

Design, synthesis and binding studies of a novel quadruple ADDA hydrogen-bond array

Supporting Information

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Additional NMR studies

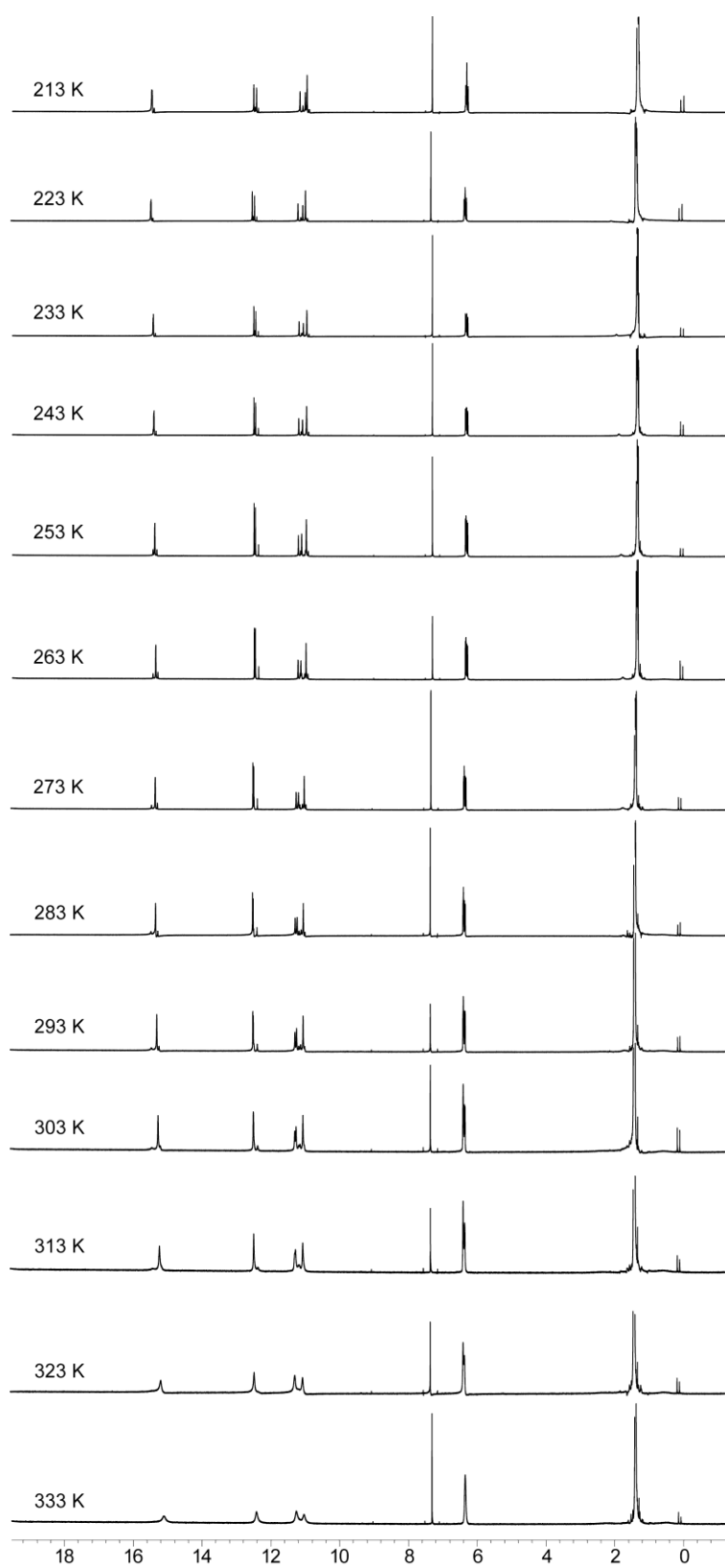


Figure ESI 1 VT NMR study on UDIM 2; ¹H NMR spectra (40 mM, 300 MHz, CDCl₃), the temperature at which each spectrum is obtained is illustrated in the lower left hand corner

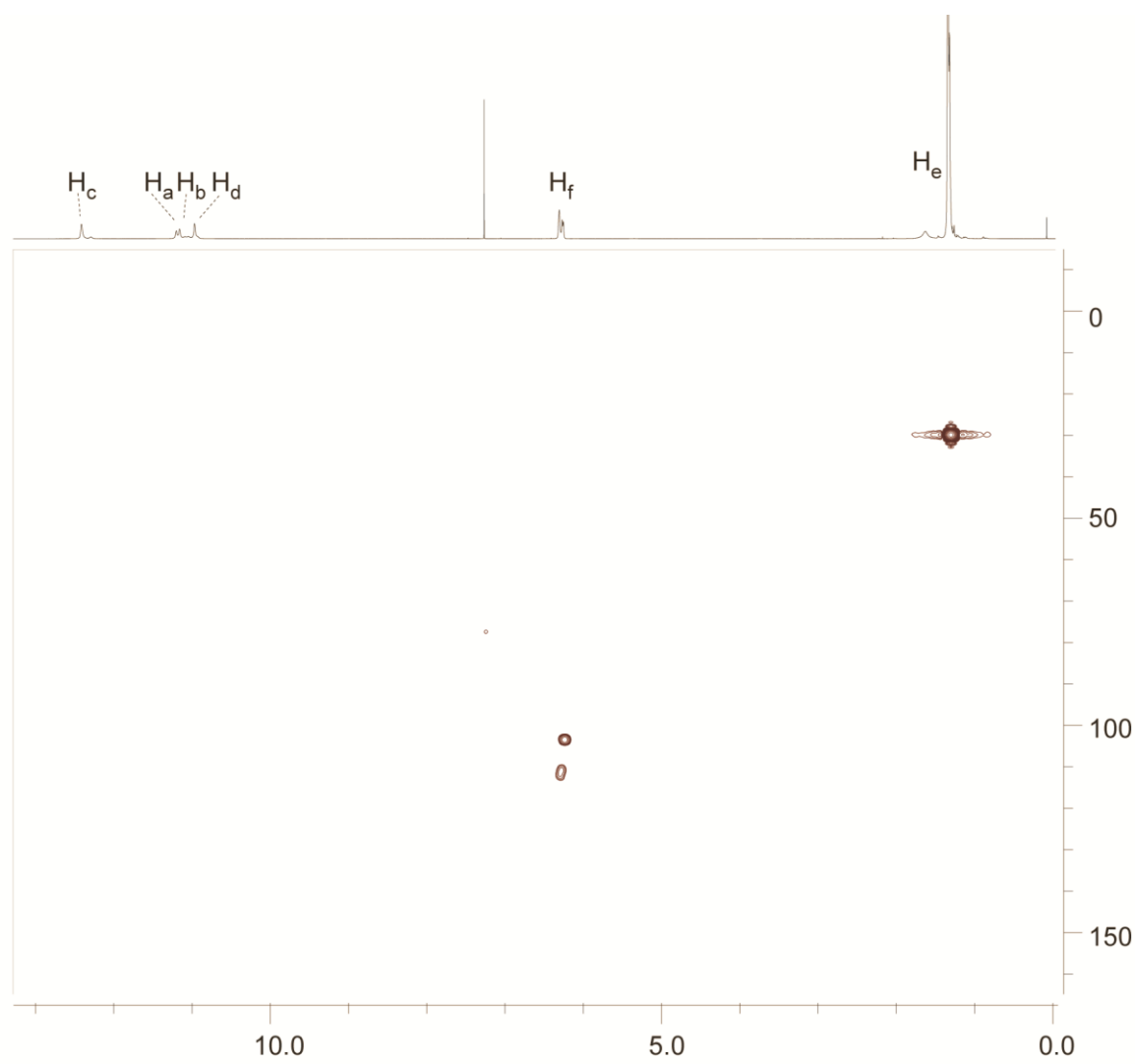


Figure ESI 2 ^1H - ^{13}C HMQC spectrum of UDIM 2 (CDCl_3 , 500 MHz)

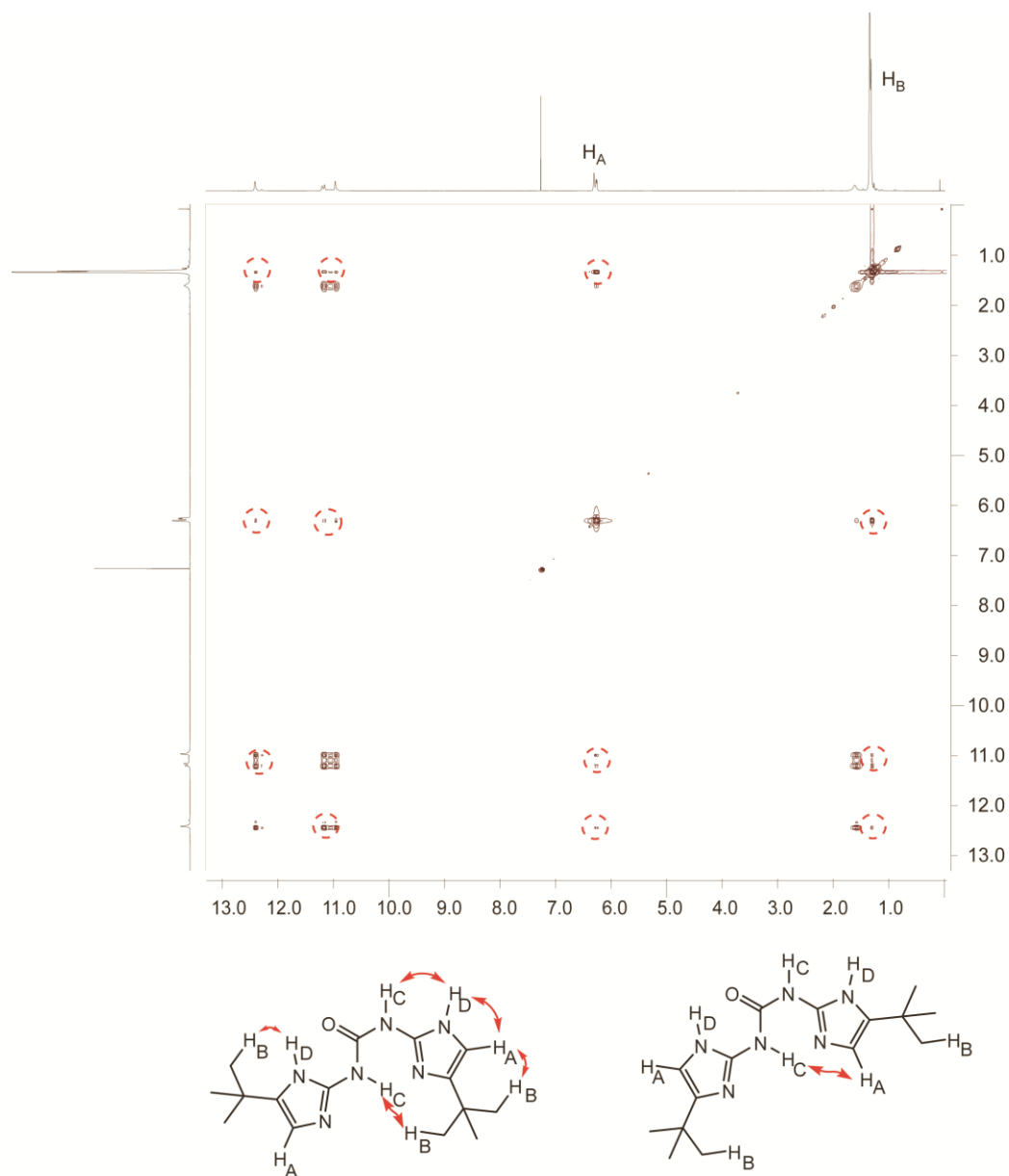


Figure ESI 3 Phase sensitive ^1H - ^1H NOESY spectrum of UDIM 2 (10 mM, CDCl_3 , 500 MHz).

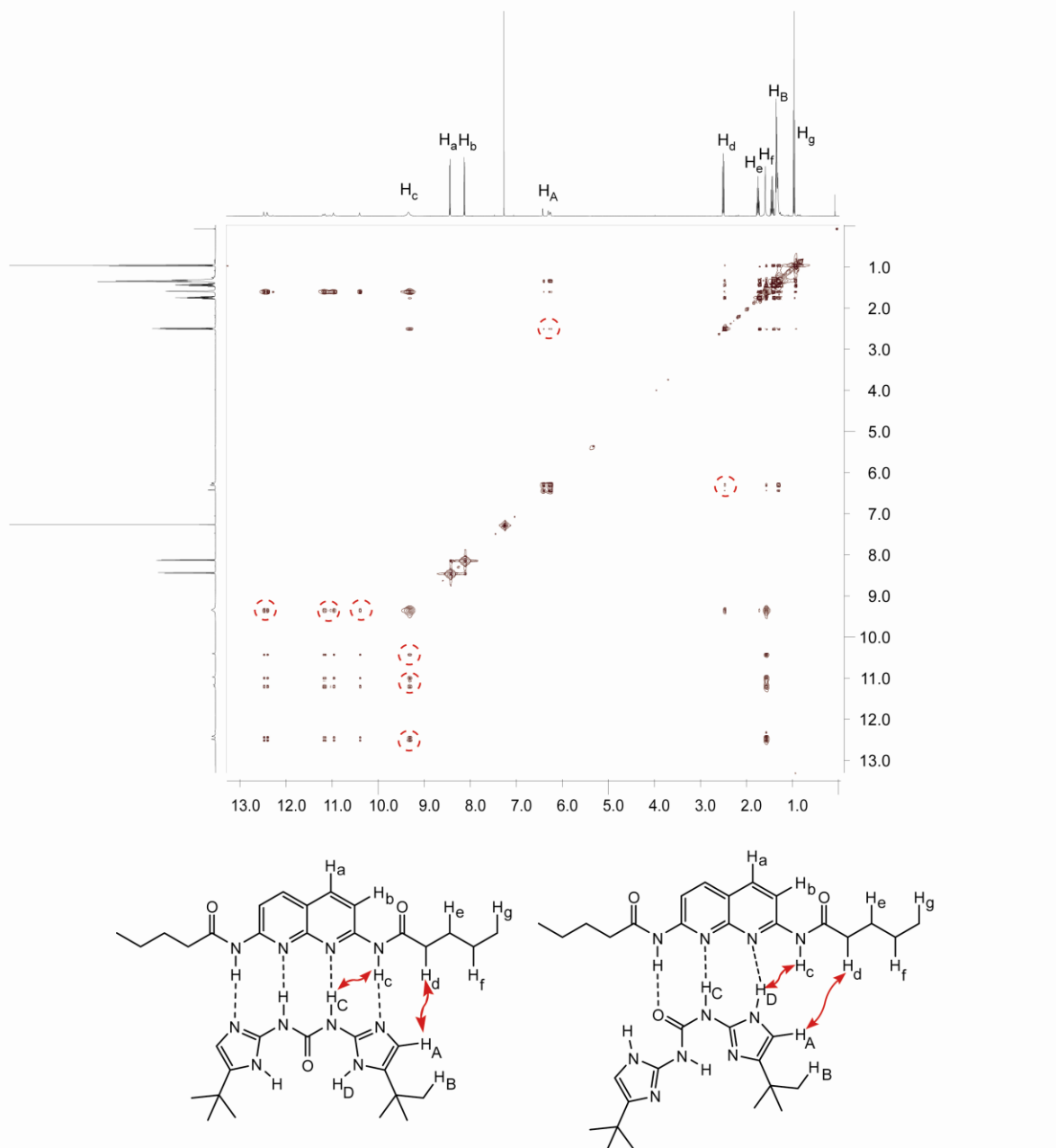


Figure ESI 3 Phase sensitive ^1H - ^1H NOESY spectrum of 1:1 mix of components UDIM 2 and DAN 3 at 10 mM concentration (with respect to each component) in CDCl_3 , 500 MHz. (note: the spectrum has been symmetrised for presentation purposes)

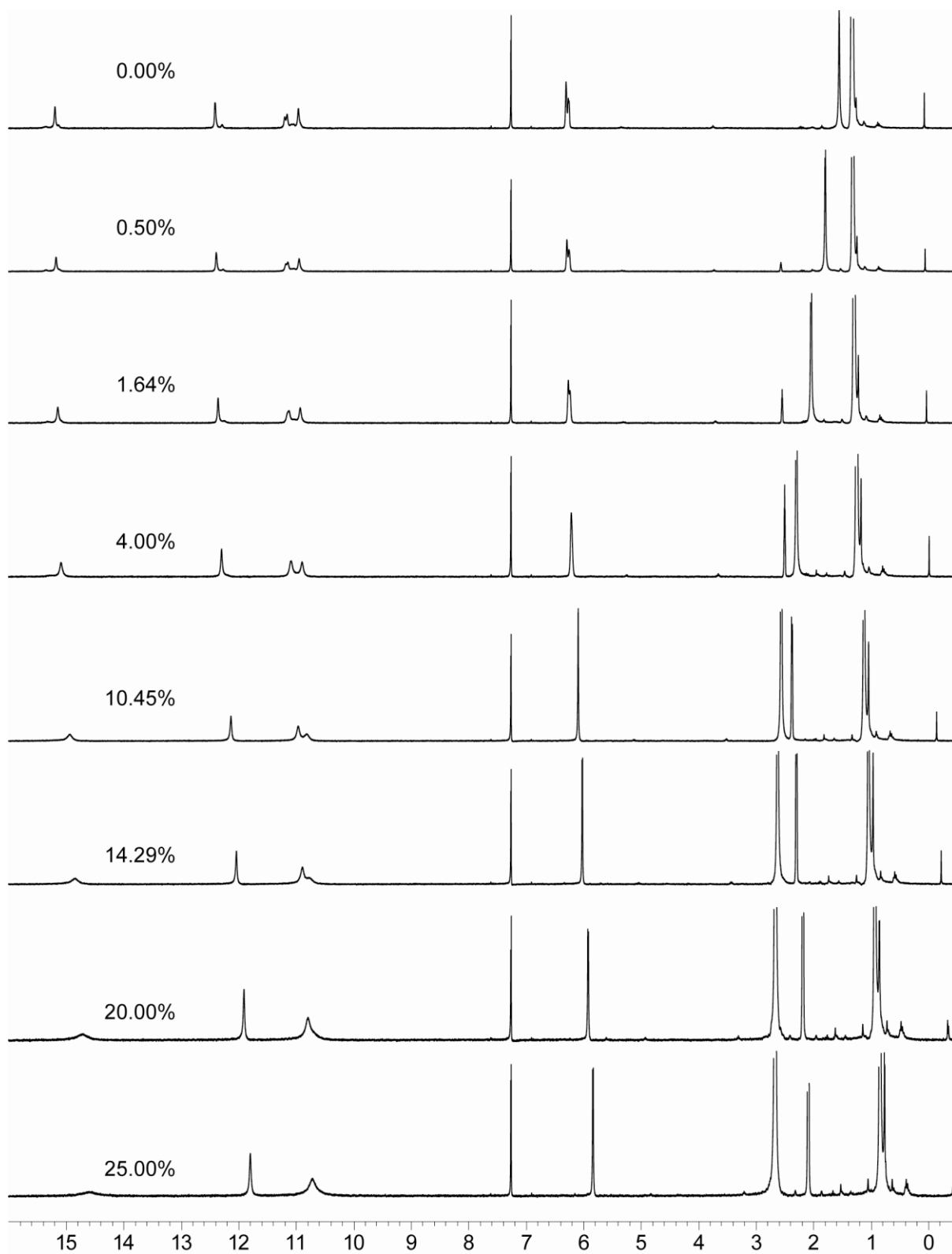


Figure ESI 4 NMR solvent study on UDIM 2; ^1H NMR spectra (10 mM, 300 MHz, CDCl_3), the % of DMSO present in each spectrum is illustrated in the lower left hand corner.

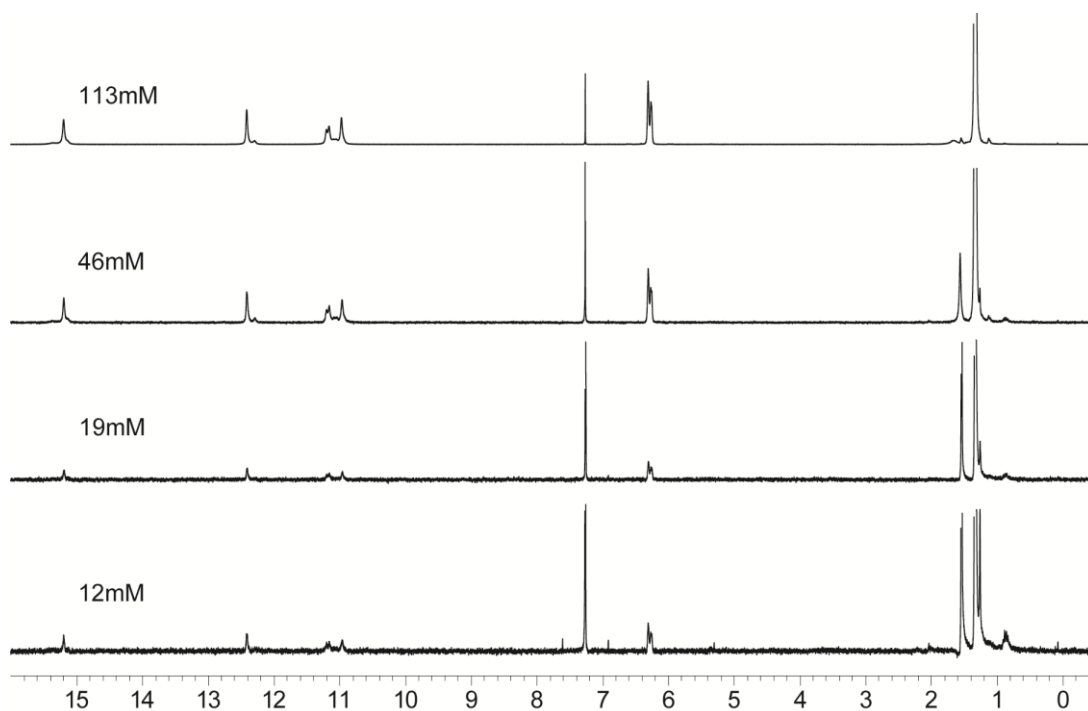


Figure ESI 5 NMR dilution study on UDIM **2**; ^1H NMR spectra (300 MHz, CDCl_3), the concentration of **2** in each spectrum is illustrated in the lower left hand corner

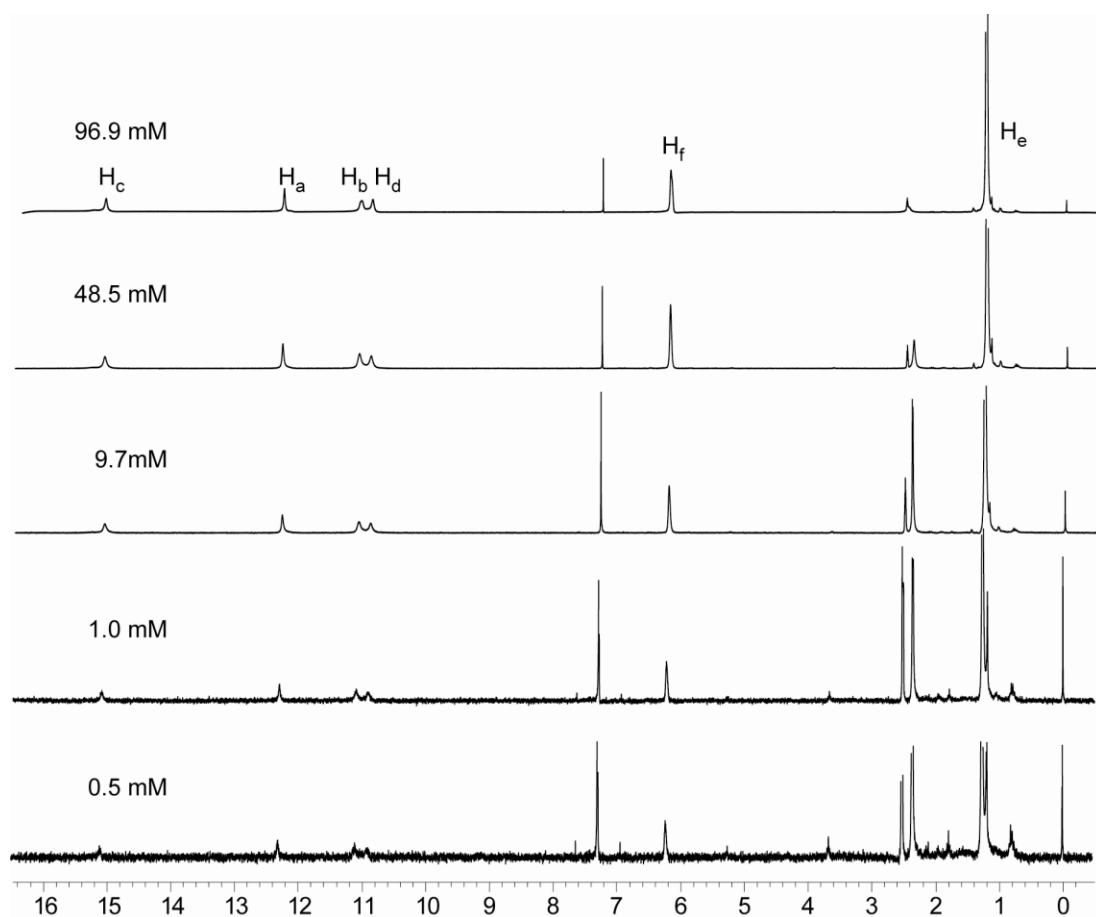


Figure ESI 6 NMR dilution study on UDIM **2**; ^1H NMR spectra (300 MHz, 5% DMSO-d_6 in CDCl_3), the concentration of **2** in each spectrum is illustrated in the lower left hand corner

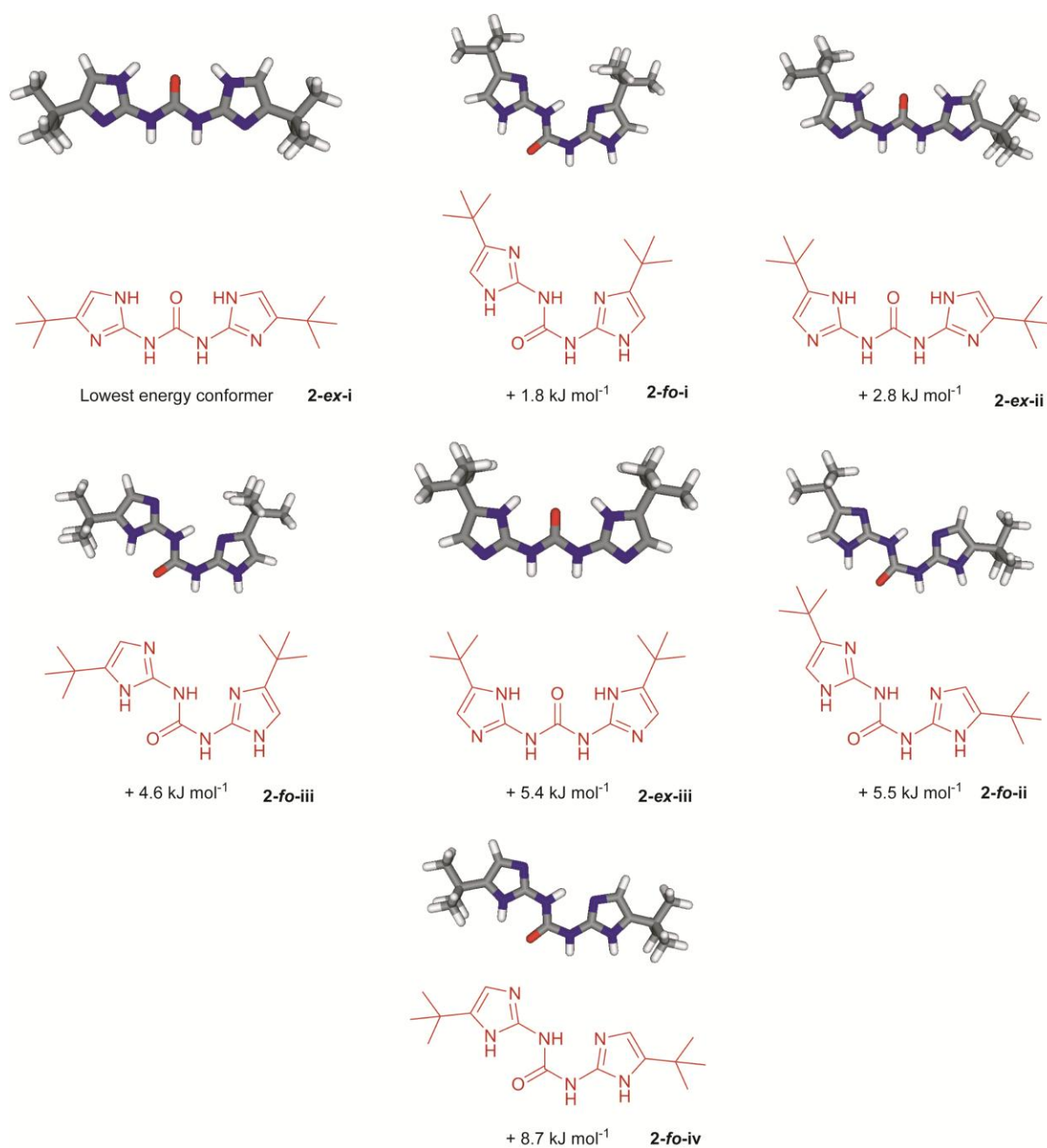
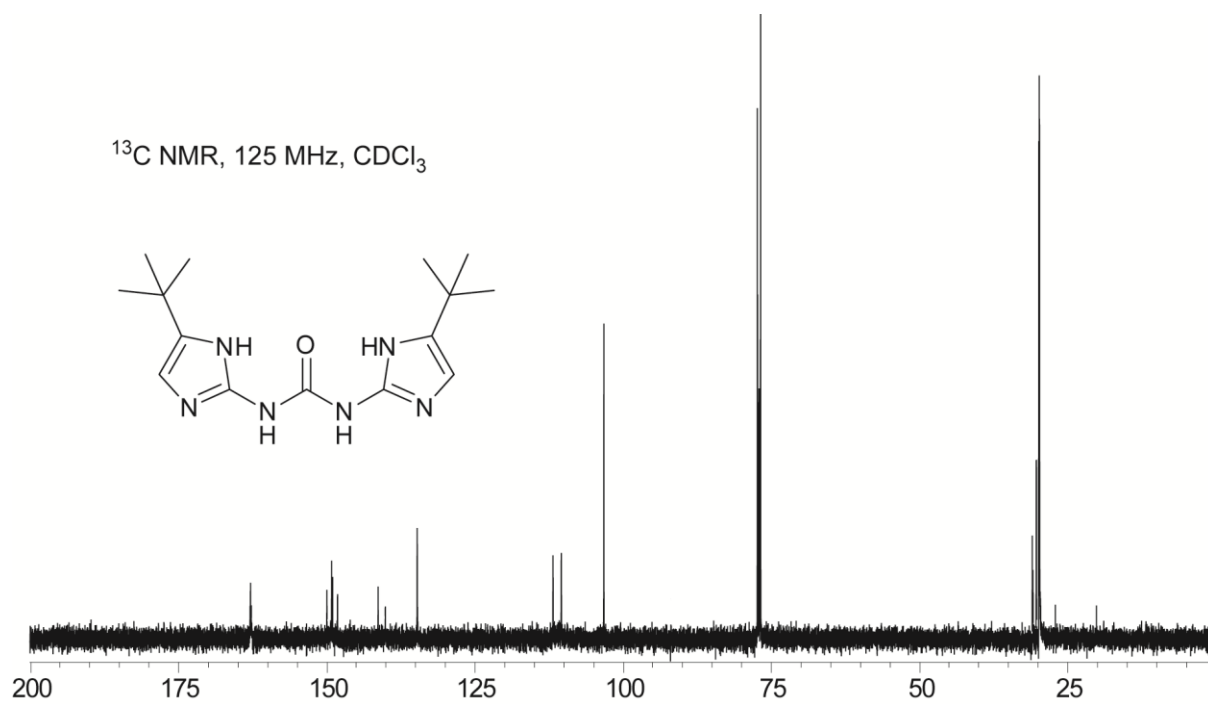
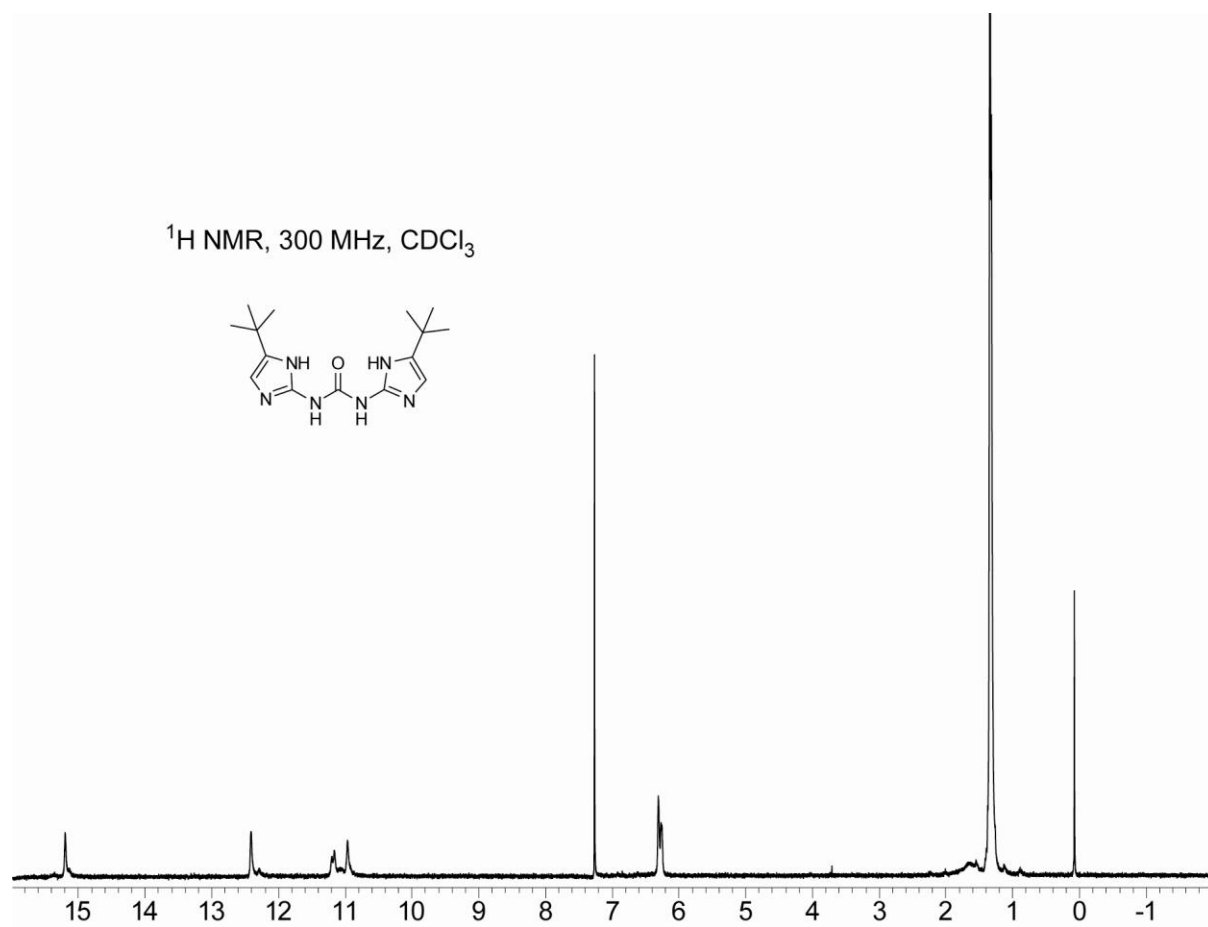
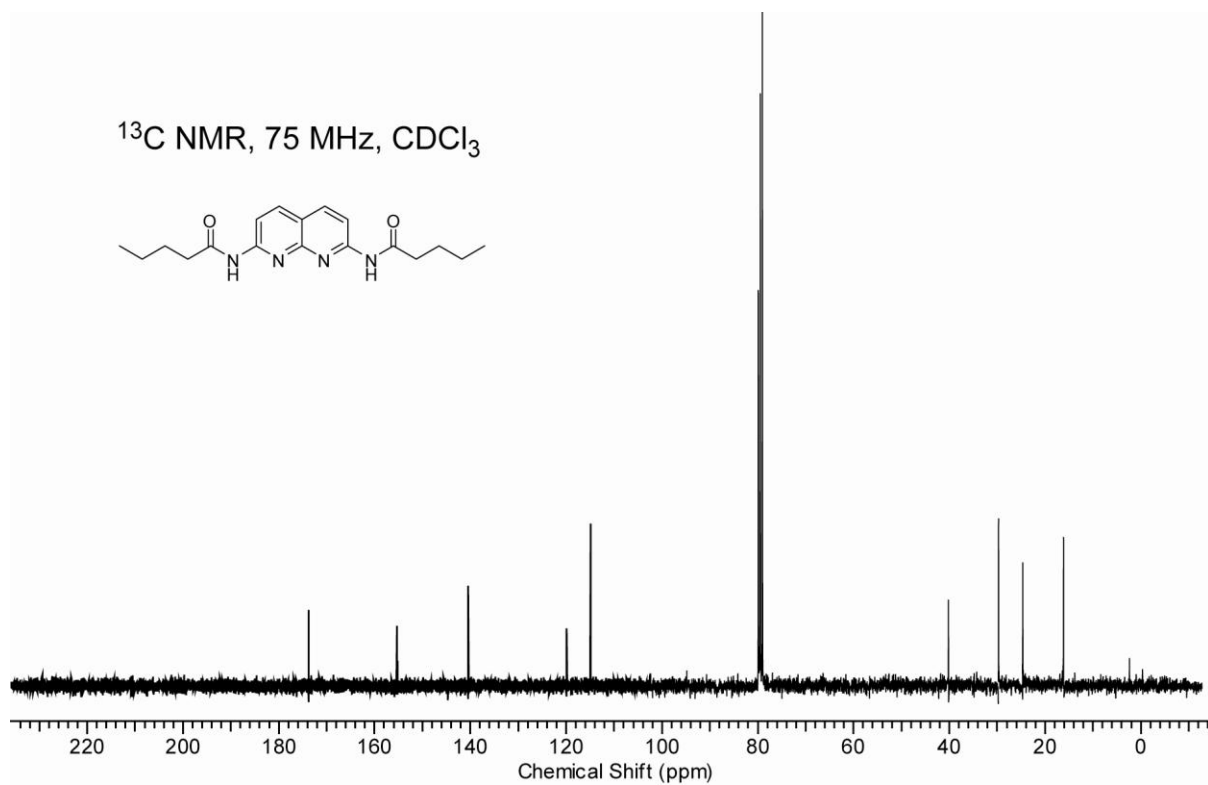
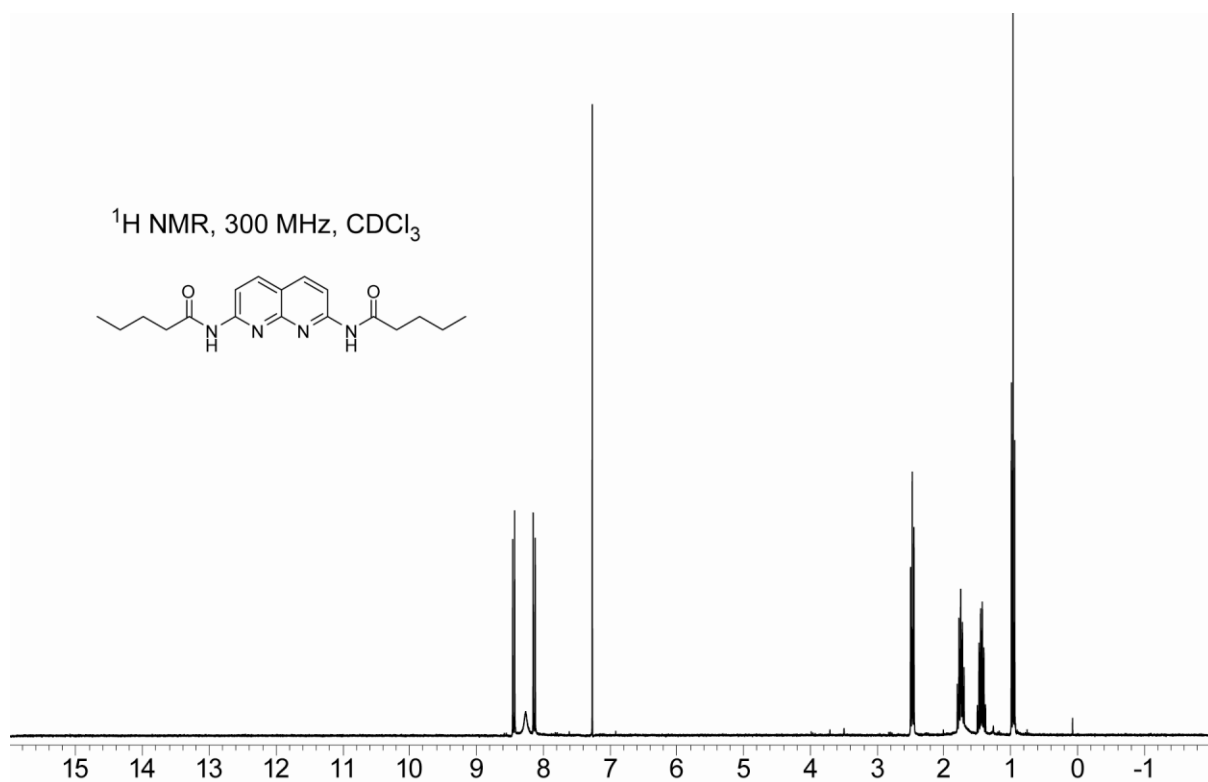
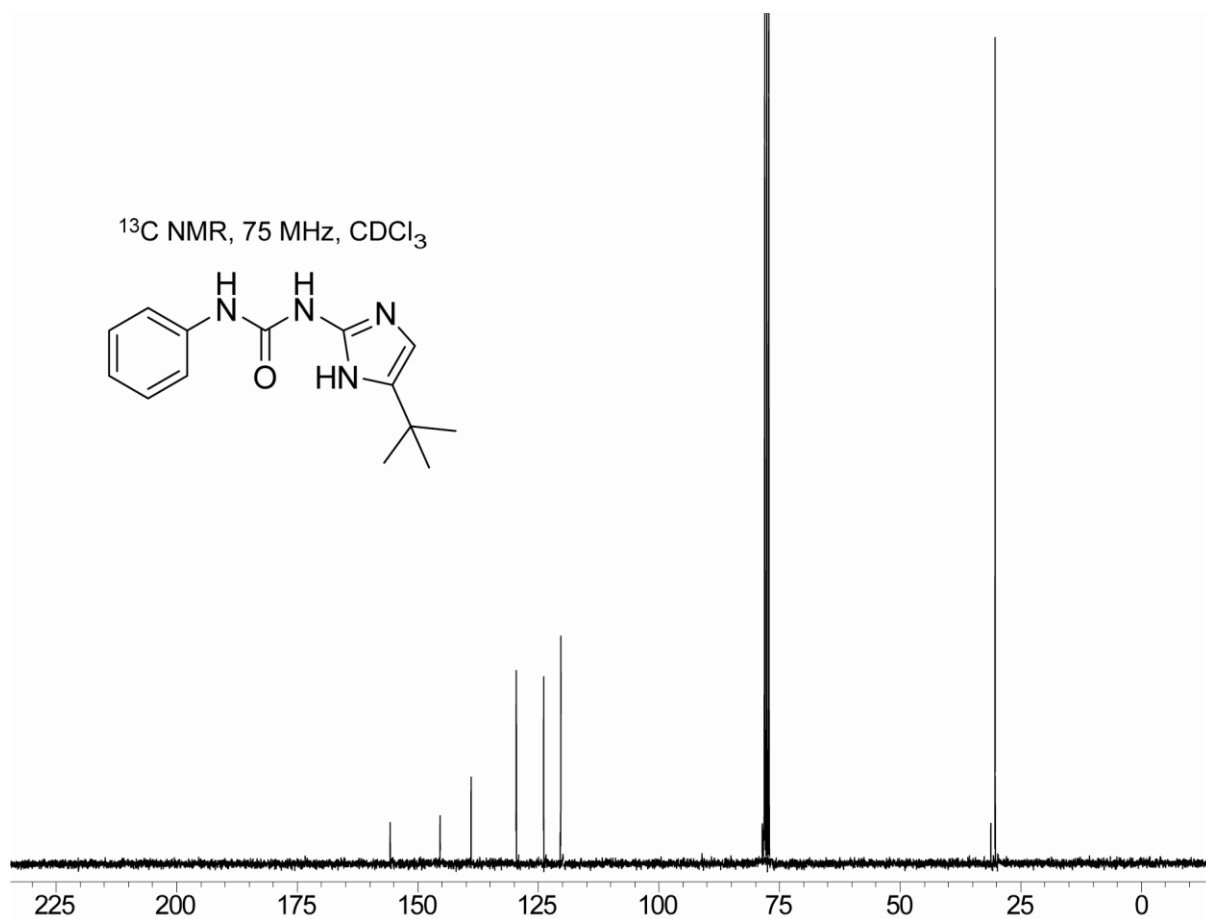
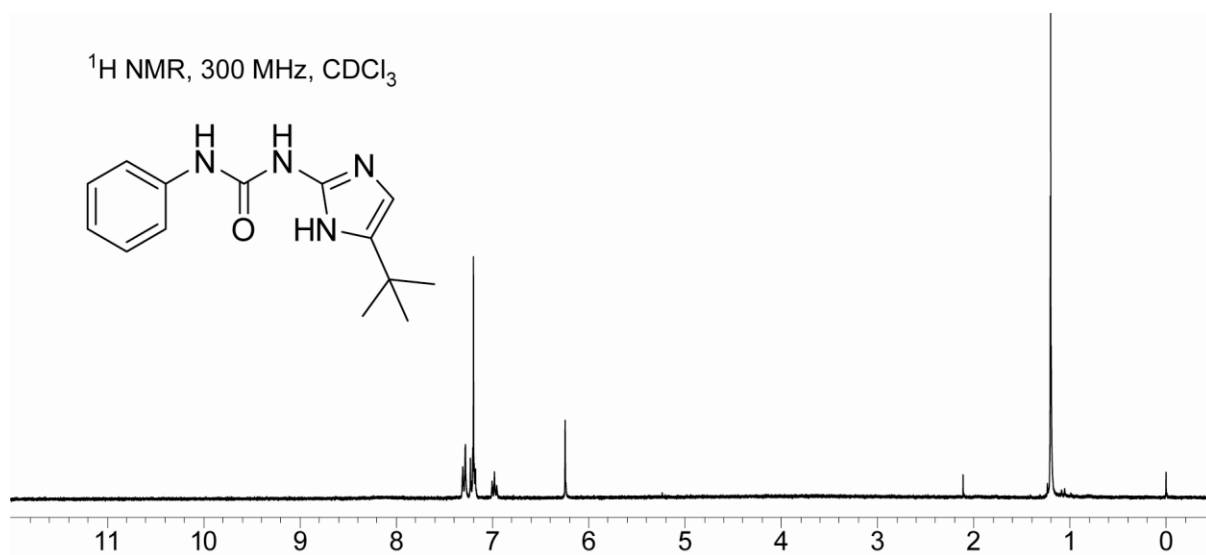


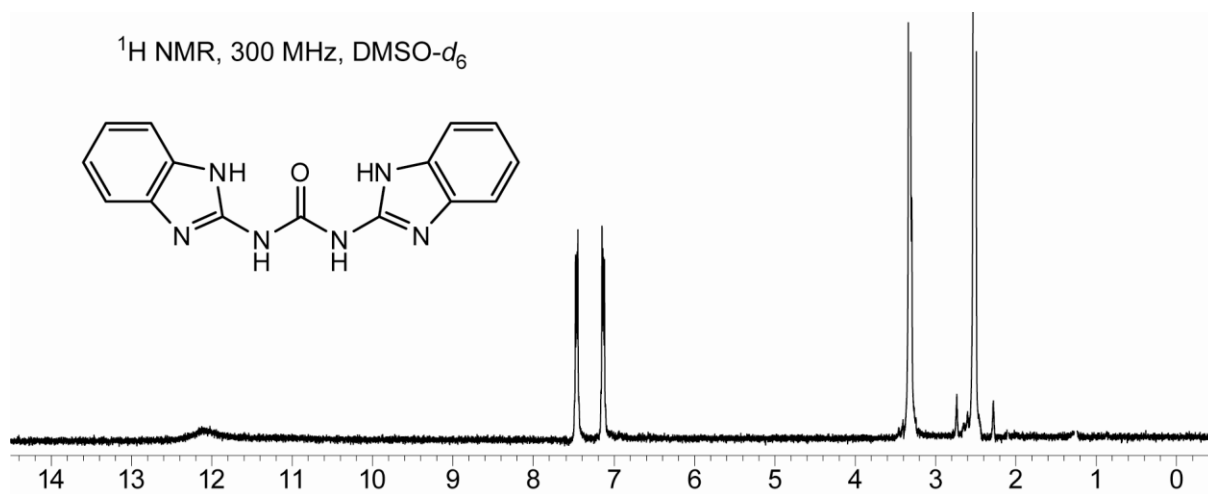
Figure ESI 7 Optimized geometries and calculated energies of monomers and compound 2 used in this work as calculated using DFT (B3LYP, C, 6-31G; N/O, 6-31G*; H, 6-31++G**).

Spectral Data for Each Compound









Details of Calculations from DOSY experiments

The measured diffusion coefficients (D) can be used to calculate the mole fraction (χ) of the complex in solution. K_a can then also be calculated. A K_a of 834 M^{-1} was calculated from the DOSY measurements, which is comparable to the K_a which was measured using ^1H NMR titrations (825 M^{-1}).

Molecule	Diffusion coefficient
DAN	10.61 ± 0.05
UDIM	9.33 ± 0.05
DAN (in complex)	10.06 ± 0.07
UDIM (in complex)	8.67 ± 0.07

$$\chi_{\text{DAN-UDIM}} = \frac{D_{\text{obs}} - D_{\text{UDIM}}}{D_{\text{DAN}} - D_{\text{UDIM}}}$$

$$\chi_{\text{DAN-UDIM}} = \frac{10.06 - 9.33}{10.61 - 9.33}$$

$$\chi_{\text{DAN-UDIM}} = 0.566$$

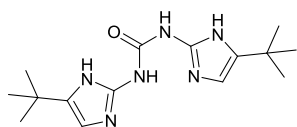
$$K_a = \frac{\chi_{\text{DAN-UDIM}} [\text{DAN}]}{[(1 - \chi_{\text{DAN-UDIM}}) [\text{DAN}]]^2}$$

$$K_a = \frac{0.566 \times 3.6 \times 10^{-3}}{(0.434 \times 3.6 \times 10^{-3})^2}$$

$$K_a = 0.834 \times 10^3 \text{ M}^{-1}$$

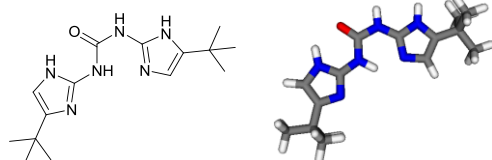
Optimised Geometries obtained from Modelling Studies

UDIM folded 1



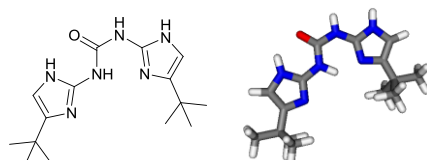
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3	6	-2.839701	4.780039	0.656953
4	1	-1.265741	2.909628	2.709691
5	1	-3.198120	5.643329	0.123423
6	7	-2.829431	1.322563	1.190823
7	1	-3.483360	0.906626	0.518683
8	6	-2.170035	0.502797	2.056648
9	7	-2.455525	-0.866053	1.941992
10	1	-1.940736	-1.423937	2.607322
11	8	-1.354405	0.873796	2.918188
12	6	-3.328730	-1.484489	1.055231
13	6	-4.455023	-3.134887	0.040060
14	1	-3.071876	-3.515261	1.651434
15	6	-4.767207	-1.908014	-0.496754
16	1	-5.450180	-1.686416	-1.297676
17	7	-4.065464	-0.887405	0.136920
18	7	-3.519628	-2.843797	1.046864
19	7	-1.823754	3.385092	2.010188
20	7	-3.297402	3.510626	0.334029
21	6	-1.138289	5.810613	2.414692
22	6	-1.497610	5.807760	3.927443
23	1	-1.265339	4.844065	4.392826
24	1	-0.929924	6.581156	4.456576
25	1	-2.564644	6.002093	4.072029
26	6	-1.484476	7.193745	1.816231
27	1	-0.920815	7.977572	2.331763
28	1	-1.232367	7.236938	0.752230
29	1	-2.550891	7.414130	1.924458
30	6	-4.916219	-4.543170	-0.264550
31	6	-5.941308	-4.504097	-1.422207
32	1	-5.498104	-4.081393	-2.328831
33	1	-6.282789	-5.517716	-1.652189
34	1	-6.816161	-3.903527	-1.155708
35	6	-5.591062	-5.168669	0.988934
36	1	-4.896995	-5.229320	1.834657
37	1	-6.453493	-4.573905	1.303403
38	1	-5.933644	-6.185165	0.769185
39	6	-3.706298	-5.423026	-0.688611
40	1	-3.218142	-5.010549	-1.576300
41	1	-2.956429	-5.491152	0.107443
42	1	-4.038051	-6.440988	-0.917969
43	6	0.386700	5.554584	2.252296
44	1	0.676465	4.583176	2.666594
45	1	0.670820	5.567372	1.195723
46	1	0.961711	6.327001	2.774911

UDIM folded 2



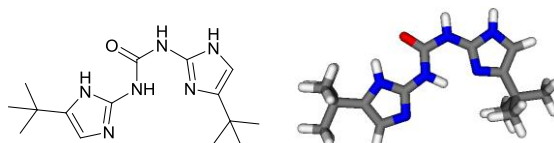
Centre Number	Atomic Number	Coordinates (Angstroms)		
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5	7	-2.941156	1.359412	1.454638
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8	7	-2.514719	-0.858163	2.083715
9	1	-2.002954	-1.439446	2.731151
10	8	-1.513068	0.853698	3.205368
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16	7	-3.473391	-2.810198	1.027768
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20	6	-3.018856	7.365885	1.052265
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22	1	-1.926135	7.385168	0.978047
23	1	-3.406339	8.251839	0.538882
24	6	-5.149709	6.109902	0.526930
25	1	-5.559831	6.969031	-0.016226
26	1	-5.575464	5.193885	0.109893
27	1	-5.462075	6.183759	1.574092
28	6	-3.203347	6.027197	-1.084993
29	1	-2.114099	6.041662	-1.198658
30	1	-3.579836	5.109020	-1.542673
31	1	-3.617378	6.886409	-1.625042
32	1	-1.680001	5.504676	2.764986
33	1	-5.358002	-1.573366	-1.313518
34	6	-4.759469	-4.469786	-0.438582
35	6	-3.504250	-5.280391	-0.869235
36	1	-2.782290	-5.373992	-0.050284
37	1	-3.791340	-6.292198	-1.173623
38	1	-2.998674	-4.796898	-1.710120
39	6	-5.456145	-5.195804	0.747038
40	1	-6.350058	-4.651577	1.065160
41	1	-5.753808	-6.207096	0.451230
42	1	-4.790892	-5.287129	1.612932
43	6	-5.742617	-4.391548	-1.629948
44	1	-6.647298	-3.838481	-1.360158
45	1	-5.281947	-3.897697	-2.490767
46	1	-6.040037	-5.398863	-1.936364

UDIM folded 3



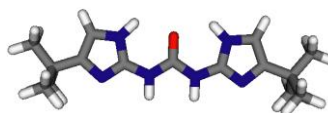
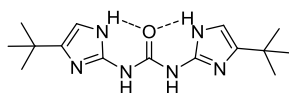
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5	7	-2.906842	1.296013	1.449398
6	1	-3.559200	0.878776	0.776583
7	6	-2.171903	0.466595	2.244272
8	7	-2.387678	-0.907276	2.055912
9	1	-1.819445	-1.474059	2.668304
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11	6	-3.256151	-1.520797	1.161649
12	6	-4.326875	-3.145871	0.083227
13	1	-2.875610	-3.569120	1.617419
14	6	-4.736693	-1.918359	-0.381066
15	7	-4.056458	-0.909852	0.304744
16	7	-3.375194	-2.881598	1.074702
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21	6	-6.352297	-2.871057	-2.050113
22	1	-6.864597	-3.462263	-1.283384
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24	1	-5.578626	-3.496383	-2.508642
25	6	-6.885247	-0.717719	-0.834539
26	1	-7.414574	-1.274201	-0.054061
27	1	-6.479978	0.193569	-0.387677
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31	1	-4.264083	-1.357719	-3.055985
32	1	-5.780137	-0.481655	-3.348462
33	6	-3.753223	5.995457	0.431670
34	6	-3.159372	7.295792	1.018594
35	1	-3.360162	7.374678	2.092534
36	1	-2.075366	7.340815	0.867586
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41	1	-5.530018	6.057553	1.718478
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44	1	-3.845893	5.004952	-1.516035
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UDIM folded 4



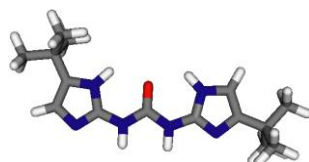
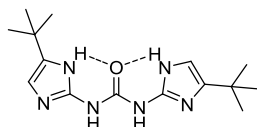
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4	1	0.391849	-1.491418	2.374857
5	7	0.086678	-0.735473	0.024425
6	1	0.044376	-0.609609	-0.976279
7	6	1.243532	-3.391524	2.266896
8	6	1.895926	-4.892028	3.646914
9	6	2.148529	-5.418009	2.394475
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12	6	-0.374821	0.270389	0.864388
13	6	-1.252652	2.214072	1.499114
14	1	-0.998285	1.710793	-0.579720
15	6	-0.929822	1.457198	2.600571
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17	7	-0.892754	1.444119	0.387008
18	7	-0.380855	0.242310	2.186237
19	7	1.717435	-4.427404	1.510937
20	7	1.331073	-3.627137	3.562204
21	6	-1.090588	1.770399	4.074019
22	6	-1.718928	3.170470	4.257904
23	1	-2.710449	3.226052	3.795695
24	1	-1.833255	3.392660	5.323139
25	1	-1.088389	3.951013	3.818570
26	6	-2.008087	0.702067	4.729301
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29	1	-2.110234	0.897402	5.802251
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32	1	0.198894	1.929426	5.834856
33	1	0.772202	0.756536	4.632208
34	6	2.741362	-6.728646	1.926512
35	6	1.709709	-7.499237	1.055179
36	1	1.425241	-6.921735	0.169369
37	1	2.132192	-8.450865	0.714446
38	1	0.800404	-7.708953	1.626429
39	6	3.112070	-7.592579	3.154386
40	1	3.542467	-8.544481	2.827800
41	1	3.848208	-7.085655	3.785916
42	1	2.230101	-7.810042	3.764751
43	6	4.021932	-6.464156	1.085373
44	1	4.771294	-5.931052	1.678165
45	1	4.457841	-7.409863	0.745075
46	1	3.799941	-5.858954	0.200189

UDIM
 unfolded 3



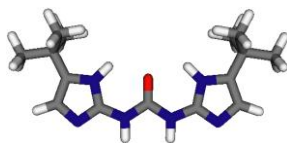
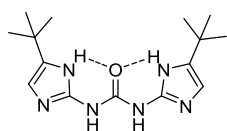
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6	1	-1.137516	-1.585159	-0.002194
7	6	0.000000	0.170174	-0.001377
8	7	1.158475	-0.574752	-0.002246
9	1	1.137517	-1.585159	-0.002166
10	8	0.000000	1.416939	-0.000353
11	6	2.449334	-0.035783	-0.001059
12	6	4.113373	1.411738	0.000543
13	1	2.007927	2.010271	0.000064
14	6	4.598811	0.119201	0.000263
15	7	3.536974	-0.782914	-0.000688
16	7	2.725417	1.297015	-0.000493
17	7	-2.725417	1.297015	-0.000752
18	7	-3.536974	-0.782914	-0.000808
19	6	6.033016	-0.371718	0.000864
20	6	6.277156	-1.239868	1.265179
21	1	5.570950	-2.073356	1.298612
22	1	7.295941	-1.643346	1.261516
23	1	6.145988	-0.646190	2.176053
24	6	7.012238	0.823531	0.002011
25	1	6.875216	1.450027	-0.885855
26	1	6.874181	1.449178	0.890314
27	1	8.045860	0.463633	0.002440
28	6	6.278620	-1.238569	-1.264122
29	1	5.572451	-2.072016	-1.299200
30	1	6.148473	-0.643902	-2.174490
31	1	7.297409	-1.642025	-1.259704
32	1	4.603440	2.367966	0.001200
33	1	-4.603440	2.367966	0.000874
34	6	-6.033016	-0.371718	0.000929
35	6	-7.012238	0.823531	0.002076
36	1	-6.875267	1.449985	-0.885827
37	1	-8.045860	0.463633	0.002584
38	1	-6.874129	1.449220	0.890342
39	6	-6.277067	-1.239797	1.265310
40	1	-5.570858	-2.073282	1.298741
41	1	-6.145836	-0.646068	2.176141
42	1	-7.295852	-1.643276	1.261741
43	6	-6.278708	-1.238639	-1.263990
44	1	-5.572543	-2.072090	-1.299070
45	1	-7.297498	-1.642094	-1.259478
46	1	-6.148625	-0.644024	-2.174402

UDIM
 unfolded 2



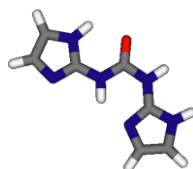
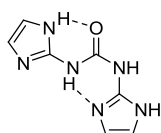
Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-4.447891	-0.281149	0.000246
2	6	-2.499724	-1.346970	-0.000269
3	6	-4.616997	-1.651746	0.000471
4	1	-2.508984	0.744713	-0.000662
5	1	-5.539414	-2.205723	0.000787
6	7	-1.121350	-1.588279	-0.000686
7	1	-0.880362	-2.569909	-0.001156
8	6	-0.154632	-0.609152	-0.001139
9	7	1.138844	-1.083177	-0.001406
10	1	1.337771	-2.074029	0.000132
11	8	-0.426218	0.608629	-0.001270
12	6	2.281541	-0.276871	-0.001155
13	6	3.591537	1.497657	-0.001668
14	1	1.406422	1.624552	-0.002702
15	6	4.346117	0.341487	-0.000144
16	7	3.505681	-0.769805	0.000183
17	7	2.261630	1.084082	-0.002517
18	7	-3.061622	-0.103197	-0.000174
19	7	-3.395672	-2.312892	0.000161
20	6	-5.420250	0.877580	0.000626
21	6	-5.206505	1.752723	1.267863
22	1	-4.193548	2.167759	1.302499
23	1	-5.911549	2.590936	1.276381
24	1	-5.359953	1.163156	2.176663
25	6	-6.867070	0.331408	0.001206
26	1	-7.580751	1.160886	0.001458
27	1	-7.058181	-0.280854	-0.885414
28	1	-7.057480	-0.280813	0.888003
29	6	-5.207530	1.752740	-1.266772
30	1	-4.194585	2.167741	-1.302250
31	1	-5.361754	1.163194	-2.175455
32	1	-5.912546	2.590981	-1.274698
33	6	5.852739	0.173616	0.001023
34	6	6.278838	-0.620119	1.265809
35	1	5.772234	-1.588015	1.296550
36	1	7.361295	-0.790121	1.264726
37	1	6.018111	-0.070409	2.176359
38	6	6.549556	1.553013	0.001536
39	1	6.280804	2.135223	-0.886530
40	1	6.279681	2.135107	0.889338
41	1	7.636728	1.425758	0.002203
42	6	6.280736	-0.620119	-1.263209
43	1	5.773937	-1.587879	-1.294808
44	1	6.021590	-0.070190	-2.174067
45	1	7.363147	-0.790385	-1.260378
46	1	3.861775	2.537585	-0.002284

UDIM
 unfolded 1



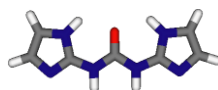
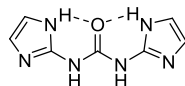
Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-4.119151	-0.038053	0.000028
2	6	-2.450389	-1.503216	0.000267
3	6	-4.583285	-1.338748	0.000037
4	1	-2.002983	0.540008	0.000171
5	1	-5.604358	-1.678141	-0.000138
6	7	-1.157778	-2.038943	0.000449
7	1	-1.136271	-3.049481	0.001009
8	6	-0.000031	-1.294714	0.000382
9	7	1.157727	-2.038917	0.000768
10	1	1.136244	-3.049456	-0.000211
11	8	-0.000044	-0.046109	0.000295
12	6	2.450336	-1.503180	-0.000002
13	6	4.119107	-0.038032	-0.000202
14	1	2.002985	0.540071	0.000679
15	6	4.583237	-1.338734	-0.001585
16	1	5.604307	-1.678139	-0.002577
17	7	3.535535	-2.250434	-0.001362
18	7	2.727378	-0.166741	0.001018
19	7	-2.727412	-0.166771	0.000089
20	7	-3.535591	-2.250460	0.000329
21	6	-4.815744	1.304865	-0.000255
22	6	-4.417370	2.113003	1.266891
23	1	-3.337819	2.293590	1.304595
24	1	-4.919752	3.086281	1.271343
25	1	-4.700628	1.573822	2.175766
26	6	-6.346647	1.087304	-0.000639
27	1	-6.862033	2.052635	-0.000907
28	1	-6.666462	0.531464	-0.887357
29	1	-6.666918	0.531653	0.886029
30	6	4.815784	1.304833	0.000126
31	6	6.346691	1.087142	-0.000342
32	1	6.666413	0.531484	-0.887190
33	1	6.862146	2.052433	-0.000293
34	1	6.666938	0.531234	0.886185
35	6	4.417407	2.112404	1.267647
36	1	3.337847	2.292908	1.305363
37	1	4.700620	1.572776	2.176275
38	1	4.919808	3.085664	1.272572
39	6	4.416810	2.113365	-1.266570
40	1	4.699604	1.574472	-2.175748
41	1	3.337236	2.294015	-1.303632
42	1	4.919184	3.086666	-1.271002
43	6	-4.416647	2.112773	-1.267339
44	1	-3.337046	2.293196	-1.304445
45	1	-4.699422	1.573411	-2.176255
46	1	-4.918950	3.086094	-1.272289

UDIM folded –
no tBu



Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.089324	1.208310	-0.000011
2	7	1.311437	1.310374	-0.000029
3	1	1.626006	2.269534	-0.000053
4	7	-0.594223	-0.057069	-0.000035
5	1	0.056576	-0.849414	-0.000104
6	6	2.242957	0.280310	-0.000005
7	6	3.211634	-1.651430	0.000125
8	6	4.227598	-0.731698	-0.000030
9	1	4.051283	1.413455	-0.000184
10	1	3.280758	-2.725422	0.000224
11	1	5.298108	-0.829279	-0.000088
12	6	-1.962850	-0.335856	-0.000022
13	6	-4.153217	-0.038870	0.000088
14	1	-2.717713	1.615616	0.000263
15	6	-3.834350	-1.378742	-0.000109
16	1	-5.092803	0.484192	0.000179
17	1	-4.504049	-2.222036	-0.000212
18	7	3.594127	0.514593	-0.000087
19	7	1.975987	-1.015622	0.000133
20	7	-2.460069	-1.560303	-0.000129
21	7	-2.933187	0.625808	0.000135
22	8	-0.763920	2.250843	-0.000021

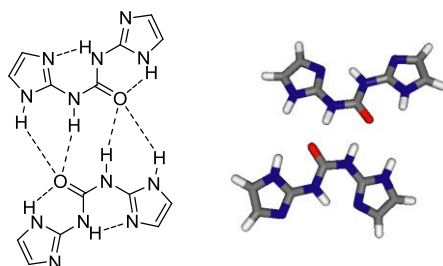
UDIM unfolded –
no tBu



Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.000028	-0.179540	-0.000003
2	7	1.158150	-0.923650	-0.000008
3	1	1.138729	-1.934157	-0.000015
4	7	-1.158195	-0.923594	-0.000008
5	1	-1.138657	-1.934105	-0.000015
6	6	2.448597	-0.383831	-0.000003
7	6	4.584193	-0.221422	0.000001
8	6	4.109634	1.070651	0.000011
9	1	2.001901	1.661375	0.000005
10	1	5.607872	-0.554958	-0.000001
11	1	4.602548	2.026211	0.000018
12	6	-2.448689	-0.383963	-0.000004
13	6	-4.109439	1.070683	-0.000022
14	1	-2.002025	1.661498	-0.000021
15	6	-4.584119	-0.221417	0.000035
16	1	-4.603067	2.025883	-0.000038
17	1	-5.607793	-0.554900	0.000067
18	7	2.723235	0.951580	0.000004
19	7	3.536940	-1.131381	-0.000003

20	7	-3.536936	-1.131403	0.000002
21	7	-2.723329	0.951692	-0.000012
22	8	0.000068	1.067936	0.000010

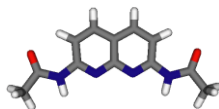
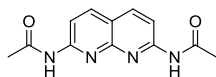
UDIM folded
dimer – no tBu



Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.060161	0.228470	-0.228104
2	7	-1.189055	1.289724	-0.073504
3	1	-0.197077	1.094337	-0.271510
4	7	-3.384707	0.493313	-0.071980
5	1	-3.660180	1.457505	0.157710
6	6	-1.522050	2.593869	0.266554
7	6	-2.539375	4.425628	0.786836
8	6	-1.201330	4.730311	0.789066
9	1	0.442213	3.384067	0.385496
10	1	-3.373796	5.072463	0.995559
11	1	-0.666013	5.641147	0.987490
12	6	-4.400670	-0.453177	-0.216547
13	6	-6.332635	-1.379946	-0.273427
14	6	-5.441577	-2.352594	-0.669491
15	1	-3.276128	-2.098623	-0.852769
16	1	-7.401824	-1.458531	-0.172826
17	1	-5.570010	-3.379228	-0.962843
18	8	-1.602087	-0.915193	-0.503724
19	7	-5.676328	-0.192938	0.009035
20	7	-4.194367	-1.740569	-0.627749
21	7	-0.552672	3.542873	0.451333
22	7	-2.734602	3.089470	0.458602
23	6	2.060369	-0.228091	-0.227107
24	7	1.188936	-1.288945	-0.071638
25	1	0.197100	-1.093644	-0.270627
26	7	3.384885	-0.493251	-0.071142
27	1	3.660209	-1.457485	0.158428
28	6	1.521662	-2.593446	0.267347
29	6	2.538382	-4.425870	0.786404
30	6	1.200244	-4.730155	0.788315
31	1	-0.442847	-3.383110	0.385320
32	1	3.372588	-5.073117	0.994735
33	1	0.664631	-5.640963	0.986070
34	6	4.401087	0.452907	0.216272
35	6	6.333317	1.379077	-0.274034
36	6	5.442376	2.351971	-0.669771
37	1	3.276787	2.098572	-0.852298
38	1	7.402572	1.457355	-0.173872
39	1	5.570994	3.378539	-0.963269
40	8	1.602576	0.915616	-0.502994

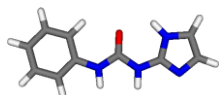
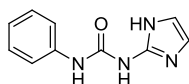
41	7	5.676767	0.192290	0.008778
42	7	4.194994	1.740341	-0.627411
43	7	0.551967	-3.542268	0.451414
44	7	2.734044	-3.089527	0.459168

DAN



Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2.306317	-0.063547	-0.011218
2	6	0.000000	-0.004731	-0.010952
3	6	0.000000	1.429002	0.002698
4	6	1.254919	2.090001	0.009060
5	6	2.421277	1.359066	0.002243
6	6	-1.254919	2.090000	0.009063
7	1	1.287691	3.173915	0.019188
8	1	3.399446	1.811236	0.006467
9	6	-2.421277	1.359066	0.002250
10	6	-2.306317	-0.063548	-0.011212
11	1	-1.287692	3.173914	0.019192
12	1	-3.399446	1.811235	0.006477
13	7	1.155506	-0.725647	-0.017752
14	7	-1.155506	-0.725647	-0.017749
15	7	3.425897	-0.914142	-0.019670
16	1	3.161457	-1.891541	-0.028959
17	7	-3.425897	-0.914142	-0.019661
18	1	-3.161457	-1.891541	-0.028951
19	6	4.772347	-0.593952	-0.005751
20	6	-4.772347	-0.593952	-0.005739
21	8	-5.206526	0.556408	0.003640
22	8	5.206526	0.556407	0.003646
23	6	-5.697761	-1.802770	0.026790
24	1	-5.214308	-2.728214	-0.294600
25	1	-6.073674	-1.941839	1.045548
26	1	-6.555214	-1.601883	-0.617013
27	6	5.697760	-1.802770	0.026800
28	1	6.073664	-1.941829	1.045563
29	1	5.214310	-2.728217	-0.294585
30	1	6.555219	-1.601890	-0.616996

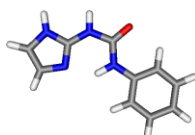
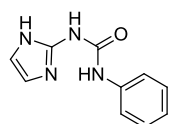
UIM unfolded –
no tBu



Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	4.861443	0.451170	-0.000001
2	6	4.520944	-0.907263	0.000001
3	6	3.180486	-1.295679	0.000001
4	6	2.156552	-0.328734	0.000000
5	6	2.493278	1.037192	-0.000001
6	6	3.841969	1.409855	-0.000002

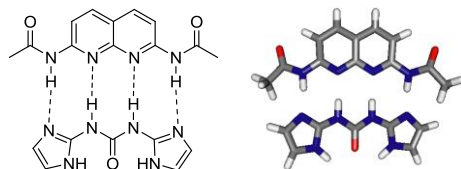
7	1	5.901214	0.755369	-0.000001
8	1	5.295161	-1.665798	0.000001
9	1	2.923861	-2.350799	0.000002
10	1	1.710188	1.777720	-0.000002
11	1	4.091710	2.464691	-0.000003
12	7	0.824664	-0.810275	0.000001
13	1	0.738088	-1.816578	0.000001
14	6	-0.348716	-0.079291	0.000001
15	7	-1.485292	-0.872706	0.000000
16	1	-1.436398	-1.881818	0.000001
17	8	-0.409377	1.158543	-0.000001
18	6	-2.792517	-0.379284	0.000000
19	6	-4.504181	1.016110	0.000002
20	1	-2.415018	1.677356	0.000005
21	6	-4.933614	-0.291541	-0.000003
22	1	-5.030590	1.953654	0.000004
23	1	-5.945312	-0.660295	-0.000007
24	7	-3.855149	-1.164746	-0.000001
25	7	-3.114473	0.945291	0.000003

UIM folded – no
tBu



Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-4.455048	-0.770787	0.000002
2	6	-3.475936	-1.772763	0.000003
3	6	-2.121816	-1.434962	0.000002
4	6	-1.723587	-0.083172	0.000000
5	6	-2.704093	0.926623	-0.000001
6	6	-4.057395	0.571016	0.000000
7	1	-5.506758	-1.032158	0.000003
8	1	-3.764205	-2.817954	0.000005
9	1	-1.366403	-2.213493	0.000003
10	1	-2.398082	1.960561	-0.000003
11	1	-4.804530	1.356748	-0.000001
12	7	-0.332444	0.168191	-0.000002
13	1	0.294341	-0.641431	0.000000
14	6	0.280681	1.389614	-0.000003
15	7	1.697414	1.340720	0.000000
16	1	2.101217	2.266025	0.000002
17	8	-0.257865	2.498771	-0.000001
18	6	2.533370	0.235613	0.000000
19	6	4.429297	-0.939478	0.000004
20	1	4.429756	1.213059	0.000011
21	6	3.340930	-1.771664	-0.000006
22	1	5.487876	-1.126434	0.000008
23	1	3.322433	-2.847896	-0.000012
24	7	2.161197	-1.035935	-0.000005
25	7	3.900812	0.354533	0.000006

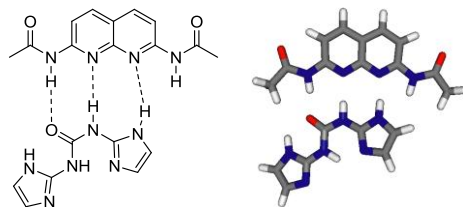
DAN-UDIM
 unfolded – no tBu



Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.000013	2.484629	-0.000274
2	7	1.124098	1.736466	0.251648
3	1	1.106954	0.708195	0.155492
4	7	-1.124090	1.736429	-0.252259
5	1	-1.106889	0.708178	-0.155974
6	6	2.352753	2.309510	0.556009
7	6	4.445903	2.545296	1.015994
8	6	3.905007	3.807480	1.059996
9	1	1.815421	4.321165	0.645510
10	1	5.465996	2.250737	1.192850
11	1	4.334062	4.771457	1.265709
12	6	-2.352885	2.309388	-0.556174
13	6	-3.905375	3.807250	-1.059759
14	1	-1.815761	4.321126	-0.645799
15	6	-4.446194	2.545044	-1.015519
16	1	-4.334560	4.771186	-1.265404
17	1	-5.466330	2.250422	-1.192003
18	7	2.556706	3.641029	0.766033
19	7	3.470198	1.609410	0.696369
20	7	-3.470321	1.609221	-0.696188
21	7	-2.556957	3.640889	-0.766263
22	8	-0.000067	3.737715	-0.000169
23	6	-2.315458	-1.968304	0.241566
24	6	0.000049	-2.014295	-0.000091
25	6	0.000080	-3.445136	-0.000103
26	6	-1.234574	-4.114823	0.171182
27	6	-2.392960	-3.394263	0.308902
28	6	1.234759	-4.114782	-0.171435
29	1	-1.254540	-5.198821	0.189619
30	1	-3.353557	-3.855739	0.460146
31	6	2.393115	-3.394179	-0.309102
32	6	2.315554	-1.968214	-0.241641
33	1	1.254730	-5.198779	-0.189939
34	1	3.353755	-3.855551	-0.460397
35	7	-1.163442	-1.296022	0.098000
36	7	1.163523	-1.295974	-0.098150
37	7	-3.473842	-1.187588	0.296612
38	1	-3.392807	-0.209297	-0.019251
39	7	3.473938	-1.187466	-0.296539
40	1	3.392862	-0.209241	0.019431
41	6	-4.753222	-1.605850	0.647121
42	6	4.753392	-1.605705	-0.646832
43	8	5.045640	-2.744792	-1.009679
44	8	-5.045391	-2.744949	1.009998
45	6	5.807510	-0.514456	-0.533888
46	1	5.450200	0.442702	-0.917855
47	1	6.081752	-0.370087	0.516739
48	1	6.690210	-0.836022	-1.084927

49	6	-5.807397	-0.514625	0.534415
50	1	-5.449982	0.442594	0.918128
51	1	-6.082011	-0.370420	-0.516136
52	1	-6.689890	-0.836158	1.085806

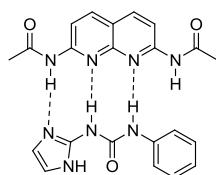
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no tBu



Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.432729	-0.634982	-0.163251
2	7	-1.100665	-0.884334	0.104532
3	1	-0.473043	-0.077763	-0.002506
4	7	-3.294245	-1.680056	-0.017028
5	1	-2.918655	-2.572591	0.328093
6	6	-0.555238	-2.066727	0.588500
7	6	-0.217761	-4.063537	1.325462
8	6	1.013065	-3.452540	1.309865
9	1	1.459187	-1.428234	0.602459
10	1	-0.466236	-5.063763	1.636431
11	1	1.988905	-3.793246	1.607313
12	6	-4.664529	-1.606850	-0.270916
13	6	-6.637957	-0.816778	-0.884617
14	1	-4.797025	0.366925	-0.949086
15	6	-6.735085	-2.125900	-0.467915
16	1	-7.366703	-0.113283	-1.245941
17	1	-7.614943	-2.744869	-0.418824
18	7	0.783744	-2.162035	0.836116
19	7	-1.198514	-3.191532	0.871764
20	7	-5.497036	-2.616785	-0.084929
21	7	-5.293037	-0.492724	-0.752486
22	8	-2.783421	0.516613	-0.529360
23	6	0.275750	2.765188	0.112040
24	6	2.110168	1.350439	-0.044716
25	6	3.023190	2.445957	0.062228
26	6	2.474153	3.744712	0.220386
27	6	1.112577	3.919674	0.248008
28	6	4.409793	2.164625	0.000765
29	1	3.137685	4.597181	0.312524
30	1	0.648986	4.884740	0.364942
31	6	4.850750	0.871627	-0.175627
32	6	3.865590	-0.151746	-0.275112
33	1	5.122339	2.977463	0.084699
34	1	5.893779	0.609716	-0.237300
35	7	0.757668	1.522636	-0.014044
36	7	2.552194	0.064865	-0.187192
37	7	-1.114722	2.856891	0.086133
38	1	-1.615839	1.984515	-0.124758
39	7	4.196215	-1.499934	-0.489421
40	1	3.391516	-2.089441	-0.659678

41	6	-1.897321	3.994555	0.271657
42	6	5.452898	-2.088074	-0.588902
43	8	6.506289	-1.477384	-0.436587
44	8	-1.447380	5.111887	0.518915
45	6	5.415546	-3.569437	-0.933000
46	1	4.459217	-4.044918	-0.703141
47	1	5.617223	-3.696971	-2.001578
48	1	6.211090	-4.074608	-0.384080
49	6	-3.388060	3.744311	0.115592
50	1	-3.677987	3.930262	-0.924670
51	1	-3.668562	2.721205	0.367958
52	1	-3.924848	4.452698	0.746598

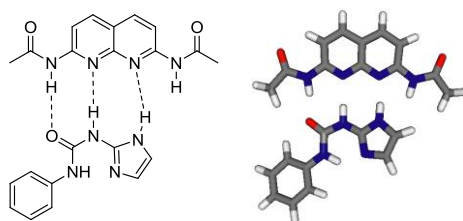
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no tBu



Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.809594	-2.241089	-0.596593
2	6	0.438838	-2.040333	-0.063112
3	6	0.553930	-3.452613	0.128236
4	6	-0.602884	-4.245408	-0.070985
5	6	-1.790362	-3.658843	-0.446728
6	6	1.824103	-3.962125	0.500751
7	1	-0.543168	-5.319376	0.065967
8	1	-2.693159	-4.219378	-0.623234
9	6	2.895293	-3.113255	0.634007
10	6	2.695257	-1.718126	0.377795
11	1	1.943965	-5.026424	0.670075
12	1	3.877654	-3.451968	0.916796
13	7	3.745799	-0.802005	0.409481
14	1	3.544513	0.126729	0.001856
15	7	-2.962881	-1.543863	-0.980732
16	1	-2.820993	-0.545099	-1.067489
17	6	5.048857	-1.028357	0.837837
18	6	-4.243337	-2.028396	-1.230971
19	6	-5.228952	-0.941265	-1.630500
20	1	-5.268128	-0.147754	-0.877843
21	1	-4.941010	-0.487871	-2.585020
22	1	-6.215009	-1.390482	-1.735551
23	6	5.968602	0.169362	0.660020
24	1	6.374191	0.171308	-0.357904
25	1	5.450841	1.116881	0.816795
26	1	6.798571	0.071848	1.359144
27	8	5.454451	-2.091424	1.306958
28	8	-4.554089	-3.213047	-1.145394
29	7	-0.750994	-1.454979	-0.390896
30	7	1.502809	-1.196785	0.065041
31	6	-5.109878	2.413739	1.776122
32	6	-4.503098	1.171425	2.001201
33	6	-3.216085	0.917601	1.521089

34	6	-2.516071	1.902146	0.793479
35	6	-3.124465	3.152510	0.567249
36	6	-4.409449	3.395131	1.064299
37	1	-6.104696	2.614926	2.155468
38	1	-5.022565	0.403141	2.562812
39	1	-2.737812	-0.033616	1.725723
40	1	-2.584783	3.911732	0.024612
41	1	-4.864580	4.363177	0.887749
42	7	-1.230965	1.557629	0.314871
43	1	-1.008853	0.561771	0.272193
44	6	-0.240866	2.426178	-0.093784
45	8	-0.382361	3.655069	-0.219388
46	7	0.959173	1.783303	-0.357349
47	1	1.077803	0.772180	-0.209124
48	6	2.109016	2.462355	-0.732942
49	6	3.472947	4.085806	-1.377132
50	1	1.337393	4.380165	-0.960396
51	6	4.158627	2.903028	-1.242071
52	1	3.784483	5.073738	-1.664570
53	1	5.205204	2.716807	-1.413202
54	7	3.302950	1.886852	-0.832204
55	7	2.154617	3.786413	-1.051908

UIM folded – no
tBu



Centre Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	4.072755	-0.356424	-0.253839
2	6	2.424384	1.264589	-0.031278
3	6	3.412250	3.412250	0.110486
4	6	4.775641	1.909715	0.071360
5	6	5.126575	0.590876	-0.117733
6	6	2.954913	3.622118	0.278128
7	1	5.542745	2.667862	0.182498
8	1	6.149179	0.255632	-0.163830
9	6	1.609485	3.894185	0.282305
10	6	0.693376	2.805080	0.113275
11	1	3.676227	4.422988	0.396027
12	1	1.213247	4.888125	0.405102
13	7	-0.684580	2.998235	0.063548
14	1	-1.246404	2.163504	-0.153860
15	7	4.309663	-1.722069	-0.486355
16	1	3.467994	-2.248254	-0.682857
17	6	-1.385408	4.190544	0.238001
18	6	5.521658	-2.397092	-0.576386
19	6	5.384883	-3.865805	-0.949924
20	1	4.386883	-4.270650	-0.766812
21	1	5.619615	-3.990450	-2.011983
22	1	6.117204	-4.439757	-0.380726

23	6	-2.885701	4.054102	0.043741
24	1	-3.139110	4.332013	-0.985437
25	1	-3.243922	3.039332	0.217114
26	1	-3.385820	4.756198	0.711615
27	8	-0.858288	5.269942	0.503756
28	8	6.614039	-1.868077	-0.394363
29	7	2.776871	-0.047273	-0.187669
30	7	1.087723	1.532450	-0.023013
31	6	-7.418745	-1.210154	-0.488932
32	6	-6.773194	-2.336663	0.037281
33	6	-5.384646	-2.353029	0.175959
34	6	-4.614182	-1.238767	-0.213361
35	6	-5.259601	-0.106879	-0.745571
36	6	-6.652760	-0.104670	-0.875670
37	1	-8.497069	-1.195717	-0.595296
38	1	-7.348963	-3.203244	0.342119
39	1	-4.888699	-3.225109	0.588237
40	1	-4.670798	0.744515	-1.045874
41	1	-7.138979	0.772824	-1.287192
42	7	-3.214557	-1.350764	-0.053155
43	1	-2.846998	-2.253402	0.267873
44	6	-2.277949	-0.369298	-0.207925
45	8	-2.510284	0.814229	-0.533942
46	7	-0.957947	-0.752541	0.013853
47	1	-0.273891	0.007452	-0.073163
48	6	-0.496659	-1.968811	0.495779
49	6	0.977731	-3.458750	1.213878
50	1	1.555675	-1.460799	0.527322
51	6	-0.289477	-3.988836	1.225160
52	1	1.929057	-3.863281	1.510886
53	1	-0.601150	-4.972924	1.531264
54	7	-1.211732	-3.053198	0.772959
55	7	0.832883	-2.154436	0.744827
