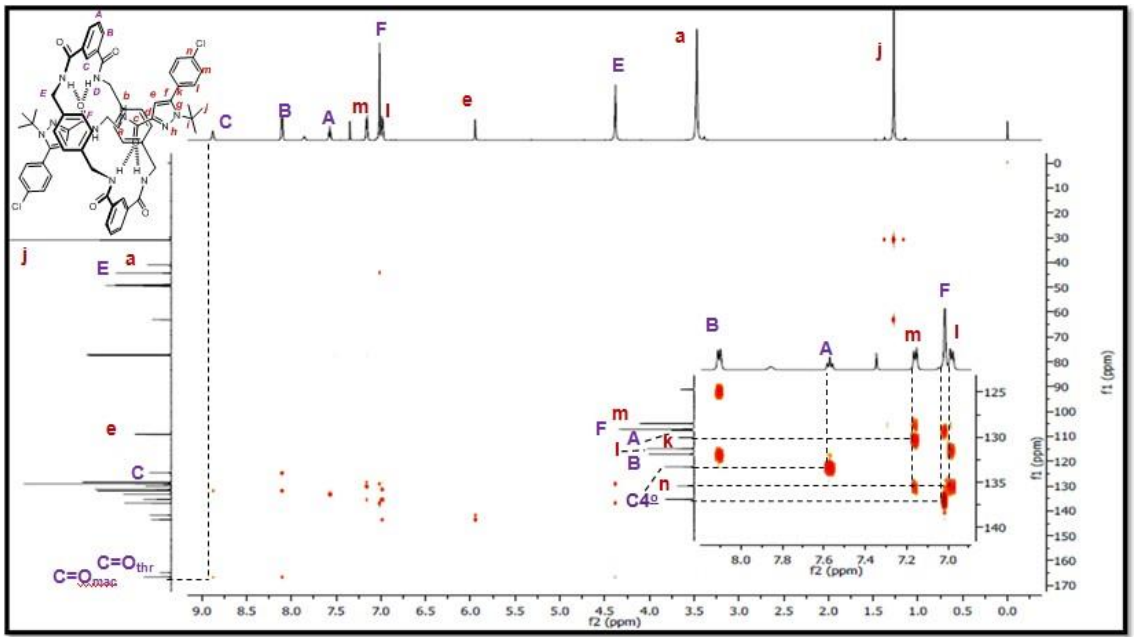


Figure S106: HMBC NMR (600 MHz. $CDCl_3$:MeOD (9:1)) spectrum of **10e**.

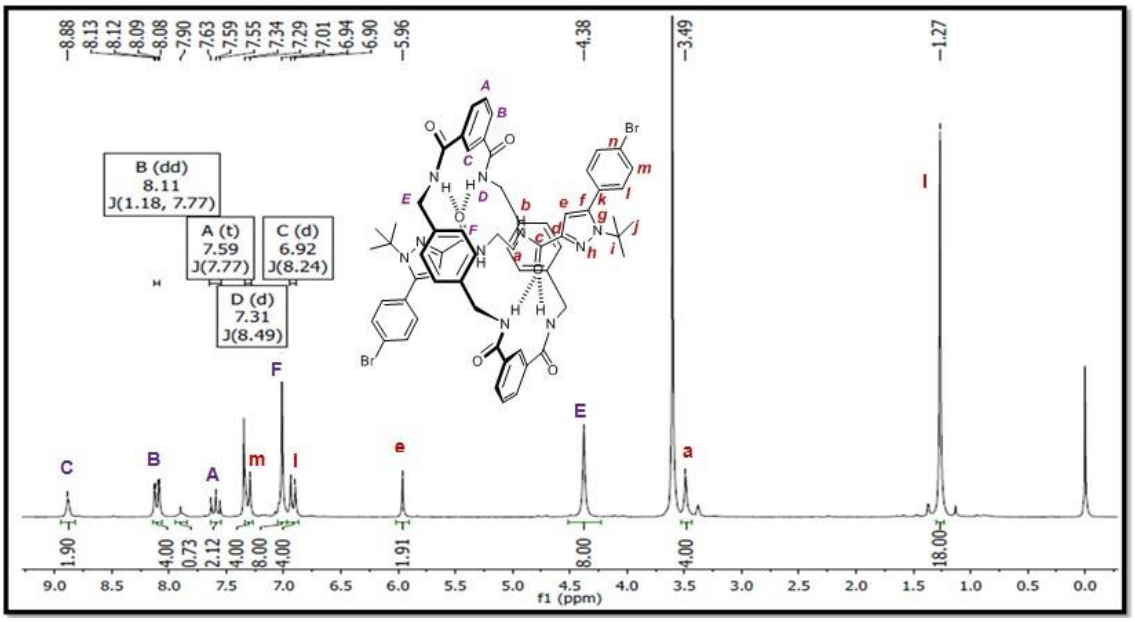


Figure S107: ^{1}H NMR (400 MHz. $CDCl_3$:MeOD (9:1)) spectrum of **10f**.

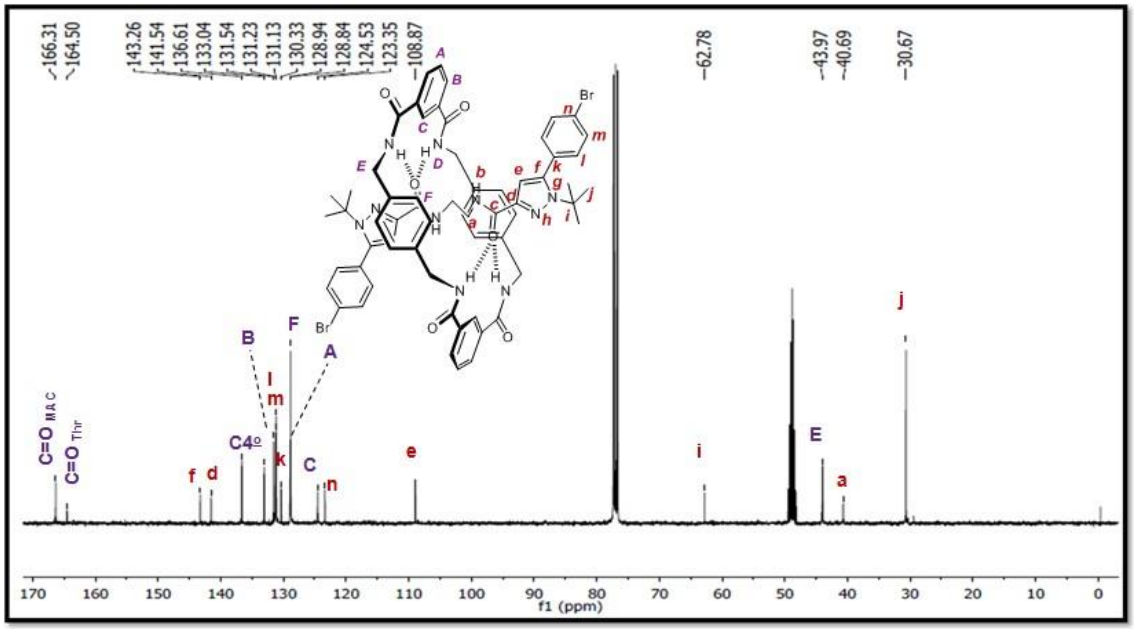


Figure S108: ^{13}C NMR (100 MHz. $CDCl_3$:MeOD (9:1)) spectrum of **10f.**

5.2 Thermogravimetric analysis

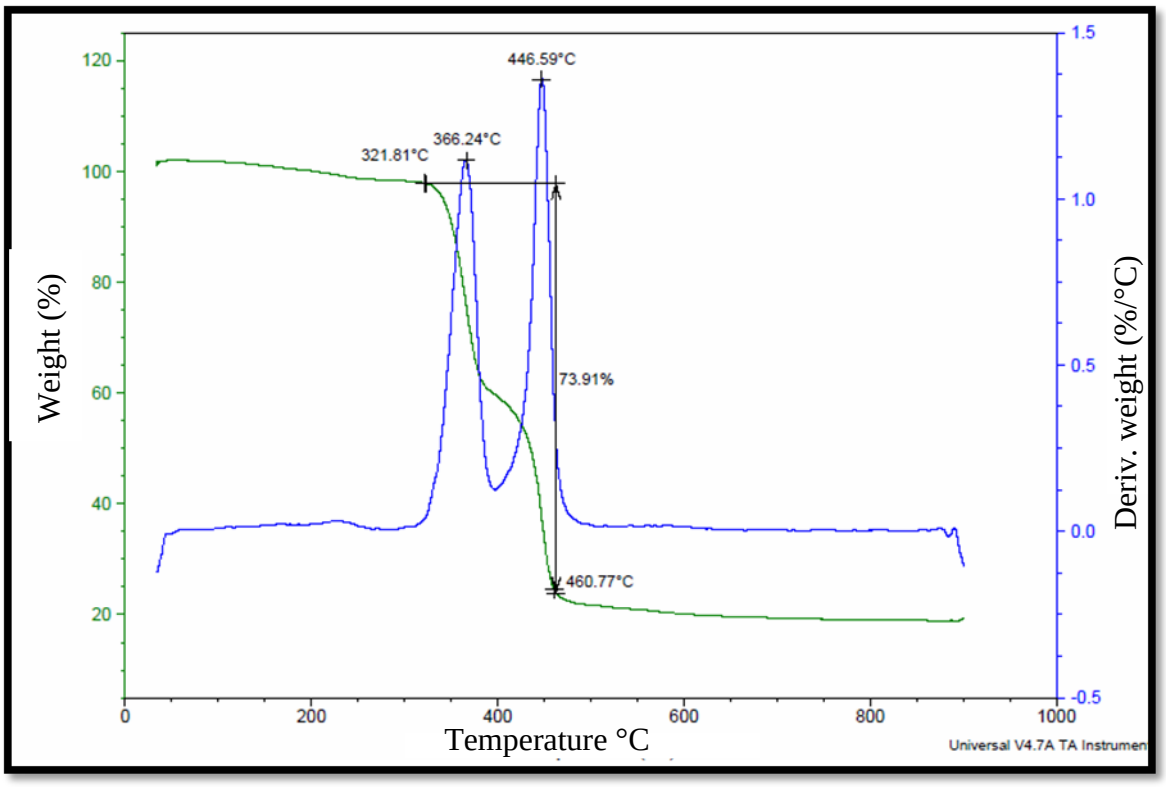


Figure S109. Thermogram of compound **10b** (10 ºC/min; N2flow).

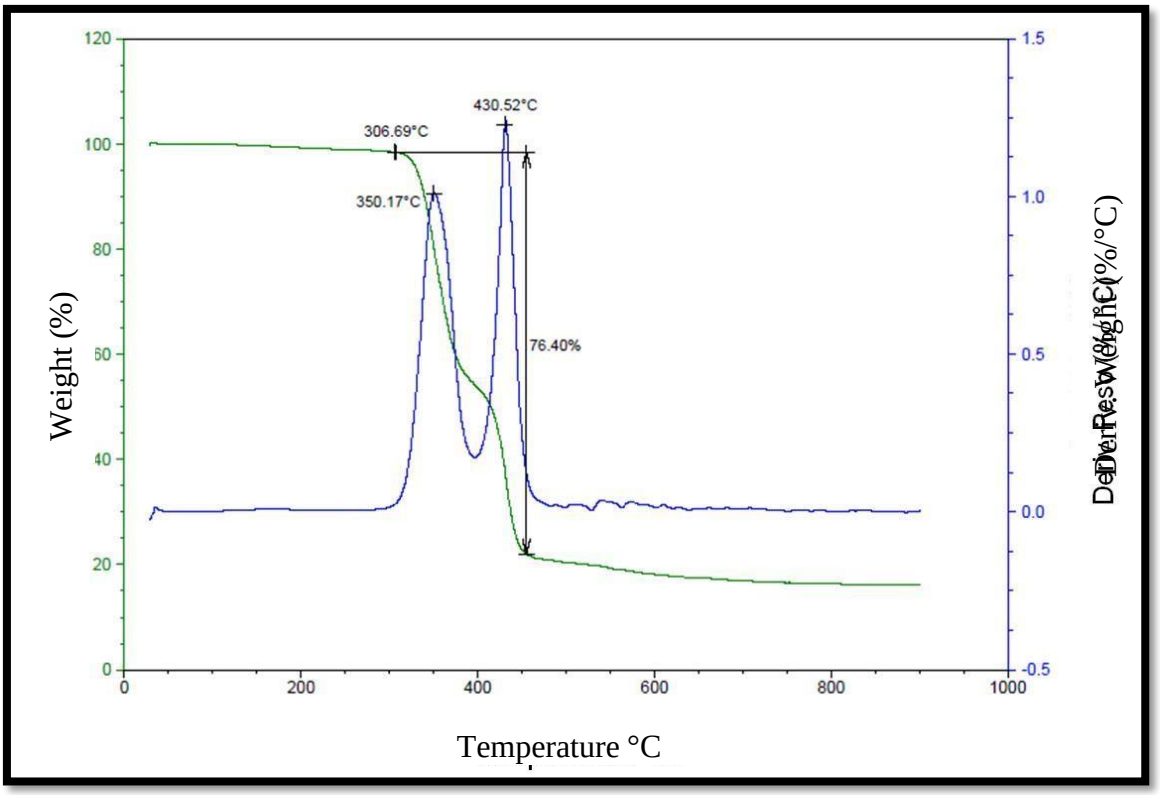


Figure S110. Thermogram of compound **10c** (10 ºC/min; N2flow).

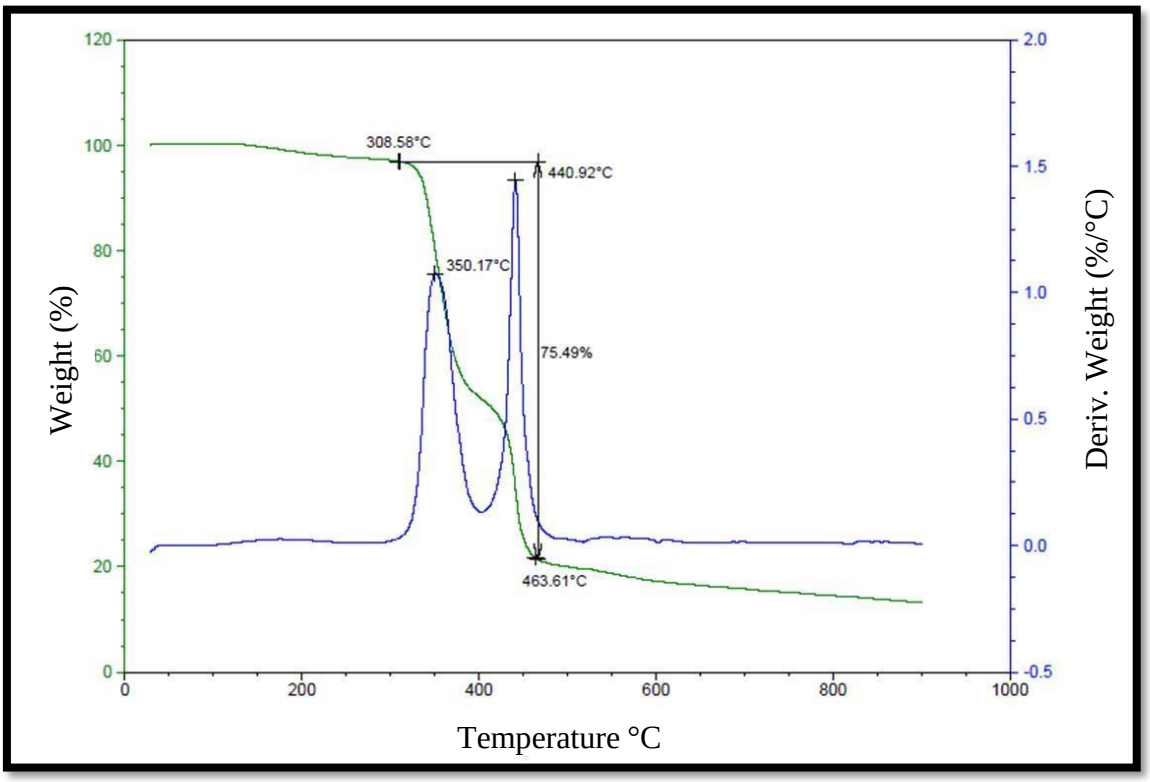


Figure S111 Thermogram of compound **10d** (10 ºC/min; N2flow).

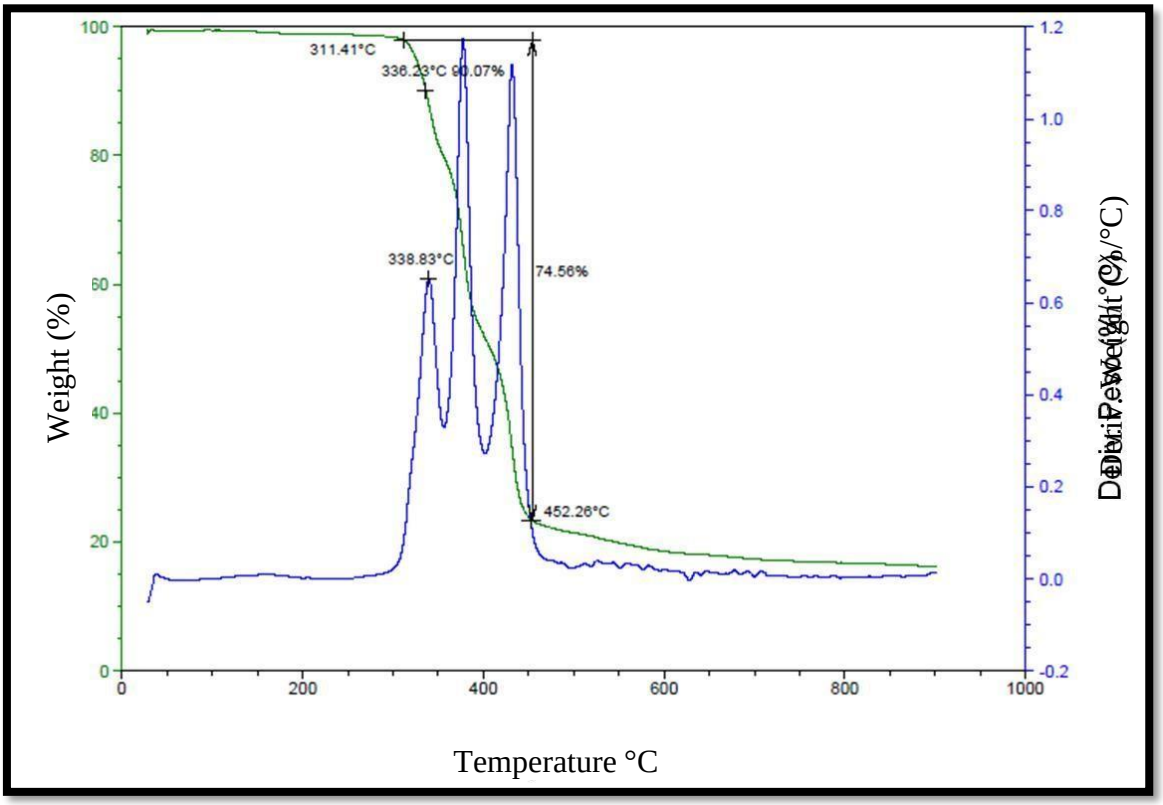


Figure S112. Thermogram of compound **10e** (10 ºC/min; N2flow).

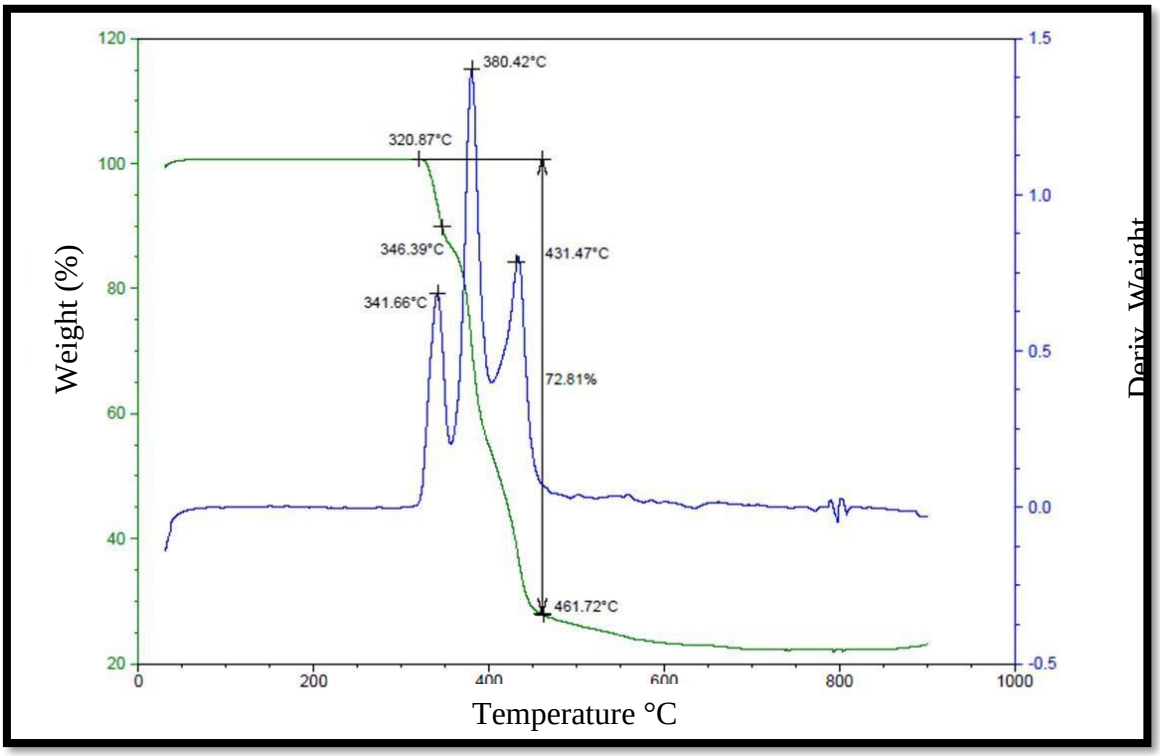


Figure S113 Thermogram of compound **10f** (10 ºC/min; N2 flow).

5.3 Mass spectra

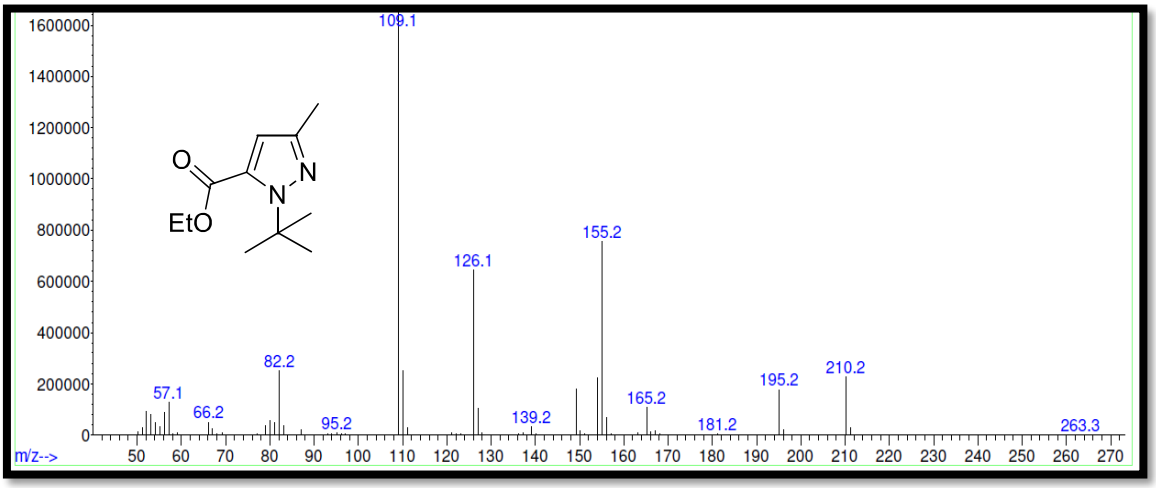


Figure S114: CG-MS Mass spectra of **3a**.

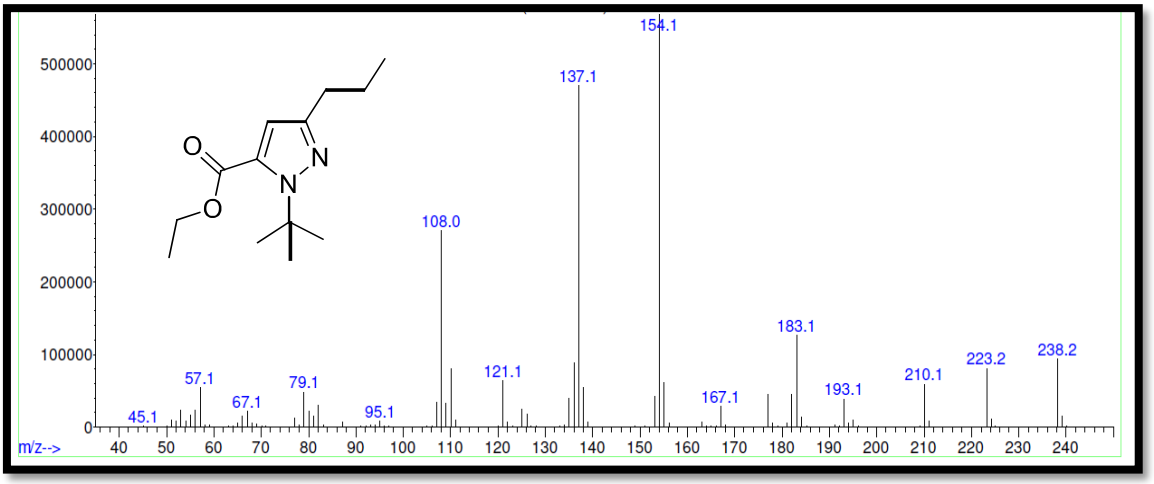


Figure S115: CG-Ms Mass spectra of **3b**.

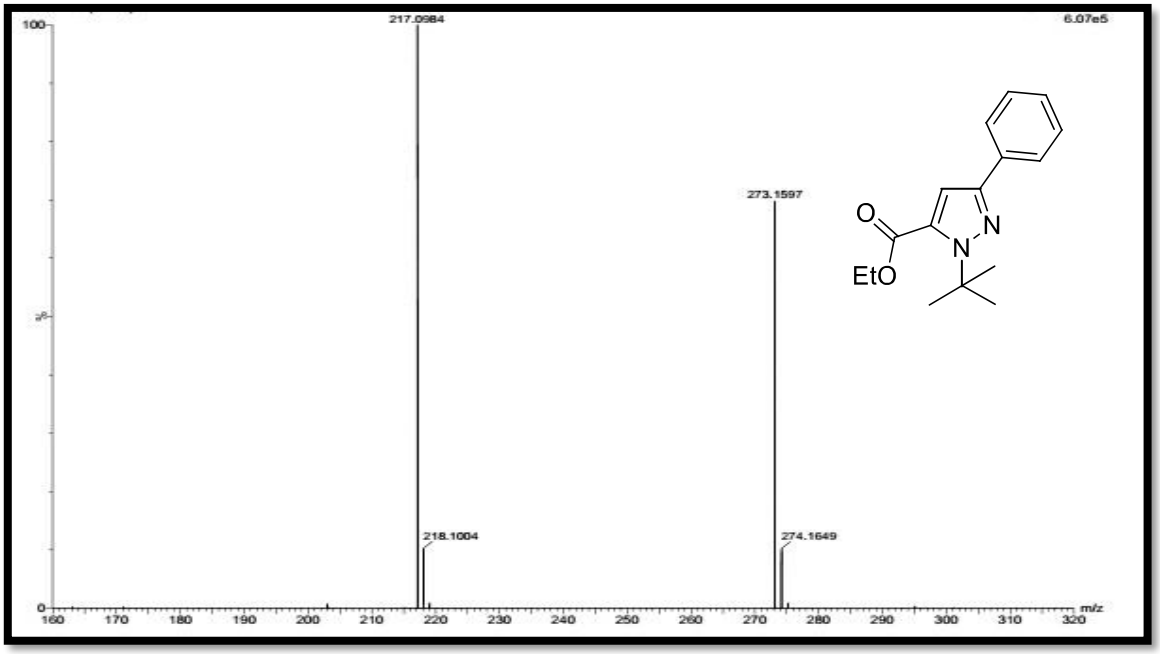


Figure S116: HRMS ESI-TOF Mass spectra of **3c**.

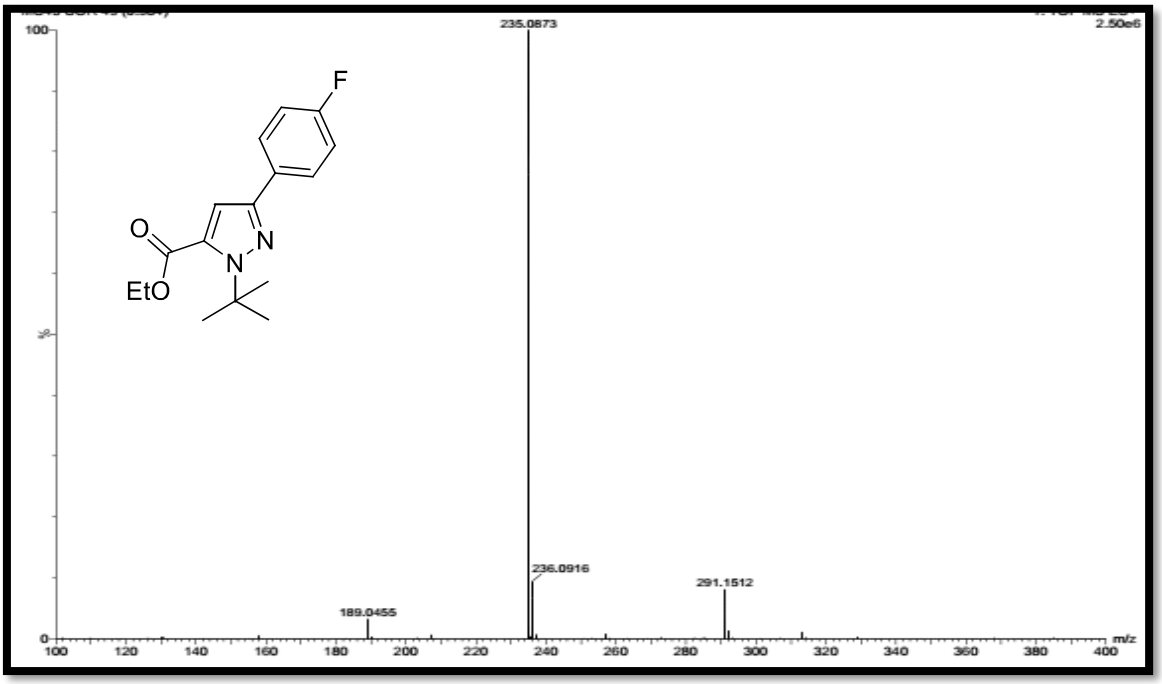


Figure S117: HRMS ESI-TOF mass spectra of **3d**.

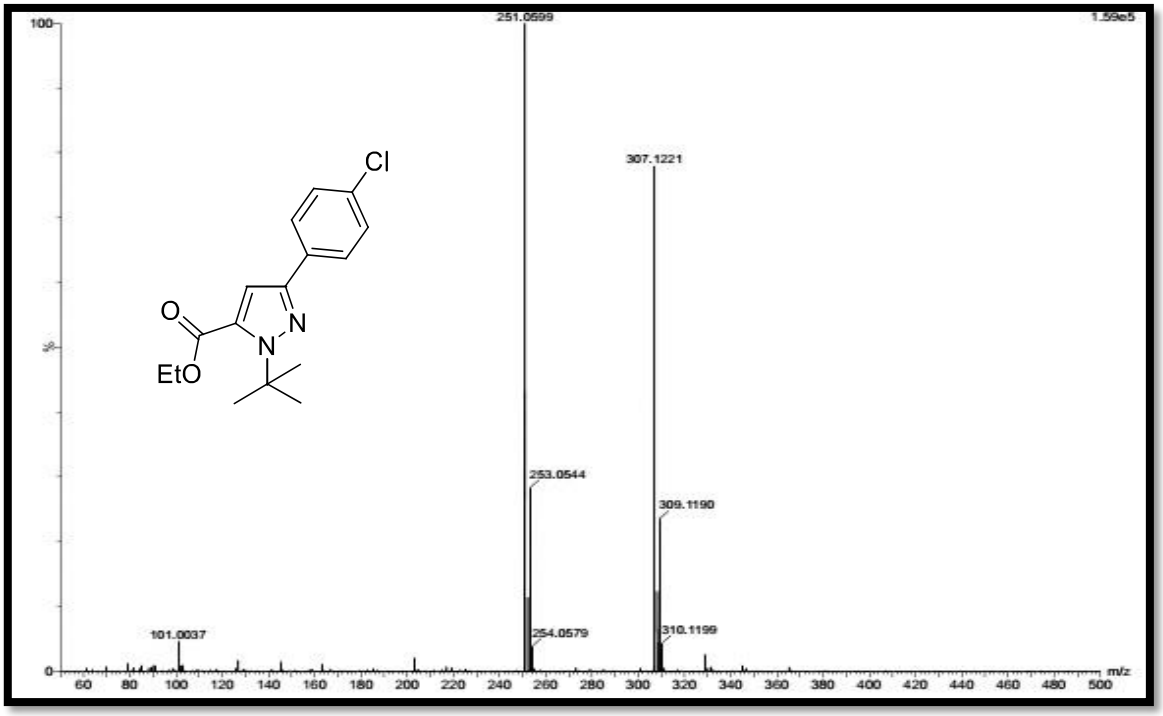


Figure S118: HRMS ESI-TOF Mass spectra of **3e**.

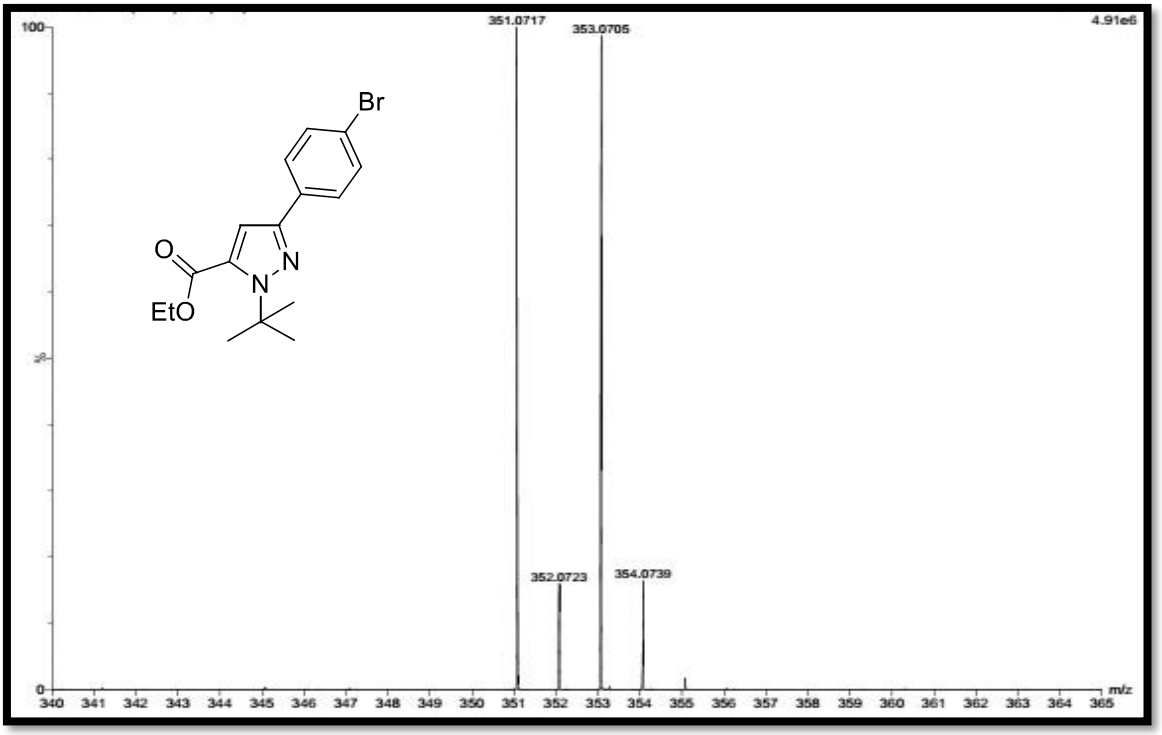


Figure S119: HRMS ESI-TOF Mass spectra of **3f**.

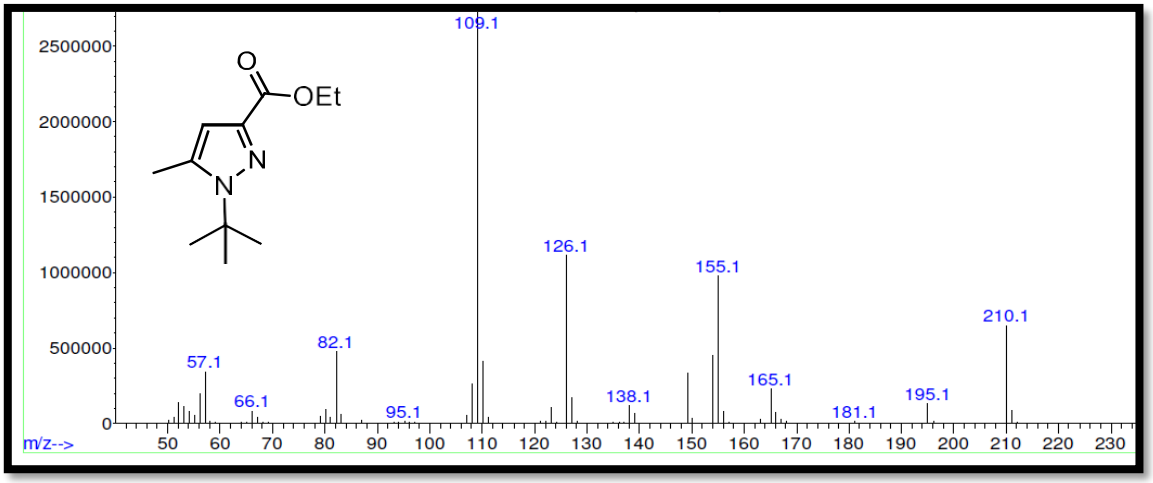


Figure S120: CG-MS Mass spectra of **4a**.

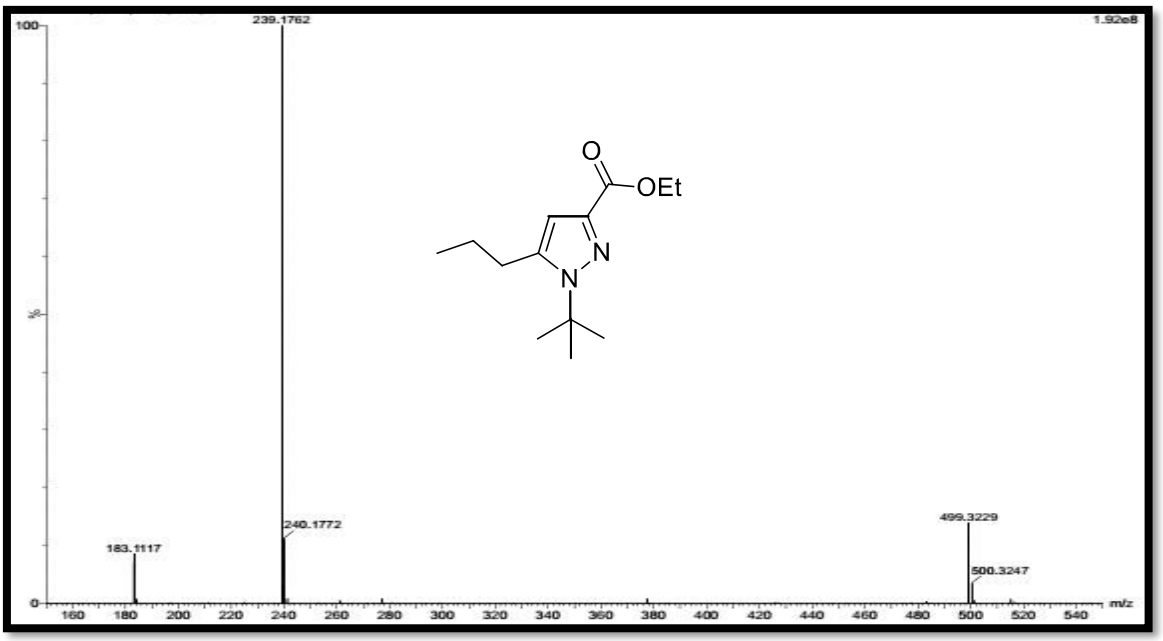


Figure S121: HRMS ESI-TOF Mass spectra of **4b**.

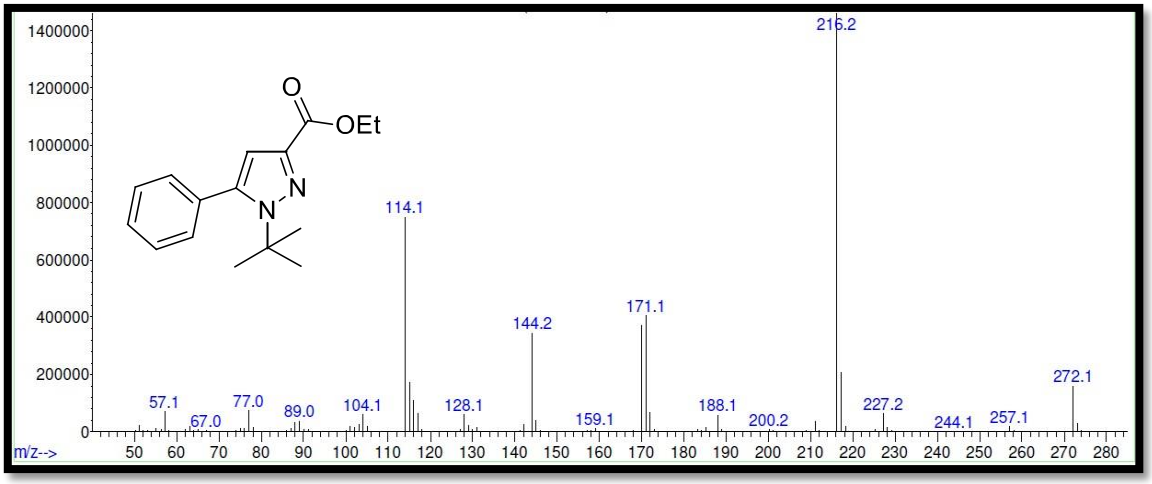


Figure S122: CG-MS Mass spectra of **4c**.

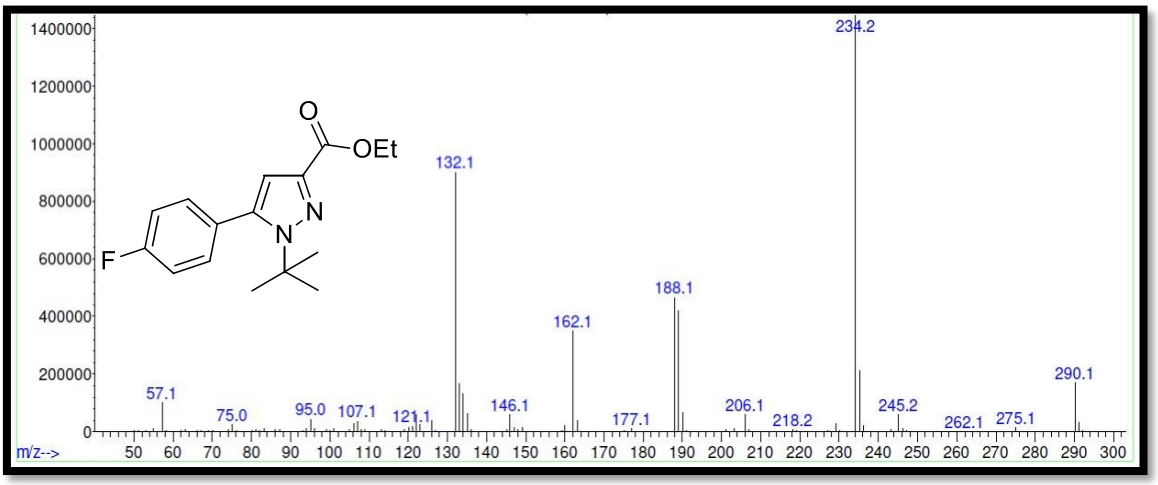


Figure S123: CG-MS Mass spectra of **4d**.

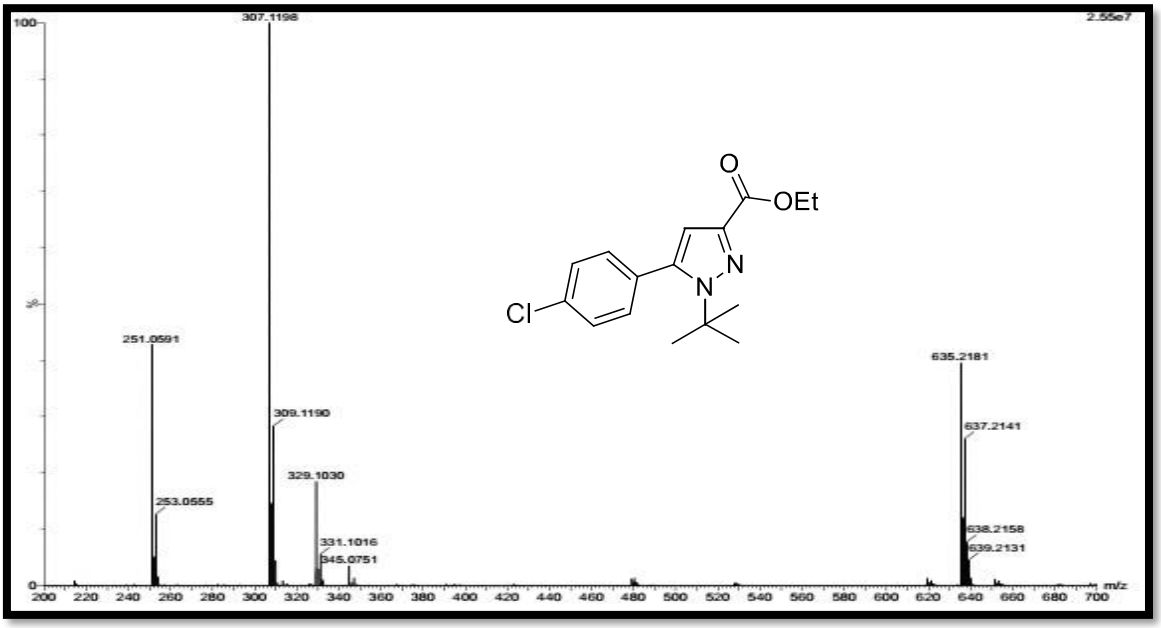


Figure S124: HRMS ESI-TOF Mass spectra of **4e**.

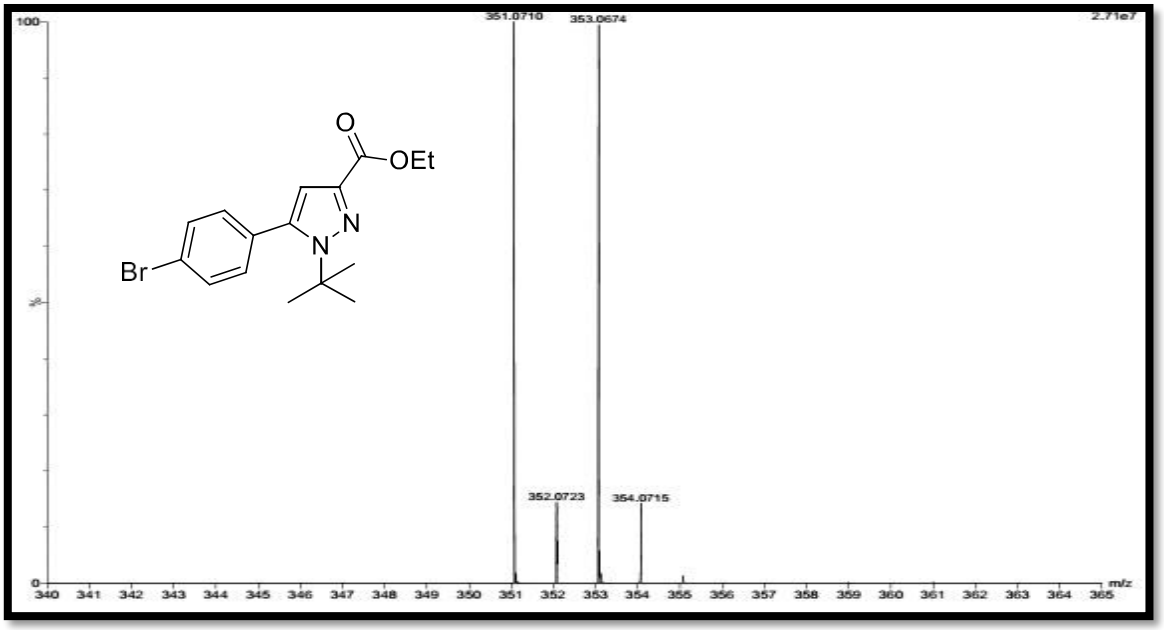


Figure S125: HRMS ESI-TOF Mass spectra of **4f**.

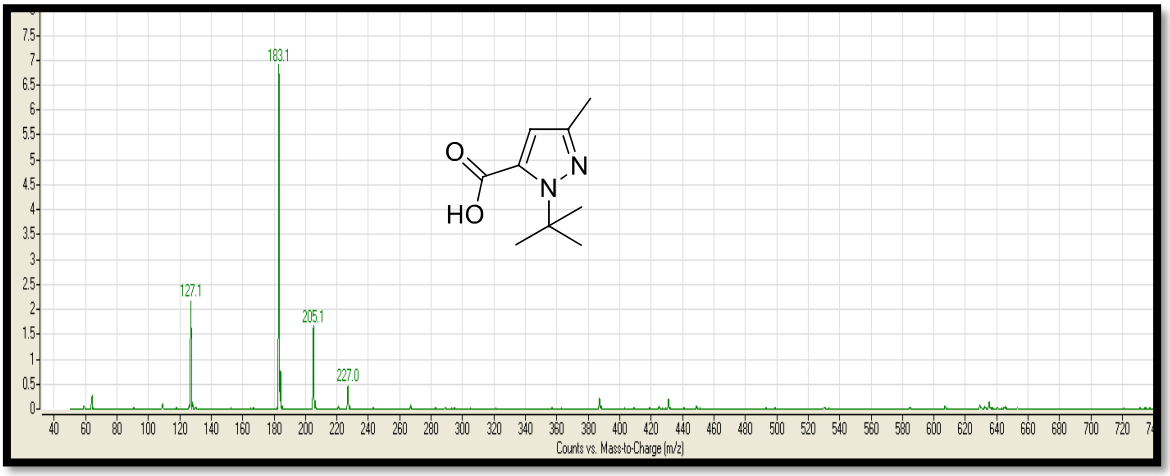


Figure S126: LC-MS Mass spectra of **5a**.

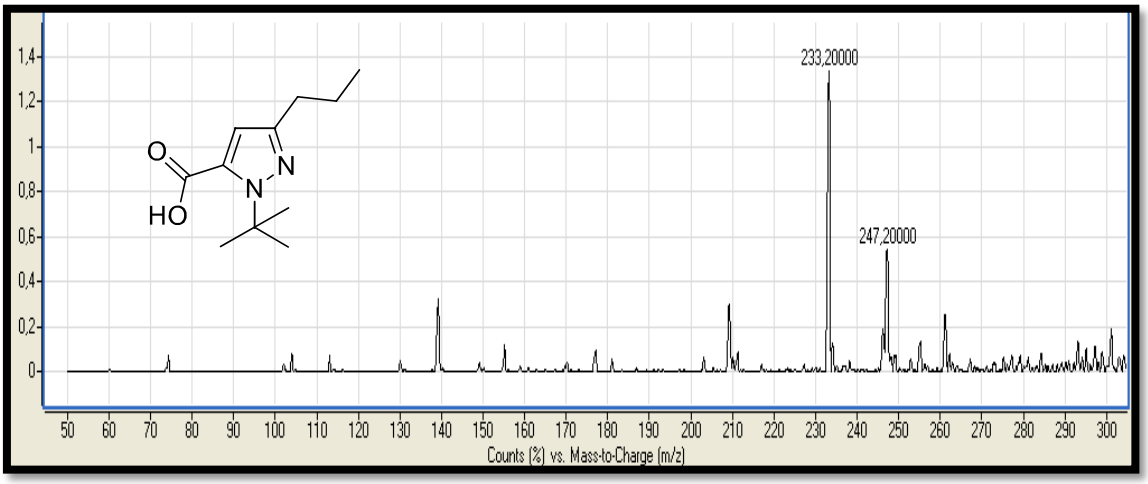


Figure S127: LC-MS Mass spectra of **5b**.

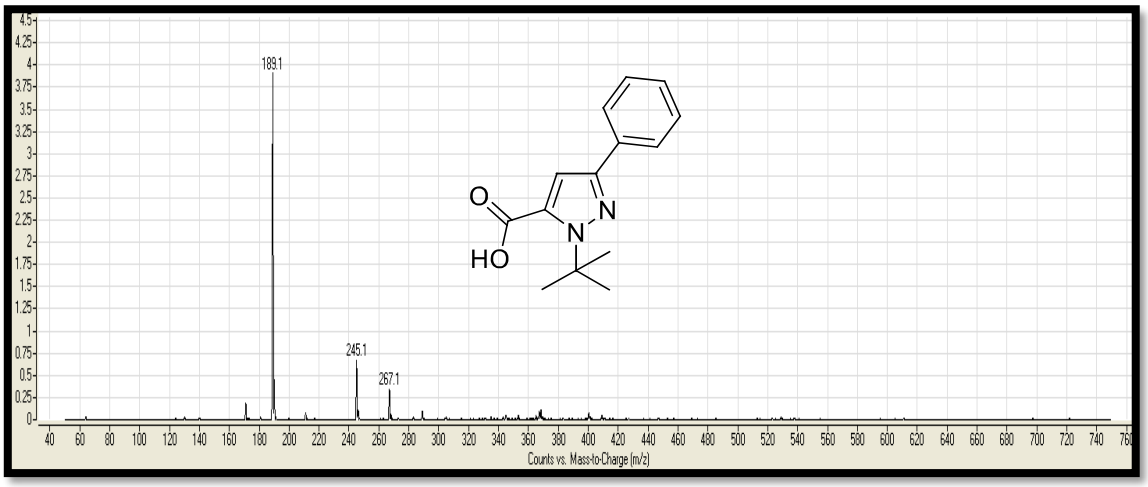


Figure S128: LC-MS Mass spectra of **5c**.

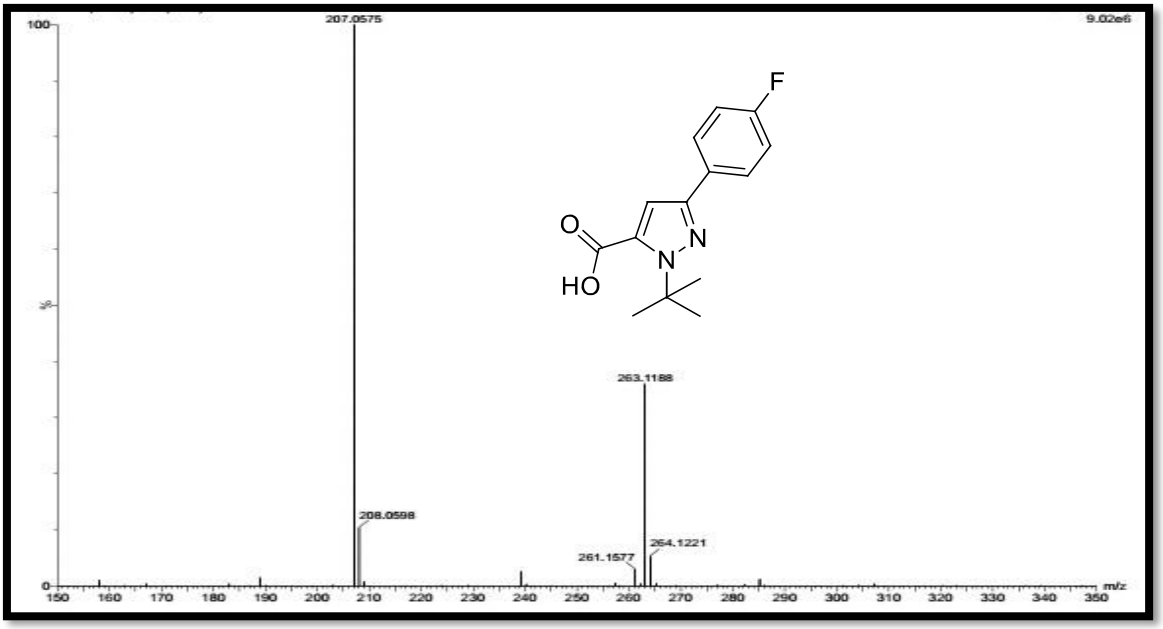


Figure S129: HRMS ESI-TOF Mass spectra of **5d**.

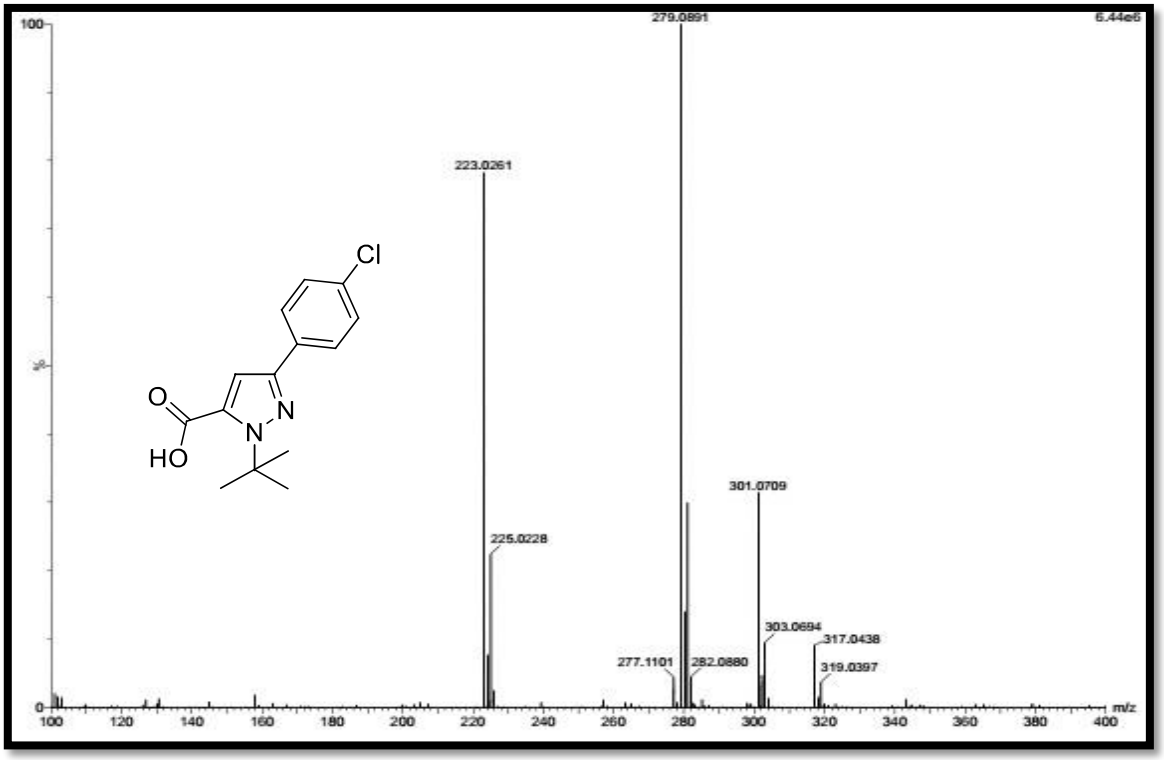


Figure S130: HRMS ESI-TOF Mass spectra of **5e**.

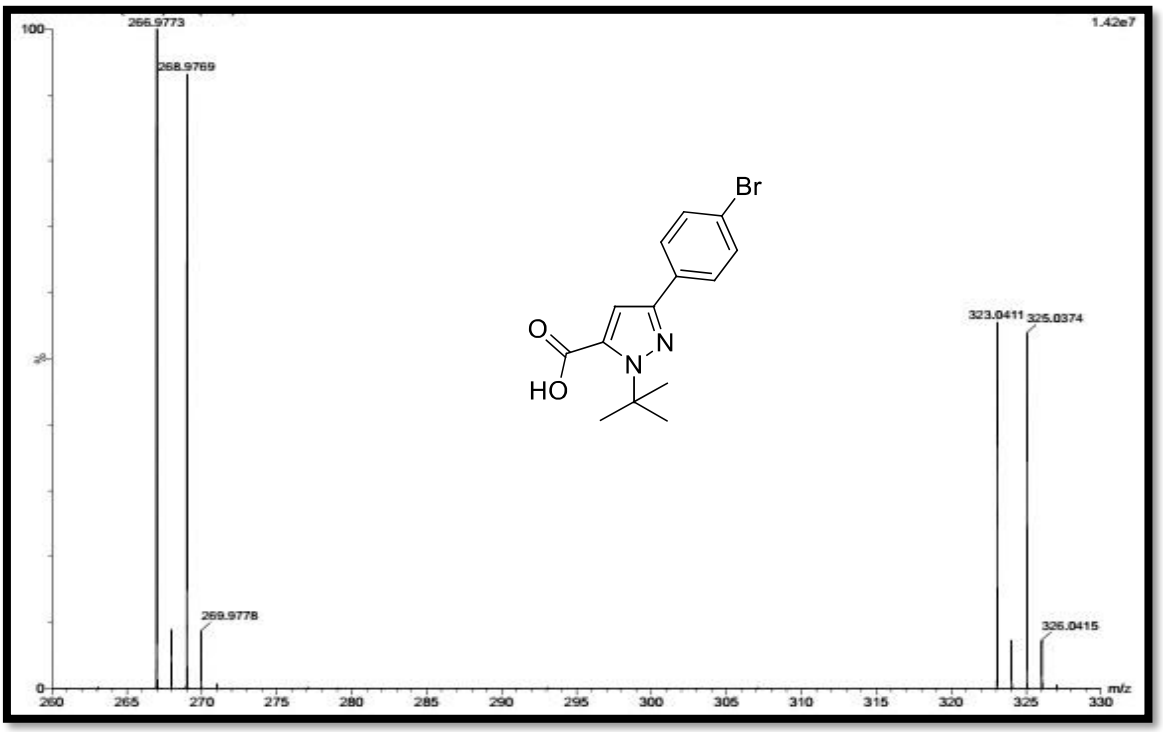


Figure S131: HRMS ESI-TOF Mass spectra of **5f**.

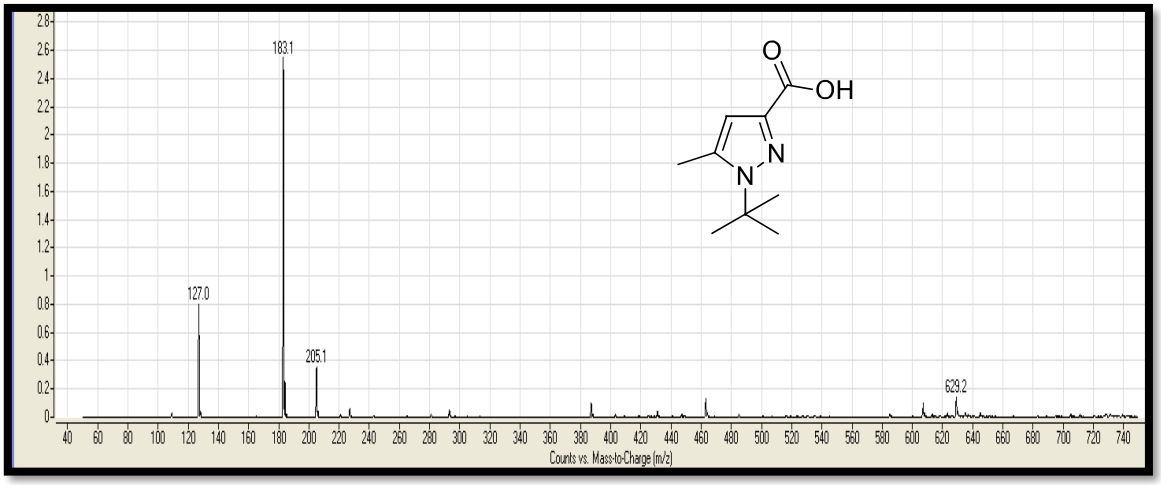


Figure S132: LC-MS Mass spectra of **6a**.

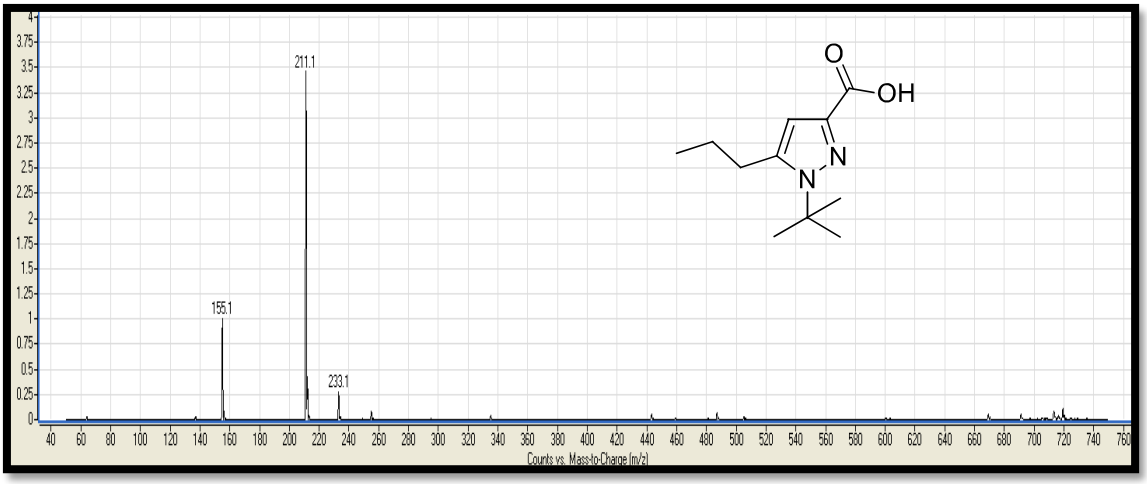


Figure S133: LC-MS Mass spectra of **6b**.

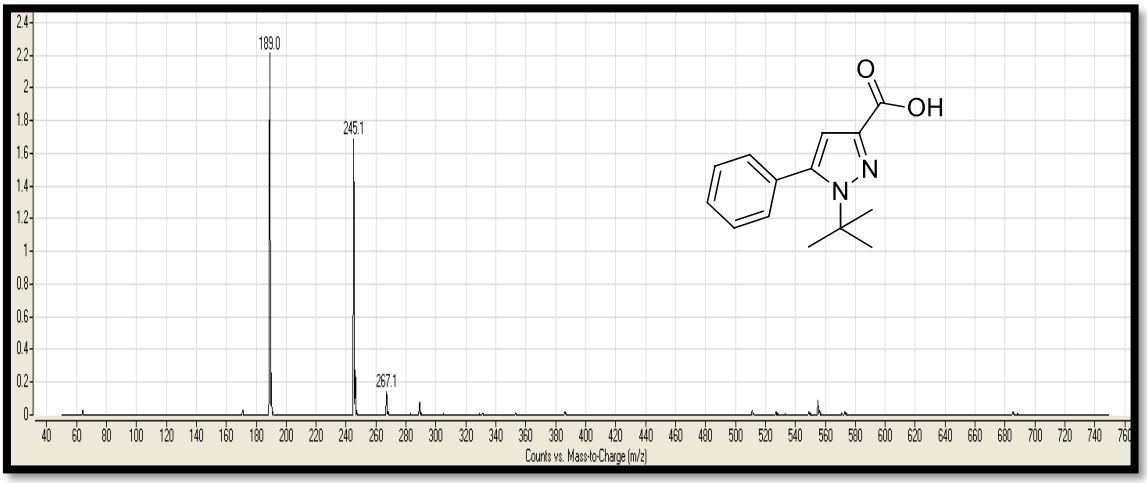


Figure S134: LC-MS Mass spectra of **6c**.

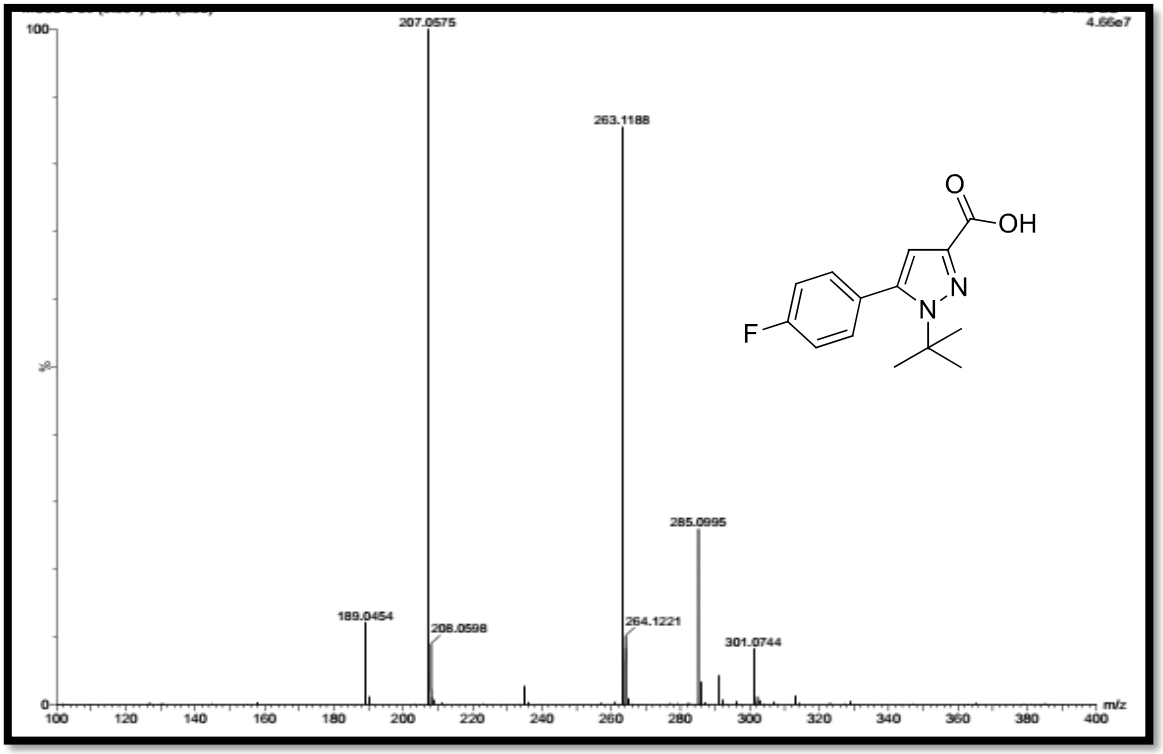


Figure S135: HRMS ESI-TOF Mass spectra of **6d**.

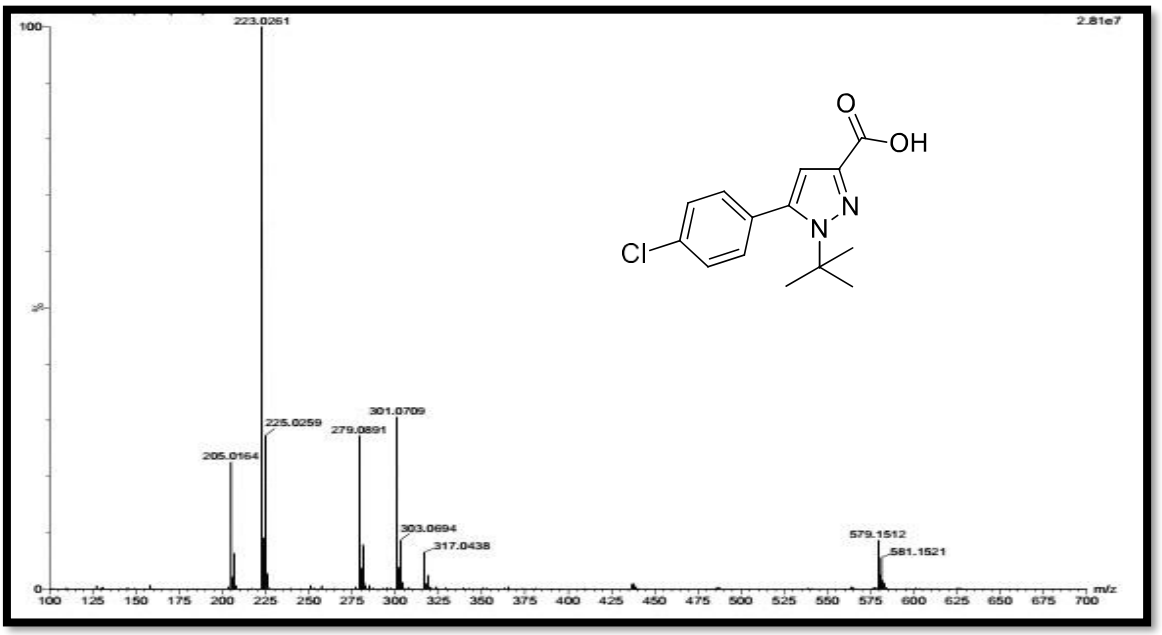


Figure S136: HRMS ESI-TOF Mass spectra of **6e**.

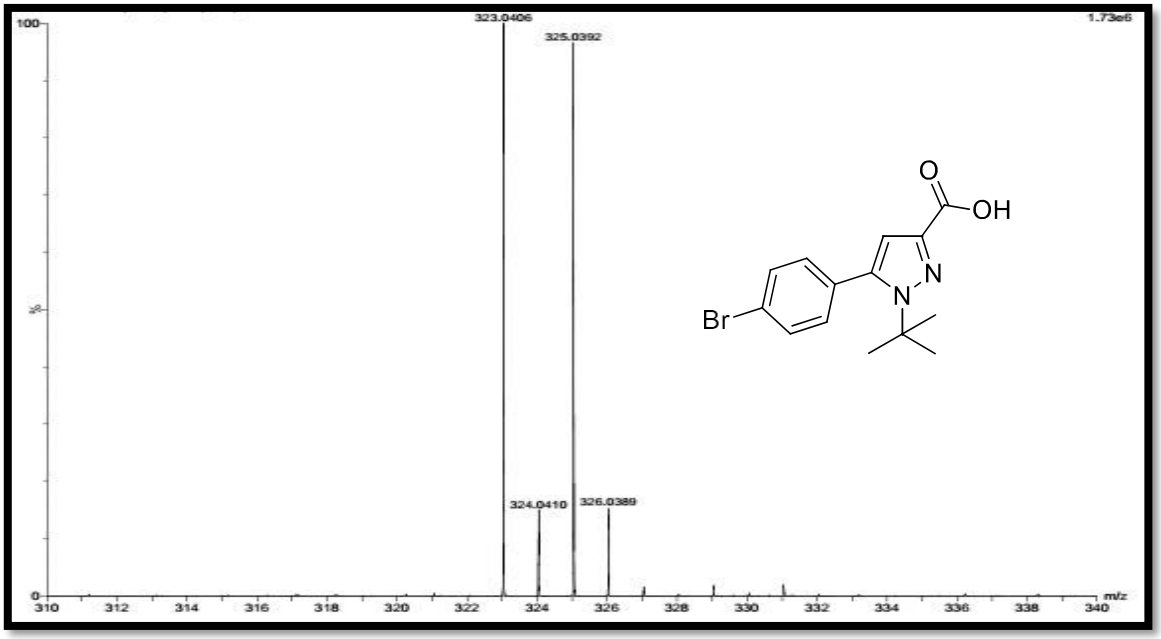


Figure S137: HRMS ESI-TOF Mass spectra of **6f**.

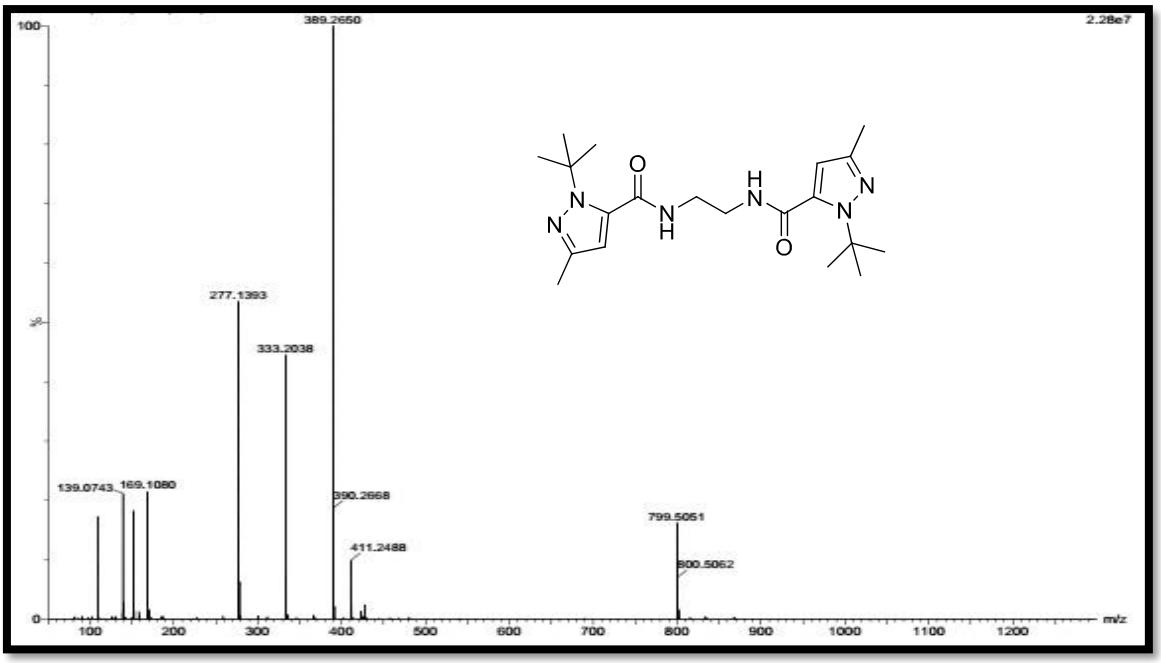


Figure S138: HRMS ESI-TOF Mass spectra of **8a.**

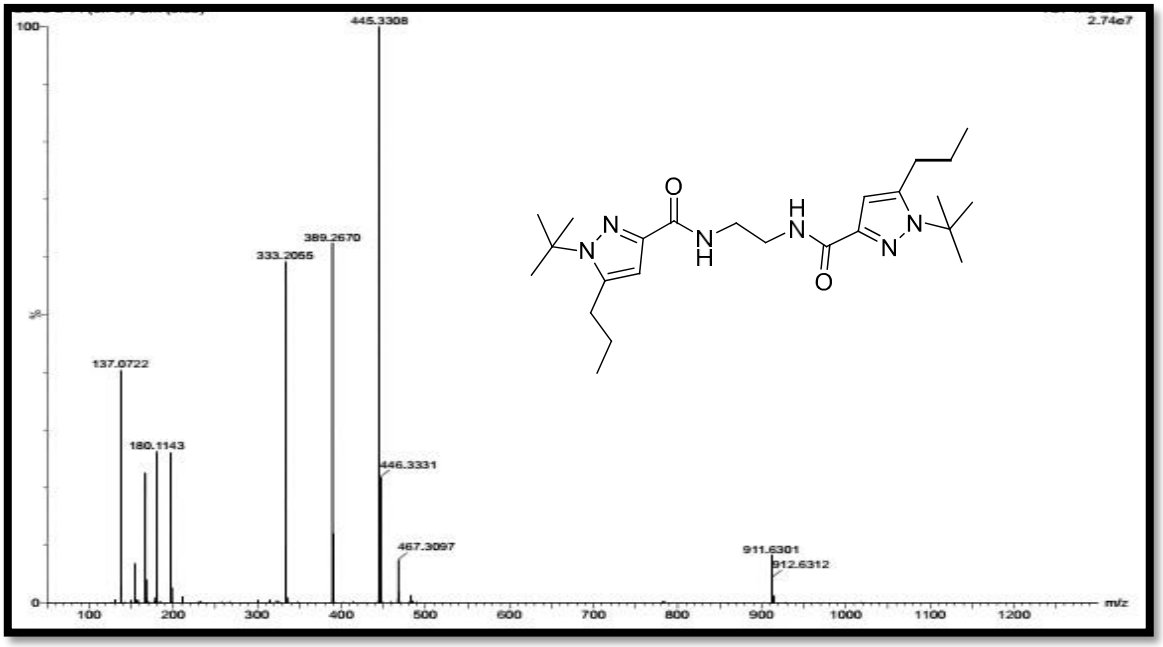


Figure S139: HRMS ESI-TOF Mass spectra of **8b.**

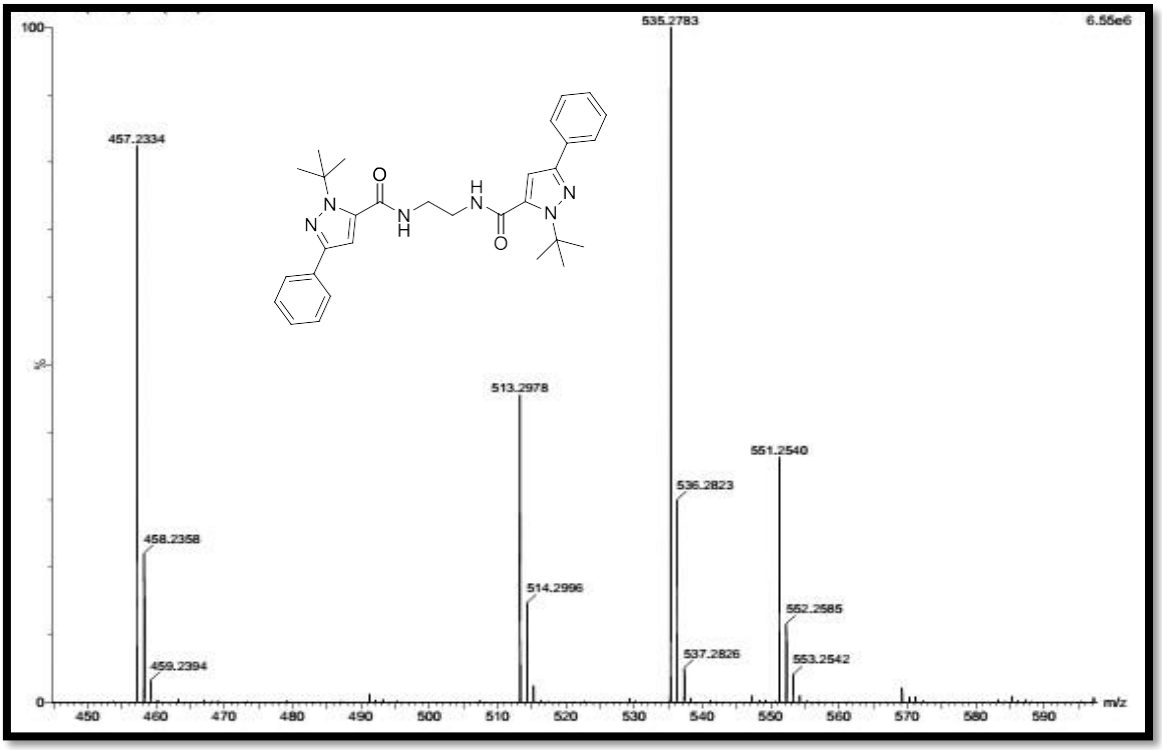


Figure S140: HRMS ESI-TOF Mass spectra of **8c.**

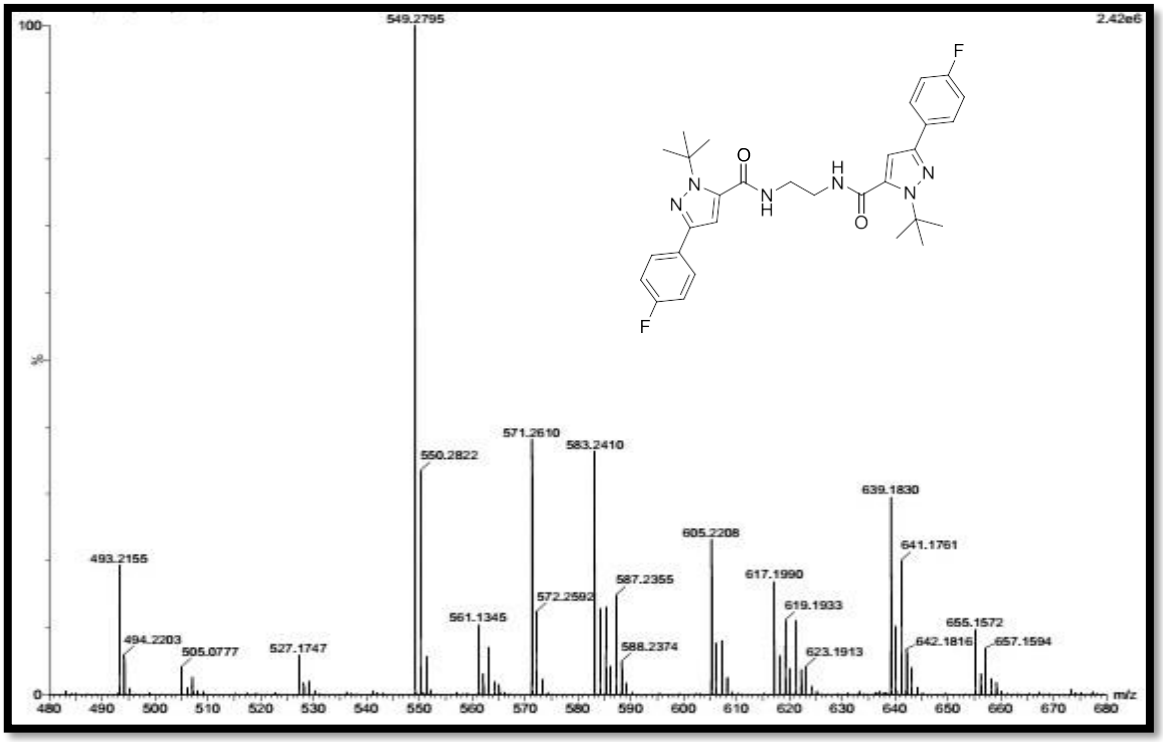


Figure S141: HRMS ESI-TOF Mass spectra of **8d.**

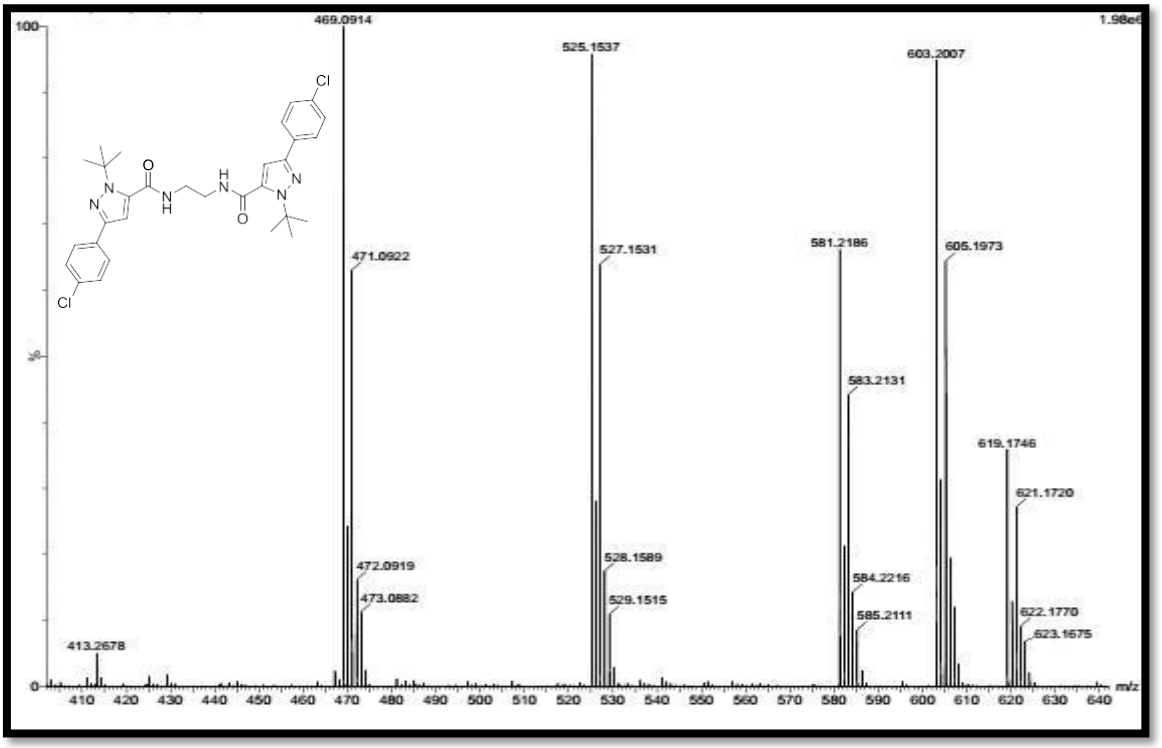


Figure S142: HRMS ESI-TOF Mass spectra of **8e.**

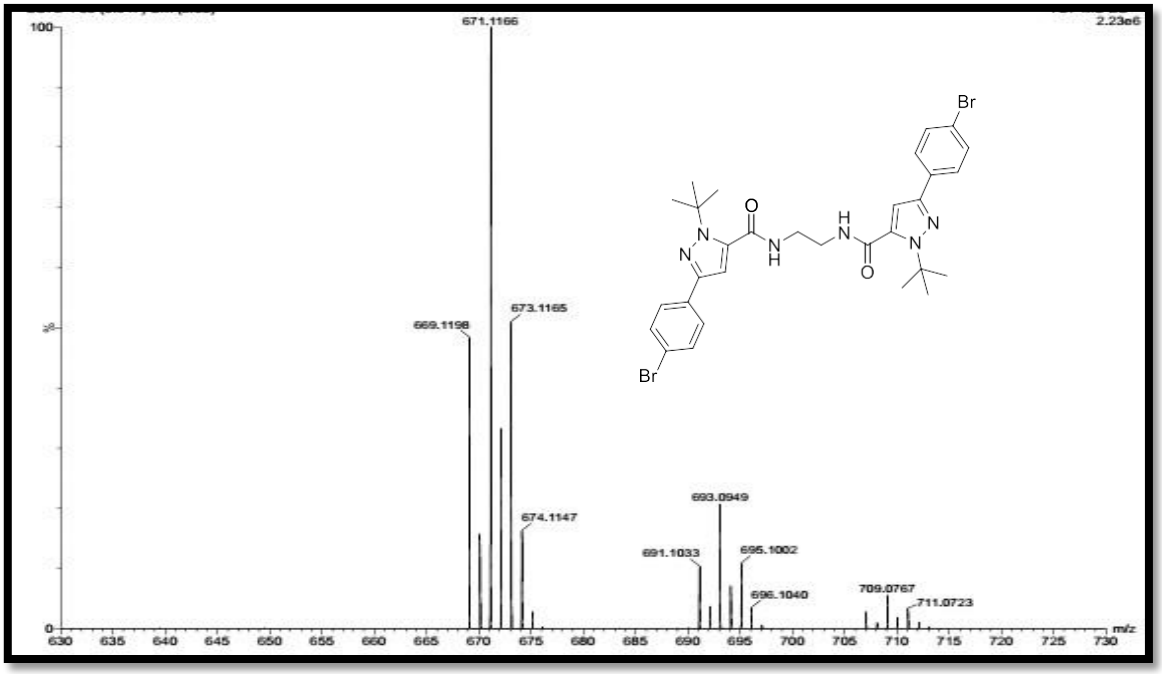


Figure S143: HRMS ESI-TOF Mass spectra of **8f.**

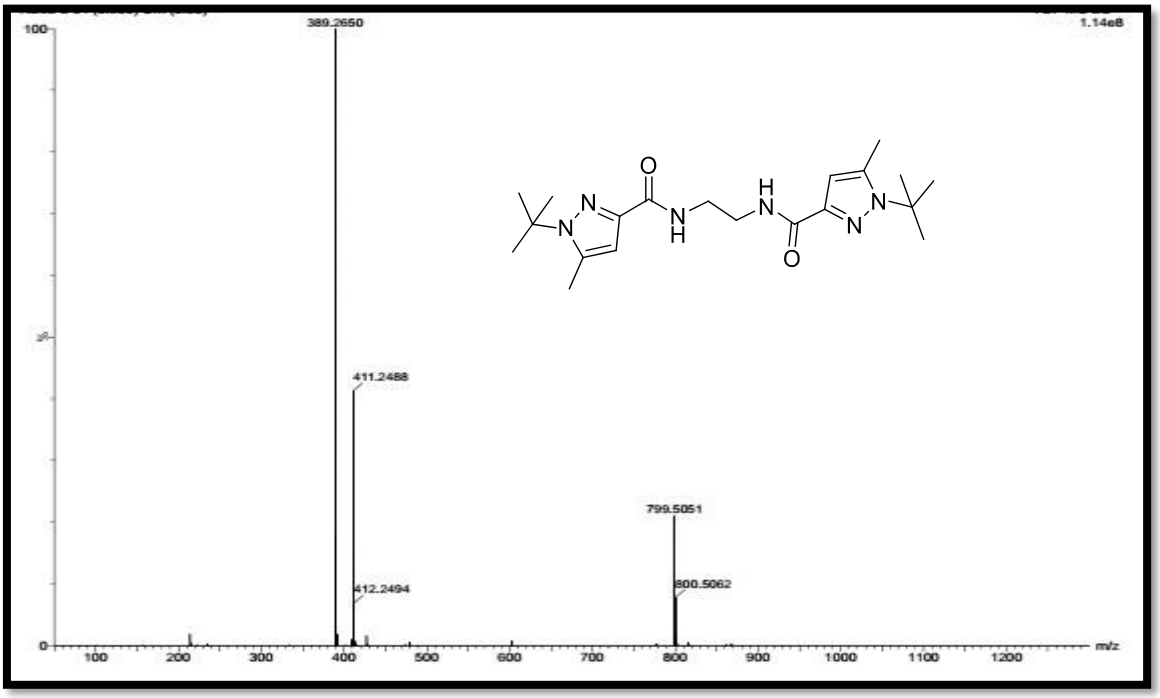


Figure S144: HRMS ESI-TOF Mass spectra of **9a.**

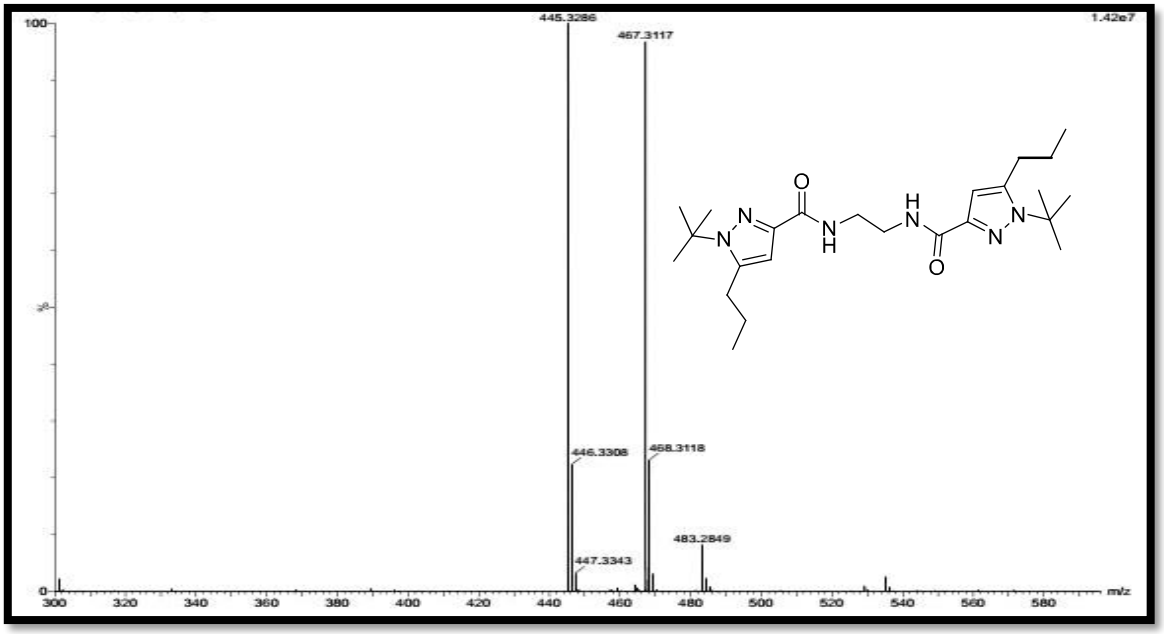


Figure S145: HRMS ESI-TOF Mass spectra of **9b.**

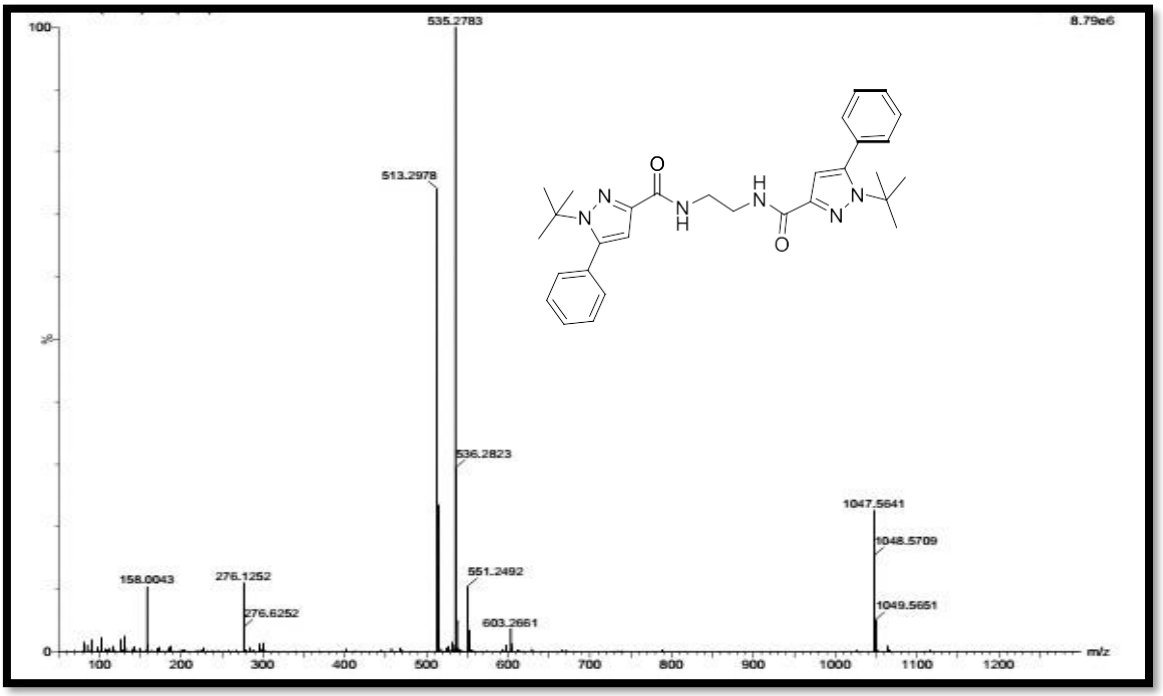


Figure S146: HRMS ESI-TOF Mass spectra of **9c.**

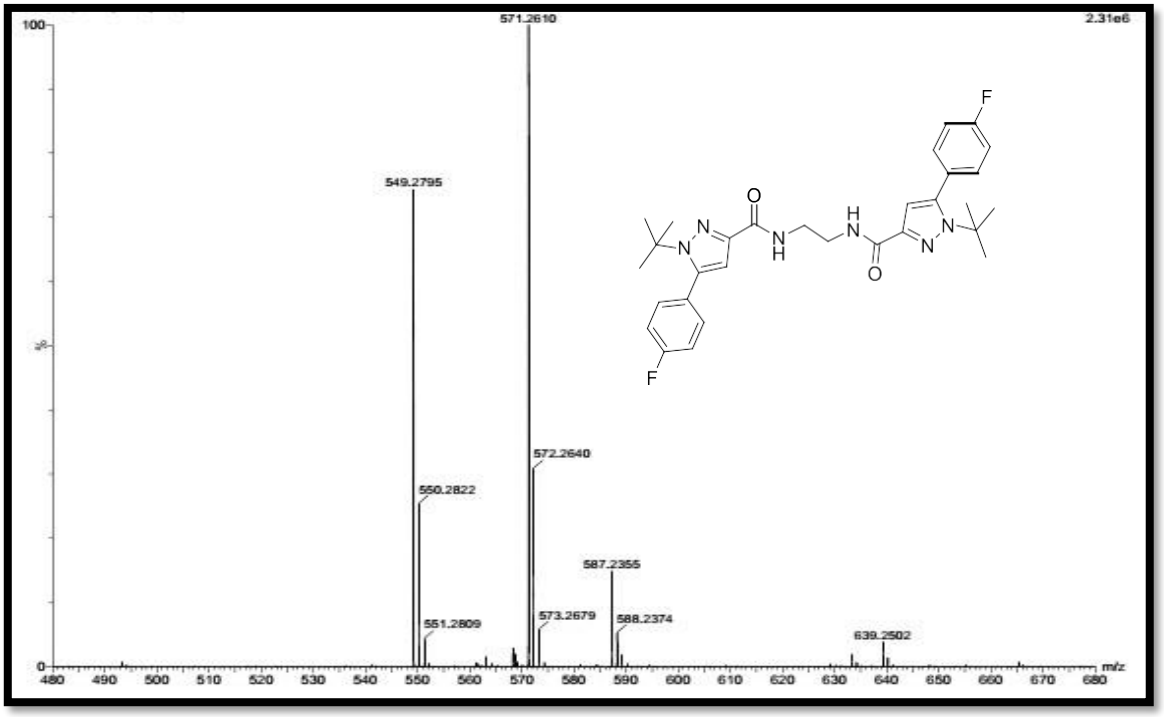


Figure S147: HRMS ESI-TOF Mass spectra of **9d.**

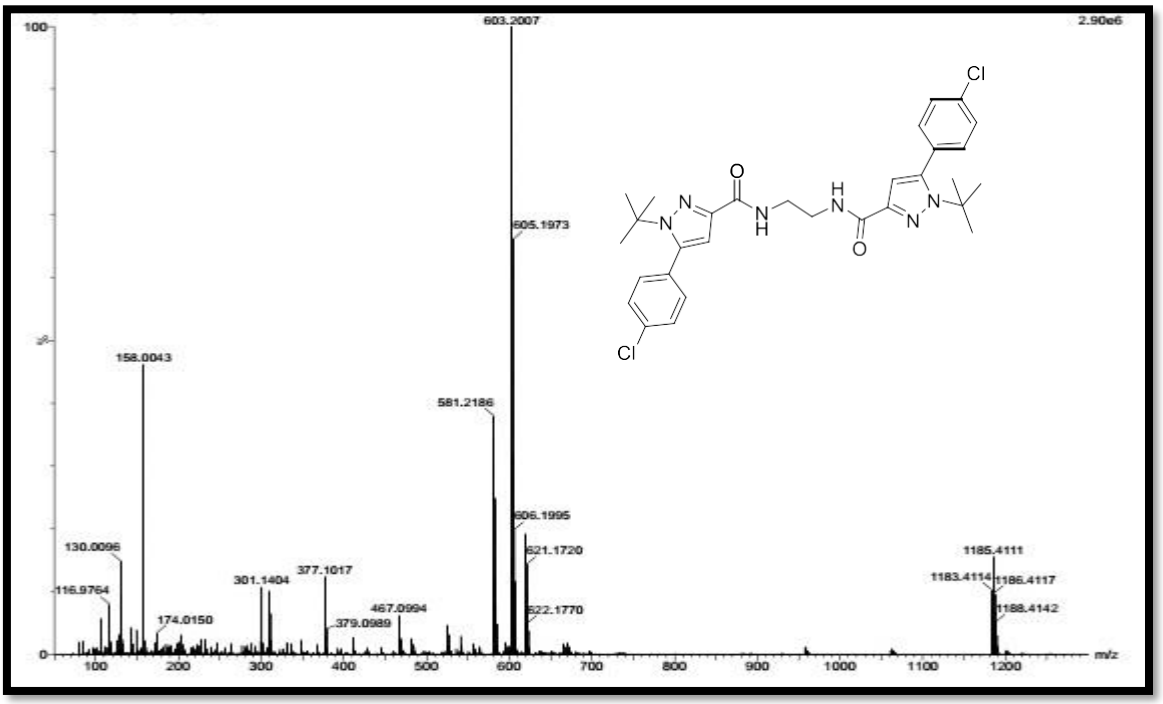


Figure S148: HRMS ESI-TOF Mass spectra of **9e**

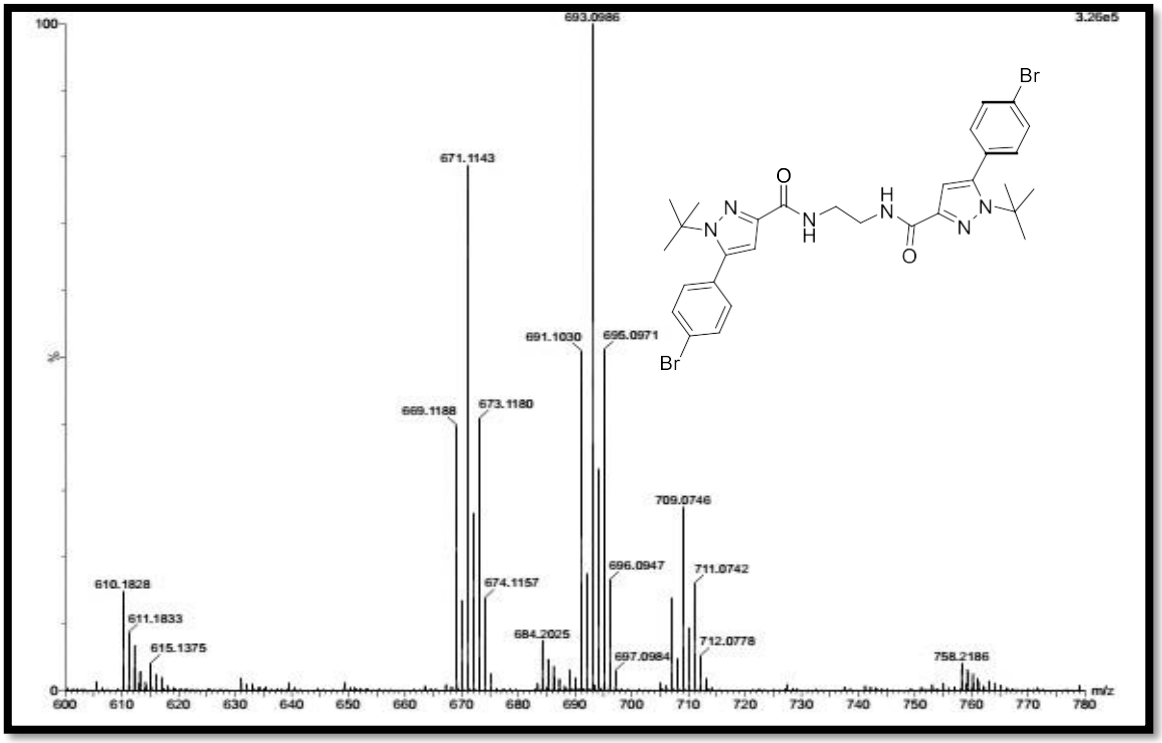


Figure S149: HRMS ESI-TOF Mass spectra of **9f.**

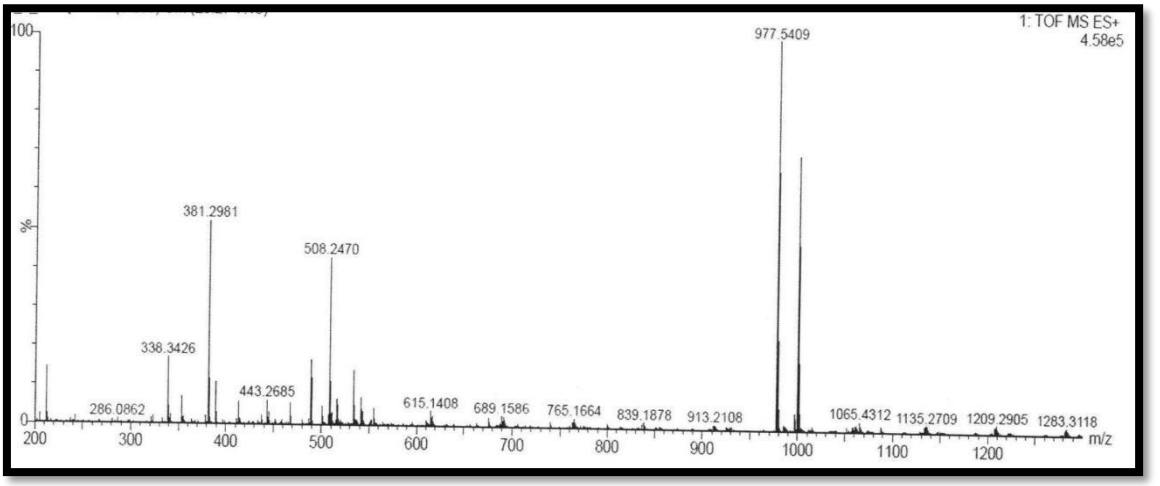


Figure S150: HRMS ESI-TOF Mass spectra of **10b.**

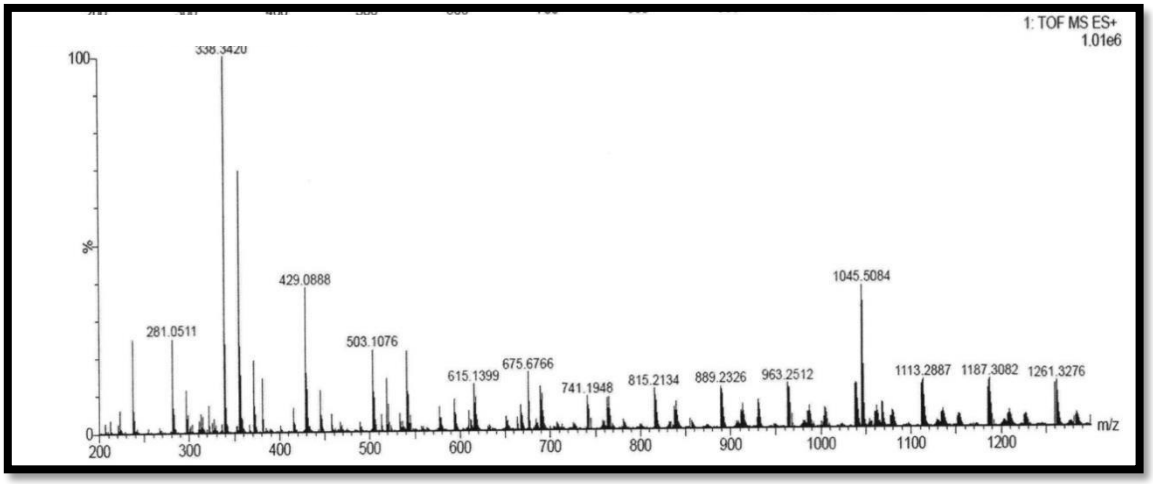


Figure S151: HRMS ESI-TOF Mass spectra of **10c.**

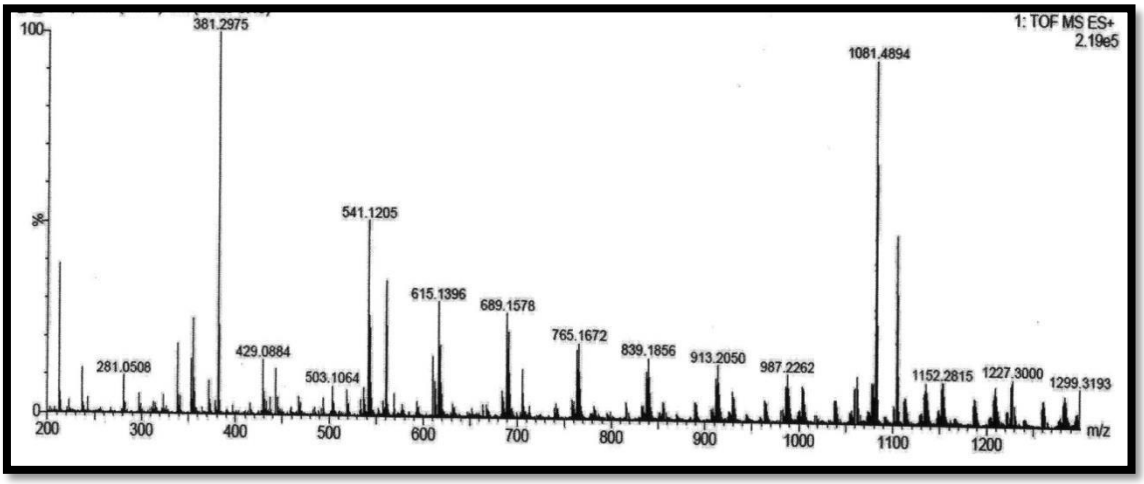


Figure S152: HRMS ESI-TOF Mass spectra of **10d.**

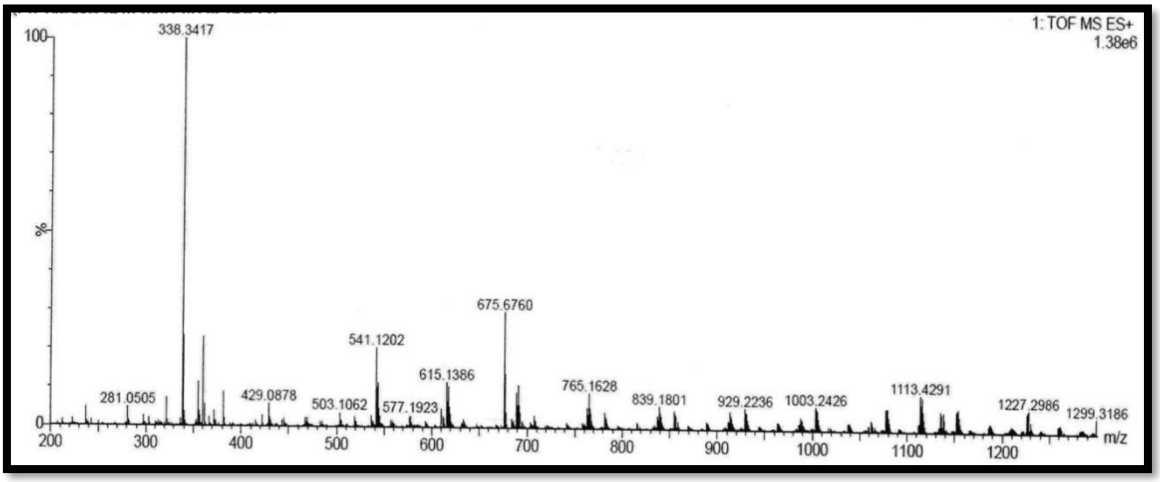


Figure S153: HRMS ESI-TOF Mass spectra of **10e.**

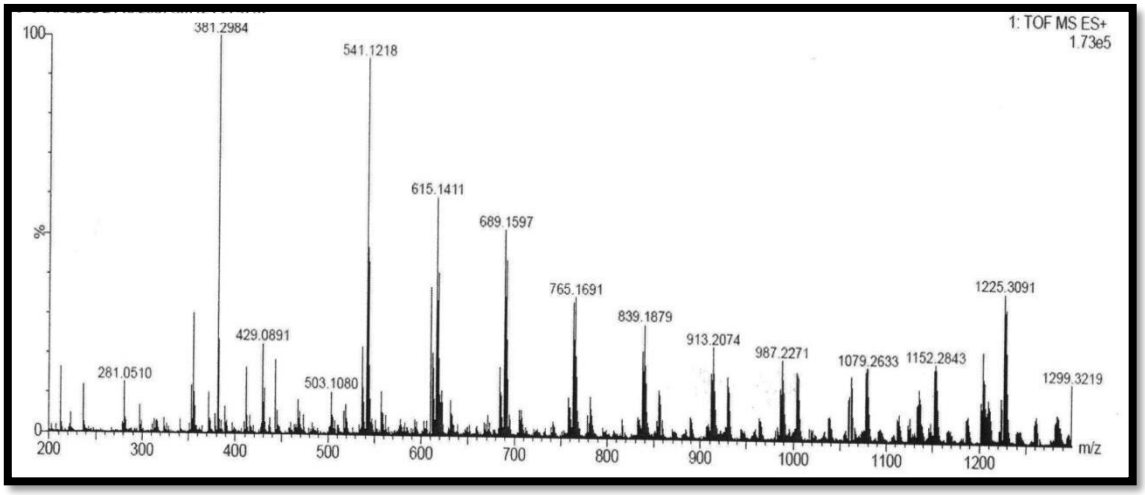


Figure S154: HRMS ESI-TOF Mass spectra of **10f.**

5.4 IR spectra of [2]rotaxanes 10a-f

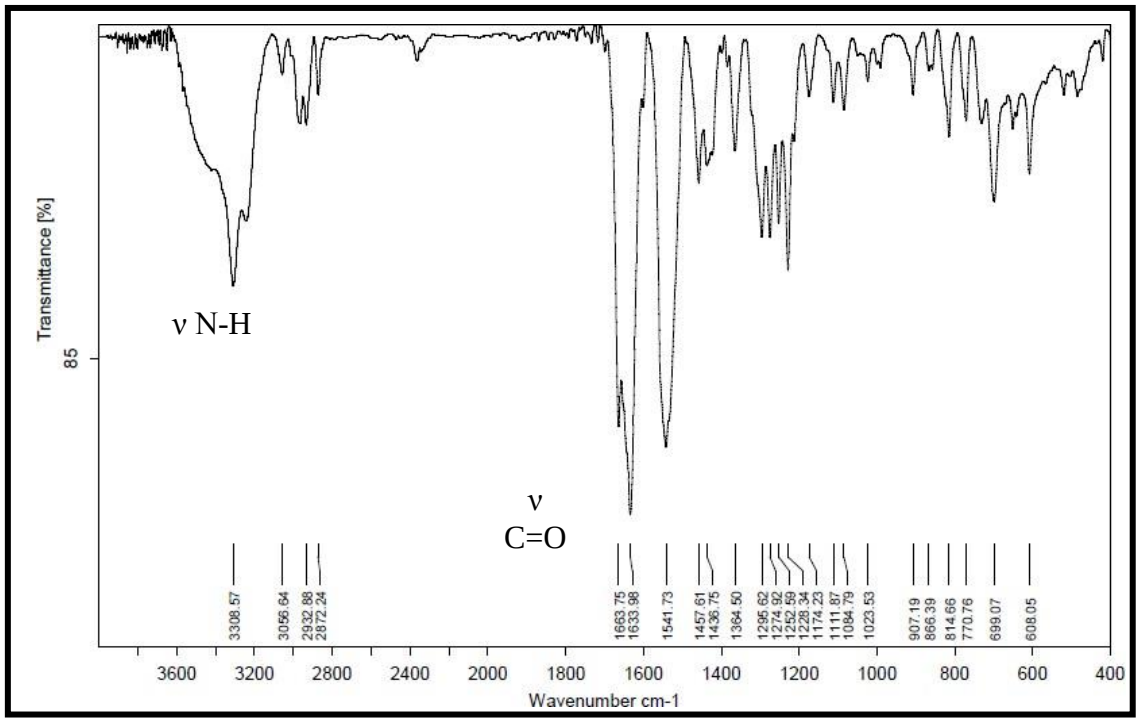


Figure S155: IR spectra of **10b.**

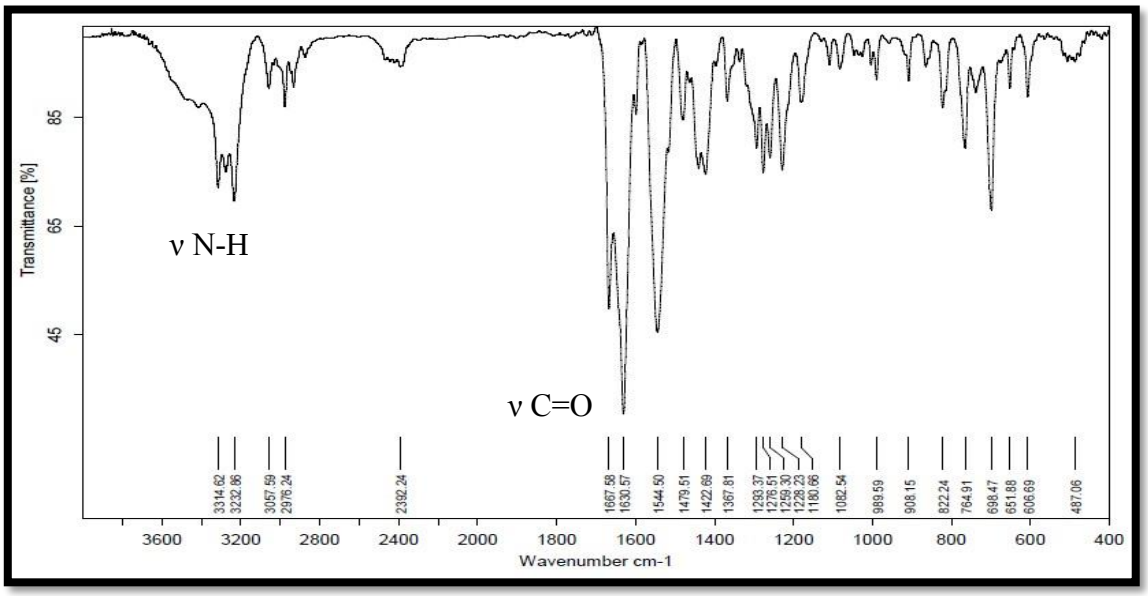


Figure S156: IR spectra of **10c.**

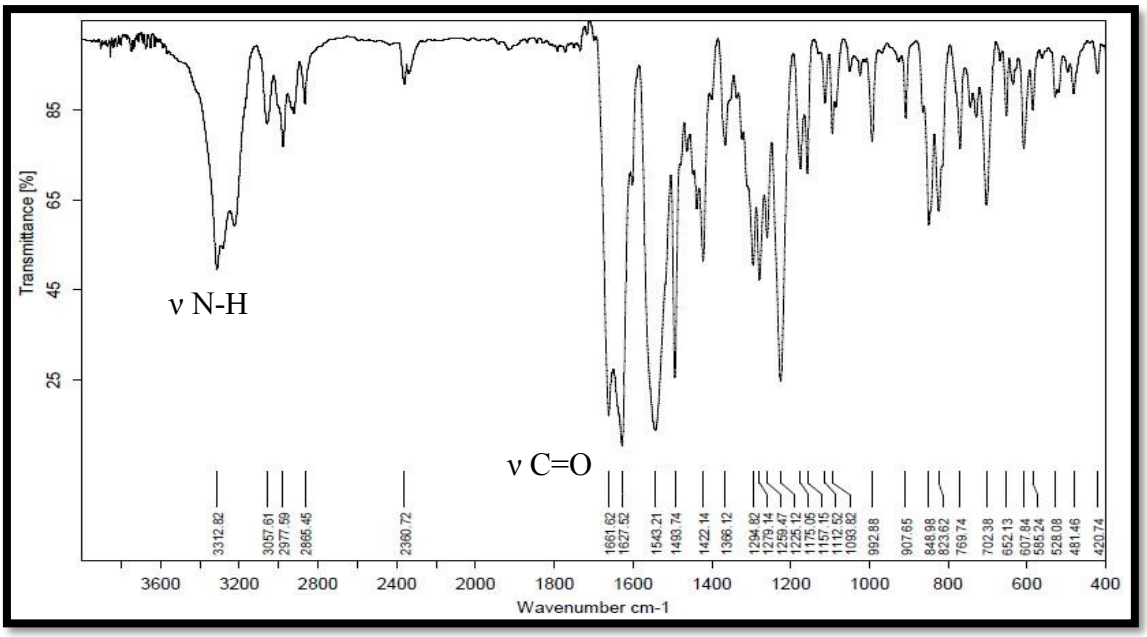


Figure S157: IR spectra of **10d.**

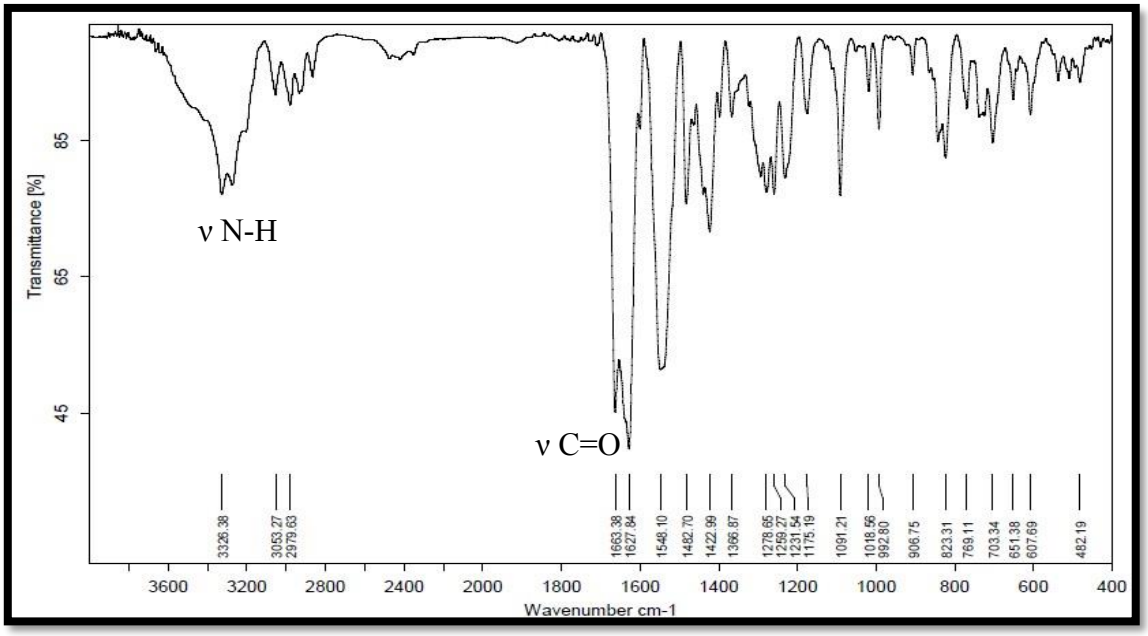


Figure S158: IR spectra of **10e.**

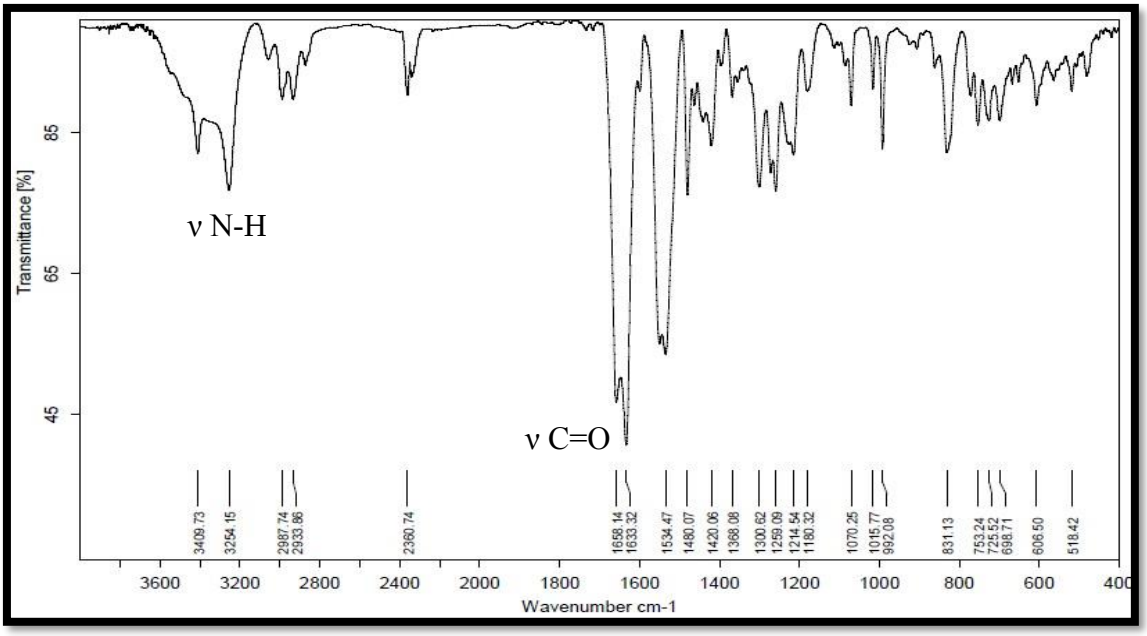


Figure S159: IR spectra of **10f.**

6. Computational Data

Table S7. Atomic coordinates used in single point calculations with a ωB97x-D/cc-pVDZ for compound **8c.**

	Atoms	Coordinates		
M1	O	6.303100	0.505100	5.191600
	O	2.225300	4.419600	7.148900
	N	9.219700	2.143000	2.503900
	N	0.902700	3.161600	9.709900
	N	8.034000	1.807200	3.041200
	N	6.596500	2.497500	6.188700
	H	7.077100	3.206800	6.264200
	N	2.996900	2.281700	7.115200
	H	2.849400	1.474400	7.374700
	C	9.326400	2.351400	4.748300
	H	9.650000	2.528100	5.601800
	N	-0.211500	2.611100	10.246100
	C	12.248500	3.378400	4.221000
	H	11.962900	3.411600	5.105600
	C	8.062800	1.913100	4.398800
	C	1.198900	5.547400	10.154000
	H	1.372800	5.712900	9.225000
	H	1.665600	6.195800	10.687000
	H	0.255900	5.616000	10.320200
	C	10.013300	2.470300	3.524300
	C	5.436800	2.315500	7.045900
	H	5.480000	2.941500	7.784600
	H	5.443300	1.417700	7.412800
	C	1.680500	4.147600	10.520000
	C	11.385800	2.909000	3.230900
	C	5.641200	2.183600	2.540700
	H	5.788200	3.131800	2.547100
	H	5.401600	1.891500	3.422700
	H	4.931900	1.973800	1.930300
	C	3.176000	3.995600	10.249200
	H	3.352900	4.172600	9.322700
	H	3.450700	3.100700	10.462400
	H	3.664500	4.617200	10.792300
	C	2.154100	3.243300	7.510700
	C	6.920300	1.473000	2.099100
	C	13.537600	3.797400	3.894800
	H	14.104800	4.106800	4.562400
	C	11.839100	2.868900	1.911200
	H	11.273800	2.561000	1.239900
	C	4.146700	2.535800	6.268300
	H	4.114900	3.448200	5.943100
	H	4.123600	1.940900	5.501500
	C	-1.996900	1.118800	9.518200
	C	6.919500	1.569400	5.285600
	C	1.075300	2.758000	8.425500
	C	1.411900	3.870800	11.990400
	H	1.719700	2.989100	12.211200
	H	0.469300	3.931200	12.160400
	H	1.876300	4.514700	12.528500
	C	7.301400	1.983500	0.710700
	H	7.414200	2.936000	0.738600
	H	6.607200	1.761600	0.085000
	H	8.124900	1.573200	0.432800
	C	0.051500	1.891300	8.119600

	H	-0.089300	1.437800	7.320100
	C	-0.732200	1.843800	9.282100
	C	-2.751600	0.646800	8.438200
	H	-2.432200	0.750000	7.570100
	C	-2.472200	0.946800	10.805000
	H	-1.971600	1.243900	11.529700
	C	13.119600	3.281900	1.591400
	H	13.410700	3.243300	0.709400
	C	13.975900	3.754600	2.583900
	H	14.833600	4.039100	2.366900
	C	6.741800	-0.042600	2.071200
	H	6.501000	-0.353100	2.946800
	H	7.565100	-0.457300	1.799600
	H	6.048200	-0.270700	1.448000
	C	-3.708400	0.324200	11.013200
	H	-4.031800	0.212200	11.877400
	C	-3.976000	0.023400	8.659000
	H	-4.471400	-0.292700	7.938200
	C	-4.451800	-0.125900	9.930600
	H	-5.276000	-0.530500	10.071500
Energy single point calculations:	-1642.7816542 a.u			
	Atoms	Coordinates		
M1···M2	O	6.303100	0.505100	5.191600
	O	2.225300	4.419600	7.148900
	N	9.219700	2.143000	2.503900
	N	0.902700	3.161600	9.709900
	N	8.034000	1.807200	3.041200
	N	6.596500	2.497500	6.188700
	H	7.077100	3.206800	6.264200
	N	2.996900	2.281700	7.115200
	H	2.849400	1.474400	7.374700
	C	9.326400	2.351400	4.748300
	H	9.650000	2.528100	5.601800
	N	-0.211500	2.611100	10.246100
	C	12.248500	3.378400	4.221000
	H	11.962900	3.411600	5.105600
	C	8.062800	1.913100	4.398800
	C	1.198900	5.547400	10.154000
	H	1.372800	5.712900	9.225000
	H	1.665600	6.195800	10.687000
	H	0.255900	5.616000	10.320200
	C	10.013300	2.470300	3.524300
	C	5.436800	2.315500	7.045900
	H	5.480000	2.941500	7.784600
	H	5.443300	1.417700	7.412800
	C	1.680500	4.147600	10.520000
	C	11.385800	2.909000	3.230900
	C	5.641200	2.183600	2.540700
	H	5.788200	3.131800	2.547100
	H	5.401600	1.891500	3.422700
	H	4.931900	1.973800	1.930300
	C	3.176000	3.995600	10.249200
	H	3.352900	4.172600	9.322700
	H	3.450700	3.100700	10.462400
	H	3.664500	4.617200	10.792300
	C	2.154100	3.243300	7.510700
	C	6.920300	1.473000	2.099100
	C	13.537600	3.797400	3.894800
	H	14.104800	4.106800	4.562400
	C	11.839100	2.868900	1.911200
	H	11.273800	2.561000	1.239900

	C	4.146700	2.535800	6.268300
	H	4.114900	3.448200	5.943100
	H	4.123600	1.940900	5.501500
	C	-1.996900	1.118800	9.518200
	C	6.919500	1.569400	5.285600
	C	1.075300	2.758000	8.425500
	C	1.411900	3.870800	11.990400
	H	1.719700	2.989100	12.211200
	H	0.469300	3.931200	12.160400
	H	1.876300	4.514700	12.528500
	C	7.301400	1.983500	0.710700
	H	7.414200	2.936000	0.738600
	H	6.607200	1.761600	0.085000
	H	8.124900	1.573200	0.432800
	C	0.051500	1.891300	8.119600
	H	-0.089300	1.437800	7.320100
	C	-0.732200	1.843800	9.282100
	C	-2.751600	0.646800	8.438200
	H	-2.432200	0.750000	7.570100
	C	-2.472200	0.946800	10.805000
	H	-1.971600	1.243900	11.529700
	C	13.119600	3.281900	1.591400
	H	13.410700	3.243300	0.709400
	C	13.975900	3.754600	2.583900
	H	14.833600	4.039100	2.366900
	C	6.741800	-0.042600	2.071200
	H	6.501000	-0.353100	2.946800
	H	7.565100	-0.457300	1.799600
	H	6.048200	-0.270700	1.448000
	C	-3.708400	0.324200	11.013200
	H	-4.031800	0.212200	11.877400
	C	-3.976000	0.023400	8.659000
	H	-4.471400	-0.292700	7.938200
	C	-4.451800	-0.125900	9.930600
	H	-5.276000	-0.530500	10.071500
	O	3.071300	-0.505100	7.499300
	O	7.149200	-4.419600	5.542000
	N	0.154700	-2.143000	10.187000
	N	8.471700	-3.161600	2.981000
	N	1.340500	-1.807200	9.649700
	N	2.778000	-2.497500	6.502200
	H	2.297400	-3.206800	6.426700
	N	6.377600	-2.281700	5.575700
	H	6.525100	-1.474400	5.316200
	C	0.048100	-2.351400	7.942600
	H	-0.275500	-2.528100	7.089100
	N	9.586000	-2.611100	2.444800
	C	-2.874100	-3.378400	8.469900
	H	-2.588500	-3.411600	7.585400
	C	1.311700	-1.913100	8.292100
	C	8.175500	-5.547400	2.536900
	H	8.001700	-5.712900	3.465900
	H	7.708800	-6.195800	2.003900
	H	9.118500	-5.616000	2.370700
	C	-0.638800	-2.470300	9.166600
	C	3.937700	-2.315500	5.645000
	H	3.894500	-2.941500	4.906300
	H	3.931100	-1.417700	5.278100
	C	7.693900	-4.147600	2.170900
	C	-2.011300	-2.909000	9.460100
	C	3.733300	-2.183600	10.150200

	H	3.586200	-3.131800	10.143800
	H	3.972900	-1.891500	9.268200
	H	4.442600	-1.973800	10.760600
	C	6.198500	-3.995600	2.441700
	H	6.021600	-4.172600	3.368200
	H	5.923800	-3.100700	2.228500
	H	5.709900	-4.617200	1.898600
	C	7.220300	-3.243300	5.180200
	C	2.454200	-1.473000	10.591800
	C	-4.163100	-3.797400	8.796100
	H	-4.730400	-4.106800	8.128500
	C	-2.464600	-2.868900	10.779700
	H	-1.899300	-2.561000	11.451000
	C	5.227700	-2.535800	6.422600
	H	5.259500	-3.448200	6.747800
	H	5.250800	-1.940900	7.189400
	C	11.371300	-1.118800	3.172700
	C	2.455000	-1.569400	7.405300
	C	8.299200	-2.758000	4.265400
	C	7.962600	-3.870800	0.700500
	H	7.654800	-2.989100	0.479700
	H	8.905200	-3.931200	0.530500
	H	7.498200	-4.514700	0.162400
	C	2.073000	-1.983500	11.980200
	H	1.960300	-2.936000	11.952300
	H	2.767300	-1.761600	12.605900
	H	1.249600	-1.573200	12.258100
	C	9.323000	-1.891300	4.571300
	H	9.463800	-1.437800	5.370800
	C	10.106700	-1.843800	3.408800
	C	12.126000	-0.646800	4.252700
	H	11.806700	-0.750000	5.120800
	C	11.846600	-0.946800	1.885900
	H	11.346000	-1.243900	1.161200
	C	-3.745100	-3.281900	11.099500
	H	-4.036200	-3.243300	11.981500
	C	-4.601400	-3.754600	10.107000
	H	-5.459100	-4.039100	10.324000
	C	2.632700	0.042600	10.619700
	H	2.873500	0.353100	9.744100
	H	1.809400	0.457300	10.891300
	H	3.326300	0.270700	11.242900
	C	13.082900	-0.324200	1.677700
	H	13.406200	-0.212200	0.813500
	C	13.350500	-0.023400	4.031900
	H	13.845900	0.292700	4.752700
	C	13.826300	0.125900	2.760300
	H	14.650500	0.530500	2.619400
Energy single point calculations:	-3285.61391446707 a.u.			
M1···M3	O	6.303100	0.505100	5.191600
	O	2.225300	4.419600	7.148900
	N	9.219700	2.143000	2.503900
	N	0.902700	3.161600	9.709900
	N	8.034000	1.807200	3.041200
	N	6.596500	2.497500	6.188700
	H	7.077100	3.206800	6.264200
	N	2.996900	2.281700	7.115200
	H	2.849400	1.474400	7.374700
	C	9.326400	2.351400	4.748300
	H	9.650000	2.528100	5.601800
	N	-0.211500	2.611100	10.246100

	C	12.248500	3.378400	4.221000
	H	11.962900	3.411600	5.105600
	C	8.062800	1.913100	4.398800
	C	1.198900	5.547400	10.154000
	H	1.372800	5.712900	9.225000
	H	1.665600	6.195800	10.687000
	H	0.255900	5.616000	10.320200
	C	10.013300	2.470300	3.524300
	C	5.436800	2.315500	7.045900
	H	5.480000	2.941500	7.784600
	H	5.443300	1.417700	7.412800
	C	1.680500	4.147600	10.520000
	C	11.385800	2.909000	3.230900
	C	5.641200	2.183600	2.540700
	H	5.788200	3.131800	2.547100
	H	5.401600	1.891500	3.422700
	H	4.931900	1.973800	1.930300
	C	3.176000	3.995600	10.249200
	H	3.352900	4.172600	9.322700
	H	3.450700	3.100700	10.462400
	H	3.664500	4.617200	10.792300
	C	2.154100	3.243300	7.510700
	C	6.920300	1.473000	2.099100
	C	13.537600	3.797400	3.894800
	H	14.104800	4.106800	4.562400
	C	11.839100	2.868900	1.911200
	H	11.273800	2.561000	1.239900
	C	4.146700	2.535800	6.268300
	H	4.114900	3.448200	5.943100
	H	4.123600	1.940900	5.501500
	C	-1.996900	1.118800	9.518200
	C	6.919500	1.569400	5.285600
	C	1.075300	2.758000	8.425500
	C	1.411900	3.870800	11.990400
	H	1.719700	2.989100	12.211200
	H	0.469300	3.931200	12.160400
	H	1.876300	4.514700	12.528500
	C	7.301400	1.983500	0.710700
	H	7.414200	2.936000	0.738600
	H	6.607200	1.761600	0.085000
	H	8.124900	1.573200	0.432800
	C	0.051500	1.891300	8.119600
	H	-0.089300	1.437800	7.320100
	C	-0.732200	1.843800	9.282100
	C	-2.751600	0.646800	8.438200
	H	-2.432200	0.750000	7.570100
	C	-2.472200	0.946800	10.805000
	H	-1.971600	1.243900	11.529700
	C	13.119600	3.281900	1.591400
	H	13.410700	3.243300	0.709400
	C	13.975900	3.754600	2.583900
	H	14.833600	4.039100	2.366900
	C	6.741800	-0.042600	2.071200
	H	6.501000	-0.353100	2.946800
	H	7.565100	-0.457300	1.799600
	H	6.048200	-0.270700	1.448000
	C	-3.708400	0.324200	11.013200
	H	-4.031800	0.212200	11.877400
	C	-3.976000	0.023400	8.659000
	H	-4.471400	-0.292700	7.938200
	C	-4.451800	-0.125900	9.930600

	H	-5.276000	-0.530500	10.071500
	O	0.322100	8.641400	5.191600
	O	-3.755700	4.726900	7.148900
	N	3.238700	7.003500	2.503900
	N	-5.078300	5.984900	9.709900
	N	2.053000	7.339300	3.041200
	N	0.615500	6.649000	6.188700
	H	1.096100	5.939700	6.264200
	N	-2.984100	6.864800	7.115200
	H	-3.131600	7.672100	7.374700
	C	3.345400	6.795100	4.748300
	H	3.669000	6.618400	5.601800
	N	-6.192500	6.535400	10.246100
	C	6.267500	5.768100	4.221000
	H	5.981900	5.734900	5.105600
	C	2.081800	7.233400	4.398800
	C	-4.782100	3.599100	10.154000
	H	-4.608200	3.433600	9.225000
	H	-4.315400	2.950700	10.687000
	H	-5.725100	3.530500	10.320200
	C	4.032300	6.676200	3.524300
	C	-0.544200	6.831000	7.045900
	H	-0.501000	6.205000	7.784600
	H	-0.537700	7.728800	7.412800
	C	-4.300500	4.998900	10.520000
	C	5.404800	6.237500	3.230900
	C	-0.339800	6.962900	2.540700
	H	-0.192800	6.014700	2.547100
	H	-0.579400	7.255000	3.422700
	H	-1.049100	7.172700	1.930300
	C	-2.805000	5.150900	10.249200
	H	-2.628100	4.973900	9.322700
	H	-2.530300	6.045800	10.462400
	H	-2.316500	4.529300	10.792300
	C	-3.826900	5.903200	7.510700
	C	0.939300	7.673500	2.099100
	C	7.556600	5.349100	3.894800
	H	8.123800	5.039700	4.562400
	C	5.858100	6.277600	1.911200
	H	5.292800	6.585500	1.239900
	C	-1.834300	6.610700	6.268300
	H	-1.866100	5.698300	5.943100
	H	-1.857400	7.205600	5.501500
	C	-7.977900	8.027700	9.518200
	C	0.938500	7.577100	5.285600
	C	-4.905700	6.388500	8.425500
	C	-4.569100	5.275700	11.990400
	H	-4.261300	6.157400	12.211200
	H	-5.511700	5.215300	12.160400
	H	-4.104700	4.631800	12.528500
	C	1.320400	7.163000	0.710700
	H	1.433200	6.210500	0.738600
	H	0.626200	7.384900	0.085000
	H	2.143900	7.573300	0.432800
	C	-5.929500	7.255200	8.119600
	H	-6.070300	7.708700	7.320100
	C	-6.713200	7.302700	9.282100
	C	-8.732600	8.499700	8.438200
	H	-8.413200	8.396500	7.570100
	C	-8.453200	8.199700	10.805000
	H	-7.952600	7.902600	11.529700

	C	7.138600	5.864600	1.591400
	H	7.429700	5.903200	0.709400
	C	7.994900	5.391900	2.583900
	H	8.852600	5.107400	2.366900
	C	0.760800	9.189100	2.071200
	H	0.520000	9.499600	2.946800
	H	1.584100	9.603800	1.799600
	H	0.067200	9.417200	1.448000
	C	-9.689400	8.822300	11.013200
	H	-10.012800	8.934300	11.877400
	C	-9.957000	9.123100	8.659000
	H	-10.452400	9.439200	7.938200
	C	-10.432800	9.272400	9.930600
	H	-11.257000	9.677000	10.071500
Energy single point calculations:	-3285.59798036374 a.u.			
M1···M4	O	6.303100	0.505100	5.191600
	O	2.225300	4.419600	7.148900
	N	9.219700	2.143000	2.503900
	N	0.902700	3.161600	9.709900
	N	8.034000	1.807200	3.041200
	N	6.596500	2.497500	6.188700
	H	7.077100	3.206800	6.264200
	N	2.996900	2.281700	7.115200
	H	2.849400	1.474400	7.374700
	C	9.326400	2.351400	4.748300
	H	9.650000	2.528100	5.601800
	N	-0.211500	2.611100	10.246100
	C	12.248500	3.378400	4.221000
	H	11.962900	3.411600	5.105600
	C	8.062800	1.913100	4.398800
	C	1.198900	5.547400	10.154000
	H	1.372800	5.712900	9.225000
	H	1.665600	6.195800	10.687000
	H	0.255900	5.616000	10.320200
	C	10.013300	2.470300	3.524300
	C	5.436800	2.315500	7.045900
	H	5.480000	2.941500	7.784600
	H	5.443300	1.417700	7.412800
	C	1.680500	4.147600	10.520000
	C	11.385800	2.909000	3.230900
	C	5.641200	2.183600	2.540700
	H	5.788200	3.131800	2.547100
	H	5.401600	1.891500	3.422700
	H	4.931900	1.973800	1.930300
	C	3.176000	3.995600	10.249200
	H	3.352900	4.172600	9.322700
	H	3.450700	3.100700	10.462400
	H	3.664500	4.617200	10.792300
	C	2.154100	3.243300	7.510700
	C	6.920300	1.473000	2.099100
	C	13.537600	3.797400	3.894800
	H	14.104800	4.106800	4.562400
	C	11.839100	2.868900	1.911200
	H	11.273800	2.561000	1.239900
	C	4.146700	2.535800	6.268300
	H	4.114900	3.448200	5.943100
	H	4.123600	1.940900	5.501500
	C	-1.996900	1.118800	9.518200
	C	6.919500	1.569400	5.285600
	C	1.075300	2.758000	8.425500
	C	1.411900	3.870800	11.990400

	H	1.719700	2.989100	12.211200
	H	0.469300	3.931200	12.160400
	H	1.876300	4.514700	12.528500
	C	7.301400	1.983500	0.710700
	H	7.414200	2.936000	0.738600
	H	6.607200	1.761600	0.085000
	H	8.124900	1.573200	0.432800
	C	0.051500	1.891300	8.119600
	H	-0.089300	1.437800	7.320100
	C	-0.732200	1.843800	9.282100
	C	-2.751600	0.646800	8.438200
	H	-2.432200	0.750000	7.570100
	C	-2.472200	0.946800	10.805000
	H	-1.971600	1.243900	11.529700
	C	13.119600	3.281900	1.591400
	H	13.410700	3.243300	0.709400
	C	13.975900	3.754600	2.583900
	H	14.833600	4.039100	2.366900
	C	6.741800	-0.042600	2.071200
	H	6.501000	-0.353100	2.946800
	H	7.565100	-0.457300	1.799600
	H	6.048200	-0.270700	1.448000
	C	-3.708400	0.324200	11.013200
	H	-4.031800	0.212200	11.877400
	C	-3.976000	0.023400	8.659000
	H	-4.471400	-0.292700	7.938200
	C	-4.451800	-0.125900	9.930600
	H	-5.276000	-0.530500	10.071500
	O	12.284100	8.641400	5.191600
	O	8.206300	4.726900	7.148900
	N	15.200700	7.003500	2.503900
	N	6.883700	5.984900	9.709900
	N	14.015000	7.339300	3.041200
	N	12.577500	6.649000	6.188700
	H	13.058100	5.939700	6.264200
	N	8.977900	6.864800	7.115200
	H	8.830400	7.672100	7.374700
	C	15.307400	6.795100	4.748300
	H	15.631000	6.618400	5.601800
	N	5.769500	6.535400	10.246100
	C	18.229500	5.768100	4.221000
	H	17.943900	5.734900	5.105600
	C	14.043800	7.233400	4.398800
	C	7.179900	3.599100	10.154000
	H	7.353800	3.433600	9.225000
	H	7.646600	2.950700	10.687000
	H	6.236900	3.530500	10.320200
	C	15.994300	6.676200	3.524300
	C	11.417800	6.831000	7.045900
	H	11.461000	6.205000	7.784600
	H	11.424300	7.728800	7.412800
	C	7.661500	4.998900	10.520000
	C	17.366800	6.237500	3.230900
	C	11.622200	6.962900	2.540700
	H	11.769200	6.014700	2.547100
	H	11.382600	7.255000	3.422700
	H	10.912900	7.172700	1.930300
	C	9.157000	5.150900	10.249200
	H	9.333900	4.973900	9.322700
	H	9.431700	6.045800	10.462400
	H	9.645500	4.529300	10.792300

	C	8.135100	5.903200	7.510700
	C	12.901300	7.673500	2.099100
	C	19.518600	5.349100	3.894800
	H	20.085800	5.039700	4.562400
	C	17.820100	6.277600	1.911200
	H	17.254800	6.585500	1.239900
	C	10.127700	6.610700	6.268300
	H	10.095900	5.698300	5.943100
	H	10.104600	7.205600	5.501500
	C	3.984100	8.027700	9.518200
	C	12.900500	7.577100	5.285600
	C	7.056300	6.388500	8.425500
	C	7.392900	5.275700	11.990400
	H	7.700700	6.157400	12.211200
	H	6.450300	5.215300	12.160400
	H	7.857300	4.631800	12.528500
	C	13.282400	7.163000	0.710700
	H	13.395200	6.210500	0.738600
	H	12.588200	7.384900	0.085000
	H	14.105900	7.573300	0.432800
	C	6.032500	7.255200	8.119600
	H	5.891700	7.708700	7.320100
	C	5.248800	7.302700	9.282100
	C	3.229400	8.499700	8.438200
	H	3.548800	8.396500	7.570100
	C	3.508800	8.199700	10.805000
	H	4.009400	7.902600	11.529700
	C	19.100600	5.864600	1.591400
	H	19.391700	5.903200	0.709400
	C	19.956900	5.391900	2.583900
	H	20.814600	5.107400	2.366900
	C	12.722800	9.189100	2.071200
	H	12.482000	9.499600	2.946800
	H	13.546100	9.603800	1.799600
	H	12.029200	9.417200	1.448000
	C	2.272600	8.822300	11.013200
	H	1.949200	8.934300	11.877400
	C	2.005000	9.123100	8.659000
	H	1.509600	9.439200	7.938200
	C	1.529200	9.272400	9.930600
	H	0.705000	9.677000	10.071500
Energy single point calculations:	-3285.59798036435 a.u.			
	O	6.303100	0.505100	5.191600
	O	2.225300	4.419600	7.148900
	N	9.219700	2.143000	2.503900
	N	0.902700	3.161600	9.709900
	N	8.034000	1.807200	3.041200
	N	6.596500	2.497500	6.188700
	H	7.077100	3.206800	6.264200
	N	2.996900	2.281700	7.115200
	H	2.849400	1.474400	7.374700
M1···M5	C	9.326400	2.351400	4.748300
	H	9.650000	2.528100	5.601800
	N	-0.211500	2.611100	10.246100
	C	12.248500	3.378400	4.221000
	H	11.962900	3.411600	5.105600
	C	8.062800	1.913100	4.398800
	C	1.198900	5.547400	10.154000
	H	1.372800	5.712900	9.225000
	H	1.665600	6.195800	10.687000
	H	0.255900	5.616000	10.320200

	C	10.013300	2.470300	3.524300
	C	5.436800	2.315500	7.045900
	H	5.480000	2.941500	7.784600
	H	5.443300	1.417700	7.412800
	C	1.680500	4.147600	10.520000
	C	11.385800	2.909000	3.230900
	C	5.641200	2.183600	2.540700
	H	5.788200	3.131800	2.547100
	H	5.401600	1.891500	3.422700
	H	4.931900	1.973800	1.930300
	C	3.176000	3.995600	10.249200
	H	3.352900	4.172600	9.322700
	H	3.450700	3.100700	10.462400
	H	3.664500	4.617200	10.792300
	C	2.154100	3.243300	7.510700
	C	6.920300	1.473000	2.099100
	C	13.537600	3.797400	3.894800
	H	14.104800	4.106800	4.562400
	C	11.839100	2.868900	1.911200
	H	11.273800	2.561000	1.239900
	C	4.146700	2.535800	6.268300
	H	4.114900	3.448200	5.943100
	H	4.123600	1.940900	5.501500
	C	-1.996900	1.118800	9.518200
	C	6.919500	1.569400	5.285600
	C	1.075300	2.758000	8.425500
	C	1.411900	3.870800	11.990400
	H	1.719700	2.989100	12.211200
	H	0.469300	3.931200	12.160400
	H	1.876300	4.514700	12.528500
	C	7.301400	1.983500	0.710700
	H	7.414200	2.936000	0.738600
	H	6.607200	1.761600	0.085000
	H	8.124900	1.573200	0.432800
	C	0.051500	1.891300	8.119600
	H	-0.089300	1.437800	7.320100
	C	-0.732200	1.843800	9.282100
	C	-2.751600	0.646800	8.438200
	H	-2.432200	0.750000	7.570100
	C	-2.472200	0.946800	10.805000
	H	-1.971600	1.243900	11.529700
	C	13.119600	3.281900	1.591400
	H	13.410700	3.243300	0.709400
	C	13.975900	3.754600	2.583900
	H	14.833600	4.039100	2.366900
	C	6.741800	-0.042600	2.071200
	H	6.501000	-0.353100	2.946800
	H	7.565100	-0.457300	1.799600
	H	6.048200	-0.270700	1.448000
	C	-3.708400	0.324200	11.013200
	H	-4.031800	0.212200	11.877400
	C	-3.976000	0.023400	8.659000
	H	-4.471400	-0.292700	7.938200
	C	-4.451800	-0.125900	9.930600
	H	-5.276000	-0.530500	10.071500
	O	18.265100	0.505100	5.191600
	O	14.187300	4.419600	7.148900
	N	21.181700	2.143000	2.503900
	N	12.864700	3.161600	9.709900
	N	19.996000	1.807200	3.041200
	N	18.558500	2.497500	6.188700

	H	19.039100	3.206800	6.264200
	N	14.958900	2.281700	7.115200
	H	14.811400	1.474400	7.374700
	C	21.288400	2.351400	4.748300
	H	21.612000	2.528100	5.601800
	N	11.750500	2.611100	10.246100
	C	24.210500	3.378400	4.221000
	H	23.924900	3.411600	5.105600
	C	20.024800	1.913100	4.398800
	C	13.160900	5.547400	10.154000
	H	13.334800	5.712900	9.225000
	H	13.627600	6.195800	10.687000
	H	12.217900	5.616000	10.320200
	C	21.975300	2.470300	3.524300
	C	17.398800	2.315500	7.045900
	H	17.442000	2.941500	7.784600
	H	17.405300	1.417700	7.412800
	C	13.642500	4.147600	10.520000
	C	23.347800	2.909000	3.230900
	C	17.603200	2.183600	2.540700
	H	17.750200	3.131800	2.547100
	H	17.363600	1.891500	3.422700
	H	16.893900	1.973800	1.930300
	C	15.138000	3.995600	10.249200
	H	15.314900	4.172600	9.322700
	H	15.412700	3.100700	10.462400
	H	15.626500	4.617200	10.792300
	C	14.116100	3.243300	7.510700
	C	18.882300	1.473000	2.099100
	C	25.499600	3.797400	3.894800
	H	26.066800	4.106800	4.562400
	C	23.801100	2.868900	1.911200
	H	23.235800	2.561000	1.239900
	C	16.108700	2.535800	6.268300
	H	16.076900	3.448200	5.943100
	H	16.085600	1.940900	5.501500
	C	9.965100	1.118800	9.518200
	C	18.881500	1.569400	5.285600
	C	13.037300	2.758000	8.425500
	C	13.373900	3.870800	11.990400
	H	13.681700	2.989100	12.211200
	H	12.431300	3.931200	12.160400
	H	13.838300	4.514700	12.528500
	C	19.263400	1.983500	0.710700
	H	19.376200	2.936000	0.738600
	H	18.569200	1.761600	0.085000
	H	20.086900	1.573200	0.432800
	C	12.013500	1.891300	8.119600
	H	11.872700	1.437800	7.320100
	C	11.229800	1.843800	9.282100
	C	9.210400	0.646800	8.438200
	H	9.529800	0.750000	7.570100
	C	9.489800	0.946800	10.805000
	H	9.990400	1.243900	11.529700
	C	25.081600	3.281900	1.591400
	H	25.372700	3.243300	0.709400
	C	25.937900	3.754600	2.583900
	H	26.795600	4.039100	2.366900
	C	18.703800	-0.042600	2.071200
	H	18.463000	-0.353100	2.946800
	H	19.527100	-0.457300	1.799600

	H	18.010200	-0.270700	1.448000
	C	8.253600	0.324200	11.013200
	H	7.930200	0.212200	11.877400
	C	7.986000	0.023400	8.659000
	H	7.490600	-0.292700	7.938200
	C	7.510200	-0.125900	9.930600
	H	6.686000	-0.530500	10.071500
Energy single point calculations:	-3285.57849664542 a.u.			
M1···M6	O	6.303100	0.505100	5.191600
	O	2.225300	4.419600	7.148900
	N	9.219700	2.143000	2.503900
	N	0.902700	3.161600	9.709900
	N	8.034000	1.807200	3.041200
	N	6.596500	2.497500	6.188700
	H	7.077100	3.206800	6.264200
	N	2.996900	2.281700	7.115200
	H	2.849400	1.474400	7.374700
	C	9.326400	2.351400	4.748300
	H	9.650000	2.528100	5.601800
	N	-0.211500	2.611100	10.246100
	C	12.248500	3.378400	4.221000
	H	11.962900	3.411600	5.105600
	C	8.062800	1.913100	4.398800
	C	1.198900	5.547400	10.154000
	H	1.372800	5.712900	9.225000
	H	1.665600	6.195800	10.687000
	H	0.255900	5.616000	10.320200
	C	10.013300	2.470300	3.524300
	C	5.436800	2.315500	7.045900
	H	5.480000	2.941500	7.784600
	H	5.443300	1.417700	7.412800
	C	1.680500	4.147600	10.520000
	C	11.385800	2.909000	3.230900
	C	5.641200	2.183600	2.540700
	H	5.788200	3.131800	2.547100
	H	5.401600	1.891500	3.422700
	H	4.931900	1.973800	1.930300
	C	3.176000	3.995600	10.249200
	H	3.352900	4.172600	9.322700
	H	3.450700	3.100700	10.462400
	H	3.664500	4.617200	10.792300
	C	2.154100	3.243300	7.510700
	C	6.920300	1.473000	2.099100
	C	13.537600	3.797400	3.894800
	H	14.104800	4.106800	4.562400
	C	11.839100	2.868900	1.911200
	H	11.273800	2.561000	1.239900
	C	4.146700	2.535800	6.268300
	H	4.114900	3.448200	5.943100
	H	4.123600	1.940900	5.501500
	C	-1.996900	1.118800	9.518200
	C	6.919500	1.569400	5.285600
	C	1.075300	2.758000	8.425500
	C	1.411900	3.870800	11.990400
	H	1.719700	2.989100	12.211200
	H	0.469300	3.931200	12.160400
	H	1.876300	4.514700	12.528500
	C	7.301400	1.983500	0.710700
	H	7.414200	2.936000	0.738600
	H	6.607200	1.761600	0.085000
	H	8.124900	1.573200	0.432800

	C	0.051500	1.891300	8.119600
	H	-0.089300	1.437800	7.320100
	C	-0.732200	1.843800	9.282100
	C	-2.751600	0.646800	8.438200
	H	-2.432200	0.750000	7.570100
	C	-2.472200	0.946800	10.805000
	H	-1.971600	1.243900	11.529700
	C	13.119600	3.281900	1.591400
	H	13.410700	3.243300	0.709400
	C	13.975900	3.754600	2.583900
	H	14.833600	4.039100	2.366900
	C	6.741800	-0.042600	2.071200
	H	6.501000	-0.353100	2.946800
	H	7.565100	-0.457300	1.799600
	H	6.048200	-0.270700	1.448000
	C	-3.708400	0.324200	11.013200
	H	-4.031800	0.212200	11.877400
	C	-3.976000	0.023400	8.659000
	H	-4.471400	-0.292700	7.938200
	C	-4.451800	-0.125900	9.930600
	H	-5.276000	-0.530500	10.071500
	O	-5.658900	0.505100	5.191600
	O	-9.736700	4.419600	7.148900
	N	-2.742300	2.143000	2.503900
	N	-11.059300	3.161600	9.709900
	N	-3.928000	1.807200	3.041200
	N	-5.365500	2.497500	6.188700
	H	-4.884900	3.206800	6.264200
	N	-8.965100	2.281700	7.115200
	H	-9.112600	1.474400	7.374700
	C	-2.635600	2.351400	4.748300
	H	-2.312000	2.528100	5.601800
	N	-12.173500	2.611100	10.246100
	C	0.286500	3.378400	4.221000
	H	0.000900	3.411600	5.105600
	C	-3.899200	1.913100	4.398800
	C	-10.763100	5.547400	10.154000
	H	-10.589200	5.712900	9.225000
	H	-10.296400	6.195800	10.687000
	H	-11.706100	5.616000	10.320200
	C	-1.948700	2.470300	3.524300
	C	-6.525200	2.315500	7.045900
	H	-6.482000	2.941500	7.784600
	H	-6.518700	1.417700	7.412800
	C	-10.281500	4.147600	10.520000
	C	-0.576200	2.909000	3.230900
	C	-6.320800	2.183600	2.540700
	H	-6.173800	3.131800	2.547100
	H	-6.560400	1.891500	3.422700
	H	-7.030100	1.973800	1.930300
	C	-8.786000	3.995600	10.249200
	H	-8.609100	4.172600	9.322700
	H	-8.511300	3.100700	10.462400
	H	-8.297500	4.617200	10.792300
	C	-9.807900	3.243300	7.510700
	C	-5.041700	1.473000	2.099100
	C	1.575600	3.797400	3.894800
	H	2.142800	4.106800	4.562400
	C	-0.122900	2.868900	1.911200
	H	-0.688200	2.561000	1.239900
	C	-7.815300	2.535800	6.268300

	H	-7.847100	3.448200	5.943100
	H	-7.838400	1.940900	5.501500
	C	-13.958900	1.118800	9.518200
	C	-5.042500	1.569400	5.285600
	C	-10.886700	2.758000	8.425500
	C	-10.550100	3.870800	11.990400
	H	-10.242300	2.989100	12.211200
	H	-11.492700	3.931200	12.160400
	H	-10.085700	4.514700	12.528500
	C	-4.660600	1.983500	0.710700
	H	-4.547800	2.936000	0.738600
	H	-5.354800	1.761600	0.085000
	H	-3.837100	1.573200	0.432800
	C	-11.910500	1.891300	8.119600
	H	-12.051300	1.437800	7.320100
	C	-12.694200	1.843800	9.282100
	C	-14.713600	0.646800	8.438200
	H	-14.394200	0.750000	7.570100
	C	-14.434200	0.946800	10.805000
	H	-13.933600	1.243900	11.529700
	C	1.157600	3.281900	1.591400
	H	1.448700	3.243300	0.709400
	C	2.013900	3.754600	2.583900
	H	2.871600	4.039100	2.366900
	C	-5.220200	-0.042600	2.071200
	H	-5.461000	-0.353100	2.946800
	H	-4.396900	-0.457300	1.799600
	H	-5.913800	-0.270700	1.448000
	C	-15.670400	0.324200	11.013200
	H	-15.993800	0.212200	11.877400
	C	-15.938000	0.023400	8.659000
	H	-16.433400	-0.292700	7.938200
	C	-16.413800	-0.125900	9.930600
	H	-17.238000	-0.530500	10.071500
Energy single point calculations:	-3285.5784966452 u.a.			
M1···M7	O	6.303100	0.505100	5.191600
	O	2.225300	4.419600	7.148900
	N	9.219700	2.143000	2.503900
	N	0.902700	3.161600	9.709900
	N	8.034000	1.807200	3.041200
	N	6.596500	2.497500	6.188700
	H	7.077100	3.206800	6.264200
	N	2.996900	2.281700	7.115200
	H	2.849400	1.474400	7.374700
	C	9.326400	2.351400	4.748300
	H	9.650000	2.528100	5.601800
	N	-0.211500	2.611100	10.246100
	C	12.248500	3.378400	4.221000
	H	11.962900	3.411600	5.105600
	C	8.062800	1.913100	4.398800
	C	1.198900	5.547400	10.154000
	H	1.372800	5.712900	9.225000
	H	1.665600	6.195800	10.687000
	H	0.255900	5.616000	10.320200
	C	10.013300	2.470300	3.524300
	C	5.436800	2.315500	7.045900
	H	5.480000	2.941500	7.784600
	H	5.443300	1.417700	7.412800
	C	1.680500	4.147600	10.520000
	C	11.385800	2.909000	3.230900

	C	5.641200	2.183600	2.540700
	H	5.788200	3.131800	2.547100
	H	5.401600	1.891500	3.422700
	H	4.931900	1.973800	1.930300
	C	3.176000	3.995600	10.249200
	H	3.352900	4.172600	9.322700
	H	3.450700	3.100700	10.462400
	H	3.664500	4.617200	10.792300
	C	2.154100	3.243300	7.510700
	C	6.920300	1.473000	2.099100
	C	13.537600	3.797400	3.894800
	H	14.104800	4.106800	4.562400
	C	11.839100	2.868900	1.911200
	H	11.273800	2.561000	1.239900
	C	4.146700	2.535800	6.268300
	H	4.114900	3.448200	5.943100
	H	4.123600	1.940900	5.501500
	C	-1.996900	1.118800	9.518200
	C	6.919500	1.569400	5.285600
	C	1.075300	2.758000	8.425500
	C	1.411900	3.870800	11.990400
	H	1.719700	2.989100	12.211200
	H	0.469300	3.931200	12.160400
	H	1.876300	4.514700	12.528500
	C	7.301400	1.983500	0.710700
	H	7.414200	2.936000	0.738600
	H	6.607200	1.761600	0.085000
	H	8.124900	1.573200	0.432800
	C	0.051500	1.891300	8.119600
	H	-0.089300	1.437800	7.320100
	C	-0.732200	1.843800	9.282100
	C	-2.751600	0.646800	8.438200
	H	-2.432200	0.750000	7.570100
	C	-2.472200	0.946800	10.805000
	H	-1.971600	1.243900	11.529700
	C	13.119600	3.281900	1.591400
	H	13.410700	3.243300	0.709400
	C	13.975900	3.754600	2.583900
	H	14.833600	4.039100	2.366900
	C	6.741800	-0.042600	2.071200
	H	6.501000	-0.353100	2.946800
	H	7.565100	-0.457300	1.799600
	H	6.048200	-0.270700	1.448000
	C	-3.708400	0.324200	11.013200
	H	-4.031800	0.212200	11.877400
	C	-3.976000	0.023400	8.659000
	H	-4.471400	-0.292700	7.938200
	C	-4.451800	-0.125900	9.930600
	H	-5.276000	-0.530500	10.071500
	O	-8.890700	-0.505100	7.499300
	O	-4.812800	-4.419600	5.542000
	N	-11.807300	-2.143000	10.187000
	N	-3.490300	-3.161600	2.981000
	N	-10.621500	-1.807200	9.649700
	N	-9.184000	-2.497500	6.502200
	H	-9.664600	-3.206800	6.426700
	N	-5.584400	-2.281700	5.575700
	H	-5.436900	-1.474400	5.316200
	C	-11.913900	-2.351400	7.942600
	H	-12.237500	-2.528100	7.089100
	N	-2.376000	-2.611100	2.444800

	C	-14.836100	-3.378400	8.469900
	H	-14.550500	-3.411600	7.585400
	C	-10.650300	-1.913100	8.292100
	C	-3.786500	-5.547400	2.536900
	H	-3.960300	-5.712900	3.465900
	H	-4.253200	-6.195800	2.003900
	H	-2.843500	-5.616000	2.370700
	C	-12.600800	-2.470300	9.166600
	C	-8.024300	-2.315500	5.645000
	H	-8.067500	-2.941500	4.906300
	H	-8.030900	-1.417700	5.278100
	C	-4.268100	-4.147600	2.170900
	C	-13.973300	-2.909000	9.460100
	C	-8.228700	-2.183600	10.150200
	H	-8.375800	-3.131800	10.143800
	H	-7.989100	-1.891500	9.268200
	H	-7.519400	-1.973800	10.760600
	C	-5.763500	-3.995600	2.441700
	H	-5.940400	-4.172600	3.368200
	H	-6.038200	-3.100700	2.228500
	H	-6.252100	-4.617200	1.898600
	C	-4.741700	-3.243300	5.180200
	C	-9.507800	-1.473000	10.591800
	C	-16.125100	-3.797400	8.796100
	H	-16.692400	-4.106800	8.128500
	C	-14.426600	-2.868900	10.779700
	H	-13.861300	-2.561000	11.451000
	C	-6.734300	-2.535800	6.422600
	H	-6.702500	-3.448200	6.747800
	H	-6.711200	-1.940900	7.189400
	C	-0.590700	-1.118800	3.172700
	C	-9.507000	-1.569400	7.405300
	C	-3.662800	-2.758000	4.265400
	C	-3.999400	-3.870800	0.700500
	H	-4.307200	-2.989100	0.479700
	H	-3.056800	-3.931200	0.530500
	H	-4.463800	-4.514700	0.162400
	C	-9.889000	-1.983500	11.980200
	H	-10.001700	-2.936000	11.952300
	H	-9.194700	-1.761600	12.605900
	H	-10.712400	-1.573200	12.258100
	C	-2.639000	-1.891300	4.571300
	H	-2.498200	-1.437800	5.370800
	C	-1.855300	-1.843800	3.408800
	C	0.164000	-0.646800	4.252700
	H	-0.155300	-0.750000	5.120800
	C	-0.115400	-0.946800	1.885900
	H	-0.616000	-1.243900	1.161200
	C	-15.707100	-3.281900	11.099500
	H	-15.998200	-3.243300	11.981500
	C	-16.563400	-3.754600	10.107000
	H	-17.421100	-4.039100	10.324000
	C	-9.329300	0.042600	10.619700
	H	-9.088500	0.353100	9.744100
	H	-10.152600	0.457300	10.891300
	H	-8.635700	0.270700	11.242900
	C	1.120900	-0.324200	1.677700
	H	1.444200	-0.212200	0.813500
	C	1.388500	-0.023400	4.031900
	H	1.883900	0.292700	4.752700
	C	1.864300	0.125900	2.760300

	H	2.688500	0.530500	2.619400
Energy single point calculations:	-3285.5701441852 a.u.			
M1···M8	O	6.303100	0.505100	5.191600
	O	2.225300	4.419600	7.148900
	N	9.219700	2.143000	2.503900
	N	0.902700	3.161600	9.709900
	N	8.034000	1.807200	3.041200
	N	6.596500	2.497500	6.188700
	H	7.077100	3.206800	6.264200
	N	2.996900	2.281700	7.115200
	H	2.849400	1.474400	7.374700
	C	9.326400	2.351400	4.748300
	H	9.650000	2.528100	5.601800
	N	-0.211500	2.611100	10.246100
	C	12.248500	3.378400	4.221000
	H	11.962900	3.411600	5.105600
	C	8.062800	1.913100	4.398800
	C	1.198900	5.547400	10.154000
	H	1.372800	5.712900	9.225000
	H	1.665600	6.195800	10.687000
	H	0.255900	5.616000	10.320200
	C	10.013300	2.470300	3.524300
	C	5.436800	2.315500	7.045900
	H	5.480000	2.941500	7.784600
	H	5.443300	1.417700	7.412800
	C	1.680500	4.147600	10.520000
	C	11.385800	2.909000	3.230900
	C	5.641200	2.183600	2.540700
	H	5.788200	3.131800	2.547100
	H	5.401600	1.891500	3.422700
	H	4.931900	1.973800	1.930300
	C	3.176000	3.995600	10.249200
	H	3.352900	4.172600	9.322700
	H	3.450700	3.100700	10.462400
	H	3.664500	4.617200	10.792300
	C	2.154100	3.243300	7.510700
	C	6.920300	1.473000	2.099100
	C	13.537600	3.797400	3.894800
	H	14.104800	4.106800	4.562400
	C	11.839100	2.868900	1.911200
	H	11.273800	2.561000	1.239900
	C	4.146700	2.535800	6.268300
	H	4.114900	3.448200	5.943100
	H	4.123600	1.940900	5.501500
	C	-1.996900	1.118800	9.518200
	C	6.919500	1.569400	5.285600
	C	1.075300	2.758000	8.425500
	C	1.411900	3.870800	11.990400
	H	1.719700	2.989100	12.211200
	H	0.469300	3.931200	12.160400
	H	1.876300	4.514700	12.528500
	C	7.301400	1.983500	0.710700
	H	7.414200	2.936000	0.738600
	H	6.607200	1.761600	0.085000
	H	8.124900	1.573200	0.432800
	C	0.051500	1.891300	8.119600
	H	-0.089300	1.437800	7.320100
	C	-0.732200	1.843800	9.282100
	C	-2.751600	0.646800	8.438200
	H	-2.432200	0.750000	7.570100
	C	-2.472200	0.946800	10.805000

	H	-1.971600	1.243900	11.529700
	C	13.119600	3.281900	1.591400
	H	13.410700	3.243300	0.709400
	C	13.975900	3.754600	2.583900
	H	14.833600	4.039100	2.366900
	C	6.741800	-0.042600	2.071200
	H	6.501000	-0.353100	2.946800
	H	7.565100	-0.457300	1.799600
	H	6.048200	-0.270700	1.448000
	C	-3.708400	0.324200	11.013200
	H	-4.031800	0.212200	11.877400
	C	-3.976000	0.023400	8.659000
	H	-4.471400	-0.292700	7.938200
	C	-4.451800	-0.125900	9.930600
	H	-5.276000	-0.530500	10.071500
	O	20.852700	0.505100	-7.499300
	O	16.774800	4.419600	-5.542000
	N	23.769300	2.143000	-10.187000
	N	15.452300	3.161600	-2.981000
	N	22.583500	1.807200	-9.649700
	N	21.146000	2.497500	-6.502200
	H	21.626600	3.206800	-6.426700
	N	17.546400	2.281700	-5.575700
	H	17.398900	1.474400	-5.316200
	C	23.875900	2.351400	-7.942600
	H	24.199500	2.528100	-7.089100
	N	14.338000	2.611100	-2.444800
	C	26.798100	3.378400	-8.469900
	H	26.512500	3.411600	-7.585400
	C	22.612300	1.913100	-8.292100
	C	15.748500	5.547400	-2.536900
	H	15.922300	5.712900	-3.465900
	H	16.215200	6.195800	-2.003900
	H	14.805500	5.616000	-2.370700
	C	24.562800	2.470300	-9.166600
	C	19.986300	2.315500	-5.645000
	H	20.029500	2.941500	-4.906300
	H	19.992900	1.417700	-5.278100
	C	16.230100	4.147600	-2.170900
	C	25.935300	2.909000	-9.460100
	C	20.190700	2.183600	-10.150200
	H	20.337800	3.131800	-10.143800
	H	19.951100	1.891500	-9.268200
	H	19.481400	1.973800	-10.760600
	C	17.725500	3.995600	-2.441700
	H	17.902400	4.172600	-3.368200
	H	18.000200	3.100700	-2.228500
	H	18.214100	4.617200	-1.898600
	C	16.703700	3.243300	-5.180200
	C	21.469800	1.473000	-10.591800
	C	28.087100	3.797400	-8.796100
	H	28.654400	4.106800	-8.128500
	C	26.388600	2.868900	-10.779700
	H	25.823300	2.561000	-11.451000
	C	18.696300	2.535800	-6.422600
	H	18.664500	3.448200	-6.747800
	H	18.673200	1.940900	-7.189400
	C	12.552700	1.118800	-3.172700
	C	21.469000	1.569400	-7.405300
	C	15.624800	2.758000	-4.265400
	C	15.961400	3.870800	-0.700500

	H	16.269200	2.989100	-0.479700
	H	15.018800	3.931200	-0.530500
	H	16.425800	4.514700	-0.162400
	C	21.851000	1.983500	-11.980200
	H	21.963700	2.936000	-11.952300
	H	21.156700	1.761600	-12.605900
	H	22.674400	1.573200	-12.258100
	C	14.601000	1.891300	-4.571300
	H	14.460200	1.437800	-5.370800
	C	13.817300	1.843800	-3.408800
	C	11.798000	0.646800	-4.252700
	H	12.117300	0.750000	-5.120800
	C	12.077400	0.946800	-1.885900
	H	12.578000	1.243900	-1.161200
	C	27.669100	3.281900	-11.099500
	H	27.960200	3.243300	-11.981500
	C	28.525400	3.754600	-10.107000
	H	29.383100	4.039100	-10.324000
	C	21.291300	-0.042600	-10.619700
	H	21.050500	-0.353100	-9.744100
	H	22.114600	-0.457300	-10.891300
	H	20.597700	-0.270700	-11.242900
	C	10.841100	0.324200	-1.677700
	H	10.517800	0.212200	-0.813500
	C	10.573500	0.023400	-4.031900
	H	10.078100	-0.292700	-4.752700
	C	10.097700	-0.125900	-2.760300
	H	9.273500	-0.530500	-2.619400
Energy single point calculations:	-3285.5683743027 a.u.			
M1···M9	O	6.303100	0.505100	5.191600
	O	2.225300	4.419600	7.148900
	N	9.219700	2.143000	2.503900
	N	0.902700	3.161600	9.709900
	N	8.034000	1.807200	3.041200
	N	6.596500	2.497500	6.188700
	H	7.077100	3.206800	6.264200
	N	2.996900	2.281700	7.115200
	H	2.849400	1.474400	7.374700
	C	9.326400	2.351400	4.748300
	H	9.650000	2.528100	5.601800
	N	-0.211500	2.611100	10.246100
	C	12.248500	3.378400	4.221000
	H	11.962900	3.411600	5.105600
	C	8.062800	1.913100	4.398800
	C	1.198900	5.547400	10.154000
	H	1.372800	5.712900	9.225000
	H	1.665600	6.195800	10.687000
	H	0.255900	5.616000	10.320200
	C	10.013300	2.470300	3.524300
	C	5.436800	2.315500	7.045900
	H	5.480000	2.941500	7.784600
	H	5.443300	1.417700	7.412800
	C	1.680500	4.147600	10.520000
	C	11.385800	2.909000	3.230900
	C	5.641200	2.183600	2.540700
	H	5.788200	3.131800	2.547100
	H	5.401600	1.891500	3.422700
	H	4.931900	1.973800	1.930300
	C	3.176000	3.995600	10.249200
	H	3.352900	4.172600	9.322700

	H	3.450700	3.100700	10.462400
	H	3.664500	4.617200	10.792300
	C	2.154100	3.243300	7.510700
	C	6.920300	1.473000	2.099100
	C	13.537600	3.797400	3.894800
	H	14.104800	4.106800	4.562400
	C	11.839100	2.868900	1.911200
	H	11.273800	2.561000	1.239900
	C	4.146700	2.535800	6.268300
	H	4.114900	3.448200	5.943100
	H	4.123600	1.940900	5.501500
	C	-1.996900	1.118800	9.518200
	C	6.919500	1.569400	5.285600
	C	1.075300	2.758000	8.425500
	C	1.411900	3.870800	11.990400
	H	1.719700	2.989100	12.211200
	H	0.469300	3.931200	12.160400
	H	1.876300	4.514700	12.528500
	C	7.301400	1.983500	0.710700
	H	7.414200	2.936000	0.738600
	H	6.607200	1.761600	0.085000
	H	8.124900	1.573200	0.432800
	C	0.051500	1.891300	8.119600
	H	-0.089300	1.437800	7.320100
	C	-0.732200	1.843800	9.282100
	C	-2.751600	0.646800	8.438200
	H	-2.432200	0.750000	7.570100
	C	-2.472200	0.946800	10.805000
	H	-1.971600	1.243900	11.529700
	C	13.119600	3.281900	1.591400
	H	13.410700	3.243300	0.709400
	C	13.975900	3.754600	2.583900
	H	14.833600	4.039100	2.366900
	C	6.741800	-0.042600	2.071200
	H	6.501000	-0.353100	2.946800
	H	7.565100	-0.457300	1.799600
	H	6.048200	-0.270700	1.448000
	C	-3.708400	0.324200	11.013200
	H	-4.031800	0.212200	11.877400
	C	-3.976000	0.023400	8.659000
	H	-4.471400	-0.292700	7.938200
	C	-4.451800	-0.125900	9.930600
	H	-5.276000	-0.530500	10.071500
	O	-8.246400	0.505100	17.882500
	O	-12.324200	4.419600	19.839800
	N	-5.329800	2.143000	15.194800
	N	-13.646800	3.161600	22.400800
	N	-6.515600	1.807200	15.732200
	N	-7.953000	2.497500	18.879600
	H	-7.472500	3.206800	18.955100
	N	-11.552600	2.281700	19.806100
	H	-11.700200	1.474400	20.065600
	C	-5.223200	2.351400	17.439200
	H	-4.899500	2.528100	18.292700
	N	-14.761000	2.611100	22.937000
	C	-2.301000	3.378400	16.911900
	H	-2.586600	3.411600	17.796500
	C	-6.486700	1.913100	17.089700
	C	-13.350600	5.547400	22.844900
	H	-13.176700	5.712900	21.915900
	H	-12.883900	6.195800	23.377900

	H	-14.293600	5.616000	23.011100
	C	-4.536300	2.470300	16.215200
	C	-9.112700	2.315500	19.736800
	H	-9.069600	2.941500	20.475500
	H	-9.106200	1.417700	20.103700
	C	-12.869000	4.147600	23.210900
	C	-3.163700	2.909000	15.921800
	C	-8.908300	2.183600	15.231600
	H	-8.761300	3.131800	15.238000
	H	-9.148000	1.891500	16.113600
	H	-9.617600	1.973800	14.621200
	C	-11.373500	3.995600	22.940100
	H	-11.196600	4.172600	22.013600
	H	-11.098800	3.100700	23.153300
	H	-10.885000	4.617200	23.483200
	C	-12.395400	3.243300	20.201600
	C	-7.629200	1.473000	14.790000
	C	-1.012000	3.797400	16.585700
	H	-0.444700	4.106800	17.253300
	C	-2.710500	2.868900	14.602200
	H	-3.275700	2.561000	13.930800
	C	-10.402800	2.535800	18.959200
	H	-10.434600	3.448200	18.634100
	H	-10.425900	1.940900	18.192400
	C	-16.546400	1.118800	22.209100
	C	-7.630000	1.569400	17.976500
	C	-13.474300	2.758000	21.116400
	C	-13.137700	3.870800	24.681300
	H	-12.829800	2.989100	24.902100
	H	-14.080300	3.931200	24.851300
	H	-12.673200	4.514700	25.219400
	C	-7.248100	1.983500	13.401600
	H	-7.135400	2.936000	13.429500
	H	-7.942300	1.761600	12.775900
	H	-6.424700	1.573200	13.123700
	C	-14.498100	1.891300	20.810500
	H	-14.638900	1.437800	20.011000
	C	-15.281700	1.843800	21.973000
	C	-17.301100	0.646800	21.129100
	H	-16.981800	0.750000	20.261000
	C	-17.021700	0.946800	23.495900
	H	-16.521100	1.243900	24.220600
	C	-1.429900	3.281900	14.282300
	H	-1.138800	3.243300	13.400300
	C	-0.573600	3.754600	15.274800
	H	0.284000	4.039100	15.057800
	C	-7.807800	-0.042600	14.762100
	H	-8.048500	-0.353100	15.637700
	H	-6.984400	-0.457300	14.490500
	H	-8.501300	-0.270700	14.138900
	C	-18.257900	0.324200	23.704100
	H	-18.581300	0.212200	24.568300
	C	-18.525600	0.023400	21.349900
	H	-19.021000	-0.292700	20.629100
	C	-19.001400	-0.125900	22.621500
	H	-19.825600	-0.530500	22.762400
Energy single point calculations:	-3285.56837651708 a.u.			
M1···M10	O	6.303100	0.505100	5.191600
	O	2.225300	4.419600	7.148900
	N	9.219700	2.143000	2.503900
	N	0.902700	3.161600	9.709900

	N	8.034000	1.807200	3.041200
	N	6.596500	2.497500	6.188700
	H	7.077100	3.206800	6.264200
	N	2.996900	2.281700	7.115200
	H	2.849400	1.474400	7.374700
	C	9.326400	2.351400	4.748300
	H	9.650000	2.528100	5.601800
	N	-0.211500	2.611100	10.246100
	C	12.248500	3.378400	4.221000
	H	11.962900	3.411600	5.105600
	C	8.062800	1.913100	4.398800
	C	1.198900	5.547400	10.154000
	H	1.372800	5.712900	9.225000
	H	1.665600	6.195800	10.687000
	H	0.255900	5.616000	10.320200
	C	10.013300	2.470300	3.524300
	C	5.436800	2.315500	7.045900
	H	5.480000	2.941500	7.784600
	H	5.443300	1.417700	7.412800
	C	1.680500	4.147600	10.520000
	C	11.385800	2.909000	3.230900
	C	5.641200	2.183600	2.540700
	H	5.788200	3.131800	2.547100
	H	5.401600	1.891500	3.422700
	H	4.931900	1.973800	1.930300
	C	3.176000	3.995600	10.249200
	H	3.352900	4.172600	9.322700
	H	3.450700	3.100700	10.462400
	H	3.664500	4.617200	10.792300
	C	2.154100	3.243300	7.510700
	C	6.920300	1.473000	2.099100
	C	13.537600	3.797400	3.894800
	H	14.104800	4.106800	4.562400
	C	11.839100	2.868900	1.911200
	H	11.273800	2.561000	1.239900
	C	4.146700	2.535800	6.268300
	H	4.114900	3.448200	5.943100
	H	4.123600	1.940900	5.501500
	C	-1.996900	1.118800	9.518200
	C	6.919500	1.569400	5.285600
	C	1.075300	2.758000	8.425500
	C	1.411900	3.870800	11.990400
	H	1.719700	2.989100	12.211200
	H	0.469300	3.931200	12.160400
	H	1.876300	4.514700	12.528500
	C	7.301400	1.983500	0.710700
	H	7.414200	2.936000	0.738600
	H	6.607200	1.761600	0.085000
	H	8.124900	1.573200	0.432800
	C	0.051500	1.891300	8.119600
	H	-0.089300	1.437800	7.320100
	C	-0.732200	1.843800	9.282100
	C	-2.751600	0.646800	8.438200
	H	-2.432200	0.750000	7.570100
	C	-2.472200	0.946800	10.805000
	H	-1.971600	1.243900	11.529700
	C	13.119600	3.281900	1.591400
	H	13.410700	3.243300	0.709400
	C	13.975900	3.754600	2.583900
	H	14.833600	4.039100	2.366900
	C	6.741800	-0.042600	2.071200

	H	6.501000	-0.353100	2.946800
	H	7.565100	-0.457300	1.799600
	H	6.048200	-0.270700	1.448000
	C	-3.708400	0.324200	11.013200
	H	-4.031800	0.212200	11.877400
	C	-3.976000	0.023400	8.659000
	H	-4.471400	-0.292700	7.938200
	C	-4.451800	-0.125900	9.930600
	H	-5.276000	-0.530500	10.071500
	O	14.871700	8.641400	-7.499300
	O	10.793800	4.726900	-5.542000
	N	17.788300	7.003500	-10.187000
	N	9.471300	5.984900	-2.981000
	N	16.602500	7.339300	-9.649700
	N	15.165000	6.649000	-6.502200
	H	15.645600	5.939700	-6.426700
	N	11.565400	6.864800	-5.575700
	H	11.417900	7.672100	-5.316200
	C	17.894900	6.795100	-7.942600
	H	18.218500	6.618400	-7.089100
	N	8.357000	6.535400	-2.444800
	C	20.817100	5.768100	-8.469900
	H	20.531500	5.734900	-7.585400
	C	16.631300	7.233400	-8.292100
	C	9.767500	3.599100	-2.536900
	H	9.941300	3.433600	-3.465900
	H	10.234200	2.950700	-2.003900
	H	8.824500	3.530500	-2.370700
	C	18.581800	6.676200	-9.166600
	C	14.005300	6.831000	-5.645000
	H	14.048500	6.205000	-4.906300
	H	14.011900	7.728800	-5.278100
	C	10.249100	4.998900	-2.170900
	C	19.954300	6.237500	-9.460100
	C	14.209700	6.962900	-10.150200
	H	14.356800	6.014700	-10.143800
	H	13.970100	7.255000	-9.268200
	H	13.500400	7.172700	-10.760600
	C	11.744500	5.150900	-2.441700
	H	11.921400	4.973900	-3.368200
	H	12.019200	6.045800	-2.228500
	H	12.233100	4.529300	-1.898600
	C	10.722700	5.903200	-5.180200
	C	15.488800	7.673500	-10.591800
	C	22.106100	5.349100	-8.796100
	H	22.673400	5.039700	-8.128500
	C	20.407600	6.277600	-10.779700
	H	19.842300	6.585500	-11.451000
	C	12.715300	6.610700	-6.422600
	H	12.683500	5.698300	-6.747800
	H	12.692200	7.205600	-7.189400
	C	6.571700	8.027700	-3.172700
	C	15.488000	7.577100	-7.405300
	C	9.643800	6.388500	-4.265400
	C	9.980400	5.275700	-0.700500
	H	10.288200	6.157400	-0.479700
	H	9.037800	5.215300	-0.530500
	H	10.444800	4.631800	-0.162400
	C	15.870000	7.163000	-11.980200
	H	15.982700	6.210500	-11.952300
	H	15.175700	7.384900	-12.605900

	H	16.693400	7.573300	-12.258100
	C	8.620000	7.255200	-4.571300
	H	8.479200	7.708700	-5.370800
	C	7.836300	7.302700	-3.408800
	C	5.817000	8.499700	-4.252700
	H	6.136300	8.396500	-5.120800
	C	6.096400	8.199700	-1.885900
	H	6.597000	7.902600	-1.161200
	C	21.688100	5.864600	-11.099500
	H	21.979200	5.903200	-11.981500
	C	22.544400	5.391900	-10.107000
	H	23.402100	5.107400	-10.324000
	C	15.310300	9.189100	-10.619700
	H	15.069500	9.499600	-9.744100
	H	16.133600	9.603800	-10.891300
	H	14.616700	9.417200	-11.242900
	C	4.860100	8.822300	-1.677700
	H	4.536800	8.934300	-0.813500
	C	4.592500	9.123100	-4.031900
	H	4.097100	9.439200	-4.752700
	C	4.116700	9.272400	-2.760300
	H	3.292500	9.677000	-2.619400
Energy single point calculations:	-3285.5681507849 a.u.			
M1···M11	O	6.303100	0.505100	5.191600
	O	2.225300	4.419600	7.148900
	N	9.219700	2.143000	2.503900
	N	0.902700	3.161600	9.709900
	N	8.034000	1.807200	3.041200
	N	6.596500	2.497500	6.188700
	H	7.077100	3.206800	6.264200
	N	2.996900	2.281700	7.115200
	H	2.849400	1.474400	7.374700
	C	9.326400	2.351400	4.748300
	H	9.650000	2.528100	5.601800
	N	-0.211500	2.611100	10.246100
	C	12.248500	3.378400	4.221000
	H	11.962900	3.411600	5.105600
	C	8.062800	1.913100	4.398800
	C	1.198900	5.547400	10.154000
	H	1.372800	5.712900	9.225000
	H	1.665600	6.195800	10.687000
	H	0.255900	5.616000	10.320200
	C	10.013300	2.470300	3.524300
	C	5.436800	2.315500	7.045900
	H	5.480000	2.941500	7.784600
	H	5.443300	1.417700	7.412800
	C	1.680500	4.147600	10.520000
	C	11.385800	2.909000	3.230900
	C	5.641200	2.183600	2.540700
	H	5.788200	3.131800	2.547100
	H	5.401600	1.891500	3.422700
	H	4.931900	1.973800	1.930300
	C	3.176000	3.995600	10.249200
	H	3.352900	4.172600	9.322700
	H	3.450700	3.100700	10.462400
	H	3.664500	4.617200	10.792300
	C	2.154100	3.243300	7.510700
	C	6.920300	1.473000	2.099100
	C	13.537600	3.797400	3.894800
	H	14.104800	4.106800	4.562400
	C	11.839100	2.868900	1.911200

	H	11.273800	2.561000	1.239900
	C	4.146700	2.535800	6.268300
	H	4.114900	3.448200	5.943100
	H	4.123600	1.940900	5.501500
	C	-1.996900	1.118800	9.518200
	C	6.919500	1.569400	5.285600
	C	1.075300	2.758000	8.425500
	C	1.411900	3.870800	11.990400
	H	1.719700	2.989100	12.211200
	H	0.469300	3.931200	12.160400
	H	1.876300	4.514700	12.528500
	C	7.301400	1.983500	0.710700
	H	7.414200	2.936000	0.738600
	H	6.607200	1.761600	0.085000
	H	8.124900	1.573200	0.432800
	C	0.051500	1.891300	8.119600
	H	-0.089300	1.437800	7.320100
	C	-0.732200	1.843800	9.282100
	C	-2.751600	0.646800	8.438200
	H	-2.432200	0.750000	7.570100
	C	-2.472200	0.946800	10.805000
	H	-1.971600	1.243900	11.529700
	C	13.119600	3.281900	1.591400
	H	13.410700	3.243300	0.709400
	C	13.975900	3.754600	2.583900
	H	14.833600	4.039100	2.366900
	C	6.741800	-0.042600	2.071200
	H	6.501000	-0.353100	2.946800
	H	7.565100	-0.457300	1.799600
	H	6.048200	-0.270700	1.448000
	C	-3.708400	0.324200	11.013200
	H	-4.031800	0.212200	11.877400
	C	-3.976000	0.023400	8.659000
	H	-4.471400	-0.292700	7.938200
	C	-4.451800	-0.125900	9.930600
	H	-5.276000	-0.530500	10.071500
	O	-2.265400	8.641400	17.882500
	O	-6.343300	4.726900	19.839800
	N	0.651200	7.003500	15.194800
	N	-7.665800	5.984900	22.400800
	N	-0.534600	7.339300	15.732200
	N	-1.972000	6.649000	18.879600
	H	-1.491500	5.939700	18.955100
	N	-5.571600	6.864800	19.806100
	H	-5.719200	7.672100	20.065600
	C	0.757800	6.795100	17.439200
	H	1.081500	6.618400	18.292700
	N	-8.780000	6.535400	22.937000
	C	3.680000	5.768100	16.911900
	H	3.394400	5.734900	17.796500
	C	-0.505700	7.233400	17.089700
	C	-7.369600	3.599100	22.844900
	H	-7.195700	3.433600	21.915900
	H	-6.902900	2.950700	23.377900
	H	-8.312600	3.530500	23.011100
	C	1.444700	6.676200	16.215200
	C	-3.131700	6.831000	19.736800
	H	-3.088600	6.205000	20.475500
	H	-3.125200	7.728800	20.103700
	C	-6.888000	4.998900	23.210900
	C	2.817300	6.237500	15.921800

	C	-2.927300	6.962900	15.231600
	H	-2.780300	6.014700	15.238000
	H	-3.167000	7.255000	16.113600
	H	-3.636600	7.172700	14.621200
	C	-5.392500	5.150900	22.940100
	H	-5.215600	4.973900	22.013600
	H	-5.117800	6.045800	23.153300
	H	-4.904000	4.529300	23.483200
	C	-6.414400	5.903200	20.201600
	C	-1.648200	7.673500	14.790000
	C	4.969000	5.349100	16.585700
	H	5.536300	5.039700	17.253300
	C	3.270500	6.277600	14.602200
	H	2.705300	6.585500	13.930800
	C	-4.421800	6.610700	18.959200
	H	-4.453600	5.698300	18.634100
	H	-4.444900	7.205600	18.192400
	C	-10.565400	8.027700	22.209100
	C	-1.649000	7.577100	17.976500
	C	-7.493300	6.388500	21.116400
	C	-7.156700	5.275700	24.681300
	H	-6.848800	6.157400	24.902100
	H	-8.099300	5.215300	24.851300
	H	-6.692200	4.631800	25.219400
	C	-1.267100	7.163000	13.401600
	H	-1.154400	6.210500	13.429500
	H	-1.961300	7.384900	12.775900
	H	-0.443700	7.573300	13.123700
	C	-8.517100	7.255200	20.810500
	H	-8.657900	7.708700	20.011000
	C	-9.300700	7.302700	21.973000
	C	-11.320100	8.499700	21.129100
	H	-11.000800	8.396500	20.261000
	C	-11.040700	8.199700	23.495900
	H	-10.540100	7.902600	24.220600
	C	4.551100	5.864600	14.282300
	H	4.842200	5.903200	13.400300
	C	5.407400	5.391900	15.274800
	H	6.265000	5.107400	15.057800
	C	-1.826800	9.189100	14.762100
	H	-2.067500	9.499600	15.637700
	H	-1.003400	9.603800	14.490500
	H	-2.520300	9.417200	14.138900
	C	-12.276900	8.822300	23.704100
	H	-12.600300	8.934300	24.568300
	C	-12.544600	9.123100	21.349900
	H	-13.040000	9.439200	20.629100
	C	-13.020400	9.272400	22.621500
	H	-13.844600	9.677000	22.762400
Energy single point calculations:	-3285.56815312301 a.u.			
	O	6.303100	0.505100	5.191600
	O	2.225300	4.419600	7.148900
	N	9.219700	2.143000	2.503900
	N	0.902700	3.161600	9.709900
	N	8.034000	1.807200	3.041200
M1···M12	N	6.596500	2.497500	6.188700
	H	7.077100	3.206800	6.264200
	N	2.996900	2.281700	7.115200
	H	2.849400	1.474400	7.374700
	C	9.326400	2.351400	4.748300
	H	9.650000	2.528100	5.601800

	N	-0.211500	2.611100	10.246100
	C	12.248500	3.378400	4.221000
	H	11.962900	3.411600	5.105600
	C	8.062800	1.913100	4.398800
	C	1.198900	5.547400	10.154000
	H	1.372800	5.712900	9.225000
	H	1.665600	6.195800	10.687000
	H	0.255900	5.616000	10.320200
	C	10.013300	2.470300	3.524300
	C	5.436800	2.315500	7.045900
	H	5.480000	2.941500	7.784600
	H	5.443300	1.417700	7.412800
	C	1.680500	4.147600	10.520000
	C	11.385800	2.909000	3.230900
	C	5.641200	2.183600	2.540700
	H	5.788200	3.131800	2.547100
	H	5.401600	1.891500	3.422700
	H	4.931900	1.973800	1.930300
	C	3.176000	3.995600	10.249200
	H	3.352900	4.172600	9.322700
	H	3.450700	3.100700	10.462400
	H	3.664500	4.617200	10.792300
	C	2.154100	3.243300	7.510700
	C	6.920300	1.473000	2.099100
	C	13.537600	3.797400	3.894800
	H	14.104800	4.106800	4.562400
	C	11.839100	2.868900	1.911200
	H	11.273800	2.561000	1.239900
	C	4.146700	2.535800	6.268300
	H	4.114900	3.448200	5.943100
	H	4.123600	1.940900	5.501500
	C	-1.996900	1.118800	9.518200
	C	6.919500	1.569400	5.285600
	C	1.075300	2.758000	8.425500
	C	1.411900	3.870800	11.990400
	H	1.719700	2.989100	12.211200
	H	0.469300	3.931200	12.160400
	H	1.876300	4.514700	12.528500
	C	7.301400	1.983500	0.710700
	H	7.414200	2.936000	0.738600
	H	6.607200	1.761600	0.085000
	H	8.124900	1.573200	0.432800
	C	0.051500	1.891300	8.119600
	H	-0.089300	1.437800	7.320100
	C	-0.732200	1.843800	9.282100
	C	-2.751600	0.646800	8.438200
	H	-2.432200	0.750000	7.570100
	C	-2.472200	0.946800	10.805000
	H	-1.971600	1.243900	11.529700
	C	13.119600	3.281900	1.591400
	H	13.410700	3.243300	0.709400
	C	13.975900	3.754600	2.583900
	H	14.833600	4.039100	2.366900
	C	6.741800	-0.042600	2.071200
	H	6.501000	-0.353100	2.946800
	H	7.565100	-0.457300	1.799600
	H	6.048200	-0.270700	1.448000
	C	-3.708400	0.324200	11.013200
	H	-4.031800	0.212200	11.877400
	C	-3.976000	0.023400	8.659000
	H	-4.471400	-0.292700	7.938200

	C	-4.451800	-0.125900 9.930600
	H	-5.276000	-0.530500 10.071500
	O	-11.478200	-0.505100 20.190200
	O	-7.400300	-4.419600 18.232900
	N	-14.394800	-2.143000 22.877900
	N	-6.077800	-3.161600 15.671900
	N	-13.209000	-1.807200 22.340600
	N	-11.771600	-2.497500 19.193100
	H	-12.252100	-3.206800 19.117600
	N	-8.172000	-2.281700 18.266600
	H	-8.024400	-1.474400 18.007100
	C	-14.501400	-2.351400 20.633500
	H	-14.825000	-2.528100 19.780000
	N	-4.963500	-2.611100 15.135700
	C	-17.423600	-3.378400 21.160800
	H	-17.138000	-3.411600 20.276300
	C	-13.237900	-1.913100 20.983000
	C	-6.374000	-5.547400 15.227800
	H	-6.547800	-5.712900 16.156800
	H	-6.840700	-6.195800 14.694800
	H	-5.431000	-5.616000 15.061600
	C	-15.188300	-2.470300 21.857500
	C	-10.611900	-2.315500 18.335900
	H	-10.655000	-2.941500 17.597200
	H	-10.618400	-1.417700 17.969000
	C	-6.855600	-4.147600 14.861800
	C	-16.560900	-2.909000 22.151000
	C	-10.816300	-2.183600 22.841100
	H	-10.963300	-3.131800 22.834700
	H	-10.576600	-1.891500 21.959100
	H	-10.107000	-1.973800 23.451500
	C	-8.351000	-3.995600 15.132600
	H	-8.528000	-4.172600 16.059100
	H	-8.625800	-3.100700 14.919400
	H	-8.839600	-4.617200 14.589500
	C	-7.329200	-3.243300 17.871100
	C	-12.095300	-1.473000 23.282700
	C	-18.712600	-3.797400 21.487000
	H	-19.279900	-4.106800 20.819400
	C	-17.014100	-2.868900 23.470600
	H	-16.448800	-2.561000 24.141900
	C	-9.321800	-2.535800 19.113500
	H	-9.290000	-3.448200 19.438700
	H	-9.298700	-1.940900 19.880300
	C	-3.178200	-1.118800 15.863600
	C	-12.094600	-1.569400 20.096200
	C	-6.250300	-2.758000 16.956300
	C	-6.586900	-3.870800 13.391400
	H	-6.894800	-2.989100 13.170600
	H	-5.644300	-3.931200 13.221400
	H	-7.051400	-4.514700 12.853300
	C	-12.476500	-1.983500 24.671100
	H	-12.589200	-2.936000 24.643200
	H	-11.782300	-1.761600 25.296800
	H	-13.299900	-1.573200 24.949000
	C	-5.226500	-1.891300 17.262200
	H	-5.085700	-1.437800 18.061700
	C	-4.442900	-1.843800 16.099700
	C	-2.423500	-0.646800 16.943600
	H	-2.742800	-0.750000 17.811700
	C	-2.702900	-0.946800 14.576800

	H	-3.203500	-1.243900	13.852100
	C	-18.294700	-3.281900	23.790400
	H	-18.585800	-3.243300	24.672400
	C	-19.151000	-3.754600	22.797900
	H	-20.008600	-4.039100	23.015000
	C	-11.916800	0.042600	23.310600
	H	-11.676100	0.353100	22.435000
	H	-12.740100	0.457300	23.582200
	H	-11.223300	0.270700	23.933800
	C	-1.466600	-0.324200	14.368600
	H	-1.143300	-0.212200	13.504400
	C	-1.199000	-0.023400	16.722800
	H	-0.703600	0.292700	17.443600
	C	-0.723200	0.125900	15.451200
	H	0.101000	0.530500	15.310300
Energy single point calculations:	-3285.56670229167 a.u.			
M1···M13	O	6.303100	0.505100	5.191600
	O	2.225300	4.419600	7.148900
	N	9.219700	2.143000	2.503900
	N	0.902700	3.161600	9.709900
	N	8.034000	1.807200	3.041200
	N	6.596500	2.497500	6.188700
	H	7.077100	3.206800	6.264200
	N	2.996900	2.281700	7.115200
	H	2.849400	1.474400	7.374700
	C	9.326400	2.351400	4.748300
	H	9.650000	2.528100	5.601800
	N	-0.211500	2.611100	10.246100
	C	12.248500	3.378400	4.221000
	H	11.962900	3.411600	5.105600
	C	8.062800	1.913100	4.398800
	C	1.198900	5.547400	10.154000
	H	1.372800	5.712900	9.225000
	H	1.665600	6.195800	10.687000
	H	0.255900	5.616000	10.320200
	C	10.013300	2.470300	3.524300
	C	5.436800	2.315500	7.045900
	H	5.480000	2.941500	7.784600
	H	5.443300	1.417700	7.412800
	C	1.680500	4.147600	10.520000
	C	11.385800	2.909000	3.230900
	C	5.641200	2.183600	2.540700
	H	5.788200	3.131800	2.547100
	H	5.401600	1.891500	3.422700
	H	4.931900	1.973800	1.930300
	C	3.176000	3.995600	10.249200
	H	3.352900	4.172600	9.322700
	H	3.450700	3.100700	10.462400
	H	3.664500	4.617200	10.792300
	C	2.154100	3.243300	7.510700
	C	6.920300	1.473000	2.099100
	C	13.537600	3.797400	3.894800
	H	14.104800	4.106800	4.562400
	C	11.839100	2.868900	1.911200
	H	11.273800	2.561000	1.239900
	C	4.146700	2.535800	6.268300
	H	4.114900	3.448200	5.943100
	H	4.123600	1.940900	5.501500
	C	-1.996900	1.118800	9.518200
	C	6.919500	1.569400	5.285600
	C	1.075300	2.758000	8.425500

	C	1.411900	3.870800	11.990400
	H	1.719700	2.989100	12.211200
	H	0.469300	3.931200	12.160400
	H	1.876300	4.514700	12.528500
	C	7.301400	1.983500	0.710700
	H	7.414200	2.936000	0.738600
	H	6.607200	1.761600	0.085000
	H	8.124900	1.573200	0.432800
	C	0.051500	1.891300	8.119600
	H	-0.089300	1.437800	7.320100
	C	-0.732200	1.843800	9.282100
	C	-2.751600	0.646800	8.438200
	H	-2.432200	0.750000	7.570100
	C	-2.472200	0.946800	10.805000
	H	-1.971600	1.243900	11.529700
	C	13.119600	3.281900	1.591400
	H	13.410700	3.243300	0.709400
	C	13.975900	3.754600	2.583900
	H	14.833600	4.039100	2.366900
	C	6.741800	-0.042600	2.071200
	H	6.501000	-0.353100	2.946800
	H	7.565100	-0.457300	1.799600
	H	6.048200	-0.270700	1.448000
	C	-3.708400	0.324200	11.013200
	H	-4.031800	0.212200	11.877400
	C	-3.976000	0.023400	8.659000
	H	-4.471400	-0.292700	7.938200
	C	-4.451800	-0.125900	9.930600
	H	-5.276000	-0.530500	10.071500
	O	8.890700	0.505100	-7.499300
	O	4.812800	4.419600	-5.542000
	N	11.807300	2.143000	-10.187000
	N	3.490300	3.161600	-2.981000
	N	10.621500	1.807200	-9.649700
	N	9.184000	2.497500	-6.502200
	H	9.664600	3.206800	-6.426700
	N	5.584400	2.281700	-5.575700
	H	5.436900	1.474400	-5.316200
	C	11.913900	2.351400	-7.942600
	H	12.237500	2.528100	-7.089100
	N	2.376000	2.611100	-2.444800
	C	14.836100	3.378400	-8.469900
	H	14.550500	3.411600	-7.585400
	C	10.650300	1.913100	-8.292100
	C	3.786500	5.547400	-2.536900
	H	3.960300	5.712900	-3.465900
	H	4.253200	6.195800	-2.003900
	H	2.843500	5.616000	-2.370700
	C	12.600800	2.470300	-9.166600
	C	8.024300	2.315500	-5.645000
	H	8.067500	2.941500	-4.906300
	H	8.030900	1.417700	-5.278100
	C	4.268100	4.147600	-2.170900
	C	13.973300	2.909000	-9.460100
	C	8.228700	2.183600	-10.150200
	H	8.375800	3.131800	-10.143800
	H	7.989100	1.891500	-9.268200
	H	7.519400	1.973800	-10.760600
	C	5.763500	3.995600	-2.441700
	H	5.940400	4.172600	-3.368200
	H	6.038200	3.100700	-2.228500

	H	6.252100	4.617200	-1.898600
	C	4.741700	3.243300	-5.180200
	C	9.507800	1.473000	-10.591800
	C	16.125100	3.797400	-8.796100
	H	16.692400	4.106800	-8.128500
	C	14.426600	2.868900	-10.779700
	H	13.861300	2.561000	-11.451000
	C	6.734300	2.535800	-6.422600
	H	6.702500	3.448200	-6.747800
	H	6.711200	1.940900	-7.189400
	C	0.590700	1.118800	-3.172700
	C	9.507000	1.569400	-7.405300
	C	3.662800	2.758000	-4.265400
	C	3.999400	3.870800	-0.700500
	H	4.307200	2.989100	-0.479700
	H	3.056800	3.931200	-0.530500
	H	4.463800	4.514700	-0.162400
	C	9.889000	1.983500	-11.980200
	H	10.001700	2.936000	-11.952300
	H	9.194700	1.761600	-12.605900
	H	10.712400	1.573200	-12.258100
	C	2.639000	1.891300	-4.571300
	H	2.498200	1.437800	-5.370800
	C	1.855300	1.843800	-3.408800
	C	-0.164000	0.646800	-4.252700
	H	0.155300	0.750000	-5.120800
	C	0.115400	0.946800	-1.885900
	H	0.616000	1.243900	-1.161200
	C	15.707100	3.281900	-11.099500
	H	15.998200	3.243300	-11.981500
	C	16.563400	3.754600	-10.107000
	H	17.421100	4.039100	-10.324000
	C	9.329300	-0.042600	-10.619700
	H	9.088500	-0.353100	-9.744100
	H	10.152600	-0.457300	-10.891300
	H	8.635700	-0.270700	-11.242900
	C	-1.120900	0.324200	-1.677700
	H	-1.444200	0.212200	-0.813500
	C	-1.388500	0.023400	-4.031900
	H	-1.883900	-0.292700	-4.752700
	C	-1.864300	-0.125900	-2.760300
	H	-2.688500	-0.530500	-2.619400
Energy single point calculations:	-3285.56669697907 a.u.			
M1···M14	O	6.303100	0.505100	5.191600
	O	2.225300	4.419600	7.148900
	N	9.219700	2.143000	2.503900
	N	0.902700	3.161600	9.709900
	N	8.034000	1.807200	3.041200
	N	6.596500	2.497500	6.188700
	H	7.077100	3.206800	6.264200
	N	2.996900	2.281700	7.115200
	H	2.849400	1.474400	7.374700
	C	9.326400	2.351400	4.748300
	H	9.650000	2.528100	5.601800
	N	-0.211500	2.611100	10.246100
	C	12.248500	3.378400	4.221000
	H	11.962900	3.411600	5.105600
	C	8.062800	1.913100	4.398800
	C	1.198900	5.547400	10.154000
	H	1.372800	5.712900	9.225000
	H	1.665600	6.195800	10.687000

	H	0.255900	5.616000	10.320200
	C	10.013300	2.470300	3.524300
	C	5.436800	2.315500	7.045900
	H	5.480000	2.941500	7.784600
	H	5.443300	1.417700	7.412800
	C	1.680500	4.147600	10.520000
	C	11.385800	2.909000	3.230900
	C	5.641200	2.183600	2.540700
	H	5.788200	3.131800	2.547100
	H	5.401600	1.891500	3.422700
	H	4.931900	1.973800	1.930300
	C	3.176000	3.995600	10.249200
	H	3.352900	4.172600	9.322700
	H	3.450700	3.100700	10.462400
	H	3.664500	4.617200	10.792300
	C	2.154100	3.243300	7.510700
	C	6.920300	1.473000	2.099100
	C	13.537600	3.797400	3.894800
	H	14.104800	4.106800	4.562400
	C	11.839100	2.868900	1.911200
	H	11.273800	2.561000	1.239900
	C	4.146700	2.535800	6.268300
	H	4.114900	3.448200	5.943100
	H	4.123600	1.940900	5.501500
	C	-1.996900	1.118800	9.518200
	C	6.919500	1.569400	5.285600
	C	1.075300	2.758000	8.425500
	C	1.411900	3.870800	11.990400
	H	1.719700	2.989100	12.211200
	H	0.469300	3.931200	12.160400
	H	1.876300	4.514700	12.528500
	C	7.301400	1.983500	0.710700
	H	7.414200	2.936000	0.738600
	H	6.607200	1.761600	0.085000
	H	8.124900	1.573200	0.432800
	C	0.051500	1.891300	8.119600
	H	-0.089300	1.437800	7.320100
	C	-0.732200	1.843800	9.282100
	C	-2.751600	0.646800	8.438200
	H	-2.432200	0.750000	7.570100
	C	-2.472200	0.946800	10.805000
	H	-1.971600	1.243900	11.529700
	C	13.119600	3.281900	1.591400
	H	13.410700	3.243300	0.709400
	C	13.975900	3.754600	2.583900
	H	14.833600	4.039100	2.366900
	C	6.741800	-0.042600	2.071200
	H	6.501000	-0.353100	2.946800
	H	7.565100	-0.457300	1.799600
	H	6.048200	-0.270700	1.448000
	C	-3.708400	0.324200	11.013200
	H	-4.031800	0.212200	11.877400
	C	-3.976000	0.023400	8.659000
	H	-4.471400	-0.292700	7.938200
	C	-4.451800	-0.125900	9.930600
	H	-5.276000	-0.530500	10.071500
	O	3.715600	0.505100	17.882500
	O	-0.362300	4.419600	19.839800
	N	6.632200	2.143000	15.194800
	N	-1.684800	3.161600	22.400800
	N	5.446400	1.807200	15.732200

	N	4.009000	2.497500	18.879600
	H	4.489500	3.206800	18.955100
	N	0.409400	2.281700	19.806100
	H	0.261800	1.474400	20.065600
	C	6.738800	2.351400	17.439200
	H	7.062500	2.528100	18.292700
	N	-2.799000	2.611100	22.937000
	C	9.661000	3.378400	16.911900
	H	9.375400	3.411600	17.796500
	C	5.475300	1.913100	17.089700
	C	-1.388600	5.547400	22.844900
	H	-1.214700	5.712900	21.915900
	H	-0.921900	6.195800	23.377900
	H	-2.331600	5.616000	23.011100
	C	7.425700	2.470300	16.215200
	C	2.849300	2.315500	19.736800
	H	2.892400	2.941500	20.475500
	H	2.855800	1.417700	20.103700
	C	-0.907000	4.147600	23.210900
	C	8.798300	2.909000	15.921800
	C	3.053700	2.183600	15.231600
	H	3.200700	3.131800	15.238000
	H	2.814000	1.891500	16.113600
	H	2.344400	1.973800	14.621200
	C	0.588500	3.995600	22.940100
	H	0.765400	4.172600	22.013600
	H	0.863200	3.100700	23.153300
	H	1.077000	4.617200	23.483200
	C	-0.433400	3.243300	20.201600
	C	4.332700	1.473000	14.790000
	C	10.950000	3.797400	16.585700
	H	11.517300	4.106800	17.253300
	C	9.251500	2.868900	14.602200
	H	8.686300	2.561000	13.930800
	C	1.559200	2.535800	18.959200
	H	1.527400	3.448200	18.634100
	H	1.536100	1.940900	18.192400
	C	-4.584400	1.118800	22.209100
	C	4.332000	1.569400	17.976500
	C	-1.512300	2.758000	21.116400
	C	-1.175700	3.870800	24.681300
	H	-0.867800	2.989100	24.902100
	H	-2.118300	3.931200	24.851300
	H	-0.711200	4.514700	25.219400
	C	4.713900	1.983500	13.401600
	H	4.826600	2.936000	13.429500
	H	4.019700	1.761600	12.775900
	H	5.537300	1.573200	13.123700
	C	-2.536100	1.891300	20.810500
	H	-2.676900	1.437800	20.011000
	C	-3.319700	1.843800	21.973000
	C	-5.339100	0.646800	21.129100
	H	-5.019800	0.750000	20.261000
	C	-5.059700	0.946800	23.495900
	H	-4.559100	1.243900	24.220600
	C	10.532100	3.281900	14.282300
	H	10.823200	3.243300	13.400300
	C	11.388400	3.754600	15.274800
	H	12.246000	4.039100	15.057800
	C	4.154200	-0.042600	14.762100
	H	3.913500	-0.353100	15.637700

	H	4.977600	-0.457300	14.490500
	H	3.460700	-0.270700	14.138900
	C	-6.295900	0.324200	23.704100
	H	-6.619300	0.212200	24.568300
	C	-6.563600	0.023400	21.349900
	H	-7.059000	-0.292700	20.629100
	C	-7.039400	-0.125900	22.621500
	H	-7.863600	-0.530500	22.762400
Energy single point calculations:	-3285.56669914999 a.u.			
M1···M15	O	6.303100	0.505100	5.191600
	O	2.225300	4.419600	7.148900
	N	9.219700	2.143000	2.503900
	N	0.902700	3.161600	9.709900
	N	8.034000	1.807200	3.041200
	N	6.596500	2.497500	6.188700
	H	7.077100	3.206800	6.264200
	N	2.996900	2.281700	7.115200
	H	2.849400	1.474400	7.374700
	C	9.326400	2.351400	4.748300
	H	9.650000	2.528100	5.601800
	N	-0.211500	2.611100	10.246100
	C	12.248500	3.378400	4.221000
	H	11.962900	3.411600	5.105600
	C	8.062800	1.913100	4.398800
	C	1.198900	5.547400	10.154000
	H	1.372800	5.712900	9.225000
	H	1.665600	6.195800	10.687000
	H	0.255900	5.616000	10.320200
	C	10.013300	2.470300	3.524300
	C	5.436800	2.315500	7.045900
	H	5.480000	2.941500	7.784600
	H	5.443300	1.417700	7.412800
	C	1.680500	4.147600	10.520000
	C	11.385800	2.909000	3.230900
	C	5.641200	2.183600	2.540700
	H	5.788200	3.131800	2.547100
	H	5.401600	1.891500	3.422700
	H	4.931900	1.973800	1.930300
	C	3.176000	3.995600	10.249200
	H	3.352900	4.172600	9.322700
	H	3.450700	3.100700	10.462400
	H	3.664500	4.617200	10.792300
	C	2.154100	3.243300	7.510700
	C	6.920300	1.473000	2.099100
	C	13.537600	3.797400	3.894800
	H	14.104800	4.106800	4.562400
	C	11.839100	2.868900	1.911200
	H	11.273800	2.561000	1.239900
	C	4.146700	2.535800	6.268300
	H	4.114900	3.448200	5.943100
	H	4.123600	1.940900	5.501500
	C	-1.996900	1.118800	9.518200
	C	6.919500	1.569400	5.285600
	C	1.075300	2.758000	8.425500
	C	1.411900	3.870800	11.990400
	H	1.719700	2.989100	12.211200
	H	0.469300	3.931200	12.160400
	H	1.876300	4.514700	12.528500
	C	7.301400	1.983500	0.710700
	H	7.414200	2.936000	0.738600
	H	6.607200	1.761600	0.085000

	H	8.124900	1.573200	0.432800
	C	0.051500	1.891300	8.119600
	H	-0.089300	1.437800	7.320100
	C	-0.732200	1.843800	9.282100
	C	-2.751600	0.646800	8.438200
	H	-2.432200	0.750000	7.570100
	C	-2.472200	0.946800	10.805000
	H	-1.971600	1.243900	11.529700
	C	13.119600	3.281900	1.591400
	H	13.410700	3.243300	0.709400
	C	13.975900	3.754600	2.583900
	H	14.833600	4.039100	2.366900
	C	6.741800	-0.042600	2.071200
	H	6.501000	-0.353100	2.946800
	H	7.565100	-0.457300	1.799600
	H	6.048200	-0.270700	1.448000
	C	-3.708400	0.324200	11.013200
	H	-4.031800	0.212200	11.877400
	C	-3.976000	0.023400	8.659000
	H	-4.471400	-0.292700	7.938200
	C	-4.451800	-0.125900	9.930600
	H	-5.276000	-0.530500	10.071500
	O	5.658900	-0.505100	-5.191600
	O	9.736700	-4.419600	-7.148900
	N	2.742300	-2.143000	-2.503900
	N	11.059300	-3.161600	-9.709900
	N	3.928000	-1.807200	-3.041200
	N	5.365500	-2.497500	-6.188700
	H	4.884900	-3.206800	-6.264200
	N	8.965100	-2.281700	-7.115200
	H	9.112600	-1.474400	-7.374700
	C	2.635600	-2.351400	-4.748300
	H	2.312000	-2.528100	-5.601800
	N	12.173500	-2.611100	-10.246100
	C	-0.286500	-3.378400	-4.221000
	H	-0.000900	-3.411600	-5.105600
	C	3.899200	-1.913100	-4.398800
	C	10.763100	-5.547400	-10.154000
	H	10.589200	-5.712900	-9.225000
	H	10.296400	-6.195800	-10.687000
	H	11.706100	-5.616000	-10.320200
	C	1.948700	-2.470300	-3.524300
	C	6.525200	-2.315500	-7.045900
	H	6.482000	-2.941500	-7.784600
	H	6.518700	-1.417700	-7.412800
	C	10.281500	-4.147600	-10.520000
	C	0.576200	-2.909000	-3.230900
	C	6.320800	-2.183600	-2.540700
	H	6.173800	-3.131800	-2.547100
	H	6.560400	-1.891500	-3.422700
	H	7.030100	-1.973800	-1.930300
	C	8.786000	-3.995600	-10.249200
	H	8.609100	-4.172600	-9.322700
	H	8.511300	-3.100700	-10.462400
	H	8.297500	-4.617200	-10.792300
	C	9.807900	-3.243300	-7.510700
	C	5.041700	-1.473000	-2.099100
	C	-1.575600	-3.797400	-3.894800
	H	-2.142800	-4.106800	-4.562400
	C	0.122900	-2.868900	-1.911200
	H	0.688200	-2.561000	-1.239900

	C	7.815300	-2.535800	-6.268300
	H	7.847100	-3.448200	-5.943100
	H	7.838400	-1.940900	-5.501500
	C	13.958900	-1.118800	-9.518200
	C	5.042500	-1.569400	-5.285600
	C	10.886700	-2.758000	-8.425500
	C	10.550100	-3.870800	-11.990400
	H	10.242300	-2.989100	-12.211200
	H	11.492700	-3.931200	-12.160400
	H	10.085700	-4.514700	-12.528500
	C	4.660600	-1.983500	-0.710700
	H	4.547800	-2.936000	-0.738600
	H	5.354800	-1.761600	-0.085000
	H	3.837100	-1.573200	-0.432800
	C	11.910500	-1.891300	-8.119600
	H	12.051300	-1.437800	-7.320100
	C	12.694200	-1.843800	-9.282100
	C	14.713600	-0.646800	-8.438200
	H	14.394200	-0.750000	-7.570100
	C	14.434200	-0.946800	-10.805000
	H	13.933600	-1.243900	-11.529700
	C	-1.157600	-3.281900	-1.591400
	H	-1.448700	-3.243300	-0.709400
	C	-2.013900	-3.754600	-2.583900
	H	-2.871600	-4.039100	-2.366900
	C	5.220200	0.042600	-2.071200
	H	5.461000	0.353100	-2.946800
	H	4.396900	0.457300	-1.799600
	H	5.913800	0.270700	-1.448000
	C	15.670400	-0.324200	-11.013200
	H	15.993800	-0.212200	-11.877400
	C	15.938000	-0.023400	-8.659000
	H	16.433400	0.292700	-7.938200
	C	16.413800	0.125900	-9.930600
	H	17.238000	0.530500	-10.071500
Energy single point calculations:	-3285.5659007737 a.u.			
M1···M16	O	6.303100	0.505100	5.191600
	O	2.225300	4.419600	7.148900
	N	9.219700	2.143000	2.503900
	N	0.902700	3.161600	9.709900
	N	8.034000	1.807200	3.041200
	N	6.596500	2.497500	6.188700
	H	7.077100	3.206800	6.264200
	N	2.996900	2.281700	7.115200
	H	2.849400	1.474400	7.374700
	C	9.326400	2.351400	4.748300
	H	9.650000	2.528100	5.601800
	N	-0.211500	2.611100	10.246100
	C	12.248500	3.378400	4.221000
	H	11.962900	3.411600	5.105600
	C	8.062800	1.913100	4.398800
	C	1.198900	5.547400	10.154000
	H	1.372800	5.712900	9.225000
	H	1.665600	6.195800	10.687000
	H	0.255900	5.616000	10.320200
	C	10.013300	2.470300	3.524300
	C	5.436800	2.315500	7.045900
	H	5.480000	2.941500	7.784600
	H	5.443300	1.417700	7.412800
	C	1.680500	4.147600	10.520000

	C	11.385800	2.909000	3.230900
	C	5.641200	2.183600	2.540700
	H	5.788200	3.131800	2.547100
	H	5.401600	1.891500	3.422700
	H	4.931900	1.973800	1.930300
	C	3.176000	3.995600	10.249200
	H	3.352900	4.172600	9.322700
	H	3.450700	3.100700	10.462400
	H	3.664500	4.617200	10.792300
	C	2.154100	3.243300	7.510700
	C	6.920300	1.473000	2.099100
	C	13.537600	3.797400	3.894800
	H	14.104800	4.106800	4.562400
	C	11.839100	2.868900	1.911200
	H	11.273800	2.561000	1.239900
	C	4.146700	2.535800	6.268300
	H	4.114900	3.448200	5.943100
	H	4.123600	1.940900	5.501500
	C	-1.996900	1.118800	9.518200
	C	6.919500	1.569400	5.285600
	C	1.075300	2.758000	8.425500
	C	1.411900	3.870800	11.990400
	H	1.719700	2.989100	12.211200
	H	0.469300	3.931200	12.160400
	H	1.876300	4.514700	12.528500
	C	7.301400	1.983500	0.710700
	H	7.414200	2.936000	0.738600
	H	6.607200	1.761600	0.085000
	H	8.124900	1.573200	0.432800
	C	0.051500	1.891300	8.119600
	H	-0.089300	1.437800	7.320100
	C	-0.732200	1.843800	9.282100
	C	-2.751600	0.646800	8.438200
	H	-2.432200	0.750000	7.570100
	C	-2.472200	0.946800	10.805000
	H	-1.971600	1.243900	11.529700
	C	13.119600	3.281900	1.591400
	H	13.410700	3.243300	0.709400
	C	13.975900	3.754600	2.583900
	H	14.833600	4.039100	2.366900
	C	6.741800	-0.042600	2.071200
	H	6.501000	-0.353100	2.946800
	H	7.565100	-0.457300	1.799600
	H	6.048200	-0.270700	1.448000
	C	-3.708400	0.324200	11.013200
	H	-4.031800	0.212200	11.877400
	C	-3.976000	0.023400	8.659000
	H	-4.471400	-0.292700	7.938200
	C	-4.451800	-0.125900	9.930600
	H	-5.276000	-0.530500	10.071500
	O	-2.909700	-8.641400	7.499300
	O	1.168200	-4.726900	5.542000
	N	-5.826300	-7.003500	10.187000
	N	2.490700	-5.984900	2.981000
	N	-4.640500	-7.339300	9.649700
	N	-3.203000	-6.649000	6.502200
	H	-3.683600	-5.939700	6.426700
	N	0.396600	-6.864800	5.575700
	H	0.544100	-7.672100	5.316200
	C	-5.932900	-6.795100	7.942600
	H	-6.256500	-6.618400	7.089100

	N	3.605000	-6.535400	2.444800
	C	-8.855100	-5.768100	8.469900
	H	-8.569500	-5.734900	7.585400
	C	-4.669300	-7.233400	8.292100
	C	2.194500	-3.599100	2.536900
	H	2.020700	-3.433600	3.465900
	H	1.727800	-2.950700	2.003900
	H	3.137500	-3.530500	2.370700
	C	-6.619800	-6.676200	9.166600
	C	-2.043300	-6.831000	5.645000
	H	-2.086500	-6.205000	4.906300
	H	-2.049900	-7.728800	5.278100
	C	1.712900	-4.998900	2.170900
	C	-7.992300	-6.237500	9.460100
	C	-2.247700	-6.962900	10.150200
	H	-2.394800	-6.014700	10.143800
	H	-2.008100	-7.255000	9.268200
	H	-1.538400	-7.172700	10.760600
	C	0.217500	-5.150900	2.441700
	H	0.040600	-4.973900	3.368200
	H	-0.057200	-6.045800	2.228500
	H	-0.271100	-4.529300	1.898600
	C	1.239300	-5.903200	5.180200
	C	-3.526800	-7.673500	10.591800
	C	-10.144100	-5.349100	8.796100
	H	-10.711400	-5.039700	8.128500
	C	-8.445600	-6.277600	10.779700
	H	-7.880300	-6.585500	11.451000
	C	-0.753300	-6.610700	6.422600
	H	-0.721500	-5.698300	6.747800
	H	-0.730200	-7.205600	7.189400
	C	5.390300	-8.027700	3.172700
	C	-3.526000	-7.577100	7.405300
	C	2.318200	-6.388500	4.265400
	C	1.981600	-5.275700	0.700500
	H	1.673800	-6.157400	0.479700
	H	2.924200	-5.215300	0.530500
	H	1.517200	-4.631800	0.162400
	C	-3.908000	-7.163000	11.980200
	H	-4.020700	-6.210500	11.952300
	H	-3.213700	-7.384900	12.605900
	H	-4.731400	-7.573300	12.258100
	C	3.342000	-7.255200	4.571300
	H	3.482800	-7.708700	5.370800
	C	4.125700	-7.302700	3.408800
	C	6.145000	-8.499700	4.252700
	H	5.825700	-8.396500	5.120800
	C	5.865600	-8.199700	1.885900
	H	5.365000	-7.902600	1.161200
	C	-9.726100	-5.864600	11.099500
	H	-10.017200	-5.903200	11.981500
	C	-10.582400	-5.391900	10.107000
	H	-11.440100	-5.107400	10.324000
	C	-3.348300	-9.189100	10.619700
	H	-3.107500	-9.499600	9.744100
	H	-4.171600	-9.603800	10.891300
	H	-2.654700	-9.417200	11.242900
	C	7.101900	-8.822300	1.677700
	H	7.425200	-8.934300	0.813500
	C	7.369500	-9.123100	4.031900
	H	7.864900	-9.439200	4.752700

	C	7.845300	-9.272400	2.760300
	H	8.669500	-9.677000	2.619400
Energy single point calculations:	-3285.56472849037			
M1···M17	O	6.303100	0.505100	5.191600
	O	2.225300	4.419600	7.148900
	N	9.219700	2.143000	2.503900
	N	0.902700	3.161600	9.709900
	N	8.034000	1.807200	3.041200
	N	6.596500	2.497500	6.188700
	H	7.077100	3.206800	6.264200
	N	2.996900	2.281700	7.115200
	H	2.849400	1.474400	7.374700
	C	9.326400	2.351400	4.748300
	H	9.650000	2.528100	5.601800
	N	-0.211500	2.611100	10.246100
	C	12.248500	3.378400	4.221000
	H	11.962900	3.411600	5.105600
	C	8.062800	1.913100	4.398800
	C	1.198900	5.547400	10.154000
	H	1.372800	5.712900	9.225000
	H	1.665600	6.195800	10.687000
	H	0.255900	5.616000	10.320200
	C	10.013300	2.470300	3.524300
	C	5.436800	2.315500	7.045900
	H	5.480000	2.941500	7.784600
	H	5.443300	1.417700	7.412800
	C	1.680500	4.147600	10.520000
	C	11.385800	2.909000	3.230900
	C	5.641200	2.183600	2.540700
	H	5.788200	3.131800	2.547100
	H	5.401600	1.891500	3.422700
	H	4.931900	1.973800	1.930300
	C	3.176000	3.995600	10.249200
	H	3.352900	4.172600	9.322700
	H	3.450700	3.100700	10.462400
	H	3.664500	4.617200	10.792300
	C	2.154100	3.243300	7.510700
	C	6.920300	1.473000	2.099100
	C	13.537600	3.797400	3.894800
	H	14.104800	4.106800	4.562400
	C	11.839100	2.868900	1.911200
	H	11.273800	2.561000	1.239900
	C	4.146700	2.535800	6.268300
	H	4.114900	3.448200	5.943100
	H	4.123600	1.940900	5.501500
	C	-1.996900	1.118800	9.518200
	C	6.919500	1.569400	5.285600
	C	1.075300	2.758000	8.425500
	C	1.411900	3.870800	11.990400
	H	1.719700	2.989100	12.211200
	H	0.469300	3.931200	12.160400
	H	1.876300	4.514700	12.528500
	C	7.301400	1.983500	0.710700
	H	7.414200	2.936000	0.738600
	H	6.607200	1.761600	0.085000
	H	8.124900	1.573200	0.432800
	C	0.051500	1.891300	8.119600
	H	-0.089300	1.437800	7.320100
	C	-0.732200	1.843800	9.282100
	C	-2.751600	0.646800	8.438200
	H	-2.432200	0.750000	7.570100

	C	-2.472200	0.946800	10.805000
	H	-1.971600	1.243900	11.529700
	C	13.119600	3.281900	1.591400
	H	13.410700	3.243300	0.709400
	C	13.975900	3.754600	2.583900
	H	14.833600	4.039100	2.366900
	C	6.741800	-0.042600	2.071200
	H	6.501000	-0.353100	2.946800
	H	7.565100	-0.457300	1.799600
	H	6.048200	-0.270700	1.448000
	C	-3.708400	0.324200	11.013200
	H	-4.031800	0.212200	11.877400
	C	-3.976000	0.023400	8.659000
	H	-4.471400	-0.292700	7.938200
	C	-4.451800	-0.125900	9.930600
	H	-5.276000	-0.530500	10.071500
	O	-2.909700	-8.641400	7.499300
	O	1.168200	-4.726900	5.542000
	N	-5.826300	-7.003500	10.187000
	N	2.490700	-5.984900	2.981000
	N	-4.640500	-7.339300	9.649700
	N	-3.203000	-6.649000	6.502200
	H	-3.683600	-5.939700	6.426700
	N	0.396600	-6.864800	5.575700
	H	0.544100	-7.672100	5.316200
	C	-5.932900	-6.795100	7.942600
	H	-6.256500	-6.618400	7.089100
	N	3.605000	-6.535400	2.444800
	C	-8.855100	-5.768100	8.469900
	H	-8.569500	-5.734900	7.585400
	C	-4.669300	-7.233400	8.292100
	C	2.194500	-3.599100	2.536900
	H	2.020700	-3.433600	3.465900
	H	1.727800	-2.950700	2.003900
	H	3.137500	-3.530500	2.370700
	C	-6.619800	-6.676200	9.166600
	C	-2.043300	-6.831000	5.645000
	H	-2.086500	-6.205000	4.906300
	H	-2.049900	-7.728800	5.278100
	C	1.712900	-4.998900	2.170900
	C	-7.992300	-6.237500	9.460100
	C	-2.247700	-6.962900	10.150200
	H	-2.394800	-6.014700	10.143800
	H	-2.008100	-7.255000	9.268200
	H	-1.538400	-7.172700	10.760600
	C	0.217500	-5.150900	2.441700
	H	0.040600	-4.973900	3.368200
	H	-0.057200	-6.045800	2.228500
	H	-0.271100	-4.529300	1.898600
	C	1.239300	-5.903200	5.180200
	C	-3.526800	-7.673500	10.591800
	C	-10.144100	-5.349100	8.796100
	H	-10.711400	-5.039700	8.128500
	C	-8.445600	-6.277600	10.779700
	H	-7.880300	-6.585500	11.451000
	C	-0.753300	-6.610700	6.422600
	H	-0.721500	-5.698300	6.747800
	H	-0.730200	-7.205600	7.189400
	C	5.390300	-8.027700	3.172700
	C	-3.526000	-7.577100	7.405300
	C	2.318200	-6.388500	4.265400

	C	1.981600	-5.275700	0.700500
	H	1.673800	-6.157400	0.479700
	H	2.924200	-5.215300	0.530500
	H	1.517200	-4.631800	0.162400
	C	-3.908000	-7.163000	11.980200
	H	-4.020700	-6.210500	11.952300
	H	-3.213700	-7.384900	12.605900
	H	-4.731400	-7.573300	12.258100
	C	3.342000	-7.255200	4.571300
	H	3.482800	-7.708700	5.370800
	C	4.125700	-7.302700	3.408800
	C	6.145000	-8.499700	4.252700
	H	5.825700	-8.396500	5.120800
	C	5.865600	-8.199700	1.885900
	H	5.365000	-7.902600	1.161200
	C	-9.726100	-5.864600	11.099500
	H	-10.017200	-5.903200	11.981500
	C	-10.582400	-5.391900	10.107000
	H	-11.440100	-5.107400	10.324000
	C	-3.348300	-9.189100	10.619700
	H	-3.107500	-9.499600	9.744100
	H	-4.171600	-9.603800	10.891300
	H	-2.654700	-9.417200	11.242900
	C	7.101900	-8.822300	1.677700
	H	7.425200	-8.934300	0.813500
	C	7.369500	-9.123100	4.031900
	H	7.864900	-9.439200	4.752700
	C	7.845300	-9.272400	2.760300
	H	8.669500	-9.677000	2.619400
Energy single point calculations:	-3285.56472829748 a.u.			

Table S8. Atomic coordinates used in single point calculations with a ωB97x-D/cc-pVDZ for compound **9c.**

Dimer	Atoms	Coordinates		
M1	N	1.305900	9.039400	5.796300
	O	3.353400	5.073800	6.360700
	N	2.231500	8.429100	6.565500
	N	3.864700	6.697200	7.839600
	H	3.654900	7.480800	8.127300
	C	0.735000	8.159100	4.916800
	C	-0.351400	8.448300	3.957200
	C	1.352000	6.946500	5.120000
	H	1.197100	6.150600	4.664500
	C	2.260000	7.166900	6.155200
	C	3.202500	6.205500	6.785100
	C	-1.664100	8.620700	4.381900
	H	-1.867900	8.566200	5.288300
	C	-0.080400	8.480800	2.601400
	H	0.790000	8.351800	2.300300
	C	4.917100	5.971000	8.519600
	C	1.066300	10.493900	6.062200
	C	-2.669100	8.872500	3.464600
	H	-3.540000	9.013300	3.759100
	C	-2.387900	8.916100	2.119700
	H	-3.064500	9.087600	1.504600
	C	-1.099800	8.705400	1.688700
	H	-0.910400	8.713600	0.777700
	C	0.537000	11.191800	4.830500

	H	-0.301600	10.799200	4.576100
	H	1.166200	11.095200	4.112800
	H	0.409300	12.124500	5.021400
	C	2.394900	11.130300	6.439800
	H	3.005800	11.057400	5.702500
	H	2.760700	10.678600	7.203900
	H	2.257300	12.056300	6.652100
	C	0.095200	10.586600	7.215800
	H	-0.739800	10.184000	6.964800
	H	-0.048500	11.509400	7.439600
	H	0.456600	10.125500	7.976700
	H	4.954400	6.249300	9.453500
	H	4.710600	5.021300	8.544800
	N	9.867000	3.142400	10.576100
	O	7.819600	7.108000	10.011800
	N	8.941400	3.752700	9.806900
	N	7.308200	5.484600	8.532800
	H	7.518000	4.701000	8.245200
	C	10.437900	4.022700	11.455600
	C	11.524300	3.733500	12.415200
	C	9.820900	5.235300	11.252500
	H	9.975800	6.031200	11.707900
	C	8.913000	5.014900	10.217200
	C	7.970400	5.976300	9.587400
	C	12.837000	3.561100	11.990500
	H	13.040800	3.615600	11.084100
	C	11.253300	3.701000	13.771000
	H	10.382900	3.830000	14.072100
	C	6.255800	6.210800	7.852900
	C	10.106600	1.687900	10.310200
	C	13.842000	3.309300	12.907900
	H	14.712900	3.168500	12.613300
	C	13.560800	3.265700	14.252700
	H	14.237400	3.094200	14.867800
	C	12.272700	3.476400	14.683800
	H	12.083300	3.468200	15.594800
	C	10.635900	0.990000	11.541900
	H	11.474500	1.382600	11.796300
	H	10.006700	1.086600	12.259700
	H	10.763600	0.057300	11.351000
	C	8.778000	1.051500	9.932700
	H	8.167100	1.124400	10.669900
	H	8.412200	1.503200	9.168600
	H	8.915600	0.125500	9.720300
	C	11.077700	1.595200	9.156600
	H	11.912700	1.997800	9.407600
	H	11.221400	0.672400	8.932800
	H	10.716300	2.056300	8.395800
	H	6.218500	5.932500	6.919000
	H	6.462300	7.160500	7.827700
Energy single point calculations:	-1642.7899296 u.a.			
	Atoms	Coordinates		
M1···M2	N	1.305900	9.039400	5.796300
	O	3.353400	5.073800	6.360700
	N	2.231500	8.429100	6.565500
	N	3.864700	6.697200	7.839600
	H	3.654900	7.480800	8.127300
	C	0.735000	8.159100	4.916800
	C	-0.351400	8.448300	3.957200
	C	1.352000	6.946500	5.120000

	H	1.197100	6.150600	4.664500
	C	2.260000	7.166900	6.155200
	C	3.202500	6.205500	6.785100
	C	-1.664100	8.620700	4.381900
	H	-1.867900	8.566200	5.288300
	C	-0.080400	8.480800	2.601400
	H	0.790000	8.351800	2.300300
	C	4.917100	5.971000	8.519600
	C	1.066300	10.493900	6.062200
	C	-2.669100	8.872500	3.464600
	H	-3.540000	9.013300	3.759100
	C	-2.387900	8.916100	2.119700
	H	-3.064500	9.087600	1.504600
	C	-1.099800	8.705400	1.688700
	H	-0.910400	8.713600	0.777700
	C	0.537000	11.191800	4.830500
	H	-0.301600	10.799200	4.576100
	H	1.166200	11.095200	4.112800
	H	0.409300	12.124500	5.021400
	C	2.394900	11.130300	6.439800
	H	3.005800	11.057400	5.702500
	H	2.760700	10.678600	7.203900
	H	2.257300	12.056300	6.652100
	C	0.095200	10.586600	7.215800
	H	-0.739800	10.184000	6.964800
	H	-0.048500	11.509400	7.439600
	H	0.456600	10.125500	7.976700
	H	4.954400	6.249300	9.453500
	H	4.710600	5.021300	8.544800
	N	9.867000	3.142400	10.576100
	O	7.819600	7.108000	10.011800
	N	8.941400	3.752700	9.806900
	N	7.308200	5.484600	8.532800
	H	7.518000	4.701000	8.245200
	C	10.437900	4.022700	11.455600
	C	11.524300	3.733500	12.415200
	C	9.820900	5.235300	11.252500
	H	9.975800	6.031200	11.707900
	C	8.913000	5.014900	10.217200
	C	7.970400	5.976300	9.587400
	C	12.837000	3.561100	11.990500
	H	13.040800	3.615600	11.084100
	C	11.253300	3.701000	13.771000
	H	10.382900	3.830000	14.072100
	C	6.255800	6.210800	7.852900
	C	10.106600	1.687900	10.310200
	C	13.842000	3.309300	12.907900
	H	14.712900	3.168500	12.613300
	C	13.560800	3.265700	14.252700
	H	14.237400	3.094200	14.867800
	C	12.272700	3.476400	14.683800
	H	12.083300	3.468200	15.594800
	C	10.635900	0.990000	11.541900
	H	11.474500	1.382600	11.796300
	H	10.006700	1.086600	12.259700
	H	10.763600	0.057300	11.351000
	C	8.778000	1.051500	9.932700
	H	8.167100	1.124400	10.669900
	H	8.412200	1.503200	9.168600
	H	8.915600	0.125500	9.720300
	C	11.077700	1.595200	9.156600

	H	11.912700	1.997800	9.407600
	H	11.221400	0.672400	8.932800
	H	10.716300	2.056300	8.395800
	H	6.218500	5.932500	6.919000
	H	6.462300	7.160500	7.827700
	N	8.274600	9.039400	5.796300
	O	10.322100	5.073800	6.360700
	N	9.200200	8.429100	6.565500
	N	10.833400	6.697200	7.839600
	H	10.623600	7.480800	8.127300
	C	7.703700	8.159100	4.916800
	C	6.617300	8.448300	3.957200
	C	8.320700	6.946500	5.120000
	H	8.165800	6.150600	4.664500
	C	9.228700	7.166900	6.155200
	C	10.171200	6.205500	6.785100
	C	5.304600	8.620700	4.381900
	H	5.100800	8.566200	5.288300
	C	6.888300	8.480800	2.601400
	H	7.758700	8.351800	2.300300
	C	11.885800	5.971000	8.519600
	C	8.035000	10.493900	6.062200
	C	4.299600	8.872500	3.464600
	H	3.428700	9.013300	3.759100
	C	4.580800	8.916100	2.119700
	H	3.904200	9.087600	1.504600
	C	5.868900	8.705400	1.688700
	H	6.058300	8.713600	0.777700
	C	7.505700	11.191800	4.830500
	H	6.667100	10.799200	4.576100
	H	8.134900	11.095200	4.112800
	H	7.378000	12.124500	5.021400
	C	9.363600	11.130300	6.439800
	H	9.974500	11.057400	5.702500
	H	9.729400	10.678600	7.203900
	H	9.226000	12.056300	6.652100
	C	7.063900	10.586600	7.215800
	H	6.228900	10.184000	6.964800
	H	6.920200	11.509400	7.439600
	H	7.425300	10.125500	7.976700
	H	11.923100	6.249300	9.453500
	H	11.679300	5.021300	8.544800
	N	16.835700	3.142400	10.576100
	O	14.788300	7.108000	10.011800
	N	15.910100	3.752700	9.806900
	N	14.276900	5.484600	8.532800
	H	14.486700	4.701000	8.245200
	C	17.406600	4.022700	11.455600
	C	18.493000	3.733500	12.415200
	C	16.789600	5.235300	11.252500
	H	16.944500	6.031200	11.707900
	C	15.881700	5.014900	10.217200
	C	14.939100	5.976300	9.587400
	C	19.805700	3.561100	11.990500
	H	20.009500	3.615600	11.084100
	C	18.222000	3.701000	13.771000
	H	17.351600	3.830000	14.072100
	C	13.224500	6.210800	7.852900
	C	17.075300	1.687900	10.310200
	C	20.810700	3.309300	12.907900
	H	21.681600	3.168500	12.613300

	C	20.529500	3.265700	14.252700
	H	21.206100	3.094200	14.867800
	C	19.241400	3.476400	14.683800
	H	19.052000	3.468200	15.594800
	C	17.604600	0.990000	11.541900
	H	18.443200	1.382600	11.796300
	H	16.975400	1.086600	12.259700
	H	17.732300	0.057300	11.351000
	C	15.746700	1.051500	9.932700
	H	15.135800	1.124400	10.669900
	H	15.380900	1.503200	9.168600
	H	15.884300	0.125500	9.720300
	C	18.046400	1.595200	9.156600
	H	18.881400	1.997800	9.407600
	H	18.190100	0.672400	8.932800
	H	17.685000	2.056300	8.395800
	H	13.187200	5.932500	6.919000
	H	13.431000	7.160500	7.827700
Energy single point calculations:	-3285.61222672753 u.a.			
M1···M3	N	1.305900	9.039400	5.796300
	O	3.353400	5.073800	6.360700
	N	2.231500	8.429100	6.565500
	N	3.864700	6.697200	7.839600
	H	3.654900	7.480800	8.127300
	C	0.735000	8.159100	4.916800
	C	-0.351400	8.448300	3.957200
	C	1.352000	6.946500	5.120000
	H	1.197100	6.150600	4.664500
	C	2.260000	7.166900	6.155200
	C	3.202500	6.205500	6.785100
	C	-1.664100	8.620700	4.381900
	H	-1.867900	8.566200	5.288300
	C	-0.080400	8.480800	2.601400
	H	0.790000	8.351800	2.300300
	C	4.917100	5.971000	8.519600
	C	1.066300	10.493900	6.062200
	C	-2.669100	8.872500	3.464600
	H	-3.540000	9.013300	3.759100
	C	-2.387900	8.916100	2.119700
	H	-3.064500	9.087600	1.504600
	C	-1.099800	8.705400	1.688700
	H	-0.910400	8.713600	0.777700
	C	0.537000	11.191800	4.830500
	H	-0.301600	10.799200	4.576100
	H	1.166200	11.095200	4.112800
	H	0.409300	12.124500	5.021400
	C	2.394900	11.130300	6.439800
	H	3.005800	11.057400	5.702500
	H	2.760700	10.678600	7.203900
	H	2.257300	12.056300	6.652100
	C	0.095200	10.586600	7.215800
	H	-0.739800	10.184000	6.964800
	H	-0.048500	11.509400	7.439600
	H	0.456600	10.125500	7.976700
	H	4.954400	6.249300	9.453500
	H	4.710600	5.021300	8.544800
	N	9.867000	3.142400	10.576100
	O	7.819600	7.108000	10.011800
	N	8.941400	3.752700	9.806900
	N	7.308200	5.484600	8.532800

	H	7.518000	4.701000	8.245200
	C	10.437900	4.022700	11.455600
	C	11.524300	3.733500	12.415200
	C	9.820900	5.235300	11.252500
	H	9.975800	6.031200	11.707900
	C	8.913000	5.014900	10.217200
	C	7.970400	5.976300	9.587400
	C	12.837000	3.561100	11.990500
	H	13.040800	3.615600	11.084100
	C	11.253300	3.701000	13.771000
	H	10.382900	3.830000	14.072100
	C	6.255800	6.210800	7.852900
	C	10.106600	1.687900	10.310200
	C	13.842000	3.309300	12.907900
	H	14.712900	3.168500	12.613300
	C	13.560800	3.265700	14.252700
	H	14.237400	3.094200	14.867800
	C	12.272700	3.476400	14.683800
	H	12.083300	3.468200	15.594800
	C	10.635900	0.990000	11.541900
	H	11.474500	1.382600	11.796300
	H	10.006700	1.086600	12.259700
	H	10.763600	0.057300	11.351000
	C	8.778000	1.051500	9.932700
	H	8.167100	1.124400	10.669900
	H	8.412200	1.503200	9.168600
	H	8.915600	0.125500	9.720300
	C	11.077700	1.595200	9.156600
	H	11.912700	1.997800	9.407600
	H	11.221400	0.672400	8.932800
	H	10.716300	2.056300	8.395800
	H	6.218500	5.932500	6.919000
	H	6.462300	7.160500	7.827700
	N	-5.662800	9.039400	5.796300
	O	-3.615300	5.073800	6.360700
	N	-4.737200	8.429100	6.565500
	N	-3.104000	6.697200	7.839600
	H	-3.313800	7.480800	8.127300
	C	-6.233700	8.159100	4.916800
	C	-7.320100	8.448300	3.957200
	C	-5.616700	6.946500	5.120000
	H	-5.771600	6.150600	4.664500
	C	-4.708700	7.166900	6.155200
	C	-3.766200	6.205500	6.785100
	C	-8.632800	8.620700	4.381900
	H	-8.836600	8.566200	5.288300
	C	-7.049100	8.480800	2.601400
	H	-6.178700	8.351800	2.300300
	C	-2.051600	5.971000	8.519600
	C	-5.902400	10.493900	6.062200
	C	-9.637800	8.872500	3.464600
	H	-10.508700	9.013300	3.759100
	C	-9.356600	8.916100	2.119700
	H	-10.033200	9.087600	1.504600
	C	-8.068500	8.705400	1.688700
	H	-7.879100	8.713600	0.777700
	C	-6.431700	11.191800	4.830500
	H	-7.270300	10.799200	4.576100
	H	-5.802500	11.095200	4.112800
	H	-6.559400	12.124500	5.021400
	C	-4.573800	11.130300	6.439800

	H	-3.962900	11.057400	5.702500
	H	-4.208000	10.678600	7.203900
	H	-4.711400	12.056300	6.652100
	C	-6.873500	10.586600	7.215800
	H	-7.708500	10.184000	6.964800
	H	-7.017200	11.509400	7.439600
	H	-6.512100	10.125500	7.976700
	H	-2.014300	6.249300	9.453500
	H	-2.258100	5.021300	8.544800
	N	2.898300	3.142400	10.576100
	O	0.850900	7.108000	10.011800
	N	1.972700	3.752700	9.806900
	N	0.339500	5.484600	8.532800
	H	0.549300	4.701000	8.245200
	C	3.469200	4.022700	11.455600
	C	4.555600	3.733500	12.415200
	C	2.852200	5.235300	11.252500
	H	3.007100	6.031200	11.707900
	C	1.944300	5.014900	10.217200
	C	1.001700	5.976300	9.587400
	C	5.868300	3.561100	11.990500
	H	6.072100	3.615600	11.084100
	C	4.284600	3.701000	13.771000
	H	3.414200	3.830000	14.072100
	C	-0.712900	6.210800	7.852900
	C	3.137900	1.687900	10.310200
	C	6.873300	3.309300	12.907900
	H	7.744200	3.168500	12.613300
	C	6.592100	3.265700	14.252700
	H	7.268700	3.094200	14.867800
	C	5.304000	3.476400	14.683800
	H	5.114600	3.468200	15.594800
	C	3.667200	0.990000	11.541900
	H	4.505800	1.382600	11.796300
	H	3.038000	1.086600	12.259700
	H	3.794900	0.057300	11.351000
	C	1.809300	1.051500	9.932700
	H	1.198400	1.124400	10.669900
	H	1.443500	1.503200	9.168600
	H	1.946900	0.125500	9.720300
	C	4.109000	1.595200	9.156600
	H	4.944000	1.997800	9.407600
	H	4.252700	0.672400	8.932800
	H	3.747600	2.056300	8.395800
	H	-0.750200	5.932500	6.919000
	H	-0.506400	7.160500	7.827700
Energy single point calculations:	-3285.61222672747 u.a.			
M1···M4	N	1.305900	9.039400	5.796300
	O	3.353400	5.073800	6.360700
	N	2.231500	8.429100	6.565500
	N	3.864700	6.697200	7.839600
	H	3.654900	7.480800	8.127300
	C	0.735000	8.159100	4.916800
	C	-0.351400	8.448300	3.957200
	C	1.352000	6.946500	5.120000
	H	1.197100	6.150600	4.664500
	C	2.260000	7.166900	6.155200
	C	3.202500	6.205500	6.785100
	C	-1.664100	8.620700	4.381900
	H	-1.867900	8.566200	5.288300

	C	-0.080400	8.480800	2.601400
	H	0.790000	8.351800	2.300300
	C	4.917100	5.971000	8.519600
	C	1.066300	10.493900	6.062200
	C	-2.669100	8.872500	3.464600
	H	-3.540000	9.013300	3.759100
	C	-2.387900	8.916100	2.119700
	H	-3.064500	9.087600	1.504600
	C	-1.099800	8.705400	1.688700
	H	-0.910400	8.713600	0.777700
	C	0.537000	11.191800	4.830500
	H	-0.301600	10.799200	4.576100
	H	1.166200	11.095200	4.112800
	H	0.409300	12.124500	5.021400
	C	2.394900	11.130300	6.439800
	H	3.005800	11.057400	5.702500
	H	2.760700	10.678600	7.203900
	H	2.257300	12.056300	6.652100
	C	0.095200	10.586600	7.215800
	H	-0.739800	10.184000	6.964800
	H	-0.048500	11.509400	7.439600
	H	0.456600	10.125500	7.976700
	H	4.954400	6.249300	9.453500
	H	4.710600	5.021300	8.544800
	N	9.867000	3.142400	10.576100
	O	7.819600	7.108000	10.011800
	N	8.941400	3.752700	9.806900
	N	7.308200	5.484600	8.532800
	H	7.518000	4.701000	8.245200
	C	10.437900	4.022700	11.455600
	C	11.524300	3.733500	12.415200
	C	9.820900	5.235300	11.252500
	H	9.975800	6.031200	11.707900
	C	8.913000	5.014900	10.217200
	C	7.970400	5.976300	9.587400
	C	12.837000	3.561100	11.990500
	H	13.040800	3.615600	11.084100
	C	11.253300	3.701000	13.771000
	H	10.382900	3.830000	14.072100
	C	6.255800	6.210800	7.852900
	C	10.106600	1.687900	10.310200
	C	13.842000	3.309300	12.907900
	H	14.712900	3.168500	12.613300
	C	13.560800	3.265700	14.252700
	H	14.237400	3.094200	14.867800
	C	12.272700	3.476400	14.683800
	H	12.083300	3.468200	15.594800
	C	10.635900	0.990000	11.541900
	H	11.474500	1.382600	11.796300
	H	10.006700	1.086600	12.259700
	H	10.763600	0.057300	11.351000
	C	8.778000	1.051500	9.932700
	H	8.167100	1.124400	10.669900
	H	8.412200	1.503200	9.168600
	H	8.915600	0.125500	9.720300
	C	11.077700	1.595200	9.156600
	H	11.912700	1.997800	9.407600
	H	11.221400	0.672400	8.932800
	H	10.716300	2.056300	8.395800
	H	6.218500	5.932500	6.919000
	H	6.462300	7.160500	7.827700

	N	15.453500	2.948500	18.762300
	O	13.406000	-1.017100	18.198000
	N	14.527900	2.338200	17.993200
	N	12.894700	0.606300	16.719100
	H	13.104400	1.389900	16.431400
	C	16.024400	2.068200	19.641900
	C	17.110700	2.357400	20.601500
	C	15.407300	0.855600	19.438700
	H	15.562300	0.059700	19.894200
	C	14.499400	1.076000	18.403500
	C	13.556800	0.114600	17.773600
	C	18.423400	2.529800	20.176800
	H	18.627200	2.475300	19.270400
	C	16.839700	2.389900	21.957300
	H	15.969400	2.260900	22.258300
	C	11.842200	-0.119900	16.039100
	C	15.693100	4.403000	18.496400
	C	19.428400	2.781600	21.094100
	H	20.299300	2.922400	20.799600
	C	19.147300	2.825200	22.438900
	H	19.823900	2.996700	23.054000
	C	17.859100	2.614500	22.870000
	H	17.669800	2.622700	23.781000
	C	16.222400	5.100900	19.728100
	H	17.061000	4.708300	19.982600
	H	15.593200	5.004300	20.445900
	H	16.350100	6.033600	19.537200
	C	14.364500	5.039400	18.118900
	H	13.753600	4.966500	18.856100
	H	13.998700	4.587700	17.354800
	H	14.502100	5.965400	17.906500
	C	16.664200	4.495700	17.342800
	H	17.499100	4.093100	17.593800
	H	16.807900	5.418500	17.119000
	H	16.302700	4.034600	16.582000
	H	11.805000	0.158400	15.105200
	H	12.048800	-1.069600	16.013900
	N	6.892400	-2.948500	13.982600
	O	8.939800	1.017100	14.546900
	N	7.818000	-2.338200	14.751700
	N	9.451100	-0.606300	16.025800
	H	9.241400	-1.389900	16.313500
	C	6.321400	-2.068200	13.103000
	C	5.235100	-2.357400	12.143400
	C	6.938500	-0.855600	13.306200
	H	6.783500	-0.059700	12.850700
	C	7.846400	-1.076000	14.341400
	C	8.789000	-0.114600	14.971300
	C	3.922400	-2.529800	12.568100
	H	3.718600	-2.475300	13.474500
	C	5.506100	-2.389900	10.787600
	H	6.376500	-2.260900	10.486600
	C	10.503600	0.119900	16.705800
	C	6.652800	-4.403000	14.248500
	C	2.917400	-2.781600	11.650800
	H	2.046500	-2.922400	11.945300
	C	3.198600	-2.825200	10.306000
	H	2.521900	-2.996700	9.690900
	C	4.486700	-2.614500	9.874900
	H	4.676000	-2.622700	8.963900
	C	6.123400	-5.100900	13.016800

	H	5.284900	-4.708300	12.762300
	H	6.752700	-5.004300	12.299000
	H	5.995700	-6.033600	13.207700
	C	7.981400	-5.039400	14.626000
	H	8.592300	-4.966500	13.888700
	H	8.347100	-4.587700	15.390100
	H	7.843800	-5.965400	14.838300
	C	5.681700	-4.495700	15.402100
	H	4.846700	-4.093100	15.151100
	H	5.537900	-5.418500	15.625900
	H	6.043100	-4.034600	16.162900
	H	10.540800	-0.158400	17.639700
	H	10.297000	1.069600	16.731000
Energy single point calculations:	-3285.59269859265 u.a.			
M1···M5	N	1.305900	9.039400	5.796300
	O	3.353400	5.073800	6.360700
	N	2.231500	8.429100	6.565500
	N	3.864700	6.697200	7.839600
	H	3.654900	7.480800	8.127300
	C	0.735000	8.159100	4.916800
	C	-0.351400	8.448300	3.957200
	C	1.352000	6.946500	5.120000
	H	1.197100	6.150600	4.664500
	C	2.260000	7.166900	6.155200
	C	3.202500	6.205500	6.785100
	C	-1.664100	8.620700	4.381900
	H	-1.867900	8.566200	5.288300
	C	-0.080400	8.480800	2.601400
	H	0.790000	8.351800	2.300300
	C	4.917100	5.971000	8.519600
	C	1.066300	10.493900	6.062200
	C	-2.669100	8.872500	3.464600
	H	-3.540000	9.013300	3.759100
	C	-2.387900	8.916100	2.119700
	H	-3.064500	9.087600	1.504600
	C	-1.099800	8.705400	1.688700
	H	-0.910400	8.713600	0.777700
	C	0.537000	11.191800	4.830500
	H	-0.301600	10.799200	4.576100
	H	1.166200	11.095200	4.112800
	H	0.409300	12.124500	5.021400
	C	2.394900	11.130300	6.439800
	H	3.005800	11.057400	5.702500
	H	2.760700	10.678600	7.203900
	H	2.257300	12.056300	6.652100
	C	0.095200	10.586600	7.215800
	H	-0.739800	10.184000	6.964800
	H	-0.048500	11.509400	7.439600
	H	0.456600	10.125500	7.976700
	H	4.954400	6.249300	9.453500
	H	4.710600	5.021300	8.544800
	N	9.867000	3.142400	10.576100
	O	7.819600	7.108000	10.011800
	N	8.941400	3.752700	9.806900
	N	7.308200	5.484600	8.532800
	H	7.518000	4.701000	8.245200
	C	10.437900	4.022700	11.455600
	C	11.524300	3.733500	12.415200
	C	9.820900	5.235300	11.252500
	H	9.975800	6.031200	11.707900

	C	8.913000	5.014900	10.217200
	C	7.970400	5.976300	9.587400
	C	12.837000	3.561100	11.990500
	H	13.040800	3.615600	11.084100
	C	11.253300	3.701000	13.771000
	H	10.382900	3.830000	14.072100
	C	6.255800	6.210800	7.852900
	C	10.106600	1.687900	10.310200
	C	13.842000	3.309300	12.907900
	H	14.712900	3.168500	12.613300
	C	13.560800	3.265700	14.252700
	H	14.237400	3.094200	14.867800
	C	12.272700	3.476400	14.683800
	H	12.083300	3.468200	15.594800
	C	10.635900	0.990000	11.541900
	H	11.474500	1.382600	11.796300
	H	10.006700	1.086600	12.259700
	H	10.763600	0.057300	11.351000
	C	8.778000	1.051500	9.932700
	H	8.167100	1.124400	10.669900
	H	8.412200	1.503200	9.168600
	H	8.915600	0.125500	9.720300
	C	11.077700	1.595200	9.156600
	H	11.912700	1.997800	9.407600
	H	11.221400	0.672400	8.932800
	H	10.716300	2.056300	8.395800
	H	6.218500	5.932500	6.919000
	H	6.462300	7.160500	7.827700
	N	15.453500	15.130300	18.762300
	O	13.406000	11.164700	18.198000
	N	14.527900	14.520000	17.993200
	N	12.894700	12.788100	16.719100
	H	13.104400	13.571700	16.431400
	C	16.024400	14.250000	19.641900
	C	17.110700	14.539200	20.601500
	C	15.407300	13.037400	19.438700
	H	15.562300	12.241500	19.894200
	C	14.499400	13.257800	18.403500
	C	13.556800	12.296400	17.773600
	C	18.423400	14.711600	20.176800
	H	18.627200	14.657100	19.270400
	C	16.839700	14.571700	21.957300
	H	15.969400	14.442700	22.258300
	C	11.842200	12.061900	16.039100
	C	15.693100	16.584800	18.496400
	C	19.428400	14.963400	21.094100
	H	20.299300	15.104200	20.799600
	C	19.147300	15.007000	22.438900
	H	19.823900	15.178500	23.054000
	C	17.859100	14.796300	22.870000
	H	17.669800	14.804500	23.781000
	C	16.222400	17.282700	19.728100
	H	17.061000	16.890100	19.982600
	H	15.593200	17.186100	20.445900
	H	16.350100	18.215400	19.537200
	C	14.364500	17.221200	18.118900
	H	13.753600	17.148300	18.856100
	H	13.998700	16.769500	17.354800
	H	14.502100	18.147200	17.906500
	C	16.664200	16.677500	17.342800
	H	17.499100	16.274900	17.593800

	H	16.807900	17.600300	17.119000
	H	16.302700	16.216400	16.582000
	H	11.805000	12.340200	15.105200
	H	12.048800	11.112200	16.013900
	N	6.892400	9.233300	13.982600
	O	8.939800	13.198900	14.546900
	N	7.818000	9.843600	14.751700
	N	9.451100	11.575500	16.025800
	H	9.241400	10.791900	16.313500
	C	6.321400	10.113600	13.103000
	C	5.235100	9.824400	12.143400
	C	6.938500	11.326200	13.306200
	H	6.783500	12.122100	12.850700
	C	7.846400	11.105800	14.341400
	C	8.789000	12.067200	14.971300
	C	3.922400	9.652000	12.568100
	H	3.718600	9.706500	13.474500
	C	5.506100	9.791900	10.787600
	H	6.376500	9.920900	10.486600
	C	10.503600	12.301700	16.705800
	C	6.652800	7.778800	14.248500
	C	2.917400	9.400200	11.650800
	H	2.046500	9.259400	11.945300
	C	3.198600	9.356600	10.306000
	H	2.521900	9.185100	9.690900
	C	4.486700	9.567300	9.874900
	H	4.676000	9.559100	8.963900
	C	6.123400	7.080900	13.016800
	H	5.284900	7.473500	12.762300
	H	6.752700	7.177500	12.299000
	H	5.995700	6.148200	13.207700
	C	7.981400	7.142400	14.626000
	H	8.592300	7.215300	13.888700
	H	8.347100	7.594100	15.390100
	H	7.843800	6.216400	14.838300
	C	5.681700	7.686100	15.402100
	H	4.846700	8.088700	15.151100
	H	5.537900	6.763300	15.625900
	H	6.043100	8.147200	16.162900
	H	10.540800	12.023400	17.639700
	H	10.297000	13.251400	16.731000
Energy single point calculations:	-3285.59269788902 u.a.			
M1···M6	N	1.305900	9.039400	5.796300
	O	3.353400	5.073800	6.360700
	N	2.231500	8.429100	6.565500
	N	3.864700	6.697200	7.839600
	H	3.654900	7.480800	8.127300
	C	0.735000	8.159100	4.916800
	C	-0.351400	8.448300	3.957200
	C	1.352000	6.946500	5.120000
	H	1.197100	6.150600	4.664500
	C	2.260000	7.166900	6.155200
	C	3.202500	6.205500	6.785100
	C	-1.664100	8.620700	4.381900
	H	-1.867900	8.566200	5.288300
	C	-0.080400	8.480800	2.601400
	H	0.790000	8.351800	2.300300
	C	4.917100	5.971000	8.519600
	C	1.066300	10.493900	6.062200
	C	-2.669100	8.872500	3.464600

	H	-3.540000	9.013300	3.759100
	C	-2.387900	8.916100	2.119700
	H	-3.064500	9.087600	1.504600
	C	-1.099800	8.705400	1.688700
	H	-0.910400	8.713600	0.777700
	C	0.537000	11.191800	4.830500
	H	-0.301600	10.799200	4.576100
	H	1.166200	11.095200	4.112800
	H	0.409300	12.124500	5.021400
	C	2.394900	11.130300	6.439800
	H	3.005800	11.057400	5.702500
	H	2.760700	10.678600	7.203900
	H	2.257300	12.056300	6.652100
	C	0.095200	10.586600	7.215800
	H	-0.739800	10.184000	6.964800
	H	-0.048500	11.509400	7.439600
	H	0.456600	10.125500	7.976700
	H	4.954400	6.249300	9.453500
	H	4.710600	5.021300	8.544800
	N	9.867000	3.142400	10.576100
	O	7.819600	7.108000	10.011800
	N	8.941400	3.752700	9.806900
	N	7.308200	5.484600	8.532800
	H	7.518000	4.701000	8.245200
	C	10.437900	4.022700	11.455600
	C	11.524300	3.733500	12.415200
	C	9.820900	5.235300	11.252500
	H	9.975800	6.031200	11.707900
	C	8.913000	5.014900	10.217200
	C	7.970400	5.976300	9.587400
	C	12.837000	3.561100	11.990500
	H	13.040800	3.615600	11.084100
	C	11.253300	3.701000	13.771000
	H	10.382900	3.830000	14.072100
	C	6.255800	6.210800	7.852900
	C	10.106600	1.687900	10.310200
	C	13.842000	3.309300	12.907900
	H	14.712900	3.168500	12.613300
	C	13.560800	3.265700	14.252700
	H	14.237400	3.094200	14.867800
	C	12.272700	3.476400	14.683800
	H	12.083300	3.468200	15.594800
	C	10.635900	0.990000	11.541900
	H	11.474500	1.382600	11.796300
	H	10.006700	1.086600	12.259700
	H	10.763600	0.057300	11.351000
	C	8.778000	1.051500	9.932700
	H	8.167100	1.124400	10.669900
	H	8.412200	1.503200	9.168600
	H	8.915600	0.125500	9.720300
	C	11.077700	1.595200	9.156600
	H	11.912700	1.997800	9.407600
	H	11.221400	0.672400	8.932800
	H	10.716300	2.056300	8.395800
	H	6.218500	5.932500	6.919000
	H	6.462300	7.160500	7.827700
	N	4.280500	15.130300	2.389900
	O	2.233100	11.164700	1.825500
	N	3.354900	14.520000	1.620700
	N	1.721800	12.788100	0.346600
	H	1.931500	13.571700	0.058900

	C	4.851500	14.250000	3.269400
	C	5.937800	14.539200	4.229000
	C	4.234400	13.037400	3.066200
	H	4.389400	12.241500	3.521700
	C	3.326500	13.257800	2.031000
	C	2.383900	12.296400	1.401200
	C	7.250500	14.711600	3.804300
	H	7.454300	14.657100	2.897900
	C	5.666800	14.571700	5.584800
	H	4.796500	14.442700	5.885900
	C	0.669300	12.061900	-0.333300
	C	4.520100	16.584800	2.124000
	C	8.255500	14.963400	4.721700
	H	9.126400	15.104200	4.427100
	C	7.974400	15.007000	6.066500
	H	8.651000	15.178500	6.681600
	C	6.686200	14.796300	6.497600
	H	6.496900	14.804500	7.408500
	C	5.049500	17.282700	3.355700
	H	5.888000	16.890100	3.610100
	H	4.420300	17.186100	4.073500
	H	5.177200	18.215400	3.164800
	C	3.191600	17.221200	1.746400
	H	2.580700	17.148300	2.483700
	H	2.825800	16.769500	0.982300
	H	3.329200	18.147200	1.534100
	C	5.491200	16.677500	0.970400
	H	6.326200	16.274900	1.221400
	H	5.635000	17.600300	0.746600
	H	5.129800	16.216400	0.209600
	H	0.632100	12.340200	-1.267200
	H	0.875900	11.112200	-0.358600
	N	-4.280500	9.233300	-2.389900
	O	-2.233100	13.198900	-1.825500
	N	-3.354900	9.843600	-1.620700
	N	-1.721800	11.575500	-0.346600
	H	-1.931500	10.791900	-0.058900
	C	-4.851500	10.113600	-3.269400
	C	-5.937800	9.824400	-4.229000
	C	-4.234400	11.326200	-3.066200
	H	-4.389400	12.122100	-3.521700
	C	-3.326500	11.105800	-2.031000
	C	-2.383900	12.067200	-1.401200
	C	-7.250500	9.652000	-3.804300
	H	-7.454300	9.706500	-2.897900
	C	-5.666800	9.791900	-5.584800
	H	-4.796500	9.920900	-5.885900
	C	-0.669300	12.301700	0.333300
	C	-4.520100	7.778800	-2.124000
	C	-8.255500	9.400200	-4.721700
	H	-9.126400	9.259400	-4.427100
	C	-7.974400	9.356600	-6.066500
	H	-8.651000	9.185100	-6.681600
	C	-6.686200	9.567300	-6.497600
	H	-6.496900	9.559100	-7.408500
	C	-5.049500	7.080900	-3.355700
	H	-5.888000	7.473500	-3.610100
	H	-4.420300	7.177500	-4.073500
	H	-5.177200	6.148200	-3.164800
	C	-3.191600	7.142400	-1.746400
	H	-2.580700	7.215300	-2.483700

	H	-2.825800	7.594100	-0.982300
	H	-3.329200	6.216400	-1.534100
	C	-5.491200	7.686100	-0.970400
	H	-6.326200	8.088700	-1.221400
	H	-5.635000	6.763300	-0.746600
	H	-5.129800	8.147200	-0.209600
	H	-0.632100	12.023400	1.267200
	H	-0.875900	13.251400	0.358600
Energy single point calculations:	-3285.59261136809 u.a.			
M1···M7	N	1.305900	9.039400	5.796300
	O	3.353400	5.073800	6.360700
	N	2.231500	8.429100	6.565500
	N	3.864700	6.697200	7.839600
	H	3.654900	7.480800	8.127300
	C	0.735000	8.159100	4.916800
	C	-0.351400	8.448300	3.957200
	C	1.352000	6.946500	5.120000
	H	1.197100	6.150600	4.664500
	C	2.260000	7.166900	6.155200
	C	3.202500	6.205500	6.785100
	C	-1.664100	8.620700	4.381900
	H	-1.867900	8.566200	5.288300
	C	-0.080400	8.480800	2.601400
	H	0.790000	8.351800	2.300300
	C	4.917100	5.971000	8.519600
	C	1.066300	10.493900	6.062200
	C	-2.669100	8.872500	3.464600
	H	-3.540000	9.013300	3.759100
	C	-2.387900	8.916100	2.119700
	H	-3.064500	9.087600	1.504600
	C	-1.099800	8.705400	1.688700
	H	-0.910400	8.713600	0.777700
	C	0.537000	11.191800	4.830500
	H	-0.301600	10.799200	4.576100
	H	1.166200	11.095200	4.112800
	H	0.409300	12.124500	5.021400
	C	2.394900	11.130300	6.439800
	H	3.005800	11.057400	5.702500
	H	2.760700	10.678600	7.203900
	H	2.257300	12.056300	6.652100
	C	0.095200	10.586600	7.215800
	H	-0.739800	10.184000	6.964800
	H	-0.048500	11.509400	7.439600
	H	0.456600	10.125500	7.976700
	H	4.954400	6.249300	9.453500
	H	4.710600	5.021300	8.544800
	N	9.867000	3.142400	10.576100
	O	7.819600	7.108000	10.011800
	N	8.941400	3.752700	9.806900
	N	7.308200	5.484600	8.532800
	H	7.518000	4.701000	8.245200
	C	10.437900	4.022700	11.455600
	C	11.524300	3.733500	12.415200
	C	9.820900	5.235300	11.252500
	H	9.975800	6.031200	11.707900
	C	8.913000	5.014900	10.217200
	C	7.970400	5.976300	9.587400
	C	12.837000	3.561100	11.990500
	H	13.040800	3.615600	11.084100
	C	11.253300	3.701000	13.771000

	H	10.382900	3.830000	14.072100
	C	6.255800	6.210800	7.852900
	C	10.106600	1.687900	10.310200
	C	13.842000	3.309300	12.907900
	H	14.712900	3.168500	12.613300
	C	13.560800	3.265700	14.252700
	H	14.237400	3.094200	14.867800
	C	12.272700	3.476400	14.683800
	H	12.083300	3.468200	15.594800
	C	10.635900	0.990000	11.541900
	H	11.474500	1.382600	11.796300
	H	10.006700	1.086600	12.259700
	H	10.763600	0.057300	11.351000
	C	8.778000	1.051500	9.932700
	H	8.167100	1.124400	10.669900
	H	8.412200	1.503200	9.168600
	H	8.915600	0.125500	9.720300
	C	11.077700	1.595200	9.156600
	H	11.912700	1.997800	9.407600
	H	11.221400	0.672400	8.932800
	H	10.716300	2.056300	8.395800
	H	6.218500	5.932500	6.919000
	H	6.462300	7.160500	7.827700
	N	4.280500	2.948500	2.389900
	O	2.233100	-1.017100	1.825500
	N	3.354900	2.338200	1.620700
	N	1.721800	0.606300	0.346600
	H	1.931500	1.389900	0.058900
	C	4.851500	2.068200	3.269400
	C	5.937800	2.357400	4.229000
	C	4.234400	0.855600	3.066200
	H	4.389400	0.059700	3.521700
	C	3.326500	1.076000	2.031000
	C	2.383900	0.114600	1.401200
	C	7.250500	2.529800	3.804300
	H	7.454300	2.475300	2.897900
	C	5.666800	2.389900	5.584800
	H	4.796500	2.260900	5.885900
	C	0.669300	-0.119900	-0.333300
	C	4.520100	4.403000	2.124000
	C	8.255500	2.781600	4.721700
	H	9.126400	2.922400	4.427100
	C	7.974400	2.825200	6.066500
	H	8.651000	2.996700	6.681600
	C	6.686200	2.614500	6.497600
	H	6.496900	2.622700	7.408500
	C	5.049500	5.100900	3.355700
	H	5.888000	4.708300	3.610100
	H	4.420300	5.004300	4.073500
	H	5.177200	6.033600	3.164800
	C	3.191600	5.039400	1.746400
	H	2.580700	4.966500	2.483700
	H	2.825800	4.587700	0.982300
	H	3.329200	5.965400	1.534100
	C	5.491200	4.495700	0.970400
	H	6.326200	4.093100	1.221400
	H	5.635000	5.418500	0.746600
	H	5.129800	4.034600	0.209600
	H	0.632100	0.158400	-1.267200
	H	0.875900	-1.069600	-0.358600
	N	-4.280500	-2.948500	-2.389900

	O	-2.233100	1.017100	-1.825500
	N	-3.354900	-2.338200	-1.620700
	N	-1.721800	-0.606300	-0.346600
	H	-1.931500	-1.389900	-0.058900
	C	-4.851500	-2.068200	-3.269400
	C	-5.937800	-2.357400	-4.229000
	C	-4.234400	-0.855600	-3.066200
	H	-4.389400	-0.059700	-3.521700
	C	-3.326500	-1.076000	-2.031000
	C	-2.383900	-0.114600	-1.401200
	C	-7.250500	-2.529800	-3.804300
	H	-7.454300	-2.475300	-2.897900
	C	-5.666800	-2.389900	-5.584800
	H	-4.796500	-2.260900	-5.885900
	C	-0.669300	0.119900	0.333300
	C	-4.520100	-4.403000	-2.124000
	C	-8.255500	-2.781600	-4.721700
	H	-9.126400	-2.922400	-4.427100
	C	-7.974400	-2.825200	-6.066500
	H	-8.651000	-2.996700	-6.681600
	C	-6.686200	-2.614500	-6.497600
	H	-6.496900	-2.622700	-7.408500
	C	-5.049500	-5.100900	-3.355700
	H	-5.888000	-4.708300	-3.610100
	H	-4.420300	-5.004300	-4.073500
	H	-5.177200	-6.033600	-3.164800
	C	-3.191600	-5.039400	-1.746400
	H	-2.580700	-4.966500	-2.483700
	H	-2.825800	-4.587700	-0.982300
	H	-3.329200	-5.965400	-1.534100
	C	-5.491200	-4.495700	-0.970400
	H	-6.326200	-4.093100	-1.221400
	H	-5.635000	-5.418500	-0.746600
	H	-5.129800	-4.034600	-0.209600
	H	-0.632100	-0.158400	1.267200
	H	-0.875900	1.069600	0.358600
Energy single point calculations:	-3285.59261096737 u.a.			
M1···M8	N	1.305900	9.039400	5.796300
	O	3.353400	5.073800	6.360700
	N	2.231500	8.429100	6.565500
	N	3.864700	6.697200	7.839600
	H	3.654900	7.480800	8.127300
	C	0.735000	8.159100	4.916800
	C	-0.351400	8.448300	3.957200
	C	1.352000	6.946500	5.120000
	H	1.197100	6.150600	4.664500
	C	2.260000	7.166900	6.155200
	C	3.202500	6.205500	6.785100
	C	-1.664100	8.620700	4.381900
	H	-1.867900	8.566200	5.288300
	C	-0.080400	8.480800	2.601400
	H	0.790000	8.351800	2.300300
	C	4.917100	5.971000	8.519600
	C	1.066300	10.493900	6.062200
	C	-2.669100	8.872500	3.464600
	H	-3.540000	9.013300	3.759100
	C	-2.387900	8.916100	2.119700
	H	-3.064500	9.087600	1.504600
	C	-1.099800	8.705400	1.688700
	H	-0.910400	8.713600	0.777700

	C	0.537000	11.191800	4.830500
	H	-0.301600	10.799200	4.576100
	H	1.166200	11.095200	4.112800
	H	0.409300	12.124500	5.021400
	C	2.394900	11.130300	6.439800
	H	3.005800	11.057400	5.702500
	H	2.760700	10.678600	7.203900
	H	2.257300	12.056300	6.652100
	C	0.095200	10.586600	7.215800
	H	-0.739800	10.184000	6.964800
	H	-0.048500	11.509400	7.439600
	H	0.456600	10.125500	7.976700
	H	4.954400	6.249300	9.453500
	H	4.710600	5.021300	8.544800
	N	9.867000	3.142400	10.576100
	O	7.819600	7.108000	10.011800
	N	8.941400	3.752700	9.806900
	N	7.308200	5.484600	8.532800
	H	7.518000	4.701000	8.245200
	C	10.437900	4.022700	11.455600
	C	11.524300	3.733500	12.415200
	C	9.820900	5.235300	11.252500
	H	9.975800	6.031200	11.707900
	C	8.913000	5.014900	10.217200
	C	7.970400	5.976300	9.587400
	C	12.837000	3.561100	11.990500
	H	13.040800	3.615600	11.084100
	C	11.253300	3.701000	13.771000
	H	10.382900	3.830000	14.072100
	C	6.255800	6.210800	7.852900
	C	10.106600	1.687900	10.310200
	C	13.842000	3.309300	12.907900
	H	14.712900	3.168500	12.613300
	C	13.560800	3.265700	14.252700
	H	14.237400	3.094200	14.867800
	C	12.272700	3.476400	14.683800
	H	12.083300	3.468200	15.594800
	C	10.635900	0.990000	11.541900
	H	11.474500	1.382600	11.796300
	H	10.006700	1.086600	12.259700
	H	10.763600	0.057300	11.351000
	C	8.778000	1.051500	9.932700
	H	8.167100	1.124400	10.669900
	H	8.412200	1.503200	9.168600
	H	8.915600	0.125500	9.720300
	C	11.077700	1.595200	9.156600
	H	11.912700	1.997800	9.407600
	H	11.221400	0.672400	8.932800
	H	10.716300	2.056300	8.395800
	H	6.218500	5.932500	6.919000
	H	6.462300	7.160500	7.827700
	N	22.422200	15.130300	18.762300
	O	20.374700	11.164700	18.198000
	N	21.496600	14.520000	17.993200
	N	19.863400	12.788100	16.719100
	H	20.073100	13.571700	16.431400
	C	22.993100	14.250000	19.641900
	C	24.079400	14.539200	20.601500
	C	22.376000	13.037400	19.438700
	H	22.531000	12.241500	19.894200
	C	21.468100	13.257800	18.403500

	C	20.525500	12.296400	17.773600
	C	25.392100	14.711600	20.176800
	H	25.595900	14.657100	19.270400
	C	23.808400	14.571700	21.957300
	H	22.938100	14.442700	22.258300
	C	18.810900	12.061900	16.039100
	C	22.661800	16.584800	18.496400
	C	26.397100	14.963400	21.094100
	H	27.268000	15.104200	20.799600
	C	26.116000	15.007000	22.438900
	H	26.792600	15.178500	23.054000
	C	24.827800	14.796300	22.870000
	H	24.638500	14.804500	23.781000
	C	23.191100	17.282700	19.728100
	H	24.029700	16.890100	19.982600
	H	22.561900	17.186100	20.445900
	H	23.318800	18.215400	19.537200
	C	21.333200	17.221200	18.118900
	H	20.722300	17.148300	18.856100
	H	20.967400	16.769500	17.354800
	H	21.470800	18.147200	17.906500
	C	23.632900	16.677500	17.342800
	H	24.467800	16.274900	17.593800
	H	23.776600	17.600300	17.119000
	H	23.271400	16.216400	16.582000
	H	18.773700	12.340200	15.105200
	H	19.017500	11.112200	16.013900
	N	13.861100	9.233300	13.982600
	O	15.908500	13.198900	14.546900
	N	14.786700	9.843600	14.751700
	N	16.419800	11.575500	16.025800
	H	16.210100	10.791900	16.313500
	C	13.290100	10.113600	13.103000
	C	12.203800	9.824400	12.143400
	C	13.907200	11.326200	13.306200
	H	13.752200	12.122100	12.850700
	C	14.815100	11.105800	14.341400
	C	15.757700	12.067200	14.971300
	C	10.891100	9.652000	12.568100
	H	10.687300	9.706500	13.474500
	C	12.474800	9.791900	10.787600
	H	13.345200	9.920900	10.486600
	C	17.472300	12.301700	16.705800
	C	13.621500	7.778800	14.248500
	C	9.886100	9.400200	11.650800
	H	9.015200	9.259400	11.945300
	C	10.167300	9.356600	10.306000
	H	9.490600	9.185100	9.690900
	C	11.455400	9.567300	9.874900
	H	11.644700	9.559100	8.963900
	C	13.092100	7.080900	13.016800
	H	12.253600	7.473500	12.762300
	H	13.721400	7.177500	12.299000
	H	12.964400	6.148200	13.207700
	C	14.950100	7.142400	14.626000
	H	15.561000	7.215300	13.888700
	H	15.315800	7.594100	15.390100
	H	14.812500	6.216400	14.838300
	C	12.650400	7.686100	15.402100
	H	11.815400	8.088700	15.151100
	H	12.506600	6.763300	15.625900

	H	13.011800	8.147200	16.162900
	H	17.509500	12.023400	17.639700
	H	17.265700	13.251400	16.731000
Energy single point calculations:	-3285.59194311546 u.a.			
M1···M9	N	1.305900	9.039400	5.796300
	O	3.353400	5.073800	6.360700
	N	2.231500	8.429100	6.565500
	N	3.864700	6.697200	7.839600
	H	3.654900	7.480800	8.127300
	C	0.735000	8.159100	4.916800
	C	-0.351400	8.448300	3.957200
	C	1.352000	6.946500	5.120000
	H	1.197100	6.150600	4.664500
	C	2.260000	7.166900	6.155200
	C	3.202500	6.205500	6.785100
	C	-1.664100	8.620700	4.381900
	H	-1.867900	8.566200	5.288300
	C	-0.080400	8.480800	2.601400
	H	0.790000	8.351800	2.300300
	C	4.917100	5.971000	8.519600
	C	1.066300	10.493900	6.062200
	C	-2.669100	8.872500	3.464600
	H	-3.540000	9.013300	3.759100
	C	-2.387900	8.916100	2.119700
	H	-3.064500	9.087600	1.504600
	C	-1.099800	8.705400	1.688700
	H	-0.910400	8.713600	0.777700
	C	0.537000	11.191800	4.830500
	H	-0.301600	10.799200	4.576100
	H	1.166200	11.095200	4.112800
	H	0.409300	12.124500	5.021400
	C	2.394900	11.130300	6.439800
	H	3.005800	11.057400	5.702500
	H	2.760700	10.678600	7.203900
	H	2.257300	12.056300	6.652100
	C	0.095200	10.586600	7.215800
	H	-0.739800	10.184000	6.964800
	H	-0.048500	11.509400	7.439600
	H	0.456600	10.125500	7.976700
	H	4.954400	6.249300	9.453500
	H	4.710600	5.021300	8.544800
	N	9.867000	3.142400	10.576100
	O	7.819600	7.108000	10.011800
	N	8.941400	3.752700	9.806900
	N	7.308200	5.484600	8.532800
	H	7.518000	4.701000	8.245200
	C	10.437900	4.022700	11.455600
	C	11.524300	3.733500	12.415200
	C	9.820900	5.235300	11.252500
	H	9.975800	6.031200	11.707900
	C	8.913000	5.014900	10.217200
	C	7.970400	5.976300	9.587400
	C	12.837000	3.561100	11.990500
	H	13.040800	3.615600	11.084100
	C	11.253300	3.701000	13.771000
	H	10.382900	3.830000	14.072100
	C	6.255800	6.210800	7.852900
	C	10.106600	1.687900	10.310200
	C	13.842000	3.309300	12.907900
	H	14.712900	3.168500	12.613300

	C	13.560800	3.265700	14.252700
	H	14.237400	3.094200	14.867800
	C	12.272700	3.476400	14.683800
	H	12.083300	3.468200	15.594800
	C	10.635900	0.990000	11.541900
	H	11.474500	1.382600	11.796300
	H	10.006700	1.086600	12.259700
	H	10.763600	0.057300	11.351000
	C	8.778000	1.051500	9.932700
	H	8.167100	1.124400	10.669900
	H	8.412200	1.503200	9.168600
	H	8.915600	0.125500	9.720300
	C	11.077700	1.595200	9.156600
	H	11.912700	1.997800	9.407600
	H	11.221400	0.672400	8.932800
	H	10.716300	2.056300	8.395800
	H	6.218500	5.932500	6.919000
	H	6.462300	7.160500	7.827700
	N	22.422200	2.948500	18.762300
	O	20.374700	-1.017100	18.198000
	N	21.496600	2.338200	17.993200
	N	19.863400	0.606300	16.719100
	H	20.073100	1.389900	16.431400
	C	22.993100	2.068200	19.641900
	C	24.079400	2.357400	20.601500
	C	22.376000	0.855600	19.438700
	H	22.531000	0.059700	19.894200
	C	21.468100	1.076000	18.403500
	C	20.525500	0.114600	17.773600
	C	25.392100	2.529800	20.176800
	H	25.595900	2.475300	19.270400
	C	23.808400	2.389900	21.957300
	H	22.938100	2.260900	22.258300
	C	18.810900	-0.119900	16.039100
	C	22.661800	4.403000	18.496400
	C	26.397100	2.781600	21.094100
	H	27.268000	2.922400	20.799600
	C	26.116000	2.825200	22.438900
	H	26.792600	2.996700	23.054000
	C	24.827800	2.614500	22.870000
	H	24.638500	2.622700	23.781000
	C	23.191100	5.100900	19.728100
	H	24.029700	4.708300	19.982600
	H	22.561900	5.004300	20.445900
	H	23.318800	6.033600	19.537200
	C	21.333200	5.039400	18.118900
	H	20.722300	4.966500	18.856100
	H	20.967400	4.587700	17.354800
	H	21.470800	5.965400	17.906500
	C	23.632900	4.495700	17.342800
	H	24.467800	4.093100	17.593800
	H	23.776600	5.418500	17.119000
	H	23.271400	4.034600	16.582000
	H	18.773700	0.158400	15.105200
	H	19.017500	-1.069600	16.013900
	N	13.861100	-2.948500	13.982600
	O	15.908500	1.017100	14.546900
	N	14.786700	-2.338200	14.751700
	N	16.419800	-0.606300	16.025800
	H	16.210100	-1.389900	16.313500
	C	13.290100	-2.068200	13.103000

	C	12.203800	-2.357400	12.143400
	C	13.907200	-0.855600	13.306200
	H	13.752200	-0.059700	12.850700
	C	14.815100	-1.076000	14.341400
	C	15.757700	-0.114600	14.971300
	C	10.891100	-2.529800	12.568100
	H	10.687300	-2.475300	13.474500
	C	12.474800	-2.389900	10.787600
	H	13.345200	-2.260900	10.486600
	C	17.472300	0.119900	16.705800
	C	13.621500	-4.403000	14.248500
	C	9.886100	-2.781600	11.650800
	H	9.015200	-2.922400	11.945300
	C	10.167300	-2.825200	10.306000
	H	9.490600	-2.996700	9.690900
	C	11.455400	-2.614500	9.874900
	H	11.644700	-2.622700	8.963900
	C	13.092100	-5.100900	13.016800
	H	12.253600	-4.708300	12.762300
	H	13.721400	-5.004300	12.299000
	H	12.964400	-6.033600	13.207700
	C	14.950100	-5.039400	14.626000
	H	15.561000	-4.966500	13.888700
	H	15.315800	-4.587700	15.390100
	H	14.812500	-5.965400	14.838300
	C	12.650400	-4.495700	15.402100
	H	11.815400	-4.093100	15.151100
	H	12.506600	-5.418500	15.625900
	H	13.011800	-4.034600	16.162900
	H	17.509500	-0.158400	17.639700
	H	17.265700	1.069600	16.731000
Energy single point calculations:	-3285.59194285223 u.a.			
M1···M10	N	1.305900	9.039400	5.796300
	O	3.353400	5.073800	6.360700
	N	2.231500	8.429100	6.565500
	N	3.864700	6.697200	7.839600
	H	3.654900	7.480800	8.127300
	C	0.735000	8.159100	4.916800
	C	-0.351400	8.448300	3.957200
	C	1.352000	6.946500	5.120000
	H	1.197100	6.150600	4.664500
	C	2.260000	7.166900	6.155200
	C	3.202500	6.205500	6.785100
	C	-1.664100	8.620700	4.381900
	H	-1.867900	8.566200	5.288300
	C	-0.080400	8.480800	2.601400
	H	0.790000	8.351800	2.300300
	C	4.917100	5.971000	8.519600
	C	1.066300	10.493900	6.062200
	C	-2.669100	8.872500	3.464600
	H	-3.540000	9.013300	3.759100
	C	-2.387900	8.916100	2.119700
	H	-3.064500	9.087600	1.504600
	C	-1.099800	8.705400	1.688700
	H	-0.910400	8.713600	0.777700
	C	0.537000	11.191800	4.830500
	H	-0.301600	10.799200	4.576100
	H	1.166200	11.095200	4.112800
	H	0.409300	12.124500	5.021400
	C	2.394900	11.130300	6.439800

	H	3.005800	11.057400	5.702500
	H	2.760700	10.678600	7.203900
	H	2.257300	12.056300	6.652100
	C	0.095200	10.586600	7.215800
	H	-0.739800	10.184000	6.964800
	H	-0.048500	11.509400	7.439600
	H	0.456600	10.125500	7.976700
	H	4.954400	6.249300	9.453500
	H	4.710600	5.021300	8.544800
	N	9.867000	3.142400	10.576100
	O	7.819600	7.108000	10.011800
	N	8.941400	3.752700	9.806900
	N	7.308200	5.484600	8.532800
	H	7.518000	4.701000	8.245200
	C	10.437900	4.022700	11.455600
	C	11.524300	3.733500	12.415200
	C	9.820900	5.235300	11.252500
	H	9.975800	6.031200	11.707900
	C	8.913000	5.014900	10.217200
	C	7.970400	5.976300	9.587400
	C	12.837000	3.561100	11.990500
	H	13.040800	3.615600	11.084100
	C	11.253300	3.701000	13.771000
	H	10.382900	3.830000	14.072100
	C	6.255800	6.210800	7.852900
	C	10.106600	1.687900	10.310200
	C	13.842000	3.309300	12.907900
	H	14.712900	3.168500	12.613300
	C	13.560800	3.265700	14.252700
	H	14.237400	3.094200	14.867800
	C	12.272700	3.476400	14.683800
	H	12.083300	3.468200	15.594800
	C	10.635900	0.990000	11.541900
	H	11.474500	1.382600	11.796300
	H	10.006700	1.086600	12.259700
	H	10.763600	0.057300	11.351000
	C	8.778000	1.051500	9.932700
	H	8.167100	1.124400	10.669900
	H	8.412200	1.503200	9.168600
	H	8.915600	0.125500	9.720300
	C	11.077700	1.595200	9.156600
	H	11.912700	1.997800	9.407600
	H	11.221400	0.672400	8.932800
	H	10.716300	2.056300	8.395800
	H	6.218500	5.932500	6.919000
	H	6.462300	7.160500	7.827700
	N	-2.688200	2.948500	2.389900
	O	-4.735600	-1.017100	1.825500
	N	-3.613800	2.338200	1.620700
	N	-5.246900	0.606300	0.346600
	H	-5.037200	1.389900	0.058900
	C	-2.117200	2.068200	3.269400
	C	-1.030900	2.357400	4.229000
	C	-2.734300	0.855600	3.066200
	H	-2.579300	0.059700	3.521700
	C	-3.642200	1.076000	2.031000
	C	-4.584800	0.114600	1.401200
	C	0.281800	2.529800	3.804300
	H	0.485600	2.475300	2.897900
	C	-1.301900	2.389900	5.584800
	H	-2.172200	2.260900	5.885900

	C	-6.299400	-0.119900	-0.333300
	C	-2.448600	4.403000	2.124000
	C	1.286800	2.781600	4.721700
	H	2.157700	2.922400	4.427100
	C	1.005700	2.825200	6.066500
	H	1.682300	2.996700	6.681600
	C	-0.282500	2.614500	6.497600
	H	-0.471800	2.622700	7.408500
	C	-1.919200	5.100900	3.355700
	H	-1.080700	4.708300	3.610100
	H	-2.548400	5.004300	4.073500
	H	-1.791500	6.033600	3.164800
	C	-3.777100	5.039400	1.746400
	H	-4.388000	4.966500	2.483700
	H	-4.142900	4.587700	0.982300
	H	-3.639500	5.965400	1.534100
	C	-1.477500	4.495700	0.970400
	H	-0.642500	4.093100	1.221400
	H	-1.333700	5.418500	0.746600
	H	-1.838900	4.034600	0.209600
	H	-6.336600	0.158400	-1.267200
	H	-6.092800	-1.069600	-0.358600
	N	-11.249200	-2.948500	-2.389900
	O	-9.201800	1.017100	-1.825500
	N	-10.323600	-2.338200	-1.620700
	N	-8.690500	-0.606300	-0.346600
	H	-8.900200	-1.389900	-0.058900
	C	-11.820200	-2.068200	-3.269400
	C	-12.906500	-2.357400	-4.229000
	C	-11.203100	-0.855600	-3.066200
	H	-11.358100	-0.059700	-3.521700
	C	-10.295200	-1.076000	-2.031000
	C	-9.352600	-0.114600	-1.401200
	C	-14.219200	-2.529800	-3.804300
	H	-14.423000	-2.475300	-2.897900
	C	-12.635500	-2.389900	-5.584800
	H	-11.765200	-2.260900	-5.885900
	C	-7.638000	0.119900	0.333300
	C	-11.488800	-4.403000	-2.124000
	C	-15.224200	-2.781600	-4.721700
	H	-16.095100	-2.922400	-4.427100
	C	-14.943100	-2.825200	-6.066500
	H	-15.619700	-2.996700	-6.681600
	C	-13.654900	-2.614500	-6.497600
	H	-13.465600	-2.622700	-7.408500
	C	-12.018200	-5.100900	-3.355700
	H	-12.856700	-4.708300	-3.610100
	H	-11.389000	-5.004300	-4.073500
	H	-12.145900	-6.033600	-3.164800
	C	-10.160300	-5.039400	-1.746400
	H	-9.549400	-4.966500	-2.483700
	H	-9.794500	-4.587700	-0.982300
	H	-10.297900	-5.965400	-1.534100
	C	-12.459900	-4.495700	-0.970400
	H	-13.294900	-4.093100	-1.221400
	H	-12.603700	-5.418500	-0.746600
	H	-12.098500	-4.034600	-0.209600
	H	-7.600800	-0.158400	1.267200
	H	-7.844600	1.069600	0.358600
Energy single point calculations:	-3285.59185568289 u.a.			

M1···M11	N	1.305900	9.039400	5.796300
	O	3.353400	5.073800	6.360700
	N	2.231500	8.429100	6.565500
	N	3.864700	6.697200	7.839600
	H	3.654900	7.480800	8.127300
	C	0.735000	8.159100	4.916800
	C	-0.351400	8.448300	3.957200
	C	1.352000	6.946500	5.120000
	H	1.197100	6.150600	4.664500
	C	2.260000	7.166900	6.155200
	C	3.202500	6.205500	6.785100
	C	-1.664100	8.620700	4.381900
	H	-1.867900	8.566200	5.288300
	C	-0.080400	8.480800	2.601400
	H	0.790000	8.351800	2.300300
	C	4.917100	5.971000	8.519600
	C	1.066300	10.493900	6.062200
	C	-2.669100	8.872500	3.464600
	H	-3.540000	9.013300	3.759100
	C	-2.387900	8.916100	2.119700
	H	-3.064500	9.087600	1.504600
	C	-1.099800	8.705400	1.688700
	H	-0.910400	8.713600	0.777700
	C	0.537000	11.191800	4.830500
	H	-0.301600	10.799200	4.576100
	H	1.166200	11.095200	4.112800
	H	0.409300	12.124500	5.021400
	C	2.394900	11.130300	6.439800
	H	3.005800	11.057400	5.702500
	H	2.760700	10.678600	7.203900
	H	2.257300	12.056300	6.652100
	C	0.095200	10.586600	7.215800
	H	-0.739800	10.184000	6.964800
	H	-0.048500	11.509400	7.439600
	H	0.456600	10.125500	7.976700
	H	4.954400	6.249300	9.453500
	H	4.710600	5.021300	8.544800
	N	9.867000	3.142400	10.576100
	O	7.819600	7.108000	10.011800
	N	8.941400	3.752700	9.806900
	N	7.308200	5.484600	8.532800
	H	7.518000	4.701000	8.245200
	C	10.437900	4.022700	11.455600
	C	11.524300	3.733500	12.415200
	C	9.820900	5.235300	11.252500
	H	9.975800	6.031200	11.707900
	C	8.913000	5.014900	10.217200
	C	7.970400	5.976300	9.587400
	C	12.837000	3.561100	11.990500
	H	13.040800	3.615600	11.084100
	C	11.253300	3.701000	13.771000
	H	10.382900	3.830000	14.072100
	C	6.255800	6.210800	7.852900
	C	10.106600	1.687900	10.310200
	C	13.842000	3.309300	12.907900
	H	14.712900	3.168500	12.613300
	C	13.560800	3.265700	14.252700
	H	14.237400	3.094200	14.867800
	C	12.272700	3.476400	14.683800
	H	12.083300	3.468200	15.594800
	C	10.635900	0.990000	11.541900

	H	11.474500	1.382600	11.796300
	H	10.006700	1.086600	12.259700
	H	10.763600	0.057300	11.351000
	C	8.778000	1.051500	9.932700
	H	8.167100	1.124400	10.669900
	H	8.412200	1.503200	9.168600
	H	8.915600	0.125500	9.720300
	C	11.077700	1.595200	9.156600
	H	11.912700	1.997800	9.407600
	H	11.221400	0.672400	8.932800
	H	10.716300	2.056300	8.395800
	H	6.218500	5.932500	6.919000
	H	6.462300	7.160500	7.827700
	N	-2.688200	15.130300	2.389900
	O	-4.735600	11.164700	1.825500
	N	-3.613800	14.520000	1.620700
	N	-5.246900	12.788100	0.346600
	H	-5.037200	13.571700	0.058900
	C	-2.117200	14.250000	3.269400
	C	-1.030900	14.539200	4.229000
	C	-2.734300	13.037400	3.066200
	H	-2.579300	12.241500	3.521700
	C	-3.642200	13.257800	2.031000
	C	-4.584800	12.296400	1.401200
	C	0.281800	14.711600	3.804300
	H	0.485600	14.657100	2.897900
	C	-1.301900	14.571700	5.584800
	H	-2.172200	14.442700	5.885900
	C	-6.299400	12.061900	-0.333300
	C	-2.448600	16.584800	2.124000
	C	1.286800	14.963400	4.721700
	H	2.157700	15.104200	4.427100
	C	1.005700	15.007000	6.066500
	H	1.682300	15.178500	6.681600
	C	-0.282500	14.796300	6.497600
	H	-0.471800	14.804500	7.408500
	C	-1.919200	17.282700	3.355700
	H	-1.080700	16.890100	3.610100
	H	-2.548400	17.186100	4.073500
	H	-1.791500	18.215400	3.164800
	C	-3.777100	17.221200	1.746400
	H	-4.388000	17.148300	2.483700
	H	-4.142900	16.769500	0.982300
	H	-3.639500	18.147200	1.534100
	C	-1.477500	16.677500	0.970400
	H	-0.642500	16.274900	1.221400
	H	-1.333700	17.600300	0.746600
	H	-1.838900	16.216400	0.209600
	H	-6.336600	12.340200	-1.267200
	H	-6.092800	11.112200	-0.358600
	N	-11.249200	9.233300	-2.389900
	O	-9.201800	13.198900	-1.825500
	N	-10.323600	9.843600	-1.620700
	N	-8.690500	11.575500	-0.346600
	H	-8.900200	10.791900	-0.058900
	C	-11.820200	10.113600	-3.269400
	C	-12.906500	9.824400	-4.229000
	C	-11.203100	11.326200	-3.066200
	H	-11.358100	12.122100	-3.521700
	C	-10.295200	11.105800	-2.031000
	C	-9.352600	12.067200	-1.401200

	C	-14.219200	9.652000	-3.804300
	H	-14.423000	9.706500	-2.897900
	C	-12.635500	9.791900	-5.584800
	H	-11.765200	9.920900	-5.885900
	C	-7.638000	12.301700	0.333300
	C	-11.488800	7.778800	-2.124000
	C	-15.224200	9.400200	-4.721700
	H	-16.095100	9.259400	-4.427100
	C	-14.943100	9.356600	-6.066500
	H	-15.619700	9.185100	-6.681600
	C	-13.654900	9.567300	-6.497600
	H	-13.465600	9.559100	-7.408500
	C	-12.018200	7.080900	-3.355700
	H	-12.856700	7.473500	-3.610100
	H	-11.389000	7.177500	-4.073500
	H	-12.145900	6.148200	-3.164800
	C	-10.160300	7.142400	-1.746400
	H	-9.549400	7.215300	-2.483700
	H	-9.794500	7.594100	-0.982300
	H	-10.297900	6.216400	-1.534100
	C	-12.459900	7.686100	-0.970400
	H	-13.294900	8.088700	-1.221400
	H	-12.603700	6.763300	-0.746600
	H	-12.098500	8.147200	-0.209600
	H	-7.600800	12.023400	1.267200
	H	-7.844600	13.251400	0.358600
Energy single point calculations:	-3285.59185567969 u.a.			
M1···M12	N	1.305900	9.039400	5.796300
	O	3.353400	5.073800	6.360700
	N	2.231500	8.429100	6.565500
	N	3.864700	6.697200	7.839600
	H	3.654900	7.480800	8.127300
	C	0.735000	8.159100	4.916800
	C	-0.351400	8.448300	3.957200
	C	1.352000	6.946500	5.120000
	H	1.197100	6.150600	4.664500
	C	2.260000	7.166900	6.155200
	C	3.202500	6.205500	6.785100
	C	-1.664100	8.620700	4.381900
	H	-1.867900	8.566200	5.288300
	C	-0.080400	8.480800	2.601400
	H	0.790000	8.351800	2.300300
	C	4.917100	5.971000	8.519600
	C	1.066300	10.493900	6.062200
	C	-2.669100	8.872500	3.464600
	H	-3.540000	9.013300	3.759100
	C	-2.387900	8.916100	2.119700
	H	-3.064500	9.087600	1.504600
	C	-1.099800	8.705400	1.688700
	H	-0.910400	8.713600	0.777700
	C	0.537000	11.191800	4.830500
	H	-0.301600	10.799200	4.576100
	H	1.166200	11.095200	4.112800
	H	0.409300	12.124500	5.021400
	C	2.394900	11.130300	6.439800
	H	3.005800	11.057400	5.702500
	H	2.760700	10.678600	7.203900
	H	2.257300	12.056300	6.652100
	C	0.095200	10.586600	7.215800
	H	-0.739800	10.184000	6.964800

	H	-0.048500	11.509400	7.439600
	H	0.456600	10.125500	7.976700
	H	4.954400	6.249300	9.453500
	H	4.710600	5.021300	8.544800
	N	9.867000	3.142400	10.576100
	O	7.819600	7.108000	10.011800
	N	8.941400	3.752700	9.806900
	N	7.308200	5.484600	8.532800
	H	7.518000	4.701000	8.245200
	C	10.437900	4.022700	11.455600
	C	11.524300	3.733500	12.415200
	C	9.820900	5.235300	11.252500
	H	9.975800	6.031200	11.707900
	C	8.913000	5.014900	10.217200
	C	7.970400	5.976300	9.587400
	C	12.837000	3.561100	11.990500
	H	13.040800	3.615600	11.084100
	C	11.253300	3.701000	13.771000
	H	10.382900	3.830000	14.072100
	C	6.255800	6.210800	7.852900
	C	10.106600	1.687900	10.310200
	C	13.842000	3.309300	12.907900
	H	14.712900	3.168500	12.613300
	C	13.560800	3.265700	14.252700
	H	14.237400	3.094200	14.867800
	C	12.272700	3.476400	14.683800
	H	12.083300	3.468200	15.594800
	C	10.635900	0.990000	11.541900
	H	11.474500	1.382600	11.796300
	H	10.006700	1.086600	12.259700
	H	10.763600	0.057300	11.351000
	C	8.778000	1.051500	9.932700
	H	8.167100	1.124400	10.669900
	H	8.412200	1.503200	9.168600
	H	8.915600	0.125500	9.720300
	C	11.077700	1.595200	9.156600
	H	11.912700	1.997800	9.407600
	H	11.221400	0.672400	8.932800
	H	10.716300	2.056300	8.395800
	H	6.218500	5.932500	6.919000
	H	6.462300	7.160500	7.827700
	N	-5.662800	21.221200	5.796300
	O	-3.615300	17.255600	6.360700
	N	-4.737200	20.610900	6.565500
	N	-3.104000	18.879000	7.839600
	H	-3.313800	19.662600	8.127300
	C	-6.233700	20.340900	4.916800
	C	-7.320100	20.630100	3.957200
	C	-5.616700	19.128300	5.120000
	H	-5.771600	18.332400	4.664500
	C	-4.708700	19.348700	6.155200
	C	-3.766200	18.387300	6.785100
	C	-8.632800	20.802500	4.381900
	H	-8.836600	20.748000	5.288300
	C	-7.049100	20.662600	2.601400
	H	-6.178700	20.533600	2.300300
	C	-2.051600	18.152800	8.519600
	C	-5.902400	22.675700	6.062200
	C	-9.637800	21.054300	3.464600
	H	-10.508700	21.195100	3.759100
	C	-9.356600	21.097900	2.119700

	H	-10.033200	21.269400	1.504600
	C	-8.068500	20.887200	1.688700
	H	-7.879100	20.895400	0.777700
	C	-6.431700	23.373600	4.830500
	H	-7.270300	22.981000	4.576100
	H	-5.802500	23.277000	4.112800
	H	-6.559400	24.306300	5.021400
	C	-4.573800	23.312100	6.439800
	H	-3.962900	23.239200	5.702500
	H	-4.208000	22.860400	7.203900
	H	-4.711400	24.238100	6.652100
	C	-6.873500	22.768400	7.215800
	H	-7.708500	22.365800	6.964800
	H	-7.017200	23.691200	7.439600
	H	-6.512100	22.307300	7.976700
	H	-2.014300	18.431100	9.453500
	H	-2.258100	17.203100	8.544800
	N	2.898300	15.324200	10.576100
	O	0.850900	19.289800	10.011800
	N	1.972700	15.934500	9.806900
	N	0.339500	17.666400	8.532800
	H	0.549300	16.882800	8.245200
	C	3.469200	16.204500	11.455600
	C	4.555600	15.915300	12.415200
	C	2.852200	17.417100	11.252500
	H	3.007100	18.213000	11.707900
	C	1.944300	17.196700	10.217200
	C	1.001700	18.158100	9.587400
	C	5.868300	15.742900	11.990500
	H	6.072100	15.797400	11.084100
	C	4.284600	15.882800	13.771000
	H	3.414200	16.011800	14.072100
	C	-0.712900	18.392600	7.852900
	C	3.137900	13.869700	10.310200
	C	6.873300	15.491100	12.907900
	H	7.744200	15.350300	12.613300
	C	6.592100	15.447500	14.252700
	H	7.268700	15.276000	14.867800
	C	5.304000	15.658200	14.683800
	H	5.114600	15.650000	15.594800
	C	3.667200	13.171800	11.541900
	H	4.505800	13.564400	11.796300
	H	3.038000	13.268400	12.259700
	H	3.794900	12.239100	11.351000
	C	1.809300	13.233300	9.932700
	H	1.198400	13.306200	10.669900
	H	1.443500	13.685000	9.168600
	H	1.946900	12.307300	9.720300
	C	4.109000	13.777000	9.156600
	H	4.944000	14.179600	9.407600
	H	4.252700	12.854200	8.932800
	H	3.747600	14.238100	8.395800
	H	-0.750200	18.114300	6.919000
	H	-0.506400	19.342300	7.827700
Energy single point calculations:	-3285.58381998741 u.a.			
M1···M13	N	1.305900	9.039400	5.796300
	O	3.353400	5.073800	6.360700
	N	2.231500	8.429100	6.565500
	N	3.864700	6.697200	7.839600
	H	3.654900	7.480800	8.127300

	C	0.735000	8.159100	4.916800
	C	-0.351400	8.448300	3.957200
	C	1.352000	6.946500	5.120000
	H	1.197100	6.150600	4.664500
	C	2.260000	7.166900	6.155200
	C	3.202500	6.205500	6.785100
	C	-1.664100	8.620700	4.381900
	H	-1.867900	8.566200	5.288300
	C	-0.080400	8.480800	2.601400
	H	0.790000	8.351800	2.300300
	C	4.917100	5.971000	8.519600
	C	1.066300	10.493900	6.062200
	C	-2.669100	8.872500	3.464600
	H	-3.540000	9.013300	3.759100
	C	-2.387900	8.916100	2.119700
	H	-3.064500	9.087600	1.504600
	C	-1.099800	8.705400	1.688700
	H	-0.910400	8.713600	0.777700
	C	0.537000	11.191800	4.830500
	H	-0.301600	10.799200	4.576100
	H	1.166200	11.095200	4.112800
	H	0.409300	12.124500	5.021400
	C	2.394900	11.130300	6.439800
	H	3.005800	11.057400	5.702500
	H	2.760700	10.678600	7.203900
	H	2.257300	12.056300	6.652100
	C	0.095200	10.586600	7.215800
	H	-0.739800	10.184000	6.964800
	H	-0.048500	11.509400	7.439600
	H	0.456600	10.125500	7.976700
	H	4.954400	6.249300	9.453500
	H	4.710600	5.021300	8.544800
	N	9.867000	3.142400	10.576100
	O	7.819600	7.108000	10.011800
	N	8.941400	3.752700	9.806900
	N	7.308200	5.484600	8.532800
	H	7.518000	4.701000	8.245200
	C	10.437900	4.022700	11.455600
	C	11.524300	3.733500	12.415200
	C	9.820900	5.235300	11.252500
	H	9.975800	6.031200	11.707900
	C	8.913000	5.014900	10.217200
	C	7.970400	5.976300	9.587400
	C	12.837000	3.561100	11.990500
	H	13.040800	3.615600	11.084100
	C	11.253300	3.701000	13.771000
	H	10.382900	3.830000	14.072100
	C	6.255800	6.210800	7.852900
	C	10.106600	1.687900	10.310200
	C	13.842000	3.309300	12.907900
	H	14.712900	3.168500	12.613300
	C	13.560800	3.265700	14.252700
	H	14.237400	3.094200	14.867800
	C	12.272700	3.476400	14.683800
	H	12.083300	3.468200	15.594800
	C	10.635900	0.990000	11.541900
	H	11.474500	1.382600	11.796300
	H	10.006700	1.086600	12.259700
	H	10.763600	0.057300	11.351000
	C	8.778000	1.051500	9.932700
	H	8.167100	1.124400	10.669900

	H	8.412200	1.503200	9.168600
	H	8.915600	0.125500	9.720300
	C	11.077700	1.595200	9.156600
	H	11.912700	1.997800	9.407600
	H	11.221400	0.672400	8.932800
	H	10.716300	2.056300	8.395800
	H	6.218500	5.932500	6.919000
	H	6.462300	7.160500	7.827700
	N	8.274600	-3.142400	5.796300
	O	10.322100	-7.108000	6.360700
	N	9.200200	-3.752700	6.565500
	N	10.833400	-5.484600	7.839600
	H	10.623600	-4.701000	8.127300
	C	7.703700	-4.022700	4.916800
	C	6.617300	-3.733500	3.957200
	C	8.320700	-5.235300	5.120000
	H	8.165800	-6.031200	4.664500
	C	9.228700	-5.014900	6.155200
	C	10.171200	-5.976300	6.785100
	C	5.304600	-3.561100	4.381900
	H	5.100800	-3.615600	5.288300
	C	6.888300	-3.701000	2.601400
	H	7.758700	-3.830000	2.300300
	C	11.885800	-6.210800	8.519600
	C	8.035000	-1.687900	6.062200
	C	4.299600	-3.309300	3.464600
	H	3.428700	-3.168500	3.759100
	C	4.580800	-3.265700	2.119700
	H	3.904200	-3.094200	1.504600
	C	5.868900	-3.476400	1.688700
	H	6.058300	-3.468200	0.777700
	C	7.505700	-0.990000	4.830500
	H	6.667100	-1.382600	4.576100
	H	8.134900	-1.086600	4.112800
	H	7.378000	-0.057300	5.021400
	C	9.363600	-1.051500	6.439800
	H	9.974500	-1.124400	5.702500
	H	9.729400	-1.503200	7.203900
	H	9.226000	-0.125500	6.652100
	C	7.063900	-1.595200	7.215800
	H	6.228900	-1.997800	6.964800
	H	6.920200	-0.672400	7.439600
	H	7.425300	-2.056300	7.976700
	H	11.923100	-5.932500	9.453500
	H	11.679300	-7.160500	8.544800
	N	16.835700	-9.039400	10.576100
	O	14.788300	-5.073800	10.011800
	N	15.910100	-8.429100	9.806900
	N	14.276900	-6.697200	8.532800
	H	14.486700	-7.480800	8.245200
	C	17.406600	-8.159100	11.455600
	C	18.493000	-8.448300	12.415200
	C	16.789600	-6.946500	11.252500
	H	16.944500	-6.150600	11.707900
	C	15.881700	-7.166900	10.217200
	C	14.939100	-6.205500	9.587400
	C	19.805700	-8.620700	11.990500
	H	20.009500	-8.566200	11.084100
	C	18.222000	-8.480800	13.771000
	H	17.351600	-8.351800	14.072100
	C	13.224500	-5.971000	7.852900

	C 17.075300 -10.493900 10.310200 C 20.810700 -8.872500 12.907900 H 21.681600 -9.013300 12.613300 C 20.529500 -8.916100 14.252700 H 21.206100 -9.087600 14.867800 C 19.241400 -8.705400 14.683800 H 19.052000 -8.713600 15.594800 C 17.604600 -11.191800 11.541900 H 18.443200 -10.799200 11.796300 H 16.975400 -11.095200 12.259700 H 17.732300 -12.124500 11.351000 C 15.746700 -11.130300 9.932700 H 15.135800 -11.057400 10.669900 H 15.380900 -10.678600 9.168600 H 15.884300 -12.056300 9.720300 C 18.046400 -10.586600 9.156600 H 18.881400 -10.184000 9.407600 H 18.190100 -11.509400 8.932800 H 17.685000 -10.125500 8.395800 H 13.187200 -6.249300 6.919000 H 13.431000 -5.021300 7.827700
Energy single point calculations:	-3285.58381998705 u.a.
M1···M14	N 1.305900 9.039400 5.796300 O 3.353400 5.073800 6.360700 N 2.231500 8.429100 6.565500 N 3.864700 6.697200 7.839600 H 3.654900 7.480800 8.127300 C 0.735000 8.159100 4.916800 C -0.351400 8.448300 3.957200 C 1.352000 6.946500 5.120000 H 1.197100 6.150600 4.664500 C 2.260000 7.166900 6.155200 C 3.202500 6.205500 6.785100 C -1.664100 8.620700 4.381900 H -1.867900 8.566200 5.288300 C -0.080400 8.480800 2.601400 H 0.790000 8.351800 2.300300 C 4.917100 5.971000 8.519600 C 1.066300 10.493900 6.062200 C -2.669100 8.872500 3.464600 H -3.540000 9.013300 3.759100 C -2.387900 8.916100 2.119700 H -3.064500 9.087600 1.504600 C -1.099800 8.705400 1.688700 H -0.910400 8.713600 0.777700 C 0.537000 11.191800 4.830500 H -0.301600 10.799200 4.576100 H 1.166200 11.095200 4.112800 H 0.409300 12.124500 5.021400 C 2.394900 11.130300 6.439800 H 3.005800 11.057400 5.702500 H 2.760700 10.678600 7.203900 H 2.257300 12.056300 6.652100 C 0.095200 10.586600 7.215800 H -0.739800 10.184000 6.964800 H -0.048500 11.509400 7.439600 H 0.456600 10.125500 7.976700 H 4.954400 6.249300 9.453500 H 4.710600 5.021300 8.544800 N 9.867000 3.142400 10.576100

	O	7.819600	7.108000	10.011800
	N	8.941400	3.752700	9.806900
	N	7.308200	5.484600	8.532800
	H	7.518000	4.701000	8.245200
	C	10.437900	4.022700	11.455600
	C	11.524300	3.733500	12.415200
	C	9.820900	5.235300	11.252500
	H	9.975800	6.031200	11.707900
	C	8.913000	5.014900	10.217200
	C	7.970400	5.976300	9.587400
	C	12.837000	3.561100	11.990500
	H	13.040800	3.615600	11.084100
	C	11.253300	3.701000	13.771000
	H	10.382900	3.830000	14.072100
	C	6.255800	6.210800	7.852900
	C	10.106600	1.687900	10.310200
	C	13.842000	3.309300	12.907900
	H	14.712900	3.168500	12.613300
	C	13.560800	3.265700	14.252700
	H	14.237400	3.094200	14.867800
	C	12.272700	3.476400	14.683800
	H	12.083300	3.468200	15.594800
	C	10.635900	0.990000	11.541900
	H	11.474500	1.382600	11.796300
	H	10.006700	1.086600	12.259700
	H	10.763600	0.057300	11.351000
	C	8.778000	1.051500	9.932700
	H	8.167100	1.124400	10.669900
	H	8.412200	1.503200	9.168600
	H	8.915600	0.125500	9.720300
	C	11.077700	1.595200	9.156600
	H	11.912700	1.997800	9.407600
	H	11.221400	0.672400	8.932800
	H	10.716300	2.056300	8.395800
	H	6.218500	5.932500	6.919000
	H	6.462300	7.160500	7.827700
	N	8.484800	2.948500	18.762300
	O	6.437300	-1.017100	18.198000
	N	7.559200	2.338200	17.993200
	N	5.926000	0.606300	16.719100
	H	6.135700	1.389900	16.431400
	C	9.055700	2.068200	19.641900
	C	10.142000	2.357400	20.601500
	C	8.438600	0.855600	19.438700
	H	8.593600	0.059700	19.894200
	C	7.530700	1.076000	18.403500
	C	6.588100	0.114600	17.773600
	C	11.454700	2.529800	20.176800
	H	11.658500	2.475300	19.270400
	C	9.871000	2.389900	21.957300
	H	9.000700	2.260900	22.258300
	C	4.873500	-0.119900	16.039100
	C	8.724400	4.403000	18.496400
	C	12.459700	2.781600	21.094100
	H	13.330600	2.922400	20.799600
	C	12.178600	2.825200	22.438900
	H	12.855200	2.996700	23.054000
	C	10.890400	2.614500	22.870000
	H	10.701100	2.622700	23.781000
	C	9.253700	5.100900	19.728100
	H	10.092300	4.708300	19.982600

	H	8.624500	5.004300	20.445900
	H	9.381400	6.033600	19.537200
	C	7.395800	5.039400	18.118900
	H	6.784900	4.966500	18.856100
	H	7.030000	4.587700	17.354800
	H	7.533400	5.965400	17.906500
	C	9.695500	4.495700	17.342800
	H	10.530400	4.093100	17.593800
	H	9.839200	5.418500	17.119000
	H	9.334000	4.034600	16.582000
	H	4.836300	0.158400	15.105200
	H	5.080100	-1.069600	16.013900
	N	-0.076300	-2.948500	13.982600
	O	1.971100	1.017100	14.546900
	N	0.849300	-2.338200	14.751700
	N	2.482400	-0.606300	16.025800
	H	2.272700	-1.389900	16.313500
	C	-0.647300	-2.068200	13.103000
	C	-1.733600	-2.357400	12.143400
	C	-0.030200	-0.855600	13.306200
	H	-0.185200	-0.059700	12.850700
	C	0.877700	-1.076000	14.341400
	C	1.820300	-0.114600	14.971300
	C	-3.046300	-2.529800	12.568100
	H	-3.250100	-2.475300	13.474500
	C	-1.462600	-2.389900	10.787600
	H	-0.592200	-2.260900	10.486600
	C	3.534900	0.119900	16.705800
	C	-0.315900	-4.403000	14.248500
	C	-4.051300	-2.781600	11.650800
	H	-4.922200	-2.922400	11.945300
	C	-3.770100	-2.825200	10.306000
	H	-4.446800	-2.996700	9.690900
	C	-2.482000	-2.614500	9.874900
	H	-2.292700	-2.622700	8.963900
	C	-0.845300	-5.100900	13.016800
	H	-1.683800	-4.708300	12.762300
	H	-0.216000	-5.004300	12.299000
	H	-0.973000	-6.033600	13.207700
	C	1.012700	-5.039400	14.626000
	H	1.623600	-4.966500	13.888700
	H	1.378400	-4.587700	15.390100
	H	0.875100	-5.965400	14.838300
	C	-1.287000	-4.495700	15.402100
	H	-2.122000	-4.093100	15.151100
	H	-1.430800	-5.418500	15.625900
	H	-0.925600	-4.034600	16.162900
	H	3.572100	-0.158400	17.639700
	H	3.328300	1.069600	16.731000
Energy single point calculations:	-3285.58262053250 u.a.			
M1···M15	N	1.305900	9.039400	5.796300
	O	3.353400	5.073800	6.360700
	N	2.231500	8.429100	6.565500
	N	3.864700	6.697200	7.839600
	H	3.654900	7.480800	8.127300
	C	0.735000	8.159100	4.916800
	C	-0.351400	8.448300	3.957200
	C	1.352000	6.946500	5.120000
	H	1.197100	6.150600	4.664500
	C	2.260000	7.166900	6.155200

	C	3.202500	6.205500	6.785100
	C	-1.664100	8.620700	4.381900
	H	-1.867900	8.566200	5.288300
	C	-0.080400	8.480800	2.601400
	H	0.790000	8.351800	2.300300
	C	4.917100	5.971000	8.519600
	C	1.066300	10.493900	6.062200
	C	-2.669100	8.872500	3.464600
	H	-3.540000	9.013300	3.759100
	C	-2.387900	8.916100	2.119700
	H	-3.064500	9.087600	1.504600
	C	-1.099800	8.705400	1.688700
	H	-0.910400	8.713600	0.777700
	C	0.537000	11.191800	4.830500
	H	-0.301600	10.799200	4.576100
	H	1.166200	11.095200	4.112800
	H	0.409300	12.124500	5.021400
	C	2.394900	11.130300	6.439800
	H	3.005800	11.057400	5.702500
	H	2.760700	10.678600	7.203900
	H	2.257300	12.056300	6.652100
	C	0.095200	10.586600	7.215800
	H	-0.739800	10.184000	6.964800
	H	-0.048500	11.509400	7.439600
	H	0.456600	10.125500	7.976700
	H	4.954400	6.249300	9.453500
	H	4.710600	5.021300	8.544800
	N	9.867000	3.142400	10.576100
	O	7.819600	7.108000	10.011800
	N	8.941400	3.752700	9.806900
	N	7.308200	5.484600	8.532800
	H	7.518000	4.701000	8.245200
	C	10.437900	4.022700	11.455600
	C	11.524300	3.733500	12.415200
	C	9.820900	5.235300	11.252500
	H	9.975800	6.031200	11.707900
	C	8.913000	5.014900	10.217200
	C	7.970400	5.976300	9.587400
	C	12.837000	3.561100	11.990500
	H	13.040800	3.615600	11.084100
	C	11.253300	3.701000	13.771000
	H	10.382900	3.830000	14.072100
	C	6.255800	6.210800	7.852900
	C	10.106600	1.687900	10.310200
	C	13.842000	3.309300	12.907900
	H	14.712900	3.168500	12.613300
	C	13.560800	3.265700	14.252700
	H	14.237400	3.094200	14.867800
	C	12.272700	3.476400	14.683800
	H	12.083300	3.468200	15.594800
	C	10.635900	0.990000	11.541900
	H	11.474500	1.382600	11.796300
	H	10.006700	1.086600	12.259700
	H	10.763600	0.057300	11.351000
	C	8.778000	1.051500	9.932700
	H	8.167100	1.124400	10.669900
	H	8.412200	1.503200	9.168600
	H	8.915600	0.125500	9.720300
	C	11.077700	1.595200	9.156600
	H	11.912700	1.997800	9.407600
	H	11.221400	0.672400	8.932800

	H	10.716300	2.056300	8.395800
	H	6.218500	5.932500	6.919000
	H	6.462300	7.160500	7.827700
	N	8.484800	15.130300	18.762300
	O	6.437300	11.164700	18.198000
	N	7.559200	14.520000	17.993200
	N	5.926000	12.788100	16.719100
	H	6.135700	13.571700	16.431400
	C	9.055700	14.250000	19.641900
	C	10.142000	14.539200	20.601500
	C	8.438600	13.037400	19.438700
	H	8.593600	12.241500	19.894200
	C	7.530700	13.257800	18.403500
	C	6.588100	12.296400	17.773600
	C	11.454700	14.711600	20.176800
	H	11.658500	14.657100	19.270400
	C	9.871000	14.571700	21.957300
	H	9.000700	14.442700	22.258300
	C	4.873500	12.061900	16.039100
	C	8.724400	16.584800	18.496400
	C	12.459700	14.963400	21.094100
	H	13.330600	15.104200	20.799600
	C	12.178600	15.007000	22.438900
	H	12.855200	15.178500	23.054000
	C	10.890400	14.796300	22.870000
	H	10.701100	14.804500	23.781000
	C	9.253700	17.282700	19.728100
	H	10.092300	16.890100	19.982600
	H	8.624500	17.186100	20.445900
	H	9.381400	18.215400	19.537200
	C	7.395800	17.221200	18.118900
	H	6.784900	17.148300	18.856100
	H	7.030000	16.769500	17.354800
	H	7.533400	18.147200	17.906500
	C	9.695500	16.677500	17.342800
	H	10.530400	16.274900	17.593800
	H	9.839200	17.600300	17.119000
	H	9.334000	16.216400	16.582000
	H	4.836300	12.340200	15.105200
	H	5.080100	11.112200	16.013900
	N	-0.076300	9.233300	13.982600
	O	1.971100	13.198900	14.546900
	N	0.849300	9.843600	14.751700
	N	2.482400	11.575500	16.025800
	H	2.272700	10.791900	16.313500
	C	-0.647300	10.113600	13.103000
	C	-1.733600	9.824400	12.143400
	C	-0.030200	11.326200	13.306200
	H	-0.185200	12.122100	12.850700
	C	0.877700	11.105800	14.341400
	C	1.820300	12.067200	14.971300
	C	-3.046300	9.652000	12.568100
	H	-3.250100	9.706500	13.474500
	C	-1.462600	9.791900	10.787600
	H	-0.592200	9.920900	10.486600
	C	3.534900	12.301700	16.705800
	C	-0.315900	7.778800	14.248500
	C	-4.051300	9.400200	11.650800
	H	-4.922200	9.259400	11.945300
	C	-3.770100	9.356600	10.306000
	H	-4.446800	9.185100	9.690900

	C	-2.482000	9.567300	9.874900
	H	-2.292700	9.559100	8.963900
	C	-0.845300	7.080900	13.016800
	H	-1.683800	7.473500	12.762300
	H	-0.216000	7.177500	12.299000
	H	-0.973000	6.148200	13.207700
	C	1.012700	7.142400	14.626000
	H	1.623600	7.215300	13.888700
	H	1.378400	7.594100	15.390100
	H	0.875100	6.216400	14.838300
	C	-1.287000	7.686100	15.402100
	H	-2.122000	8.088700	15.151100
	H	-1.430800	6.763300	15.625900
	H	-0.925600	8.147200	16.162900
	H	3.572100	12.023400	17.639700
	H	3.328300	13.251400	16.731000
Energy single point calculations:	-3285.58262046724 u.a.			
M1···M16	N	1.305900	9.039400	5.796300
	O	3.353400	5.073800	6.360700
	N	2.231500	8.429100	6.565500
	N	3.864700	6.697200	7.839600
	H	3.654900	7.480800	8.127300
	C	0.735000	8.159100	4.916800
	C	-0.351400	8.448300	3.957200
	C	1.352000	6.946500	5.120000
	H	1.197100	6.150600	4.664500
	C	2.260000	7.166900	6.155200
	C	3.202500	6.205500	6.785100
	C	-1.664100	8.620700	4.381900
	H	-1.867900	8.566200	5.288300
	C	-0.080400	8.480800	2.601400
	H	0.790000	8.351800	2.300300
	C	4.917100	5.971000	8.519600
	C	1.066300	10.493900	6.062200
	C	-2.669100	8.872500	3.464600
	H	-3.540000	9.013300	3.759100
	C	-2.387900	8.916100	2.119700
	H	-3.064500	9.087600	1.504600
	C	-1.099800	8.705400	1.688700
	H	-0.910400	8.713600	0.777700
	C	0.537000	11.191800	4.830500
	H	-0.301600	10.799200	4.576100
	H	1.166200	11.095200	4.112800
	H	0.409300	12.124500	5.021400
	C	2.394900	11.130300	6.439800
	H	3.005800	11.057400	5.702500
	H	2.760700	10.678600	7.203900
	H	2.257300	12.056300	6.652100
	C	0.095200	10.586600	7.215800
	H	-0.739800	10.184000	6.964800
	H	-0.048500	11.509400	7.439600
	H	0.456600	10.125500	7.976700
	H	4.954400	6.249300	9.453500
	H	4.710600	5.021300	8.544800
	N	9.867000	3.142400	10.576100
	O	7.819600	7.108000	10.011800
	N	8.941400	3.752700	9.806900
	N	7.308200	5.484600	8.532800
	H	7.518000	4.701000	8.245200
	C	10.437900	4.022700	11.455600

	C	11.524300	3.733500	12.415200
	C	9.820900	5.235300	11.252500
	H	9.975800	6.031200	11.707900
	C	8.913000	5.014900	10.217200
	C	7.970400	5.976300	9.587400
	C	12.837000	3.561100	11.990500
	H	13.040800	3.615600	11.084100
	C	11.253300	3.701000	13.771000
	H	10.382900	3.830000	14.072100
	C	6.255800	6.210800	7.852900
	C	10.106600	1.687900	10.310200
	C	13.842000	3.309300	12.907900
	H	14.712900	3.168500	12.613300
	C	13.560800	3.265700	14.252700
	H	14.237400	3.094200	14.867800
	C	12.272700	3.476400	14.683800
	H	12.083300	3.468200	15.594800
	C	10.635900	0.990000	11.541900
	H	11.474500	1.382600	11.796300
	H	10.006700	1.086600	12.259700
	H	10.763600	0.057300	11.351000
	C	8.778000	1.051500	9.932700
	H	8.167100	1.124400	10.669900
	H	8.412200	1.503200	9.168600
	H	8.915600	0.125500	9.720300
	C	11.077700	1.595200	9.156600
	H	11.912700	1.997800	9.407600
	H	11.221400	0.672400	8.932800
	H	10.716300	2.056300	8.395800
	H	6.218500	5.932500	6.919000
	H	6.462300	7.160500	7.827700
	N	11.249200	15.130300	2.389900
	O	9.201800	11.164700	1.825500
	N	10.323600	14.520000	1.620700
	N	8.690500	12.788100	0.346600
	H	8.900200	13.571700	0.058900
	C	11.820200	14.250000	3.269400
	C	12.906500	14.539200	4.229000
	C	11.203100	13.037400	3.066200
	H	11.358100	12.241500	3.521700
	C	10.295200	13.257800	2.031000
	C	9.352600	12.296400	1.401200
	C	14.219200	14.711600	3.804300
	H	14.423000	14.657100	2.897900
	C	12.635500	14.571700	5.584800
	H	11.765200	14.442700	5.885900
	C	7.638000	12.061900	-0.333300
	C	11.488800	16.584800	2.124000
	C	15.224200	14.963400	4.721700
	H	16.095100	15.104200	4.427100
	C	14.943100	15.007000	6.066500
	H	15.619700	15.178500	6.681600
	C	13.654900	14.796300	6.497600
	H	13.465600	14.804500	7.408500
	C	12.018200	17.282700	3.355700
	H	12.856700	16.890100	3.610100
	H	11.389000	17.186100	4.073500
	H	12.145900	18.215400	3.164800
	C	10.160300	17.221200	1.746400
	H	9.549400	17.148300	2.483700
	H	9.794500	16.769500	0.982300

	H	10.297900	18.147200	1.534100
	C	12.459900	16.677500	0.970400
	H	13.294900	16.274900	1.221400
	H	12.603700	17.600300	0.746600
	H	12.098500	16.216400	0.209600
	H	7.600800	12.340200	-1.267200
	H	7.844600	11.112200	-0.358600
	N	2.688200	9.233300	-2.389900
	O	4.735600	13.198900	-1.825500
	N	3.613800	9.843600	-1.620700
	N	5.246900	11.575500	-0.346600
	H	5.037200	10.791900	-0.058900
	C	2.117200	10.113600	-3.269400
	C	1.030900	9.824400	-4.229000
	C	2.734300	11.326200	-3.066200
	H	2.579300	12.122100	-3.521700
	C	3.642200	11.105800	-2.031000
	C	4.584800	12.067200	-1.401200
	C	-0.281800	9.652000	-3.804300
	H	-0.485600	9.706500	-2.897900
	C	1.301900	9.791900	-5.584800
	H	2.172200	9.920900	-5.885900
	C	6.299400	12.301700	0.333300
	C	2.448600	7.778800	-2.124000
	C	-1.286800	9.400200	-4.721700
	H	-2.157700	9.259400	-4.427100
	C	-1.005700	9.356600	-6.066500
	H	-1.682300	9.185100	-6.681600
	C	0.282500	9.567300	-6.497600
	H	0.471800	9.559100	-7.408500
	C	1.919200	7.080900	-3.355700
	H	1.080700	7.473500	-3.610100
	H	2.548400	7.177500	-4.073500
	H	1.791500	6.148200	-3.164800
	C	3.777100	7.142400	-1.746400
	H	4.388000	7.215300	-2.483700
	H	4.142900	7.594100	-0.982300
	H	3.639500	6.216400	-1.534100
	C	1.477500	7.686100	-0.970400
	H	0.642500	8.088700	-1.221400
	H	1.333700	6.763300	-0.746600
	H	1.838900	8.147200	-0.209600
	H	6.336600	12.023400	1.267200
	H	6.092800	13.251400	0.358600
Energy single point calculations:	-3285.58253317670 u.a.			
M1···M17	N	1.305900	9.039400	5.796300
	O	3.353400	5.073800	6.360700
	N	2.231500	8.429100	6.565500
	N	3.864700	6.697200	7.839600
	H	3.654900	7.480800	8.127300
	C	0.735000	8.159100	4.916800
	C	-0.351400	8.448300	3.957200
	C	1.352000	6.946500	5.120000
	H	1.197100	6.150600	4.664500
	C	2.260000	7.166900	6.155200
	C	3.202500	6.205500	6.785100
	C	-1.664100	8.620700	4.381900
	H	-1.867900	8.566200	5.288300
	C	-0.080400	8.480800	2.601400
	H	0.790000	8.351800	2.300300

	C	4.917100	5.971000	8.519600
	C	1.066300	10.493900	6.062200
	C	-2.669100	8.872500	3.464600
	H	-3.540000	9.013300	3.759100
	C	-2.387900	8.916100	2.119700
	H	-3.064500	9.087600	1.504600
	C	-1.099800	8.705400	1.688700
	H	-0.910400	8.713600	0.777700
	C	0.537000	11.191800	4.830500
	H	-0.301600	10.799200	4.576100
	H	1.166200	11.095200	4.112800
	H	0.409300	12.124500	5.021400
	C	2.394900	11.130300	6.439800
	H	3.005800	11.057400	5.702500
	H	2.760700	10.678600	7.203900
	H	2.257300	12.056300	6.652100
	C	0.095200	10.586600	7.215800
	H	-0.739800	10.184000	6.964800
	H	-0.048500	11.509400	7.439600
	H	0.456600	10.125500	7.976700
	H	4.954400	6.249300	9.453500
	H	4.710600	5.021300	8.544800
	N	9.867000	3.142400	10.576100
	O	7.819600	7.108000	10.011800
	N	8.941400	3.752700	9.806900
	N	7.308200	5.484600	8.532800
	H	7.518000	4.701000	8.245200
	C	10.437900	4.022700	11.455600
	C	11.524300	3.733500	12.415200
	C	9.820900	5.235300	11.252500
	H	9.975800	6.031200	11.707900
	C	8.913000	5.014900	10.217200
	C	7.970400	5.976300	9.587400
	C	12.837000	3.561100	11.990500
	H	13.040800	3.615600	11.084100
	C	11.253300	3.701000	13.771000
	H	10.382900	3.830000	14.072100
	C	6.255800	6.210800	7.852900
	C	10.106600	1.687900	10.310200
	C	13.842000	3.309300	12.907900
	H	14.712900	3.168500	12.613300
	C	13.560800	3.265700	14.252700
	H	14.237400	3.094200	14.867800
	C	12.272700	3.476400	14.683800
	H	12.083300	3.468200	15.594800
	C	10.635900	0.990000	11.541900
	H	11.474500	1.382600	11.796300
	H	10.006700	1.086600	12.259700
	H	10.763600	0.057300	11.351000
	C	8.778000	1.051500	9.932700
	H	8.167100	1.124400	10.669900
	H	8.412200	1.503200	9.168600
	H	8.915600	0.125500	9.720300
	C	11.077700	1.595200	9.156600
	H	11.912700	1.997800	9.407600
	H	11.221400	0.672400	8.932800
	H	10.716300	2.056300	8.395800
	H	6.218500	5.932500	6.919000
	H	6.462300	7.160500	7.827700
	N	11.249200	2.948500	2.389900
	O	9.201800	-1.017100	1.825500

	N	10.323600	2.338200	1.620700
	N	8.690500	0.606300	0.346600
	H	8.900200	1.389900	0.058900
	C	11.820200	2.068200	3.269400
	C	12.906500	2.357400	4.229000
	C	11.203100	0.855600	3.066200
	H	11.358100	0.059700	3.521700
	C	10.295200	1.076000	2.031000
	C	9.352600	0.114600	1.401200
	C	14.219200	2.529800	3.804300
	H	14.423000	2.475300	2.897900
	C	12.635500	2.389900	5.584800
	H	11.765200	2.260900	5.885900
	C	7.638000	-0.119900	-0.333300
	C	11.488800	4.403000	2.124000
	C	15.224200	2.781600	4.721700
	H	16.095100	2.922400	4.427100
	C	14.943100	2.825200	6.066500
	H	15.619700	2.996700	6.681600
	C	13.654900	2.614500	6.497600
	H	13.465600	2.622700	7.408500
	C	12.018200	5.100900	3.355700
	H	12.856700	4.708300	3.610100
	H	11.389000	5.004300	4.073500
	H	12.145900	6.033600	3.164800
	C	10.160300	5.039400	1.746400
	H	9.549400	4.966500	2.483700
	H	9.794500	4.587700	0.982300
	H	10.297900	5.965400	1.534100
	C	12.459900	4.495700	0.970400
	H	13.294900	4.093100	1.221400
	H	12.603700	5.418500	0.746600
	H	12.098500	4.034600	0.209600
	H	7.600800	0.158400	-1.267200
	H	7.844600	-1.069600	-0.358600
	N	2.688200	-2.948500	-2.389900
	O	4.735600	1.017100	-1.825500
	N	3.613800	-2.338200	-1.620700
	N	5.246900	-0.606300	-0.346600
	H	5.037200	-1.389900	-0.058900
	C	2.117200	-2.068200	-3.269400
	C	1.030900	-2.357400	-4.229000
	C	2.734300	-0.855600	-3.066200
	H	2.579300	-0.059700	-3.521700
	C	3.642200	-1.076000	-2.031000
	C	4.584800	-0.114600	-1.401200
	C	-0.281800	-2.529800	-3.804300
	H	-0.485600	-2.475300	-2.897900
	C	1.301900	-2.389900	-5.584800
	H	2.172200	-2.260900	-5.885900
	C	6.299400	0.119900	0.333300
	C	2.448600	-4.403000	-2.124000
	C	-1.286800	-2.781600	-4.721700
	H	-2.157700	-2.922400	-4.427100
	C	-1.005700	-2.825200	-6.066500
	H	-1.682300	-2.996700	-6.681600
	C	0.282500	-2.614500	-6.497600
	H	0.471800	-2.622700	-7.408500
	C	1.919200	-5.100900	-3.355700
	H	1.080700	-4.708300	-3.610100
	H	2.548400	-5.004300	-4.073500

	H	1.791500	-6.033600	-3.164800
	C	3.777100	-5.039400	-1.746400
	H	4.388000	-4.966500	-2.483700
	H	4.142900	-4.587700	-0.982300
	H	3.639500	-5.965400	-1.534100
	C	1.477500	-4.495700	-0.970400
	H	0.642500	-4.093100	-1.221400
	H	1.333700	-5.418500	-0.746600
	H	1.838900	-4.034600	-0.209600
	H	6.336600	-0.158400	1.267200
	H	6.092800	1.069600	0.358600
Energy single point calculations:	-3285.58253289386 u.a.			
M1···M18	N	1.305900	9.039400	5.796300
	O	3.353400	5.073800	6.360700
	N	2.231500	8.429100	6.565500
	N	3.864700	6.697200	7.839600
	H	3.654900	7.480800	8.127300
	C	0.735000	8.159100	4.916800
	C	-0.351400	8.448300	3.957200
	C	1.352000	6.946500	5.120000
	H	1.197100	6.150600	4.664500
	C	2.260000	7.166900	6.155200
	C	3.202500	6.205500	6.785100
	C	-1.664100	8.620700	4.381900
	H	-1.867900	8.566200	5.288300
	C	-0.080400	8.480800	2.601400
	H	0.790000	8.351800	2.300300
	C	4.917100	5.971000	8.519600
	C	1.066300	10.493900	6.062200
	C	-2.669100	8.872500	3.464600
	H	-3.540000	9.013300	3.759100
	C	-2.387900	8.916100	2.119700
	H	-3.064500	9.087600	1.504600
	C	-1.099800	8.705400	1.688700
	H	-0.910400	8.713600	0.777700
	C	0.537000	11.191800	4.830500
	H	-0.301600	10.799200	4.576100
	H	1.166200	11.095200	4.112800
	H	0.409300	12.124500	5.021400
	C	2.394900	11.130300	6.439800
	H	3.005800	11.057400	5.702500
	H	2.760700	10.678600	7.203900
	H	2.257300	12.056300	6.652100
	C	0.095200	10.586600	7.215800
	H	-0.739800	10.184000	6.964800
	H	-0.048500	11.509400	7.439600
	H	0.456600	10.125500	7.976700
	H	4.954400	6.249300	9.453500
	H	4.710600	5.021300	8.544800
	N	9.867000	3.142400	10.576100
	O	7.819600	7.108000	10.011800
	N	8.941400	3.752700	9.806900
	N	7.308200	5.484600	8.532800
	H	7.518000	4.701000	8.245200
	C	10.437900	4.022700	11.455600
	C	11.524300	3.733500	12.415200
	C	9.820900	5.235300	11.252500
	H	9.975800	6.031200	11.707900
	C	8.913000	5.014900	10.217200
	C	7.970400	5.976300	9.587400

	C	12.837000	3.561100	11.990500
	H	13.040800	3.615600	11.084100
	C	11.253300	3.701000	13.771000
	H	10.382900	3.830000	14.072100
	C	6.255800	6.210800	7.852900
	C	10.106600	1.687900	10.310200
	C	13.842000	3.309300	12.907900
	H	14.712900	3.168500	12.613300
	C	13.560800	3.265700	14.252700
	H	14.237400	3.094200	14.867800
	C	12.272700	3.476400	14.683800
	H	12.083300	3.468200	15.594800
	C	10.635900	0.990000	11.541900
	H	11.474500	1.382600	11.796300
	H	10.006700	1.086600	12.259700
	H	10.763600	0.057300	11.351000
	C	8.778000	1.051500	9.932700
	H	8.167100	1.124400	10.669900
	H	8.412200	1.503200	9.168600
	H	8.915600	0.125500	9.720300
	C	11.077700	1.595200	9.156600
	H	11.912700	1.997800	9.407600
	H	11.221400	0.672400	8.932800
	H	10.716300	2.056300	8.395800
	H	6.218500	5.932500	6.919000
	H	6.462300	7.160500	7.827700
	N	15.243300	-3.142400	5.796300
	O	17.290800	-7.108000	6.360700
	N	16.168900	-3.752700	6.565500
	N	17.802100	-5.484600	7.839600
	H	17.592300	-4.701000	8.127300
	C	14.672400	-4.022700	4.916800
	C	13.586000	-3.733500	3.957200
	C	15.289400	-5.235300	5.120000
	H	15.134500	-6.031200	4.664500
	C	16.197400	-5.014900	6.155200
	C	17.139900	-5.976300	6.785100
	C	12.273300	-3.561100	4.381900
	H	12.069500	-3.615600	5.288300
	C	13.857000	-3.701000	2.601400
	H	14.727400	-3.830000	2.300300
	C	18.854500	-6.210800	8.519600
	C	15.003700	-1.687900	6.062200
	C	11.268300	-3.309300	3.464600
	H	10.397400	-3.168500	3.759100
	C	11.549500	-3.265700	2.119700
	H	10.872900	-3.094200	1.504600
	C	12.837600	-3.476400	1.688700
	H	13.027000	-3.468200	0.777700
	C	14.474400	-0.990000	4.830500
	H	13.635800	-1.382600	4.576100
	H	15.103600	-1.086600	4.112800
	H	14.346700	-0.057300	5.021400
	C	16.332300	-1.051500	6.439800
	H	16.943200	-1.124400	5.702500
	H	16.698100	-1.503200	7.203900
	H	16.194700	-0.125500	6.652100
	C	14.032600	-1.595200	7.215800
	H	13.197600	-1.997800	6.964800
	H	13.888900	-0.672400	7.439600
	H	14.394000	-2.056300	7.976700

	H	18.891800	-5.932500	9.453500
	H	18.648000	-7.160500	8.544800
	N	23.804400	-9.039400	10.576100
	O	21.757000	-5.073800	10.011800
	N	22.878800	-8.429100	9.806900
	N	21.245600	-6.697200	8.532800
	H	21.455400	-7.480800	8.245200
	C	24.375300	-8.159100	11.455600
	C	25.461700	-8.448300	12.415200
	C	23.758300	-6.946500	11.252500
	H	23.913200	-6.150600	11.707900
	C	22.850400	-7.166900	10.217200
	C	21.907800	-6.205500	9.587400
	C	26.774400	-8.620700	11.990500
	H	26.978200	-8.566200	11.084100
	C	25.190700	-8.480800	13.771000
	H	24.320300	-8.351800	14.072100
	C	20.193200	-5.971000	7.852900
	C	24.044000	-10.493900	10.310200
	C	27.779400	-8.872500	12.907900
	H	28.650300	-9.013300	12.613300
	C	27.498200	-8.916100	14.252700
	H	28.174800	-9.087600	14.867800
	C	26.210100	-8.705400	14.683800
	H	26.020700	-8.713600	15.594800
	C	24.573300	-11.191800	11.541900
	H	25.411900	-10.799200	11.796300
	H	23.944100	-11.095200	12.259700
	H	24.701000	-12.124500	11.351000
	C	22.715400	-11.130300	9.932700
	H	22.104500	-11.057400	10.669900
	H	22.349600	-10.678600	9.168600
	H	22.853000	-12.056300	9.720300
	C	25.015100	-10.586600	9.156600
	H	25.850100	-10.184000	9.407600
	H	25.158800	-11.509400	8.932800
	H	24.653700	-10.125500	8.395800
	H	20.155900	-6.249300	6.919000
	H	20.399700	-5.021300	7.827700
Energy single point calculations:	-3285.58069348353 u.a.			
M1···M19	N	1.305900	9.039400	5.796300
	O	3.353400	5.073800	6.360700
	N	2.231500	8.429100	6.565500
	N	3.864700	6.697200	7.839600
	H	3.654900	7.480800	8.127300
	C	0.735000	8.159100	4.916800
	C	-0.351400	8.448300	3.957200
	C	1.352000	6.946500	5.120000
	H	1.197100	6.150600	4.664500
	C	2.260000	7.166900	6.155200
	C	3.202500	6.205500	6.785100
	C	-1.664100	8.620700	4.381900
	H	-1.867900	8.566200	5.288300
	C	-0.080400	8.480800	2.601400
	H	0.790000	8.351800	2.300300
	C	4.917100	5.971000	8.519600
	C	1.066300	10.493900	6.062200
	C	-2.669100	8.872500	3.464600
	H	-3.540000	9.013300	3.759100
	C	-2.387900	8.916100	2.119700

	H	-3.064500	9.087600	1.504600
	C	-1.099800	8.705400	1.688700
	H	-0.910400	8.713600	0.777700
	C	0.537000	11.191800	4.830500
	H	-0.301600	10.799200	4.576100
	H	1.166200	11.095200	4.112800
	H	0.409300	12.124500	5.021400
	C	2.394900	11.130300	6.439800
	H	3.005800	11.057400	5.702500
	H	2.760700	10.678600	7.203900
	H	2.257300	12.056300	6.652100
	C	0.095200	10.586600	7.215800
	H	-0.739800	10.184000	6.964800
	H	-0.048500	11.509400	7.439600
	H	0.456600	10.125500	7.976700
	H	4.954400	6.249300	9.453500
	H	4.710600	5.021300	8.544800
	N	9.867000	3.142400	10.576100
	O	7.819600	7.108000	10.011800
	N	8.941400	3.752700	9.806900
	N	7.308200	5.484600	8.532800
	H	7.518000	4.701000	8.245200
	C	10.437900	4.022700	11.455600
	C	11.524300	3.733500	12.415200
	C	9.820900	5.235300	11.252500
	H	9.975800	6.031200	11.707900
	C	8.913000	5.014900	10.217200
	C	7.970400	5.976300	9.587400
	C	12.837000	3.561100	11.990500
	H	13.040800	3.615600	11.084100
	C	11.253300	3.701000	13.771000
	H	10.382900	3.830000	14.072100
	C	6.255800	6.210800	7.852900
	C	10.106600	1.687900	10.310200
	C	13.842000	3.309300	12.907900
	H	14.712900	3.168500	12.613300
	C	13.560800	3.265700	14.252700
	H	14.237400	3.094200	14.867800
	C	12.272700	3.476400	14.683800
	H	12.083300	3.468200	15.594800
	C	10.635900	0.990000	11.541900
	H	11.474500	1.382600	11.796300
	H	10.006700	1.086600	12.259700
	H	10.763600	0.057300	11.351000
	C	8.778000	1.051500	9.932700
	H	8.167100	1.124400	10.669900
	H	8.412200	1.503200	9.168600
	H	8.915600	0.125500	9.720300
	C	11.077700	1.595200	9.156600
	H	11.912700	1.997800	9.407600
	H	11.221400	0.672400	8.932800
	H	10.716300	2.056300	8.395800
	H	6.218500	5.932500	6.919000
	H	6.462300	7.160500	7.827700
	N	-12.631500	21.221200	5.796300
	O	-10.584000	17.255600	6.360700
	N	-11.705900	20.610900	6.565500
	N	-10.072700	18.879000	7.839600
	H	-10.282500	19.662600	8.127300
	C	-13.202400	20.340900	4.916800
	C	-14.288800	20.630100	3.957200

	C	-12.585400	19.128300	5.120000
	H	-12.740300	18.332400	4.664500
	C	-11.677400	19.348700	6.155200
	C	-10.734900	18.387300	6.785100
	C	-15.601500	20.802500	4.381900
	H	-15.805300	20.748000	5.288300
	C	-14.017800	20.662600	2.601400
	H	-13.147400	20.533600	2.300300
	C	-9.020300	18.152800	8.519600
	C	-12.871100	22.675700	6.062200
	C	-16.606500	21.054300	3.464600
	H	-17.477400	21.195100	3.759100
	C	-16.325300	21.097900	2.119700
	H	-17.001900	21.269400	1.504600
	C	-15.037200	20.887200	1.688700
	H	-14.847800	20.895400	0.777700
	C	-13.400400	23.373600	4.830500
	H	-14.239000	22.981000	4.576100
	H	-12.771200	23.277000	4.112800
	H	-13.528100	24.306300	5.021400
	C	-11.542500	23.312100	6.439800
	H	-10.931600	23.239200	5.702500
	H	-11.176700	22.860400	7.203900
	H	-11.680100	24.238100	6.652100
	C	-13.842200	22.768400	7.215800
	H	-14.677200	22.365800	6.964800
	H	-13.985900	23.691200	7.439600
	H	-13.480800	22.307300	7.976700
	H	-8.983000	18.431100	9.453500
	H	-9.226800	17.203100	8.544800
	N	-4.070400	15.324200	10.576100
	O	-6.117800	19.289800	10.011800
	N	-4.996000	15.934500	9.806900
	N	-6.629200	17.666400	8.532800
	H	-6.419400	16.882800	8.245200
	C	-3.499500	16.204500	11.455600
	C	-2.413100	15.915300	12.415200
	C	-4.116500	17.417100	11.252500
	H	-3.961600	18.213000	11.707900
	C	-5.024400	17.196700	10.217200
	C	-5.967000	18.158100	9.587400
	C	-1.100400	15.742900	11.990500
	H	-0.896600	15.797400	11.084100
	C	-2.684100	15.882800	13.771000
	H	-3.554500	16.011800	14.072100
	C	-7.681600	18.392600	7.852900
	C	-3.830800	13.869700	10.310200
	C	-0.095400	15.491100	12.907900
	H	0.775500	15.350300	12.613300
	C	-0.376600	15.447500	14.252700
	H	0.300000	15.276000	14.867800
	C	-1.664700	15.658200	14.683800
	H	-1.854100	15.650000	15.594800
	C	-3.301500	13.171800	11.541900
	H	-2.462900	13.564400	11.796300
	H	-3.930700	13.268400	12.259700
	H	-3.173800	12.239100	11.351000
	C	-5.159400	13.233300	9.932700
	H	-5.770300	13.306200	10.669900
	H	-5.525200	13.685000	9.168600
	H	-5.021800	12.307300	9.720300

	C	-2.859700	13.777000	9.156600
	H	-2.024700	14.179600	9.407600
	H	-2.716000	12.854200	8.932800
	H	-3.221100	14.238100	8.395800
	H	-7.718900	18.114300	6.919000
	H	-7.475100	19.342300	7.827700
Energy single point calculations:	-3285.58069348339 u.a.			

Table S9. Atomic coordinates used in single point calculations with a ωB97x-D/cc-pVDZ for intramolecular energy interactions to compound **10e.**

	Atoms	Coordinates		
Thread	C	11.376200	0.836900	6.530100
	C	12.588300	0.151100	4.515700
	C	12.817300	-0.889400	3.486000
	C	13.909200	-0.934100	2.618400
	H	14.607700	-0.321900	2.557800
	C	13.733500	-2.073200	1.875400
	C	14.708800	-2.616600	0.891100
	C	14.784200	-2.082900	-0.388400
	H	14.161400	-1.448000	-0.659400
	C	15.783300	-2.488800	-1.270100
	H	15.826600	-2.139200	-2.130600
	C	16.709500	-3.423800	-0.838600
	C	16.652400	-3.968000	0.422000
	H	17.280800	-4.599500	0.689300
	C	15.646400	-3.563900	1.294300
	H	15.600200	-3.927400	2.149100
	C	11.893800	-3.908600	1.841200
	C	12.633900	-5.090900	2.455900
	H	13.544900	-5.091100	2.153400
	H	12.208300	-5.908700	2.189000
	H	12.614800	-5.017500	3.412400
	C	11.918900	-3.974900	0.320700
	H	12.828500	-3.974100	0.015700
	H	11.459900	-3.213200	-0.039900
	H	11.483600	-4.779700	0.028500
	C	10.448900	-3.899100	2.319400
	H	10.429400	-3.855400	3.278500
	H	10.009000	-4.701700	2.026600
	H	9.996100	-3.135600	1.955400
	N	11.677500	-0.106400	5.463600
	H	11.256200	-0.855500	5.441800
	N	12.561800	-2.640600	2.301500
	N	11.998300	-1.925000	3.296900
	O	13.236900	1.200200	4.489900
	Cl	18.004400	-3.900400	-1.901200
	H	11.408800	1.789300	6.176700
	H	10.458500	0.707100	6.847500
	C	12.329400	0.689500	7.711900
	C	11.117400	1.375300	9.726200
	C	10.888400	2.415800	10.755900
	C	9.796500	2.460500	11.623500
	H	9.098000	1.848300	11.684100
	C	9.972200	3.599600	12.366500
	C	8.996800	4.143100	13.350800
	C	8.921500	3.609300	14.630300
	H	9.544300	2.974400	14.901300
	C	7.922400	4.015200	15.512000

	H	7.879100	3.665600	16.372500
	C	6.996200	4.950300	15.080500
	C	7.053300	5.494500	13.819900
	H	6.424900	6.125900	13.552600
	C	8.059300	5.090300	12.947600
	H	8.105500	5.453800	12.092800
	C	11.811900	5.435000	12.400700
	C	11.071800	6.617300	11.786000
	H	10.160800	6.617500	12.088500
	H	11.497400	7.435200	12.052900
	H	11.090900	6.543900	10.829500
	C	11.786800	5.501300	13.921200
	H	10.877200	5.500500	14.226200
	H	12.245800	4.739700	14.281800
	H	12.222100	6.306100	14.213400
	C	13.256800	5.425500	11.922500
	H	13.276200	5.381800	10.963400
	H	13.696700	6.228100	12.215300
	H	13.709600	4.662000	12.286500
	N	12.028200	1.632900	8.778300
	H	12.449500	2.381900	8.800100
	N	11.143900	4.167000	11.940400
	N	11.707400	3.451400	10.945000
	O	10.468800	0.326200	9.752000
	Cl	5.701300	5.426800	16.143100
	H	12.296900	-0.262900	8.065200
	H	13.247200	0.819300	7.394400
Energy single point calculations	-1755.2178279 u.a.			
	Atoms	Coordinates		
Macrocycle	C	8.535300	4.458800	8.828100
	C	9.885200	5.435000	7.025000
	H	9.904200	6.187200	7.636500
	H	9.473800	5.735200	6.199500
	C	11.304100	4.996300	6.738300
	C	11.709500	4.710200	5.439000
	H	11.100300	4.780700	4.739700
	C	13.012700	4.320200	5.177800
	H	13.267400	4.127900	4.303900
	C	13.944500	4.212700	6.202100
	C	13.537100	4.500500	7.506500
	H	14.144800	4.431100	8.206200
	C	12.232800	4.889000	7.764400
	H	11.975600	5.080100	8.637700
	C	15.382100	3.837400	5.925800
	H	15.713100	4.366000	5.182600
	H	15.921600	4.048000	6.703700
	C	16.754600	1.900100	5.451200
	C	16.868000	0.461700	5.070700
	C	17.991100	0.091100	4.330700
	H	18.634000	0.728100	4.117300
	C	18.154400	-1.218800	3.911300
	H	18.898400	-1.456600	3.405200
	C	17.213200	-2.172100	4.244500
	H	17.313600	-3.046500	3.942200
	C	16.113600	-1.834000	5.029200
	C	15.937500	-0.509000	5.435000
	H	15.198300	-0.274300	5.948800
	N	9.072900	4.370500	7.603000
	H	8.933700	3.659500	7.140900
	N	15.530900	2.418300	5.607900

	H	14.835800	1.918900	5.521600
	O	8.745500	5.411800	9.589900
	O	17.782100	2.581500	5.596800
	C	15.170400	-2.932400	5.413800
	C	13.820500	-3.908600	7.216900
	H	13.801500	-4.660800	6.605400
	H	14.231900	-4.208700	8.042400
	C	12.401600	-3.469900	7.503600
	C	11.996200	-3.183700	8.802900
	H	12.605400	-3.254200	9.502200
	C	10.693000	-2.793800	9.064100
	H	10.438300	-2.601400	9.938000
	C	9.761200	-2.686200	8.039800
	C	10.168600	-2.974000	6.735400
	H	9.560900	-2.904700	6.035700
	C	11.472900	-3.362500	6.477500
	H	11.730100	-3.553700	5.604200
	C	8.323500	-2.311000	8.316100
	H	7.992600	-2.839600	9.059300
	H	7.784100	-2.521600	7.538200
	C	6.951100	-0.373700	8.790700
	C	6.837700	1.064800	9.171200
	C	5.714600	1.435300	9.911200
	H	5.071700	0.798300	10.124600
	C	5.551200	2.745200	10.330700
	H	4.807300	2.983000	10.836700
	C	6.492500	3.698500	9.997400
	H	6.392100	4.572900	10.299700
	C	7.592100	3.360500	9.212700
	C	7.768200	2.035400	8.806900
	H	8.507400	1.800700	8.293100
	N	14.632800	-2.844100	6.638900
	H	14.772000	-2.133100	7.101000
	N	8.174800	-0.891800	8.634000
	H	8.869900	-0.392500	8.720300
	O	5.923500	-1.055100	8.645100
	O	14.960200	-3.885300	4.652000
Energy single point calculations	-2562.06029668 u.a.			
	Atoms	Coordinates		
[2]Rotaxane	C	8.535300	4.458800	8.828100
	C	9.885200	5.435000	7.025000
	H	9.904200	6.187200	7.636500
	H	9.473800	5.735200	6.199500
	C	11.304100	4.996300	6.738300
	C	11.709500	4.710200	5.439000
	H	11.100300	4.780700	4.739700
	C	13.012700	4.320200	5.177800
	H	13.267400	4.127900	4.303900
	C	13.944500	4.212700	6.202100
	C	13.537100	4.500500	7.506500
	H	14.144800	4.431100	8.206200
	C	12.232800	4.889000	7.764400
	H	11.975600	5.080100	8.637700
	C	15.382100	3.837400	5.925800
	H	15.713100	4.366000	5.182600
	H	15.921600	4.048000	6.703700
	C	16.754600	1.900100	5.451200
	C	16.868000	0.461700	5.070700
	C	17.991100	0.091100	4.330700
	H	18.634000	0.728100	4.117300

	C	18.154400	-1.218800	3.911300
	H	18.898400	-1.456600	3.405200
	C	17.213200	-2.172100	4.244500
	H	17.313600	-3.046500	3.942200
	C	16.113600	-1.834000	5.029200
	C	15.937500	-0.509000	5.435000
	H	15.198300	-0.274300	5.948800
	N	9.072900	4.370500	7.603000
	H	8.933700	3.659500	7.140900
	N	15.530900	2.418300	5.607900
	H	14.835800	1.918900	5.521600
	O	8.745500	5.411800	9.589900
	O	17.782100	2.581500	5.596800
	C	15.170400	-2.932400	5.413800
	C	13.820500	-3.908600	7.216900
	H	13.801500	-4.660800	6.605400
	H	14.231900	-4.208700	8.042400
	C	12.401600	-3.469900	7.503600
	C	11.996200	-3.183700	8.802900
	H	12.605400	-3.254200	9.502200
	C	10.693000	-2.793800	9.064100
	H	10.438300	-2.601400	9.938000
	C	9.761200	-2.686200	8.039800
	C	10.168600	-2.974000	6.735400
	H	9.560900	-2.904700	6.035700
	C	11.472900	-3.362500	6.477500
	H	11.730100	-3.553700	5.604200
	C	8.323500	-2.311000	8.316100
	H	7.992600	-2.839600	9.059300
	H	7.784100	-2.521600	7.538200
	C	6.951100	-0.373700	8.790700
	C	6.837700	1.064800	9.171200
	C	5.714600	1.435300	9.911200
	H	5.071700	0.798300	10.124600
	C	5.551200	2.745200	10.330700
	H	4.807300	2.983000	10.836700
	C	6.492500	3.698500	9.997400
	H	6.392100	4.572900	10.299700
	C	7.592100	3.360500	9.212700
	C	7.768200	2.035400	8.806900
	H	8.507400	1.800700	8.293100
	N	14.632800	-2.844100	6.638900
	H	14.772000	-2.133100	7.101000
	N	8.174800	-0.891800	8.634000
	H	8.869900	-0.392500	8.720300
	O	5.923500	-1.055100	8.645100
	O	14.960200	-3.885300	4.652000
	C	11.376200	0.836900	6.530100
	C	12.588300	0.151100	4.515700
	C	12.817300	-0.889400	3.486000
	C	13.909200	-0.934100	2.618400
	H	14.607700	-0.321900	2.557800
	C	13.733500	-2.073200	1.875400
	C	14.708800	-2.616600	0.891100
	C	14.784200	-2.082900	-0.388400
	H	14.161400	-1.448000	-0.659400
	C	15.783300	-2.488800	-1.270100
	H	15.826600	-2.139200	-2.130600
	C	16.709500	-3.423800	-0.838600
	C	16.652400	-3.968000	0.422000
	H	17.280800	-4.599500	0.689300

	C	15.646400	-3.563900	1.294300
	H	15.600200	-3.927400	2.149100
	C	11.893800	-3.908600	1.841200
	C	12.633900	-5.090900	2.455900
	H	13.544900	-5.091100	2.153400
	H	12.208300	-5.908700	2.189000
	H	12.614800	-5.017500	3.412400
	C	11.918900	-3.974900	0.320700
	H	12.828500	-3.974100	0.015700
	H	11.459900	-3.213200	-0.039900
	H	11.483600	-4.779700	0.028500
	C	10.448900	-3.899100	2.319400
	H	10.429400	-3.855400	3.278500
	H	10.009000	-4.701700	2.026600
	H	9.996100	-3.135600	1.955400
	N	11.677500	-0.106400	5.463600
	H	11.256200	-0.855500	5.441800
	N	12.561800	-2.640600	2.301500
	N	11.998300	-1.925000	3.296900
	O	13.236900	1.200200	4.489900
	Cl	18.004400	-3.900400	-1.901200
	H	11.408800	1.789300	6.176700
	H	10.458500	0.707100	6.847500
	C	12.329400	0.689500	7.711900
	C	11.117400	1.375300	9.726200
	C	10.888400	2.415800	10.755900
	C	9.796500	2.460500	11.623500
	H	9.098000	1.848300	11.684100
	C	9.972200	3.599600	12.366500
	C	8.996800	4.143100	13.350800
	C	8.921500	3.609300	14.630300
	H	9.544300	2.974400	14.901300
	C	7.922400	4.015200	15.512000
	H	7.879100	3.665600	16.372500
	C	6.996200	4.950300	15.080500
	C	7.053300	5.494500	13.819900
	H	6.424900	6.125900	13.552600
	C	8.059300	5.090300	12.947600
	H	8.105500	5.453800	12.092800
	C	11.811900	5.435000	12.400700
	C	11.071800	6.617300	11.786000
	H	10.160800	6.617500	12.088500
	H	11.497400	7.435200	12.052900
	H	11.090900	6.543900	10.829500
	C	11.786800	5.501300	13.921200
	H	10.877200	5.500500	14.226200
	H	12.245800	4.739700	14.281800
	H	12.222100	6.306100	14.213400
	C	13.256800	5.425500	11.922500
	H	13.276200	5.381800	10.963400
	H	13.696700	6.228100	12.215300
	H	13.709600	4.662000	12.286500
	N	12.028200	1.632900	8.778300
	H	12.449500	2.381900	8.800100
	N	11.143900	4.167000	11.940400
	N	11.707400	3.451400	10.945000
	O	10.468800	0.326200	9.752000
	Cl	5.701300	5.426800	16.143100
	H	12.296900	-0.262900	8.065200
	H	13.247200	0.819300	7.394400
Energy single point calculations	-4317.34774739 u.a.			