

Table 1 Naph-SAC4A@2ASP corresponding xyz bidet.

corresponding atom	X-axis coordinates	Y-axis coordinates	Y-axis coordinates
S	-1.79034	7.498	-0.47924
S	1.95151	4.40486	-3.60563
S	8.12979	-2.3843	-0.06474
S	5.18816	1.58887	3.82962
O	-6.16561	-4.18346	-0.6848
H	-5.74231	-4.74161	-1.42025
O	-4.86895	-5.71963	-2.2817
O	-3.78935	-6.62655	-0.0543
H	-4.17367	-6.33889	-0.94403
O	-5.30219	-5.36971	1.87754
H	-4.86395	-5.99453	1.2509
O	-2.62027	8.27852	-1.44891
O	-0.3238	7.66571	-0.70203
O	-2.19436	7.72861	0.94616
O	3.14396	4.25663	-4.49734
O	2.24107	3.99443	-2.18996
O	1.32063	5.75399	-3.69474
O	8.95422	-3.6241	0.06793
O	7.90333	-1.69755	1.24862
O	8.63116	-1.46643	-1.12891
O	6.48385	1.12818	3.24948
O	5.20841	1.67688	5.32382
O	4.68788	2.85037	3.19346
N	-5.80466	1.31483	-1.40489
N	-5.10863	1.86737	-0.51019
N	-0.83494	-2.57341	-4.32587
N	-1.02936	-1.32209	-4.20998
N	1.81127	-6.45335	0.25068
N	2.27665	-5.29464	0.15526
N	-1.69153	-1.27484	3.04189
N	-0.53739	-1.57751	3.45569
C	-6.08986	-2.84824	-0.89297
C	-6.17873	-2.01735	0.24895
C	-6.12232	-0.63744	0.08722
H	-6.15267	0.01319	0.95535
C	-5.98666	-0.07582	-1.19012
C	-5.94117	-0.90576	-2.317
H	-5.82618	-0.45631	-3.29966
C	-5.95596	-2.29471	-2.18563
C	-5.72516	-3.19122	-3.38964

Table 1 Naph-SAC4A@2ASP corresponding xyz bidet.

H	-6.41815	-4.0393	-3.36861
H	-5.93916	-2.6173	-4.2964
C	-4.29458	-3.71249	-3.46502
C	-3.28606	-2.90044	-3.95573
H	-3.5155	-1.88657	-4.26952
C	-1.95569	-3.36167	-4.03252
C	-1.68095	-4.69662	-3.6912
H	-0.65663	-5.05237	-3.77416
C	-2.65244	-5.5115	-3.12893
C	-3.97247	-5.00981	-2.94191
C	-2.27893	-6.87337	-2.56911
H	-1.56338	-7.35889	-3.23993
H	-3.16661	-7.51119	-2.51924
C	-1.63903	-6.74453	-1.19572
C	-0.24339	-6.68953	-1.09775
H	0.36102	-6.79947	-1.99355
C	0.37379	-6.47301	0.1298
C	-0.39435	-6.34281	1.28589
H	0.09582	-6.18314	2.24201
C	-1.78941	-6.40866	1.22653
C	-2.41028	-6.58768	-0.02557
C	-2.59678	-6.16521	2.4929
H	-1.95682	-6.36711	3.35681
H	-3.44414	-6.85317	2.55133
C	-3.07848	-4.72391	2.55477
C	-2.18762	-3.71295	2.88868
H	-1.17478	-3.96652	3.18265
C	-2.5625	-2.36145	2.79097
C	-3.85687	-2.04	2.35935
H	-4.12842	-1.00353	2.18267
C	-4.79682	-3.03482	2.08075
C	-4.39443	-4.37958	2.1664
C	-6.19849	-2.63128	1.63696
H	-6.85772	-3.50014	1.6656
H	-6.59333	-1.89322	2.34239
C	-4.97598	3.27683	-0.61365
C	-6.07392	4.09782	-0.44759
H	-7.06047	3.6572	-0.34445
C	-5.8897	5.49243	-0.3311
H	-6.75467	6.1303	-0.17383
C	-4.63148	6.05214	-0.40105
H	-4.5185	7.12418	-0.30841

Table 1 Naph-SAC4A@2ASP corresponding xyz bidet.

C	-3.4838	5.23993	-0.6294
C	-2.15239	5.75332	-0.77736
C	-1.09773	4.92268	-1.08105
H	-0.10468	5.33277	-1.21057
C	-1.29414	3.53093	-1.20083
H	-0.44549	2.90173	-1.43902
C	-2.54238	2.98863	-1.01432
H	-2.67936	1.91839	-1.09595
C	-3.66065	3.82031	-0.74094
C	0.11705	-0.50386	-4.25343
C	-0.11494	0.91095	-4.3573
C	-1.41109	1.43478	-4.61114
H	-2.23523	0.74454	-4.74817
C	-1.62135	2.79227	-4.68051
H	-2.61509	3.18263	-4.87814
C	-0.55879	3.69147	-4.43714
H	-0.74854	4.75798	-4.4151
C	0.70604	3.21847	-4.1681
C	0.9869	1.81293	-4.17005
C	2.28715	1.27235	-3.97758
H	3.13354	1.93626	-3.86523
C	2.48222	-0.09202	-3.92245
H	3.47976	-0.48015	-3.74286
C	1.40265	-0.98338	-4.03583
H	1.55587	-2.04937	-3.90994
C	3.65536	-5.1487	0.48114
C	4.15998	-5.71512	1.63683
H	3.5305	-6.37569	2.22356
C	5.45137	-5.36543	2.08253
H	5.83025	-5.79612	3.00431
C	6.21588	-4.45441	1.38581
H	7.18818	-4.17583	1.76887
C	5.74154	-3.87398	0.17444
C	6.49134	-2.93391	-0.60485
C	5.98922	-2.42803	-1.7843
H	6.57598	-1.71592	-2.35277
C	4.71845	-2.82909	-2.25504
H	4.34549	-2.43086	-3.19315
C	3.95864	-3.71714	-1.53037
H	2.97534	-4.00995	-1.88216
C	4.43947	-4.24396	-0.30196
C	0.29579	-0.47098	3.74825

Table 1 Naph-SAC4A@2ASP corresponding xyz bidet.

C	1.70393	-0.64334	3.52022
C	2.23704	-1.87169	3.04935
H	1.56613	-2.70347	2.8708
C	3.58511	-2.00916	2.81427
H	3.98225	-2.95456	2.46398
C	4.46045	-0.91834	3.0031
H	5.516	-1.03532	2.78432
C	3.98045	0.28758	3.47024
C	2.5914	0.4584	3.7802
C	2.05162	1.64694	4.34687
H	2.70448	2.48224	4.56194
C	0.7074	1.74377	4.63335
H	0.31554	2.65049	5.08409
C	-0.18137	0.69475	4.3252
H	-1.23107	0.80057	4.5761
C	-0.42373	-1.30372	-0.5136
C	0.65827	-2.14758	-0.15053
C	1.9364	-1.63785	-0.06175
C	2.24007	-0.29	-0.35349
C	1.15887	0.54453	-0.72708
C	-0.13131	0.06205	-0.79738
C	3.61377	0.13015	-0.32114
C	4.116	1.29271	-0.83382
C	5.50384	1.66235	-0.81295
C	6.49333	0.97977	-0.06828
C	7.80387	1.38782	-0.10025
N	8.19211	2.45854	-0.83965
C	7.27067	3.14595	-1.57012
C	5.94932	2.77782	-1.57239
C	9.60536	2.87376	-0.89139
N	-1.69418	-1.78365	-0.58146
C	-1.93371	-3.22105	-0.53631
C	-2.81568	-0.88438	-0.79578
H	0.49519	-3.19251	0.0803
H	2.739	-2.29753	0.23641
H	1.34037	1.58278	-0.98095
H	-0.91969	0.70639	-1.15989
H	4.30325	-0.59467	0.10758
H	3.45425	1.98628	-1.34189
H	6.2505	0.13029	0.55397
H	8.57531	0.8752	0.45663
H	7.64748	3.98719	-2.1392

Table 1 Naph-SAC4A@2ASP corresponding xyz bidet.

H	5.24743	3.34832	-2.17188
H	10.17641	2.28503	-0.17486
H	9.67835	3.93303	-0.63834
H	9.99434	2.70717	-1.89838
H	-1.74004	-3.62721	0.45833
H	-2.9723	-3.42234	-0.79559
H	-1.29419	-3.74287	-1.251
H	-2.8286	-0.45597	-1.80727
H	-3.73113	-1.44461	-0.64327
H	-2.7946	-0.06354	-0.07072
C	-6.31876	2.18536	3.22458
C	-5.85039	3.49713	2.92746
C	-4.50811	3.7514	2.72956
C	-3.53781	2.72707	2.82321
C	-3.99551	1.43965	3.18397
C	-5.33801	1.16984	3.39262
C	-2.14001	2.92052	2.52385
C	-1.50262	4.10767	2.32462
C	-0.12206	4.2451	1.93677
C	0.7311	3.15915	1.61951
C	2.02333	3.38129	1.21599
N	2.52119	4.64092	1.09799
C	1.73309	5.70858	1.37915
C	0.43654	5.53787	1.80262
C	3.9084	4.81144	0.63082
N	-7.65632	1.9168	3.34635
C	-8.67714	2.83756	2.85455
C	-8.1167	0.60347	3.78072
H	-6.55251	4.31738	2.83867
H	-4.20912	4.75988	2.45927
H	-3.27101	0.63141	3.28539
H	-5.63297	0.15682	3.63857
H	-1.56512	2.00172	2.43929
H	-2.04799	5.04184	2.43146
H	0.38933	2.13387	1.66678
H	2.70311	2.57628	0.97063
H	2.17745	6.686	1.24236
H	-0.16919	6.41646	1.99118
H	4.12035	5.8742	0.51836
H	4.01256	4.31751	-0.33326
H	4.58165	4.36561	1.3652
H	-8.28261	3.47176	2.05796

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H	-9.50334	2.25947	2.43117
H	-9.07784	3.48018	3.64986
H	-7.57041	0.26784	4.66731
H	-9.17309	0.67231	4.04671
H	-8.00648	-0.15624	2.99378

Table 2 Naph-SAC4A@2ADY-G corresponding xyz bidet.

corresponding atom	X-axis coordinates	Y-axis coordinates	Y-axis coordinates
C	-2.58909	-2.02938	5.1385
C	-1.83049	2.97735	4.56451
C	3.2019	2.07542	4.4302
C	2.42705	-2.97298	4.59511
H	-2.32851	-1.88202	6.18775
H	-3.44636	-2.70972	5.09799
H	-1.69986	3.00752	5.65264
H	-2.43607	3.84505	4.28605
H	3.13232	2.05851	5.52206
H	4.06503	2.69689	4.17498
H	2.4669	-2.93268	5.68746
H	2.97009	-3.87205	4.2896
C	3.45399	0.67311	3.89751
C	4.23448	0.49224	2.75651
C	4.48136	-0.78221	2.23145
C	3.91427	-1.90685	2.85817
C	3.11973	-1.76481	3.98691
C	2.89654	-0.46788	4.50449
H	4.67599	1.35342	2.26296
H	4.09114	-2.89336	2.44398
O	2.1427	-0.36951	5.64394
N	5.29985	-0.81724	1.08573
N	5.55946	-1.97001	0.63308
C	6.37756	-1.98438	-0.52467
C	6.74671	-3.2576	-0.98235
C	6.82354	-0.84101	-1.2125
C	7.55767	-3.39639	-2.10567
H	6.39522	-4.13046	-0.44073
C	7.62915	-0.97916	-2.33517
H	6.5362	0.14221	-0.85833
C	7.99848	-2.25558	-2.77978
H	7.85582	-4.38115	-2.44917

Table 2 Naph-SAC4A@2ADY-G corresponding xyz bidet.

H	7.98467	-0.1007	-2.86343
C	0.98618	-3.08997	4.1167
C	0.72043	-3.65509	2.87173
C	-0.58871	-3.76009	2.38389
C	-1.65036	-3.25517	3.1537
C	-1.42373	-2.6702	4.39326
C	-0.09712	-2.60742	4.88183
H	1.53713	-4.03417	2.2634
H	-2.66014	-3.30207	2.76042
O	0.10301	-2.09247	6.13428
H	0.91794	-1.53741	6.11396
N	-0.72049	-4.37363	1.12234
N	-1.90566	-4.49597	0.69573
C	-2.02406	-5.12212	-0.57037
C	-3.33481	-5.26037	-1.04877
C	-0.94779	-5.59868	-1.34181
C	-3.57884	-5.87591	-2.27411
H	-4.15407	-4.88009	-0.44624
C	-1.19057	-6.21213	-2.56336
H	0.06559	-5.48344	-0.97509
C	-2.50557	-6.3543	-3.02768
H	-4.59268	-5.97811	-2.64562
H	-0.36357	-6.5745	-3.16538
C	-2.9769	-0.70348	4.504
C	-3.93792	-0.64535	3.50931
C	-4.24901	0.55695	2.83978
C	-3.54573	1.73172	3.19727
C	-2.58426	1.71402	4.18703
C	-2.27734	0.48967	4.87997
H	-4.47381	-1.54538	3.21659
H	-3.77899	2.65993	2.68474
O	-1.39543	0.46219	5.83912
N	-5.24036	0.47324	1.87054
N	-5.54238	1.55754	1.2685
C	-6.54799	1.42053	0.28503
C	-6.96675	2.61429	-0.32448
C	-7.12941	0.20295	-0.1219
C	-7.95354	2.60492	-1.3067
H	-6.50557	3.54696	-0.01326
C	-8.11034	0.19217	-1.10461
H	-6.79956	-0.72288	0.33512
C	-8.52643	1.39255	-1.697

Table 2 Naph-SAC4A@2ADY-G corresponding xyz bidet.

H	-8.26955	3.53039	-1.77608
H	-8.54703	-0.74804	-1.42655
C	-0.47216	3.11504	3.89239
C	-0.34932	3.82735	2.70186
C	0.89123	4.00004	2.07113
C	2.04198	3.44017	2.6562
C	1.95668	2.71387	3.83435
C	0.69105	2.53718	4.44677
H	-1.22877	4.27783	2.24964
H	3.00465	3.57563	2.1751
O	0.63953	1.82647	5.60386
H	-0.58461	1.25114	5.71332
N	0.87054	4.7513	0.88226
N	1.99609	4.93807	0.33209
C	1.95721	5.69284	-0.8664
C	3.20482	5.95136	-1.45132
C	0.78693	6.17235	-1.48494
C	3.29471	6.68612	-2.63146
H	4.09826	5.56786	-0.96803
C	0.87569	6.90119	-2.66291
H	-0.17816	5.96346	-1.03805
C	2.12937	7.16013	-3.23534
H	4.25982	6.88102	-3.08587
H	-0.02574	7.26	-3.14953
S	-9.85484	1.36838	-2.90894
O	-11.1263	1.36299	-2.11943
O	-9.68566	2.60785	-3.72718
S	-2.81084	-7.24289	-4.56426
O	-2.86218	-8.68802	-4.18054
O	-4.11499	-6.72844	-5.07997
S	8.99204	-2.42858	-4.27239
O	9.8306	-1.19319	-4.34166
O	9.79274	-3.67498	-4.07811
S	2.22594	8.16456	-4.72705
O	2.11432	9.58338	-4.26474
O	3.55107	7.85399	-5.34299
O	-9.65728	0.11211	-3.69526
O	-1.6535	-6.91985	-5.4525
O	1.06657	7.73693	-5.56773
O	8.01409	-2.5326	-5.39973
H	1.65432	0.50197	5.68014
C	-3.97076	-1.06896	-3.51944

Table 2 Naph-SAC4A@2ADY-G corresponding xyz bidet.

C	-3.22454	-0.53314	-4.52853
C	-1.95914	0.08188	-4.25731
C	-1.49257	0.12986	-2.90772
C	-2.30549	-0.44239	-1.87586
C	-3.50422	-1.0229	-2.17291
C	-0.25982	0.7283	-2.62548
C	0.5238	1.27872	-3.64556
C	0.0581	1.22908	-4.99535
C	0.87374	1.79622	-6.02783
H	0.50423	1.75077	-7.06342
C	2.0745	2.37285	-5.73128
C	2.53884	2.42305	-4.3842
C	1.78915	1.89368	-3.37423
H	-3.57313	-0.56264	-5.5719
H	-1.93503	-0.39867	-0.84057
H	0.09945	0.76514	-1.58544
H	2.1361	1.92585	-2.33037
C	-4.38236	-1.63895	-1.06794
H	-5.30562	-1.1018	-1.00511
H	-4.58133	-2.66422	-1.30059
H	-3.87024	-1.57886	-0.13037
C	3.90018	3.08385	-4.09834
H	4.67777	2.51387	-4.56243
H	3.90349	4.07868	-4.49229
H	4.06515	3.11811	-3.04169
N	2.91535	2.95523	-6.78708
H	3.15724	2.2463	-7.44958
N	-5.26805	-1.70377	-3.79322
H	-5.88572	-1.03496	-4.20695
H	-5.13787	-2.47068	-4.42163
N	-1.17588	0.63293	-5.27727
H	-1.50283	0.60023	-6.22174
H	3.74866	3.33006	-6.38076

Table 3 SAC4A@ASP corresponding xyz bidet.

corresponding atom	X-axis coordinates	Y-axis coordinates	Y-axis coordinates
C	-2.58909	-2.02938	5.1385
C	-1.83049	2.97735	4.56451
C	3.2019	2.07542	4.4302
C	2.42705	-2.97298	4.59511

Table 3 SAC4A@ASP corresponding xyz bidet.

H	-2.32851	-1.88202	6.18775
H	-3.44636	-2.70972	5.09799
H	-1.69986	3.00752	5.65264
H	-2.43607	3.84505	4.28605
H	3.13232	2.05851	5.52206
H	4.06503	2.69689	4.17498
H	2.4669	-2.93268	5.68746
H	2.97009	-3.87205	4.2896
C	3.45399	0.67311	3.89751
C	4.23448	0.49224	2.75651
C	4.48136	-0.78221	2.23145
C	3.91427	-1.90685	2.85817
C	3.11973	-1.76481	3.98691
C	2.89654	-0.46788	4.50449
H	4.67599	1.35342	2.26296
H	4.09114	-2.89336	2.44398
O	2.1427	-0.36951	5.64394
N	5.29985	-0.81724	1.08573
N	5.55946	-1.97001	0.63308
C	6.37756	-1.98438	-0.52467
C	6.74671	-3.2576	-0.98235
C	6.82354	-0.84101	-1.2125
C	7.55767	-3.39639	-2.10567
H	6.39522	-4.13046	-0.44073
C	7.62915	-0.97916	-2.33517
H	6.5362	0.14221	-0.85833
C	7.99848	-2.25558	-2.77978
H	7.85582	-4.38115	-2.44917
H	7.98467	-0.1007	-2.86343
C	0.98618	-3.08997	4.1167
C	0.72043	-3.65509	2.87173
C	-0.58871	-3.76009	2.38389
C	-1.65036	-3.25517	3.1537
C	-1.42373	-2.6702	4.39326
C	-0.09712	-2.60742	4.88183
H	1.53713	-4.03417	2.2634
H	-2.66014	-3.30207	2.76042
O	0.10301	-2.09247	6.13428
H	0.91794	-1.53741	6.11396
N	-0.72049	-4.37363	1.12234
N	-1.90566	-4.49597	0.69573
C	-2.02406	-5.12212	-0.57037

Table 3 SAC4A@ASP corresponding xyz bidet.

C	-3.33481	-5.26037	-1.04877
C	-0.94779	-5.59868	-1.34181
C	-3.57884	-5.87591	-2.27411
H	-4.15407	-4.88009	-0.44624
C	-1.19057	-6.21213	-2.56336
H	0.06559	-5.48344	-0.97509
C	-2.50557	-6.3543	-3.02768
H	-4.59268	-5.97811	-2.64562
H	-0.36357	-6.5745	-3.16538
C	-2.9769	-0.70348	4.504
C	-3.93792	-0.64535	3.50931
C	-4.24901	0.55695	2.83978
C	-3.54573	1.73172	3.19727
C	-2.58426	1.71402	4.18703
C	-2.27734	0.48967	4.87997
H	-4.47381	-1.54538	3.21659
H	-3.77899	2.65993	2.68474
O	-1.39543	0.46219	5.83912
N	-5.24036	0.47324	1.87054
N	-5.54238	1.55754	1.2685
C	-6.54799	1.42053	0.28503
C	-6.96675	2.61429	-0.32448
C	-7.12941	0.20295	-0.1219
C	-7.95354	2.60492	-1.3067
H	-6.50557	3.54696	-0.01326
C	-8.11034	0.19217	-1.10461
H	-6.79956	-0.72288	0.33512
C	-8.52643	1.39255	-1.697
H	-8.26955	3.53039	-1.77608
H	-8.54703	-0.74804	-1.42655
C	-0.47216	3.11504	3.89239
C	-0.34932	3.82735	2.70186
C	0.89123	4.00004	2.07113
C	2.04198	3.44017	2.6562
C	1.95668	2.71387	3.83435
C	0.69105	2.53718	4.44677
H	-1.22877	4.27783	2.24964
H	3.00465	3.57563	2.1751
O	0.63953	1.82647	5.60386
H	-0.58461	1.25114	5.71332
N	0.87054	4.7513	0.88226
N	1.99609	4.93807	0.33209

Table 3 SAC4A@ASP corresponding xyz bidet.

C	1.95721	5.69284	-0.8664
C	3.20482	5.95136	-1.45132
C	0.78693	6.17235	-1.48494
C	3.29471	6.68612	-2.63146
H	4.09826	5.56786	-0.96803
C	0.87569	6.90119	-2.66291
H	-0.17816	5.96346	-1.03805
C	2.12937	7.16013	-3.23534
H	4.25982	6.88102	-3.08587
H	-0.02574	7.26	-3.14953
S	-9.85484	1.36838	-2.90894
O	-11.1263	1.36299	-2.11943
O	-9.68566	2.60785	-3.72718
S	-2.81084	-7.24289	-4.56426
O	-2.86218	-8.68802	-4.18054
O	-4.11499	-6.72844	-5.07997
S	8.99204	-2.42858	-4.27239
O	9.8306	-1.19319	-4.34166
O	9.79274	-3.67498	-4.07811
S	2.22594	8.16456	-4.72705
O	2.11432	9.58338	-4.26474
O	3.55107	7.85399	-5.34299
O	-9.65728	0.11211	-3.69526
O	-1.6535	-6.91985	-5.4525
O	1.06657	7.73693	-5.56773
O	8.01409	-2.5326	-5.39973
H	1.65432	0.50197	5.68014
C	1.33445	-2.51485	-3.38871
C	1.1276	-2.48835	-1.98209
C	0.31054	-1.53389	-1.40786
C	-0.35116	-0.54667	-2.17454
C	-0.15631	-0.59054	-3.57697
C	0.66019	-1.52893	-4.16742
C	-1.07309	0.49885	-1.50349
C	-1.71869	1.55546	-2.08182
C	-2.3146	2.64892	-1.3668
C	-2.23643	2.82903	0.04101
C	-2.81821	3.91557	0.64219
N	-3.47661	4.86276	-0.08202
C	-3.56771	4.73206	-1.43199
C	-3.00526	3.66115	-2.0816
C	-4.13708	5.98663	0.60641

Table 3 SAC4A@ASP corresponding xyz bidet.

N	2.14751	-3.43819	-3.97452
C	2.40313	-3.38844	-5.40952
C	2.88843	-4.38933	-3.15493
H	1.61005	-3.21672	-1.34296
H	0.18545	-1.53127	-0.32832
H	-0.6259	0.1516	-4.21393
H	0.8014	-1.49295	-5.23962
H	-1.05221	0.43635	-0.41725
H	-1.78053	1.62323	-3.16517
H	-1.70554	2.12615	0.67082
H	-2.77576	4.07947	1.71224
H	-4.10272	5.51543	-1.95441
H	-3.09683	3.60268	-3.16102
H	-4.23503	6.82128	-0.08762
H	-3.52822	6.28928	1.45897
H	-5.12574	5.67353	0.95155
H	1.46744	-3.37423	-5.97448
H	2.99097	-2.50572	-5.68449
H	2.94355	-4.28313	-5.70194
H	3.62595	-3.88208	-2.51628
H	2.21267	-4.96906	-2.51678
H	3.41454	-5.08678	-3.80454

Table 4 SAC4A@ADY-G corresponding xyz bidet.

corresponding atom	X-axis coordinates	Y-axis coordinates	Y-axis coordinates
C	-2.58909	-2.02938	5.1385
C	-1.83049	2.97735	4.56451
C	3.2019	2.07542	4.4302
C	2.42705	-2.97298	4.59511
H	-2.32851	-1.88202	6.18775
H	-3.44636	-2.70972	5.09799
H	-1.69986	3.00752	5.65264
H	-2.43607	3.84505	4.28605
H	3.13232	2.05851	5.52206
H	4.06503	2.69689	4.17498
H	2.4669	-2.93268	5.68746
H	2.97009	-3.87205	4.2896
C	3.45399	0.67311	3.89751
C	4.23448	0.49224	2.75651
C	4.48136	-0.78221	2.23145
C	3.91427	-1.90685	2.85817

Table 4 SAC4A@ADY-G corresponding xyz bidet.

C	3.11973	-1.76481	3.98691
C	2.89654	-0.46788	4.50449
H	4.67599	1.35342	2.26296
H	4.09114	-2.89336	2.44398
O	2.1427	-0.36951	5.64394
N	5.29985	-0.81724	1.08573
N	5.55946	-1.97001	0.63308
C	6.37756	-1.98438	-0.52467
C	6.74671	-3.2576	-0.98235
C	6.82354	-0.84101	-1.2125
C	7.55767	-3.39639	-2.10567
H	6.39522	-4.13046	-0.44073
C	7.62915	-0.97916	-2.33517
H	6.5362	0.14221	-0.85833
C	7.99848	-2.25558	-2.77978
H	7.85582	-4.38115	-2.44917
H	7.98467	-0.1007	-2.86343
C	0.98618	-3.08997	4.1167
C	0.72043	-3.65509	2.87173
C	-0.58871	-3.76009	2.38389
C	-1.65036	-3.25517	3.1537
C	-1.42373	-2.6702	4.39326
C	-0.09712	-2.60742	4.88183
H	1.53713	-4.03417	2.2634
H	-2.66014	-3.30207	2.76042
O	0.10301	-2.09247	6.13428
H	0.91794	-1.53741	6.11396
N	-0.72049	-4.37363	1.12234
N	-1.90566	-4.49597	0.69573
C	-2.02406	-5.12212	-0.57037
C	-3.33481	-5.26037	-1.04877
C	-0.94779	-5.59868	-1.34181
C	-3.57884	-5.87591	-2.27411
H	-4.15407	-4.88009	-0.44624
C	-1.19057	-6.21213	-2.56336
H	0.06559	-5.48344	-0.97509
C	-2.50557	-6.3543	-3.02768
H	-4.59268	-5.97811	-2.64562
H	-0.36357	-6.5745	-3.16538
C	-2.9769	-0.70348	4.504
C	-3.93792	-0.64535	3.50931
C	-4.24901	0.55695	2.83978

Table 4 SAC4A@ADY-G corresponding xyz bidet.

C	-3.54573	1.73172	3.19727
C	-2.58426	1.71402	4.18703
C	-2.27734	0.48967	4.87997
H	-4.47381	-1.54538	3.21659
H	-3.77899	2.65993	2.68474
O	-1.39543	0.46219	5.83912
N	-5.24036	0.47324	1.87054
N	-5.54238	1.55754	1.2685
C	-6.54799	1.42053	0.28503
C	-6.96675	2.61429	-0.32448
C	-7.12941	0.20295	-0.1219
C	-7.95354	2.60492	-1.3067
H	-6.50557	3.54696	-0.01326
C	-8.11034	0.19217	-1.10461
H	-6.79956	-0.72288	0.33512
C	-8.52643	1.39255	-1.697
H	-8.26955	3.53039	-1.77608
H	-8.54703	-0.74804	-1.42655
C	-0.47216	3.11504	3.89239
C	-0.34932	3.82735	2.70186
C	0.89123	4.00004	2.07113
C	2.04198	3.44017	2.6562
C	1.95668	2.71387	3.83435
C	0.69105	2.53718	4.44677
H	-1.22877	4.27783	2.24964
H	3.00465	3.57563	2.1751
O	0.63953	1.82647	5.60386
H	-0.58461	1.25114	5.71332
N	0.87054	4.7513	0.88226
N	1.99609	4.93807	0.33209
C	1.95721	5.69284	-0.8664
C	3.20482	5.95136	-1.45132
C	0.78693	6.17235	-1.48494
C	3.29471	6.68612	-2.63146
H	4.09826	5.56786	-0.96803
C	0.87569	6.90119	-2.66291
H	-0.17816	5.96346	-1.03805
C	2.12937	7.16013	-3.23534
H	4.25982	6.88102	-3.08587
H	-0.02574	7.26	-3.14953
S	-9.85484	1.36838	-2.90894
O	-11.1263	1.36299	-2.11943

Table 4 SAC4A@ADY-G corresponding xyz bidet.

O	-9.68566	2.60785	-3.72718
S	-2.81084	-7.24289	-4.56426
O	-2.86218	-8.68802	-4.18054
O	-4.11499	-6.72844	-5.07997
S	8.99204	-2.42858	-4.27239
O	9.8306	-1.19319	-4.34166
O	9.79274	-3.67498	-4.07811
S	2.22594	8.16456	-4.72705
O	2.11432	9.58338	-4.26474
O	3.55107	7.85399	-5.34299
O	-9.65728	0.11211	-3.69526
O	-1.6535	-6.91985	-5.4525
O	1.06657	7.73693	-5.56773
O	8.01409	-2.5326	-5.39973
H	1.65432	0.50197	5.68014
C	-3.97076	-1.06896	-3.51944
C	-3.22454	-0.53314	-4.52853
C	-1.95914	0.08188	-4.25731
C	-1.49257	0.12986	-2.90772
C	-2.30549	-0.44239	-1.87586
C	-3.50422	-1.0229	-2.17291
C	-0.25982	0.7283	-2.62548
C	0.5238	1.27872	-3.64556
C	0.0581	1.22908	-4.99535
C	0.87374	1.79622	-6.02783
H	0.50423	1.75077	-7.06342
C	2.0745	2.37285	-5.73128
C	2.53884	2.42305	-4.3842
C	1.78915	1.89368	-3.37423
H	-3.57313	-0.56264	-5.5719
H	-1.93503	-0.39867	-0.84057
H	0.09945	0.76514	-1.58544
H	2.1361	1.92585	-2.33037
C	-4.38236	-1.63895	-1.06794
H	-5.30562	-1.1018	-1.00511
H	-4.58133	-2.66422	-1.30059
H	-3.87024	-1.57886	-0.13037
C	3.90018	3.08385	-4.09834
H	4.67777	2.51387	-4.56243
H	3.90349	4.07868	-4.49229
H	4.06515	3.11811	-3.04169
N	2.91535	2.95523	-6.78708

Table 4 SAC4A@ADY-G corresponding xyz bidet.

H	3.15724	2.2463	-7.44958
N	-5.26805	-1.70377	-3.79322
H	-5.88572	-1.03496	-4.20695
H	-5.13787	-2.47068	-4.42163
N	-1.17588	0.63293	-5.27727
H	-1.50283	0.60023	-6.22174
H	3.74866	3.33006	-6.38076