Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supplementary materials: Cartesian coordinates of optimized short peptides Ac-X-OMe and their N-methylated analogues.

X = Gly

0 1

N	-1.03839800	0.27740600	-0.00021100
H	-0.81229300	1.26100500	-0.00031100
C	0.07589600	-0.64040000	-0.00011100
H	0.05609300	-1.29980000	0.87428900
H	0.05609300	-1.30010000	-0.87431100
C	1.37040100	0.14419200	-0.00021100
O	1.44450800	1.34939200	-0.00021100
O	2.42709600	-0.67901400	0.00008900
C	-2.32510100	-0.17168700	-0.00041100
C	3.72180000	-0.04362100	0.00018900
H	3.84000300	0.57687900	0.88938900
H	3.84040300	0.57667900	-0.88901100
H	4.44229500	-0.85762500	0.00048900
O	-2.59500800	-1.36148500	0.00038900
C	-3.39559500	0.90631900	0.00018900
H	-2.99668900	1.92251700	0.00038900
H	-4.02699600	0.76912300	0.88028900
H	-4.02729600	0.76952300	-0.87971100

X = (NMe) Gly

0 1

N	-1.07490700	0.41439300	-0.46719400
C	-1.31111300	1.82429200	-0.17629400
C	0.21929500	0.05939800	-1.00719400
H	0.16439900	-0.94870200	-1.41829400
H	0.49379200	0.74190000	-1.81649400
C	1.32729500	0.07820300	0.04000600
O	1.18379300	0.32520300	1.21090600

O	2.50549600	-0.21909100	-0.53249400
C	-1.88610200	-0.60771100	-0.02999400
C	3.64889600	-0.25188600	0.34610600
H	3.53189900	-1.03418700	1.09800600
H	3.78009200	0.71091400	0.84240600
H	4.50169700	-0.46878300	-0.29379400
O	-1.57939700	-1.78171000	-0.18839400
C	-3.19140400	-0.21871700	0.63840600
H	-3.83030700	0.36538000	-0.02969400
H	-3.01810700	0.37408400	1.54060600
H	-3.70970000	-1.13621900	0.90980600
H	-0.86301600	2.42899400	-0.96839400
H	-0.86991500	2.12449400	0.77970600
H	-2.37681400	2.04468700	-0.15989400

X = Val

0 1

N	-1.07040300	-0.53060000	0.13458900
C	-2.38133900	-0.36655400	-0.21243000
C	-0.02663300	0.31896700	-0.42279700
H	-0.32811600	0.58708600	-1.43783500
C	1.29446700	-0.42834400	-0.53941400
O	2.20177900	-0.09492800	-1.25682500
C	0.13180700	1.65386800	0.37382000
H	-0.89083800	2.03981400	0.42836100
C	0.64193600	1.42776600	1.80183400
H	0.59778600	2.35929500	2.37196400
H	0.03852800	0.68595300	2.33091000
H	1.68317200	1.08903100	1.80929400
C	0.98166100	2.68100500	-0.38245700
H	0.99040400	3.63058100	0.15984900
H	2.01407900	2.34530900	-0.50009700
H	0.57731900	2.86935200	-1.38062600
O	1.36064200	-1.49838000	0.28816200

O	-2.75485900	0.52079900	-0.96177100
C	-3.35014600	-1.36252000	0.40300100
H	-0.78819300	-1.30873100	0.70738600
C	2.59424100	-2.24378100	0.25100200
H	3.43278600	-1.60271900	0.52455700
H	2.76293200	-2.64580500	-0.74859000
H	2.47137300	-3.04699100	0.97373100
H	-4.09886400	-0.81064100	0.97463800
H	-2.87354400	-2.09728800	1.05506100
H	-3.87246600	-1.88241600	-0.40260700

X = (NMe) Val

0 1

N	-0.89103800	-0.79784200	0.52319600
C	-1.65573700	-0.44046200	-0.55789000
C	0.50548900	-0.33709100	0.61500100
H	0.70776800	-0.26352200	1.69075800
C	0.68032700	1.10570800	0.12183800
O	1.59330900	1.51304400	-0.54808900
C	1.52385000	-1.35698600	0.04277400
H	1.20874700	-2.31956500	0.46804700
C	1.50257500	-1.49986100	-1.48526600
H	2.17777600	-2.30724900	-1.78499700
H	0.50551200	-1.73485900	-1.85855500
H	1.82976900	-0.57828500	-1.96666200
C	2.94415200	-1.07756300	0.56046300
H	3.61801400	-1.88524100	0.26217600
H	3.33191400	-0.14294100	0.15351700
H	2.96958700	-1.01376700	1.65374400
O	-0.26038600	1.90371100	0.66784000
O	-1.18607500	0.20604500	-1.48322600
C	-3.11329600	-0.87496000	-0.57591800
C	-0.22965100	3.27404100	0.23229900

H	-0.40350600	3.32474100	-0.84339700
H	0.73313200	3.73107400	0.46508300
H	-1.03244700	3.77045700	0.77336000
H	-3.66670100	-0.47359200	0.27699500
H	-3.21330600	-1.96356300	-0.56282100
H	-3.54917000	-0.49176800	-1.49577800
C	-1.41184600	-1.47215900	1.70596900
H	-2.34326000	-1.98624800	1.48373600
H	-1.58981200	-0.76333300	2.52414200
H	-0.69671900	-2.22384500	2.05046000

X = Leu

0 1

N	-1.66330700	0.38660400	-0.31959300
H	-1.81210600	1.11070400	-1.00649300
C	-0.28980700	0.16990300	0.10790700
H	-0.29600700	-0.03619700	1.17890700
C	0.46869400	1.46270300	-0.15479300
O	0.14859500	2.28230300	-0.98319300
C	0.33939200	-1.03559700	-0.63989300
H	-0.35360800	-1.86849700	-0.48519300
H	0.32919300	-0.80499700	-1.71119300
C	1.75239200	-1.47829800	-0.21709300
H	2.44509300	-0.64559900	-0.38429300
C	1.82679200	-1.86169800	1.26780700
H	2.81999200	-2.24669900	1.51650700
H	1.63579200	-1.00629800	1.91920700
H	1.09559100	-2.64039800	1.50850700
C	2.20509100	-2.64709900	-1.10499300
H	3.22569100	-2.95349900	-0.85919300
H	1.55439100	-3.51719800	-0.96759300
H	2.18209200	-2.37739900	-2.16509300
O	1.55129400	1.57780200	0.62930700
C	-2.70710700	-0.28879500	0.23960700

C	2.36189500	2.75220100	0.41630700
H	1.77629600	3.65360200	0.59960700
H	2.74079500	2.77250100	-0.60619300
H	3.17899500	2.67190100	1.12890700
O	-2.55100800	-1.13709500	1.10400700
C	-4.08310700	0.08230600	-0.28699300
H	-4.06570600	0.85050600	-1.06249300
H	-4.69240700	0.43070600	0.54940700
H	-4.55740700	-0.81719400	-0.68429300

X = (Nme) Leu

0 1

N	-1.64190600	0.34818300	0.12343200
C	-2.09930400	1.68482100	-0.26027800
C	-0.21315200	0.12931600	0.40563900
H	-0.17411300	-0.11003100	1.46495000
C	0.54977300	1.43685400	0.18450600
O	0.06278700	2.54294600	0.22669200
C	0.38330700	-1.01815600	-0.42675700
H	-0.22753100	-1.90879800	-0.23753900
H	0.28700500	-0.77926300	-1.49026100
C	1.86079400	-1.34326700	-0.12998700
H	2.45331100	-0.44567200	-0.35038400
C	2.10124800	-1.72612900	1.33762500
H	3.14822500	-1.99919900	1.49740300
H	1.86870000	-0.90650100	2.02103700
H	1.48600900	-2.58600800	1.62361000
C	2.34669300	-2.45510300	-1.07058700
H	3.40926600	-2.66340500	-0.91702700
H	1.79696600	-3.38547500	-0.89147000
H	2.20723400	-2.18037200	-2.12010800
O	1.85154300	1.21044300	-0.06160500
C	-2.46432700	-0.76036200	0.08774000

C	2.66898400	2.38102700	-0.25809300
H	2.65991500	3.00456900	0.63693800
H	2.30212100	2.96517100	-1.10318200
H	3.67008500	2.00505000	-0.45432500
O	-2.06118600	-1.88524800	0.33711300
C	-3.92088600	-0.51586100	-0.27600300
H	-4.02446400	0.00258600	-1.23230700
H	-4.42272900	0.08853400	0.48483400
H	-4.40842300	-1.48629200	-0.33500600
H	-1.38517500	2.41769400	0.10892800
H	-3.06396600	1.90922600	0.19609500
H	-2.19302000	1.79694000	-1.34664500

X = Ile

0 1

N	-1.47851200	-0.54231500	0.21082400
C	-2.62623400	-0.04578500	-0.33458200
C	-0.16770700	-0.16806900	-0.29462500
H	-0.23582400	-0.05065400	-1.37945800
C	0.77106800	-1.32740500	0.01461600
O	0.53631200	-2.19763800	0.82041800
C	0.31415200	1.19842400	0.29224400
H	-0.54382400	1.85752400	0.12298000
C	1.49979700	1.78905300	-0.49274400
H	2.40248400	1.20047000	-0.30328900
H	1.29240300	1.68999900	-1.56407000
C	0.57201200	1.11215000	1.80143400
H	0.72887500	2.10419800	2.22921900
H	-0.27796400	0.66323000	2.32046900
H	1.45969800	0.51099000	2.02553700
C	1.76955800	3.26508500	-0.17913900
H	2.57355900	3.65291100	-0.81038900
H	0.88048500	3.87628500	-0.36250100

H	2.07064400	3.41673500	0.86065200
O	1.89929100	-1.26860900	-0.70767700
O	-2.62049400	0.79624300	-1.21871000
C	-3.91754100	-0.60399400	0.23935800
H	-1.50277500	-1.30958500	0.86647700
C	2.85957700	-2.31666100	-0.46162900
H	3.18631900	-2.29804300	0.57871600
H	3.69095100	-2.10867400	-1.13058600
H	2.42068400	-3.29032000	-0.68184700
H	-4.51304900	0.22579600	0.62500700
H	-3.76523600	-1.33536400	1.03528600
H	-4.48680900	-1.06605200	-0.56983000

X = (NMe) Ile

0 1

N	1.37042300	-0.47097500	-0.62852200
C	2.05823300	-0.70684800	0.54595400
C	-0.03080300	-0.03918300	-0.56322800
H	-0.35987500	0.00084800	-1.60567700
C	-0.10733200	1.42460700	-0.10630500
O	0.82542100	2.09998100	0.24312800
C	-1.00715700	-1.04277800	0.15422600
H	-0.40611200	-1.93880100	0.32726600
C	-2.15080600	-1.42254800	-0.81216400
H	-2.73943800	-0.52436100	-1.03436400
H	-1.71033100	-1.74772100	-1.76308200
C	-1.53819200	-0.57486100	1.51767500
H	-1.99063300	-1.41388200	2.05077900
H	-0.72235800	-0.19988400	2.13348100
H	-2.29863800	0.20156900	1.40526000
C	-3.07477600	-2.53129800	-0.30044200
H	-3.80507700	-2.80940800	-1.06532300
H	-2.50636800	-3.43069500	-0.04208400
H	-3.63114000	-2.22317800	0.58747700

O	-1.36527000	1.89609800	-0.23253900
O	1.49473200	-0.75645200	1.62566100
C	3.55750800	-0.94513500	0.44685700
C	2.06348200	-0.13361700	-1.87098700
C	-1.55701000	3.27354700	0.14234900
H	-1.31224100	3.41777300	1.19543200
H	-2.60922900	3.48073000	-0.03868400
H	-0.92532100	3.92475100	-0.46332000
H	4.07829900	-0.04710000	0.10416600
H	3.80260600	-1.76209500	-0.23670700
H	3.90657700	-1.19725200	1.44570600
H	3.00342300	-0.67434100	-1.94857900
H	2.27026900	0.94098600	-1.94466900
H	1.44468600	-0.42943900	-2.72103400

X = Phe

0 1

N	-2.40137600	0.04599100	-0.22100600
C	-3.12842300	-1.04534500	0.15195800
C	-0.98897600	0.16255600	0.09271900
H	-0.81474700	-0.23519700	1.09347200
C	-0.63959900	1.64294200	0.06751300
O	-1.24116500	2.46719600	-0.58199200
C	-0.11703300	-0.64609400	-0.91797500
H	-0.58893400	-1.62887500	-0.98272800
H	-0.20068300	-0.17404900	-1.90118000
C	1.33195300	-0.80812000	-0.52299700
C	1.68256800	-1.68373100	0.51161500
H	0.90461400	-2.24632200	1.01831800
C	2.34810800	-0.10543500	-1.17568500
H	2.09424300	0.56890500	-1.98770900

C	3.01283000	-1.84498100	0.88733700
H	3.26657900	-2.52984400	1.68893300
C	3.68179600	-0.26736900	-0.80477900
H	4.45753500	0.28166500	-1.32734800
C	4.01776700	-1.13623400	0.23019900
H	5.05471600	-1.26556700	0.51927000
O	0.42490800	1.91425000	0.82807500
C	-4.59929800	-1.01435100	-0.22453300
O	-2.62994700	-1.98729900	0.74914000
H	-2.82246100	0.82387700	-0.70738000
C	0.88497500	3.28092400	0.81166500
H	0.10645200	3.94629200	1.18673400
H	1.15474800	3.57852200	-0.20217100
H	1.75554600	3.29843300	1.46214200
H	-4.81481200	-1.87674700	-0.85859400
H	-4.90091400	-0.10307600	-0.74433100
H	-5.19262100	-1.12171500	0.68560800

X = (Nme) Phe

0 1

N	-2.09923400	-0.38306600	-0.41508900
C	-2.68999800	-1.30657300	0.41906200
C	-0.75949300	0.07738200	-0.06770800
H	-0.51198600	-0.45974200	0.85142200
C	-0.78983000	1.55799100	0.31482400
O	-1.78739700	2.19750000	0.53769400
C	0.30383800	-0.29051700	-1.14266700
H	-0.06295400	-1.19983100	-1.62840600
H	0.35695300	0.48159000	-1.91448700
C	1.69310400	-0.55906100	-0.60013300
C	1.90659400	-1.60612300	0.30456600
H	1.06634700	-2.20672300	0.63965700
C	2.79187800	0.19621100	-1.01522100

H	2.64293800	1.01372400	-1.71276100
C	3.18398400	-1.88615200	0.78141900
H	3.32898000	-2.70160900	1.48136300
C	4.07276800	-0.08338900	-0.54259400
H	4.91320900	0.51453800	-0.87805900
C	4.27308400	-1.12561300	0.35868000
H	5.26844000	-1.34459600	0.72859200
O	0.45374400	2.06074400	0.40633600
C	-4.12540700	-1.69891100	0.11162000
O	-2.09156700	-1.80512200	1.36181300
C	-2.79728300	0.26159800	-1.52505500
C	0.54922800	3.43090700	0.83886400
H	0.10911700	3.54761500	1.83006200
H	0.03208800	4.08931500	0.13938800
H	1.61350300	3.65243200	0.86272700
H	-4.19786600	-2.22858900	-0.84253200
H	-4.78384400	-0.82838000	0.06295400
H	-4.45823100	-2.36167900	0.90710100
H	-3.47955700	-0.43598100	-2.00824900
H	-2.06719700	0.57065400	-2.27513300
H	-3.34833900	1.14725400	-1.19868900

X = Met

O 1

N	1.98571400	-0.24176300	0.38296400
C	2.74273000	-1.25121200	-0.13734200
C	0.76957900	0.21181400	-0.26786300
H	0.91129800	0.15184000	-1.34991800
C	0.56275600	1.66602400	0.13288200
O	1.05485000	2.17823300	1.11025600
C	-0.44086500	-0.68363500	0.11966900
H	-0.10900400	-1.71383600	-0.01948900
H	-0.64469300	-0.54674300	1.18627800

C	-1.70219600	-0.45614600	-0.71470600
H	-2.07966600	0.56326600	-0.62537300
H	-1.48812200	-0.62892600	-1.77238000
S	-3.07017400	-1.61715300	-0.32846400
C	-3.63666500	-0.95676200	1.27778600
H	-4.50510700	-1.54962600	1.56653700
H	-2.87473900	-1.05758200	2.05146400
H	-3.94040800	0.08781300	1.18501100
O	-0.24950400	2.30979000	-0.71866300
O	2.41630900	-1.85727100	-1.14512500
C	4.01571300	-1.57331700	0.62575800
H	2.29400100	0.28971300	1.18379200
C	-0.53047000	3.68973700	-0.40075300
H	3.97996200	-2.61953400	0.93582100
H	4.17207900	-0.94438200	1.50415200
H	4.86446900	-1.46193200	-0.05189000
H	0.39441200	4.26659400	-0.37732500
H	-1.02435000	3.76397100	0.56881200
H	-1.18408300	4.04110200	-1.19514200

X = (NMe) Met

0 1

N	1.77338300	-0.54556600	0.34908800
C	2.77053400	-0.92272500	-0.52491100
C	0.56611400	0.04431600	-0.21501400
H	0.68803800	-0.03317700	-1.29784500
C	0.50555000	1.53911300	0.11297700
O	1.24091200	2.12646900	0.86479900
C	-0.71896500	-0.72580900	0.19966600
H	-0.44434300	-1.77901300	0.29422000
H	-1.05778400	-0.39878300	1.18769500
C	-1.86222100	-0.61519600	-0.81295500
H	-2.15454000	0.42115200	-0.97872700
H	-1.54846900	-1.02478500	-1.77625300

S	-3.35537700	-1.58175700	-0.35935400
C	-4.06955400	-0.51526100	0.94028000
H	-5.01127600	-0.97772500	1.23755800
H	-3.42322500	-0.45028800	1.81646100
H	-4.27583100	0.48404200	0.55284800
O	-0.49690900	2.13950300	-0.56200100
O	2.67244100	-0.75884100	-1.73171400
C	4.01112600	-1.55880800	0.07964600
C	1.86397200	-0.71991400	1.79682400
C	-0.63848900	3.55756900	-0.34364400
H	3.76869400	-2.38933700	0.74665300
H	4.58559300	-0.82555700	0.65296600
H	4.62496700	-1.91962200	-0.74255400
H	0.27202200	4.07839100	-0.64157700
H	-0.84024300	3.76401000	0.70830100
H	-1.47679800	3.86484400	-0.96447900
H	2.88193500	-0.54895600	2.14256900
H	1.54550800	-1.71905700	2.11676700
H	1.23814700	0.02418100	2.28555600

X = Cys

O 1

N	-1.32839200	-0.84549100	-0.05673400
C	-2.54434200	-0.21860300	-0.15817100
C	-0.08831200	-0.09448700	-0.23472100
H	-0.06351000	0.21637500	-1.28298700
C	1.10671900	-1.05440800	-0.06543200
O	0.97514200	-2.23326900	0.13507800
C	-0.05852000	1.17300700	0.63754400
H	-1.05752600	1.60978900	0.62661800
H	0.19540500	0.93104400	1.66573700
S	1.02980300	2.51626700	0.01250600
H	2.19872000	1.91053300	0.29393600

O	2.29440100	-0.44510100	-0.21363900
O	-2.63905300	0.92946500	-0.55562700
C	-3.74445000	-1.04309700	0.26422600
H	-1.27743500	-1.71284400	0.45284600
C	3.45067500	-1.29091000	-0.04480600
H	-3.99699800	-0.78752100	1.29724400
H	-3.56836500	-2.11898300	0.20346500
H	-4.59153900	-0.77477900	-0.36600900
H	3.43740700	-2.10294600	-0.77251500
H	3.46158200	-1.70732100	0.96258800
H	4.30962500	-0.64295900	-0.20222500

X = (NMe) Cys

0 1

N	-1.35505100	0.14272400	0.39981800
C	-2.33136000	0.24176700	-0.57599000
C	0.03190300	0.27966000	-0.03246300
H	-0.02711200	0.62913500	-1.06728400
C	0.69954100	-1.09993200	-0.08582600
O	0.11041900	-2.14925000	-0.05859100
C	0.80115900	1.33439400	0.79408800
H	0.09003200	2.10894300	1.08276700
H	1.23078100	0.91587500	1.70452400
S	2.11049500	2.25762600	-0.10855800
H	2.91653700	1.20138900	-0.32522000
O	2.04135700	-1.00632200	-0.19356300
O	-2.06667000	0.56087200	-1.72276900
C	-3.76154300	-0.04368800	-0.15149100
C	-1.61765300	-0.39498700	1.73355800
C	2.74897900	-2.25895400	-0.30729800
H	-4.10144100	0.65827000	0.61479900
H	-3.86788300	-1.05534200	0.24788600
H	-4.38891000	0.06310400	-1.03336400

H	2.42064400	-2.79865900	-1.19596500
H	2.57105600	-2.87643700	0.57368400
H	3.80037000	-1.99253900	-0.38505500
H	-2.57360300	-0.03585500	2.11073400
H	-0.84839300	-0.04216000	2.42222700
H	-1.61164200	-1.48876400	1.74038500

X = Ser

0 1

N	-1.20022400	-0.47978200	0.25869500
H	-1.03855700	-1.38955400	0.66590200
C	-0.02073100	0.26111600	-0.14150200
H	-0.12006000	0.58823200	-1.18237200
C	1.16990500	-0.67711600	-0.02522100
O	1.11573600	-1.82255100	0.34893800
C	0.16828000	1.55003800	0.70527300
H	-0.79120200	2.06537100	0.70812800
H	0.41674800	1.26940700	1.73985100
O	1.10753900	2.44565700	0.15105400
H	1.93576600	1.96650400	0.03769900
O	2.32272800	-0.06279400	-0.36404800
C	-2.44663600	-0.12727700	-0.18215200
C	3.51937500	-0.86885600	-0.27195600
O	-2.64398000	0.88260500	-0.83563100
C	-3.56713600	-1.07675400	0.20439100
H	-3.25147200	-1.87827600	0.87470600
H	-3.98255300	-1.51454000	-0.70618600
H	-4.36101100	-0.49997400	0.68152900
H	4.33076200	-0.21711000	-0.58592700
H	3.44008300	-1.73215000	-0.93249600
H	3.66852300	-1.20967400	0.75279900

X = (NMe) Ser

0 1

N	-1.20677400	0.02593600	0.34053300
C	-1.38647800	-0.29458300	1.75409800
C	0.10175400	0.46728700	-0.11299200
H	-0.01172900	0.70926800	-1.17326900
C	1.11144900	-0.67843900	-0.02756800
O	0.86705400	-1.82119000	0.25346300
C	0.57994600	1.76248500	0.59166000
H	-0.27263300	2.44262400	0.63410500
H	0.89225600	1.54716800	1.62436400
O	1.59528800	2.43536000	-0.12330400
H	2.31170900	1.80345000	-0.25487800
O	2.36464000	-0.24281400	-0.32205900
C	-2.21063600	-0.07640100	-0.60192900
C	3.40084400	-1.24821000	-0.30874900
O	-2.01980700	0.18275400	-1.77898400
C	-3.57646800	-0.52570100	-0.11033200
H	-3.93226400	0.07305200	0.73144200
H	-3.55411100	-1.57215600	0.20699600
H	-4.26860800	-0.42723100	-0.94345600
H	4.31654900	-0.72574400	-0.57508600
H	3.17614700	-2.02784900	-1.03667000
H	3.48421800	-1.69434800	0.68271200
H	-2.12293900	-1.08568800	1.87991300
H	-1.70274000	0.57541100	2.34144300
H	-0.44831100	-0.67102900	2.16059500

X = Asp

0 1

N	-1.13282800	-0.81478900	-0.57980300
C	0.09084100	-0.22930400	-0.07878500

H	0.15266200	-0.56104300	0.96432700
C	0.05123900	1.29894400	-0.01304600
O	1.04128500	1.97542700	0.19356100
C	1.33205600	-0.73420700	-0.86545800
H	1.10752000	-1.73214200	-1.23633300
H	1.52176100	-0.08916700	-1.73090700
C	2.64080600	-0.87522600	-0.07425800
O	3.04807500	0.19520500	0.62227400
O	3.27714800	-1.89421400	-0.09414600
O	-1.15861500	1.81689700	-0.18735000
C	-2.07689200	-1.33794700	0.27430600
H	2.43394400	0.94932600	0.49742800
C	-1.26049500	3.25553800	-0.06467100
H	-0.62948700	3.74224400	-0.80826500
H	-0.95245900	3.56690500	0.93323300
H	-2.30952300	3.48214300	-0.23479200
O	-1.89610400	-1.41126400	1.47452300
C	-3.35378000	-1.81696800	-0.38874900
H	-3.27595600	-1.90565900	-1.47416300
H	-4.15698300	-1.11605000	-0.14765100
H	-3.62152400	-2.78487500	0.03542500
H	-1.37713600	-0.66953700	-1.54661800

X = (Nme)Asp

0 1

N	1.09758000	-0.73367900	0.40904700
C	1.52168700	-0.53031000	1.78979700
C	-0.18806300	-0.18875800	-0.00685100
H	-0.27729400	-0.47694700	-1.06076000
C	-0.22054200	1.34015300	-0.01778200
O	-1.25179600	1.98562200	-0.01416300
C	-1.37561700	-0.78825800	0.79330000
H	-1.09578000	-1.79113100	1.11025100
H	-1.58235500	-0.19088000	1.68745300
C	-2.68711500	-0.95435000	0.01458300

O	-3.20958900	0.15831800	-0.52384600
O	-3.23020600	-2.02069200	-0.09218200
O	0.98442900	1.89995500	-0.06936600
C	1.93980400	-1.19347700	-0.59007800
H	-2.64645100	0.93412600	-0.32330200
C	1.01425800	3.34189900	-0.18536100
H	0.53418500	3.79927000	0.67981000
H	0.49916600	3.65385200	-1.09367800
H	2.06822500	3.60276400	-0.22934300
O	1.59071800	-1.21963900	-1.75766800
C	3.31360400	-1.68349300	-0.16894900
H	3.24495600	-2.53608800	0.51190900
H	3.88713400	-0.89851300	0.33050800
H	3.83725400	-1.99232900	-1.07060400
H	0.66209400	-0.63069000	2.45434200
H	1.96439200	0.46061000	1.94112600
H	2.24488200	-1.28724200	2.08480100

X = His

0 1

N	1.86754100	-0.57754300	0.30728000
H	2.58186400	0.03917600	0.65746200
C	0.56550300	-0.00851900	-0.01524300
H	0.31424700	-0.31066800	-1.04024000
C	0.62829600	1.51579400	-0.00601500
O	-0.32299700	2.24373800	0.15847200
C	-0.55430900	-0.55977500	0.91305800
H	-0.31082700	-1.60931400	1.07788800
H	-0.49143700	-0.05489200	1.88388300
C	-1.94658900	-0.51996100	0.36824300
N	-2.66592400	0.63532400	0.13380700
H	-2.27406200	1.56356100	0.21191800
C	-2.81120800	-1.53769300	0.03842800

H	-2.62200400	-2.59941100	0.08984500
C	-3.89481500	0.26472300	-0.32533900
H	-4.65177000	0.98540100	-0.59620400
N	-4.01993600	-1.04172200	-0.39011000
O	1.87025500	1.98558000	-0.21483000
C	2.22133500	-1.81656000	-0.15843800
C	2.00385900	3.42334800	-0.26301400
H	1.67500900	3.86564400	0.67759400
H	1.40688300	3.82822700	-1.08030000
H	3.06189900	3.60831300	-0.43036600
O	1.43805000	-2.52909100	-0.76053600
C	3.64777700	-2.24457100	0.13798000
H	3.62137100	-3.20191800	0.66121400
H	4.20880000	-1.52483300	0.73728700
H	4.16669500	-2.40424100	-0.80962400

X = (NMe) His

0 1

N	1.67468700	-0.63310400	0.37971700
C	2.21152200	-0.34774000	1.70653400
C	0.35719900	-0.10957700	0.03283500
H	0.19302700	-0.42593200	-1.00199200
C	0.35778000	1.42147100	0.02123300
O	-0.55495900	2.12136800	0.40427200
C	-0.76926800	-0.70139400	0.91873900
H	-0.52291000	-1.75490400	1.06796800
H	-0.74928500	-0.22531000	1.90554800
C	-2.15064000	-0.65156200	0.34552100
N	-2.88063900	0.50803500	0.17972500
H	-2.50757200	1.43153200	0.35306200
C	-2.99249300	-1.65349800	-0.07791700
H	-2.79316400	-2.71468500	-0.09648800
C	-4.09408600	0.15684100	-0.33307700
H	-4.85570700	0.88556200	-0.56641600

N	-4.19828000	-1.14262800	-0.49729400
O	1.48988100	1.91791300	-0.49068500
C	2.32855300	-1.41271100	-0.55378000
C	1.55415700	3.35337400	-0.61413000
H	1.45486500	3.82475900	0.36437300
H	0.75896400	3.71285800	-1.26815000
H	2.52984700	3.56131000	-1.04598100
O	1.84780800	-1.64801600	-1.64947600
C	3.68540900	-1.96720500	-0.15309300
H	3.64896400	-2.50524700	0.79717000
H	4.42300600	-1.16528100	-0.05570800
H	4.00604000	-2.64500800	-0.94081700
H	1.75130500	0.56224700	2.09511200
H	3.28601700	-0.17203000	1.66467800
H	2.01559200	-1.15410500	2.42251400