



**Figure S1.** Side and top representations of the relaxed AAA...RuC complexes (AAA; tryptophan (TRP), histidine (HIS), tyrosine (TYR), and phenylalanine (PHE)) at all possible adsorption sites on the RuC nanosheet. The adsorption energies ( $E_{ads}$ ) and the equilibrium adsorption distances ( $d$ ) between the AAA molecules and the RuC nanosheet are in kcal/mol and Å, respectively.

**Table S1.** The atomic coordinates of the relaxed AAA···RuC/···GN complexes.

<i>TRP···RuC</i>			
Ru	0.0243501193	0.2460819278	0.4194738572
C	1.6250885367	1.1580986246	-0.0694209976
Ru	-1.8066249602	3.3792341645	0.3826998873
C	-0.1959694083	4.3056317310	-0.0386756851
Ru	-3.6384450365	6.5554015450	0.4050313304
C	-2.0245205635	7.4919014765	0.0109384979
Ru	-5.4403208735	9.7064958951	0.4257219057
C	-3.8429461927	10.6275337578	-0.0512782122
Ru	3.2867935908	0.0279593543	-0.2866165566
C	4.8867054482	0.9522604390	-0.7652644057
Ru	1.4702018154	3.1620529381	-0.2882627403
C	3.0679836657	4.0987865720	-0.7329208310
Ru	-0.3302097505	6.3710768356	-0.1089877705
C	1.2700891147	7.2866670361	-0.7067912631
Ru	-2.1815662445	9.5003827386	-0.2576682744
C	-0.5813589956	10.4090988875	-0.7570922180
Ru	6.5529391684	-0.1827490400	-0.9859805897
C	8.1545087321	0.7410691479	-1.4531163099
Ru	4.7369519784	2.9547710411	-0.9900993197
C	6.3297083806	3.8947107837	-1.4481559761
Ru	2.9617594063	6.1478510366	-0.8556287732
C	4.5329618951	7.0499266379	-1.4404451100
Ru	1.0923750311	9.2853893252	-0.9994042500
C	2.6990584598	10.1978228896	-1.4627018130
Ru	9.8219653241	-0.3957097979	-1.6818403480
C	11.4179171282	0.5214396439	-2.1805995813
Ru	8.0036569017	2.7556652931	-1.6723756021
C	9.5888647444	3.6779620749	-2.1781465978
Ru	6.1870696088	5.9045651727	-1.6976017818
C	7.7731140034	6.8326479367	-2.1831845161
Ru	4.3624609663	9.0644163366	-1.7025603992
C	5.9609127170	9.9832357636	-2.1611502937
N	0.3236768861	4.7924510169	2.9518443428
C	0.4992145875	6.8663199576	2.0470469470
C	1.8253434822	6.2806293674	2.1372036290
C	1.6735115159	4.9718356088	2.6421601002
C	-0.3811678410	5.8928646789	2.5789211994
C	3.0965446978	6.7057149470	1.6881273462
C	2.7341359303	4.0620042068	2.7255889452
C	4.1732435414	5.8026343881	1.8070869968
C	3.9913238733	4.5053865486	2.3146492481
H	-1.4494574146	5.9631730436	2.7538206046
H	-0.1025894783	3.8860743798	3.1291376536
H	3.2756654803	7.7461630536	1.4210277712

H	2.5875530716	3.0483139564	3.0984136477
H	5.1695263145	6.1247424642	1.5053580836
H	4.8395235879	3.8225623645	2.3531119198
H	0.2775540539	7.9288958488	2.0272843021
<b><i>HIS...RuC</i></b>			
Ru	-0.2202035667	0.0303643653	0.3299492252
C	1.3781580448	0.9476873821	-0.1563239929
Ru	-2.0318099954	3.1864389717	0.3386012508
C	-0.4393358404	4.1057045147	-0.1578261502
Ru	-3.8588157677	6.3335670816	0.3289117135
C	-2.2668160033	7.2597155985	-0.1601340706
Ru	-5.6819108050	9.4815435830	0.3181111396
C	-4.0824152901	10.4061391100	-0.1399777793
Ru	3.0449522255	-0.1909204772	-0.3687250667
C	4.6439318292	0.7271084935	-0.8534870818
Ru	1.2256694189	2.9493449735	-0.3796842148
C	2.8409488997	3.8648211017	-0.8091417473
Ru	-0.6101448436	6.1259658493	-0.3853627510
C	0.9912065512	7.0659150205	-0.8163586154
Ru	-2.4194580647	9.2726979898	-0.3702417294
C	-0.8257413174	10.1988044147	-0.8566794727
Ru	6.3107727846	-0.3987576153	-1.0796194840
C	7.9147935718	0.5262218081	-1.5481967268
Ru	4.5000495044	2.7351107197	-1.0716623029
C	6.0956739423	3.6726351839	-1.5451943723
Ru	2.7101865115	5.9238172427	-0.9164765091
C	4.3007496872	6.8393674841	-1.5275633276
Ru	0.8407343968	9.0683634077	-1.0769281372
C	2.4535477081	9.9794508814	-1.5454251550
Ru	9.5798868054	-0.6108967736	-1.7713582273
C	11.1803255114	0.3124671191	-2.2418045719
Ru	7.7630715723	2.5367147281	-1.7723764862
C	9.3624823692	3.4616682745	-2.2426969913
Ru	5.9492016019	5.6876684139	-1.7780703513
C	7.5435755942	6.6087355523	-2.2599266001
Ru	4.1243536469	8.8456712812	-1.7790276131
C	5.7188391530	9.7667982082	-2.2600505675
N	3.1806282185	7.0079153103	3.1396127948
N	3.1293811058	6.1695377736	1.1154036203
C	4.0094055924	5.9019764761	3.1555444864
C	3.9718628144	5.3871628118	1.8866642305
C	2.6647179203	7.1456772442	1.8941891640
H	2.9830230167	7.6202698897	3.9235644443
H	4.4781540079	4.5245637489	1.4684243139
H	1.9841614208	7.9304463918	1.5821272535
H	4.5404610671	5.5867334647	4.0445164589

**TYR---RuC**

Ru	0.6191477680	0.2688764074	0.3374833404
C	2.2221910971	1.1926610447	-0.1436235147
Ru	-1.2000585433	3.4358427673	0.3464831790
C	0.4129640094	4.3645549065	-0.0699405362
Ru	-3.0088381871	6.5866030932	0.3648356014
C	-1.4102647847	7.5109685473	-0.1155580019
Ru	-4.8296799337	9.7285831477	0.3572282533
C	-3.2312897826	10.6551104288	-0.1104638835
Ru	3.8981783325	0.0580272173	-0.3411372079
C	5.4918136123	0.9930558487	-0.8179533976
Ru	2.0991869551	3.2381057272	-0.2427414711
C	3.6801612550	4.1468114862	-0.8300302523
Ru	0.2558660892	6.3771873662	-0.3252292980
C	1.8541538743	7.2941037656	-0.8154760405
Ru	-1.5621505550	9.5202234090	-0.3389668015
C	0.0354876464	10.4457899833	-0.8142680096
Ru	7.1595685030	-0.1465306742	-1.0428551647
C	8.7560119744	0.7764197057	-1.5169374007
Ru	5.3506186305	3.0054186434	-1.0560317825
C	6.9455883947	3.9268185621	-1.5262439070
Ru	3.5186232040	6.1596869837	-1.0681486456
C	5.1192259533	7.0791025704	-1.5339544450
Ru	1.7029217861	9.3083006290	-1.0419745502
C	3.3021738631	10.2306501045	-1.5180344837
Ru	10.4223465685	-0.3594511489	-1.7428745773
C	12.0173800879	0.5625333007	-2.2351972722
Ru	8.6080543057	2.7897478289	-1.7469673584
C	10.1993426662	3.7161205290	-2.2305062750
Ru	6.7869289770	5.9386327526	-1.7549421367
C	8.3859616132	6.8614170031	-2.2206004568
Ru	4.9665322268	9.0879392183	-1.7497573665
C	6.5647843440	10.0081125837	-2.2312877901
O	1.3241205341	1.3338764457	2.8534580742
C	5.0318503263	3.1562605022	2.3083035224
C	3.8779106895	3.9251735512	2.1971156300
C	4.9217640560	1.7870011193	2.5943343062
C	2.5987616613	3.3374993175	2.3262126288
C	3.6760340607	1.1881823915	2.7783604468
C	2.5169444189	1.9678615058	2.6742375050
H	3.9442292836	4.9931119933	1.9900649592
H	5.8206911343	1.1747843890	2.6688393950
H	1.7125869011	3.9702444223	2.3977026985
H	3.5810798652	0.1285811238	3.0126618788
H	0.5807352356	1.9386007296	2.6423013617
H	6.0113538818	3.6161617705	2.1832222466

**PHE...RuC**

Ru	-0.1150295614	-0.0650656235	0.2636293804
C	1.4930324220	0.8531367667	-0.1800929874
Ru	-1.9413844103	3.0988929962	0.2646669529
C	-0.3413099830	4.0323387280	-0.1775296183
Ru	-3.7643404915	6.2442605017	0.2684174482
C	-2.1727448720	7.1700460869	-0.2237091788
Ru	-5.5790845334	9.3872270206	0.2679243282
C	-3.9815760811	10.3022398592	-0.2250522892
Ru	3.1458974867	-0.2980152142	-0.4528732038
C	4.7413828888	0.6383626605	-0.9104014761
Ru	1.3560120113	2.8934845213	-0.3227052217
C	2.9227546842	3.7972872658	-0.9419054099
Ru	-0.5120383255	6.0392247908	-0.4501360445
C	1.0964755420	6.9517983730	-0.9102849156
Ru	-2.3146819932	9.1763081952	-0.4488551745
C	-0.7123589167	10.1010791827	-0.9176103332
Ru	6.4138115690	-0.4900200829	-1.1345569219
C	8.0132785950	0.4365485841	-1.6048723380
Ru	4.5933012112	2.6574628263	-1.1452790980
C	6.1885508006	3.5826934228	-1.6139607270
Ru	2.7698296462	5.8147905288	-1.1473140374
C	4.3687489389	6.7343901992	-1.6145644185
Ru	0.9548315706	8.9650825912	-1.1347305764
C	2.5563477277	9.8878169272	-1.6053921779
Ru	9.6843543972	-0.7002430306	-1.8281306858
C	11.2816323199	0.2218545654	-2.3083782277
Ru	7.8576212049	2.4469998040	-1.8384234123
C	9.4529424408	3.3703634452	-2.3244536719
Ru	6.0339881747	5.5946766509	-1.8523403938
C	7.6321890896	6.5172067418	-2.3135538086
Ru	4.2198163125	8.7475217089	-1.8386805170
C	5.8171262634	9.6670399577	-2.3249957414
C	4.3963911546	4.6079644046	2.1322098215
C	3.1939981075	5.3221036936	2.1734292037
C	4.3919745048	3.2091557574	2.1728881418
C	1.9810733263	4.6358024888	2.2512960601
C	3.1802067217	2.5209532704	2.2520231345
C	1.9617543493	3.2273093852	2.2700466437
H	3.2028721992	6.4120086723	2.1470958579
H	5.3313502169	2.6563798085	2.1470170447
H	1.0403653856	5.1860332777	2.2799596806
H	3.1688204290	1.4311729576	2.2809092998
H	5.3424896434	5.1445854615	2.0531438431
H	1.0242218324	2.6959018714	2.4418467652

AAA...GN Complexes

*TRP...GN*

C	1.2199482047	0.7071500660	0.3715137954
C	-0.0128543995	1.4188478821	0.3695699798
C	-0.0128032413	2.8414955667	0.3555829616
C	-1.2448815430	3.5525076331	0.3634347762
C	-1.2448342653	4.9754565634	0.3636906963
C	-2.4773729606	5.6870275510	0.3780359965
C	-2.4777954982	7.1105761691	0.3800177027
C	-3.7103539358	7.8226782871	0.3815219072
C	3.6840260389	0.7065636482	0.3663652449
C	2.4520980768	1.4184252859	0.3599160294
C	2.4515479182	2.8412863271	0.3478372125
C	1.2194552435	3.5528377232	0.3445175072
C	1.2191140360	4.9751146773	0.3448440973
C	-0.0127481668	5.6866245993	0.3555037655
C	-0.0130570986	7.1095554714	0.3676191283
C	-1.2452372161	7.8222858322	0.3737296166
C	6.1488878099	0.7060545784	0.3765819986
C	4.9163419303	1.4177520830	0.3673174280
C	4.9159727973	2.8407202956	0.3634355380
C	3.6835194281	3.5521376573	0.3516289565
C	3.6832842274	4.9751185927	0.3573209118
C	2.4511158350	5.6865489245	0.3532142240
C	2.4515922779	7.1096588544	0.3690816762
C	1.2192022867	7.8214392662	0.3727582886
C	8.6147015043	0.7066174140	0.3791069029
C	7.3818110596	1.4178105677	0.3790881632
C	7.3823445044	2.8411240809	0.3751752423
C	6.1488531214	3.5519498986	0.3741328701
C	6.1493168887	4.9755150756	0.3792071198
C	4.9160642392	5.6870287122	0.3753204641
C	4.9167954571	7.1106655450	0.3811588370
C	3.6839445330	7.8220601723	0.3787505574
N	4.0058114294	4.0853579295	3.7626040804
C	3.0287124990	2.0564182315	3.8121020198
C	1.9963516253	3.0531656098	3.8347381803
C	2.6454906260	4.3251702689	3.7997382662
C	4.2322195277	2.7199806011	3.7622445067
C	0.5902809010	3.0139474788	3.8571381848
C	1.9347304524	5.5295430942	3.7919145722
C	-0.1188273990	4.2099744162	3.8453152847
C	0.5450175509	5.4547188756	3.8151092366
H	5.2446571036	2.3314072225	3.7169804617
H	4.7229997039	4.7947582315	3.6733578256
H	0.0655036077	2.0569455917	3.8688280282

H	2.4470701342	6.4922150362	3.7518158211
H	-1.2098433556	4.1893797469	3.8481930409
H	-0.0402198155	6.3750962148	3.7949266796
H	2.8984353154	0.9788694492	3.8184762156
<b><i>HIS...GN</i></b>			
C	1.0322254676	0.8652713286	0.6252574906
C	-0.2005075678	1.5771921216	0.6258593487
C	-0.2008564946	3.0005875238	0.6258986387
C	-1.4336541517	3.7120493923	0.6229820994
C	-1.4333950267	5.1350532956	0.6245687050
C	-2.6658308813	5.8460684395	0.6210472364
C	-2.6652719109	7.2691363271	0.6241078590
C	-3.8976249585	7.9808736789	0.6247248879
C	3.4982027079	0.8657612039	0.6128440430
C	2.2652900218	1.5771585553	0.6179689836
C	2.2654719010	3.0008383130	0.6128380348
C	1.0321814104	3.7121288853	0.6228640494
C	1.0321602353	5.1354169059	0.6239842307
C	-0.2007486212	5.8466317439	0.6264498119
C	-0.2001807796	7.2699050460	0.6237862837
C	-1.4327432229	7.9813351297	0.6220514941
C	5.9623448052	0.8660667238	0.6101918575
C	4.7303654943	1.5777599522	0.6027714456
C	4.7306589557	3.0006794248	0.5968045825
C	3.4983375241	3.7120582472	0.6014480268
C	3.4980737417	5.1350405887	0.6089810065
C	2.2652655671	5.8466583980	0.6196075613
C	2.2649327686	7.2700234615	0.6223538788
C	1.0323188544	7.9820336234	0.6200066270
C	8.4267935896	0.8657421932	0.6231302037
C	7.1943175896	1.5777134335	0.6147446553
C	7.1939749770	3.0006973886	0.6130552451
C	5.9622707924	3.7122056178	0.6032017320
C	5.9624030980	5.1345052525	0.6110050308
C	4.7306543678	5.8460814196	0.6128300506
C	4.7300161185	7.2692047894	0.6219419161
C	3.4975630746	7.9813626418	0.6230082309
N	3.7146311078	2.7503590662	3.9338829948
N	5.5472496607	4.0084267676	4.0358708895
C	4.7791785725	1.8736062305	4.0048416128
C	5.8990849390	2.6719059352	4.0698356499
C	4.2264640661	4.0208966770	3.9522341200
H	2.7375450089	2.4940109774	3.8361542144
H	6.9372009367	2.3602570413	4.1314149594
H	3.5968921799	4.9038471146	3.8938119841
H	4.6398290806	0.7986901436	3.9921103280

**TYR...GN**

C	1.2432143961	0.8708329220	0.2526740646
C	0.0110501034	1.5816544328	0.2522637447
C	0.0116428304	3.0045796791	0.2464812128
C	-1.2211391721	3.7161976600	0.2691232672
C	-1.2216214734	5.1398835100	0.2747684350
C	-2.4546504957	5.8514735481	0.2827410376
C	-2.4547010570	7.2749743970	0.2778163785
C	-3.6871730604	7.9867268393	0.2710679147
C	3.7074459722	0.8709596117	0.2594264843
C	2.4754837801	1.5824948002	0.2422940266
C	2.4758581022	3.0050930496	0.2297102779
C	1.2437801432	3.7164469510	0.2318810884
C	1.2435492983	5.1394120684	0.2425422721
C	0.0113901592	5.8511716972	0.2641568634
C	0.0105376793	7.2746886231	0.2728978565
C	-1.2221152332	7.9867152824	0.2731579679
C	6.1727667204	0.8703942766	0.2759005751
C	4.9399764094	1.5822827201	0.2653689491
C	4.9396408392	3.0051915852	0.2588626530
C	3.7076849469	3.7165951249	0.2400551654
C	3.7078016084	5.1392846626	0.2484869703
C	2.4756575846	5.8508956231	0.2492747203
C	2.4757482606	7.2741640203	0.2671599399
C	1.2431172896	7.9861185457	0.2732330228
C	8.6388032183	0.8702983360	0.2682772345
C	7.4059411586	1.5813249689	0.2757514673
C	7.4054084370	3.0047234084	0.2780070730
C	6.1722722869	3.7163515573	0.2753930073
C	6.1725671003	5.1396872408	0.2789108026
C	4.9397849398	5.8511468502	0.2694529777
C	4.9404809604	7.2745936729	0.2729411392
C	3.7081704009	7.9862586052	0.2709344359
O	-0.0871625646	2.1172034152	3.6089143943
C	3.7344311807	3.7891692768	3.7305400562
C	2.6206691686	4.6292604293	3.6674946657
C	3.5479236108	2.4038828557	3.7604066694
C	1.3319923053	4.0938241385	3.6324288651
C	2.2658664034	1.8568469884	3.7265712678
C	1.1550465065	2.7053667399	3.6594950187
H	2.7517074086	5.7118356124	3.6316147063
H	4.4109755725	1.7371334049	3.7971518625
H	0.4621812202	4.7528714073	3.5653355602
H	2.1079669808	0.7780556756	3.7336774540
H	-0.7607705533	2.8108635446	3.4894407354
H	4.7395216266	4.2115582412	3.7418677187



**PHE...GN**

C	1.2331538110	0.7098371920	0.2821643256
C	0.0003989054	1.4211848909	0.2875696765
C	0.0006856775	2.8444486770	0.2828403261
C	-1.2323993239	3.5556831113	0.2866103207
C	-1.2323862941	4.9789634818	0.2864831357
C	-2.4652900128	5.6903265055	0.2848663818
C	-2.4648995817	7.1137618060	0.2860593073
C	-3.6974163807	7.8253891328	0.2862977514
C	3.6976027567	0.7101695739	0.2706616038
C	2.4654291876	1.4217095140	0.2666836091
C	2.4656368242	2.8443998301	0.2560714393
C	1.2334074499	3.5556102755	0.2683752718
C	1.2332632903	4.9785651841	0.2733504284
C	0.0005165331	5.6903237155	0.2846277319
C	0.0001256871	7.1137518010	0.2859064322
C	-1.2323819887	7.8258335491	0.2833580597
C	6.1620770085	0.7098447981	0.2821137684
C	4.9297925670	1.4217188920	0.2667103879
C	4.9296080531	2.8444097039	0.2562332209
C	3.6976138909	3.5557109708	0.2499336019
C	3.6976435250	4.9783208446	0.2579559356
C	2.4656341540	5.6899597285	0.2694860843
C	2.4652012458	7.1131535282	0.2834898849
C	1.2326842038	7.8253883222	0.2861579829
C	8.6276145827	0.7095055443	0.2918876893
C	7.3948386111	1.4211849303	0.2876246444
C	7.3945425451	2.8444539132	0.2830672432
C	6.1617987621	3.5556245834	0.2687187026
C	6.1619965020	4.9785793117	0.2737266944
C	4.9296361883	5.6899623645	0.2696978547
C	4.9300713578	7.1131671498	0.2835723987
C	3.6976469892	7.8250659002	0.2880988128
C	4.9453628788	4.0738196971	3.7140868144
C	3.7835532234	4.8502078496	3.7129834885
C	4.8533423311	2.6794282979	3.7157947041
C	2.5299691405	4.2326021672	3.7148969898
C	3.6000667228	2.0614966985	3.7175746233
C	2.4384891662	2.8383453573	3.7167409636
H	3.8548195334	5.9391109611	3.6959975175
H	5.7606584829	2.0731604348	3.7005430768
H	1.6228921826	4.8389619361	3.6996591475
H	3.5283969504	0.9726932447	3.7049333673
H	5.9241158473	4.5560199578	3.6980700268
H	1.4598488133	2.3555136719	3.7026365722