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Conformational change in association of heterocyclic urea derivative forming two intramolecular hydrogen bonds in polar solvent

Supporting Information

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Cartesian coordinates for optimized compounds

1'a

E(a.u.)= -790.8611918

C 2.5496452517 -1.6258467236 -0.1578145832
C 1.4187986759 -0.7878296440 -0.1577749594
N 1.5385641933 0.5346892549 -0.1555495743
C 2.7819066236 1.0332824653 -0.1534341428
N 3.9123473884 0.3370746274 -0.1532352274
C 3.7653515985 -0.9956515856 -0.1554691860
N 2.8303937699 2.4090404763 -0.1511572967
C 3.8973448576 3.3211365176 -0.1500094892
N 5.1372289948 2.8125041424 -0.1516610871
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N -1.2376530260 0.5183578387 -0.1595314234
C -2.5280490709 1.1705506917 -0.1606811050
O -2.0739235341 -1.5933550944 -0.1638000694
O 3.6364681433 4.5180354889 -0.1482273057
C 6.3050086841 3.6635133406 -0.1500984404
H 2.4663396602 -2.7021653637 -0.1596173417
H 4.6813662379 -1.5747015103 -0.1553375703
H 1.9345272190 2.8646910211 -0.1508732236
H 5.2239363892 1.8066628152 -0.1508324759
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H -0.3847400366 1.0554222159 -0.1575000984
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H -3.1044436331 0.9030126222 -1.0460968727
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H 6.3187167902 4.3168829700 -1.0222858967
H 6.3430421289 4.2839350612 0.7454297316

1'b

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C 2.6017962230 -1.6254557545 -0.2359740290
C 1.4854978538 -0.7735789746 -0.2122944178
N 1.6277622018 0.5471390013 -0.2112236296
C 2.8804103492 1.0263293232 -0.2468005940
N 3.9991197625 0.3201779412 -0.2905698288
C 3.8264199244 -1.0083858630 -0.2757389073
N 2.9316902362 2.4061167008 -0.2796664107
C 4.0183512576 3.2542771040 -0.0262405981
N 3.7547813029 4.5435112310 -0.3597913294
N 0.2273648101 -1.3241959131 -0.1859278495
C -1.0610379994 -0.7617653653 -0.1336724553
N -1.1462649833 0.5753506687 -0.1192106793
C -2.4224657347 1.2506956104 -0.0488531302
O -2.0210556839 -1.5204576841 -0.1069173302
O 5.0662267313 2.8930536976 0.4725971720
C 4.7447826867 5.5823849784 -0.1797635335
H 2.5043973724 -2.7003053329 -0.2292221527

H 4.7317664702 -1.6047725611 -0.3049738768
H 2.0290643182 2.8357062299 -0.3818552709
H 2.9609057253 4.7478122782 -0.9378575177
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H 4.2743621767 6.5429402354 -0.3713151843
H 5.1175401399 5.5748088830 0.8424642141
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1'c

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N	1.7122917616	0.1930495468	-0.1589104903
C	2.8614842834	0.8692050597	-0.1589105009
N	4.0874193760	0.3495075556	-0.1589103758
C	4.1335992620	-0.9867476008	-0.1589102051
N	2.7044371858	2.2398865649	-0.1589106937
C	3.6198468585	3.3003073391	-0.1589108859
N	4.9232249927	2.9845110607	-0.1589106499
N	0.5647011765	-1.7611886490	-0.1589103457
C	0.2828200702	-3.1298959809	-0.1589102986
N	-1.0406848646	-3.4070057015	-0.1589106613
C	-1.5232107292	-4.7710243471	-0.1589110672
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H	3.0966814016	-2.8727146863	-0.1589099891
H	5.1248092019	-1.4257872532	-0.1589101097
H	1.7486831981	2.5510304377	-0.1589108468
H	5.1598434510	2.0030379844	-0.1589107371
H	-0.2058830399	-1.1139269620	-0.1589105177
H	-1.7143021395	-2.6645025482	-0.1589117165
H	-2.6089514273	-4.7488029441	-0.1589092976
H	-1.1832027176	-5.3084025603	-1.0439124509
H	-1.1831999244	-5.3084038100	0.7260884416
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E(a.u.)=-790. 857226

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N	3.8341091754	0.7383340178	-0.1717026559
C	4.0230652335	-0.5796332265	-0.1758886034
N	2.3715228605	2.4875170298	-0.1623710698

C	1.2349459076	3.3058738435	-0.1538087800
N	0.0389220603	2.6983994956	-0.1578303986
N	0.5615883403	-1.7478416489	-0.1702915928
C	0.4306690219	-3.1400214793	-0.1797558172
N	-0.8556378070	-3.5579322751	-0.1862773730
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O	1.3827255120	-3.9010573704	-0.1733820414
O	1.3922892592	4.5211113296	-0.1455961728
C	-1.1936669861	3.4522770445	-0.1378751885
H	3.1989341307	-2.5727607885	-0.1781054273
H	5.0557646818	-0.9112817064	-0.1796345100
H	3.2278884976	3.0141264326	-0.1612215076
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H	-2.2640775664	-5.0660363305	-0.1220755418
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N	1.8846727557	0.2629413446	-0.1268444038
C	3.0540985995	0.9039256838	-0.0682429649
N	4.2601221815	0.3545665298	0.0148023896
C	4.2604762154	-0.9815770766	0.0182786028
N	2.9196334079	2.2814273655	-0.0534764306
C	3.8828371166	3.2655046175	-0.3015373677
N	3.4297690852	4.5148187969	-0.0193973954
N	0.6737184258	-1.6541318007	-0.1608054462
C	0.3445513386	-3.0108752591	-0.1383826093
N	-0.9858393384	-3.2419459429	-0.2270818479
C	-1.5188752576	-4.5867610291	-0.2475316834
O	1.1729650332	-3.9003727001	-0.0393402480
O	4.9893472743	3.0434155313	-0.7544863332
C	4.2686227922	5.6780195126	-0.2045754054
H	3.1702721556	-2.8412017830	-0.0280763742
H	5.2355351353	-1.4532455963	0.0800560023
H	1.9619363761	2.5804138801	0.0075018406
H	2.5953197714	4.6212908789	0.5268042888
H	-0.0737242599	-0.9821894489	-0.2081262989
H	-1.6207092041	-2.4795678383	-0.3711075134
H	-2.6030919007	-4.5237415734	-0.2386797338
H	-1.2041729649	-5.1286691712	-1.1399969574
H	-1.1933127753	-5.1436442842	0.6296074719
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C	2.5027764270	1.2181386812	-0.1589099987
N	3.7414781853	0.7231460698	-0.1589094649
C	3.8098659573	-0.6125145357	-0.1589091806
N	2.4371294844	2.5977023765	-0.1589101648
C	1.3096119397	3.4249145710	-0.1589104274
N	1.6234244992	4.7429124983	-0.1589106281
N	0.3039274465	-1.5273076664	-0.1589101751
C	-1.0507054387	-1.1355628452	-0.1589108348
N	-1.3195296348	0.1769348557	-0.1589114668
C	-2.6809516954	0.6615707327	-0.1589124328
O	-1.8992110674	-2.0198681538	-0.1589109191
O	0.1598522372	3.0186867019	-0.1589103410
C	0.5993232392	5.7641766311	-0.1589112522
H	2.8081181773	-2.5167587431	-0.1589090768
H	4.8074457996	-1.0374134825	-0.1589086895
H	3.3440810432	3.0309066257	-0.1589099094
H	2.5825217198	5.0336130932	-0.1589115951
H	0.3987620758	-2.5282188117	-0.1589098238
H	-0.5489118564	0.8346333980	-0.1589117234
H	-2.6492984547	1.7477440332	-0.1589118448
H	-3.2238741901	0.3257185816	-1.0427666516
H	-3.2238757332	0.3257176416	0.7249404590
H	1.0866540537	6.7347951647	-0.1589101680
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1'g

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C	1.3747811246	-0.7937528868	-0.1762126610
N	1.3888198458	0.5306981778	-0.1694221882
C	2.5725583173	1.1319228484	-0.1477632715
N	3.7704831568	0.5433719410	-0.1362001171
C	3.7302352445	-0.7919983308	-0.1456770083
N	2.5918616474	2.5091695300	-0.1365502761
C	1.5656746815	3.4667793853	-0.1261442743
N	0.2996218504	3.0246288319	-0.1307518232
N	0.1670782391	-1.4528462531	-0.1992799868
C	-1.1270387787	-0.9068489501	-0.1980932682
N	-2.0947724264	-1.8516062305	-0.2579564376
C	-3.4958568959	-1.4914890829	-0.2892229373
O	-1.3657882289	0.2856252850	-0.1389009913
O	1.8844967235	4.6515348733	-0.1126887754
C	-0.8150282490	3.9431678363	-0.1179214582
H	2.5843956376	-2.6099981062	-0.1701710413

H	4.6893887731	-1.2980184789	-0.1371285078
H	3.5092399582	2.9198745327	-0.1245098130
H	0.1318668432	2.0261651305	-0.1411751039
H	0.2350069055	-2.4552010746	-0.2108648133
H	-1.8530424695	-2.8180166782	-0.3717129044
H	-4.0834601576	-2.4042942455	-0.2602943376
H	-3.7558608774	-0.8797999516	0.5733022766
H	-3.7463268254	-0.9388828533	-1.1953226762
H	-1.7310202666	3.3585032954	-0.1291311057
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C	-0.7928253967	0.3261025196	-0.0123284899
N	-1.4191899962	1.4976241843	0.0505600770
C	-0.6155556420	2.5685478263	0.0968402986
N	-1.5353024406	-0.8352805518	-0.0698842264
C	-2.9145026203	-1.0813857519	-0.0789587403
N	-3.7271452389	-0.0158561571	-0.0251609669
N	2.6671579156	1.0623927099	-0.0061503078
C	3.4476361032	-0.0928736516	0.1820368569
N	4.7439743587	0.0979345682	-0.1660935650
C	5.7200478496	-0.9620951561	-0.0380698944
O	3.0207684800	-1.1309155402	0.6455451030
O	-3.2987013741	-2.2441528561	-0.1344802589
C	-5.1646211268	-0.1591277276	-0.0282635807
H	1.3713039430	3.3729625929	0.1363421579
H	-1.1083698006	3.5326580749	0.1462744649
H	-0.9885472647	-1.6777580552	-0.1117414568
H	-3.2916632454	0.8941645850	0.0194796711
H	3.1688451794	1.9284929075	-0.0935434123
H	4.9965572048	0.9041594821	-0.7065260735
H	6.7100738847	-0.5376583012	-0.1799122955
H	5.6670054948	-1.4011462836	0.9556736827
H	5.5631985292	-1.7511159659	-0.7755361395
H	-5.6064297932	0.8312580515	0.0369364162
H	-5.5141732200	-0.6387355904	-0.9428054583
H	-5.5053030388	-0.7506909390	0.8215099785

A

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N	-0.1714852598	0.6153043954	0.0000000000
C	-0.1449397084	1.9460244605	0.0000000000
C	1.0390722600	2.6827189754	0.0000000000
C	2.2230386027	1.9629379177	0.0000000000
C	2.2239707541	0.5773472162	0.0000000000
C	0.9798349605	-0.0525155043	0.0000000000
N	-1.4209385956	2.5158085937	0.0000000000

C	-1.7978441808	3.8360816376	0.0000000000
O	-1.0059752904	4.7608405670	0.0000000000
C	-3.2904833539	4.0347729287	0.0000000000
N	0.8047877601	-1.4389445819	0.0000000000
C	1.7378250194	-2.4462275953	0.0000000000
O	2.9392425332	-2.2491700078	0.0000000000
C	1.1331410363	-3.8252878229	0.0000000000
H	1.0181190303	3.7584113566	0.0000000000
H	3.1660521014	2.4936634851	0.0000000000
H	3.1326372660	0.0012587075	0.0000000000
H	-2.1564338447	1.8291260747	0.0000000000
H	-3.5098387427	5.0972832843	0.0000000000
H	-3.7382870872	3.5729964353	-0.8802137710
H	-3.7382870872	3.5729964353	0.8802137710
H	-0.1638613683	-1.7113499397	0.0000000000
H	1.9275875683	-4.5641381207	0.0000000000
H	0.5060328139	-3.9684694425	0.8802137836
H	0.5060328139	-3.9684694425	-0.8802137836

B

E(a.u.)=-478.4474635

C	1.2621518014	-2.3274190398	-0.2744471679
N	1.4306419422	-0.9522558785	-0.2680378328
C	2.6221149126	-0.2465342832	-0.3083523616
C	3.8721455447	-1.0707048586	-0.4218615846
C	3.7743302384	-2.4768447906	0.1781774378
C	2.5170792261	-3.1439275586	-0.3885914005
O	0.1482062364	-2.8025472006	-0.2158680175
O	2.6108595635	0.9655257923	-0.2778359286
C	3.6942342573	-2.3999710455	1.7059870159
C	5.0043580066	-3.2872789103	-0.2229031334
H	0.5875748926	-0.4002582378	-0.2074395981
H	4.6820050216	-0.4970131762	0.0259459243
H	4.0893857108	-1.1352519207	-1.4926282452
H	2.3237063987	-4.1058417642	0.0834799612
H	2.6475447718	-3.3405707233	-1.4573446188
H	2.8307199389	-1.8298498176	2.0523110831
H	3.6229018239	-3.3995446944	2.1359860773
H	4.5874030527	-1.9242491099	2.1122851650
H	5.9149414247	-2.8231699736	0.1587968466
H	4.9505765971	-4.2986509720	0.1826678340
H	5.0934686379	-3.3630618371	-1.3073774561

C

E(a.u.)=-889. 6801589

N	-4.6945173139	-1.3728752639	0.5218909856
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C	-3.6638591414	-0.5830954867	0.1451903089
C	-3.8636092628	0.7622386838	-0.2663065378
C	-5.1716030680	1.2721543277	-0.2771768136
C	-6.2065000620	0.4601672753	0.1072181096
N	-2.4343791120	-1.1478980917	0.1827581508

C	-1.3971983819	-0.4328394743	-0.1705268600
C	-1.4929340938	0.9292902791	-0.5994484148
C	-2.7187954103	1.5082324679	-0.6422772902
N	-0.1319037677	-0.9771770024	-0.1436310041
C	0.3477506604	-2.2348870316	0.2073127799
N	1.6522684111	-2.3344928067	0.0854233596
C	2.2506706167	-3.5035279544	0.3937833105
N	3.5970802311	-3.5510920485	0.2500547230
C	4.2017188039	-4.6764600590	0.5435025537
C	3.5567616866	-5.8448252189	0.9986299912
C	2.1968555578	-5.8121759362	1.1487645411
C	1.5037324669	-4.6262169679	0.8461161238
C	0.1039505891	-4.4760817090	0.9627650077
C	-0.4936785713	-3.2931261797	0.6497727038
H	-6.7081429607	-1.5180842936	0.8060367921
H	-5.3458514052	2.2959699352	-0.5876686514
H	-7.2301302222	0.8079761367	0.1152489558
H	-0.6033600584	1.4771970564	-0.8812761597
H	-2.8321599668	2.5374194855	-0.9616333076
H	0.6219538377	-0.3748463915	-0.4276775679
H	5.2817512308	-4.6844297698	0.4184778722
H	4.1327276841	-6.7331401662	1.2185750447
H	1.6472572809	-6.6798346324	1.4951124392
H	-0.4948498084	-5.3121135457	1.3045212501
H	-1.5569739786	-3.1400882192	0.7255096469

D

E(a.u.)=-554.1086563

C	-1.1851113648	-1.8486310325	0.0000000000
C	-1.1813952149	-0.4638381257	0.0000000000
C	-0.0007581745	0.2782296113	0.0000000000
C	1.1925377750	-0.4433051145	0.0000000000
C	1.2202060810	-1.8278262007	0.0000000000
C	0.0239400689	-2.5773400985	0.0000000000
H	-2.1335353608	-2.3658681716	0.0000000000
H	-2.1243104235	0.0679331100	0.0000000000
C	-0.0139022684	1.7977901719	0.0000000000
H	2.1261133321	0.1046971007	0.0000000000
H	2.1774347311	-2.3285811596	0.0000000000
N	0.0358150083	-3.9501982802	0.0000000000
O	1.0996302644	2.3790423948	0.0000000000
O	-1.1373227327	2.3596930069	0.0000000000
C	-1.2058289557	-4.6901564219	0.0000000000
C	1.2900731842	-4.6685674031	0.0000000000
H	-1.8111083554	-4.4713521801	-0.8848016175
H	-1.8111083554	-4.4713521801	0.8848016175
H	-0.9883645012	-5.7538521780	0.0000000000
H	1.8914770321	-4.4393255784	0.8848016204
H	1.8914770321	-4.4393255784	-0.8848016204
H	1.0910411987	-5.7358656970	0.0000000000

E

E(a.u.)=-534.7045184

C	-1.1672313656	-1.9707390564	0.0367550096
C	-1.1771192702	-0.5798065799	0.0135734847
C	-0.0036847458	0.1657878605	-0.0011304942
C	1.2064079657	-0.5337012495	0.0081463731
C	1.2429902992	-1.9155371879	0.0311042721
C	0.0522986597	-2.6476946419	0.0456709131
H	-2.1040693559	-2.5088370152	0.0475498857
H	-2.1229717373	-0.0548566231	0.0066552360
C	-0.0329052964	1.6906650490	-0.0264132163
H	2.1293097540	0.0306173200	-0.0030503313
H	2.1844121651	-2.4501774135	0.0381718493
O	1.0754643456	2.2771920871	-0.0379440120
O	-1.1622199129	2.2367178946	-0.0335680613
O	0.1824906608	-3.9965726744	0.0679430839
C	-0.9847158731	-4.7970652150	0.0840604474
H	-1.5909185341	-4.6329306872	-0.8088015107
H	-1.5871812270	-4.6024631680	0.9733211347
H	-0.6423565317	-5.8275986991	0.1009559361

F

E(a.u.)=-459.5004914

C	-1.1798660459	-1.9529683595	0.0355155015
C	-1.1873969684	-0.5630251238	0.0129374008
C	0.0000838681	0.1634808398	-0.0009549395
C	1.1988035566	-0.5502154239	0.0085334176
C	1.2084253207	-1.9370527963	0.0310281081
C	0.0173768733	-2.6673410791	0.0449873842
H	-2.1208333301	-2.4917848764	0.0459502895
H	-2.1247296298	-0.0223550005	0.0058123383
C	-0.0080047756	1.6916519989	-0.0257607034
H	2.1290971633	0.0024878157	-0.0020571289
H	2.1559755213	-2.4651835973	0.0379417967
O	1.1077344321	2.2626713307	-0.0365594590
O	-1.1301073933	2.2508961283	-0.0332602821
C	0.0372521476	-4.1677093423	0.0692151375
H	0.5625745520	-4.5396999158	0.9508737575
H	0.5574394070	-4.5680559051	-0.8030335743
H	-0.9698246988	-4.5817966933	0.0788309554

G

E(a.u.)=-420.207905

C	-1.2220969029	-1.9153351748	0.0000000000
C	-1.2127272091	-0.5257174332	0.0000000000
C	-0.0123988031	0.1838562922	0.0000000000
C	1.1826037306	-0.5345230580	0.0000000000
C	1.1817138486	-1.9242649269	0.0000000000
C	-0.0227490186	-2.6196694067	0.0000000000
H	-2.1642749881	-2.4500075850	0.0000000000
H	-2.1401201404	0.0314403598	0.0000000000

C	-0.0061401141	1.7148017944	0.0000000000
H	2.1147480536	0.0147601918	0.0000000000
H	2.1198339201	-2.4660342246	0.0000000000
H	-0.0266615750	-3.7025549247	0.0000000000
O	1.1147071997	2.2739525250	0.0000000000
O	-1.1234380013	2.2822955708	0.0000000000

H

E(a.u.)=-519.459546

C	-1.2006842044	-1.9759561107	0.0355204732
C	-1.1920442575	-0.5876272522	0.0132130434
C	0.0014015683	0.1324669585	-0.0005294136
C	1.2013043627	-0.5766235782	0.0088090650
C	1.2225351168	-1.9647912565	0.0311023052
C	0.0140711589	-2.6355002329	0.0439498704
H	-2.1232443771	-2.5409642711	0.0462259023
H	-2.1254795977	-0.0413286845	0.0060670717
C	-0.0066220095	1.6624285130	-0.0251695731
H	2.1297959000	-0.0218734478	-0.0017617782
H	2.1502668484	-2.5213619179	0.0384378615
O	1.1105783517	2.2289171838	-0.0367526249
O	-1.1285184291	2.2185562295	-0.0318536803
F	0.0206395684	-3.9843421331	0.0657414773

I

E(a.u.)=-879.8422039

C	-1.2019853482	-1.9454119276	0.0348415457
C	-1.1929605100	-0.5573615476	0.0125482867
C	0.0002685038	0.1614314933	-0.0012140960
C	1.1983894063	-0.5491783971	0.0079364185
C	1.2169566130	-1.9371644251	0.0301382386
C	0.0098434760	-2.6214631510	0.0433852450
H	-2.1338074368	-2.4935338822	0.0454003412
H	-2.1269576806	-0.0122704139	0.0055510243
C	-0.0050712476	1.6924353486	-0.0257527677
H	2.1287510119	0.0021183293	-0.0026359800
H	2.1525245542	-2.4789397112	0.0370527921
O	1.1129510451	2.2556364667	-0.0364461707
O	-1.1268334128	2.2479167794	-0.0332071909
Cl	0.0159310256	-4.3692149616	0.0714023130

J

E(a.u.)=-757.2683376

C	-1.1951623367	-2.0823355357	0.0673327050
C	-1.1900460396	-0.6968733486	0.0105861877
C	0.0057502926	0.0167960177	-0.0267709607
C	1.2043109980	-0.6927591276	-0.0046285527
C	1.2147932528	-2.0781906098	0.0517833018
C	0.0112195934	-2.7744780192	0.0914365150
H	-2.1328722742	-2.6209494817	0.0991956376
H	-2.1212105189	-0.1477075342	-0.0036644067
C	0.0025247000	1.5494448996	-0.0892072049

H	2.1334107613	-0.1404880536	-0.0305663386
H	2.1546881888	-2.6136080008	0.0714694236
O	1.1214672856	2.1080723525	-0.1154900425
O	-1.1188919097	2.1034764145	-0.1089179823
C	0.0140431801	-4.2697173054	0.0988756969
F	-1.0569498677	-4.7853137191	0.7158269422
F	0.0093895170	-4.7780878820	-1.1493639399
F	1.0925351772	-4.7812810666	0.7061030186

K

E(a.u.)=-624.7011285

C	-1.2395017288	-2.1201507182	0.0412904448
C	-1.2077705472	-0.7367208802	0.0016803758
C	0.0030729842	-0.0453660975	-0.0262387524
C	1.1944317823	-0.7701499657	-0.0136523554
C	1.1882862355	-2.1539881808	0.0258172163
C	-0.0348404441	-2.8102803187	0.0527785081
H	-2.1726664458	-2.6619703483	0.0630435755
H	-2.1276342948	-0.1698176103	-0.0082311377
C	0.0243849637	1.4907147044	-0.0701328728
H	2.1296410485	-0.2291393960	-0.0353864123
O	1.1530090811	2.0269979131	-0.0918849582
O	-1.0887730520	2.0583855913	-0.0798878533
N	-0.0550109512	-4.2795748420	0.0948062825
O	-1.1370630561	-4.8386670921	0.1165996980
O	1.0111237796	-4.8687246673	0.1056287692
H	2.1063106450	-2.7215480917	0.0357694718

1’c: B

E(a.u.)=-1269.3220085

C	-2.4145274946	0.2110436802	-0.0172455081
N	-3.5541808712	0.8935320349	0.0833673900
C	-3.4275970127	2.2220765891	0.1441148707
C	-2.2263879600	2.8844704484	0.1079562732
C	-1.0870167450	2.0732075653	-0.0019935436
N	-1.1839365314	0.7387110667	-0.0640052684
N	-2.4620086814	-1.1645648537	-0.0808380232
C	-3.5416592218	-2.0620652243	-0.0643825371
N	-4.7784776921	-1.5486323013	0.0210440100
C	-5.9479191826	-2.3956335216	0.0489422740
N	0.1942885834	2.5539199540	-0.0578303017
C	0.6355731394	3.8795495157	0.0086102225
N	1.9813609346	3.9821440857	-0.0794049752
C	2.6463182815	5.2638089206	-0.0089632977
O	-0.1059526603	4.8407556053	0.1309406947
O	-3.3034182757	-3.2627662296	-0.1308329400
H	-4.3524836027	2.7821104676	0.2262035776
H	-2.1546101384	3.9550632873	0.1588063978
H	-1.5715561336	-1.6447924487	-0.1454938255
H	-4.8575482330	-0.5440385040	0.0782066408
H	-6.8290255287	-1.7601333262	0.0732741156
H	-5.9981550052	-3.0292723951	-0.8364643546

H	-5.9558714028	-3.0377865447	0.9305334712
H	0.9205020601	1.8528655365	-0.1470391439
H	2.5380255996	3.1496950944	-0.1603096777
H	3.7117688893	5.1038414229	-0.1466229231
H	2.2889965538	5.9340350911	-0.7900463837
H	2.4857098469	5.7430624870	0.9573876449
C	1.2373856673	-2.3351232283	-0.2766153894
N	1.4180376238	-0.9648329136	-0.2659870086
C	2.6164591476	-0.2923848555	-0.3039252261
C	3.8575854569	-1.1249673090	-0.4080810708
C	3.7380082324	-2.5294282699	0.1917071536
C	2.4726938663	-3.1774507385	-0.3796917789
O	0.1112219162	-2.7896240032	-0.2287481970
O	2.6284482834	0.9275929166	-0.2774645945
C	3.6537193731	-2.4496360177	1.7190523841
C	4.9581502865	-3.3562691018	-0.2047611563
H	0.5655836605	-0.4046066285	-0.2061151629
H	4.6701222870	-0.5592973713	0.0444547711
H	4.0806631618	-1.1909964750	-1.4777081101
H	2.2577400506	-4.1336677490	0.0943737909
H	2.6055913450	-3.3800202838	-1.4472097828
H	2.7988220138	-1.8645386038	2.0621278987
H	3.5636789433	-3.4472841589	2.1498696747
H	4.5538137169	-1.9887790526	2.1271160675
H	5.8726067086	-2.9042079288	0.1817355495
H	4.8887416315	-4.3664366963	0.2008508804
H	5.0518337454	-3.4337738783	-1.2886698406

1'd:A

E(a.u.)=-1454.9756173

C	2.8427540873	-1.5381340684	0.4985369489
C	1.6245623769	-0.9838572217	0.0957798277
N	1.5321019119	0.2978505257	-0.2779747559
C	2.6443600986	1.0235727075	-0.2612115016
N	3.8648515157	0.5906248628	0.0763301880
C	3.9245706303	-0.6859028265	0.4568650840
N	2.5928550186	2.3543236303	-0.6126979198
C	1.5479164636	3.1682417643	-1.0467973799
N	0.3408630489	2.6156802087	-1.2129911563
N	0.4319465038	-1.6609084532	0.0453056758
C	0.1791957210	-3.0033361329	0.3515182893
N	-1.1205641592	-3.3469473736	0.2140455086
C	-1.5815829947	-4.6861200242	0.5114977080
O	1.0480290461	-3.7838920223	0.6990227871
O	1.7870713009	4.3578909667	-1.2608642521
C	-0.7966535075	3.3907895242	-1.6558224258
H	2.9277393800	-2.5632515079	0.8084580433
H	4.9044635706	-1.0524488591	0.7423111506
H	3.4708569113	2.8564632278	-0.5177505652
H	0.2451338218	1.6384380067	-0.9849955148
H	-0.3385280570	-1.0925801815	-0.2639203453
H	-1.8040631412	-2.6518179023	-0.0204577319

H	-2.6347744761	-4.7491709210	0.2545243671
H	-1.0329634286	-5.4214159405	-0.0748061044
H	-1.4614309597	-4.9234316815	1.5689005948
H	-1.6685949577	2.7431200472	-1.6594988917
H	-0.9851081191	4.2306500008	-0.9876649827
H	-0.6433417584	3.7786308605	-2.6627624322
N	5.2573782942	4.0517772212	-0.1794499738
C	5.1647740346	5.3408926748	0.1630126549
C	6.2794659597	6.1282206332	0.4503771122
C	7.5221725556	5.5247601940	0.3691598369
C	7.6433573322	4.1929356787	0.0142161399
C	6.4681223637	3.4929478706	-0.2544060051
N	3.8583019456	5.8381099784	0.1692214417
C	3.3931752887	6.9979373127	0.7307896341
O	4.0930152398	7.7858670409	1.3464959775
C	1.9196930208	7.2430607384	0.5396511392
N	6.4568970572	2.1348127590	-0.5914907295
C	7.4807070168	1.3905560017	-1.1172225337
O	8.5852619567	1.8395328875	-1.3731768200
C	7.1423893360	-0.0595714863	-1.3431241788
H	6.1626409797	7.1623251825	0.7220642350
H	8.4111551468	6.1024296246	0.5862343944
H	8.5997422829	3.7055047579	-0.0561385032
H	3.1733639256	5.2521305819	-0.3009787165
H	1.7977760292	8.1877020983	0.0101487756
H	1.4119046025	6.4540684432	-0.0077029555
H	1.4621145063	7.3600824211	1.5215220841
H	5.5700320119	1.6611683472	-0.4395256415
H	7.7718928580	-0.4478861583	-2.1383281785
H	7.3657079351	-0.6162230740	-0.4309199112
H	6.0952924725	-0.2172029459	-1.5903094917

1’e:C

E(a.u.)=-1680.5720057

C	-1.0708490457	2.6427610102	-0.4076999286
N	-1.2212042471	3.9635638117	-0.3642112090
C	-0.1692094652	4.6354125327	0.1078374328
C	0.9950506283	4.0505231000	0.5463980554
C	1.0496812300	2.6532524001	0.4508934694
N	0.0149276068	1.9519524745	-0.0291297123
N	-2.1307312152	1.8681818000	-0.8305854000
C	-3.2021893028	2.2776724448	-1.6370066225
N	-4.2916441184	1.4943536197	-1.4876321688
C	-5.4655726333	1.6690631451	-2.3087254612
N	2.1562917219	1.9107508109	0.7816898862
C	3.2816535743	2.3522023268	1.4915308809
N	4.3191090717	1.4942089276	1.4219551561
C	5.5610934181	1.7739285369	2.1041910084
O	3.3010981758	3.3937417499	2.1319743994
O	-3.1404660512	3.2086829228	-2.4252891583
H	-0.2724961338	5.7152088038	0.1425769694
H	1.8175272416	4.6251320923	0.9317110091

H	-2.1373385981	0.9069965430	-0.5003080900
H	-4.3244928077	0.8081002068	-0.7403298322
H	-6.1792739319	0.8893192621	-2.0536146848
H	-5.9363129534	2.6396855560	-2.1431732925
H	-5.2234719177	1.5842125919	-3.3683826902
H	2.1527012464	0.9450886682	0.4613272108
H	4.3167794187	0.7502514313	0.7294546046
H	6.2210771684	0.9196253915	1.9750371077
H	6.0550958520	2.6622346684	1.7059982616
H	5.3934216380	1.9252853542	3.1698451807
N	4.5230941382	-0.7478956077	-0.5517724384
C	5.6925002811	-1.2015246084	-0.9536260067
C	3.4400906938	-1.5455141850	-0.7079721676
C	3.5474778590	-2.8392491104	-1.2767099778
C	4.8124766717	-3.2848901904	-1.6961708800
C	5.8972182727	-2.4621975302	-1.5384469765
N	2.2595896573	-1.0401307708	-0.2775998256
C	1.1738151118	-1.7791701643	-0.3942004139
C	1.1788602241	-3.0821706703	-0.9690466044
C	2.3602771245	-3.5974267630	-1.4009926674
N	-0.0016059020	-1.1765953938	0.0075477941
C	-1.1820889290	-1.7590175538	0.4232893972
N	-2.2586895351	-1.0075038019	0.3036956316
C	-3.4442059192	-1.4883774766	0.7474665021
N	-4.5158929508	-0.6751235260	0.5906156653
C	-5.6889089625	-1.1081638092	1.0043921670
C	-5.9087213122	-2.3601344993	1.6026096832
C	-4.8353552597	-3.1970649554	1.7628752969
C	-3.5665775761	-2.7742169277	1.3311896055
C	-2.3893576211	-3.5476262318	1.4574669342
C	-1.2025327027	-3.0547223623	1.0140543852
H	6.5386483285	-0.5372628160	-0.8093182889
H	4.9130164373	-4.2689455674	-2.1369717070
H	6.8885357157	-2.7617104732	-1.8461993776
H	0.2579439523	-3.6284031931	-1.0998418027
H	2.3969140179	-4.5769826331	-1.8601226932
H	0.0042268506	-0.1573849671	-0.0060797745
H	-6.5263123473	-0.4329540962	0.8594896306
H	-6.9025579656	-2.6417065351	1.9191192186
H	-4.9476191724	-4.1747951521	2.2148530265
H	-2.4375508137	-4.5214904692	1.9275828507
H	-0.2893341972	-3.6132423395	1.1469364569

1'f:C

E(a.u.)=-1264.0004363

C	2.6419792887	-1.5172213044	0.2215602122
C	1.4064549007	-0.8563569422	0.1489832452
N	1.3332067857	0.4574480764	-0.0111845186
C	2.4678283704	1.1351897465	-0.1344449186
N	3.6982029320	0.6097778963	-0.1002941256
C	3.7493596661	-0.7132208016	0.0879838948
N	2.4121685470	2.4996032923	-0.2942673708

C	1.2693602027	3.2889846057	-0.5025762921
N	1.5386665588	4.6099156126	-0.4764427334
N	0.2349124499	-1.5633044094	0.2482383593
C	-1.1122425697	-1.1664633224	0.1215912006
N	-1.3595586487	0.1264675228	-0.1241802412
C	-2.7113353060	0.6111044659	-0.2828358289
O	-1.9739520658	-2.0305303295	0.2390533353
O	0.1519270260	2.8361540122	-0.7082733742
C	0.4945744702	5.5836086939	-0.6917196387
H	2.7238708220	-2.5843806823	0.3618833439
H	4.7421616900	-1.1487268668	0.1248428192
H	3.3160942041	2.9683420338	-0.2877124876
H	2.4564497603	4.9538219129	-0.2031885402
H	0.3162117738	-2.5545531617	0.3934437497
H	-0.5792523304	0.7682724809	-0.2070635217
H	-2.6639235975	1.6819216678	-0.4615176007
H	-3.2094756074	0.1349658398	-1.1279346708
H	-3.3069054657	0.4291626390	0.6121377264
H	0.9493787384	6.5710432942	-0.7159062353
H	-0.0129058000	5.4121033274	-1.6406292700
H	-0.2527759298	5.5625807104	0.1037064468
N	5.2269785830	3.9752229963	-0.2820098959
C	5.2953581340	5.2988680065	-0.0019674744
C	6.5216196940	6.0134696142	0.0270279365
C	7.7079351198	5.2913911302	-0.2695815994
C	7.6350588204	3.9704451507	-0.5558683240
C	6.3536441427	3.3266592745	-0.5434800460
N	4.1185730086	5.9178710754	0.2539210550
C	4.1360945341	7.2055322090	0.5459680029
C	5.2952476303	7.9887585859	0.6091714967
C	6.4973697491	7.3783453446	0.3410851159
N	6.2771854300	2.0096819845	-0.8321326272
H	8.6607205403	5.8057966604	-0.2627857011
H	8.5197625142	3.3930320795	-0.7867587947
H	3.1718666127	7.6633424928	0.7454373656
H	5.2310465405	9.0383427711	0.8569743590
H	7.4258025845	7.9357391259	0.3682905141
H	7.1226009196	1.4723036052	-0.8684938671
H	5.4136545792	1.5174878839	-0.6200504851

1'b:AcO$^-$

E(a.u.)=-10 19.452671

C 2.5036899153 -1.5322569465 -0.3196906350
C 1.4203055916 -0.6466576097 -0.1931439398
N 1.6033036504 0.6613477968 -0.1271906758
C 2.8659618085 1.1208691927 -0.1967506315
N 3.9594801334 0.3764185454 -0.3340717957
C 3.7425559194 -0.9433120646 -0.3867344800
N 2.9328356161 2.4904876191 -0.1358439531
C 4.0560009319 3.3181850000 -0.0238153059
N 3.7364583543 4.6269526449 -0.1346479876

N 0.1413498635 -1.1505621480 -0.1339685832
C -1.1176855182 -0.5365440861 -0.0165677252
N -1.1593200089 0.8008596627 0.0412102763
C -2.4153365251 1.5059352369 0.1579978316
O -2.1059139656 -1.2624738985 0.0243091046
O 5.1955456607 2.9185218597 0.1689756227
C 4.7397363935 5.6510028325 0.0187556314
H 2.3746179844 -2.6031361737 -0.3679974552
H 4.6267683865 -1.5632958654 -0.4944333032
H 2.0120341899 2.9456859809 -0.1279791260
H 2.7726030336 4.9262216464 -0.2953416415
H 0.0555934473 -2.1508775408 -0.1806683590
H -0.2949704863 1.3230132616 -0.0050480035
H -2.1931208010 2.5682811747 0.1848133395
H -3.0673908887 1.2989210621 -0.6911791383
H -2.9438051380 1.2274584177 1.0703687695
H 4.2550372505 6.6188983908 -0.0880406504
H 5.2155184196 5.6077354929 1.0001240228
H 5.5208513694 5.5694072085 -0.7390081673
C 0.1806678022 4.9003799142 -0.3401831232
C -1.2469385405 5.4289226688 -0.3827230669
O 1.1176124708 5.7119856783 -0.5408827168
O 0.3241876261 3.6731709349 -0.1041530474
H -1.8131901955 4.8951633093 -1.1473729285
H -1.7378992238 5.2345472550 0.5718227932
H -1.2798245271 6.4954935468 -0.5917109518

1'd:AcO$^-$

E(a.u.)=-1019.4600863

C	2.9206504361	-1.5048397793	-0.1426239918
C	1.6079200558	-1.0115745599	-0.1576455945
N	1.3787497022	0.3099332728	-0.1655089291
C	2.4261430557	1.1189596037	-0.1589109607
N	3.7155204885	0.7642905694	-0.1449132153
C	3.9199604226	-0.5549327785	-0.1371355224
N	2.2080354468	2.4835709632	-0.1668745808
C	1.0455407920	3.2634851711	-0.1818969283
N	-0.1357092962	2.6286174845	-0.1904968020
N	0.4679626835	-1.7634331693	-0.1660383796
C	0.3596430704	-3.1570244633	-0.1604957631
N	-0.9192317044	-3.5805531565	-0.1759545154
C	-1.2373160769	-4.9877137290	-0.1735090859
O	1.3269906185	-3.9100646123	-0.1430549598
O	1.1702392027	4.4854774207	-0.1862437379
C	-1.3823120638	3.3581488335	-0.2059292200
H	3.1288291152	-2.5590737638	-0.1358714133
H	4.9574715914	-0.8725823873	-0.1256888243
H	3.0461775403	3.0379114788	-0.1611874255
H	-0.1478571226	1.6183087605	-0.1862852438
H	-0.4013330825	-1.2110878903	-0.1779712788
H	-1.6964418501	-2.9149775537	-0.1928434500
H	-2.3198665972	-5.0895476605	-0.1871470016

H -0.8296366653 -5.4952412376 -1.0493051179
H -0.8527391834 -5.4867076424 0.7174577047
H -2.1885497352 2.6304734298 -0.2105028209
H -1.4822314020 3.9947787206 0.6739147427
H -1.4650073928 3.9868057742 -1.0932464420
C -3.0112734629 -0.6766205148 -0.2194281715
C -4.2037397155 0.2693734764 -0.2387772168
O -1.8699995220 -0.1481298990 -0.1979541364
O -3.2346625757 -1.9125009747 -0.2247914202
H -5.1490790886 -0.2670278490 -0.2705276116
H -4.1805539364 0.9038862231 0.6484145400
H -4.1343937482 0.9294024391 -1.1044472263

1'c:AcO$^-$

E(a.u.)=-1019.4571616
C 2.8942212015 -1.7933878313 -0.1747010605
C 1.6392475456 -1.1532435609 -0.1688877915
N 1.5572464286 0.1816261447 -0.1744714761
C 2.6975803277 0.8673640741 -0.1803742286
N 3.9321127953 0.3682998738 -0.1844204324
C 3.9913219103 -0.9699013990 -0.1821802760
N 2.5254196705 2.2402780878 -0.1827405373
C 3.4289257657 3.3077855467 -0.1693804430
N 4.7359098096 3.0038322300 -0.1600582923
N 0.4314474212 -1.7937238454 -0.1566185674
C 0.2002519795 -3.1750776627 -0.1508045566
N -1.1078945025 -3.4931320922 -0.1513182031
C -1.5315133154 -4.8724678911 -0.1499725967
O 1.0981017433 -4.0099925726 -0.1448085213
O 2.9851401399 4.4516071373 -0.1658031057
C 5.7532215688 4.0285684026 -0.1413512736
H 2.9799490081 -2.8639676794 -0.1709887803
H 4.9875214537 -1.3983244119 -0.1857004391
H 1.5661075686 2.5399663295 -0.1816521352
H 4.9787243324 2.0231632547 -0.1671530614
H -0.3916816863 -1.1771970425 -0.1364491814
H -1.8407576432 -2.7796073753 -0.1762171121
H -2.6187413750 -4.8903932002 -0.1533776723
H -1.1710124321 -5.4064289223 -1.0305872351
H -1.1769400963 -5.4015848595 0.7357549314
H 6.7249852860 3.5440788399 -0.1042055803
H 5.7079657191 4.6522096060 -1.0346365071
H 5.6505558105 4.6725809726 0.7320947466
C -3.0827582102 -0.5831374799 -0.1725460476
C -4.2028365652 0.4464082401 -0.2322587881
O -1.9108802610 -0.1402171987 -0.0638070563
O -3.3906693678 -1.7990025652 -0.2433977855
H -5.1853614021 -0.0193553086 -0.2415192466
H -4.1301771069 1.1255739453 0.6174969932
H -4.0878635217 1.0501902138 -1.1338586804

1'e-left:AcO$^-$

E(a.u.)=-1019.4468484

C	3.0240350524	-1.8283171678	-0.1763709281
C	1.7917221453	-1.1511607039	-0.1731905925
N	1.7539972290	0.1849944558	-0.1766106881
C	2.9180444624	0.8363786889	-0.1844910450
N	4.1344006959	0.3062569298	-0.1923995792
C	4.1446063410	-1.0331035537	-0.1860110331
N	2.7500916022	2.2148087233	-0.2014821771
C	3.6820845319	3.2470297856	-0.1025883218
N	3.1101115799	4.4780086763	-0.1926641802
N	0.5610164513	-1.7509288483	-0.1660200754
C	0.2813155461	-3.1210310365	-0.1561173232
N	-1.0381675297	-3.3922949658	-0.1641815067
C	-1.5118046486	-4.7549900921	-0.1530655763
O	1.1481770305	-3.9886629239	-0.1412301438
O	4.8777874604	3.0891637864	0.0631346534
C	3.9081840789	5.6825489214	-0.1497004713
H	3.0788949915	-2.9011294245	-0.1721315975
H	5.1265336659	-1.4954973747	-0.1909990793
H	1.7787055915	2.4704643495	-0.2333252164
H	2.1402937226	4.5659044772	-0.4303769943
H	-0.2387942825	-1.1047906174	-0.1542073967
H	-1.7428368402	-2.6516365543	-0.1918766381
H	-2.5978076598	-4.7351514578	-0.2047558645
H	-1.1324463412	-5.3196831358	-1.0055811607
H	-1.2171762860	-5.2783581952	0.7580807984
H	3.2385742387	6.5373527823	-0.1859579031
H	4.4855275019	5.7321265305	0.7725422172
H	4.5982415783	5.7403913447	-0.9928489189
C	-2.8931088203	-0.3938696270	-0.2055419515
C	-3.9685789611	0.6822003908	-0.2668653584
O	-1.7027350356	0.0000912269	-0.1096275620
O	-3.2525280472	-1.5959540688	-0.2633082010
H	-4.9704833155	0.2600163787	-0.2488254069
H	-3.8500272362	1.3758490236	0.5656170306
H	-3.8445504936	1.2601232758	-1.1842018086

1'e-right: AcO^-

E(a.u.)=-1019.4457238

C	-2.2425064754	-1.9466930749	0.4605359095
C	-1.9157838065	-0.6540051648	0.0379571155
N	-0.6551706081	-0.2844864452	-0.1743902636
C	0.3032003084	-1.1911691853	0.0546721607
N	0.1109586457	-2.4405338001	0.4842904540
C	-1.1648926675	-2.7825117931	0.6645888549
N	1.5785127006	-0.7188879120	-0.1428281665
C	2.7530191907	-1.4652648404	-0.3065689677
N	3.8640089680	-0.7176284026	-0.1373812845
N	-2.8308736704	0.3505406252	-0.2058525256
C	-4.2172663366	0.3217580652	-0.0701590149
N	-4.8145625316	1.4979838116	-0.3772281996
C	-6.2463085485	1.6689568631	-0.2636091391

O	-4.8377990716	-0.6673082448	0.2847518281
O	2.7758507291	-2.6510703567	-0.6079889842
C	5.1760343471	-1.2687727620	-0.3683002133
H	-3.2583402206	-2.2580019150	0.6226310436
H	-1.3378533592	-3.7979515382	1.0076140025
H	1.6598277996	0.2983112438	-0.2478399691
H	3.7966222752	0.2537999176	0.1734343877
H	-2.3966174207	1.2069303265	-0.5069091343
H	-4.2599832018	2.2974301383	-0.6180605470
H	-6.4984276789	2.6686845789	-0.6052129844
H	-6.7744489713	0.9445873117	-0.8819434006
H	-6.5812681396	1.5544267720	0.7677215989
H	5.9055479067	-0.4692050374	-0.2599697115
H	5.4193116422	-2.0578034674	0.3459668070
H	5.2636099394	-1.6848448146	-1.3729903482
C	2.9158720669	2.6503675059	0.1815049852
C	2.9273088410	4.1661486985	0.3283300929
O	3.8695227768	2.0167890980	0.7012578266
O	1.9472157207	2.1288472493	-0.4255726941
H	2.2800205685	4.6465088653	-0.4021354840
H	2.5623558409	4.4207554132	1.3257988104
H	3.9397313483	4.5580524751	0.2432115285

1'f:AcO$^-$

E(a.u.)=-1019.4541979

C	2.7495256885	-1.4452343911	-0.1828598277
C	1.5142011342	-0.7839983625	-0.1829207120
N	1.4365063783	0.5383921025	-0.1835797507
C	2.5712782138	1.2322654004	-0.1836382192
N	3.8051249380	0.7101714889	-0.1833144010
C	3.8555678807	-0.6237498453	-0.1830839940
N	2.5149417110	2.6039808152	-0.1844087569
C	1.3730284245	3.4160823363	-0.1833600191
N	1.6695459190	4.7322574008	-0.1878564140
N	0.3398076584	-1.4999136746	-0.1823415548
C	-1.0062578356	-1.0876745777	-0.1799726812
N	-1.2567137474	0.2284753450	-0.1785494479
C	-2.6113614064	0.7299214488	-0.1754925875
O	-1.8703974773	-1.9589854970	-0.1792546992
O	0.2218296845	2.9934670115	-0.1777697911
C	0.6229521440	5.7247848900	-0.1900344113
H	2.8364656607	-2.5211862841	-0.1824741816
H	4.8487171913	-1.0609620705	-0.1829491867
H	3.4264691713	3.0762203556	-0.1850423614
H	2.6328626955	5.0738791828	-0.2009884258
H	0.4198986694	-2.5018353623	-0.1822383534
H	-0.4771168197	0.8780987239	-0.1793051003
H	-2.5659263946	1.8155996258	-0.1755861633
H	-3.1613475413	0.4012088774	-1.0578662840
H	-3.1574116371	0.4011808989	0.7093152971
H	1.0904847955	6.7066545315	-0.1786093672

H	-0.0056124633	5.6498035977	-1.0790941563
H	-0.0198853993	5.6357084659	0.6870153038
C	5.1492145963	5.2481544635	-0.2058844059
C	6.5670491101	5.8035095667	-0.1839682050
O	5.0274690865	3.9967943932	-0.1845208010
O	4.1956105618	6.0651021430	-0.2262571079
H	6.5900375089	6.8653568885	-0.4181149623
H	6.9867544985	5.6583720669	0.8135189712
H	7.2013774021	5.2579380444	-0.8817732463

1'g:AcO$^-$

E(a.u.)=-1019.4573095

C	2.4252961541	-1.6998396294	-0.2126441900
C	1.2555498115	-0.9163611240	-0.2004731633
N	1.3339635260	0.4110263680	-0.1941158805
C	2.5427847311	0.9579931100	-0.1992240583
N	3.7158685157	0.3232692285	-0.2111800609
C	3.6152541733	-1.0124961137	-0.2177133761
N	2.6186199015	2.3373509810	-0.1917144725
C	1.6306029759	3.3312638491	-0.1706842907
N	0.3487117818	2.9367078940	-0.1623497145
N	0.0381207674	-1.5333944991	-0.1957205560
C	-1.2333618368	-0.9380830360	-0.1854691219
N	-2.2242023574	-1.8529747655	-0.1897430737
C	-3.6088655562	-1.4484627807	-0.1810749072
O	-1.4300052476	0.2707747952	-0.1736054023
O	1.9919821951	4.5053181929	-0.1620890513
C	-0.7305300531	3.8953210463	-0.1336034900
H	2.3838127717	-2.7780579926	-0.2180908792
H	4.5530586352	-1.5578828579	-0.2274984637
H	3.5513923481	2.7111943979	-0.1955130117
H	0.1466344576	1.9430990013	-0.1678686772
H	0.0743373575	-2.5614939565	-0.2010774134
H	-2.0206481966	-2.8554160314	-0.2018852342
H	-4.2234388388	-2.3456181665	-0.1840703001
H	-3.8527855110	-0.8635800426	0.7071154842
H	-3.8608287557	-0.8521810947	-1.0594595665
H	-1.6677181346	3.3460245988	-0.1675150574
H	-0.7096861171	4.4965516891	0.7763487837
H	-0.6875063767	4.5700508821	-0.9887759181
C	-0.6851184787	-5.0892902509	-0.2088030424
C	-0.4664682698	-6.5952186931	-0.1896043451
O	-1.8748294811	-4.6864200517	-0.2187692545
O	0.3291457964	-4.3447800971	-0.2052189708
H	0.5857198617	-6.8561571009	-0.2734294260
H	-0.8600314799	-7.0026453822	0.7430369623
H	-1.0237810694	-7.0619523668	-1.0018968637

1'h: AcO$^-$

E(a.u.)=-1019.4536

C	1.1734940456	0.4985783575	0.0664578074
C	1.3817638779	-0.8977946424	-0.0260486296

N	2.6093928945	-1.3989693940	-0.1222743439
C	3.6188301304	-0.5240117099	-0.1224276439
N	3.5422292835	0.7997997132	-0.0372630034
C	2.2921833007	1.2839849643	0.0550404231
N	4.8620877665	-1.1228577385	-0.2282934793
C	6.1611467798	-0.6099278193	-0.2879418050
N	6.2966667360	0.7233900701	-0.2185294230
N	0.2785363166	-1.7026675626	-0.0301223956
C	0.2026574172	-3.1055866972	-0.0125769017
N	-1.0661463686	-3.5459168805	-0.1522456167
C	-1.3692262042	-4.9553477515	-0.1097918224
O	1.1635705776	-3.8465055085	0.1287120399
O	7.0975982096	-1.3949548539	-0.3984866486
C	7.5918475133	1.3591530287	-0.2817451909
H	0.1801358515	0.9135896563	0.1402572549
H	2.2053927854	2.3625849335	0.1232849071
H	4.8339460522	-2.1257635698	-0.2872022830
H	5.4493682608	1.2663907152	-0.1343270236
H	-0.6161861479	-1.1964631232	-0.0278945602
H	-1.8428036839	-2.8959417373	-0.2909807882
H	-2.4420832352	-5.0756131150	-0.2408225694
H	-0.8588231037	-5.5027947847	-0.9035871457
H	-1.0846240079	-5.4005777990	0.8452108231
H	7.4499895369	2.4321295471	-0.1875242834
H	8.2399381883	1.0201228076	0.5265590083
H	8.0905068935	1.1547983137	-1.2296849838
C	-3.2014679942	-0.6862367429	-0.3254474094
C	-4.4040952289	0.2426164039	-0.4057322074
O	-2.0969966906	-0.1593290064	-0.0287055009
O	-3.3800818114	-1.9087487042	-0.5463010435
H	-5.2843972595	-0.2650863039	-0.7925106749
H	-4.6268906179	0.6248192122	0.5920549035
H	-4.1724600639	1.1031377214	-1.0331097897

1'd:AcO$^-$:A

E(a.u.)=-1683.5792628

C	2.8087474375	-1.6244327161	0.5954929329
C	1.5639901065	-1.0769832303	0.2466898021
N	1.4656609025	0.2132083563	-0.1065843278
C	2.5702100894	0.9399538717	-0.1260662230
N	3.8090410683	0.5159823721	0.1554458411
C	3.8835672475	-0.7681416240	0.5196027912
N	2.4839787534	2.2749323157	-0.4631658579
C	1.4001210956	3.0756316586	-0.8168164410
N	0.1904632525	2.5158442742	-0.9252719683
N	0.3738990192	-1.7414998923	0.2246887013
C	0.1353010895	-3.0848893612	0.5364182894
N	-1.1608300927	-3.4257494293	0.4081223253
C	-1.6068530313	-4.7702285597	0.6821242390
O	1.0149783715	-3.8622972746	0.8885205479
O	1.6116663121	4.2754223104	-1.0203954793
C	-0.9730417868	3.2973117642	-1.2784165796

H	2.9122826876	-2.6519775057	0.8922021211
H	4.8751658983	-1.1345676734	0.7631486599
H	3.3559428809	2.7913666357	-0.4081383696
H	0.0854937175	1.5338316325	-0.7098087151
H	-0.4276570830	-1.1617436348	-0.0642736680
H	-1.8606151487	-2.7410079507	0.1097274241
H	-2.6838048323	-4.8055720179	0.5359480580
H	-1.1409216132	-5.4943398073	0.0120682772
H	-1.3852625617	-5.0655952076	1.7085231620
H	-1.8267859745	2.6265062457	-1.2851997646
H	-1.1505997197	4.0951439180	-0.5563593461
H	-0.8631196348	3.7474103451	-2.2652427339
C	-2.9356352628	-0.4966952954	-0.6410838067
C	-4.0236606110	0.4871617447	-1.0478723257
O	-1.7604155103	-0.0504493225	-0.5845281965
O	-3.2706479858	-1.6807850219	-0.3914354333
H	-5.0107542652	0.0315029488	-1.0324622692
H	-4.0120568570	1.3474105559	-0.3773950914
H	-3.8188401062	0.8620131261	-2.0519503119
N	5.1482608470	3.9970777397	-0.1578105177
C	5.0629533426	5.2864737909	0.1847550513
C	6.1848439601	6.0856050897	0.4019118876
C	7.4264566661	5.4924169883	0.2534252841
C	7.5393421781	4.1593839610	-0.1001708615
C	6.3569448036	3.4479330438	-0.2994976959
N	3.7539000993	5.7704084584	0.2664326634
C	3.3099133597	6.9197977765	0.8647421771
O	4.0360391654	7.7128106069	1.4427336991
C	1.8239568301	7.1452273895	0.7692306854
N	6.3385772426	2.0884123302	-0.6300030000
C	7.3349461470	1.3554700260	-1.2201520850
O	8.4154008820	1.8172177293	-1.5479725942
C	6.9985833676	-0.0988823835	-1.4218836233
H	6.0759675868	7.1205161441	0.6737256031
H	8.3210292769	6.0794705755	0.4163763979
H	8.4945232716	3.6794805931	-0.2202491327
H	3.0474443729	5.1753328593	-0.1604213448
H	1.6550423219	8.1052173486	0.2819421449
H	1.2976160669	6.3649471666	0.2268022238
H	1.4247072140	7.2197618320	1.7803518281
H	5.4661891124	1.6053463622	-0.4240846483
H	7.6239977603	-0.4991017760	-2.2143010102
H	7.2227782738	-0.6422759894	-0.5019261117
H	5.9495779984	-0.2587262138	-1.6612132837

Geometry of transition states

TS1

E(a.u.)=-790.8460531

C	0.8535055649	2.2528574312	-1.1536502864
C	1.3501234042	1.0409312799	-0.6448402643
N	0.5361203356	0.0552074497	-0.2826582670
C	-0.7791483924	0.2783184961	-0.4132708265
N	-1.3589807506	1.3811227439	-0.8817476649
C	-0.5131407090	2.3505739173	-1.2470650098
N	-1.5959035431	-0.7288002926	0.0281664762
C	-2.9586662360	-0.8418804535	-0.4342387865
N	-3.8454630067	-0.6558160250	0.5498944671
N	2.7093476424	0.8775840117	-0.5259265880
C	3.5071089337	-0.1818336404	-0.0581621883
N	2.8745757275	-1.2886844126	0.3553221665
C	3.6006154054	-2.4320812104	0.8604868002
O	4.7222768531	-0.0328861312	-0.0583754812
O	-3.2393595155	-1.1143713651	-1.5836687298
C	-5.2746134064	-0.7472093651	0.3414431594
H	1.5055831147	3.0585421153	-1.4553815468
H	-0.9658916677	3.2567949178	-1.6342725675
H	-1.1329094978	-1.6045881201	0.2085651401
H	-3.4911929956	-0.3994625025	1.4524828415
H	3.2736685453	1.6569959180	-0.8158005191
H	1.8668739988	-1.2889321969	0.3149266686
H	4.1395712393	-2.1888235155	1.7764719807
H	2.8859361167	-3.2215688062	1.0747397628
H	4.3172132151	-2.7978656600	0.1258510521
H	-5.6356793675	0.0771919505	-0.2738581305
H	-5.5252653143	-1.6847894035	-0.1512666518
H	-5.7687506940	-0.7111881307	1.3075899931

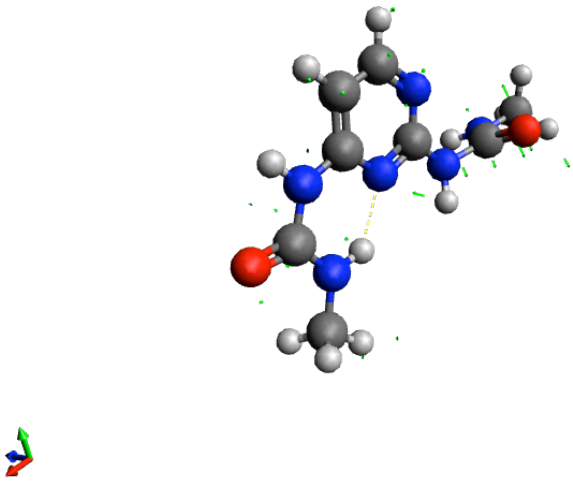


Figure S1. Geometry of transition states of **TS1**

1'a-TS-1'h

E(a.u.)=-790.8473858

C	0.6092536979	2.4490996890	1.1890279073
C	1.2132627795	1.1965780913	0.9617834171

N	0.5158100599	0.1599486479	0.5059764837
C	-0.7831725600	0.3663579566	0.2716352477
N	-1.4557104098	1.5003677264	0.4437372462
C	-0.7278334076	2.5285206155	0.9065397080
N	-1.4452788317	-0.7503866810	-0.1968494661
C	-2.7778682628	-0.9819201808	-0.5606952005
N	-3.6268495067	0.0516847488	-0.4638383756
N	2.5486774983	1.0191592593	1.1643742467
C	3.1317190622	-0.2991633829	1.2847212613
N	3.9039048363	-0.6120003110	0.2394122389
C	4.6160210657	-1.8690598499	0.1446050888
O	2.9471240411	-1.0027501239	2.2556518299
O	-3.0916611149	-2.1032981172	-0.9442020848
C	-5.0231763260	-0.0780985601	-0.8104989655
H	1.1649515563	3.2962182033	1.5618177797
H	-1.2631979878	3.4593278810	1.0556121079
H	-0.8673959159	-1.5667682755	-0.2954993424
H	-3.2498094659	0.9266579308	-0.1295563658
H	3.0374487074	1.7488871739	1.6556528468
H	3.9553938673	0.0449295604	-0.5168063149
H	5.2463722072	-1.8432657009	-0.7388338067
H	5.2410003986	-2.0190071062	1.0234225861
H	3.9220343881	-2.7054285895	0.0630118089
H	-5.1474555995	-0.3690723886	-1.8537711111
H	-5.5207248227	-0.8198697595	-0.1854494310
H	-5.5029299543	0.8846815430	-0.6577313406

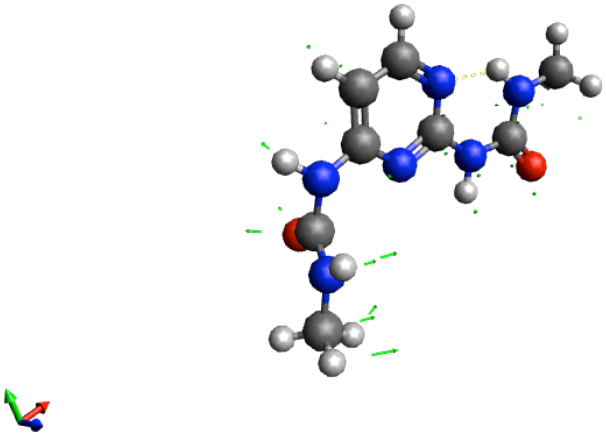


Figure S2. Geometry of transition state for **1'a** → **1'h** rotation

1'h-TS-1'g

E(a.u.)=-790.8315628

C -0.62936 2.56701 0.51077
C -0.90795 1.23544 0.16269
N 0.03682 0.44853 -0.34784
C 1.23638 0.99049 -0.52323
N 1.61381 2.22511 -0.23247
C 0.65241 3.00251 0.29038
N 2.23189 0.14879 -1.09119
C 2.80607 -0.94371 -0.46949
N 2.70536 -0.98479 0.88220
N -2.16627 0.73435 0.39109
C -2.75846 -0.41770 -0.16444
N -3.89812 -0.77086 0.47565
C -4.68008 -1.91020 0.04692
O -2.32010 -0.99879 -1.13613
O 3.39049 -1.80185 -1.12184
C 3.37720 -2.00362 1.65825
H -1.38245 3.22136 0.92493
H 0.93459 4.01980 0.53566
H 2.21369 0.06100 -2.09319
H 2.35570 -0.18247 1.37139
H -2.77220 1.33102 0.92621
H -4.10800 -0.36594 1.36918
H -5.62427 -1.90091 0.58398
H -4.88393 -1.84609 -1.01975
H -4.16721 -2.85229 0.24694
H 3.06223 -1.90938 2.69396
H 3.10376 -2.99458 1.30163
H 4.46323 -1.90575 1.60952

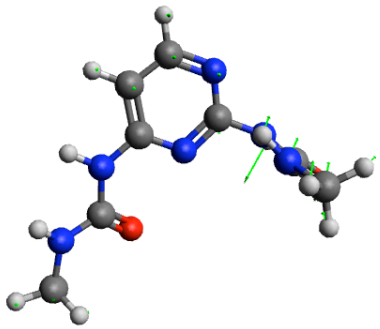


Figure S3. Geometry of transition state for **1'h** → **1'g** rotation

TS2

E(a.u.)=-790.8426122

C 0.76528 2.15765 0.06852
C 1.15199 0.86886 0.41061
N 0.29421 -0.13490 0.48795
C -0.98434 0.14915 0.21310
N -1.46834 1.34591 -0.12325
C -0.58128 2.33522 -0.18939
N -1.83570 -0.92741 0.30434
C -3.21930 -1.06873 0.11447

N -3.90715 0.02997 -0.22740
N 2.51102 0.60052 0.71887
C 3.27617 -0.17775 -0.13684
N 4.42132 -0.66344 0.40710
C 5.42283 -1.31680 -0.40771
O 2.94437 -0.38115 -1.29607
O -3.71488 -2.17753 0.27136
C -5.33549 -0.00951 -0.44436
H 1.47632 2.96575 0.00814
H -0.96928 3.30950 -0.46295
H -1.38990 -1.79175 0.56006
H -3.39031 0.89018 -0.33029
H 2.72347 0.57280 1.70231
H 4.69872 -0.34707 1.31763
H 4.97774 -2.13437 -0.97058
H 5.89325 -0.62653 -1.11067
H 6.18661 -1.72429 0.24903
H -5.59385 -0.68386 -1.26078
H -5.86262 -0.33611 0.45199
H -5.66878 0.99225 -0.70003

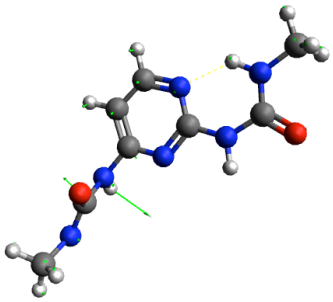


Figure S4. Geometry of transition states of **TS2**

TS3

E(a.u.)=-790.8383373

C	-0.9278712661	1.5704158712	-0.0962055732
C	-1.0182340064	0.1751493457	-0.0278325659
N	0.0819313786	-0.5847771927	0.0318018263
C	1.2512683060	0.0381280047	0.0204878143
N	1.4588741936	1.3449949440	-0.0485453220
C	0.3457804840	2.0899837027	-0.1020181531
N	2.4087314938	-0.7821179779	0.0998957543
C	2.8594242684	-1.6277871294	-0.8963820858
N	2.4055072899	-1.3724238012	-2.1487294662
N	-2.1881627150	-0.5424230880	-0.0130720902
C	-3.5025811947	-0.0650610668	-0.0506663914
N	-4.4314367279	-1.0463555148	-0.0482191803
C	-5.8457046080	-0.7436013983	-0.0991627245
O	-3.7789526847	1.1220508773	-0.0760555188
O	3.6422268099	-2.5362140081	-0.6415290045
C	2.9106603601	-2.0962515174	-3.2948597612
H	-1.8038815866	2.1923289277	-0.1401824212
H	0.4898815942	3.1630797391	-0.1539777727

H	2.6665008260	-1.0928577771	1.0213247098
H	1.9059659928	-0.5206586262	-2.3225900959
H	-2.0390604742	-1.5364917059	0.0417407856
H	-4.1513419677	-2.0085474641	-0.0835387034
H	-6.3972911251	-1.6754093399	-0.0156160385
H	-6.1302994438	-0.0922611436	0.7257057126
H	-6.1148737116	-0.2564615183	-1.0365357389
H	2.3207275044	-1.8176913482	-4.1638854550
H	3.9599216927	-1.8693941188	-3.4927738073
H	2.8125693172	-3.1683956755	-3.1383087330

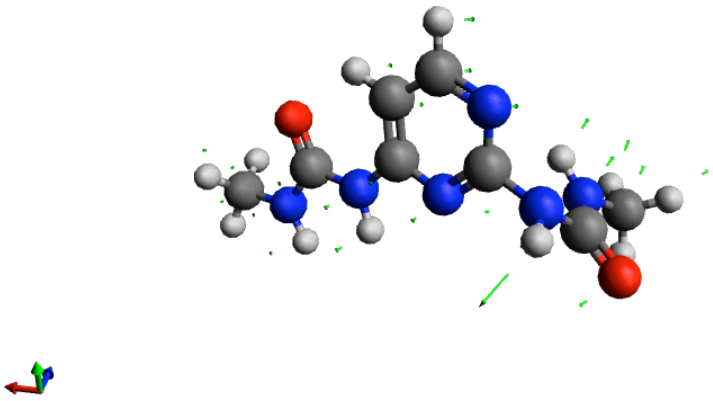


Figure S5. Geometry of transition states of **TS3**

TS4

E(a.u.)=-1019.4340831

C	2.9769741047	-1.6828491312	-0.1833559395
C	1.7098539311	-1.0737970973	-0.1535055516
N	1.6062974061	0.2647643561	-0.2130332670
C	2.7266277367	0.9628051383	-0.2971027271
N	3.9670901893	0.4974170660	-0.3274139651
C	4.0581996767	-0.8409775210	-0.2726869026
N	2.5874132443	2.3779952856	-0.3751898623
C	2.1571210556	3.1992431115	0.6473922076
N	2.2289152550	2.6854586559	1.9004187839
N	0.5168107370	-1.7309247071	-0.0725634927
C	0.3141775012	-3.1158535216	-0.0024800660
N	-0.9861845643	-3.4581041628	0.0384781534
C	-1.3840611931	-4.8435008491	0.1076992108
O	1.2313779818	-3.9291790296	0.0211864708
O	1.7603424893	4.3371096665	0.4159750498
C	1.9340175119	3.4895084007	3.0652277442
H	3.0851134070	-2.7512185494	-0.1381775258
H	5.0609398370	-1.2527340810	-0.3010940853

H	2.3852432460	2.7519005852	-1.2867926444
H	2.6874319982	1.8056304770	2.0443854815
H	-0.3171704656	-1.1265427181	-0.0668650865
H	-1.7321461161	-2.7582258656	-0.0010681200
H	-2.4705087318	-4.8809541891	0.1322417396
H	-1.0357972172	-5.4075134238	-0.7590302844
H	-0.9988895793	-5.3285276396	1.0056356739
H	1.9073897186	2.8384163890	3.9348399140
H	2.6843890850	4.2654756912	3.2288375241
H	0.9620120809	3.9666775855	2.9589167767
C	-2.9922100819	-0.5655922717	-0.0424079523
C	-4.1535128180	0.4185112682	-0.0380442660
O	-1.8243681820	-0.1017943178	-0.0367605640
O	-3.2830087504	-1.7886713520	-0.0520297593
H	-4.7886132958	0.2314597906	0.8286542614
H	-3.8129527593	1.4509289182	-0.0177533439
H	-4.7693144386	0.2606580423	-0.9245335862

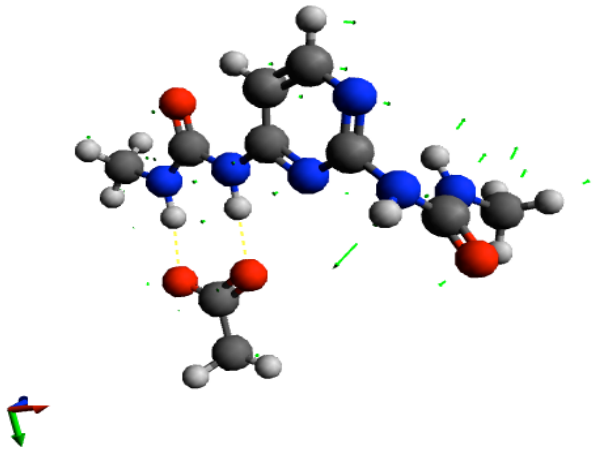


Figure S6. Geometry of transition states of **TS4**

TS5

E(a.u.)=-1019.4380378

C	-0.1769721833	-1.7681319180	0.3805672512
C	-0.2839721845	-0.5391768901	-0.3110304413
N	0.7131434561	-0.0939291050	-1.0703937764
C	1.8125784732	-0.8504624667	-1.1243808826
N	2.0270751123	-2.0097569820	-0.5109500152
C	1.0004250803	-2.4478420900	0.2367734663
N	2.8054313673	-0.3190376630	-1.9287671811
C	4.0909042205	-0.7554625802	-2.2627055918
N	4.5017304866	-1.9156782349	-1.7278308999
N	-1.4541015332	0.1546285731	-0.2002205734
C	-1.7324351383	1.4729743300	-0.6027616357
N	-3.0598734100	1.7255870183	-0.6027478667
C	-3.5947247869	3.0362895100	-0.8768897680
O	-0.8712860646	2.2912493047	-0.8874302125
O	4.7687905927	-0.0636257759	-3.0158549274
C	5.8119320633	-2.4565947249	-2.0040345536
H	-0.9864147543	-2.1421626595	0.9882796049
H	1.1524679537	-3.3949894469	0.7423153895

H	2.5649601432	0.5572151640	-2.3582452857
H	3.8517478883	-2.3973778836	-1.1231517075
H	-2.2109537237	-0.3503638449	0.2799130088
H	-3.7235440862	0.9862017423	-0.3613647139
H	-4.1440532372	3.4213666020	-0.0159859516
H	-2.7785882434	3.7157127462	-1.1032292455
H	-4.2715046972	3.0073840601	-1.7321949005
H	5.9233515771	-3.3820234509	-1.4457651937
H	5.9389975608	-2.6718337567	-3.0654152717
H	6.5984539165	-1.7667299879	-1.6977831290
C	-4.6422560317	-1.1445695855	0.8435838650
C	-5.6637617954	-2.1009697531	1.4416143632
O	-3.4356848041	-1.3470529900	1.1414893188
O	-5.0559256869	-0.2188802230	0.1037823915
H	-6.6690513615	-1.9027821667	1.0774444255
H	-5.3890383491	-3.1303290296	1.2096661579
H	-5.6533578204	-2.0052958416	2.5285244819

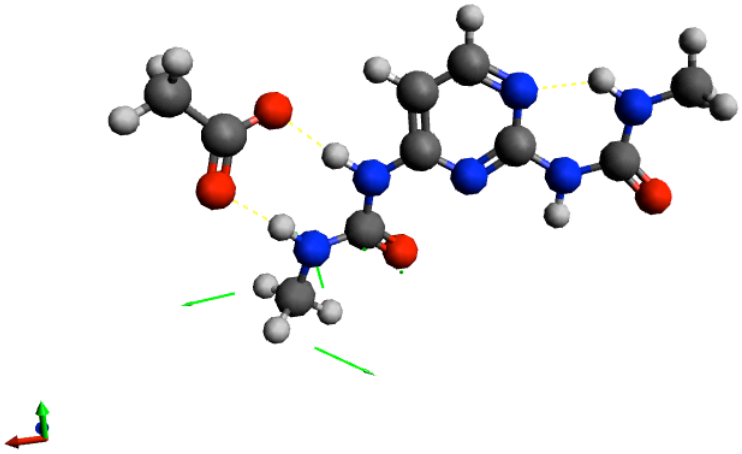


Figure S7. Geometry of transition states of **TS5**

TS6

E(a.u.)=-1019.4528698

C	0.0996752267	-1.5952053583	0.2570014257
C	-0.0172403517	-0.1891047792	0.2247648067
N	1.0749241992	0.5750730920	0.1263555932
C	2.2442921668	-0.0504531915	0.0744453128
N	2.4717845198	-1.3531046561	0.0943161993
C	1.3645425008	-2.1130307237	0.1876014863
N	3.3981391258	0.7822858235	-0.0097948384
C	3.7500472123	1.5504256997	-1.1013300887
N	3.1852526503	1.2069185557	-2.2847684039
N	-1.2665751795	0.3545844087	0.2675088926
C	-1.6389111581	1.7012063371	0.4361340669
N	-2.9532745424	1.8934809325	0.2016549681
C	-3.5601070829	3.1882748474	0.3920068832
O	-0.8728738331	2.5875555860	0.7814879986
O	4.5544414892	2.4709238205	-0.9908735806
C	3.5626384394	1.8546718551	-3.5208026906
H	-0.7733322814	-2.2262625597	0.3314234588
H	1.5193548264	-3.1857453073	0.2076729127

H	3.7241952398	1.1710593384	0.8589296636
H	2.6207022553	0.3807835786	-2.3403193246
H	-2.0345462915	-0.3285414504	0.2065771325
H	-3.5525601422	1.1218483287	-0.1000709891
H	-4.6254168286	3.0960440463	0.1938691146
H	-3.4259123657	3.5485822937	1.4129514720
H	-3.1440549312	3.9335666391	-0.2879304957
H	2.9035359495	1.5008624028	-4.3089124433
H	3.4534277571	2.9341648037	-3.4354836347
H	4.5945396989	1.6326047278	-3.7994809186
C	-4.4001999275	-1.3251408419	-0.3358044125
C	-5.3828001844	-2.4660988054	-0.5544122272
O	-3.2586053353	-1.6359997427	0.0958105857
O	-4.7761112510	-0.1575396311	-0.6016134135
H	-5.0049708661	-3.1194825879	-1.3425295809
H	-5.4601477135	-3.0691098134	0.3504641893
H	-6.3688029912	-2.1051176687	-0.8365191204

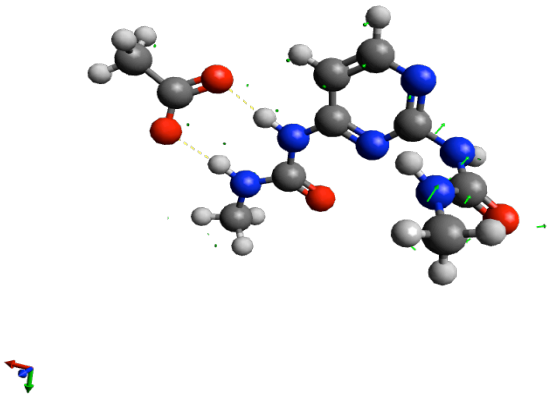


Figure S8. Geometry of transition states of **TS6**

QTAIM based charts representing bond paths and bond critical points for investigated molecules and complexes

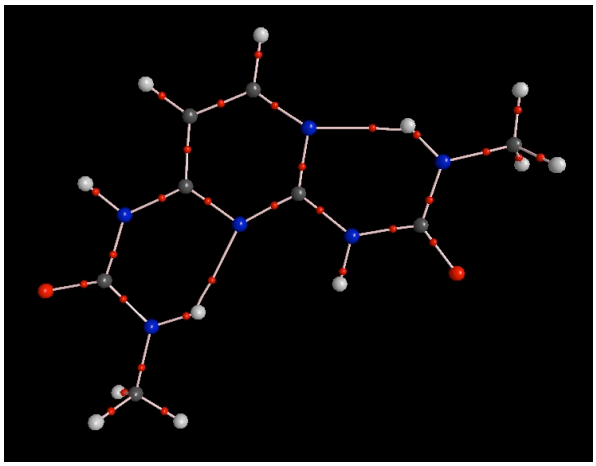


Figure S9. QTAIM-based bond paths in **1'a**

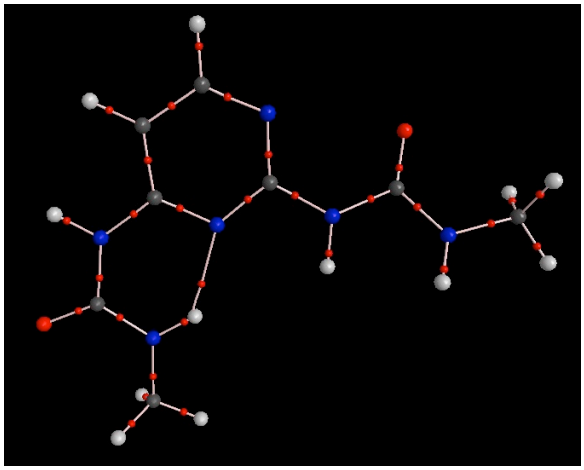


Figure S10. QTAIM-based bond paths in **1'b**

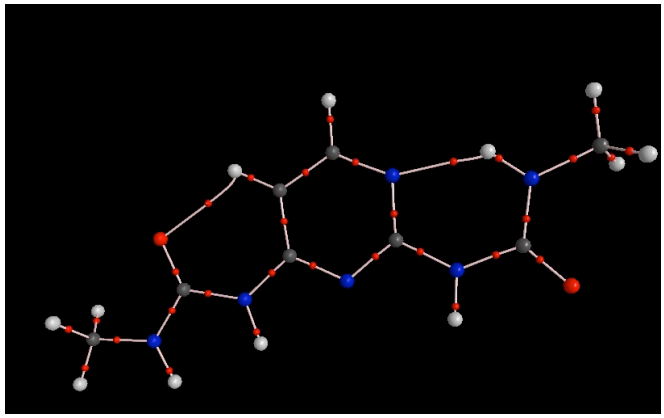


Figure S11. QTAIM-based bond paths in **1'c**

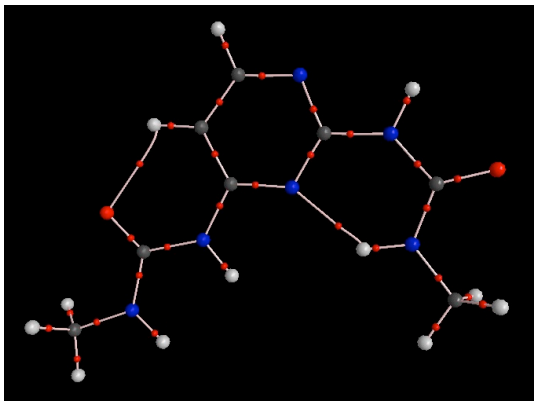


Figure S12. QTAIM-based bond paths in **1'd**

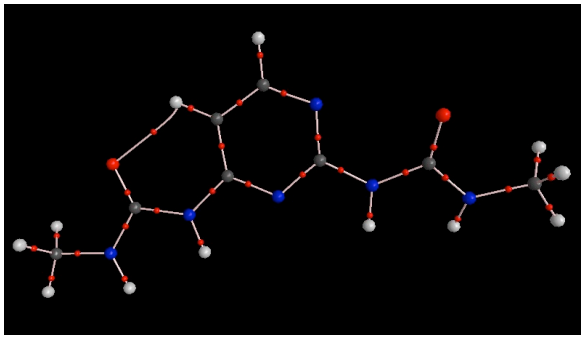


Figure S13. QTAIM-based bond paths in **1'e**

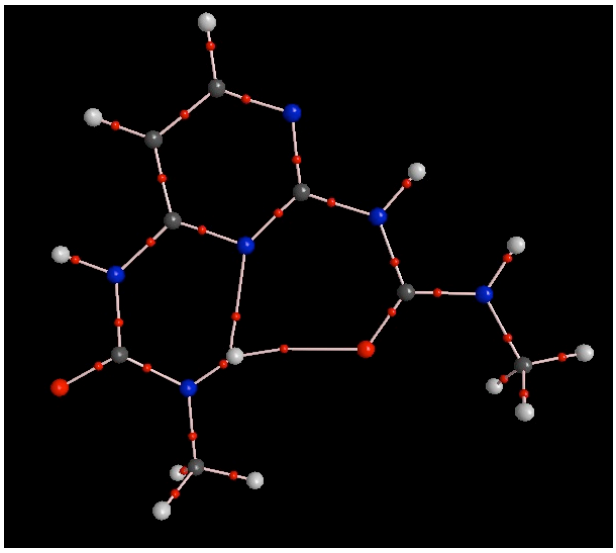


Figure S14. QTAIM-based bond paths in **1'f**

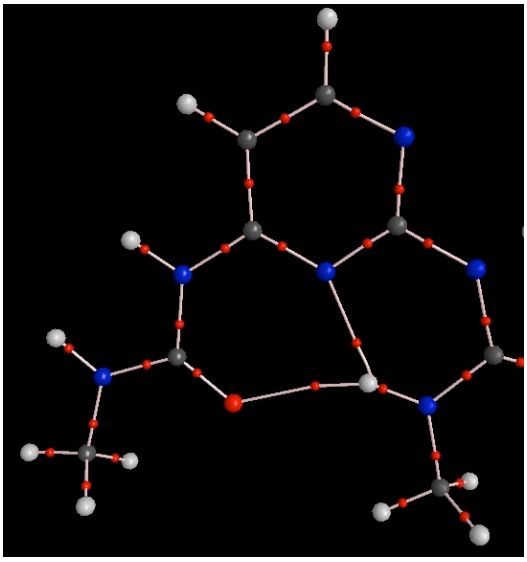


Figure S15. QTAIM-based bond paths in **1'g**

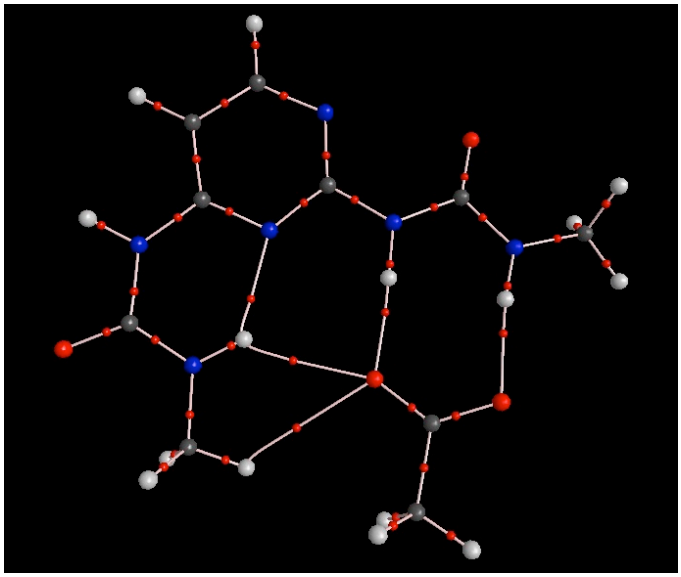


Figure S16. QTAIM-based bond paths in **1'b:AcO**$^{-}$

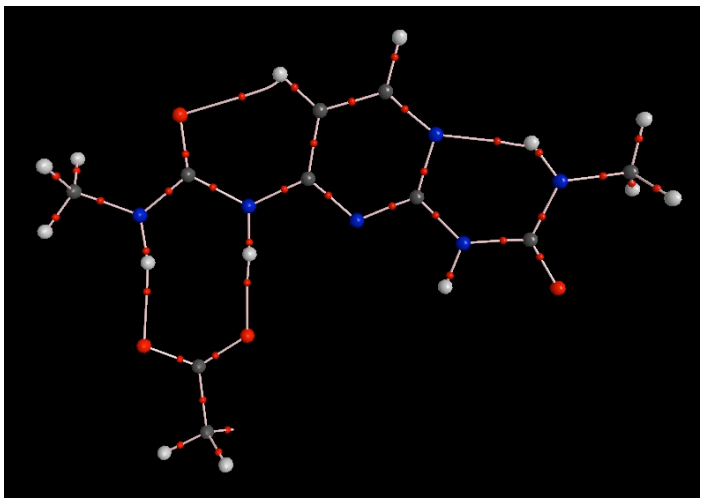


Figure S17. QTAIM-based bond paths in **1'c:AcO**$^{-}$

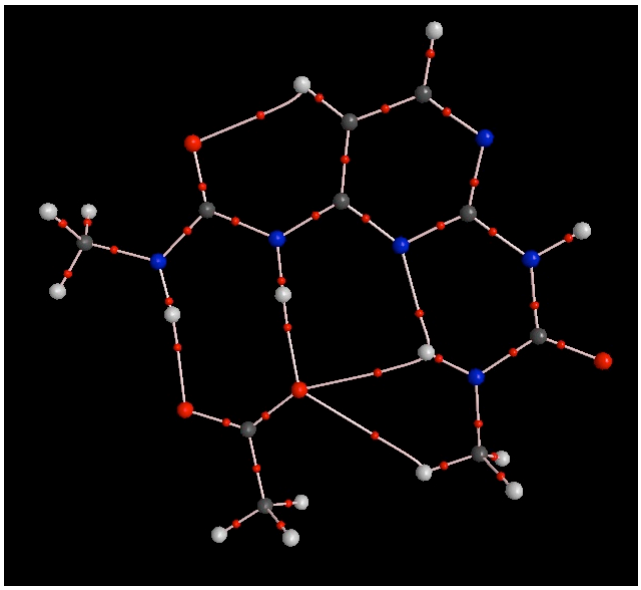


Figure S18. QTAIM-based bond paths in **1'd:AcO$^-$**

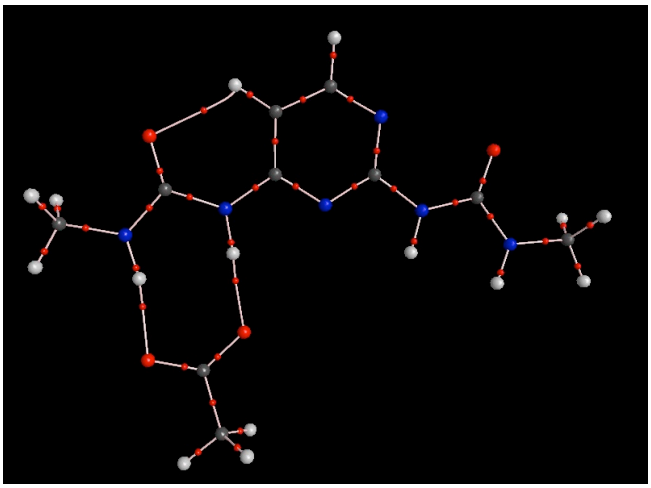


Figure S19. QTAIM-based bond paths in **1'e:AcO$^-$ left**

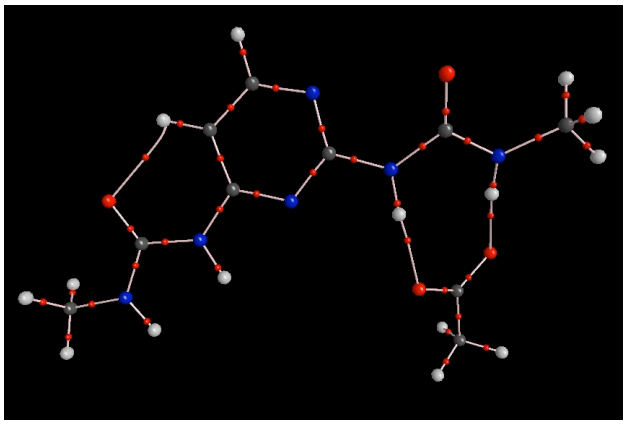


Figure S20. QTAIM-based bond paths in **1'f:AcO$^-$ right**

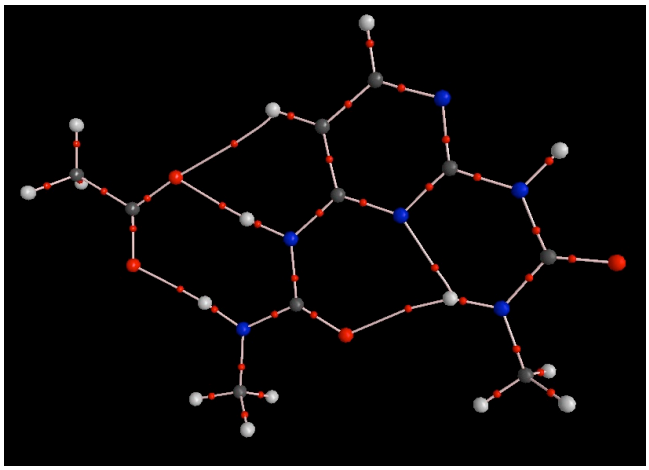


Figure S21. QTAIM-based bond paths in **1'g:AcO$^-$**

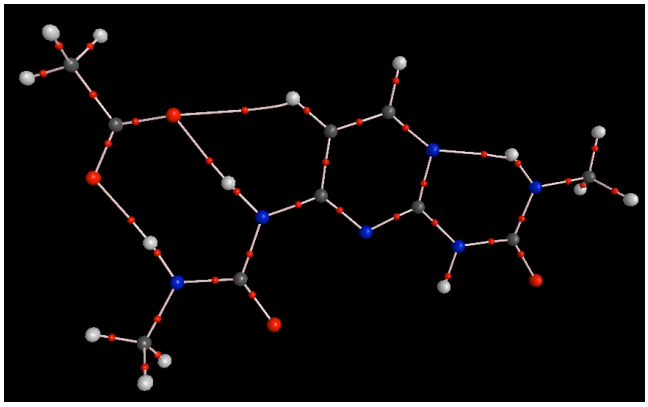


Figure S22. QTAIM-based bond paths in **1'h:AcO**$^-$

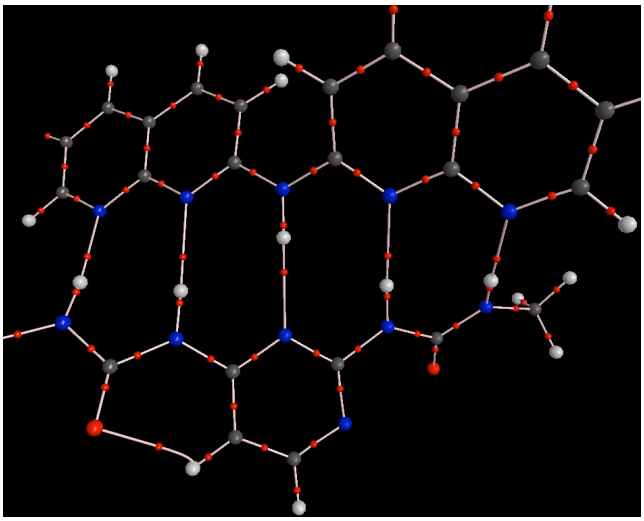


Figure S23. QTAIM-based bond paths in **1'e:C**

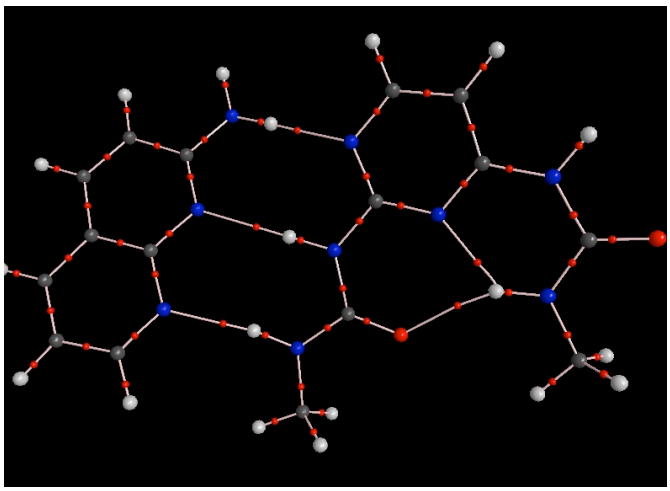


Figure S24. QTAIM-based bond paths in **1'f:C**

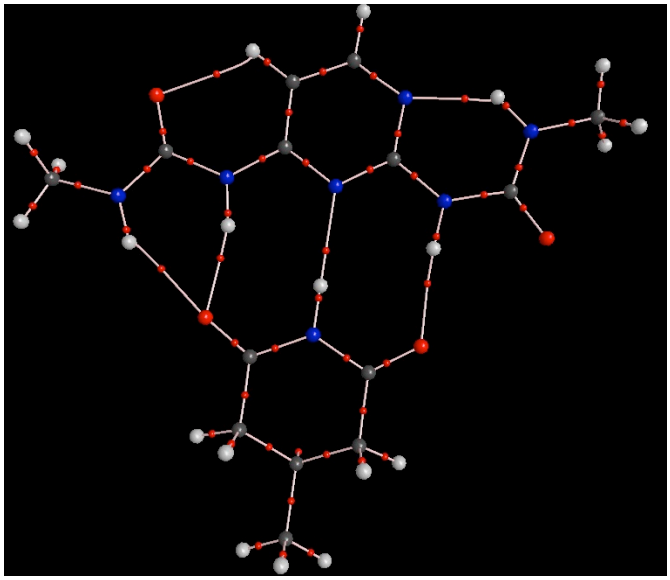


Figure S25. QTAIM-based bond paths in **1'c:B**

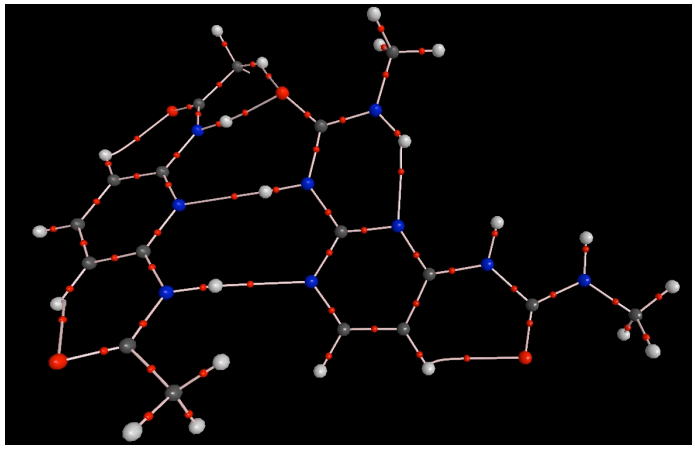


Figure S26. QTAIM-based bond paths in **1'd:A**

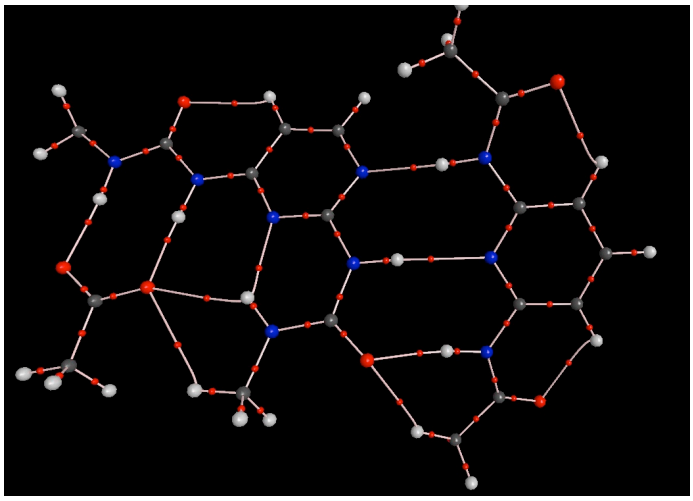


Figure S27. QTAIM-based bond paths in **1'd:AcO$^-$:A**

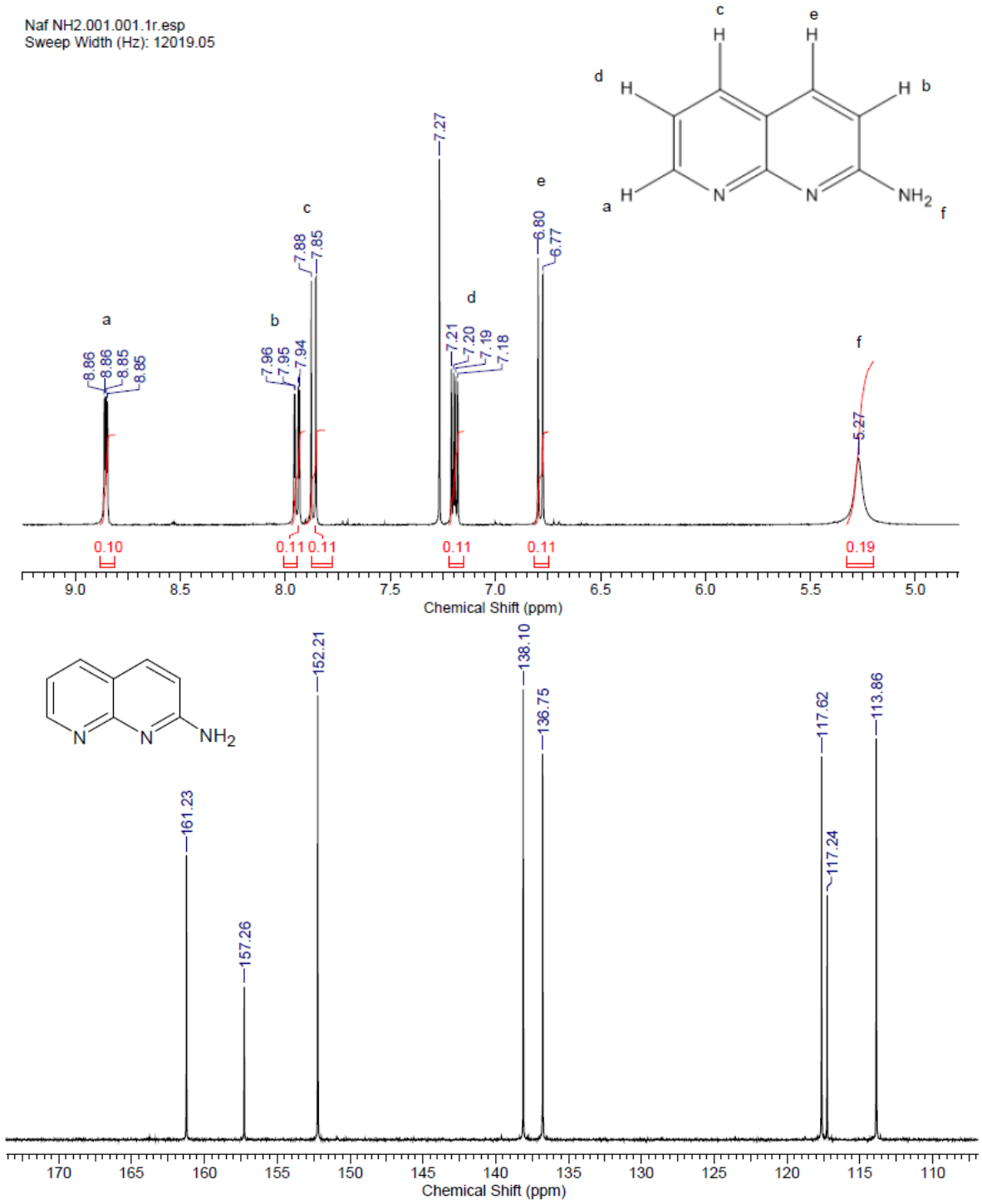


Figure S28. ^{1}H and ^{13}C NMR (TMS, $CDCl_3$) spectra of 2-Amino-1,8-naphthyridine

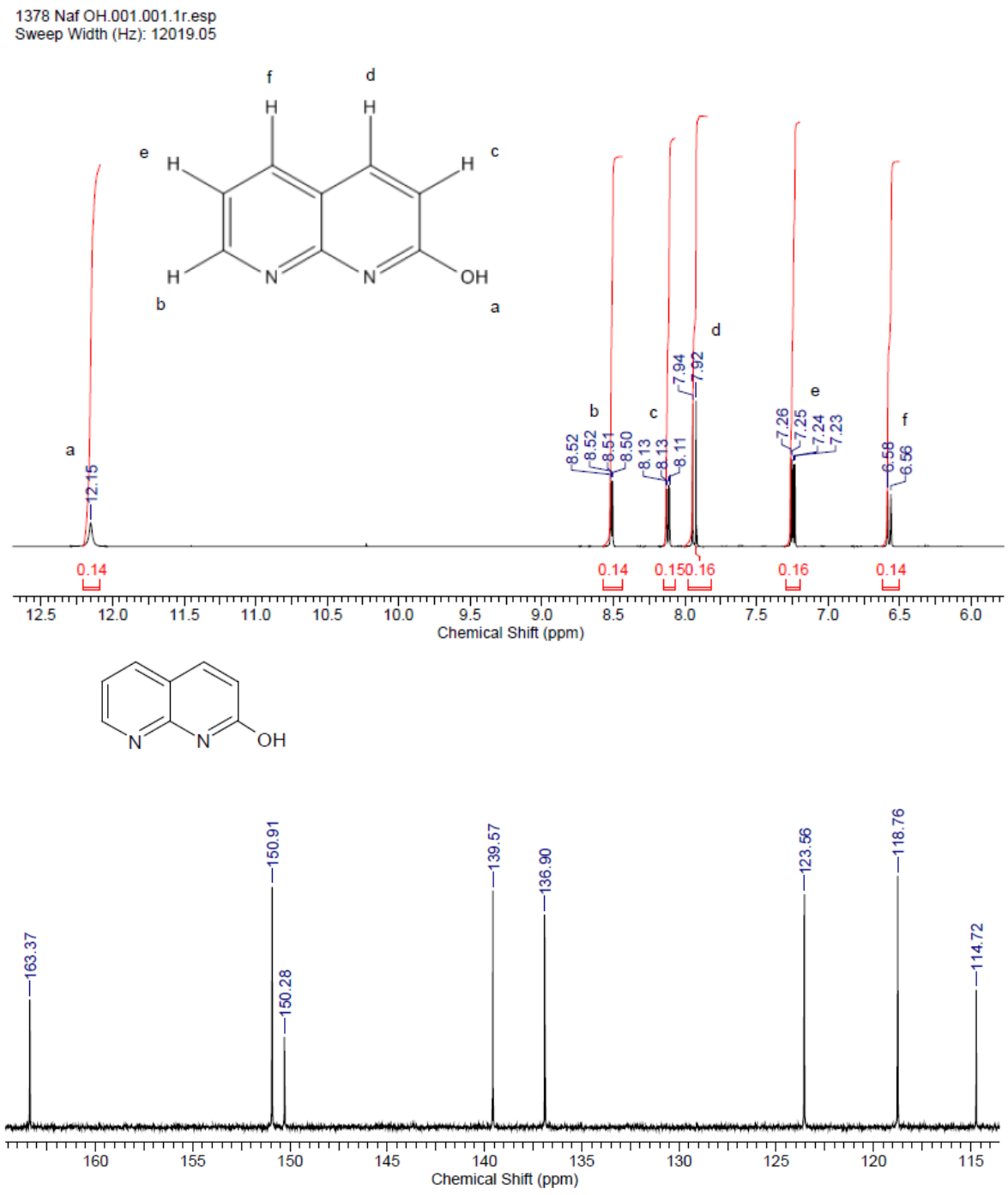


Figure S29. ^{1}H and ^{13}C NMR (TMS, $CDCl_3$) spectra of 2-hydroxy-1,8-naphthyridine

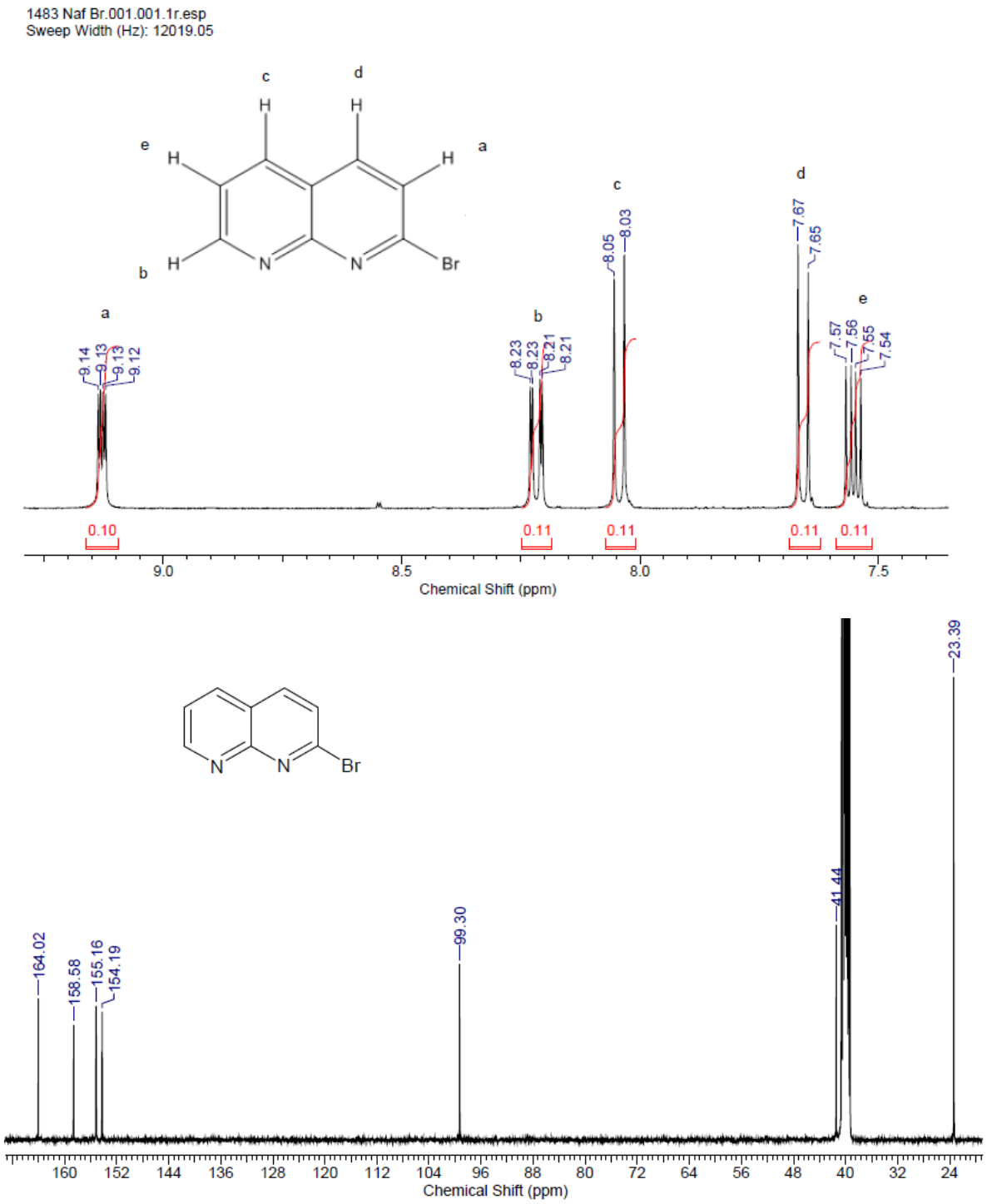


Figure S30. ^{1}H and ^{13}C NMR (TMS, $CDCl_3$) spectra of 2-Bromo-1,8-naphthyridine

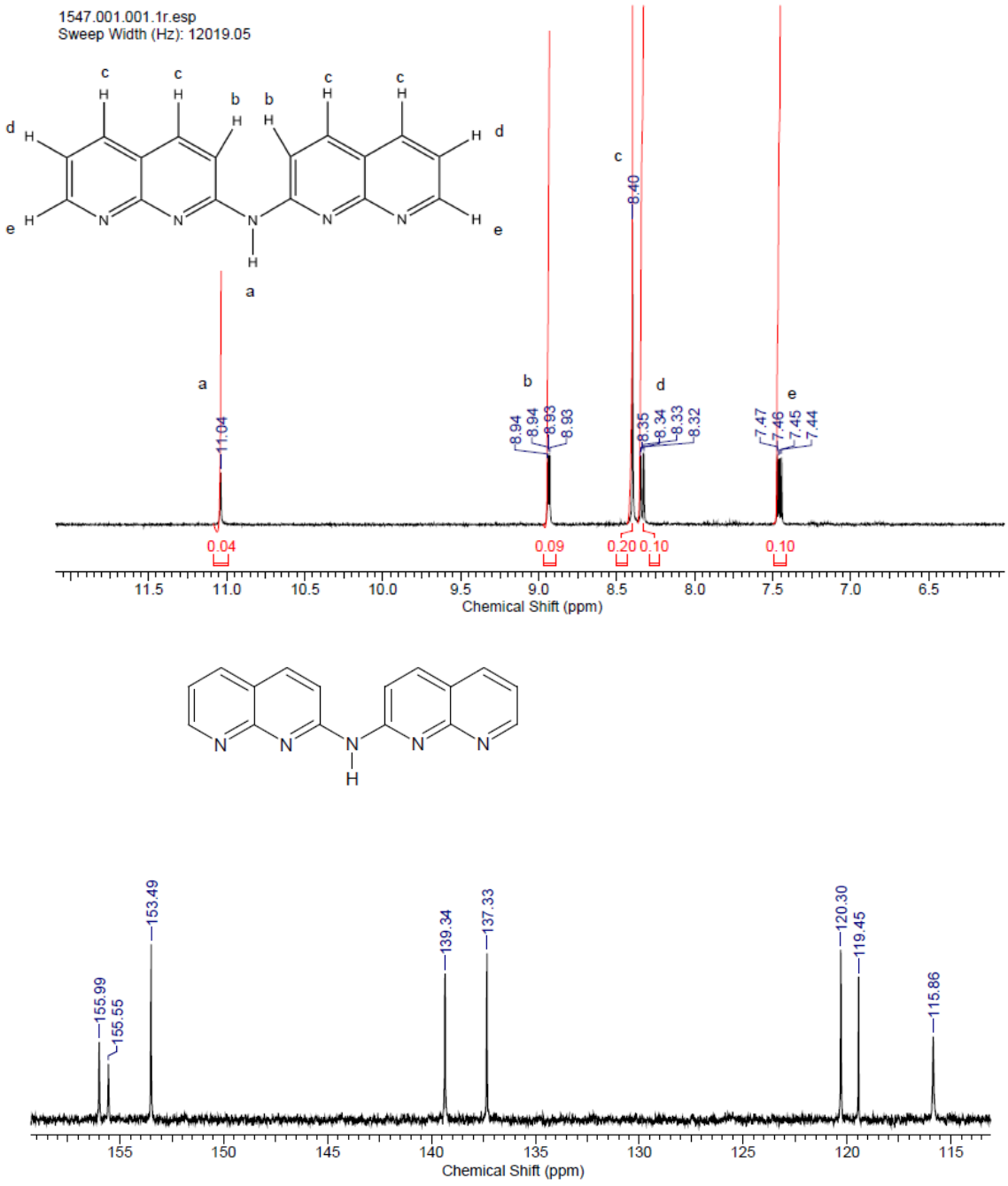


Figure S31. ^{1}H and ^{13}C NMR (TMS, $CDCl_3$) spectra of Bis(1,8-naphthyridin-2-yl)amine (**C**)

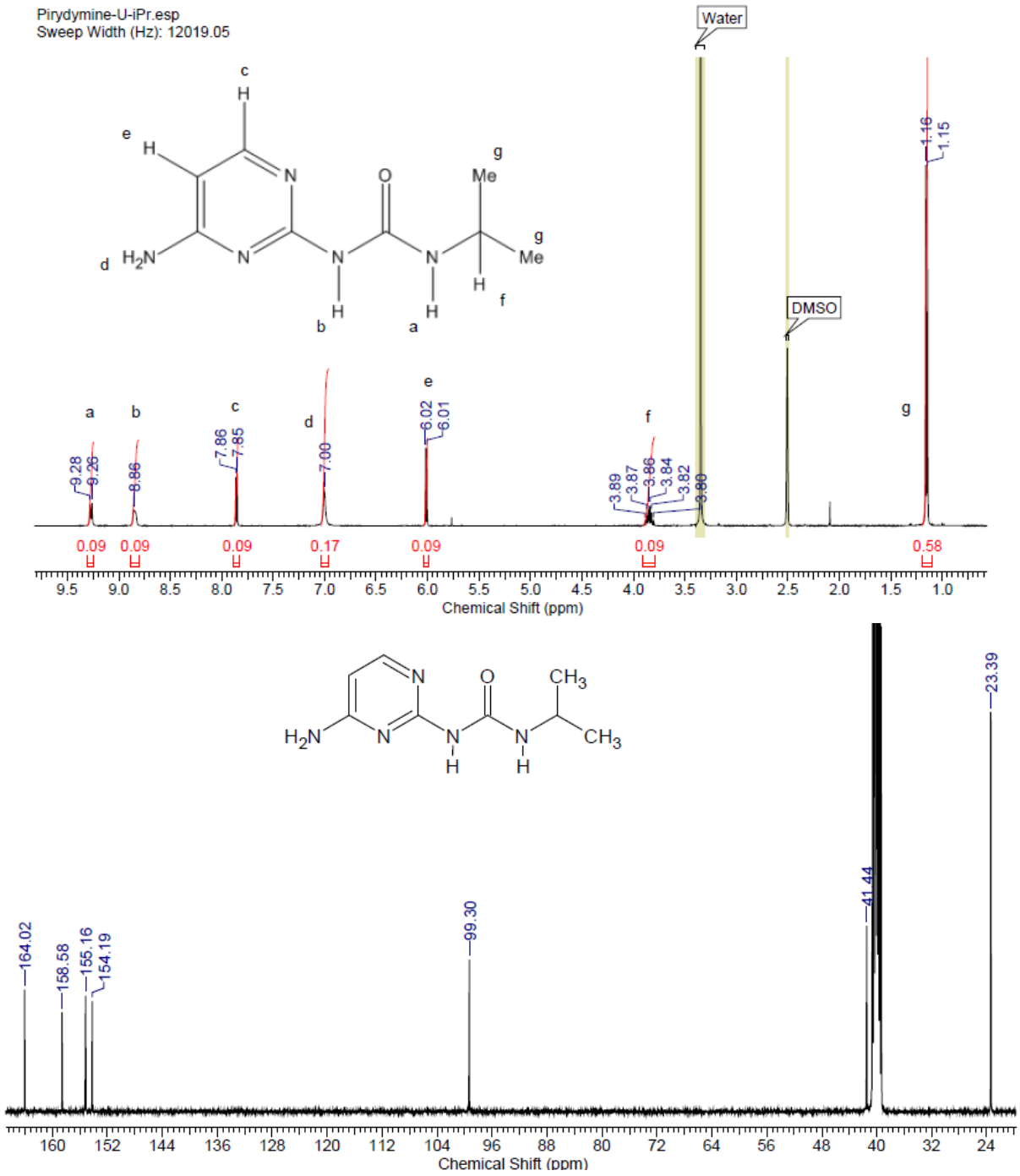


Figure S32. ^{1}H and ^{13}C NMR (TMS, $CDCl_3$) spectra of 1-(4-aminopyrimidin-2-yl)-3-isopropylurea

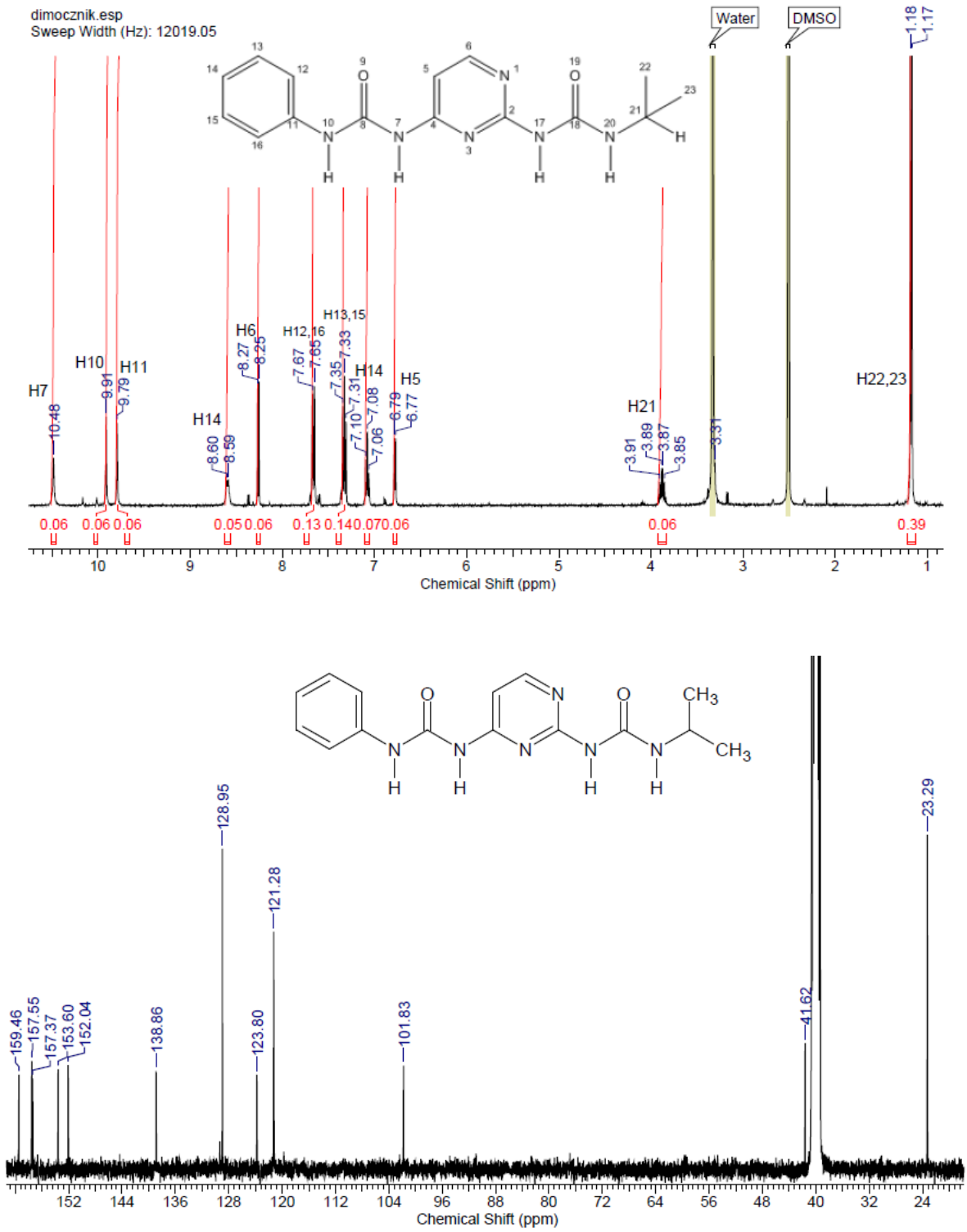


Figure S33. ^{1}H and ^{13}C NMR (TMS, $CDCl_3$) spectra of 1-(2-(3-isopropylureido)pyrimidin-4-yl)-3-phenylurea (**1**)

Example of titration experiment in DMSO

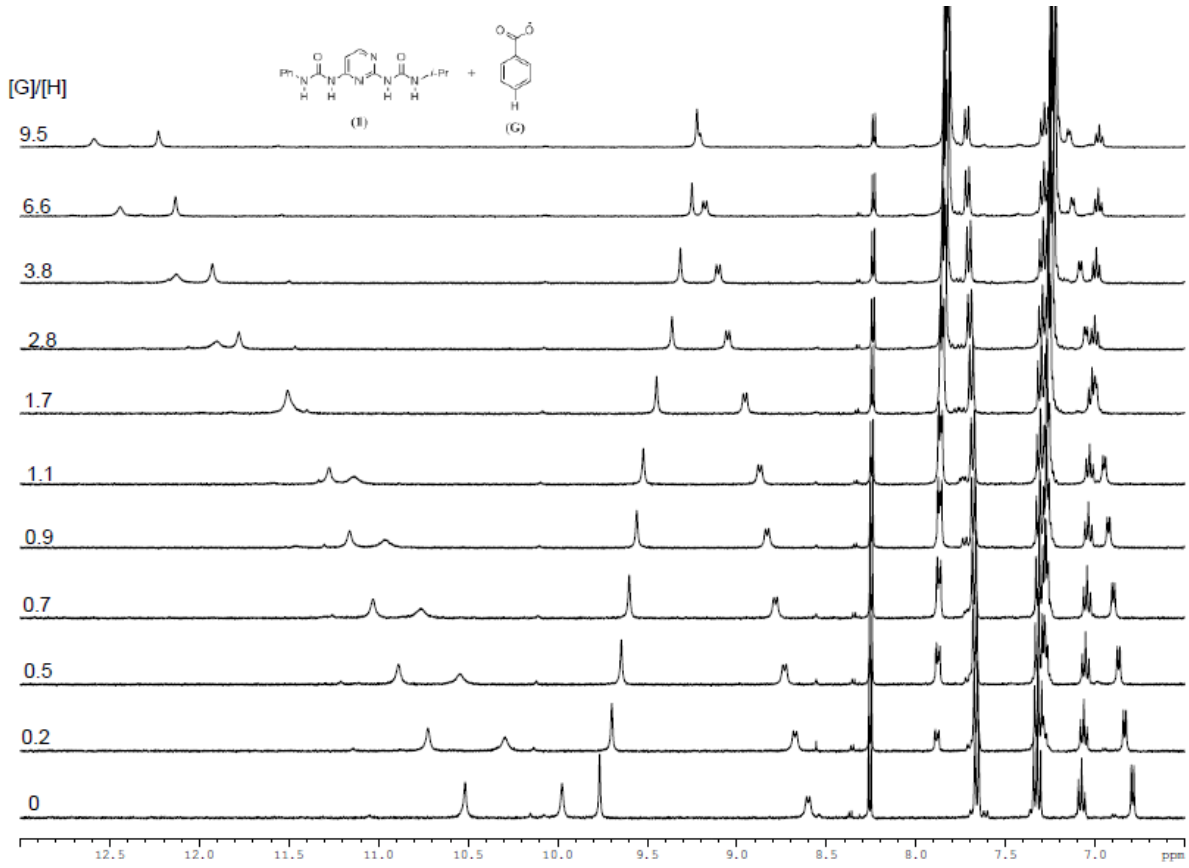
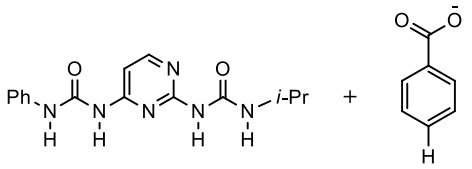


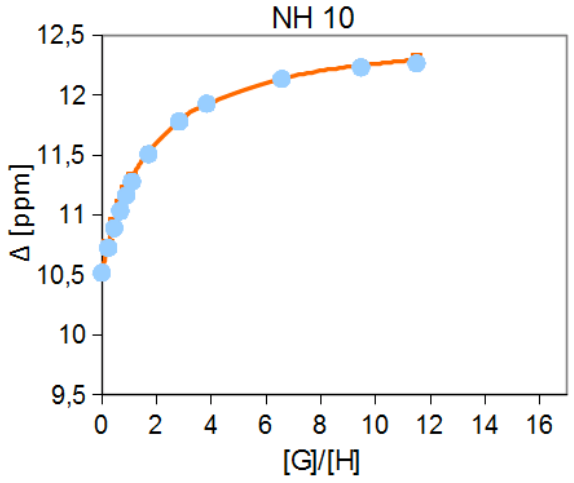
Figure S34. Stacked representative ^{1}H NMR (25 °C, DMSO) titration of (**1**) with (**G**)

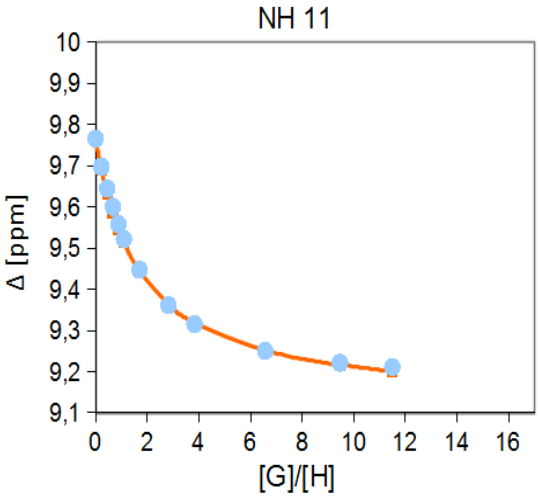
Titration curves

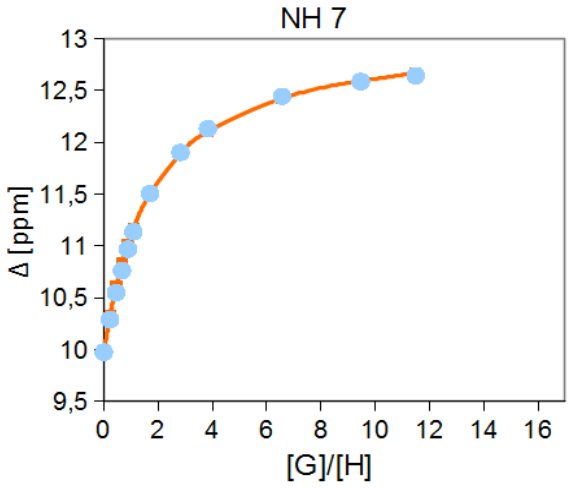
Complex **1:G**. The [G]/[H] on the x-axis refers to the guest-to-host molar ratio.

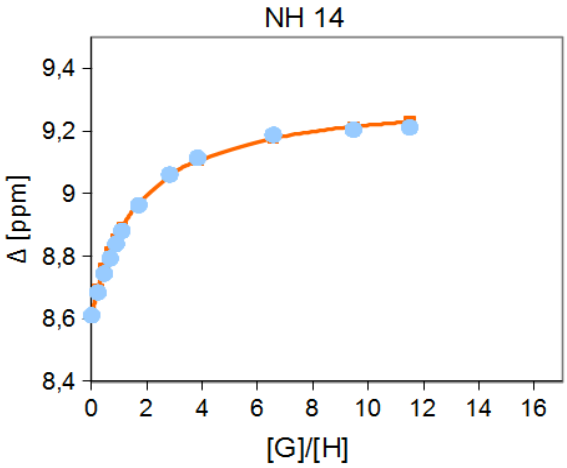


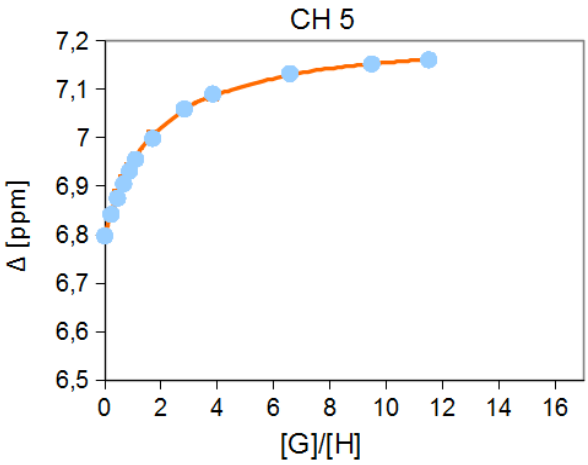
(1) **(G)**



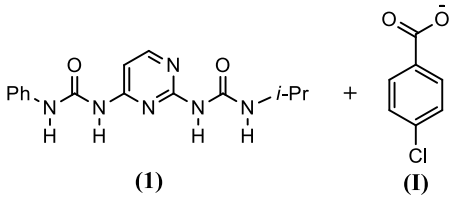




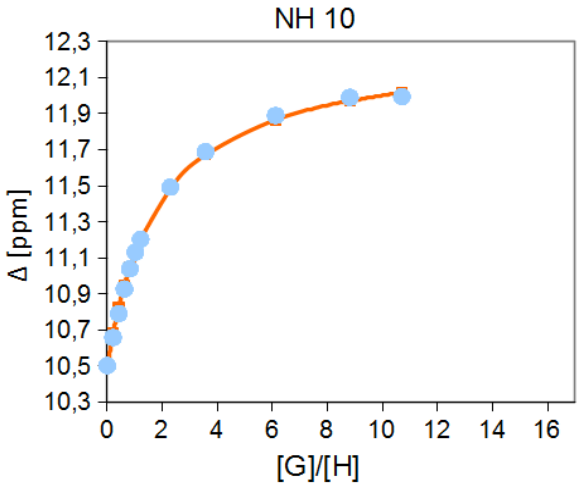


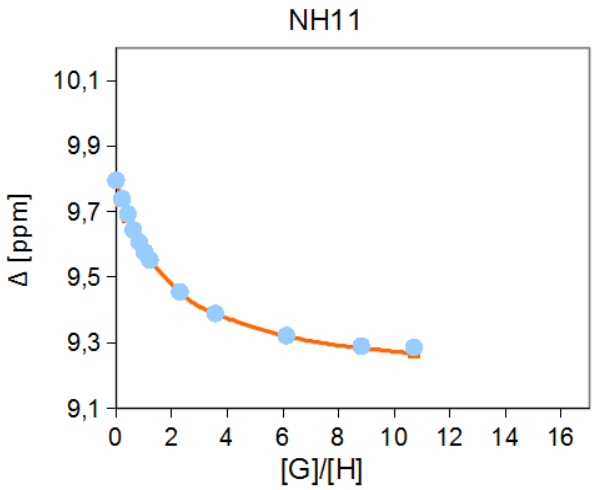


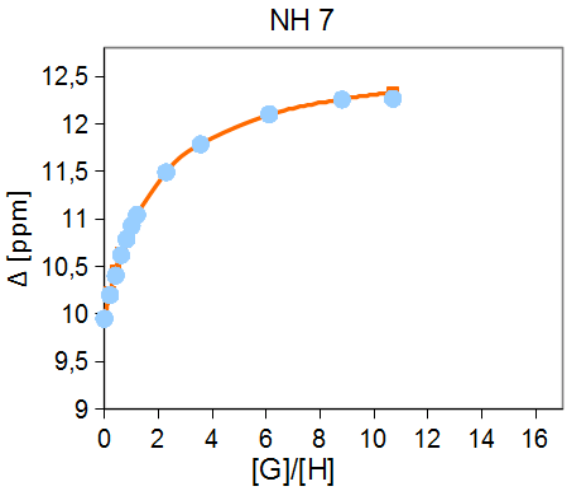
Complex **1:I**. The [G]/[H] on the x-axis refers to the guest-to-host molar ratio.

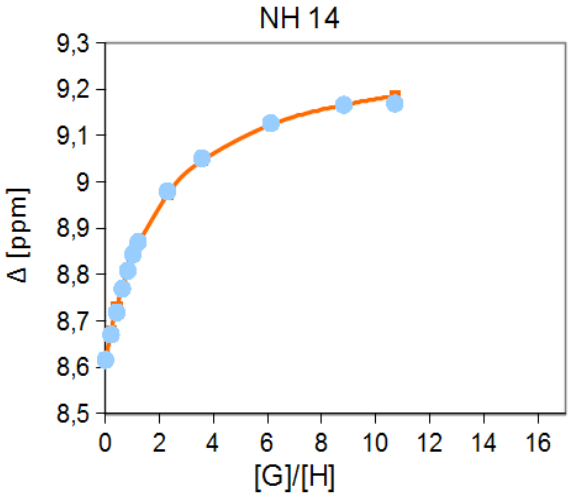


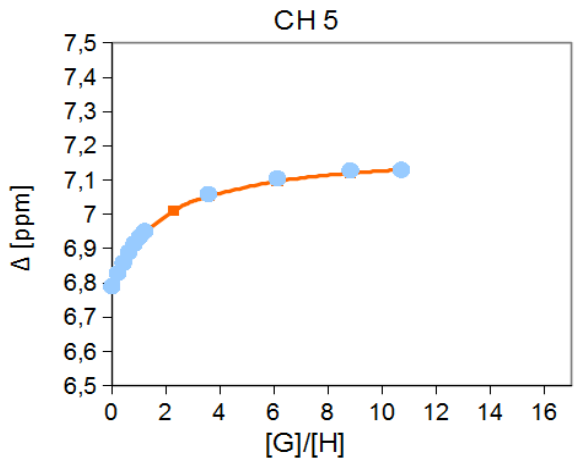
(1) **(I)**



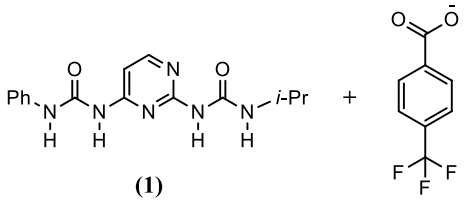




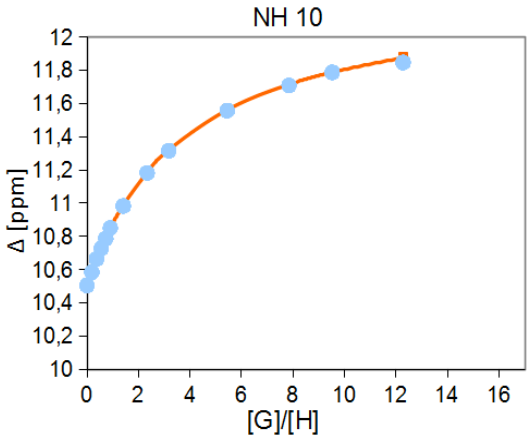


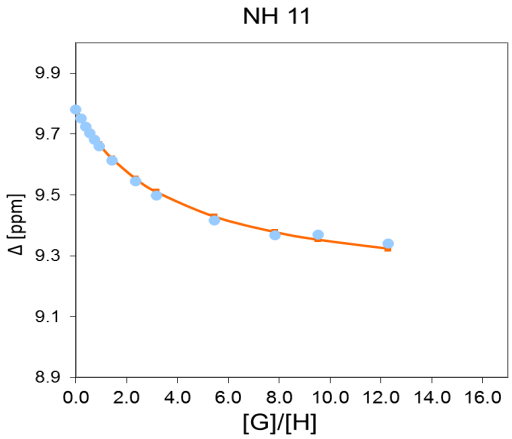


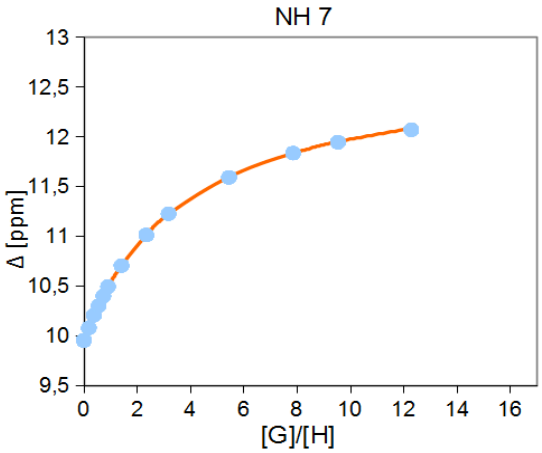
Complex **1:J**. The [G]/[H] on the x-axis refers to the guest-to-host molar ratio.

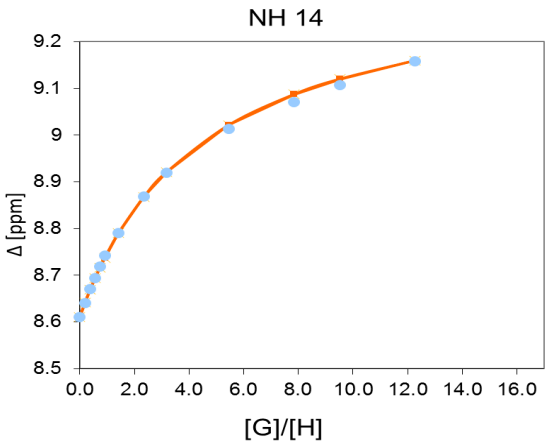


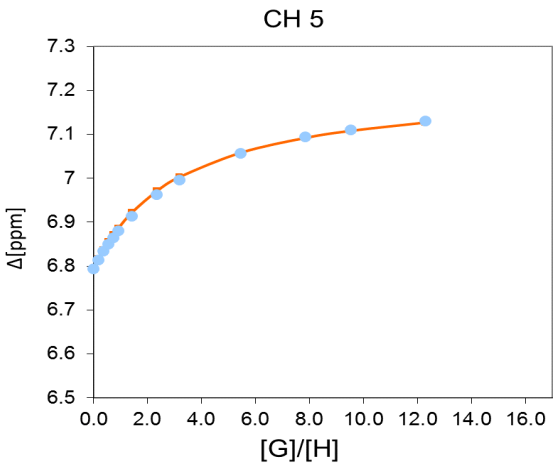
(1) **(J)**



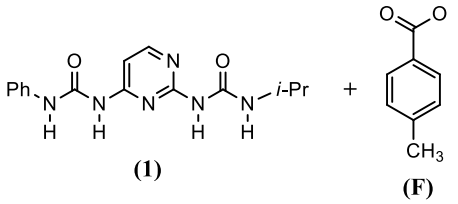




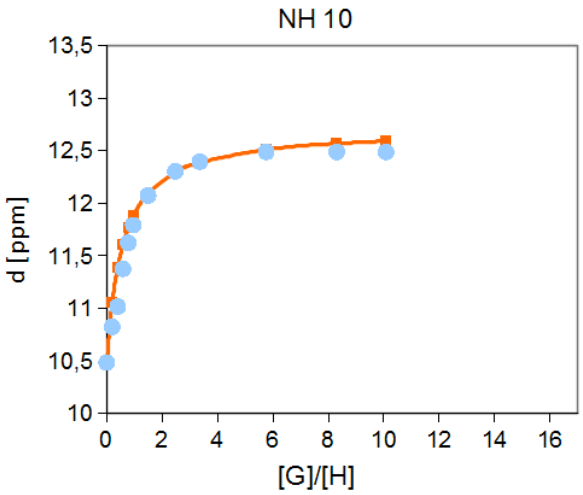


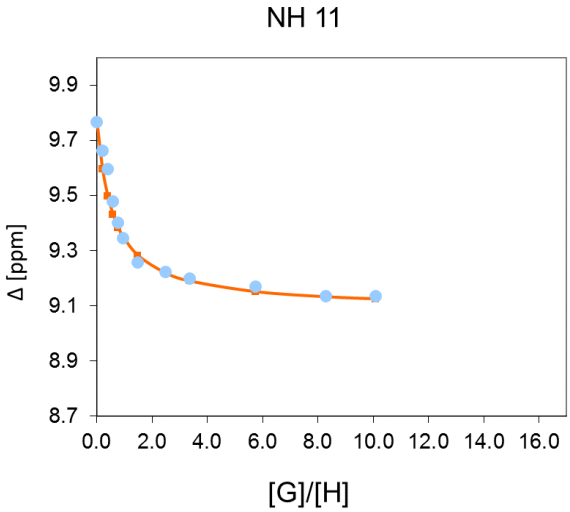


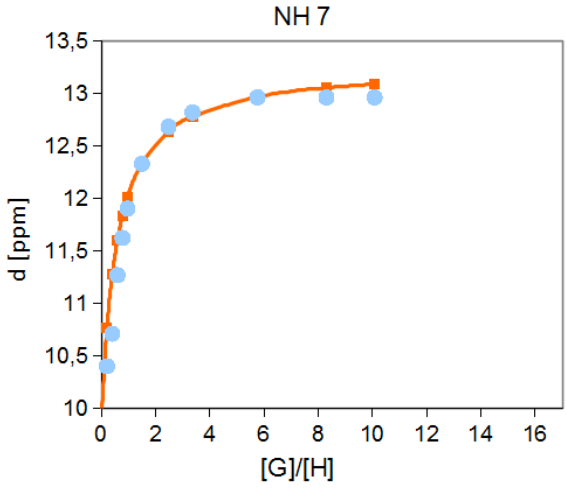
Complex **1:F**. The [G]/[H] on the x-axis refers to the guest-to-host molar ratio.

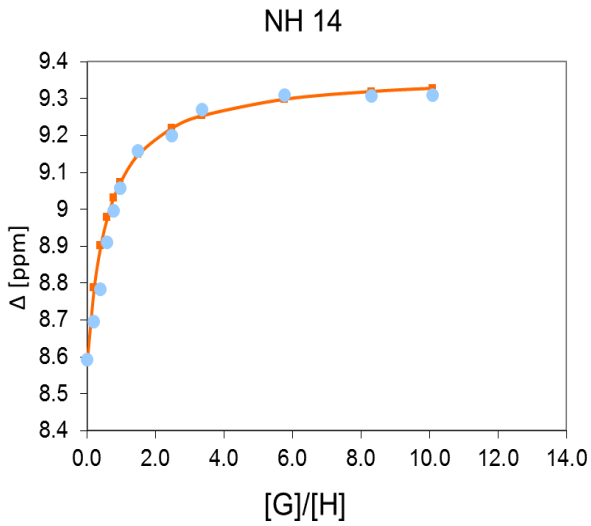


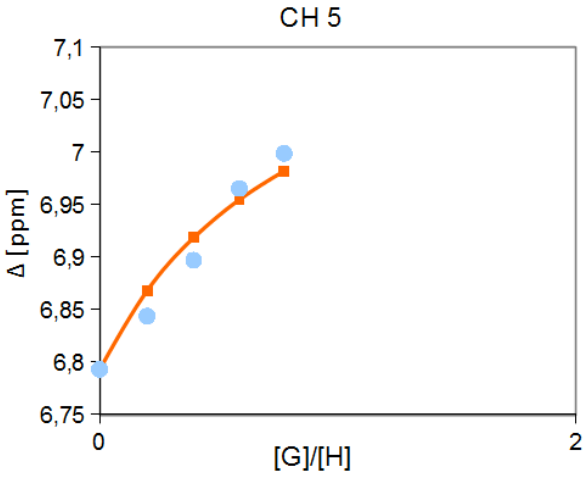
(1) (F)



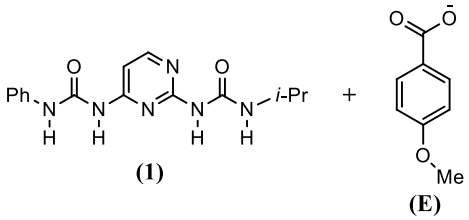




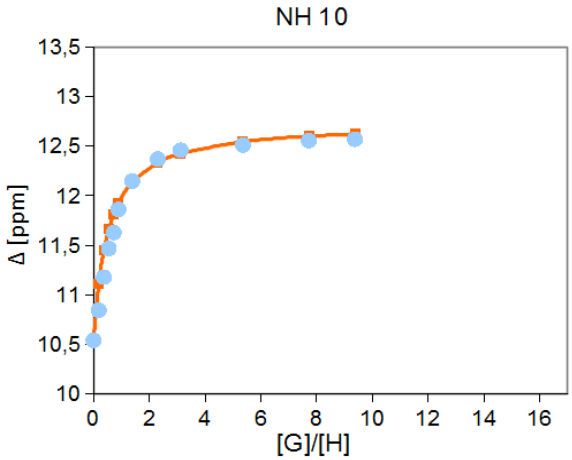


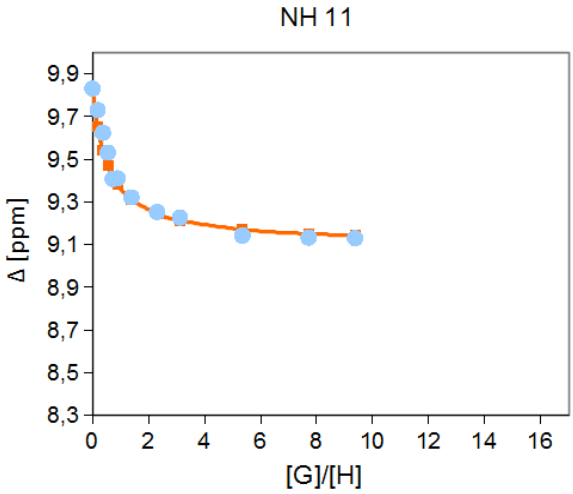


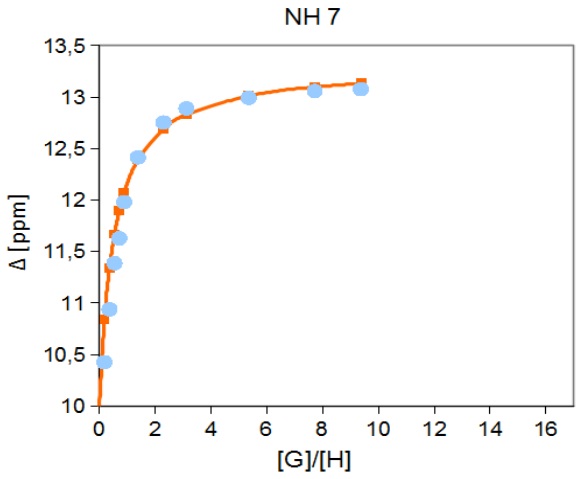
Complex **1:E**. The [G]/[H] on the x-axis refers to the guest-to-host molar ratio.

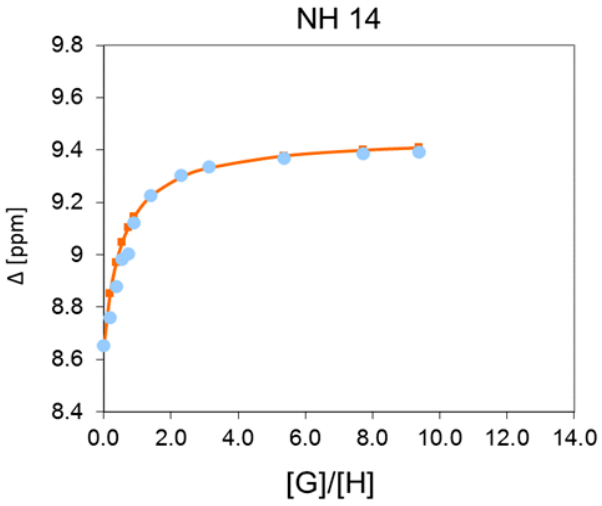


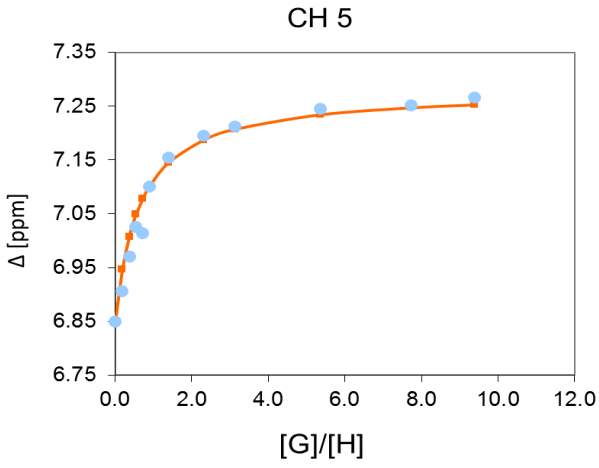
(1) (E)



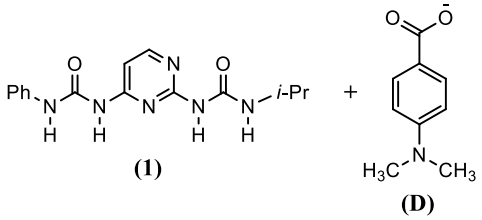


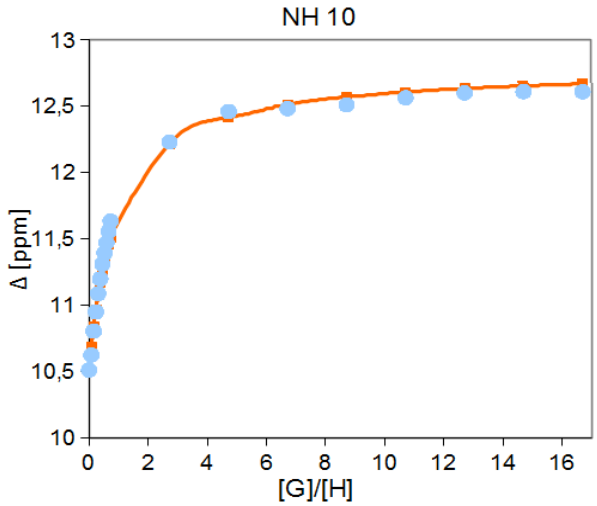


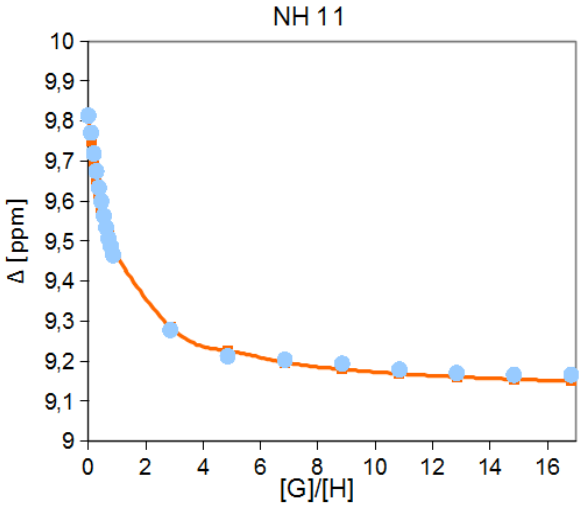


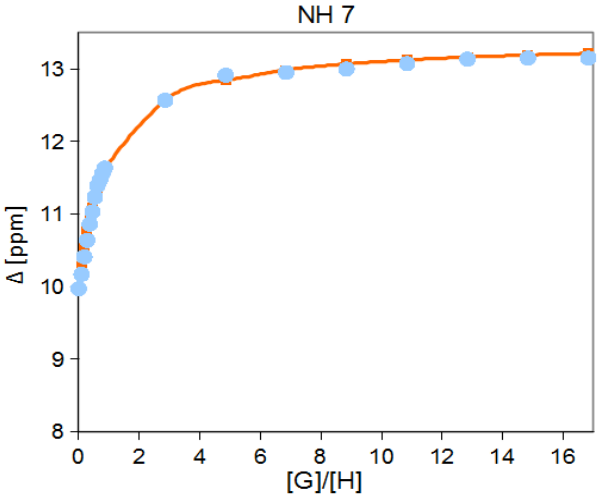


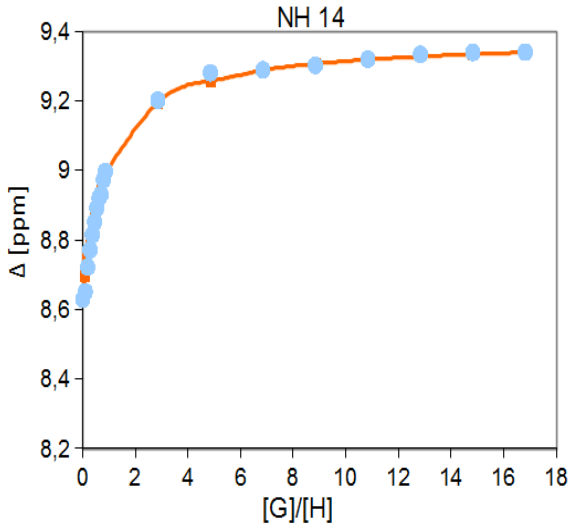
Complex **1:D**. The [G]/[H] on the x-axis refers to the guest-to-host molar ratio

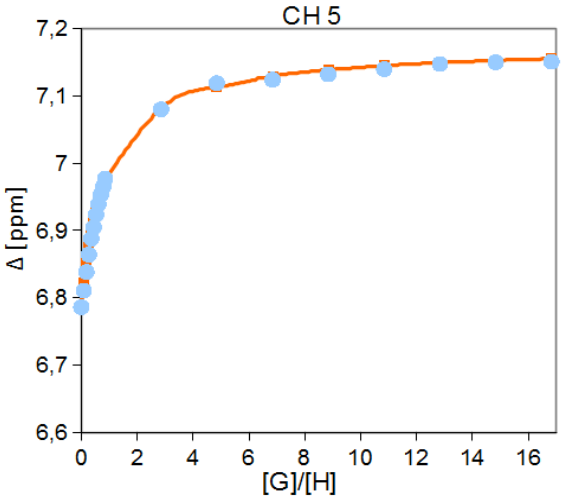




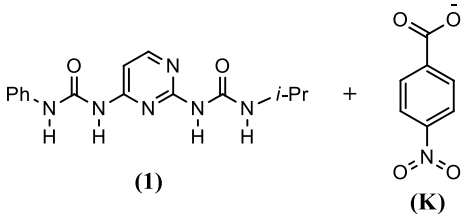




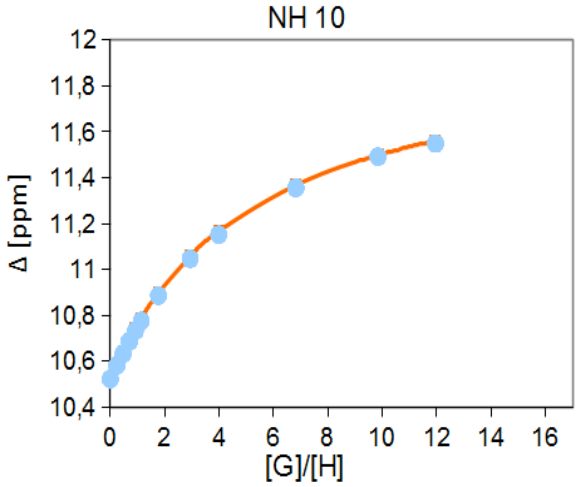


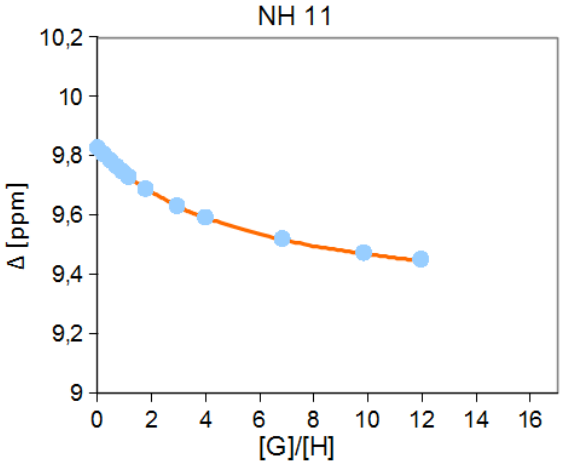


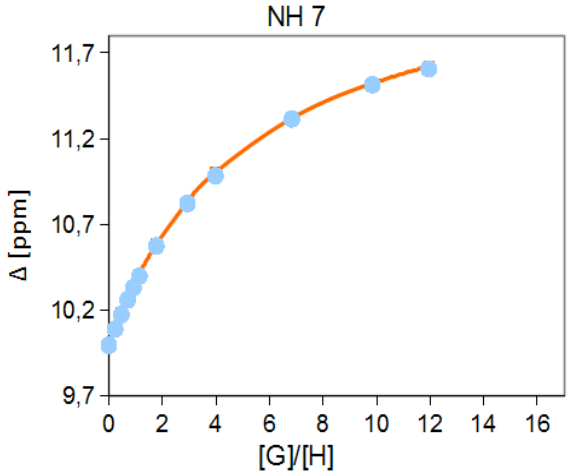
Complex **1:K**. The [G]/[H] on the x-axis refers to the guest-to-host molar ratio.

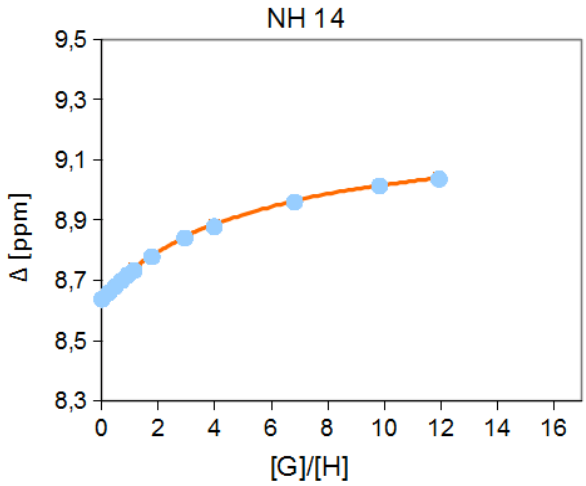


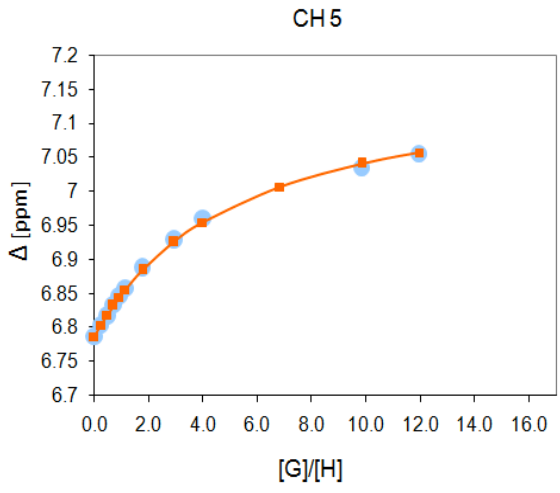
(1) **(K)**



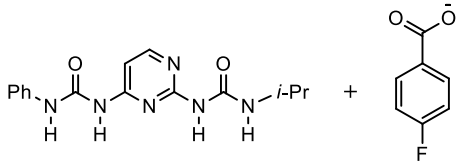




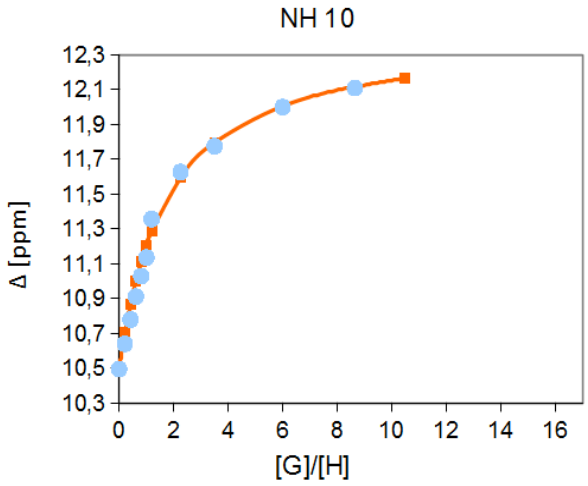


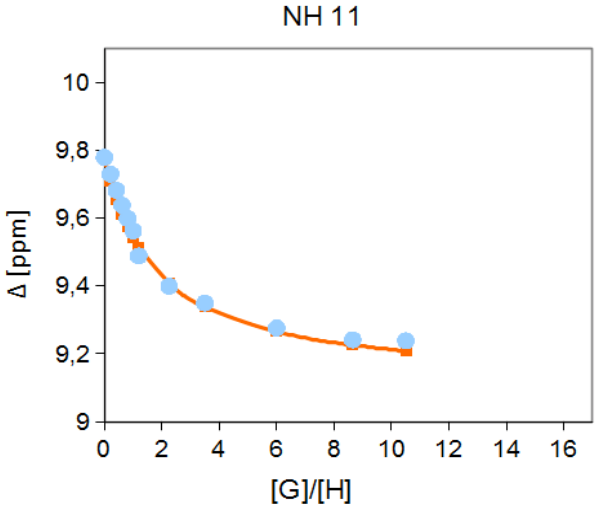


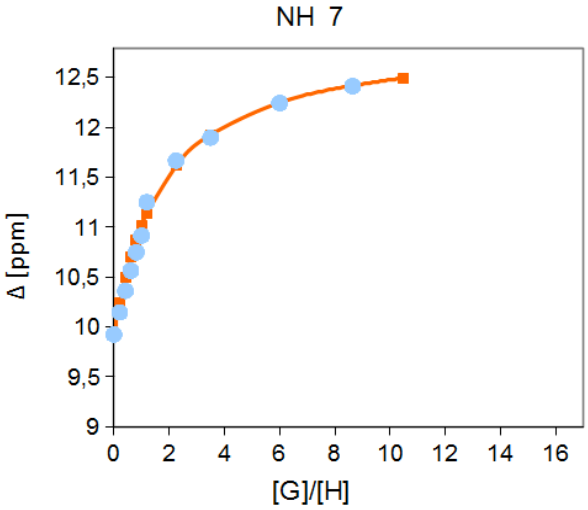
Complex **1:H**. The [G]/[H] on the x-axis refers to the guest-to-host molar ratio.

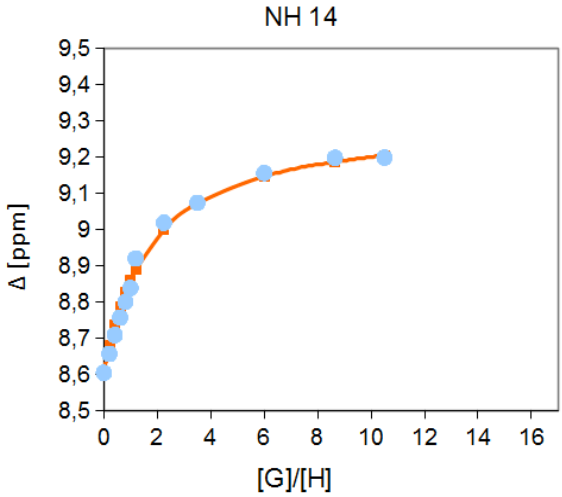


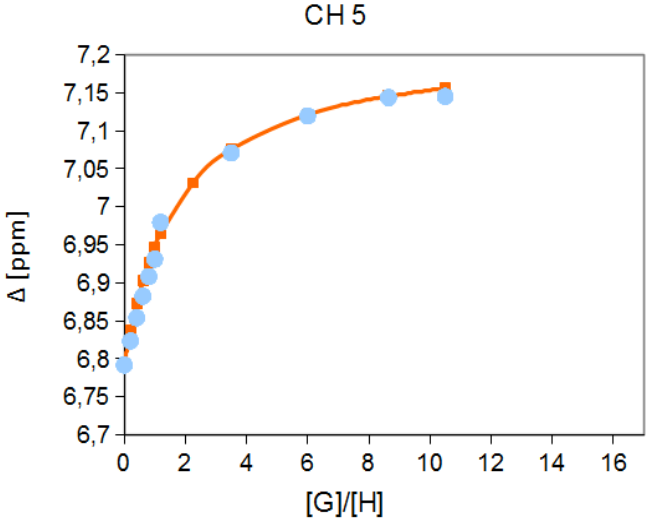
(1) **(H)**











Titration curves of **1** (Host) by benzoates with extreme substituents and unsubstituted one

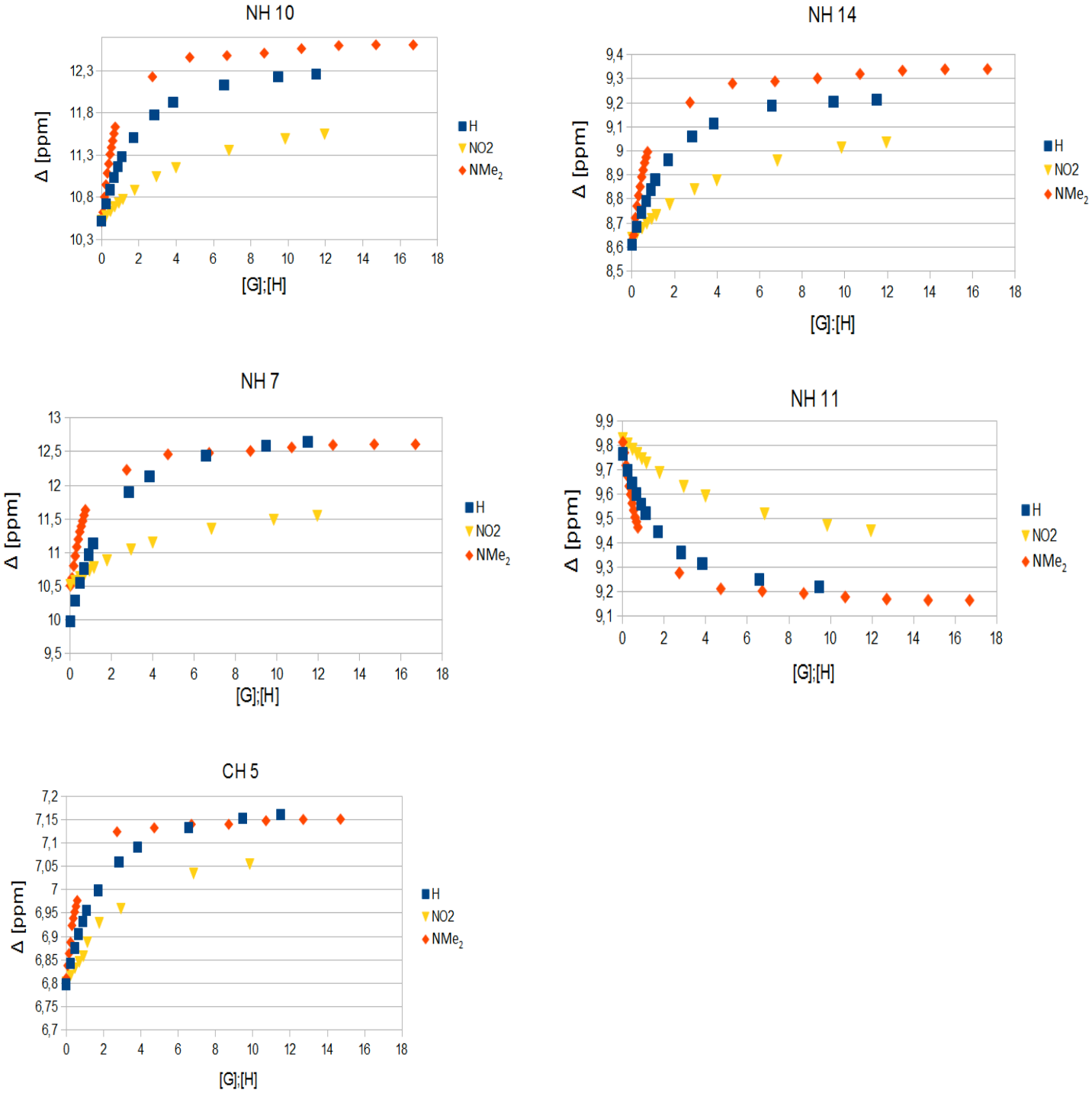


Figure S35. Chemical shift data from the ^{1}H NMR (25 °C, DMSO) titration of **1** (Host) by benzoates with extreme substituents and unsubstituted one

Collective correlations between K_{assoc} of **1**:**D-K** and substituent constants

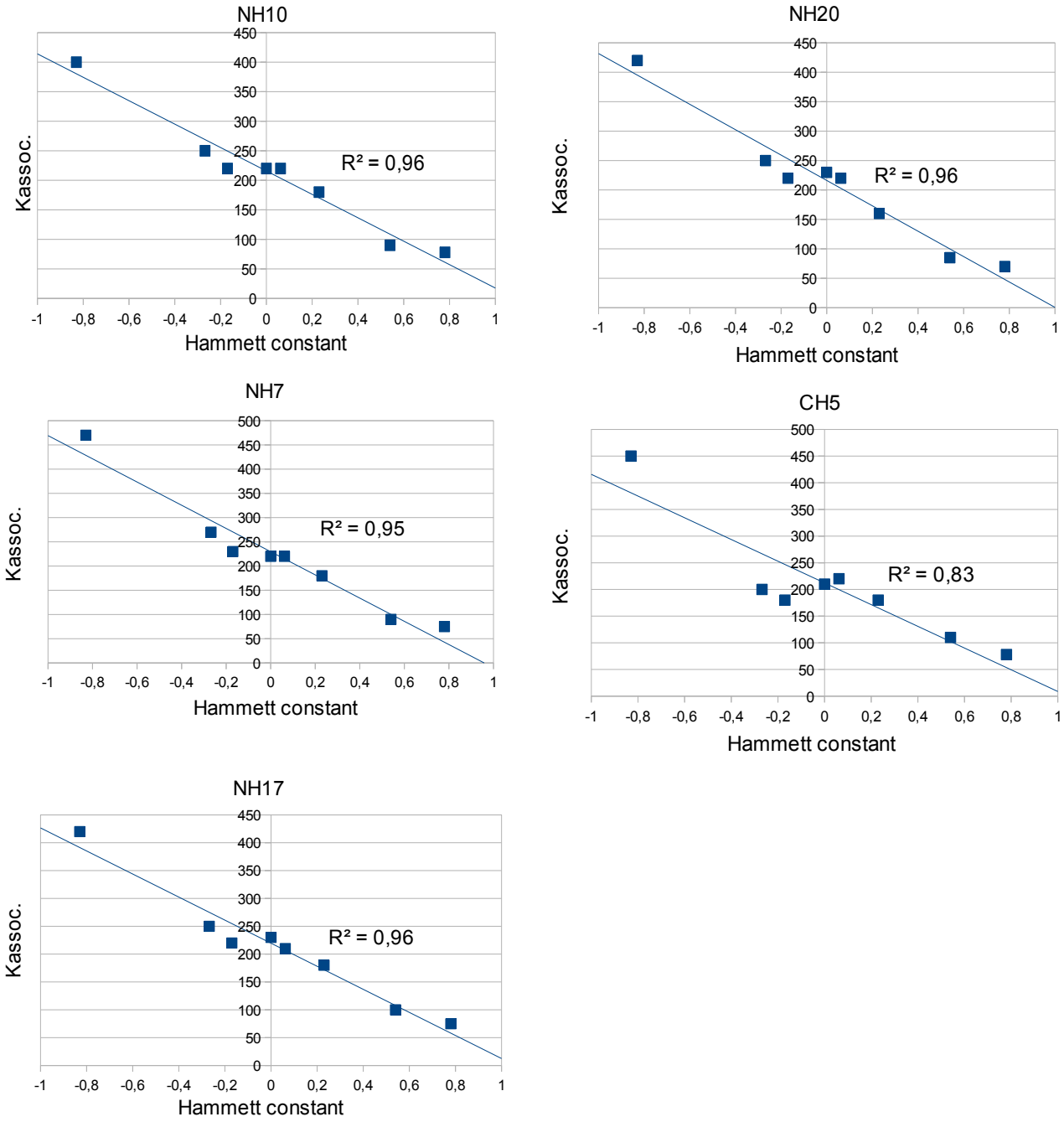


Figure S36. Collected correlation plots between K_{assoc} of **1**:**D-K** and substituent constants

Collective correlations between CIS of **1**:**D-K** and substituent constants

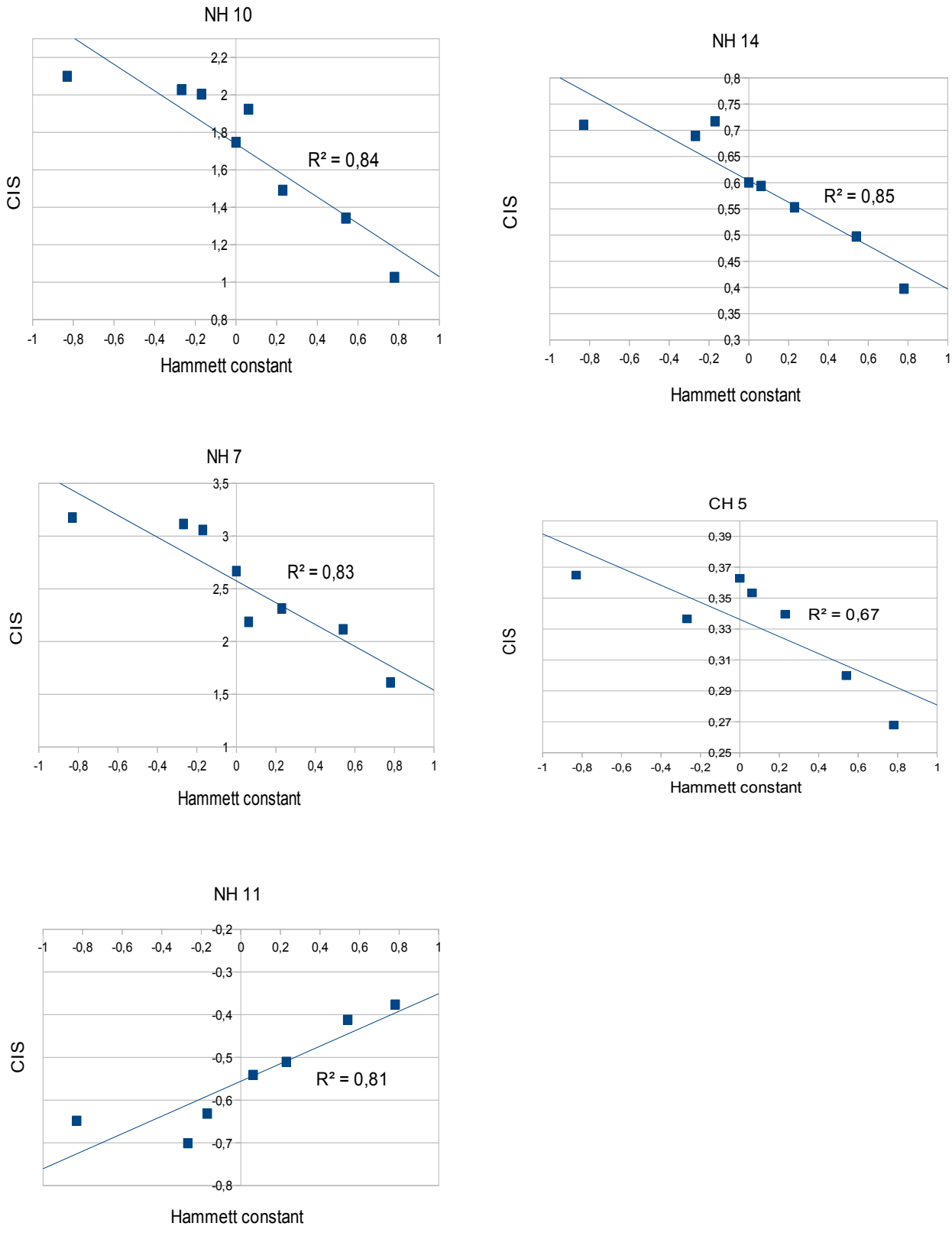


Figure S37. Collected correlation plots between CIS of 1:D-K and substituent constants

Table S1 collects the obtained data for interaction energy and energy of each individual hydrogen bond calculated with the use of QTAIM while Fig. 6 and 7 in the main text show considered complexes.

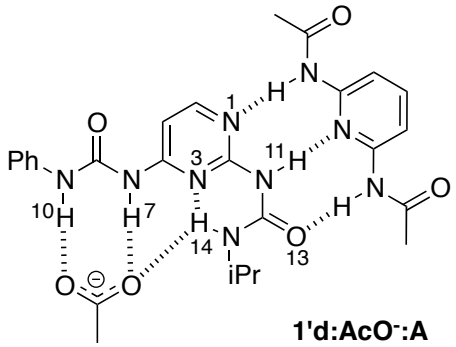


Figure S38. The triple **1'd:AcO⁻:A** complex and atom numbering

Table S1. The energy of interaction (E_{int}, kJ/mol) and energy of hydrogen bonds (E_{HB}, kJ/mol) for three- and five-hydrogen bonded neutral complexes of **1'**

Complex	E_{int}	E_{HB}[a]	ΣE_{HB} intermolecular
1'e:C	-63.7	-24.1, -16.3, -16.7, -18.3, -22.7	-98.1
1'f:C[b]	-41.7	-22.0, -14.6, -24.8, -30.0	-61.3
1'c:B	-34.2	-11.0, -25.3, -17.4, -18.6[c]	-72.4
1'd:A	-31.1	-18.3, -14.1, -27.0, -26.3[d]	-59.4
1'd:AcO⁻:A[e]	-89.5	-19.0, -14.2, -27.7, -25.6, -36.3, -34.3, -7.4	-138.8

[a] - the energy of hydrogen bond are given from left to right or from top to bottom as drawn in Fig. 6. For example in **1'e:C** the order is H10, H7, **C**'s NH, H11, H14, [b] - in computations 2-amino-1,8-naphthyridine was used for simplicity, c - intramolecular hydrogen bond (H14···N1) energy equals to -

30.6 kJ/mol, [d] - intramolecular hydrogen bond (H14···N3), [e] - the order of hydrogen bonds is N1···H, H11···N, O13···H, H14···N3, H7···O, H10···O, H14···O (Fig. 7 in the main text)

The difference between E_{int} and ΣE_{HB} may be explained by the existence of secondary repulsion interactions.[1] Also, it is worth to mention that the E_{int} for **1'e:C** is in fact not so high when keeping in mind the **1'e** energy with respect to the lowest in energy **1'a** (Table 6 in the main text). The solvation of the neutral **C** that is able to form hydrogen bond with basic solvent (DMSO) may hinder association although the $E_{int.}$ for **1'e:C** is relatively high. The solvation of anions is different from neutral hydrogen bonding molecules and this is especially true for polar aprotic solvents. The polar and basic DMSO causes that benzoates still can bind by hydrogen bonding donors because anionic counterparts can efficiently compete with neutral solvent molecules for double hydrogen bonding sites as urea derivatives.

The relatively high interaction energy for **1'd**:AcO-:**A** triple complex (in the light of E_{int} or ΣE_{HB}) is possible if only entropy of the system allows that together with solvation of constituents. In the real situation compounds that carry NH or OH groups are solvated much better that other ones in dimethylsulfoxide and do not associate easily. This, in fact, was observed in our case. It is also worth to mention that simple N-(pyridin-2-yl),N'-substituted ureas[2] interacts with 2-amino-1,8-naphthyridine in $CDCl_3$ solution forming three intermolecular hydrogen bonds while the **1e**:**C** complex did not form in DMSO although five hydrogen bonds would stabilize that complex. Also, 2,4-bis(acylamino)pyrimidines are able to change the geometry to fit to the counterpart used forming three and four hydrogen bonds but that was realized in chloroform and without breaking intramolecular hydrogen bonds.[3] The lack of interaction of **1** with **C** in chloroform is caused by formation of two intramolecular hydrogen bonds, while the same compounds do not associate in DMSO, most probably, due to efficient solvation of neutral molecules that carry hydrogen bond donors (NH groups).

1. W. L. Jorgensen and J. Pranata, *J. Am. Chem. Soc.*, 1990, **112**, 2008-2010.
2. B. Ośmiałowski, K. Mroczyńska, E. Kolehmainen, M. Kowalska, A. Valkonen, M. Pietrzak and K. Rissanen, *J. Org. Chem.*, 2013, **78**, 7582-7593.
3. B. Ośmiałowski, E. Kolehmainen, S. Ikonen, A. Valkonen, A. Kwiatkowski, I. Grela and E. Haapaniemi, *J. Org. Chem.*, 2012, **77**, 9609-9619.