Supporting Information
A generalized energy-based fragmentation approach for computing the ground-state energies and properties of large molecules

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Contents

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I. CARTESIAN COORDINATES

A. Water clusters

1. $(H_2O)_{32}$ [1]

O -5.297633 -3.258368 -2.917500
H -4.555640 -3.526640 -3.471568
H -6.055243 -3.669168 -3.337921
O -3.588127 -2.893849 -0.229710
H -4.452484 -2.978549 -0.643675
H -2.996644 -2.777467 -0.980941
O -3.554748 -0.454520 -2.421492
H -2.754291 -0.738168 -2.877459
H -4.211370 -1.089780 -2.722408
O -3.024122 1.063887 4.026190
H -2.822590 1.697258 4.723008
H -3.385422 1.620990 3.330426
O -3.238103 4.544063 -3.257114
H -2.759243 4.402619 -2.435988
H -4.116349 4.210806 -3.056105
O -2.675500 2.985631 1.319092
H -3.356776 3.394501 0.775814
H -2.457465 2.192649 0.816724
O -4.109121 2.322147 -1.327362
H -3.281001 2.011155 -1.711593
H -4.668281 1.541861 -1.380198
O -0.781796 -1.971094 -1.598127
H -0.172816 -2.130956 -0.870159
H -0.426945 -1.176684 -2.009621
O -2.352805 -3.016056 -4.129675
H -1.902521 -2.362473 -4.672843
H -1.638454 -3.366377 -3.585369
O 0.834124 -3.761010 -3.760759
H 1.005170 -2.866589 -3.447948
H 1.477278 -3.879841 -4.461444
O 1.020191 -4.406299 -0.533764
H 0.349125 -4.873497 -0.024875
H 0.755876 -4.557847 -1.447470
O -1.350176 -4.339044 1.659902
H -2.152735 -4.143643 1.166077
H -1.568078 -4.045035 2.550107
O 0.697262 -1.977076 1.667690
H -0.221438 -1.832216 1.916250
H 0.721298 -2.920518 1.476300
O -1.909568 -1.906240 3.666101

H -2.595426 -1.253128 3.842346
H -1.238959 -1.699346 4.325595
O -0.842879 -0.165719 -4.379869
H -1.258131 0.636468 -4.713693
H 0.095368 0.022073 -4.479475
O 0.919325 0.311615 -0.422476
H 0.214093 0.409977 0.227969
H 1.577420 -0.204264 0.058915
O -2.198138 -0.223738 0.725036
H -2.411490 -0.431272 -0.191527
H -2.632323 -0.935160 1.208287
O 1.054676 -1.039049 4.747887
H 1.674686 -1.024208 5.483345
H 1.571709 -1.417272 4.028162
O -0.051243 1.290185 2.607374
H -1.000641 1.161940 2.498164
H 0.199062 0.549528 3.168569
O -0.918578 2.713964 -1.703671
H -0.229069 2.044037 -1.768975
H -0.500164 3.391373 -1.162345
O -1.225036 3.042061 -5.005655
H -1.891383 3.658458 -5.324070
H -1.268909 3.164251 -4.051712
O 0.413567 4.146167 0.934236
H 0.687219 4.736721 1.642533
H -0.229077 3.573610 1.367561
O -2.264274 4.037848 4.411603
H -2.303950 4.095271 3.453016
H -1.446255 4.492034 4.630767
O 0.899772 4.118701 4.006384
H 0.694817 3.179281 3.943300
H 1.723096 4.120213 4.503020
O 3.279768 -2.000381 -0.352667
H 2.782826 -2.822022 -0.283881
H 3.430354 -1.910810 -1.297361
O 2.272756 -0.845359 -3.206127
H 2.001410 -0.186264 -2.557468
H 2.621860 -0.306284 -3.923821
O 3.564222 -0.769200 2.600096
H 3.172042 -1.416973 2.002870
H 3.854944 -0.079062 1.994083
O 4.099726 -0.805882 5.754151
H 4.350227 -0.971897 4.838300
H 4.792437 -1.233490 6.261513
O 2.227638 3.059248 -1.531546
H 2.537039 2.331914 -0.981469
H 2.064947 3.756121 -0.888618
O 1.703820 1.869214 -4.507871
H 1.118729 2.410711 -5.047858
H 1.995957 2.478613 -3.820612
O 2.939002 2.142339 1.444049
H 3.207154 2.631047 2.226794
H 1.978369 2.125582 1.513459
O 2.867207 1.866062 4.610181
H 2.701152 1.056959 4.114986
H 3.310663 1.544391 5.400608

2. $(H_2O)_{40}$ [2]

O -4.45183800 -1.89774700 -1.07247800
O -4.53101300 0.19580200 -4.32052800
O -4.55650900 1.58831900 -1.34644400
O -5.00972500 2.66106600 2.91209800
O -0.86516300 -4.62923600 -3.16570000
O -2.57074100 -4.21079400 -0.01441600
O -1.33869000 -4.57643800 2.98757700
O -1.87182400 -1.59995600 -3.51198600
O -1.46702200 -1.52781700 1.98478300
O -3.03884900 -1.05242000 4.57128400
O -1.82244100 1.63275500 -3.52009400
O -1.92333000 -0.05407400 -0.70645000
O -1.98701600 3.08331000 0.07603000
O -1.85704700 1.61335600 3.16156400
O -4.31715200 0.04611100 1.53570900
O -0.95533500 0.52471200 6.39530500
O -3.48045500 4.36725200 -2.74712500
O -2.64653400 6.21470100 -0.05839500
O -1.84199000 4.89361400 2.96292700
O 0.08982400 -5.79774800 -0.41423100
O 3.07973500 -4.44773900 0.28886200
O 2.09611700 -3.35987300 -2.86452400
O 0.99807500 -1.08061100 -4.94954300
O 0.09126700 -2.57082800 -0.63272300
O 1.78820700 -1.85973000 1.90371700
O 0.20519900 -2.15282800 4.79556200
O 1.12257100 2.92441000 -3.81130800
O 0.91971600 0.16893400 -2.09085200
O 0.51368600 0.97623100 0.97212200
O 1.03836500 3.16232200 3.11107900
O 2.04810700 1.62569500 5.73385400
O 2.63404900 4.81220900 -1.63991400
O 0.41516200 5.19022800 0.66429000
O 4.05806700 -3.74429400 3.15702300
O 3.58077600 -1.33658300 -0.81375200
O 3.39283000 -1.25770100 5.01883900
O 3.58554100 0.86704700 -3.71601000
O 3.38945500 1.77221800 -0.43075500
O 3.36098100 0.97159400 2.73134100
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H -4.09903000 1.92064100 -0.56760500
H -4.60841700 0.64135200 -1.17298700
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H -4.13520500 2.35056300 2.65614000
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H -2.17508500 -1.42349200 4.35459300
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H -1.01507000 -0.30002800 -0.49968400
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H -2.09875200 0.73513900 2.84942100
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H -0.67290400 -0.35774700 6.13480000
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H -3.32210300 5.03987800 -2.07668100
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H -1.99640700 4.05933500 3.42065200
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H 3.51860900 -3.60037000 0.42402000
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H 1.99820500 -1.19280100 1.24024900
H 1.44259700 -2.58551500 1.37427000
H 0.88109200 -1.82724200 4.18834400
H 0.62455500 -2.92701200 5.18565800
H 0.94992300 3.32747000 -4.66837200
H 1.15936100 3.68511000 -3.22179500
H 1.26775700 0.69988300 -1.36501200
H 0.61466200 0.83383800 -2.71768700
H 1.29718200 1.43450200 1.29271800
H -0.20314300 1.53536200 1.28962300
H 0.30670300 2.86093700 3.66039500
H 1.58957900 3.64862000 3.73360100
H 1.14539800 1.56628200 6.06367100
H 2.33858500 2.49208900 6.03646800
H 3.44505100 5.32478600 -1.56775100
H 2.93431900 3.91378300 -1.46095000
H 1.30866400 4.91720600 0.43057900
H 0.23628200 4.68276600 1.46261300
H 4.58794900 -3.72808900 3.95892200
H 3.56341900 -2.91831000 3.20727100
H 3.04930500 -1.13609900 -1.59235700
H 4.46141000 -1.46262300 -1.18098300
H 3.02981100 -0.50701700 5.49945400
H 3.85978200 -1.75389900 5.69836900
H 3.45313000 1.80917800 -3.86976300
H 2.75723700 0.48269700 -4.02310100
H 3.57345800 1.09664800 0.23157000
H 3.93315000 1.49389000 -1.17582900
H 3.58890300 0.05941400 2.94215200
H 2.65287000 1.16301000 3.35665500
H 4.25668800 4.26612300 0.74766000
H 3.28787900 3.39160000 1.50448800

3. $(H_2O)_{48}$ [2]

O -4.45183800 -1.89774700 -1.07247800
O -4.55708800 -3.05497300 2.35995000
O -4.53101300 0.19580200 -4.32052800
O -4.55650900 1.58831900 -1.34644400
O -5.00972500 2.66106600 2.91209800
O -4.00001800 -5.11993600 -2.80813700
O -0.86516300 -4.62923600 -3.16570000
O -2.57074100 -4.21079400 -0.01441600
O -1.33869000 -4.57643800 2.98757700
O -1.87182400 -1.59995600 -3.51198600
O -1.46702200 -1.52781700 1.98478300
O -3.03884900 -1.05242000 4.57128400
O -1.82244100 1.63275500 -3.52009400
O -1.92333000 -0.05407400 -0.70645000
O -1.98701600 3.08331000 0.07603000
O -1.85704700 1.61335600 3.16156400
O -4.31715200 0.04611100 1.53570900
O -0.95533500 0.52471200 6.39530500
O -3.48045500 4.36725200 -2.74712500
O -2.64653400 6.21470100 -0.05839500
O -1.84199000 4.89361400 2.96292700
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O 2.09611700 -3.35987300 -2.86452400
O 0.99807500 -1.08061100 -4.94954300
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O 1.78820700 -1.85973000 1.90371700
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O 3.61347800 4.29909800 1.46421600

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H -3.32210300 5.03987800 -2.07668100
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H -0.95191500 6.46783800 -1.75155700
H 1.30866400 4.91720600 0.43057900
H 0.23628200 4.68276600 1.46261300
H 2.41661400 5.89385000 2.85317900
H 1.22568900 6.77799500 2.58172800
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H 3.56341900 -2.91831000 3.20727100
H 5.82103200 -2.38013100 -3.83293300
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H 3.02981100 -0.50701700 5.49945400
H 3.85978200 -1.75389900 5.69836900
H 3.45313000 1.80917800 -3.86976300
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H 3.57345800 1.09664800 0.23157000
H 3.93315000 1.49389000 -1.17582900
H 3.58890300 0.05941400 2.94215200
H 2.65287000 1.16301000 3.35665500
H 5.61437000 4.07270200 -2.24692300
H 6.09638500 3.30860400 -1.04294300
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H 3.28787900 3.39160000 1.50448800
H 4.28200700 2.78452700 4.27400400

4. $(H_3O^+)_5(HO^-)_5(H_2O)_{22}$

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O -3.58812700 -2.89384900 -0.22971000
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O -3.02412200 1.06388700 4.02619000
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O -2.67550000 2.98563100 1.31909200
O -4.10912100 2.32214700 -1.32736200
O -0.78179600 -1.97109400 -1.59812700
O -2.35280500 -3.01605600 -4.12967500
O 0.83412400 -3.76101000 -3.76075900
O 1.02019100 -4.40629900 -0.53376400
O -1.35017600 -4.33904400 1.65990200
O 0.69726200 -1.97707600 1.66769000
O -1.90956800 -1.90624000 3.66610100

O -0.84287900 -0.16571900 -4.37986900
O 0.91932500 0.31161500 -0.42247600
O -2.19813800 -0.22373800 0.72503600
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O -0.05124300 1.29018500 2.60737400
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O 0.41356700 4.14616700 0.93423600
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O 0.89977200 4.11870100 4.00638400
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O 2.27275600 -0.84535900 -3.20612700
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O 2.22763800 3.05924800 -1.53154600
O 1.70382000 1.86921400 -4.50787100
O 2.93900200 2.14233900 1.44404900
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H -6.13064131 -3.61173720 -3.23816706
H -4.45248400 -2.97854900 -0.64367500
H -2.99664400 -2.77746700 -0.98094100
H -2.75429100 -0.73816800 -2.87745900
H -4.21137000 -1.08978000 -2.72240800
H -3.38542200 1.62099000 3.33042600
H -2.75924300 4.40261900 -2.43598800
H -4.11634900 4.21080600 -3.05610500
H -3.35677600 3.39450100 0.77581400
H -2.45746500 2.19264900 0.81672400
H -3.23521837 2.14766795 -1.68436516
H -4.77124933 1.62709776 -1.31773789
H -0.17281600 -2.13095600 -0.87015900
H -0.42694500 -1.17668400 -2.00962100
H -1.90252100 -2.36247300 -4.67284300
H -1.63845400 -3.36637700 -3.58536900
H 1.00517000 -2.86658900 -3.44794800
H 0.34912500 -4.87349700 -0.02487500
H 0.75587600 -4.55784700 -1.44747000
H -2.15273500 -4.14364300 1.16607700
H -1.56807800 -4.04503500 2.55010700
H -0.18108934 -1.69525066 1.93353469
H 0.86004459 -2.89722999 1.44764805
H -2.59542600 -1.25312800 3.84234600
H -1.23895900 -1.69934600 4.32559500
H -1.25813100 0.63646800 -4.71369300
H 0.09536800 0.02207300 -4.47947500
H 0.21409300 0.40997700 0.22796900
H -2.41149000 -0.43127200 -0.19152700
H -2.63232300 -0.93516000 1.20828700
H 1.67468600 -1.02420800 5.48334500
H 1.57170900 -1.41727200 4.02816200
H -0.99223074 1.28190455 2.41744372
H 0.33323356 0.60464822 3.15857006
H -0.22906900 2.04403700 -1.76897500
H -0.50016400 3.39137300 -1.16234500
H -1.89138300 3.65845800 -5.32407000
H -1.26890900 3.16425100 -4.05171200
H 0.68721900 4.73672100 1.64253300
H -2.30395000 4.09527100 3.45301600
H -1.44625500 4.49203400 4.63076700
H 0.69481700 3.17928100 3.94330000
H 1.72309600 4.12021300 4.50302000
H 2.78405128 -2.79634642 -0.14698767
H 3.49743671 -1.79258597 -1.26428181
H 2.00141000 -0.18626400 -2.55746800
H 2.62186000 -0.30628400 -3.92382100
H 3.17204200 -1.41697300 2.00287000
H 3.85494400 -0.07906200 1.99408300
H 4.35022700 -0.97189700 4.83830000
H 2.53703900 2.33191400 -0.98146900
H 2.06494700 3.75612100 -0.88861800
H 1.11872900 2.41071100 -5.04785800
H 1.99595700 2.47861300 -3.82061200
H 3.20715400 2.63104700 2.22679400
H 1.97836900 2.12558200 1.51345900
H 2.70115200 1.05695900 4.11498600
H -5.28047362 -2.70911862 -2.13033377
H -4.32089530 3.19167529 -0.97998296
H 1.41283075 -1.33874734 1.62188726
H 0.50526818 1.98400223 2.24610823
H 3.55781601 -1.41221062 0.35326848

B. Ice-like water clusters

1. $(H_2O)_{32}$

O 0.02750038 1.32388057 8.27761339
H 0.02749115 2.26670075 7.94427047
H -0.78901046 0.85247847 7.94427047
O 0.02750038 3.91664095 7.36093417
H 0.02750960 3.91664628 6.36092047
H 0.84401122 4.38805370 7.69426202
O 2.27289673 5.21302114 8.27761339
H 2.27290596 6.15584132 7.94427047
H 3.08940757 4.74161904 7.94427047
O 2.27289673 7.80578152 7.36093417
H 1.45639512 8.27719960 7.69427709
H 3.08939835 8.27719960 7.69427709
O 0.02750038 9.10216171 8.27761339
H 0.02749115 10.04498189 7.94427047
H -0.78901046 8.63075961 7.94427047
O 0.02750038 11.69492209 7.36093417
H 0.84400199 12.16634017 7.69427709
H -0.78900124 12.16634017 7.69427709
O 4.51829309 1.32388057 8.27761339
H 5.33480393 0.85247847 7.94427047
H 4.51830231 2.26670075 7.94427047
O 4.51829309 3.91664095 7.36093417
H 4.51830231 3.91664628 6.36092047
H 5.33480393 4.38805370 7.69426202
O 6.76368945 5.21302114 8.27761339
H 7.58020029 4.74160839 7.94428554
H 6.76369867 5.21301581 9.27762709

O 6.76368945 7.80578152 7.36093417
H 6.76368022 6.86296134 7.69427709
H 5.94717860 8.27718362 7.69427709
O 4.51829309 9.10216171 8.27761339
H 4.51829309 10.04498722 7.94428554
H 4.51829309 9.10217236 9.27762709
O 4.51829309 11.69492209 7.36093417
H 3.70179147 12.16634017 7.69427709
H 5.33479471 12.16634017 7.69427709
O 9.00908580 1.32388057 8.27761339
H 9.82559664 0.85247847 7.94427047
H 9.00909503 2.26670075 7.94427047
O 9.00908580 3.91664095 7.36093417
H 9.00909503 3.91664628 6.36092047
H 9.82559664 4.38805370 7.69426202
O 9.00908580 9.10216171 8.27761339
H 8.19257496 8.63074896 7.94428554
H 9.00907658 9.10215639 9.27762709
O 9.00908580 11.69492209 7.36093417
H 9.00908580 11.69491144 6.36092047
H 9.00908580 10.75209659 7.69426202
O 0.02750038 1.32388057 11.02765106
H 0.02749115 1.32387524 10.02763736
H -0.78901046 0.85246781 11.36097892
O 0.02750038 3.91664095 11.94433029
H 0.02750960 2.97382077 11.61098737
H 0.84401122 4.38804305 11.61098737
O 2.27289673 5.21302114 11.02765106
H 2.27289673 5.21303179 10.02763736
H 2.27289673 6.15584665 11.36097892
O 2.27289673 7.80578152 11.94433029
H 2.27290596 7.80578685 12.94434399
H 3.08940757 8.27719428 11.61100243
O 0.02750038 9.10216171 11.02765106
H 0.02750960 9.10215639 10.02763736
H 0.84401122 8.63074896 11.36097892
O 0.02750038 11.69492209 11.94433029
H 0.02750960 10.75210191 11.61098737
H 0.84401122 12.16632420 11.61098737
O 4.51829309 1.32388057 11.02765106
H 4.51830231 1.32387524 10.02763736
H 5.33480393 0.85246781 11.36097892
O 4.51829309 3.91664095 11.94433029
H 3.70178225 4.38804305 11.61098737
H 4.51828386 2.97382077 11.61098737
O 6.76368945 5.21302114 11.02765106
H 5.94718783 4.74160306 11.36099398
H 7.58019106 4.74160306 11.36099398
O 6.76368945 7.80578152 11.94433029
H 6.76368945 7.80577087 12.94434399
H 6.76368945 6.86295601 11.61100243
O 4.51829309 9.10216171 11.02765106
H 5.33480393 8.63075961 11.36099398
H 4.51830231 10.04498189 11.36099398
O 4.51829309 11.69492209 11.94433029
H 4.51830231 11.69492742 12.94434399
H 5.33480393 12.16633485 11.61100243
O 9.00908580 1.32388057 11.02765106
H 9.00908580 1.32389122 10.02763736
H 9.00908580 2.26670608 11.36097892
O 9.00908580 3.91664095 11.94433029
H 9.00909503 3.91664628 12.94434399
H 9.82559664 4.38805370 11.61100243
O 9.00908580 9.10216171 11.02765106
H 8.19258419 8.63074363 11.36099398
H 9.82558742 8.63074363 11.36099398
O 9.00908580 11.69492209 11.94433029
H 9.00909503 10.75210191 11.61098737
H 9.82559664 12.16632420 11.61098737

2. $(H_2O)_{48}$

O 0.02750038 1.32388057 3.69421727
H 0.84400199 0.85246249 4.02756019
H -0.78900124 0.85246249 4.02756019
O 0.02750038 3.91664095 4.61089650
H 0.02749115 2.97382077 4.27755358
H -0.78901046 4.38804305 4.27755358
O 2.27289673 5.21302114 3.69421727
H 1.45638589 4.74161904 4.02756019
H 2.27288751 6.15584132 4.02756019
O 2.27289673 7.80578152 4.61089650
H 3.08940757 8.27719428 4.27756864
H 2.27290596 7.80578685 5.61091020
O 0.02750038 9.10216171 3.69421727
H 0.84401122 8.63075961 4.02756019
H 0.02750960 10.04498189 4.02756019
O 0.02750038 11.69492209 4.61089650
H 0.84401122 12.16633485 4.27756864
H 0.02750960 11.69492742 5.61091020
O 4.51829309 1.32388057 3.69421727
H 4.51828386 1.32387524 2.69420357
H 3.70178225 0.85246781 4.02754513
O 4.51829309 3.91664095 4.61089650
H 3.70178225 4.38804305 4.27755358
H 4.51828386 2.97382077 4.27755358
O 6.76368945 5.21302114 3.69421727
H 6.76368022 5.21301581 2.69420357
H 5.94717860 4.74160839 4.02754513
O 6.76368945 7.80578152 4.61089650
H 6.76368945 6.86295601 4.27756864
H 6.76368945 7.80577087 5.61091020
O 4.51829309 9.10216171 3.69421727
H 5.33480393 8.63075961 4.02756019
H 4.51830231 10.04498189 4.02756019
O 4.51829309 11.69492209 4.61089650
H 5.33480393 12.16633485 4.27756864
H 4.51830231 11.69492742 5.61091020
O 9.00908580 1.32388057 3.69421727
H 8.19257496 0.85247847 4.02756019
H 9.00907658 2.26670075 4.02756019
O 9.00908580 3.91664095 4.61089650
H 8.19258419 4.38805903 4.27755358
H 9.82558742 4.38805903 4.27755358

O 9.00908580 9.10216171 3.69421727
H 9.00907658 9.10215639 2.69420357
H 8.19257496 8.63074896 4.02754513
O 9.00908580 11.69492209 4.61089650
H 8.19257496 12.16632420 4.27755358
H 9.00907658 10.75210191 4.27755358
O 0.02750038 1.32388057 8.27761339
H 0.02749115 2.26670075 7.94427047
H -0.78901046 0.85247847 7.94427047
O 0.02750038 3.91664095 7.36093417
H 0.02750960 3.91664628 6.36092047
H 0.84401122 4.38805370 7.69426202
O 2.27289673 5.21302114 8.27761339
H 2.27290596 6.15584132 7.94427047
H 3.08940757 4.74161904 7.94427047
O 2.27289673 7.80578152 7.36093417
H 1.45639512 8.27719960 7.69427709
H 3.08939835 8.27719960 7.69427709
O 0.02750038 9.10216171 8.27761339
H 0.02749115 10.04498189 7.94427047
H -0.78901046 8.63075961 7.94427047
O 0.02750038 11.69492209 7.36093417
H 0.84400199 12.16634017 7.69427709
H -0.78900124 12.16634017 7.69427709
O 4.51829309 1.32388057 8.27761339
H 5.33480393 0.85247847 7.94427047
H 4.51830231 2.26670075 7.94427047
O 4.51829309 3.91664095 7.36093417
H 4.51830231 3.91664628 6.36092047
H 5.33480393 4.38805370 7.69426202
O 6.76368945 5.21302114 8.27761339
H 7.58020029 4.74160839 7.94428554
H 6.76369867 5.21301581 9.27762709
O 6.76368945 7.80578152 7.36093417
H 6.76368022 6.86296134 7.69427709
H 5.94717860 8.27718362 7.69427709
O 4.51829309 9.10216171 8.27761339
H 4.51829309 10.04498722 7.94428554
H 4.51829309 9.10217236 9.27762709
O 4.51829309 11.69492209 7.36093417
H 3.70179147 12.16634017 7.69427709
H 5.33479471 12.16634017 7.69427709
O 9.00908580 1.32388057 8.27761339
H 9.82559664 0.85247847 7.94427047
H 9.00909503 2.26670075 7.94427047
O 9.00908580 3.91664095 7.36093417
H 9.00909503 3.91664628 6.36092047
H 9.82559664 4.38805370 7.69426202
O 9.00908580 9.10216171 8.27761339
H 8.19257496 8.63074896 7.94428554
H 9.00907658 9.10215639 9.27762709
O 9.00908580 11.69492209 7.36093417
H 9.00908580 11.69491144 6.36092047
H 9.00908580 10.75209659 7.69426202
O 0.02750038 1.32388057 11.02765106
H 0.02749115 1.32387524 10.02763736
H -0.78901046 0.85246781 11.36097892
O 0.02750038 3.91664095 11.94433029
H 0.02750960 2.97382077 11.61098737
H 0.84401122 4.38804305 11.61098737
O 2.27289673 5.21302114 11.02765106
H 2.27289673 5.21303179 10.02763736
H 2.27289673 6.15584665 11.36097892
O 2.27289673 7.80578152 11.94433029
H 2.27290596 7.80578685 12.94434399
H 3.08940757 8.27719428 11.61100243
O 0.02750038 9.10216171 11.02765106
H 0.02750960 9.10215639 10.02763736
H 0.84401122 8.63074896 11.36097892
O 0.02750038 11.69492209 11.94433029
H 0.02750960 10.75210191 11.61098737
H 0.84401122 12.16632420 11.61098737
O 4.51829309 1.32388057 11.02765106
H 4.51830231 1.32387524 10.02763736
H 5.33480393 0.85246781 11.36097892
O 4.51829309 3.91664095 11.94433029
H 3.70178225 4.38804305 11.61098737
H 4.51828386 2.97382077 11.61098737
O 6.76368945 5.21302114 11.02765106
H 5.94718783 4.74160306 11.36099398
H 7.58019106 4.74160306 11.36099398
O 6.76368945 7.80578152 11.94433029
H 6.76368945 7.80577087 12.94434399
H 6.76368945 6.86295601 11.61100243
O 4.51829309 9.10216171 11.02765106
H 5.33480393 8.63075961 11.36099398
H 4.51830231 10.04498189 11.36099398
O 4.51829309 11.69492209 11.94433029
H 4.51830231 11.69492742 12.94434399
H 5.33480393 12.16633485 11.61100243
O 9.00908580 1.32388057 11.02765106
H 9.00908580 1.32389122 10.02763736
H 9.00908580 2.26670608 11.36097892
O 9.00908580 3.91664095 11.94433029
H 9.00909503 3.91664628 12.94434399
H 9.82559664 4.38805370 11.61100243
O 9.00908580 9.10216171 11.02765106
H 8.19258419 8.63074363 11.36099398
H 9.82558742 8.63074363 11.36099398
O 9.00908580 11.69492209 11.94433029
H 9.00909503 10.75210191 11.61098737
H 9.82559664 12.16632420 11.61098737

3. $(H_2O)_{64}$

O 0.02750038 1.32388057 0.94417960
H -0.78901046 0.85246781 0.61085174
H 0.02749115 1.32387524 1.94419330
O 0.02750038 3.91664095 0.02750038
H 0.02750038 2.97381544 0.36082823
H 0.02750038 3.91663030 -0.97251332
O 2.27289673 5.21302114 0.94417960
H 1.45638589 4.74160839 0.61085174
H 2.27288751 5.21301581 1.94419330

O 2.27289673 7.80578152 0.02750038
H 2.27288751 6.86296134 0.36084330
H 1.45638589 8.27718362 0.36084330
O 0.02750038 9.10216171 0.94417960
H -0.78901046 8.63074896 0.61085174
H 0.02749115 9.10215639 1.94419330
O 0.02750038 11.69492209 0.02750038
H 0.02750038 10.75209659 0.36082823
H 0.02750038 11.69491144 -0.97251332
O 4.51829309 1.32388057 0.94417960
H 3.70178225 0.85247847 0.61083668
H 4.51828386 2.26670075 0.61083668
O 4.51829309 3.91664095 0.02750038
H 3.70178225 4.38805370 0.36082823
H 4.51828386 3.91664628 -0.97251332
O 6.76368945 5.21302114 0.94417960
H 5.94717860 4.74161904 0.61083668
H 6.76368022 6.15584132 0.61083668
O 6.76368945 7.80578152 0.02750038
H 5.94718783 8.27719960 0.36084330
H 7.58019106 8.27719960 0.36084330
O 4.51829309 9.10216171 0.94417960
H 3.70178225 8.63074896 0.61085174
H 4.51828386 9.10215639 1.94419330
O 4.51829309 11.69492209 0.02750038
H 3.70178225 12.16632420 0.36084330
H 4.51828386 10.75210191 0.36084330
O 9.00908580 1.32388057 0.94417960
H 8.19257496 0.85246781 0.61085174
H 9.00907658 1.32387524 1.94419330
O 9.00908580 3.91664095 0.02750038
H 8.19257496 4.38804305 0.36084330
H 9.00907658 2.97382077 0.36084330
O 9.00908580 9.10216171 0.94417960
H 9.82559664 8.63075961 0.61083668
H 9.00909503 10.04498189 0.61083668
O 9.00908580 11.69492209 0.02750038
H 9.82559664 12.16633485 0.36082823
H 9.00909503 11.69492742 -0.97251332
O 0.02750038 1.32388057 3.69421727
H 0.84400199 0.85246249 4.02756019
H -0.78900124 0.85246249 4.02756019
O 0.02750038 3.91664095 4.61089650
H 0.02749115 2.97382077 4.27755358
H -0.78901046 4.38804305 4.27755358
O 2.27289673 5.21302114 3.69421727
H 1.45638589 4.74161904 4.02756019
H 2.27288751 6.15584132 4.02756019
O 2.27289673 7.80578152 4.61089650
H 3.08940757 8.27719428 4.27756864
H 2.27290596 7.80578685 5.61091020
O 0.02750038 9.10216171 3.69421727
H 0.84401122 8.63075961 4.02756019
H 0.02750960 10.04498189 4.02756019
O 0.02750038 11.69492209 4.61089650
H 0.84401122 12.16633485 4.27756864
H 0.02750960 11.69492742 5.61091020
O 4.51829309 1.32388057 3.69421727
H 4.51828386 1.32387524 2.69420357
H 3.70178225 0.85246781 4.02754513
O 4.51829309 3.91664095 4.61089650
H 3.70178225 4.38804305 4.27755358
H 4.51828386 2.97382077 4.27755358
O 6.76368945 5.21302114 3.69421727
H 6.76368022 5.21301581 2.69420357
H 5.94717860 4.74160839 4.02754513
O 6.76368945 7.80578152 4.61089650
H 6.76368945 6.86295601 4.27756864
H 6.76368945 7.80577087 5.61091020
O 4.51829309 9.10216171 3.69421727
H 5.33480393 8.63075961 4.02756019
H 4.51830231 10.04498189 4.02756019
O 4.51829309 11.69492209 4.61089650
H 5.33480393 12.16633485 4.27756864
H 4.51830231 11.69492742 5.61091020
O 9.00908580 1.32388057 3.69421727
H 8.19257496 0.85247847 4.02756019
H 9.00907658 2.26670075 4.02756019
O 9.00908580 3.91664095 4.61089650
H 8.19258419 4.38805903 4.27755358
H 9.82558742 4.38805903 4.27755358
O 9.00908580 9.10216171 3.69421727
H 9.00907658 9.10215639 2.69420357
H 8.19257496 8.63074896 4.02754513
O 9.00908580 11.69492209 4.61089650
H 8.19257496 12.16632420 4.27755358
H 9.00907658 10.75210191 4.27755358
O 0.02750038 1.32388057 8.27761339
H 0.02749115 2.26670075 7.94427047
H -0.78901046 0.85247847 7.94427047
O 0.02750038 3.91664095 7.36093417
H 0.02750960 3.91664628 6.36092047
H 0.84401122 4.38805370 7.69426202
O 2.27289673 5.21302114 8.27761339
H 2.27290596 6.15584132 7.94427047
H 3.08940757 4.74161904 7.94427047
O 2.27289673 7.80578152 7.36093417
H 1.45639512 8.27719960 7.69427709
H 3.08939835 8.27719960 7.69427709
O 0.02750038 9.10216171 8.27761339
H 0.02749115 10.04498189 7.94427047
H -0.78901046 8.63075961 7.94427047
O 0.02750038 11.69492209 7.36093417
H 0.84400199 12.16634017 7.69427709
H -0.78900124 12.16634017 7.69427709
O 4.51829309 1.32388057 8.27761339
H 5.33480393 0.85247847 7.94427047
H 4.51830231 2.26670075 7.94427047
O 4.51829309 3.91664095 7.36093417
H 4.51830231 3.91664628 6.36092047
H 5.33480393 4.38805370 7.69426202
O 6.76368945 5.21302114 8.27761339
H 7.58020029 4.74160839 7.94428554
H 6.76369867 5.21301581 9.27762709
O 6.76368945 7.80578152 7.36093417
H 6.76368022 6.86296134 7.69427709

H 5.94717860 8.27718362 7.69427709
O 4.51829309 9.10216171 8.27761339
H 4.51829309 10.04498722 7.94428554
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O 9.00908580 3.91664095 7.36093417
H 9.00909503 3.91664628 6.36092047
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O 9.00908580 9.10216171 8.27761339
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H 9.00907658 9.10215639 9.27762709
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H 9.00908580 10.75209659 7.69426202
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H 0.02749115 1.32387524 10.02763736
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O 0.02750038 3.91664095 11.94433029
H 0.02750960 2.97382077 11.61098737
H 0.84401122 4.38804305 11.61098737
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H 2.27289673 5.21303179 10.02763736
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H 0.02750960 9.10215639 10.02763736
H 0.84401122 8.63074896 11.36097892
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H -0.78900124 12.16634017 7.69427709
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O 4.51829309 3.91664095 7.36093417
H 4.51830231 3.91664628 6.36092047
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H 5.33479471 12.16634017 7.69427709
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O 9.00908580 3.91664095 7.36093417
H 9.00909503 3.91664628 6.36092047
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H 2.27289673 5.21303179 10.02763736
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H 4.51830231 1.32387524 10.02763736
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H 6.76368945 7.80577087 12.94434399
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H 4.51830231 11.69492742 12.94434399
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H 7.58020029 12.51990018 11.36099398
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H 9.00908580 1.32389122 10.02763736
H 9.00908580 2.26670608 11.36097892
O 9.00908580 3.91664095 11.94433029
H 9.00909503 3.91664628 12.94434399
H 9.82559664 4.38805370 11.61100243
O 9.00908580 9.10216171 11.02765106
H 8.19258419 8.63074363 11.36099398
H 9.82558742 8.63074363 11.36099398
O 9.00908580 11.69492209 11.94433029
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5. $(H_2O)_{96}$ [3]

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H 0.02750960 10.04498189 4.02756019
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H 0.02750960 11.69492742 5.61091020
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H 3.70178225 4.38804305 4.27755358
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H 6.76368022 5.21301581 2.69420357
H 5.94717860 4.74160839 4.02754513
O 6.76368945 7.80578152 4.61089650
H 6.76368945 6.86295601 4.27756864
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H 5.33480393 8.63075961 4.02756019
H 4.51830231 10.04498189 4.02756019
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H 5.33480393 12.16633485 4.27756864
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H 9.00907658 2.26670075 4.02756019
O 9.00908580 3.91664095 4.61089650
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H 9.82558742 4.38805903 4.27755358
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H -0.78900124 12.16634017 7.69427709
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H 2.27289673 13.93412779 7.94428554
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H 4.51828386 2.97382077 11.61098737
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H 7.58019106 4.74160306 11.36099398
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O 9.00908580 9.10216171 11.02765106
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O 9.00908580 11.69492209 11.94433029
H 9.00909503 10.75210191 11.61098737
H 9.82559664 12.16632420 11.61098737
O 11.25448216 12.99130228 11.02765106
H 12.07099300 12.51990018 11.36099398
H 11.25449138 13.93412247 11.36099398

C. Alanine peptides

1. *β-strand acetyl(ala)$_{10}NH_2$ [4]*

C 19.402172 0.699285 0.029799
C 18.238889 -0.208126 -0.288508
O 18.412171 -1.275953 -0.881556
N 17.007717 0.238073 0.111294
H 16.889771 1.106059 0.626212
C 15.781659 -0.518634 -0.130092
C 14.609950 0.433887 0.225555
O 14.798597 1.489028 0.839493
N 13.389367 0.012283 -0.179811
H 13.253932 -0.855679 -0.693441
C 12.151384 0.734404 0.116665
C 10.994941 -0.236568 -0.242392
O 11.208976 -1.286924 -0.856628
N 9.767987 0.160193 0.162951
H 9.613295 1.028097 0.672244
C 8.541805 -0.583275 -0.133026
C 7.371989 0.369421 0.234049
O 7.576818 1.425989 0.841386
N 6.148317 -0.048264 -0.157047
H 6.001282 -0.921822 -0.659358
C 4.913080 0.677926 0.145581
C 3.755818 -0.294678 -0.209909
O 3.974854 -1.352620 -0.809871
N 2.527970 0.107973 0.182746
H 2.369736 0.984351 0.676878
C 1.301429 -0.636741 -0.110719
C 0.133253 0.324462 0.240563
O 0.341887 1.390771 0.829480
N -1.091124 -0.096697 -0.142897
H -1.241189 -0.979649 -0.627833
C -2.324901 0.637335 0.147437
C -3.483568 -0.339872 -0.190823
O -3.265140 -1.409857 -0.769241
N -4.711386 0.072353 0.191606
H -4.869242 0.959048 0.667055
C -5.938254 -0.676819 -0.089176
C -7.105862 0.292953 0.239003
O -6.897634 1.371495 0.805053
N -8.330430 -0.134822 -0.137526
H -8.480518 -1.027734 -0.603534
C -9.562568 0.608329 0.135623
C -10.723596 -0.373557 -0.178137
O -10.510318 -1.456246 -0.733433
N -11.950764 0.049539 0.197711
H -12.104313 0.945132 0.656653
C -13.176828 -0.707539 -0.063903
C -14.346138 0.267324 0.236098
O -14.146768 1.357749 0.780620
N -15.570334 -0.169113 -0.139310
H -15.716627 -1.072551 -0.584543
C -16.798422 0.582414 0.121123
C -17.966199 -0.397434 -0.161175
O -17.774663 -1.490702 -0.687448
N -19.198694 0.034879 0.228478
C 15.663972 -1.801296 0.658395
H 15.730442 -0.777389 -1.198517
C 11.990453 2.037674 -0.627503
H 12.118152 0.955001 1.194242
C 8.406545 -1.891575 0.606619
H 8.508525 -0.799291 -1.211460
C 4.752962 1.981212 -0.597711
H 4.884205 0.896862 1.223519
C 1.160380 -1.936014 0.643179
H 1.272324 -0.864276 -1.186861
C -2.482477 1.927632 -0.618526
H -2.353076 0.874889 1.221431
C -6.082791 -1.959817 0.691437
H -5.964988 -0.926796 -1.160393
C -9.718126 1.880173 -0.661125
H -9.589242 0.871913 1.203596
C -13.321934 -1.969280 0.750863
H -13.201472 -0.986772 -1.127939
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H -16.819394 0.872425 1.182673
H 16.556800 -2.448419 0.463332
H 14.750137 -2.360802 0.342818
H 15.601219 -1.605248 1.755875
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H 11.078587 2.573061 -0.267194
H 11.897028 1.873976 -1.728205
H 9.305433 -2.531294 0.414857
H 7.503518 -2.441993 0.246476
H 8.312839 -1.733827 1.708179
H 5.644083 2.634609 -0.416101

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H 0.258642 -2.489458 0.284318
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H -2.584436 1.745305 -1.715572
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H -6.984345 -2.519585 0.342037
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H -19.346725 0.953517 0.621320
H -19.999726 -0.542620 0.010082
H 19.496293 0.847917 1.132449
H 20.340084 0.227643 -0.352574
H 19.272350 1.693968 -0.460793

2. 3_{10}-helix acetyl(ala)$_{10}NH_2$ [4]

C -10.564903 -0.552887 -2.122609
C -9.373722 0.097093 -1.476607
O -8.225039 -0.185696 -1.831842
N -9.628469 0.995523 -0.465759
H -10.594068 1.253579 -0.295692
C -8.558263 1.896287 0.017721
H -8.072675 2.365936 -0.848328
C -7.401487 1.159534 0.738413
O -6.283005 1.680074 0.789355
C -9.086481 2.976176 0.924896
H -8.229172 3.606928 1.272287
H -9.810359 3.633203 0.382825
H -9.596684 2.552362 1.824232
N -7.685249 -0.049394 1.280790
H -8.613687 -0.432129 1.155182
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H -6.121526 -0.276403 2.662228
C -5.492476 -1.262499 0.907145
O -4.382480 -1.572282 1.358355
C -7.168570 -2.126406 2.532973
H -6.313351 -2.709747 2.959340
H -7.875500 -1.876872 3.361850
H -7.701081 -2.774633 1.794736
N -5.774397 -1.218431 -0.415016
H -6.680855 -0.896200 -0.752607
C -4.715473 -1.459532 -1.412335
H -4.225613 -2.414545 -1.184777
C -3.560837 -0.423092 -1.345067
O -2.446996 -0.720349 -1.796055
C -5.255570 -1.507424 -2.816986
H -4.399475 -1.569993 -3.534225
H -5.904372 -2.406990 -2.955548
H -5.864364 -0.600978 -3.060940
N -3.830113 0.767491 -0.758217
H -4.740770 0.954486 -0.340812
C -2.757703 1.752103 -0.535768
H -2.241569 1.934322 -1.486876
C -1.633244 1.238912 0.404429
O -0.513367 1.766188 0.360152
C -3.283873 3.059979 -0.006029
H -2.420168 3.717635 0.263464
H -3.897731 3.576977 -0.783876
H -3.923678 2.915291 0.900496
N -1.932625 0.202887 1.222393
H -2.846816 -0.247265 1.191771
C -0.885824 -0.430414 2.041451
H -0.375715 0.344990 2.627008
C 0.254879 -1.067749 1.201950
O 1.360262 -1.263077 1.725829
C -1.444255 -1.466409 2.981156
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H -2.071568 -0.980661 3.768309
H -2.080378 -2.215174 2.445406
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H -0.919542 -1.139345 -0.506163
C 1.054269 -1.831310 -0.989664
H 1.548189 -2.696798 -0.530070
C 2.204832 -0.803807 -1.174031
O 3.318889 -1.195740 -1.546438
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H -0.092568 -1.418758 -2.803509
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H 1.015932 0.773304 -0.537724
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H 3.528106 1.437463 -1.873853
C 4.109123 1.263214 0.140076
O 5.216146 1.795902 -0.008819
C 2.459006 2.903670 -0.751984
H 3.317001 3.612702 -0.642430
H 1.861766 3.199739 -1.648976
H 1.799199 2.992787 0.147543
N 3.809894 0.446075 1.178300
H 2.901929 -0.012702 1.243866
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H 5.361746 0.954017 2.496945
C 5.989489 -0.801663 1.521803
O 7.064927 -0.908644 2.124831
C 4.276145 -0.684299 3.328321
H 5.116713 -1.076064 3.953368
H 3.655816 0.004456 3.952558
H 3.629650 -1.541797 3.013206
N 5.744534 -1.374669 0.319618
H 4.852478 -1.236887 -0.153331
C 6.805687 -2.077360 -0.420609

H 7.340725 -2.730418 0.280903
C 7.923231 -1.146547 -0.981010
O 8.944364 -1.648599 -1.451817
C 6.257306 -2.910400 -1.549359
H 7.109593 -3.308183 -2.154822
H 5.668485 -3.771598 -1.149058
H 5.587176 -2.313729 -2.218369
N 7.706682 0.192424 -0.876607
H 6.816872 0.551743 -0.538463
C 8.744657 1.174263 -1.210644
H 9.455653 0.678304 -1.883590
C 9.597182 1.631352 0.010401
O 10.494072 2.461915 -0.139077
C 8.192315 2.403846 -1.885306
H 9.013555 3.153756 -2.004909
H 7.787582 2.149021 -2.894824
H 7.369418 2.865960 -1.284004
N 9.298100 1.059771 1.208484
H 8.580041 0.352954 1.334176
H 9.878510 1.315321 1.995080
H -11.068082 0.180893 -2.799634
H -10.215931 -1.421632 -2.733908
H -11.302760 -0.916689 -1.367816

3. α-helix acetyl(ala)$_{10}$NH$_2$ [4]

C -8.239178 -1.239415 -1.849390
C -7.289526 -0.112832 -1.349117
N -7.768934 0.677662 -0.355326
C -6.898097 1.681692 0.289336
C -5.722158 1.024159 1.062348
N -6.045801 -0.037551 1.840157
C -4.995280 -0.799732 2.546067
C -3.937454 -1.381896 1.565064
N -4.423288 -1.977479 0.451115
C -3.511087 -2.525930 -0.570582
C -2.596532 -1.433243 -1.192399
N -3.197243 -0.266752 -1.516998
C -2.420093 0.864976 -2.057113
C -1.323502 1.352033 -1.068638
N -1.689448 1.450233 0.228669
C -0.706534 1.834547 1.258659
C 0.454186 0.806459 1.377799
N 0.097849 -0.496251 1.317816
C 1.119921 -1.557170 1.356598
C 2.110637 -1.467606 0.163104
N 1.562794 -1.258255 -1.055642
C 2.426637 -1.143250 -2.243572
C 3.320291 0.129860 -2.224056
N 2.739554 1.256871 -1.747976
C 3.483362 2.526693 -1.730182
C 4.597958 2.593503 -0.646573
N 4.380531 1.856937 0.479717
C 5.340075 1.890839 1.591872
C 6.364289 0.718797 1.606011
N 6.010501 -0.407119 0.918153
C 6.837892 -1.620011 0.969901
C 7.327156 -2.124924 -0.414444
N 6.938388 -1.410182 -1.502735
O -6.191690 0.045175 -1.887421
C -7.664284 2.586768 1.215775
O -4.573459 1.458553 0.945776
C -5.570207 -1.918133 3.374536
O -2.733425 -1.279657 1.815309
C -4.257037 -3.231820 -1.672735
O -1.396148 -1.661229 -1.374223
C -3.306776 2.026460 -2.423677
O -0.194279 1.634286 -1.483310
C -1.347382 2.009214 2.610790
O 1.619997 1.190243 1.517767
C 0.501657 -2.931255 1.376615
O 3.325478 -1.593831 0.348782
C 1.632149 -1.153516 -3.524110
O 4.479554 0.086288 -2.648245
C 2.574920 3.715874 -1.548068
O 5.585653 3.303002 -0.831391
C 4.669503 1.939059 2.942410
O 7.422641 0.850458 2.222065
O 8.042141 -3.127470 -0.485516
H -8.559366 0.342843 0.185407
H -6.420135 2.274514 -0.497515
H -7.021513 -0.304856 1.949501
H -4.423929 -0.121005 3.191655
H -5.425248 -2.120035 0.346411
H -2.810876 -3.225621 -0.096611
H -4.205782 -0.162679 -1.424872
H -1.861194 0.535791 -2.942183
H -2.654224 1.275679 0.505869
H -0.212515 2.768259 0.961294
H -0.885183 -0.759879 1.278691
H 1.751812 -1.424351 2.243859
H 0.550302 -1.241974 -1.168168
H 3.141278 -1.975613 -2.247687
H 1.752220 1.261192 -1.496586
H 4.030294 2.629638 -2.675748
H 3.456801 1.463609 0.648056
H 5.957981 2.787475 1.464047
H 5.041416 -0.524664 0.629999
H 7.746245 -1.348179 1.521954
C 6.170700 -2.778201 1.671994
H 6.256268 -0.661327 -1.471346
H 7.208965 -1.767350 -2.408439
H -6.950103 3.288667 1.713969
H -8.414017 3.190194 0.647746
H -8.201730 2.004128 2.006516
H -4.733678 -2.494634 3.842156
H -6.218470 -1.513590 4.190194
H -6.180428 -2.619210 2.750096
H 2.331609 -1.040945 -4.388873
H 1.076225 -2.116344 -3.637321
H 0.891787 -0.315101 -3.551245
H -2.674627 2.861573 -2.814007
H -4.038973 1.731012 -3.215231
H -3.881245 2.395747 -1.536474

H 1.313951 -3.699053 1.371005
H -0.117403 -3.072457 2.296468
H -0.153664 -3.095289 0.483510
H 3.194038 4.646467 -1.525976
H 1.844917 3.788960 -2.391069
H 1.997163 3.646142 -0.593094
H -0.558181 2.266566 3.359464
H -2.100636 2.834578 2.588086
H -1.862733 1.071742 2.940885
H 5.446788 1.853015 3.741360
H 4.126390 2.906613 3.073939
H 3.930386 1.108666 3.065063
H -3.523237 -3.608776 -2.427559
H -4.830845 -4.102082 -1.269133
H -4.974914 -2.544042 -2.186857
H 6.823632 -3.682192 1.589747
H 6.016560 -2.544289 2.753259
H 5.175112 -3.009937 1.217229
H -8.538029 -1.847786 -1.021457
H -7.727757 -1.843367 -2.569522
H -9.104765 -0.801773 -2.301197

4. β-strand acetyl(ala)$_{18}$NH$_2$ [4]

C -29.093450 -0.473930 0.203276
O -29.282421 -1.483994 0.888797
N -27.871738 -0.075276 -0.221177
H -27.736574 0.754966 -0.793940
C -26.632130 -0.766803 0.135358
C -25.478366 0.181336 -0.288044
O -25.694628 1.183273 -0.977838
N -24.251696 -0.178841 0.150540
H -24.095515 -1.006859 0.722114
C -23.027025 0.546425 -0.193102
C -21.855454 -0.371093 0.250473
O -22.060120 -1.380740 0.933129
N -20.631318 0.022223 -0.163216
H -20.484977 0.856729 -0.728371
C -19.394351 -0.673328 0.198688
C -18.239759 0.273815 -0.227833
O -18.461934 1.282166 -0.906982
N -17.011602 -0.093231 0.196651
H -16.851356 -0.929262 0.756002
C -15.786063 0.629964 -0.150182
C -14.616891 -0.297976 0.279539
O -14.826598 -1.316794 0.947162
N -13.392053 0.096180 -0.129121
H -13.241686 0.940197 -0.679247
C -12.156960 -0.609310 0.220740
C -11.000362 0.341504 -0.192903
O -11.222745 1.363968 -0.850751
N -9.771962 -0.038191 0.218378
H -9.611520 -0.887501 0.757520
C -8.544852 0.686792 -0.119622
C -7.378221 -0.256036 0.284446
O -7.591107 -1.290474 0.926669
N -6.152817 0.143028 -0.117015
H -5.999464 1.001497 -0.643558
C -4.919812 -0.576050 0.212298
C -3.760541 0.382229 -0.176205
O -3.981057 1.424855 -0.802346
N -2.532570 -0.013982 0.220124
H -2.373286 -0.881093 0.730568
C -1.303652 0.716315 -0.099624
C -0.139654 -0.244216 0.268991
O -0.355184 -1.299459 0.875524
N 1.086365 0.163625 -0.121447
H 1.242431 1.040431 -0.616017
C 2.317205 -0.571043 0.180580
C 3.479313 0.397402 -0.172693
O 3.261583 1.463892 -0.758316
N 4.706440 -0.017454 0.206790
H 4.863901 -0.904664 0.682014
C 5.937176 0.720698 -0.087001
C 7.098658 -0.257551 0.240577
O 6.880875 -1.335488 0.804899
N 8.325367 0.161464 -0.135748
H 8.483717 1.057308 -0.594085
C 9.554150 -0.588503 0.135485
C 10.718979 0.390160 -0.178204
O 10.504533 1.479969 -0.720425
N 11.945018 -0.042929 0.184377
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C 14.336780 -0.289452 0.207989
O 14.117384 -1.387946 0.730346
N 15.564302 0.140986 -0.153084
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C 17.958629 0.364625 -0.186923
O 17.748350 1.473683 -0.690044
N 19.183310 -0.084151 0.162023
H 19.334934 -1.004415 0.571288
C 20.417036 0.669709 -0.073045
C 21.575052 -0.333355 0.181559
O 21.355815 -1.447814 0.668480
N 22.803464 0.107234 -0.165942
H 22.963269 1.031064 -0.563533
C 24.028039 -0.666322 0.051518
C 25.198838 0.324630 -0.189336
O 24.996008 1.447638 -0.662472
N 26.421654 -0.137162 0.153242
H 26.566705 -1.066408 0.542898
C 27.655456 0.624482 -0.053250
C 28.814467 -0.382127 0.173271
O 28.603103 -1.508089 0.634654
N 30.043492 0.068205 -0.168149
H 30.200016 1.001323 -0.543206
C 31.263444 -0.713164 0.037054
C 32.441574 0.273366 -0.168566
O 32.262127 1.404823 -0.611872
N 33.668684 -0.199113 0.190028
H -26.604212 -0.906611 1.226538
H -22.988107 0.681679 -1.284432

H -19.367908 -0.807641 1.290481
H -15.753340 0.772253 -1.240774
H -12.129501 -0.759930 1.310346
H -8.516875 0.851567 -1.207162
H -4.891944 -0.756333 1.297363
H -1.279370 0.915718 -1.181432
H 2.344742 -0.791368 1.258230
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H 24.051461 -1.008111 1.097151
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H 34.475823 0.385482 0.017855
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O -32.895040 1.135655 -1.049796
H -31.373533 -1.130109 0.628356
C 31.410568 -1.901223 -0.882596
H 30.507593 -2.558762 -0.802732
H 32.305222 -2.502212 -0.589658
H 31.525140 -1.585676 -1.947751
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H 26.922241 2.492012 0.754734
H 28.721180 2.403832 0.559363
H 27.913652 1.518193 1.922042
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H 23.271230 -2.535237 -0.731338
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H 24.275987 -1.590223 -1.910897
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H 12.445029 2.618957 0.607920
H 14.242482 2.522263 0.403806
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H 8.803682 -2.511252 -0.511296
H 10.602898 -2.424200 -0.319123
H 9.807089 -1.650605 -1.754853
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H 5.199816 2.660251 0.523513
H 6.997476 2.560171 0.323071
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H 1.572206 -2.520686 -0.387256
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H -0.250353 2.574016 0.240173
H -1.043200 1.890150 1.722318
C -4.763539 -1.905009 -0.484503
H -5.658095 -2.547866 -0.283216
H -3.859632 -2.435261 -0.097133
H -4.658319 -1.780675 -1.589320
C -8.400862 2.026959 0.558007
H -9.299949 2.659653 0.345105
H -7.500065 2.558454 0.165142
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C -11.995182 -1.956293 -0.439322
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H -11.089328 -2.472080 -0.037274
H -11.889990 -1.861860 -1.547097
C -15.651307 1.984777 0.499824
H -16.551521 2.609208 0.268104
H -14.750079 2.511262 0.101287
H -15.554436 1.901275 1.609235
C -19.226741 -2.029765 -0.440522
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H -18.318863 -2.535447 -0.030363
H -19.121660 -1.951943 -1.549592
C -22.901769 1.906761 0.447772
H -23.802286 2.526162 0.204012
H -21.999041 2.433102 0.052582
H -22.813743 1.831887 1.558516
C -26.460080 -2.120840 -0.508947
H -27.346348 -2.765727 -0.279604
H -25.548332 -2.623435 -0.103883
H -26.359707 -2.038745 -1.618117
C -30.163485 1.779332 0.471311
H -29.249070 2.320827 0.127272
H -30.111263 1.659556 1.580263
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C -33.882719 -0.778055 -0.013333
H -33.989501 -0.843553 1.096235
H -33.741020 -1.806057 -0.425677
H -34.818634 -0.343043 -0.441285

5. 3_{10}-helix acetyl(ala)$_{18}NH_2$ [4]

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H -18.33744200 -1.43676100 -2.57784400
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C -16.64178100 1.81847500 -0.08687500
H -16.33275600 2.47518600 -0.90015400
C -15.45368600 1.00665000 0.40960000
O -14.34590800 1.14728700 -0.10143600
C -17.16398600 2.64431900 1.08306700

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H -17.99570000 3.26351700 0.74868300
H -17.50377200 1.97743000 1.87616700
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H -16.62353600 0.08539500 1.78597900
C -14.64159000 -0.67534300 1.97117800
H -14.31419800 -0.18797000 2.88979800
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O -12.35797600 -0.39522400 1.31468900
C -15.15670300 -2.07793100 2.27756900
H -14.35023000 -2.67790600 2.69717900
H -15.97461800 -2.01603400 2.99502400
H -15.51407200 -2.54219400 1.35839900
N -13.73037600 -1.39201600 -0.16774400
H -14.66876500 -1.71079000 -0.36112300
C -12.70277100 -1.57866400 -1.17215600
H -12.37337500 -2.61419500 -1.09393600
C -11.52970100 -0.63736400 -0.93688100
O -10.40953700 -1.08401600 -0.70081400
C -13.24568100 -1.30545600 -2.57053500
H -12.45280400 -1.45312700 -3.30389000
H -14.06762800 -1.98985300 -2.78085100
H -13.60497900 -0.27802400 -2.62659100
N -11.79045800 0.66997300 -1.00224700
H -12.73299300 0.97338900 -1.20016900
C -10.75830800 1.66718600 -0.79706500
H -10.44856400 2.00520400 -1.78620200
C -9.57020100 1.08026700 -0.04905900
O -8.45955100 1.04067800 -0.57506700
C -11.28676600 2.84333700 0.01717500
H -10.49179900 3.57595900 0.15529400
H -12.11940800 3.30757700 -0.51238200
H -11.62698300 2.48873600 0.99036100
N -9.80552100 0.62293700 1.18299900
H -10.74115600 0.68464800 1.55797600
C -8.75725500 0.04144300 1.99698400
H -8.43424900 0.81601900 2.69190700
C -7.58484400 -0.41240300 1.13816600
O -6.47234900 0.08726200 1.28865100
C -9.26898900 -1.17206900 2.76572100
H -8.46112500 -1.58853000 3.36792200
H -10.08978900 -0.87024400 3.41666900
H -9.62250600 -1.92572200 2.06200600
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C -6.80684400 -1.88041000 -0.64002300
H -6.47386800 -2.82500500 -0.21053000
C -5.63678700 -0.91208600 -0.74125000
O -4.51571500 -1.24589200 -0.36386800
C -7.34679100 -2.10752900 -2.04876600
H -6.55076000 -2.49508600 -2.68482600
H -8.16462400 -2.82537500 -2.01255000
H -7.70885200 -1.16355400 -2.45546300
N -5.90078100 0.29227800 -1.25323400
H -6.84352900 0.50587300 -1.54463400
C -4.87290200 1.30339600 -1.40173900
H -4.56075700 1.28225500 -2.44606200
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H -2.26310300 -3.32378100 -0.99266700
H -1.80967500 -1.91321900 -1.97989200
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H 1.33119700 0.39815400 -2.80548800
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H 0.13153200 2.55022900 -1.00119300
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H 5.31699600 -2.24037100 1.52628800
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O 7.26877500 -1.11840200 0.39360500
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N 5.88277500 -0.52931400 -1.28257100
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H 9.19757000 2.79249300 0.42218200
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O 11.17803200 1.23542600 0.36342300
C 8.37123100 1.86303200 2.18578500
H 9.17443700 2.19073200 2.84550700
H 7.54251100 2.56903100 2.24445200
H 8.02979100 0.87497200 2.49202400
N 9.83161400 -0.41237000 1.10199600
H 8.89762300 -0.67033100 1.38588000
C 10.87412500 -1.41792000 1.11866500
H 11.20693100 -1.50759400 2.15315800
C 12.04105000 -1.01181000 0.22821900
O 13.15961700 -0.83577800 0.70695700
C 10.35191000 -2.75977600 0.61895000
H 11.15606000 -3.49500400 0.64206300
H 9.53581500 -3.09408200 1.25990400
H 9.98906800 -2.65087400 -0.40329000
N 11.77647600 -0.86449000 -1.07192100
H 10.83568000 -1.02376400 -1.40282800
C 12.80126100 -0.48044200 -2.02228600
H 13.12452100 -1.39458600 -2.51978900
C 13.98069600 0.17728100 -1.32077800
O 15.09818700 -0.33022800 -1.37061900
C 12.25674500 0.50862000 -3.04632200
H 13.04717900 0.77818700 -3.74717800
H 11.43046500 0.05109700 -3.59087700
H 11.90325500 1.40388100 -2.53469200
N 13.72874700 1.31325100 -0.66544900
H 12.78693700 1.67962200 -0.66306500
C 14.76664200 2.03492700 0.04136300
H 15.07586400 2.85422000 -0.60747400
C 15.95309700 1.13159600 0.34589600
O 17.06183700 1.37944700 -0.12340100
C 14.24759600 2.58458000 1.36640000
H 15.04770200 3.12192500 1.87521300
H 13.41680600 3.26507600 1.17730100
H 13.90786600 1.76088000 1.99290400
N 15.71754200 0.08129600 1.13472700
H 14.78321800 -0.06765400 1.48822800
C 16.76379700 -0.85426500 1.49717500
H 17.09364500 -0.58115800 2.50039200
C 17.93069100 -0.77464500 0.52410600
O 19.04793500 -0.44046600 0.91474200
C 16.24619800 -2.28839300 1.48851400
H 17.05270000 -2.96749500 1.76532400
H 15.42871200 -2.38414200 2.20384800
H 15.88608700 -2.53884100 0.49046600
N 17.67075500 -1.08389000 -0.74788900
H 16.73132700 -1.35071900 -1.00557800
H 18.37876000 -1.05849500 -1.45364000
H -19.46659700 -0.55689700 -1.54801500

6. α-helix $acetyl(ala)_{18}NH_2$ [4]

C 12.98677500 -0.51314500 -1.81705000
C 11.87201900 -1.02213700 -0.87032300
N 12.24586300 -1.38290400 0.38246700
C 11.24661600 -1.86670300 1.35635700
C 10.19196000 -0.78588800 1.72908600
N 10.62477100 0.49857400 1.75973500
C 9.67929400 1.61121500 1.98639900
C 8.65322600 1.74849500 0.82901400
N 9.15717500 1.64286800 -0.42411200
C 8.26755800 1.63258700 -1.60211700
C 7.23061900 0.47529600 -1.53677900
N 7.71431300 -0.73560200 -1.17650900
C 6.81634100 -1.89697400 -1.02272300
C 5.71765500 -1.65073400 0.04856300
N 6.12981100 -1.10265800 1.21221100
C 5.16522800 -0.76635000 2.27649700
C 4.09130000 0.24763100 1.79372500
N 4.54432100 1.29920600 1.07805300
C 3.61119800 2.29133800 0.51319400
C 2.59714000 1.64909500 -0.47370300
N 3.10737900 0.77081600 -1.36305300
C 2.23059600 0.04353500 -2.29891000
C 1.17221600 -0.82052700 -1.55858800
N 1.62484200 -1.54727500 -0.51491500
C 0.70094300 -2.34737400 0.30890300
C -0.39721600 -1.47304600 0.97654400
N 0.02419600 -0.32235900 1.54201100
C -0.93256900 0.62758600 2.13815000
C -1.97932300 1.13310500 1.10666800
N -1.49625500 1.49421500 -0.10088900
C -2.40088800 1.92284400 -1.18237000
C -3.42160200 0.81629500 -1.57091900
N -2.92262200 -0.43278600 -1.68405300
C -3.79846900 -1.58172000 -1.97459400
C -4.88639300 -1.78702800 -0.88363100
N -4.47048000 -1.68651400 0.39677200
C -5.42972400 -1.78317300 1.51140900
C -6.50421400 -0.65959300 1.46519100
N -6.05091700 0.57779200 1.16922200
C -6.98405900 1.70915800 1.03236000
C -8.02192400 1.48486100 -0.10171300
N -7.53931800 0.99160700 -1.26383800
C -8.45083900 0.72588300 -2.38980700
C -9.45558800 -0.42525300 -2.09839400
N -8.95609600 -1.49410100 -1.43572200
C -9.80741300 -2.65891900 -1.14728700
C -10.87918200 -2.40522500 -0.04835400
N -10.54795500 -1.49232800 0.90760700
C -11.46355900 -1.21027900 2.02096800
C -12.37758100 0.03264800 1.81394600

N -11.94815300 0.95777600 0.90599100
C -12.65979000 2.22951700 0.72356900
C -13.17024400 2.48162500 -0.72103500
N -12.85623700 1.54852200 -1.65688400
O 10.70924900 -1.09636900 -1.27416300
O 9.03972800 -1.12990900 2.00517800
O 7.45681600 1.93595700 1.06634400
O 6.04311400 0.68700100 -1.80170800
O 4.54214000 -1.95320100 -0.18655000
O 2.89919000 0.07127500 2.07299700
O 1.39829300 1.95084100 -0.41898100
O -0.00664300 -0.82103900 -1.93519800
O -1.57809400 -1.84386800 0.96963400
O -3.17738000 1.19084700 1.41192900
O -4.61036100 1.10385900 -1.76067500
O -6.05508800 -2.03241400 -1.20743500
O -7.69162400 -0.91670700 1.69568100
O -9.21347000 1.76475900 0.07453600
O -10.62720200 -0.34747300 -2.48511800
O -11.93915700 -3.02988900 -0.07359600
O -13.42064400 0.13005800 2.46259000
O -13.84250100 3.48637100 -0.96842600
N 14.02299800 0.27230900 -1.10772900
H 12.46240800 0.13648400 -2.53052900
H 13.21864000 -1.29831300 0.65026000
H 10.66263600 -2.66896900 0.88906900
H 11.52341700 0.72905700 1.34718500
H 9.07571300 1.37863100 2.87033200
H 10.15320600 1.49618900 -0.55297300
H 7.65972000 2.54561200 -1.60366900
H 8.71741000 -0.86647100 -1.06259100
H 6.25726700 -2.05397500 -1.95402800
H 7.12166700 -0.94864100 1.38594500
H 4.59154100 -1.66161800 2.54854300
H 5.54493400 1.42741800 0.93350000
H 2.98531200 2.70378300 1.31491100
H 4.11351000 0.61147700 -1.40556500
H 1.63716900 0.76126400 -2.87982700
H 2.62003000 -1.55795800 -0.29213400
H 0.14161200 -3.03928000 -0.33391500
H 1.02028000 -0.10419700 1.57785000
H -1.53100300 0.11651600 2.90340300
H -0.48996600 1.49601800 -0.27050500
H -3.02496300 2.75530600 -0.83219400
H -1.91956900 -0.59256100 -1.58772000
H -4.36866300 -1.38704800 -2.89210700
H -3.47966700 -1.56073700 0.60539000
H -6.00585900 -2.71289700 1.41956400
H -5.05036000 0.74975600 1.07132400
H -7.59155300 1.79656000 1.94219400
H -6.53548000 0.86146100 -1.38966300
H -9.08638200 1.60519800 -2.55374600
H -7.96025100 -1.54900300 -1.22436700
H -10.39843800 -2.89686700 -2.04064200
H -9.58406400 -1.17118700 0.97783900
H -12.16368600 -2.05109000 2.09171100
H -10.98348800 0.92013100 0.58204200
H -13.56059500 2.17005300 1.34698600
H -12.20973800 0.78346400 -1.49922800
H -13.13786500 1.74014100 -2.60824200
C 13.67740800 1.44381200 -0.47677000
O 12.49785500 1.74877600 -0.25895000
H 14.99283300 0.15184000 -1.37968200
C 14.80323100 2.33093800 -0.02451100
H 14.38249300 3.17789200 0.57233700
H 15.53248900 1.77109100 0.61009900
H 15.34122800 2.75124300 -0.90972500
C 13.57217300 -1.68466200 -2.56040300
H 12.74481200 -2.24624200 -3.06321400
H 14.10789000 -2.38641600 -1.87523200
H 14.28902900 -1.34037900 -3.34625300
C 11.87796300 -2.38896000 2.61885400
H 11.06840700 -2.73078400 3.31226600
H 12.54532500 -3.25875700 2.40086100
H 12.47721500 -1.60295800 3.14044200
C 10.38779800 2.92428700 2.18492700
H 9.62784500 3.73931600 2.27946000
H 11.00139400 2.90390800 3.11881700
H 11.06184600 3.16230700 1.32304200
C 9.03900000 1.53811100 -2.89173000
H 8.31923400 1.47882500 -3.74555300
H 9.68202200 2.44104800 -3.03488400
H 9.69257200 0.62899200 -2.91284300
C 7.57448900 -3.15110600 -0.67420100
H 6.84925200 -3.99044900 -0.53362500
H 8.28148600 -3.42723500 -1.49478400
H 8.16166100 -3.02534100 0.27092400
C 5.85114200 -0.21584500 3.49939500
H 5.08056900 0.04758200 4.26513900
H 6.54564400 -0.97419400 3.93814100
H 6.44340000 0.70276200 3.25580800
C 4.33856800 3.41042500 -0.18541500
H 3.59138900 4.11460800 -0.62732200
H 4.97861300 3.97603900 0.53565800
H 4.99364500 3.02059000 -1.00585200
C 3.01748600 -0.83600900 -3.23533600
H 2.30990900 -1.39585700 -3.89505100
H 3.69440400 -0.22151200 -3.87844600
H 3.64307600 -1.57410300 -2.67118900
C 1.42964400 -3.12381400 1.37460900
H 0.68641600 -3.68088000 1.99631100
H 2.13360500 -3.86018000 0.91462900
H 2.01889800 -2.44410300 2.04197500
C -0.23390500 1.81291500 2.75218900
H -0.99821900 2.52180300 3.15518100
H 0.42996100 1.48849200 3.59095000
H 0.39340100 2.35162600 1.99652600
C -1.64100900 2.34405700 -2.41339000
H -2.36726400 2.62294300 -3.21580000
H -0.99348200 3.22838200 -2.19415000
H -0.98811500 1.51596500 -2.79097100
C -3.01214300 -2.85778200 -2.12978600
H -3.71833100 -3.70459500 -2.31177900
H -2.30927500 -2.78536200 -2.99588400
H -2.41306800 -3.07987200 -1.20965600
C -4.73905000 -1.74512900 2.84993600

H -5.50760700 -1.78267900 3.66049900
H -4.05374000 -2.62037700 2.96595200
H -4.13624200 -0.80878500 2.96918400
C -6.25802400 3.00578600 0.78157000
H -7.00568000 3.82560000 0.64810500
H -5.59687800 3.26118800 1.64586200
H -5.62307300 2.94405900 -0.13912800
C -7.70250800 0.39987500 -3.65681700
H -8.43767900 0.18257500 -4.47023200
H -7.06434600 1.26150300 -3.97204800
H -7.04299800 -0.49400700 -3.52134200
C -8.99858900 -3.86679500 -0.74731800
H -9.69374500 -4.71410200 -0.52753700
H -8.30809500 -4.17119600 -1.57166100
H -8.38262200 -3.66154000 0.16345700
C -10.74864400 -1.04716800 3.33944900
H -11.48503400 -0.73349800 4.11986800
H -10.28339900 -2.01334800 3.65323000
H -9.93865000 -0.27858500 3.27603400
C -11.85571000 3.43667500 1.14318400
H -12.42465100 4.36417700 0.88598400
H -11.67356600 3.42160900 2.24510100
H -10.86485700 3.46502700 0.62422700

D. Proteins from protein data bank (PDB)

1. α-conotoxin pnib (1akg) [5]

N 0.50400000 -0.49400000 0.92400000
C 1.27200000 0.58900000 0.27700000
C 1.70000000 1.61400000 1.30100000
O 1.43400000 1.46000000 2.49600000
N 2.26500000 2.70800000 0.81800000
C 2.76400000 3.78400000 1.66900000
C 3.16200000 4.96900000 0.79200000
S 3.95200000 6.32600000 1.71100000
C 1.81200000 4.29800000 2.74300000
O 2.19600000 4.46700000 3.91100000
N 0.56300000 4.53300000 2.36200000
C -0.38300000 5.11000000 3.29700000
C -1.53600000 5.76800000 2.53800000
S -0.92100000 6.87800000 1.22000000
C -0.84300000 4.23000000 4.45100000
O -1.43300000 4.73400000 5.40500000
N -0.53700000 2.93500000 4.39500000
C -0.88500000 2.02200000 5.48300000
C -1.56500000 0.75200000 4.94700000
O -2.62500000 1.05700000 4.06400000
C 0.36200000 1.66100000 6.30800000
O 0.29700000 0.84300000 7.22600000
N 1.49200000 2.27900000 5.97100000
C 2.76800000 2.05300000 6.65300000
C 3.82900000 1.65100000 5.61700000
C 5.25300000 1.31600000 6.07800000
C 5.23000000 0.10800000 7.02100000
C 6.13600000 1.02600000 4.86000000
C 3.12800000 3.38800000 7.31300000
O 3.61300000 4.30700000 6.64600000
N 2.94300000 3.50000000 8.64100000
C 3.24200000 4.74400000 9.36500000
C 2.51600000 2.43900000 9.57900000
C 3.25500000 4.29900000 10.83000000
C 2.20000000 3.22700000 10.84500000
C 4.49900000 5.53600000 8.96000000
O 4.39800000 6.72300000 8.65800000
N 5.68200000 4.89200000 8.91500000
C 6.90100000 5.62200000 8.53300000
C 5.99900000 3.48500000 9.21900000
C 7.97200000 4.53000000 8.54900000
C 7.46100000 3.55200000 9.53800000
C 6.80000000 6.25400000 7.14200000
O 7.29400000 7.36000000 6.92300000
N 6.16100000 5.55500000 6.20700000
C 6.02400000 6.08600000 4.85200000
C 5.66300000 4.98500000 3.85400000
S 5.78000000 5.54800000 2.11900000
C 5.00100000 7.22000000 4.79200000
O 5.25600000 8.26200000 4.18500000
N 3.85600000 7.03400000 5.44600000
C 2.81600000 8.05700000 5.46000000
C 1.60800000 7.57300000 6.24900000
C 3.34800000 9.35800000 6.05700000
O 3.02800000 10.44700000 5.58400000
N 4.17700000 9.23200000 7.08900000
C 4.76300000 10.38500000 7.76200000
C 5.60200000 9.91400000 8.95200000
C 6.04200000 10.95900000 9.97600000
C 4.82800000 11.46100000 10.73900000
C 7.06200000 10.35300000 10.93900000
C 5.63500000 11.21500000 6.81500000
O 5.61300000 12.44800000 6.86400000
N 6.38700000 10.53300000 5.95100000
C 7.27700000 11.19100000 4.99700000
C 8.49600000 10.30600000 4.72600000
O 9.15300000 9.95100000 5.93000000
C 6.61400000 11.58400000 3.67400000
O 7.21900000 12.27000000 2.84400000
N 5.37700000 11.14800000 3.46800000
C 4.64200000 11.47000000 2.24100000
C 4.52200000 10.22100000 1.34700000
C 5.86600000 9.72400000 0.84700000
O 6.27500000 10.03900000 -0.27200000
N 6.55600000 8.93700000 1.66400000
C 3.25000000 11.93500000 2.65500000
O 2.24600000 11.44600000 2.13900000
N 3.17600000 12.97900000 3.50000000
C 1.87800000 13.47600000 3.97000000
C 4.27700000 13.83700000 3.97900000
C 2.27000000 14.53900000 5.00200000
C 3.55500000 15.08300000 4.45200000
C 0.88700000 14.01000000 2.94100000
O -0.30000000 13.72800000 3.03200000
N 1.36000000 14.80300000 1.98400000
C 0.45900000 15.36900000 0.98200000

C 1.13400000 16.55200000 0.28800000
C 1.46200000 17.67900000 1.26100000
O 0.52700000 18.21600000 1.89400000
O 2.65300000 18.01700000 1.41200000
C -0.00400000 14.31800000 -0.01700000
O -1.10600000 14.38800000 -0.55300000
N 0.86100000 13.35000000 -0.26600000
C 0.58800000 12.24800000 -1.17200000
C 1.89300000 11.45700000 -1.32600000
C 1.85900000 10.15400000 -2.10300000
C 1.98300000 10.14000000 -3.49700000
C 1.81000000 8.92800000 -1.43500000
C 2.06300000 8.92400000 -4.20700000
C 1.88900000 7.71700000 -2.13500000
C 2.01700000 7.72500000 -3.51500000
O 2.08300000 6.52300000 -4.18400000
C -0.53600000 11.38200000 -0.59100000
O -1.48200000 11.03700000 -1.30100000
N -0.44800000 11.07300000 0.70300000
C -1.46400000 10.25300000 1.35900000
C -0.88100000 9.55800000 2.59300000
S 0.27300000 8.21200000 2.18300000
C -2.71800000 11.03600000 1.74600000
O -3.80500000 10.42400000 1.75400000
O -2.62200000 12.21000000 2.20400000
H 0.43400000 -1.32900000 0.29900000
H -0.46100000 -0.14600000 1.18200000
H 0.98200000 -0.79700000 1.81100000
H 0.62900000 1.07300000 -0.44500000
H 2.16700000 0.15200000 -0.14500000
H 2.39500000 2.85900000 -0.16200000
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H 2.26700000 5.36800000 0.26300000
H 3.86800000 4.62100000 0.00600000
H 0.28000000 4.47100000 1.41100000
H 0.12900000 5.92800000 3.79100000
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H -2.18100000 4.98700000 2.08100000
H -0.03600000 2.55600000 3.62000000
H -1.57500000 2.48700000 6.17000000
H -1.94500000 0.13800000 5.79700000
H -0.81600000 0.13700000 4.39800000
H -3.38200000 1.22800000 4.66900000
H 1.49500000 2.98100000 5.26000000
H 2.67700000 1.25900000 7.37700000
H 3.89000000 2.46100000 4.85500000
H 3.43300000 0.75700000 5.08100000
H 5.68900000 2.20200000 6.57800000
H 4.77000000 -0.76900000 6.51800000
H 4.65500000 0.32600000 7.94500000
H 6.26600000 -0.16700000 7.31600000
H 6.15200000 1.89200000 4.16600000
H 5.75600000 0.14000000 4.30800000
H 7.17900000 0.81300000 5.18000000
H 2.41700000 5.41300000 9.15800000
H 3.34700000 1.71900000 9.73900000
H 1.60500000 1.91500000 9.20800000
H 2.95500000 5.15200000 11.48300000
H 4.22100000 3.92500000 11.20500000
H 2.22000000 2.59900000 11.75900000
H 1.18900000 3.68800000 10.73900000
H 7.06500000 6.42000000 9.24500000
H 5.81200000 2.87100000 8.32600000
H 5.44600000 3.05000000 10.07100000
H 8.96700000 4.94700000 8.82400000
H 8.06700000 4.03600000 7.55400000
H 7.96100000 2.56100000 9.46300000
H 7.60100000 3.94600000 10.57300000
H 5.65700000 4.72900000 6.44800000
H 6.97400000 6.51200000 4.55500000
H 4.65300000 4.58200000 4.08200000
H 6.38700000 4.15300000 3.99600000
H 3.66400000 6.17300000 5.92300000
H 2.52400000 8.27200000 4.43900000
H 1.87600000 7.35800000 7.30600000
H 1.21000000 6.63700000 5.80300000
H 0.79400000 8.33300000 6.24000000
H 4.39300000 8.32600000 7.45500000
H 3.95500000 11.02400000 8.09400000
H 6.50700000 9.38900000 8.56800000
H 5.01200000 9.14700000 9.50500000
H 6.52400000 11.81600000 9.44500000
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H 4.10900000 11.96900000 10.06200000
H 5.13800000 12.19400000 11.51500000
H 7.95700000 9.99600000 10.38500000
H 6.61800000 9.49400000 11.48500000
H 7.39000000 11.11100000 11.68200000
H 6.40100000 9.53700000 5.98000000
H 7.64000000 12.10900000 5.43900000
H 9.21100000 10.84700000 4.06100000
H 8.17500000 9.37500000 4.20500000
H 10.11600000 9.98800000 5.72400000
H 4.90700000 10.61000000 4.16800000
H 5.10900000 12.28100000 1.69700000
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H 4.00700000 9.40300000 1.89300000
H 6.15800000 8.70100000 2.55200000
H 7.43500000 8.61000000 1.33400000
H 1.36300000 12.64800000 4.43200000
H 5.01400000 14.06600000 3.17800000
H 4.77100000 13.34500000 4.84200000
H 2.45800000 14.04100000 5.98200000
H 1.49200000 15.32000000 5.14300000
H 3.35700000 15.77100000 3.59900000
H 4.13700000 15.64100000 5.21800000
H 2.30500000 15.10500000 1.98700000
H -0.43600000 15.72400000 1.48100000
H 0.45100000 16.98300000 -0.47600000
H 2.07200000 16.23700000 -0.20800000
H 1.74400000 13.35900000 0.20200000
H 0.24200000 12.63200000 -2.12200000
H 2.25700000 11.21900000 -0.30700000
H 2.65800000 12.11000000 -1.79800000
H 2.03600000 11.07800000 -4.02900000
H 1.71900000 8.92200000 -0.35700000

H 2.15800000 8.94400000 -5.28200000
H 1.83100000 6.81600000 -1.55600000
H 2.12700000 6.73800000 -5.12100000
H 0.25500000 11.47000000 1.28500000
H -1.80600000 9.50100000 0.66200000
H -1.72200000 9.14300000 3.19000000
H -0.37700000 10.32800000 3.21900000

2. crambin (1cnr) [5]

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H -12.86200000 3.17100000 3.35800000
H -13.67500000 1.86900000 6.75200000
H -14.47400000 2.56500000 5.75500000
H -12.13400000 1.30400000 5.27300000
H -13.33200000 1.12500000 4.41000000
H -10.33400000 3.84400000 6.54600000
H -9.05000000 4.28600000 8.37500000
H -10.22300000 3.83700000 9.33500000
H -9.74600000 1.55500000 6.99500000
H -9.09400000 -0.55000000 8.40100000
H -8.16400000 -0.19500000 5.74000000
H -10.06800000 -0.03700000 5.08800000
H -9.01000000 -2.59000000 7.11300000
H -8.53800000 -2.56900000 5.57400000
H -7.47300000 -2.27400000 6.75600000
H -4.86200000 0.06000000 9.58500000
H -7.65800000 -2.45200000 9.40800000
H -8.13400000 -1.20900000 10.22900000
H -4.78500000 -2.74400000 9.73100000
H -4.23300000 -1.82100000 10.70900000
H -6.40800000 -2.82700000 11.16800000
H -6.31100000 -1.42400000 11.65400000
H -2.89500000 0.16600000 8.57300000
H -2.87200000 -0.09200000 5.89100000
H -0.72800000 0.23300000 7.73800000
H -0.47600000 0.09200000 6.17300000
H -1.86500000 2.13700000 5.88600000
H -1.92800000 2.19800000 7.45400000
H -1.70600000 -2.27600000 8.30400000
H -0.52300000 -4.02300000 6.73800000
H -1.75100000 -4.60200000 9.22500000
H -0.85400000 -5.66600000 8.44800000
H -0.20400000 -4.30400000 8.98500000
H -3.88700000 -3.92000000 7.37700000
H -4.52500000 -6.22500000 6.00400000
H -6.18800000 -4.23000000 7.19100000
H -6.84000000 -5.35800000 6.22900000
H -5.38300000 -6.01900000 8.58400000
H -8.21600000 -5.73800000 8.44500000
H -7.42500000 -6.40900000 9.68000000
H -7.21000000 -4.84200000 9.32800000
H -7.04500000 -7.63200000 6.91800000
H -5.45500000 -7.82100000 7.14100000
H -6.48600000 -8.12800000 8.35400000
H -4.48900000 -2.90000000 5.18600000
H -5.65000000 -3.17800000 2.72600000
H -4.13000000 -0.98500000 3.62200000
H -4.83500000 -1.02400000 2.19900000
H -2.45500000 -3.47200000 3.83700000
H -1.10700000 -3.64700000 1.52600000
H 0.05100000 -3.29900000 3.50800000
H -0.31000000 -4.77300000 3.99900000
H 0.65100000 -4.57100000 2.74100000
H -2.24800000 -6.32100000 3.43500000
H -1.57800000 -8.22300000 1.61100000
H -2.96900000 -9.74000000 2.77000000
H -4.45700000 -8.35700000 3.52400000
H -0.96800000 -8.36800000 4.34000000
H -1.53300000 -9.81700000 4.75300000
H -0.65500000 -9.63700000 3.40600000
H -4.43400000 -6.40300000 1.94800000
H -5.99600000 -7.72200000 0.23300000
H -7.05900000 -6.42300000 1.63600000
H -6.11600000 -5.16600000 1.38000000
H -8.66700000 -7.09500000 -0.39600000
H -6.94500000 -3.38500000 0.11400000
H -10.28000000 -6.15100000 -1.85400000
H -8.56100000 -2.44100000 -1.35300000
H -10.29000000 -2.68300000 -2.55500000
H -3.65700000 -5.35000000 -0.46200000
H -4.33800000 -5.16200000 -3.15700000
H -3.12300000 -3.17200000 -3.22600000
H -2.96500000 -3.41000000 -0.48800000
H -5.53800000 -3.09700000 -2.59000000
H -5.04200000 -3.02500000 -1.06400000
H -4.69500000 -1.81900000 -2.06900000
H -1.72600000 -6.29400000 -1.37800000
H 0.20800000 -7.21500000 -2.18100000
H -0.07500000 -6.60000000 -3.60900000
H -0.54500000 -4.12700000 -1.56900000
H 1.89000000 -2.87500000 -1.87300000
H -0.24400000 -2.01300000 -0.25300000
H 1.05100000 -1.15700000 -0.55200000
H 3.10700000 -2.12500000 0.09600000
H 3.26400000 -4.03000000 2.12600000
H 5.50200000 -4.24000000 2.02600000
H 4.24700000 -4.85400000 -0.46400000
H 5.71300000 -5.43800000 -0.04900000
H 4.40200000 -5.84400000 0.80800000
H 5.52400000 -2.62100000 -0.30900000
H 6.06000000 -2.11100000 1.13100000
H 7.74100000 -3.81600000 0.99900000
H 7.34400000 -4.00500000 -0.58400000
H 7.93700000 -2.57500000 -0.01900000
H 4.22700000 -3.34600000 4.07000000
H 4.47900000 -0.61600000 4.54200000
H 4.11700000 -2.63300000 6.47400000
H 5.52500000 -0.95000000 7.31800000
H 4.39000000 0.16100000 6.99700000
H 4.11900000 -0.99100000 8.12100000
H 2.32400000 -0.48900000 6.02000000
H 2.09600000 -1.93300000 5.32200000

H 1.90900000 -2.91500000 7.45900000
H 1.96700000 -1.42500000 8.14600000
H 0.71900000 -1.86300000 7.16400000
H 6.58000000 0.12900000 4.97300000
H 8.51900000 -1.72500000 5.70400000
H 10.23100000 -0.69900000 4.57800000
H 9.09200000 -2.53900000 3.57500000
H 8.20900000 -1.48600000 2.71800000
H 9.82000000 -1.58600000 2.48800000
H 8.27900000 0.81800000 3.16000000
H 9.16100000 1.47300000 4.34700000
H 11.11300000 1.09200000 3.11200000
H 10.21900000 0.52900000 1.85300000
H 10.10400000 2.09700000 2.34600000
H 9.16300000 1.11200000 8.83600000
H 10.87600000 -1.63300000 6.62800000
H 9.70500000 -2.14100000 7.52900000
H 11.48900000 0.40300000 9.79800000
H 10.27700000 -0.31900000 10.14800000
H 12.09100000 -1.09300000 8.32200000
H 11.32300000 -2.05600000 9.15000000
H 11.56300000 1.11700000 6.49600000
H 12.46900000 3.61900000 6.95800000
H 12.86700000 2.71200000 5.72200000
H 12.70000000 4.65700000 4.39700000
H 10.12300000 5.53400000 3.77000000
H 12.33600000 7.27300000 4.10000000
H 10.96000000 7.73000000 3.43500000
H 10.99900000 7.28500000 4.97000000
H 12.65700000 4.01600000 2.56000000
H 12.54800000 5.09600000 0.00100000
H 14.63900000 3.48900000 1.06800000
H 15.78600000 5.49300000 1.01700000
H 14.64600000 3.49100000 -1.37900000
H 14.69400000 5.09700000 -1.33200000
H 15.95100000 4.25000000 -0.79000000
H 10.83900000 4.06400000 -1.02400000
H 10.36400000 1.40800000 -0.83900000
H 9.31200000 3.25800000 -2.68600000
H 8.80800000 1.76100000 -2.59100000
H 13.24800000 0.04900000 -3.78900000
H 10.00800000 -0.65800000 -1.70800000
H 11.37200000 -0.71000000 -0.94200000
H 12.70300000 -2.45900000 -3.90700000
H 13.27900000 -1.94200000 -2.67200000
H 10.61400000 -2.25700000 -3.10700000
H 11.28800000 -2.83900000 -1.91300000
H 13.41600000 -0.90200000 -5.99300000
H 11.91500000 0.56800000 -7.65800000
H 12.95800000 -0.52200000 -8.12800000
H 11.28700000 -2.52400000 -6.52800000
H 9.48800000 -3.12900000 -8.56600000
H 9.34100000 -5.28400000 -7.82700000
H 10.80500000 -4.88300000 -8.16900000
H 9.29800000 -1.47100000 -5.84600000
H 6.53200000 -1.67600000 -5.65900000
H 8.13500000 -1.59100000 -3.33900000
H 6.58500000 -1.22200000 -3.30700000
H 8.87000000 -3.97400000 -3.77400000
H 4.89100000 -2.97600000 -3.40600000
H 8.32800000 -6.26100000 -3.54500000
H 4.34800000 -5.28200000 -3.17600000
H 6.71000000 -7.77200000 -3.49100000
H 7.13800000 0.00500000 -7.33600000
H 8.38600000 2.29200000 -6.46300000
H 7.65300000 1.41700000 -9.05100000
H 8.29300000 2.85700000 -8.80900000
H 9.13000000 1.53600000 -8.46200000
H 5.23600000 1.49000000 -6.55800000
H 4.27100000 4.02500000 -7.21600000
H 2.85700000 1.61600000 -7.64400000
H 2.26400000 3.05700000 -7.93900000
H 4.50700000 3.73400000 -10.60900000
H 3.90300000 4.46900000 -9.33200000

3. epidermal growth factor subdomain (1fgd) [5]

N -1.84200000 -7.03800000 0.76300000
C -1.12100000 -6.02400000 1.54600000
C -0.92000000 -4.76000000 0.69300000
S 0.51900000 -4.98600000 -0.38400000
C -1.92700000 -5.67900000 2.83000000
O -3.09000000 -5.31400000 2.73000000
N -1.29200000 -5.82600000 4.00400000
C -1.94500000 -5.55200000 5.32300000
C 0.12000000 -6.27600000 4.13100000
C -1.03000000 -6.27500000 6.32400000
C 0.35000000 -6.41800000 5.64500000
C -2.03600000 -4.03100000 5.64500000
O -1.72900000 -3.18800000 4.80800000
N -2.47200000 -3.69800000 6.86800000
C -2.61800000 -2.25600000 7.32000000
C -2.93300000 -2.21400000 8.82500000
C -4.45700000 -2.26200000 9.03500000
C -5.07600000 -0.87400000 8.77800000
O -5.44100000 -0.60700000 7.64200000
O -5.17500000 -0.10500000 9.72100000
C -1.33200000 -1.45200000 7.03900000
O -0.22400000 -1.92300000 7.28500000
N -1.48500000 -0.25400000 6.48500000
C -0.30000000 0.60600000 6.12100000
C 0.02500000 0.40000000 4.62900000
O 0.25700000 1.35700000 3.90500000
N 0.01100000 -0.85100000 4.17800000
C 0.28000000 -1.19800000 2.74600000
C 0.80300000 -2.65800000 2.67000000
C 1.98300000 -2.87900000 3.60000000
C 3.28400000 -2.66700000 3.14000000
C 1.77000000 -3.30600000 4.91900000
C 4.37200000 -2.87800000 3.99700000
C 2.85700000 -3.51600000 5.77300000
C 4.15900000 -3.30100000 5.31200000
O 5.23400000 -3.50000000 6.15300000
C -1.06100000 -1.05200000 1.97800000

O -1.83700000 -1.99900000 1.86500000
N -1.35600000 0.15100000 1.49600000
C -2.67000000 0.40900000 0.77300000
C -3.29400000 1.78800000 1.21700000
C -2.96000000 2.10000000 2.68600000
C -2.84400000 2.98900000 0.33300000
C -1.32400000 3.02900000 0.15500000
C -2.50400000 0.32200000 -0.77100000
O -1.43200000 0.00700000 -1.28400000
N -3.57700000 0.60600000 -1.50000000
C -3.55700000 0.56700000 -2.99700000
C -4.84200000 -0.10000000 -3.54400000
C -4.86100000 -1.64300000 -3.35800000
C -3.81600000 -2.30100000 -4.25700000
C -4.59500000 -2.04500000 -1.90000000
C -3.48600000 2.01600000 -3.51300000
O -4.39900000 2.80600000 -3.28200000
N -2.41500000 2.36400000 -4.20000000
C -2.25400000 3.76600000 -4.74200000
C -1.07800000 4.45400000 -4.01500000
C -1.50600000 5.84000000 -3.51600000
O -1.44900000 6.77800000 -4.29800000
O -1.88200000 5.94000000 -2.35800000
C -2.01200000 3.73900000 -6.27100000
O -2.13000000 2.69300000 -6.89900000
N -1.69200000 4.89800000 -6.86000000
C -1.43400000 5.03000000 -8.34500000
C -0.14300000 4.26100000 -8.72500000
C 1.06200000 4.81900000 -7.95100000
O 1.64800000 5.78500000 -8.41500000
O 1.38300000 4.26400000 -6.91100000
C -2.66200000 4.53000000 -9.15100000
O -3.54500000 5.31600000 -9.46800000
N -2.73300000 3.23600000 -9.44600000
C -3.89800000 2.64800000 -10.19000000
C -4.36300000 1.36700000 -9.48000000
O -4.60000000 0.36100000 -10.12900000
N -4.46900000 1.40500000 -8.14500000
C -4.89500000 0.21600000 -7.32600000
C -6.24000000 -0.35000000 -7.84800000
C -6.90400000 -1.17500000 -6.76400000
C -7.76000000 -0.56300000 -5.84000000
C -6.66200000 -2.55200000 -6.68700000
C -8.37100000 -1.32700000 -4.84000000
C -7.27400000 -3.31600000 -5.68700000
C -8.12800000 -2.70300000 -4.76400000
C -3.76800000 -0.85000000 -7.33600000
O -3.92300000 -1.95500000 -7.84600000
N -2.63000000 -0.50200000 -6.75300000
C -1.45300000 -1.45000000 -6.67600000
C -0.37800000 -1.10700000 -7.74400000
C -0.82200000 -1.67000000 -9.10100000
C -0.16300000 0.41500000 -7.87900000
C 0.62300000 0.94700000 -6.67800000
C -0.84600000 -1.41900000 -5.25500000
O -0.95500000 -0.42500000 -4.54100000
N -0.22500000 -2.51800000 -4.84200000
C 0.38600000 -2.61500000 -3.46200000
C 0.94700000 -4.02900000 -3.22400000
S -0.24400000 -4.99200000 -2.25400000
C 1.50100000 -1.56300000 -3.30100000
O 2.55900000 -1.65900000 -3.91300000
N 1.23700000 -0.55200000 -2.49200000
C 2.22700000 0.56600000 -2.25500000
C 1.46800000 1.88500000 -1.98600000
O 0.39200000 2.01800000 -2.90600000
C 2.41000000 3.08000000 -2.15500000
C 3.13000000 0.23600000 -1.04800000
O 2.71100000 -0.43800000 -0.10800000
N 4.36700000 0.72100000 -1.07500000
C 5.33800000 0.47000000 0.04500000
C 6.76700000 0.78700000 -0.43900000
C 7.14600000 -0.11400000 -1.62600000
O 7.59900000 -1.22300000 -1.38500000
O 6.98000000 0.32300000 -2.75500000
C 4.98900000 1.33600000 1.29000000
O 3.95800000 2.00400000 1.33300000
N 5.85200000 1.30900000 2.30300000
C 5.62200000 2.09600000 3.57900000
C 4.32700000 1.59600000 4.28100000
C 4.39900000 0.09100000 4.56700000
C 4.10000000 2.35600000 5.60100000
C 2.77900000 1.90900000 6.23300000
C 6.84400000 1.98300000 4.53000000
O 7.32400000 2.99500000 5.01600000
N 7.32600000 0.76200000 4.79800000
C 8.49800000 0.53100000 5.71800000
C 9.75500000 1.23100000 5.14100000
C 10.12400000 0.61600000 3.78000000
O 9.60700000 1.08700000 2.77400000
O 10.91200000 -0.31600000 3.76400000
C 8.13400000 1.03500000 7.14200000
O 8.79100000 1.90700000 7.70200000
N 7.05600000 0.46600000 7.69700000
C 6.52000000 0.82500000 9.07400000
C 7.64600000 0.80900000 10.14800000
C 7.72800000 -0.57700000 10.82800000
C 8.08800000 -1.66900000 9.79800000
O 9.26300000 -1.81100000 9.49300000
O 7.18100000 -2.34600000 9.33400000
C 5.81900000 2.15200000 9.04000000
O 6.16500000 3.05000000 9.80600000
O 4.82000000 2.35700000 8.18000000
H -1.29100000 -7.27500000 -0.06100000
H -1.97800000 -7.87900000 1.32500000
H -2.77300000 -6.65200000 0.48600000
H -0.15600000 -6.42000000 1.82200000
H -1.79800000 -4.58300000 0.09000000
H -0.75200000 -3.91400000 1.33700000
H -2.92700000 -5.99400000 5.35200000
H 0.79400000 -5.53900000 3.71700000
H 0.25200000 -7.22800000 3.64100000
H -0.93900000 -5.69500000 7.23300000
H -1.42700000 -7.25300000 6.54800000
H 1.01500000 -5.64000000 5.99500000
H 0.76900000 -7.38800000 5.86000000

H -2.71400000 -4.41200000 7.49400000
H -3.43500000 -1.80400000 6.77600000
H -2.47500000 -3.06200000 9.31300000
H -2.54300000 -1.30100000 9.25100000
H -4.88800000 -2.98100000 8.35300000
H -4.66800000 -2.56400000 10.05000000
H -2.39000000 0.06900000 6.28000000
H -0.53800000 1.64500000 6.30300000
H 0.55500000 0.32100000 6.71500000
H -0.20100000 -1.57800000 4.79300000
H 1.01500000 -0.52000000 2.33400000
H 0.00800000 -3.33100000 2.95200000
H 1.10200000 -2.87100000 1.66200000
H 3.44800000 -2.33700000 2.12700000
H 0.76500000 -3.47100000 5.27700000
H 5.37600000 -2.70800000 3.64600000
H 2.69100000 -3.84400000 6.78800000
H 5.41000000 -4.44300000 6.19600000
H -0.72800000 0.89100000 1.63600000
H -3.36000000 -0.37200000 1.06400000
H -4.37100000 1.69700000 1.14000000
H -3.11600000 1.21600000 3.28800000
H -1.92900000 2.41100000 2.76500000
H -3.60200000 2.89400000 3.04000000
H -3.30900000 2.90900000 -0.63800000
H -3.16800000 3.90900000 0.79900000
H -0.84300000 2.96100000 1.11900000
H -1.02200000 2.19900000 -0.46100000
H -1.04200000 3.95500000 -0.32600000
H -4.40300000 0.85600000 -1.05200000
H -2.69400000 0.02100000 -3.33200000
H -5.69800000 0.33000000 -3.05700000
H -4.90500000 0.12100000 -4.59000000
H -5.83700000 -2.00800000 -3.64600000
H -3.13400000 -1.55300000 -4.61600000
H -3.27100000 -3.04700000 -3.69800000
H -4.30800000 -2.77000000 -5.09600000
H -5.24700000 -1.48700000 -1.24500000
H -4.78100000 -3.10100000 -1.78000000
H -3.56600000 -1.83600000 -1.65000000
H -1.70700000 1.69900000 -4.36200000
H -3.16000000 4.32400000 -4.54900000
H -0.77900000 3.85300000 -3.17200000
H -0.24300000 4.55900000 -4.69200000
H -1.62200000 5.70400000 -6.30800000
H -1.28900000 6.07600000 -8.57100000
H -0.26300000 3.21500000 -8.48700000
H 0.03300000 4.36900000 -9.78100000
H -2.01600000 2.64000000 -9.14800000
H -4.71000000 3.36100000 -10.21800000
H -3.59700000 2.40700000 -11.19400000
H -4.24200000 2.23500000 -7.66900000
H -5.03300000 0.54800000 -6.30700000
H -6.88900000 0.46600000 -8.12600000
H -6.05800000 -0.97300000 -8.71200000
H -7.94700000 0.49900000 -5.89900000
H -5.99800000 -3.02400000 -7.40000000
H -9.03100000 -0.85500000 -4.12700000
H -7.08700000 -4.37800000 -5.62800000
H -8.60100000 -3.29300000 -3.99200000
H -2.54900000 0.39100000 -6.35100000
H -1.81500000 -2.45400000 -6.86200000
H 0.55600000 -1.57700000 -7.46200000
H -1.88700000 -1.87000000 -9.08100000
H -0.60700000 -0.95300000 -9.87900000
H -0.28900000 -2.58700000 -9.30100000
H 0.39100000 0.61700000 -8.78400000
H -1.11800000 0.91100000 -7.93100000
H 0.95500000 0.11700000 -6.06600000
H 1.48100000 1.50500000 -7.02700000
H -0.01400000 1.59600000 -6.09400000
H -0.17100000 -3.28500000 -5.44500000
H -0.38700000 -2.41700000 -2.72900000
H 1.11600000 -4.51700000 -4.17300000
H 1.88000000 -3.96400000 -2.68400000
H 0.36300000 -0.51300000 -2.04300000
H 2.84300000 0.68600000 -3.13600000
H 1.08100000 1.87800000 -0.97700000
H -0.41500000 1.74200000 -2.46400000
H 2.93600000 2.99400000 -3.09400000
H 1.83500000 3.99500000 -2.14800000
H 3.12100000 3.09700000 -1.34200000
H 4.66000000 1.25600000 -1.84000000
H 5.28600000 -0.57100000 0.31900000
H 6.82400000 1.82200000 -0.74000000
H 7.45500000 0.61200000 0.36900000
H 6.65500000 0.76600000 2.21600000
H 5.49400000 3.13200000 3.32100000
H 3.49300000 1.77900000 3.62200000
H 4.88700000 -0.40900000 3.74600000
H 4.95600000 -0.07800000 5.47700000
H 3.39800000 -0.30000000 4.68200000
H 4.91300000 2.14700000 6.28400000
H 4.06200000 3.41700000 5.40500000
H 2.57600000 0.88200000 5.94700000
H 2.85300000 1.97500000 7.30800000
H 1.97900000 2.54600000 5.88600000
H 6.90300000 -0.01200000 4.39500000
H 8.68500000 -0.53400000 5.77400000
H 9.55100000 2.28200000 5.01600000
H 10.58000000 1.10600000 5.82600000
H 6.57300000 -0.21500000 7.18100000
H 5.78800000 0.07200000 9.34300000
H 8.59300000 1.03200000 9.68500000
H 7.43300000 1.55800000 10.89700000
H 8.48900000 -0.55000000 11.59500000
H 6.77700000 -0.81200000 11.28400000

4. μ-conotoxin giiib (1gib) [5]

N -1.63500000 -4.47300000 -16.76800000
C -0.90700000 -5.53100000 -16.01400000
C 0.28000000 -6.04900000 -16.85500000
C 0.87700000 -7.31800000 -16.20200000

C 1.93200000 -7.92100000 -17.14300000
N 2.36000000 -9.23700000 -16.58200000
C 2.54000000 -10.25600000 -17.37800000
N 1.58000000 -11.12900000 -17.51000000
N 3.67200000 -10.36900000 -18.01600000
C -0.38900000 -4.94800000 -14.69300000
O 0.02300000 -3.80400000 -14.64000000
N -0.43000000 -5.76900000 -13.67000000
C 0.03400000 -5.37000000 -12.30300000
C 1.57900000 -5.19800000 -12.33500000
C 2.11300000 -5.10200000 -10.89300000
O 2.05200000 -4.00600000 -10.36000000
O 2.55300000 -6.13100000 -10.40500000
C -0.65100000 -4.06900000 -11.84500000
O -0.13400000 -2.98100000 -12.02800000
N -1.81100000 -4.24100000 -11.26100000
C -2.59500000 -3.07300000 -10.76100000
C -3.47000000 -2.50700000 -11.88500000
S -2.66700000 -1.54800000 -13.18800000
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O -3.50100000 -2.79000000 -8.58300000
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5. Bovine lactoferricin (1lfc) [5]

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6. α-conotoxin mii (1m2c) [5]

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H 10.35000000 22.38000000 -7.80700000
H 13.83300000 22.94800000 -5.98700000
H 13.96400000 19.80400000 -8.23000000
H 14.31000000 19.74700000 -6.51400000
H 16.63900000 20.44600000 -5.32500000
H 16.06100000 23.27700000 -4.17200000
H 16.16000000 20.66800000 -2.60100000
H 16.08500000 22.24400000 -1.84100000
H 13.97700000 21.19900000 -3.81400000
H 14.00900000 19.85500000 -1.70600000
H 13.85300000 21.33400000 -0.72900000
H 12.53200000 20.82600000 -1.81100000
H 13.88400000 23.66700000 -1.91900000
H 13.97600000 23.75000000 -3.68700000
H 12.53000000 23.08900000 -2.91600000
H 18.73700000 20.86600000 -3.86100000
H 20.93400000 22.42200000 -3.35700000
H 20.14200000 20.54500000 -5.68800000
H 21.71300000 21.16900000 -5.51500000
H 22.11800000 20.05000000 -3.34200000
H 20.43300000 19.53800000 -3.29300000
H 22.11000000 16.61800000 -4.24100000
H 18.96000000 23.04600000 -6.14700000
H 20.27000000 25.70700000 -6.51700000
H 22.39100000 22.37500000 -8.06400000
H 25.09000000 25.62000000 -7.30800000
H 24.76800000 23.04000000 -7.33400000
H 22.63900000 26.62600000 -7.78200000
H 20.16400000 23.68600000 -8.77300000
H 20.35100000 25.42600000 -9.03600000
H 18.03600000 25.44600000 -5.39500000
H 15.79600000 25.41200000 -6.70700000
H 16.19100000 25.59900000 -4.14200000
H 16.08200000 27.34600000 -4.34600000
H 14.01600000 26.86700000 -4.05900000
H 17.58800000 27.96700000 -6.87800000
H 16.10100000 29.95300000 -8.55900000
H 18.21900000 30.72800000 -9.28200000
H 18.33200000 30.46300000 -7.55100000
H 21.32400000 29.04400000 -9.60100000
H 20.21400000 30.43200000 -10.05700000
H 17.58800000 26.89300000 -9.19500000
H 16.99900000 27.10100000 -12.17700000
H 18.53300000 24.87200000 -10.77200000
H 18.28400000 25.02400000 -12.49700000
H 19.94300000 26.97000000 -10.78200000
H 20.97800000 24.67100000 -11.17000000
H 20.82400000 24.92100000 -12.92100000
H 21.89000000 25.97700000 -11.96000000
H 19.50200000 26.97800000 -13.84700000
H 18.97000000 28.22900000 -12.70100000
H 20.69600000 27.97100000 -12.97800000
H 15.38000000 25.85400000 -9.49800000
H 13.46100000 24.44700000 -11.43700000
H 14.02000000 23.22400000 -9.19300000
H 13.21500000 24.55200000 -8.39900000

7. *ω-conotoxin mviia (1omg) [5]*

N -1.66700000 -8.43300000 4.89900000
C -1.70400000 -7.33600000 3.88900000
C -0.29000000 -6.90600000 3.51100000
S 0.83800000 -8.31800000 3.61000000
C -2.39000000 -7.81500000 2.61900000
O -2.89400000 -8.91700000 2.53400000
N -2.37600000 -6.98500000 1.62400000
C -2.98000000 -7.34200000 0.32300000
C -4.06800000 -6.32300000 -0.02400000
C -5.20200000 -6.42000000 0.99800000
C -6.52400000 -6.03500000 0.32900000
C -7.04300000 -4.73100000 0.93700000
N -8.39800000 -4.95600000 1.51200000
C -1.86900000 -7.31700000 -0.71900000
O -0.72000000 -7.56900000 -0.42100000
N -2.19700000 -7.01600000 -1.92700000
C -1.16300000 -6.97200000 -2.98700000
C -1.29300000 -5.67600000 -3.78700000
O -1.43200000 -4.59700000 -3.24300000
N -1.23900000 -5.78400000 -5.07800000
C -1.33600000 -4.58100000 -5.93900000
C -0.82700000 -4.91500000 -7.34200000
C 0.30700000 -3.95700000 -7.71300000
C 0.10000000 -3.44500000 -9.13900000
C 1.41500000 -2.86900000 -9.66800000
N 1.44700000 -2.98700000 -11.15400000
C -2.78500000 -4.10600000 -6.02700000
O -3.71200000 -4.89100000 -6.00800000
N -2.98300000 -2.82200000 -6.13400000
C -4.36500000 -2.28400000 -6.23600000
C -5.02200000 -2.28000000 -4.85600000
O -6.13800000 -1.82600000 -4.69300000
N -4.34800000 -2.78300000 -3.85700000
C -4.95500000 -2.80000000 -2.49900000
C -4.23100000 -3.81600000 -1.62500000
C -4.83900000 -1.41800000 -1.86100000
O -3.77800000 -0.83000000 -1.81600000
N -5.92000000 -0.90100000 -1.35900000
C -5.87100000 0.44200000 -0.71700000
C -7.25300000 0.79500000 -0.16300000
C -7.50600000 2.29500000 -0.32900000
C -7.85000000 2.91000000 1.02900000
C -6.59800000 3.54300000 1.63800000
N -6.71400000 5.02700000 1.58100000

C -4.85300000 0.41000000 0.42200000
O -4.90500000 -0.44300000 1.28700000
N -3.91700000 1.32100000 0.43300000
C -2.90000000 1.31200000 1.51900000
C -1.72200000 0.43600000 1.09500000
S -0.79100000 1.25600000 -0.22400000
C -2.39800000 2.73100000 1.79800000
O -2.79700000 3.68300000 1.15700000
N -1.51500000 2.86800000 2.74900000
C -0.96000000 4.21000000 3.08100000
C -1.52300000 4.68400000 4.42100000
O -0.77900000 4.09300000 5.47900000
C 0.56500000 4.09900000 3.17400000
O 1.09200000 3.32000000 3.94200000
N 1.27400000 4.85700000 2.38000000
C 2.76500000 4.78300000 2.40100000
C 3.36000000 6.04800000 1.77000000
C 2.57700000 7.28600000 2.22100000
C 2.51300000 8.28900000 1.06700000
N 3.61900000 9.28000000 1.20500000
C 3.34700000 10.53000000 1.46500000
N 2.64700000 10.83700000 2.52200000
N 3.77400000 11.47100000 0.66800000
C 3.27200000 4.64100000 3.83900000
O 4.01100000 3.72800000 4.15300000
N 2.88900000 5.52600000 4.71400000
C 3.36200000 5.41900000 6.12300000
C 2.67300000 6.48200000 6.97900000
C 3.48600000 6.71000000 8.25500000
C 4.13400000 8.09500000 8.20700000
C 2.56200000 6.62300000 9.47000000
C 3.02800000 4.02700000 6.66500000
O 3.90200000 3.26100000 7.01700000
N 1.76900000 3.69200000 6.72600000
C 1.37700000 2.34500000 7.23700000
C 0.14300000 2.47500000 8.13300000
C 0.50900000 3.24200000 9.40600000
S -0.59300000 2.73600000 10.75000000
C 0.67000000 2.59000000 12.03700000
C 1.05200000 1.43600000 6.05100000
O -0.00400000 0.83700000 5.98400000
N 1.94800000 1.33700000 5.10700000
C 1.69000000 0.48000000 3.91700000
C 2.98600000 0.29000000 3.13100000
C 3.89400000 -0.66700000 3.87000000
C 4.45400000 -0.29100000 5.09700000
C 4.17400000 -1.92800000 3.32900000
C 5.29400000 -1.17500000 5.78300000
C 5.01500000 -2.81200000 4.01600000
C 5.57600000 -2.43500000 5.24300000
O 6.40500000 -3.30500000 5.92000000
C 1.15800000 -0.88500000 4.35200000
O 1.82200000 -1.63500000 5.04100000
N -0.03100000 -1.21900000 3.94200000
C -0.60600000 -2.53800000 4.31000000
C -2.09800000 -2.37800000 4.60700000
C -2.27900000 -1.74600000 5.98800000
O -1.63200000 -2.20400000 6.91500000
O -3.05900000 -0.81500000 6.09400000
C -0.41100000 -3.50600000 3.14000000
O -1.07900000 -4.51500000 3.03900000
N 0.50500000 -3.20500000 2.25400000
C 0.74900000 -4.10800000 1.09300000
C 1.23900000 -3.28600000 -0.10600000
S 0.28700000 -1.74800000 -0.22600000
C 1.81500000 -5.13900000 1.47800000
O 2.76000000 -4.83400000 2.17800000
N 1.67400000 -6.35800000 1.03000000
C 2.68300000 -7.39800000 1.37700000
C 2.18500000 -8.77500000 0.92500000
S 0.65900000 -9.20300000 1.80300000
C 3.99400000 -7.08100000 0.66100000
O 5.03900000 -6.97900000 1.27200000
N 3.94500000 -6.93300000 -0.63300000
C 5.18300000 -6.63200000 -1.39400000
C 5.83300000 -7.94100000 -1.82300000
O 4.83800000 -8.81800000 -2.33400000
C 6.52300000 -8.59000000 -0.62200000
C 4.82800000 -5.80600000 -2.63200000
O 4.07000000 -6.23400000 -3.47900000
N 5.36800000 -4.62400000 -2.74200000
C 5.06000000 -3.77100000 -3.92300000
C 5.32900000 -2.30800000 -3.57700000
O 6.45800000 -1.90200000 -3.38600000
N 4.30100000 -1.51100000 -3.49300000
C 4.50300000 -0.07500000 -3.15900000
C 4.68300000 0.72700000 -4.44900000
O 5.93700000 0.40000000 -5.03500000
C 3.29100000 0.45100000 -2.39400000
O 2.46000000 -0.30400000 -1.92900000
N 3.18400000 1.74200000 -2.25800000
C 2.03100000 2.32300000 -1.52400000
C 2.13900000 1.99000000 -0.03900000
S 0.56700000 2.37300000 0.76800000
C 2.05200000 3.83500000 -1.71100000
O 2.78700000 4.54200000 -1.05000000
N 1.26900000 4.33700000 -2.61900000
C 1.26800000 5.80100000 -2.85700000
C 2.34500000 6.12800000 -3.89300000
C 2.13100000 7.54400000 -4.43500000
C 3.47100000 8.28300000 -4.47800000
N 3.23100000 9.75400000 -4.43400000
C 4.24100000 10.58200000 -4.46700000
N 5.45600000 10.13500000 -4.30000000
N 4.03500000 11.85500000 -4.66700000
C -0.10800000 6.22900000 -3.36700000
O -0.78600000 5.48400000 -4.04600000
N -0.53400000 7.41500000 -3.03500000
C -1.87400000 7.87300000 -3.49200000
C -2.03700000 7.57800000 -4.98300000
O -2.23900000 8.79700000 -5.68500000
C -2.95400000 7.12400000 -2.70900000
O -4.13400000 7.28700000 -2.95000000
N -2.55900000 6.30200000 -1.77400000
C -3.55900000 5.54300000 -0.97800000
C -3.80400000 4.17700000 -1.62500000

O -4.84900000 3.58400000 -1.45400000
N -2.85700000 3.67000000 -2.37200000
C -3.05700000 2.35000000 -3.02100000
C -3.53500000 2.56300000 -4.45200000
C -4.96000000 3.11800000 -4.43800000
C -5.83100000 2.31800000 -5.40700000
C -6.79800000 3.26200000 -6.12300000
N -6.16800000 3.75700000 -7.38000000
C -1.73200000 1.58900000 -3.03900000
O -0.67900000 2.16300000 -2.86800000
N -1.77700000 0.30200000 -3.25100000
C -0.51300000 -0.49100000 -3.28300000
C -0.81900000 -1.97300000 -3.04700000
S -1.33700000 -2.22900000 -1.32900000
C 0.15600000 -0.32600000 -4.64900000
O -0.24400000 -0.94300000 -5.61700000
O 1.19000000 0.40500000 -4.72000000
H -1.39000000 -9.32200000 4.43700000
H -0.97800000 -8.20100000 5.64000000
H -2.61100000 -8.54400000 5.32400000
H -2.23200000 -6.48800000 4.28700000
H -0.30400000 -6.53000000 2.49900000
H 0.04000000 -6.12800000 4.17500000
H -1.93900000 -6.11400000 1.72800000
H -3.40700000 -8.32800000 0.36200000
H -3.64500000 -5.33100000 0.00200000
H -4.45900000 -6.52500000 -1.00900000
H -5.26700000 -7.43200000 1.36800000
H -5.00900000 -5.74700000 1.81800000
H -6.36600000 -5.90200000 -0.73200000
H -7.25000000 -6.81900000 0.49000000
H -6.37000000 -4.40300000 1.71500000
H -7.10000000 -3.97400000 0.16800000
H -8.56900000 -5.97700000 1.60700000
H -8.45500000 -4.50800000 2.44900000
H -9.11400000 -4.54100000 0.88400000
H -3.11700000 -6.82100000 -2.13600000
H -0.18300000 -7.01900000 -2.53500000
H -1.29300000 -7.81300000 -3.65000000
H -1.12400000 -6.65700000 -5.48000000
H -0.72900000 -3.80300000 -5.51800000
H -0.46300000 -5.93200000 -7.36000000
H -1.63300000 -4.80800000 -8.05200000
H 0.31100000 -3.12300000 -7.02600000
H 1.25100000 -4.47700000 -7.65200000
H -0.21800000 -4.26000000 -9.77200000
H -0.65400000 -2.67300000 -9.13800000
H 1.49100000 -1.82900000 -9.38800000
H 2.24300000 -3.41800000 -9.24500000
H 0.85900000 -3.79200000 -11.45100000
H 1.07600000 -2.11400000 -11.57900000
H 2.42700000 -3.13700000 -11.46800000
H -2.21700000 -2.20900000 -6.15300000
H -4.33100000 -1.27600000 -6.62200000
H -4.94400000 -2.90500000 -6.90300000
H -3.44700000 -3.15000000 -3.99900000
H -5.99700000 -3.07400000 -2.57600000
H -3.53800000 -4.38100000 -2.23000000
H -3.69100000 -3.29900000 -0.84600000
H -4.95200000 -4.48600000 -1.18000000
H -6.76300000 -1.39900000 -1.39700000
H -5.57200000 1.18000000 -1.44800000
H -8.00900000 0.24000000 -0.70000000
H -7.29700000 0.54000000 0.88600000
H -6.62000000 2.76600000 -0.72400000
H -8.33000000 2.44800000 -1.01000000
H -8.61000000 3.66700000 0.89800000
H -8.21900000 2.14000000 1.69000000
H -6.49900000 3.22800000 2.66700000
H -5.72700000 3.22900000 1.08100000
H -7.68400000 5.28900000 1.31200000
H -6.49400000 5.42800000 2.51700000
H -6.04800000 5.40100000 0.87800000
H -3.88000000 1.99800000 -0.27500000
H -3.33900000 0.90400000 2.41600000
H -1.07400000 0.27700000 1.93800000
H -2.09000000 -0.51400000 0.73900000
H -1.20500000 2.07800000 3.24200000
H -1.22400000 4.91400000 2.30600000
H -1.44400000 5.75600000 4.48800000
H -2.56300000 4.39700000 4.49500000
H -0.75200000 4.71800000 6.20700000
H 0.82500000 5.46500000 1.75600000
H 3.08200000 3.92200000 1.83100000
H 4.39200000 6.14700000 2.07400000
H 3.31200000 5.96700000 0.69500000
H 1.57700000 7.00000000 2.50600000
H 3.07600000 7.74100000 3.06200000
H 2.61500000 7.76600000 0.12800000
H 1.56400000 8.80400000 1.09100000
H 4.55000000 8.99200000 1.10200000
H 2.31900000 10.11600000 3.13200000
H 2.43800000 11.79500000 2.72200000
H 4.31000000 11.23400000 -0.14300000
H 3.56600000 12.42800000 0.86700000
H 2.29300000 6.25700000 4.44700000
H 4.43200000 5.56900000 6.15500000
H 2.60800000 7.40600000 6.42300000
H 1.68100000 6.14800000 7.24100000
H 4.25500000 5.95500000 8.32900000
H 3.79900000 8.62000000 7.32600000
H 3.85300000 8.65400000 9.08700000
H 5.20800000 7.98700000 8.17600000
H 1.76700000 5.92100000 9.26800000
H 3.12700000 6.29000000 10.32900000
H 2.14100000 7.59700000 9.67300000
H 1.07900000 4.32100000 6.42900000
H 2.19400000 1.92200000 7.80300000
H -0.63200000 3.00900000 7.60200000
H -0.21400000 1.49200000 8.39900000
H 1.53200000 3.02500000 9.67700000
H 0.40100000 4.30200000 9.23100000
H 1.63900000 2.46200000 11.57600000
H 0.67600000 3.48500000 12.64000000
H 0.44800000 1.73800000 12.66300000
H 2.78800000 1.83600000 5.17700000

H 0.96000000 0.96200000 3.28400000
H 2.75800000 -0.11300000 2.15400000
H 3.47900000 1.24200000 3.02100000
H 4.23600000 0.68000000 5.51400000
H 3.74000000 -2.22000000 2.38400000
H 5.72700000 -0.88500000 6.72900000
H 5.23100000 -3.78500000 3.59900000
H 6.80600000 -2.82500000 6.64900000
H -0.54200000 -0.60500000 3.38300000
H -0.10200000 -2.92100000 5.18400000
H -2.54900000 -1.74300000 3.85700000
H -2.57400000 -3.34700000 4.59100000
H 1.03400000 -2.38700000 2.35500000
H -0.16700000 -4.61700000 0.83400000
H 2.28700000 -3.04700000 0.02300000
H 1.11200000 -3.86200000 -1.01200000
H 0.90800000 -6.58700000 0.46400000
H 2.84600000 -7.40200000 2.44300000
H 1.99200000 -8.75500000 -0.13700000
H 2.94200000 -9.51600000 1.13900000
H 3.09600000 -7.02500000 -1.10500000
H 5.86700000 -6.07700000 -0.77300000
H 6.55900000 -7.73800000 -2.58500000
H 5.10400000 -9.08400000 -3.21700000
H 7.05900000 -7.83700000 -0.06400000
H 5.78100000 -9.04900000 0.01400000
H 7.21600000 -9.34300000 -0.96800000
H 5.97600000 -4.29600000 -2.04700000
H 5.68500000 -4.06800000 -4.75400000
H 4.02200000 -3.88900000 -4.19200000
H 3.39700000 -1.85500000 -3.65100000
H 5.38200000 0.03100000 -2.54400000
H 3.89500000 0.48200000 -5.14100000
H 4.64500000 1.78400000 -4.22500000
H 6.06900000 -0.54700000 -4.94500000
H 3.86500000 2.33600000 -2.64200000
H 1.11500000 1.91900000 -1.91700000
H 2.35600000 0.94100000 0.07800000
H 2.92800000 2.57500000 0.40800000
H 0.68600000 3.75100000 -3.15000000
H 1.48700000 6.31700000 -1.93400000
H 3.31900000 6.05900000 -3.42800000
H 2.28700000 5.41700000 -4.70500000
H 1.71800000 7.48900000 -5.43200000
H 1.44900000 8.07800000 -3.79000000
H 4.07000000 7.99000000 -3.62900000
H 3.99100000 8.03100000 -5.39000000
H 2.31600000 10.10000000 -4.37900000
H 5.61400000 9.16100000 -4.14400000
H 6.22900000 10.76900000 -4.32800000
H 3.10500000 12.19700000 -4.79600000
H 4.80800000 12.48800000 -4.69200000
H 0.02200000 7.99800000 -2.47700000
H -1.97200000 8.93500000 -3.32100000
H -1.14700000 7.09700000 -5.35700000
H -2.88500000 6.92200000 -5.12900000
H -2.94600000 8.66100000 -6.31900000
H -1.60500000 6.18400000 -1.59300000
H -3.18900000 5.40700000 0.02700000
H -4.48800000 6.09400000 -0.94900000
H -2.01700000 4.15700000 -2.51000000
H -3.79500000 1.78200000 -2.47400000
H -2.87800000 3.26000000 -4.94800000
H -3.52000000 1.62500000 -4.97300000
H -5.36600000 3.04200000 -3.44000000
H -4.94600000 4.15400000 -4.74300000
H -5.20000000 1.82500000 -6.13400000
H -6.39400000 1.57800000 -4.85800000
H -7.70800000 2.73300000 -6.36100000
H -7.02500000 4.10000000 -5.48000000
H -5.18000000 3.43200000 -7.42400000
H -6.69200000 3.38900000 -8.19900000
H -6.19300000 4.79600000 -7.39400000
H -2.64000000 -0.13700000 -3.39600000
H 0.15400000 -0.13600000 -2.51200000
H -1.61000000 -2.28800000 -3.71200000
H 0.06700000 -2.55500000 -3.24400000

8. α-conotoxin pni1 (1pen) [5]

N -4.78800000 -8.93500000 3.45300000
C -4.21800000 -10.29400000 3.31200000
C -3.81500000 -10.53400000 1.87000000
O -4.27600000 -9.83600000 0.96500000
N -3.04500000 -11.59400000 1.65400000
C -2.53100000 -11.94500000 0.33700000
C -1.89500000 -13.33300000 0.37700000
S -1.01600000 -13.75200000 -1.15800000
C -3.48500000 -11.92200000 -0.84400000
O -3.22800000 -11.26300000 -1.85300000
N -4.59800000 -12.62700000 -0.70900000
C -5.52200000 -12.75800000 -1.81900000
C -6.44000000 -13.95800000 -1.58900000
S -5.49200000 -15.45100000 -1.11400000
C -6.26500000 -11.51700000 -2.28700000
O -6.83200000 -11.51300000 -3.38200000
N -6.25000000 -10.45900000 -1.48600000
C -6.89400000 -9.21200000 -1.88500000
C -7.68900000 -8.60700000 -0.72500000
O -6.86700000 -8.39100000 0.40700000
C -5.84400000 -8.21200000 -2.37400000
O -6.18600000 -7.13500000 -2.86100000
N -4.57100000 -8.58800000 -2.26800000
C -3.46200000 -7.73100000 -2.67400000
C -2.38200000 -7.76800000 -1.58700000
C -1.24500000 -6.75400000 -1.67900000
C -1.77900000 -5.34100000 -1.46900000
C -0.20100000 -7.09500000 -0.63400000
C -2.91300000 -8.25100000 -4.00900000
O -2.30100000 -9.31900000 -4.05700000
N -3.08600000 -7.48300000 -5.10200000
C -2.60900000 -7.90200000 -6.42800000
C -3.72500000 -6.15300000 -5.17000000
C -2.68800000 -6.61100000 -7.24800000

C -3.88900000 -5.93700000 -6.67000000
C -1.24800000 -8.61300000 -6.54700000
O -1.19000000 -9.74300000 -7.03700000
N -0.15100000 -7.99600000 -6.06100000
C 1.15900000 -8.65800000 -6.16800000
C -0.03000000 -6.69300000 -5.38800000
C 2.11000000 -7.67400000 -5.47900000
C 1.41800000 -6.36900000 -5.56900000
C 1.21200000 -10.00800000 -5.45700000
O 1.86500000 -10.94300000 -5.92600000
N 0.55200000 -10.10000000 -4.30900000
C 0.56800000 -11.34200000 -3.55600000
C 0.12500000 -11.11600000 -2.11600000
S 0.59000000 -12.51900000 -1.05700000
C -0.27000000 -12.44000000 -4.19700000
O 0.19100000 -13.57900000 -4.33400000
N -1.48700000 -12.09300000 -4.61400000
C -2.38300000 -13.05600000 -5.24200000
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9. tertiapin (1ter) [5]

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H -6.61700000 -0.33200000 -5.88800000
H -8.01800000 -1.36800000 -5.94200000
H -9.00800000 -0.37300000 -4.12200000
H -7.45600000 0.17700000 -3.43900000
H -7.44200000 1.51100000 -5.52800000
H -9.04800000 1.26100000 -5.49600000
H -8.28500000 1.97700000 -4.21800000
H -2.81300000 -1.76500000 -1.51500000
H -1.73700000 -4.36400000 -1.48300000
H -0.60000000 -2.34400000 -0.87300000
H -1.61900000 -2.14100000 0.55900000
H -4.14800000 -2.68800000 0.48100000
H -6.31900000 -3.62000000 1.20400000
H -5.54200000 -5.24900000 1.31200000
H -5.13200000 -1.90200000 2.06100000
H -3.50600000 -2.55400000 4.52200000
H -2.85200000 -2.78300000 1.71500000
H -1.48200000 -2.12400000 2.70500000
H -2.73500000 -4.24000000 4.16800000
H -2.08100000 -4.81300000 2.59200000
H -0.22600000 -5.01200000 3.81400000
H -0.06400000 -3.29800000 3.50400000
H -0.99900000 -4.73300000 5.95900000
H 0.25700000 -3.47200000 5.81600000
H -1.66000000 -2.13400000 5.06700000
H -2.55200000 -3.27100000 5.87000000
H -1.41700000 -2.41100000 6.65000000
H -1.83100000 -0.33200000 2.48600000
H -0.36300000 1.27400000 3.48100000
H -2.44600000 2.43700000 4.54400000
H -2.16700000 1.35000000 5.92100000
H 0.07900000 2.19900000 6.22400000
H -0.08400000 3.26800000 4.80600000
H -1.80000000 4.53200000 5.94000000
H -1.87600000 3.38700000 7.24700000
H -0.35100000 4.50200000 8.35100000
H 0.82400000 4.24200000 7.03400000
H -1.14500000 6.25400000 6.77100000
H 0.10300000 6.49700000 7.78100000
H 0.37300000 6.15500000 6.18900000

10. vacuolar targeting peptide (1vtp) [5]

N -10.09700000 6.94100000 10.12000000
C -8.60900000 6.96600000 10.20700000
C -8.07900000 5.58000000 10.64200000
O -8.52100000 5.44900000 11.98500000
C -8.03800000 7.32700000 8.83200000
O -7.50600000 8.40300000 8.63200000
N -8.17400000 6.40700000 7.91200000
C -7.66500000 6.61800000 6.52000000
C -7.32300000 5.22400000 5.91900000
C -8.54600000 4.26100000 5.96600000
C -9.03300000 3.96400000 4.53600000
O -8.34700000 3.20000000 3.87700000
O -10.06200000 4.51700000 4.18000000
C -8.70300000 7.35400000 5.66000000
O -8.85200000 7.10100000 4.47900000
N -9.38500000 8.26100000 6.30800000
C -10.44100000 9.07300000 5.63700000
C -11.53300000 9.40600000 6.67900000
C -12.91900000 9.16000000 6.06200000
C -13.49800000 10.10200000 5.23200000
C -13.60600000 7.99300000 6.32800000
C -14.74200000 9.87800000 4.67800000
C -14.84900000 7.77100000 5.77400000
C -15.42600000 8.71000000 4.94600000
O -16.67000000 8.48400000 4.39300000
C -9.89900000 10.37000000 5.02000000
O -10.47200000 10.87400000 4.07300000
N -8.82200000 10.87500000 5.56700000
C -8.21100000 12.13900000 5.04000000
C -8.94800000 13.34200000 5.65800000
C -6.71500000 12.21100000 5.38200000
O -6.08100000 13.22700000 5.16900000
N -6.20000000 11.12700000 5.90300000
C -4.75600000 11.05000000 6.28000000
C -4.63700000 10.42300000 7.68100000
O -5.46700000 11.23700000 8.49600000
C -4.08800000 10.16500000 5.22400000
O -3.25100000 10.59900000 4.45500000
N -4.50100000 8.92400000 5.22000000
C -3.94700000 7.93600000 4.24700000
C -4.55400000 6.55300000 4.55100000
C -3.44200000 5.55900000 4.94900000
C -2.86900000 5.93600000 6.34600000
C -3.08500000 4.78100000 7.33600000
N -2.65800000 5.19900000 8.70000000
C -4.26600000 8.35000000 2.80500000
O -3.62500000 7.89300000 1.88400000
N -5.24200000 9.20700000 2.65500000
C -5.66900000 9.70400000 1.31500000
C -6.70200000 10.83200000 1.54900000

C -7.91700000 10.24500000 2.29100000
C -6.07700000 12.01600000 2.32300000
C -4.47500000 10.21000000 0.49400000
O -4.37200000 9.97000000 -0.69400000
N -3.61500000 10.89800000 1.19600000
C -2.38500000 11.48100000 0.58300000
C -2.07900000 12.83000000 1.27700000
C -1.78800000 13.88900000 0.20000000
O -0.68900000 13.83600000 -0.32800000
O -2.68000000 14.68900000 -0.03500000
C -1.17900000 10.54200000 0.71300000
O -0.42800000 10.37300000 -0.22600000
N -1.02400000 9.95800000 1.87200000
C 0.12700000 9.02200000 2.10500000
C 0.09400000 8.56600000 3.58200000
C 0.20200000 9.78700000 4.52900000
C 1.65000000 10.31300000 4.54700000
O 2.39500000 9.83200000 5.38600000
O 1.93200000 11.16700000 3.72100000
C 0.09800000 7.78900000 1.17700000
O 1.13000000 7.25000000 0.82800000
N -1.09000000 7.38900000 0.81100000
C -1.31100000 6.21200000 -0.08600000
C -2.55800000 5.48300000 0.42100000
C -2.67000000 4.07700000 -0.18800000
C -1.99400000 3.00800000 0.36800000
C -3.45600000 3.86300000 -1.30300000
C -2.10800000 1.75200000 -0.18400000
C -3.56800000 2.60500000 -1.85500000
C -2.89300000 1.53900000 -1.29700000
O -2.99800000 0.27500000 -1.84100000
C -1.49100000 6.64200000 -1.55200000
O -1.44700000 5.81500000 -2.44300000
N -1.69400000 7.92100000 -1.76700000
C -1.88400000 8.46000000 -3.16100000
C -1.71400000 10.01900000 -3.12300000
C -0.22700000 10.45700000 -3.10000000
C -2.39200000 10.63800000 -4.36600000
C -0.90100000 7.83500000 -4.17700000
O -1.27200000 7.53000000 -5.29300000
N 0.32700000 7.65400000 -3.75600000
C 1.36500000 7.05500000 -4.65300000
C 0.89000000 5.68500000 -5.16500000
O 0.88600000 5.42600000 -6.35300000
N 0.49200000 4.83600000 -4.25100000
C 0.00900000 3.47800000 -4.64600000
C -0.31300000 2.68500000 -3.36900000
C 0.99200000 2.03700000 -2.85000000
C 0.69400000 1.21200000 -1.58900000
O 0.01800000 0.20700000 -1.74500000
O 1.15500000 1.62800000 -0.53800000
C -1.23700000 3.61100000 -5.53500000
O -1.38900000 2.86500000 -6.48100000
N -2.09700000 4.55300000 -5.22400000
C -3.33400000 4.73800000 -6.05700000
C -4.15800000 5.96900000 -5.56300000
C -5.47500000 6.06900000 -6.37800000
C -4.50300000 5.79900000 -4.07500000
C -2.89000000 4.97800000 -7.50500000
O -3.37000000 4.33800000 -8.41900000
N -1.97200000 5.89800000 -7.66200000
C -1.44200000 6.23400000 -9.01000000
C -0.31000000 7.27600000 -8.86100000
C 0.28900000 7.62400000 -10.25400000
C 1.59200000 6.82700000 -10.47600000
O 2.56000000 7.18800000 -9.82400000
O 1.56200000 5.90600000 -11.27600000
C -0.91200000 4.96200000 -9.68000000
O -1.19900000 4.70100000 -10.82900000
N -0.15400000 4.20400000 -8.93000000
C 0.42900000 2.93200000 -9.46000000
C 1.16500000 2.22100000 -8.30900000
C 2.11200000 1.17000000 -8.89800000
O 1.70700000 0.08500000 -9.26800000
N 3.38100000 1.45500000 -9.00300000
C -0.68600000 2.03600000 -10.02800000
O -0.60000000 1.54100000 -11.13600000
N -1.71300000 1.87000000 -9.23200000
C -2.87400000 1.02200000 -9.65200000
C -3.94600000 1.01800000 -8.53600000
C -5.01000000 -0.08500000 -8.76900000
O -5.46800000 -0.22900000 -9.89500000
O -5.31700000 -0.73800000 -7.78500000
C -3.48300000 1.58300000 -10.94000000
O -3.71500000 0.85600000 -11.88400000
N -3.71900000 2.86800000 -10.92800000
C -4.31100000 3.56500000 -12.10200000
C -4.32000000 5.08800000 -11.80900000
C -5.77800000 5.58100000 -11.63500000
C -5.76800000 6.97900000 -10.97800000
C -6.46500000 5.66900000 -13.01700000
C -3.49700000 3.25400000 -13.35500000
O -4.04600000 2.86100000 -14.36200000
N -2.21000000 3.44600000 -13.22600000
C -1.24200000 3.19200000 -14.33900000
C 0.18200000 3.12800000 -13.73500000
C 1.20300000 3.73400000 -14.71300000
C 2.61800000 3.41200000 -14.21600000
O 3.35200000 2.66700000 -14.83500000
N 3.04500000 3.94800000 -13.10600000
C -1.58400000 1.87000000 -15.05300000
O -1.75000000 1.82400000 -16.25700000
N -1.67700000 0.84000000 -14.25100000
C -2.00400000 -0.53200000 -14.75200000
C -1.80900000 -1.53400000 -13.59800000
C -0.35100000 -1.47500000 -13.07800000
C -0.28100000 -2.03800000 -11.64000000
C -0.34800000 -3.58300000 -11.66000000
N 0.54500000 -4.13600000 -10.60300000
C -3.44200000 -0.65000000 -15.29200000
O -3.64700000 -1.08900000 -16.40700000
N -4.38400000 -0.24900000 -14.47300000
C -5.83600000 -0.29600000 -14.82600000
C -6.62200000 0.41800000 -13.69600000
O -6.87200000 -0.60700000 -12.74100000
C -6.14100000 0.34800000 -16.18800000

O -6.86700000 -0.20900000 -16.98800000
N -5.56900000 1.50500000 -16.39800000
C -5.75300000 2.26800000 -17.66800000
C -6.68800000 3.46700000 -17.37400000
C -7.27500000 4.02500000 -18.69700000
C -8.68000000 4.60900000 -18.42000000
C -9.30600000 5.10700000 -19.73300000
N -10.48200000 5.97000000 -19.43100000
C -4.35500000 2.71700000 -18.11800000
O -3.92400000 3.82500000 -17.86300000
N -3.69400000 1.80300000 -18.78300000
C -2.31400000 2.04400000 -19.30800000
C -1.58500000 0.65400000 -19.32100000
C -2.27600000 -0.35000000 -20.28700000
C -0.08900000 0.82100000 -19.69500000
C -2.38000000 2.69700000 -20.70400000
O -1.77700000 2.24000000 -21.65700000
N -3.13100000 3.77100000 -20.76400000
C -3.32000000 4.54500000 -22.03400000
C -1.97300000 5.22600000 -22.38900000
C -3.79700000 3.63800000 -23.18800000
O -3.47700000 3.86800000 -24.33900000
N -4.55500000 2.63100000 -22.81800000
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C -5.97900000 2.36800000 -24.88100000
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C -6.96500000 3.35800000 -24.21000000
C -4.01400000 0.80500000 -24.46300000
O -2.85700000 1.18300000 -24.46200000
N -4.40800000 -0.31100000 -25.02500000
C -3.43300000 -1.20700000 -25.72100000
C -4.15700000 -2.48500000 -26.17700000
O -4.59000000 -3.08700000 -24.96600000
C -2.81900000 -0.49900000 -26.94500000
O -3.57400000 0.18200000 -27.62200000
O -1.62800000 -0.68100000 -27.13300000
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H -8.31400000 7.72300000 10.91800000
H -8.49800000 4.77900000 10.04900000
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H -6.78700000 7.24100000 6.57300000
H -6.98400000 5.34600000 4.90100000
H -6.51400000 4.79100000 6.48800000
H -8.25400000 3.32800000 6.43000000
H -9.36100000 4.68400000 6.53900000
H -9.19200000 8.40600000 7.25600000
H -10.85500000 8.47100000 4.84000000
H -11.42300000 8.77800000 7.55200000
H -11.46700000 10.43900000 6.99300000
H -12.97800000 11.02300000 5.01100000
H -13.16900000 7.24500000 6.97500000
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H -15.37500000 6.85400000 5.99200000
H -17.14400000 9.31900000 4.37400000
H -8.40400000 10.42800000 6.33200000
H -8.30100000 12.15200000 3.95700000
H -10.00900000 13.27100000 5.46800000
H -8.78600000 13.37100000 6.72600000
H -8.57900000 14.25900000 5.22400000
H -6.76800000 10.34400000 6.05500000
H -4.30600000 12.03200000 6.26100000
H -5.00400000 9.40700000 7.70700000
H -3.62200000 10.46500000 8.04800000
H -4.98100000 12.04000000 8.69700000
H -5.18400000 8.64700000 5.86600000
H -2.87600000 7.91000000 4.36700000
H -5.24400000 6.64900000 5.37100000
H -5.09600000 6.17700000 3.69500000
H -3.85200000 4.55900000 4.95800000
H -2.64900000 5.58900000 4.21500000
H -1.81000000 6.13300000 6.25400000
H -3.34400000 6.82600000 6.73300000
H -4.12800000 4.50300000 7.37400000
H -2.50000000 3.92300000 7.04000000
H -1.79600000 5.77600000 8.63200000
H -3.41400000 5.75700000 9.14500000
H -2.46500000 4.35500000 9.27600000
H -5.71700000 9.54400000 3.43800000
H -6.13500000 8.88400000 0.79100000
H -7.04700000 11.23600000 0.62400000
H -8.24400000 9.33500000 1.80900000
H -7.66500000 10.02100000 3.31700000
H -8.73200000 10.95100000 2.27000000
H -5.54300000 11.66300000 3.19000000
H -5.38700000 12.54800000 1.68400000
H -6.83900000 12.71500000 2.63100000
H -3.79900000 11.02500000 2.14900000
H -2.57200000 11.64500000 -0.46600000
H -2.92400000 13.15000000 1.87200000
H -1.21900000 12.74900000 1.92700000
H -1.66400000 10.13800000 2.59100000
H 1.04500000 9.55700000 1.91200000
H -0.83200000 8.04600000 3.77400000
H 0.91000000 7.88400000 3.77100000
H -0.46000000 10.58200000 4.21600000
H -0.07500000 9.49200000 5.53000000
H -1.87500000 7.87100000 1.13200000
H -0.45600000 5.55500000 -0.02100000
H -2.51300000 5.39500000 1.49600000
H -3.43900000 6.05100000 0.15800000
H -1.37300000 3.15400000 1.24000000
H -3.99100000 4.68900000 -1.74300000
H -1.57700000 0.92600000 0.26200000
H -4.18800000 2.45700000 -2.72500000
H -2.11900000 -0.10900000 -1.80800000
H -1.72800000 8.52400000 -0.99600000
H -2.89100000 8.21900000 -3.47100000
H -2.20800000 10.40300000 -2.24300000
H 0.34200000 9.83900000 -2.42300000
H 0.20700000 10.37900000 -4.08600000
H -0.15500000 11.48300000 -2.77300000
H -3.43100000 10.34500000 -4.41400000

H -2.34000000 11.71700000 -4.31500000
H -1.89700000 10.31100000 -5.26800000
H 0.56000000 7.91800000 -2.84300000
H 1.52900000 7.71300000 -5.49500000
H 2.28400000 6.93400000 -4.10000000
H 0.50500000 5.08400000 -3.30300000
H 0.78100000 2.98400000 -5.22200000
H -0.72400000 3.33700000 -2.61300000
H -1.03700000 1.91700000 -3.59100000
H 1.40800000 1.38200000 -3.60200000
H 1.72100000 2.80200000 -2.61700000
H -1.92000000 5.12100000 -4.44700000
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H -3.59400000 6.88000000 -5.69700000
H -5.95100000 5.10200000 -6.45100000
H -6.16200000 6.75700000 -5.90700000
H -5.27100000 6.42700000 -7.37700000
H -4.79600000 4.77900000 -3.87500000
H -3.64100000 6.03900000 -3.47300000
H -5.31200000 6.45500000 -3.79000000
H -1.63300000 6.37200000 -6.88200000
H -2.25700000 6.63400000 -9.58800000
H -0.70100000 8.17000000 -8.39900000
H 0.46000000 6.88500000 -8.21400000
H -0.41100000 7.39000000 -11.04500000
H 0.51600000 8.67900000 -10.30400000
H 0.02900000 4.48100000 -8.01100000
H 1.12300000 3.18000000 -10.25200000
H 1.74500000 2.93600000 -7.74300000
H 0.47400000 1.73200000 -7.63800000
H 4.00200000 0.79700000 -9.37900000
H 3.71300000 2.32800000 -8.70500000
H -1.70600000 2.30900000 -8.35500000
H -2.52100000 0.02000000 -9.83600000
H -3.46200000 0.85800000 -7.58300000
H -4.45000000 1.97200000 -8.50100000
H -3.50300000 3.38200000 -10.13100000
H -5.30500000 3.17100000 -12.23500000
H -3.77500000 5.27600000 -10.89600000
H -3.83600000 5.63600000 -12.60600000
H -6.32700000 4.89800000 -11.00200000
H -5.17300000 7.66800000 -11.56000000
H -6.77600000 7.36100000 -10.91000000
H -5.35500000 6.91800000 -9.98200000
H -5.92700000 6.34900000 -13.66100000
H -6.49200000 4.69600000 -13.48400000
H -7.47800000 6.02500000 -12.90300000
H -1.88100000 3.77200000 -12.36500000
H -1.32200000 4.00400000 -15.04900000
H 0.21600000 3.68000000 -12.80700000
H 0.45200000 2.10300000 -13.52400000
H 1.07700000 3.31600000 -15.70200000
H 1.08700000 4.80700000 -14.76600000
H 3.94800000 3.74500000 -12.78600000
H 2.47100000 4.54900000 -12.58900000
H -1.52000000 0.98100000 -13.29500000
H -1.32100000 -0.77400000 -15.55200000
H -2.49600000 -1.28900000 -12.80100000
H -2.03100000 -2.53400000 -13.94300000
H 0.29200000 -2.04400000 -13.73400000
H 0.00300000 -0.45400000 -13.06200000
H 0.64600000 -1.71900000 -11.18500000
H -1.09600000 -1.64900000 -11.04700000
H -1.35700000 -3.91500000 -11.46400000
H -0.02900000 -3.97900000 -12.61300000
H 0.92800000 -3.34900000 -10.04200000
H 0.00400000 -4.77700000 -9.98800000
H 1.32600000 -4.65800000 -11.05000000
H -4.13700000 0.09600000 -13.59600000
H -6.12100000 -1.33500000 -14.87200000
H -6.04100000 1.20400000 -13.23500000
H -7.56400000 0.81200000 -14.04300000
H -6.43000000 -0.40600000 -11.91100000
H -5.00400000 1.88900000 -15.70200000
H -6.17500000 1.62200000 -18.42500000
H -7.49000000 3.13000000 -16.73200000
H -6.15100000 4.24900000 -16.85600000
H -6.62700000 4.80100000 -19.07900000
H -7.35100000 3.24400000 -19.44000000
H -9.31400000 3.84400000 -17.99500000
H -8.60500000 5.42500000 -17.71600000
H -8.59400000 5.68300000 -20.30600000
H -9.64000000 4.26900000 -20.32700000
H -11.01400000 5.56600000 -18.63400000
H -10.15400000 6.92500000 -19.18000000
H -11.09600000 6.02200000 -20.26800000
H -4.12100000 0.93500000 -18.94100000
H -1.79500000 2.71800000 -18.64200000
H -1.63500000 0.24200000 -18.32200000
H -3.34600000 -0.21000000 -20.28900000
H -1.91400000 -0.23200000 -21.29700000
H -2.06700000 -1.36000000 -19.96500000
H 0.26100000 1.81200000 -19.44400000
H 0.50400000 0.10300000 -19.14800000
H 0.06900000 0.66100000 -20.75200000
H -3.58400000 4.07800000 -19.95200000
H -4.07300000 5.29900000 -21.86100000
H -1.54100000 5.67200000 -21.50500000
H -1.27400000 4.50900000 -22.79200000
H -2.13600000 6.00300000 -23.12200000
H -4.75800000 2.52900000 -21.86500000
H -5.75400000 0.95200000 -23.22500000
H -5.33600000 2.91100000 -25.55800000
H -7.16300000 0.54700000 -25.05800000
H -7.64600000 1.81200000 -26.17200000
H -6.18100000 0.90200000 -26.46900000
H -7.54800000 2.85200000 -23.45400000
H -6.42700000 4.17200000 -23.74800000
H -7.63900000 3.77200000 -24.94700000
H -5.35400000 -0.56100000 -24.99000000
H -2.64600000 -1.46600000 -25.02500000
H -5.01400000 -2.26600000 -26.79700000
H -3.48700000 -3.15800000 -26.69100000
H -3.84200000 -3.55500000 -24.58700000

11. trypsin inhibitor II (2eti) [5]

N 10.34000000 0.13600000 -1.96700000
C 9.71100000 -1.19000000 -1.86600000
C 8.30300000 -1.08300000 -1.29900000
O 7.61200000 -0.08600000 -1.49300000
N 7.81300000 -2.11900000 -0.61500000
C 6.42100000 -2.25000000 -0.23200000
C 6.12300000 -3.66400000 0.26100000
S 4.72100000 -3.80900000 1.39600000
C 5.94900000 -1.19200000 0.75500000
O 5.01400000 -0.45300000 0.45800000
N 6.53200000 -1.10800000 1.95500000
C 6.22100000 -0.05700000 2.90000000
C 7.53400000 -2.01200000 2.48400000
C 6.85500000 -0.52800000 4.20400000
C 8.08300000 -1.28700000 3.71000000
C 6.78200000 1.26900000 2.40400000
O 7.49300000 1.31900000 1.40400000
N 6.51300000 2.34900000 3.14100000
C 6.90700000 3.73300000 2.96400000
C 8.42000000 3.91000000 2.86100000
C 9.26200000 3.27900000 3.96700000
C 8.87500000 3.81500000 5.34200000
N 7.83700000 2.98000000 5.94700000
C 7.44200000 3.14700000 7.21700000
N 6.63500000 2.26500000 7.82000000
N 7.86800000 4.21700000 7.90200000
C 6.07200000 4.34900000 1.85000000
O 5.91500000 3.75900000 0.78500000
N 5.42700000 5.48800000 2.11700000
C 4.12900000 5.80900000 1.55900000
C 3.24900000 6.55300000 2.55900000
C 2.67300000 5.58400000 3.58600000
C 3.87200000 7.76100000 3.25300000
C 2.82300000 8.68400000 3.86700000
C 4.19100000 6.49800000 0.20200000
O 4.34000000 7.71400000 0.10900000
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C 3.84200000 6.12500000 -2.22900000
C 5.10300000 6.77200000 -2.79600000
C 6.41500000 6.14700000 -2.33100000
C 6.41200000 4.62500000 -2.42700000
C 7.61400000 6.65000000 -3.13100000
C 3.28300000 5.01300000 -3.10500000
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C 2.10800000 1.76400000 -3.17700000
C 3.36500000 1.39100000 -3.95900000
S 5.00000000 1.81700000 -3.31100000
C 4.66900000 1.75800000 -1.53200000
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N -3.48600000 3.14100000 -1.64900000
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C -4.18200000 0.84800000 -1.10300000
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C -5.87500000 2.49700000 -1.79600000
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C -9.52200000 2.87200000 -2.62100000
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C -11.42500000 2.19400000 -4.13500000
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C -7.66200000 -2.81600000 -3.62100000
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N 2.92100000 -3.05500000 -5.27400000
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C 5.26300000 -3.69700000 -5.61700000
C 5.69000000 -2.88800000 -4.39500000
C 7.05200000 -3.35500000 -3.88800000
C 5.77600000 -1.39600000 -4.70800000
C 3.56200000 -5.28000000 -4.68500000
O 3.33100000 -5.00400000 -3.51000000
N 3.58500000 -6.53800000 -5.13100000
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C 3.10200000 -8.97300000 -5.02700000
C 4.36200000 -7.76900000 -3.15500000
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N 4.13000000 -8.72900000 -2.25900000
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C 2.43800000 -5.77100000 0.06400000
C 2.79800000 -4.52500000 -0.73700000
S 3.08800000 -3.13100000 0.37900000
C 0.92500000 -5.90700000 0.15600000
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C 2.70900000 -0.90200000 5.36300000
O 1.64600000 -0.51400000 5.89900000
O 3.84200000 -0.72700000 5.86000000
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H 11.31700000 0.06100000 -2.21100000
H 9.82600000 0.72800000 -2.60200000
H 9.67500000 -1.66100000 -2.84800000
H 10.37800000 -1.75300000 -1.21200000
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H 5.95300000 -4.33100000 -0.61500000
H 5.14200000 0.03700000 3.02200000
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H 7.04500000 -2.93400000 2.79800000
H 7.12700000 0.28200000 4.88100000
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H 8.81500000 -0.53600000 3.41400000
H 8.53600000 -1.98500000 4.41600000
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H 6.57100000 4.21200000 3.88500000
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H 8.65700000 4.97200000 2.91400000
H 9.17800000 2.19400000 3.92700000
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H 9.75800000 3.82200000 5.98000000
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H 6.34200000 2.38800000 8.77900000
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H 7.57200000 4.36000000 8.85700000
H 5.77700000 6.11200000 2.82900000
H 3.62400000 4.86400000 1.35500000
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H 3.38200000 5.33500000 4.37500000

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H -2.92700000 -0.48100000 0.86900000

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H -3.00000000 10.14200000 5.83700000
H -5.33500000 4.44000000 3.93300000
H -5.49800000 3.86800000 1.68700000
H -5.50400000 5.59600000 1.32800000
H -3.17300000 3.32500000 2.90700000
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H -0.54500000 4.39700000 3.45700000
H 0.60700000 3.71100000 2.33800000
H -0.63900000 6.78300000 3.45000000
H 0.76300000 4.77800000 -0.07100000
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H 1.04700000 6.98900000 -1.15600000
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H 0.29600000 2.04000000 0.92100000
H -0.52300000 -0.59600000 1.93400000
H 0.48100000 0.39700000 -0.51200000
H 1.83800000 -0.49700000 0.18500000
H 0.75500000 -1.88300000 2.97000000
H 2.46600000 -2.74300000 4.28400000
H 3.53200000 -1.57200000 3.51200000

II. COMPLEMENTARY DETAILS

A. Radius of element

TABLE I: Radiuses of all elements in our calculations. ($\mathring{A}$)

Elem.	Rad.	Elem.	Rad.	Elem.	Rad.	Elem.	Rad.	Elem.	Rad.
H	0.30	He	1.16	Li	1.23	Be	0.89	B	0.88
C	0.77	N	0.70	O	0.66	F	0.58	Ne	0.55
Na	1.40	Mg	1.36	Al	1.25	Si	1.17	P	1.10
S	1.11	Cl	0.99	Ar	1.58	K	2.03	Ca	1.74
Sc	1.44	Ti	1.32	V	1.20	Cr	1.13	Mn	1.17
Fe	1.16	Co	1.16	Ni	1.15	Cu	1.17	Zn	1.25
Ga	1.25	Ge	1.22	As	1.21	Se	1.17	Br	1.14
Kr	1.89	Rb	2.25	Sr	1.92	Y	1.62	Zr	1.45
Nb	1.34	Mo	1.29	Tc	1.23	Ru	1.24	Rh	1.25
Pd	1.28	Ag	1.34	Cd	1.41	In	1.50	Sn	1.40
Sb	1.41	Te	1.37	I	1.33	Xe	2.09	Cs	2.35
Ba	1.98	La	1.69	Ce	1.65	Pr	1.65	Nd	1.64
Pm	1.64	Sm	1.66	Eu	1.85	Gd	1.61	Tb	1.59
Dy	1.59	Ho	1.58	Er	1.57	Tm	1.56	Yb	1.70
Lu	1.56	Hf	1.44	Ta	1.34	W	1.30	Re	1.28
Os	1.26	Ir	1.26	Pt	1.29	Au	1.34	Hg	1.44
Tl	1.55	Pb	1.54	Bi	1.52	Po	1.53	At	1.52
Rn	1.53	Fr	2.45	Ra	2.02	Ac	1.70	Th	1.63
Pa	1.46	U	1.40	Np	1.36	Pu	1.25	Am	1.57
Cm	1.58	Bk	1.54	Cf	1.53	Es	1.84	Fm	1.61
Md	1.50	No	1.49	Lr	1.38	Rf	1.36	Db	1.26
Sg	1.20	Bh	1.16	Hs	1.14	Mt	1.06		

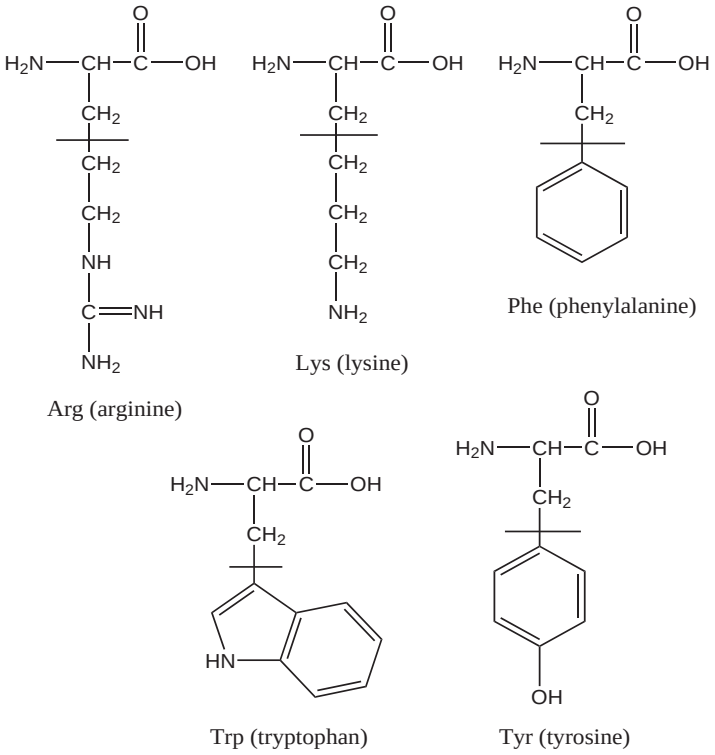

FIG. 1: Fragmentation scheme for five residues

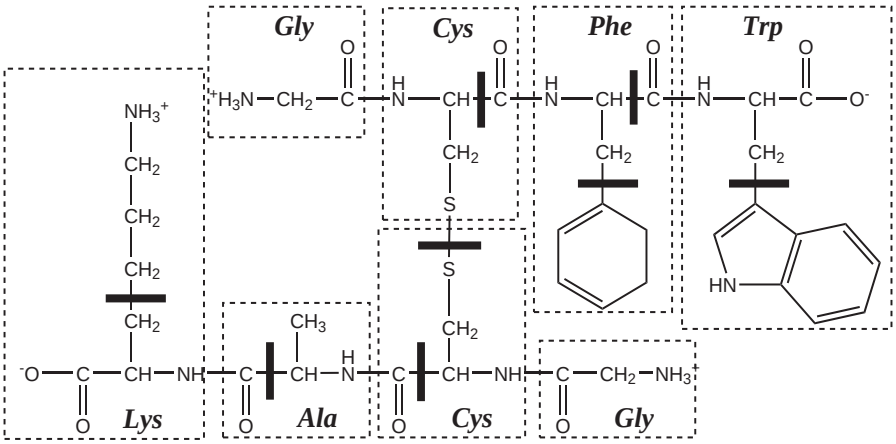

FIG. 2: Illustration of fragmentation for a protein

B. Fragmentation for proteins

C-C bond between α-carbon and the carbonyl group in the central residues, the S-S bond between two residues, and the C-C bond between β- and γ-carbons in five residues with large side chains (Arg, Lys, Phe, Trp, Tyr). See FIG.1-2

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