
The interaction of carbohydrates and amino acids with aromatic systems studied by density functional and semi-empirical molecular orbital calculations with dispersion corrections.

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Supporting Information

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Figure S1 Starting geometries for amino acid-pyrene complexes optimisations.

Figure S2 DFT-D optimised geometries.

Figure S3 PM3-D* optimised geometries.

Table S1 Interaction distances (Å) for carbohydrate-benzene complexes^{a,b}

Complex	PM3-D	PM3-D*	DFT-D
<i>Beta Galactose</i>			
ccG-g-	3.767	4.178	4.161
ccG+g-	3.753	4.422	4.155
ccTg+	3.754	4.082	4.179
<i>Beta Glucose</i>			
ccG+g-	3.764	3.900	4.137
ccG-g+	3.769	4.208	4.148
ccTg+	3.770	3.899	4.146
<i>Alpha Glucose</i>			
g+ttG+g-	3.962	4.611	4.401
g+ttG-g+	4.270	4.660	4.422
g+ttTg+	3.950	4.605	4.409
<i>Statistics</i>			
MUE	0.38	0.17	

^a MUE (Mean unsigned error). ^b Distance from geometric centre of sugar ring to centre of benzene ring.

Table S2 Interaction distances (Å) for optimised S22 complexes^a

No.	Complex (symmetry)	PM3-D	PM3-D*	Database ^b
<i>Hydrogen bonded complexes (7)</i>				
1	(NH ₃) ₂ (C _{2h})	2.726	2.894	2.504
2	(H ₂ O) ₂ (C _s)	1.769	2.043	1.952
3	Formic acid dimer (C _{2h})	1.737	1.624	1.670
4	Formamide dimer (C _{2h})	1.763	2.046	1.841
5	Uracil dimer (C _{2h})	1.744	1.720	1.775
6	2-pyridoxine-2-aminopyridine (C ₁)	1.722, 1.768	1.901, 1.996	1.859, 1.874
7	Adenine-thymine WC (C ₁)	1.708, 1.768	1.723, 2.118	1.819, 1.929
MUE		0.12	0.14	
<i>Complexes with predominant dispersion contribution (8)</i>				
8	(CH ₄) ₂ (D _{3d})	3.160	3.424	3.718
9	(C ₂ H ₄) ₂ (D _{2d})	3.469	3.579	3.718
10	Benzene·CH ₄ (C ₃)	3.450	3.620	3.716
11	Benzene dimer (C _{2h})	3.499	3.458	3.765
12	Pyrazine dimer (C _s)	3.437	3.403	3.479
13	Uracil dimer (C ₂)	3.406	3.436	3.166
14	Indole·benzene (C ₁)	3.415	3.404	3.444
15	Adenine-thymine stack (C ₁)	3.280	3.490	3.172
MUE		0.22	0.19	
<i>Mixed complexes (7)</i>				
16	Ethene·ethine (C _{2v})	2.366	2.563	2.752
17	Benzene·H ₂ O (C _s)	3.196	3.134	3.435
18	Benzene·NH ₃ (C _s)	3.069	3.499	3.592
19	Benzene·HCN (C _s)	3.343	3.495	3.387
20	Benzene dimer (C _{2v})	3.370	3.517	3.513
21	Indole·benzene T-shape (C ₁)	3.233	3.389	3.210
22	Phenol dimer (C ₁)	1.778	2.129	1.937, 4.921
MUE		0.24	0.15	
<i>Statistics</i>				
MUE		0.19	0.15	

^a MUE (Mean unsigned error). ^b S22 database.

Table S3 Interaction distances (Å) and angles (°) for peptide bond-aromatic ring interactions^a

Complex	PM3-D ^b		PM3-D ^{a,b}		MP2/cc-pVTZ ^c	
	NM ^d	Θ ^e	NM ^d	Θ ^e	NM ^d	Θ ^e
FMA_T	3.313	79	3.420	90	3.274	83
FMA_S	3.306	79	3.427	90	3.259	68
NMF_T	3.231	68	3.324	90	3.210	74
NMF_S	3.160	32	3.215	25	3.144	55
NMA_T	3.160	56	3.269	34	3.221	89
NMA_S	3.213	35	3.263	32	3.188	52
<i>Statistics</i>						
MUE	0.035	15.9	0.104	24.8		

^a Formamide (FMA), N-methylformamide (NMF) and N-methylacetamide (NMA); T-shaped (T) and stacked (S). MUE (Mean unsigned error).
^b Optimised semi-empirical values. ^c Bendová *et al.*³² ^d NM is the distance between nitrogen and M, centre of the benzene ring. ^e Θ is the angle between the plane of the benzene ring and the NCO plane of the peptide bond moiety.

Table S4 Cartesian co-ordinates (Å) of the DFT-D optimised amino acid-pyrene complexes.

ALA_T (1):

6	0.030501	0.878969	0.309513
6	0.011241	0.468379	1.644597
6	1.208768	0.167853	2.323451
6	2.453546	0.288747	1.622228
6	2.462881	0.706486	0.250517
6	1.238547	0.997292	-0.382539
6	1.232495	-0.244333	3.700423
6	3.682217	0.013760	2.294298
6	3.673941	-0.387565	3.671327
6	2.409060	-0.509542	4.343848
6	4.901101	-0.642059	4.314953
1	4.899670	-0.944413	5.360496
6	6.110176	-0.508066	3.627921
6	6.128501	-0.119043	2.286292
6	4.928904	0.147432	1.596813
6	4.904616	0.559151	0.219246
6	3.727608	0.828323	-0.422320
1	3.731814	1.144855	-1.463942
1	5.851501	0.660278	-0.308224
1	0.286079	-0.335325	4.230419
1	-0.903900	1.112215	-0.195330
1	-0.935506	0.383189	2.174494
1	1.241430	1.322765	-1.420977
1	2.404976	-0.814626	5.388785
1	7.046865	-0.706994	4.143242
1	7.076644	-0.016120	1.761921
1	3.780470	3.690993	0.898610
7	3.685774	3.677389	1.914342
6	2.250634	3.738255	2.289664
1	1.644591	2.985567	1.755569
6	2.087933	3.504724	3.793463
6	1.666837	5.088210	1.858510
1	2.649265	4.253005	4.363251
1	1.034144	3.561381	4.082533
1	2.462291	2.507157	4.048408
8	1.928626	5.341563	0.527312
8	1.015601	5.850238	2.544980
1	4.055902	2.777121	2.220314
1	1.523894	6.210547	0.333293

ALA_S (2):

6	-0.082185	0.017772	-0.220081
6	-0.171742	0.023260	1.174156
6	0.987987	0.101572	1.969542
6	2.266941	0.183091	1.327180
6	2.347553	0.187170	-0.104403
6	1.159839	0.098168	-0.855430
6	0.936791	0.114791	3.405721
6	3.455887	0.277675	2.110728
6	3.373260	0.286216	3.542364
6	2.075774	0.198344	4.156793
6	4.560115	0.399407	4.293375
1	4.502038	0.407774	5.380231
6	5.800604	0.503091	3.658773
6	5.890829	0.496840	2.264468
6	4.733453	0.386490	1.468619
6	4.781641	0.391124	0.031526
6	3.642481	0.295667	-0.719135
1	3.701131	0.305777	-1.806067
1	5.751798	0.477713	-0.454691
1	-0.036598	0.067765	3.889586
1	-0.989012	-0.050106	-0.817067
1	-1.144553	-0.026710	1.658619
1	1.217147	0.100358	-1.942299
1	2.014830	0.212428	5.243543
1	6.705159	0.589799	4.256319
1	6.862435	0.579975	1.780908
1	3.355872	2.928223	0.710971
7	3.381361	3.742138	1.324722
6	2.294969	3.673950	2.322029
1	2.374872	2.793351	2.981674
6	2.330271	4.923083	3.223661
6	0.910259	3.507575	1.688147
1	2.231973	5.833883	2.622204
1	1.524862	4.885478	3.963092
1	3.290370	4.960059	3.753203
8	0.952227	3.284244	0.337390
8	-0.133198	3.519432	2.317145
1	4.273707	3.700434	1.818798
1	0.033182	3.084763	0.067967

GLY_T (3):

6	0.043032	0.203369	0.006044
6	0.053540	0.239082	1.402943
6	1.261572	0.116258	2.117961
6	2.486148	-0.045628	1.389447
6	2.465386	-0.078423	-0.043907
6	1.231097	0.046092	-0.711638
6	1.316741	0.161171	3.554061
6	3.726051	-0.149657	2.089702
6	3.748810	-0.099522	3.523377
6	2.503396	0.056274	4.224783
6	4.986464	-0.194362	4.189545
1	5.008619	-0.155799	5.277021
6	6.176539	-0.331870	3.470567
6	6.164872	-0.376940	2.074445
6	4.953518	-0.287164	1.360487
6	4.899444	-0.318566	-0.075981
6	3.711969	-0.219724	-0.746149
1	3.694073	-0.242013	-1.834405
1	5.832561	-0.419772	-0.627392
1	0.385780	0.284371	4.104714
1	-0.899022	0.303111	-0.527759
1	-0.877814	0.366869	1.951339
1	1.211118	0.025562	-1.799565
1	2.522541	0.095119	5.312555
1	7.122089	-0.400489	4.003239
1	7.098820	-0.478617	1.525010
7	3.485476	3.421558	1.767391
1	3.097214	3.757627	2.649805
6	2.434865	3.417990	0.741100
6	1.671382	4.730385	0.730520
1	2.880686	3.250862	-0.246137
1	1.663107	2.637303	0.870488
8	1.574133	5.506493	1.661671
8	1.028193	4.926884	-0.471192
1	3.804993	2.466691	1.923253
1	0.514945	5.753843	-0.370846

GLY_S (4):

6	0.090849	0.138419	0.295178
6	0.268798	0.303544	1.671549
6	1.539085	0.141738	2.259800
6	2.653065	-0.193821	1.421709
6	2.460135	-0.364223	0.010833
6	1.170020	-0.192190	-0.528435
6	1.764140	0.312315	3.668428
6	3.954184	-0.341515	1.988763
6	4.148339	-0.149204	3.396005
6	3.009894	0.173140	4.210796
6	5.449060	-0.265575	3.925631
1	5.602317	-0.118576	4.993335
6	6.533811	-0.571723	3.098535
6	6.351349	-0.769369	1.727913
6	5.072470	-0.656912	1.149327
6	4.846782	-0.827148	-0.260142
6	3.599901	-0.687614	-0.804045
1	3.451969	-0.813722	-1.875134
1	5.697593	-1.065227	-0.896206
1	0.917208	0.571536	4.300927
1	-0.896231	0.274325	-0.140225
1	-0.578634	0.564971	2.302407
1	1.021568	-0.309391	-1.599961
1	3.161993	0.322503	5.278100
1	7.529619	-0.659494	3.527215
1	7.203599	-1.003401	1.092889
7	2.300727	3.273619	0.066937
1	1.998458	4.066124	0.635626
6	3.732450	3.050800	0.259838
6	4.216804	2.974510	1.714110
1	4.030726	2.125457	-0.245905
1	4.300147	3.858763	-0.224743
8	3.540955	3.184510	2.702838
8	5.550184	2.646768	1.772947
1	1.778901	2.468347	0.413707
1	5.778114	2.550343	2.719725

HIS_T (5):

7	-0.470224	2.889100	-1.332938
6	0.654929	3.204929	-0.585801
6	0.430335	3.009575	0.763491
7	-0.883454	2.567133	0.833173
6	-1.374832	2.503698	-0.449506
6	1.279734	3.174371	1.989339
6	2.710509	3.652055	1.681446
6	2.811454	5.087947	1.139505
8	3.698855	5.461462	0.393321
7	3.524009	3.615062	2.926063
8	1.838710	5.926607	1.610246
6	1.768721	-0.313848	1.373294
6	0.758781	-0.708558	2.310873
6	-0.533597	-1.009780	1.834745
6	-0.830391	-0.920259	0.473031
6	0.143043	-0.520416	-0.445385
6	1.448681	-0.211812	-0.019740
6	3.087491	-0.011151	1.828285
6	3.406151	-0.103898	3.223888
6	2.369737	-0.495105	4.140528
6	1.105968	-0.782768	3.704101
6	4.094273	0.394832	0.891356
6	3.739672	0.494139	-0.499395
6	2.476559	0.206719	-0.933339
6	5.386241	0.694478	1.366222
6	5.690632	0.592876	2.726564
6	4.717004	0.198653	3.647661
1	4.963781	0.126575	4.705199
1	2.222493	0.303713	-1.986622
1	4.502089	0.815638	-1.206516
1	0.336945	-1.080140	4.415278
1	-1.833017	-1.156117	0.123682
1	-1.300767	-1.321357	2.541816
1	-0.107240	-0.425928	-1.499047
1	2.611406	-0.559831	5.199999
1	6.695134	0.825946	3.071941
1	6.151563	1.009146	0.659427
1	4.489898	3.851958	2.691435
1	3.130787	3.016695	0.889571
1	1.362495	2.207572	2.506109
1	0.812897	3.870255	2.698851
1	-1.359026	2.261327	1.672215
1	1.564985	3.548320	-1.059543
1	-2.382888	2.173694	-0.666065
1	3.553133	2.650467	3.260577
1	2.026655	6.806167	1.224813

HIS_S (6):

7	-1.101895	2.875215	5.357551
6	0.109534	3.536408	5.233100
6	0.436567	3.737969	3.904748
7	-0.621287	3.181433	3.199992
6	-1.508749	2.670886	4.113593
6	1.646555	4.348888	3.264511
6	2.548722	3.336546	2.467987
6	2.256089	3.275478	0.970925
8	0.903841	3.235162	0.692465
7	3.978769	3.631941	2.666409
8	3.088571	3.225714	0.087759
6	3.166482	-0.084114	2.075972
6	1.872592	-0.081020	1.473318
6	0.698350	-0.014158	2.293298
6	0.855489	0.044683	3.721176
6	2.095062	0.040758	4.297570
6	3.292338	-0.019376	3.503105
6	1.747385	-0.118182	0.044826
6	0.460063	-0.085066	-0.527263
6	-0.679648	-0.020199	0.280274
6	-0.566147	0.013654	1.672077
6	4.341268	-0.117818	1.255408
6	4.181862	-0.173476	-0.171876
6	2.943957	-0.174682	-0.749506
6	5.606426	-0.084515	1.874274
6	5.720614	-0.017366	3.265273
6	4.581019	0.015291	4.073323
1	4.681155	0.066055	5.156027
1	2.845849	-0.203897	-1.833199
1	5.075447	-0.201037	-0.792568
1	-0.033822	0.125836	4.341648
1	-1.664992	-0.002537	-0.180299
1	-1.458690	0.062099	2.292277
1	0.358990	-0.118388	-1.610777
1	2.191648	0.105126	5.379630
1	6.706512	0.009949	3.723509
1	6.501254	-0.108109	1.255237
1	4.496761	3.356683	1.830832
1	2.278664	2.338300	2.835130
1	2.279234	4.750050	4.062096
1	1.377675	5.199313	2.623612
1	-0.639192	3.072209	2.192654
1	0.682035	3.838680	6.101304
1	-2.424638	2.175896	3.815647
1	4.337298	3.069852	3.437580
1	0.827112	3.080545	-0.269926

HIS_SR (7):

6	0.218449	-0.047967	-0.215543
6	-0.058225	-0.417673	1.104015
6	0.977492	-0.518328	2.054803
6	2.320577	-0.215774	1.653568
6	2.592579	0.171220	0.300864
6	1.525351	0.239737	-0.615578
6	0.740561	-0.918915	3.415965
6	3.383695	-0.291022	2.601411
6	3.116810	-0.688986	3.952916
6	1.762919	-1.007573	4.320212
6	4.181592	-0.738241	4.874103
1	3.983729	-1.034265	5.902556
6	5.477656	-0.391793	4.485137
6	5.747396	-0.007202	3.169811
6	4.720015	0.044348	2.206418
6	4.959036	0.431938	0.843942
6	3.943419	0.490607	-0.067248
1	4.140692	0.810869	-1.087547
1	5.973029	0.696669	0.550399
1	-0.278115	-1.158453	3.716626
1	-0.592075	0.012573	-0.938514
1	-1.079290	-0.648155	1.403430
1	1.728825	0.533387	-1.643169
1	1.562418	-1.319774	5.344057
1	6.283167	-0.418596	5.214701
1	6.761258	0.260417	2.878787
1	2.182003	2.880271	6.321328
7	2.942984	2.341060	5.902698
6	3.209341	2.847072	4.537151
1	2.634419	1.371061	5.840167
1	3.996982	2.225328	4.104499
6	1.966215	2.833776	3.608873
6	3.744947	4.274812	4.720161
1	1.541738	1.822985	3.664966
1	1.220084	3.518542	4.040992
6	2.230114	3.194015	2.175555
8	3.091240	5.205689	5.151473
8	5.064122	4.389490	4.367432
7	1.215679	3.185513	1.224888
6	3.352295	3.592564	1.475598
1	5.312535	5.322879	4.530089
1	0.272205	2.850001	1.371669
6	1.766068	3.556860	0.021354
7	3.055944	3.817604	0.138428
1	4.354493	3.725124	1.858694
1	1.180292	3.614317	-0.887127

HIS_TR (8):

6	-0.533181	-0.525247	0.811567
6	-0.243028	-0.546347	2.178234
6	1.080217	-0.395491	2.637570
6	2.133526	-0.231236	1.678465
6	1.824716	-0.198509	0.278778
6	0.483934	-0.346740	-0.129894
6	1.416159	-0.386334	4.034967
6	3.483134	-0.086014	2.117006
6	3.786022	-0.079922	3.516810
6	2.707257	-0.228687	4.454162
6	5.124153	0.077069	3.924926
1	5.355666	0.099911	4.987688
6	6.146755	0.214882	2.984650
6	5.861414	0.213385	1.617365
6	4.536968	0.073892	1.158893
6	4.195231	0.113568	-0.236740
6	2.899147	-0.007802	-0.657295
1	2.660810	0.033835	-1.718522
1	4.995246	0.247352	-0.963421
1	0.613720	-0.500438	4.761883
1	-1.561836	-0.642228	0.478065
1	-1.045351	-0.673440	2.902678
1	0.246736	-0.319039	-1.191681
1	2.939960	-0.211497	5.517290
1	7.173914	0.335513	3.320657
1	6.665250	0.330813	0.892480
1	0.012293	5.121470	1.658428
6	-0.016685	4.229351	1.024257
7	-1.442501	3.948496	0.713504
6	0.580042	3.027038	1.789993
6	0.742974	4.530740	-0.277264
1	-1.506287	3.151446	0.076332
1	-1.870427	4.748111	0.244712
1	-0.070281	2.850797	2.652789
1	0.508195	2.141943	1.147311
6	1.983475	3.208387	2.277068
8	1.305695	3.714294	-0.990533
8	0.642226	5.857253	-0.622342
7	3.100345	3.131984	1.453936
6	2.498136	3.460658	3.534011
1	1.080394	5.953624	-1.492668
1	3.079590	2.897097	0.468003
6	4.208635	3.326508	2.238732
7	3.880891	3.533680	3.504835
1	1.942753	3.580256	4.456150
1	5.212836	3.288270	1.838229

LEU_T (9):

6	-0.520217	-0.939997	0.191705
6	-0.404422	-0.971951	1.583284
6	0.816967	-0.659246	2.211731
6	1.944393	-0.303628	1.400826
6	1.812793	-0.262512	-0.026172
6	0.571203	-0.588539	-0.606291
6	0.977126	-0.679502	3.640241
6	3.194920	0.010339	2.012900
6	3.327018	-0.032365	3.440263
6	2.175426	-0.381501	4.226778
6	4.574055	0.276333	4.019699
1	4.678288	0.248067	5.102667
6	5.668543	0.617893	3.220563
6	5.547247	0.668509	1.829314
6	4.321293	0.371583	1.201916
6	4.152789	0.422026	-0.225242
6	2.955935	0.117562	-0.811195
1	2.850123	0.159825	-1.893823
1	5.005626	0.709359	-0.837481
1	0.116823	-0.939185	4.254500
1	-1.471749	-1.183446	-0.274891
1	-1.263981	-1.237963	2.195444
1	0.466332	-0.557632	-1.689078
1	2.274809	-0.402666	5.310580
1	6.621542	0.856958	3.686149
1	6.401994	0.951622	1.218737
7	3.881163	3.796711	2.572300
1	3.892314	4.254503	3.486426
6	2.542031	3.960838	1.967090
1	2.571924	3.498126	0.976286
6	1.381424	3.330942	2.794227
6	2.297912	5.461342	1.798401
1	1.604220	2.260153	2.881804
1	1.434973	3.755881	3.806825
6	-0.057492	3.504808	2.251994
8	2.448881	6.295952	2.670889
8	1.838747	5.781243	0.542576
1	-0.281433	4.581184	2.217912
6	-0.235988	2.938983	0.829463
6	-1.060513	2.855791	3.227176
1	0.006839	1.871433	0.802440
1	-1.277540	3.054207	0.502517
1	0.399032	3.457633	0.103536
1	-0.964825	3.280224	4.234829
1	-2.092192	3.012459	2.887007
1	-0.885693	1.773923	3.294996
1	4.053887	2.805160	2.735120
1	1.678437	6.747427	0.549754

LEU_S (10):

6	-0.361100	-0.705785	0.970091
6	0.113310	-0.651875	2.282615
6	1.489357	-0.502949	2.543791
6	2.400774	-0.403697	1.441781
6	1.905527	-0.473628	0.098297
6	0.520632	-0.621927	-0.110595
6	2.014385	-0.412750	3.879925
6	3.793957	-0.211345	1.680720
6	4.285176	-0.105263	3.023173
6	3.348576	-0.216366	4.108288
6	5.661730	0.109241	3.232544
1	6.037123	0.197604	4.250210
6	6.540111	0.214178	2.151893
6	6.071410	0.107263	0.839585
6	4.703242	-0.104062	0.577115
6	4.179294	-0.204647	-0.758029
6	2.843016	-0.376529	-0.986453
1	2.464528	-0.437339	-2.005330
1	4.872935	-0.131495	-1.594184
1	1.320676	-0.491779	4.715213
1	-1.427921	-0.810271	0.787473
1	-0.582856	-0.708184	3.116733
1	0.138520	-0.662680	-1.128736
1	3.723902	-0.138489	5.127165
1	7.599221	0.381536	2.333316
1	6.766255	0.187708	0.005338
7	0.793631	2.847092	3.367667
1	1.116497	3.673911	3.875975
6	1.109717	3.010993	1.938204
1	0.843029	2.079229	1.432134
6	0.242749	4.163526	1.361400
6	2.605610	3.276652	1.685492
1	-0.792208	3.930582	1.647896
1	0.517711	5.089395	1.888831
6	0.298034	4.417471	-0.162935
8	3.361540	3.845404	2.452117
8	3.018314	2.798907	0.464288
1	1.331679	4.662111	-0.441517
6	-0.130266	3.184784	-0.983604
6	-0.576926	5.638302	-0.512518
1	-1.145039	2.868131	-0.703136
1	-0.135026	3.421879	-2.055272
1	0.546811	2.338577	-0.831204
1	-0.254089	6.529841	0.040206
1	-0.521371	5.863265	-1.585047
1	-1.629879	5.447342	-0.261459
1	1.329051	2.063332	3.744696
1	3.976646	2.987165	0.398931

LYS_T (11):

6	-0.923052	-0.147982	1.361197
6	-0.465856	-0.390506	2.658386

6	0.908095	-0.333410	2.960653
6	1.837893	-0.029018	1.912992
6	1.359911	0.218557	0.584204
6	-0.025424	0.155033	0.334861
6	1.416282	-0.557770	4.286321
6	3.235293	0.036007	2.193322
6	3.711933	-0.191706	3.526548
6	2.754408	-0.488604	4.557509
6	5.096252	-0.111050	3.779951
1	5.462342	-0.280696	4.790697
6	5.994974	0.182308	2.750579
6	5.538814	0.408130	1.449559
6	4.164550	0.343272	1.145547
6	3.654503	0.590272	-0.175430
6	2.315180	0.531832	-0.443001
1	1.949249	0.731184	-1.448411
1	4.360116	0.836754	-0.966487
1	0.708045	-0.782888	5.081759
1	-1.988902	-0.188324	1.150416
1	-1.175756	-0.617233	3.451353
1	-0.393481	0.348333	-0.670827
1	3.117697	-0.657291	5.569676
1	7.059201	0.240529	2.965979
1	6.247234	0.642070	0.657148
7	4.264924	3.481428	2.833750
1	4.926004	3.460230	2.055408
6	2.879943	3.548141	2.290128
1	2.707238	2.805840	1.496853
6	1.859047	3.306987	3.413432
6	2.778172	4.909703	1.584150
1	2.105384	2.339390	3.871157
1	1.982910	4.070223	4.191175
6	0.398269	3.263027	2.935270
8	2.288605	5.914966	2.378691
8	3.134306	5.103780	0.435176
1	0.123410	4.232245	2.496255
1	0.296889	2.512541	2.140753
6	-0.586624	2.930365	4.067980
1	-0.312571	1.964210	4.516012
1	-0.502805	3.685070	4.865032
6	-2.050928	2.859977	3.596741
1	-2.345263	3.829668	3.172027
1	-2.132001	2.124914	2.785838
7	-3.052539	2.501389	4.626925
1	-3.010746	3.179887	5.390569
1	-2.799886	1.602518	5.043609
1	4.377215	2.589319	3.317559
1	2.325904	6.728460	1.835910

LYS_S (12):

6	2.313063	-1.032152	-1.204132
6	1.325578	-1.480179	-0.323355
6	1.339935	-1.096333	1.032283
6	2.389092	-0.238152	1.499874
6	3.396743	0.219916	0.588106
6	3.336042	-0.190234	-0.759214
6	0.331152	-1.519910	1.964409
6	2.422310	0.170782	2.866335
6	1.404276	-0.272307	3.773411
6	0.361642	-1.125685	3.273048
6	1.456362	0.150522	5.116473
1	0.682597	-0.178498	5.807312
6	2.482883	0.985701	5.563353
6	3.477965	1.422608	4.686220
6	3.468351	1.032414	3.333388
6	4.464028	1.474673	2.395853
6	4.429680	1.088286	1.084930
1	5.191335	1.438454	0.390530
1	5.254116	2.133858	2.751165
1	-0.472026	-2.160092	1.604603
1	2.282868	-1.336983	-2.247465
1	0.530099	-2.130406	-0.682394
1	4.097499	0.156546	-1.455158
1	-0.417103	-1.450976	3.960266
1	2.503866	1.305121	6.602391
1	4.267913	2.079861	5.044272
7	0.229842	1.957499	-0.458607
1	-0.355503	1.170093	-0.742602
6	-0.039485	2.268712	0.972772
1	-0.023218	1.368664	1.605051
6	1.009784	3.257328	1.505651
6	-1.495808	2.758018	1.021718
1	1.996107	2.806491	1.331197
1	0.972345	4.183118	0.918908
6	0.873617	3.568816	3.005320
8	-1.630691	4.119416	0.922566
8	-2.456925	2.013171	1.100055
1	-0.099644	4.041387	3.197992
1	0.891665	2.631237	3.575698
6	1.988321	4.492140	3.523683
1	2.965582	4.026655	3.329911
1	1.972278	5.441280	2.966212
6	1.873610	4.793777	5.029435
1	0.911603	5.284747	5.231446
1	1.865741	3.847712	5.585611
7	2.938910	5.643770	5.608877
1	2.960948	6.540569	5.118472
1	3.848241	5.211063	5.432064
1	1.193567	1.630304	-0.540134
1	-2.593638	4.293666	0.910445

PHE_T (13):

6	-0.031819	-0.242880	0.226241
6	0.059792	-0.257776	1.620261
6	1.315034	-0.276212	2.259561
6	2.503205	-0.280959	1.455787
6	2.399319	-0.257665	0.025165
6	1.119782	-0.243754	-0.564405
6	1.453518	-0.289132	3.690668
6	3.788524	-0.283367	2.078702
6	3.891955	-0.304094	3.508807
6	2.683564	-0.306797	4.287162
6	5.170513	-0.305134	4.101017
1	5.255297	-0.319630	5.185091
6	6.321178	-0.254466	3.310875
6	6.229617	-0.221813	1.917818
6	4.975560	-0.245061	1.276666
6	4.837857	-0.231639	-0.153408
6	3.608895	-0.241746	-0.750782
1	3.527618	-0.228094	-1.836163
1	5.741075	-0.208013	-0.760375
1	0.550311	-0.285377	4.298510
1	-1.010137	-0.228479	-0.248443
1	-0.844721	-0.253642	2.225599
1	1.035300	-0.229561	-1.649423
1	2.767296	-0.316301	5.372344
1	7.297248	-0.230097	3.788979
1	7.134758	-0.186499	1.314561
7	3.252828	3.033744	1.561302
1	2.427119	3.453550	1.134326
6	3.525539	3.680842	2.859873
1	2.750634	3.451364	3.616181
6	4.889917	3.186336	3.391430
6	3.402412	5.195731	2.642760
1	4.922185	2.103490	3.221978
1	5.689759	3.617864	2.777415
6	5.235302	3.339943	4.870102
8	2.671474	5.710116	1.815386
8	4.168165	5.938338	3.501799
6	6.494487	2.864212	5.283946
6	4.373735	3.846004	5.855758
1	7.168609	2.444902	4.538470
6	6.883467	2.896313	6.624550
6	4.756305	3.875527	7.203831
1	3.399091	4.242006	5.587048
1	7.865154	2.525563	6.912194
6	6.011288	3.402796	7.596202
1	4.069023	4.275717	7.946157
1	6.307969	3.430035	8.641939
1	3.067749	2.040553	1.696174
1	3.975801	6.875118	3.292707

PHE_S (14):

6	1.491419	-0.229828	-0.906023
6	0.820036	-0.767457	0.194390
6	1.398255	-0.733654	1.478474
6	2.690911	-0.136278	1.642464
6	3.370876	0.417016	0.507377
6	2.751294	0.355505	-0.756001
6	0.734068	-1.264202	2.637756
6	3.287628	-0.067669	2.936711
6	2.600291	-0.605786	4.074491
6	1.309317	-1.206784	3.876570
6	3.202151	-0.504756	5.344910
1	2.683127	-0.910340	6.211517
6	4.442775	0.117162	5.500132
6	5.115738	0.651492	4.399484
6	4.560503	0.569649	3.108804
6	5.215626	1.120409	1.952937
6	4.650508	1.041257	0.709920
1	5.161405	1.467343	-0.151821
1	6.176610	1.612494	2.088894
1	-0.249164	-1.713654	2.510539
1	1.026317	-0.261614	-1.888470
1	-0.165190	-1.211809	0.067211
1	3.261819	0.778257	-1.619318
1	0.788041	-1.611885	4.742275
1	4.884690	0.197956	6.490285
1	6.068454	1.156717	4.536336
7	2.063896	3.162644	2.214201
1	1.514279	2.584716	1.579564
6	1.578190	2.988636	3.590111
1	1.973116	2.080817	4.077882
6	1.996981	4.200894	4.482845
6	0.064760	2.771858	3.563994
1	1.650644	5.114232	3.983779
1	1.487798	4.121945	5.448495
6	3.496561	4.257861	4.711081
8	-0.610792	2.603497	2.566603
8	-0.474926	2.732284	4.829946
6	4.364409	4.805603	3.748901
6	4.055311	3.733890	5.889054
1	3.947211	5.214172	2.831467
6	5.747710	4.818765	3.955730
6	5.436681	3.756020	6.104370
1	3.400807	3.303641	6.645198
1	6.401895	5.246424	3.198910
6	6.289820	4.295196	5.135485
1	5.846631	3.350346	7.026831
1	7.364589	4.315406	5.301328
1	3.032397	2.855971	2.148540

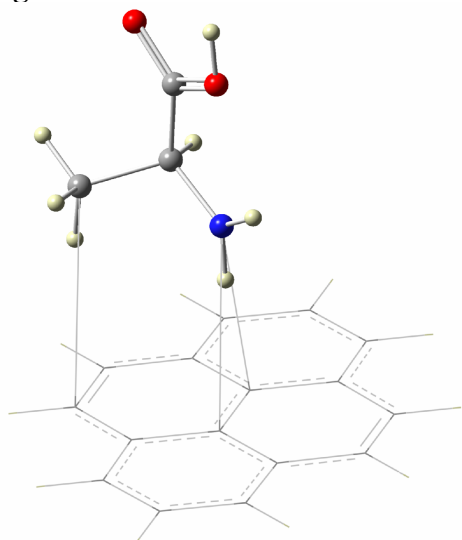
PHE_SR (15):

6	0.175004	0.033402	0.118181
6	0.169415	-0.040987	1.512554
6	1.373071	-0.172536	2.231329
6	2.610078	-0.225106	1.511306
6	2.606828	-0.137090	0.081671
6	1.376571	-0.012925	-0.591739
6	1.409098	-0.259411	3.664863
6	3.841941	-0.369488	2.215611
6	3.843812	-0.481028	3.644422
6	2.588167	-0.411479	4.340060
6	5.072688	-0.647763	4.314744
1	5.076426	-0.744883	5.399391
6	6.275087	-0.693115	3.604598
6	6.283642	-0.570456	2.212603
6	5.081149	-0.412642	1.495623
6	5.047026	-0.297324	0.063348
6	3.864925	-0.171112	-0.611293
1	3.860713	-0.091549	-1.697147
1	5.989537	-0.319617	-0.481071
1	0.468807	-0.207776	4.211231
1	-0.765025	0.132652	-0.419729
1	-0.772244	0.002463	2.056757
1	1.370194	0.053900	-1.678177
1	2.591833	-0.484546	5.426465
1	7.214017	-0.813052	4.139573
1	7.226863	-0.597978	1.670570
1	6.454860	3.228065	5.763924
7	6.688947	2.556345	5.029309
6	5.952910	2.911289	3.789654
1	6.366479	1.639986	5.342962
1	6.172246	2.128628	3.060108
6	4.423266	3.041374	3.986172
6	6.574901	4.228987	3.306262
1	4.109061	2.150731	4.545513
1	4.241565	3.902201	4.646125
6	3.539395	3.161820	2.750903
8	6.449833	5.301080	3.867148
8	7.326728	4.069579	2.168968
6	2.151795	3.297662	2.940942
6	4.023104	3.121919	1.433762
1	7.694502	4.952513	1.958368
1	1.754717	3.322373	3.954712
6	1.277005	3.389851	1.857858
6	3.148066	3.222866	0.345267
1	5.083286	3.005152	1.232904
6	1.773944	3.355067	0.550025
1	0.207622	3.482705	2.032676
1	3.547198	3.182042	-0.665344
1	1.095332	3.418204	-0.296556

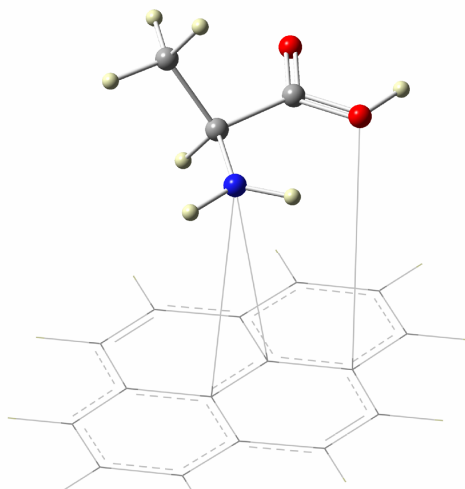
PHE_TR (16):

6	0.624414	0.421761	-0.554231
6	0.434292	0.038180	0.774959
6	1.530718	-0.109662	1.645954
6	2.850947	0.139175	1.148792
6	3.035771	0.538146	-0.214583
6	1.907323	0.670521	-1.046344
6	1.376107	-0.496653	3.020749
6	3.978354	-0.009550	2.009579
6	3.793838	-0.413911	3.372310
6	2.456251	-0.642219	3.845559
6	4.923958	-0.565856	4.199460
1	4.787224	-0.869516	5.235534
6	6.207834	-0.321468	3.707002
6	6.397226	0.084282	2.383089
6	5.299093	0.246532	1.514667
6	5.451323	0.657639	0.145786
6	4.370552	0.794415	-0.679990
1	4.508172	1.104615	-1.714592
1	6.454798	0.855943	-0.227695
1	0.370746	-0.672133	3.399933
1	-0.235269	0.531381	-1.211441
1	-0.570592	-0.146956	1.150138
1	2.043876	0.975303	-2.082407
1	2.316848	-0.935138	4.884762
1	7.067489	-0.443432	4.361997
1	7.402165	0.273840	2.009555
1	6.581780	4.788776	5.897488
7	6.124157	3.926409	5.596930
6	4.965680	4.257412	4.718530
1	6.811313	3.409530	5.045485
1	5.231030	4.965153	3.916155
6	4.407670	2.969143	4.078271
6	3.928860	4.951655	5.618321
1	5.256682	2.437005	3.630562
1	4.004629	2.328146	4.867783
6	3.366230	3.221882	3.005061
8	2.943364	4.452310	6.119187
8	4.284839	6.267029	5.836188
6	1.996747	3.072141	3.270311
6	3.759691	3.615183	1.714462
1	3.617725	6.632637	6.452025
1	1.678292	2.772675	4.265029
6	1.046627	3.302431	2.270281
6	2.812832	3.850830	0.715070
1	4.819324	3.714392	1.484159
6	1.450347	3.692568	0.990109
1	-0.009991	3.167232	2.489547
1	3.138349	4.137761	-0.282112
1	0.712202	3.856517	0.209159

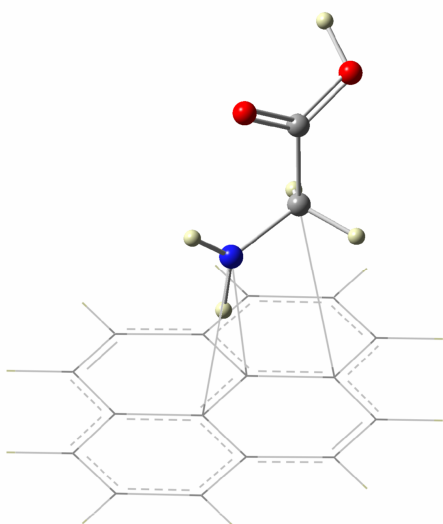
Figure S1 Initial structures for amino acid-pyrene complex optimisations.



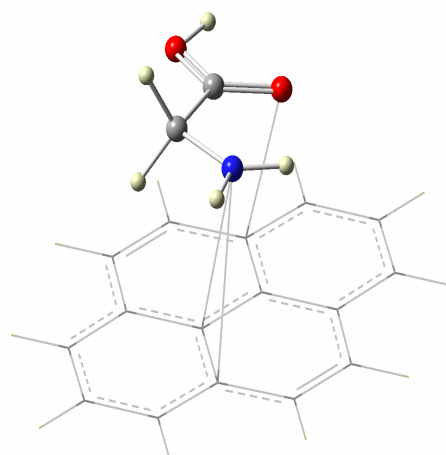
i) ALA_T (1)



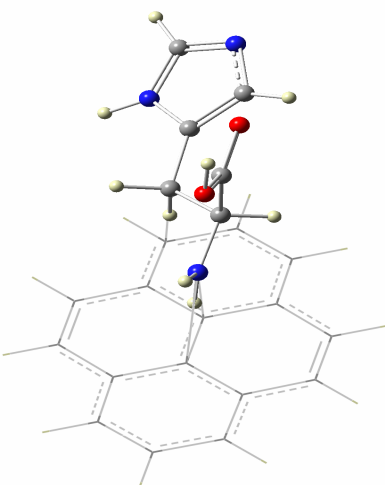
ii) ALA_S (2)



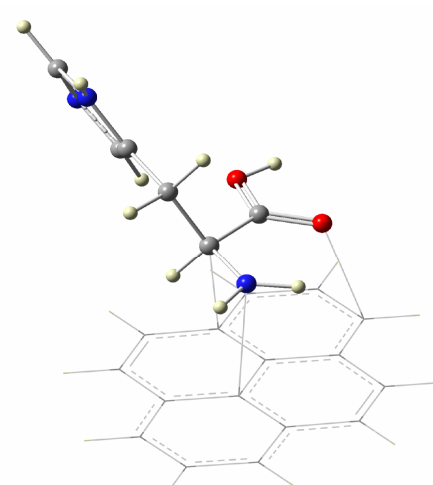
iii) GLY_T (3)



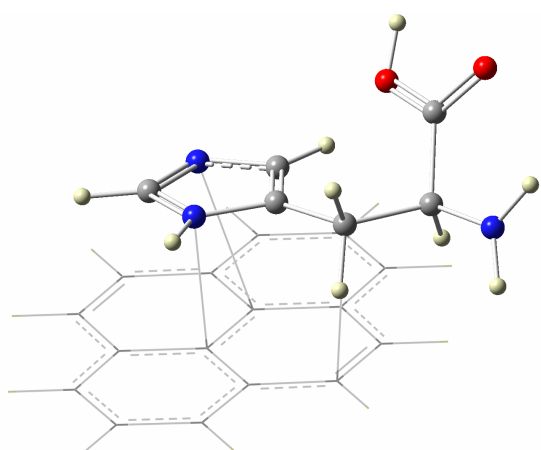
iv) GLY_S (4)



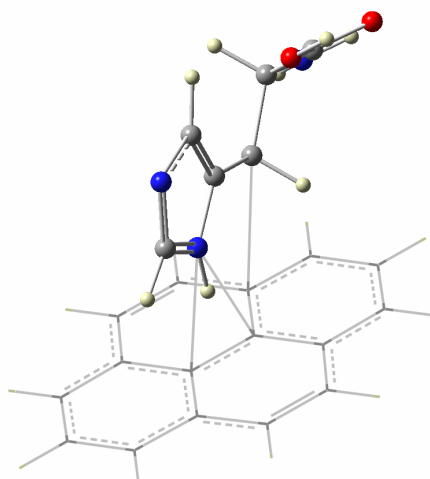
v) HIS_T (5)



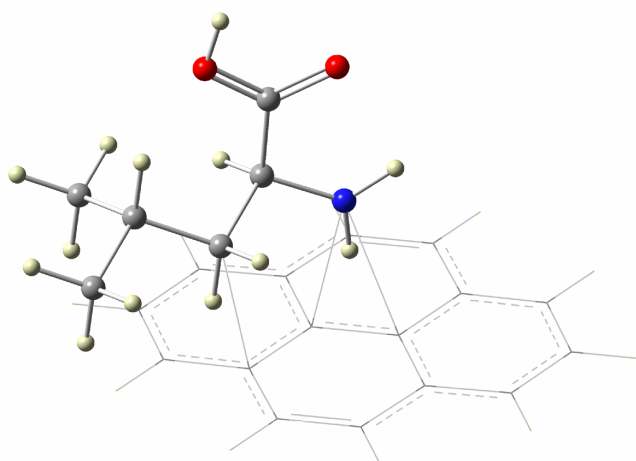
vi) HIS_S (6)



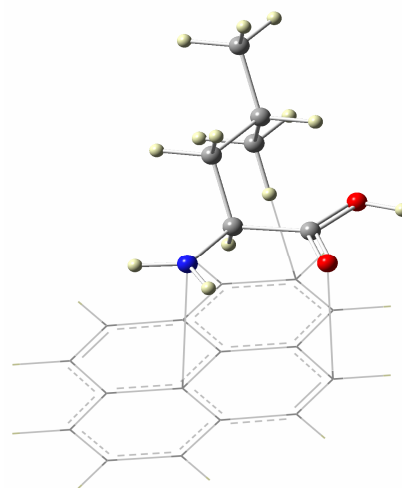
vii) HIS_SR (7)



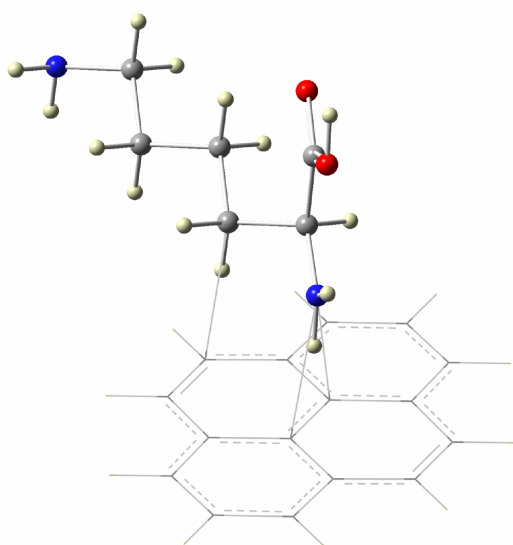
viii) HIS_TR (8)



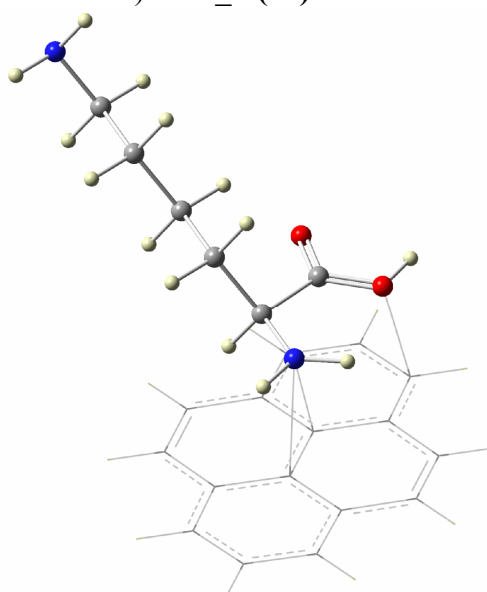
ix) LEU_T (9)



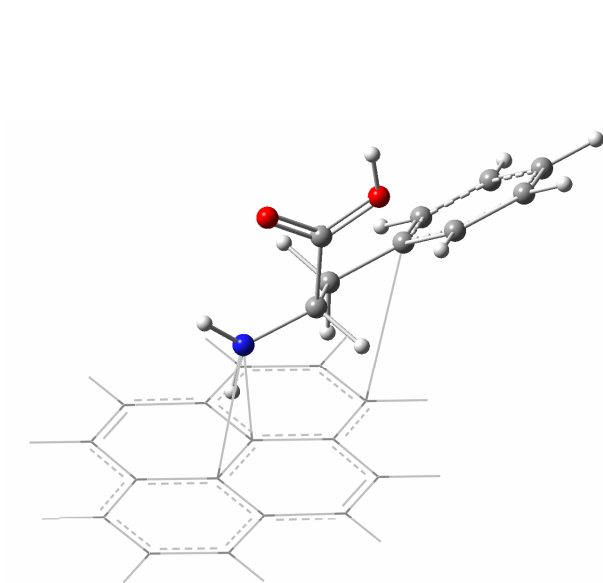
x) LEU_S (10)



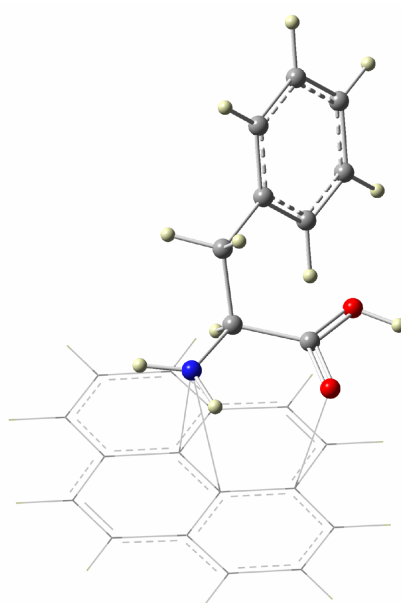
xi) LYS_T (11)



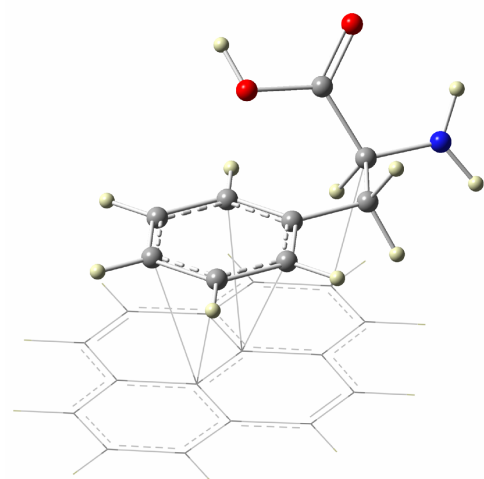
xii) LYS_S (12)



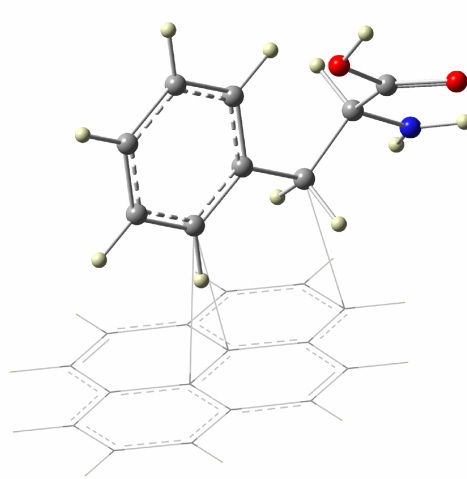
xiii) PHE_T (13)



xiv) PHE_S (14)

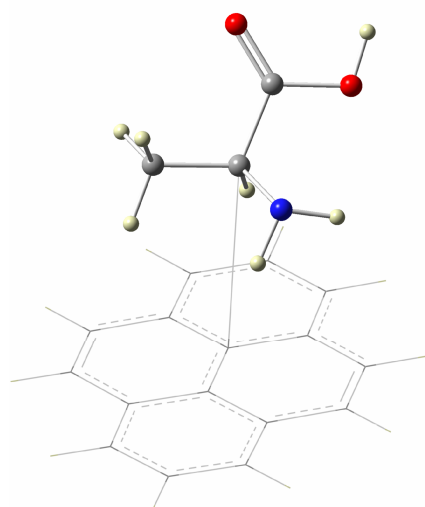


xv) PHE_SR (15)

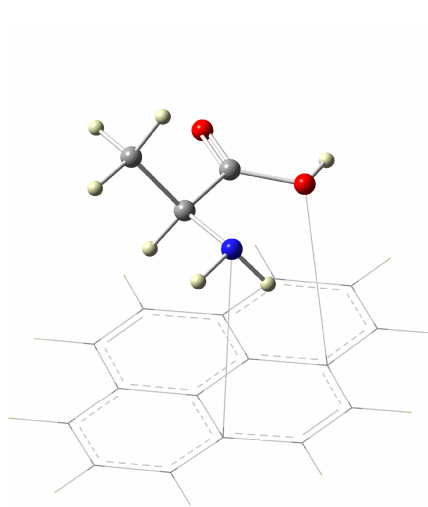


xvi) PHE_TR (16)

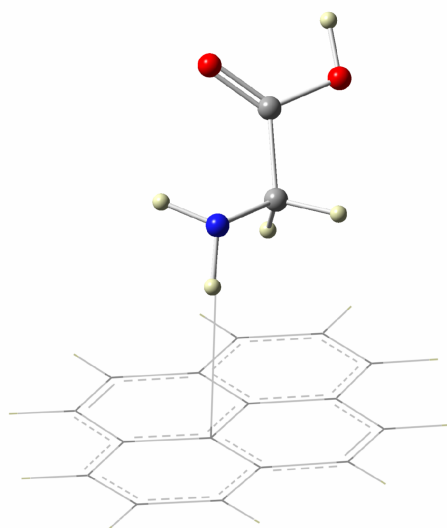
Figure S2 DFT-D optimised amino acid-pyrene complexes.



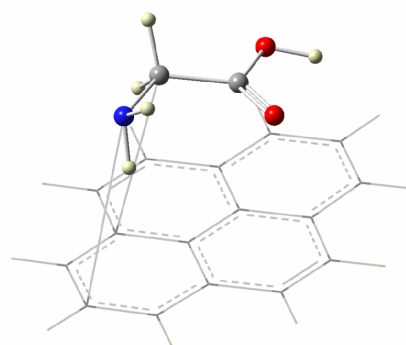
i) ALA_T (1)



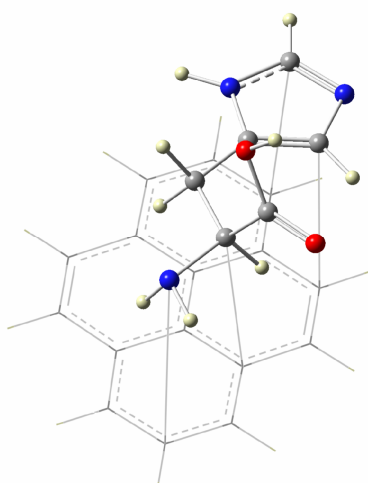
ii) ALA_S (2)



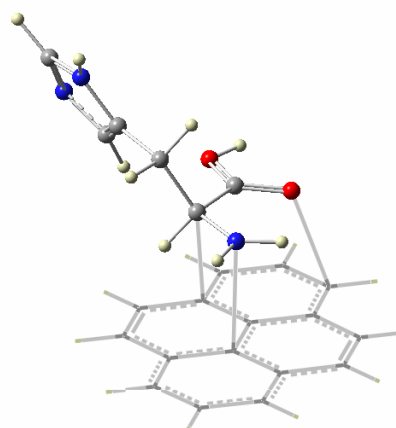
iii) GLY_T (3)



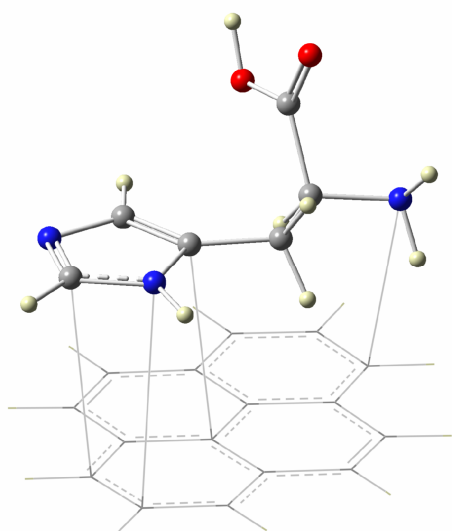
iv) GLY_S (4)



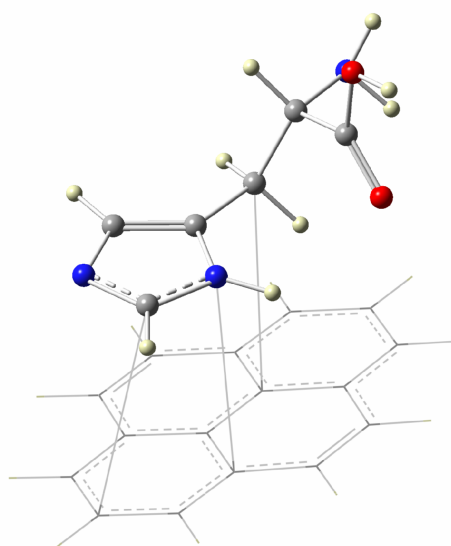
v) HIS_T (5)



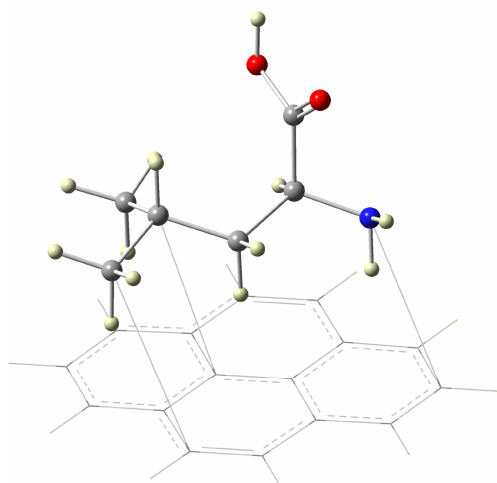
vi) HIS_S (6)



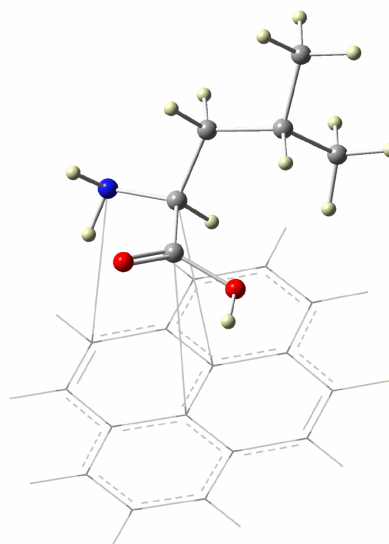
vii) HIS_SR (7)



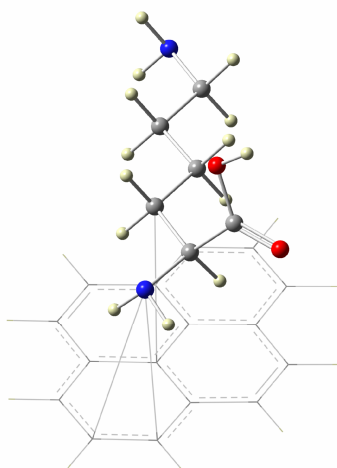
viii) HIS_TR (8)



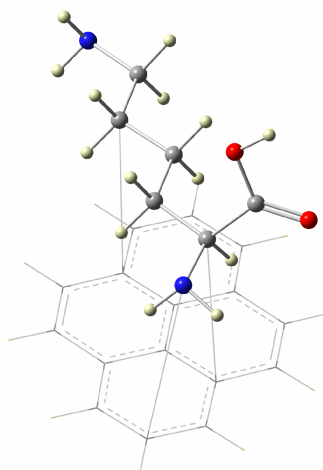
ix) LEU_T (9)



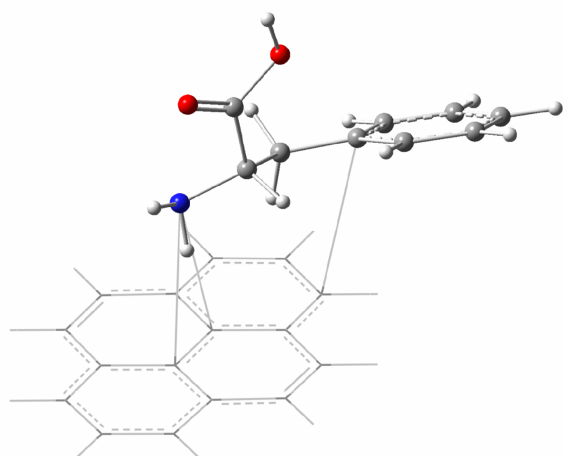
x) LEU_S (10)



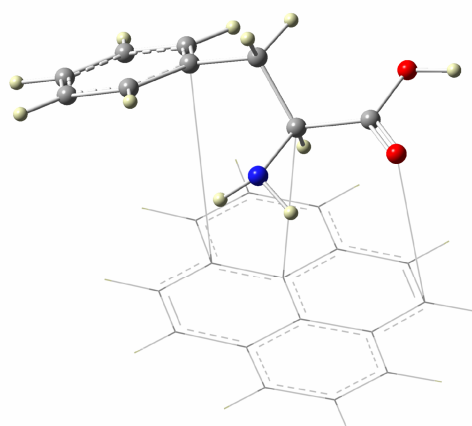
xi) LYS_T (11)



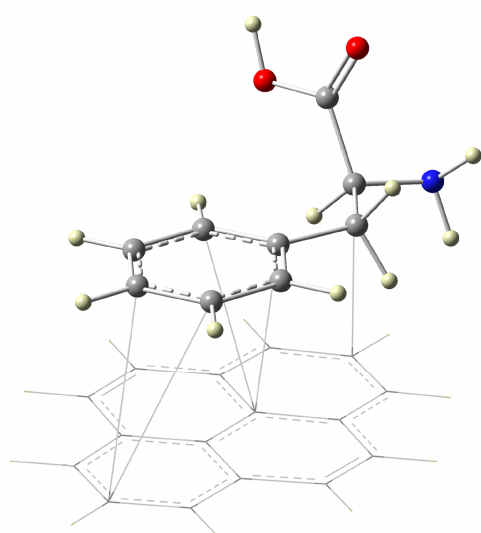
xii) LYS_S (12)



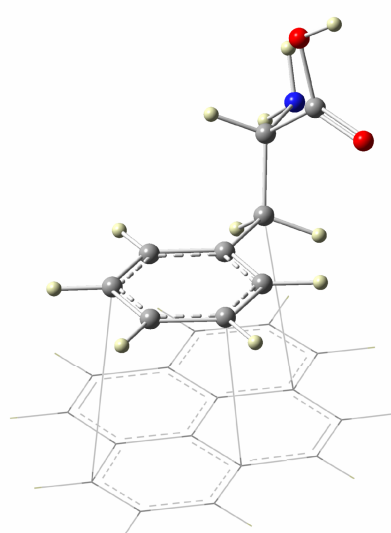
xiii) PHE_T (13)



xiv) PHE_S (14)

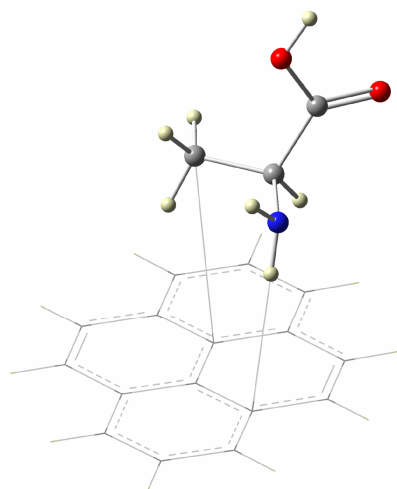


xv) PHE_SR (15)

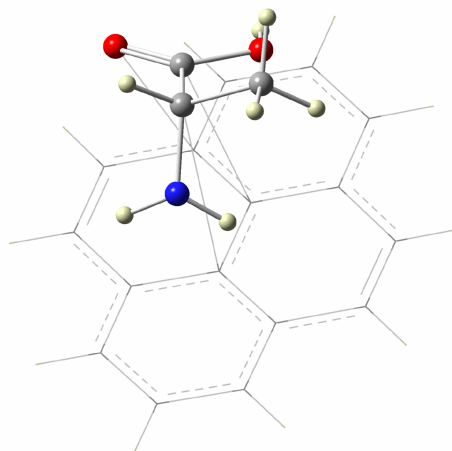


xvi) PHE_TR (16)

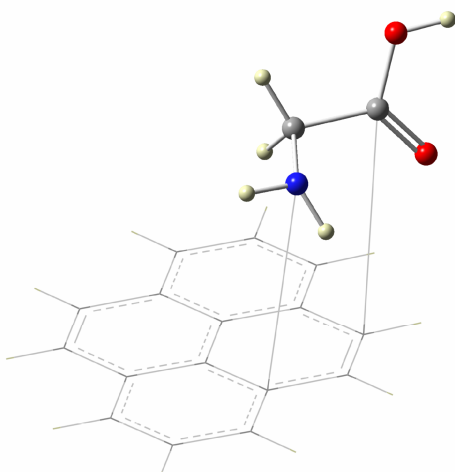
Figure S3 PM3-D* optimised amino-acid pyrene complexes.



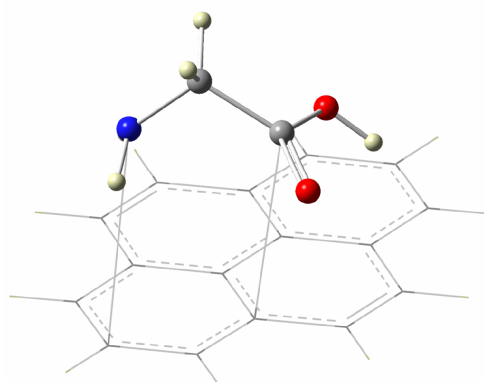
i) ALA_T (1)



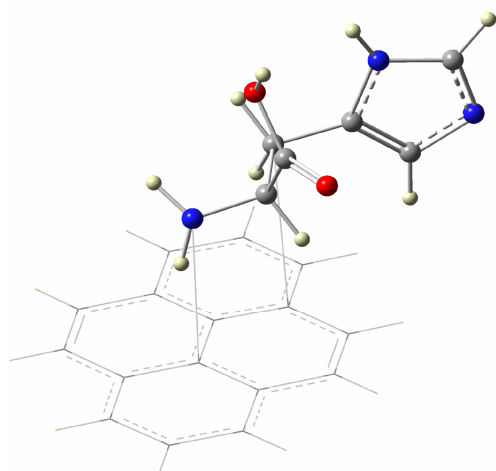
ii) ALA_S (2)



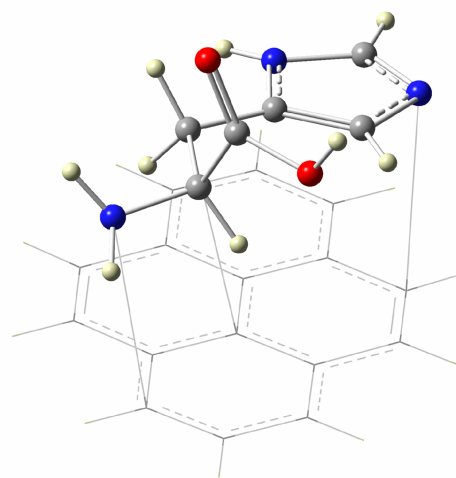
iii) GLY_T (3)



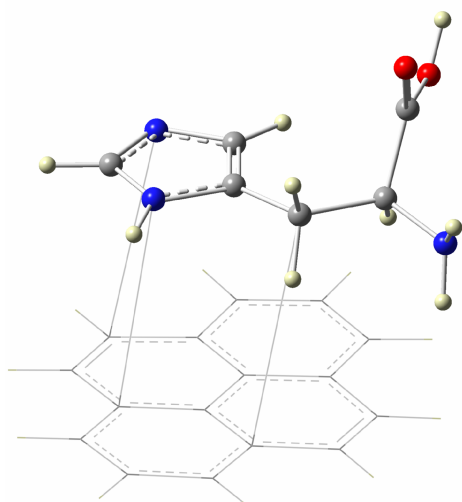
iv) GLY_S (4)



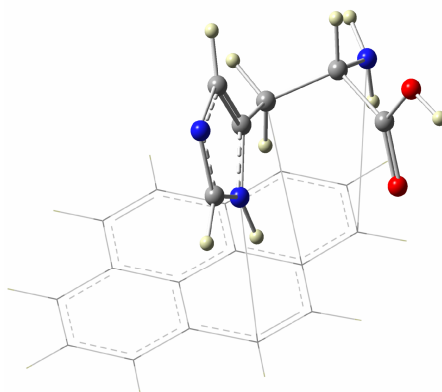
v) HIS_T (5)



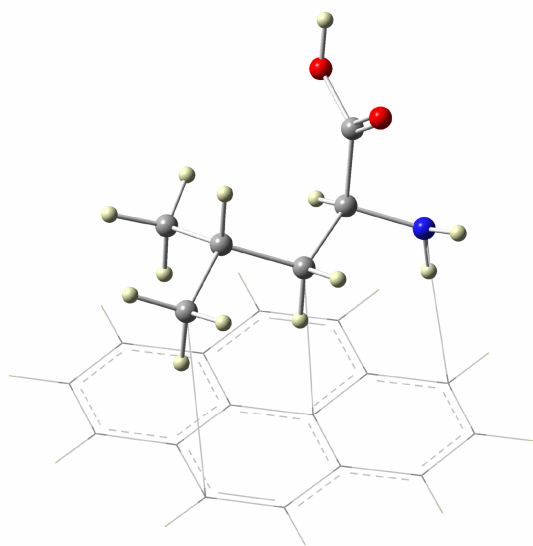
vi) HIS_S (6)



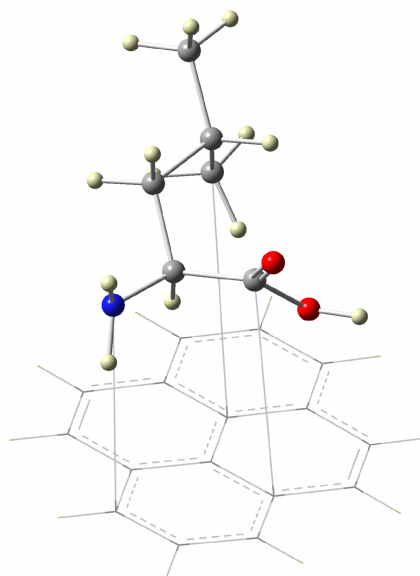
vii) HIS_SR (7)



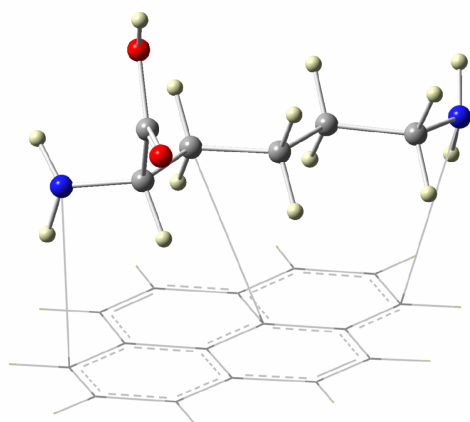
viii) HIS_TR (8)



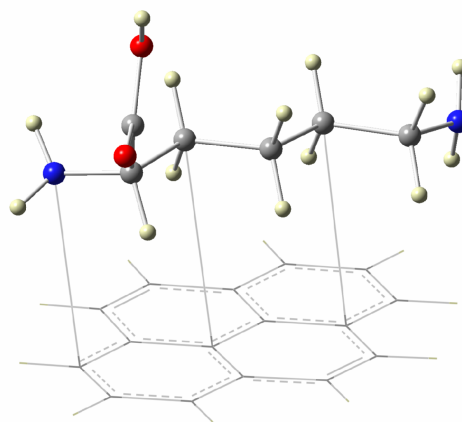
ix) LEU_T (9)



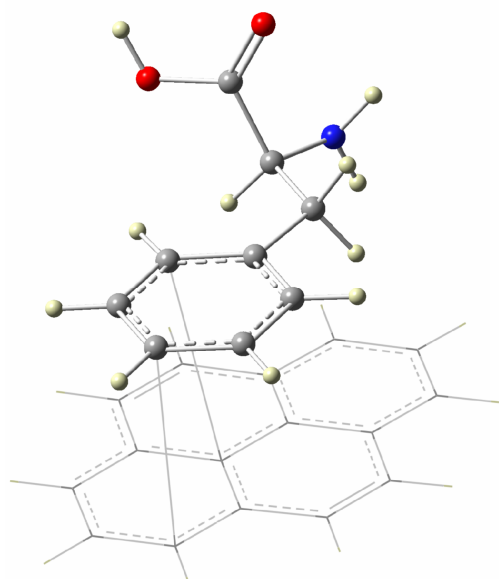
x) LEU_S (10)



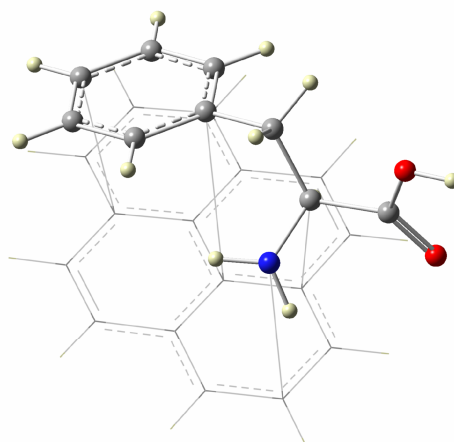
xi) LYS_T (11)



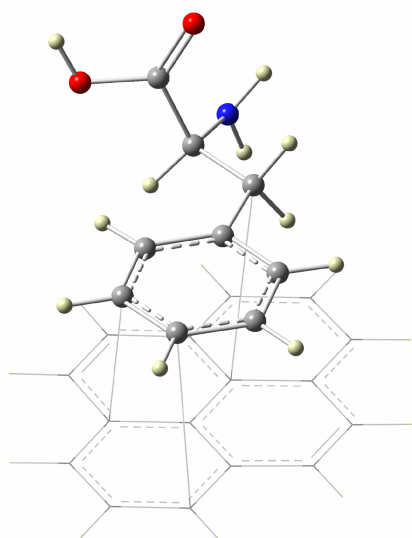
xii) LYS_S (12)



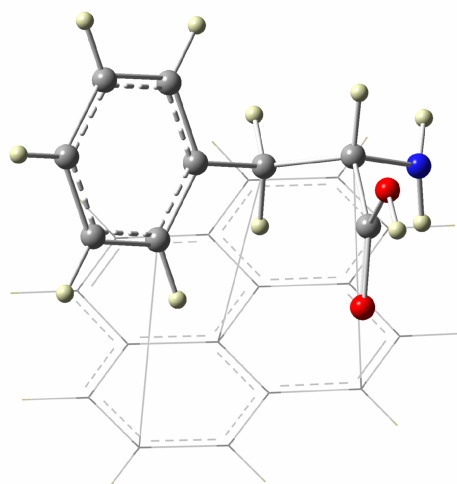
xiii) PHE_T (13)



xiv) PHE_S (14)



xv) PHE_SR (15)



xvi) PHE_S (16)