

Supplementary information for “Attractive acceptor—acceptor interactions in self-complementary quadruple hydrogen bonds for molecular self-assembly”

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1. Interaction energies at SAPT and coupled cluster levels

The total interaction energies between the dimers were computed at four different levels of theory: SAPT, CCSD, CCSD(T), and Goodson’s continued-fraction extrapolation towards Full Configuration Interaction (FCI), CCSD(T)-cf. The interaction energies are extrapolated to the basis-set limit, using the two-point formula by Halkier *et al.*, based on aug-cc-pVTZ and aug-cc-pVQZ energies. Table S1.1 shows the interaction energies for the DDAA dimers, and Table S1.2 for the DADA dimers.

Table S1.1. Comparison of hydrogen-bonding energies (in kJ/mol) for the DDAA-AADD arrays. The average hydrogen-binding energy is reported for the dimers DDAA02-DDAA08.

Molecule	SAPT	CCSD	CCSD(T)	CCSD(T)-cf
DDAA01	-216.6	-	-	-
DDAA02	-250.5	-220.5	-222.7	-223.1
DDAA03	-157.7	-137.6	-141.0	-141.7
DDAA04	-140.0	-125.2	-129.0	-129.8
DDAA05	-164.1	-149.8	-153.0	-153.4
DDAA06	-334.3	-292.6	-293.3	-293.6
DDAA07	-257.6	-227.3	-229.0	-229.5
DDAA08	-235.2	-207.9	-211.0	-211.6

Average	-219.9	-194.4	-197.0	-197.5
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Table S1.2. Comparison of hydrogen-bonding energies (in kJ/mol) for the DDAA-AADD arrays. The average hydrogen-binding energy is reported for the dimers DDAA01-DDA06 and DDAA08.

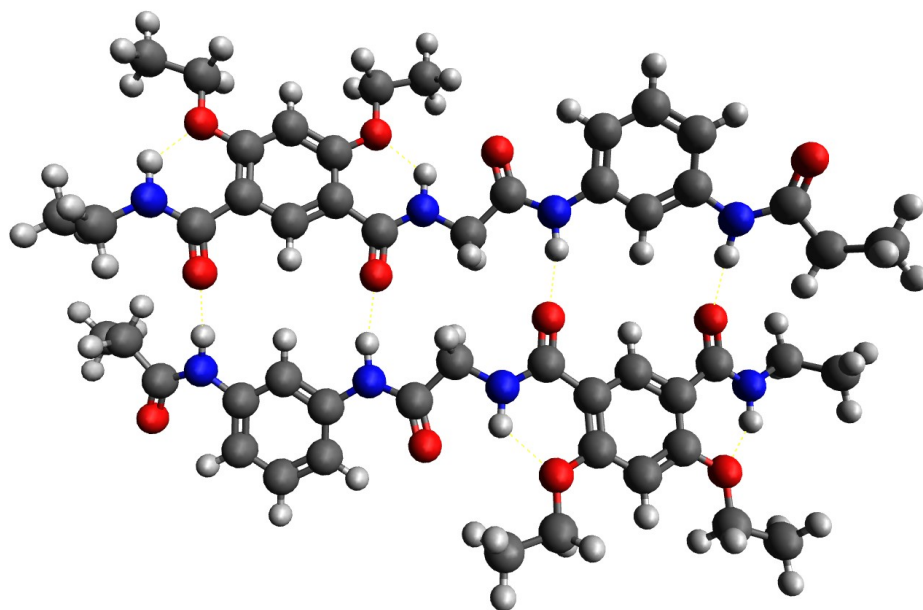
Molecule	SAPT	CCSD	CCSD(T)	CCSD(T)-cf
DADA01	-152.5	-131.4	-132.8	-133.2
DADA02	-132.9	-120.4	-122.3	-122.8
DADA03	-127.3	-115.3	-118.0	-118.6
DADA04	-149.6	-126.6	-129.6	-130.4
DADA05	-152.0	-129.6	-131.4	-131.9
DADA06	-153.1	-130.8	-132.3	-132.7
DADA07	-208.8	-	-	-
DADA08	-137.9	-120.5	-124.2	-124.9
Average	-143.6	-124.9	-127.2	-127.8

2. Molecular structures

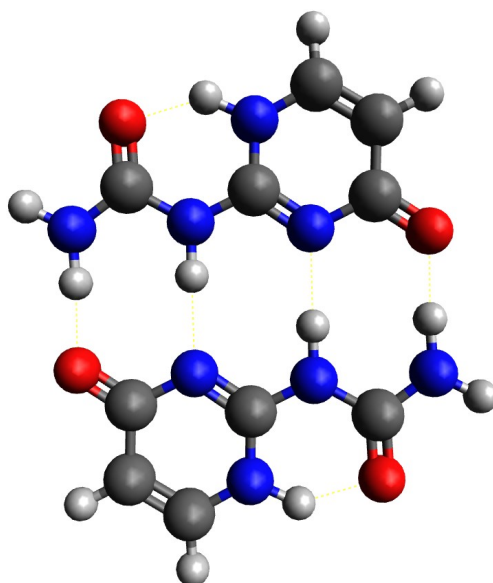
Molecular structures of the studied dimers.

2.1 DDAA dimers

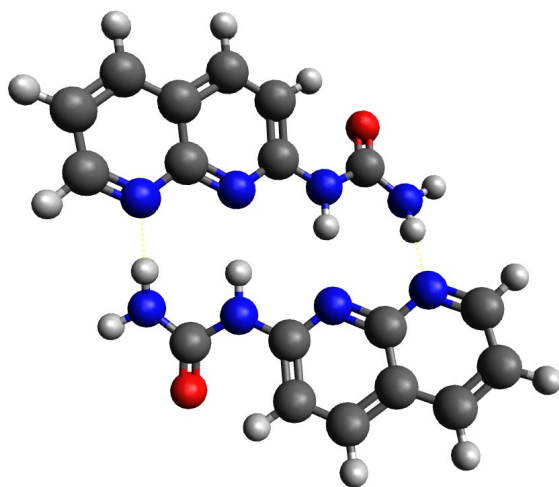
DDAA01



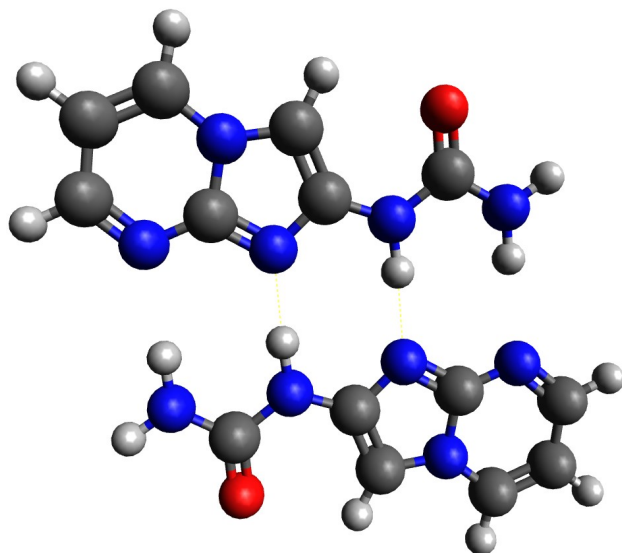
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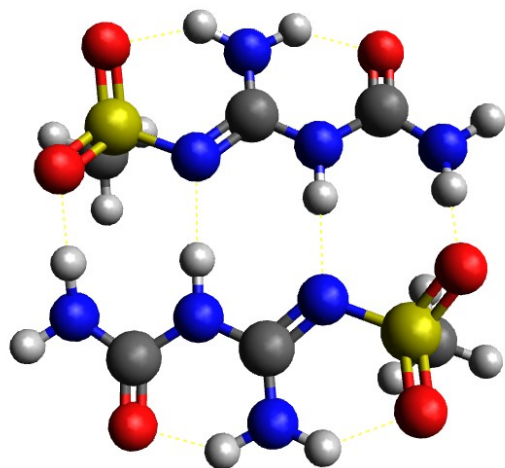
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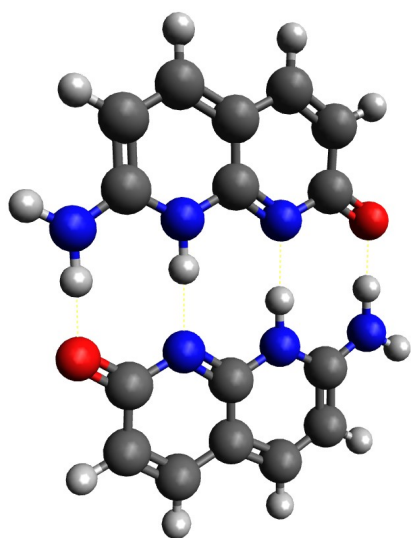
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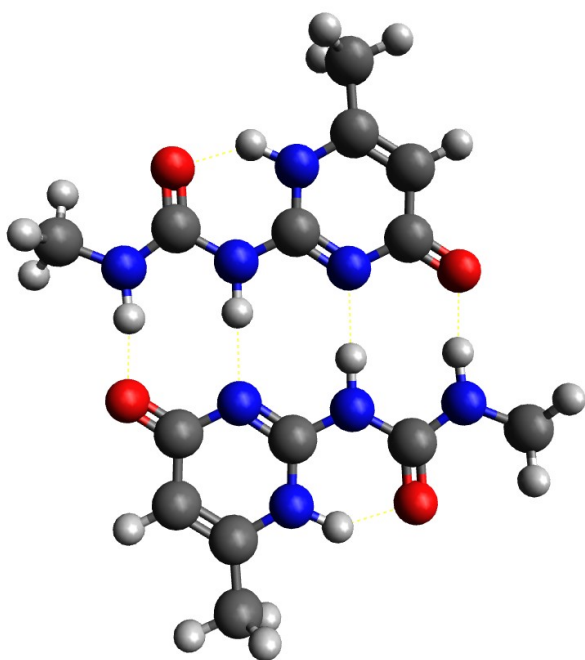
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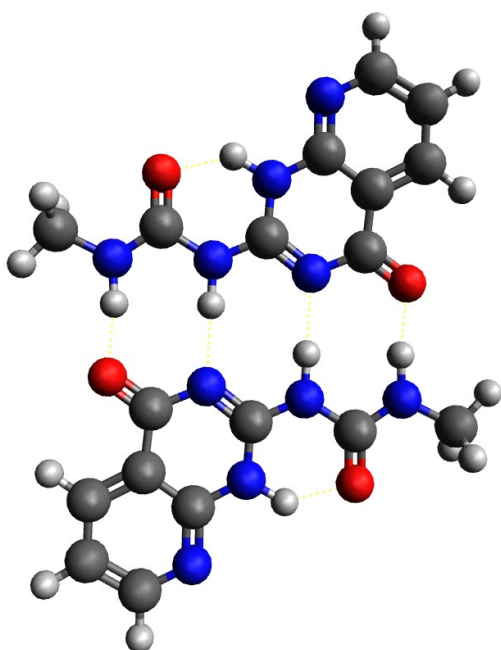
DDAA06



DDAA07

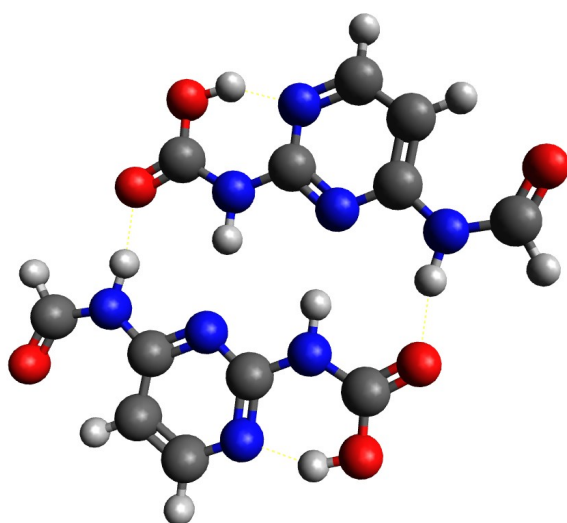


DDAA08

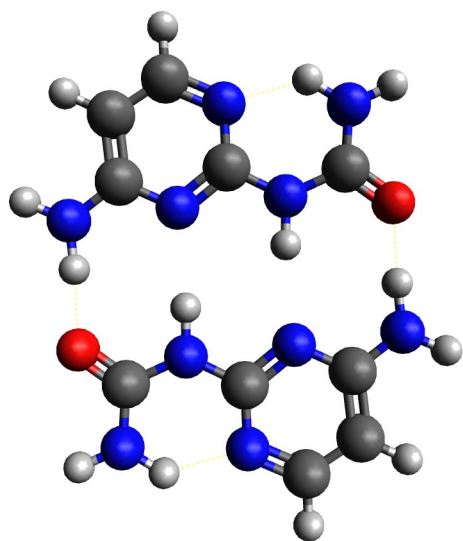


2.2 DADA dimers

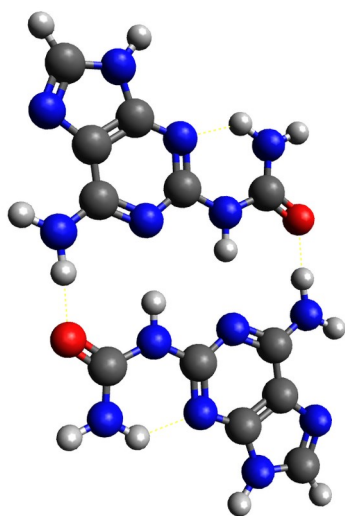
DADA01



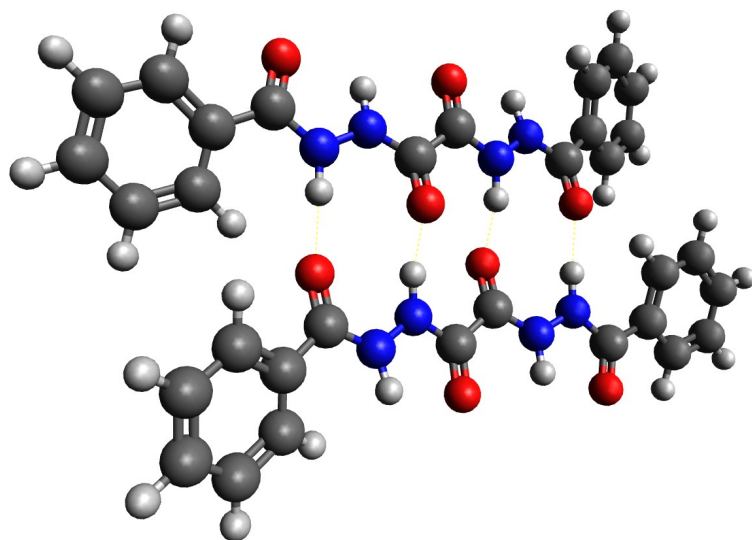
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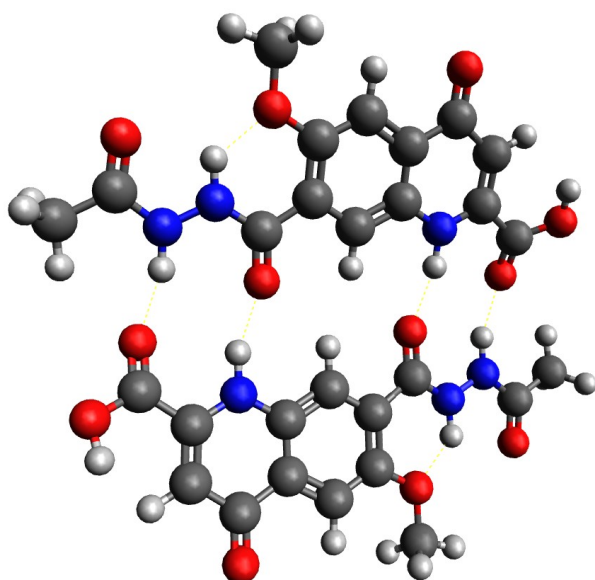
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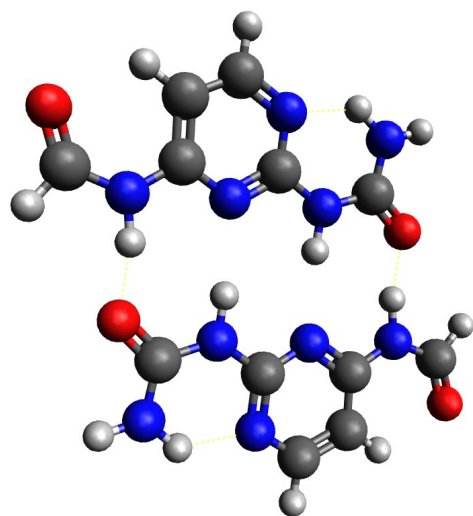
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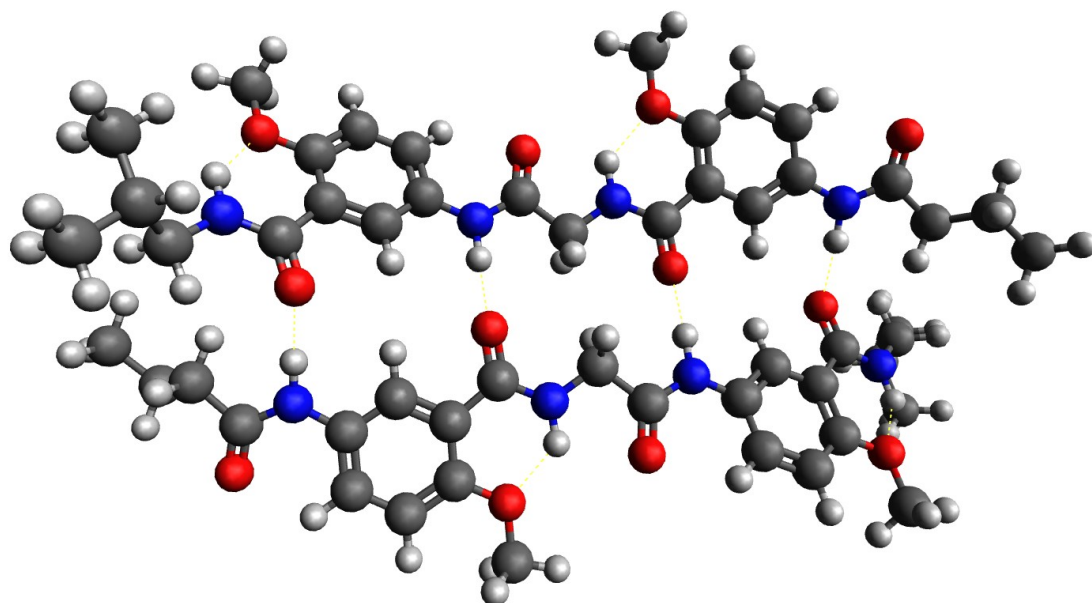
DADA05



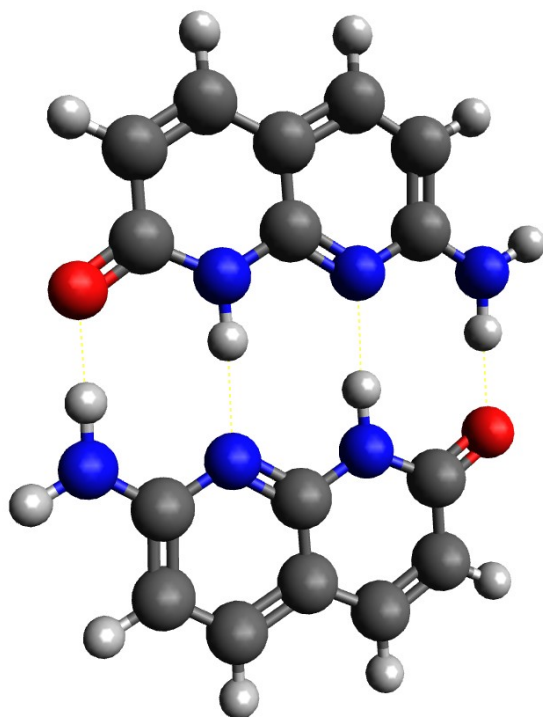
DADA06



DADA07



DADA08



2.3 Cartesian coordinates

DDAA01

134

C	-4.4372625	3.5304096	-3.6110366
C	-5.6365908	2.8546721	-3.4031632
C	-3.2719725	3.1339481	-2.9539893
C	-5.6995494	1.7728307	-2.5039867
C	-3.2953830	2.0386579	-2.0651458
C	-4.5178314	1.4113434	-1.8662220
O	-2.0989380	3.7795068	-3.1407287
O	-6.7794917	3.2196360	-4.0489638
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O	1.2486341	2.6164107	-2.9323730
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C	4.0384503	2.1857576	-3.5370374
C	5.3055572	2.2979183	-4.0954544
C	6.4296266	1.7270491	-3.5139924

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C	5.6995494	-1.7728307	2.5039867
C	3.2953830	-2.0386579	2.0651458
C	4.5178314	-1.4113434	1.8662220
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C	9.2145991	-0.3234191	2.7659087
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H	9.0494410	0.3233104	1.9066949
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H	10.5585238	-1.9111081	3.3987415
H	11.3108787	-0.6809365	2.3784643
H	-9.9053854	2.3015966	2.1052327
H	-11.0077137	0.9951065	2.5411346
H	-11.1970545	1.8352890	0.9891369

DDAA02

34

C	1.1118360	4.1944160	-0.0422388
N	-0.0581903	3.4933381	-0.0257443
C	2.2915122	3.5425181	-0.0347372
C	-0.0329496	2.1380244	0.0011063
C	2.2978338	2.0917759	-0.0069341
N	1.0779940	1.4336871	0.0098277
N	-1.2326224	1.4877161	0.0192392
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N	-3.5177818	1.2754401	0.0638818
O	3.3576520	1.4474370	0.0028757
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H	-3.4222648	0.2430844	0.0439150
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C	-2.2978338	-2.0917759	-0.0069341
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C	-1.1118360	-4.1944160	-0.0422388
N	1.2326224	-1.4877161	0.0192392
C	2.4844910	-2.1200286	0.0312069
N	3.5177818	-1.2754401	0.0638818
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H	1.1810800	-0.4511300	0.0271505
H	3.4222648	-0.2430844	0.0439150
H	4.4318898	-1.6951537	0.0559161
O	-3.3576520	-1.4474370	0.0028757
H	-3.2344618	-4.0674379	-0.0473167
H	-1.0127163	-5.2709604	-0.0620257
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DDAA03

44

C	-3.8849678	3.7567598	0.8396547
C	-4.9073648	2.8341448	1.0349610
C	-2.6100947	3.3060884	0.4248711
C	-4.6270886	1.4715057	0.7816800
C	-2.4083433	1.8922199	0.2296740
N	-3.4388725	1.0142864	0.3956363
C	-1.4965162	4.1614528	0.1704678
C	-0.2914463	3.6279451	-0.2140052
C	-0.1679390	2.1921703	-0.3307840
N	-1.2091709	1.3659224	-0.1331099
N	1.0344942	1.5984023	-0.6124257
C	2.2049820	2.2649696	-1.0724020
N	3.2911112	1.4490061	-1.0752034
O	2.2134723	3.4376327	-1.4487797
N	3.4476255	-1.0076849	0.3391677
C	2.4133249	-1.8880132	0.2146095

C	4.6441717	-1.4577941	0.7074022
C	2.6190481	-3.2977425	0.4344051
C	4.9298220	-2.8151798	0.9819780
C	3.9029091	-3.7408072	0.8291678
N	1.2064479	-1.3684693	-0.1318648
C	0.1608045	-2.1979032	-0.2888835
C	0.2863630	-3.6309751	-0.1446544
C	1.4996843	-4.1573567	0.2233870
N	-1.0474259	-1.6093413	-0.5561765
C	-2.2266667	-2.2845286	-0.9797726
N	-3.3133636	-1.4694006	-0.9740796
H	-3.3390499	-0.5628181	-0.4464740
H	-4.1855102	-1.9225505	-1.2431024
O	-2.2418096	-3.4635645	-1.3353333
H	-1.0827650	-0.5656365	-0.4470452
H	4.1578740	1.8975394	-1.3683488
H	3.3279766	0.5533086	-0.5299643
H	1.0726114	0.5570999	-0.4832011
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H	-5.9107812	3.1427489	1.3602839
H	-5.4249559	0.7151675	0.8950955
H	-1.6123992	5.2502857	0.2897485
H	0.5884205	4.2398142	-0.4431207
H	5.4445071	-0.6998042	0.7877125
H	5.9403598	-3.1178203	1.2904408
H	4.0709470	-4.8150570	1.0073091
H	-0.5985895	-4.2468524	-0.3409434
H	1.6179390	-5.2435742	0.3626072

DDAA04

40

C	-4.0076986	3.2290573	0.0000000
C	-3.5053168	4.5418992	0.0000000
N	-3.2289840	2.1542907	0.0000000
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C	-1.9120046	2.3553588	0.0000000
N	-1.3391743	3.6499296	0.0000000
N	-0.9594222	1.4387236	0.0000000
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C	0.2288217	2.1191731	0.0000000
N	1.3806276	1.3917520	0.0000000
C	2.6517048	1.9467068	0.0000000
N	3.6443226	1.0157420	0.0000000
O	2.8483979	3.1558699	0.0000000
H	-5.0766605	3.0504221	0.0000000
H	-4.1728865	5.3911215	0.0000000
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C	4.0076986	-3.2290573	0.0000000
N	3.2289840	-2.1542907	0.0000000
C	3.5053168	-4.5418992	0.0000000
C	1.9120046	-2.3553588	0.0000000
C	2.1469249	-4.7390285	0.0000000
N	1.3391743	-3.6499296	0.0000000
N	0.9594222	-1.4387236	0.0000000
C	-0.0281624	-3.4937098	0.0000000
C	-0.2288217	-2.1191731	0.0000000

N	-1.3806276	-1.3917520	0.0000000
C	-2.6517048	-1.9467068	0.0000000
N	-3.6443226	-1.0157420	0.0000000
O	-2.8483979	-3.1558699	0.0000000
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H	4.1728865	-5.3911215	0.0000000
H	1.6684682	-5.7080849	0.0000000
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H	-3.4906373	-0.0118556	0.0000000
H	-4.5854159	-1.3659833	0.0000000
H	-1.2582241	-0.3650296	0.0000000

DDAA05

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S	-2.3906043	2.2719308	0.6013863
O	-3.2901753	1.3733313	1.3007449
O	-2.3165679	3.6401578	1.0829363
N	-0.9531313	1.5241564	0.5439539
C	0.1509392	2.2280299	0.2906138
N	0.2195346	3.5407439	0.0889844
H	-0.5863392	4.0925016	0.3575179
H	1.1568008	3.9207482	-0.0501658
N	1.3076496	1.4964852	0.2213638
C	2.5874961	2.0393220	0.0253852
H	1.1973362	0.4889715	0.3899489
N	3.5848274	1.1334311	0.0999505
H	3.4744514	0.2398709	0.5853896
H	4.5100144	1.5290883	0.0588417
O	2.7752060	3.2270190	-0.2325869
N	-3.5848274	-1.1334311	0.0999505
C	-2.5874961	-2.0393220	0.0253852
H	-4.5100144	-1.5290883	0.0588417
H	-3.4744514	-0.2398709	0.5853896
N	-1.3076496	-1.4964852	0.2213638
C	-0.1509392	-2.2280299	0.2906138
H	-1.1973362	-0.4889715	0.3899489
N	0.9531313	-1.5241564	0.5439539
N	-0.2195346	-3.5407439	0.0889844
H	0.5863392	-4.0925016	0.3575179
H	-1.1568008	-3.9207482	-0.0501658
S	2.3906043	-2.2719308	0.6013863
O	3.2901753	-1.3733313	1.3007449
O	2.3165679	-3.6401578	1.0829363
O	-2.7752060	-3.2270190	-0.2325869
C	2.9215116	-2.3382055	-1.0994095
H	2.9925652	-1.3228068	-1.4849029
H	2.1979973	-2.9219116	-1.6670245
H	3.8957798	-2.8252151	-1.1113118
C	-2.9215116	2.3382055	-1.0994095
H	-3.8957798	2.8252151	-1.1113118
H	-2.9925652	1.3228068	-1.4849029
H	-2.1979973	2.9219116	-1.6670245

DDAA06

38

N	1.5063512	-1.1103757	0.0000000
C	2.1722103	-2.2911404	0.0000000
C	3.5867416	-2.2734164	0.0000000
C	4.2417543	-1.0680081	0.0000000
C	3.3626153	2.5472057	0.0000000
C	1.9180662	2.4354621	0.0000000
N	1.3404621	1.1873400	0.0000000
C	2.1277164	0.1169531	0.0000000
C	3.5442119	0.1500279	0.0000000
C	4.1432105	1.4379137	0.0000000
N	1.4531482	-3.4114259	0.0000000
H	4.1200252	-3.2138128	0.0000000
H	5.3264340	-1.0472450	0.0000000
H	0.3977119	-3.4097765	0.0000000
H	5.2256056	1.5139348	0.0000000
H	3.7769621	3.5461449	0.0000000
O	1.2008732	3.4646497	0.0000000
H	1.9455360	-4.2875749	0.0000000
H	0.4523327	-1.1216411	0.0000000
N	-1.5063512	1.1103757	0.0000000
C	-2.1722103	2.2911404	0.0000000
C	-3.5867416	2.2734164	0.0000000
C	-4.2417543	1.0680081	0.0000000
C	-3.3626153	-2.5472057	0.0000000
C	-1.9180662	-2.4354621	0.0000000
N	-1.3404621	-1.1873400	0.0000000
C	-2.1277164	-0.1169531	0.0000000
C	-3.5442119	-0.1500279	0.0000000
C	-4.1432105	-1.4379137	0.0000000
N	-1.4531482	3.4114259	0.0000000
H	-4.1200252	3.2138128	0.0000000
H	-5.3264340	1.0472450	0.0000000
H	-0.3977119	3.4097765	0.0000000
H	-5.2256056	-1.5139348	0.0000000
H	-3.7769621	-3.5461449	0.0000000
O	-1.2008732	-3.4646497	0.0000000
H	-1.9455360	4.2875749	0.0000000
H	-0.4523327	1.1216411	0.0000000

DDAA07

46

H	4.8479511	-2.8567145	0.9228588
C	3.8944425	-3.3873159	0.7359036
N	2.8011630	-2.4589794	0.5281782
C	2.4137346	-2.1066319	-0.7053687
O	2.9253952	-2.5473524	-1.7490709
N	1.3467597	-1.1806727	-0.7300305
C	0.7710671	-0.6816744	-1.8667281
N	-0.2209975	0.1818470	-1.7681536
C	-0.8064284	0.6855768	-2.9235082
O	-1.7445855	1.4951466	-2.8563121
N	1.2635117	-1.1134733	-3.0638204
C	0.7426027	-0.6596561	-4.2532793

17

C	-0.2845832	0.2334125	-4.2075433
C	1.3717260	-1.2060822	-5.5006370
H	3.6672356	-4.0191621	1.6104720
H	4.0135679	-4.0173484	-0.1587801
H	2.3545319	-2.0376733	1.3748124
H	0.9399581	-0.8240057	0.1711376
H	2.0495164	-1.7961777	-2.9740482
H	-0.7398706	0.6292164	-5.1162302
H	2.4500561	-0.9638438	-5.5296780
H	0.8897024	-0.7836067	-6.3950543
H	1.2779184	-2.3072318	-5.5325876
H	-4.8479511	2.8567145	-0.9228588
C	-3.8944425	3.3873159	-0.7359036
N	-2.8011630	2.4589794	-0.5281782
C	-2.4137346	2.1066319	0.7053687
O	-2.9253952	2.5473524	1.7490709
N	-1.3467597	1.1806727	0.7300305
C	-0.7710671	0.6816744	1.8667281
N	0.2209975	-0.1818470	1.7681536
C	0.8064284	-0.6855768	2.9235082
O	1.7445855	-1.4951466	2.8563121
N	-1.2635117	1.1134733	3.0638204
C	-0.7426027	0.6596561	4.2532793
C	0.2845832	-0.2334125	4.2075433
C	-1.3717260	1.2060822	5.5006370
H	-3.6672356	4.0191621	-1.6104720
H	-4.0135679	4.0173484	0.1587801
H	-2.3545319	2.0376733	-1.3748124
H	-0.9399581	0.8240057	-0.1711376
H	-2.0495164	1.7961777	2.9740482
H	0.7398706	-0.6292164	5.1162302
H	-2.4500561	0.9638438	5.5296780
H	-0.8897024	0.7836067	6.3950543
H	-1.2779184	2.3072318	5.5325876

DDAA08

50

C	-2.3795454	6.1873472	0.0000000
C	-3.6350620	5.5527593	0.0000000
C	-3.6731055	4.1606264	0.0000000
N	-1.2143491	5.5406775	0.0000000
C	-1.2709523	4.2050976	0.0000000
C	-2.4624376	3.4556297	0.0000000
N	-0.0802832	3.5136225	0.0000000
C	-2.3873151	1.9810048	0.0000000
C	-0.0526811	2.1555345	0.0000000
N	-1.1424358	1.3951882	0.0000000
N	1.1677484	1.5489476	0.0000000
C	2.4087824	2.2346679	0.0000000
N	3.4781070	1.4286761	0.0000000
O	2.4809811	3.4702680	0.0000000
O	-3.4254799	1.3054176	0.0000000
C	4.8121525	1.9974864	0.0000000
H	4.9788008	2.6257950	-0.8929561
H	5.5326475	1.1657652	0.0000000
H	4.9788008	2.6257950	0.8929561
C	2.4624376	-3.4556297	0.0000000

C	1.2709523	-4.2050976	0.0000000
C	3.6731055	-4.1606264	0.0000000
N	1.2143491	-5.5406775	0.0000000
C	3.6350620	-5.5527593	0.0000000
C	2.3795454	-6.1873472	0.0000000
C	2.3873151	-1.9810048	0.0000000
N	0.0802832	-3.5136225	0.0000000
C	0.0526811	-2.1555345	0.0000000
N	1.1424358	-1.3951882	0.0000000
N	-1.1677484	-1.5489476	0.0000000
C	-2.4087824	-2.2346679	0.0000000
N	-3.4781070	-1.4286761	0.0000000
C	-4.8121525	-1.9974864	0.0000000
H	-4.9788008	-2.6257950	-0.8929561
H	-5.5326475	-1.1657652	0.0000000
H	-4.9788008	-2.6257950	0.8929561
O	-2.4809811	-3.4702680	0.0000000
O	3.4254799	-1.3054176	0.0000000
H	-4.5515092	6.1483217	0.0000000
H	-4.6089026	3.5957359	0.0000000
H	-2.3161844	7.2823337	0.0000000
H	4.6089026	-3.5957359	0.0000000
H	4.5515092	-6.1483217	0.0000000
H	2.3161844	-7.2823337	0.0000000
H	-0.8487800	-3.9854879	0.0000000
H	-1.1500020	-0.5005675	0.0000000
H	-3.3796809	-0.3918097	0.0000000
H	1.1500020	0.5005675	0.0000000
H	3.3796809	0.3918097	0.0000000
H	0.8487800	3.9854879	0.0000000

DADA01

38

C	0.9794353	4.2796257	0.0000000
N	-0.1584407	3.5720738	0.0000000
C	2.2229912	3.6949296	0.0000000
C	-0.0320073	2.2404277	0.0000000
C	2.2492717	2.2884329	0.0000000
N	1.1163299	1.5596814	0.0000000
N	3.4064031	1.5556922	0.0000000
C	4.7027775	2.0284253	0.0000000
O	5.0474968	3.1902662	0.0000000
N	-1.1898964	1.4927503	0.0000000
C	-2.5022605	1.9640371	0.0000000
O	-3.4342575	1.1738647	0.0000000
H	5.4160457	1.1911271	0.0000000
H	0.8673746	5.3574152	0.0000000
H	3.1376113	4.2631216	0.0000000
H	-1.0994941	0.4705564	0.0000000
H	3.3089875	0.5244519	0.0000000
O	-2.6811431	3.2655575	0.0000000
H	-1.7679406	3.7060051	0.0000000
O	3.4342575	-1.1738647	0.0000000
C	2.5022605	-1.9640371	0.0000000
N	1.1898964	-1.4927503	0.0000000
O	2.6811431	-3.2655575	0.0000000

C	0.0320073	-2.2404277	0.0000000
N	-1.1163299	-1.5596814	0.0000000
N	0.1584407	-3.5720738	0.0000000
H	1.7679406	-3.7060051	0.0000000
C	-2.2492717	-2.2884329	0.0000000
N	-3.4064031	-1.5556922	0.0000000
C	-0.9794353	-4.2796257	0.0000000
C	-2.2229912	-3.6949296	0.0000000
C	-4.7027775	-2.0284253	0.0000000
H	-5.4160457	-1.1911271	0.0000000
O	-5.0474968	-3.1902662	0.0000000
H	-0.8673746	-5.3574152	0.0000000
H	-3.1376113	-4.2631216	0.0000000
H	1.0994941	-0.4705564	0.0000000
H	-3.3089875	-0.5244519	0.0000000

DADA02

36

C	4.1549460	1.4904225	0.0000000
C	3.3991125	2.6287686	0.0000000
N	3.6275654	0.2537732	0.0000000
C	1.9909345	2.4627565	0.0000000
C	2.2917135	0.1940943	0.0000000
N	1.4422803	1.2296952	0.0000000
N	1.1680746	3.5160620	0.0000000
N	1.6871920	-1.0496210	0.0000000
C	2.2685982	-2.3146056	0.0000000
O	1.5483926	-3.3198603	0.0000000
N	3.6088659	-2.3843501	0.0000000
H	5.2388486	1.5399923	0.0000000
H	1.5604270	4.4406410	0.0000000
H	0.1429917	3.4040035	0.0000000
H	4.1387663	-1.5124844	0.0000000
H	4.0188749	-3.3012571	0.0000000
H	0.6622370	-1.0557211	0.0000000
N	-1.4422803	-1.2296952	0.0000000
C	-2.2917135	-0.1940943	0.0000000
C	-1.9909345	-2.4627565	0.0000000
N	-3.6275654	-0.2537732	0.0000000
C	-3.3991125	-2.6287686	0.0000000
C	-4.1549460	-1.4904225	0.0000000
N	-1.1680746	-3.5160620	0.0000000
N	-1.6871920	1.0496210	0.0000000
C	-2.2685982	2.3146056	0.0000000
O	-1.5483926	3.3198603	0.0000000
N	-3.6088659	2.3843501	0.0000000
H	-5.2388486	-1.5399923	0.0000000
H	-0.6622370	1.0557211	0.0000000
H	-0.1429917	-3.4040035	0.0000000
H	-1.5604270	-4.4406410	0.0000000
H	-4.1387663	1.5124844	0.0000000
H	-4.0188749	3.3012571	0.0000000
H	3.8473298	3.6130484	0.0000000
H	-3.8473298	-3.6130484	0.0000000

DADA03

42

C	1.1797795	4.2305816	0.0000000
N	-0.0381453	3.6766595	0.0000000
C	2.3905840	3.5593943	0.0000000
C	0.0176829	2.3375075	0.0000000
C	2.3301813	2.1466270	0.0000000
N	1.1140092	1.5559767	0.0000000
N	3.4338340	1.4054181	0.0000000
N	-1.1769829	1.6336069	0.0000000
C	-2.4832164	2.1072209	0.0000000
O	-3.4300755	1.3123074	0.0000000
N	-2.6679888	3.4386452	0.0000000
N	-1.1140092	-1.5559767	0.0000000
C	-2.3301813	-2.1466270	0.0000000
C	-0.0176829	-2.3375075	0.0000000
C	-2.3905840	-3.5593943	0.0000000
N	0.0381453	-3.6766595	0.0000000
C	-1.1797795	-4.2305816	0.0000000
N	1.1769829	-1.6336069	0.0000000
C	2.4832164	-2.1072209	0.0000000
O	3.4300755	-1.3123074	0.0000000
N	2.6679888	-3.4386452	0.0000000
N	-3.4338340	-1.4054181	0.0000000
N	1.5148431	5.5617892	0.0000000
N	3.4562195	4.4415202	0.0000000
C	2.8962787	5.6223993	0.0000000
H	3.4188263	6.5659703	0.0000000
N	-3.4562195	-4.4415202	0.0000000
N	-1.5148431	-5.5617892	0.0000000
C	-2.8962787	-5.6223993	0.0000000
H	-3.4188263	-6.5659703	0.0000000
H	-1.8523241	4.0459564	0.0000000
H	-3.6178203	3.7648353	0.0000000
H	-1.0956850	0.6132933	0.0000000
H	0.8740915	6.3385409	0.0000000
H	4.3178360	1.8860201	0.0000000
H	3.4013258	0.3752859	0.0000000
H	1.0956850	-0.6132933	0.0000000
H	-3.4013258	-0.3752859	0.0000000
H	-4.3178360	-1.8860201	0.0000000
H	-0.8740915	-6.3385409	0.0000000
H	1.8523241	-4.0459564	0.0000000
H	3.6178203	-3.7648353	0.0000000

DADA04

76

C	-5.5136815	1.7413585	-2.7363477
C	-6.8372688	1.9279270	-3.1157464
C	-5.0954784	0.5026518	-2.2434239
C	-7.7500303	0.8835043	-3.0005818
C	-6.0122313	-0.5453258	-2.1403048
C	-7.3353493	-0.3530216	-2.5123815

C	-3.6893733	0.2303840	-1.8416953
N	-2.9991169	1.3013517	-1.3960124
N	-1.6868159	1.2129970	-1.0023268
C	-1.1344362	2.3696380	-0.5870748
C	0.2735543	2.2002154	-0.0496438
N	0.6845930	3.2955523	0.5884712
N	1.9136973	3.3917433	1.1864439
C	2.2432505	4.6448720	1.6313276
C	3.5174039	4.8007747	2.3802359
C	4.0097632	6.1020355	2.5142901
C	4.2055532	3.7365838	2.9675292
C	5.1859677	6.3348174	3.2125848
C	5.3797528	3.9767184	3.6721993
C	5.8740030	5.2718362	3.7931008
O	-3.1839135	-0.8934770	-1.8940363
O	-1.7180766	3.4520659	-0.6398937
O	0.9283074	1.1633566	-0.1780850
O	1.4923572	5.5875118	1.3882602
H	-7.1536764	2.8857673	-3.5094686
H	-8.7814815	1.0319762	-3.2961166
H	-4.8052401	2.5524448	-2.8600787
H	-5.6738728	-1.5006357	-1.7620723
H	-8.0433574	-1.1676294	-2.4213544
H	3.4510400	6.9123424	2.0649367
H	5.5654784	7.3448437	3.3082758
H	6.7892721	5.4539325	4.3435876
H	3.8315937	2.7242046	2.8909137
H	5.9038479	3.1479362	4.1328747
C	-3.5174039	-4.8007747	-2.3802359
C	-4.2055532	-3.7365838	-2.9675292
C	-4.0097632	-6.1020355	-2.5142901
C	-5.3797528	-3.9767184	-3.6721993
C	-5.1859677	-6.3348174	-3.2125848
C	-5.8740030	-5.2718362	-3.7931008
C	-2.2432505	-4.6448720	-1.6313276
N	-1.9136973	-3.3917433	-1.1864439
N	-0.6845930	-3.2955523	-0.5884712
C	-0.2735543	-2.2002154	0.0496438
C	1.1344362	-2.3696380	0.5870748
N	1.6868159	-1.2129970	1.0023268
N	2.9991169	-1.3013517	1.3960124
C	3.6893733	-0.2303840	1.8416953
O	-1.4923572	-5.5875118	-1.3882602
O	-0.9283074	-1.1633566	0.1780850
O	1.7180766	-3.4520659	0.6398937
O	3.1839135	0.8934770	1.8940363
C	5.0954784	-0.5026518	2.2434239
C	6.0122313	0.5453258	2.1403048
C	5.5136815	-1.7413585	2.7363477
C	7.3353493	0.3530216	2.5123815
C	6.8372688	-1.9279270	3.1157464
C	7.7500303	-0.8835043	3.0005818
H	-5.9038479	-3.1479362	-4.1328747
H	-6.7892721	-5.4539325	-4.3435876
H	-3.4510400	-6.9123424	-2.0649367
H	-5.5654784	-7.3448437	-3.3082758
H	-3.8315937	-2.7242046	-2.8909137

H	5.6738728	1.5006357	1.7620723
H	8.0433574	1.1676294	2.4213544
H	8.7814815	-1.0319762	3.2961166
H	4.8052401	-2.5524448	2.8600787
H	7.1536764	-2.8857673	3.5094686
H	-3.3783550	2.2337978	-1.2776497
H	-1.3360022	0.2812256	-0.7310595
H	0.1591923	4.1677864	0.5847878
H	2.3954894	2.5090493	1.3682017
H	-2.3954894	-2.5090493	-1.3682017
H	-0.1591923	-4.1677864	-0.5847878
H	1.3360022	-0.2812256	0.7310595
H	3.3783550	-2.2337978	1.2776497

DADA05

72

C	-2.7912620	4.8735013	-0.4647286
C	-3.9729554	4.0544627	-0.3126676
C	-1.5279812	4.1318074	-0.3002255
C	-3.8929752	2.7118591	-0.0579800
C	-1.5202850	2.7516114	-0.0374297
N	-2.7118763	2.0665294	0.0795690
C	-0.3162750	4.8182205	-0.3990061
C	0.8868248	4.1613418	-0.2390321
C	0.9056083	2.7592804	0.0216118
C	-0.2986588	2.0833333	0.1118366
C	2.1347267	1.9285866	0.2197490
N	3.2902738	2.6005425	0.2793766
N	4.4971118	1.9867517	0.4778073
C	5.5959467	2.7938957	0.4567905
C	6.9119627	2.1013673	0.6900987
H	6.8041899	1.0239917	0.8021181
H	7.3694660	2.5207044	1.5876347
H	7.5720446	2.3210042	-0.1500503
O	2.0793677	0.6931998	0.3467732
O	5.4771689	4.0000545	0.2632507
O	-2.8263688	6.0833928	-0.7005309
C	-5.0984122	1.8576091	0.1379912
O	-6.2656195	2.3344471	-0.3166641
O	-5.0562291	0.7802326	0.6869591
H	-4.9265548	4.5662882	-0.3590457
H	-0.3745903	5.8783605	-0.6015519
H	-0.2888047	1.0217377	0.3119123
O	2.0836957	4.8032673	-0.3225954
N	2.7118763	-2.0665294	0.0795690
C	1.5202850	-2.7516114	-0.0374297
C	3.8929752	-2.7118591	-0.0579800
C	1.5279812	-4.1318074	-0.3002255
C	3.9729554	-4.0544627	-0.3126676
C	2.7912620	-4.8735013	-0.4647286
C	5.0984122	-1.8576091	0.1379912
O	6.2656195	-2.3344471	-0.3166641
O	5.0562291	-0.7802326	0.6869591
C	0.2986588	-2.0833333	0.1118366
C	-0.9056083	-2.7592804	0.0216118

C	-0.8868248	-4.1613418	-0.2390321
C	0.3162750	-4.8182205	-0.3990061
C	-2.1347267	-1.9285866	0.2197490
N	-3.2902738	-2.6005425	0.2793766
N	-4.4971118	-1.9867517	0.4778073
C	-5.5959467	-2.7938957	0.4567905
C	-6.9119627	-2.1013673	0.6900987
O	-5.4771689	-4.0000545	0.2632507
O	-2.0793677	-0.6931998	0.3467732
H	4.9265548	-4.5662882	-0.3590457
H	0.3745903	-5.8783605	-0.6015519
H	0.2888047	-1.0217377	0.3119123
O	-2.0836957	-4.8032673	-0.3225954
C	-2.0948841	-6.2117068	-0.5644555
H	-1.6322650	-6.4371516	-1.5275838
H	-3.1455202	-6.4879466	-0.5752644
H	-1.5710384	-6.7407837	0.2344092
C	2.0948841	6.2117068	-0.5644555
H	1.6322650	6.4371516	-1.5275838
H	3.1455202	6.4879466	-0.5752644
H	1.5710384	6.7407837	0.2344092
H	-2.6941926	1.0536200	0.2471799
H	3.3593461	3.6077431	0.1412330
H	4.4979989	0.9803024	0.6212394
H	-4.4979989	-0.9803024	0.6212394
H	-3.3593461	-3.6077431	0.1412330
H	2.6941926	-1.0536200	0.2471799
H	-6.1180800	3.1678682	-0.7887285
H	6.1180800	-3.1678682	-0.7887285
H	-6.8041899	-1.0239917	0.8021181
H	-7.3694660	-2.5207044	1.5876347
H	-7.5720446	-2.3210042	-0.1500503
O	2.8263688	-6.0833928	-0.7005309

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C	1.0152836	4.3255086	0.0000000
N	-0.1406299	3.6501668	0.0000000
C	2.2488753	3.7191610	0.0000000
C	-0.0401174	2.3171815	0.0000000
C	2.2429087	2.3142826	0.0000000
N	1.0974774	1.6094095	0.0000000
N	3.3893313	1.5596491	0.0000000
C	4.6902465	2.0063334	0.0000000
O	5.0658438	3.1605825	0.0000000
N	-1.1997261	1.5662250	0.0000000
C	-2.5275576	1.9873385	0.0000000
O	-3.4299841	1.1417363	0.0000000
H	5.3863987	1.1539695	0.0000000
H	0.9299469	5.4067309	0.0000000
H	3.1752012	4.2680398	0.0000000
H	-1.0896542	0.5496190	0.0000000
H	3.2753227	0.5285757	0.0000000
N	-2.7667894	3.3055080	0.0000000
O	3.4299841	-1.1417363	0.0000000

C	2.5275576	-1.9873385	0.0000000
N	1.1997261	-1.5662250	0.0000000
N	2.7667894	-3.3055080	0.0000000
C	0.0401174	-2.3171815	0.0000000
N	-1.0974774	-1.6094095	0.0000000
N	0.1406299	-3.6501668	0.0000000
C	-2.2429087	-2.3142826	0.0000000
N	-3.3893313	-1.5596491	0.0000000
C	-1.0152836	-4.3255086	0.0000000
C	-2.2488753	-3.7191610	0.0000000
C	-4.6902465	-2.0063334	0.0000000
H	-5.3863987	-1.1539695	0.0000000
O	-5.0658438	-3.1605825	0.0000000
H	-0.9299469	-5.4067309	0.0000000
H	-3.1752012	-4.2680398	0.0000000
H	1.0896542	-0.5496190	0.0000000
H	-3.2753227	-0.5285757	0.0000000
H	-1.9737448	3.9449972	0.0000000
H	-3.7281267	3.5978583	0.0000000
H	3.7281267	-3.5978583	0.0000000
H	1.9737448	-3.9449972	0.0000000

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C	-4.9535472	4.4948261	0.8983411
C	-6.1328183	3.7958315	0.6728674
C	-3.7211966	3.8486032	0.9281871
C	-3.6606681	2.4550390	0.7122583
C	-6.0915907	2.4140307	0.4748980
C	-4.8544094	1.7731670	0.4935091
O	-2.5500350	4.5168362	1.1541547
N	-7.2293333	1.6229949	0.2576719
C	-8.4929053	2.0434245	-0.0468701
C	-9.4888411	0.9101010	-0.2322788
C	-10.4132800	1.1443264	-1.4254346
C	-11.4647176	0.0454925	-1.5548350
O	-8.8221523	3.2179088	-0.1628450
C	-2.4132718	1.6304172	0.6582107
N	-1.2533974	2.2311631	0.9610990
C	0.0115969	1.5528552	0.8966411
C	1.1071904	2.5610910	1.2266591
N	2.3547694	2.1025566	0.9572645
C	3.5631869	2.7962412	1.1304503
C	3.6929607	3.9413993	1.9176811
C	4.9297632	4.5645064	2.0293308
C	6.0508820	4.0727339	1.3680272
C	5.9378853	2.9124537	0.5758343
C	4.6897654	2.3028332	0.4781329
C	7.0279650	2.2642423	-0.2234113
N	8.2068721	2.9130699	-0.3142062
C	9.2903548	2.4765316	-1.1757443
C	9.5341858	3.4182554	-2.3612727
C	9.8818352	4.8340948	-1.9008937
O	6.8254068	1.1840906	-0.7944029

O	-2.4507400	0.4282496	0.3404221
O	0.8394086	3.6647455	1.6904202
O	7.2786396	4.6815195	1.4594561
C	-2.5930323	5.9182157	1.3931427
C	7.3925427	5.8523482	2.2618349
C	10.6412843	2.8367645	-3.2406388
H	-5.0081384	5.5633916	1.0519894
H	-7.0799780	4.3109438	0.6426893
H	-4.7987456	0.7061660	0.3308730
H	-7.0876170	0.6172227	0.3510647
H	-8.9658867	-0.0427005	-0.3314349
H	-10.0878084	0.8531198	0.6841968
H	-10.8873820	2.1207200	-1.3118049
H	-9.8136940	1.1945461	-2.3393946
H	-12.0821700	-0.0132914	-0.6538629
H	-10.9977587	-0.9330065	-1.7015497
H	-12.1277913	0.2278859	-2.4031362
H	-1.2354430	3.2079818	1.2364554
H	0.0575615	0.7249105	1.6126735
H	0.1860840	1.1230326	-0.0910988
H	2.4208482	1.1867827	0.5051118
H	2.8326027	4.3464457	2.4259468
H	5.0049580	5.4494956	2.6449973
H	4.6113882	1.4263434	-0.1504782
H	8.2903256	3.7769790	0.2026295
H	10.2069243	2.3902919	-0.5819200
H	9.0252897	1.4848747	-1.5360380
H	8.6067049	3.4572495	-2.9426481
H	10.0604901	5.4882180	-2.7568789
H	10.7898574	4.8294032	-1.2890468
H	9.0747445	5.2778967	-1.3126607
H	-3.1910640	6.1437569	2.2800793
H	-2.9998763	6.4484157	0.5279318
H	-1.5592747	6.2116952	1.5571302
H	7.1456260	5.6346808	3.3037886
H	6.7446519	6.6476617	1.8848919
H	8.4334908	6.1575256	2.1862937
H	11.5807969	2.7656890	-2.6839233
H	10.8187524	3.4673327	-4.1142913
H	10.3825134	1.8353922	-3.5923178
C	2.5930323	-5.9182157	-1.3931427
C	-7.3925427	-5.8523482	-2.2618349
C	-4.9297632	-4.5645064	-2.0293308
O	2.5500350	-4.5168362	-1.1541547
C	-3.6929607	-3.9413993	-1.9176811
O	-0.8394086	-3.6647455	-1.6904202
C	4.9535472	-4.4948261	-0.8983411
O	-7.2786396	-4.6815195	-1.4594561
C	3.7211966	-3.8486032	-0.9281871
C	-6.0508820	-4.0727339	-1.3680272
C	6.1328183	-3.7958315	-0.6728674
C	-9.8818352	-4.8340948	1.9008937
C	-1.1071904	-2.5610910	-1.2266591
C	-3.5631869	-2.7962412	-1.1304503
N	1.2533974	-2.2311631	-0.9610990
C	3.6606681	-2.4550390	-0.7122583
N	-2.3547694	-2.1025566	-0.9572645

C	-5.9378853	-2.9124537	-0.5758343
C	-0.0115969	-1.5528552	-0.8966411
C	-4.6897654	-2.3028332	-0.4781329
C	6.0915907	-2.4140307	-0.4748980
C	2.4132718	-1.6304172	-0.6582107
C	-9.5341858	-3.4182554	2.3612727
O	8.8221523	-3.2179088	0.1628450
C	4.8544094	-1.7731670	-0.4935091
C	-7.0279650	-2.2642423	0.2234113
C	8.4929053	-2.0434245	0.0468701
N	7.2293333	-1.6229949	-0.2576719
O	-6.8254068	-1.1840906	0.7944029
N	-8.2068721	-2.9130699	0.3142062
C	-10.6412843	-2.8367645	3.2406388
O	2.4507400	-0.4282496	-0.3404221
C	9.4888411	-0.9101010	0.2322788
C	-9.2903548	-2.4765316	1.1757443
C	10.4132800	-1.1443264	1.4254346
C	11.4647176	-0.0454925	1.5548350
H	2.9998763	-6.4484157	-0.5279318
H	3.1910640	-6.1437569	-2.2800793
H	1.5592747	-6.2116952	-1.5571302
H	-6.7446519	-6.6476617	-1.8848919
H	-7.1456260	-5.6346808	-3.3037886
H	-8.4334908	-6.1575256	-2.1862937
H	-5.0049580	-5.4494956	-2.6449973
H	-2.8326027	-4.3464457	-2.4259468
H	5.0081384	-5.5633916	-1.0519894
H	7.0799780	-4.3109438	-0.6426893
H	-9.0747445	-5.2778967	1.3126607
H	-10.7898574	-4.8294032	1.2890468
H	-10.0604901	-5.4882180	2.7568789
H	1.2354430	-3.2079818	-1.2364554
H	-2.4208482	-1.1867827	-0.5051118
H	-0.0575615	-0.7249105	-1.6126735
H	-0.1860840	-1.1230326	0.0910988
H	-4.6113882	-1.4263434	0.1504782
H	-8.6067049	-3.4572495	2.9426481
H	4.7987456	-0.7061660	-0.3308730
H	7.0876170	-0.6172227	-0.3510647
H	-8.2903256	-3.7769790	-0.2026295
H	-11.5807969	-2.7656890	2.6839233
H	-10.3825134	-1.8353922	3.5923178
H	-10.8187524	-3.4673327	4.1142913
H	8.9658867	0.0427005	0.3314349
H	10.0878084	-0.8531198	-0.6841968
H	-10.2069243	-2.3902919	0.5819200
H	-9.0252897	-1.4848747	1.5360380
H	10.8873820	-2.1207200	1.3118049
H	9.8136940	-1.1945461	2.3393946
H	10.9977587	0.9330065	1.7015497
H	12.0821700	0.0132914	0.6538629
H	12.1277913	-0.2278859	2.4031362

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N	1.5406905	-1.0479636	0.0000000
C	2.2744162	-2.1768296	0.0000000
C	3.6984566	-2.1505023	0.0000000
C	4.3383755	-0.9430295	0.0000000
C	3.3621863	2.6671236	0.0000000
C	1.9251931	2.5494553	0.0000000
N	1.4264813	1.2562942	0.0000000
C	2.1895701	0.1222806	0.0000000
C	3.5961490	0.2537143	0.0000000
C	4.1510813	1.5605630	0.0000000
N	1.6128477	-3.3447529	0.0000000
H	4.2488498	-3.0826744	0.0000000
H	5.4216619	-0.8942676	0.0000000
H	0.5821678	-3.3858169	0.0000000
H	5.2317577	1.6617388	0.0000000
H	3.7660982	3.6692842	0.0000000
O	1.1488318	3.5180306	0.0000000
H	2.1342396	-4.2029866	0.0000000
H	0.3961150	1.1527608	0.0000000
N	-1.5406905	1.0479636	0.0000000
C	-2.2744162	2.1768296	0.0000000
C	-3.6984566	2.1505023	0.0000000
C	-4.3383755	0.9430295	0.0000000
C	-3.3621863	-2.6671236	0.0000000
C	-1.9251931	-2.5494553	0.0000000
N	-1.4264813	-1.2562942	0.0000000
C	-2.1895701	-0.1222806	0.0000000
C	-3.5961490	-0.2537143	0.0000000
C	-4.1510813	-1.5605630	0.0000000
N	-1.6128477	3.3447529	0.0000000
H	-4.2488498	3.0826744	0.0000000
H	-5.4216619	0.8942676	0.0000000
H	-0.5821678	3.3858169	0.0000000
H	-5.2317577	-1.6617388	0.0000000
H	-3.7660982	-3.6692842	0.0000000
O	-1.1488318	-3.5180306	0.0000000
H	-2.1342396	4.2029866	0.0000000
H	-0.3961150	-1.1527608	0.0000000

3. Detailed SAPT analysis

Here, we report the full SAPT analysis for all dimers.

Table S3.1. Full SAPT analysis for the DDAA dimers. Yellow rows mark direct hydrogen bonds, blue rows diagonal interactions. Energies in kJ/mol.

DDAA01							
Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
D1	A3	-40.06	42.57	-6.35	-7.65	-20.80	-32.28
D1	A4	-4.52	0.00	-0.34	-0.63	-0.27	-5.75
D1	D3	0.71	0.00	0.08	-0.10	-0.05	0.65
D1	D4	0.24	0.00	0.03	0.03	0.00	0.29
D2	A3	-5.49	5.30	-1.56	-2.35	-8.82	-12.92
D2	A4	-47.05	41.54	-10.74	-8.07	-15.87	-40.19
D2	D3	1.48	9.02	0.11	0.11	-5.87	4.84
D2	D4	0.71	0.00	-0.10	0.08	-0.05	0.65
A1	A3	-3.66	0.00	-0.35	-0.46	-0.25	-4.72
A1	A4	-24.05	0.38	-2.62	-2.62	-1.45	-30.36
A1	D3	-47.05	41.54	-8.07	-10.74	-15.87	-40.19
A1	D4	-4.52	0.00	-0.63	-0.34	-0.27	-5.75
A2	A3	-0.44	0.00	-0.21	-0.21	-0.10	-0.96
A2	A4	-3.66	0.00	-0.46	-0.35	-0.25	-4.72
A2	D3	-5.49	5.30	-2.35	-1.56	-8.82	-12.92
A2	D4	-40.06	42.57	-7.65	-6.35	-20.80	-32.28
D1	All	-43.63	42.57	-6.57	-8.35	-21.11	-37.09
D2	All	-50.36	55.86	-12.30	-10.23	-30.61	-47.63
A1	All	-79.28	41.93	-11.66	-14.17	-17.84	-81.01
A2	All	-49.64	47.87	-10.67	-8.47	-29.97	-50.88
All	A3	-49.64	47.87	-8.47	-10.67	-29.97	-50.88
All	A4	-79.28	41.93	-14.17	-11.66	-17.84	-81.01
All	D3	-50.36	55.86	-10.23	-12.30	-30.61	-47.63
All	D4	-43.63	42.57	-8.35	-6.57	-21.11	-37.09
All	All	-222.90	188.23	-41.21	-41.21	-99.52	-216.61
direct H-bonds		-174.21	168.22	-32.80	-32.80	-73.34	-144.94
direct diagonal		-42.60	20.01	-7.39	-7.39	-25.49	-62.85
the rest		-6.10	0.01	-1.01	-1.01	-0.70	-8.81

DDAA02

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
D1	A3	-50.12	77.89	-8.92	-16.98	-12.14	-10.27
D1	A4	1.08	0.86	-1.03	-1.12	-1.95	-2.16
D1	D3	0.22	0.00	-0.06	-0.11	-0.19	-0.14
D1	D4	0.04	0.00	-0.01	-0.01	-0.03	0.00
D2	A3	-6.79	2.27	-0.40	-5.47	-3.02	-13.40
D2	A4	-77.95	59.79	-9.31	-17.94	-11.42	-56.84
D2	D3	11.09	0.36	-0.41	-0.41	-1.50	9.13
D2	D4	0.22	0.00	-0.11	-0.06	-0.19	-0.14
A1	A3	-22.32	0.11	-2.43	-2.76	-0.65	-28.05
A1	A4	-22.43	2.31	-5.68	-5.68	-3.57	-35.06
A1	D3	-77.96	59.80	-17.95	-9.31	-11.42	-56.84
A1	D4	1.08	0.86	-1.12	-1.03	-1.95	-2.15
A2	A3	-0.66	0.00	-1.06	-1.06	-0.11	-2.89
A2	A4	-22.32	0.11	-2.76	-2.43	-0.65	-28.05
A2	D3	-6.79	2.27	-5.47	-0.39	-3.02	-13.40
A2	D4	-50.11	77.87	-16.97	-8.91	-12.14	-10.26
D1	All	-48.78	78.75	-10.00	-18.21	-14.31	-12.56
D2	All	-73.43	62.42	-10.23	-23.88	-16.12	-61.24
A1	All	-121.64	63.08	-27.18	-18.79	-17.59	-122.11
A2	All	-79.88	80.25	-26.25	-12.79	-15.92	-54.59
All	A3	-79.90	80.27	-12.80	-26.26	-15.92	-54.61
All	A4	-121.63	63.07	-18.78	-27.17	-17.59	-122.10
All	D3	-73.44	62.44	-23.88	-10.23	-16.12	-61.24
All	D4	-48.77	78.73	-18.21	-10.00	-14.30	-12.55
All	All	-323.73	284.50	-73.67	-73.67	-63.94	-250.49
direct H-bonds		-256.15	275.35	-53.14	-53.14	-47.12	-134.20
direct diagonal		-22.76	8.93	-14.10	-14.10	-15.00	-57.04
the rest		-44.83	0.23	-6.42	-6.42	-1.82	-59.26

DDAA03

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
D1	A3	-78.85	62.41	-8.77	-16.07	-13.03	-54.30
D1	A4	4.16	1.75	1.89	-5.84	-4.77	-2.81
D1	D3	1.81	0.03	0.14	-0.05	-0.39	1.53
D1	D4	6.41	0.00	0.20	0.20	-0.17	6.63
D2	A3	4.39	0.89	-2.37	0.24	-1.66	1.49
D2	A4	-28.36	43.40	-3.28	-7.29	-9.59	-5.12
D2	D3	1.73	0.67	-0.01	-0.01	-1.27	1.12
D2	D4	1.80	0.03	-0.05	0.14	-0.39	1.53
A1	A3	-10.84	0.01	-1.44	-1.51	-0.74	-14.52
A1	A4	-10.37	2.12	-3.09	-3.09	-4.79	-19.23
A1	D3	-28.36	43.39	-7.29	-3.28	-9.59	-5.12
A1	D4	4.15	1.75	-5.84	1.89	-4.77	-2.81
A2	A3	1.24	0.00	0.06	0.06	-0.09	1.27
A2	A4	-10.84	0.01	-1.51	-1.44	-0.74	-14.52
A2	D3	4.39	0.89	0.24	-2.37	-1.66	1.50
A2	D4	-78.84	62.41	-16.07	-8.77	-13.03	-54.30
D1	All	-66.48	64.19	-6.55	-21.76	-18.36	-48.95
D2	All	-20.44	44.98	-5.71	-6.92	-12.90	-0.98
A1	All	-45.41	47.27	-17.66	-5.99	-19.89	-41.68
A2	All	-84.05	63.31	-17.28	-12.52	-15.52	-66.05
All	A3	-84.06	63.31	-12.52	-17.28	-15.52	-66.06
All	A4	-45.41	47.28	-5.99	-17.66	-19.89	-41.68
All	D3	-20.43	44.97	-6.92	-5.71	-12.90	-0.98
All	D4	-66.48	64.20	-21.76	-6.55	-18.36	-48.94
All	All	-216.38	219.76	-47.19	-47.19	-66.67	-157.66
direct H-bonds		-214.41	211.61	-35.41	-35.41	-45.23	-118.84
direct diagonal		8.46	8.07	-9.18	-9.18	-18.91	-20.75
the rest		-10.43	0.08	-2.60	-2.60	-2.52	-18.07

DDAA04

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
D1	A3	-47.78	21.49	-4.98	-6.70	-6.72	-44.70
D1	A4	-12.19	1.84	0.63	-4.89	-3.63	-18.23
D1	D3	7.40	0.09	0.45	-0.34	-0.66	6.95
D1	D4	5.82	0.00	0.10	0.10	-0.12	5.90
D2	A3	-0.45	0.19	-1.75	-0.39	-1.29	-3.69
D2	A4	-50.22	73.81	-7.94	-13.44	-13.13	-10.93
D2	D3	14.61	0.72	1.36	1.36	-2.63	15.42
D2	D4	7.40	0.09	-0.34	0.45	-0.66	6.95
A1	A3	-3.26	0.00	-0.93	-0.07	-0.43	-4.68
A1	A4	-3.66	2.38	-1.47	-1.47	-3.32	-7.54
A1	D3	-50.22	73.81	-13.44	-7.94	-13.13	-10.93
A1	D4	-12.19	1.84	-4.89	0.63	-3.63	-18.23
A2	A3	-2.83	0.00	-0.15	-0.15	-0.09	-3.21
A2	A4	-3.26	0.00	-0.07	-0.93	-0.43	-4.68
A2	D3	-0.45	0.19	-0.39	-1.75	-1.29	-3.69
A2	D4	-47.78	21.49	-6.70	-4.98	-6.72	-44.70
D1	All	-46.74	23.42	-3.80	-11.82	-11.13	-50.08
D2	All	-28.66	74.81	-8.67	-12.03	-17.71	7.76
A1	All	-69.32	78.02	-20.73	-8.86	-20.51	-41.39
A2	All	-54.32	21.68	-7.31	-7.80	-8.53	-56.28
All	A3	-54.32	21.68	-7.80	-7.31	-8.53	-56.28
All	A4	-69.32	78.02	-8.86	-20.72	-20.51	-41.38
All	D3	-28.66	74.82	-12.03	-8.67	-17.71	7.76
All	D4	-46.74	23.42	-11.82	-3.80	-11.13	-50.08
All	All	-199.04	197.93	-40.51	-40.50	-57.87	-139.99
direct H-bonds		-195.99	190.59	-33.07	-33.07	-39.71	-111.25
direct diagonal		-14.32	7.16	-6.51	-6.51	-15.78	-35.96
the rest		11.28	0.18	-0.93	-0.93	-2.38	7.22

DDAA05

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
D1	A3	-45.65	62.12	-4.72	-11.29	-12.56	-12.10
D1	A4	1.49	0.40	-0.97	-0.18	-1.42	-0.67
D1	D3	0.44	0.00	0.03	0.06	-0.15	0.38
D1	D4	0.08	0.00	0.04	0.04	-0.02	0.14
D2	A3	18.52	2.16	1.79	-5.06	-4.04	13.38
D2	A4	-71.64	35.28	-6.37	-10.16	-8.27	-61.15
D2	D3	9.61	0.23	-0.10	-0.10	-1.21	8.44
D2	D4	0.44	0.00	0.06	0.03	-0.15	0.38
A1	A3	-19.99	0.14	-0.88	-1.67	-0.97	-23.36
A1	A4	-14.41	1.87	-3.26	-3.26	-3.06	-22.12
A1	D3	-71.64	35.28	-10.15	-6.37	-8.27	-61.15
A1	D4	1.50	0.40	-0.18	-0.97	-1.42	-0.67
A2	A3	18.38	0.00	-0.83	-0.83	-0.28	16.43
A2	A4	-19.98	0.14	-1.67	-0.88	-0.96	-23.36
A2	D3	18.52	2.16	-5.06	1.79	-4.04	13.38
A2	D4	-45.65	62.11	-11.29	-4.72	-12.56	-12.10
D1	All	-43.64	62.52	-5.61	-11.37	-14.15	-12.25
D2	All	-43.07	37.68	-4.61	-15.28	-13.66	-38.95
A1	All	-104.54	37.68	-14.47	-12.26	-13.72	-107.30
A2	All	-28.73	64.41	-18.85	-4.64	-17.84	-5.65
All	A3	-28.74	64.42	-4.64	-18.85	-17.85	-5.65
All	A4	-104.54	37.68	-12.26	-14.47	-13.71	-107.31
All	D3	-43.07	37.68	-15.28	-4.61	-13.66	-38.95
All	D4	-43.63	62.51	-11.37	-5.61	-14.15	-12.25
All	All	-219.97	202.29	-43.54	-43.55	-59.37	-164.15
direct H-bonds		-234.58	194.78	-32.53	-32.53	-41.65	-146.51
direct diagonal		35.24	7.23	-7.77	-7.77	-15.19	11.74
the rest		-20.63	0.27	-3.25	-3.25	-2.53	-29.38

DDAA06 (tautomer)

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
D1	A3	-69.60	107.11	-12.84	-24.08	-12.76	-12.18
D1	A4	5.03	2.93	-1.10	-4.25	-4.62	-2.02
D1	D3	-0.83	0.04	-2.08	-1.05	-0.99	-4.91
D1	D4	-0.02	0.00	-0.07	-0.07	-0.05	-0.20
D2	A3	-21.48	1.99	-3.14	-5.79	-2.15	-30.57
D2	A4	-104.60	84.54	-16.07	-29.39	-15.32	-80.84
D2	D3	8.46	2.93	-8.00	-8.00	-8.36	-12.96
D2	D4	-0.83	0.04	-1.05	-2.08	-0.99	-4.91
A1	A3	-10.87	0.00	-1.89	-1.69	-0.12	-14.57
A1	A4	-19.08	2.40	-5.26	-5.26	-1.94	-29.14
A1	D3	-104.60	84.54	-29.39	-16.07	-15.32	-80.84
A1	D4	5.03	2.93	-4.25	-1.10	-4.62	-2.02
A2	A3	-0.85	0.00	-0.50	-0.50	0.00	-1.85
A2	A4	-10.87	0.00	-1.69	-1.89	-0.12	-14.57
A2	D3	-21.48	1.99	-5.79	-3.14	-2.15	-30.57
A2	D4	-69.60	107.11	-24.08	-12.84	-12.76	-12.18
D1	All	-65.42	110.08	-16.10	-29.45	-18.42	-19.30
D2	All	-118.45	89.50	-28.25	-45.25	-26.83	-129.28
A1	All	-129.52	89.86	-40.79	-24.12	-21.99	-126.57
A2	All	-102.81	109.09	-32.06	-18.38	-15.02	-59.17
All	A3	-102.81	109.09	-18.38	-32.06	-15.02	-59.17
All	A4	-129.52	89.86	-24.12	-40.79	-21.99	-126.57
All	D3	-118.45	89.50	-45.25	-28.25	-26.83	-129.28
All	D4	-65.42	110.08	-29.45	-16.10	-18.42	-19.30
All	All	-416.20	398.54	-117.20	-117.20	-82.26	-334.32
direct H-bonds		-348.39	383.29	-82.39	-82.39	-56.16	-186.04
direct diagonal		-43.53	15.16	-27.54	-27.54	-23.84	-107.28
the rest		-24.28	0.08	-7.28	-7.28	-2.26	-41.02

DDAA07

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
D1	A3	-49.99	81.31	-10.72	-16.32	-13.68	-9.40
D1	A4	3.47	0.99	-1.65	-0.68	-2.38	-0.26
D1	D3	-0.49	0.00	0.00	-0.12	-0.24	-0.84
D1	D4	0.08	0.00	-0.03	-0.03	-0.05	-0.03
D2	A3	-7.06	2.23	-0.24	-5.59	-3.10	-13.76
D2	A4	-82.73	64.43	-10.47	-19.65	-12.12	-60.53
D2	D3	10.89	0.38	-0.44	-0.44	-1.56	8.83
D2	D4	-0.49	0.00	-0.12	0.00	-0.24	-0.84
A1	A3	-22.91	0.12	-2.51	-2.74	-0.67	-28.71
A1	A4	-22.81	2.43	-6.05	-6.05	-3.75	-36.21
A1	D3	-82.73	64.43	-19.65	-10.47	-12.12	-60.53
A1	D4	3.47	0.99	-0.68	-1.65	-2.38	-0.26
A2	A3	-0.91	0.00	-1.08	-1.08	-0.12	-3.17
A2	A4	-22.91	0.12	-2.74	-2.51	-0.67	-28.71
A2	D3	-7.06	2.23	-5.59	-0.24	-3.10	-13.76
A2	D4	-49.99	81.31	-16.32	-10.72	-13.68	-9.40
D1	All	-46.94	82.30	-12.40	-17.14	-16.34	-10.53
D2	All	-79.40	67.05	-11.27	-25.68	-17.01	-66.30
A1	All	-124.98	67.97	-28.89	-20.91	-18.92	-125.72
A2	All	-80.87	83.65	-25.72	-14.55	-17.57	-55.05
All	A3	-80.87	83.65	-14.55	-25.72	-17.57	-55.05
All	A4	-124.98	67.97	-20.91	-28.89	-18.92	-125.72
All	D3	-79.40	67.05	-25.68	-11.27	-17.01	-66.30
All	D4	-46.94	82.30	-17.14	-12.40	-16.34	-10.53
All	All	-332.18	300.96	-78.27	-78.27	-69.84	-257.60
direct H-bonds		-265.44	291.48	-57.16	-57.16	-51.59	-139.87
direct diagonal		-19.12	9.25	-14.65	-14.65	-16.26	-55.43
the rest		-47.63	0.24	-6.47	-6.47	-1.99	-62.31

DDAA08

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
D1	A3	-47.32	78.40	-8.49	-15.72	-13.91	-7.04
D1	A4	3.01	0.94	-2.04	-0.50	-2.12	-0.70
D1	D3	-0.49	0.00	-0.02	-0.11	-0.24	-0.85
D1	D4	0.08	0.00	-0.03	-0.03	-0.05	-0.03
D2	A3	-0.57	2.18	0.73	-6.12	-3.37	-7.15
D2	A4	-81.24	58.07	-9.97	-17.34	-11.19	-61.68
D2	D3	9.58	0.39	-0.46	-0.46	-1.52	7.51
D2	D4	-0.49	0.00	-0.11	-0.02	-0.24	-0.85
A1	A3	-22.88	0.13	-1.88	-2.64	-0.83	-28.09
A1	A4	-22.59	2.08	-5.30	-5.30	-3.29	-34.41
A1	D3	-81.23	58.06	-17.33	-9.97	-11.19	-61.66
A1	D4	3.01	0.94	-0.50	-2.04	-2.12	-0.70
A3	A3	5.34	0.01	-1.16	-1.16	-0.32	2.71
A3	A4	-22.87	0.13	-2.64	-1.88	-0.83	-28.09
A3	D3	-0.58	2.18	-6.12	0.73	-3.37	-7.15
A3	D4	-47.32	78.39	-15.72	-8.49	-13.91	-7.05
D1	All	-44.72	79.34	-10.58	-16.36	-16.31	-8.62
D2	All	-72.73	60.63	-9.82	-23.93	-16.32	-62.17
A1	All	-123.69	61.21	-25.01	-19.95	-17.42	-124.87
A3	All	-65.44	80.70	-25.63	-10.80	-18.42	-39.58
All	A3	-65.43	80.71	-10.80	-25.63	-18.42	-39.58
All	A4	-123.70	61.21	-19.95	-25.01	-17.42	-124.88
All	D3	-72.72	60.63	-23.93	-9.82	-16.32	-62.16
All	D4	-44.72	79.34	-16.36	-10.58	-16.31	-8.63
All	All	-306.57	281.89	-71.04	-71.04	-68.47	-235.24
direct H-bonds		-257.12	272.92	-51.52	-51.52	-50.20	-137.43
direct diagonal		-8.15	8.70	-13.69	-13.69	-15.78	-42.61
the rest		-41.30	0.27	-5.84	-5.84	-2.49	-55.20

DDAA Average							
Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
D1	A3	-52.97	67.97	-8.25	-14.50	-13.28	-21.04
D1	A4	0.50	1.18	-0.74	-2.06	-2.58	-3.70
D1	D3	0.92	0.02	-0.16	-0.21	-0.35	0.21
D1	D4	1.42	0.00	0.02	0.02	-0.06	1.41
D2	A3	-2.17	2.15	-0.69	-4.07	-3.42	-8.20
D2	A4	-69.45	57.66	-9.35	-15.62	-12.01	-48.77
D2	D3	8.56	1.68	-0.94	-0.94	-2.83	5.54
D2	D4	0.92	0.02	-0.21	-0.16	-0.35	0.21
A1	A3	-15.51	0.07	-1.58	-1.80	-0.61	-19.42
A1	A4	-18.00	2.00	-4.23	-4.23	-3.16	-27.61
A1	D3	-69.45	57.66	-15.62	-9.35	-12.01	-48.77
A1	D4	0.50	1.18	-2.06	-0.74	-2.58	-3.70
A2	A3	2.73	0.00	-0.68	-0.68	-0.16	1.23
A2	A4	-15.51	0.07	-1.80	-1.58	-0.61	-19.42
A2	D3	-2.17	2.15	-4.07	-0.69	-3.42	-8.20
A2	D4	-52.96	67.96	-14.50	-8.25	-13.28	-21.03
D1	All	-50.12	69.17	-9.13	-16.76	-16.27	-23.11
D2	All	-62.14	61.51	-11.19	-20.79	-18.61	-51.22
A1	All	-102.45	60.91	-23.49	-16.11	-18.37	-99.50
A2	All	-67.91	70.19	-21.04	-11.19	-17.47	-47.43
All	A3	-67.91	70.19	-11.19	-21.05	-17.47	-47.43
All	A4	-102.45	60.91	-16.11	-23.49	-18.37	-99.50
All	D3	-62.14	61.51	-20.79	-11.19	-18.61	-51.21
All	D4	-50.12	69.16	-16.76	-9.13	-16.27	-23.11
All	All	-282.61	261.78	-64.85	-64.85	-70.71	-221.25
direct H-bonds		-244.82	251.24	-47.72	-47.73	-50.58	-139.61
direct diagonal		-12.77	10.36	-12.72	-12.72	-18.00	-45.86
the rest		-25.02	0.18	-4.40	-4.40	-2.13	-35.78

Table S3.2. Full SAPT analysis for the DADA dimers. Yellow rows mark direct hydrogen bonds, blue rows diagonal interactions. Energies in kJ/mol.

DADA01							
Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
D1	A3	-63.30	74.96	-9.05	-19.15	-13.03	-29.58
D1	D3	4.21	0.64	0.27	-0.12	-1.52	3.49
D1	A4	2.74	0.05	0.51	-0.90	-0.56	1.85
D1	D4	1.88	0.00	-0.09	-0.09	-0.05	1.66
A1	A3	-29.08	2.01	-3.82	-3.18	-3.20	-37.28
A1	D3	-27.30	38.68	-7.42	-2.33	-8.52	-6.89
A1	A4	-14.81	0.80	0.09	0.09	-3.59	-17.42
A1	D4	2.74	0.05	-0.90	0.51	-0.56	1.85
D2	A3	1.31	0.03	0.48	0.06	-0.28	1.61
D2	D3	0.88	0.68	0.00	0.00	-1.15	0.40
D2	A4	-27.30	38.68	-2.33	-7.42	-8.52	-6.89
D2	D4	4.21	0.64	-0.12	0.27	-1.52	3.49
A2	A3	-2.07	0.00	-0.72	-0.72	-0.09	-3.59
A2	D3	1.31	0.03	0.06	0.48	-0.28	1.61
A2	A4	-29.08	2.01	-3.18	-3.82	-3.20	-37.28
A2	D4	-63.30	74.96	-19.15	-9.05	-13.03	-29.58
D1	All	-54.46	75.66	-8.36	-20.26	-15.15	-22.59
A1	All	-68.44	41.55	-12.05	-4.92	-15.87	-59.73
D2	All	-20.90	40.04	-1.98	-7.10	-11.46	-1.39
A2	All	-93.14	77.01	-23.00	-13.11	-16.60	-68.84
All	A3	-93.14	77.01	-13.11	-23.00	-16.60	-68.84
All	D3	-20.90	40.04	-7.10	-1.98	-11.46	-1.39
All	A4	-68.44	41.55	-4.92	-12.05	-15.87	-59.73
All	D4	-54.46	75.66	-20.26	-8.36	-15.15	-22.59
All	All	-236.94	234.27	-45.38	-45.38	-59.09	-152.54
direct H-bonds		-181.19	227.29	-37.96	-37.96	-43.11	-72.93
direct diagonal		-63.66	6.79	-6.77	-6.77	-14.18	-84.60
the rest		7.91	0.17	-0.65	-0.65	-1.80	4.98

DADA02

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
D1	A3	-52.26	76.57	-10.13	-16.92	-12.11	-14.84
D1	D3	2.30	0.64	0.25	-0.18	-1.29	1.73
D1	A4	1.66	0.03	0.70	-0.14	-0.43	1.83
D1	D4	0.06	0.00	-0.03	-0.03	-0.03	-0.03
A1	A3	-32.56	1.96	-3.00	-3.75	-3.06	-40.41
A1	D3	-22.30	30.32	-5.43	-2.60	-7.31	-7.33
A1	A4	-10.20	0.93	0.08	0.08	-3.49	-12.61
A1	D4	1.66	0.03	-0.14	0.70	-0.43	1.83
D2	A3	0.84	0.02	0.47	0.03	-0.24	1.11
D2	D3	0.98	0.37	0.04	0.04	-0.91	0.54
D2	A4	-22.30	30.31	-2.60	-5.43	-7.31	-7.32
D2	D4	2.30	0.64	-0.18	0.25	-1.29	1.73
A2	A3	-3.75	0.00	-0.56	-0.56	-0.09	-4.96
A2	D3	0.84	0.02	0.03	0.47	-0.24	1.11
A2	A4	-32.56	1.96	-3.75	-3.00	-3.06	-40.41
A2	D4	-52.26	76.57	-16.92	-10.13	-12.11	-14.85
D1	All	-48.24	77.25	-9.21	-17.26	-13.86	-11.32
A1	All	-63.40	33.24	-8.49	-5.58	-14.29	-58.52
D2	All	-18.18	31.34	-2.26	-5.11	-9.74	-3.95
A2	All	-87.73	78.54	-21.19	-13.21	-15.50	-59.09
All	A3	-87.73	78.55	-13.22	-21.19	-15.50	-59.09
All	D3	-18.18	31.34	-5.11	-2.26	-9.74	-3.95
All	A4	-63.39	33.24	-5.58	-8.49	-14.29	-58.51
All	D4	-48.24	77.25	-17.26	-9.21	-13.86	-11.32
All	All	-217.54	220.37	-41.16	-41.16	-53.39	-132.88
direct H-bonds		-149.12	213.76	-35.08	-35.08	-38.82	-44.34
direct diagonal		-69.73	6.51	-6.56	-6.56	-13.09	-89.43
the rest		1.30	0.10	0.48	0.48	-1.47	0.90

DADA03

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
D1	A3	-53.24	77.74	-10.13	-17.23	-12.28	-15.13
D1	D3	2.11	0.62	0.22	-0.22	-1.26	1.46
D1	A4	1.62	0.03	0.78	-0.11	-0.44	1.87
D1	D4	0.03	0.00	-0.04	-0.04	-0.03	-0.08
A1	A3	-29.82	1.89	-2.91	-3.47	-3.08	-37.38
A1	D3	-20.01	25.12	-4.49	-2.31	-6.66	-8.35
A1	A4	-7.78	0.82	0.20	0.20	-3.55	-10.11
A1	D4	1.62	0.03	-0.11	0.78	-0.44	1.87
D2	A3	0.78	0.01	0.43	0.02	-0.23	1.00
D2	D3	1.06	0.31	0.07	0.07	-0.84	0.66
D2	A4	-20.01	25.12	-2.31	-4.49	-6.66	-8.35
D2	D4	2.11	0.62	-0.22	0.22	-1.26	1.46
A2	A3	-3.61	0.00	-0.54	-0.54	-0.08	-4.77
A2	D3	0.78	0.01	0.02	0.43	-0.23	1.00
A2	A4	-29.82	1.89	-3.47	-2.91	-3.08	-37.38
A2	D4	-53.24	77.73	-17.22	-10.13	-12.28	-15.13
D1	All	-49.48	78.39	-9.17	-17.59	-14.02	-11.87
A1	All	-55.98	27.86	-7.31	-4.79	-13.73	-53.97
D2	All	-16.05	26.05	-2.03	-4.19	-8.99	-5.22
A2	All	-85.89	79.64	-21.22	-13.15	-15.66	-56.28
All	A3	-85.89	79.65	-13.15	-21.22	-15.66	-56.29
All	D3	-16.05	26.05	-4.19	-2.03	-8.99	-5.22
All	A4	-55.99	27.86	-4.79	-7.31	-13.73	-53.97
All	D4	-49.48	78.38	-17.59	-9.17	-14.01	-11.87
All	All	-207.41	211.93	-39.73	-39.73	-52.40	-127.34
direct H-bonds		-146.49	205.71	-34.15	-34.16	-37.87	-46.96
direct diagonal		-62.13	6.13	-6.12	-6.12	-13.06	-81.29
the rest		1.21	0.10	0.54	0.54	-1.46	0.91

DADA04

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
D1	A3	-56.97	56.36	-8.67	-12.19	-24.54	-46.01
D1	D3	8.61	0.12	1.35	0.34	-0.83	9.60
D1	A4	-2.18	0.01	-0.12	-0.20	-0.27	-2.75
D1	D4	0.36	0.00	0.06	0.06	-0.08	0.40
A1	A3	-4.16	7.83	-1.83	-2.93	-5.36	-6.45
A1	D3	-65.25	48.08	-13.85	-4.71	-10.80	-46.51
A1	A4	16.16	7.51	0.85	0.85	-3.67	21.70
A1	D4	-2.18	0.01	-0.20	-0.12	-0.27	-2.75
D2	A3	-3.36	0.06	0.21	-0.06	-0.49	-3.64
D2	D3	23.13	0.25	1.15	1.15	-0.88	24.80
D2	A4	-65.23	48.08	-4.71	-13.84	-10.79	-46.50
D2	D4	8.60	0.12	0.34	1.35	-0.83	9.59
A2	A3	-3.71	0.00	-0.52	-0.52	-0.19	-4.94
A2	D3	-3.36	0.06	-0.06	0.21	-0.49	-3.64
A2	A4	-4.16	7.83	-2.93	-1.83	-5.36	-6.45
A2	D4	-56.97	56.37	-12.19	-8.67	-24.54	-46.00
D1	All	-50.19	56.50	-7.38	-11.99	-25.71	-38.77
A1	All	-55.43	63.43	-15.02	-6.91	-20.09	-34.02
D2	All	-36.86	48.51	-3.01	-11.40	-12.98	-15.75
A2	All	-68.20	64.26	-15.70	-10.81	-30.58	-61.03
All	A3	-68.20	64.26	-10.81	-15.70	-30.58	-61.04
All	D3	-36.87	48.52	-11.40	-3.01	-12.99	-15.76
All	A4	-55.42	63.42	-6.91	-15.01	-20.09	-34.01
All	D4	-50.19	56.50	-11.99	-7.38	-25.71	-38.76
All	All	-210.68	232.70	-41.11	-41.11	-89.36	-149.56
direct H-bonds		-244.42	208.89	-39.41	-39.41	-70.67	-185.02
direct diagonal		48.17	23.66	-1.06	-1.06	-16.91	52.79
the rest		-14.43	0.16	-0.64	-0.64	-1.79	-17.33

DADA05

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
D1	A3	-45.44	40.41	-4.32	-8.91	-11.88	-30.14
D1	D3	17.26	0.19	1.17	1.08	-1.77	17.93
D1	A4	-0.51	0.00	0.26	-0.07	-0.08	-0.40
D1	D4	0.42	0.00	-0.04	-0.04	-0.02	0.32
A1	A3	-0.98	2.89	-0.84	-0.95	-2.76	-2.65
A1	D3	-72.43	43.04	-12.25	-8.94	-14.67	-65.26
A1	A4	-2.43	0.05	-0.31	-0.31	-0.66	-3.66
A1	D4	-0.51	0.00	-0.07	0.26	-0.08	-0.40
D2	A3	-4.76	0.01	0.46	-0.50	-0.32	-5.11
D2	D3	24.66	2.99	0.90	0.90	-5.42	24.02
D2	A4	-72.43	43.04	-8.94	-12.25	-14.67	-65.25
D2	D4	17.27	0.19	1.08	1.17	-1.77	17.94
A2	A3	-1.27	0.00	-0.12	-0.12	0.00	-1.50
A2	D3	-4.76	0.01	-0.50	0.46	-0.32	-5.11
A2	A4	-0.98	2.89	-0.95	-0.84	-2.76	-2.64
A2	D4	-45.44	40.40	-8.91	-4.32	-11.88	-30.14
D1	All	-28.27	40.60	-2.93	-7.95	-13.74	-12.29
A1	All	-76.35	45.97	-13.47	-9.94	-18.17	-71.96
D2	All	-35.27	46.23	-6.50	-10.68	-22.19	-28.40
A2	All	-52.45	43.30	-10.48	-4.81	-14.96	-39.40
All	A3	-52.45	43.31	-4.81	-10.48	-14.96	-39.40
All	D3	-35.27	46.23	-10.68	-6.50	-22.19	-28.40
All	A4	-76.35	45.97	-9.94	-13.47	-18.17	-71.95
All	D4	-28.26	40.59	-7.95	-2.93	-13.74	-12.29
All	All	-192.33	176.10	-33.38	-33.38	-69.06	-152.04
direct H-bonds		-235.74	166.88	-34.41	-34.41	-53.11	-190.79
direct diagonal		54.79	9.20	1.05	1.05	-15.13	50.95
the rest		-11.39	0.02	-0.01	-0.01	-0.82	-12.20

DADA06

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
D1	A3	-71.84	83.00	-10.78	-21.11	-14.18	-34.91
D1	D3	4.07	0.63	0.41	-0.20	-1.44	3.48
D1	A4	3.18	0.04	0.78	-0.77	-0.54	2.69
D1	D4	2.14	0.00	-0.02	-0.02	-0.05	2.05
A1	A3	-25.35	2.05	-3.13	-3.12	-3.20	-32.74
A1	D3	-20.49	25.96	-4.48	-1.82	-6.74	-7.58
A1	A4	-11.97	0.63	0.37	0.37	-3.22	-13.82
A1	D4	3.18	0.04	-0.77	0.78	-0.54	2.69
D2	A3	0.95	0.02	0.25	0.04	-0.26	1.01
D2	D3	0.86	0.49	0.04	0.04	-0.97	0.46
D2	A4	-20.49	25.95	-1.82	-4.48	-6.74	-7.58
D2	D4	4.07	0.63	-0.20	0.41	-1.44	3.48
A2	A3	-4.11	0.00	-0.72	-0.73	-0.09	-5.65
A2	D3	0.95	0.02	0.04	0.25	-0.26	1.01
A2	A4	-25.35	2.05	-3.12	-3.13	-3.20	-32.73
A2	D4	-71.84	82.99	-21.11	-10.78	-14.18	-34.91
D1	All	-62.45	83.66	-9.61	-22.10	-16.20	-26.70
A1	All	-54.62	28.67	-8.01	-3.79	-13.69	-51.44
D2	All	-14.60	27.09	-1.73	-3.99	-9.41	-2.64
A2	All	-100.34	85.06	-24.90	-14.38	-17.72	-72.29
All	A3	-100.34	85.07	-14.38	-24.91	-17.73	-72.29
All	D3	-14.60	27.09	-3.99	-1.73	-9.41	-2.63
All	A4	-54.62	28.67	-3.79	-8.01	-13.69	-51.44
All	D4	-62.45	83.65	-22.09	-9.61	-16.20	-26.71
All	All	-232.01	224.48	-44.25	-44.26	-57.03	-153.07
direct H-bonds		-184.65	217.90	-38.19	-38.20	-41.83	-84.98
direct diagonal		-53.66	6.48	-5.61	-5.61	-13.47	-71.88
the rest		6.30	0.11	-0.45	-0.45	-1.73	3.78

DADA07

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
D1	A3	-59.21	53.53	-9.95	-10.10	-26.00	-51.73
D1	D3	14.42	3.53	1.09	0.64	-7.39	12.29
D1	A4	-1.14	0.00	0.34	-0.14	-0.21	-1.14
D1	D4	1.39	0.00	-0.09	-0.09	-0.09	1.11
A1	A3	-3.11	0.02	-0.50	-0.51	-0.55	-4.65
A1	D3	-57.27	46.43	-10.96	-11.85	-16.54	-50.19
A1	A4	-19.92	0.27	-1.96	-1.96	-1.15	-24.71
A1	D4	-1.14	0.00	-0.14	0.34	-0.21	-1.14
D2	A3	0.13	0.00	0.22	0.01	-0.08	0.28
D2	D3	1.97	9.95	0.23	0.23	-6.13	6.25
D2	A4	-57.27	46.43	-11.85	-10.96	-16.53	-50.19
D2	D4	14.42	3.53	0.64	1.09	-7.39	12.29
A2	A3	-1.00	0.00	-0.07	-0.07	-0.01	-1.13
A2	D3	0.13	0.00	0.01	0.22	-0.08	0.28
A2	A4	-3.11	0.02	-0.51	-0.50	-0.55	-4.65
A2	D4	-59.21	53.53	-10.10	-9.95	-26.00	-51.73
D1	All	-44.54	57.06	-8.62	-9.69	-33.68	-39.47
A1	All	-81.44	46.72	-13.55	-13.98	-18.44	-80.69
D2	All	-40.75	59.90	-10.76	-9.63	-30.13	-31.38
A2	All	-63.19	53.55	-10.67	-10.30	-26.64	-57.24
All	A3	-63.19	53.55	-10.30	-10.67	-26.64	-57.24
All	D3	-40.75	59.90	-9.63	-10.76	-30.13	-31.38
All	A4	-81.44	46.72	-13.98	-13.55	-18.44	-80.69
All	D4	-44.54	57.06	-9.69	-8.62	-33.68	-39.47
All	All	-229.92	217.23	-43.60	-43.60	-108.89	-208.78
direct H-bonds		-232.96	199.91	-42.86	-42.86	-85.07	-203.84
direct diagonal		4.67	17.32	-1.01	-1.01	-23.15	-3.18
the rest		-1.62	0.00	0.27	0.27	-0.68	-1.75

DADA08 (tautomer)							
Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
D1	A3	-50.79	67.61	-8.87	-13.63	-9.20	-14.88
D1	D3	5.90	1.92	0.10	-1.56	-3.82	2.55
D1	A4	1.20	0.04	0.03	-0.18	-0.53	0.56
D1	D4	0.03	0.00	-0.06	-0.06	-0.04	-0.14
A1	A3	-27.43	1.76	-2.28	-2.88	-1.83	-32.66
A1	D3	-39.25	54.43	-11.49	-5.02	-12.36	-13.69
A1	A4	-20.09	1.73	-1.25	-1.25	-4.36	-25.22
A1	D4	1.20	0.04	-0.18	0.03	-0.53	0.56
D2	A3	2.97	0.00	0.19	0.37	-0.15	3.38
D2	D3	0.37	0.80	-0.15	-0.15	-1.95	-1.06
D2	A4	-39.25	54.43	-5.02	-11.49	-12.36	-13.69
D2	D4	5.90	1.92	-1.56	0.10	-3.82	2.55
A2	A3	-1.56	0.00	-0.23	-0.23	0.00	-2.01
A2	D3	2.97	0.00	0.37	0.19	-0.15	3.38
A2	A4	-27.43	1.76	-2.88	-2.28	-1.83	-32.66
A2	D4	-50.79	67.61	-13.63	-8.87	-9.20	-14.88
D1	All	-43.66	69.58	-8.80	-15.43	-13.59	-11.91
A1	All	-85.57	57.97	-15.21	-9.12	-19.09	-71.02
D2	All	-30.00	57.15	-6.54	-11.16	-18.28	-8.82
A2	All	-76.81	69.38	-16.36	-11.19	-11.19	-46.17
All	A3	-76.81	69.38	-11.19	-16.36	-11.19	-46.17
All	D3	-30.00	57.15	-11.16	-6.54	-18.28	-8.82
All	A4	-85.57	57.97	-9.12	-15.21	-19.09	-71.02
All	D4	-43.66	69.58	-15.43	-8.80	-13.59	-11.91
All	All	-236.04	254.08	-46.91	-46.91	-62.14	-137.92
direct H-bonds		-180.07	244.09	-39.01	-39.01	-43.14	-57.15
direct diagonal		-62.78	9.90	-8.02	-8.02	-17.61	-86.51
the rest		6.81	0.08	0.13	0.13	-1.40	5.73

DADA Average							
Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
D1	A3	-56.63	66.27	-8.99	-14.90	-15.40	-29.65
D1	D3	7.36	1.04	0.61	-0.03	-2.41	6.57
D1	A4	0.82	0.03	0.41	-0.31	-0.38	0.56
D1	D4	0.79	0.00	-0.04	-0.04	-0.05	0.66
A1	A3	-19.06	2.55	-2.29	-2.60	-2.88	-24.28
A1	D3	-40.54	39.01	-8.80	-4.95	-10.45	-25.72
A1	A4	-8.88	1.59	-0.24	-0.24	-2.96	-10.73
A1	D4	0.82	0.03	-0.31	0.41	-0.38	0.56
D2	A3	-0.14	0.02	0.34	0.00	-0.26	-0.05
D2	D3	6.74	1.98	0.28	0.28	-2.28	7.01
D2	A4	-40.53	39.00	-4.95	-8.80	-10.45	-25.72
D2	D4	7.36	1.04	-0.03	0.61	-2.41	6.57
A2	A3	-2.63	0.00	-0.43	-0.43	-0.07	-3.57
A2	D3	-0.14	0.02	0.00	0.34	-0.26	-0.05
A2	A4	-19.06	2.55	-2.60	-2.29	-2.88	-24.28
A2	D4	-56.63	66.27	-14.90	-8.99	-15.40	-29.65
D1	All	-47.66	67.34	-8.01	-15.28	-18.24	-21.86
A1	All	-67.65	43.18	-11.64	-7.38	-16.67	-60.17
D2	All	-26.58	42.04	-4.35	-7.91	-15.40	-12.19
A2	All	-78.47	68.84	-17.94	-11.37	-18.61	-57.54
All	A3	-78.47	68.85	-11.37	-17.94	-18.61	-57.54
All	D3	-26.58	42.04	-7.91	-4.35	-15.40	-12.19
All	A4	-67.65	43.17	-7.38	-11.64	-16.67	-60.17
All	D4	-47.66	67.33	-15.28	-8.01	-18.24	-21.86
All	All	-220.36	221.39	-41.94	-41.94	-68.92	-151.77
direct H-bonds		-194.33	210.55	-37.64	-37.64	-51.70	-110.75
direct diagonal		-25.54	10.75	-4.26	-4.26	-15.83	-39.14
the rest		-0.49	0.09	-0.04	-0.04	-1.39	-1.87

Table S3.3. Full SAPT analysis for the DDAA06 dimer in a simulated solution phase. Average over 21 snapshots. Yellow rows mark direct hydrogen bonds, blue rows diagonal interactions. Energies in kJ/mol.

Frag1	Frag2	Average					Total
		Elst	Exch	IndAB	IndBA	Disp	
D1	A3	-67.00	111.03	-15.11	-21.83	-13.03	-5.94
D1	A4	3.67	3.20	-2.62	-3.14	-4.69	-3.57
D1	D3	-0.49	0.04	-2.84	-0.65	-1.02	-4.95
D1	D4	-0.01	0.00	-0.05	-0.05	-0.05	-0.16
D2	A3	-22.36	2.12	-3.49	-5.41	-2.11	-31.25
D2	A4	-107.69	84.39	-17.66	-28.39	-15.31	-84.67
D2	D3	3.33	2.94	-8.78	-8.31	-8.39	-19.22
D2	D4	-0.55	0.04	-0.69	-2.69	-1.02	-4.91
A1	A3	-12.16	0.00	-1.97	-1.61	-0.11	-15.85
A1	A4	-23.10	2.34	-5.62	-5.37	-1.91	-33.66
A1	D3	-108.08	84.34	-28.91	-17.25	-15.30	-85.20
A1	D4	3.90	3.18	-3.22	-2.46	-4.69	-3.29
A2	A3	-0.82	0.00	-0.50	-0.48	0.00	-1.80
A2	A4	-12.23	0.00	-1.68	-1.92	-0.11	-15.93
A2	D3	-22.84	2.11	-5.62	-3.36	-2.11	-31.82
A2	D4	-67.10	110.63	-21.90	-14.90	-13.00	-6.27
D1	All	-63.82	114.27	-20.62	-25.66	-18.79	-14.63
D2	All	-127.28	89.48	-30.61	-44.80	-26.84	-140.05
A1	All	-139.44	89.86	-39.72	-26.68	-22.02	-138.00
A2	All	-103.00	112.75	-29.69	-20.65	-15.22	-55.82
All	A3	-102.35	113.15	-21.07	-29.33	-15.26	-54.85
All	A4	-139.35	89.93	-27.57	-38.81	-22.02	-137.83
All	D3	-128.07	89.43	-46.15	-29.57	-26.83	-141.19
All	D4	-63.76	113.85	-25.86	-20.09	-18.77	-14.62
All	All	-433.54	406.36	-120.64	-117.80	-82.87	-348.49
direct H-bonds		-349.87	390.39	-83.57	-82.37	-56.65	-182.08
direct diagonal		-57.40	15.89	-29.34	-28.04	-23.91	-122.81
the rest		-26.26	0.09	-7.73	-7.38	-2.31	-43.60

Table S3.4. Full SAPT analysis for the DADA08 dimer in a simulated solution phase. Average over 21 snapshots. Yellow rows mark direct hydrogen bonds, blue rows diagonal interactions. Energies in kJ/mol.

Frag1	Frag2	Average					Total
		Elst	Exch	IndAB	IndBA	Disp	
D1	A3	-48.97	69.77	-10.55	-12.58	-9.34	-11.67
D1	D3	3.68	2.07	-1.74	-1.31	-3.87	-1.17
D1	A4	1.22	0.04	0.99	-0.14	-0.54	1.57
D1	D4	0.01	0.00	-0.04	-0.05	-0.05	-0.13
A1	A3	-26.59	1.86	-2.80	-2.38	-1.80	-31.71
A1	D3	-46.05	55.00	-12.69	-5.75	-12.43	-21.91
A1	A4	-13.20	1.78	0.06	-0.13	-4.41	-15.92
A1	D4	1.09	0.04	-0.15	0.82	-0.54	1.26
D2	A3	-0.48	0.00	0.23	-0.09	-0.15	-0.48
D2	D3	3.07	0.79	0.44	0.35	-1.94	2.72
D2	A4	-46.22	55.20	-5.79	-12.85	-12.41	-22.08
D2	D4	4.03	2.05	-1.25	-1.55	-3.87	-0.58
A2	A3	-1.60	0.00	-0.22	-0.21	0.00	-2.03
A2	D3	-1.12	0.00	-0.17	0.24	-0.15	-1.19
A2	A4	-25.74	1.88	-2.27	-2.77	-1.80	-30.69
A2	D4	-48.11	69.49	-12.38	-10.38	-9.33	-10.70
D1	All	-44.06	71.89	-11.34	-14.08	-13.81	-11.40
A1	All	-84.75	58.68	-15.58	-7.45	-19.18	-68.28
D2	All	-39.60	58.04	-6.36	-14.14	-18.37	-20.43
A2	All	-76.56	71.37	-15.03	-13.12	-11.28	-44.62
All	A3	-77.63	71.64	-13.33	-15.27	-11.30	-45.89
All	D3	-40.42	57.87	-14.16	-6.46	-18.39	-21.56
All	A4	-83.94	58.90	-7.00	-15.90	-19.17	-67.12
All	D4	-42.97	71.58	-13.82	-11.16	-13.78	-10.16
All	All	-244.97	259.98	-48.32	-48.79	-62.64	-144.73
direct H-bonds		-189.34	249.46	-41.41	-41.55	-43.52	-66.36
direct diagonal		-54.74	10.43	-7.56	-7.80	-17.70	-77.36
the rest		-0.88	0.09	0.65	0.56	-1.43	-1.00

4. SAPT partitioning

Figure S4.1. The SAPT partitioning of the DDAA molecules is shown with the green lines.

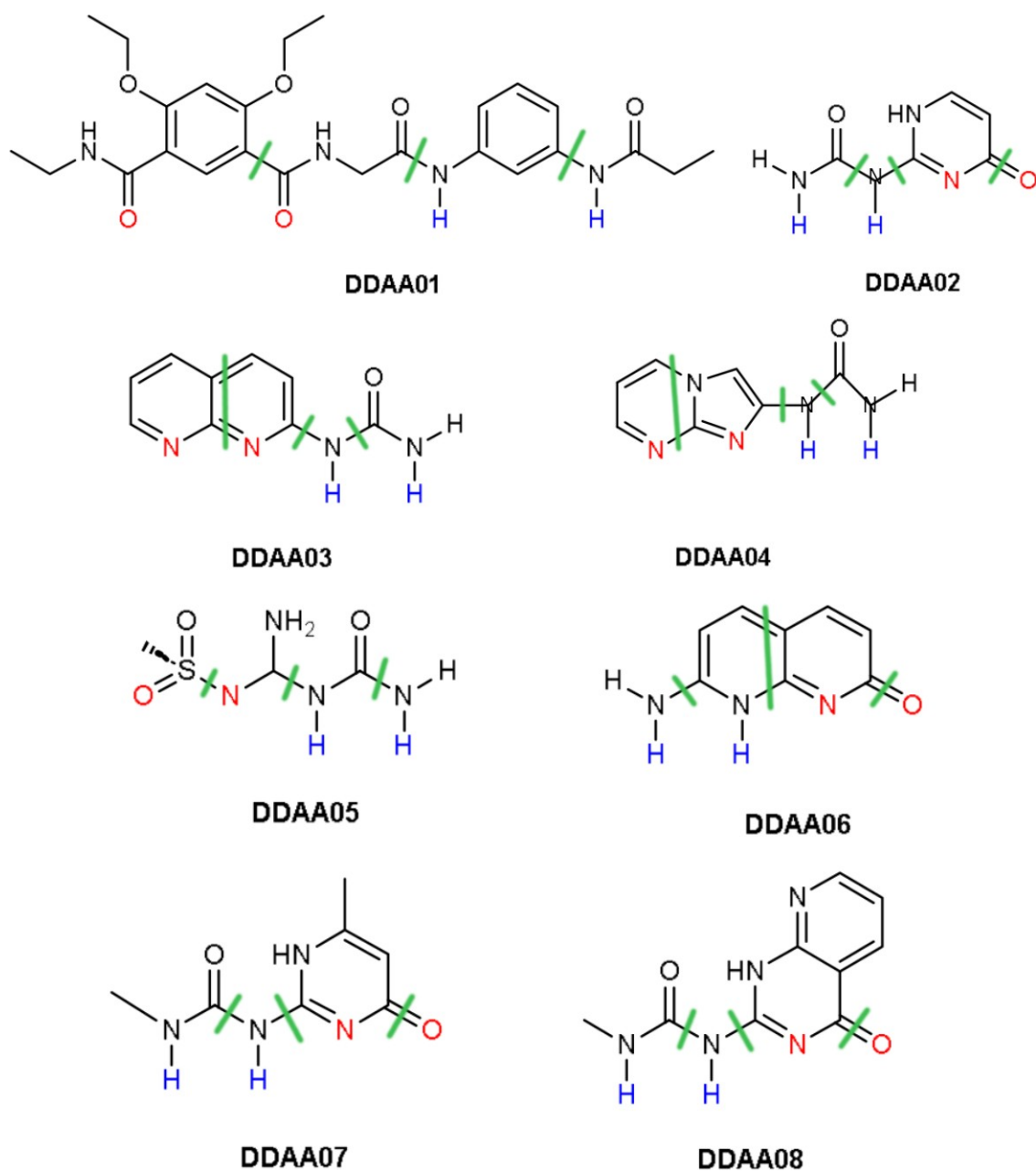


Figure S4.2. The SAPT partitioning of the DADA molecules is shown with the green lines.

