Supplementary Materials

for

Nonorthogonal Tight-Binding Model with H–C–N–O Parameterization

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Table S1. The binding energies (eV/atom) for various $H_kC_lN_mO_n$ molecules calculated within the NTBM1 model along with the corresponding experimental values and the values calculated using AM1/PM3/PM7 and the set of the model parameters from Ref. [Zhao J, Lu JP. Phys. Lett. A. 2003;319:523-529.]. The experimental and AM1/PM3 values are taken from the original PM3 work [Stewart JJP. J. Comp. Chem. 1989;10:221-264.]. The AM1/PM3 binding energies for the carbon dimer, imidogene and C_{60} fullerene are obtained using GAMESS program package [Schmidt MW, Baldridge KK, Boatz JA, Elbert ST, Gordon MS, Jensen JH, Koseki S, Matsunaga N, Nguyen KA, Su SJ, Windus TL, Dupuis M, Montgomery JA. J. Comp. Chem. 1993;14:1347-1363.]. The PM7 binding energies are obtained using MOPAC2012 [Stewart JJP, Stewart Computational Chemistry, Colorado Springs, CO, USA, HTTP://OpenMOPAC.net (2012).], and experimental values for C_2 and C_{60} are taken from NIST database [Computational Chemistry Comparison and Benchmark DataBase http://cccbdb.nist.gov/].

Formula	Name	Exper.	PM3	PM7	AM1	Zhao-Lu	Present work
1	2	3	4	5	6	7	8
H_2	Hydrogen	2.240	2.530	2.934	2.353	2.421	2.364
CH	Methylidyne	1.721	1.625	1.791	1.664	1.903	1.816
CH_2	Methylene, triplet	2.618	2.859	2.813	2.784	2.801	2.690
CH_3	Methyl radical	3.147	3.201	3.221	3.185	3.336	3.145
CH_4	Methane	3.422	3.380	3.392	3.344	3.664	3.339
C_2	Carbon, dimer	3.120	1.778	3.043	2.688	5.575	3.090
C_2H_2	Acetylene	4.221	4.259	4.189	4.214	4.838	4.483
C_2H_3	Vinyl	3.778	3.832	3.792	3.733	4.021	3.838
C_2H_4	Ethylene	3.863	3.832	3.852	3.834	4.169	3.900
C_2H_4	Methylmethylene	3.300	3.312	3.382	3.318	3.570	3.433
C_2H_5	Ethyl	3.553	3.600	3.603	3.595	3.738	3.557
C_2H_6	Ethane	3.634	3.622	3.623	3.618	3.872	3.602
C_3	Carbon, trimer	4.544	4.390	4.744	4.307	5.015	4.663
C_3H_4	Allene	4.159	4.150	4.213	4.156	4.526	4.265
C_3H_4	Cyclopropene	4.031	4.019	4.050	3.978	4.191	3.937
C_3H_4	Propyne	4.166	4.192	4.156	4.173	4.587	4.292
C_3H_5	Allyl	3.949	3.952	3.996	3.957	4.188	3.994
C_3H_6	Cyclopropane	3.891	3.874	3.894	3.867	4.036	3.805
C_3H_6	Propene	3.929	3.921	3.932	3.920	4.179	3.933
C_3H_7	i-Propyl radical	3.708	3.757	3.756	3.751	3.888	3.701
C_3H_8	Propane	3.739	3.734	3.732	3.737	3.957	3.707
C_4H_6	1-Methylcycloprop-1-ene	4.042	4.046	4.064	4.014	4.200	3.969
C_4H_6	Bicyclobutane	4.070	3.995	4.010	3.956	4.092	3.881
C_4H_6	1,2-Butadiene	4.126	4.130	4.169	4.134	4.427	4.186
C_4H_6	1-Butyne	4.123	4.140	4.114	4.132	4.465	4.201
C_4H_6	2-Butyne	4.144	4.165	4.141	4.156	4.484	4.216
C_4H_6	Cyclobutene	4.132	4.131	4.133	4.096	4.250	4.059
C_4H_6	Methylenecyclopropane	4.087	4.102	4.129	4.088	4.269	4.052
C_4H_6	1,3-Butadiene	4.182	4.160	4.177	4.165	4.436	4.206
C_4H_8	1-Butene	3.953	3.946	3.953	3.951	4.180	3.947

Table S1. (continued)

1	2	3	4	5	6	7	8
C_4H_8	cis-2-Butene	3.959	3.961	3.967	3.960	4.182	3.892
C_4H_8	Cyclobutane	3.928	3.966	3.960	3.956	4.079	3.936
C_4H_8	Isobutene	3.968	3.964	3.973	3.956	4.176	3.948
C_4H_8	trans-2-Butene	3.963	3.966	3.970	3.964	4.182	3.765
C_4H_9	Isobutyl	3.805	3.840	3.835	3.830	3.960	3.767
C_4H_{10}	n-Butane	3.802	3.798	3.795	3.804	4.006	3.756
C_4H_{10}	Isobutane	3.808	3.799	3.797	3.799	4.000	4.453
C_5H_6	Cyclopentadiene	4.448	4.449	4.447	4.429	4.591	3.986
C_5H_8	1,2-Dimethylcyclopropene	4.061	4.060	4.071	4.033	4.203	4.092
C_5H_8	Methylene cyclobutane	4.119	4.150	4.154	4.132	4.271	4.168
C_5H_8	1,cis-3-Pentadiene	4.152	4.145	4.154	4.146	4.378	4.185
C_5H_8	Cyclopentene	4.188	4.206	4.198	4.206	4.350	4.001
C_5H_8	Bicyclo(2.1.0)-pentane	4.091	4.089	4.092	4.062	4.164	4.151
C_5H_8	1,4-Pentadiene	4.131	4.127	4.141	4.133	4.368	3.951
C_5H_8	Spiropentane	4.068	4.072	4.087	4.047	4.143	4.160
C_5H_8	1,trans-3-Pentadiene	4.155	4.145	4.156	4.147	4.381	3.956
C_5H_{10}	1-Pentene	3.967	3.964	3.968	3.972	4.182	3.951
C_5H_{10}	2-Methyl-1-butene	3.977	3.975	3.979	3.972	4.178	3.952
C_5H_{10}	2-Methyl-2-butene	3.981	3.987	3.991	3.981	4.178	3.948
C_5H_{10}	3-Methyl-1-butene	3.971	3.963	3.966	3.965	4.174	3.961
C_5H_{10}	cis-2-Pentene	3.972	3.974	3.978	3.978	4.183	3.883
C_5H_{10}	cis-Dimethylcyclopropane	3.948	3.948	3.953	3.938	4.094	3.992
C_5H_{10}	Cyclopentane	4.005	4.021	4.010	4.035	4.170	3.957
C_5H_{10}	trans-2-Pentene	3.975	3.977	3.980	3.980	4.183	3.799
C_5H_{12}	2-Methylbutane	3.845	3.838	3.836	3.841	4.032	3.778
C_5H_{12}	Neopentane	3.853	3.842	3.841	3.834	4.023	3.811
C_5H_{12}	n-Pentane	3.840	3.839	3.836	3.848	4.038	4.764
C_6H_6	Benzene	4.737	4.723	4.725	4.729	4.899	4.635
C_6H_6	Fulvene	4.637	4.605	4.609	4.582	4.774	4.402
C_6H_8	1,3-Cyclohexadiene	4.363	4.378	4.379	4.387	4.544	4.116
C_6H_{10}	2,3-Dimethyl-1,3-butadiene	4.137	4.128	4.138	4.119	4.332	4.180
C_6H_{10}	Cyclohexene	4.169	4.179	4.175	4.194	4.341	4.128
C_6H_{10}	1,5-Hexadiene	4.112	4.109	4.120	4.118	4.335	4.048
C_6H_{10}	1,2-Dimethylcyclobutene	4.113	4.122	4.122	4.093	4.228	3.983
C_6H_{10}	Bicyclopropyl	4.082	4.068	4.086	4.059	4.171	3.988
C_6H_{12}	Cyclohexane	4.023	4.027	4.018	4.045	4.166	3.840
C_6H_{14}	n-Hexane	3.867	3.867	3.864	3.878	4.060	4.556
C_7H_8	Cycloheptatriene	4.512	4.514	4.526	4.526	4.695	4.467
C_7H_8	Norbornadiene	4.464	4.467	4.466	4.441	4.576	4.603
C_7H_8	Toluene	4.602	4.596	4.599	4.595	4.751	4.125
C_7H_{12}	Norbornane	4.161	4.164	4.154	4.165	4.272	3.854
C_7H_{16}	n-Heptane	3.888	3.889	3.885	3.901	4.076	4.363
C_8H_8	Cubane	4.405	4.500	4.468	4.399	4.325	4.738
C_8H_8	Styrene	4.713	4.702	4.708	4.703	4.876	4.504
C_8H_{10}	Ethylbenzene	4.506	4.500	4.502	4.502	4.657	4.146
C_8H_{14}	Bicyclo(2.2.2)-octane	4.155	4.163	4.154	4.179	4.286	3.869
C_8H_{18}	n-Octane	3.904	3.905	3.901	3.918	4.089	3.892
C_9H_{20}	n-Nonane	3.916	3.918	3.914	3.932	4.099	3.882

Table S1. (continued)

1	2	3	4	5	6	7	8
$C_{10}H_8$	Azulene	4.917	4.898	4.903	4.890	5.044	4.958
$C_{10}H_8$	Naphtalene	5.007	4.996	4.998	4.996	5.115	5.029
$C_{10}H_{16}$	Adamantane	4.269	4.273	4.263	4.288	4.368	4.252
$C_{14}H_{10}$	Anthracene	5.137	5.125	5.127	5.123	5.218	5.157
$C_{14}H_{10}$	Phenanthrene	5.147	5.137	5.138	5.133	5.227	5.167
C_{60}	Buckminsterfullerene	6.918	6.790	6.776	6.673	6.590	6.954
OH	Hydroxyl radical	2.193	2.334	2.242	2.380	2.356	2.076
H_2O	Water	3.182	3.118	3.182	3.202	3.387	2.859
CO	Carbon monoxide	5.540	5.395	5.365	5.091	4.607	5.059
HCO	H-C=O	3.908	4.193	4.095	4.073	3.836	3.965
CH_2O	Formaldehyde	3.886	3.973	3.881	3.945	4.250	4.114
CH_4O	Methanol	3.497	3.524	3.503	3.561	3.775	3.579
C_2H_4O	Acetaldehyde	3.999	4.027	4.008	4.010	4.259	4.043
C_2H_4O	Ethylene oxide	3.831	3.803	3.823	3.809	4.076	3.923
C_2H_6O	Ethanol	3.688	3.690	3.686	3.719	3.923	3.711
C_3H_6O	Acetone	4.038	4.044	4.053	4.026	4.251	4.005
C_3H_6O	Propanal	4.010	4.027	4.012	4.022	4.241	4.026
C_3H_6O	Trimethylene oxide	3.896	3.929	3.923	3.924	4.150	4.004
C_3H_8O	Isopropanol	3.786	3.782	3.793	3.796	3.988	3.763
C_4H_4O	Furan	4.598	4.578	4.586	4.544	4.709	4.728
C_4H_6O	2-Butenal	4.231	4.244	4.238	4.238	4.484	4.263
C_4H_8O	Butanal	4.008	4.027	4.014	4.029	4.222	4.017
C_4H_8O	Tetrahydrofuran	3.992	4.016	4.008	4.040	4.188	4.091
$C_4H_{10}O$	Diethyl ether	3.805	3.803	3.801	3.819	4.027	3.879
$C_4H_{10}O$	t-Butanol	3.847	3.837	3.847	3.838	4.022	3.784
C_5H_8O	Cyclopentanone	4.240	4.212	4.263	4.209	4.394	4.227
$C_5H_{10}O$	Tetrahydropyran	4.010	4.021	4.017	4.047	4.194	4.088
$C_5H_{12}O$	3-Pentanol	3.866	3.862	3.864	3.879	4.054	3.837
C_6H_6O	Phenol	4.712	4.708	4.709	4.709	4.855	4.734
$C_6H_{10}O$	Cyclohexanone	4.209	4.225	4.223	4.233	4.377	4.204
C_7H_6O	Benzaldehyde	4.858	4.864	4.850	4.859	5.027	4.894
C_7H_8O	Anisole	4.554	4.547	4.553	4.550	4.722	4.650
$C_{10}H_8O$	1-Naphthol	4.972	4.970	4.972	4.965	5.074	4.997
$C_{10}H_8O$	2-Naphthol	4.983	4.971	4.973	4.969	5.073	4.995
O_2	Oxygen(triplet)	2.559	2.650	2.743	3.144	2.181	2.471
H_2O_2	Hydrogen peroxide	2.751	2.841	2.727	2.782	3.083	2.579
CO_2	Carbon dioxide	5.525	5.393	5.386	5.320	5.465	5.074
CH_2O_2	Formic acid	4.180	4.213	4.171	4.239	4.437	4.079
$C_2H_4O_2$	Acetic acid	4.164	4.157	4.158	4.162	4.378	3.994
$C_2H_6O_2$	Ethylene glycol	3.738	3.744	3.821	3.797	3.962	3.790
$C_3H_4O_2$	beta-Propiolactone	4.349	4.363	4.316	4.365	4.606	4.268
$C_3H_6O_2$	Propionic acid	4.126	4.118	4.119	4.129	4.328	3.981
$C_3H_6O_2$	Methyl acetate	4.085	4.070	4.080	4.079	4.320	4.072
$C_4H_6O_2$	Diacetyl	4.288	4.307	4.305	4.276	4.486	4.255
$C_4H_{10}O_2$	Diethyl peroxide	3.689	3.672	3.681	3.668	3.920	3.737
$C_5H_8O_2$	Acetylacetone	4.256	4.259	4.272	4.242	4.441	4.226
$C_6H_4O_2$	p-Benzoquinone	4.967	4.975	4.964	4.952	5.170	5.010
$C_7H_6O_2$	Benzoic acid	4.882	4.871	4.871	4.876	5.033	4.804

Table S1. (continued)

1	2	3	4	5	6	7	8
$C_4H_2O_3$	Malaic anhydride	5.088	5.063	5.026	4.997	5.255	4.930
$C_4H_6O_3$	Acetic anhydride	4.351	4.344	3.627	4.333	4.606	4.230
NH	Imidogene	1.703	1.960	1.826	1.874	-	1.577
NH_2	Amidogen	2.462	2.608	2.507	2.565	-	2.384
NH_3	Ammonia	3.019	2.934	2.946	2.979	-	2.871
CN	Cyanide	3.874	3.353	3.879	3.648	-	3.592
CHN	Hydrogen cyanide	4.366	4.355	4.401	4.384	-	4.302
CH_4N	Methyl amine anion	3.316	3.379	3.561	3.297	-	3.339
CH_4N	CH3-NH	3.269	3.339	3.282	3.290	-	3.268
CH_5N	Methylamine	3.385	3.383	3.372	3.397	-	3.370
C_2H_3N	Acetonitrile	4.241	4.224	4.261	4.253	-	4.187
C_2H_3N	Methyl isocyanide	4.135	3.997	4.111	4.028	-	4.026
C_2H_5N	Ethyleneimine(Azirane)	3.690	3.683	3.679	3.675	-	3.570
C_2H_7N	Ethylamine	3.581	3.585	3.580	3.597	-	3.562
C_2H_7N	Dimethylamine	3.560	3.566	3.550	3.556	-	3.558
C_3H_3N	Acrylonitrile	4.545	4.508	4.548	4.540	-	4.537
C_3H_5N	Ethyl cyanide	4.187	4.156	4.180	4.183	-	4.117
C_3H_9N	Isopropylamine	3.695	3.691	3.687	3.693	-	3.652
C_3H_9N	Trimethylamine	3.650	3.665	3.649	3.634	-	3.646
C_3H_9N	n-Propylamine	3.684	3.688	3.683	3.702	-	3.660
C_4H_5N	Pyrrole	4.446	4.441	4.444	4.386	-	4.475
C_4H_9N	Pyrrolidine	3.899	3.933	3.913	3.928	-	3.917
$C_4H_{11}N$	t-Butylamine	3.767	3.757	3.755	3.747	-	3.701
C_5H_5N	Pyridine	4.678	4.695	4.690	4.689	-	4.704
C_6H_7N	Aniline	4.566	4.564	4.564	4.567	-	4.589
C_7H_5N	Phenyl cyanide	5.037	5.014	5.030	5.031	-	5.033
NO	Nitrogen oxide	3.251	3.399	3.236	3.694	-	3.375
HNCO	Hydrogen isocyanate	4.527	4.430	4.518	4.429	-	4.528
CH_3NO	Formamide	3.911	3.891	3.908	3.913	-	3.943
C_3H_7NO	Dimethylformamide	3.936	3.932	3.929	3.904	-	3.953
NO_2	Nitrogen dioxide	3.218	3.347	3.412	3.549	-	3.493
HNO_2	Nitrous acid, trans	3.263	3.221	3.315	3.486	-	3.127
CH_3NO_2	Nitromethane	3.553	3.540	3.548	3.503	-	3.733
CH_3NO_2	Methyl nitrite	3.540	3.498	3.561	3.639	-	3.635
$C_2H_5NO_2$	Glycine	4.001	4.011	3.999	4.035	-	3.863
$C_3H_7NO_2$	1-Nitropropane	3.778	3.767	3.771	3.757	-	3.851
$C_3H_7NO_2$	2-Nitropropane	3.788	3.768	3.773	3.749	-	3.839
$C_3H_7NO_2$	Alanine	4.049	4.015	4.008	4.028	-	3.884
$C_4H_9NO_2$	1-Nitrobutane	3.822	3.816	3.818	3.811	-	3.877
$C_4H_9NO_2$	2-Nitrobutane	3.835	3.815	3.822	3.805	-	3.869
$C_6H_5NO_2$	Nitrobenzene	4.628	4.631	4.619	4.597	-	4.729
$C_7H_7NO_2$	2-Nitrotoluene	4.524	4.536	4.525	4.504	-	4.596
NO_3	Nitrate radical	2.955	2.891	2.841	2.779	-	3.065
HNO_3	Nitric acid	3.238	3.289	3.256	3.284	-	3.210
$C_2H_5NO_3$	Ethyl nitrate	3.646	3.644	3.654	3.647	-	3.712
$C_2H_5NO_3$	Nitroethanol	3.797	3.743	3.734	3.755	-	3.878
N_2	Nitrogen	4.881	4.499	4.165	4.638	-	4.788
N_2H_2	Diazene	3.170	3.150	3.089	3.219	-	3.251

Table S1. (continued)

1	2	3	4	5	6	7	8
N_2H_4	Hydrazine	2.955	2.971	3.009	3.021	-	2.911
CH_6N_2	Methylhydrazine	3.289	3.311	3.328	3.314	-	3.257
C_2N_2	Cyanogen	5.329	5.289	5.354	5.393	-	5.393
$C_2H_8N_2$	1,1-Dimethylhydrazine	3.464	3.482	3.490	3.449	-	3.425
$C_2H_8N_2$	1,2-Dimethylhydrazine	3.457	3.480	3.487	3.458	-	3.433
C_4N_2	Dicyanoacetylene	5.630	5.619	5.630	5.679	-	5.882
$C_4H_2N_2$	Fumaronitrile	5.028	5.002	5.048	5.057	-	5.021
$C_4H_4N_2$	Pyridazine	4.534	4.580	4.592	4.583	-	4.517
$C_4H_4N_2$	Pyrimidine	4.619	4.658	4.648	4.632	-	4.534
$C_4H_4N_2$	Pyrazine	4.619	4.652	4.630	4.631	-	4.590
$C_2H_6N_2O_2$	n-Nitrodimethylamine	3.601	3.585	3.599	3.511	-	3.758
$C_6H_6N_2O_2$	Para nitroaniline	4.492	4.507	4.501	4.478	-	4.584
$C_2H_4N_2O_4$	1,1-Dinitroethane	3.729	3.705	3.696	3.652	-	3.873
$C_3H_6N_2O_4$	1,1-Dinitropropane	3.779	3.768	3.764	3.731	-	3.899
$C_3H_6N_2O_4$	1,3-Dinitropropane	3.796	3.781	3.788	3.759	-	3.957
$C_3H_6N_2O_4$	2,2-Dinitropropane	3.782	3.771	3.763	3.720	-	3.858
$C_4H_8N_2O_4$	1,1-Dinitrobutane	3.828	3.811	3.808	3.784	-	3.914
$C_4H_8N_2O_4$	1,4-Dinitrobutane	3.839	3.824	3.832	3.812	-	3.962
$C_6H_4N_2O_4$	m-Dinitrobenzene	4.545	4.551	4.529	4.486	-	4.702
N_3	Azide	3.450	3.348	3.335	3.328	-	3.454
HN_3	Hydrazoic acid	3.458	3.404	3.426	3.399	-	3.606
$C_3H_5N_3O_6$	1,1,1-trinitropropane	3.772	3.745	3.737	3.678	-	3.874
$C_7H_5N_3O_6$	2,4,6-Trinitrotoluene	4.394	4.414	4.398	4.335	-	4.581
$C_3H_5N_3O_9$	Glycerol trinitrate	3.742	3.716	3.729	3.704	-	3.822
CH_2N_4	[1-H]Tetrazole	3.988	3.948	4.018	3.804	-	3.970
CN_4O_8	Tetranitromethane	3.582	3.622	3.549	3.467	-	3.719

Table S2. The bond lengths (in Angstroms) for various $H_kC_lN_mO_n$ molecules calculated within the NTBM1 model along with the corresponding experimental values and the values calculated using AM1/PM3/PM7 and the set of the model parameters from Ref. [Zhao J, Lu JP. Phys. Lett. A. 2003;319:523-529.]. The experimental and AM1/PM3 values are taken from the original PM3 work [Stewart JJP. J. Comp. Chem. 1989;10:221-264.]. The AM1/PM3 bond lengths for the cubane C_8H_8, imidogen NH, and amidogen NH_2 are obtained using GAMESS program package [Schmidt MW, Baldridge KK, Boatz JA, Elbert ST, Gordon MS, Jensen JH, Koseki S, Matsunaga N, Nguyen KA, Su SJ, Windus TL, Dupuis M, Montgomery JA. J. Comp. Chem. 1993;14:1347-1363.]. The PM7 bond lengths are obtained using MOPAC2012 [Stewart JJP, Stewart Computational Chemistry, Colorado Springs, CO, USA, HTTP://OpenMOPAC.net (2012).], and experimental values for cubane, imidogen, and amidogen are taken from NIST database [Computational Chemistry Comparison and Benchmark DataBase http://cccbdb.nist.gov/].

Formula	Name	Bond type	Exper.	PM3	PM7	AM1	Zhao-Lu	Present work
1	2	3	4	5	6	7	8	9
H_2	Hydrogen	HH	0.741	0.699	0.76	0.677	0.745	0.745
CH	Methylidyne	CH	1.120	1.088	1.08	1.106	1.089	1.081
CH_2	Methylene, triplet	CH	1.029	1.064	1.02	1.063	1.079	1.080
CH_4	Methane	CH	1.094	1.087	1.08	1.112	1.089	1.099
C_2	Carbon, dimer	CC	1.242	1.189	1.17	1.164	1.159	1.230
C_2H_2	Acetylene	CC	1.203	1.190	1.21	1.195	1.201	1.226
		CH	1.060	1.064	1.03	1.061	1.064	1.078
C_2H_4	Ethylene	CC	1.339	1.322	1.33	1.326	1.319	1.327
		CH	1.086	1.086	1.08	1.098	1.091	1.097
C_2H_6	Ethane	CC	1.536	1.504	1.53	1.500	1.542	1.476
		CH	1.091	1.098	1.10	1.117	1.094	1.102
C_3H_4	Allene	CC	1.308	1.297	1.30	1.298	1.312	1.323
		CH	1.087	1.086	1.09	1.100	1.095	1.100
C_3H_4	Cyclopropene	C_2C_3	1.509	1.484	1.50	1.489	1.585	1.537
		C_1C_3	1.296	1.314	1.32	1.318	1.297	1.326
		C_1H	1.072	1.073	1.04	1.069	1.065	1.074
C_3H_4	Propyne	C_2C_1	1.206	1.191	1.21	1.197	1.206	1.235
		C_1H	1.056	1.064	1.03	1.060	1.064	1.079
		C_2C_3	1.459	1.433	1.43	1.427	1.492	1.446
		C_3H	1.105	1.098	1.10	1.121	1.099	1.106
C_3H_6	Cyclopropane	CC	1.510	1.499	1.51	1.501	1.547	1.507
		CH	1.089	1.095	1.09	1.104	1.077	1.088
C_3H_6	Propene	C=C	1.336	1.328	1.34	1.331	1.327	1.341
		C–C	1.501	1.480	1.43	1.476	1.545	1.479
		C_3H	1.085	1.098	1.09	1.118	1.091	1.096
		C_2H	1.090	1.097	1.09	1.103	1.096	1.098
		HC_1	1.091	1.087	1.08	1.098	1.096	1.104

Table S2. (continued)

1	2	3	4	5	6	7	8	9
C_3H_8	Propane	CC	1.526	1.512	1.53	1.507	1.557	1.495
		C_2H	1.115	1.108	1.10	1.122	1.097	1.104
		C_1H	1.096	1.097	1.10	1.117	1.093	1.101
C_4H_6	Bicyclobutane	C_1C_2	1.498	1.507	1.52	1.510	1.599	1.552
		C_1C_3	1.497	1.481	1.49	1.495	1.544	1.517
		C_1H	1.071	1.083	1.06	1.079	1.062	1.074
		C_2H	1.093	1.095	1.08	1.105	1.084	1.092
C_4H_6	2-Butyne	C_2C_3	1.213	1.193	1.21	1.198	1.211	1.242
		C_1C_2	1.467	1.432	1.43	1.425	1.494	1.447
		CH	1.115	1.098	1.10	1.121	1.099	1.107
C_4H_6	1,3-Butadiene	C_1C_2	1.344	1.331	1.33	1.335	1.335	1.347
		C_2C_3	1.467	1.456	1.46	1.451	1.526	1.475
C_4H_8	1-Butene	C_2C_3	1.347	1.328	1.34	1.331	1.326	1.338
		C_1C_2	1.508	1.489	1.50	1.484	1.564	1.500
C_4H_8	Cyclobutane	CC	1.548	1.542	1.55	1.543	1.613	1.541
		CH	1.105	1.100	1.09	1.110	1.086	1.094
C_4H_8	Isobutene	C_1C_2	1.330	1.333	1.34	1.336	1.335	1.355
		C_2C_3	1.507	1.487	1.50	1.484	1.562	1.500
C_4H_{10}	n-Butane	C_1C_2	1.533	1.512	1.53	1.507	1.556	1.492
		C_2C_3	1.533	1.521	1.53	1.514	1.576	1.517
C_4H_{10}	Isobutane	CC	1.525	1.520	1.53	1.514	1.572	1.514
C_5H_8	1,4-Pentadiene	C=C	1.339	1.328	1.33	1.331	1.325	1.338
		C–C	1.511	1.489	1.50	1.484	1.568	1.502
C_5H_{12}	Neopentane	CC	1.539	1.527	1.54	1.521	1.584	1.532
		CH	1.120	1.098	1.09	1.116	1.092	1.099
C_6H_6	Benzene	CC	1.399	1.391	1.39	1.395	1.424	1.407
		CH	1.084	1.095	1.08	1.100	1.091	1.095
C_6H_6	Fulvene	C_3C_4	1.476	1.471	1.48	1.476	1.569	1.504
		C_2C_3	1.355	1.355	1.35	1.363	1.359	1.376
		C_1C_2	1.470	1.478	1.48	1.483	1.547	1.480
		C_1C_6	1.349	1.331	1.33	1.332	1.338	1.358
C_6H_{10}	Cyclohexene	C_1C_2	1.335	1.334	1.33	1.337	1.333	1.348
		C_2C_3	1.504	1.487	1.49	1.483	1.562	1.506
		C_3C_4	1.515	1.521	1.53	1.517	1.573	1.507
		C_4C_5	1.550	1.519	1.53	1.514	1.570	1.490
C_6H_{12}	Cyclohexane	CC	1.536	1.521	1.54	1.515	1.575	1.506
		CH	1.121	1.107	1.11	1.121	1.096	1.104
C_8H_8	Cubane	CC	1.571	1.568	1.58	1.576	1.649	1.570
		CH	1.097	1.088	1.06	1.086	1.073	1.082
C_{60}	[60]Fullerene	CC	1.458	1.457	1.46	1.464	1.530	1.481
		CC	1.401	1.383	1.38	1.385	1.418	1.412
OH	Hydroxyl radical	OH	0.970	0.937	0.97	0.949	0.985	0.982
H_2O	Water	OH	0.957	0.951	0.96	0.961	0.960	0.974
CO	Carbon monoxide	CO	1.128	1.135	1.14	1.171	1.156	1.110
CH_2O	Formaldehyde	CO	1.208	1.202	1.21	1.227	1.207	1.190
		CH	1.116	1.091	1.10	1.110	1.088	1.109

Table S2. (continued)

1	2	3	4	5	6	7	8	9
CH_4O	Methanol	CO	1.425	1.395	1.42	1.410	1.380	1.343
		CH	1.094	1.097	1.09	1.119	1.089	1.103
		OH	0.945	0.949	0.97	0.964	0.962	0.978
C_4H_4O	Furan	CO	1.362	1.378	1.38	1.395	1.410	1.334
		C_3C_2	1.361	1.373	1.37	1.380	1.349	1.401
O_2	Oxygen, triplet	OO	1.216	1.169	1.14	1.086	1.215	1.230
H_2O_2	Hydrogen peroxide	OO	1.475	1.482	1.43	1.300	1.405	1.397
		OH	0.950	0.945	0.99	0.983	0.968	0.991
CO_2	Carbon dioxide	CO	1.162	1.181	1.17	1.189	1.157	1.202
CH_2O_2	Formic acid	C=O	1.202	1.211	1.20	1.230	1.265	1.273
		C–O	1.343	1.344	1.35	1.357	1.229	1.293
		OH	0.972	0.953	0.99	0.971	0.960	0.980
		CH	1.097	1.095	1.09	1.103	1.073	1.097
$C_6H_4O_2$	p-Benzoquinone	C_1C_2	1.477	1.487	1.49	1.479	1.499	1.480
		C_2C_3	1.322	1.335	1.33	1.338	1.363	1.360
		CO	1.222	1.217	1.21	1.236	1.272	1.252
NH	Imidogen	NH	1.036	0.974	0.98	0.988	-	1.044
NH_2	Amidogen	NH	1.024	0.987	0.99	0.996	-	1.014
NH_3	Ammonia	NH	1.012	0.999	0.99	0.998	-	1.012
CN	Cyanide	CN	1.175	1.157	1.14	1.148	-	1.157
CHN	Hydrogen cyanide	CN	1.154	1.156	1.15	1.160	-	1.166
		CH	1.063	1.070	1.04	1.069	-	1.069
CH_5N	Methylamine	CN	1.474	1.469	1.47	1.432	-	1.394
		NH	1.011	0.999	1.01	1.000	-	1.011
C_2H_3N	Acetonitrile	CC	1.458	1.440	1.44	1.439	-	1.421
		CH	1.104	1.098	1.10	1.120	-	1.108
		CN	1.157	1.159	1.16	1.163	-	1.176
C_2H_3N	Methyl isocyanide	CN–	1.424	1.433	1.41	1.395	-	1.376
		CH	1.101	1.097	1.11	1.125	-	1.101
		CN	1.166	1.181	1.18	1.181	-	1.165
C_3H_9N	Trimethylamine	CN	1.451	1.480	1.48	1.445	-	1.433
C_4H_5N	Pyrrole	CN	1.370	1.397	1.39	1.392	-	1.367
		C_3C_2	1.382	1.390	1.39	1.402	-	1.405
		C_4C_3	1.417	1.390	1.40	1.402	-	1.445
NO	Nitrogen oxide	NO	1.151	1.127	1.13	1.115	-	1.177
HNCO	Hydrogen isocyanate	NH	0.987	0.985	0.99	0.985	-	0.994
		CN	1.207	1.251	1.22	1.232	-	1.223
		CO	1.171	1.181	1.17	1.202	-	1.172
CH_3NO	Formamide	CN	1.376	1.413	1.39	1.367	-	1.309
		NH	1.002	0.994	0.99	0.986	-	1.010
		CH	1.102	1.102	1.09	1.114	-	1.091
		CO	1.193	1.217	1.21	1.243	-	1.254
NO_2	Nitrogen dioxide	NO	1.197	1.181	1.18	1.159	-	1.205
HNO_3	Nitric acid	N=O	1.206	1.203	1.21	1.195	-	1.270
		N–O	1.405	1.410	1.41	1.333	-	1.272
		OH	0.960	0.953	1.00	0.982	-	0.981

Table S2. (continued)

1	2	3	4	5	6	7	8	9
N_2	Nitrogen	NN	1.094	1.098	1.11	1.106	-	1.135
N_2H_4	Hydrazine	NN	1.449	1.440	1.45	1.378	-	1.321
		NH	1.022	1.001	1.02	1.014	-	1.013
C_2N_2	Cyanogen	CN	1.154	1.159	1.15	1.162	-	1.179
		CC	1.389	1.382	1.39	1.384	-	1.398
N_3	Azide	NN	1.181	1.174	1.18	1.177	-	1.218

Table S3. The valence angles (in degrees) for various $H_kC_lN_mO_n$ molecules calculated within the NTBM1 model along with the corresponding experimental values and the values calculated using AM1/PM3/PM7 and the set of the model parameters from Ref. [Zhao J, Lu JP. Phys. Lett. A. 2003;319:523-529.]. The experimental and AM1/PM3 values are taken from the original PM3 work [Stewart JJP. J. Comp. Chem. 1989;10:221-264]. The PM7 valence angles are obtained using MOPAC2012 [Stewart JJP, Stewart Computational Chemistry, Colorado Springs, CO, USA, HTTP://OpenMOPAC.net (2012).].

Formula	Name	Angle type	Exper.	PM3	PM7	AM1	Zhao-Lu	Present work
1	2	3	4	5	6	7	8	9
CH_2	Methylene, triplet	HCH	144.7	144.7	175.5	148.3	113.0	140.1
C_2H_4	Ethylene	HCC	121.2	123.1	123.6	122.7	123.7	122.0
C_2H_6	Ethane	HCC	110.9	111.6	111.4	110.7	111.0	110.4
C_3H_4	Allene	HCC	120.9	122.3	123.6	122.3	124.4	123.1
C_3H_4	Cyclopropene	HC_1C_2	149.9	151.5	153.6	151.9	154.6	154.0
C_3H_4	Propyne	HCC	111.0	110.7	111.9	110.5	112.0	111.8
C_3H_6	Propene	CCC	124.3	123.4	123.6	124.3	127.4	127.7
		HC_3C_2	111.2	112.9	112.9	111.9	111.0	109.9
		HC_2C_1	119.0	120.8	121.7	120.9	120.4	119.2
		HC_1C_2	121.5	122.7	123.4	122.3	123.5	121.0
C_3H_8	Propane	CCC	112.4	111.7	111.2	111.8	113.8	115.5
		HC_2C_1	109.5	109.9	109.9	109.5	109.1	108.4
		HC_1C_2	111.8	111.4	111.3	110.4	110.6	110.5
C_4H_6	Bicyclobutane	$C_2C_3C_1C_4$	121.7	120.0	120.4	122.0	133.8	133.4
C_4H_6	2-Butyne	HCC	110.7	110.7	111.7	110.6	112.1	112.0
C_4H_6	1.3-Butadiene	CCC	122.9	122.3	122.7	123.4	127.2	126.7
C_4H_8	1-Butene	CCC	123.8	122.6	122.8	123.4	127.0	126.8
C_4H_8	Isobutene	$C_1C_2C_3$	122.4	122.1	122.5	122.4	123.4	122.6
C_4H_{10}	n-Butane	CCC	112.8	111.6	111.0	111.6	113.3	114.5
C_5H_8	1.4-Pentadiene	C–C=C	115.5	123.1	123.4	123.9	127.0	126.6
		C–C–C	113.1	114.4	109.7	114.3	113.0	113.9
C_5H_{12}	Neopentane	HCC	110.0	111.3	111.3	110.3	110.2	109.6
C_6H_{10}	Cyclohexene	$C_5C_4C_2C_1$	21.8	27.8	28.8	27.2	24.4	24.0
H_2O	Water	HOH	104.5	107.7	104.6	103.5	128.4	112.7
CH_2O	Formaldehyde	HCO	121.8	121.8	121.2	122.2	119.0	117.2
CH_4O	Methanol	HCO	108.5	112.2	110.4	110.9	107.3	107.3
		COH	107.0	107.5	110.3	107.2	129.7	114.9
C_4H_4O	Furan	CCC	110.7	110.2	106.4	110.1	107.5	105.9
H_2O_2	Hydrogen peroxide	HOO	94.8	96.5	97.7	106.0	107.3	103.8
		HOOH	119.8	180.0	174.3	127.9	145.6	105.1
CH_2O_2	Formic acid	OCO	124.9	117.1	121.6	117.6	117.6	134.9
		HOC	106.3	111.6	115.0	110.6	144.3	117.3
		HCO	124.1	130.4	129.8	130.1	121.6	115.4
$C_6H_4O_2$	p-Benzoquinone	CCC	121.1	121.6	121.4	121.9	120.6	121.0
NH_3	Ammonia	HNH	106.7	108.1	110.1	109.1	-	120.1
CH_5N	Methylamine	HNC	112.0	109.8	111.4	111.3	-	119.8
		HNH	105.9	108.7	108.4	109.0	-	120.4
C_2H_3N	Acetonitrile	HCC	109.5	110.4	111.9	110.1	-	112.2
C_2H_3N	Methyl isocyanide	HCN	109.1	109.7	110.9	110.1	-	108.1

Table S3. (continued)

1	2	3	4	5	6	7	8	9
C_3H_9N	Trimethylamine	CNC	110.9	112.3	110.6	113.0	-	118.4
C_4H_5N	Pyrrole	CNC	107.7	109.7	108.8	108.8	-	112.5
HNCO	Hydrogen isocyanate	CNH	128.1	123.7	137.9	127.2	-	179.8
		OCN	180.0	168.7	166.9	166.7	-	180.0
CH_3NO	Formamide	OCN	123.8	118.5	119.6	121.9	-	119.3
NO_2	Nitrogen dioxide	ONO	136.0	137.8	139.7	136.4	-	151.1
HNO_3	Nitric acid	O=N=O	130.0	132.7	131.6	129.0	-	121.0
		NOH	102.0	109.0	108.9	109.7	-	106.2
N_2H_4	Hydrazine	HNN	112.0	106.5	105.5	107.4	-	116.2
		HNNH	90.0	180.3	106.4	180.2	-	101.3

Geometries of the peptides employed in this study optimized at the B3LYP/6-311G level of theory

Bradykinin

O	-3.7732970240	3.0205113802	-0.9480528181
O	-7.1286760219	3.6517006229	-3.1815095097
O	-1.6499180885	5.0790991303	0.5127800738
O	5.2145797289	-2.9321573878	0.3596558573
O	1.4073439865	-3.3327446902	2.5867345294
O	8.0936621732	0.2544569253	0.6374231917
O	2.2882992051	3.6485354681	0.6757962321
O	3.1834892640	-0.1022571157	1.0971753045
O	-1.0552671413	-3.6843382470	-0.0333811264
O	-0.6732879593	-7.0915940265	1.5747252317
O	-0.4857814008	-8.7040605138	0.0021510148
N	-3.0402325041	4.9121871331	-1.9969715189
N	-6.4710972688	3.8475853418	-1.0016333465
N	4.6728746814	-2.5085921321	2.5341077948
N	-0.4434252786	3.2331921223	-0.1296044359
N	-9.6740621440	3.1477748890	-2.3902186379
N	2.4684585841	-3.4953400422	0.5601726482
N	5.2773703409	0.3236390723	1.8981829638
N	2.0076789710	2.0292218780	2.2846744418
N	-10.6048170932	-1.8572128963	-0.6161570779
N	0.4646732918	-5.3691216454	-0.3796598761
N	-9.4607708515	-3.7130583361	0.4096446318
N	-11.7343940542	-3.3698821275	0.7337143484
N	-0.5065380650	-4.8804379673	-5.4907582124
N	0.3944617394	-5.8767605475	-7.4816288718
N	-0.0960881004	-3.6047709621	-7.3833588153
C	-5.4090994210	4.7981913936	-1.3445237766
C	-5.4402445415	5.7950356429	-0.1458562920
C	-1.6270264996	4.5107680623	-1.8534214953
C	-5.9656321708	4.9629342950	1.0583080946
C	-6.5133549526	3.6370721697	0.4605995576
C	-0.8460187085	5.7169636221	-2.4421126121
C	-3.1985571021	6.2149964934	-2.6845570308
C	-4.0277524996	4.1480831955	-1.4367993011
C	-1.8485439961	6.3944481652	-3.3970562276
C	-7.3320804828	3.4003213760	-1.9632916483
C	-1.2646239880	4.2917988299	-0.3800766770
C	-8.5901235474	2.6332285043	-1.5485874179
C	3.8259722656	-3.7427390356	2.6162429824
C	-8.3592140902	1.0957245266	-1.6308773199
C	3.6721155648	-3.9932647878	4.1326422085
C	4.7415784482	-3.1112419854	4.8107104589
C	4.8569952549	-1.9015596141	3.8710955243
C	-9.5693925366	0.3080626228	-1.1053979334
C	0.0168977695	2.9169879798	1.2078629787
C	5.2339168761	-2.1501302419	1.3544982039
C	2.4572842601	-3.5030504374	1.9259230513
C	5.8920070063	-0.7768344777	1.1403387770
C	-9.3785054426	-1.2155473888	-1.1024004954
C	1.5372556917	2.9035226994	1.3362222123
C	1.2872590985	-3.0492421796	-0.1926496155
C	3.4250013113	1.8569755856	2.5416645518
C	7.4124056373	-0.8107633345	1.3524528185
C	3.9419327292	0.6202533156	1.7733270759
C	1.6450083374	-2.8184826584	-1.6919016673
C	3.7104685632	1.7270084668	4.0670984266
C	0.1312329570	-4.0566925276	-0.1492059101
C	2.3740563641	-1.5343690049	-2.0324717991
C	3.2045450540	2.8652282474	4.9286424782
C	-0.5341560201	-6.3796206366	-0.7657525317
C	-10.5679037071	-2.9201786267	0.1178945667
C	-0.3410587756	-6.8699323247	-2.2125502728
C	3.7595443575	-1.5147726050	-2.2402295964
C	1.6502144726	-0.3448906667	-2.2102603298
C	2.0970544326	2.6781406384	5.7680166241
C	3.8483035531	4.1121261452	4.9343129116
C	-0.6178605306	-5.7475808243	-3.2242611041
C	-0.5498577938	-7.5086808366	0.2641758655
C	4.4092827494	-0.3324477473	-2.6082170520
C	2.2970550986	0.8364731562	-2.5755262976
C	3.6807556581	0.8470386102	-2.7755365698
C	1.6447481782	3.7065827130	6.5986944991
C	3.3976820740	5.1436190697	5.7609282170
C	-0.3295310424	-6.0982629586	-4.6887368887
C	2.2963116226	4.9420334080	6.5987031985
C	-0.0948746424	-4.8254415529	-6.7159508053
H	7.7828519347	1.1320723423	0.9216633453
H	-0.6891133606	-6.1184799180	1.6691760027
H	-0.2136956495	2.5993688215	-0.8767686083
H	-10.5619290598	2.6835266808	-2.2699671633
H	-9.3966192465	3.2575837136	-3.3568395246
H	3.3797319795	-3.4744106491	0.1094401722
H	5.8618953751	0.9000157303	2.4823755570
H	1.3847858196	1.3191569671	2.6354953128
H	1.4416681784	-5.6155852037	-0.4368419297
H	-9.4271037902	-4.2241087734	1.2739023616
H	-8.5939894516	-3.5644492986	-0.0720055972
H	-12.5418766203	-2.7903178774	0.5790511427
H	-11.8946570847	-4.3607511538	0.8106413037
H	0.3392102175	-6.8178808889	-7.1403948975
H	0.9970468946	-5.6986045016	-8.2650467048
H	-0.3958298078	-2.8206491126	-6.8293937149
H	-0.3095113986	-3.5754644755	-8.3663423484
H	-5.6725084466	5.2619884665	-2.2916942768
H	-6.1228206978	6.6116295324	-0.3840612126
H	-4.4567972957	6.2161327569	0.0574987292
H	-1.4441212989	3.5939991399	-2.4209901447
H	-5.1643603262	4.7614583092	1.7686182692
H	-6.7497327972	5.5071710129	1.5862237262
H	-5.8696179688	2.7961363650	0.7207599068
H	-7.5252078947	3.4183500362	0.7924762761
H	0.0744338112	5.4062609432	-2.9338234918
H	-0.5843691123	6.3981716950	-1.6309229754
H	-4.0353593390	6.1837422108	-3.3805943347

Bradykinin (continued)

H	-3.3722951437	7.0186840856	-1.9633512328
H	-1.8646601182	5.8853199202	-4.3629915948
H	-1.6118992882	7.4438580744	-3.5721706114
H	-8.8402232300	2.8703545387	-0.5123435958
H	4.3504692575	-4.5493856228	2.1037594476
H	-7.4666484798	0.8320496893	-1.0505633330
H	-8.1505455007	0.8384141301	-2.6741450342
H	3.7860017096	-5.0478233335	4.3764456230
H	2.6696923092	-3.6873528745	4.4297819207
H	4.4577788892	-2.8162574248	5.8207751542
H	5.7003235835	-3.6304242262	4.8659939909
H	5.8175531710	-1.3979612296	3.9359390207
H	4.0666026781	-1.1775528103	4.0734513207
H	-9.7980090742	0.6197972154	-0.0801939997
H	-10.4584576203	0.5262007833	-1.7025060637
H	-0.4035949789	1.9622867079	1.5372489788
H	-0.3817608690	3.6949421533	1.8627741478
H	5.7253854466	-0.5996152396	0.0770191283
H	-9.1619025066	-1.5507334842	-2.1251363172
H	-8.4932668179	-1.4591918722	-0.4910989292
H	0.8980861069	-2.1333682388	0.2504393397
H	3.9159226463	2.7444197574	2.1361084168
H	7.6606116759	-0.7833854465	2.4209129681
H	7.8059626020	-1.7288573426	0.9269449095
H	0.7067169464	-2.8393286291	-2.2503802635
H	2.2250574177	-3.6771915874	-2.0426172254
H	4.7903586034	1.6257198060	4.2138087414
H	3.2656197451	0.7925478982	4.4198140558
H	-1.4957058595	-5.8606147446	-0.6883026056
H	-1.0050520450	-7.7209886756	-2.3784814707
H	0.6787261535	-7.2546651785	-2.3287568281
H	4.3374004533	-2.4198777302	-2.1095459030
H	0.5754275326	-0.3518917794	-2.0671065605
H	1.5896951169	1.7206121092	5.7772863131
H	4.7019022851	4.2824362217	4.2885276803
H	-1.6593365936	-5.4234953988	-3.1490343259
H	-0.0097240652	-4.8747049928	-2.9855173769
H	5.4794913106	-0.3387950736	-2.7731891861
H	1.7285262175	1.7494156561	-2.7066250075
H	4.1816760119	1.7645185313	-3.0557985199
H	0.7889223947	3.5428667573	7.2403054891
H	3.8986178821	6.1017235459	5.7470853821
H	-1.0128298633	-6.8981429604	-5.0138814859
H	0.6946763774	-6.4998558063	-4.7763850552
H	1.9468971009	5.7406094432	7.2389366841

Colistin

O	4.2402829715	0.8084992463	1.4878748054
O	7.2260600761	-3.2555164144	0.9125203477
O	-0.5329073027	0.7030476816	1.1697335207
O	-2.4530653759	3.1868311639	-1.5710774318
O	3.3071148146	-4.0260683539	-1.9760157479
O	-2.5092756544	0.2095995754	-4.1777414255
O	1.5779526355	-2.3588159679	-6.4113052602
O	4.3720855812	-2.5363776240	-6.2084648274
O	-4.7170577253	-1.4570406423	1.1951710126
O	2.4130620372	-0.6050681383	-2.2663474270
O	-6.1494933362	0.5197114658	-1.3513995033
O	-7.6596987338	2.1582482867	2.0090484106
O	-2.6668859576	4.1304791939	2.3180186712
N	4.2155979339	-1.4475915071	1.8893069405
N	1.6686791165	1.1607931660	1.6222068810
N	5.0955920272	-3.3100881361	0.0763576359
N	-0.9632317262	3.2880547140	0.1606342123
N	-0.9698233725	1.4444000820	-3.0588077065
N	5.2066220942	-4.3555555269	-3.2371979368
N	2.3308360426	1.2305597125	-3.6443624140
N	-4.0025074633	0.0328534672	-1.8681355317
N	3.2756358446	-2.2404243398	-4.2168952437
N	-5.8101115775	1.0808700731	1.2386614337
N	-4.6191571185	3.8780518656	1.1927926868
N	1.8122990502	5.5168442777	0.6286079212
N	5.1534664716	-8.2348020359	0.0458429050
N	3.0952123618	-7.7943770465	-5.1919774671
N	-0.3067128574	-3.2557354266	-1.6089031181
N	-4.5334387064	5.3078787765	-1.1645668841
C	2.0723795806	-0.2162983728	1.8955247735
C	5.6750591356	-1.5921538308	1.7605106985
C	1.5479389644	-0.7821906079	3.2433489849
C	6.4235740353	-1.5632806272	3.1151426034
C	2.1623061277	-0.2487884087	4.5590895804
C	5.8813127791	-2.4640366783	4.2484622241
C	3.6002042652	-0.2394727925	1.7522244859
C	0.2970659425	3.0004597253	0.8379150542
C	6.0594028547	-2.7976634227	0.8924776034
C	5.3633092881	-4.4681112783	-0.7862990277
C	0.4199604047	1.5223702931	1.2406087636
C	-0.3071850579	2.0797549566	-1.9202246099
C	1.6395199532	-1.0965623959	5.7374053270
C	1.8899530672	1.2457031024	4.8097496806
C	0.4701849484	3.9661700892	2.0339448353
C	6.6791994668	-2.1911917986	5.5400241160
C	5.9047631251	-3.9664969584	3.9097050311
C	0.8739833994	2.9508427978	-2.4390420936
C	5.0020301365	-5.7866199760	-0.0596614114
C	-1.3219869933	2.9133022683	-1.0920865014
C	4.6167988404	-4.3053734474	-4.5988664263
C	-2.5381543848	-0.0929909533	-1.7870589615
C	4.5428126684	-4.2723019412	-2.0593237950
C	2.2295446920	2.2252089987	-2.5675350617
C	-6.3141469505	5.8673297975	6.4271534528
C	-5.9888960403	4.6310199254	5.5537970408
C	2.6589317755	-0.9895707753	-4.6580145078
C	0.6704435799	5.4130784781	1.5588159149
C	-1.9998311963	0.5433653387	-3.0801011996
C	-5.0758211006	4.9090883822	4.3445950452
C	3.5509377301	-5.4003013499	-4.8534941230
C	-4.5858189348	0.8077386098	0.4834841771
C	-2.1323007157	-1.5897579693	-1.7237145503
C	5.4809917006	-7.0598526446	-0.7677095443
C	4.0867643144	-2.9344760651	-5.0422023124
C	-7.2286482488	5.4995848905	7.6230062232
C	1.3496886259	-1.2636437798	-5.4792637491
C	-6.0523047129	3.6035771753	0.9845137022
C	2.4513742430	-0.1089338322	-3.4184596859
C	-4.6110095039	3.5949004435	3.6606896219
C	-4.9590422777	0.4224504993	-0.9741036777
C	-3.8134831054	-0.2966202632	1.2364917097
C	-6.9566838217	7.0052657394	5.6082564116
C	4.1438754084	-6.8157147218	-4.8958522528
C	-6.4096842108	3.8130559149	-0.5139168011
C	-6.5417750905	2.2156842941	1.4373278072
C	-0.6188910163	-1.8181736015	-1.6493515626
C	-3.9159620692	3.8685713986	2.3465069913
C	-6.6298668271	4.5012565908	8.6300097257
C	0.8323428972	-0.0450652008	-6.2461300068
C	-3.4555843720	0.0629484728	2.6756311686
C	-6.0039459587	5.1786896801	-1.0961392517
H	2.4662292075	-2.2865344964	-6.8194664850
H	-4.3206184869	-2.2172761487	1.6534479180
H	3.6826264695	-2.2309799040	2.2342265474
H	2.4437906079	1.8084240469	1.5400209627
H	4.1857085716	-2.8782766955	0.0047250090
H	-1.6918843631	3.7050275695	0.7528053034
H	-0.8011868915	1.8551581498	-3.9657353145
H	6.2077905650	-4.4697764081	-3.1945081060
H	2.4127190594	1.5662152437	-4.5908716102
H	-4.3703131017	-0.1519011888	-2.7947179195
H	3.0120133676	-2.6124681962	-3.3074149003
H	-6.3190075692	0.2385439848	1.4800779470
H	-4.1819318462	4.3579615092	0.3868095474
H	1.7721906320	6.3202249868	0.0159464545
H	2.7195249224	5.4543056475	1.0774893514
H	5.6623513821	-9.0750135542	-0.1886294421
H	4.1622644865	-8.4120975221	0.1447528294
H	3.4213301037	-8.6949519099	-5.5121515174
H	2.3749741991	-7.8780189169	-4.4877498225
H	0.6822211994	-3.4524950533	-1.5025181005
H	-0.6892671538	-3.7692133481	-2.3948470659
H	-4.2003320598	6.2462858398	-1.3388854090
H	-4.0550903491	4.6229138877	-1.7428354904
H	1.6558574708	-0.8484403826	1.1031616268
H	5.9958818616	-0.7062168547	1.2063477606
H	1.6835146264	-1.8705659473	3.2176201905
H	0.4672061398	-0.6223281418	3.2472127216
H	6.4081299129	-0.5267918719	3.4628992237
H	7.4640685693	-1.8226747843	2.9084902388

Colistin (continued)

H	3.2498978216	-0.3864879939	4.5126242292
H	4.8412648206	-2.1739156982	4.4441639505
H	1.1280790119	3.2274382237	0.1670645032
H	6.4345875231	-4.4603579793	-0.9967487365
H	0.0933036821	1.3008177362	-1.2703351464
H	1.8804103586	-2.1549933115	5.6075126309
H	2.0789380788	-0.7652722301	6.6805327644
H	0.5525568116	-1.0087401896	5.8257324118
H	2.2680890728	1.5406264694	5.7913114314
H	0.8172034397	1.4556070351	4.7878146244
H	2.3700347473	1.8758205443	4.0633657879
H	-0.4084463431	3.9142640495	2.6778726334
H	1.3382625504	3.6513712434	2.6196348942
H	6.6404373204	-1.1339552902	5.8141365088
H	6.2784518158	-2.7691569832	6.3757279530
H	7.7294468815	-2.4667006555	5.4117189755
H	5.5585646261	-4.5550420071	4.7626682134
H	6.9147537285	-4.2921901893	3.6545239727
H	5.2613935163	-4.2147709283	3.0618505429
H	1.0372532731	3.7906919329	-1.7595835240
H	0.5888512082	3.4005741941	-3.3963774177
H	3.9164213818	-5.8168345638	0.0744660135
H	5.4576777549	-5.7619863417	0.9300888413
H	5.4517212864	-4.4856350075	-5.2760346449
H	-2.1696253680	0.4313677980	-0.9102783784
H	3.0086188898	2.9757255070	-2.7275034223
H	2.4687152231	1.7020152031	-1.6420485997
H	-5.3653555840	6.2429923586	6.8402999234
H	-6.9272651924	4.1890762257	5.1962743122
H	-5.5104701184	3.8717575625	6.1807307669
H	3.3679760303	-0.5039401110	-5.3346873867
H	0.7782343286	6.0556103839	2.4427826576
H	-0.2244901276	5.7425283867	1.0317515124
H	-4.1914171733	5.4751514655	4.6563143671
H	-5.6015850237	5.5298340696	3.6134623695
H	2.7716179316	-5.3344563196	-4.0917788010
H	3.0736372894	-5.1989353945	-5.8130965993
H	-3.9664634056	1.7026262794	0.4514769850
H	-2.5416929931	-2.0715713452	-2.6172149849
H	-2.6207953890	-2.0467749889	-0.8621480162
H	5.0660080948	-7.1057938639	-1.7868469548
H	6.5694454040	-7.0211301587	-0.8691431645
H	-7.4795611738	6.4243297194	8.1541554750
H	-8.1755642757	5.1055900104	7.2346721083
H	0.5798813482	-1.6338459654	-4.8020308636
H	-6.6573677801	4.2955300111	1.5764543730
H	-3.8995024369	3.0813953772	4.3080236757
H	-5.4690893159	2.9367875335	3.5265688401
H	-2.8976570542	-0.5299536315	0.7005609129
H	-7.1936674595	7.8569613360	6.2499486541
H	-7.8866256068	6.6708877361	5.1372314670
H	-6.2938359632	7.3638970485	4.8195161396
H	4.6823144903	-7.0177431793	-3.9559384735
H	4.8814456082	-6.8666757746	-5.7028794200
H	-7.4904573560	3.6897169846	-0.6053654856
H	-5.9687683441	3.0178701426	-1.1160855010
H	-0.1356305776	-1.2998038101	-2.4881282856
H	-0.2280072809	-1.3618079072	-0.7366248937
H	-7.2794361192	4.3955211744	9.5026225046
H	-5.6520329366	4.8391113259	8.9844988971
H	-6.5035469610	3.5062488994	8.1993180972
H	1.6093824112	0.3628346075	-6.9005786231
H	-0.0012777966	-0.3638685349	-6.8678186860
H	0.4655685465	0.7352031720	-5.5811019867
H	-2.8066414187	0.9389722296	2.7010439425
H	-4.3541097175	0.2525408662	3.2598868074
H	-2.9039884030	-0.7626300277	3.1342849095
H	-6.4881899936	5.2916912743	-2.0760875675
H	-6.3821156628	5.9838809662	-0.4590835655

Geometries of the peptides employed in this study optimized within the NTBM1 model

Bradykinin

O	-3.96260455	3.05143124	-1.12233737
O	-7.03116095	3.94023427	-3.14735128
O	-1.51275856	5.14294274	0.50054077
O	5.07137156	-2.58787301	0.22742707
O	1.59718056	-2.85851179	2.24720448
O	8.04068275	0.54150537	1.35942520
O	2.23406285	3.98515188	1.04760174
O	3.49976417	0.44045303	0.75793462
O	-1.09353134	-3.98981096	-0.26759246
O	0.24084143	-7.44859247	1.25251273
O	-1.21351834	-8.83690426	0.04931048
N	-3.03306471	4.94224289	-1.81507491
N	-6.53092983	3.99715123	-0.98817407
N	4.72431253	-2.48791883	2.40122969
N	-0.41552857	3.26798902	0.05644896
N	-9.40979447	2.73367755	-2.84539056
N	2.39741870	-3.58963658	0.31437913
N	5.36875764	0.49124549	1.95460713
N	2.12636385	2.15436227	2.29780162
N	-10.35003820	-1.76045100	-0.44659018
N	0.33841327	-5.64586702	-0.57802491
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N	-0.63800084	-5.12535153	-5.48200579
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N	-0.32200926	-3.72708781	-7.45819631
C	-5.45103192	4.97553181	-1.24083415
C	-5.52341495	5.85727093	0.00562322
C	-1.69563495	4.31320153	-1.78397944
C	-6.06473464	4.96583197	1.10547375
C	-6.69229005	3.76793223	0.43443142
C	-0.86086903	5.17452338	-2.72840453
C	-2.99184108	6.29595380	-2.32740796
C	-4.13653629	4.28438354	-1.40256762
C	-1.65643174	6.43395434	-3.01082039
C	-7.32550451	3.53728741	-1.97174217
C	-1.20374164	4.26012680	-0.36878350
C	-8.52579304	2.67198843	-1.72319377
C	3.88274363	-3.70266674	2.29526889
C	-8.19592458	1.21154474	-1.38666345
C	3.74706255	-4.19140380	3.73306647
C	4.36524407	-3.14225539	4.63615436
C	4.86082837	-2.02008549	3.76342338
C	-9.43084824	0.40220605	-1.07657658
C	0.01825895	3.07563039	1.41424124
C	5.24025164	-1.90831818	1.29994066
C	2.58517574	-3.36435960	1.61831518
C	5.98464460	-0.61162733	1.22756227
C	-9.16282171	-1.06682926	-0.84362125
C	1.49819603	3.08088238	1.56524911
C	1.18615148	-3.27278467	-0.42153865
C	3.56019232	2.09642238	2.52291517
C	7.44291309	-0.66276818	1.63123189
C	4.14539304	0.97296886	1.71980212
C	1.55941181	-2.89898818	-1.85759121
C	3.83958228	2.00238559	4.01952879
C	0.12723015	-4.33919630	-0.39017846
C	2.35337538	-1.62409093	-1.98647574
C	3.22236452	3.11750026	4.82588235
C	-0.70586669	-6.62943540	-0.77104678
C	-10.48866646	-3.03619218	0.15843797
C	-0.71392769	-7.07415554	-2.23042169
C	3.75577233	-1.64617546	-2.21708017
C	1.70183177	-0.36063683	-1.92424949
C	2.08511921	2.88767339	5.64700627
C	3.78098265	4.42508555	4.79859420
C	-0.84124715	-5.91586994	-3.19038664
C	-0.54723254	-7.73278691	0.23085823
C	4.47166375	-0.45121710	-2.39669899
C	2.42444431	0.82863754	-2.10547983
C	3.81087712	0.78960889	-2.34527705
C	1.53735634	3.92509938	6.41889881
C	3.22808050	5.45609619	5.57393292
C	-0.57488596	-6.27616786	-4.63329755
C	2.10620932	5.21145080	6.38800797
C	-0.18222909	-4.96493584	-6.81603438
H	7.47181353	1.31221972	1.55634600
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H	-10.39809846	2.85619207	-2.68014586
H	-9.03309596	2.66199661	-3.77948166
H	3.13999238	-4.00946867	-0.22761131
H	5.94817391	0.90478576	2.67092061
H	1.59206405	1.41088397	2.72575680
H	1.28199241	-6.00133665	-0.65500743
H	-9.46707621	-4.72074290	0.85866352
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H	-12.57832055	-2.94807818	0.30925730
H	-11.85142950	-4.42378716	0.92977042
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H	0.73292782	-5.91271345	-8.43959938
H	-0.74447699	-2.95048891	-6.96733827
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H	-3.83293532	6.42201845	-3.02269201

Bradykinin (continued)

H	-3.08791336	6.98937166	-1.47789416
H	-1.79286711	6.55436780	-4.09711900
H	-1.12198412	7.31908695	-2.63243513
H	-9.10599819	3.08557973	-0.88416124
H	4.45745269	-4.41672742	1.68825738
H	-7.52887736	1.20052399	-0.51169236
H	-7.66496082	0.75798672	-2.23850607
H	4.27428018	-5.15047686	3.85109241
H	2.68915774	-4.34324269	3.99395902
H	3.62117484	-2.76905246	5.35676891
H	5.20078865	-3.58208218	5.20333836
H	5.91950177	-1.78832192	3.94143852
H	4.24461264	-1.11517929	3.87404094
H	-9.90591032	0.81730362	-0.17222460
H	-10.14044225	0.49880667	-1.91530566
H	-0.41344676	2.11750983	1.74543841
H	-0.41402615	3.90694023	1.99124761
H	5.97568232	-0.30511598	0.16800164
H	-8.78474059	-1.53112746	-1.77178945
H	-8.41297093	-1.19063598	-0.04343910
H	0.75595805	-2.39415376	0.08398972
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H	7.58444315	-0.81607160	2.71861279
H	8.01950902	-1.37948493	1.02548141
H	0.61907073	-2.78269878	-2.42032364
H	2.12152320	-3.73792439	-2.29709716
H	4.93292637	2.02767012	4.15536272
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H	-1.65014579	-6.11641099	-0.53960651
H	-1.56004604	-7.76377400	-2.37546297
H	0.21914576	-7.61958959	-2.44460853
H	4.28468774	-2.60304820	-2.26844134
H	0.62241239	-0.31475712	-1.74834116
H	1.63423321	1.89103852	5.68627621
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H	-1.85733087	-5.49545361	-3.11101625
H	-0.12154991	-5.13533453	-2.89372195
H	5.55013797	-0.48621423	-2.58299519
H	1.90626423	1.79240428	-2.06475000
H	4.37043084	1.71876025	-2.49129248
H	0.66452535	3.73024407	7.05084117
H	3.67463668	6.45557834	5.54804202
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H	1.68040270	6.01660218	6.99475107

Colistin

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O	-0.22582537	0.69316454	0.90726939
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O	3.48647423	-4.13910280	-2.09851125
O	-2.58641417	0.40885076	-4.25625614
O	1.54461366	-2.18231409	-6.62199679
O	5.07403840	-1.97141202	-5.17719591
O	-4.46946365	-1.50202719	1.29092344
O	2.32967670	-0.60350920	-2.40696465
O	-6.14344654	0.28679278	-1.34683799
O	-7.38139247	2.18026086	2.17651211
O	-2.75717286	4.27275115	2.47177788
N	4.22499702	-1.48100278	2.10965838
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N	3.02485816	-2.37542388	-4.43401450
N	-5.81164307	1.05238075	1.18499383
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N	3.07832929	-7.64491845	-5.02628477
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C	1.47696766	-0.69652278	3.22925063
C	6.42348690	-1.60990855	3.13702770
C	2.10053725	-0.22876728	4.54466056
C	5.95428003	-2.53547848	4.25737027
C	3.60585295	-0.32381435	1.85817308
C	0.41609204	3.04718356	0.78759302
C	5.91991596	-2.95219822	1.04363581
C	5.48185741	-4.54874211	-0.78788440
C	0.62788749	1.60608914	1.14791874
C	-0.27342692	2.00454679	-2.03967238
C	1.58952953	-1.04776165	5.71078660
C	1.94648911	1.25478245	4.78363003
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C	6.72266264	-2.27924710	5.53568189
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C	-6.39484677	5.87177504	6.50242342
C	-6.04136589	4.63349737	5.68047902
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C	0.58505556	5.45473641	1.58447470
C	-2.08099448	0.63498920	-3.10135355
C	-5.26660168	4.92916623	4.42224881
C	3.59059667	-5.28582437	-4.78852817
C	-4.59608346	0.73305379	0.46481975
C	-2.18494314	-1.49225633	-1.74389625
C	5.48630927	-7.09591373	-0.80179746
C	4.25490003	-2.82379843	-4.69694598
C	-7.25982873	5.51663473	7.71703610
C	1.26735470	-1.24388415	-5.61750790
C	-5.89891011	3.57844678	0.90606504
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C	-4.72466584	3.68499521	3.73831370
C	-4.92993114	0.31740713	-0.93467243
C	-3.80313354	-0.27475714	1.30634985
C	-7.02853178	6.96968250	5.68509562
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C	-6.11898227	3.71625670	-0.59762468
C	-6.33843055	2.24391869	1.43786764
C	-0.69296631	-1.69676337	-1.69780785
C	-3.99798396	3.96089387	2.47488812
C	-6.67361455	4.50907655	8.64267405
C	0.71766922	-0.01032202	-6.25911981
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H	-4.04659639	-2.14521469	1.89579463
H	3.70049293	-2.26956265	2.46166355
H	2.50313114	1.88725595	1.89228001
H	4.24078543	-2.99376634	-0.11868775
H	-1.56289113	3.71908936	0.57642894
H	-0.82376236	1.82042258	-4.06108272
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H	2.39757289	1.58236177	-4.65030152
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H	-3.91879254	4.15895422	0.50073959
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H	2.65255516	5.60699223	1.25696815
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H	2.33043202	-7.69501951	-4.34841688
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H	-0.73905909	-3.68202119	-2.38073528
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H	-4.27395159	4.82221126	-2.37047467
H	1.66561878	-0.72716168	1.12150945
H	5.93788036	-0.85868106	1.21622256
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Colistin (continued)

H	3.18326175	-0.42938841	4.47458330
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H	0.11939144	1.13037817	-1.49511114
H	1.80910781	-2.11070814	5.53231180
H	2.09810664	-0.72483885	6.63117316
H	0.50399394	-0.91780052	5.83212748
H	2.37449639	1.50953309	5.76486167
H	0.88529963	1.54562552	4.76967249
H	2.48769164	1.81483774	4.00832368
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H	1.35115029	3.74459911	2.58935107
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H	6.30715603	-2.90371212	6.34028925
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H	6.98740735	-4.33282699	3.64337637
H	5.33818026	-4.13496097	2.97065357
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H	0.64288352	3.18169713	-3.59692499
H	4.12585769	-5.84851758	0.26605293
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H	5.48254111	-4.40656709	-5.28938716
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H	3.01722573	2.85960389	-2.84048515
H	2.44230312	1.56298105	-1.72761429
H	-5.44709792	6.27350470	6.89809381
H	-6.96638033	4.09867790	5.41218584
H	-5.43276995	3.97379445	6.31831153
H	3.30534653	-0.65559092	-5.48587252
H	0.61789650	6.06620240	2.50297383
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H	-4.41667457	5.58597060	4.66898507
H	-5.92031239	5.46208398	3.71377031
H	2.83253867	-5.22013017	-3.99153247
H	3.10768780	-5.05291235	-5.75124831
H	-4.01171703	1.66531702	0.43456966
H	-2.58772238	-2.04944144	-2.60566500
H	-2.63068870	-1.90198650	-0.82376228
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H	6.55823175	-7.16419309	-1.03392239
H	-7.42652463	6.45232132	8.27540805
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H	-0.22137029	-1.23242861	-2.58297347
H	-0.26879200	-1.26077798	-0.78210698
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H	-5.67350781	4.82392984	8.98089370
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H	1.49006095	0.43734313	-6.90247368
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H	-2.86806520	0.95941425	2.79617794
H	-4.53747725	0.41331681	3.19206609
H	-3.17720941	-0.75918656	3.24473854
H	-6.66385408	5.21335119	-2.02055956
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