Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting information

THEORETICAL STUDY OF THE CARBOHYDRATES DISPERSION INTERACTIONS WITH CONDENSED AROMATIC MOIETIES

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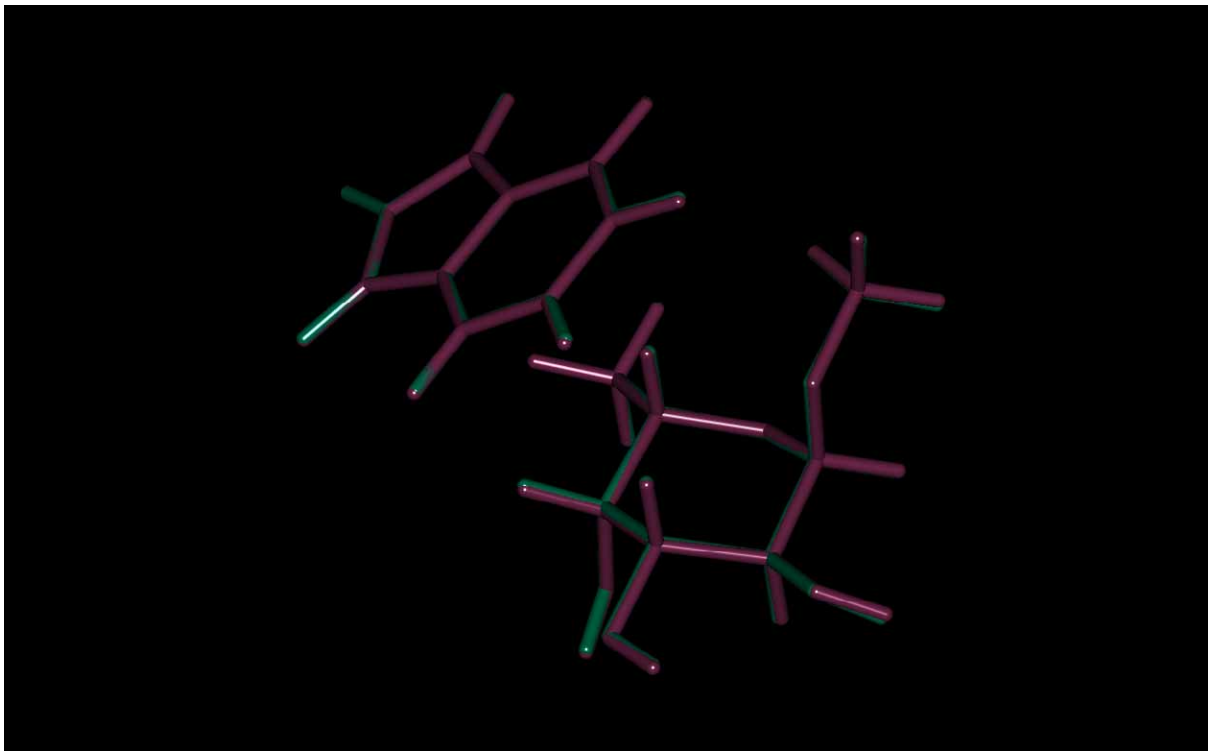
Contents: Cartesian coordinates and Boltzmann weighted populations of 46 carbohydrate (glucose, mannose and fucose) – naphtalene complexes used for study on CH/π interaction additive properties. Total 26 of these complexes contains interaction of naphtalene with one CH-hydrogen of carbohydrate (monodentate complexes) and the rest (20 complexes) involve interaction of naphtalene with two CH-hydrogens of the carbohydrate (bidentate complexes). Each structure contains table with DFT-D BP/def2-TZVPP optimized and CCSD(T)/CBS energies of benzene and carbohydrate monomers and counterpoise corrected BSSE energy of complex. Comparison of the CH – π complex geometry optimized using ri-DFT-D (BP/def2-TZVPP) and ri-MP2 (MP2/def2-TZVPP) methods.

Abbrevations: Glc = glucose, Man = mannose, Fuc = fucose, a = above face, b = below face, c = clockwise –OH orientation of carbohydrate, cc = counter-clockwise –OH orientation of carbohydrate, H*n* = complex with naphtalene bound to carbohydrate hydrogen #*n*.

Table S1: Boltzmann weighted populations of monodentate and bidentate saccharide-naphtalene complexes

Saccharide-naphtalene complex	Hn	Population (%)
Glc(a,c)	2	4.81
	4	8.02
	6	0.25
	2,4	52.45
	4,6	34.46
Glc(b,c)	1	0.51
	3	2.27
	5	1.27
	1,3	26.99
	1,5	16.37
	3,5	52.60
Glc(a,cc)	2	14.91
	4	2.45
	6	0.30
	2,4	58.42
	4,6	23.93
Glc(b,cc)	1	4.02
	3	1.93
	5	2.12
	1,3	31.99
	1,5	26.62
	3,5	33.32
Man(b,c)	1	0.36
	3	1.49
	5	1.56
	1,3	21.35
	1,5	33.96
	3,5	41.27
Man(b,cc)	1	2.66
	3	0.79
	5	0.74
	1,3	39.74
	1,5	24.69
	3,5	31.37
Fuc(a,c)	3	3.37
	4	2.47
	5	3.39
	6	0.26
	3,5	75.68
	4,6	14.83
Fuc(a,cc)	3	3.58
	4	1.86
	5	11.23
	6	0.35
	3,5	70.23
	4,6	12.75

Figure S1: On the base of referee note, overlaid structures of the CH/π complex (α-L-Me-Fucoside with indol) optimized geometry at the ri-DFT-D (BP/def2-TZVPP) coloured in purple and ri-MP2 (MP2/def2-TZVPP) coloured in green are shown. Optimization was done by TURBOMOLE 6.0 program package. The differences in the geometry are negligible.



Glc (a,c) H2:

C	0.9823564	0.8222355	-1.7619887
C	0.2658381	-0.4631952	-1.3262714
C	-1.1681969	-0.4881045	-1.8454033
C	-1.9152923	0.7759198	-1.4480616
C	-1.1111443	1.9931894	-1.9206390
O	0.1950666	1.9560199	-1.3321168
O	1.0068381	-1.5827952	-1.8215714
O	-1.7898671	-1.6668485	-1.3199420
O	-3.2106521	0.6953000	-2.0680443
C	-1.7295037	3.3099963	-1.4761167
O	-0.9746866	4.4350680	-1.9061062
O	2.2488213	0.9487237	-1.2112115
H	0.5068381	-2.3767952	-1.5696714
H	-2.7071601	-1.6547944	-1.6410833
H	-0.0496353	4.2390360	-1.6740887
H	1.0950209	0.8503683	-2.8611186
H	0.2424381	-0.4608952	-0.2246714
H	-1.1385941	-0.5349296	-2.9518045
H	-2.0022275	0.8074745	-0.3473126
H	-1.0321794	1.9707113	-3.0256161
H	-3.7865451	1.3516516	-1.6478137
H	-2.7322038	3.4116664	-1.9177902
H	-1.8274468	3.2868830	-0.3713846
H	2.1743051	0.7123491	-0.2663182
C	0.4373001	-2.9907932	1.9698313
C	-0.8357949	-0.8588115	2.0874568
C	2.8498508	-1.5447556	1.8994638
C	1.5714330	0.5875638	2.0025916
C	1.6458798	-3.6524659	1.8855905
C	-0.8509259	0.5222376	2.1003825
C	2.8614194	-2.9237796	1.8513207
C	0.3612888	1.2527804	2.0507450
C	0.3904813	-1.5727106	2.0242026
C	1.6239062	-0.8334711	1.9844727
H	-0.5021987	-3.5453835	1.9898680
H	-1.7679340	-1.4251429	2.0987761
H	3.7827530	-0.9794476	1.8633192
H	2.5088385	1.1482504	1.9789929
H	1.6704923	-4.7415591	1.8421299
H	-1.8000964	1.0575183	2.1420395
H	3.8086803	-3.4585104	1.7791878
H	0.3365780	2.3419032	2.0416916

Table S2: Energy values for Glc(a,c) H2 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.622184	-386.0598013	-687.5504688
CCSD(T)/CBS	-1071.789138	-385.3111028	-686.4671864

Glc (a,c) H4:

C	2.7267439	-0.1918468	-1.8005696
C	1.9746571	-1.4196636	-1.2741987
C	0.5291236	-1.3632379	-1.7429411
C	-0.0995952	-0.0440095	-1.3088548
C	0.7626588	1.1189242	-1.8223561
O	2.1015537	0.9851570	-1.3126956
O	2.6596109	-2.5777861	-1.7605848
O	-0.1492023	-2.4968371	-1.1908390
O	-1.4244952	-0.0386095	-1.8651548
C	0.2647226	2.4719054	-1.3426006
O	1.0493697	3.5474824	-1.8472385
O	4.0507843	-0.1408384	-1.3384401
H	2.1066389	-3.3445225	-1.5354772
H	-1.0946401	-2.3652315	-1.3782796
H	1.9742671	3.3204322	-1.6479160
H	2.6900422	-0.1896011	-2.9134259
H	1.9939104	-1.3794510	-0.1705234
H	0.5096179	-1.4097844	-2.8496382
H	-0.1359952	-0.0223095	-0.2084548
H	0.7803439	1.0972966	-2.9298412
H	-1.9295952	0.6910905	-1.4446548
H	-0.7610131	2.6308246	-1.7075317
H	0.2517943	2.4597866	-0.2368546
H	4.3805181	-1.0565176	-1.3489057
C	-0.0915693	-1.4185222	2.0522778
C	-2.5468114	-1.4481140	1.6659842
C	-0.1321447	1.3924442	2.1021907
C	-2.5871889	1.3634497	1.7004902
C	1.0780454	-0.7060337	2.2251586
C	-3.7311260	-0.7661164	1.4698703
C	1.0590443	0.7109677	2.2488595
C	-3.7513249	0.6515555	1.4848178
C	-1.3321761	-0.7467318	1.8877006
C	-1.3529231	0.6914867	1.9091210
H	-0.0782371	-2.5081738	2.0082561
H	-2.5226690	-2.5392603	1.6498740
H	-0.1523280	2.4833597	2.1167922
H	-2.5983051	2.4548005	1.7194172
H	2.0272152	-1.2313717	2.3350269
H	-4.6575993	-1.3157721	1.3017964
H	1.9930332	1.2593283	2.3675634
H	-4.6932069	1.1785905	1.3299560

Table S3: Energy values for Glc(a,c) H4 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.622007	-386.0597784	-687.5502139
CCSD(T)/CBS	-1071.789900	-385.3110730	-686.4675048

Glc (a,c) H6:

C	2.3814036	-1.4259094	-1.5054285
C	1.5982378	-2.6962979	-1.1523956
C	0.2916678	-2.7124923	-1.9321760
C	-0.4877689	-1.4324612	-1.6618432
C	0.4006835	-0.2116188	-1.9505766
O	1.6050887	-0.2913464	-1.1662902
O	2.4316139	-3.8134816	-1.4658936
O	-0.4306793	-3.8817224	-1.5317653
O	-1.6483306	-1.4723313	-2.5093697
C	-0.2664219	1.0922495	-1.5443698
O	0.5291781	2.2255495	-1.8715698
O	3.5683523	-1.3095439	-0.7648204
H	1.8836455	-4.6099998	-1.3654138
H	-1.2835610	-3.8472704	-1.9971205
H	1.3952781	2.0697495	-1.4574698
H	2.5885123	-1.4176961	-2.5995365
H	1.3730647	-2.6601688	-0.0701204
H	0.5245945	-2.7581937	-3.0139499
H	-0.7819077	-1.4108610	-0.6003991
H	0.6555347	-0.1913738	-3.0281270
H	-2.2958906	-0.8468940	-2.1496345
H	-1.2150068	1.2033986	-2.0894143
H	-0.4747219	1.0436495	-0.4592698
H	3.9475317	-2.2041056	-0.7078203
C	-2.4162277	0.6466862	1.6675023
C	-2.1254620	3.1078392	1.8739127
C	0.3520683	0.2899903	2.0155430
C	0.6434462	2.7513628	2.2129705
C	-1.8703577	-0.6218600	1.6622585
C	-1.2990619	4.1985769	2.0542182
C	-0.4746469	-0.8003401	1.8397012
C	0.0967741	4.0188211	2.2239893
C	-1.5952321	1.7904937	1.8588410
C	-0.1794564	1.6073666	2.0364229
H	-3.4900072	0.7909185	1.5324061
H	-3.2006622	3.2406452	1.7400210
H	1.4291087	0.1564378	2.1214404
H	1.7176277	2.6066973	2.3409268
H	-2.5107168	-1.4932188	1.5197064
H	-1.7179428	5.2050742	2.0639235
H	-0.0546008	-1.8064603	1.8195465
H	0.7388071	4.8891148	2.3615937

Table S4: Energy values for Glc (a,c) H6 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.618845	-386.0598671	-687.5504272
CCSD(T)/CBS	-1071.787231	-385.3111515	-686.4679641

Glc (a,c) H2&H4:

C	1.7716690	0.2096000	-1.7100257
C	1.0397690	-1.0535000	-1.2426257
C	-0.3954215	-1.0240736	-1.7429928
C	-1.0614342	0.2579573	-1.2574539
C	-0.2338822	1.4607059	-1.7390375
O	1.0996103	1.3554870	-1.2067864
O	1.7744967	-2.1754367	-1.7436279
O	-1.0529131	-2.1966621	-1.2537963
O	-2.4017779	0.2699472	-1.7812871
C	-0.7809682	2.7906968	-1.2507050
O	-0.0162421	3.8952456	-1.7253128
O	3.0813690	0.2865000	-1.2159257
H	1.2790240	-2.9681310	-1.4790352
H	-1.9929379	-2.0870167	-1.4787012
H	0.9111036	3.6877093	-1.5173396
H	1.7626600	0.2459182	-2.8232484
H	1.0359402	-1.0530298	-0.1420336
H	-0.3943200	-1.0229746	-2.8508562
H	-1.0796503	0.2554151	-0.1587246
H	-0.1935955	1.4600677	-2.8463594
H	-2.9603742	0.7233968	-1.1317207
H	-1.8024396	2.9181636	-1.6358614
H	-0.8157647	2.7649455	-0.1456505
H	3.4386690	-0.6278000	-1.2442257
C	0.2778970	-2.2912698	2.0709782
C	-1.8685776	-1.0394601	2.0387099
C	1.6934729	0.1391716	2.1462514
C	-0.4556602	1.3886391	2.1490756
C	1.6578900	-2.2884548	2.1087850
C	-2.5500854	0.1620390	2.0584851
C	2.3709567	-1.0630905	2.1401858
C	-1.8367549	1.3869297	2.1180781
C	-0.4495720	-1.0714867	2.0849482
C	0.2738283	0.1700687	2.1333341
H	-0.2770501	-3.2288477	2.0216488
H	-2.4081207	-1.9862098	1.9868562
H	2.2388763	1.0832865	2.1413839
H	0.0988478	2.3278336	2.1789934
H	2.2062178	-3.2309703	2.0994485
H	-3.6406434	0.1731222	2.0338231
H	3.4609187	-1.0728334	2.1432894
H	-2.3842743	2.3299498	2.1347656

Table S5: Energy values for Glc (a,c) H2&H4 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.624184	-386.0598067	-687.5499126
CCSD(T)/CBS	-1071.791557	-385.3111173	-686.4673770

Glc (a,c) H4&H6:

C	2.1789521	-0.5908470	-1.6602571
C	1.4423100	-1.8870776	-1.3013989
C	0.0161067	-1.8416684	-1.8297054
C	-0.6727462	-0.5758758	-1.3340789
C	0.1705653	0.6386450	-1.7523920
O	1.4704475	0.5229723	-1.1440290
O	2.1968682	-2.9670104	-1.8609289
O	-0.6393462	-3.0342453	-1.3864906
O	-1.9891602	-0.5611159	-1.9141234
C	-0.4281040	1.9526581	-1.2772174
O	0.3993159	3.0693533	-1.5884579
O	3.4545487	-0.5333626	-1.0721510
H	1.6741270	-3.7741228	-1.7209133
H	-1.5747297	-2.9342796	-1.6330159
H	1.2811820	2.8514121	-1.2398965
H	2.2438565	-0.5028027	-2.7682592
H	1.4054908	-1.9572942	-0.2012072
H	0.0429087	-1.8103073	-2.9369072
H	-0.7345029	-0.6028392	-0.2352468
H	0.2803481	0.6531897	-2.8548329
H	-2.5521796	-0.0234783	-1.3364175
H	-1.3838087	2.1090152	-1.7969544
H	-0.6194343	1.8871773	-0.1932586
H	3.8411277	-1.4210725	-1.1723863
C	-2.0595572	-0.5763593	2.1066908
C	-2.0395050	1.9133712	2.1064624
C	0.7511403	-0.5949339	2.0380939
C	0.7717846	1.8894088	2.0262721
C	-1.3709296	-1.7731360	2.0910390
C	-1.3317193	3.0988423	2.0835715
C	0.0458659	-1.7811474	2.0607604
C	0.0854585	3.0869068	2.0423271
C	-1.3636534	0.6632315	2.0940334
C	0.0739023	0.6525421	2.0567087
H	-3.1509776	-0.5637283	2.1340131
H	-3.1308059	1.9183485	2.1368572
H	1.8404003	-0.5936949	1.9820039
H	1.8612345	1.8699271	1.9756613
H	-1.9144184	-2.7177939	2.0923051
H	-1.8618366	4.0515343	2.0885109
H	0.5761869	-2.7328538	2.0358512
H	0.6287250	4.0309888	2.0090935

Table S6: Energy values for Glc (a,c) H4&H6 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.623849	-386.0598342	-687.5499095
CCSD(T)/CBS	-1071.791321	-385.3111426	-686.4675048

Glc (a,cc) H2:

C	0.9896301	0.9660023	-1.6960608
C	0.2710238	-0.3056381	-1.2454714
C	-1.1490421	-0.2943625	-1.7919496
C	-1.8697964	0.9753464	-1.3580361
C	-1.0467530	2.1966064	-1.7825685
O	0.2780519	2.1122787	-1.2193199
O	0.9008238	-1.4884381	-1.7478714
O	-1.9124346	-1.4094187	-1.3213579
O	-3.1600061	1.0772238	-1.9627173
C	-1.6460491	3.4976922	-1.2739798
O	-0.8952386	4.6358033	-1.6912516
O	2.2717242	0.9619604	-1.1302186
H	1.7637238	-1.5469381	-1.3064714
H	-1.3627497	-2.1989051	-1.4660540
H	0.0206665	4.4690137	-1.4128327
H	1.0344065	1.0030253	-2.8053662
H	0.2390238	-0.3080381	-0.1456714
H	-1.1020878	-0.3078760	-2.8991825
H	-1.9467148	0.9669432	-0.2549746
H	-0.9806477	2.2230491	-2.8876019
H	-3.5903790	0.2146806	-1.8357737
H	-2.6592703	3.6055163	-1.6804221
H	-1.7111003	3.4395170	-0.1704020
H	2.8003234	1.6462530	-1.5705547
C	0.1934039	-3.2030095	1.7672718
C	-1.0668726	-1.0796859	2.0597385
C	2.6115990	-1.7667599	1.7693075
C	1.3519456	0.3551865	2.0805985
C	1.3956139	-3.8645675	1.6117545
C	-1.0690778	0.2942830	2.1932104
C	2.6151902	-3.1392918	1.6091985
C	0.1481736	1.0178162	2.2043074
C	0.1555379	-1.7924511	1.9335265
C	1.3924121	-1.0574058	1.9408175
H	-0.7501866	-3.7528616	1.7621630
H	-2.0031370	-1.6379026	2.0265407
H	3.5474915	-1.2045049	1.7656321
H	2.2910844	0.9074431	2.0555147
H	1.4111895	-4.9485288	1.4883816
H	-2.0142040	0.8289212	2.2804784
H	3.5592419	-3.6725050	1.4851502
H	0.1296632	2.1030126	2.2856077

Table S7: Energy values for Glc (a,cc) H2 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.624583	-386.0597645	-687.5548315
CCSD(T)/CBS	-1071.794515	-385.3110555	-686.4730628

Glc (a,cc) H4:

C	2.6459387	-0.0410726	-1.7859606
C	1.9583599	-1.3260745	-1.3220917
C	0.5115256	-1.3193239	-1.7930168
C	-0.1945810	-0.0502643	-1.3270690
C	0.6030339	1.1701237	-1.7997746
O	1.9487261	1.0964748	-1.2801497
O	2.5791743	-2.4899956	-1.8766970
O	-0.2198231	-2.4411002	-1.2870176
O	-1.5087810	0.0403357	-1.8802690
C	0.0130100	2.4769438	-1.2969411
O	0.7475191	3.6107956	-1.7593497
O	3.9475433	-0.0493551	-1.2617620
H	3.5035537	-2.4831441	-1.5775136
H	0.2733841	-3.2344226	-1.5542425
H	1.6693893	3.4596489	-1.4910360
H	2.6539891	0.0009470	-2.8959698
H	1.9818493	-1.3416407	-0.2190325
H	0.5044999	-1.3315134	-2.9008149
H	-0.2287810	-0.0467643	-0.2241690
H	0.6366402	1.1786473	-2.9066870
H	-1.9419810	-0.8077643	-1.6853690
H	-1.0116475	2.5714411	-1.6761523
H	-0.0196579	2.4369074	-0.1929657
H	4.4523210	0.6609342	-1.6890255
C	-0.1292640	-1.4841544	2.0251122
C	-2.6094212	-1.5114633	1.8501829
C	-0.1695684	1.3228461	2.1637265
C	-2.6502958	1.2964214	2.0011292
C	1.0489851	-0.7735662	2.1371474
C	-3.8079345	-0.8277829	1.8054556
C	1.0306614	0.6420942	2.1991872
C	-3.8286637	0.5877540	1.8823167
C	-1.3799235	-0.8127359	1.9794911
C	-1.4012068	0.6232276	2.0548668
H	-0.1187827	-2.5719534	1.9503352
H	-2.5865427	-2.6006059	1.7863011
H	-0.1919381	2.4130609	2.2116595
H	-2.6593215	2.3861311	2.0532385
H	2.0039422	-1.2991465	2.1681808
H	-4.7463371	-1.3750675	1.7105749
H	1.9702552	1.1906240	2.2625486
H	-4.7821407	1.1155137	1.8443639

Table S8: Energy values for Glc (a,cc) H4 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.624223	-386.0598559	-687.5550450
CCSD(T)/CBS	-1071.793135	-385.3111813	-686.4732318

Glc (a,cc) H6:

C	2.2647848	-1.4915896	-1.6689074
C	1.5216835	-2.7711570	-1.2826600
C	0.1590267	-2.7723546	-1.9612027
C	-0.6087529	-1.4970373	-1.6321970
C	0.2469675	-0.2676054	-1.9583065
O	1.5089070	-0.3560163	-1.2612388
O	2.2104696	-3.9460438	-1.7155681
O	-0.6483603	-3.8771695	-1.5403122
O	-1.8145945	-1.4108662	-2.3923229
C	-0.4134550	1.0185324	-1.4858650
O	0.3694450	2.1678324	-1.8028650
O	3.4910516	-1.4930562	-0.9865403
H	3.0907040	-3.9219917	-1.3051045
H	-0.1336581	-4.6824814	-1.7159384
H	1.2077450	2.0521324	-1.3256650
H	2.4106537	-1.4600528	-2.7701500
H	1.3893771	-2.7624354	-0.1852970
H	0.3180258	-2.8112096	-3.0566010
H	-0.8249439	-1.4867019	-0.5485297
H	0.4310641	-0.2250982	-3.0492874
H	-2.2702425	-2.2620022	-2.2775442
H	-1.3814453	1.1277202	-1.9891539
H	-0.5778550	0.9340324	-0.3978650
H	4.0417568	-0.7825092	-1.3523454
C	-2.1528792	0.4321321	1.8793159
C	-2.3377619	2.9097477	1.9762478
C	0.6492424	0.6366693	1.9740095
C	0.4645471	3.1154623	2.0710198
C	-1.3699138	-0.7047285	1.8555321
C	-1.7318743	4.1479256	2.0413717
C	0.0427249	-0.6005351	1.9004691
C	-0.3188284	4.2517524	2.0890471
C	-1.5612474	1.7209191	1.9565166
C	-0.1272576	1.8255745	2.0071758
H	-3.2406531	0.3582700	1.8342296
H	-3.4248891	2.8242157	1.9361800
H	1.7372043	0.7183580	1.9902164
H	1.5534012	3.1894832	2.1075680
H	-1.8359660	-1.6883008	1.7905538
H	-2.3394753	5.0531335	2.0538875
H	0.6525285	-1.5030613	1.8607504
H	0.1476546	5.2360531	2.1373829

Table S9: Energy values forGlc (a,cc) H6complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.622431	-386.0598749	-687.5547458
CCSD(T)/CBS	-1071.791197	-385.3112039	-686.4732294

Glc (a,cc) H2&H4:

C	1.7121591	0.2359712	-1.7163340
C	0.9920706	-1.0285737	-1.2478137
C	-0.4354100	-1.0127559	-1.7733088
C	-1.1380044	0.2655542	-1.3303842
C	-0.3174509	1.4755284	-1.7895632
O	1.0149909	1.3902277	-1.2403756
O	1.6161664	-2.2165252	-1.7454811
O	-1.1964189	-2.1238000	-1.2883835
O	-2.4420713	0.3685857	-1.9047993
C	-0.9010152	2.7897718	-1.2978463
O	-0.1371472	3.9134844	-1.7358991
O	3.0010163	0.2267714	-1.1650531
H	2.4906949	-2.2625967	-1.3260129
H	-0.6629843	-2.9177902	-1.4622046
H	0.7780309	3.7363237	-1.4610510
H	1.7442461	0.2646193	-2.8266531
H	0.9791386	-1.0204643	-0.1488965
H	-0.4061361	-1.0295691	-2.8811639
H	-1.1933892	0.2748561	-0.2285622
H	-0.2601800	1.4828113	-2.8957914
H	-2.8879708	-0.4735062	-1.7126066
H	-1.9138286	2.9017255	-1.7037479
H	-0.9634194	2.7453009	-0.1951189
H	3.5244649	0.9130794	-1.6085397
C	0.1108452	-2.3411374	1.9718570
C	-1.9803884	-0.9977310	1.9835860
C	1.6287622	0.0163237	2.1651704
C	-0.4622088	1.3608579	2.1822466
C	1.4895647	-2.4022722	2.0199765
C	-2.6071047	0.2306134	2.0431735
C	2.2550762	-1.2129591	2.1162804
C	-1.8409066	1.4199037	2.1444538
C	-0.5641849	-1.0934559	2.0333141
C	0.2121989	0.1119000	2.1338650
H	-0.4842015	-3.2503660	1.8786424
H	-2.5611642	-1.9159169	1.8881297
H	2.2140590	0.9352810	2.2129314
H	0.1340290	2.2728840	2.2440571
H	1.9958255	-3.3666214	1.9715915
H	-3.6948838	0.2937969	2.0022943
H	3.3432515	-1.2702350	2.1345601
H	-2.3466107	2.3853841	2.1790628

Table S10: Energy values for Glc (a,cc) H2&H4 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.627318	-386.0598418	-687.5548464
CCSD(T)/CBS	-1071.795923	-385.3111755	-686.4730843

Glc (a,cc) H4&H6:

C	2.1520493	-0.5943300	-1.6430400
C	1.4399815	-1.8916599	-1.2592699
C	0.0224498	-1.8746886	-1.8121639
C	-0.7094064	-0.6100086	-1.3751592
C	0.1166924	0.6144048	-1.7819996
O	1.4181177	0.5292415	-1.1610249
O	2.0937315	-3.0408690	-1.8085786
O	-0.7388804	-2.9986848	-1.3560507
O	-1.9908195	-0.5156886	-1.9997905
C	-0.5152675	1.9156594	-1.3150724
O	0.2826442	3.0507276	-1.6530278
O	3.4143755	-0.6119496	-1.0282333
H	2.9977200	-3.0435319	-1.4533556
H	-0.2391098	-3.7925267	-1.6092607
H	1.1465002	2.8982028	-1.2351646
H	2.2386239	-0.5260637	-2.7488379
H	1.3975783	-1.9376491	-0.1583106
H	0.0785496	-1.8779780	-2.9184346
H	-0.8065533	-0.6171237	-0.2758305
H	0.2385428	0.6299051	-2.8829587
H	-2.4346688	-1.3644693	-1.8335390
H	-1.4836042	2.0340084	-1.8159761
H	-0.6853931	1.8574158	-0.2283284
H	3.9436977	0.1099955	-1.4032215
C	-2.1488308	-0.6186269	2.0306479
C	-2.1658608	1.8687105	2.0252618
C	0.6622870	-0.5972424	2.0871591
C	0.6448073	1.8880463	2.0771906
C	-1.4435644	-1.8050832	2.0450110
C	-1.4773651	3.0649412	2.0346018
C	-0.0266668	-1.7934747	2.0774499
C	-0.0598970	3.0748902	2.0617571
C	-1.4712199	0.6298814	2.0481654
C	-0.0338313	0.6402718	2.0748306
H	-3.2395112	-0.6201154	1.9979888
H	-3.2564623	1.8555978	1.9943730
H	1.7536451	-0.5810656	2.0866811
H	1.7360134	1.8866517	2.0837499
H	-1.9725397	-2.7572739	2.0165635
H	-2.0217709	4.0088465	2.0099278
H	0.5169988	-2.7386408	2.0758727
H	0.4713261	4.0265980	2.0582990

Table S11: Energy values forGlc (a,cc) H4&H6complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.626721	-386.0598536	-687.5548814
CCSD(T)/CBS	-1071.795194	-385.3111859	-686.4731726

Glc (b,c) H1:

C	0.5890688	-1.2250717	-0.1979190
C	0.0618603	-1.5809498	-1.5929737
C	-1.4064200	-1.1973463	-1.6934187
C	-2.1973342	-1.8523959	-0.5662905
C	-1.5401222	-1.5057617	0.7797831
O	-0.1714186	-1.9454522	0.7687977
O	0.8662168	-0.8941130	-2.5559640
O	-1.8650198	-1.6037162	-2.9874846
O	-3.5388782	-1.3448961	-0.6683270
C	-2.1967981	-2.2076907	1.9569786
O	-1.5967296	-1.8494520	3.1966970
O	1.9187688	-1.6367717	-0.0206190
H	0.4563030	-1.0524018	-3.4232932
H	-2.8126879	-1.3913786	-3.0230687
H	-0.6393797	-1.9791237	3.0763444
H	0.4748688	-0.1371717	-0.0060190
H	0.1577379	-2.6767917	-1.7138944
H	-1.4901018	-0.1010124	-1.5791857
H	-2.1814438	-2.9482748	-0.7062126
H	-1.5781231	-0.4102733	0.9274823
H	-4.1209470	-1.9308574	-0.1615734
H	-3.2522914	-1.9041179	2.0177460
H	-2.1481432	-3.3021709	1.7878091
H	2.3657688	-1.5100717	-0.8755190
C	0.5202091	2.3125038	-1.2185563
C	2.9517813	2.3413430	-0.7036005
C	-0.0594989	2.0843466	1.5234504
C	2.3728214	2.1331886	2.0416350
C	-0.7886623	2.2599737	-0.7846001
C	3.9723632	2.3221193	0.2257593
C	-1.0822346	2.1398344	0.5966033
C	3.6813767	2.2196686	1.6104621
C	1.5948497	2.2704139	-0.2919217
C	1.2989490	2.1588081	1.1117044
H	0.7515673	2.3792421	-2.2814982
H	3.1722374	2.4187715	-1.7690005
H	-0.2816393	1.9797356	2.5874281
H	2.1414238	2.0482740	3.1050027
H	-1.6037859	2.3019725	-1.5067437
H	5.0091076	2.3857320	-0.1078760
H	-2.1200189	2.0856167	0.9248544
H	4.4992248	2.2068863	2.3321745

Table S12: Energy values for Glc (b,c) H1 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.619272	-386.0598419	-687.5504343
CCSD(T)/CBS	-1071.787510	-385.3111379	-686.4678621

Glc (b,c) H3:

C	2.0841075	-1.4180667	0.8524428
C	1.5452159	-1.7220061	-0.5488628
C	0.0710038	-1.3459421	-0.6153810
C	-0.6963602	-2.0555146	0.4938413
C	-0.0309151	-1.7558593	1.8464063
O	1.3441934	-2.1766138	1.8039456
O	2.3317074	-0.9781639	-1.4836956
O	-0.3941962	-1.7189421	-1.9162810
O	-2.0514782	-1.5777689	0.4317697
C	-0.6674477	-2.5189196	2.9954431
O	-0.0659269	-2.2083611	4.2468380
O	3.4241702	-1.8028426	1.0093769
H	1.8681239	-1.0245706	-2.3373449
H	-1.3464962	-1.5246421	-1.9316810
H	0.8914254	-2.3292760	4.1200767
H	1.9486134	-0.3373200	1.0670837
H	1.6511103	-2.8091618	-0.7238785
H	-0.0124962	-0.2518421	-0.4710810
H	-0.6588992	-3.1445933	0.3086242
H	-0.0883743	-0.6686257	2.0374463
H	-2.6116337	-2.2112550	0.9048432
H	-1.7276096	-2.2361621	3.0747849
H	-0.6029853	-3.6031343	2.7737320
H	3.8519814	-1.6894642	0.1429309
C	1.1755406	2.2246593	-0.1493950
C	0.5394345	2.3352781	-2.5492949
C	-1.5193757	1.8207503	0.5465989
C	-2.1554743	1.9320651	-1.8547912
C	0.8130753	2.0653316	1.1730549
C	-0.4319250	2.2811488	-3.5284730
C	-0.5456873	1.8617791	1.5239342
C	-1.7908051	2.0779901	-3.1785093
C	0.1973464	2.1939033	-1.1785749
C	-1.1809490	1.9873423	-0.8227536
H	2.2216149	2.3598874	-0.4266955
H	1.5880031	2.4856426	-2.8114592
H	-2.5625599	1.6422619	0.8095456
H	-3.1994029	1.7727620	-1.5789133
H	1.5736871	2.0852440	1.9539015
H	-0.1570432	2.3933319	-4.5777805
H	-0.8168383	1.7264694	2.5712659
H	-2.5487007	2.0381458	-3.9615540

Table S13: Energy values for Glc (b,c) H3 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.620251	-386.0598483	-687.5503638
CCSD(T)/CBS	-1071.788813	-385.3111554	-686.4677588

Glc (b,c) H5:

C	2.1494538	-1.2015396	-1.0431419
C	1.5716773	-1.4926858	-2.4327222
C	0.1220067	-1.0332176	-2.4813065
C	-0.6727580	-1.6745772	-1.3495606
C	0.0341400	-1.3912892	-0.0137725
O	1.3812259	-1.8976516	-0.0697450
O	2.3848321	-0.8016605	-3.3858930
O	-0.3919139	-1.3758198	-3.7735017
O	-1.9888108	-1.0997699	-1.4101888
C	-0.6302257	-2.0926940	1.1574888
O	-0.0117257	-1.7767940	2.3990888
O	3.4656814	-1.6685352	-0.9026013
H	1.9478693	-0.9004467	-4.2484840
H	-1.3291875	-1.1187918	-3.7719231
H	0.9425743	-1.9099940	2.2622888
H	2.0856479	-0.1119829	-0.8402186
H	1.6146993	-2.5853666	-2.5964475
H	0.0939747	0.0618227	-2.3319257
H	-0.7153298	-2.7671434	-1.5132552
H	0.0484683	-0.3015924	0.1632469
H	-2.5666459	-1.6095934	-0.8223055
H	-1.6729724	-1.7481036	1.2360553
H	-0.6276257	-3.1863940	0.9744888
H	3.8956960	-1.5516762	-1.7676025
C	1.2532960	2.0436510	1.0604000
C	-0.0417146	1.5926946	3.1322233
C	-1.1338372	2.0973457	-0.4227202
C	-2.4314717	1.6454315	1.6504402
C	1.2838327	2.2790948	-0.2998148
C	-1.2530553	1.3872092	3.7581326
C	0.0792683	2.3083094	-1.0471287
C	-2.4580238	1.4143576	3.0115325
C	0.0213365	1.8367929	1.7356038
C	-1.1998707	1.8632617	0.9765419
H	2.1779217	2.0094855	1.6387483
H	0.8904131	1.5642422	3.6982563
H	-2.0611301	2.0874408	-0.9971510
H	-3.3564533	1.6715230	1.0709350
H	2.2363199	2.4359696	-0.8061724
H	-1.2893350	1.1938220	4.8302923
H	0.1171992	2.4873101	-2.1219381
H	-3.4094471	1.2519193	3.5193799

Table S14: Energy values for Glc (b,c) H5 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.619824	-386.0598559	-687.5504042
CCSD(T)/CBS	-1071.788210	-385.3111784	-686.4676746

Glc (b,c) H1&H3:

C	1.5117876	-1.2092947	0.1380353
C	1.0063345	-1.5015359	-1.2791526
C	-0.4700831	-1.1415092	-1.3614633
C	-1.2465067	-1.9006440	-0.2907413
C	-0.6141242	-1.6142090	1.0806163
O	0.7708246	-2.0019876	1.0605450
O	1.7990660	-0.7343262	-2.1892528
O	-0.9169037	-1.4611137	-2.6842167
O	-2.6090939	-1.4460832	-0.3647525
C	-1.2550660	-2.4050070	2.2071718
O	-0.6912447	-2.0833612	3.4742216
O	2.8561281	-1.5735263	0.3140755
H	1.3647252	-0.8031926	-3.0562302
H	-1.8555854	-1.2122766	-2.7177857
H	0.2724822	-2.1598813	3.3622482
H	1.3558156	-0.1386454	0.3722062
H	1.1305115	-2.5846022	-1.4672636
H	-0.5845206	-0.0601265	-1.1723553
H	-1.1837134	-2.9834046	-0.5016436
H	-0.6960819	-0.5326762	1.2900165
H	-3.1680177	-2.1183847	0.0526772
H	-2.3246756	-2.1544772	2.2625806
H	-1.1527041	-3.4852561	1.9818607
H	3.3094112	-1.3618879	-0.5202179
C	0.2378444	1.8545540	1.8533406
C	-1.6621894	1.9727509	0.2538173
C	2.0378506	2.3466847	-0.2491496
C	0.1377775	2.4626029	-1.8487631
C	1.5951579	1.9067791	2.0963595
C	-2.1265947	2.1414031	-1.0350437
C	2.5029602	2.1578787	1.0366855
C	-1.2192915	2.3906379	-2.0954342
C	-0.2741579	2.0487520	0.5420584
C	0.6466164	2.2972220	-0.5332525
H	-0.4634002	1.6493828	2.6632425
H	-2.3549756	1.7640142	1.0698138
H	2.7321672	2.5207543	-1.0728478
H	0.8433047	2.6387236	-2.6625343
H	1.9758725	1.7432245	3.1043268
H	-3.1942301	2.0712024	-1.2429823
H	3.5734279	2.1844970	1.2399203
H	-1.5969055	2.5163450	-3.1107367

Table S15: Energy values for Glc (b,c) H1&H3 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.623501	-386.0598355	-687.5503613
CCSD(T)/CBS	-1071.791245	-385.3111745	-686.4678775

Glc (b,c) H1&H5:

C	1.4537995	-1.2383983	-0.3337545
C	0.9069664	-1.6041928	-1.7186685
C	-0.5408808	-1.1462907	-1.8215272
C	-1.3517966	-1.7542067	-0.6824035
C	-0.6846190	-1.3930797	0.6548591
O	0.6661463	-1.8911316	0.6553373
O	1.7446678	-0.9769456	-2.6933106
O	-1.0275284	-1.5433305	-3.1080827
O	-2.6829037	-1.2239286	-0.8016213
C	-1.3724387	-2.0415546	1.8444567
O	-0.7343357	-1.7274462	3.0764827
O	2.7665119	-1.6990204	-0.1434509
H	1.3340277	-1.1408173	-3.5586226
H	-1.9729569	-1.3179660	-3.1229037
H	0.2141337	-1.8930325	2.9335239
H	1.3907783	-0.1424763	-0.1873477
H	0.9457354	-2.7049825	-1.8167465
H	-0.5737480	-0.0459277	-1.7153884
H	-1.3585754	-2.8536644	-0.7963096
H	-0.6840870	-0.2971220	0.7768978
H	-3.2740105	-1.7809237	-0.2732016
H	-2.4022322	-1.6605267	1.9132894
H	-1.4072039	-3.1373413	1.6774370
H	3.2265350	-1.5683984	-0.9909097
C	0.8274362	2.3194376	-1.2112684
C	-1.4218487	2.1468065	-0.1667410
C	2.0246250	1.9693871	1.3078776
C	-0.2258598	1.7933723	2.3525162
C	2.2018780	2.3006304	-1.0900266
C	-2.2032772	1.9629880	0.9565543
C	2.8055110	2.1256459	0.1803991
C	-1.6003871	1.7844726	2.2262686
C	-0.0053018	2.1637435	-0.0713810
C	0.6068707	1.9823252	1.2179967
H	0.3581010	2.4393107	-2.1892033
H	-1.8817670	2.2687935	-1.1489767
H	2.4849057	1.8204818	2.2857955
H	0.2412196	1.6345161	3.3250089
H	2.8283421	2.4062055	-1.9753810
H	-3.2893314	1.9418629	0.8661120
H	3.8920673	2.1018077	0.2622645
H	-2.2251688	1.6209172	3.1041497

Table S16: Energy values for Glc (b,c) H1&H5 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.622934	-386.059808	-687.5503448
CCSD(T)/CBS	-1071.790700	-385.3110781	-686.4678922

Glc (b,c) H3&H5:

C	1.9773163	-1.1816661	-0.0624765
C	1.4535413	-1.5003147	-1.4669037
C	-0.0124578	-1.0992820	-1.5561883
C	-0.8056281	-1.7946889	-0.4548369
C	-0.1576407	-1.4677857	0.8995947
O	1.2123636	-1.9145477	0.8885084
O	2.2671779	-0.7895645	-2.4031327
O	-0.4701761	-1.4543863	-2.8660480
O	-2.1557986	-1.3100457	-0.5497841
C	-0.8251467	-2.1764189	2.0644018
O	-0.2203046	-1.8497327	3.3109475
O	3.3102771	-1.5809171	0.1190237
H	1.8281562	-0.8707399	-3.2667616
H	-1.4020210	-1.1824643	-2.9080692
H	0.7374853	-1.9599729	3.1773390
H	1.8532297	-0.0972018	0.1359813
H	1.5416086	-2.5923641	-1.6205550
H	-0.0950646	-0.0087218	-1.4065819
H	-0.7708383	-2.8868833	-0.6210545
H	-0.1940600	-0.3788744	1.0629653
H	-2.7217478	-1.9134765	-0.0452163
H	-1.8742961	-1.8506754	2.1258365
H	-0.7989207	-3.2690473	1.8783986
H	3.7483670	-1.4968659	-0.7453813
C	-1.8700318	1.6692761	1.3634506
C	-1.7442552	2.1127407	-1.0803285
C	0.9153471	1.9855645	1.5649258
C	1.0419600	2.4221711	-0.8806492
C	-1.2386702	1.5204523	2.5814551
C	-0.9920352	2.3933710	-2.2040090
C	0.1667005	1.6784780	2.6825392
C	0.4138683	2.5453498	-2.1032864
C	-1.1278698	1.9802040	0.1922333
C	0.2961713	2.1430037	0.2949948
H	-2.9494876	1.5355066	1.2748344
H	-2.8246572	1.9774275	-1.1522792
H	1.9984140	2.0977641	1.6354209
H	2.1248312	2.5243029	-0.8014791
H	-1.8139283	1.2623060	3.4701798
H	-1.4765651	2.4905627	-3.1761043
H	0.6541308	1.5388613	3.6468040
H	1.0006554	2.7492954	-2.9987093

Table S17: Energy values for Glc (b,c) H3&H5 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.623964	-386.0598261	-687.5503074
CCSD(T)/CBS	-1071.791696	-385.3111746	-686.4677092

Glc (b,cc) H1:

C	0.4247752	-0.0080938	1.3138914
C	-0.2287592	-1.3256176	1.7363932
C	-1.6618675	-1.3437870	1.2244594
C	-2.4200635	-0.1046197	1.6910971
C	-1.6367878	1.1513414	1.2926900
O	-0.3099901	1.0872377	1.8618549
O	0.4351386	-2.4608530	1.1701782
O	-2.3877974	-2.4893265	1.6861599
O	-3.7107803	-0.0331011	1.0831575
C	-2.2705849	2.4294131	1.8119096
O	-1.5593374	3.5893110	1.3800625
O	1.7298752	-0.0046938	1.8344914
H	1.3703309	-2.3947453	1.4255738
H	-1.8666703	-3.2693350	1.4329553
H	-0.6364131	3.4533486	1.6525066
H	0.4244752	0.0600062	0.2099914
H	-0.2227374	-1.3703233	2.8405560
H	-1.6286066	-1.3289018	0.1188822
H	-2.5055967	-0.1370731	2.7943365
H	-1.5578859	1.1941974	0.1909359
H	-4.1180223	-0.9073786	1.2072535
H	-3.2915811	2.5052131	1.4178353
H	-2.3205819	2.3749571	2.9163147
H	2.0902752	0.8995062	1.7087914
C	2.7835578	-1.3829395	-1.6639949
C	0.3423769	-1.2867207	-2.1175138
C	2.8910610	1.4269004	-1.6375348
C	0.4457288	1.5238805	-2.0852662
C	3.9781642	-0.7338848	-1.4257351
C	-0.8054957	-0.5445645	-2.3098843
C	4.0327396	0.6829773	-1.4136568
C	-0.7540334	0.8722622	-2.2923769
C	1.5918932	-0.6480341	-1.8999650
C	1.6453683	0.7895045	-1.8837906
H	2.7327666	-2.4730291	-1.6701138
H	0.3048704	-2.3765200	-2.1045447
H	2.9273425	2.5180188	-1.6322278
H	0.4860757	2.6140524	-2.0597724
H	4.8861634	-1.3094458	-1.2437986
H	-1.7614001	-1.0451930	-2.4652030
H	4.9833226	1.1840427	-1.2280521
H	-1.6694961	1.4465972	-2.4346576

Table S18: Energy values for Glc (b,cc) H1 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.624736	-386.0598296	-687.5540794
CCSD(T)/CBS	-1071.794013	-385.3111145	-686.4723368

Glc (b,cc) H3:

C	2.0633870	0.8575790	1.4749774
C	1.3769165	-0.4346241	1.9192789
C	-0.0509305	-0.4494107	1.3952052
C	-0.7943138	0.8110340	1.8270045
C	0.0050965	2.0416009	1.3876786
O	1.3299268	1.9843190	1.9625147
O	2.0357276	-1.5946879	1.4023161
O	-0.7935305	-1.5660107	1.8983052
O	-2.0872274	0.8769425	1.2223958
C	-0.6146029	3.3442308	1.8609778
O	0.1133224	4.4808187	1.3964033
O	3.3457797	0.8684316	2.0443330
H	2.9456557	-1.5696308	1.7415514
H	-0.2887305	-2.3640107	1.6685052
H	1.0299360	4.3488181	1.6913509
H	2.1029220	0.8980516	0.3675405
H	1.3636163	-0.4438742	3.0244787
H	-0.0335305	-0.4624107	0.2897052
H	-0.8778851	0.8137687	2.9310867
H	0.0793951	2.0414992	0.2850241
H	-2.4668417	-0.0159859	1.2945234
H	-1.6324810	3.4197589	1.4587767
H	-0.6714409	3.3260773	2.9662103
H	3.8527898	1.5896133	1.6386467
C	-2.4607689	-1.4293464	-1.8388464
C	-1.0183851	0.5794571	-2.0768504
C	-0.1741445	-3.0650683	-1.7714894
C	1.2695513	-1.0559152	-2.0194709
C	-2.5861893	-2.7967028	-1.6974546
C	0.2398493	1.1381371	-2.1741744
C	-1.4332493	-3.6213575	-1.6620984
C	1.3929131	0.3130307	-2.1465673
C	-1.1809121	-0.8260833	-1.9571312
C	-0.0114328	-1.6624405	-1.9250578
H	-3.3431868	-0.7876953	-1.8606029
H	-1.9078123	1.2101694	-2.0713485
H	0.7174459	-3.6937759	-1.7400557
H	2.1537929	-1.6927531	-1.9728294
H	-3.5746377	-3.2485752	-1.6098058
H	0.3513110	2.2193473	-2.2611312
H	-1.5456846	-4.7000334	-1.5478255
H	2.3818147	0.7670934	-2.2208410

Table S19: Energy values for Glc (b,cc) H3 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.624863	-386.0598342	-687.5549503
CCSD(T)/CBS	-1071.794128	-385.3111377	-686.4731093

Glc (b,cc) H5:

C	2.0182934	-0.8287966	1.3222654
C	1.3621142	-2.1275078	1.7936091
C	-0.1040240	-2.1222911	1.3848858
C	-0.8024203	-0.8603811	1.8805065
C	-0.0212754	0.3677162	1.4002458
O	1.3332008	0.2872104	1.8970640
O	1.9615859	-3.2781358	1.1890457
O	-0.8151380	-3.2460706	1.9192659
O	-2.1360374	-0.7808245	1.3730195
C	-0.6071043	1.6715174	1.9123367
O	0.1218957	2.8075174	1.4481367
O	3.3453467	-0.8378340	1.7782127
H	2.9006138	-3.2645480	1.4378284
H	-0.3355993	-4.0403706	1.6307919
H	1.0450957	2.6587174	1.7128367
H	1.9630412	-0.7551901	0.2166641
H	1.4425455	-2.1669184	2.8950866
H	-0.1539753	-2.1242063	0.2803956
H	-0.8046046	-0.8676528	2.9875915
H	-0.0046227	0.3801115	0.2978782
H	-2.5440830	-1.6446546	1.5545809
H	-1.6309261	1.7655504	1.5290462
H	-0.6422043	1.6397174	3.0182367
H	3.8234410	-0.1225876	1.3291028
C	-2.4088846	1.0566092	-1.6727803
C	-0.9163473	-0.8934711	-2.0465340
C	-0.2092978	2.7900295	-1.9353030
C	1.2851281	0.8356180	-2.2942491
C	-2.5749350	2.4205415	-1.5437520
C	0.3480189	-1.4042331	-2.2609049
C	-1.4669013	3.2942543	-1.6775342
C	1.4595777	-0.5318053	-2.3837097
C	-1.1286473	0.5066135	-1.9416046
C	-0.0030315	1.3925941	-2.0715724
H	-3.2528094	0.3772488	-1.5499588
H	-1.7732741	-1.5584451	-1.9317581
H	0.6504624	3.4568707	-2.0167507
H	2.1368521	1.5124371	-2.3879082
H	-3.5614493	2.8319574	-1.3283312
H	0.5005155	-2.4817203	-2.3255173
H	-1.6095189	4.3681865	-1.5571789
H	2.4536610	-0.9478499	-2.5516569

Table S20: Energy values for Glc (b,cc) H5 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.624635	-386.0597783	-687.5549768
CCSD(T)/CBS	-1071.794151	-385.3110962	-686.4730874

Glc (b,cc) H1&H3:

C	1.3438586	0.2052557	1.4414417
C	0.6781515	-1.1079042	1.8602173
C	-0.7486686	-1.1064735	1.3285962
C	-1.5011522	0.1257059	1.8211569
C	-0.7137197	1.3823725	1.4339934
O	0.6173066	1.3068142	1.9914734
O	1.3407308	-2.2461810	1.3005324
O	-1.4889549	-2.2582630	1.7500104
O	-2.7976146	0.2134657	1.2283285
C	-1.3391057	2.6566999	1.9705423
O	-0.6375676	3.8205117	1.5318154
O	2.6489586	0.2086557	1.9620417
H	2.2625278	-2.2088608	1.6040274
H	-1.0085294	-3.0304022	1.4084291
H	0.2896000	3.6862300	1.7898138
H	1.3435586	0.2733557	0.3375417
H	0.6708490	-1.1535175	2.9642528
H	-0.7080263	-1.0691371	0.2272777
H	-1.5787036	0.0774936	2.9246672
H	-0.6454878	1.4354529	0.3330499
H	-3.1745323	-0.6822862	1.2703773
H	-2.3668219	2.7330687	1.5942245
H	-1.3706362	2.5968515	3.0752342
H	3.0093586	1.1128557	1.8363417
C	0.5451063	1.5023292	-2.0012085
C	-1.4651558	0.0410110	-2.0782397
C	2.1959013	-0.7729044	-1.9363511
C	0.1863269	-2.2341653	-2.0123588
C	1.9180773	1.6387819	-1.9423285
C	-2.0189779	-1.2229552	-2.0964277
C	2.7506776	0.4910919	-1.9123224
C	-1.1865463	-2.3699214	-2.0657098
C	-0.0560211	0.2148960	-2.0372982
C	0.7882338	-0.9480090	-2.0017022
H	-0.1003719	2.3823235	-2.0117625
H	-2.1030681	0.9258029	-2.0775783
H	2.8301814	-1.6595000	-1.8972728
H	0.8317009	-3.1121598	-1.9673720
H	2.3658562	2.6326588	-1.9170982
H	-3.1021912	-1.3417500	-2.1197772
H	3.8331819	0.6111339	-1.8628506
H	-1.6373717	-3.3626371	-2.0744994

Table S21: Energy values for Glc (b,cc) H1&H3 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.627628	-386.0598403	-687.5539997
CCSD(T)/CBS	-1071.795911	-385.3111626	-686.4722631

Glc (b,cc) H1&H5:

C	1.3836633	-0.4384667	1.3653271
C	0.7147813	-1.7427599	1.8051851
C	-0.7326431	-1.7401064	1.3314013
C	-1.4566974	-0.4948178	1.8351094
C	-0.6770972	0.7479517	1.3942065
O	0.6679591	0.6692401	1.9194692
O	1.3424019	-2.8953919	1.2343772
O	-1.4549207	-2.8808036	1.8097711
O	-2.7801023	-0.4124024	1.3046997
C	-1.2770368	2.0365875	1.9280808
O	-0.5379225	3.1851942	1.5130507
O	2.6887633	-0.4350667	1.8859271
H	2.2707675	-2.8793412	1.5188701
H	-0.9372990	-3.6632459	1.5563701
H	0.3890491	3.0009274	1.7402039
H	1.3833633	-0.3703667	0.2614271
H	0.7430659	-1.7802719	2.9093667
H	-0.7361969	-1.7167914	0.2258074
H	-1.4800192	-0.5252713	2.9416324
H	-0.6418341	0.7844511	0.2946127
H	-3.1862995	-1.2832370	1.4532654
H	-2.2950789	2.1403080	1.5326234
H	-1.3307717	1.9726692	3.0319671
H	3.0491633	0.4691333	1.7602271
C	0.7181354	-1.4158065	-2.1371482
C	-1.4715854	-0.2417428	-2.0378097
C	2.0506699	1.0515468	-1.9463273
C	-0.1393587	2.2272163	-1.8505341
C	2.0972242	-1.3695814	-2.1177877
C	-2.1897614	0.9315549	-1.9247628
C	2.7699693	-0.1249722	-2.0233276
C	-1.5185989	2.1754873	-1.8328114
C	-0.0521095	-0.2248197	-2.0598180
C	0.6294931	1.0385564	-1.9606641
H	0.1974935	-2.3728797	-2.1958920
H	-1.9852456	-1.2027307	-2.0914729
H	2.5613856	2.0135173	-1.8713979
H	0.3794350	3.1816583	-1.7532852
H	2.6739792	-2.2930160	-2.1627798
H	-3.2780914	0.9020513	-1.8833717
H	3.8599768	-0.1023897	-2.0064868
H	-2.0948105	3.0939474	-1.7240877

Table S22: Energy values for Glc (b,cc) H1&H5 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.627079	-386.0597823	-687.5540363
CCSD(T)/CBS	-1071.795770	-385.3111251	-686.4723304

Glc (b,cc) H3&H5:

C	1.7218490	-0.0946013	1.4657891
C	1.0231946	-1.4032026	1.8392391
C	-0.3865279	-1.3947726	1.2639411
C	-1.1408741	-0.1501434	1.7199916
C	-0.3248219	1.0892718	1.3398303
O	0.9730596	1.0121425	1.9736279
O	1.6985554	-2.5407300	1.2943934
O	-1.1433852	-2.5360316	1.6861185
O	-2.4219185	-0.0633020	1.0939794
C	-0.9630474	2.3845096	1.8067740
O	-0.2040549	3.5261206	1.4074053
O	2.9890424	-0.1056917	2.0694341
H	2.5984935	-2.5278247	1.6595268
H	-0.6429275	-3.3172346	1.3980810
H	0.7042344	3.3586401	1.7104374
H	1.7904762	-0.0072810	0.3629743
H	0.9750133	-1.4576880	2.9420482
H	-0.3150202	-1.3750475	0.1627804
H	-1.2448378	-0.1821462	2.8219240
H	-0.1949411	1.1189551	0.2462836
H	-2.8141913	-0.9506162	1.1635459
H	-1.9555827	2.4732876	1.3478698
H	-1.0828300	2.3468693	2.9066147
H	3.5051860	0.6292778	1.7017756
C	-1.4454126	1.3885815	-2.0249764
C	-1.6985179	-1.0806620	-2.1556003
C	1.3500595	1.1024568	-2.0263822
C	1.0965685	-1.3697436	-2.1524554
C	-0.6325306	2.5005101	-1.9453413
C	-1.1282276	-2.3369183	-2.2103339
C	0.7778394	2.3558500	-1.9463494
C	0.2816759	-2.4827086	-2.2058553
C	-0.8884465	0.0838644	-2.1035699
C	0.5410172	-0.0639679	-2.1038448
H	-2.5312141	1.4901472	-2.0039549
H	-2.7826143	-0.9608912	-2.1394513
H	2.4356208	0.9848790	-2.0290998
H	2.1819652	-1.4789200	-2.1329531
H	-1.0689822	3.4946573	-1.8568295
H	-1.7622576	-3.2232254	-2.2445607
H	1.4070739	3.2426807	-1.8724155
H	0.7222389	-3.4793507	-2.2304119

Table S23: Energy values for Glc (b,cc) H3&H5 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.628261	-386.0598104	-687.5549136
CCSD(T)/CBS	-1071.796787	-385.3111599	-686.4731047

Man (b,c) H1:

C	0.4987367	-0.1202786	1.1949586
C	-0.2246708	-1.4078217	1.6196016
C	-1.6795503	-1.3652451	1.1686098
C	-2.3642146	-0.0851357	1.6275093
C	-1.5406077	1.1209035	1.1439133
O	-0.2104826	1.0488722	1.6549719
H	0.5647367	-0.0894786	0.0956586
H	-1.5356019	1.1221103	0.0362598
C	-2.0863440	2.4459584	1.6611492
H	-1.4236680	3.2642165	1.3329849
H	-2.0951961	2.4113513	2.7647315
O	-3.4214801	2.6235889	1.1383197
H	-3.8287840	3.3674084	1.6072834
H	-2.3866949	-0.0635234	2.7333142
O	-3.6875502	-0.1175069	1.0807443
H	-4.0251664	0.7999392	1.1268676
H	-1.6990676	-1.3755166	0.0629509
O	-2.3279745	-2.5325597	1.6942224
H	-3.2836361	-2.3818025	1.5936682
H	0.2800157	-2.2544144	1.1182060
O	-0.1078883	-1.5263540	3.0395515
H	-0.7522373	-2.2040438	3.3068493
O	1.7928367	-0.0584786	1.7009586
H	1.7334367	-0.3128786	2.6406586
C	3.1040798	-1.5453847	-1.9096869
C	0.6287815	-1.5240386	-2.1535708
C	3.1347395	1.2657115	-1.9828181
C	0.6598020	1.2853493	-2.2223587
C	4.2969567	-0.8581648	-1.8155691
C	-0.5500307	-0.8179636	-2.2899671
C	4.3124942	0.5589166	-1.8528927
C	-0.5343894	0.5994132	-2.3238624
C	1.8746233	-0.8486279	-2.0506309
C	1.8903048	0.5888822	-2.0870007
H	3.0860742	-2.6363601	-1.8768374
H	0.6217090	-2.6149905	-2.1213721
H	3.1393349	2.3568571	-2.0049732
H	0.6771462	2.3762083	-2.2415802
H	5.2343543	-1.4042558	-1.7073685
H	-1.4997538	-1.3474603	-2.3686762
H	5.2617633	1.0894359	-1.7733656
H	-1.4724549	1.1456650	-2.4276184

Table S24: Energy values for Man (b,c) H1 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.623306	-386.0599007	-687.5547551
CCSD(T)/CBS	-1071.791359	-385.3112023	-686.4723158

Man (b,c) H3:

C	2.2051804	0.6780259	1.4085938
C	1.4741541	-0.6132731	1.8115995
C	0.0201483	-0.5626345	1.3570086
C	-0.6608896	0.7157857	1.8247297
C	0.1651171	1.9231702	1.3502671
O	1.4943047	1.8445587	1.8673373
H	2.2833902	0.7150151	0.3081036
H	0.1693191	1.9287189	0.2427351
C	-0.3776513	3.2455297	1.8782529
H	0.2876082	4.0652567	1.5614977
H	-0.3925100	3.2010589	2.9806386
O	-1.7109619	3.4344970	1.3524550
H	-2.1203545	4.1668804	1.8363938
H	-0.6807198	0.7303731	2.9311491
O	-1.9870036	0.6937444	1.2848945
H	-2.3175444	1.6134606	1.3355726
H	0.0017483	-0.5749345	0.2514086
O	-0.6290517	-1.7288345	1.8836086
H	-1.5846517	-1.5777345	1.7824086
H	1.9762031	-1.4558658	1.3014659
O	1.5895809	-0.7506212	3.2301696
H	0.9298010	-1.4179221	3.4878603
O	3.4932355	0.7322111	1.9303363
H	3.4230449	0.4610853	2.8647223
C	-2.1683119	-1.3181719	-2.0155611
C	-0.6183079	0.6159011	-2.1975602
C	0.0290411	-3.0726322	-1.9455899
C	1.5791176	-1.1360734	-2.1169750
C	-2.3656252	-2.6797201	-1.9027281
C	0.6694540	1.1101085	-2.2534564
C	-1.2581585	-3.5641572	-1.8692624
C	1.7780580	0.2268103	-2.2119812
C	-0.8571267	-0.7810650	-2.1033855
C	0.2668594	-1.6777876	-2.0628424
H	-3.0154388	-0.6307297	-2.0285852
H	-1.4741817	1.2924532	-2.2070966
H	0.8856029	-3.7478262	-1.9102914
H	2.4291511	-1.8194247	-2.0778614
H	-3.3773010	-3.0807926	-1.8340556
H	0.8397323	2.1850269	-2.3216693
H	-1.4280260	-4.6370149	-1.7754073
H	2.7904827	0.6298432	-2.2502226

Table S25: Energy values for Man (b,c) H3 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.623306	-386.0599007	-687.5547551
CCSD(T)/CBS	-1071.792604	-385.3111529	-686.4722982

Man (b,c) H5:

C	2.0181000	-1.0441412	1.3394811
C	1.2946847	-2.3591503	1.6801800
C	-0.1557187	-2.2998228	1.2129776
C	-0.8528284	-1.0433099	1.7166917
C	-0.0234647	0.1825443	1.2982613
O	1.2934943	0.0905816	1.8452573
H	2.1008278	-0.9503691	0.2419433
H	0.0121042	0.2253489	0.1934767
C	-0.5816436	1.4925317	1.8418045
H	0.0802564	2.3105317	1.5138045
H	-0.5920724	1.4440004	2.9438365
O	-1.9165436	1.6707317	1.3170045
H	-2.3264436	2.4103317	1.7893045
H	-0.8958900	-1.0698446	2.8219222
O	-2.1679393	-1.0553408	1.1481668
H	-2.4995969	-0.1360963	1.2152362
H	-0.1650346	-2.2580349	0.1085041
O	-0.8055946	-3.4929832	1.6759426
H	-1.7606404	-3.3397376	1.5727798
H	1.8109969	-3.1767216	1.1432347
O	1.3958812	-2.5536004	3.0924130
H	0.7622873	-3.2577531	3.3132360
O	3.3038692	-1.0058350	1.8688811
H	3.2320422	-1.3154265	2.7908963
C	-0.8127073	-0.6505635	-2.2168540
C	-1.9642435	1.5489400	-2.1049754
C	1.6762829	0.6573393	-2.3049169
C	0.5225518	2.8581717	-2.2193504
C	0.3571670	-1.3802292	-2.2900677
C	-1.9005329	2.9271580	-2.0864398
C	1.6118729	-0.7212740	-2.3298489
C	-0.6472619	3.5875868	-2.1483073
C	-0.7809864	0.7689265	-2.1925729
C	0.4916874	1.4378234	-2.2414917
H	-1.7803544	-1.1500225	-2.1555874
H	-2.9239433	1.0334172	-2.0441631
H	2.6395981	1.1686981	-2.3317244
H	1.4901527	3.3621554	-2.2605723
H	0.3203963	-2.4697990	-2.3075149
H	-2.8162584	3.5161133	-2.0199772
H	2.5283089	-1.3088336	-2.3804362
H	-0.6135653	4.6777539	-2.1400939

Table S26: Energy values for Man (b,c) H5 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.623882	-386.0598532	-687.5546750
CCSD(T)/CBS	-1071.792650	-385.3111525	-686.4723020

Man (b,c) H1&H3:

C	1.5079722	0.1048038	1.2867884
C	0.7773954	-1.2086679	1.6104049
C	-0.6752802	-1.1338424	1.1565153
C	-1.3587901	0.1144807	1.6981187
C	-0.5334386	1.3430021	1.2782507
O	0.7888958	1.2434475	1.8053681
H	1.6006911	0.2095148	0.1946054
H	-0.5148304	1.3934621	0.1726917
C	-1.0846879	2.6444783	1.8456836
H	-0.4057160	3.4718772	1.5815692
H	-1.1331114	2.5565371	2.9444670
O	-2.4008835	2.8615297	1.2874814
H	-2.8213442	3.5766687	1.7875906
H	-1.3686659	0.0745813	2.8039563
O	-2.6896326	0.1162735	1.1698643
H	-3.0105016	1.0381356	1.2350259
H	-0.6975093	-1.0779757	0.0553755
O	-1.3258927	-2.3329160	1.6055259
H	-2.2796529	-2.1805019	1.4919478
H	1.2846984	-2.0166129	1.0520665
O	0.8868208	-1.4314504	3.0194935
H	0.2282191	-2.1150287	3.2338267
O	2.7901619	0.1322062	1.8253869
H	2.7096700	-0.1915682	2.7419524
C	0.1527138	-2.2354133	-2.2141035
C	2.3136188	-1.0093061	-2.0839629
C	-1.2316917	0.2104974	-2.2514631
C	0.9291083	1.4354197	-2.1296621
C	-1.2264762	-2.2158908	-2.2812700
C	3.0057142	0.1840138	-2.0258161
C	-1.9242166	-0.9823673	-2.2967648
C	2.3068693	1.4174891	-2.0490680
C	0.8951654	-1.0250519	-2.1682264
C	0.1866929	0.2258672	-2.1920364
H	0.6945578	-3.1825357	-2.1874525
H	2.8462954	-1.9616493	-2.0569095
H	-1.7664817	1.1612219	-2.2429024
H	0.3858412	2.3816237	-2.1388496
H	-1.7844780	-3.1522360	-2.3058215
H	4.0925846	0.1817729	-1.9447254
H	-3.0134468	-0.9786964	-2.3260122
H	2.8630419	2.3528066	-1.9889106

Table S27: Energy values for Man (b,c) H1&H3 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.627541	-386.0598409	-687.5546749
CCSD(T)/CBS	-1071.795039	-385.3111677	-686.4722526

Man (b,c) H1&H5:

C	1.4615508	-0.3568278	1.2853594
C	0.7424835	-1.6623087	1.6664634
C	-0.7079475	-1.6246510	1.1983154
C	-1.4088581	-0.3596545	1.6748358
C	-0.5948758	0.8553268	1.1977495
O	0.7256902	0.7956921	1.7401876
H	1.5654772	-0.3075647	0.1903842
H	-0.5713301	0.8568475	0.0932628
C	-1.1567755	2.1782412	1.7019353
H	-0.5113998	3.0008156	1.3532955
H	-1.1540199	2.1599538	2.8051150
O	-2.5022242	2.3354950	1.1943522
H	-2.9276205	3.0427431	1.7010750
H	-1.4248154	-0.3483353	2.7812579
O	-2.7359084	-0.4039280	1.1392888
H	-3.0692014	0.5161697	1.1656978
H	-0.7184337	-1.6115400	0.0934514
O	-1.3512142	-2.8093097	1.6924349
H	-2.3074695	-2.6578410	1.5970069
H	1.2637507	-2.4913468	1.1535696
O	0.8399468	-1.8141705	3.0853076
H	0.1929556	-2.4993505	3.3271843
O	2.7383989	-0.2907490	1.8342005
H	2.6512359	-0.5678826	2.7653129
C	2.3938572	0.8005885	-2.0451836
C	0.2571616	2.0695908	-2.1654177
C	0.9616218	-1.6168458	-2.1278338
C	-1.1733355	-0.3484864	-2.2561162
C	3.0615616	-0.4062738	-1.9939556
C	-1.1216765	2.0769535	-2.2324218
C	2.3390870	-1.6255091	-2.0338367
C	-1.8430099	0.8577587	-2.2769533
C	0.9770410	0.8452085	-2.1382072
C	0.2445912	-0.3913646	-2.1848197
H	2.9441497	1.7412401	-1.9983438
H	0.8173360	3.0049110	-2.1231241
H	0.3999742	-2.5526804	-2.1524989
H	-1.7257397	-1.2894930	-2.2745982
H	4.1474285	-0.4264144	-1.9052435
H	-1.6641291	3.0221311	-2.2376660
H	2.8766644	-2.5724303	-1.9810342
H	-2.9319788	0.8752906	-2.3097898

Table S28: Energy values for Man (b,c) H1&H5 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.627855	-386.0598336	-687.5546753
CCSD(T)/CBS	-1071.795459	-385.3111672	-686.4722427

Man (b,c) H3&H5:

C	1.8967540	-0.1039309	1.3309818
C	1.1634945	-1.4057849	1.6987535
C	-0.2793773	-1.3558505	1.2129934
C	-0.9789702	-0.0893998	1.6872337
C	-0.1527181	1.1229524	1.2269318
O	1.1653515	1.0519415	1.7787881
H	2.0086197	-0.0518383	0.2353539
H	-0.1198009	1.1325709	0.1228504
C	-0.7069048	2.4470021	1.7378621
H	-0.0563079	3.2676260	1.3940607
H	-0.7026677	2.4224517	2.8407843
O	-2.0516791	2.6174551	1.2330775
H	-2.4747814	3.3167975	1.7525858
H	-1.0123355	-0.0831533	2.7932568
O	-2.2978527	-0.1182745	1.1299991
H	-2.6283882	0.8020776	1.1731580
H	-0.2773535	-1.3459247	0.1100474
O	-0.9343513	-2.5385490	1.6969596
H	-1.8863370	-2.3941608	1.5591535
H	1.6813947	-2.2385338	1.1887221
O	1.2475567	-1.5619118	3.1181569
H	0.5877774	-2.2374038	3.3526920
O	3.1691561	-0.0480201	1.8918071
H	3.0717384	-0.3272741	2.8212553
C	1.4279169	-1.3773989	-2.0879084
C	1.4423916	1.1093010	-2.1069397
C	-1.3779388	-1.3626186	-2.2621880
C	-1.3640272	1.1234095	-2.2623387
C	0.7254392	-2.5649904	-2.1177179
C	0.7528595	2.3046170	-2.1454471
C	-0.6896454	-2.5580802	-2.2095855
C	-0.6625722	2.3118413	-2.2221205
C	0.7503786	-0.1304318	-2.1501804
C	-0.6843360	-0.1229091	-2.2335011
H	2.5163627	-1.3773756	-2.0115410
H	2.5308876	1.0986786	-2.0349405
H	-2.4678647	-1.3487623	-2.3109812
H	-2.4543131	1.1220817	-2.3028496
H	1.2567382	-3.5153178	-2.0642109
H	1.2963367	3.2488688	-2.1073272
H	-1.2328470	-3.5030775	-2.2229039
H	-1.1977840	3.2612999	-2.2347832

Table S29: Energy values for Man (b,c) H3&H5 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.628083	-386.0598452	-687.5546766
CCSD(T)/CBS	-1071.795682	-385.3111882	-686.4722641

Man (b,cc) H1:

C	0.5428948	-0.1710419	1.3694133
C	-0.1167618	-1.4787412	1.8246555
C	-1.5869291	-1.4495377	1.4143276
C	-2.2739877	-0.1627630	1.8883730
C	-1.4892656	1.0473463	1.3645440
O	-0.1431203	0.9754280	1.8626772
H	0.5556948	-0.1415419	0.2638133
H	-1.4804220	1.0122600	0.2594467
C	-2.0871821	2.3624467	1.8119531
H	-1.8939294	2.4851884	2.8937289
H	-3.1759838	2.3166421	1.6430777
O	-1.4834409	3.4190476	1.0510676
H	-1.8756553	4.2523337	1.3513460
H	-2.2638886	-0.1394417	2.9941078
O	-3.6095338	-0.1048362	1.3825360
H	-3.9814619	-0.9937360	1.5243803
H	-1.6431666	-1.4734765	0.3149353
O	-2.3047079	-2.5997220	1.8793054
H	-2.0529994	-2.7122122	2.8138164
H	0.3933372	-2.3174280	1.3156681
O	-0.0652394	-1.6467998	3.2429159
H	0.7889280	-1.2846847	3.5369189
O	1.8430948	-0.1508419	1.9089133
H	2.2101948	0.7313581	1.7317133
C	2.7412263	-1.5270156	-1.9076174
C	0.2641526	-1.5443687	-2.1262042
C	2.7146341	1.2844951	-1.8329982
C	0.2383214	1.2673546	-2.0601656
C	3.9202767	-0.8224638	-1.7735161
C	-0.9301434	-0.8560416	-2.2077936
C	3.9068879	0.5948586	-1.7348240
C	-0.9426434	0.5612696	-2.1759652
C	1.4977540	-0.8491205	-2.0107823
C	1.4838027	0.5895028	-1.9758325
H	2.7453068	-2.6179779	-1.9320754
H	0.2780972	-2.6354899	-2.1439540
H	2.6972510	2.3755026	-1.8042209
H	0.2279019	2.3570483	-2.0087465
H	4.8683040	-1.3548663	-1.6934456
H	-1.8711723	-1.4003366	-2.2909555
H	4.8455340	1.1395917	-1.6282658
H	-1.8926025	1.0933216	-2.2276085

Table S30: Energy values for Man (b,cc) H1 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.621157	-386.0598555	-687.5507676
CCSD(T)/CBS	-1071.790535	-385.3111325	-686.4693080

Man (b,cc) H3:

C	2.1452633	0.7982278	1.2770022
C	1.4858237	-0.5161708	1.7172023
C	0.0204564	-0.4888162	1.2920726
C	-0.6737607	0.7953117	1.7626205
C	0.1121635	2.0124152	1.2593942
O	1.4544197	1.9364753	1.7745480
H	2.1581648	0.8365987	0.1673971
H	0.1311444	1.9864515	0.1544964
C	-0.4943571	3.3201977	1.7148905
H	-0.3148456	3.4307310	2.8003851
H	-1.5808900	3.2709812	1.5332736
O	0.1140116	4.3866812	0.9731635
H	-0.3006953	5.2136164	1.2606377
H	-0.6739258	0.8117886	2.8688915
O	-2.0065748	0.8522111	1.2489527
H	-2.3568998	-0.0530182	1.3341489
H	-0.0266436	-0.5223162	0.1925726
O	-0.7031436	-1.6337162	1.7602726
H	-0.4610436	-1.7381162	2.6982726
H	2.0008543	-1.3525268	1.2093463
O	1.5258841	-0.6867402	3.1349972
H	2.3816717	-0.3351699	3.4363855
O	3.4450349	0.8175755	1.8200675
H	3.7787949	1.7258033	1.7262549
C	-2.4525048	-1.6917482	-1.8767929
C	-1.1643436	0.4227545	-2.0907954
C	-0.0633333	-3.1655959	-2.0452540
C	1.2266522	-1.0484170	-2.2487126
C	-2.4778187	-3.0702276	-1.8140824
C	0.0449324	1.0727587	-2.2320298
C	-1.2735352	-3.8131563	-1.9008302
C	1.2506735	0.3309662	-2.3095249
C	-1.2252322	-0.9948778	-2.0325975
C	-0.0027340	-1.7484666	-2.1141891
H	-3.3749944	-1.1130048	-1.8073504
H	-2.0912889	0.9896930	-2.0015928
H	0.8675609	-3.7326036	-2.1065089
H	2.1530640	-1.6232123	-2.3045812
H	-3.4261908	-3.5948205	-1.6941337
H	0.0795846	2.1616937	-2.2691305
H	-1.3065266	-4.9016831	-1.8471217
H	2.1997237	0.8571743	-2.4174706

Table S31: Energy values for Man (b,cc) H3 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.620063	-386.0598637	-687.5507790
CCSD(T)/CBS	-1071.789465	-385.3111687	-686.4693209

Man (b,cc) H5:

C	2.0883202	-0.9766384	1.3525531
C	1.4163818	-2.2702483	1.8351646
C	-0.0566143	-2.2319199	1.4337448
C	-0.7221824	-0.9237950	1.8771424
C	0.0769316	0.2667264	1.3275846
O	1.4225598	0.1813696	1.8353343
H	2.0839823	-0.9566321	0.2422183
H	0.0897032	0.2183162	0.2242649
C	-0.5123464	1.5883276	1.7642671
H	-0.3326464	1.7118276	2.8482671
H	-1.5989406	1.5466128	1.5814066
O	0.0985536	2.6441276	1.0092671
H	-0.3067464	3.4762276	1.2954671
H	-0.7048058	-0.8734113	2.9821077
O	-2.0618393	-0.8641194	1.3815388
H	-2.4417982	-1.7438061	1.5561478
H	-0.1275638	-2.2817773	0.3370940
O	-0.7863004	-3.3588461	1.9359362
H	-0.5316384	-3.4475187	2.8722223
H	1.9134763	-3.1271788	1.3433073
O	1.4747681	-2.4074345	3.2557995
H	2.3370480	-2.0538385	3.5363036
O	3.3972701	-0.9670920	1.8744560
H	3.7453891	-0.0680614	1.7493739
C	-0.9918446	-0.8890425	-2.0009474
C	-2.3346468	1.2001811	-1.9088352
C	1.3489482	0.6299059	-2.3393460
C	0.0034113	2.7180159	-2.2840604
C	0.2320250	-1.5150134	-2.1274226
C	-2.3984093	2.5774590	-1.9682185
C	1.4143031	-0.7491029	-2.2916179
C	-1.2204110	3.3422261	-2.1621445
C	-1.0925862	0.5266549	-2.0478450
C	0.1033373	1.3034003	-2.2299196
H	-1.9009044	-1.4709360	-1.8472473
H	-3.2353815	0.6059845	-1.7510920
H	2.2553148	1.2255665	-2.4640121
H	0.9167998	3.3012780	-2.4121852
H	0.2954534	-2.6032609	-2.0937386
H	-3.3586149	3.0839076	-1.8648307
H	2.3763367	-1.2545559	-2.3842892
H	-1.2849951	4.4300460	-2.2057877

Table S32: Energy values for Man (b,cc) H5 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.619717	-386.0598458	-687.5508118
CCSD(T)/CBS	-1071.789380	-385.3111739	-686.4692920

Man (b,cc) H1&H3:

C	1.4392649	0.1131744	1.2110211
C	0.7417710	-1.1711577	1.6780650
C	-0.7353457	-1.0912936	1.3021259
C	-1.3642832	0.2197379	1.7896673
C	-0.5505824	1.3977170	1.2380719
O	0.8009801	1.2827412	1.7148411
H	1.4406855	0.1476920	0.1051627
H	-0.5643197	1.3494055	0.1339797
C	-1.0967947	2.7362593	1.6809931
H	-0.8692959	2.8691951	2.7546779
H	-2.1908758	2.7194173	1.5442148
O	-0.4865672	3.7640221	0.8863834
H	-0.8317777	4.6135647	1.1987767
H	-1.3192475	0.2497630	2.8946089
O	-2.7125047	0.3231139	1.3267743
H	-3.0959474	-0.5645258	1.4438876
H	-0.8259102	-1.1230269	0.2075355
O	-1.4810550	-2.2133342	1.7928727
H	-1.2177862	-2.3217030	2.7247543
H	1.2073410	-2.0280734	1.1572750
O	0.8224387	-1.3416348	3.0954972
H	1.6874395	-0.9898734	3.3700949
O	2.7479300	0.0891381	1.7325497
H	3.1308946	0.9683485	1.5747392
C	-1.4983061	-0.0059898	-2.1348777
C	0.6208690	1.2910638	-2.2216229
C	-0.0307281	-2.4032549	-2.0749807
C	2.0902729	-1.1062372	-2.1702881
C	-2.1498371	-1.2209124	-2.0713741
C	2.0011493	1.3190973	-2.2455366
C	-1.4105422	-2.4295186	-2.0416266
C	2.7422385	0.1100052	-2.2227996
C	-0.0801057	0.0556868	-2.1772593
C	0.6710022	-1.1701912	-2.1452451
H	-2.0627690	0.9272643	-2.1344106
H	0.0474293	2.2192400	-2.2194462
H	0.5435029	-3.3305733	-2.0419151
H	2.6564473	-2.0388481	-2.1426414
H	-3.2380009	-1.2531465	-2.0257784
H	2.5254386	2.2746477	-2.2748012
H	-1.9365629	-3.3815011	-1.9758336
H	3.8320501	0.1445008	-2.2381327

Table S33: Energy values for Man (b,cc) H1&H3 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.624515	-386.0598411	-687.5507266
CCSD(T)/CBS	-1071.793070	-385.3111573	-686.4693103

Man (b,cc) H1&H5:

C	1.4388782	-0.3291090	1.1762340
C	0.7958789	-1.6363137	1.6566534
C	-0.6938172	-1.6015889	1.3207669
C	-1.3480054	-0.3085806	1.8227272
C	-0.5855260	0.8962260	1.2535228
O	0.7794120	0.8172840	1.7024347
H	1.4057734	-0.2934047	0.0714291
H	-0.6248947	0.8630391	0.1503242
C	-1.1636304	2.2080410	1.7356019
H	-0.9674475	2.2951663	2.8202151
H	-2.2536743	2.1777139	1.5698197
O	-0.5525179	3.2829707	1.0086691
H	-0.8703891	4.1100775	1.3999381
H	-1.2690739	-0.2778795	2.9258458
O	-2.7130334	-0.2511259	1.4037859
H	-3.0749570	-1.1383577	1.5784043
H	-0.8113001	-1.6327270	0.2278386
O	-1.3908770	-2.7449025	1.8336492
H	-1.0878749	-2.8507612	2.7537082
H	1.2771258	-2.4751057	1.1214027
O	0.9156527	-1.8100384	3.0710016
H	1.7751199	-1.4326096	3.3277421
O	2.7627861	-0.3170842	1.6572650
H	3.1244789	0.5647101	1.4678347
C	-0.1206434	1.9358628	-2.2457166
C	2.0524698	0.7267755	-2.2768611
C	-1.4834357	-0.5186701	-2.0960308
C	0.6897994	-1.7267747	-2.1202204
C	-1.4988294	1.9057445	-2.1784854
C	2.7571801	-0.4599377	-2.2363728
C	-2.1857118	0.6694416	-2.1018609
C	2.0695221	-1.6976686	-2.1549672
C	0.6315159	0.7321715	-2.2384758
C	-0.0654688	-0.5236578	-2.1619902
H	0.4124670	2.8866544	-2.2771797
H	2.5755407	1.6832292	-2.3320566
H	-2.0075187	-1.4727553	-2.0213426
H	0.1557093	-2.6762235	-2.0526941
H	-2.0623433	2.8381546	-2.1608795
H	3.8470542	-0.4502722	-2.2604275
H	-3.2725680	0.6597794	-2.0262749
H	2.6371734	-2.6274938	-2.1149782

Table S34: Energy values for Man (b,cc) H1&H5 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.623909	-386.0597998	-687.5506928
CCSD(T)/CBS	-1071.792545	-385.311131	-686.4692522

Man (b,cc) H3&H5:

C	1.8893538	-0.0616772	1.2003069
C	1.2373121	-1.3777260	1.6483094
C	-0.2400895	-1.3443550	1.2662292
C	-0.9144566	-0.0588762	1.7607024
C	-0.1398799	1.1531673	1.2258828
O	1.2123766	1.0750826	1.7176510
H	1.8798342	-0.0135170	0.0923207
H	-0.1401403	1.1278615	0.1224197
C	-0.7377056	2.4604770	1.6943579
H	-0.5738650	2.5486609	2.7842621
H	-1.8221371	2.4236514	1.4964848
O	-0.1117498	3.5390547	0.9852263
H	-0.4504174	4.3646562	1.3619495
H	-0.8715294	-0.0371359	2.8661348
O	-2.2657675	-0.0012416	1.2988089
H	-2.6182528	-0.9009172	1.4217133
H	-0.3231863	-1.3722294	0.1716760
O	-0.9496568	-2.4946811	1.7451008
H	-0.6835645	-2.6050864	2.6758672
H	1.7350387	-2.2113501	1.1197002
O	1.3182149	-1.5600672	3.0636438
H	2.1825323	-1.2092441	3.3413277
O	3.2015999	-0.0476873	1.7163872
H	3.5280729	0.8640261	1.6315460
C	-1.7287048	-1.4440353	-2.0269470
C	-1.6706463	1.0406818	-2.0996905
C	1.0757341	-1.5150146	-2.1861932
C	1.1333928	0.9707281	-2.2799101
C	-1.0616699	-2.6525266	-2.0145042
C	-0.9471841	2.2135251	-2.1672308
C	0.3534036	-2.6879211	-2.0913128
C	0.4668625	2.1786901	-2.2591864
C	-1.0153226	-0.2192558	-2.1189845
C	0.4186530	-0.2556116	-2.2064293
H	-2.8163039	-1.4080344	-1.9493517
H	-2.7573519	1.0607328	-2.0081497
H	2.1657033	-1.5366917	-2.2424119
H	2.2227477	0.9375585	-2.3424625
H	-1.6194935	-3.5845685	-1.9273014
H	-1.4579267	3.1750701	-2.1281430
H	0.8702984	-3.6473873	-2.0682674
H	1.0258715	3.1132146	-2.2915323

Table S35: Energy values for Man (b,cc) H3&H5 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-1073.624013	-386.0598032	-687.5507436
CCSD(T)/CBS	-1071.792863	-385.3111633	-686.4693156

Fuc (a,c) H3:

C	1.5849588	1.1023856	-2.2549569
C	0.6979516	-0.1554007	-2.3090504
C	-0.3179122	-0.1436463	-1.1638220
C	-1.1224211	1.1487192	-1.1690019
C	-0.1492133	2.3392308	-1.1613530
O	0.7855383	2.2676720	-2.2548495
C	-0.8596479	3.6757109	-1.2832994
O	2.4307981	1.0867102	-1.1130331
O	1.5466428	-1.3038896	-2.1995415
O	-1.1389122	-1.3186463	-1.2209220
O	-1.9683270	1.1006895	-2.3298298
H	2.4749450	0.1620165	-0.8040160
H	2.1928717	1.1846660	-3.1710130
H	0.1599311	-0.1466408	-3.2725742
H	0.2282878	-0.2003463	-0.2136220
H	-1.7326819	1.1928465	-0.2473264
H	0.4044666	2.2833487	-0.2077287
H	-0.1355514	4.4987813	-1.2279032
H	-1.5944284	3.7930909	-0.4733151
H	-1.3738871	3.7495889	-2.2546940
H	0.9612804	-2.0398321	-1.9432956
H	-1.7872122	-1.1555463	-1.9299220
H	-2.4932879	1.9151075	-2.3536735
C	1.8749622	-1.0164583	1.7044030
C	0.6184090	-3.1628627	1.7203791
C	-0.4820458	0.3675818	2.3514439
C	-1.7394728	-1.7778997	2.3709283
C	1.8948136	0.3560112	1.8573950
C	-0.5673350	-3.8476440	1.8911801
C	0.7042282	1.0536916	2.1828750
C	-1.7563379	-3.1495345	2.2194528
C	0.6703393	-1.7522423	1.8723080
C	-0.5356951	-1.0443892	2.2047757
H	2.7876528	-1.5604665	1.4534605
H	1.5377940	-3.6953143	1.4706140
H	-1.4004493	0.9019337	2.6027809
H	-2.6526980	-1.2346358	2.6198584
H	2.8203738	0.9119349	1.7136262
H	-0.5945980	-4.9313149	1.7727824
H	0.7321030	2.1373340	2.3001683
H	-2.6875599	-3.7017718	2.3477517

Table S36: Energy values for Fuc (a,c) H3 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-998.3669278	-386.0598949	-612.2966716
CCSD(T)/CBS	-996.6385396	-385.3112086	-611.3176117

Fuc (a,c) H4:

C	2.7204903	-0.2194784	-2.4676291
C	1.8072225	-1.4562718	-2.3842552
C	0.9207911	-1.3723462	-1.1405540
C	0.1363195	-0.0673366	-1.1425317
C	1.1132542	1.1086549	-1.2883942
O	1.9652397	0.9647749	-2.4459762
C	0.3941777	2.4365969	-1.4320492
O	3.6565192	-0.2195105	-1.3889690
O	2.6495386	-2.6145758	-2.3274822
O	0.0822385	-2.5313389	-1.0454044
O	-0.8131805	-0.1681366	-2.2229317
H	3.8962059	-1.1551137	-1.2532186
H	3.2519695	-0.2024871	-3.4337994
H	1.1703906	-1.4733562	-3.2849275
H	1.5639272	-1.3796607	-0.2491434
H	-0.3892805	0.0413634	-0.1805317
H	1.7385749	1.1105719	-0.3805916
H	1.1181509	3.2587985	-1.5003100
H	-0.2533480	2.6013887	-0.5580134
H	-0.2156697	2.4396630	-2.3478526
H	2.0832250	-3.3384822	-2.0059737
H	-0.6618980	-2.3633097	-1.6525634
H	-1.4324805	0.5721634	-2.1399317
C	-0.2368036	-1.1853559	2.1907341
C	-2.7214041	-1.1782378	2.1196796
C	-0.2259591	1.6251209	2.1229295
C	-2.7126071	1.6329572	2.0578602
C	0.9566225	-0.4921265	2.2108164
C	-3.9107695	-0.4791472	2.0725120
C	0.9629444	0.9251624	2.1745676
C	-3.9062709	0.9393367	2.0421819
C	-1.4769376	-0.4943722	2.1425241
C	-1.4721096	0.9433433	2.1082840
H	-0.2471835	-2.2758874	2.1929051
H	-2.7156312	-2.2689900	2.1419483
H	-0.2269384	2.7160503	2.0952394
H	-2.7016012	2.7243145	2.0374732
H	1.9020946	-1.0343044	2.2457075
H	-4.8595737	-1.0158316	2.0594602
H	1.9135432	1.4595525	2.1830816
H	-4.8523104	1.4804031	2.0092023

Table S37: Energy values for Fuc (a,c) H4 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-998.3676933	-386.0598796	-612.2972995
CCSD(T)/CBS	-996.6393435	-385.3111761	-611.3187369

Fuc (a,c) H5:

C	1.2745162	-0.9043605	-2.3032923
C	0.3767140	-2.1526602	-2.3960717
C	-0.6346116	-2.1615427	-1.2480486
C	-1.4359268	-0.8671654	-1.2450009
C	-0.4618585	0.3195951	-1.1926268
O	0.5038139	0.2682469	-2.2665138
C	-1.1674585	1.6575951	-1.3049268
O	2.1100687	-0.9803985	-1.1478656
O	1.2279201	-3.3042926	-2.3275227
O	-1.4565986	-3.3359153	-1.3148736
O	-2.2609912	-0.8976739	-2.4233976
H	2.3237769	-1.9279930	-1.0460895
H	1.8919260	-0.8111413	-3.2128876
H	-0.1635454	-2.1156293	-3.3574458
H	-0.0844577	-2.2201411	-0.2983484
H	-2.0619893	-0.8304794	-0.3360003
H	0.0673415	0.2501951	-0.2294268
H	-0.4408585	2.4763951	-1.2274268
H	-1.8974819	1.7598888	-0.4896598
H	-1.6782235	1.7457864	-2.2766180
H	0.6446381	-4.0537581	-2.1103831
H	-2.1170087	-3.1565463	-2.0088964
H	-2.8050656	-0.0955962	-2.4265815
C	2.2912654	1.5817066	1.9926682
C	1.0723997	-0.5834308	2.0840541
C	-0.1519445	2.9642003	2.1646713
C	-1.3698942	0.7992700	2.2522728
C	2.2694297	2.9619532	1.9935138
C	-0.1171997	-1.2778840	2.1685240
C	1.0379480	3.6589935	2.0807444
C	-1.3493219	-0.5810703	2.2520426
C	1.0854334	0.8368881	2.0841425
C	-0.1639379	1.5441997	2.1703564
H	3.2351869	1.0403656	1.9136096
H	2.0211725	-1.1153872	2.0035275
H	-1.1032267	3.4960930	2.2303303
H	-2.3148473	1.3402262	2.3203200
H	3.2024584	3.5220619	1.9231883
H	-0.1170297	-2.3680348	2.1680370
H	1.0341380	4.7488909	2.0790527
H	-2.2812006	-1.1430973	2.3187743

Table S38: Energy values for Fuc (a,c) H5 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-998.3676285	-386.0598881	-612.2973665
CCSD(T)/CBS	-996.6395328	-385.3112073	-611.3186025

Fuc (a,c) H6:

C	2.2390781	-1.9040168	-2.3480197
C	1.2601637	-3.0860874	-2.2155837
C	0.3990183	-2.9194607	-0.9621040
C	-0.3098893	-1.5709925	-0.9886120
C	0.7331564	-0.4582430	-1.1763076
O	1.5510074	-0.6798935	-2.3450314
C	0.0967954	0.9096616	-1.3276585
O	3.1939855	-1.9277851	-1.2869492
O	2.0395858	-4.2862076	-2.1373439
O	-0.5004811	-4.0273216	-0.8206368
O	-1.2779180	-1.6451789	-2.0498878
H	3.3857707	-2.8719341	-1.1298731
H	2.7521811	-1.9426851	-3.3239115
H	0.6085309	-3.0929117	-3.1054704
H	1.0609605	-2.9450935	-0.0840394
H	-0.8140061	-1.3998643	-0.0217598
H	1.3747324	-0.4725489	-0.2796233
H	0.8721115	1.6801886	-1.4205884
H	-0.5171080	1.1351178	-0.4447807
H	-0.5254315	0.9453890	-2.2352008
H	1.4417287	-4.9696153	-1.7847859
H	-1.2288261	-3.8561362	-1.4450214
H	-1.7699030	-0.8100295	-2.0607598
C	-1.4438617	0.4644692	2.2300645
C	-2.7427909	2.5686881	1.9618700
C	0.9519184	1.9045099	1.9362939
C	-0.3454100	4.0085501	1.6662071
C	-0.2276125	-0.1865742	2.2880817
C	-2.7703360	3.9343537	1.7602594
C	0.9810838	0.5396132	2.1389337
C	-1.5610049	4.6599436	1.6107564
C	-1.5079579	1.8690074	2.0243188
C	-0.2816876	2.6053095	1.8745842
H	-2.3767858	-0.0909219	2.3457569
H	-3.6703844	2.0047468	2.0788612
H	1.8791728	2.4669655	1.8166037
H	0.5873488	4.5634447	1.5525157
H	-0.1934335	-1.2645258	2.4484385
H	-3.7248768	4.4590510	1.7160521
H	1.9354258	0.0149602	2.1800321
H	-1.5958932	5.7382376	1.4525163

Table S39: Energy values for Fuc (a,c) H6 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-998.3652395	-386.0599065	-612.2973799
CCSD(T)/CBS	-996.6372638	-385.3111990	-611.3187210

Fuc (a,c) H3&H5:

C	1.0037144	0.0303245	-2.4722348
C	0.0381818	-1.1674627	-2.4037154
C	-0.7539231	-1.1386953	-1.0941699
C	-1.4635644	0.1974551	-0.9294338
C	-0.4301955	1.3264963	-1.0573596
O	0.3047796	1.2408932	-2.2972372
C	-1.0634799	2.7042073	-1.0179579
O	2.0320341	-0.0942224	-1.4946633
O	0.8197285	-2.3665679	-2.4831147
O	-1.6437924	-2.2624580	-1.0291926
O	-2.4983871	0.2357848	-1.9278317
H	2.1049380	-1.0469266	-1.2955678
H	1.4482498	0.1076298	-3.4782683
H	-0.6588482	-1.0898319	-3.2553943
H	-0.0509621	-1.2587495	-0.2603817
H	-1.9016696	0.2492557	0.0837782
H	0.2704228	1.2120388	-0.2161885
H	-0.2872039	3.4785545	-1.0647318
H	-1.6272863	2.8274459	-0.0823935
H	-1.7356916	2.8478282	-1.8785396
H	0.2427445	-3.0787504	-2.1529417
H	-2.4000980	-2.0339722	-1.5994150
H	-2.9640305	1.0816063	-1.8432921
C	2.0663486	1.0432853	1.6317188
C	1.9456792	-1.4342559	1.4796274
C	-0.6112396	1.1205555	2.4867312
C	-0.7300545	-1.3596673	2.3361196
C	1.4596258	2.2503331	1.9138077
C	1.2232746	-2.6038573	1.6133912
C	0.1094559	2.2891302	2.3452032
C	-0.1266210	-2.5659972	2.0450163
C	1.3543082	-0.1769872	1.7742005
C	-0.0144079	-0.1391844	2.2107429
H	3.0946357	1.0075204	1.2713135
H	2.9834508	-1.4545637	1.1425227
H	-1.6515530	1.1445894	2.8167566
H	-1.7731061	-1.3250115	2.6550675
H	2.0142902	3.1809599	1.7937459
H	1.6867315	-3.5622025	1.3780356
H	-0.3595670	3.2498255	2.5599596
H	-0.6929096	-3.4930408	2.1287495

Table S40: Energy values for Fuc (a,c) H3&H5 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-998.3711789	-386.0598530	-612.2969880
CCSD(T)/CBS	-996.6418904	-385.3111840	-611.3181030

Fuc (a,c) H4&H6:

C	2.4042788	-0.6478842	-2.2953333
C	1.5270224	-1.9127999	-2.3333743
C	0.5211379	-1.8859476	-1.1822813
C	-0.3004439	-0.6052888	-1.2325963
C	0.6463682	0.6038690	-1.2558674
O	1.6143721	0.5122200	-2.3246487
C	-0.0991745	1.9109739	-1.4424939
O	3.2273967	-0.6487471	-1.1271886
O	2.3959020	-3.0476836	-2.2195354
O	-0.2855625	-3.0724047	-1.1928891
O	-1.1378369	-0.7069972	-2.4015487
H	3.4798311	-1.5812690	-0.9888239
H	3.0308271	-0.5913456	-3.2014970
H	0.9842462	-1.9242494	-3.2937008
H	1.0739674	-1.8958980	-0.2329540
H	-0.9227518	-0.5393898	-0.3271413
H	1.1776161	0.6063339	-0.2903491
H	0.6019576	2.7547484	-1.4232264
H	-0.8295619	2.0440891	-0.6318046
H	-0.6147615	1.9175162	-2.4150600
H	1.8227604	-3.7964095	-1.9749786
H	-0.9732843	-2.9137838	-1.8650891
H	-1.7559358	0.0390091	-2.3834578
C	-2.4529675	-0.4654053	1.7774620
C	-2.4736461	2.0194855	1.6386999
C	0.3325326	-0.4192626	2.1517009
C	0.3105808	2.0631099	2.0244142
C	-1.7502489	-1.6445774	1.9253583
C	-1.7924997	3.2204652	1.6679708
C	-0.3455344	-1.6206827	2.1133214
C	-0.3884785	3.2422450	1.8635936
C	-1.7845034	0.7884856	1.8067955
C	-0.3603693	0.8117745	2.0023212
H	-3.5336604	-0.4781992	1.6260425
H	-3.5545817	1.9974309	1.4880427
H	1.4156483	-0.3956719	2.2839650
H	1.3928296	2.0727428	2.1649253
H	-2.2693038	-2.6017420	1.8835817
H	-2.3334588	4.1581067	1.5368810
H	0.1980252	-2.5601217	2.2132091
H	0.1387810	4.1963860	1.8790353

Table S41: Energy values for Fuc (a,c) H4&H6 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-998.3700828	-386.0598741	-612.297318
CCSD(T)/CBS	-996.6409677	-385.3111848	-611.318691

Fuc (a,cc) H3:

C	1.4654591	1.1793480	-2.3588356
C	0.6555373	-0.1244621	-2.3417291
C	-0.2808122	-0.1547756	-1.1345463
C	-1.1673488	1.0886646	-1.1258155
C	-0.2754823	2.3317795	-1.1618081
O	0.6357045	2.3142779	-2.2932749
C	-1.0655211	3.6227039	-1.2653050
O	2.3875005	1.0998798	-1.2624603
O	1.4933092	-1.2860452	-2.3668484
O	-1.1344122	-1.3060756	-1.1862463
O	-2.0662216	1.0950301	-2.2349734
H	3.0317749	1.8159507	-1.3754418
H	2.0147131	1.2772355	-3.3086418
H	0.0493588	-0.1533692	-3.2568294
H	0.3218878	-0.1605756	-0.2115463
H	-1.7265138	1.1088836	-0.1700824
H	0.3215330	2.3097304	-0.2330566
H	-0.3857447	4.4848849	-1.2816540
H	-1.7399469	3.7149525	-0.4020431
H	-1.6676942	3.6178068	-2.1828622
H	2.1494333	-1.1516062	-1.6591073
H	-0.5651122	-2.0480756	-1.4565463
H	-2.4106313	0.1858745	-2.2941350
C	1.8175707	-0.9834660	1.8265803
C	0.5888001	-3.1441868	1.7600638
C	-0.5943505	0.3732007	2.3073153
C	-1.8243425	-1.7867647	2.2451325
C	1.8098905	0.3890433	1.9763441
C	-0.5978633	-3.8432190	1.8510355
C	0.5933121	1.0733411	2.2189091
C	-1.8149466	-3.1584708	2.0965602
C	0.6139969	-1.7328389	1.9135066
C	-0.6204455	-1.0388319	2.1608323
H	2.7519823	-1.5158124	1.6385903
H	1.5291123	-3.6661423	1.5756347
H	-1.5341486	0.8964818	2.4921614
H	-2.7587210	-1.2531797	2.4278084
H	2.7395124	0.9518641	1.8983165
H	-0.6038256	-4.9278495	1.7362986
H	0.5986108	2.1576701	2.3352144
H	-2.7463069	-3.7212540	2.1624838

Table S42: Energy values for Fuc (a,cc) H3 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-998.3688448	-386.0599001	-612.3001872
CCSD(T)/CBS	-996.6419701	-385.3112161	-611.3221468

Fuc (a,cc) H4:

C	2.8569668	0.0740945	-2.2440063
C	2.0367168	-1.2224597	-2.2891552
C	1.0517947	-1.2577241	-1.1214861
C	0.1650073	-0.0134659	-1.1612024
C	1.0582390	1.2277115	-1.1395512
O	2.0383268	1.2167159	-2.2140459
C	0.2713638	2.5167341	-1.2716925
O	3.7101754	-0.0344771	-1.0924818
O	2.8651109	-2.3916451	-2.3048832
O	0.2104803	-2.4159725	-1.1969086
O	-0.6583927	-0.0060659	-2.3311024
H	4.3614550	0.6823754	-1.1473266
H	3.4656701	0.1761137	-3.1562927
H	1.4663457	-1.2272699	-3.2272451
H	1.6125787	-1.2509842	-0.1701007
H	-0.4546927	0.0126341	-0.2484024
H	1.5953976	1.2036560	-0.1767111
H	0.9468911	3.3820230	-1.2366010
H	-0.4466702	2.5851485	-0.4422717
H	-0.2810058	2.5221268	-2.2197583
H	3.5210290	-2.2614673	-1.5961552
H	0.7835705	-3.1445542	-1.4958135
H	-1.0391927	-0.9001659	-2.3847024
C	-0.4078953	-1.3421311	2.0739984
C	-2.8673504	-1.3886586	1.7157924
C	-0.4760060	1.4668255	2.1767016
C	-2.9372903	1.4208334	1.8233990
C	0.7542565	-0.6234504	2.2678852
C	-4.0629781	-0.7147536	1.5690013
C	0.7205451	0.7926977	2.3179774
C	-4.0986910	0.7016957	1.6239494
C	-1.6556447	-0.6795659	1.9281779
C	-1.6911572	0.7575713	1.9811589
H	-0.3842396	-2.4301644	2.0082988
H	-2.8322334	-2.4779086	1.6667502
H	-0.5064561	2.5574927	2.2109230
H	-2.9580626	2.5117432	1.8623644
H	1.7069911	-1.1424226	2.3743250
H	-4.9867327	-1.2707827	1.4066743
H	1.6465741	1.3489832	2.4659262
H	-5.0493877	1.2222605	1.5043293

Table S43: Energy values for Fuc (a,cc) H4 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-998.3691804	-386.0598758	-612.3002342
CCSD(T)/CBS	-996.6412665	-385.3111782	-611.3220869

Fuc (a,cc) H5:

C	1.0129069	-1.0231635	-2.2754320
C	0.2029178	-2.3244665	-2.2070813
C	-0.7290320	-2.2982866	-0.9952152
C	-1.6225120	-1.0577668	-1.0497545
C	-0.7301585	0.1791610	-1.1370024
O	0.1816561	0.1088199	-2.2712079
C	-1.4972585	1.4779610	-1.2866024
O	1.9180700	-1.0570791	-1.1606154
O	1.0350789	-3.4913029	-2.1900668
O	-1.5726665	-3.4576600	-0.9744817
O	-2.5137840	-1.1090392	-2.1641988
H	2.4464899	-0.2430518	-1.1950593
H	1.5769051	-0.9664136	-3.2204240
H	-0.4079780	-2.3872651	-3.1172795
H	-0.1199224	-2.2420360	-0.0752544
H	-2.1865101	-0.9878641	-0.1000555
H	-0.1234585	0.1947610	-0.2184024
H	-0.7995585	2.3246610	-1.3337024
H	-2.1567862	1.6118134	-0.4178776
H	-2.1076541	1.4511527	-2.1984781
H	1.7217417	-3.3201694	-1.5207237
H	-1.0132428	-4.2031676	-1.2568522
H	-2.8726700	-2.0141543	-2.1695192
C	2.4004537	1.5960141	1.4840977
C	1.1395460	-0.4784162	2.0227839
C	0.0252230	3.0881010	1.6702908
C	-1.2349999	1.0154165	2.2125029
C	2.4134991	2.9583485	1.2592355
C	-0.0565417	-1.1043351	2.3102152
C	1.2154188	3.7103681	1.3524311
C	-1.2545408	-0.3513718	2.4049932
C	1.1921909	0.9251439	1.8115687
C	-0.0224943	1.6892610	1.9080864
H	3.3205593	1.0117760	1.4209966
H	2.0602578	-1.0556360	1.9302898
H	-0.9008819	3.6613036	1.7384940
H	-2.1551921	1.5986423	2.2804058
H	3.3474669	3.4627453	1.0110664
H	-0.0872022	-2.1842135	2.4586840
H	1.2375885	4.7847305	1.1705398
H	-2.1931772	-0.8596548	2.6282890

Table S44: Energy values for Fuc (a,cc) H5 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-998.3705013	-386.0598556	-612.2999476
CCSD(T)/CBS	-996.6426691	-385.3111606	-611.3218410

Fuc (a,cc) H6:

C	2.1564082	-1.8387493	-2.3675020
C	1.2375770	-3.0532790	-2.1784679
C	0.3921850	-2.8782827	-0.9169316
C	-0.3906731	-1.5670238	-1.0015652
C	0.5943516	-0.4164641	-1.2161370
O	1.4374689	-0.6315957	-2.3819692
C	-0.0947890	0.9195974	-1.4029948
O	3.1245524	-1.9039157	-1.3072471
O	1.9625227	-4.2882157	-2.1482415
O	-0.5447855	-3.9526759	-0.7751144
O	-1.3447847	-1.6063602	-2.0632695
H	3.8237271	-1.2644957	-1.5145099
H	2.6628319	-1.8884377	-3.3440870
H	0.5643662	-3.1034861	-3.0439497
H	1.0632036	-2.8315652	-0.0384833
H	-0.8931863	-1.3856091	-0.0337194
H	1.2387820	-0.3858065	-0.3215476
H	0.6507577	1.7127980	-1.5458455
H	-0.6877468	1.1508297	-0.5077852
H	-0.7589972	0.8798131	-2.2756963
H	2.7056277	-4.1464452	-1.5340854
H	-0.0716585	-4.7601703	-1.0439451
H	-1.7890577	-2.4688147	-1.9814050
C	-1.5163263	0.4477132	2.2515759
C	-2.7916524	2.5629691	1.9637797
C	0.8941048	1.8556764	1.9234536
C	-0.3802436	3.9715525	1.6351825
C	-0.3083240	-0.2171652	2.3092544
C	-2.8049144	3.9253129	1.7446597
C	0.9076255	0.4930593	2.1438529
C	-1.5889157	4.6359547	1.5789109
C	-1.5651645	1.8498042	2.0285817
C	-0.3318135	2.5701915	1.8610453
H	-2.4545597	-0.0957624	2.3755887
H	-3.7244358	2.0107138	2.0906042
H	1.8272766	2.4067173	1.7920516
H	0.5582857	4.5143680	1.5075890
H	-0.2848835	-1.2935970	2.4803700
H	-3.7532437	4.4615836	1.6969648
H	1.8554600	-0.0438621	2.1890368
H	-1.6132016	5.7121514	1.4061001

Table S45: Energy values for Fuc (a,cc) H6 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-998.3670353	-386.0599096	-612.3002531
CCSD(T)/CBS	-996.6397939	-385.3112119	-611.3221308

Fuc (a,cc) H3&H5:

C	0.8733692	0.1606793	-2.5261340
C	0.0736935	-1.1416274	-2.3813141
C	-0.6554497	-1.1680595	-1.0386604
C	-1.5288337	0.0754492	-0.8921288
C	-0.6495121	1.3147894	-1.0629572
O	0.0695304	1.2970400	-2.3285488
C	-1.4391621	2.6081313	-1.0298163
O	1.9568694	0.0730833	-1.5885131
O	0.8938775	-2.3064976	-2.5374461
O	-1.5024855	-2.3215065	-0.9454437
O	-2.5879880	0.0824798	-1.8509872
H	2.5351647	0.8354221	-1.7482041
H	1.2677917	0.2590146	-3.5501507
H	-0.6705285	-1.1696368	-3.1879346
H	0.0905582	-1.1712964	-0.2280287
H	-1.9342985	0.1002558	0.1374187
H	0.0872608	1.2944619	-0.2444617
H	-0.7639578	3.4668482	-1.1428639
H	-1.9586849	2.6909248	-0.0652305
H	-2.1813039	2.6165702	-1.8381014
H	1.6602522	-2.1683849	-1.9516437
H	-0.9830781	-3.0627144	-1.3041449
H	-2.9454677	-0.8231731	-1.8497350
C	-0.6256696	-1.3199652	2.3770395
C	-0.6965964	1.1638081	2.4657705
C	2.0527967	-1.2120569	1.5304694
C	1.9814345	1.2712986	1.6222967
C	0.0698139	-2.4833857	2.1200444
C	-0.0690058	2.3810126	2.2957591
C	1.4205150	-2.4289553	1.6933042
C	1.2823141	2.4356567	1.8700007
C	-0.0037556	-0.0526430	2.2227260
C	1.3657944	0.0028270	1.7905938
H	-1.6702326	-1.3560394	2.6903152
H	-1.7380441	1.1156624	2.7890172
H	3.0874055	-1.1632659	1.1884459
H	3.0201006	1.3056763	1.2896756
H	-0.4228735	-3.4490600	2.2298637
H	-0.6128157	3.3071850	2.4821692
H	1.9573773	-3.3553796	1.4871527
H	1.7652152	3.4036432	1.7342302

Table S46: Energy values for Fuc (a,cc) H3&H5 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-998.3727751	-386.0598771	-612.3001507
CCSD(T)/CBS	-996.6447323	-385.3112224	-611.3221422

Fuc (a,cc) H4&H6:

C	2.4654243	-0.4166658	-2.1534896
C	1.6725856	-1.7276868	-2.2394244
C	0.6417039	-1.7872503	-1.1138472
C	-0.2670172	-0.5601575	-1.1856675
C	0.5990100	0.6985149	-1.1191603
O	1.6263469	0.7098780	-2.1503396
C	-0.2051456	1.9724281	-1.2800664
O	3.2745523	-0.5184668	-0.9684244
O	2.5226264	-2.8814528	-2.2267377
O	-0.1717299	-2.9622912	-1.2272954
O	-1.0407496	-0.5622915	-2.3891952
H	3.9230377	0.2020616	-0.9994315
H	3.1096670	-0.2985404	-3.0390256
H	1.1410245	-1.7375774	-3.2000236
H	1.1628752	-1.7726720	-0.1399855
H	-0.9281121	-0.5559550	-0.3031695
H	1.0954686	0.6832308	-0.1346108
H	0.4552469	2.8474163	-1.2171669
H	-0.9519033	2.0356614	-0.4770701
H	-0.7184079	1.9689414	-2.2499835
H	3.1488704	-2.7409402	-1.4934121
H	0.4277553	-3.6767196	-1.5083363
H	-1.4073586	-1.4611582	-2.4583613
C	-2.6056262	-0.5821696	1.7226333
C	-2.6363072	1.9058212	1.7166601
C	0.1553297	-0.5456194	2.2476755
C	0.1233710	1.9404554	2.2472464
C	-1.9040653	-1.7647591	1.8471684
C	-1.9664041	3.1061497	1.8448807
C	-0.5121842	-1.7458482	2.1124254
C	-0.5745890	3.1234670	2.1130331
C	-1.9481766	0.6705846	1.8541445
C	-0.5364973	0.6888746	2.1251788
H	-3.6756178	-0.5909725	1.5086626
H	-3.7065609	1.8863668	1.5039568
H	1.2295241	-0.5255412	2.4405981
H	1.1964446	1.9471844	2.4473459
H	-2.4142690	-2.7199233	1.7259770
H	-2.5053434	4.0473742	1.7343353
H	0.0313759	-2.6871721	2.1909370
H	-0.0559400	4.0778592	2.2058296

Table S47: Energy values for Fuc (a,cc) H4&H6 complex.

	E_dimer BSSE (Hartree)	E_naphtalene (Hartree)	E_saccharide (Hartree)
DFT-D BP/def2-TZVPP	-998.3714780	-386.0598761	-612.3002135
CCSD(T)/CBS	-996.6430551	-385.311202	-611.3220677