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Supporting Information

THEORETICAL-EXPERIMENTAL PREDICTION OF THE SELECTIVITY BETWEEN POLYAMIDOAMINE DENDRIMERS AND BIOACTIVE PEPTIDES DERIVED FROM AMARANTH SEED.

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Contents of supporting information:

1. **Table S1.** Final Z matriz between YLAGKPQQEH and PAMAM. With their absolute energies (Hartrees).

Electronic energy = -5694.929030 Hartrees.

N																			
C	1	B1			H	59	B62 58	A61 53	D60 0	N	122	B123 119	A122 116	D121 0	C	176	B184 168	A183 165	D182 0
C	2	B2 1	A1		C	59	B63 58	A62 53	D61 0	H	124	B124 122	A123 119	D122 0	H	185	B185 176	A184 168	D183 0
O	3	B3 2	A2 1	D1 0	H	64	B64 59	A63 58	D62 0	H	124	B125 122	A124 119	D123 0	H	185	B186 176	A185 168	D184 0
H	1	B4 2	A3 3	D2 0	H	64	B65 59	A64 58	D63 0	N	112	B126 111	A125 110	D124 0	C	170	B187 169	A186 163	D185 0
H	2	B5 1	A4 3	D3 0	C	64	B66 59	A65 58	D64 0	C	127	B127 112	A126 111	D125 0	H	188	B188 170	A187 169	D186 0
C	2	B6 1	A5 3	D4 0	H	67	B67 64	A66 59	D65 0	C	128	B128 127	A127 112	D126 0	H	188	B189 170	A188 169	D187 0
C	7	B7 2	A6 1	D5 0	H	67	B68 64	A67 59	D66 0	O	129	B129 128	A128 127	D127 0	C	173	B190 169	A189 163	D188 0
H	7	B8 2	A7 1	D6 0	C	67	B69 64	A68 59	D67 0	H	127	B130 112	A129 111	D128 0	H	191	B191 173	A190 169	D189 0
H	7	B9 2	A8 1	D7 0	H	70	B70 67	A69 64	D68 0	H	128	B131 127	A130 112	D129 0	H	191	B192 173	A191 169	D190 0
C	8	B10 7	A9 2	D8 0	C	70	B71 67	A70 64	D69 0	C	128	B132 127	A131 112	D130 0	C	188	B193 170	A192 169	D191 0
C	8	B11 7	A10 2	D9 0	H	70	B72 67	A71 64	D70 0	C	133	B133 128	A132 127	D131 0	C	191	B194 173	A193 169	D192 0
C	8	B12 7	A11 2	D10 0	H	72	B73 70	A72 67	D71 0	H	133	B134 128	A133 127	D132 0	C	182	B195 179	A194 168	D193 0
C	13	B13 8	A12 7	D11 0	H	72	B74 70	A73 67	D72 0	H	133	B135 128	A134 127	D133 0	C	185	B196 176	A195 168	D194 0
C	12	B14 8	A13 7	D12 0	N	72	B75 70	A74 67	D73 0	H	134	B136 133	A135 128	D134 0	O	197	B197 185	A196 176	D195 0
H	12	B15 8	A14 7	D13 0	H	76	B76 72	A75 70	D74 0	H	134	B137 133	A136 128	D135 0	O	196	B198 182	A197 179	D196 0
H	13	B16 8	A15 7	D14 0	H	76	B77 72	A76 70	D75 0	C	134	B138 133	A137 128	D136 0	O	195	B199 191	A198 173	D197 0
H	14	B17 13	A16 8	D15 0	N	60	B78 59	A77 58	D76 0	O	139	B139 134	A138 133	D137 0	O	194	B200 188	A199 170	D198 0
H	15	B18 12	A17 8	D16 0	C	79	B79 60	A78 59	D77 0	O	139	B140 134	A139 133	D138 0	N	196	B201 182	A200 179	D199 0
O	11	B19 8	A18 7	D17 0	C	80	B80 79	A79 60	D78 0	H	141	B141 139	A140 134	D139 0	H	202	B202 196	A201 182	D200 0
H	20	B20 11	A19 8	D18 0	O	81	B81 80	A80 79	D79 0	N	129	B142 128	A141 127	D140 0	N	195	B203 191	A202 173	D201 0
N	3	B21 2	A20 1	D19 0	C	79	B82 60	A81 59	D80 0	C	143	B143 129	A142 128	D141 0	H	204	B204 195	A203 191	D202 0
C	22	B22 3	A21 2	D20 0	C	80	B83 79	A82 60	D81 0	C	144	B144 143	A143 129	D142 0	N	194	B205 188	A204 170	D203 0
C	23	B23 22	A22 3	D21 0	H	84	B84 80	A83 79	D82 0	O	145	B145 144	A144 143	D143 0	H	206	B206 194	A205 188	D204 0
O	24	B24 23	A23 22	D22 0	C	83	B85 79	A84 60	D83 0	H	143	B146 129	A145 128	D144 0	N	197	B207 185	A206 176	D205 0
H	22	B25 3	A24 2	D23 0	H	84	B86 80	A85 79	D84 0	H	144	B147 143	A146 129	D145 0	H	208	B208 197	A207 185	D206 0
H	23	B26 22	A25 3	D24 0	H	86	B87 83	A86 79	D85 0	C	144	B148 143	A147 129	D146 0	C	202	B209 196	A208 182	D207 0
C	23	B27 22	A26 3	D25 0	H	86	B88 83	A87 79	D86 0	C	149	B149 144	A148 143	D147 0	H	210	B210 202	A209 196	D208 0
C	28	B28 23	A27 22	D26 0	H	83	B89 79	A88 60	D87 0	H	149	B150 144	A149 143	D148 0	H	210	B211 202	A210 196	D209 0
H	28	B29 23	A28 22	D27 0	H	83	B90 79	A89 60	D88 0	H	149	B151 144	A150 143	D149 0	C	210	B212 202	A211 196	D210 0
C	29	B30 28	A29 23	D28 0	H	80	B91 79	A90 60	D89 0	C	150	B152 149	A151 144	D150 0	H	213	B213 210	A212 202	D211 0
H	31	B31 29	A30 28	D29 0	N	81	B92 80	A91 79	D90 0	N	150	B153 149	A152 144	D151 0	H	213	B214 210	A213 202	D212 0
H	28	B32 23	A31 22	D30 0	C	93	B93 81	A92 80	D91 0	H	153	B154 150	A153 149	D152 0	N	213	B215 210	A214 202	D213 0
C	31	B33 29	A32 28	D31 0	C	94	B94 93	A93 81	D92 0	H	153	B155 150	A154 149	D153 0	H	216	B216 213	A215 210	D214 0
H	34	B34 31	A33 29	D32 0	O	95	B95 94	A94 93	D93 0	C	154	B156 150	A155 149	D154 0	H	216	B217 213	A216 210	D215 0
H	34	B35 31	A34 29	D33 0	H	93	B96 81	A95 80	D94 0	N	157	B157 154	A156 150	D155 0	C	204	B218 195	A217 191	D216 0
H	34	B36 31	A35 29	D34 0	H	94	B97 93	A96 81	D95 0	H	157	B158 154	A157 150	D156 0	H	219	B219 204	A218 195	D217 0
H	29	B37 28	A36 23	D35 0	C	94	B98 93	A97 81	D96 0	H	1	B159 2	A158 3	D157 0	H	219	B220 204	A219 195	D218 0
H	29	B38 28	A37 23	D36 0	H	99	B99 94	A98 93	D97 0	H	145	B160 144	A159 143	D158 0	C	219	B221 204	A220 195	D219 0
H	29	B39 28	A38 23	D37 0	H	99	B100 94	A99 93	D98 0	H	72	B161 70	A160 67	D159 0	H	222	B222 219	A221 204	D220 0
N	24	B40 23	A39 22	D38 0	C	99	B101 94	A100 93	D99 0	C	70	B162 67	A161 64	D160 0	H	222	B223 219	A222 204	D221 0
C	41	B41 24	A40 23	D39 0	H	102	B102 99	A101 94	D100 0	H	163	B163 70	A162 67	D161 0	N	222	B224 219	A223 204	D222 0
C	42	B42 41	A41 24	D40 0	H	102	B103 99	A102 94	D101 0	C	163	B164 70	A163 67	D162 0	H	225	B225 222	A224 219	D223 0
O	43	B43 42	A42 41	D41 0	C	102	B104 99	A103 94	D102 0	H	165	B165 163	A164 70	D163 0	H	225	B226 222	A225 219	D224 0
H	41	B44 24	A43 23	D42 0	O	105	B105 102	A104 99	D103 0	H	165	B166 163	A165 70	D164 0	C	206	B227 194	A226 188	D225 0
H	42	B45 41	A44 24	D43 0	N	105	B106 102	A105 99	D104 0	N	165	B167 163	A166 70	D165 0	H	228	B228 206	A227 194	D226 0
C	42	B46 41	A45 24	D44 0	H	107	B107 105	A106 102	D105 0	N	163	B168 70	A167 67	D166 0	H	228	B229 206	A228 194	D227 0
H	47	B47 42	A46 41	D45 0	H	107	B108 105	A107 102	D106 0	C	169	B169 163	A168 70	D167 0	C	228	B230 206	A229 194	D228 0
H	47	B48 42	A47 41	D46 0	N	95	B109 94	A108 93	D107 0	H	170	B170 169	A169 163	D168 0	H	231	B231 228	A230 206	D229 0
H	47	B49 42	A48 41	D47 0	C	110	B110 95	A109 94	D108 0	H	170	B171 169	A170 163	D169 0	H	231	B232 228	A231 206	D230 0
N	43	B50 42	A49 41	D48 0	C	111	B111 110	A110 95	D109 0	C	169	B172 163	A171 70	D170 0	N	231	B233 228	A232 206	D231 0
C	51	B51 43	A50 42	D49 0	O	112	B112 111	A111 110	D110 0	H	173	B173 169	A172 163	D171 0	H	234	B234 231	A233 228	D232 0
C	52	B52 51	A51 43	D50 0	H	110	B113 95	A112 94	D111 0	H	173	B174 169	A173 163	D172 0	H	234	B235 231	A234 228	D233 0
O	53	B53 52	A52 51	D51 0	H	111	B114 110	A113 95	D112 0	C	168	B175 165	A174 163	D173 0	C	208	B236 197	A235 185	D234 0
H	51	B54 43	A53 42	D52 0	C	111	B115 110	A114 95	D113 0	H	176	B176 168	A175 165	D174 0	H	237	B237 208	A236 197	D235 0
H	52	B55 51	A54 43	D53 0	H	116	B116 111	A115 110	D114 0	H	176	B177 168	A176 165	D175 0	H	237	B238 208	A237 197	D236 0
H	52	B56 51	A55 43	D54 0	H	116	B117 111	A116 110	D115 0	C	168	B178 165	A177 163	D176 0	C	237	B239 208	A238 197	D237 0
N	53	B57 52	A56 51	D55 0	C	116	B118 111	A117 110	D116 0	H	179	B179 168	A178 165	D177 0	H	240	B240 237	A239 208	D238 0
C	58	B58 53	A57 52	D56 0	H	119	B119 116	A118 111	D117 0	H	179	B180 168	A179 165	D178 0	H	240	B241 237	A240 208	D239 0
C	59	B59 58	A58 53	D57 0	H	119	B120 116	A119 111	D118 0	C	179	B181 168	A180 165	D179 0	N	240	B242 237	A241 208	D240 0
O	60	B60 59	A59 58	D58 0	C	119	B121 116	A120 111	D119 0	H	182	B182 179	A181 168	D180 0	H	243	B243 240	A242 237	D241 0
H	58	B61 53	A60 52	D59 0	O	122	B122 119	A121 116	D120 0	H	182	B183 179	A182 168	D181 0	H	243	B244 240	A243 237	D242 0

Continuation

1	2	3	4	5	6	7
B1 1.46343576	B53 1.232608860	B105 1.22487504	B157 1.35860219	B209 1.46109822	A17 121.15633196	A69 109.95214663
B2 1.53316605	B54 1.01357880	B106 1.36158904	B158 1.08073403	B210 1.09787219	A18 176.68561060	A70 114.1971150
B3 1.2412576	B55 1.08956100	B107 1.01488824	B159 1.01673162	B211 1.09236778	A19 110.96786804	A71 109.34598355
B4 1.01756932	B56 1.09949884	B108 1.00767613	B160 1.10920957	B212 1.53783590	A20 115.57531355	A72 109.45283234
B5 1.09937545	B57 1.36097180	B109 1.34953912	B161 4.13440477	B213 1.09563293	A21 121.90535392	A73 109.89416907
B6 1.55025873	B58 1.45817439	B110 1.46475890	B162 4.96790694	B214 1.09850693	A22 114.86516309	A74 110.33642695
B7 1.51249489	B59 1.54155860	B111 1.54186254	B163 1.09691672	B215 1.45946601	A23 119.16642997	A75 109.72469577
B8 1.09331102	B60 1.24024705	B112 1.22418404	B164 1.54757928	B216 1.01813254	A24 113.75497930	A76 108.86250640
B9 1.09661123	B61 1.01475933	B113 1.01829524	B165 1.09756522	B217 1.01803335	A25 107.32532863	A77 121.81103738
B10 2.83604456	B62 1.09622777	B114 1.09173181	B166 1.09319555	B218 1.45101247	A26 112.50250203	A78 118.06944015
B11 1.40354096	B63 1.53831842	B115 1.55081214	B167 1.46758526	B219 1.09312066	A27 102.16164285	A79 114.27020272
B12 1.40353970	B64 1.09817640	B116 1.09352188	B168 1.46687351	B220 1.09724755	A28 105.14090326	A80 118.79517395
B13 1.39203096	B65 1.09467868	B117 1.09420675	B169 1.46515810	B221 1.53385304	A29 33.03654775	A81 128.27329408
B14 1.39328014	B66 1.53491640	B118 1.52763735	B170 1.01431651	B222 1.09497278	A30 107.97477019	A82 103.94260264
B15 1.08797678	B67 1.09751800	B119 1.09524991	B171 1.09148532	B223 1.09639491	A31 108.20329660	A83 109.85076400
B16 1.08790801	B68 1.09833694	B120 1.09283713	B172 1.46546583	B224 1.48230607	A32 110.18472734	A84 102.68224242
B17 1.08570266	B69 1.53616691	B121 1.52507272	B173 1.09613792	B225 1.01870718	A33 111.43793766	A85 111.58050219
B18 1.08505223	B70 1.09760362	B122 1.22921849	B174 1.09338607	B226 1.01930731	A34 110.96676151	A86 109.06828168
B19 1.34706738	B71 1.52882780	B123 1.36274559	B175 1.46373170	B227 1.45772562	A35 111.05394762	A87 111.36872234
B20 1.00137446	B72 1.09991189	B124 1.01673300	B176 1.01348179	B228 1.09409500	A36 95.99872660	A88 110.67937849
B21 1.35150538	B73 1.09475244	B125 1.00810426	B177 1.0981891	B229 1.09525788	A37 91.45705142	A89 111.05169953
B22 1.46730538	B74 1.10146882	B126 1.38387528	B178 1.46570720	B230 1.54115894	A38 143.44072871	A90 109.82364545
B23 1.53889625	B75 1.47952925	B127 1.46442299	B179 1.10592215	B231 1.09213387	A39 117.02643048	A91 117.97377996
B24 1.22639867	B76 1.01787443	B128 1.53703048	B180 1.09069529	B232 1.09546294	A40 122.92918490	A92 123.23678776
B25 1.01736885	B77 1.01995295	B129 1.23390773	B181 1.53752179	B233 1.46763354	A41 113.30822819	A93 111.56130395
B26 1.09588682	B78 1.35559868	B130 1.01875011	B182 1.09628746	B234 1.01773994	A42 120.16837978	A94 123.35879615
B27 1.54376430	B79 1.47385010	B131 1.09565311	B183 1.09242699	B235 1.01859208	A43 117.95882494	A95 119.79187373
B28 2.58526194	B80 1.53037516	B132 1.54108615	B184 1.53916486	B236 1.45300856	A44 105.44012976	A96 108.25167232
B29 1.09439013	B81 1.24582189	B133 1.53407191	B185 1.09470003	B237 1.09361484	A45 111.69298265	A97 110.08968723
B30 1.53708502	B82 1.48289668	B134 1.09298121	B186 1.09282867	B238 1.09985590	A46 110.48414004	A98 108.43058772
B31 1.09833320	B83 1.54885146	B135 1.09349704	B187 1.53955836	B239 1.54051622	A47 109.24474114	A99 108.24374312
B32 1.09915044	B84 1.09577967	B136 1.09158075	B188 1.09495394	B240 1.09582955	A48 111.14906160	A100 112.89684813
B33 1.53695131	B85 1.53113342	B137 1.09912032	B189 1.09493949	B241 1.09660913	A49 115.97442999	A101 110.99446771
B34 1.09463027	B86 1.09072556	B138 1.50754972	B190 1.54884243	B242 1.46272740	A50 121.15788553	A102 110.05940087
B35 1.09454341	B87 1.0954790	B139 1.21619719	B191 1.09395598	B243 1.01805396	A51 113.29881494	A103 114.00038106
B36 1.09689775	B88 1.09207842	B140 1.35557696	B192 1.09667306	B244 1.01797611	A52 121.52729968	A104 122.66898696
B37 1.09400606	B89 1.09526338	B141 0.97272133	B193 1.52305334	A1 111.41239234	A53 119.88872849	A105 113.78805140
B38 1.09769713	B90 1.08842408	B142 1.35905838	B194 1.52244019	A2 121.03761882	A54 107.48299449	A106 120.84227645
B39 1.09467598	B91 1.09251052	B143 1.45547277	B195 1.52656409	A3 109.50793546	A55 110.59994388	A107 118.03679848
B40 1.36023540	B92 1.34611910	B144 1.53218978	B196 1.52776496	A4 114.02041471	A56 116.55307134	A108 113.17201555
B41 1.45862397	B93 1.47154493	B145 1.21063749	B197 1.24004438	A5 110.08119679	A57 119.93740691	A109 123.59939896
B42 1.54784192	B94 1.55590743	B146 1.01318512	B198 1.24689334	A6 115.46255777	A58 116.94432129	A110 105.08703313
B43 1.22379434	B95 1.23293833	B147 1.09990118	B199 1.23209180	A7 107.02474611	A59 116.90677804	A111 119.19457257
B44 1.01024061	B96 1.01917575	B148 1.53562474	B200 1.22820656	A8 107.54772748	A60 120.02275902	A112 116.7120261
B45 1.09485795	B97 1.09651230	B149 1.50089750	B201 1.34398074	A9 175.03318092	A61 105.71288702	A113 108.76708790
B46 1.53004449	B98 1.53146852	B150 1.09568615	B202 1.02506464	A10 121.38236068	A62 112.48534382	A114 114.27099945
B47 1.09289159	B99 1.09271184	B151 1.09698088	B203 1.36111071	A11 120.91389655	A63 107.24752085	A115 106.98677581
B48 1.09042684	B100 1.09408087	B152 1.37359704	B204 1.02546463	A12 121.46277298	A64 106.68825628	A116 109.28908648
B49 1.09635570	B101 1.55007409	B153 1.38823450	B205 1.36888340	A13 121.55457389	A65 117.4710117	A117 115.64109945
B50 1.36509455	B102 1.09132471	B154 1.08009639	B206 1.00948713	A14 119.35102030	A66 110.36282154	A118 112.17060083
B51 1.45335398	B103 1.09631460	B155 2.13476793	B207 1.35647617	A15 119.60261761	A67 110.49812737	A119 110.60746042
B52 1.53287533	B104 1.53276557	B156 1.31843256	B208 1.02596054	A16 120.26676072	A68 110.29474603	A120 112.38487749

8	9	10	11	12	13	14
A121 123.70151220	A173 110.13795742	A225 109.62077226	D34 -62.95231395	D86 -158.59118510	D138 -148.40184809	D190 67.17346411
A122 113.78024441	A174 112.03964294	A226 119.61338474	D35 1.65689077	D87 100.05041530	D139 -177.55863392	D191 -62.82176696
A123 121.39800488	A175 113.57964048	A227 107.22681925	D36 -106.63762495	D88 -20.55633698	D140 13.92420508	D192 -174.43026622
A124 117.52213572	A176 106.47167378	A228 108.84862779	D37 131.25145936	D89 49.14531651	D141 170.52909239	D193 159.22019374
A125 118.32894906	A177 115.23449560	A229 111.87994478	D38 -20.80418903	D90 -21.35537253	D142 -121.41875110	D194 163.12965590
A126 117.53882824	A178 113.48187726	A230 107.19762551	D39 175.29497850	D91 -167.66968162	D143 -151.18707324	D195 61.56094752
A127 114.2707350	A179 108.07562446	A231 110.28285222	D40 -100.72558218	D92 -82.963906623	D144 -2.90079519	D196 -54.5119802662
A128 119.37520967	A180 112.00651631	A232 115.56991266	D41 -166.0917376	D93 -116.33270572	D145 -8.669550349	D197 -46.01860789
A129 119.84737651	A181 107.37179437	A233 110.95044156	D42 0.64048197	D94 13.12288084	D146 112.44153300	D198 -63.21546593
A130 103.74859483	A182 111.94227248	A234 109.88523894	D43 14.65743461	D95 33.27973150	D147 -78.68473835	D199 128.28584385
A131 114.86213784	A183 113.34240752	A235 122.79869857	D44 133.77738363	D96 152.67112290	D148 159.20307087	D200 -8.08693618
A132 115.37458317	A184 109.98425728	A236 107.05953340	D45 -62.38516971	D97 69.38721480	D149 45.29773937	D201 133.44366815
A133 107.54730747	A185 109.15372031	A237 109.22905809	D46 176.93731056	D98 -45.91893738	D150 0.85929884	D202 -1.22945396
A134 107.75622685	A186 111.92237003	A238 113.48121448	D47 58.19002360	D99 -167.47508100	D151 -177.76844133	D203 115.94304659
A135 111.13803801	A187 108.63858264	A239 109.14303334	D48 15.33275942	D100 101.41623888	D152 2.70898745	D204 -11.08116527
A136 110.79679824	A188 111.69252043	A240 109.42800020	D49 -179.27316980	D101 -17.52095030	D153 -179.21828624	D205 -116.46394409
A137 112.17604002	A189 116.39455693	A241 114.82828043	D50 -128.83280420	D102 -137.99087625	D154 179.07497875	D206 -6.39589839
A138 125.995922523	A190 111.14469146	A242 110.00767502	D51 113.96636576	D103 -119.55810228	D155 -0.26317441	D207 176.66343917
A139 112.44765558	A191 109.76303969	A243 109.88621361	D52 -6.12872300	D104 61.05041905	D156 179.68793408	D208 90.11321122
A140 105.79601893	A192 109.15752526	D1 164.58275053	D53 -10.0257782	D105 2.69380177	D157 -86.07292950	D209 -27.08510174
A141 117.52796751	A193 110.72914798	D2 156.41460584	D54 108.53382881	D106 178.43922724	D158 31.23492707	D210 -147.03580935
A142 122.70147926	A194 112.62968449	D3 120.53670767	D55 -68.37781946	D107 64.57297901	D159 101.81469219	D211 50.69943013
A143 109.31066553	A195 110.00194281	D4 -117.34780179	D56 -170.10456894	D108 177.77897888	D160 -82.81316807	D212 -65.8677380
A144 124.20036081	A196 121.49381947	D5 -68.69749976	D57 -68.55877292	D109 -149.91970831	D161 59.90307852	D213 171.58347192
A145 119.55582533	A197 120.07486373	D6 168.80612619	D58 160.51251520	D110 96.51674777	D162 -28.25548998	D214 -65.25209758
A146 105.48834341	A198 121.91065504	D7 54.13848651	D59 9.53306479	D111 -4.40708733	D163 -97.47019470	D215 51.65163729
A147 115.17967190	A199 121.32697244	D8 -158.08789762	D60 42.53523440	D112 -40.45844591	D164 146.29589022	D216 -177.1263424
A148 115.79391649	A200 116.15614708	D9 111.74450395	D61 158.97342554	D113 78.28840666	D165 23.5742574	D217 158.34919734
A149 107.05624408	A201 119.51959848	D10 -71.80272981	D62 -50.7551392	D114 -88.88431626	D166 149.58306841	D218 40.97707743
A150 108.43197521	A202 115.22160909	D11 -174.74851066	D63 -164.23564848	D115 156.78299646	D167 123.53802137	D219 -80.00274190
A151 130.29412993	A203 120.49098723	D12 174.28642612	D64 73.84408944	D116 31.61857698	D168 -79.63106649	D220 -56.11605186
A152 120.13166486	A204 116.61551159	D13 -3.55467755	D65 63.63877088	D117 65.20048112	D169 38.80754995	D221 61.81971992
A153 131.33692596	A205 117.96322803	D14 4.33494976	D66 -53.57780198	D118 -53.28683203	D170 -8.91394515	D222 -174.35286605
A154 128.01892934	A206 114.86359858	D15 -179.74251983	D67 -174.46960180	D119 -175.01553736	D171 -52.86195031	D223 -168.84796100
A155 106.05406259	A207 118.52934568	D16 -178.11590554	D68 -48.7022348	D120 -18.90870559	D172 -167.72797625	D224 -53.57280487
A156 111.13484826	A208 123.14890706	D17 -40.09204912	D69 -170.72201706	D121 161.85523622	D173 -54.14375194	D225 -167.87123450
A157 125.94849405	A209 109.51369096	D18 100.51085630	D70 66.94167763	D122 1.36094782	D174 69.87446250	D226 -46.63082635
A158 111.01559624	A210 107.76166537	D19 -19.28043047	D71 68.7173548	D123 176.37088767	D175 -46.86684520	D227 -163.34187389
A159 113.96503755	A211 111.36281099	D20 -158.55149028	D72 -47.42576460	D124 -76.17405053	D176 79.68320236	D228 72.93688140
A160 88.29014439	A212 108.96260572	D21 -71.67011280	D73 -171.7479181	D125 172.58169102	D177 -56.19020613	D229 -47.1134343
A161 103.54116875	A213 109.40957552	D22 159.83720302	D74 -168.08763875	D126 -129.06012817	D178 -173.85595045	D230 69.04370626
A162 54.93892267	A214 114.84489909	D23 -0.00437526	D75 76.82826414	D127 -169.51929878	D179 68.86513957	D231 -167.81638332
A163 125.58500062	A215 108.57122948	D24 42.39593116	D76 -13.38888525	D128 -30.68990104	D180 42.17025500	D232 -66.40846170
A164 109.76053972	A216 110.12311648	D25 160.28639735	D77 168.98388094	D129 -15.86902612	D181 -75.57483438	D233 51.00439928
A165 108.97197037	A217 120.95315261	D26 43.94946417	D78 -70.21978835	D130 99.25576210	D182 -166.25734085	D234 177.52866304
A166 114.92923294	A218 108.09987089	D27 -164.68792946	D79 163.10329596	D131 78.57759729	D183 -78.58193991	D235 -9.25305824
A167 119.66329710	A219 108.61707900	D28 124.71654611	D80 -29.69641080	D132 -44.33470791	D184 40.72810280	D236 -125.69974025
A168 115.09848518	A220 113.15249734	D29 -119.69733919	D81 168.26916965	D133 -159.55013375	D185 156.09742707	D237 112.57104449
A169 113.21597585	A221 109.67845034	D30 -51.25838372	D82 90.33690146	D134 76.13177627	D186 179.99810897	D238 -59.82035386
A170 108.40870175	A222 108.38597232	D31 123.08763652	D83 -141.68800585	D135 -42.68386119	D187 61.78197149	D239 56.27422764
A171 111.68478793	A223 110.15434500	D32 176.85173959	D84 -150.62148528	D136 -160.74511338	D188 69.32888695	D240 178.17306925
A172 107.28756636	A224 109.32951096	D33 56.85490219	D85 80.52638441	D137 33.56281149	D189 -51.17453962	D241 -58.75313677
						D242 57.87313264

2. **Table S2.** Final Z matriz between AMINO ACID TYROSINE and PAMAM. With their absolute energies (Hartrees).

Electronic energy = -2402.193743 Hartrees.

H
C 1 B1
H 2 B2 1 A1
C 2 B3 1 A2 3 D1 0
H 4 B4 2 A3 1 D2 0
H 4 B5 2 A4 1 D3 0
N 4 B6 2 A5 1 D4 0
N 2 B7 1 A6 4 D5 0
C 8 B8 2 A7 1 D6 0
H 9 B9 8 A8 2 D7 0
H 9 B10 8 A9 2 D8 0
C 8 B11 2 A10 1 D9 0
H 12 B12 8 A11 2 D10 0
H 12 B13 8 A12 2 D11 0
C 7 B14 4 A13 2 D12 0
H 15 B15 7 A14 4 D13 0
H 15 B16 7 A15 4 D14 0
C 7 B17 4 A16 2 D15 0
H 18 B18 7 A17 4 D16 0
H 18 B19 7 A18 4 D17 0
C 18 B20 7 A19 4 D18 0
H 21 B21 18 A20 7 D19 0
H 21 B22 18 A21 7 D20 0
C 15 B23 7 A22 4 D21 0
H 24 B24 15 A23 7 D22 0
H 24 B25 15 A24 7 D23 0
C 9 B26 8 A25 2 D24 0
H 27 B27 9 A26 8 D25 0
H 27 B28 9 A27 8 D26 0
C 12 B29 8 A28 2 D27 0
H 30 B30 12 A29 8 D28 0
H 30 B31 12 A30 8 D29 0
C 27 B32 9 A31 8 D30 0
C 30 B33 12 A32 8 D31 0
C 21 B34 18 A33 7 D32 0
C 24 B35 15 A34 7 D33 0
O 36 B36 24 A35 15 D34 0
O 35 B37 21 A36 18 D35 0
O 34 B38 30 A37 12 D36 0
O 33 B39 27 A38 9 D37 0
N 35 B40 21 A39 18 D38 0
H 41 B41 35 A40 21 D39 0
N 34 B42 30 A41 12 D40 0
H 43 B43 34 A42 30 D41 0
N 33 B44 27 A43 9 D42 0
H 45 B45 33 A44 27 D43 0
N 36 B46 24 A45 15 D44 0
H 47 B47 36 A46 24 D45 0
C 41 B48 35 A47 21 D46 0
H 49 B49 41 A48 35 D47 0
H 49 B50 41 A49 35 D48 0
C 49 B51 41 A50 35 D49 0
H 52 B52 49 A51 41 D50 0
H 52 B53 49 A52 41 D51 0
N 52 B54 49 A53 41 D52 0
H 55 B55 52 A54 49 D53 0
H 55 B56 52 A55 49 D54 0
C 43 B57 34 A56 30 D55 0
H 58 B58 43 A57 34 D56 0
H 58 B59 43 A58 34 D57 0
C 58 B60 43 A59 34 D58 0
H 61 B61 58 A60 43 D59 0
H 61 B62 58 A61 43 D60 0
N 61 B63 58 A62 43 D61 0
H 64 B64 61 A63 58 D62 0
H 64 B65 61 A64 58 D63 0
C 45 B66 33 A65 27 D64 0
H 67 B67 45 A66 33 D65 0
H 67 B68 45 A67 33 D66 0
C 67 B69 45 A68 33 D67 0
H 70 B70 67 A69 45 D68 0
H 70 B71 67 A70 45 D69 0
N 70 B72 67 A71 45 D70 0
H 73 B73 70 A72 67 D71 0
H 73 B74 70 A73 67 D72 0
C 47 B75 36 A74 24 D73 0
H 76 B76 47 A75 36 D74 0
H 76 B77 47 A76 36 D75 0
C 76 B78 47 A77 36 D76 0
H 79 B79 76 A78 47 D77 0
H 79 B80 76 A79 47 D78 0
N 79 B81 76 A80 47 D79 0
H 82 B82 79 A81 76 D80 0
H 82 B83 79 A82 76 D81 0
N 82 B84 79 A83 76 D82 0
C 85 B85 82 A84 79 D83 0
C 86 B86 85 A85 82 D84 0
O 87 B87 86 A86 85 D85 0
H 85 B88 82 A87 79 D86 0
H 85 B89 82 A88 79 D87 0
H 86 B90 85 A89 82 D88 0
C 86 B91 85 A90 82 D89 0
C 92 B92 86 A91 85 D90 0
H 92 B93 86 A92 85 D91 0
H 92 B94 86 A93 85 D92 0
C 93 B95 92 A94 86 D93 0
C 93 B96 92 A95 86 D94 0
C 93 B97 92 A96 86 D95 0
C 98 B98 93 A97 92 D96 0
C 97 B99 93 A98 92 D97 0
H 97 B100 93 A99 92 D98 0
H 98 B101 93 A100 92 D99 0
H 99 B102 98 A101 93 D100 0
H 100 B103 97 A102 93 D101 0
O 96 B104 93 A103 92 D102 0
H 105 B105 96 A104 93 D103 0
O 87 B106 86 A105 85 D104 0
H 107 B107 87 A106 86 D105 0

Continuation

1	2	3	4	5	6	7	8
B1 1.10737064	B43 1.01670181	B85 1.46444710	A20 108.00467605	A62 109.67684542	A104 111.69969323	D40 39.73505596	D82 153.25897155
B2 1.09252607	B44 1.37587872	B86 1.52414086	A21 111.66989666	A63 108.88112145	A105 113.18646027	D41 2.19240600	D83 -33.71119440
B3 1.53547475	B45 1.00939883	B87 1.21150990	A22 112.82911635	A64 109.31363031	A106 105.84242291	D42 -117.27127307	D84 83.22815471
B4 1.11081880	B46 1.37048103	B88 1.01638965	A23 109.57089324	A65 122.12247400	D1 -116.04069517	D43 -7.90198676	D85 -167.71515154
B5 1.09203422	B47 1.00977219	B89 1.01716471	A24 110.64552952	A66 109.53053012	D2 -54.50757850	D44 162.18205371	D86 106.82460507
B6 1.46200632	B48 1.45651043	B90 1.10698411	A25 113.46026852	A67 106.64400166	D3 -170.91656381	D45 -9.19679931	D87 -146.38476332
B7 1.47009909	B49 1.09649715	B91 1.54975966	A26 108.72177893	A68 113.03268618	D4 69.97053437	D46 175.14604999	D88 -161.06976964
B8 1.46523379	B50 1.09161128	B92 1.51431879	A27 109.75969800	A69 108.29682999	D5 -126.66867698	D47 154.51504210	D89 -42.02233093
B9 1.10551075	B51 1.53478895	B93 1.09768267	A28 115.12885501	A70 109.52076873	D6 56.13125534	D48 37.77688341	D90 65.36294251
B10 1.09274349	B52 1.09436253	B94 1.09354516	A29 110.69077159	A71 110.79676508	D7 -88.38300629	D49 -83.00570499	D91 -58.07983080
B11 1.47242172	B53 1.10523655	B95 2.83155323	A30 108.73003031	A72 110.37396816	D8 28.22545135	D50 63.84679156	D92 -171.68255928
B12 1.09537030	B54 1.46434263	B96 1.40511127	A31 112.87153742	A73 109.13672710	D9 -69.87505454	D51 -51.98004113	D93 139.72271421
B13 1.10736537	B55 1.01768601	B97 1.40077274	A32 117.39487237	A74 121.24902336	D10 164.91766040	D52 -178.18189741	D94 -83.77417628
B14 1.46803351	B56 1.01610709	B98 1.39567744	A33 111.53511139	A75 107.60247553	D11 49.57407710	D53 75.71362579	D95 97.03250193
B15 1.10476473	B57 1.45701050	B99 1.39223590	A34 112.18781462	A76 108.81443186	D12 166.67383146	D54 -167.42676383	D96 179.81786588
B16 1.09204257	B58 1.09347699	B100 1.08662437	A35 122.75079468	A77 112.31860668	D13 93.32556135	D55 174.39226807	D97 -179.41886441
B17 1.46616247	B59 1.09350295	B101 1.08625978	A36 122.39324983	A78 107.74449265	D14 -24.17688103	D56 164.02928436	D98 1.19607992
B18 1.10425753	B60 1.53494156	B102 1.08717484	A37 120.19366600	A79 109.02076034	D15 -62.95222381	D57 46.52699068	D99 -1.23850735
B19 1.09342084	B61 1.10181946	B103 1.08548133	A38 122.72751752	A80 111.02150010	D16 -25.67690899	D58 -74.99391060	D100 178.65813319
B20 1.53767427	B62 1.09392496	B104 1.35569891	A39 115.37797073	A81 109.95130054	D17 -142.31505942	D59 -48.14820934	D101 179.54090104
B21 1.09715013	B63 1.46942038	B105 0.98872422	A40 118.39234668	A82 110.55209383	D18 98.82506915	D60 68.20607806	D102 163.34498731
B22 1.09455090	B64 1.01897007	B106 1.35380521	A41 116.22023912	A83 123.81812923	D19 48.44230242	D61 -173.33724246	D103 169.56863746
B23 1.53499689	B65 1.01713530	B107 0.97235621	A42 119.55421139	A84 148.16316332	D20 -68.32488131	D62 78.77922232	D104 16.05226453
B24 1.09827904	B66 1.45934522	A1 107.03867698	A43 115.48532907	A85 112.01182653	D21 -144.35919415	D63 -166.25640578	D105 177.66266541
B25 1.09713977	B67 1.09650534	A2 111.05565699	A44 118.08973279	A86 124.32892554	D22 -158.46282747	D64 -172.85742115	
B26 1.54547343	B68 1.09225062	A3 109.89922211	A45 114.99682245	A87 94.44262880	D23 -41.76164587	D65 122.10976668	
B27 1.09662232	B69 1.53029027	A4 107.63137190	A46 117.69793799	A88 81.44244992	D24 149.22702656	D66 4.91818872	
B28 1.09484301	B70 1.09571562	A5 112.96557371	A47 122.10330050	A89 112.31338254	D25 163.54520289	D67 -115.94852692	
B29 1.53492510	B71 1.10285988	A6 110.62195865	A48 108.18751977	A90 111.94639532	D26 46.58672748	D68 -177.50882588	
B30 1.09691341	B72 1.47007936	A7 113.17658014	A49 108.21028846	A91 116.62166711	D27 -74.29230767	D69 -61.26122591	
B31 1.09335813	B73 1.01730769	A8 111.24458581	A50 113.20711324	A92 106.65566196	D28 53.59696883	D70 63.74698974	
B32 1.52370836	B74 1.01867041	A9 109.04256763	A51 107.78673575	A93 106.71193934	D29 169.83424634	D71 -177.39936823	
B33 1.53423031	B75 1.45972924	A10 111.80715880	A52 109.08475920	A94 179.46739488	D30 -72.75961667	D72 -60.57286722	
B34 1.52736302	B76 1.09046907	A11 107.83659250	A53 109.68386046	A95 121.67508267	D31 -70.59661892	D73 -168.89635701	
B35 1.53130480	B77 1.09669341	A12 110.30536261	A54 110.14707570	A96 120.70819247	D32 167.00160493	D74 -34.00036729	
B36 1.22656070	B78 1.53669590	A13 111.80410291	A55 110.15213763	A97 121.44011596	D33 80.43327540	D75 -150.86695173	
B37 1.22784760	B79 1.09311276	A14 111.17574898	A56 121.75373213	A98 121.69846537	D34 -17.79927760	D76 85.88588627	
B38 1.23082625	B80 1.10642299	A15 108.77940422	A57 107.00476134	A99 119.72093694	D35 -34.11262874	D77 -55.72862883	
B39 1.22539415	B81 1.46246899	A16 115.22158047	A58 109.49077648	A100 119.22906240	D36 -141.39253083	D78 59.51865625	
B40 1.36759792	B82 1.02030353	A17 111.29592434	A59 112.75736633	A101 120.03769313	D37 61.48447613	D79 -173.67792361	
B41 1.00876047	B83 1.01704609	A18 109.65836953	A60 108.68443905	A102 121.27047229	D38 146.33563720	D80 158.39930155	
B42 1.35602550	B84 3.24659390	A19 113.71034455	A61 108.07643918	A103 177.32618847	D39 4.81117060	D81 -83.11256747	

3. **Table S3.** Final Z matriz of PAMAM. With their absolute energies (Hartrees).

Electronic energy = -1715.758156 Hartrees.

H
C 1 B1
H 2 B2 1 A1
C 2 B3 1 A2 3 D1 0
H 4 B4 2 A3 1 D2 0
H 4 B5 2 A4 1 D3 0
N 4 B6 2 A5 1 D4 0
N 2 B7 1 A6 4 D5 0
C 8 B8 2 A7 1 D6 0
H 9 B9 8 A8 2 D7 0
H 9 B10 8 A9 2 D8 0
C 8 B11 2 A10 1 D9 0
H 12 B12 8 A11 2 D10 0
H 12 B13 8 A12 2 D11 0
C 7 B14 4 A13 2 D12 0
H 15 B15 7 A14 4 D13 0
H 15 B16 7 A15 4 D14 0
C 7 B17 4 A16 2 D15 0
H 18 B18 7 A17 4 D16 0
H 18 B19 7 A18 4 D17 0
C 18 B20 7 A19 4 D18 0
H 21 B21 18 A20 7 D19 0
H 21 B22 18 A21 7 D20 0
C 15 B23 7 A22 4 D21 0
H 24 B24 15 A23 7 D22 0
H 24 B25 15 A24 7 D23 0
C 9 B26 8 A25 2 D24 0
H 27 B27 9 A26 8 D25 0
H 27 B28 9 A27 8 D26 0
C 12 B29 8 A28 2 D27 0
H 30 B30 12 A29 8 D28 0
H 30 B31 12 A30 8 D29 0
C 27 B32 9 A31 8 D30 0
C 30 B33 12 A32 8 D31 0
C 21 B34 18 A33 7 D32 0
C 24 B35 15 A34 7 D33 0
O 36 B36 24 A35 15 D34 0
O 35 B37 21 A36 18 D35 0
O 34 B38 30 A37 12 D36 0
O 33 B39 27 A38 9 D37 0
N 35 B40 21 A39 18 D38 0
H 41 B41 35 A40 21 D39 0
N 34 B42 30 A41 12 D40 0
H 43 B43 34 A42 30 D41 0
N 33 B44 27 A43 9 D42 0
H 45 B45 33 A44 27 D43 0
N 36 B46 24 A45 15 D44 0
H 47 B47 36 A46 24 D45 0
C 41 B48 35 A47 21 D46 0
H 49 B49 41 A48 35 D47 0
H 49 B50 41 A49 35 D48 0
C 49 B51 41 A50 35 D49 0
H 52 B52 49 A51 41 D50 0
H 52 B53 49 A52 41 D51 0
N 52 B54 49 A53 41 D52 0
H 55 B55 52 A54 49 D53 0
H 55 B56 52 A55 49 D54 0
C 43 B57 34 A56 30 D55 0
H 58 B58 43 A57 34 D56 0
H 58 B59 43 A58 34 D57 0
C 58 B60 43 A59 34 D58 0
H 61 B61 58 A60 43 D59 0
H 61 B62 58 A61 43 D60 0
N 61 B63 58 A62 43 D61 0
H 64 B64 61 A63 58 D62 0
H 64 B65 61 A64 58 D63 0
C 45 B66 33 A65 27 D64 0
H 67 B67 45 A66 33 D65 0
H 67 B68 45 A67 33 D66 0
C 67 B69 45 A68 33 D67 0
H 70 B70 67 A69 45 D68 0
H 70 B71 67 A70 45 D69 0
N 70 B72 67 A71 45 D70 0
H 73 B73 70 A72 67 D71 0
H 73 B74 70 A73 67 D72 0
C 47 B75 36 A74 24 D73 0
H 76 B76 47 A75 36 D74 0
H 76 B77 47 A76 36 D75 0
C 76 B78 47 A77 36 D76 0
H 79 B79 76 A78 47 D77 0
H 79 B80 76 A79 47 D78 0
N 79 B81 76 A80 47 D79 0
H 82 B82 79 A81 76 D80 0
H 82 B83 79 A82 76 D81 0

Continuation

1	2	3	4	5	6
B1 1.10522732	B46 1.36762206	A8 113.24258695	A53 115.16468501	D16 -52.84912860	D61 -179.11919779
B2 1.09575325	B47 1.00871849	A9 107.89885195	A54 109.61292199	D17 -169.85010147	D62 172.06982574
B3 1.55096965	B48 1.45433018	A10 113.50246033	A55 110.05594928	D18 71.78143519	D63 -71.70917480
B4 1.09577328	B49 1.09739074	A11 107.67651723	A56 122.35094717	D19 51.88534986	D64 -167.39426499
B5 1.09375303	B50 1.09495936	A12 109.59302276	A57 109.40376693	D20 -65.84490209	D65 -41.72938461
B6 1.46527024	B51 1.54111043	A13 113.55952177	A58 106.83037578	D21 -149.57350190	D66 -158.51566931
B7 1.46686960	B52 1.09466002	A14 112.73361753	A59 113.15714519	D22 -63.71990022	D67 77.76698265
B8 1.46376001	B53 1.09733320	A15 108.84236498	A60 109.10239720	D23 53.35080289	D68 -46.26260459
B9 1.10510442	B54 1.46333068	A16 114.79621632	A61 108.33692040	D24 156.35197674	D69 69.79532475
B10 1.09171161	B55 1.01808224	A17 112.73750023	A62 109.34519308	D25 -176.20509474	D70 -167.25628523
B11 1.45997670	B56 1.01844313	A18 108.88375041	A63 110.02935806	D26 65.81426218	D71 -62.83151831
B12 1.09692883	B57 1.45594073	A19 113.24126594	A64 109.60541983	D27 65.82842917	D72 54.01804327
B13 1.09284252	B58 1.09399853	A20 108.22785892	A65 119.59920409	D28 -67.15557241	D73 -179.26661534
B14 1.46377144	B59 1.09357563	A21 111.78456301	A66 106.90584957	D29 51.13475553	D74 -32.27010251
B15 1.10546634	B60 1.53392570	A22 112.37849909	A67 109.10511745	D30 -58.80883044	D75 -148.72619937
B16 1.09301301	B61 1.09708561	A23 111.46189454	A68 111.91265523	D31 168.47253858	D76 88.49997026
B17 1.46344524	B62 1.10242841	A24 108.27847381	A69 107.58783991	D32 170.03446808	D77 -57.21016583
B18 1.10665263	B63 1.46487929	A25 112.38119671	A70 110.20264552	D33 172.11344794	D78 58.83843519
B19 1.09179343	B64 1.01656990	A26 108.47291480	A71 115.53060581	D34 -35.74783980	D79 -178.82363673
B20 1.53423348	B65 1.01805212	A27 111.75613148	A72 110.60658777	D35 -44.70386617	D80 -57.51530492
B21 1.09663760	B66 1.45611694	A28 117.25554348	A73 109.58147930	D36 -45.52924601	D81 59.35443732
B22 1.09313190	B67 1.09361513	A29 111.15580630	A74 121.97864758	D37 -60.62286452	
B23 1.53437600	B68 1.09579013	A30 109.67537426	A75 107.09218678	D38 135.34026214	
B24 1.09553861	B69 1.54125523	A31 109.22971107	A76 108.61666946	D39 0.60892614	
B25 1.09688059	B70 1.09285058	A32 110.12326336	A77 113.44633926	D40 133.83919866	
B26 1.53923594	B71 1.09605511	A33 110.69734866	A78 108.27047564	D41 4.18413193	
B27 1.09512669	B72 1.46916335	A34 111.24413916	A79 109.47713663	D42 118.73175472	
B28 1.09489040	B73 1.01814048	A35 122.32212010	A80 115.10227893	D43 -10.19946187	
B29 1.54840065	B74 1.01875917	A36 121.20106144	A81 110.25973801	D44 146.02797119	
B30 1.09552436	B75 1.45586184	A37 121.54116548	A82 109.87088369	D45 -7.08322376	
B31 1.09685245	B76 1.09381297	A38 121.62110976	D1 -117.07520992	D46 177.47990830	
B32 1.52325168	B77 1.09708622	A39 115.92355711	D2 -41.07865994	D47 152.85390196	
B33 1.52522155	B78 1.54126996	A40 120.86159235	D3 -156.74330949	D48 36.03887055	
B34 1.52810504	B79 1.09504784	A41 115.92600128	D4 80.78479149	D49 -84.98717084	
B35 1.52596529	B80 1.09744081	A42 118.63471375	D5 -126.72246873	D50 56.98837545	
B36 1.22803378	B81 1.46164722	A43 116.35186880	D6 58.03336843	D51 -59.09120203	
B37 1.23229461	B82 1.01805548	A44 118.00400310	D7 -79.16231833	D52 178.50855489	
B38 1.22913287	B83 1.01785690	A45 115.42699933	D8 38.89509387	D53 -60.33188659	
B39 1.22722524	A1 106.28004599	A46 118.66831927	D9 -76.48089478	D54 55.98657257	
B40 1.36027927	A2 109.62073260	A47 120.75601107	D10 -56.98011860	D55 177.44398781	
B41 1.02295958	A3 110.17494413	A48 108.23862507	D11 -172.27745934	D56 146.94861623	
B42 1.36515662	A4 108.01336281	A49 108.04086577	D12 -62.55279620	D57 30.09910791	
B43 1.00870859	A5 115.86454485	A50 113.44412893	D13 86.47732949	D58 -90.72114142	
B44 1.37100287	A6 112.61810401	A51 108.24855884	D14 -31.12422180	D59 -61.10961758	
B45 1.00953171	A7 114.40528752	A52 109.38117203	D15 70.39944283	D60 55.02776730	

4. **Table S4.** Final Z matriz of YLAGKPQQEH. With their absolute energies (Hartrees).

Electronic energy -3979.12754 Hartrees.

N
C 1 B1
C 2 B2 1 A1
O 3 B3 2 A2 1 D1 0
H 1 B4 2 A3 3 D2 0
H 2 B5 1 A4 3 D3 0
C 2 B6 1 A5 3 D4 0
C 7 B7 2 A6 1 D5 0
H 7 B8 2 A7 1 D6 0
H 7 B9 2 A8 1 D7 0
C 8 B10 7 A9 2 D8 0
C 8 B11 7 A10 2 D9 0
C 8 B12 7 A11 2 D10 0
C 13 B13 8 A12 7 D11 0
C 12 B14 8 A13 7 D12 0
H 12 B15 8 A14 7 D13 0
H 13 B16 8 A15 7 D14 0
H 14 B17 13 A16 8 D15 0
H 15 B18 12 A17 8 D16 0
O 11 B19 8 A18 7 D17 0
H 20 B20 11 A19 8 D18 0
N 3 B21 2 A20 1 D19 0
C 22 B22 3 A21 2 D20 0
C 23 B23 22 A22 3 D21 0
O 24 B24 23 A23 22 D22 0
H 22 B25 3 A24 2 D23 0
H 23 B26 22 A25 3 D24 0
C 23 B27 22 A26 3 D25 0
C 28 B28 23 A27 22 D26 0
H 28 B29 23 A28 22 D27 0
C 29 B30 28 A29 23 D28 0
H 31 B31 29 A30 28 D29 0
H 28 B32 23 A31 22 D30 0
C 31 B33 29 A32 28 D31 0
H 34 B34 31 A33 29 D32 0
H 34 B35 31 A34 29 D33 0
H 34 B36 31 A35 29 D34 0
H 29 B37 28 A36 23 D35 0
H 29 B38 28 A37 23 D36 0
H 29 B39 28 A38 23 D37 0
N 24 B40 23 A39 22 D38 0
C 41 B41 24 A40 23 D39 0
C 42 B42 41 A41 24 D40 0
O 43 B43 42 A42 41 D41 0
H 41 B44 24 A43 23 D42 0
H 42 B45 41 A44 24 D43 0
C 42 B46 41 A45 24 D44 0
H 47 B47 42 A46 41 D45 0
H 47 B48 42 A47 41 D46 0
H 47 B49 42 A48 41 D47 0
N 43 B50 42 A49 41 D48 0
C 51 B51 43 A50 42 D49 0
C 52 B52 51 A51 43 D50 0
O 53 B53 52 A52 51 D51 0
H 51 B54 43 A53 42 D52 0
H 52 B55 51 A54 43 D53 0
H 52 B56 51 A55 43 D54 0
N 53 B57 52 A56 51 D55 0
C 58 B58 53 A57 52 D56 0
C 59 B59 58 A58 53 D57 0
O 60 B60 59 A59 58 D58 0
H 58 B61 53 A60 52 D59 0
H 59 B62 58 A61 53 D60 0
C 59 B63 58 A62 53 D61 0
H 64 B64 59 A63 58 D62 0
H 64 B65 59 A64 58 D63 0
C 64 B66 59 A65 58 D64 0
H 67 B67 64 A66 59 D65 0
H 67 B68 64 A67 59 D66 0
C 67 B69 64 A68 59 D67 0
H 70 B70 67 A69 64 D68 0
C 70 B71 67 A70 64 D69 0
H 70 B72 67 A71 64 D70 0
H 72 B73 70 A72 67 D71 0
H 72 B74 70 A73 67 D72 0
N 72 B75 70 A74 67 D73 0
H 76 B76 72 A75 70 D74 0
H 76 B77 72 A76 70 D75 0
N 60 B78 59 A77 58 D76 0
C 79 B79 60 A78 59 D77 0
C 80 B80 79 A79 60 D78 0
O 81 B81 80 A80 79 D79 0
C 79 B82 60 A81 59 D80 0
C 80 B83 79 A82 60 D81 0
H 84 B84 80 A83 79 D82 0
C 83 B85 79 A84 60 D83 0
H 84 B86 80 A85 79 D84 0
H 86 B87 83 A86 79 D85 0
H 86 B88 83 A87 79 D86 0
H 83 B89 79 A88 60 D87 0
H 83 B90 79 A89 60 D88 0
H 80 B91 79 A90 60 D89 0
N 81 B92 80 A91 79 D90 0
C 93 B93 81 A92 80 D91 0
C 94 B94 93 A93 81 D92 0
O 95 B95 94 A94 93 D93 0
H 93 B96 81 A95 80 D94 0
H 94 B97 93 A96 81 D95 0
C 94 B98 93 A97 81 D96 0
H 99 B99 94 A98 93 D97 0
H 99 B100 94 A99 93 D98 0
C 99 B101 94 A100 93 D99 0
H 102 B102 99 A101 94 D100 0
H 102 B103 99 A102 94 D101 0
C 102 B104 99 A103 94 D102 0
O 105 B105 102 A104 99 D103 0
N 105 B106 102 A105 99 D104 0
H 107 B107 105 A106 102 D105 0
H 107 B108 105 A107 102 D106 0
N 95 B109 94 A108 93 D107 0
C 110 B110 95 A109 94 D108 0
C 111 B111 110 A110 95 D109 0
O 112 B112 111 A111 110 D110 0
H 110 B113 95 A112 94 D111 0
H 111 B114 110 A113 95 D112 0
C 111 B115 110 A114 95 D113 0
H 116 B116 111 A115 110 D114 0
H 116 B117 111 A116 110 D115 0
C 116 B118 111 A117 110 D116 0
H 119 B119 116 A118 111 D117 0
H 119 B120 116 A119 111 D118 0
C 119 B121 116 A120 111 D119 0
O 122 B122 119 A121 116 D120 0
N 122 B123 119 A122 116 D121 0
H 124 B124 122 A123 119 D122 0
H 124 B125 122 A124 119 D123 0
N 112 B126 111 A125 110 D124 0
C 127 B127 112 A126 111 D125 0
C 128 B128 127 A127 112 D126 0
O 129 B129 128 A128 127 D127 0
H 127 B130 112 A129 111 D128 0
H 128 B131 127 A130 112 D129 0
C 128 B132 127 A131 112 D130 0
C 133 B133 128 A132 127 D131 0
H 133 B134 128 A133 127 D132 0
H 133 B135 128 A134 127 D133 0
H 134 B136 133 A135 128 D134 0
H 134 B137 133 A136 128 D135 0
C 134 B138 133 A137 128 D136 0
O 139 B139 134 A138 133 D137 0
O 139 B140 134 A139 133 D138 0
H 141 B141 139 A140 134 D139 0
N 129 B142 128 A141 127 D140 0
C 143 B143 129 A142 128 D141 0
C 144 B144 143 A143 129 D142 0
O 145 B145 144 A144 143 D143 0
H 143 B146 129 A145 128 D144 0
H 144 B147 143 A146 129 D145 0
C 144 B148 143 A147 129 D146 0
C 149 B149 144 A148 143 D147 0
H 149 B150 144 A149 143 D148 0
H 149 B151 144 A150 143 D149 0
C 150 B152 149 A151 144 D150 0
N 150 B153 149 A152 144 D151 0
H 153 B154 150 A153 149 D152 0
H 153 B155 150 A154 149 D153 0
C 154 B156 150 A155 149 D154 0
N 157 B157 154 A156 150 D155 0
H 157 B158 154 A157 150 D156 0
H 145 B159 144 A158 143 D157 0
H 1 B160 2 A159 3 D158 0

Continuation

1	2	3	4	5	6	7	8
B1 1.46634367	B46 1.53102789	B91 1.09188505	B136 1.09901251	A21 121.19422194	A66 109.47629015	A111 118.75501499	A156 111.57958535
B2 1.53401885	B47 1.09352655	B92 1.35540970	B137 1.09247014	A22 113.61066485	A67 110.92120563	A112 118.88065880	A157 126.01005305
B3 1.23505219	B48 1.09107924	B93 1.45826240	B138 1.50957412	A23 119.77818840	A68 111.56966502	A113 105.17915536	A158 113.99592630
B4 1.01754515	B49 1.09589292	B94 1.54436299	B139 1.21724703	A24 113.85148731	A69 109.85436121	A114 112.86000841	A159 110.75313356
B5 1.09952258	B50 1.34976323	B95 1.22510952	B140 1.35209841	A25 107.98639187	A70 112.89660530	A115 107.29897680	D1 168.77093189
B6 1.55239576	B51 1.44947204	B96 1.00981763	B141 0.97239912	A26 112.93540844	A71 109.50232285	A116 108.57379376	D2 155.11276659
B7 1.51272622	B52 1.53463981	B97 1.09423940	B142 1.35930349	A27 102.33525030	A72 109.09106366	A117 114.48963380	D3 119.21733873
B8 1.09396996	B53 1.23373080	B98 1.53855364	B143 1.45641046	A28 105.40039927	A73 108.99526394	A118 109.93689911	D4 -119.79815832
B9 1.09645573	B54 1.01855550	B99 1.09698438	B144 1.52846853	A29 33.06296493	A74 110.84333178	A119 110.87934941	D5 -63.72916962
B10 2.82029598	B55 1.09235445	B100 1.09182950	B145 1.20992114	A30 107.97512035	A75 109.56472726	A120 110.91640117	D6 173.72593990
B11 1.40512841	B56 1.09358403	B101 1.54185516	B146 1.01509346	A31 107.93593238	A76 110.08847532	A121 122.34073250	D7 58.32950114
B12 1.39968360	B57 1.35625143	B102 1.09424131	B147 1.09972781	A32 110.18530969	A77 122.95157031	A122 114.84121848	D8 -6.64914381
B13 1.39646332	B58 1.46353256	B103 1.09517649	B148 1.53592445	A33 111.47788367	A78 117.70780266	A123 121.88252230	D9 -75.35341332
B14 1.38894541	B59 1.54425892	B104 1.52639470	B149 1.50174643	A34 110.96663566	A79 114.10745180	A124 116.66168898	D10 103.85829839
B15 1.08736579	B60 1.24402520	B105 1.22289568	B150 1.09619460	A35 111.02709575	A80 121.01470186	A125 118.83685567	D11 -179.00854619
B16 1.08745090	B61 1.01449090	B106 1.37040666	B151 1.09376492	A36 95.63428002	A81 129.70254341	A126 119.01683882	D12 179.02986010
B17 1.08769116	B62 1.09078085	B107 1.01406231	B152 1.37684633	A37 91.55350946	A82 104.30623164	A127 114.59103825	D13 -1.66606648
B18 1.08473507	B63 1.54600739	B108 1.01009347	B153 1.38712937	A38 143.48001677	A83 110.34365642	A128 119.00067200	D14 2.05530061
B19 1.36315129	B64 1.09747838	B109 1.36250925	B154 1.07943977	A39 117.62457894	A84 102.76175080	A129 119.29520641	D15 -179.53955566
B20 0.96637428	B65 1.09525727	B110 1.45649847	B155 2.13735171	A40 121.85971633	A85 110.55018445	A130 104.69909143	D16 179.45088195
B21 1.35925258	B66 1.53525991	B111 1.54036503	B156 1.31758662	A41 113.67469943	A86 110.09509089	A131 113.88394093	D17 -69.98558834
B22 1.46198672	B67 1.09831957	B112 1.22567387	B157 1.36214122	A42 118.63506432	A87 112.16189064	A132 113.43671358	D18 -177.71392042
B23 1.53538011	B68 1.09706803	B113 1.01190094	B158 1.08139278	A43 117.95386526	A88 109.87529155	A133 107.45007010	D19 -12.40977624
B24 1.23302196	B69 1.53530692	B114 1.09282596	B159 1.11221094	A44 108.07597323	A89 111.91562841	A134 107.84257845	D20 -162.83430616
B25 1.01753758	B70 1.09544190	B115 1.54419832	B160 1.01672817	A45 110.65307890	A90 108.85919130	A135 109.33232259	D21 -67.77983028
B26 1.09675890	B71 1.52950641	B116 1.09591872	A1 111.01662607	A46 110.72013097	A91 116.02869486	A136 112.07977061	D22 158.34722141
B27 1.54432407	B72 1.10040286	B117 1.09264028	A2 121.22224148	A47 109.19509582	A92 122.81550292	A137 115.72571760	D23 -5.05786148
B28 2.58460413	B73 1.09866320	B118 1.53565757	A3 109.49244381	A48 111.16747841	A93 114.54926730	A138 125.01588377	D24 45.85215675
B29 1.09482108	B74 1.10714318	B119 1.09665026	A4 113.43691188	A49 117.79275905	A94 118.62899614	A139 113.45953115	D25 164.44522417
B30 1.53700305	B75 1.46665049	B120 1.09324947	A5 110.67729373	A50 120.66267861	A95 118.04359768	A140 106.03359931	D26 42.92702492
B31 1.09886454	B76 1.01825058	B121 1.52713177	A6 113.13501391	A51 116.04512596	A96 107.49585673	A141 118.15255620	D27 -165.22433538
B32 1.09876569	B77 1.01749815	B122 1.22462462	A7 107.19561750	A52 118.15647369	A97 110.44915038	A142 121.40944561	D28 124.53302173
B33 1.53706147	B78 1.35537340	B123 1.36595710	A8 108.22439805	A53 121.23827908	A98 107.84484456	A143 109.72182399	D29 -119.79421867
B34 1.09475253	B79 1.48374388	B124 1.01282796	A9 179.12419502	A54 110.90791122	A99 107.96584738	A144 124.27537707	D30 -51.96387714
B35 1.09442686	B80 1.52934197	B125 1.00923885	A10 120.82869841	A55 108.20897802	A100 114.85052356	A145 120.67153967	D31 123.04503904
B36 1.09668841	B81 1.23186654	B126 1.37460337	A11 121.35637181	A56 118.65714401	A101 109.59439715	A146 104.99172064	D32 176.79566631
B37 1.09375567	B82 1.48060165	B127 1.45802813	A12 121.40889440	A57 119.35473959	A102 112.57502381	A147 114.60259717	D33 56.56840638
B38 1.09739014	B83 1.54499894	B128 1.53695106	A13 121.51127631	A58 115.32294286	A103 110.15482578	A148 115.09493819	D34 -63.01748487
B39 1.09464150	B84 1.09578997	B129 1.23371062	A14 119.51113431	A59 117.02503929	A104 122.03106686	A149 107.15451552	D35 0.95153682
B40 1.35468088	B85 1.53201127	B130 1.01346802	A15 119.60823333	A60 119.84545012	A105 115.49010820	A150 108.32281363	D36 -107.23597149
B41 1.45797031	B86 1.09034296	B131 1.09526158	A16 120.05758416	A61 104.96296297	A106 123.00459724	A151 129.81058852	D37 130.38112514
B42 1.54281204	B87 1.09486501	B132 1.54401200	A17 121.35598731	A62 114.31701211	A107 115.67690370	A152 120.34709848	D38 -21.33256928
B43 1.23546951	B88 1.09338099	B133 1.53417655	A18 177.06544969	A63 106.71961044	A108 117.09401482	A153 131.74179336	D39 174.09401249
B44 1.01015205	B89 1.09622482	B134 1.09445030	A19 109.51602099	A64 106.53744391	A109 121.27406915	A154 127.91482860	D40 -64.28852974
B45 1.09413664	B90 1.08653221	B135 1.09126140	A20 115.41881968	A65 118.51189558	A110 114.95851533	A155 105.73186214	D41 166.03878750

9	10	11
042 3.39709132	087 94.25256647	0132 -56.13914843
043 51.09019053	088 -25.94577630	0133 -171.94822974
044 170.85298449	089 53.30791323	0134 63.06326173
045 -60.81471749	090 -30.32353922	0135 -54.90315372
046 179.44360842	091 -177.84542589	0136 -177.15938230
047 60.2143126l	092 -72.45579539	0137 151.35640578
048 -13.74346365	093 168.36184792	0138 -30.49911685
049 175.71725913	094 4.64780101	0139 -179.19837727
050 -73.57593935	095 42.29467542	0140 8.98638208
051 163.82610487	096 160.41993205	0141 176.68085243
052 -1.40605751	097 -60.63350669	0142 -119.37801413
053 47.69193180	098 -176.30648769	0143 -153.24444587
054 165.72345305	099 62.18936361	0144 -5.12144145
055 -18.10821535	0100 69.11486318	0145 -6.53439307
056 -173.97790486	0101 -49.40539148	0146 114.40295602
057 -86.22100888	0102 -172.81634353	0147 -65.86385740
058 140.24972382	0103 -66.34416065	0148 171.18867255
059 2.72050555	0104 113.32014782	0149 57.14224237
060 24.95434371	0105 -13.75565956	0150 -20.62404981
061 140.85437415	0106 -171.74622053	0151 162.10371283
062 -51.20235072	0107 -11.59337558	0152 5.48096412
063 -164.19760292	0108 176.13774780	0153 -177.69091812
064 73.23444353	0109 -117.29228643	0154 177.46996343
065 52.87571696	0110 162.83942898	0155 0.18756771
066 -64.92342136	0111 -3.35028833	0156 -179.39226328
067 172.55334443	0112 -3.14081661	0157 28.16626719
068 -58.37098719	0113 113.73623252	0158 -87.89010300
069 179.63131360	0114 -63.04457303	
070 57.87099608	0115 -178.82181255	
071 54.66207899	0116 58.65727148	
072 -60.67653857	0117 64.03722825	
073 172.95038352	0118 -54.68263081	
074 61.00699550	0119 -177.55782858	
075 177.23383001	0120 -56.03853413	
076 -39.76171286	0121 124.63091769	
077 -172.72775942	0122 -10.96721647	
078 -65.39219189	0123 -173.96813447	
079 152.28686254	0124 -16.73923972	
080 -5.84358454	0125 -176.38312266	
081 171.46940729	0126 -137.73621329	
082 94.25022989	0127 -172.41784394	
083 -147.06017578	0128 -15.23952063	
084 -144.94794972	0129 -22.58019149	
085 81.98608224	0130 93.33916285	
086 -157.37067871	0131 66.34762538	

5. Table S5. Final Z matriz AMINO ACID TYROSINE. With their absolute energies (Hartrees). Electronic energy = -686.38578225 Hartrees.

	1	2
N	B1 1.45919932	A17 130.62621889
C 1 B1	B2 1.53215016	A18 121.29482725
C 2 B2 1 A1	B3 1.21221889	A19 117.54892749
O 3 B3 2 A2 1 D1 0	B4 1.01802645	A20 119.41301167
H 1 B4 2 A3 3 D2 0	B5 1.01942244	A21 119.21686895
H 1 B5 2 A4 3 D3 0	B6 1.09640625	A22 120.56951030
H 2 B6 1 A5 3 D4 0	B7 1.54732325	A23 119.65774456
C 2 B7 1 A6 3 D5 0	B8 1.50453946	A24 112.38407872
C 8 B8 2 A7 1 D6 0	B9 1.09442720	A25 106.38197603
H 8 B9 2 A8 1 D7 0	B10 1.10091633	D1 -11.79674963
H 8 B10 2 A9 1 D8 0	B11 1.37389360	D2 -60.27459097
C 9 B11 8 A10 2 D9 0	B12 1.44416188	D3 53.27506892
C 9 B12 8 A11 2 D10 0	B13 1.07903911	D4 118.30232193
H 12 B13 9 A12 8 D11 0	B14 1.38305324	D5 -123.29024936
N 12 B14 9 A13 8 D12 0	B15 1.37866446	D6 -66.98668930
C 15 B15 12 A14 9 D13 0	B16 1.00635634	D7 171.41423213
H 15 B16 12 A15 9 D14 0	B17 1.40586504	D8 57.38004934
C 13 B17 9 A16 8 D15 0	B18 1.39858182	D9 38.31840257
C 16 B18 15 A17 12 D16 0	B19 1.08653750	D10 -142.59422170
H 19 B19 16 A18 15 D17 0	B20 1.39004819	D11 -0.77363027
C 19 B20 16 A19 15 D18 0	B21 1.08600320	D12 179.47119966
H 21 B21 19 A20 16 D19 0	B22 1.38914561	D13 -0.14851595
C 18 B22 13 A21 9 D20 0	B23 1.08665536	D14 179.20406290
H 18 B23 13 A22 9 D21 0	B24 1.08605905	D15 0.63329189
H 23 B24 18 A23 13 D22 0	B25 1.35440064	D16 179.86468892
O 3 B25 2 A24 1 D23 0	B26 0.97248676	D17 0.10292729
H 26 B26 3 A25 2 D24 0	A1 112.09271595	D18 -179.95684809
	A2 124.99311942	D19 -179.94551825
	A3 109.18153268	D20 179.68520880
	A4 108.26130259	D21 -0.41628406
	A5 108.64717565	D22 -179.98342989
	A6 111.25995093	D23 168.51990233
	A7 114.81999299	D24 178.96622506
	A8 107.94132153	
	A9 107.81936109	
	A10 128.32489620	
	A11 125.27477706	
	A12 128.49172984	
	A13 109.82358005	
	A14 109.49190745	
	A15 125.02669930	
	A16 134.08025258	