

SUPPORTING INFORMATION

Stereochemical analysis of natural products: bisindole alkaloids of *Strychnos-Strychnos* type

**Dmitry A. Grigoriev,^a Valentin A. Semenov,^a Luc Angenot,^b
and Leonid B. Krivdin ^{*a}**

^a *A.E. Favorsky Irkutsk Institute of Chemistry, Siberian Branch of the Russian Academy of Sciences, 664033 Irkutsk, Russia.*

^{*} *Correspondence: semenov@irioch.irk.ru*

^b *Laboratory of Pharmacognosy, Center of Interdisciplinary Research on Medicines, Faculty of Medicine, University of Liège, Liège, Belgium.*

TABLE OF CONTENTS

Figure S1. Correlation plot of calculated vs. experimental ^1H and ^{13}C NMR chemical shifts of strychnobiline (**6**), ppm. Points that are out the region of mathematical expectation are shown in red. S4

Figure S2. Spatial arrangement of principal non-valent intramolecular interactions and (3,–1) bond critical points in the second subunit of panganensine X (**16**). Bond critical points are shown as green spheres with corresponding numerical values of electron density in a.u. S5

Cartesian coordinates (Angstroms) of main conformers of **1-17**, optimized at the M06-2X/pecG-2 level in the liquid phase of particular solvent, modulated within the IEF-PCM scheme: S6

Compound: 1-boat	S6
Compound: 1-half-chair	S8
Compound: 2-chair	S10
Compound: 2-boat	S12
Compound: 3	S14
Compound: 4	S16
Compound: 5-twist-boat	S18
Compound: 5-true-chair	S20
Compound: 6a	S22
Compound: 6b	S25
Compound: 7a	S28
Compound: 7b	S31
Compound: 7c	S34
Compound: 7d	S37
Compound: 8a	S40
Compound: 8b	S43
Compound: 8c	S46
Compound: 9a	S49
Compound: 9b	S52
Compound: 10a	S55
Compound: 10b	S58
Compound: 11-tub	S61
Compound: 11-crown	S64
Compound: 12-boat-like	S67
Compound: 12-chair-like	S70

Compound: 13-boat-like	S73
Compound: 13-chair-like	S76
Compound: 14a	S79
Compound: 14b	S82
Compound: 14c	S85
Compound: 14d	S88
Compound: 15a	S91
Compound: 15b	S94
Compound: 15c	S97
Compound: 15d	S100
Compound: 16a	S103
Compound: 16b	S106
Compound: 16c	S109
Compound: 16d	S112
Compound: 16e	S115
Compound: 16f	S118
Compound: 17a	S121
Compound: 17b	S124
Compound: 17c	S127
Compound: 17d	S130

Figure S1. Correlation plot of calculated vs. experimental ^1H and ^{13}C NMR chemical shifts of strychnobiline (**6**), ppm. Points that are out the region of mathematical expectation are shown in red.

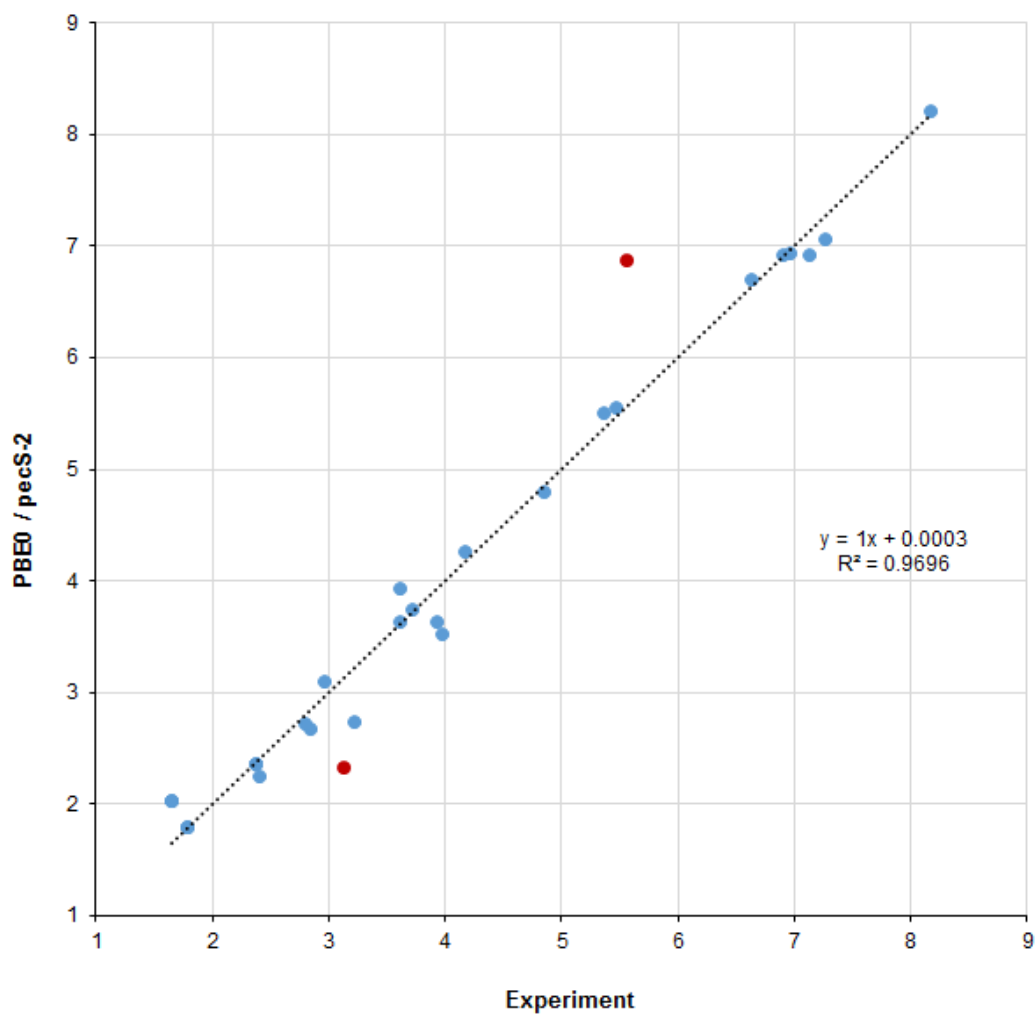
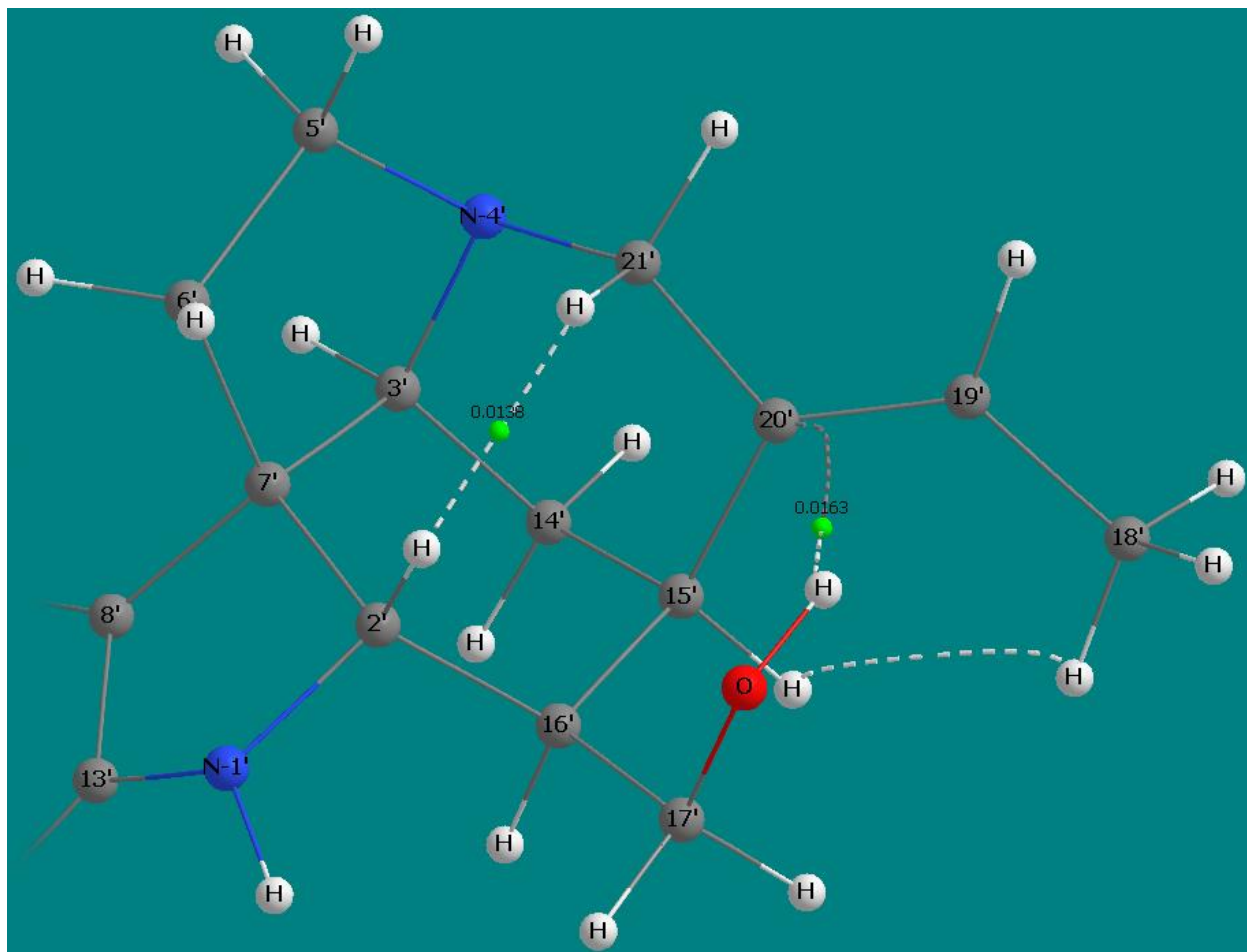
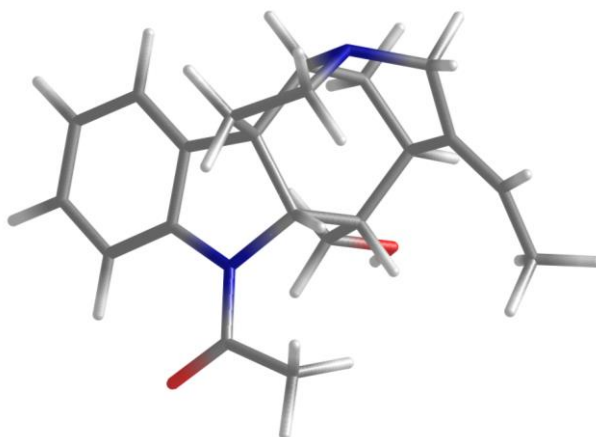


Figure S2. Spatial arrangement of principal non-valent intramolecular interactions and (3,-1) bond critical points in the second subunit of panganensine X (**16**). Bond critical points are shown as green spheres with corresponding numerical values of electron density in a.u.



Cartesian coordinates (Angstroms) of main conformers of **1-17**, optimized at the M06-2X/pecG-2 level in the liquid phase of particular solvent, modulated within the IEF-PCM scheme:

Compound: **1-boat**

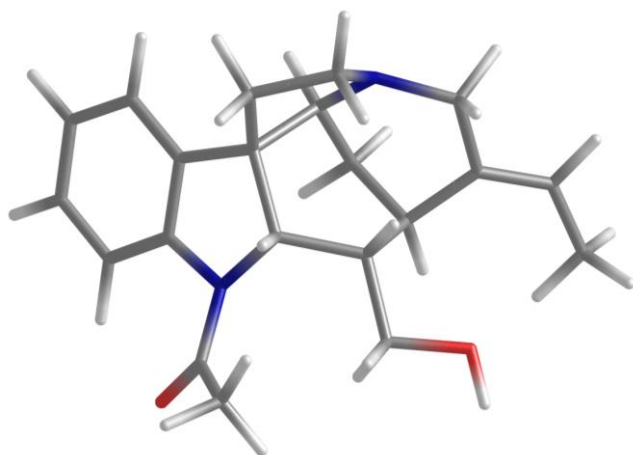


symmetry c1

N	-1.227740000	1.011492000	-0.711066000
C	0.083771000	0.367406000	-0.495553000
C	0.714856000	-2.038631000	0.263244000
N	1.788334000	-2.295945000	-0.725235000
C	1.301618000	-1.924676000	-2.060965000
C	-0.199231000	-1.715463000	-1.890214000
C	-0.291552000	-1.137884000	-0.467471000
C	-1.705116000	-1.093829000	0.044949000
C	-2.484864000	-2.087774000	0.598549000
C	-3.806624000	-1.799691000	0.937547000
C	-4.324873000	-0.534605000	0.707144000
C	-3.550595000	0.478883000	0.143815000
C	-2.236237000	0.179177000	-0.175867000
C	1.266524000	-1.436792000	1.544115000
C	1.899185000	-0.085013000	1.216052000
C	0.795404000	0.897040000	0.767947000
C	-0.154309000	1.244070000	1.910741000
C	3.861023000	2.086430000	0.253855000
C	3.782575000	0.685648000	-0.275502000
C	2.967381000	-0.277709000	0.146667000
C	3.075102000	-1.691693000	-0.380669000
C	-1.435097000	2.220604000	-1.308630000
C	-0.219687000	2.896405000	-1.896838000
H	0.728355000	0.569854000	-1.346875000

H	1.779287000	-0.999666000	-2.403947000
H	1.530828000	-2.699005000	-2.792218000
H	-0.731518000	-2.666164000	-1.921564000
H	-0.632053000	-1.055099000	-2.640225000
H	-2.081475000	-3.077321000	0.765664000
H	-4.428376000	-2.565291000	1.378108000
H	-5.350964000	-0.321774000	0.971110000
H	-3.954161000	1.460042000	-0.034774000
H	0.209721000	-2.981517000	0.488283000
H	1.997746000	-2.112327000	1.985580000
H	0.464825000	-1.331314000	2.272914000
H	2.356865000	0.336044000	2.110343000
H	1.279812000	1.835613000	0.497198000
H	-0.868409000	1.997848000	1.572257000
H	-0.727963000	0.375970000	2.242554000
H	3.341201000	2.198072000	1.203190000
H	4.901454000	2.373617000	0.401927000
H	3.435431000	2.804318000	-0.450561000
H	4.491969000	0.436265000	-1.058503000
H	3.716414000	-1.723973000	-1.259700000
H	3.559622000	-2.312208000	0.376685000
H	0.053809000	2.044033000	3.677872000
H	0.573373000	3.015449000	-1.162170000
H	-0.523669000	3.869784000	-2.263601000
H	0.175185000	2.307301000	-2.723925000
O	0.636327000	1.757460000	2.972030000
O	-2.543450000	2.720189000	-1.388155000

Compound: **1-half-chair**

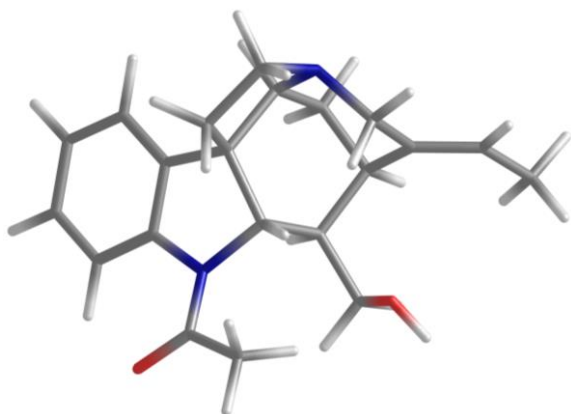


symmetry c1

N	1.383857000	1.146436000	0.149826000
C	0.333257000	0.403195000	0.898043000
C	-0.314157000	-1.842003000	-0.205441000
N	-1.400792000	-2.223000000	0.696444000
C	-0.925563000	-2.187536000	2.078172000
C	0.580144000	-1.933713000	1.975209000
C	0.702280000	-1.105459000	0.697681000
C	2.031260000	-1.056088000	0.012231000
C	2.859493000	-2.108227000	-0.327829000
C	3.994691000	-1.861198000	-1.093300000
C	4.266471000	-0.571517000	-1.524108000
C	3.436996000	0.497105000	-1.194404000
C	2.325529000	0.238459000	-0.402614000
C	-0.730164000	-0.956086000	-1.358085000
C	-1.677074000	0.099743000	-0.793443000
C	-1.133439000	0.739771000	0.516987000
C	-1.439994000	2.229699000	0.518226000
C	-4.521019000	0.676619000	-2.006738000
C	-4.133513000	-0.437636000	-1.086297000
C	-2.951461000	-0.654415000	-0.521834000
C	-2.776301000	-1.801018000	0.466755000
C	1.756353000	2.458420000	0.374538000
C	1.276146000	3.188037000	1.607878000
H	0.445090000	0.632972000	1.958733000
H	-1.412436000	-1.375790000	2.634472000
H	-1.144091000	-3.113067000	2.612753000
H	1.112949000	-2.874847000	1.839128000
H	0.986957000	-1.437843000	2.853772000
H	2.624695000	-3.114254000	-0.005372000

H	4.653550000	-2.673743000	-1.362351000
H	5.139224000	-0.382550000	-2.133028000
H	3.653265000	1.491889000	-1.538760000
H	0.191912000	-2.735472000	-0.585419000
H	-1.239093000	-1.519845000	-2.138592000
H	0.163212000	-0.517558000	-1.804920000
H	-1.843992000	0.881512000	-1.528624000
H	-1.714903000	0.331373000	1.346090000
H	-1.210611000	2.664797000	1.490339000
H	-0.843036000	2.737826000	-0.247010000
H	-3.701350000	1.361005000	-2.200434000
H	-4.884137000	0.287122000	-2.958889000
H	-5.336119000	1.255904000	-1.569985000
H	-4.932192000	-1.132488000	-0.838704000
H	-3.177898000	-1.479705000	1.433329000
H	-3.401997000	-2.638751000	0.148599000
H	-3.020971000	3.320636000	0.185500000
H	0.652969000	4.028310000	1.312270000
H	2.173451000	3.594798000	2.068342000
H	0.747836000	2.583347000	2.333016000
O	-2.822598000	2.384186000	0.243487000
O	2.532179000	3.023746000	-0.370726000

Compound: **2-chair**

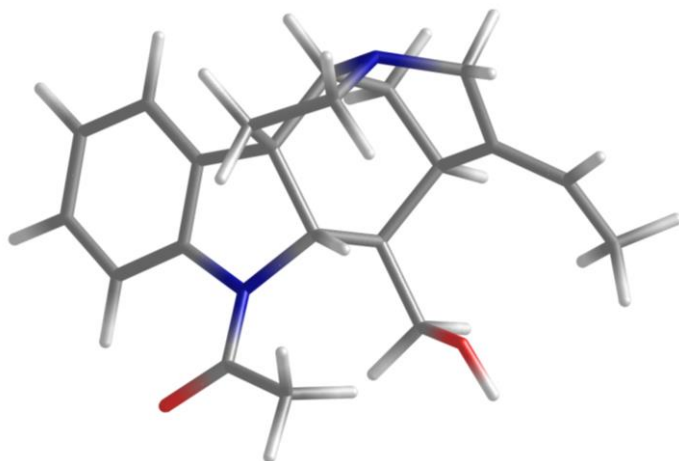


symmetry c1

N	1.457300000	1.157812000	0.163341000
C	0.134672000	0.511800000	0.315775000
C	-0.562996000	-1.989553000	0.071186000
N	-1.556427000	-2.053621000	1.143615000
C	-0.724261000	-2.136756000	2.347757000
C	0.576221000	-1.324624000	2.064769000
C	0.502748000	-0.983398000	0.554865000
C	1.827774000	-1.076217000	-0.160195000
C	2.529356000	-2.190385000	-0.577627000
C	3.765575000	-2.019441000	-1.197124000
C	4.281995000	-0.745517000	-1.384793000
C	3.587814000	0.386648000	-0.964989000
C	2.358666000	0.198026000	-0.353845000
C	-1.160198000	-1.672198000	-1.278430000
C	-1.821020000	-0.297068000	-1.195065000
C	-0.711776000	0.751976000	-0.953302000
C	-1.234641000	2.176496000	-1.019473000
C	-4.834039000	0.428279000	-1.597161000
C	-4.197695000	-0.149973000	-0.371752000
C	-2.910292000	-0.403378000	-0.153891000
C	-2.458003000	-0.888500000	1.199982000
C	1.855766000	2.355786000	0.694430000
C	0.867682000	3.092246000	1.564067000
H	-0.366669000	0.936595000	1.177034000
H	-1.274208000	-1.774698000	3.213171000
H	-0.470304000	-3.180496000	2.527580000
H	1.455468000	-1.929273000	2.276194000
H	0.651127000	-0.422140000	2.669727000
H	2.132144000	-3.184569000	-0.422183000
H	4.322788000	-2.881870000	-1.532846000
H	5.240786000	-0.623256000	-1.868072000
H	3.988849000	1.375280000	-1.105257000

H	-0.082052000	-2.970957000	0.040556000
H	-1.892169000	-2.433312000	-1.545392000
H	-0.373721000	-1.675782000	-2.034804000
H	-2.264072000	-0.057838000	-2.159116000
H	-0.027676000	0.644113000	-1.801087000
H	-0.396555000	2.878114000	-1.084459000
H	-1.833955000	2.291853000	-1.925687000
H	-4.120815000	0.659124000	-2.382950000
H	-5.580536000	-0.253411000	-2.006351000
H	-5.358880000	1.350587000	-1.343536000
H	-4.884457000	-0.350645000	0.444797000
H	-1.983546000	-0.047093000	1.723009000
H	-3.325933000	-1.165851000	1.796687000
H	-2.515891000	3.254144000	-0.006826000
H	1.257442000	4.089245000	1.735778000
H	0.791389000	2.575517000	2.522027000
H	-0.130769000	3.141510000	1.140932000
O	-2.018143000	2.446470000	0.133422000
O	2.980145000	2.788565000	0.512988000

Compound: **2-boat**

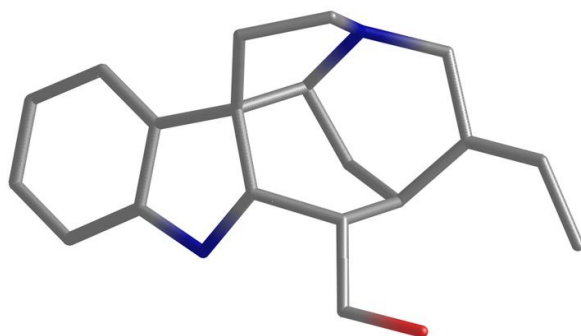


symmetry c1

N	1.344993000	1.157927000	0.226765000
C	0.066904000	0.412658000	0.268723000
C	-0.430260000	-2.128376000	0.034714000
N	-1.435750000	-2.218668000	1.109651000
C	-0.916121000	-1.559201000	2.312495000
C	0.564896000	-1.330113000	2.018446000
C	0.544882000	-1.045442000	0.509438000
C	1.902854000	-1.032531000	-0.137731000
C	2.706268000	-2.078671000	-0.545974000
C	3.960255000	-1.796454000	-1.084610000
C	4.390183000	-0.483037000	-1.201859000
C	3.590717000	0.581737000	-0.791028000
C	2.346729000	0.283562000	-0.261194000
C	-1.058286000	-1.847875000	-1.319331000
C	-1.787132000	-0.504413000	-1.255324000
C	-0.697811000	0.580784000	-1.053000000
C	-1.151906000	2.012183000	-1.274244000
C	-4.475579000	1.115725000	-1.179328000
C	-4.029204000	0.069262000	-0.210251000
C	-2.897944000	-0.630202000	-0.215308000
C	-2.782184000	-1.833378000	0.714786000
C	1.633278000	2.346056000	0.846773000
C	0.542531000	2.975866000	1.672678000
H	-0.547420000	0.772094000	1.090137000
H	-1.424543000	-0.603849000	2.487678000
H	-1.070610000	-2.175063000	3.198385000
H	1.144836000	-2.233453000	2.208798000
H	0.999074000	-0.515057000	2.596034000
H	2.373130000	-3.102821000	-0.445553000
H	4.598883000	-2.603862000	-1.412246000

H	5.363751000	-0.275820000	-1.622997000
H	3.926082000	1.600635000	-0.877692000
H	0.126113000	-3.069217000	-0.016151000
H	-1.742298000	-2.653491000	-1.584777000
H	-0.275984000	-1.825005000	-2.078600000
H	-2.244225000	-0.296784000	-2.224366000
H	0.028437000	0.398768000	-1.853022000
H	-0.270080000	2.658999000	-1.328732000
H	-1.665270000	2.077058000	-2.237475000
H	-3.759504000	1.274322000	-1.980656000
H	-5.429081000	0.825029000	-1.623587000
H	-4.633893000	2.070043000	-0.677574000
H	-4.755678000	-0.179480000	0.559089000
H	-3.369638000	-1.665550000	1.616075000
H	-3.244676000	-2.684097000	0.206615000
H	-2.358796000	3.299409000	-0.445369000
H	0.885962000	3.956279000	1.982400000
H	0.362997000	2.366226000	2.559493000
H	-0.397119000	3.051508000	1.133284000
O	-2.003702000	2.436356000	-0.223318000
O	2.738255000	2.852335000	0.763652000

Compound: **3**

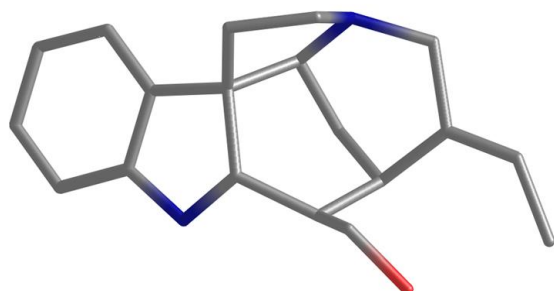


symmetry c1

N	1.228431000	1.691614000	0.099331000
C	0.375051000	0.740456000	0.843438000
C	0.223731000	-1.339116000	-0.668249000
N	-0.725292000	-2.268347000	-0.018981000
C	-0.585294000	-2.196883000	1.433183000
C	0.828363000	-1.669680000	1.627138000
C	0.979652000	-0.651828000	0.495388000
C	2.391493000	-0.283654000	0.118417000
C	3.499437000	-1.084542000	-0.074446000
C	4.705808000	-0.499429000	-0.455682000
C	4.780910000	0.874685000	-0.645689000
C	3.666862000	1.689293000	-0.469567000
C	2.473570000	1.092254000	-0.088535000
C	-0.474783000	-0.317671000	-1.562489000
C	-1.633253000	0.308722000	-0.778005000
C	-1.120354000	0.942020000	0.555673000
C	-1.420471000	2.431140000	0.630782000
C	-4.774311000	0.646720000	-0.642448000
C	-3.984266000	-0.611517000	-0.465186000
C	-2.667295000	-0.781570000	-0.546667000
C	-2.086737000	-2.188491000	-0.513667000
H	1.250367000	2.630555000	0.468328000
H	0.523936000	0.901852000	1.918123000
H	-1.319039000	-1.518956000	1.887047000
H	-0.732154000	-3.179308000	1.882627000
H	1.544980000	-2.478376000	1.480792000
H	1.000187000	-1.234119000	2.609189000
H	3.437010000	-2.154810000	0.076441000
H	5.583159000	-1.112751000	-0.599545000
H	5.720995000	1.322678000	-0.936147000
H	3.730355000	2.757383000	-0.624172000
H	0.947841000	-1.909156000	-1.256523000
H	-0.857782000	-0.796502000	-2.463631000

H	0.247181000	0.434064000	-1.877284000
H	-2.087456000	1.105262000	-1.366798000
H	-1.665794000	0.488920000	1.383916000
H	-0.913412000	2.863637000	1.501552000
H	-1.040707000	2.926525000	-0.267155000
H	-4.161629000	1.475794000	-0.978051000
H	-5.578539000	0.481352000	-1.360418000
H	-5.239967000	0.951037000	0.296359000
H	-4.577104000	-1.503915000	-0.278731000
H	-2.716965000	-2.844762000	0.085982000
H	-2.101597000	-2.591771000	-1.529873000
H	-3.024917000	3.541687000	0.653741000
O	-2.819948000	2.609420000	0.746432000

Compound: **4**

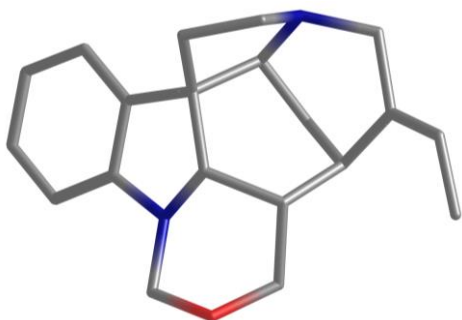


symmetry c1

N	-1.368461000	-1.787342000	-0.003501000
C	-0.409587000	-0.904922000	0.693007000
C	-0.244575000	1.307759000	-0.634610000
N	0.730936000	2.151687000	0.088318000
C	0.604010000	1.934845000	1.526864000
C	-0.821253000	1.438858000	1.683646000
C	-0.996771000	0.527951000	0.466933000
C	-2.429086000	0.233010000	0.100593000
C	-3.498894000	1.092702000	-0.050062000
C	-4.744212000	0.577330000	-0.406468000
C	-4.895861000	-0.788220000	-0.612343000
C	-3.821137000	-1.661566000	-0.479838000
C	-2.587694000	-1.131963000	-0.126696000
C	0.410095000	0.363363000	-1.638386000
C	1.575586000	-0.364479000	-0.960045000
C	1.028831000	-1.240179000	0.219829000
C	1.992586000	-1.426740000	1.389868000
C	4.705673000	-0.741096000	-1.046926000
C	3.943891000	0.484415000	-0.651306000
C	2.627282000	0.676393000	-0.616667000
C	2.086267000	2.085576000	-0.420109000
H	-1.394886000	-2.741440000	0.323360000
H	-0.466777000	-1.099555000	1.770003000
H	1.312055000	1.183258000	1.896780000
H	0.797523000	2.857568000	2.074125000
H	-1.514358000	2.277151000	1.607883000
H	-1.006850000	0.924831000	2.624290000
H	-3.377156000	2.155838000	0.115796000
H	-5.591333000	1.238152000	-0.516599000
H	-5.865446000	-1.182854000	-0.882545000
H	-3.943718000	-2.722103000	-0.649774000
H	-0.964192000	1.946862000	-1.153001000
H	0.775479000	0.917917000	-2.502538000
H	-0.338741000	-0.342760000	-1.999083000

H	2.020949000	-1.054833000	-1.672449000
H	0.920794000	-2.242320000	-0.204100000
H	1.463484000	-1.915556000	2.213458000
H	2.379748000	-0.479918000	1.756732000
H	4.058731000	-1.548684000	-1.374969000
H	5.400374000	-0.495401000	-1.851938000
H	5.295158000	-1.118207000	-0.211968000
H	4.563573000	1.346663000	-0.414889000
H	2.736826000	2.657342000	0.241500000
H	2.110083000	2.594715000	-1.387642000
H	2.850122000	-3.046758000	0.733254000
O	3.136290000	-2.179819000	1.030861000

Compound: **5-twist-boat**

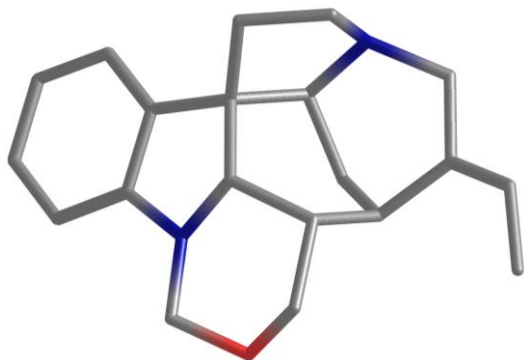


symmetry c1

N	1.242908000	1.368505000	0.093059000
C	0.185313000	0.574456000	0.728004000
C	-0.208887000	-1.552790000	-0.698182000
N	-1.285217000	-2.319212000	-0.021809000
C	-1.173793000	-2.121695000	1.424107000
C	0.302308000	-1.831394000	1.620560000
C	0.608610000	-0.902313000	0.444322000
C	2.072574000	-0.748864000	0.108050000
C	3.047133000	-1.707391000	-0.063384000
C	4.347989000	-1.311056000	-0.383484000
C	4.647780000	0.035823000	-0.524405000
C	3.671062000	1.017206000	-0.363608000
C	2.380654000	0.603882000	-0.061154000
C	-0.751813000	-0.506687000	-1.667108000
C	-1.818783000	0.321459000	-0.949016000
C	-1.180581000	1.106150000	0.227610000
C	-0.957166000	2.565611000	-0.196319000
C	-4.549807000	1.295102000	0.029545000
C	-4.127205000	-0.139103000	-0.064081000
C	-2.955205000	-0.585639000	-0.504157000
C	-2.619413000	-2.057141000	-0.545607000
C	1.282478000	2.764602000	0.446423000
H	0.230608000	0.730743000	1.813557000
H	0.443674000	-2.245341000	-1.234860000
H	-1.775500000	-1.268680000	1.770583000
H	-1.515315000	-3.007009000	1.959625000
H	0.877707000	-2.751937000	1.515834000
H	0.538988000	-1.382499000	2.582489000
H	2.812076000	-2.757494000	0.056781000
H	5.122029000	-2.053098000	-0.512390000
H	5.659348000	0.335025000	-0.761103000
H	3.914903000	2.064087000	-0.474975000
H	-1.174709000	-0.983474000	-2.550355000
H	0.070499000	0.124975000	-2.006692000

H	-2.224733000	1.056428000	-1.647802000
H	-1.871201000	1.100579000	1.070327000
H	-0.593874000	2.604241000	-1.228597000
H	-1.885325000	3.129687000	-0.137388000
H	-3.880417000	1.958296000	-0.513805000
H	-5.554445000	1.429597000	-0.370178000
H	-4.575847000	1.627761000	1.069297000
H	-4.854564000	-0.871726000	0.272010000
H	-3.344383000	-2.631593000	0.030317000
H	-2.665686000	-2.427981000	-1.571913000
H	1.832021000	2.944599000	1.377901000
H	1.756595000	3.324456000	-0.367575000
O	-0.033221000	3.210500000	0.663934000

Compound: **5-true-chair**

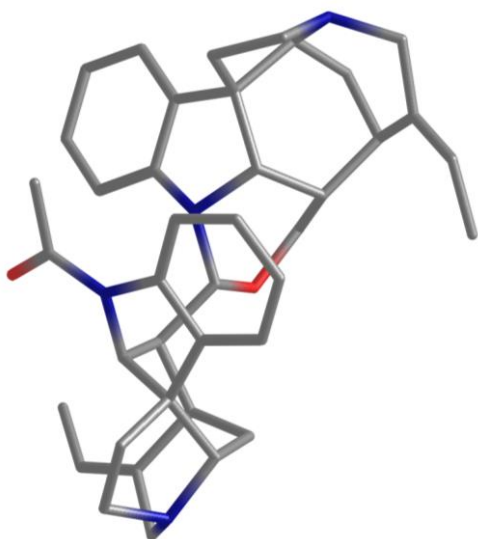


symmetry c1

N	1.163440000	1.358756000	0.142459000
C	0.235006000	0.495196000	0.871716000
C	-0.087347000	-1.467125000	-0.753100000
N	-1.153947000	-2.327052000	-0.189014000
C	-1.057480000	-2.338968000	1.270302000
C	0.398953000	-1.987105000	1.536441000
C	0.698791000	-0.932018000	0.473645000
C	2.155238000	-0.681264000	0.154345000
C	3.195396000	-1.566384000	-0.019739000
C	4.456874000	-1.080743000	-0.374482000
C	4.648049000	0.280890000	-0.554174000
C	3.604813000	1.190748000	-0.388827000
C	2.357473000	0.692636000	-0.039216000
C	-0.655963000	-0.334366000	-1.602747000
C	-1.742939000	0.385115000	-0.797823000
C	-1.205251000	0.915880000	0.566238000
C	-1.275376000	2.440503000	0.698262000
C	-4.631199000	1.165198000	-0.080897000
C	-4.121424000	-0.236533000	-0.231415000
C	-2.885308000	-0.592956000	-0.566100000
C	-2.486439000	-2.048935000	-0.706189000
C	0.986124000	2.769508000	0.282981000
H	0.405848000	0.623619000	1.952900000
H	0.591609000	-2.076546000	-1.354166000
H	-1.723224000	-1.599200000	1.733822000
H	-1.333787000	-3.316433000	1.665304000
H	1.026084000	-2.862189000	1.363827000
H	0.581996000	-1.628946000	2.547325000
H	3.040760000	-2.628998000	0.117662000
H	5.282634000	-1.764441000	-0.504049000
H	5.627825000	0.650968000	-0.821991000
H	3.772817000	2.249351000	-0.524048000
H	-1.086605000	-0.731202000	-2.521576000

H	0.143377000	0.344747000	-1.889471000
H	-2.104241000	1.237926000	-1.373330000
H	-1.841776000	0.526034000	1.360678000
H	-2.250987000	2.810274000	0.393118000
H	-1.113616000	2.719216000	1.747204000
H	-4.040241000	1.878269000	-0.652102000
H	-5.664144000	1.239825000	-0.416069000
H	-4.612272000	1.482242000	0.964460000
H	-4.838220000	-1.028055000	-0.036130000
H	-3.203626000	-2.689366000	-0.193930000
H	-2.510393000	-2.335511000	-1.759943000
H	1.142382000	3.094342000	1.324868000
H	1.677533000	3.296863000	-0.368770000
O	-0.320517000	3.108703000	-0.108127000

Compound: **6a**



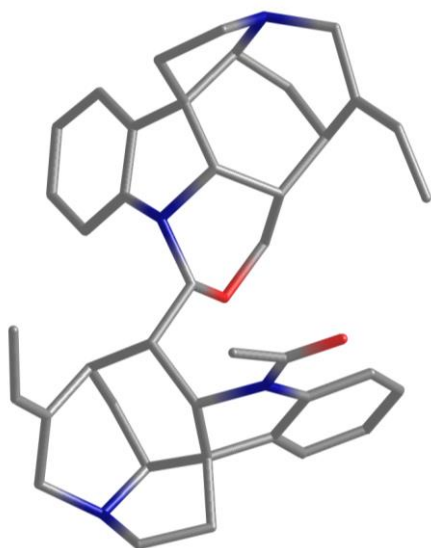
symmetry c1

N	0.583381000	0.767489000	0.012289000
C	1.826811000	-0.045311000	-0.127485000
C	4.327173000	0.701488000	-0.239351000
N	4.959404000	-0.441808000	0.459057000
C	4.175191000	-0.747575000	1.662108000
C	3.295208000	0.478103000	1.867389000
C	2.947427000	0.876128000	0.423616000
C	2.330810000	2.240823000	0.296969000
C	2.927169000	3.478389000	0.431323000
C	2.153615000	4.628846000	0.293468000
C	0.797260000	4.511489000	0.032876000
C	0.181826000	3.268271000	-0.089593000
C	0.958841000	2.123483000	0.045521000
C	4.262566000	0.487505000	-1.741394000
C	3.424421000	-0.758984000	-2.022309000
C	1.969304000	-0.509334000	-1.598579000
C	1.255110000	0.476670000	-2.518261000
C	2.525027000	-3.692206000	-2.339607000
C	3.600167000	-3.202583000	-1.416575000
C	4.028715000	-1.949891000	-1.285489000
C	5.198954000	-1.603847000	-0.393226000
N	-1.633343000	0.197118000	1.833213000
C	-2.534462000	0.094639000	0.673713000
C	-3.423696000	-1.921760000	-0.689149000
N	-4.863791000	-1.560327000	-0.680136000
C	-5.263905000	-1.235141000	0.696691000
C	-4.093072000	-1.675348000	1.565231000
C	-2.879810000	-1.409652000	0.654789000
C	-1.628851000	-2.009305000	1.237771000

C	-1.141780000	-3.296611000	1.162152000
C	0.012197000	-3.632234000	1.870599000
C	0.633186000	-2.680242000	2.661651000
C	0.149779000	-1.374601000	2.746878000
C	-0.973789000	-1.036395000	2.008233000
C	-2.728849000	-1.341487000	-1.910524000
C	-2.779001000	0.185644000	-1.820105000
C	-1.908478000	0.650786000	-0.624790000
C	-0.445047000	0.245670000	-0.867084000
C	-3.742072000	3.104256000	-1.771803000
C	-4.623882000	1.897105000	-1.647334000
C	-4.232006000	0.626646000	-1.688088000
C	-5.222696000	-0.514551000	-1.641426000
C	-1.424851000	1.432961000	2.379194000
C	-0.397525000	1.585883000	3.462965000
H	1.727027000	-0.931539000	0.501117000
H	4.904767000	1.604870000	-0.029363000
H	4.825258000	-0.945624000	2.513818000
H	3.550230000	-1.636587000	1.507215000
H	3.856024000	1.286641000	2.337698000
H	2.414615000	0.269191000	2.469233000
H	3.986457000	3.556516000	0.638493000
H	2.607397000	5.604248000	0.388734000
H	0.193496000	5.401575000	-0.074780000
H	-0.879188000	3.224404000	-0.263145000
H	5.267496000	0.379912000	-2.147108000
H	3.829561000	1.370224000	-2.209998000
H	3.423039000	-0.968933000	-3.094809000
H	1.437417000	-1.456094000	-1.691242000
H	1.685582000	1.476935000	-2.435293000
H	1.339569000	0.155623000	-3.556287000
H	2.842411000	-4.609346000	-2.834272000
H	1.609397000	-3.928261000	-1.792985000
H	2.277233000	-2.963352000	-3.108746000
H	4.089929000	-3.964968000	-0.818873000
H	5.457180000	-2.450116000	0.241304000
H	6.074586000	-1.405253000	-1.015510000
H	-3.416062000	0.695542000	0.875748000
H	-3.335005000	-3.011341000	-0.693936000
H	-6.191028000	-1.740369000	0.965508000
H	-5.432802000	-0.158582000	0.805345000
H	-4.144578000	-2.743240000	1.778797000
H	-4.031437000	-1.138004000	2.510042000
H	-1.650640000	-4.039523000	0.562720000

H	0.412120000	-4.633790000	1.812593000
H	1.518446000	-2.942783000	3.223589000
H	0.667487000	-0.666510000	3.368057000
H	-1.704391000	-1.703858000	-1.969940000
H	-3.226099000	-1.692611000	-2.813354000
H	-2.358466000	0.622804000	-2.722599000
H	-1.965850000	1.729704000	-0.559388000
H	-0.373956000	-0.834466000	-0.726474000
H	-2.795741000	2.870187000	-2.257480000
H	-4.238526000	3.878274000	-2.354753000
H	-3.520076000	3.535369000	-0.792435000
H	-5.685005000	2.093055000	-1.530702000
H	-5.299416000	-0.961925000	-2.634666000
H	-6.216875000	-0.148324000	-1.392078000
H	0.596296000	1.482712000	3.025179000
H	-0.498049000	2.583151000	3.875758000
H	-0.517797000	0.843325000	4.247847000
O	-0.137996000	0.551505000	-2.222696000
O	-2.068692000	2.389429000	1.979528000

Compound: **6b**



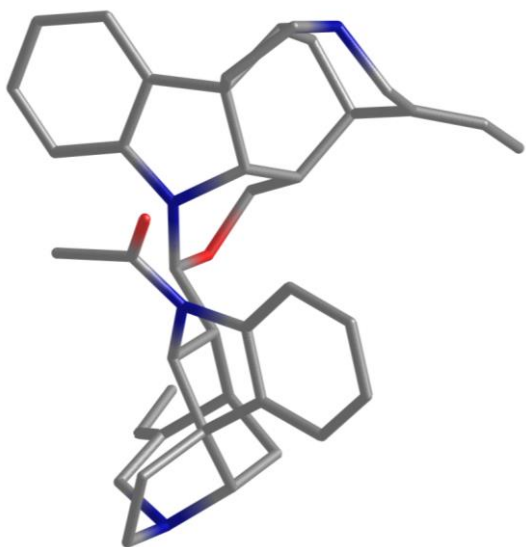
symmetry c1

N	-0.938613000	-1.222294000	0.389905000
C	-2.159991000	-0.371284000	0.533583000
C	-4.578170000	-0.726536000	-0.365719000
N	-5.335223000	-0.108816000	0.743072000
C	-4.785311000	-0.596688000	2.015136000
C	-3.927232000	-1.800162000	1.632637000
C	-3.333745000	-1.352296000	0.289242000
C	-2.675197000	-2.421760000	-0.533860000
C	-3.261971000	-3.425057000	-1.277730000
C	-2.462218000	-4.253759000	-2.062052000
C	-1.095801000	-4.032794000	-2.107430000
C	-0.494076000	-3.030695000	-1.348370000
C	-1.286522000	-2.249809000	-0.516770000
C	-4.244228000	0.262937000	-1.468530000
C	-3.399341000	1.392157000	-0.882516000
C	-2.036524000	0.852057000	-0.420420000
C	-1.098346000	0.548776000	-1.594153000
C	-2.549128000	3.974002000	0.547575000
C	-3.745190000	3.140373000	0.897707000
C	-4.153823000	2.037253000	0.275848000
C	-5.444907000	1.345109000	0.653914000
N	1.883221000	1.787273000	0.913176000
C	2.556423000	0.480995000	0.772852000
C	3.860946000	-0.577665000	-1.210938000
N	5.040229000	-1.088989000	-0.468802000
C	5.538730000	-0.032668000	0.422095000
C	4.827962000	1.233152000	-0.034967000
C	3.449350000	0.707585000	-0.476338000

C	2.683861000	1.760244000	-1.230012000
C	2.770779000	2.153869000	-2.546708000
C	1.973174000	3.209652000	-2.991484000
C	1.122722000	3.857912000	-2.110573000
C	1.031035000	3.474920000	-0.771555000
C	1.817530000	2.414917000	-0.353761000
C	2.755029000	-1.617675000	-1.300474000
C	2.284385000	-1.949858000	0.117941000
C	1.569689000	-0.727962000	0.715376000
C	0.190248000	-0.326797000	0.174485000
C	2.131209000	-3.046145000	3.000799000
C	3.388499000	-2.835718000	2.210340000
C	3.479332000	-2.391650000	0.959266000
C	4.799451000	-2.352563000	0.225242000
C	1.348503000	2.285650000	2.065372000
C	1.583847000	1.485713000	3.324151000
H	-2.197447000	0.005282000	1.555611000
H	-5.169667000	-1.543768000	-0.785615000
H	-5.581491000	-0.856651000	2.711862000
H	-4.167061000	0.172710000	2.493373000
H	-4.547873000	-2.683039000	1.475963000
H	-3.165819000	-2.038096000	2.373012000
H	-4.335862000	-3.556895000	-1.268454000
H	-2.907520000	-5.040723000	-2.652581000
H	-0.474996000	-4.639447000	-2.751667000
H	0.561723000	-2.862400000	-1.454681000
H	-5.159220000	0.655120000	-1.910570000
H	-3.711026000	-0.259891000	-2.262210000
H	-3.211942000	2.148134000	-1.649142000
H	-1.562013000	1.654649000	0.144921000
H	-1.514042000	-0.222875000	-2.244799000
H	-0.944601000	1.454144000	-2.182390000
H	-2.806105000	5.032342000	0.579136000
H	-1.731138000	3.823598000	1.256344000
H	-2.168726000	3.749244000	-0.448141000
H	-4.343852000	3.499306000	1.729067000
H	-5.813543000	1.723711000	1.605950000
H	-6.206764000	1.588624000	-0.090757000
H	3.191736000	0.313329000	1.638950000
H	4.175383000	-0.296087000	-2.218598000
H	6.622905000	0.053843000	0.359994000
H	5.287677000	-0.255685000	1.465797000
H	5.328187000	1.669156000	-0.899729000
H	4.756937000	1.995805000	0.739104000

H	3.442792000	1.652548000	-3.230137000
H	2.023151000	3.523961000	-4.023837000
H	0.512377000	4.678195000	-2.461628000
H	0.371838000	3.981102000	-0.088287000
H	1.938128000	-1.209616000	-1.891126000
H	3.123502000	-2.506571000	-1.812076000
H	1.573813000	-2.773606000	0.119252000
H	1.339951000	-0.974168000	1.750999000
H	-0.057682000	0.517680000	0.818538000
H	1.243903000	-3.068315000	2.370480000
H	2.183226000	-3.990474000	3.540861000
H	1.992633000	-2.263775000	3.750293000
H	4.311046000	-3.112979000	2.710686000
H	4.822227000	-3.164632000	-0.504707000
H	5.624881000	-2.532459000	0.911753000
H	2.646149000	1.326444000	3.499466000
H	1.157945000	2.038838000	4.153082000
H	1.103146000	0.510615000	3.263322000
O	0.200472000	0.114421000	-1.160977000
O	0.713271000	3.326475000	2.085556000

Compound: **7a**



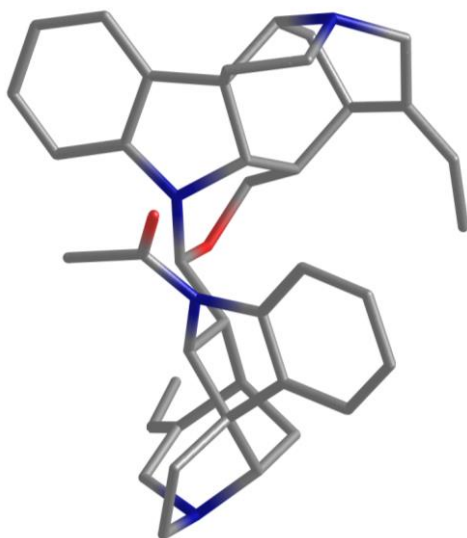
symmetry c1

N	0.718196000	-1.147380000	-0.448133000
C	1.572529000	-0.037159000	0.033329000
C	4.182378000	0.173217000	-0.100845000
N	4.345705000	1.625049000	-0.182881000
C	4.037162000	1.888615000	-1.590690000
C	2.894391000	0.911642000	-1.985694000
C	2.862308000	-0.148116000	-0.849269000
C	2.784276000	-1.569950000	-1.346006000
C	3.727261000	-2.323715000	-2.014439000
C	3.422821000	-3.635465000	-2.379311000
C	2.181088000	-4.168721000	-2.067121000
C	1.216776000	-3.415212000	-1.401401000
C	1.530123000	-2.107745000	-1.057100000
C	4.252567000	-0.351421000	1.312672000
C	3.121622000	0.282616000	2.120761000
C	1.753127000	-0.169196000	1.574053000
C	1.465139000	-1.613390000	1.981232000
C	3.235922000	2.204148000	4.584044000
C	3.386794000	2.572747000	3.140772000
C	3.310545000	1.780106000	2.074411000
C	3.415425000	2.361866000	0.687853000
N	-1.288709000	0.739760000	-1.576325000
C	-2.139159000	-0.064946000	-0.677052000
C	-4.127065000	0.636308000	0.867384000
N	-5.032530000	-0.478525000	0.583363000
C	-5.596531000	-0.099938000	-0.715763000
C	-4.471811000	0.642400000	-1.499045000
C	-3.358820000	0.882258000	-0.445107000

C	-2.692514000	2.231431000	-0.561736000
C	-3.112226000	3.472711000	-0.126668000
C	-2.316971000	4.586345000	-0.392664000
C	-1.126410000	4.445556000	-1.090646000
C	-0.693442000	3.199281000	-1.539386000
C	-1.493157000	2.103253000	-1.261180000
C	-3.250061000	0.395543000	2.069417000
C	-2.360835000	-0.808655000	1.778741000
C	-1.397026000	-0.436712000	0.626014000
C	-0.355740000	-1.549240000	0.412146000
C	-2.198932000	-3.592334000	3.200561000
C	-3.195891000	-3.154245000	2.174386000
C	-3.268633000	-1.993292000	1.524623000
C	-4.363819000	-1.790048000	0.500055000
C	-0.680120000	0.319171000	-2.728114000
C	-0.853581000	-1.118308000	-3.151597000
H	1.063122000	0.899959000	-0.186859000
H	4.992363000	-0.259701000	-0.692659000
H	3.773265000	2.934288000	-1.733755000
H	4.927042000	1.682894000	-2.184414000
H	3.098830000	0.442551000	-2.945761000
H	1.933338000	1.409880000	-2.081413000
H	4.696212000	-1.905382000	-2.254982000
H	4.155271000	-4.236582000	-2.897361000
H	1.952730000	-5.189211000	-2.340365000
H	0.257808000	-3.851597000	-1.161855000
H	5.215749000	-0.093156000	1.750911000
H	4.174184000	-1.438525000	1.301459000
H	3.184145000	-0.056530000	3.152668000
H	0.991985000	0.447334000	2.057701000
H	2.171998000	-2.297373000	1.504349000
H	1.564481000	-1.725364000	3.059631000
H	4.159844000	2.401654000	5.129048000
H	2.462476000	2.816683000	5.048149000
H	2.970498000	1.162191000	4.735222000
H	3.571084000	3.626918000	2.957757000
H	2.408333000	2.392236000	0.244423000
H	3.753568000	3.395320000	0.745522000
H	-2.443994000	-0.963096000	-1.199506000
H	-4.762435000	1.509645000	1.036538000
H	-6.433882000	0.576099000	-0.549220000
H	-5.974198000	-0.976490000	-1.236680000
H	-4.838645000	1.588292000	-1.890940000
H	-4.096690000	0.066769000	-2.344312000

H	-4.045183000	3.586114000	0.409081000
H	-2.629686000	5.563105000	-0.053482000
H	-0.518389000	5.315897000	-1.291801000
H	0.224702000	3.090835000	-2.092242000
H	-3.870373000	0.209095000	2.945240000
H	-2.643405000	1.281152000	2.265161000
H	-1.741061000	-1.014788000	2.643636000
H	-0.874690000	0.464114000	0.959362000
H	-0.865241000	-2.404086000	-0.039653000
H	-1.656650000	-4.470290000	2.846214000
H	-1.464628000	-2.829653000	3.433900000
H	-2.711296000	-3.887324000	4.116984000
H	-3.957598000	-3.892562000	1.940566000
H	-3.950423000	-1.947770000	-0.504678000
H	-5.123081000	-2.559836000	0.630871000
H	0.002877000	-1.387388000	-3.762232000
H	-0.940133000	-1.820097000	-2.331863000
H	-1.751769000	-1.183912000	-3.767494000
O	-0.062916000	1.097517000	-3.433747000
O	0.136899000	-2.009151000	1.672155000

Compound: **7b**



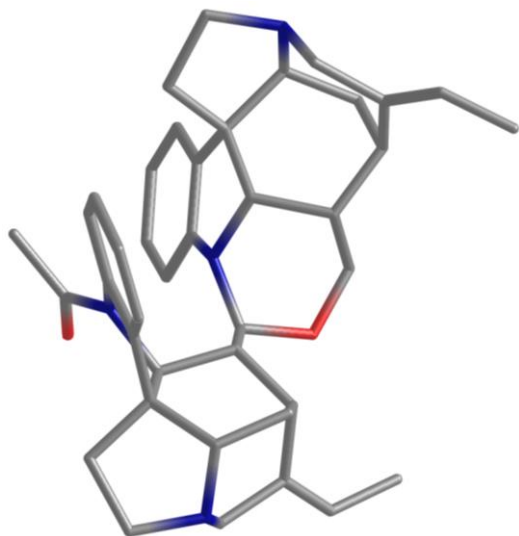
symmetry c1

N	0.861990000	-1.141609000	-0.426999000
C	1.640706000	-0.006342000	0.127680000
C	4.235250000	0.331722000	0.220053000
N	4.305876000	1.804508000	0.078160000
C	3.388100000	2.214977000	-0.993130000
C	3.076449000	0.930069000	-1.747343000
C	3.012571000	-0.103999000	-0.610878000
C	3.029990000	-1.530461000	-1.087622000
C	4.057121000	-2.271912000	-1.634974000
C	3.816881000	-3.589881000	-2.024262000
C	2.554722000	-4.140171000	-1.858359000
C	1.507531000	-3.399006000	-1.315172000
C	1.758266000	-2.085952000	-0.943172000
C	4.174871000	-0.099355000	1.675239000
C	2.919865000	0.498313000	2.309640000
C	1.669854000	-0.123622000	1.669936000
C	1.465637000	-1.582283000	2.066235000
C	0.886064000	2.462121000	3.553170000
C	2.031322000	2.835613000	2.660144000
C	2.939786000	2.014162000	2.140365000
C	4.102965000	2.533814000	1.327693000
N	-1.158367000	0.640125000	-1.666547000
C	-2.032769000	-0.163875000	-0.792114000
C	-4.074185000	0.529733000	0.682974000
N	-4.964527000	-0.585899000	0.357677000
C	-5.480898000	-0.200390000	-0.959282000
C	-4.331770000	0.554831000	-1.693657000
C	-3.258001000	0.785090000	-0.598395000

C	-2.580262000	2.131964000	-0.681796000
C	-2.998060000	3.371332000	-0.239922000
C	-2.181694000	4.479177000	-0.465155000
C	-0.972534000	4.335249000	-1.130051000
C	-0.540914000	3.090874000	-1.585873000
C	-1.361763000	2.001576000	-1.347572000
C	-3.245224000	0.281415000	1.917202000
C	-2.334967000	-0.912360000	1.648703000
C	-1.332837000	-0.516210000	0.538135000
C	-0.245072000	-1.592899000	0.369909000
C	-2.183669000	-3.719465000	3.024435000
C	-3.155690000	-3.273128000	1.978248000
C	-3.222200000	-2.101798000	1.346628000
C	-4.290186000	-1.895869000	0.292600000
C	-0.494367000	0.213057000	-2.781689000
C	-0.636990000	-1.232502000	-3.188053000
H	1.148112000	0.928379000	-0.148063000
H	5.117183000	-0.110764000	-0.249741000
H	2.466951000	2.640723000	-0.574412000
H	3.842169000	2.975027000	-1.628086000
H	3.899335000	0.669317000	-2.414507000
H	2.160002000	0.980912000	-2.331273000
H	5.041570000	-1.840158000	-1.759598000
H	4.614112000	-4.182720000	-2.447577000
H	2.375203000	-5.165197000	-2.150450000
H	0.534549000	-3.850931000	-1.186231000
H	5.070808000	0.229040000	2.200088000
H	4.164274000	-1.187414000	1.726513000
H	2.894879000	0.260004000	3.376085000
H	0.807039000	0.413736000	2.059156000
H	2.253497000	-2.218972000	1.656710000
H	1.479509000	-1.683696000	3.151123000
H	0.792726000	3.180255000	4.366647000
H	-0.061612000	2.476661000	3.009265000
H	1.007927000	1.472683000	3.990019000
H	2.130897000	3.894248000	2.442324000
H	3.963083000	3.587782000	1.093241000
H	5.015675000	2.467020000	1.924195000
H	-2.317777000	-1.066453000	-1.318527000
H	-4.718032000	1.400461000	0.833352000
H	-6.328085000	0.469440000	-0.819716000
H	-5.833302000	-1.074955000	-1.500771000
H	-4.687874000	1.504546000	-2.086286000
H	-3.924994000	-0.008699000	-2.532387000

H	-3.944263000	3.487839000	0.271362000
H	-2.492779000	5.454266000	-0.119676000
H	-0.348717000	5.201304000	-1.298980000
H	0.392721000	2.975973000	-2.111278000
H	-3.899948000	0.080144000	2.764201000
H	-2.654272000	1.169154000	2.148579000
H	-1.747647000	-1.123129000	2.535316000
H	-0.858247000	0.404622000	0.886018000
H	-0.701898000	-2.456008000	-0.119884000
H	-1.618135000	-4.581702000	2.667693000
H	-1.467401000	-2.952125000	3.295462000
H	-2.718682000	-4.041537000	3.918484000
H	-3.902111000	-4.015139000	1.709348000
H	-3.850189000	-2.051988000	-0.700744000
H	-5.051081000	-2.667420000	0.401883000
H	-1.547815000	-1.337820000	-3.779302000
H	0.213108000	-1.483989000	-3.814045000
H	-0.682527000	-1.921518000	-2.353645000
O	0.149645000	0.988364000	-3.467987000
O	0.197088000	-2.068708000	1.642858000

Compound: **7c**



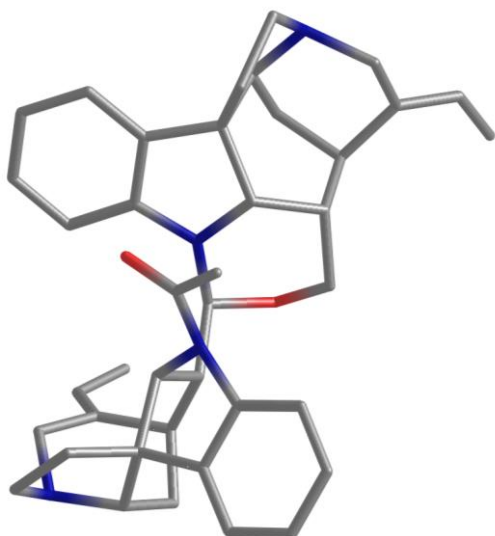
symmetry c1

N	0.765855000	0.281580000	1.128755000
C	1.600499000	0.012067000	-0.062044000
C	4.202283000	-0.252878000	-0.202346000
N	4.331797000	-1.181300000	-1.326683000
C	4.017468000	-2.466841000	-0.701044000
C	2.891840000	-2.190676000	0.336305000
C	2.892031000	-0.647109000	0.525603000
C	2.840753000	-0.213119000	1.969064000
C	3.802515000	-0.312179000	2.955008000
C	3.514096000	0.149897000	4.238230000
C	2.266170000	0.694407000	4.511450000
C	1.284776000	0.788826000	3.529623000
C	1.587152000	0.326923000	2.256037000
C	4.278558000	1.196351000	-0.618671000
C	3.132251000	1.485671000	-1.587467000
C	1.774813000	1.327949000	-0.873848000
C	1.514667000	2.516482000	0.050758000
C	3.209260000	2.333553000	-4.595745000
C	3.354312000	0.950406000	-4.041277000
C	3.292735000	0.560648000	-2.770164000
C	3.387901000	-0.902935000	-2.421552000
N	-1.532652000	-1.591209000	0.834005000
C	-2.260642000	-0.334136000	0.582255000
C	-3.995209000	0.316002000	-1.239110000
N	-4.936482000	1.055768000	-0.395326000
C	-5.684424000	-0.020385000	0.259687000
C	-4.680855000	-1.187390000	0.497920000
C	-3.428535000	-0.796839000	-0.332515000
C	-2.789293000	-1.970038000	-1.034705000

C	-3.148533000	-2.603292000	-2.206522000
C	-2.402180000	-3.695226000	-2.647771000
C	-1.311496000	-4.132606000	-1.913632000
C	-0.937656000	-3.502034000	-0.727863000
C	-1.695278000	-2.426456000	-0.291668000
C	-2.955838000	1.208336000	-1.872924000
C	-2.123140000	1.847187000	-0.763074000
C	-1.338063000	0.716077000	-0.063204000
C	-0.300950000	1.227947000	0.958564000
C	-1.789545000	4.860310000	0.015456000
C	-2.914172000	3.945668000	0.385695000
C	-3.065784000	2.652675000	0.103290000
C	-4.292581000	1.925341000	0.609013000
C	-1.079939000	-1.878165000	2.093641000
C	-0.407818000	-3.204000000	2.318871000
H	1.084747000	-0.716836000	-0.684496000
H	5.024615000	-0.481355000	0.479699000
H	3.735877000	-3.200168000	-1.453462000
H	4.908363000	-2.832074000	-0.191710000
H	3.098389000	-2.698686000	1.275979000
H	1.920861000	-2.534211000	-0.018393000
H	4.771836000	-0.742901000	2.738375000
H	4.259267000	0.085275000	5.017319000
H	2.046335000	1.051386000	5.507810000
H	0.312098000	1.194536000	3.762627000
H	5.234819000	1.387286000	-1.104043000
H	4.223258000	1.830735000	0.265812000
H	3.201867000	2.517439000	-1.925254000
H	0.995101000	1.353995000	-1.640041000
H	2.243700000	2.535087000	0.865755000
H	1.608039000	3.449292000	-0.504778000
H	2.425928000	2.352923000	-5.353912000
H	2.960827000	3.074194000	-3.841624000
H	4.129817000	2.647276000	-5.089522000
H	3.520217000	0.177414000	-4.785451000
H	2.380647000	-1.267151000	-2.169138000
H	3.706975000	-1.470313000	-3.294519000
H	-2.611173000	0.025640000	1.541714000
H	-4.594756000	-0.168152000	-2.014752000
H	-6.478387000	-0.350496000	-0.408941000
H	-6.146893000	0.339819000	1.175475000
H	-5.097980000	-2.128627000	0.146627000
H	-4.426024000	-1.316033000	1.549072000
H	-3.999688000	-2.259701000	-2.778967000

H	-2.669711000	-4.195521000	-3.566765000
H	-0.729029000	-4.971753000	-2.265643000
H	-0.074089000	-3.850569000	-0.185437000
H	-3.450003000	1.974700000	-2.468966000
H	-2.320204000	0.620007000	-2.537045000
H	-1.387982000	2.512733000	-1.202709000
H	-0.802210000	0.209110000	-0.870104000
H	-0.798663000	1.364554000	1.918055000
H	-1.043314000	4.384598000	-0.611091000
H	-2.177688000	5.740309000	-0.498630000
H	-1.282117000	5.214538000	0.913859000
H	-3.705976000	4.414908000	0.962523000
H	-4.025853000	1.348247000	1.502995000
H	-5.031223000	2.655900000	0.935696000
H	0.582552000	-3.191035000	1.863754000
H	-0.299112000	-3.341429000	3.388615000
H	-0.974338000	-4.026900000	1.889760000
O	-1.214940000	-1.076142000	3.000990000
O	0.202158000	2.512344000	0.586843000

Compound: **7d**



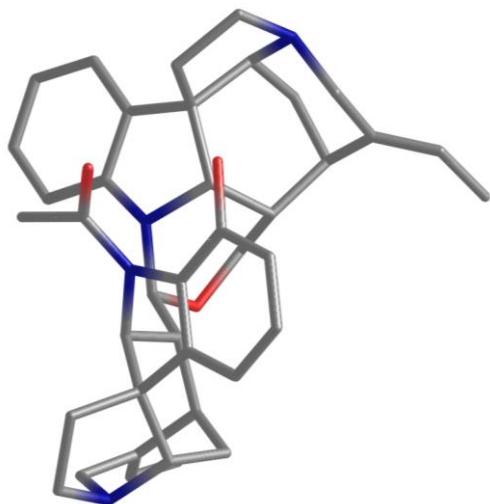
symmetry c1

N	0.777507000	-0.674332000	0.017542000
C	1.751317000	0.366471000	-0.324527000
C	4.068455000	-0.807997000	-0.524656000
N	5.116546000	0.155347000	-0.868501000
C	4.844861000	0.407489000	-2.285860000
C	3.309117000	0.526450000	-2.406187000
C	2.763441000	-0.357779000	-1.266403000
C	1.994897000	-1.590666000	-1.671093000
C	2.289693000	-2.537145000	-2.624248000
C	1.486747000	-3.677121000	-2.733003000
C	0.420032000	-3.850254000	-1.865566000
C	0.107844000	-2.898900000	-0.893856000
C	0.899911000	-1.760033000	-0.818963000
C	3.850289000	-0.992933000	0.959369000
C	3.555710000	0.374684000	1.579101000
C	2.316073000	1.052626000	0.934157000
C	1.178331000	1.192568000	1.934991000
C	5.372959000	1.684554000	3.782077000
C	5.562057000	1.740978000	2.297767000
C	4.788262000	1.213814000	1.352776000
C	5.097413000	1.414149000	-0.106299000
N	-1.433138000	1.264504000	-0.984551000
C	-2.048825000	0.095889000	-0.309004000
C	-4.393875000	-0.152394000	0.843930000
N	-4.728600000	-1.500477000	0.386729000
C	-5.160789000	-1.264080000	-0.995145000
C	-4.304865000	-0.081668000	-1.545589000
C	-3.567987000	0.473675000	-0.299656000
C	-3.483436000	1.979892000	-0.238655000

C	-4.430048000	2.909377000	0.148093000
C	-4.091248000	4.260967000	0.153554000
C	-2.816059000	4.665096000	-0.212776000
C	-1.855378000	3.735860000	-0.605044000
C	-2.215470000	2.400709000	-0.633542000
C	-3.717846000	-0.132083000	2.192453000
C	-2.387556000	-0.862254000	2.059996000
C	-1.467966000	-0.064768000	1.104320000
C	-0.043107000	-0.677143000	1.196025000
C	-1.214274000	-3.450799000	3.343313000
C	-2.203916000	-3.368939000	2.222892000
C	-2.685468000	-2.280308000	1.624258000
C	-3.590939000	-2.435691000	0.422207000
C	-0.827027000	1.106022000	-2.217043000
C	-0.441984000	2.356730000	-2.966711000
H	1.247155000	1.147583000	-0.903808000
H	4.368720000	-1.755350000	-0.975942000
H	5.376516000	1.292056000	-2.630456000
H	5.199962000	-0.447113000	-2.863168000
H	2.941712000	0.207054000	-3.378970000
H	2.990674000	1.560141000	-2.265080000
H	3.141019000	-2.404604000	-3.281398000
H	1.702113000	-4.422647000	-3.484063000
H	-0.193610000	-4.737068000	-1.944658000
H	-0.737498000	-3.043964000	-0.234824000
H	4.738514000	-1.420013000	1.423635000
H	3.021338000	-1.684217000	1.117386000
H	3.368666000	0.245959000	2.641858000
H	2.587265000	2.068548000	0.646106000
H	1.533334000	1.638991000	2.861806000
H	0.397664000	1.840548000	1.519943000
H	4.451769000	1.189474000	4.074761000
H	6.203614000	1.157950000	4.253651000
H	5.362679000	2.691100000	4.201328000
H	6.442009000	2.284987000	1.968176000
H	4.352797000	2.107766000	-0.524423000
H	6.067670000	1.895412000	-0.222040000
H	-1.835726000	-0.771942000	-0.923388000
H	-5.338741000	0.395179000	0.893700000
H	-6.212749000	-0.982762000	-0.987607000
H	-5.062000000	-2.172331000	-1.584509000
H	-4.946729000	0.679260000	-1.984668000
H	-3.596525000	-0.395331000	-2.311056000
H	-5.421944000	2.598469000	0.447060000

H	-4.820991000	4.996514000	0.458818000
H	-2.555775000	5.713225000	-0.185016000
H	-0.860027000	4.057858000	-0.868713000
H	-4.355102000	-0.618548000	2.930005000
H	-3.557658000	0.899500000	2.509092000
H	-1.887209000	-0.877692000	3.025686000
H	-1.418777000	0.940053000	1.530091000
H	-0.157763000	-1.725308000	1.477176000
H	-1.642651000	-3.976646000	4.197039000
H	-0.343123000	-4.026480000	3.025864000
H	-0.863107000	-2.479977000	3.681847000
H	-2.541919000	-4.329758000	1.845947000
H	-2.982350000	-2.330680000	-0.486474000
H	-3.987126000	-3.450176000	0.399834000
H	-1.300294000	3.006876000	-3.121583000
H	0.309125000	2.919789000	-2.415194000
H	-0.030756000	2.051997000	-3.922200000
O	-0.584623000	0.006354000	-2.669485000
O	0.642566000	-0.073763000	2.277632000

Compound: **8a**



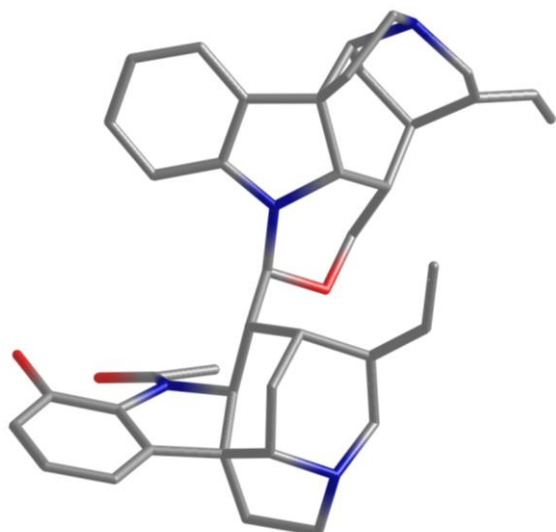
symmetry c1

N	0.716670000	-1.157699000	-0.529547000
C	1.594766000	-0.110387000	0.045286000
C	4.206318000	0.073261000	-0.066960000
N	4.377884000	1.526101000	-0.042644000
C	4.072258000	1.897996000	-1.426432000
C	2.938995000	0.945712000	-1.903475000
C	2.886576000	-0.182944000	-0.838359000
C	2.785298000	-1.562843000	-1.436045000
C	3.718775000	-2.285667000	-2.151051000
C	3.385513000	-3.554765000	-2.624267000
C	2.124495000	-4.075938000	-2.374729000
C	1.170395000	-3.352031000	-1.662951000
C	1.514196000	-2.087455000	-1.206594000
C	4.268869000	-0.553931000	1.304686000
C	3.138551000	0.026022000	2.153445000
C	1.768689000	-0.371537000	1.568853000
C	1.469966000	-1.842023000	1.853967000
C	3.259704000	1.755018000	4.754519000
C	3.419505000	2.229976000	3.343612000
C	3.339718000	1.521297000	2.219918000
C	3.454596000	2.206050000	0.881826000
N	-1.299836000	0.909622000	-1.417600000
C	-2.126655000	-0.049329000	-0.647411000
C	-4.198411000	0.352160000	0.886930000
N	-5.008059000	-0.787485000	0.454176000
C	-5.554507000	-0.319010000	-0.823377000
C	-4.473715000	0.598760000	-1.473818000
C	-3.412012000	0.791130000	-0.361568000
C	-2.836137000	2.183701000	-0.281636000

C	-3.345500000	3.312798000	0.329310000
C	-2.584291000	4.479374000	0.298406000
C	-1.353328000	4.509272000	-0.333403000
C	-0.831189000	3.374252000	-0.956667000
C	-1.603077000	2.215057000	-0.923113000
C	-3.334825000	0.059120000	2.086751000
C	-2.365673000	-1.057211000	1.716478000
C	-1.397865000	-0.541805000	0.621916000
C	-0.354336000	-1.625611000	0.301177000
C	-2.118383000	-3.925837000	2.949066000
C	-3.088475000	-3.465662000	1.907260000
C	-3.193854000	-2.266061000	1.337746000
C	-4.248757000	-2.038453000	0.278642000
C	-0.696708000	0.683838000	-2.606599000
C	-0.670131000	-0.692903000	-3.209495000
H	1.108916000	0.854165000	-0.097843000
H	5.014840000	-0.320895000	-0.687513000
H	3.795432000	2.948218000	-1.486839000
H	4.964807000	1.747963000	-2.032626000
H	3.163757000	0.537708000	-2.886692000
H	1.982923000	1.454052000	-1.975843000
H	4.701625000	-1.875519000	-2.344561000
H	4.109901000	-4.132674000	-3.178764000
H	1.872863000	-5.063690000	-2.734134000
H	0.196483000	-3.779557000	-1.473673000
H	5.231665000	-0.333016000	1.763702000
H	4.185675000	-1.636985000	1.214333000
H	3.193263000	-0.390741000	3.156855000
H	1.010554000	0.208463000	2.099904000
H	2.172538000	-2.489393000	1.322943000
H	1.565875000	-2.044311000	2.919555000
H	4.183353000	1.901946000	5.315770000
H	2.490315000	2.338233000	5.261204000
H	2.983984000	0.707227000	4.826165000
H	3.613965000	3.293178000	3.241387000
H	3.807728000	3.226814000	1.019462000
H	2.451061000	2.287863000	0.438738000
H	-2.359370000	-0.888719000	-1.289128000
H	-4.902339000	1.155104000	1.119730000
H	-5.831713000	-1.163142000	-1.450137000
H	-6.454986000	0.261003000	-0.627619000
H	-4.905913000	1.555495000	-1.757840000
H	-4.034881000	0.163355000	-2.370830000
H	-4.303788000	3.295872000	0.828156000

H	-2.954145000	5.374606000	0.777119000
H	-0.758798000	5.411061000	-0.354603000
H	-3.958437000	-0.243890000	2.926717000
H	-2.792064000	0.960957000	2.374675000
H	-1.751747000	-1.300901000	2.575610000
H	-0.889241000	0.323046000	1.056188000
H	-0.871957000	-2.431223000	-0.225539000
H	-2.656592000	-4.312859000	3.815017000
H	-1.512637000	-4.746050000	2.561059000
H	-1.439297000	-3.145494000	3.273603000
H	-3.797697000	-4.222502000	1.584641000
H	-3.776972000	-2.069590000	-0.712942000
H	-4.957901000	-2.864858000	0.293772000
H	0.347894000	-0.880094000	-3.544787000
H	-0.970200000	-1.496733000	-2.551343000
H	-1.314530000	-0.674506000	-4.087988000
O	-0.179375000	1.608856000	-3.241063000
O	0.139370000	-2.201344000	1.510666000
O	0.389473000	3.436497000	-1.526712000
H	0.367281000	2.794825000	-2.279955000

Compound: **8b**



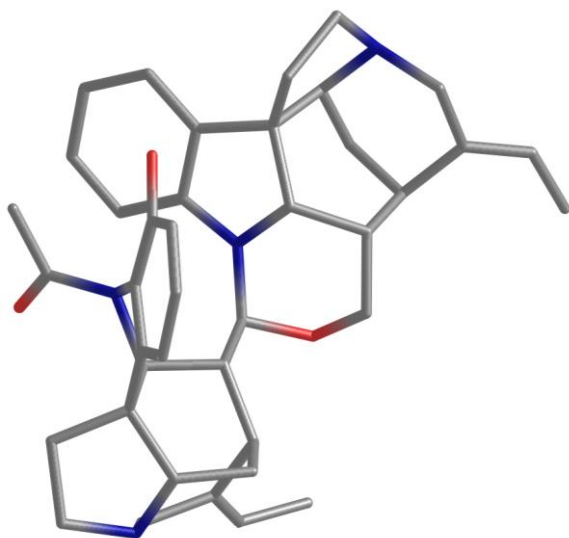
symmetry c1

N	-0.967351000	0.746943000	-0.148345000
C	-2.251004000	0.070108000	-0.395928000
C	-4.499687000	1.400506000	-0.090008000
N	-5.527415000	0.609994000	-0.771183000
C	-5.281896000	0.946810000	-2.174483000
C	-3.742919000	0.971256000	-2.345228000
C	-3.191539000	1.225715000	-0.914442000
C	-2.319044000	2.451948000	-0.811698000
C	-2.620808000	3.765753000	-1.094091000
C	-1.646146000	4.750452000	-0.910871000
C	-0.388117000	4.395967000	-0.448594000
C	-0.063602000	3.069973000	-0.165566000
C	-1.048737000	2.104478000	-0.349348000
C	-4.329458000	1.068530000	1.374732000
C	-4.037908000	-0.424829000	1.510735000
C	-2.688374000	-0.777780000	0.846548000
C	-1.588950000	-0.726597000	1.897865000
C	-5.905847000	-2.529945000	2.912127000
C	-5.973267000	-2.053706000	1.494488000
C	-5.181577000	-1.177468000	0.882919000
C	-5.368721000	-0.836973000	-0.566958000
N	3.089657000	0.481342000	1.232477000
C	2.478092000	-0.711355000	0.600001000
C	3.221252000	-2.151262000	-1.406249000
N	2.769621000	-3.434710000	-0.860200000
C	3.800661000	-3.760553000	0.133112000
C	4.392261000	-2.413186000	0.650230000
C	3.666403000	-1.333826000	-0.180713000
C	4.497227000	-0.112003000	-0.484146000

C	5.468991000	0.066515000	-1.449268000
C	6.067566000	1.319646000	-1.556971000
C	5.699582000	2.357803000	-0.719046000
C	4.716640000	2.189940000	0.258932000
C	4.135222000	0.928104000	0.366121000
C	2.200365000	-1.454325000	-2.278697000
C	0.931540000	-1.238358000	-1.447966000
C	1.298290000	-0.273155000	-0.294392000
C	0.120312000	0.147212000	0.579383000
C	-1.624736000	-2.681156000	-2.590484000
C	-0.618817000	-3.224971000	-1.623372000
C	0.450693000	-2.628297000	-1.100037000
C	1.416853000	-3.425547000	-0.265571000
C	2.974677000	0.834156000	2.535093000
C	2.081432000	0.017692000	3.431095000
H	-2.114483000	-0.633790000	-1.212669000
H	-4.799038000	2.445171000	-0.193796000
H	-5.776441000	0.236698000	-2.833690000
H	-5.696465000	1.935865000	-2.368666000
H	-3.431082000	1.751995000	-3.034557000
H	-3.373540000	0.026153000	-2.740013000
H	-3.604279000	4.035367000	-1.459903000
H	-1.871387000	5.783009000	-1.132250000
H	0.366075000	5.158008000	-0.310929000
H	0.931172000	2.813416000	0.172442000
H	-5.232849000	1.324749000	1.926156000
H	-3.509394000	1.667112000	1.778760000
H	-3.962793000	-0.678921000	2.566707000
H	-2.736016000	-1.815860000	0.511880000
H	-1.573550000	0.243814000	2.409751000
H	-1.741984000	-1.504979000	2.641854000
H	-6.824305000	-2.276743000	3.442840000
H	-5.816381000	-3.616237000	2.942319000
H	-5.071389000	-2.109268000	3.465145000
H	-6.771889000	-2.490572000	0.902870000
H	-4.498260000	-1.219917000	-1.127719000
H	-6.247427000	-1.336957000	-0.970599000
H	2.131457000	-1.374443000	1.381744000
H	4.119891000	-2.363624000	-1.992054000
H	3.375168000	-4.369602000	0.927220000
H	4.586760000	-4.343095000	-0.344938000
H	5.462558000	-2.370827000	0.459302000
H	4.246823000	-2.263808000	1.719325000
H	5.753153000	-0.738961000	-2.111439000

H	6.825260000	1.490577000	-2.308034000
H	6.155529000	3.333225000	-0.807406000
H	1.978005000	-2.063583000	-3.153149000
H	2.611062000	-0.502971000	-2.620718000
H	0.183472000	-0.722281000	-2.046154000
H	1.625055000	0.642754000	-0.797985000
H	0.472538000	0.910983000	1.290920000
H	-1.370819000	-1.693953000	-2.967007000
H	-1.703795000	-3.350383000	-3.447600000
H	-2.620315000	-2.634742000	-2.142255000
H	-0.775860000	-4.264273000	-1.352819000
H	1.423625000	-3.036905000	0.759180000
H	1.079893000	-4.458971000	-0.200135000
H	2.616349000	-0.889374000	3.716748000
H	1.888389000	0.600554000	4.324434000
H	1.148254000	-0.283158000	2.965983000
O	3.611456000	1.778429000	3.003828000
O	-0.331614000	-0.973241000	1.294372000
O	4.356078000	3.246791000	1.011670000
H	4.022868000	2.884290000	1.867175000

Compound: **8c**



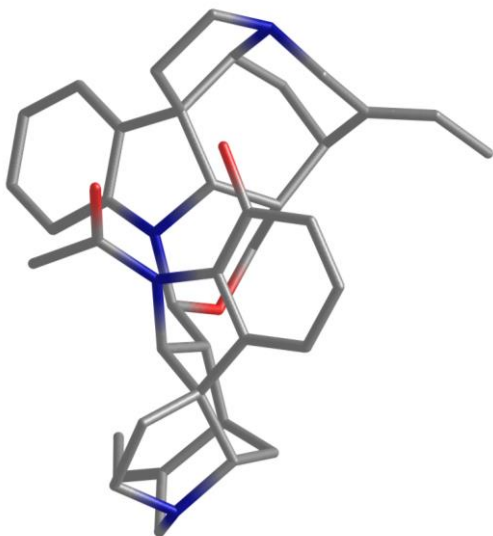
symmetry c1

N	-0.855606000	0.119688000	-0.849336000
C	-1.695069000	-0.027618000	0.344248000
C	-4.043232000	-0.646450000	-0.596507000
N	-5.033008000	-0.759918000	0.474182000
C	-4.673032000	-2.037409000	1.090990000
C	-3.130141000	-2.055278000	1.159333000
C	-2.677824000	-1.178049000	-0.027010000
C	-1.937491000	-1.854457000	-1.155556000
C	-2.210795000	-3.048656000	-1.791911000
C	-1.520543000	-3.378201000	-2.959344000
C	-0.587863000	-2.488408000	-3.476668000
C	-0.296624000	-1.283417000	-2.844422000
C	-0.963191000	-0.981592000	-1.662907000
C	-3.923577000	0.738772000	-1.185128000
C	-3.605963000	1.714266000	-0.050092000
C	-2.315961000	1.328793000	0.729776000
C	-1.248673000	2.412989000	0.599433000
C	-5.474581000	4.125454000	0.703178000
C	-5.595208000	2.705524000	1.162642000
C	-4.797349000	1.680991000	0.874374000
C	-5.030518000	0.320362000	1.474147000
N	1.757686000	-1.365228000	-0.293751000
C	2.318789000	0.002533000	-0.342735000
C	3.955405000	1.269234000	1.258877000
N	4.894443000	1.779020000	0.258327000
C	5.729463000	0.604284000	-0.006281000
C	4.790447000	-0.635979000	0.067049000
C	3.482691000	-0.090396000	0.704258000

C	2.852305000	-1.028973000	1.711709000
C	3.102616000	-1.213398000	3.056579000
C	2.293405000	-2.105822000	3.762385000
C	1.242029000	-2.764420000	3.147763000
C	0.979149000	-2.567347000	1.791188000
C	1.833626000	-1.740982000	1.082639000
C	2.856308000	2.255924000	1.564209000
C	2.004430000	2.424381000	0.308572000
C	1.289912000	1.070705000	0.052289000
C	0.092243000	1.201965000	-0.923084000
C	1.389104000	4.820454000	-1.599389000
C	2.631803000	3.988050000	-1.563222000
C	2.910562000	2.934251000	-0.796495000
C	4.244940000	2.235804000	-0.986827000
C	2.106945000	-2.238962000	-1.318338000
C	1.782151000	-3.693786000	-1.120818000
H	-1.074040000	-0.367586000	1.186957000
H	-4.349863000	-1.354713000	-1.368373000
H	-5.149943000	-2.147369000	2.062551000
H	-5.026727000	-2.844245000	0.447636000
H	-2.728797000	-3.064024000	1.101888000
H	-2.775692000	-1.627620000	2.097851000
H	-2.967365000	-3.714817000	-1.394980000
H	-1.716658000	-4.313504000	-3.461853000
H	-0.055689000	-2.740028000	-4.383423000
H	0.461994000	-0.629618000	-3.247328000
H	-4.860287000	1.028897000	-1.659932000
H	-3.143598000	0.744966000	-1.945666000
H	-3.474262000	2.707781000	-0.469770000
H	-2.555673000	1.281227000	1.792099000
H	-1.700132000	3.398148000	0.705109000
H	-0.506154000	2.305165000	1.394986000
H	-4.585980000	4.304936000	0.105147000
H	-6.344122000	4.410643000	0.109758000
H	-5.446040000	4.799369000	1.559903000
H	-6.440510000	2.504475000	1.813693000
H	-5.985982000	0.299907000	1.996587000
H	-4.256223000	0.139942000	2.234095000
H	2.668817000	0.165562000	-1.353690000
H	4.543004000	1.070646000	2.159244000
H	6.233257000	0.701509000	-0.964841000
H	6.491906000	0.538103000	0.768599000
H	5.228181000	-1.413181000	0.689941000
H	4.596394000	-1.068436000	-0.912298000

H	3.892171000	-0.674354000	3.560683000
H	2.468073000	-2.266728000	4.816356000
H	0.590960000	-3.420879000	3.706537000
H	3.298416000	3.206192000	1.861562000
H	2.244930000	1.893135000	2.392051000
H	1.244890000	3.174305000	0.494747000
H	0.883247000	0.762031000	1.018874000
H	0.455349000	1.280011000	-1.948490000
H	0.944456000	4.785167000	-2.595185000
H	0.633548000	4.491758000	-0.894542000
H	1.631585000	5.865482000	-1.402603000
H	3.401479000	4.297864000	-2.264331000
H	4.113976000	1.393197000	-1.675866000
H	4.929804000	2.920493000	-1.484947000
H	2.012542000	-4.045236000	-0.119018000
H	0.716746000	-3.843475000	-1.307897000
H	2.339121000	-4.262251000	-1.857265000
O	2.603630000	-1.837709000	-2.351092000
O	-0.620600000	2.402713000	-0.672741000
O	-0.096002000	-3.180870000	1.237906000
H	-0.286068000	-2.811652000	0.363498000

Compound: **9a**



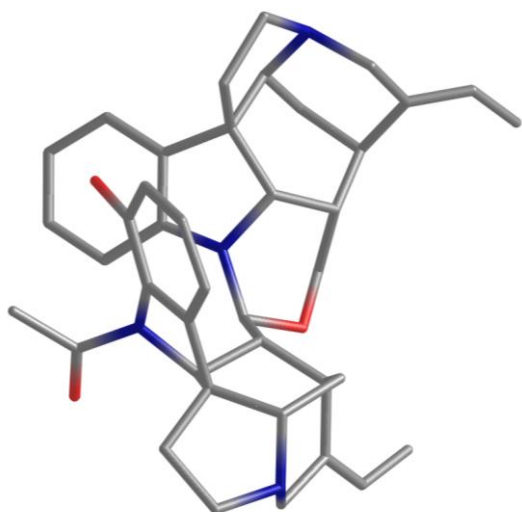
symmetry c1

N	-0.607313000	1.300173000	-0.238083000
C	-1.544411000	0.188394000	0.067162000
C	-4.154844000	0.128633000	-0.050663000
N	-4.339952000	-1.280764000	-0.403644000
C	-4.022169000	-1.302847000	-1.836126000
C	-2.958049000	-0.194943000	-2.082082000
C	-2.837719000	0.560496000	-0.735068000
C	-2.672567000	2.044060000	-0.931175000
C	-3.580780000	2.981519000	-1.379496000
C	-3.178910000	4.309015000	-1.525379000
C	-1.873307000	4.670742000	-1.229684000
C	-0.946137000	3.731290000	-0.783698000
C	-1.361213000	2.414755000	-0.639275000
C	-4.204677000	0.381493000	1.436544000
C	-3.086403000	-0.422502000	2.098027000
C	-1.706927000	0.062506000	1.608529000
C	-1.360102000	1.404797000	2.245917000
C	-3.290376000	-2.734784000	4.194546000
C	-3.451640000	-2.840471000	2.709637000
C	-3.337246000	-1.879533000	1.796035000
C	-3.456254000	-2.204038000	0.330037000
N	1.250995000	-0.656784000	-1.491967000
C	2.181127000	0.004729000	-0.549208000
C	4.128203000	-0.963369000	0.885838000
N	5.156441000	0.022993000	0.494492000
C	5.176543000	0.136092000	-0.970352000
C	4.302322000	-1.011838000	-1.466631000

C	3.246568000	-1.112957000	-0.354922000
C	2.398830000	-2.352173000	-0.451985000
C	2.619826000	-3.621514000	0.041563000
C	1.659918000	-4.600664000	-0.209501000
C	0.528308000	-4.310936000	-0.950097000
C	0.299635000	-3.029966000	-1.459406000
C	1.253389000	-2.052833000	-1.184497000
C	3.370091000	-0.534378000	2.130052000
C	2.611693000	0.758296000	1.824443000
C	1.514847000	0.400257000	0.775101000
C	0.474727000	1.525071000	0.679832000
C	2.280825000	3.949919000	1.865753000
C	3.455302000	3.144455000	1.406079000
C	3.631887000	1.822650000	1.407976000
C	5.044592000	1.294848000	1.193233000
C	0.799928000	-0.124783000	-2.648410000
C	1.126017000	1.310133000	-2.959509000
H	-1.116823000	-0.731741000	-0.327283000
H	-4.960847000	0.678048000	-0.544689000
H	-3.674122000	-2.290656000	-2.129162000
H	-4.925571000	-1.079585000	-2.402331000
H	-3.299712000	0.490417000	-2.855239000
H	-2.000701000	-0.588740000	-2.402750000
H	-4.596375000	2.692808000	-1.617742000
H	-3.882812000	5.053325000	-1.867042000
H	-1.563985000	5.700255000	-1.341516000
H	0.063777000	4.039061000	-0.555256000
H	-5.171057000	0.070426000	1.831571000
H	-4.096761000	1.449441000	1.627123000
H	-3.118085000	-0.264404000	3.173934000
H	-0.969398000	-0.657486000	1.969358000
H	-2.035570000	2.187713000	1.891986000
H	-1.455139000	1.342543000	3.328523000
H	-2.988532000	-1.745180000	4.524146000
H	-4.221723000	-2.991360000	4.700983000
H	-2.539975000	-3.445648000	4.541715000
H	-3.679721000	-3.838105000	2.346989000
H	-2.451006000	-2.214418000	-0.113442000
H	-3.849428000	-3.212380000	0.206724000
H	2.614875000	0.883049000	-1.019700000
H	4.610802000	-1.927465000	1.066023000
H	6.193461000	0.077007000	-1.356290000
H	4.762412000	1.098853000	-1.291122000
H	4.865543000	-1.943802000	-1.507596000

H	3.869499000	-0.832276000	-2.449849000
H	3.507550000	-3.853390000	0.611894000
H	1.798548000	-5.600832000	0.174818000
H	-0.214779000	-5.068629000	-1.153005000
H	4.063108000	-0.399773000	2.959366000
H	2.675018000	-1.322971000	2.418294000
H	2.087360000	1.098256000	2.714671000
H	1.004540000	-0.485323000	1.163178000
H	0.995217000	2.426132000	0.354280000
H	2.618973000	4.688965000	2.593032000
H	1.838837000	4.515897000	1.042953000
H	1.503433000	3.347702000	2.324486000
H	4.312580000	3.738614000	1.101291000
H	5.645244000	2.032605000	0.664728000
H	5.501133000	1.185480000	2.180442000
H	2.156746000	1.374227000	-3.311205000
H	0.464658000	1.635824000	-3.754869000
H	1.010433000	1.959894000	-2.098709000
O	0.164648000	-0.801681000	-3.461722000
O	-0.015082000	1.786594000	2.000679000
O	-0.829095000	-2.796993000	-2.158678000
H	-0.621659000	-2.052781000	-2.776373000

Compound: **9b**



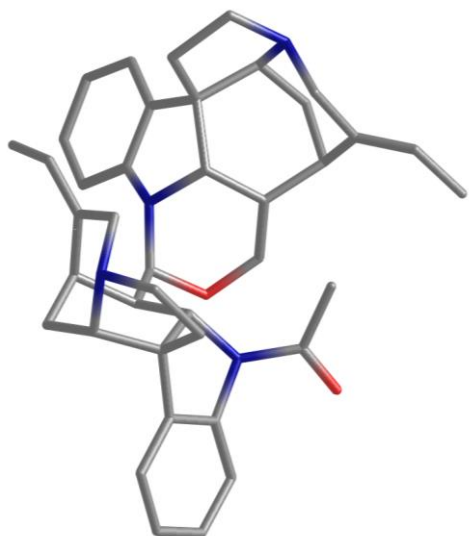
symmetry c1

N	-0.716832000	-0.207914000	-0.865132000
C	-1.761349000	0.147082000	0.108130000
C	-4.196712000	-0.825635000	0.051513000
N	-4.666820000	-0.620859000	1.422285000
C	-4.018196000	-1.722641000	2.135901000
C	-2.601742000	-1.877990000	1.517489000
C	-2.677669000	-1.128271000	0.157881000
C	-2.183455000	-1.940291000	-1.012571000
C	-2.664516000	-3.132471000	-1.511047000
C	-2.034864000	-3.724879000	-2.607093000
C	-0.935787000	-3.105199000	-3.183112000
C	-0.429519000	-1.905146000	-2.685312000
C	-1.063163000	-1.331135000	-1.587311000
C	-4.525250000	0.311842000	-0.887380000
C	-3.931112000	1.601951000	-0.324393000
C	-2.391077000	1.525053000	-0.293985000
C	-1.802907000	1.949395000	-1.635165000
C	-5.526445000	4.115549000	0.673451000
C	-5.202560000	2.876967000	1.449495000
C	-4.511841000	1.812463000	1.050640000
C	-4.243696000	0.668760000	1.988179000
N	2.099453000	-1.332409000	-0.436655000
C	2.491569000	0.089592000	-0.360623000
C	3.645206000	1.507469000	1.468661000
N	4.620216000	2.183065000	0.610137000
C	5.653958000	1.160062000	0.433984000
C	4.926571000	-0.217382000	0.398989000
C	3.476911000	0.103304000	0.843913000

C	2.844997000	-0.965133000	1.713392000
C	2.916374000	-1.188380000	3.073500000
C	2.139454000	-2.213745000	3.616880000
C	1.282328000	-2.963723000	2.828324000
C	1.195380000	-2.728677000	1.455604000
C	2.037839000	-1.773000000	0.912974000
C	2.376546000	2.314886000	1.623852000
C	1.692314000	2.416866000	0.257607000
C	1.274238000	0.979271000	-0.114998000
C	0.244626000	0.787214000	-1.250761000
C	1.004344000	4.851355000	-1.571314000
C	2.337359000	4.192352000	-1.404829000
C	2.654550000	3.127465000	-0.669980000
C	4.086563000	2.623444000	-0.695795000
C	2.502388000	-2.088255000	-1.514822000
C	2.502334000	-3.586206000	-1.365424000
H	-1.299582000	0.272807000	1.087349000
H	-4.674982000	-1.741216000	-0.303194000
H	-4.000116000	-1.527034000	3.205726000
H	-4.596987000	-2.630488000	1.969010000
H	-2.351325000	-2.925554000	1.370247000
H	-1.826298000	-1.454283000	2.154179000
H	-3.519475000	-3.612046000	-1.051094000
H	-2.402149000	-4.659261000	-3.004153000
H	-0.449135000	-3.560221000	-4.034576000
H	0.437550000	-1.452162000	-3.141637000
H	-5.605082000	0.410853000	-0.988637000
H	-4.116362000	0.087909000	-1.874592000
H	-4.203499000	2.433553000	-0.971239000
H	-2.035586000	2.262348000	0.429346000
H	-2.110925000	1.272170000	-2.438798000
H	-2.135780000	2.953308000	-1.891779000
H	-5.094378000	4.121899000	-0.322672000
H	-6.606284000	4.231697000	0.574187000
H	-5.164481000	4.997766000	1.202284000
H	-5.581939000	2.863660000	2.466661000
H	-3.167455000	0.657547000	2.228610000
H	-4.771295000	0.816048000	2.928974000
H	2.959119000	0.339215000	-1.304140000
H	4.126293000	1.378370000	2.442363000
H	6.329157000	1.195281000	1.287926000
H	6.237827000	1.357574000	-0.461571000
H	5.396481000	-0.916887000	1.086961000
H	4.939153000	-0.672755000	-0.590887000

H	3.541693000	-0.578253000	3.709932000
H	2.177558000	-2.406904000	4.679172000
H	0.643881000	-3.720389000	3.260929000
H	2.629635000	3.304799000	2.001990000
H	1.714985000	1.835959000	2.346761000
H	0.784674000	3.003905000	0.349703000
H	0.785090000	0.599667000	0.785881000
H	0.749123000	0.432893000	-2.153524000
H	0.231298000	4.410060000	-0.951822000
H	1.080586000	5.914901000	-1.342645000
H	0.674611000	4.772611000	-2.608460000
H	3.142405000	4.654365000	-1.969127000
H	4.168634000	1.815567000	-1.432041000
H	4.730824000	3.421663000	-1.061992000
H	3.216192000	-3.984765000	-2.078473000
H	2.749974000	-3.910738000	-0.358933000
H	1.515343000	-3.973452000	-1.619782000
O	2.820106000	-1.557852000	-2.565123000
O	-0.392809000	2.023057000	-1.547495000
O	0.295768000	-3.432141000	0.722198000
H	0.110461000	-2.974770000	-0.110166000

Compound: **10a**



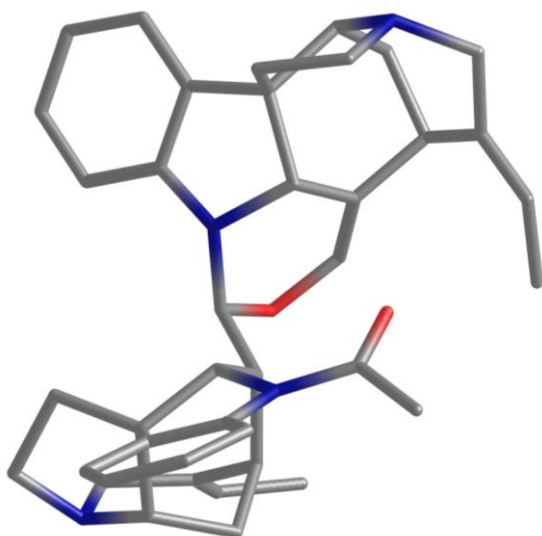
symmetry c1

N	-1.165019000	-1.076360000	-0.850954000
C	-1.642989000	0.039553000	-0.022584000
C	-4.080545000	0.891824000	0.368648000
N	-3.958887000	1.412869000	1.730600000
C	-4.010755000	0.193451000	2.540780000
C	-3.289014000	-0.920851000	1.727249000
C	-3.126963000	-0.329534000	0.302718000
C	-3.444488000	-1.285563000	-0.819330000
C	-4.658498000	-1.817360000	-1.202573000
C	-4.706883000	-2.713839000	-2.270131000
C	-3.538328000	-3.060615000	-2.932014000
C	-2.305430000	-2.538640000	-2.548165000
C	-2.271541000	-1.653800000	-1.480184000
C	-3.854550000	1.944042000	-0.693872000
C	-2.424194000	2.481667000	-0.541353000
C	-1.493648000	1.319308000	-0.811458000
C	-0.671423000	1.339509000	-1.858247000
C	-1.672541000	5.441737000	0.151264000
C	-2.080091000	4.364341000	1.107150000
C	-2.351656000	3.088116000	0.845689000
C	-2.704158000	2.145585000	1.967504000
N	2.401898000	1.174877000	-0.650755000
C	1.913155000	0.057461000	0.181418000
C	3.239578000	-1.857248000	1.401794000
N	2.525652000	-1.830430000	2.678883000
C	3.105031000	-0.657848000	3.341925000
C	3.441565000	0.376909000	2.225306000

C	3.228330000	-0.400320000	0.901772000
C	4.245860000	-0.089444000	-0.170883000
C	5.532334000	-0.560021000	-0.342314000
C	6.282780000	-0.094108000	-1.421498000
C	5.743362000	0.829574000	-2.304167000
C	4.446476000	1.313889000	-2.140700000
C	3.717889000	0.839365000	-1.066193000
C	2.680583000	-2.866029000	0.427912000
C	1.257699000	-2.433631000	0.077285000
C	1.349360000	-1.087745000	-0.689246000
C	0.071720000	-0.897202000	-1.535719000
C	-1.384490000	-4.028349000	0.610513000
C	-0.598522000	-3.221414000	1.592378000
C	0.481518000	-2.471486000	1.380760000
C	1.065665000	-1.693774000	2.538752000
C	1.991918000	2.485032000	-0.636886000
C	1.000561000	2.951491000	0.400123000
H	-1.055599000	0.064517000	0.898137000
H	-5.096576000	0.498711000	0.280049000
H	-3.564780000	0.366857000	3.517511000
H	-5.054578000	-0.077670000	2.693012000
H	-3.890381000	-1.827598000	1.702710000
H	-2.320546000	-1.185167000	2.147900000
H	-5.567154000	-1.545822000	-0.680647000
H	-5.651537000	-3.132976000	-2.583258000
H	-3.578728000	-3.750586000	-3.762973000
H	-1.408680000	-2.835498000	-3.072303000
H	-4.579615000	2.747956000	-0.571881000
H	-3.986724000	1.501931000	-1.681633000
H	-2.238986000	3.244936000	-1.292723000
H	-0.565015000	2.208583000	-2.495091000
H	-0.734040000	5.894844000	0.473918000
H	-1.537491000	5.086574000	-0.866474000
H	-2.415528000	6.239837000	0.134640000
H	-2.147778000	4.678787000	2.144099000
H	-1.866485000	1.448245000	2.123305000
H	-2.810308000	2.703571000	2.896548000
H	1.180038000	0.428068000	0.882222000
H	4.277772000	-2.106019000	1.637880000
H	2.420948000	-0.270232000	4.093014000
H	4.020324000	-0.959421000	3.848795000
H	4.473188000	0.710520000	2.311787000
H	2.810661000	1.264128000	2.267845000
H	5.959654000	-1.274917000	0.347927000

H	7.288880000	-0.457748000	-1.571722000
H	6.334152000	1.180171000	-3.138217000
H	4.022894000	2.033335000	-2.820430000
H	2.680783000	-3.854526000	0.885071000
H	3.305383000	-2.902022000	-0.465061000
H	0.822402000	-3.155682000	-0.610615000
H	2.120418000	-1.246379000	-1.449293000
H	0.126911000	-1.681760000	-2.286977000
H	-2.406066000	-3.646370000	0.544654000
H	-0.971391000	-4.009472000	-0.393057000
H	-1.452951000	-5.065767000	0.939524000
H	-0.983807000	-3.248741000	2.607493000
H	0.784210000	-0.635137000	2.442771000
H	0.605477000	-2.035366000	3.465099000
H	1.579244000	3.464851000	1.169827000
H	0.395165000	2.185210000	0.866607000
H	0.343888000	3.678645000	-0.065402000
O	2.486972000	3.299572000	-1.394679000
O	0.112876000	0.320889000	-2.291514000

Compound: **10b**



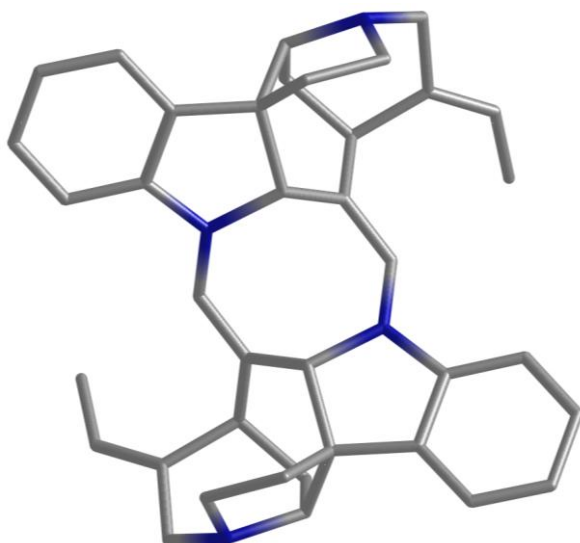
symmetry c1

N	0.943178000	-0.946340000	-0.609434000
C	1.904930000	0.104774000	-0.224140000
C	4.362312000	0.525764000	-0.969575000
N	4.344040000	2.006935000	-0.980740000
C	3.127147000	2.454574000	-1.675512000
C	2.599555000	1.211239000	-2.385803000
C	2.941376000	0.099746000	-1.383223000
C	2.797654000	-1.298881000	-1.919859000
C	3.592860000	-2.003754000	-2.800087000
C	3.218431000	-3.293905000	-3.176799000
C	2.055295000	-3.852491000	-2.668608000
C	1.239880000	-3.148538000	-1.785400000
C	1.621681000	-1.865646000	-1.422366000
C	4.814950000	-0.026392000	0.373060000
C	3.816581000	0.423115000	1.447827000
C	2.506464000	-0.236316000	1.110983000
C	1.952607000	-1.170704000	1.873990000
C	2.193598000	2.093524000	3.434038000
C	2.990723000	2.646547000	2.294427000
C	3.721112000	1.947692000	1.432033000
C	4.525959000	2.614252000	0.339152000
N	-1.962944000	1.813485000	0.069726000
C	-1.622203000	0.384209000	-0.233387000
C	-3.838688000	-0.802859000	0.477818000
N	-3.909249000	-2.247597000	0.255951000
C	-3.958612000	-2.346630000	-1.203345000
C	-2.891433000	-1.355450000	-1.702720000

C	-2.985628000	-0.192772000	-0.700474000
C	-3.679253000	1.031100000	-1.224028000
C	-4.772886000	1.116831000	-2.062638000
C	-5.276110000	2.368612000	-2.400747000
C	-4.666635000	3.510403000	-1.903355000
C	-3.561719000	3.434596000	-1.061062000
C	-3.087682000	2.177539000	-0.704776000
C	-3.309605000	-0.415408000	1.840484000
C	-1.897142000	-0.982956000	1.992938000
C	-0.930762000	-0.364885000	0.927949000
C	0.086448000	-1.414370000	0.434807000
C	-0.754717000	-2.977389000	4.089338000
C	-1.625020000	-3.306249000	2.918532000
C	-2.065030000	-2.486181000	1.967551000
C	-2.805493000	-3.063044000	0.785445000
C	-1.140210000	2.678917000	0.739129000
C	-1.733187000	3.953158000	1.291036000
H	1.395218000	1.065536000	-0.160197000
H	5.044344000	0.175048000	-1.749361000
H	2.383773000	2.822663000	-0.958547000
H	3.349893000	3.265945000	-2.368057000
H	3.137669000	1.035836000	-3.318128000
H	1.534000000	1.263828000	-2.605171000
H	4.499839000	-1.564534000	-3.194837000
H	3.836150000	-3.859589000	-3.858637000
H	1.773272000	-4.855398000	-2.956828000
H	0.339943000	-3.606880000	-1.400257000
H	5.822989000	0.322061000	0.596605000
H	4.846162000	-1.114605000	0.324892000
H	4.144272000	0.078899000	2.430843000
H	2.373314000	-1.481179000	2.822259000
H	2.503415000	1.086202000	3.701924000
H	2.290007000	2.729191000	4.313789000
H	1.135930000	2.058975000	3.164832000
H	2.956171000	3.724364000	2.167771000
H	4.267579000	3.669840000	0.269313000
H	5.587379000	2.572349000	0.595114000
H	-0.940695000	0.392556000	-1.086842000
H	-4.856097000	-0.427125000	0.356869000
H	-3.792890000	-3.370439000	-1.530810000
H	-4.948320000	-2.039047000	-1.545090000
H	-3.052506000	-1.029103000	-2.727973000
H	-1.899824000	-1.810043000	-1.663392000
H	-5.225896000	0.218538000	-2.461615000

H	-6.126881000	2.451422000	-3.060837000
H	-5.039911000	4.484458000	-2.185091000
H	-3.090254000	4.344476000	-0.733369000
H	-3.953542000	-0.824727000	2.618315000
H	-3.320257000	0.669908000	1.939853000
H	-1.514695000	-0.705108000	2.969351000
H	-0.326604000	0.373267000	1.448622000
H	-0.420394000	-2.300584000	0.072583000
H	-0.417604000	-1.945428000	4.088747000
H	-1.270276000	-3.178487000	5.029469000
H	0.133485000	-3.610345000	4.072485000
H	-1.893596000	-4.355000000	2.828525000
H	-2.077016000	-3.256674000	-0.013266000
H	-3.202223000	-4.041157000	1.058539000
H	-2.809675000	3.905890000	1.419507000
H	-1.250933000	4.123059000	2.249634000
H	-1.482208000	4.792741000	0.644978000
O	0.030572000	2.417703000	0.956624000
O	0.825311000	-1.876157000	1.577022000

Compound: **11-tub**



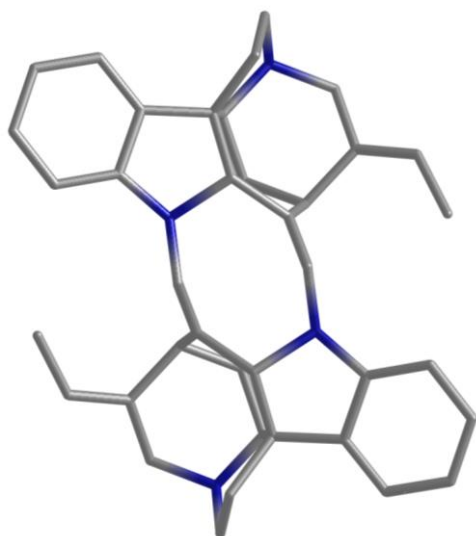
symmetry c2

N	1.328419000	1.098337000	-0.225435000
N	-1.950942000	4.159464000	-0.370753000
N	-1.328419000	-1.098337000	-0.225435000
N	1.950942000	-4.159464000	-0.370753000
C	-0.062789000	1.496756000	-0.558365000
C	0.062789000	3.002528000	-0.973624000
C	-1.063084000	1.183100000	0.530771000
C	1.676137000	0.003999000	0.545875000
C	0.062789000	-1.496756000	-0.558365000
C	-0.062789000	-3.002528000	-0.973624000
C	1.063084000	-1.183100000	0.530771000
C	-1.676137000	-0.003999000	0.545875000
C	-0.552290000	3.968611000	0.064699000
C	-1.390370000	2.219148000	1.603385000
C	-0.441395000	3.410740000	1.476538000
C	-0.794746000	3.299194000	-2.206183000
C	0.552290000	-3.968611000	0.064699000
C	1.390370000	-2.219148000	1.603385000
C	0.441395000	-3.410740000	1.476538000
C	0.794746000	-3.299194000	-2.206183000
C	1.549137000	3.196852000	-1.104222000
C	2.223389000	2.078649000	-0.612117000
C	-2.186792000	3.401917000	-1.599284000
C	-2.818602000	2.727012000	1.487760000
C	-2.947915000	4.003523000	0.671850000
C	-1.549137000	-3.196852000	-1.104222000
C	-2.223389000	-2.078649000	-0.612117000

C	2.186792000	-3.401917000	-1.599284000
C	2.818602000	-2.727012000	1.487760000
C	2.947915000	-4.003523000	0.671850000
C	2.258192000	4.291944000	-1.549622000
C	3.610991000	2.034412000	-0.566539000
C	-3.876701000	2.190879000	2.088470000
C	3.653563000	4.267768000	-1.508275000
C	4.312926000	3.149733000	-1.016981000
C	-3.913354000	1.027994000	3.033291000
C	-2.258192000	-4.291944000	-1.549622000
C	-3.610991000	-2.034412000	-0.566539000
C	3.876701000	-2.190879000	2.088470000
C	-3.653563000	-4.267768000	-1.508275000
C	-4.312926000	-3.149733000	-1.016981000
C	3.913354000	-1.027994000	3.033291000
H	-0.383766000	0.951190000	-1.447269000
H	-0.013359000	4.917392000	-0.000195000
H	-1.252251000	1.759172000	2.580157000
H	-0.695874000	4.168486000	2.216489000
H	0.592119000	3.112454000	1.662131000
H	-0.706591000	2.536592000	-2.976407000
H	0.383766000	-0.951190000	-1.447269000
H	0.013359000	-4.917392000	-0.000195000
H	1.252251000	-1.759172000	2.580157000
H	0.695874000	-4.168486000	2.216489000
H	-0.592119000	-3.112454000	1.662131000
H	0.706591000	-2.536592000	-2.976407000
H	-0.503013000	4.260142000	-2.631433000
H	-2.894648000	3.922501000	-2.243499000
H	-2.588116000	2.398967000	-1.396309000
H	-2.860196000	4.854167000	1.353303000
H	-3.938521000	4.070245000	0.223234000
H	1.738893000	5.164716000	-1.924831000
H	0.503013000	-4.260142000	-2.631433000
H	2.894648000	-3.922501000	-2.243499000
H	2.588116000	-2.398967000	-1.396309000
H	2.860196000	-4.854167000	1.353303000
H	3.938521000	-4.070245000	0.223234000
H	-1.738893000	-5.164716000	-1.924831000
H	4.131111000	1.154737000	-0.214603000
H	-4.839127000	2.658494000	1.899061000
H	4.219492000	5.116921000	-1.861469000
H	5.393512000	3.134950000	-0.993499000
H	-2.920480000	0.673096000	3.300148000

H	-4.432438000	1.302666000	3.951813000
H	-4.464090000	0.189266000	2.602956000
H	-4.131111000	-1.154737000	-0.214603000
H	4.839127000	-2.658494000	1.899061000
H	-4.219492000	-5.116921000	-1.861469000
H	-5.393512000	-3.134950000	-0.993499000
H	2.920480000	-0.673096000	3.300148000
H	4.432438000	-1.302666000	3.951813000
H	4.464090000	-0.189266000	2.602956000
H	2.499887000	0.184760000	1.228969000
H	-2.499887000	-0.184760000	1.228969000

Compound: **11-crown**



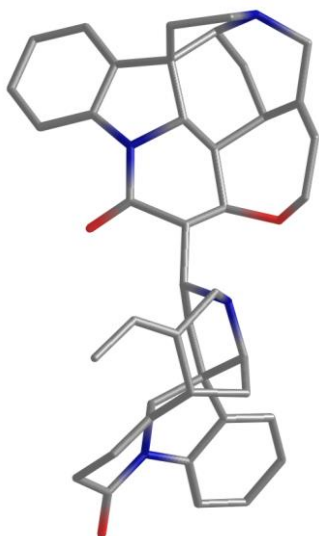
symmetry c2

N	-1.043969000	-1.572792000	-0.693162000
N	1.892376000	-3.918359000	1.633949000
C	0.421170000	-1.948270000	-0.925959000
C	0.477478000	-3.328152000	-0.278930000
C	1.262445000	-0.828133000	-0.381924000
C	-1.305254000	-0.260669000	-1.166480000
C	0.634481000	-3.236809000	1.297452000
C	1.663584000	-0.962445000	1.067781000
C	0.634481000	-1.806554000	1.837021000
C	1.679533000	-4.165676000	-0.729936000
C	-0.886644000	-3.849708000	-0.681271000
C	-1.733497000	-2.760619000	-0.945656000
C	2.119133000	-4.872347000	0.554001000
C	3.014195000	-1.692482000	1.145449000
C	3.001644000	-3.001489000	1.907046000
C	-1.352140000	-5.138687000	-0.807896000
C	-3.033741000	-2.959870000	-1.377741000
C	4.158754000	-1.194031000	0.687704000
C	-2.670939000	-5.352482000	-1.219846000
C	-3.490307000	-4.272583000	-1.505881000
C	4.356703000	0.152930000	0.072922000
H	0.563781000	-2.045682000	-2.010224000
H	-1.124155000	-0.116135000	-2.231977000
H	-0.190339000	-3.796242000	1.740927000
H	1.779685000	0.026039000	1.510355000
H	0.886339000	-1.826818000	2.896859000
H	-0.358242000	-1.383699000	1.744365000

H	2.475768000	-3.504125000	-1.077110000
H	1.427510000	-4.848326000	-1.538962000
H	1.488551000	-5.747748000	0.728186000
H	3.154060000	-5.205501000	0.541237000
H	2.972553000	-2.755480000	2.972209000
H	3.937828000	-3.531633000	1.743551000
H	-0.700916000	-5.979887000	-0.606396000
H	-3.674599000	-2.126089000	-1.619913000
H	5.047832000	-1.807956000	0.791640000
H	-3.045626000	-6.359440000	-1.329862000
H	-4.502479000	-4.444755000	-1.844074000
H	3.561906000	0.844452000	0.342303000
H	5.305805000	0.582176000	0.391395000
H	4.380525000	0.085567000	-1.017149000
N	1.043969000	1.572792000	-0.693162000
N	-1.892376000	3.918359000	1.633949000
C	-0.421170000	1.948270000	-0.925959000
C	-0.477478000	3.328152000	-0.278930000
C	-1.262445000	0.828133000	-0.381924000
C	1.305254000	0.260669000	-1.166480000
C	-0.634481000	3.236809000	1.297452000
C	-1.663584000	0.962445000	1.067781000
C	-0.634481000	1.806554000	1.837021000
C	-1.679533000	4.165676000	-0.729936000
C	0.886644000	3.849708000	-0.681271000
C	1.733497000	2.760619000	-0.945656000
C	-2.119133000	4.872347000	0.554001000
C	-3.014195000	1.692482000	1.145449000
C	-3.001644000	3.001489000	1.907046000
C	1.352140000	5.138687000	-0.807896000
C	3.033741000	2.959870000	-1.377741000
C	-4.158754000	1.194031000	0.687704000
C	2.670939000	5.352482000	-1.219846000
C	3.490307000	4.272583000	-1.505881000
C	-4.356703000	-0.152930000	0.072922000
H	-0.563781000	2.045682000	-2.010224000
H	1.124155000	0.116135000	-2.231977000
H	0.190339000	3.796242000	1.740927000
H	-1.779685000	-0.026039000	1.510355000
H	-0.886339000	1.826818000	2.896859000
H	0.358242000	1.383699000	1.744365000
H	-2.475768000	3.504125000	-1.077110000
H	-1.427510000	4.848326000	-1.538962000
H	-1.488551000	5.747748000	0.728186000

H	-3.154060000	5.205501000	0.541237000
H	-2.972553000	2.755480000	2.972209000
H	-3.937828000	3.531633000	1.743551000
H	0.700916000	5.979887000	-0.606396000
H	3.674599000	2.126089000	-1.619913000
H	-5.047832000	1.807956000	0.791640000
H	3.045626000	6.359440000	-1.329862000
H	4.502479000	4.444755000	-1.844074000
H	-3.561906000	-0.844452000	0.342303000
H	-5.305805000	-0.582176000	0.391395000
H	-4.380525000	-0.085567000	-1.017149000

Compound: **12-boat-like**



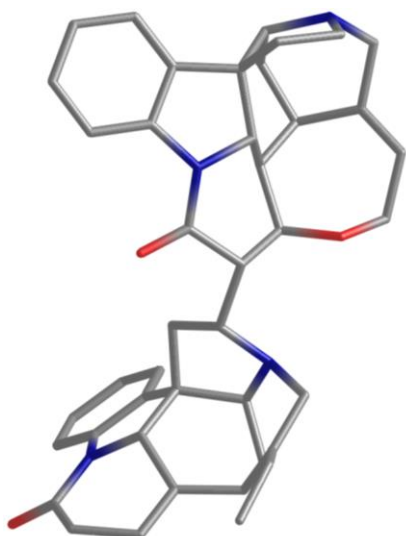
symmetry c1

N	2.644005000	1.381567000	-0.271495000
C	3.356385000	0.157844000	0.137847000
C	5.706150000	-0.773665000	-0.369254000
N	6.002466000	-1.372859000	0.956989000
C	5.703959000	-0.379622000	1.999714000
C	5.494333000	0.933869000	1.254430000
C	4.850563000	0.477887000	-0.065867000
C	4.783961000	1.588893000	-1.080984000
C	5.785346000	2.142594000	-1.853541000
C	5.491593000	3.239506000	-2.661090000
C	4.211026000	3.773515000	-2.674661000
C	3.189821000	3.232036000	-1.897427000
C	3.495569000	2.132380000	-1.111966000
C	5.045966000	-1.797758000	-1.279537000
C	3.696781000	-2.197390000	-0.670760000
C	2.817111000	-0.954923000	-0.756889000
C	1.313157000	-1.177097000	-0.490827000
C	1.431730000	-2.648159000	1.436713000
C	2.910844000	-2.789758000	1.655199000
C	3.896122000	-2.626792000	0.778848000
C	5.347328000	-2.668829000	1.193528000
C	1.277317000	1.311114000	-0.375193000
C	0.704925000	0.042139000	0.252213000
N	-4.903391000	0.475174000	-1.131392000
C	-3.784537000	0.647158000	-0.175047000
C	-2.629442000	-1.307522000	1.117497000
N	-1.314722000	-0.722954000	1.476026000

C	-0.821757000	0.076822000	0.342826000
C	-1.593682000	-0.475914000	-0.843834000
C	-2.992041000	-0.693855000	-0.253374000
C	-3.859466000	-1.557728000	-1.127040000
C	-3.686482000	-2.883385000	-1.475104000
C	-4.589233000	-3.477109000	-2.353040000
C	-5.641728000	-2.736693000	-2.873719000
C	-5.826161000	-1.398978000	-2.537279000
C	-4.921378000	-0.828602000	-1.652438000
C	-3.689524000	-1.060140000	2.182273000
C	-3.809925000	0.447240000	2.429856000
C	-4.342028000	1.080866000	1.169724000
C	-5.305884000	1.990842000	1.124494000
C	-3.304966000	3.296393000	3.472330000
C	-2.253032000	2.251150000	3.261362000
C	-2.448846000	1.006062000	2.838141000
C	-1.317294000	0.013125000	2.735926000
C	-5.921965000	1.375553000	-1.195081000
C	-5.773433000	2.514483000	-0.207181000
H	3.156498000	-0.057909000	1.184507000
H	6.641138000	-0.430292000	-0.818833000
H	6.513680000	-0.318970000	2.725683000
H	4.793744000	-0.654106000	2.544545000
H	4.873712000	1.643482000	1.799005000
H	6.448341000	1.412706000	1.033237000
H	6.786561000	1.733351000	-1.830282000
H	6.264792000	3.678488000	-3.274379000
H	3.995401000	4.627399000	-3.300836000
H	2.194772000	3.643377000	-1.907408000
H	5.705468000	-2.655360000	-1.399402000
H	4.897643000	-1.370365000	-2.270723000
H	3.245685000	-3.006100000	-1.245141000
H	2.897071000	-0.573415000	-1.778793000
H	0.825634000	-1.247645000	-1.460597000
H	0.937799000	-3.574442000	1.734036000
H	1.030681000	-1.876097000	2.102397000
H	3.170286000	-3.047860000	2.678006000
H	5.882509000	-3.443182000	0.643243000
H	5.443149000	-2.907438000	2.250718000
H	1.082220000	0.027067000	1.276576000
H	-3.144976000	1.454195000	-0.546167000
H	-2.509973000	-2.383365000	0.970644000
H	-1.104139000	1.129975000	0.475530000
H	-1.588833000	0.186885000	-1.707265000

H	-1.199924000	-1.447910000	-1.139508000
H	-2.856306000	-3.452111000	-1.076743000
H	-4.466882000	-4.512960000	-2.633410000
H	-6.335628000	-3.203594000	-3.558122000
H	-6.640168000	-0.822314000	-2.940684000
H	-3.431708000	-1.583512000	3.101505000
H	-4.642013000	-1.464295000	1.837034000
H	-4.530192000	0.641552000	3.225823000
H	-5.781202000	2.358827000	2.023140000
H	-3.438186000	3.911629000	2.580357000
H	-4.271302000	2.856511000	3.709865000
H	-3.023184000	3.960245000	4.287040000
H	-1.234209000	2.543826000	3.494354000
H	-0.360632000	0.523094000	2.851450000
H	-1.383025000	-0.705931000	3.555515000
H	-5.041396000	3.221334000	-0.613108000
H	-6.727882000	3.025725000	-0.147834000
O	0.600665000	2.160112000	-0.920469000
O	1.016884000	-2.420526000	0.107600000
O	-6.874628000	1.266376000	-1.944205000

Compound: **12-chair-like**



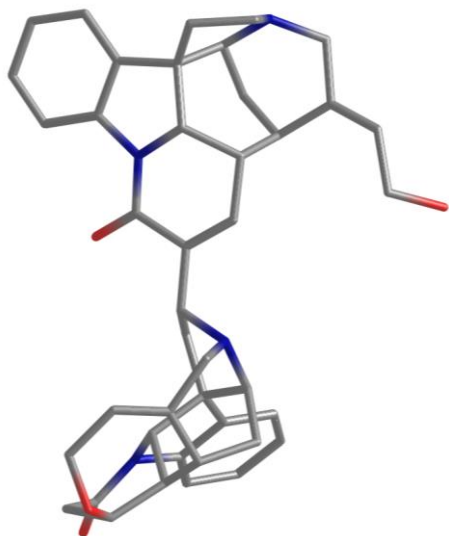
symmetry c1

N	-2.496496000	0.770115000	-1.351853000
C	-3.335378000	-0.109307000	-0.510769000
C	-5.454343000	0.459953000	0.884832000
N	-6.204746000	-0.819913000	0.811757000
C	-6.150372000	-1.322856000	-0.568332000
C	-5.718839000	-0.123979000	-1.398085000
C	-4.720989000	0.587619000	-0.468652000
C	-4.402176000	1.978274000	-0.942475000
C	-5.204584000	3.102700000	-0.947865000
C	-4.727486000	4.274670000	-1.528485000
C	-3.466071000	4.300083000	-2.106059000
C	-2.647328000	3.174132000	-2.115129000
C	-3.131809000	2.019836000	-1.516025000
C	-4.531938000	0.497869000	2.094987000
C	-3.521686000	-0.647522000	1.973601000
C	-2.592923000	-0.271015000	0.813960000
C	-1.374206000	-1.152578000	0.541120000
C	-2.165313000	-3.222286000	1.444772000
C	-3.658582000	-3.115845000	1.585699000
C	-4.274078000	-1.959066000	1.796644000
C	-5.774383000	-1.818423000	1.793961000
C	-1.142176000	0.584769000	-1.393105000
C	-0.627569000	-0.690870000	-0.730212000
N	4.687639000	1.398184000	0.178606000
C	3.764294000	0.392531000	-0.396778000
C	2.552338000	-1.451013000	0.988818000
N	1.421976000	-1.810678000	0.100967000

C	0.890086000	-0.598471000	-0.527087000
C	1.355706000	0.513451000	0.402102000
C	2.775714000	0.058739000	0.763681000
C	3.353560000	0.802250000	1.935871000
C	2.928816000	0.809608000	3.250319000
C	3.584461000	1.622108000	4.171241000
C	4.646452000	2.417640000	3.763519000
C	5.084356000	2.424396000	2.442645000
C	4.423981000	1.599631000	1.542451000
C	3.794098000	-2.290633000	0.720715000
C	4.169692000	-2.167476000	-0.759257000
C	4.576364000	-0.736555000	-1.009224000
C	5.641267000	-0.360016000	-1.704690000
C	4.275897000	-2.608991000	-3.797738000
C	3.057841000	-2.773964000	-2.941369000
C	2.991422000	-2.614011000	-1.623206000
C	1.721363000	-2.874026000	-0.850077000
C	5.804059000	1.793865000	-0.491160000
C	5.968081000	1.104192000	-1.830383000
H	-3.422360000	-1.089966000	-0.981371000
H	-6.168552000	1.283842000	0.948892000
H	-7.116776000	-1.719829000	-0.875906000
H	-5.413946000	-2.130229000	-0.661285000
H	-5.277704000	-0.395048000	-2.355532000
H	-6.562928000	0.540787000	-1.583239000
H	-6.194810000	3.072810000	-0.513025000
H	-5.343223000	5.162061000	-1.536277000
H	-3.105591000	5.211198000	-2.561846000
H	-1.670683000	3.194720000	-2.565554000
H	-5.117378000	0.418151000	3.008947000
H	-4.017437000	1.458134000	2.129628000
H	-2.917566000	-0.711384000	2.883023000
H	-2.188179000	0.714141000	1.072340000
H	-0.692355000	-1.102145000	1.395577000
H	-1.658609000	-2.853810000	2.344243000
H	-1.868842000	-4.258239000	1.301021000
H	-4.245470000	-4.017987000	1.459320000
H	-6.134878000	-1.527439000	2.781334000
H	-6.248374000	-2.767234000	1.550152000
H	-0.821214000	-1.479281000	-1.464085000
H	3.204861000	0.874390000	-1.204559000
H	2.247502000	-1.585777000	2.029713000
H	1.341056000	-0.438302000	-1.514607000
H	1.328847000	1.494762000	-0.062774000

H	0.747822000	0.540643000	1.309329000
H	2.093656000	0.195671000	3.561494000
H	3.263222000	1.636990000	5.202332000
H	5.147416000	3.049195000	4.483244000
H	5.906655000	3.040774000	2.123555000
H	3.612443000	-3.330187000	0.988108000
H	4.609746000	-1.932871000	1.350548000
H	5.032883000	-2.796460000	-0.981134000
H	6.299099000	-1.080689000	-2.170190000
H	4.352830000	-1.592332000	-4.188181000
H	5.190464000	-2.813208000	-3.244687000
H	4.236043000	-3.283457000	-4.650575000
H	2.147364000	-3.067169000	-3.454139000
H	0.875752000	-2.989843000	-1.526749000
H	1.806170000	-3.814745000	-0.302231000
H	5.286869000	1.583891000	-2.541871000
H	6.981647000	1.281976000	-2.171982000
O	-0.393532000	1.368128000	-1.948145000
O	-1.690539000	-2.513201000	0.311361000
O	6.607846000	2.595454000	-0.052714000

Compound: **13-boat-like**



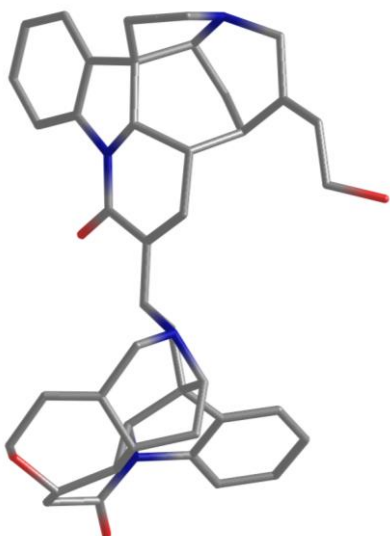
symmetry c1

N	2.622664000	-1.597567000	0.092560000
C	3.500807000	-0.733009000	-0.722632000
C	5.385886000	0.045894000	0.853509000
N	6.229646000	0.988247000	0.086014000
C	6.300391000	0.564636000	-1.312062000
C	6.007872000	-0.927017000	-1.247155000
C	4.924034000	-1.021091000	-0.172463000
C	4.733848000	-2.368508000	0.473965000
C	5.687499000	-3.251814000	0.938885000
C	5.276744000	-4.420806000	1.573970000
C	3.924098000	-4.681887000	1.743514000
C	2.949626000	-3.799195000	1.286957000
C	3.378128000	-2.643912000	0.647207000
C	4.198292000	0.737709000	1.514465000
C	3.491347000	1.598553000	0.465892000
C	3.023044000	0.717947000	-0.747048000
C	1.529626000	0.751588000	-0.884319000
C	2.652764000	4.247333000	-0.876843000
C	4.058297000	3.815611000	-0.593948000
C	4.439671000	2.695551000	0.012810000
C	5.900275000	2.390968000	0.280330000
C	1.269989000	-1.467191000	0.133713000
C	0.723769000	-0.232709000	-0.496181000
N	-4.600501000	-0.614821000	1.235610000
C	-3.797311000	-0.379700000	0.021233000
C	-2.369456000	1.641009000	-0.753148000
N	-1.261919000	0.921479000	-1.430445000

C	-0.781967000	-0.154099000	-0.557996000
C	-1.430484000	0.126800000	0.802248000
C	-2.791978000	0.726531000	0.419376000
C	-3.481762000	1.354435000	1.602499000
C	-3.205030000	2.538174000	2.257213000
C	-3.929653000	2.866639000	3.400728000
C	-4.905959000	2.004263000	3.878998000
C	-5.194551000	0.804021000	3.234596000
C	-4.475194000	0.500939000	2.089073000
C	-3.474772000	1.966281000	-1.745866000
C	-4.064147000	0.648285000	-2.263579000
C	-4.785296000	0.022681000	-1.073210000
C	-5.732839000	-1.146204000	-1.393946000
C	-4.242687000	-2.432269000	-2.829976000
C	-3.040483000	-1.549689000	-2.989834000
C	-2.935159000	-0.244500000	-2.769578000
C	-1.591814000	0.442551000	-2.782863000
C	-5.712803000	-1.410867000	1.126067000
C	-5.797100000	-2.132696000	-0.205725000
H	3.452559000	-1.110380000	-1.749042000
H	5.992260000	-0.451772000	1.613524000
H	7.282783000	0.782459000	-1.729601000
H	5.559060000	1.078108000	-1.938559000
H	5.696601000	-1.352294000	-2.198575000
H	6.896599000	-1.459090000	-0.908346000
H	6.740877000	-3.037515000	0.815818000
H	6.011807000	-5.123959000	1.937095000
H	3.614185000	-5.590793000	2.239144000
H	1.901202000	-4.001070000	1.418318000
H	4.530920000	1.364330000	2.340915000
H	3.526456000	-0.009152000	1.936440000
H	2.606986000	2.051372000	0.912055000
H	3.435920000	1.162449000	-1.651303000
H	1.078125000	1.649613000	-1.288395000
H	1.930985000	3.618300000	-0.351043000
H	2.437972000	4.166398000	-1.943317000
H	4.817778000	4.519785000	-0.920922000
H	6.141076000	2.662676000	1.310556000
H	6.539386000	2.997246000	-0.359750000
H	-3.271348000	-1.293000000	-0.251861000
H	-1.976866000	2.565394000	-0.322473000
H	-1.144817000	-1.126100000	-0.912935000
H	-1.507648000	-0.764737000	1.419253000
H	-0.851961000	0.877008000	1.344720000

H	-2.432333000	3.201175000	1.891332000
H	-3.726307000	3.791796000	3.919741000
H	-5.457987000	2.264928000	4.770674000
H	-5.951620000	0.133336000	3.603346000
H	-3.072492000	2.576287000	-2.552320000
H	-4.248081000	2.557426000	-1.256803000
H	-4.778690000	0.840979000	-3.064143000
H	-5.409519000	0.804094000	-0.630206000
H	-6.729683000	-0.734633000	-1.537400000
H	-4.041027000	-3.155101000	-2.030440000
H	-4.372619000	-3.023524000	-3.736788000
H	-2.150014000	-2.092952000	-3.292234000
H	-0.804581000	-0.239657000	-3.098799000
H	-1.581924000	1.285165000	-3.473665000
H	-4.955725000	-2.824394000	-0.255271000
H	-6.713519000	-2.712317000	-0.225636000
H	2.670556000	5.740165000	0.372123000
O	0.540131000	-2.284472000	0.675143000
O	-6.549687000	-1.516208000	1.999766000
O	2.448802000	5.615834000	-0.553921000
O	-5.477736000	-1.782255000	-2.631569000

Compound: **13-chair-like**



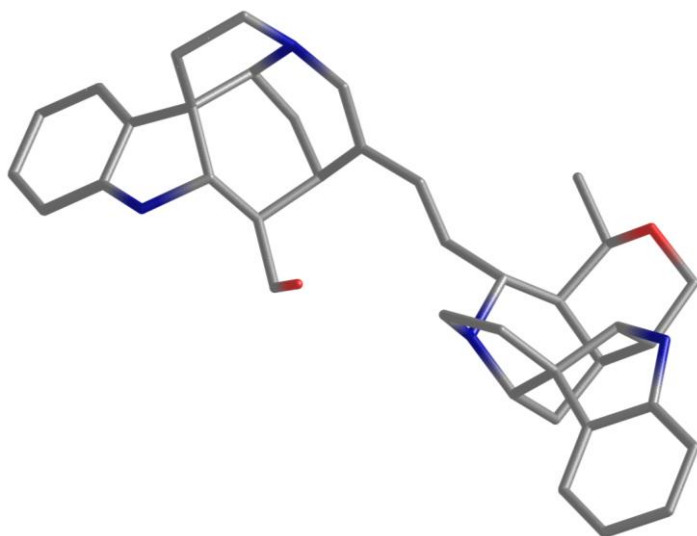
symmetry c1

N	2.589011000	-1.581004000	0.175323000
C	3.473202000	-0.752808000	-0.670200000
C	5.367675000	0.061262000	0.876757000
N	6.217972000	0.970817000	0.077393000
C	6.282155000	0.500832000	-1.306160000
C	5.977568000	-0.985396000	-1.191602000
C	4.894924000	-1.034906000	-0.112840000
C	4.693952000	-2.358206000	0.578597000
C	5.640424000	-3.234243000	1.071154000
C	5.220166000	-4.376911000	1.746670000
C	3.865522000	-4.619215000	1.927822000
C	2.898256000	-3.743472000	1.443455000
C	3.336084000	-2.614675000	0.764018000
C	4.187150000	0.784331000	1.516513000
C	3.485797000	1.616352000	0.441391000
C	3.008635000	0.700786000	-0.742058000
C	1.515369000	0.743454000	-0.879103000
C	2.666249000	4.229766000	-0.980022000
C	4.068801000	3.794437000	-0.687866000
C	4.442206000	2.690318000	-0.047849000
C	5.900775000	2.381851000	0.226243000
C	1.237625000	-1.435745000	0.217203000
C	0.701168000	-0.219123000	-0.455402000
N	-4.688220000	-0.519073000	1.254918000
C	-3.795021000	-0.419446000	0.079894000
C	-2.434083000	1.619182000	-0.787041000
N	-1.274396000	0.934439000	-1.408584000

C	-0.803582000	-0.129078000	-0.518160000
C	-1.448644000	0.198545000	0.830446000
C	-2.824660000	0.743080000	0.421551000
C	-3.528430000	1.434788000	1.556982000
C	-3.232017000	2.640174000	2.163149000
C	-3.979782000	3.047913000	3.264520000
C	-5.000189000	2.241553000	3.749274000
C	-5.307888000	1.021608000	3.153841000
C	-4.562065000	0.638348000	2.048300000
C	-3.558644000	1.831622000	-1.789030000
C	-4.014272000	0.465705000	-2.309001000
C	-4.707760000	-0.230980000	-1.133369000
C	-5.420650000	-1.564794000	-1.386484000
C	-4.211459000	-2.273350000	-3.334940000
C	-2.915747000	-1.511117000	-3.361352000
C	-2.816007000	-0.279928000	-2.877135000
C	-1.510384000	0.465347000	-2.776469000
C	-5.819991000	-1.284105000	1.163494000
C	-5.859019000	-2.193497000	-0.046669000
H	3.419710000	-1.163840000	-1.683357000
H	5.971309000	-0.416266000	1.651720000
H	7.265342000	0.696773000	-1.732615000
H	5.543574000	0.999454000	-1.947707000
H	5.661140000	-1.439292000	-2.127994000
H	6.862528000	-1.513252000	-0.836749000
H	6.695502000	-3.034354000	0.938590000
H	5.949420000	-5.074185000	2.132181000
H	3.548234000	-5.507803000	2.454639000
H	1.848267000	-3.930967000	1.583309000
H	4.526520000	1.434765000	2.321523000
H	3.509887000	0.057282000	1.963570000
H	2.605655000	2.090387000	0.873498000
H	3.424596000	1.111655000	-1.660657000
H	1.071895000	1.631843000	-1.312517000
H	1.940400000	3.624941000	-0.431903000
H	2.446949000	4.116430000	-2.042628000
H	4.833454000	4.481430000	-1.038467000
H	6.146076000	2.685058000	1.246602000
H	6.543621000	2.961499000	-0.434441000
H	-3.239718000	-1.351773000	-0.036997000
H	-2.107155000	2.586905000	-0.399799000
H	-1.176502000	-1.107006000	-0.850038000
H	-1.501545000	-0.663643000	1.489640000
H	-0.883596000	0.988474000	1.329194000

H	-2.425152000	3.258434000	1.792439000
H	-3.760801000	3.989636000	3.746029000
H	-5.571476000	2.562301000	4.608677000
H	-6.097633000	0.394979000	3.530012000
H	-3.216644000	2.471653000	-2.600269000
H	-4.384173000	2.349574000	-1.301028000
H	-4.752740000	0.598169000	-3.104563000
H	-5.499868000	0.457136000	-0.819128000
H	-6.295778000	-1.375114000	-2.015829000
H	-4.100326000	-3.234939000	-3.829095000
H	-5.001100000	-1.720052000	-3.856019000
H	-2.036104000	-2.012388000	-3.746837000
H	-0.677443000	-0.172372000	-3.068716000
H	-1.507166000	1.321694000	-3.452408000
H	-5.161712000	-3.010008000	0.150624000
H	-6.855133000	-2.618733000	-0.103774000
H	2.698733000	5.761257000	0.220817000
O	0.502673000	-2.224249000	0.792516000
O	-6.708767000	-1.261011000	1.992840000
O	2.476120000	5.609898000	-0.700996000
O	-4.626536000	-2.557585000	-2.007359000

Compound: **14a**



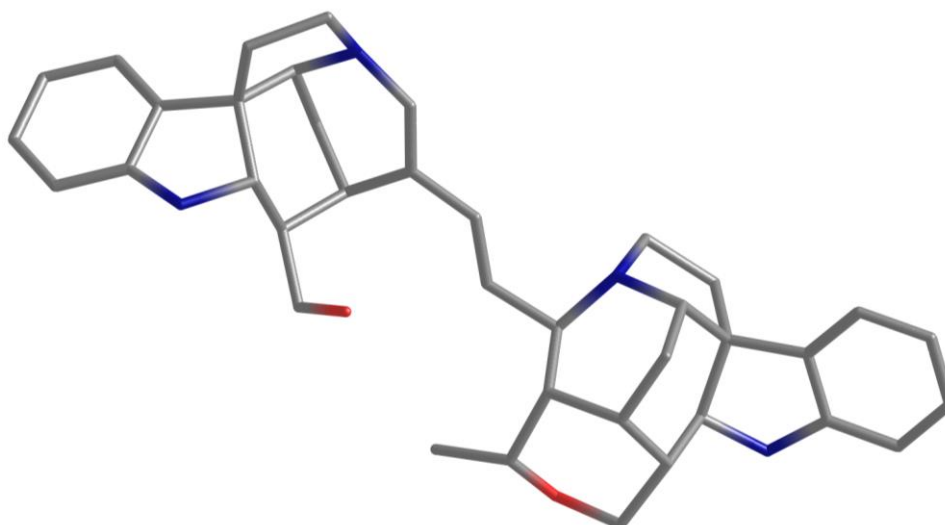
symmetry c1

N	-4.871800000	-2.191676000	0.152680000
C	-4.112010000	-0.955404000	0.406792000
C	-4.859806000	1.510625000	0.577402000
N	-4.053683000	1.810429000	1.761917000
C	-4.739742000	1.178960000	2.898332000
C	-5.557130000	0.006132000	2.293821000
C	-5.250688000	0.040461000	0.776157000
C	-6.389158000	-0.494514000	-0.054804000
C	-7.579110000	0.082277000	-0.445158000
C	-8.495127000	-0.675590000	-1.177371000
C	-8.205442000	-1.995610000	-1.494439000
C	-7.009373000	-2.590940000	-1.099689000
C	-6.105996000	-1.825279000	-0.378386000
C	-4.103980000	1.814275000	-0.697705000
C	-2.843545000	0.949599000	-0.720924000
C	-3.295284000	-0.525991000	-0.824131000
C	-2.173605000	-1.523029000	-1.119796000
C	0.224647000	0.924065000	-0.480287000
C	-0.586034000	1.221100000	0.538779000
C	-2.038005000	1.269615000	0.520662000
C	-2.689493000	1.613107000	1.649483000
N	5.957130000	0.405910000	1.283985000
C	4.681319000	0.566408000	0.562376000
C	3.316932000	-1.106582000	-0.871741000
N	1.980147000	-0.680196000	-0.454797000
C	1.841154000	-1.319182000	0.860732000
C	3.259948000	-1.359660000	1.499716000

C	4.212724000	-0.905989000	0.365130000
C	5.530741000	-1.638614000	0.348683000
C	5.846248000	-2.917431000	-0.062858000
C	7.161012000	-3.369045000	0.060555000
C	8.132809000	-2.536137000	0.598702000
C	7.824523000	-1.247088000	1.025762000
C	6.514416000	-0.810916000	0.894538000
C	3.792142000	-0.411052000	-2.121388000
C	3.837879000	1.073864000	-1.832930000
C	4.873403000	1.370865000	-0.739168000
C	4.835875000	2.863486000	-0.434078000
C	1.331690000	3.827328000	-0.719674000
C	2.586951000	3.088289000	-1.131040000
C	2.436503000	1.595825000	-1.476452000
C	1.719123000	0.782534000	-0.377117000
H	-4.378571000	-2.944467000	-0.301657000
H	-3.433989000	-1.103256000	1.245206000
H	-5.767213000	2.117839000	0.636846000
H	-5.404792000	1.899168000	3.371264000
H	-4.011413000	0.853833000	3.635988000
H	-5.297798000	-0.957433000	2.726571000
H	-6.621092000	0.167287000	2.455058000
H	-7.804628000	1.110020000	-0.190303000
H	-9.427752000	-0.235177000	-1.497661000
H	-8.918825000	-2.575830000	-2.062865000
H	-6.791889000	-3.619187000	-1.352459000
H	-3.846049000	2.872401000	-0.726138000
H	-4.741127000	1.596870000	-1.555245000
H	-2.259947000	1.188680000	-1.610801000
H	-3.963714000	-0.571428000	-1.691852000
H	-1.572199000	-1.151091000	-1.954390000
H	-2.607519000	-2.467598000	-1.449435000
H	-0.179260000	0.690114000	-1.460519000
H	-0.129203000	1.450941000	1.499128000
H	-2.137492000	1.791130000	2.565163000
H	6.573052000	1.206011000	1.279959000
H	3.983792000	1.104471000	1.200731000
H	3.249455000	-2.183928000	-1.048787000
H	1.117703000	-0.785382000	1.473172000
H	1.466877000	-2.332675000	0.719752000
H	3.502888000	-2.371141000	1.818439000
H	3.349313000	-0.712231000	2.369965000
H	5.086014000	-3.566481000	-0.478399000
H	7.423158000	-4.365157000	-0.264263000

H	9.149934000	-2.891239000	0.688185000
H	8.585762000	-0.605043000	1.446312000
H	3.110941000	-0.626430000	-2.945144000
H	4.781049000	-0.783830000	-2.393234000
H	4.157670000	1.614632000	-2.727606000
H	5.857349000	1.116772000	-1.144304000
H	5.476002000	3.121352000	0.409785000
H	5.176765000	3.432783000	-1.306587000
H	1.544261000	4.893070000	-0.663685000
H	0.530602000	3.661269000	-1.437722000
H	0.989259000	3.491069000	0.255535000
H	2.992625000	3.565759000	-2.033464000
H	1.832137000	1.530174000	-2.386257000
H	2.034830000	1.177564000	0.596687000
O	-1.352990000	-1.837422000	-0.012165000
O	3.529228000	3.271728000	-0.080826000
H	-0.728499000	-1.114481000	0.115544000

Compound: **14b**



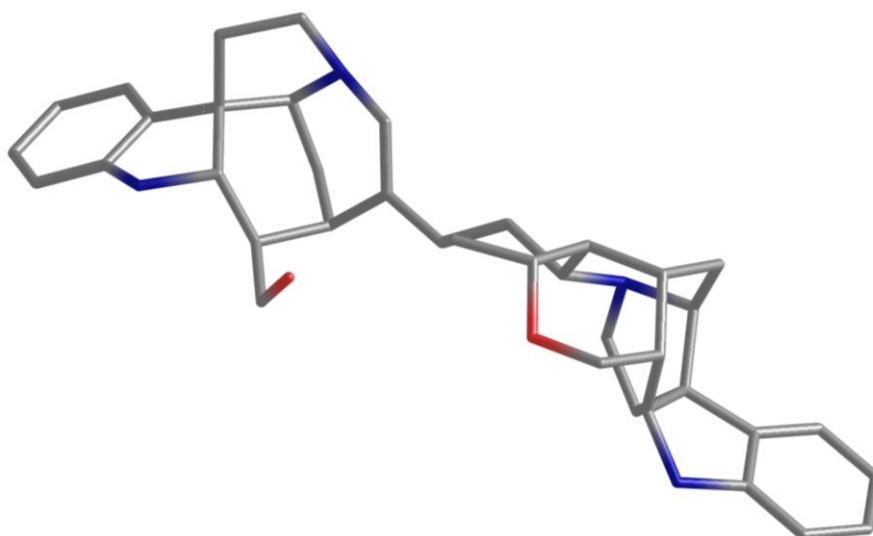
symmetry c1

N	5.466516000	1.120202000	1.278906000
C	4.434204000	0.188231000	0.793378000
C	4.575663000	-1.882369000	-0.738897000
N	3.695771000	-2.707990000	0.089252000
C	4.481298000	-3.103717000	1.267416000
C	5.579271000	-2.017512000	1.419654000
C	5.300589000	-1.001273000	0.285875000
C	6.547122000	-0.284346000	-0.166031000
C	7.574542000	-0.682060000	-0.995130000
C	8.654942000	0.178125000	-1.200492000
C	8.688649000	1.411955000	-0.565416000
C	7.659708000	1.821353000	0.279817000
C	6.589877000	0.960178000	0.470078000
C	3.796300000	-1.138573000	-1.801862000
C	2.775543000	-0.241066000	-1.101309000
C	3.567351000	0.822958000	-0.306639000
C	2.708221000	1.959778000	0.239653000
C	-0.246754000	0.172020000	-0.502137000
C	0.467211000	-0.864917000	-0.048040000
C	1.883564000	-1.126297000	-0.255015000
C	2.414226000	-2.234910000	0.300818000
N	-6.191486000	0.824448000	-1.217245000
C	-4.804210000	0.750065000	-0.723796000
C	-3.603653000	-1.029458000	0.718993000
N	-2.307443000	-0.975659000	0.049361000
C	-2.539706000	-1.767001000	-1.165502000
C	-4.029128000	-1.551745000	-1.567151000
C	-4.643130000	-0.760751000	-0.384630000

C	-6.064778000	-1.148727000	-0.065368000
C	-6.575056000	-2.260513000	0.573243000
C	-7.957384000	-2.392057000	0.714397000
C	-8.802434000	-1.413056000	0.209350000
C	-8.299706000	-0.290838000	-0.444187000
C	-6.924014000	-0.172405000	-0.574984000
C	-3.682209000	-0.113788000	1.912415000
C	-3.451922000	1.297093000	1.419231000
C	-4.581115000	1.709878000	0.462306000
C	-4.285969000	3.110857000	-0.057138000
C	-0.667823000	3.296459000	-0.401864000
C	-1.957587000	2.879906000	0.267992000
C	-2.053009000	1.433376000	0.788925000
C	-1.739388000	0.347096000	-0.275900000
H	5.171019000	2.063990000	1.474818000
H	3.793703000	-0.117720000	1.618686000
H	5.310541000	-2.547354000	-1.200907000
H	4.934035000	-4.078969000	1.098443000
H	3.833088000	-3.175775000	2.136327000
H	5.565681000	-1.535420000	2.394480000
H	6.564659000	-2.457244000	1.279289000
H	7.547769000	-1.647539000	-1.484113000
H	9.463018000	-0.115220000	-1.854160000
H	9.527490000	2.073496000	-0.730850000
H	7.693999000	2.784874000	0.768694000
H	3.297222000	-1.852639000	-2.455932000
H	4.484654000	-0.547410000	-2.406261000
H	2.173905000	0.275868000	-1.850545000
H	4.247040000	1.290134000	-1.028599000
H	2.080554000	2.343046000	-0.571924000
H	3.343108000	2.787702000	0.555861000
H	0.236875000	0.926446000	-1.108566000
H	-0.062772000	-1.612423000	0.531841000
H	1.811561000	-2.859790000	0.949552000
H	-6.606021000	1.744593000	-1.242018000
H	-4.129884000	1.033250000	-1.529310000
H	-3.737467000	-2.067558000	1.038704000
H	-1.839113000	-1.478931000	-1.944618000
H	-2.366915000	-2.819616000	-0.940576000
H	-4.533786000	-2.508531000	-1.684996000
H	-4.138281000	-1.007037000	-2.503105000
H	-5.914446000	-3.024227000	0.963491000
H	-8.369808000	-3.253615000	1.218496000
H	-9.871917000	-1.519622000	0.325532000

H	-8.963946000	0.466519000	-0.836407000
H	-2.926976000	-0.398279000	2.645664000
H	-4.662913000	-0.205313000	2.382050000
H	-3.482194000	1.992228000	2.262350000
H	-5.506319000	1.735625000	1.045725000
H	-4.994638000	3.418316000	-0.826337000
H	-4.339812000	3.835021000	0.763907000
H	-0.677070000	4.372726000	-0.562006000
H	0.183259000	3.039077000	0.225704000
H	-0.563840000	2.816142000	-1.372829000
H	-2.103178000	3.518548000	1.149706000
H	-1.324294000	1.327285000	1.597788000
H	-2.153001000	0.714895000	-1.225900000
O	1.925083000	1.624898000	1.369033000
O	-3.004731000	3.162129000	-0.652010000
H	1.263256000	0.975537000	1.102442000

Compound: **14c**



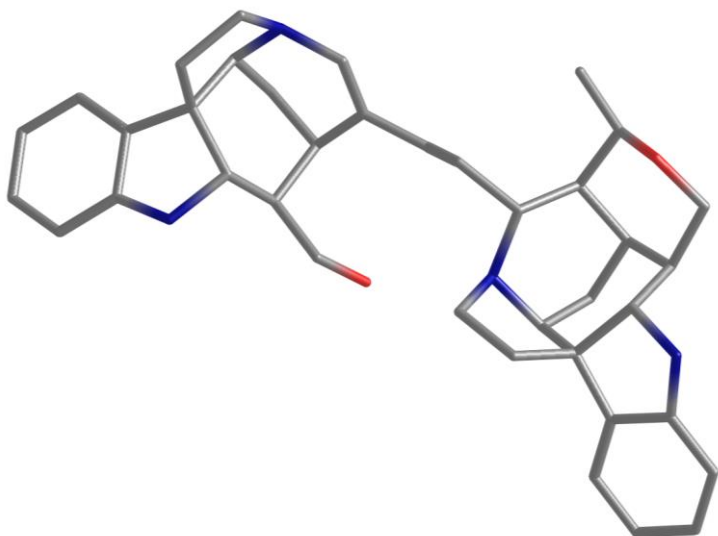
symmetry c1

N	5.752881000	1.102566000	-1.365615000
C	4.655448000	0.640299000	-0.497886000
C	4.574083000	-1.075634000	1.407678000
N	3.703425000	-0.228422000	2.229036000
C	4.528193000	0.886785000	2.724730000
C	5.757480000	0.943935000	1.782669000
C	5.431681000	-0.056334000	0.653724000
C	6.658007000	-0.550547000	-0.065896000
C	7.597541000	-1.497902000	0.283270000
C	8.682541000	-1.724381000	-0.565079000
C	8.808967000	-0.993425000	-1.738653000
C	7.870017000	-0.029306000	-2.097948000
C	6.794349000	0.182625000	-1.248883000
C	3.789001000	-2.019917000	0.524247000
C	2.843299000	-1.184046000	-0.333562000
C	3.687665000	-0.283153000	-1.262722000
C	2.830728000	0.524523000	-2.241331000
C	-0.499529000	-0.054678000	1.078866000
C	0.517472000	-0.242168000	0.238591000
C	1.924775000	-0.417728000	0.597707000
C	2.440784000	0.063576000	1.745165000
N	-5.748074000	0.395508000	-1.814525000
C	-4.613589000	0.454565000	-0.874821000
C	-4.115614000	-0.923746000	1.267682000
N	-2.665980000	-1.044431000	1.116318000
C	-2.547082000	-2.121743000	0.127441000
C	-3.750094000	-1.970784000	-0.849157000

C	-4.680533000	-0.932939000	-0.166941000
C	-6.148473000	-1.258693000	-0.285383000
C	-6.916401000	-2.204438000	0.363006000
C	-8.269412000	-2.322672000	0.041792000
C	-8.827018000	-1.497468000	-0.925684000
C	-8.060525000	-0.545753000	-1.593084000
C	-6.717719000	-0.438299000	-1.261902000
C	-4.517983000	0.260578000	2.107903000
C	-4.016619000	1.507327000	1.413168000
C	-4.723732000	1.675372000	0.060932000
C	-4.152545000	2.908386000	-0.628245000
C	-0.607798000	2.941361000	0.207301000
C	-2.080142000	2.743829000	0.502997000
C	-2.483763000	1.476307000	1.279709000
C	-1.929795000	0.166865000	0.671713000
H	5.499069000	1.390458000	-2.298554000
H	4.104525000	1.498342000	-0.117106000
H	5.223034000	-1.639364000	2.083625000
H	4.839597000	0.701413000	3.751103000
H	3.948377000	1.806072000	2.707299000
H	5.948117000	1.941874000	1.394311000
H	6.651702000	0.611583000	2.307094000
H	7.497343000	-2.062552000	1.201464000
H	9.422305000	-2.468700000	-0.310085000
H	9.650702000	-1.176182000	-2.391880000
H	7.976736000	0.534176000	-3.014252000
H	3.226163000	-2.723330000	1.136437000
H	4.485918000	-2.587639000	-0.093708000
H	2.244477000	-1.838650000	-0.968460000
H	4.294972000	-0.962796000	-1.870197000
H	2.068443000	-0.133858000	-2.670718000
H	3.439776000	0.884890000	-3.070288000
H	-0.336817000	-0.110589000	2.151008000
H	0.296320000	-0.258413000	-0.828379000
H	1.851902000	0.708017000	2.388421000
H	-6.067949000	1.279462000	-2.182550000
H	-3.692266000	0.543738000	-1.445916000
H	-4.446776000	-1.848674000	1.748567000
H	-1.580721000	-2.080730000	-0.367802000
H	-2.612594000	-3.078048000	0.645474000
H	-4.262828000	-2.922291000	-0.973247000
H	-3.447110000	-1.632158000	-1.838254000
H	-6.478900000	-2.849333000	1.114436000
H	-8.883070000	-3.053883000	0.547002000

H	-9.876582000	-1.591682000	-1.166936000
H	-8.500860000	0.091078000	-2.347496000
H	-4.084819000	0.167729000	3.104214000
H	-5.604035000	0.285851000	2.211476000
H	-4.262635000	2.388697000	2.011375000
H	-5.785008000	1.843307000	0.266761000
H	-4.540674000	3.026839000	-1.639952000
H	-4.408864000	3.808585000	-0.057603000
H	-0.445552000	3.954527000	-0.154867000
H	-0.001315000	2.778582000	1.096968000
H	-0.285044000	2.248315000	-0.565743000
H	-2.429648000	3.588252000	1.112606000
H	-2.075222000	1.569542000	2.290630000
H	-1.963342000	0.260703000	-0.421303000
O	2.231252000	1.680590000	-1.680777000
O	-2.748271000	2.806649000	-0.751497000
H	1.841548000	1.448892000	-0.831954000

Compound: **14d**



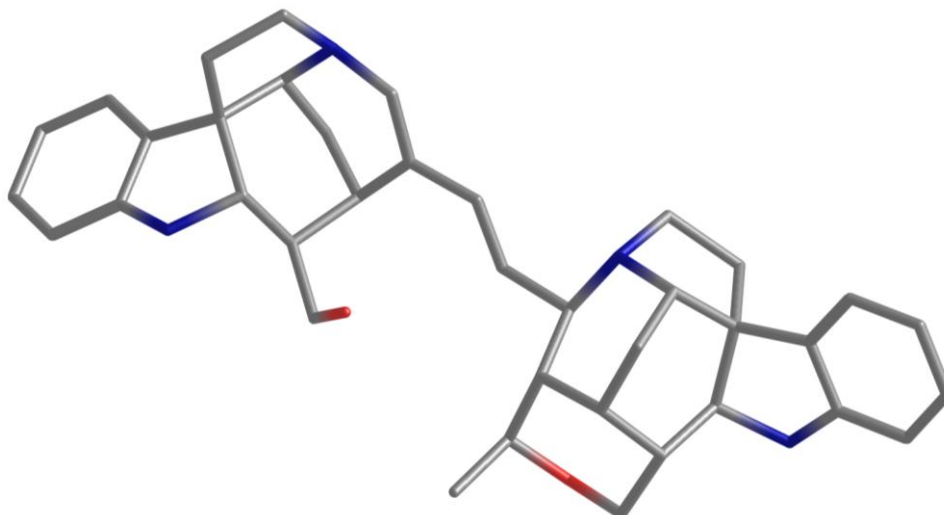
symmetry c1

N	4.494435000	-1.884834000	-1.127039000
C	3.885497000	-0.624993000	-0.658830000
C	4.913214000	1.425755000	0.540555000
N	4.171909000	2.436322000	-0.219235000
C	4.784386000	2.464661000	-1.556687000
C	5.458880000	1.079028000	-1.752454000
C	5.134588000	0.287013000	-0.463485000
C	6.193655000	-0.727766000	-0.118089000
C	7.438776000	-0.578885000	0.457438000
C	8.250659000	-1.701705000	0.623465000
C	7.805111000	-2.948017000	0.203784000
C	6.553884000	-3.108620000	-0.385842000
C	5.755938000	-1.985085000	-0.540497000
C	4.189513000	1.010957000	1.801592000
C	2.827391000	0.460830000	1.402030000
C	3.018075000	-0.841080000	0.598760000
C	1.688356000	-1.461759000	0.155712000
C	-0.236161000	1.505887000	-0.355653000
C	0.627452000	1.427660000	0.650346000
C	2.087168000	1.500434000	0.591199000
C	2.777632000	2.353875000	-0.175350000
N	-5.966132000	-0.078293000	-1.260356000
C	-4.666838000	0.369920000	-0.727768000
C	-2.922918000	-0.877130000	0.739388000
N	-1.697818000	-0.339159000	0.137491000
C	-1.585916000	-1.130385000	-1.101358000
C	-3.033497000	-1.423506000	-1.585550000

C	-3.941920000	-0.973807000	-0.411199000
C	-5.111709000	-1.892798000	-0.158651000
C	-5.165953000	-3.140664000	0.428469000
C	-6.391926000	-3.801519000	0.513654000
C	-7.538318000	-3.204885000	0.005740000
C	-7.494306000	-1.950464000	-0.596575000
C	-6.269075000	-1.304616000	-0.672371000
C	-3.378652000	-0.079533000	1.934923000
C	-3.679455000	1.328698000	1.466781000
C	-4.849977000	1.319586000	0.473596000
C	-5.064427000	2.743321000	-0.026919000
C	-1.718508000	4.165640000	-0.326194000
C	-2.813445000	3.366682000	0.347545000
C	-2.414809000	1.981946000	0.886578000
C	-1.694741000	1.123775000	-0.174383000
H	3.911180000	-2.706149000	-1.070152000
H	3.253024000	-0.212571000	-1.446609000
H	5.889309000	1.854982000	0.783079000
H	5.531781000	3.254873000	-1.603145000
H	4.026188000	2.674593000	-2.306556000
H	5.107062000	0.557270000	-2.639934000
H	6.536870000	1.197052000	-1.843817000
H	7.785359000	0.394502000	0.780297000
H	9.223976000	-1.602077000	1.080749000
H	8.438126000	-3.813809000	0.339050000
H	6.214111000	-4.082455000	-0.709470000
H	4.075877000	1.869157000	2.462939000
H	4.781571000	0.257079000	2.322283000
H	2.242127000	0.215318000	2.287631000
H	3.537338000	-1.548506000	1.254028000
H	1.874520000	-2.450417000	-0.275834000
H	1.262199000	-0.840919000	-0.635796000
H	0.114055000	1.719860000	-1.359381000
H	0.235711000	1.133354000	1.622082000
H	2.269568000	3.088043000	-0.789706000
H	-6.702986000	0.611798000	-1.269959000
H	-4.138568000	0.908789000	-1.510926000
H	-2.680274000	-1.899554000	1.043827000
H	-0.983926000	-0.602052000	-1.836966000
H	-1.077165000	-2.066232000	-0.867081000
H	-3.158924000	-2.486029000	-1.781451000
H	-3.284960000	-0.890733000	-2.500454000
H	-4.270894000	-3.605456000	0.821861000
H	-6.449724000	-4.775226000	0.977234000

H	-8.485404000	-3.720878000	0.079103000
H	-8.390301000	-1.493039000	-0.992238000
H	-2.596197000	-0.078580000	2.694966000
H	-4.267191000	-0.543436000	2.365955000
H	-3.990149000	1.941303000	2.317112000
H	-5.740491000	0.997211000	1.020987000
H	-5.821394000	2.789330000	-0.809928000
H	-5.389294000	3.386106000	0.799311000
H	-2.092167000	5.159346000	-0.564682000
H	-0.849860000	4.254950000	0.322687000
H	-1.407711000	3.686726000	-1.253155000
H	-3.183733000	3.936154000	1.210573000
H	-1.726197000	2.142485000	1.718861000
H	-2.205774000	1.292553000	-1.127386000
O	0.763230000	-1.597430000	1.215560000
O	-3.875875000	3.259379000	-0.592849000
H	-0.038015000	-1.089256000	0.990096000

Compound: **15a**



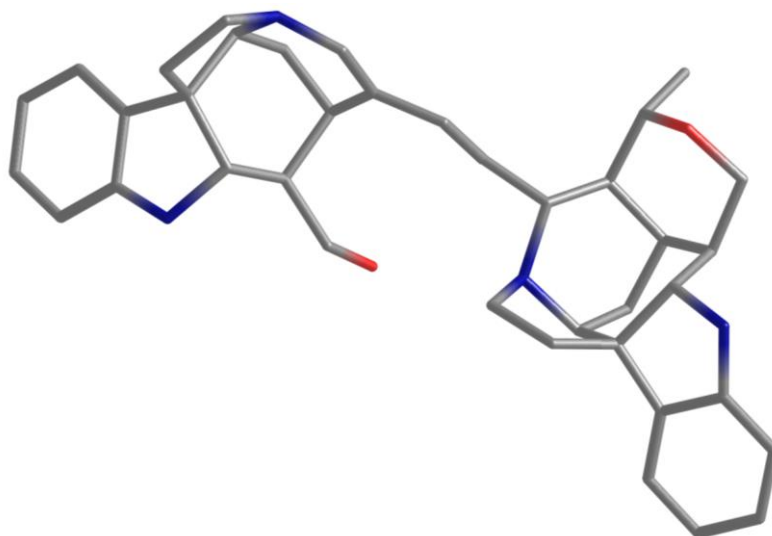
symmetry c1

N	5.230329000	1.182257000	1.278416000
C	4.302898000	0.161631000	0.760639000
C	4.682896000	-1.893414000	-0.750658000
N	3.850442000	-2.792080000	0.051933000
C	4.626256000	-3.107790000	1.261116000
C	5.616953000	-1.927291000	1.442423000
C	5.289203000	-0.946197000	0.291287000
C	6.481486000	-0.121421000	-0.122074000
C	7.568035000	-0.425464000	-0.914681000
C	8.574175000	0.527552000	-1.084907000
C	8.476599000	1.758925000	-0.451829000
C	7.386754000	2.074683000	0.356301000
C	6.391446000	1.121997000	0.511208000
C	3.879003000	-1.224914000	-1.844402000
C	2.758815000	-0.418301000	-1.187284000
C	3.420765000	0.717025000	-0.370721000
C	2.451073000	1.779786000	0.148916000
C	-0.255121000	-0.199731000	-0.663813000
C	0.491466000	-1.191462000	-0.167196000
C	1.921512000	-1.374297000	-0.363065000
C	2.526265000	-2.428192000	0.220724000
N	-6.094026000	0.877660000	-1.276640000
C	-4.697680000	0.727204000	-0.826946000
C	-3.638043000	-1.016101000	0.798750000
N	-2.337509000	-1.196340000	0.151697000
C	-2.671696000	-2.106335000	-0.951920000
C	-4.095487000	-1.710482000	-1.443000000
C	-4.643261000	-0.758826000	-0.344454000

C	-6.086349000	-1.009406000	0.016883000
C	-6.664792000	-2.031452000	0.742219000
C	-8.048855000	-2.046511000	0.918005000
C	-8.829139000	-1.042413000	0.360695000
C	-8.258541000	-0.012220000	-0.381647000
C	-6.880893000	-0.009589000	-0.546616000
C	-3.622592000	0.037527000	1.876253000
C	-3.252245000	1.356113000	1.230836000
C	-4.335365000	1.787845000	0.235589000
C	-3.870086000	3.073279000	-0.440257000
C	-1.168094000	3.692679000	0.758114000
C	-1.546354000	2.549540000	-0.172639000
C	-1.867323000	1.247829000	0.578411000
C	-1.718023000	0.030714000	-0.369287000
H	4.846832000	2.095511000	1.466187000
H	3.664720000	-0.199361000	1.565054000
H	5.489788000	-2.492367000	-1.182096000
H	3.955764000	-3.232215000	2.107131000
H	5.168929000	-4.040436000	1.117681000
H	6.641958000	-2.278464000	1.341323000
H	5.524946000	-1.443198000	2.412124000
H	7.644869000	-1.389709000	-1.401101000
H	9.427430000	0.306553000	-1.709082000
H	9.258218000	2.492984000	-0.589865000
H	7.317694000	3.037171000	0.843556000
H	3.467095000	-1.981990000	-2.510784000
H	4.533557000	-0.578081000	-2.429337000
H	2.144112000	0.037068000	-1.964567000
H	4.080738000	1.240559000	-1.072045000
H	1.794072000	2.093672000	-0.669739000
H	3.007473000	2.666484000	0.453332000
H	0.201713000	0.531682000	-1.319858000
H	-0.001948000	-1.926514000	0.460647000
H	1.959737000	-3.092423000	0.863236000
H	-6.435057000	1.824739000	-1.353974000
H	-4.044344000	0.867393000	-1.684968000
H	-3.893970000	-1.985873000	1.234795000
H	-1.916633000	-2.049943000	-1.731666000
H	-2.682362000	-3.126826000	-0.569688000
H	-4.726433000	-2.591855000	-1.536714000
H	-4.078072000	-1.217658000	-2.413427000
H	-6.055502000	-2.815445000	1.173792000
H	-8.513144000	-2.837351000	1.488669000
H	-9.900547000	-1.057353000	0.504209000

H	-8.872550000	0.763815000	-0.816922000
H	-2.901744000	-0.234080000	2.647949000
H	-4.608790000	0.100032000	2.339769000
H	-3.195491000	2.131204000	1.997672000
H	-5.240662000	2.001047000	0.811830000
H	-4.549227000	3.379903000	-1.236270000
H	-3.826938000	3.886457000	0.290927000
H	-1.911791000	3.872236000	1.531820000
H	-0.225640000	3.449490000	1.247536000
H	-1.039706000	4.609252000	0.184810000
H	-0.703331000	2.382675000	-0.842222000
H	-1.138299000	1.130227000	1.384131000
H	-2.182509000	0.316890000	-1.323033000
O	1.696414000	1.393732000	1.281177000
O	-2.609575000	2.895815000	-1.060193000
H	1.101701000	0.682119000	1.017626000

Compound: **15b**



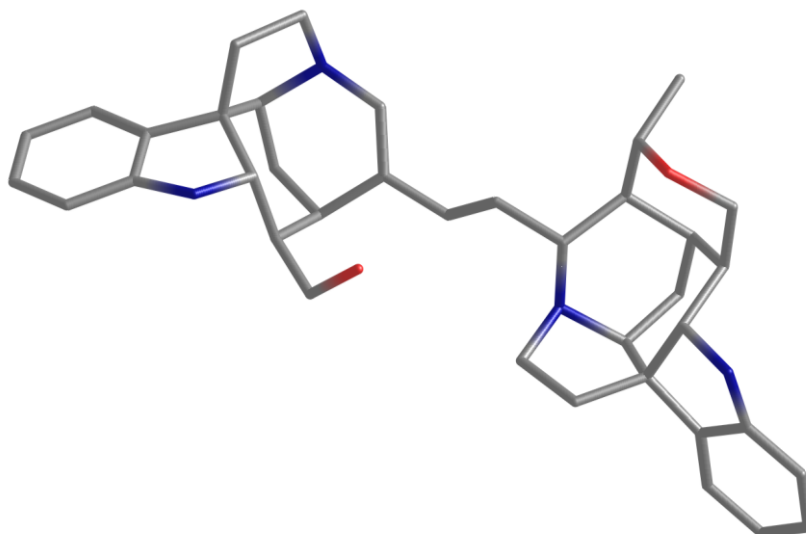
symmetry c1

N	-4.704107000	-2.156816000	0.514698000
C	-4.040742000	-0.844406000	0.641985000
C	-4.929249000	1.557089000	0.309551000
N	-4.237042000	2.107167000	1.477460000
C	-4.968680000	1.622202000	2.657940000
C	-5.700461000	0.332015000	2.199872000
C	-5.259902000	0.121639000	0.732628000
C	-6.287523000	-0.615979000	-0.085140000
C	-7.465563000	-0.188562000	-0.661991000
C	-8.263753000	-1.110292000	-1.340401000
C	-7.872431000	-2.440068000	-1.420847000
C	-6.689516000	-2.883501000	-0.835222000
C	-5.903541000	-1.955749000	-0.168850000
C	-4.099825000	1.667107000	-0.949162000
C	-2.784820000	0.929179000	-0.722302000
C	-3.083424000	-0.576536000	-0.537152000
C	-1.824187000	-1.418848000	-0.344783000
C	0.194505000	1.223793000	-0.388289000
C	-0.646164000	1.527307000	0.601068000
C	-2.098191000	1.528920000	0.486179000
C	-2.855163000	1.993513000	1.497187000
N	5.773821000	0.055707000	1.476743000
C	4.538411000	0.392203000	0.744414000
C	3.100534000	-1.023542000	-0.892578000
N	1.779876000	-0.539782000	-0.469146000
C	1.557703000	-1.271547000	0.791193000
C	2.950321000	-1.503460000	1.440562000

C	3.965705000	-1.011389000	0.381072000
C	5.225011000	-1.839299000	0.317759000
C	5.456633000	-3.087741000	-0.222652000
C	6.728651000	-3.651512000	-0.117375000
C	7.742491000	-2.958983000	0.531125000
C	7.518628000	-1.702385000	1.087010000
C	6.249826000	-1.153350000	0.972764000
C	3.677617000	-0.245063000	-2.048685000
C	3.836462000	1.198180000	-1.614900000
C	4.836142000	1.311630000	-0.457874000
C	4.875447000	2.767696000	-0.005927000
C	2.923366000	4.238502000	-1.768784000
C	2.621073000	3.201666000	-0.696728000
C	2.465833000	1.780880000	-1.257336000
C	1.657615000	0.932607000	-0.256603000
H	-4.128020000	-2.915326000	0.182512000
H	-3.470268000	-0.813482000	1.572140000
H	-5.869873000	2.103857000	0.198234000
H	-4.273871000	1.446600000	3.474934000
H	-5.689558000	2.371192000	2.981176000
H	-6.778176000	0.478884000	2.236477000
H	-5.461548000	-0.532624000	2.815356000
H	-7.769968000	0.848230000	-0.594894000
H	-9.184228000	-0.789151000	-1.805309000
H	-8.494272000	-3.147306000	-1.951711000
H	-6.390806000	-3.920226000	-0.903678000
H	-3.914832000	2.715512000	-1.180580000
H	-4.654918000	1.229371000	-1.779876000
H	-2.158998000	1.032493000	-1.606002000
H	-3.578488000	-0.916319000	-1.453622000
H	-2.103687000	-2.453940000	-0.124336000
H	-1.281009000	-1.045139000	0.525820000
H	-0.191084000	1.025590000	-1.380989000
H	-0.240258000	1.738992000	1.588269000
H	-2.392526000	2.354227000	2.409237000
H	6.447819000	0.801599000	1.570964000
H	3.865040000	0.914130000	1.420886000
H	2.961471000	-2.069652000	-1.180011000
H	0.875873000	-0.715026000	1.429657000
H	1.090046000	-2.230335000	0.562671000
H	3.100564000	-2.561553000	1.644428000
H	3.070419000	-0.968836000	2.380678000
H	4.664570000	-3.626895000	-0.726752000
H	6.924839000	-4.624750000	-0.542734000

H	8.726568000	-3.400231000	0.606859000
H	8.312439000	-1.170161000	1.592417000
H	3.016079000	-0.318404000	-2.912640000
H	4.642126000	-0.674491000	-2.324901000
H	4.241171000	1.781865000	-2.444380000
H	5.820889000	1.036689000	-0.847430000
H	5.493948000	2.895371000	0.883056000
H	5.299162000	3.394514000	-0.796537000
H	3.104990000	5.206603000	-1.305726000
H	3.789088000	3.977846000	-2.374716000
H	2.067088000	4.329411000	-2.434965000
H	1.689543000	3.483344000	-0.204073000
H	1.887186000	1.840574000	-2.183416000
H	1.985290000	1.197897000	0.754423000
O	-1.001375000	-1.412309000	-1.495680000
O	3.585314000	3.225135000	0.357129000
H	-0.102187000	-1.140990000	-1.253149000

Compound: **15c**



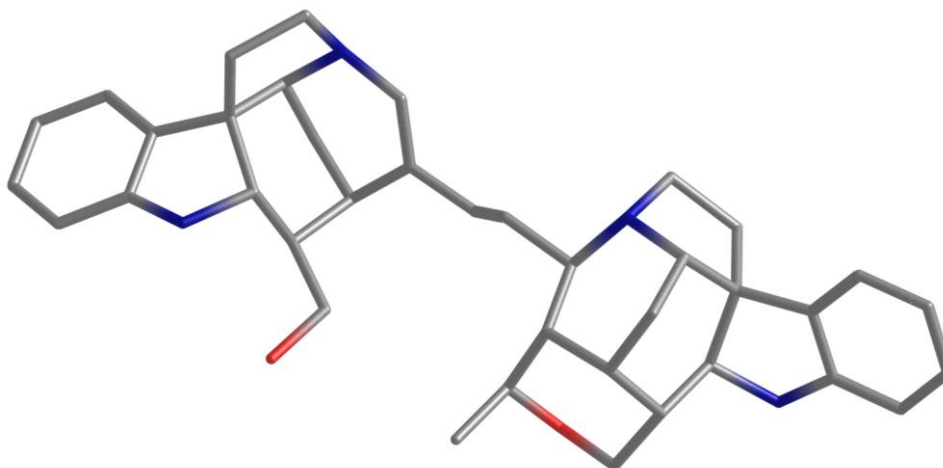
symmetry c1

N	5.054051000	-1.168578000	-1.700064000
C	4.224080000	-0.395429000	-0.760135000
C	4.837191000	0.999622000	1.326554000
N	3.947835000	2.119807000	1.012331000
C	4.590318000	2.851934000	-0.090018000
C	5.504379000	1.822574000	-0.808814000
C	5.287795000	0.491250000	-0.049520000
C	6.496691000	-0.408400000	-0.095649000
C	7.678218000	-0.379385000	0.614872000
C	8.669343000	-1.319551000	0.327111000
C	8.461399000	-2.262349000	-0.670326000
C	7.274835000	-2.297316000	-1.399189000
C	6.296641000	-1.361077000	-1.100012000
C	4.151166000	-0.029632000	2.197170000
C	2.936989000	-0.550612000	1.435136000
C	3.440599000	-1.314813000	0.191549000
C	2.338608000	-2.073803000	-0.557386000
C	-0.244826000	0.957185000	0.129799000
C	0.595242000	0.382645000	0.992947000
C	2.040641000	0.617956000	1.083856000
C	2.595990000	1.820104000	0.864531000
N	-5.790151000	-0.416256000	-1.664817000
C	-4.577937000	0.091717000	-0.996707000
C	-3.498573000	-0.562923000	1.274967000
N	-2.092496000	-0.443718000	0.889030000
C	-1.862596000	-1.693221000	0.149677000
C	-3.196153000	-2.042543000	-0.574248000

C	-4.234222000	-1.049684000	0.010077000
C	-5.593935000	-1.658739000	0.246629000
C	-6.033384000	-2.526901000	1.225385000
C	-7.356382000	-2.970159000	1.201297000
C	-8.212954000	-2.542052000	0.195876000
C	-7.778871000	-1.673748000	-0.802217000
C	-6.461831000	-1.239787000	-0.764094000
C	-4.052830000	0.699022000	1.884924000
C	-3.949906000	1.800746000	0.850997000
C	-4.830001000	1.476646000	-0.363331000
C	-4.624745000	2.572110000	-1.403387000
C	-2.637888000	4.483086000	-0.195544000
C	-2.395183000	3.055858000	-0.668577000
C	-2.479627000	2.025132000	0.469779000
C	-1.736552000	0.724807000	0.072347000
H	4.620049000	-1.971600000	-2.129234000
H	3.519513000	0.220946000	-1.313719000
H	5.710280000	1.412199000	1.839676000
H	3.833372000	3.275373000	-0.744679000
H	5.186875000	3.669612000	0.310673000
H	6.546633000	2.124135000	-0.725324000
H	5.273048000	1.716673000	-1.866321000
H	7.839330000	0.360729000	1.388372000
H	9.596565000	-1.314552000	0.880832000
H	9.232559000	-2.988546000	-0.886308000
H	7.121223000	-3.035931000	-2.173386000
H	3.847962000	0.428649000	3.137854000
H	4.849724000	-0.836571000	2.420638000
H	2.379247000	-1.254119000	2.056676000
H	4.134497000	-2.076494000	0.564009000
H	1.676624000	-2.551431000	0.172890000
H	2.780998000	-2.873159000	-1.151553000
H	0.152462000	1.654540000	-0.601326000
H	0.187715000	-0.361672000	1.670616000
H	1.982789000	2.673049000	0.600096000
H	-6.348057000	0.269819000	-2.152106000
H	-3.789936000	0.191484000	-1.739548000
H	-3.544471000	-1.376795000	2.004262000
H	-1.023417000	-1.588446000	-0.533976000
H	-1.612119000	-2.479221000	0.862357000
H	-3.488096000	-3.068489000	-0.360335000
H	-3.122704000	-1.942854000	-1.655437000
H	-5.363324000	-2.862956000	2.006422000
H	-7.714656000	-3.644004000	1.965509000

H	-9.237585000	-2.886498000	0.185261000
H	-8.450259000	-1.347367000	-1.584122000
H	-3.488228000	0.954152000	2.782116000
H	-5.092792000	0.537689000	2.173512000
H	-4.326359000	2.732445000	1.277433000
H	-5.870263000	1.500551000	-0.025664000
H	-5.142722000	2.345744000	-2.335479000
H	-5.014999000	3.523417000	-1.029672000
H	-3.570191000	4.593741000	0.354176000
H	-1.826531000	4.788705000	0.462918000
H	-2.660699000	5.155256000	-1.051242000
H	-1.403395000	3.021824000	-1.116843000
H	-1.973871000	2.438224000	1.346072000
H	-1.977267000	0.539801000	-0.984122000
O	1.591397000	-1.293358000	-1.472721000
O	-3.256618000	2.694318000	-1.746784000
H	1.087206000	-0.636152000	-0.979252000

Compound: **15d**



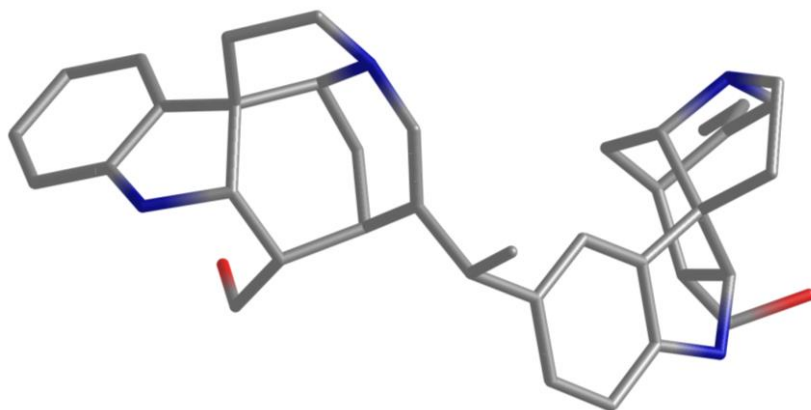
symmetry c1

N	5.108382000	1.190650000	1.181186000
C	4.191627000	0.214329000	0.566883000
C	4.635486000	-1.933667000	-0.809542000
N	3.625968000	-2.757554000	-0.142797000
C	4.186341000	-3.088004000	1.175556000
C	5.186792000	-1.949422000	1.513727000
C	5.137763000	-0.993604000	0.295842000
C	6.448827000	-0.288218000	0.058064000
C	7.619669000	-0.720577000	-0.528918000
C	8.718974000	0.139160000	-0.569794000
C	8.626681000	1.408522000	-0.015156000
C	7.452063000	1.852872000	0.587069000
C	6.365231000	0.991116000	0.616706000
C	4.073143000	-1.239913000	-2.031110000
C	2.926877000	-0.343229000	-1.575954000
C	3.507503000	0.781307000	-0.691807000
C	2.434270000	1.800074000	-0.320145000
C	-0.327153000	-0.763379000	0.187898000
C	0.500347000	-0.767878000	-0.854457000
C	1.909205000	-1.181094000	-0.830543000
C	2.320597000	-2.265748000	-0.158541000
N	-5.848809000	0.815787000	-1.488104000
C	-4.554967000	0.593772000	-0.816532000
C	-3.932828000	-0.988569000	1.156844000
N	-2.592607000	-1.389921000	0.725560000
C	-2.887956000	-2.408306000	-0.289481000
C	-4.186336000	-1.952508000	-1.018185000
C	-4.747995000	-0.800990000	-0.140670000
C	-6.245790000	-0.842445000	0.037567000

C	-7.037297000	-1.675988000	0.801561000
C	-8.423700000	-1.519516000	0.770729000
C	-8.992941000	-0.536163000	-0.027340000
C	-8.205816000	0.304432000	-0.809743000
C	-6.829162000	0.137640000	-0.768145000
C	-3.923147000	0.204290000	2.079240000
C	-3.322066000	1.373515000	1.326750000
C	-4.215720000	1.756799000	0.140251000
C	-3.525471000	2.878872000	-0.627277000
C	-0.911469000	3.393899000	0.801979000
C	-1.327697000	2.162197000	0.010545000
C	-1.889097000	1.036690000	0.893065000
C	-1.759628000	-0.313479000	0.150636000
H	4.756165000	2.136817000	1.203957000
H	3.417666000	-0.065892000	1.282591000
H	5.459042000	-2.594765000	-1.092736000
H	3.387123000	-3.182784000	1.905630000
H	4.708559000	-4.041613000	1.120589000
H	6.191699000	-2.352191000	1.622595000
H	4.938517000	-1.426638000	2.434793000
H	7.690186000	-1.712900000	-0.955974000
H	9.639788000	-0.182083000	-1.033810000
H	9.481441000	2.069452000	-0.052055000
H	7.389253000	2.842533000	1.017390000
H	3.719053000	-1.983485000	-2.744143000
H	4.860251000	-0.656512000	-2.509845000
H	2.447077000	0.119739000	-2.441065000
H	4.269863000	1.296717000	-1.288574000
H	1.756968000	1.372688000	0.419617000
H	1.838997000	2.049040000	-1.204111000
H	0.030700000	-1.070948000	1.166737000
H	0.126639000	-0.402564000	-1.810083000
H	1.612424000	-2.873454000	0.391373000
H	-6.056216000	1.769414000	-1.746779000
H	-3.777835000	0.539663000	-1.574955000
H	-4.354649000	-1.853412000	1.676262000
H	-2.040098000	-2.534657000	-0.958271000
H	-3.062000000	-3.359359000	0.212466000
H	-4.898641000	-2.772492000	-1.078216000
H	-3.996593000	-1.611330000	-2.034247000
H	-6.592494000	-2.444102000	1.421327000
H	-9.053435000	-2.160874000	1.369530000
H	-10.067322000	-0.417279000	-0.043133000
H	-8.655589000	1.065635000	-1.431773000

H	-3.339479000	-0.025880000	2.970974000
H	-4.943580000	0.431952000	2.392221000
H	-3.275195000	2.243843000	1.984638000
H	-5.156659000	2.135088000	0.550458000
H	-4.065460000	3.136684000	-1.538643000
H	-3.471879000	3.779096000	-0.007462000
H	-1.706023000	3.774304000	1.441418000
H	-0.061434000	3.146784000	1.436725000
H	-0.607476000	4.185599000	0.119315000
H	-0.449166000	1.786899000	-0.512065000
H	-1.278792000	0.975902000	1.798946000
H	-2.025923000	-0.135234000	-0.898184000
O	2.956771000	2.985951000	0.268275000
O	-2.232598000	2.483320000	-1.046347000
H	3.399644000	3.494968000	-0.415207000

Compound: **16a**



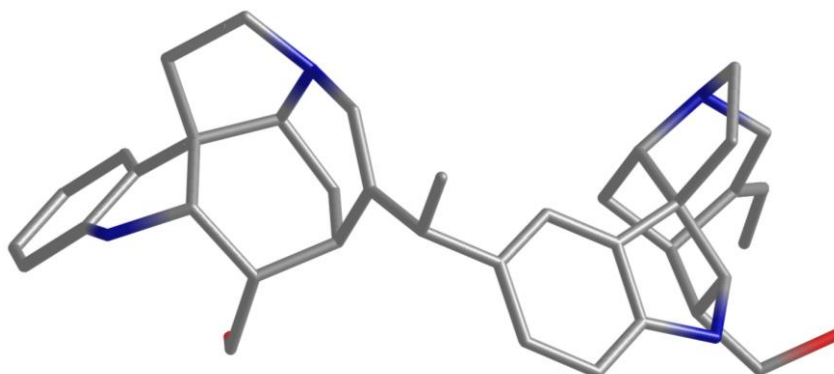
symmetry c1

N	-5.910041000	-0.430093000	-0.724212000
C	-4.589969000	-0.786037000	-0.183198000
C	-2.976542000	0.451478000	1.411795000
N	-2.710599000	-0.723119000	2.246394000
C	-3.933403000	-0.962454000	3.029165000
C	-5.082201000	-0.256918000	2.262743000
C	-4.430894000	0.257373000	0.958806000
C	-5.174900000	1.433311000	0.381233000
C	-5.136242000	2.779706000	0.680207000
C	-5.971212000	3.656003000	-0.016698000
C	-6.833215000	3.168380000	-0.989403000
C	-6.887447000	1.809928000	-1.296236000
C	-6.049278000	0.950639000	-0.601852000
C	-1.969685000	0.574217000	0.290758000
C	-2.071264000	-0.680233000	-0.575665000
C	-3.456744000	-0.791992000	-1.250612000
C	-3.610202000	0.147080000	-2.454665000
C	-1.077644000	-4.315907000	0.536245000
C	-1.115413000	-3.060975000	-0.335503000
C	-1.809944000	-1.883781000	0.304104000
C	-2.172546000	-1.840978000	1.588893000
N	4.209379000	-1.648696000	-1.741425000
C	4.511607000	-0.620030000	-0.728063000
C	3.068983000	0.223718000	1.285669000
N	4.110447000	0.433314000	2.294012000
C	4.372225000	-0.932791000	2.757276000
C	4.226225000	-1.864384000	1.518851000
C	3.537068000	-0.983383000	0.440137000
C	2.428486000	-1.686795000	-0.304080000
C	1.150658000	-2.012650000	0.097578000
C	0.290902000	-2.684704000	-0.778081000

C	0.757037000	-3.015844000	-2.044728000
C	2.050037000	-2.704101000	-2.462764000
C	2.880021000	-2.035814000	-1.577911000
C	2.759492000	1.471352000	0.493628000
C	4.019942000	1.889760000	-0.260410000
C	4.339866000	0.798737000	-1.305995000
C	5.532273000	1.176380000	-2.184986000
C	5.768704000	4.475331000	-0.043218000
C	5.794842000	3.286024000	0.867254000
C	5.093085000	2.155453000	0.772089000
C	5.340724000	1.033517000	1.752439000
H	-6.165473000	-0.839804000	-1.609622000
H	-4.632094000	-1.785145000	0.246157000
H	-2.938220000	1.332455000	2.059034000
H	-4.099031000	-2.031526000	3.137696000
H	-3.828870000	-0.536480000	4.025853000
H	-5.453761000	0.589962000	2.836912000
H	-5.924507000	-0.913620000	2.055884000
H	-4.461014000	3.156928000	1.437170000
H	-5.941837000	4.714061000	0.196737000
H	-7.470556000	3.854525000	-1.528923000
H	-7.554045000	1.440518000	-2.062779000
H	-0.966211000	0.643737000	0.713475000
H	-2.162576000	1.474797000	-0.284141000
H	-1.315253000	-0.645437000	-1.363488000
H	-3.508870000	-1.784155000	-1.712811000
H	-2.859497000	-0.153231000	-3.185382000
H	-4.586917000	-0.009190000	-2.921962000
H	-0.619130000	-5.135457000	-0.013748000
H	-0.482398000	-4.145401000	1.433509000
H	-2.079923000	-4.617778000	0.839022000
H	-1.671364000	-3.307750000	-1.246570000
H	-2.035154000	-2.693580000	2.241448000
H	4.506416000	-1.443551000	-2.683839000
H	5.544643000	-0.741155000	-0.414637000
H	2.176549000	-0.094517000	1.830834000
H	3.624474000	-1.192900000	3.505348000
H	5.351038000	-0.994183000	3.227557000
H	5.184963000	-2.236140000	1.162276000
H	3.612415000	-2.728888000	1.761359000
H	0.792677000	-1.742538000	1.084873000
H	0.092876000	-3.527348000	-2.730469000
H	2.389447000	-2.970805000	-3.454025000
H	2.432998000	2.262503000	1.167870000

H	1.949435000	1.266901000	-0.208329000
H	3.817691000	2.804406000	-0.813657000
H	3.464604000	0.771372000	-1.964195000
H	5.369660000	2.177961000	-2.595978000
H	5.611802000	0.493334000	-3.030933000
H	6.766473000	4.665211000	-0.441261000
H	5.091437000	4.358799000	-0.883885000
H	5.476749000	5.370103000	0.507124000
H	6.489913000	3.365106000	1.697609000
H	5.931196000	1.404661000	2.589028000
H	5.957408000	0.273300000	1.252799000
H	-4.101045000	1.883083000	-1.701320000
H	6.763315000	1.729691000	-0.783359000
O	-3.390099000	1.530145000	-2.245157000
O	6.780683000	1.108056000	-1.518151000

Compound: **16b**



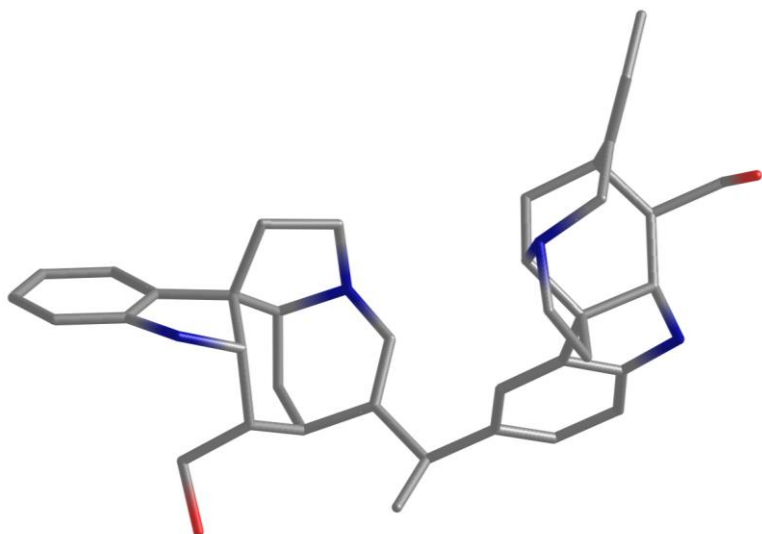
symmetry c1

N	-5.545269000	1.442140000	-1.422809000
C	-4.617685000	0.325879000	-1.097995000
C	-4.618558000	-1.475817000	0.798164000
N	-4.168371000	-2.622078000	0.007695000
C	-5.337845000	-3.025710000	-0.777385000
C	-6.160535000	-1.734117000	-1.025149000
C	-5.452975000	-0.632265000	-0.188354000
C	-6.458062000	0.325566000	0.402077000
C	-7.294030000	0.195803000	1.494994000
C	-8.214441000	1.207175000	1.766485000
C	-8.296575000	2.321274000	0.941757000
C	-7.451024000	2.462529000	-0.155598000
C	-6.536390000	1.456006000	-0.406984000
C	-3.446404000	-0.755493000	1.428818000
C	-2.568797000	-0.219509000	0.301690000
C	-3.322198000	0.883523000	-0.463911000
C	-3.535793000	2.118663000	0.420516000
C	-0.640310000	-2.291433000	-2.419880000
C	-0.871830000	-1.223079000	-1.351060000
C	-2.181094000	-1.360162000	-0.612592000
C	-2.987730000	-2.418016000	-0.726153000
N	3.666486000	-0.937159000	2.062324000
C	4.590662000	-0.127848000	1.246136000
C	4.208113000	1.031135000	-1.067941000
N	4.966737000	2.269197000	-0.878919000
C	4.049109000	3.073610000	-0.066107000
C	3.312906000	2.089734000	0.889273000
C	3.622602000	0.677740000	0.318723000
C	2.423358000	-0.237790000	0.273369000
C	1.326454000	-0.237377000	-0.566028000
C	0.309660000	-1.179627000	-0.393308000

C	0.425264000	-2.102613000	0.642464000
C	1.517826000	-2.109528000	1.504285000
C	2.515859000	-1.165926000	1.308754000
C	5.024814000	-0.064022000	-1.710615000
C	6.189736000	-0.405150000	-0.783888000
C	5.610998000	-1.018408000	0.510168000
C	6.708119000	-1.491477000	1.463860000
C	9.280027000	-0.152496000	-1.199698000
C	8.322886000	0.942570000	-0.840906000
C	7.011156000	0.853810000	-0.614557000
C	6.242384000	2.075737000	-0.169918000
H	-5.930854000	1.391799000	-2.355872000
H	-4.343403000	-0.187873000	-2.015874000
H	-5.293062000	-1.860349000	1.567798000
H	-5.024791000	-3.519011000	-1.693610000
H	-5.928025000	-3.733956000	-0.197669000
H	-7.184697000	-1.866216000	-0.682868000
H	-6.201951000	-1.458719000	-2.077814000
H	-7.247096000	-0.679982000	2.128975000
H	-8.868714000	1.122967000	2.621954000
H	-9.014981000	3.097960000	1.161728000
H	-7.495620000	3.339892000	-0.785543000
H	-2.883044000	-1.455145000	2.046175000
H	-3.806348000	0.042826000	2.076923000
H	-1.659835000	0.220291000	0.716927000
H	-2.690308000	1.227297000	-1.287430000
H	-4.369267000	1.971732000	1.113091000
H	-2.638953000	2.279135000	1.019753000
H	0.290114000	-2.090700000	-2.947722000
H	-0.557547000	-3.279397000	-1.966526000
H	-1.453403000	-2.309845000	-3.145073000
H	-0.892971000	-0.252053000	-1.857478000
H	-2.752276000	-3.238560000	-1.391256000
H	4.068595000	-1.736608000	2.528686000
H	5.132826000	0.543339000	1.906207000
H	3.364934000	1.286858000	-1.714709000
H	3.329904000	3.552539000	-0.729248000
H	4.591988000	3.856231000	0.459003000
H	3.654954000	2.175582000	1.918863000
H	2.242478000	2.282387000	0.885405000
H	1.242933000	0.492986000	-1.363345000
H	-0.363857000	-2.831088000	0.782530000
H	1.582592000	-2.830852000	2.307128000
H	5.390042000	0.271917000	-2.680458000

H	4.398005000	-0.942963000	-1.868193000
H	6.801904000	-1.174819000	-1.249236000
H	5.074267000	-1.915908000	0.183879000
H	7.402593000	-2.137522000	0.917119000
H	6.280257000	-2.091552000	2.267327000
H	9.745515000	0.048826000	-2.164911000
H	10.087185000	-0.199875000	-0.467518000
H	8.814826000	-1.132526000	-1.245826000
H	8.773659000	1.925433000	-0.743116000
H	6.851854000	2.965072000	-0.324415000
H	6.077862000	1.999872000	0.914052000
H	-4.447386000	3.087052000	-0.950516000
H	7.832349000	0.096399000	1.423721000
O	-3.733668000	3.300094000	-0.335003000
O	7.406386000	-0.436960000	2.102492000

Compound: **16c**



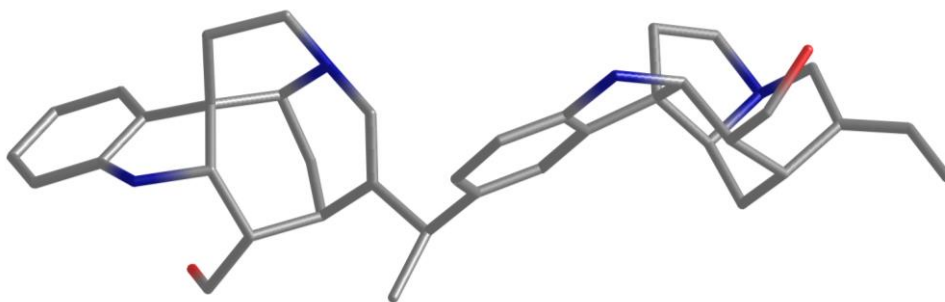
symmetry c1

N	4.202290000	-1.293193000	1.667489000
C	3.466472000	-0.435400000	0.724183000
C	3.529338000	-0.227804000	-1.844992000
N	2.073660000	-0.232182000	-2.003796000
C	1.623433000	-1.605167000	-1.725940000
C	2.755580000	-2.269462000	-0.901946000
C	3.768992000	-1.134688000	-0.630664000
C	5.155184000	-1.669734000	-0.379824000
C	6.143990000	-2.089319000	-1.243684000
C	7.336236000	-2.594224000	-0.719231000
C	7.508459000	-2.680100000	0.655101000
C	6.512245000	-2.266740000	1.538040000
C	5.338703000	-1.758952000	1.004532000
C	4.058861000	1.182561000	-1.708064000
C	3.415630000	1.814450000	-0.473999000
C	3.875743000	1.056535000	0.794921000
C	5.358761000	1.300406000	1.064413000
C	1.465961000	3.322578000	1.319446000
C	1.116099000	2.975490000	-0.135102000
C	1.911531000	1.789767000	-0.654063000
C	1.365764000	0.789077000	-1.353400000
N	-4.488683000	2.218919000	-0.648502000
C	-4.653018000	0.885697000	-0.038933000
C	-2.888004000	-0.644192000	1.139210000
N	-3.703638000	-1.223533000	2.208354000
C	-3.751168000	-0.132511000	3.186873000
C	-3.795521000	1.197264000	2.378715000

C	-3.425749000	0.789624000	0.925906000
C	-2.445792000	1.721637000	0.255617000
C	-1.090150000	1.879346000	0.446271000
C	-0.377998000	2.820567000	-0.307836000
C	-1.074361000	3.590821000	-1.230748000
C	-2.449364000	3.459103000	-1.422748000
C	-3.126481000	2.515197000	-0.669827000
C	-2.854356000	-1.499366000	-0.104600000
C	-4.276272000	-1.614093000	-0.650148000
C	-4.726898000	-0.212736000	-1.118120000
C	-6.109426000	-0.240622000	-1.770569000
C	-6.133976000	-4.106137000	-1.006195000
C	-5.871903000	-3.346067000	0.257778000
C	-5.120476000	-2.257007000	0.427711000
C	-5.064629000	-1.585850000	1.779475000
H	4.334585000	-0.928595000	2.598870000
H	2.399704000	-0.491017000	0.935587000
H	3.961443000	-0.715423000	-2.723835000
H	0.677389000	-1.580497000	-1.189873000
H	1.467159000	-2.146564000	-2.657920000
H	3.240333000	-3.049071000	-1.486944000
H	2.403317000	-2.719310000	0.023910000
H	6.004156000	-2.026052000	-2.315233000
H	8.124337000	-2.917657000	-1.383106000
H	8.434501000	-3.071065000	1.052835000
H	6.656464000	-2.332389000	2.607501000
H	3.799617000	1.756011000	-2.597519000
H	5.145518000	1.160404000	-1.639011000
H	3.747069000	2.847724000	-0.377722000
H	3.353093000	1.478835000	1.655508000
H	5.664631000	0.780625000	1.974643000
H	5.988145000	0.930853000	0.252735000
H	0.905965000	4.201737000	1.634032000
H	1.213324000	2.501565000	1.990668000
H	2.527569000	3.537424000	1.432300000
H	1.418689000	3.838803000	-0.738060000
H	0.295461000	0.729111000	-1.502740000
H	-4.997158000	2.379565000	-1.505310000
H	-5.582086000	0.877912000	0.523784000
H	-1.877324000	-0.548708000	1.544801000
H	-2.844081000	-0.169046000	3.788788000
H	-4.600441000	-0.257438000	3.854758000
H	-4.774543000	1.671411000	2.411553000
H	-3.075908000	1.909831000	2.775426000

H	-0.562347000	1.261179000	1.163503000
H	-0.529974000	4.314645000	-1.823766000
H	-2.967553000	4.075360000	-2.144234000
H	-2.452569000	-2.483268000	0.135545000
H	-2.202147000	-1.036414000	-0.847348000
H	-4.270101000	-2.252007000	-1.531364000
H	-4.016959000	0.065174000	-1.904790000
H	-6.123718000	-1.014651000	-2.544575000
H	-6.315464000	0.709093000	-2.264816000
H	-7.205730000	-4.143494000	-1.205883000
H	-5.648125000	-3.674989000	-1.876372000
H	-5.798969000	-5.138866000	-0.906286000
H	-6.377522000	-3.736712000	1.135607000
H	-5.490466000	-2.247164000	2.532780000
H	-5.711593000	-0.698056000	1.746701000
H	6.453195000	2.881005000	1.406831000
H	-7.051195000	-1.289352000	-0.429265000
O	5.527931000	2.702506000	1.229343000
O	-7.172145000	-0.433786000	-0.853450000

Compound: **16d**



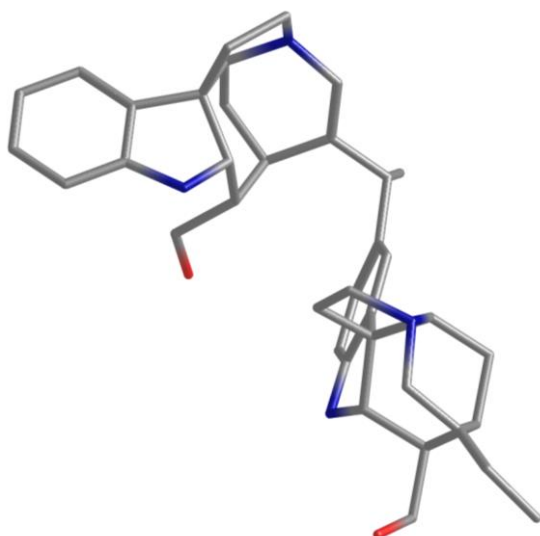
symmetry c1

N	-6.045198000	-1.352007000	1.060196000
C	-4.748765000	-0.817791000	0.616791000
C	-3.988242000	1.532598000	-0.098001000
N	-2.767633000	1.492646000	0.710220000
C	-3.180662000	1.588077000	2.120048000
C	-4.684839000	1.218245000	2.148018000
C	-4.990615000	0.712037000	0.722024000
C	-6.457372000	0.797904000	0.392293000
C	-7.240823000	1.847803000	-0.040873000
C	-8.605896000	1.637642000	-0.248518000
C	-9.160582000	0.387728000	-0.009314000
C	-8.381979000	-0.679234000	0.435603000
C	-7.026767000	-0.460228000	0.631837000
C	-3.738672000	1.027824000	-1.500365000
C	-3.231519000	-0.413063000	-1.404778000
C	-4.311108000	-1.333737000	-0.784799000
C	-5.417109000	-1.701064000	-1.783965000
C	-1.294996000	-2.787900000	-1.136941000
C	-0.829723000	-1.331947000	-1.006802000
C	-1.954526000	-0.401682000	-0.586675000
C	-1.835937000	0.491997000	0.401943000
N	3.804093000	-0.517658000	2.173158000
C	4.739485000	0.052698000	1.185766000
C	4.359212000	0.658960000	-1.330614000
N	5.158114000	1.881804000	-1.437377000
C	4.276743000	2.881617000	-0.826451000
C	3.524913000	2.169476000	0.335488000
C	3.782961000	0.654406000	0.104202000
C	2.553970000	-0.203922000	0.281721000
C	1.445524000	-0.361392000	-0.525560000
C	0.400257000	-1.203405000	-0.134885000
C	0.506490000	-1.866664000	1.084567000

C	1.611700000	-1.711080000	1.916939000
C	2.633712000	-0.870574000	1.503283000
C	5.133502000	-0.581136000	-1.708115000
C	6.300944000	-0.736502000	-0.736058000
C	5.722955000	-1.015484000	0.668850000
C	6.819102000	-1.289905000	1.698546000
C	9.391769000	-0.686761000	-1.221873000
C	8.472774000	0.491580000	-1.117038000
C	7.162286000	0.499882000	-0.867421000
C	6.436576000	1.815172000	-0.710164000
H	-6.214566000	-2.332503000	0.895058000
H	-3.973239000	-1.110519000	1.322955000
H	-4.337995000	2.568940000	-0.124423000
H	-2.578064000	0.915208000	2.725768000
H	-3.031250000	2.599993000	2.493761000
H	-5.288108000	2.102363000	2.347758000
H	-4.927149000	0.471521000	2.901215000
H	-6.804081000	2.819944000	-0.229049000
H	-9.229062000	2.445847000	-0.601204000
H	-10.216459000	0.232093000	-0.179601000
H	-8.820848000	-1.651677000	0.609185000
H	-2.982695000	1.651285000	-1.977838000
H	-4.652306000	1.091164000	-2.083407000
H	-3.010934000	-0.787397000	-2.407644000
H	-3.842812000	-2.300979000	-0.585679000
H	-4.937317000	-2.249053000	-2.595353000
H	-6.123048000	-2.390779000	-1.312564000
H	-0.466414000	-3.418631000	-1.454838000
H	-1.673610000	-3.172052000	-0.190307000
H	-2.089535000	-2.879173000	-1.876134000
H	-0.533580000	-1.015866000	-2.013946000
H	-0.950002000	0.523113000	1.022865000
H	4.188724000	-1.205101000	2.803864000
H	5.310380000	0.839950000	1.669748000
H	3.515153000	0.786181000	-2.013202000
H	3.562784000	3.217308000	-1.577404000
H	4.850305000	3.746301000	-0.500428000
H	3.884082000	2.479277000	1.315050000
H	2.460752000	2.390736000	0.294513000
H	1.370734000	0.170118000	-1.467723000
H	-0.295107000	-2.517423000	1.407105000
H	1.668388000	-2.234342000	2.861371000
H	5.494378000	-0.490577000	-2.732021000
H	4.478285000	-1.451715000	-1.653654000

H	6.883043000	-1.612260000	-1.014957000
H	5.156052000	-1.946902000	0.562782000
H	7.487320000	-2.065361000	1.310372000
H	6.385582000	-1.675524000	2.621641000
H	8.894842000	-1.637144000	-1.051849000
H	9.859306000	-0.718673000	-2.206314000
H	10.200267000	-0.597540000	-0.495010000
H	8.954232000	1.455620000	-1.249990000
H	7.070213000	2.625501000	-1.068082000
H	6.283784000	1.994603000	0.363266000
H	-6.665503000	-0.198006000	-1.761898000
H	7.988092000	0.210113000	1.286214000
O	-6.120384000	-0.646877000	-2.415586000
O	7.555746000	-0.138690000	2.072386000

Compound: **16e**



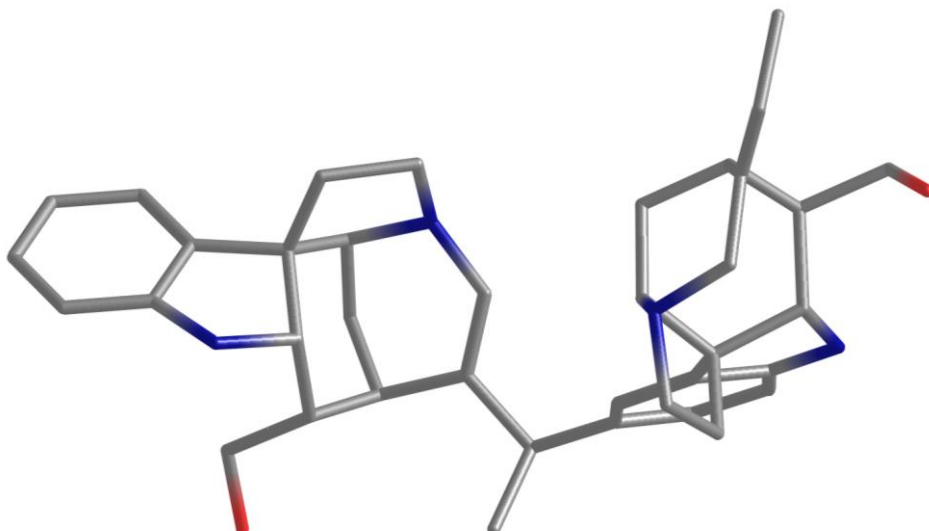
symmetry c1

N	2.346652000	-2.010687000	0.000386000
C	2.563730000	-0.602186000	-0.372205000
C	4.699862000	0.728949000	-0.959789000
N	4.136888000	1.377630000	-2.147388000
C	4.043038000	0.334648000	-3.180373000
C	4.022331000	-1.021120000	-2.427282000
C	4.015860000	-0.645565000	-0.927431000
C	4.618604000	-1.726914000	-0.067561000
C	5.930210000	-2.042186000	0.218656000
C	6.202888000	-3.147824000	1.026853000
C	5.161322000	-3.920223000	1.521830000
C	3.832706000	-3.615937000	1.232400000
C	3.576090000	-2.511352000	0.436300000
C	4.497365000	1.569200000	0.282469000
C	2.994756000	1.755529000	0.489906000
C	2.338656000	0.386706000	0.796151000
C	2.743124000	-0.113938000	2.185253000
C	1.727316000	4.705355000	-0.021881000
C	1.267139000	3.372829000	-0.616498000
C	2.426981000	2.405834000	-0.752990000
C	2.982776000	2.147078000	-1.939200000
N	-2.539345000	0.231578000	2.166303000
C	-3.342916000	-0.321327000	1.060452000
C	-3.097775000	0.007559000	-1.522447000
N	-3.437243000	-1.337304000	-1.992341000
C	-2.199726000	-2.080151000	-1.736731000
C	-1.586925000	-1.497621000	-0.429028000

C	-2.382762000	-0.189272000	-0.166335000
C	-1.506885000	0.962543000	0.260458000
C	-0.614465000	1.722156000	-0.461513000
C	0.156614000	2.704687000	0.172996000
C	-0.026404000	2.911545000	1.534414000
C	-0.919986000	2.143775000	2.285710000
C	-1.648418000	1.159171000	1.637317000
C	-4.290212000	0.932703000	-1.482903000
C	-5.306699000	0.368264000	-0.492669000
C	-4.684856000	0.422507000	0.920082000
C	-5.669940000	-0.023453000	2.000705000
C	-8.230770000	-0.658858000	-0.916758000
C	-6.961038000	-1.399657000	-1.204582000
C	-5.705311000	-1.003017000	-0.991584000
C	-4.562330000	-1.951268000	-1.267272000
H	1.551093000	-2.196038000	0.593636000
H	1.873470000	-0.324857000	-1.169014000
H	5.766309000	0.571496000	-1.145098000
H	3.153427000	0.492733000	-3.784934000
H	4.908986000	0.385355000	-3.838671000
H	4.922191000	-1.590476000	-2.652520000
H	3.165366000	-1.639686000	-2.685543000
H	6.740925000	-1.440454000	-0.171683000
H	7.224537000	-3.400853000	1.269016000
H	5.381072000	-4.772344000	2.149607000
H	3.026783000	-4.218410000	1.627846000
H	4.978946000	2.537887000	0.151255000
H	4.971460000	1.079856000	1.131975000
H	2.817488000	2.399173000	1.351549000
H	1.255406000	0.529012000	0.855974000
H	2.298064000	-1.092751000	2.377297000
H	3.820018000	-0.227185000	2.294014000
H	0.881879000	5.370082000	0.154675000
H	2.248817000	4.564709000	0.924510000
H	2.417714000	5.192245000	-0.707449000
H	0.887314000	3.569868000	-1.621741000
H	2.575975000	2.579454000	-2.846848000
H	-3.041154000	0.499023000	2.999733000
H	-3.547619000	-1.366263000	1.275278000
H	-2.353863000	0.397096000	-2.222271000
H	-1.516863000	-1.914385000	-2.568923000
H	-2.401064000	-3.147131000	-1.677597000
H	-1.669545000	-2.181868000	0.413660000
H	-0.529963000	-1.279251000	-0.573512000

H	-0.466353000	1.541990000	-1.521344000
H	0.550962000	3.671029000	2.043532000
H	-1.039084000	2.319497000	3.346264000
H	-4.725499000	1.011962000	-2.478407000
H	-3.970915000	1.927993000	-1.170583000
H	-6.182541000	1.013244000	-0.474588000
H	-4.482540000	1.483709000	1.101734000
H	-5.279578000	0.211581000	2.991147000
H	-6.604252000	0.534996000	1.884413000
H	-8.801882000	-0.510969000	-1.833634000
H	-8.862264000	-1.243784000	-0.246643000
H	-8.068277000	0.311962000	-0.458329000
H	-7.099214000	-2.390331000	-1.626739000
H	-4.922467000	-2.793750000	-1.856040000
H	-4.225526000	-2.368134000	-0.307847000
H	1.413640000	1.030884000	3.030023000
H	-6.308867000	-1.657825000	1.160083000
O	2.336195000	0.803824000	3.189757000
O	-5.919303000	-1.418028000	2.007053000

Compound: **16f**



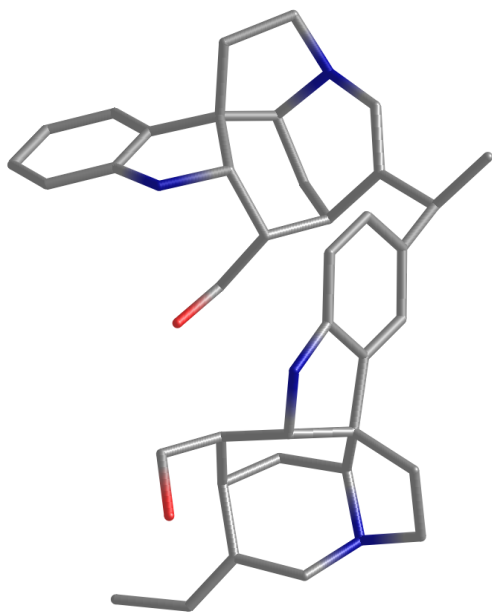
symmetry c1

N	4.196743000	-1.292972000	1.667448000
C	3.463845000	-0.431676000	0.725447000
C	3.530943000	-0.220675000	-1.843885000
N	2.076541000	-0.220000000	-2.008793000
C	1.623665000	-1.594275000	-1.742004000
C	2.745190000	-2.260542000	-0.904879000
C	3.763742000	-1.130526000	-0.630433000
C	5.147495000	-1.672181000	-0.379986000
C	6.133955000	-2.095921000	-1.244730000
C	7.323127000	-2.608307000	-0.721049000
C	7.494579000	-2.697404000	0.653257000
C	6.500805000	-2.280170000	1.536779000
C	5.330226000	-1.764850000	1.003989000
C	4.064295000	1.188156000	-1.703211000
C	3.419816000	1.816737000	-0.467261000
C	3.881723000	1.058598000	0.799748000
C	5.371386000	1.294081000	1.075665000
C	1.462677000	3.316329000	1.333979000
C	1.118294000	2.977339000	-0.123799000
C	1.915053000	1.794950000	-0.648775000
C	1.369860000	0.797546000	-1.353302000
N	-4.484038000	2.217806000	-0.654090000
C	-4.650775000	0.885705000	-0.042766000
C	-2.888913000	-0.643698000	1.140735000
N	-3.706677000	-1.221333000	2.209080000
C	-3.755231000	-0.129228000	3.186277000
C	-3.798255000	1.199545000	2.376447000

C	-3.425628000	0.790182000	0.924830000
C	-2.443923000	1.721384000	0.256066000
C	-1.088986000	1.879746000	0.450758000
C	-0.375238000	2.821351000	-0.301358000
C	-1.068911000	3.590826000	-1.226861000
C	-2.443163000	3.458143000	-1.423228000
C	-3.122198000	2.514258000	-0.671868000
C	-2.853520000	-1.500373000	-0.102002000
C	-4.274561000	-1.615209000	-0.649822000
C	-4.723682000	-0.214285000	-1.120466000
C	-6.105320000	-0.242233000	-1.774803000
C	-6.132086000	-4.107388000	-1.005643000
C	-5.872274000	-3.345434000	0.257649000
C	-5.120905000	-2.256316000	0.427418000
C	-5.067179000	-1.583303000	1.778307000
H	4.328777000	-0.933039000	2.600664000
H	2.396927000	-0.483666000	0.937367000
H	3.965290000	-0.706742000	-2.722297000
H	0.669801000	-1.572342000	-1.220170000
H	1.482101000	-2.131356000	-2.678716000
H	3.229371000	-3.046806000	-1.481196000
H	2.382640000	-2.702615000	0.020700000
H	5.994499000	-2.030587000	-2.316231000
H	8.109686000	-2.934649000	-1.385306000
H	8.418673000	-3.093354000	1.050496000
H	6.645231000	-2.347110000	2.606063000
H	3.808501000	1.764207000	-2.591861000
H	5.151190000	1.158312000	-1.633809000
H	3.734276000	2.858449000	-0.375806000
H	3.361769000	1.481236000	1.661527000
H	5.667824000	0.771088000	1.982330000
H	6.006762000	0.917816000	0.272738000
H	0.896583000	4.189908000	1.652912000
H	1.213862000	2.489381000	1.999064000
H	2.522248000	3.537602000	1.453209000
H	1.420502000	3.844850000	-0.721125000
H	0.299431000	0.738823000	-1.501601000
H	-4.991256000	2.378823000	-1.511547000
H	-5.580982000	0.879630000	0.518093000
H	-1.878910000	-0.548251000	1.548028000
H	-2.848964000	-0.165247000	3.789449000
H	-4.605443000	-0.253092000	3.853149000
H	-4.777474000	1.673461000	2.406796000
H	-3.079653000	1.912802000	2.773744000

H	-0.563413000	1.262157000	1.170090000
H	-0.523211000	4.314979000	-1.818288000
H	-2.959448000	4.073994000	-2.146401000
H	-2.452521000	-2.484118000	0.140060000
H	-2.199931000	-1.038604000	-0.844291000
H	-4.267186000	-2.254283000	-1.530189000
H	-4.012453000	0.062065000	-1.906538000
H	-6.119109000	-1.017516000	-2.547563000
H	-6.309979000	0.706846000	-2.270861000
H	-5.796611000	-5.139775000	-0.903757000
H	-7.203525000	-4.145650000	-1.206774000
H	-5.645235000	-3.677186000	-1.875738000
H	-6.379581000	-3.734698000	1.135116000
H	-5.494737000	-2.243280000	2.531787000
H	-5.713457000	-0.695088000	1.743187000
H	5.702475000	3.130683000	0.487460000
H	-7.050000000	-1.288327000	-0.433477000
O	5.640279000	2.666907000	1.324146000
O	-7.169389000	-0.433098000	-0.858813000

Compound: **17a**



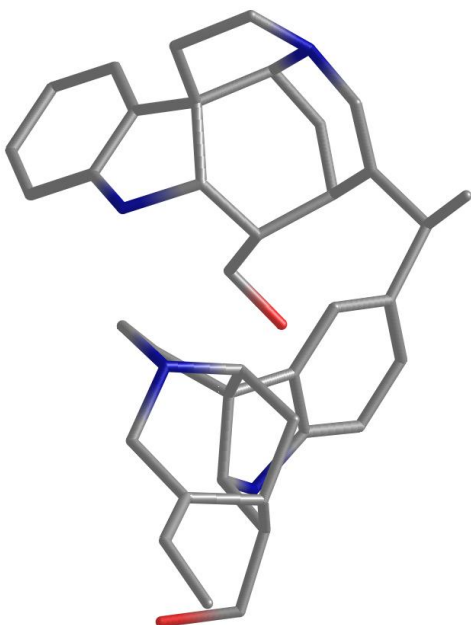
symmetry c1

N	2.363404000	1.530000000	1.342671000
C	2.681937000	0.252509000	0.649435000
C	4.452567000	-0.375931000	-1.171519000
N	4.870618000	-1.681137000	-0.663024000
C	5.739254000	-1.384269000	0.476889000
C	5.197974000	-0.072375000	1.099997000
C	4.129541000	0.448217000	0.095477000
C	4.196715000	1.950910000	-0.025766000
C	5.080814000	2.760852000	-0.713048000
C	4.984699000	4.144161000	-0.568087000
C	4.021775000	4.696867000	0.265709000
C	3.121960000	3.886881000	0.953837000
C	3.222357000	2.516796000	0.792470000
C	3.317483000	-0.529400000	-2.163452000
C	2.118917000	-1.109648000	-1.412674000
C	1.606258000	-0.051007000	-0.412265000
C	1.078920000	1.191513000	-1.143518000
C	2.023583000	-4.810090000	-0.032219000
C	1.491840000	-3.484432000	-0.570671000
C	2.547790000	-2.412580000	-0.760559000
C	3.826265000	-2.586677000	-0.414046000
N	-2.667922000	-0.979442000	2.361540000
C	-3.465653000	-0.430352000	1.247161000
C	-3.300671000	-0.866943000	-1.322993000
N	-4.725703000	-0.887550000	-1.659772000

C	-5.135111000	-2.222910000	-1.211780000
C	-4.286290000	-2.561904000	0.050578000
C	-3.198421000	-1.456594000	0.100111000
C	-1.822544000	-1.952294000	0.472603000
C	-0.866634000	-2.606869000	-0.279623000
C	0.364904000	-2.937846000	0.287898000
C	0.583614000	-2.640816000	1.630548000
C	-0.371436000	-1.993721000	2.406624000
C	-1.570531000	-1.634519000	1.806197000
C	-2.670760000	0.493906000	-1.483941000
C	-3.363732000	1.461174000	-0.527436000
C	-3.048073000	1.015196000	0.917777000
C	-3.597204000	1.994678000	1.952967000
C	-5.057994000	4.030964000	-1.084626000
C	-5.515635000	2.607817000	-1.182691000
C	-4.827097000	1.498530000	-0.907776000
C	-5.514511000	0.154269000	-0.981131000
H	2.416314000	1.469950000	2.350318000
H	2.666464000	-0.560066000	1.372461000
H	5.323499000	0.075059000	-1.654284000
H	5.751213000	-2.219741000	1.171561000
H	6.755164000	-1.230324000	0.115617000
H	5.999585000	0.653975000	1.214263000
H	4.758552000	-0.230029000	2.083728000
H	5.846642000	2.333742000	-1.347222000
H	5.664654000	4.789479000	-1.104926000
H	3.958329000	5.770341000	0.372175000
H	2.356136000	4.315186000	1.585278000
H	3.633187000	-1.202733000	-2.959778000
H	3.085251000	0.432593000	-2.617532000
H	1.305870000	-1.322716000	-2.111889000
H	0.741306000	-0.448877000	0.121205000
H	1.889382000	1.848646000	-1.468342000
H	0.541020000	0.872386000	-2.038453000
H	1.209782000	-5.528729000	0.041261000
H	2.789827000	-5.221787000	-0.687350000
H	2.454263000	-4.694266000	0.961970000
H	1.061986000	-3.680607000	-1.558275000
H	4.162019000	-3.501844000	0.055161000
H	-2.473705000	-0.343830000	3.120984000
H	-4.511538000	-0.439433000	1.539425000
H	-2.819278000	-1.578943000	-1.999023000
H	-4.915670000	-2.936949000	-2.004564000
H	-6.206685000	-2.249582000	-1.027407000

H	-4.877894000	-2.568522000	0.964021000
H	-3.831737000	-3.545157000	-0.050337000
H	-1.048044000	-2.835692000	-1.323615000
H	1.542949000	-2.880832000	2.072586000
H	-0.175560000	-1.758738000	3.443799000
H	-2.774399000	0.830869000	-2.515190000
H	-1.609215000	0.443208000	-1.240366000
H	-2.925901000	2.449356000	-0.649951000
H	-1.955601000	1.060025000	0.984656000
H	-3.264931000	3.005943000	1.696923000
H	-3.197656000	1.769423000	2.942245000
H	-4.033814000	4.129069000	-0.737696000
H	-5.137344000	4.524871000	-2.053389000
H	-5.699212000	4.585604000	-0.397927000
H	-6.544792000	2.482233000	-1.505451000
H	-6.460515000	0.259188000	-1.511046000
H	-5.769011000	-0.154908000	0.041913000
H	0.598232000	2.052158000	0.494702000
H	-5.398663000	2.171715000	1.238951000
O	0.154961000	1.924772000	-0.355288000
O	-5.008017000	1.954202000	2.091558000

Compound: **17b**



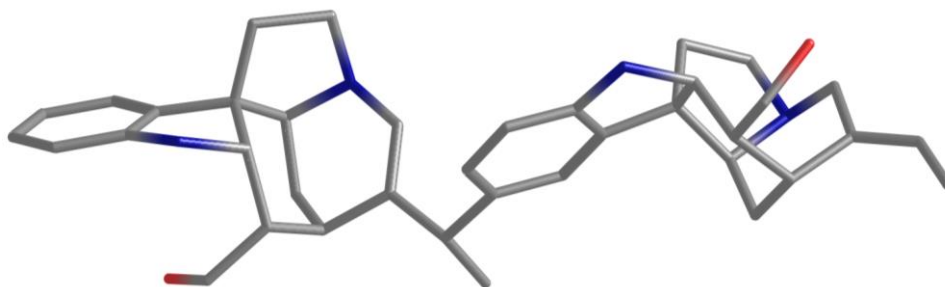
symmetry c1

N	2.356298000	-1.941593000	-0.215837000
C	2.572289000	-0.493428000	-0.379282000
C	4.698287000	0.909854000	-0.800447000
N	4.113453000	1.726149000	-1.866783000
C	3.990342000	0.848231000	-3.040928000
C	3.995290000	-0.604212000	-2.497377000
C	4.014020000	-0.455204000	-0.958866000
C	4.628123000	-1.652392000	-0.279919000
C	5.943438000	-2.008370000	-0.067664000
C	6.226099000	-3.223524000	0.559380000
C	5.190568000	-4.061417000	0.949393000
C	3.858312000	-3.715644000	0.732768000
C	3.591810000	-2.502960000	0.117915000
C	4.519033000	1.559509000	0.553895000
C	3.020108000	1.713240000	0.809854000
C	2.370098000	0.312325000	0.925080000
C	2.799910000	-0.384537000	2.218454000
C	0.784461000	4.331171000	-1.116957000
C	1.282296000	3.472437000	0.041728000
C	2.433310000	2.549800000	-0.309394000
C	2.972000000	2.470524000	-1.529328000
N	-2.529996000	-0.101511000	2.239200000
C	-3.308684000	-0.499919000	1.051985000
C	-3.038723000	0.220168000	-1.448173000
N	-3.353960000	-1.040232000	-2.123863000

C	-2.109191000	-1.798423000	-1.968397000
C	-1.522090000	-1.418948000	-0.577214000
C	-2.336422000	-0.174135000	-0.128425000
C	-1.479175000	0.909793000	0.476838000
C	-0.580513000	1.769078000	-0.115320000
C	0.168140000	2.654071000	0.669720000
C	-0.036866000	2.658896000	2.043322000
C	-0.933518000	1.785998000	2.663200000
C	-1.644014000	0.902977000	1.864914000
C	-4.244210000	1.114213000	-1.282501000
C	-5.266342000	0.390501000	-0.408484000
C	-4.664871000	0.231011000	1.005098000
C	-5.654646000	-0.400237000	1.984540000
C	-8.169053000	-0.584086000	-1.050397000
C	-6.884754000	-1.261266000	-1.418979000
C	-5.638534000	-0.890567000	-1.120633000
C	-4.477494000	-1.771913000	-1.515073000
H	1.572032000	-2.211692000	0.359824000
H	1.870037000	-0.099936000	-1.114831000
H	5.761118000	0.783781000	-1.026582000
H	3.081213000	1.087828000	-3.586975000
H	4.834351000	1.001666000	-3.711794000
H	4.896213000	-1.123514000	-2.819014000
H	3.139371000	-1.187632000	-2.830148000
H	6.749196000	-1.355335000	-0.377551000
H	7.250833000	-3.511252000	0.742560000
H	5.418255000	-4.999140000	1.436556000
H	3.057080000	-4.370529000	1.045767000
H	5.001018000	2.536604000	0.556722000
H	5.005577000	0.952254000	1.315594000
H	2.857738000	2.226862000	1.758021000
H	1.288320000	0.438720000	1.026297000
H	2.361833000	-1.383638000	2.271515000
H	3.878639000	-0.505756000	2.293392000
H	-0.028519000	4.971374000	-0.780102000
H	1.581750000	4.962717000	-1.505457000
H	0.410454000	3.719766000	-1.937727000
H	1.646946000	4.148580000	0.821862000
H	2.573087000	3.037080000	-2.360607000
H	-3.048971000	0.038722000	3.092895000
H	-3.495571000	-1.568521000	1.108349000
H	-2.292348000	0.721585000	-2.069794000
H	-1.418046000	-1.496440000	-2.754236000
H	-2.295604000	-2.864021000	-2.079063000

H	-1.608251000	-2.225562000	0.148732000
H	-0.465934000	-1.170722000	-0.670023000
H	-0.412171000	1.731984000	-1.186016000
H	0.538132000	3.341115000	2.657043000
H	-1.067341000	1.801750000	3.736323000
H	-4.667353000	1.343406000	-2.259773000
H	-3.942287000	2.051955000	-0.813815000
H	-6.151162000	1.014659000	-0.303662000
H	-4.488458000	1.253518000	1.356165000
H	-6.599969000	0.149959000	1.941222000
H	-5.283502000	-0.316994000	3.006329000
H	-8.028541000	0.303281000	-0.440563000
H	-8.718878000	-0.296822000	-1.947053000
H	-8.810657000	-1.271648000	-0.497816000
H	-7.001923000	-2.176325000	-1.991416000
H	-4.815358000	-2.522977000	-2.227698000
H	-4.146244000	-2.321052000	-0.622485000
H	1.479119000	0.614057000	3.243053000
H	-6.248842000	-1.893563000	0.887616000
O	2.405494000	0.373701000	3.352804000
O	-5.871739000	-1.783143000	1.766371000

Compound: **17c**



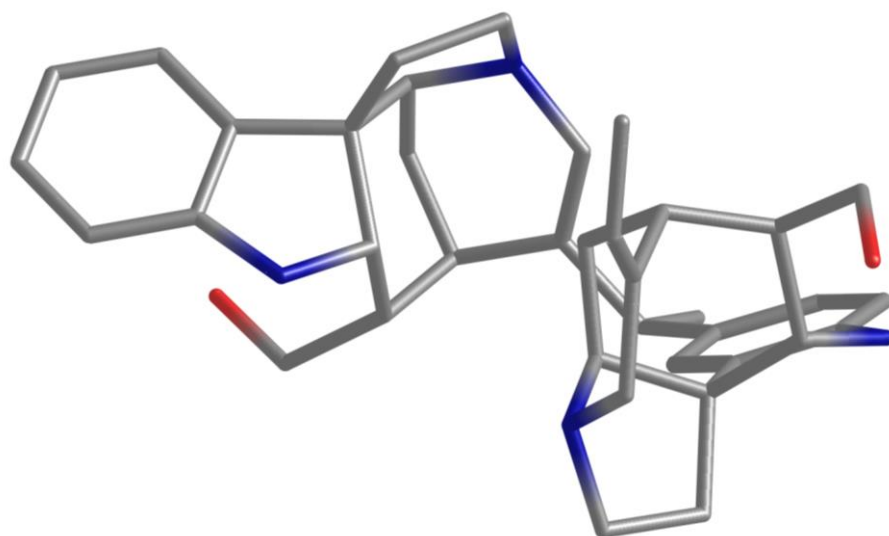
symmetry c1

N	5.362820000	1.981430000	-0.287408000
C	4.337386000	0.931946000	-0.191877000
C	4.291544000	-1.340884000	1.041170000
N	2.950222000	-1.151068000	1.599246000
C	3.084624000	-0.140107000	2.659840000
C	4.382317000	0.648853000	2.344470000
C	4.874112000	0.079749000	0.993808000
C	6.361469000	0.244261000	0.816291000
C	7.427545000	-0.500834000	1.276789000
C	8.727179000	-0.092536000	0.968704000
C	8.934911000	1.055368000	0.216227000
C	7.867362000	1.821127000	-0.249029000
C	6.581630000	1.402503000	0.058854000
C	4.243940000	-2.054894000	-0.290493000
C	3.426028000	-1.200364000	-1.257948000
C	4.108328000	0.160757000	-1.525231000
C	5.291580000	0.053746000	-2.496803000
C	0.478324000	-2.225640000	-2.153569000
C	0.885622000	-0.850792000	-1.614228000
C	2.053869000	-0.984765000	-0.658184000
C	1.924010000	-0.926542000	0.669443000
N	-3.399035000	2.031881000	0.764282000
C	-4.506431000	1.061314000	0.680973000
C	-4.515700000	-1.412847000	-0.165904000
N	-5.446354000	-2.015960000	0.790727000
C	-4.604701000	-2.182646000	1.979793000
C	-3.632166000	-0.967857000	2.018142000
C	-3.761533000	-0.312342000	0.615185000
C	-2.439346000	0.095786000	0.010428000
C	-1.435856000	-0.673744000	-0.551632000
C	-0.269921000	-0.067974000	-1.023113000
C	-0.152309000	1.317000000	-0.907283000

C	-1.145889000	2.104238000	-0.340481000
C	-2.294313000	1.475070000	0.121576000
C	-5.196870000	-0.941751000	-1.428293000
C	-6.204629000	0.143964000	-1.057166000
C	-5.423805000	1.363443000	-0.519805000
C	-6.342267000	2.547991000	-0.219406000
C	-9.319601000	0.235557000	-1.335659000
C	-8.526222000	-0.459049000	-0.271649000
C	-7.202737000	-0.476777000	-0.104960000
C	-6.608010000	-1.166132000	1.100496000
H	5.348170000	2.560493000	-1.112984000
H	3.385844000	1.379471000	0.088825000
H	4.872231000	-1.920290000	1.764678000
H	2.202570000	0.495155000	2.677740000
H	3.167756000	-0.627408000	3.630051000
H	5.133578000	0.459759000	3.109192000
H	4.225782000	1.724094000	2.291308000
H	7.262315000	-1.396944000	1.860685000
H	9.570743000	-0.673360000	1.310695000
H	9.943759000	1.359611000	-0.024102000
H	8.037863000	2.707344000	-0.843961000
H	3.761693000	-3.024120000	-0.161746000
H	5.252172000	-2.219529000	-0.657898000
H	3.330954000	-1.717056000	-2.215600000
H	3.392172000	0.772971000	-2.085857000
H	4.889697000	-0.304473000	-3.444376000
H	5.705316000	1.048612000	-2.685174000
H	-0.331569000	-2.141808000	-2.877835000
H	1.323237000	-2.707450000	-2.642397000
H	0.155573000	-2.877339000	-1.342837000
H	1.252034000	-0.269033000	-2.467692000
H	0.964067000	-0.711826000	1.123834000
H	-3.626000000	2.986288000	0.527643000
H	-5.094907000	1.134327000	1.590986000
H	-3.786024000	-2.188936000	-0.410898000
H	-4.037377000	-3.106503000	1.874841000
H	-5.220064000	-2.268382000	2.872481000
H	-3.883554000	-0.257360000	2.803288000
H	-2.612072000	-1.301295000	2.195758000
H	-1.557641000	-1.746417000	-0.625615000
H	0.750969000	1.791993000	-1.272183000
H	-1.027932000	3.176320000	-0.265526000
H	-5.695759000	-1.781286000	-1.911283000
H	-4.451626000	-0.544949000	-2.119198000

H	-6.721417000	0.473048000	-1.956245000
H	-4.775734000	1.673926000	-1.346709000
H	-5.754449000	3.448284000	-0.038860000
H	-6.968552000	2.745338000	-1.095340000
H	-10.031964000	0.925836000	-0.881688000
H	-8.705627000	0.800404000	-2.030700000
H	-9.904595000	-0.485628000	-1.906976000
H	-9.121075000	-1.000598000	0.457542000
H	-7.365475000	-1.790220000	1.572746000
H	-6.340906000	-0.395800000	1.837259000
H	6.811064000	-0.515741000	-1.406425000
H	-7.708872000	1.607407000	0.796991000
O	6.332356000	-0.849485000	-2.171507000
O	-7.143204000	2.373724000	0.936356000

Compound: **17d**



symmetry c1

N	2.612185000	-1.697655000	1.128541000
C	2.472503000	-0.412376000	0.428893000
C	3.559901000	0.504604000	-1.742015000
N	2.320107000	1.025982000	-2.321232000
C	1.572922000	-0.150917000	-2.783389000
C	2.051678000	-1.343033000	-1.911974000
C	3.108775000	-0.738216000	-0.954422000
C	4.157164000	-1.745856000	-0.556804000
C	5.298016000	-2.180483000	-1.199560000
C	6.088454000	-3.160560000	-0.595287000
C	5.718181000	-3.691989000	0.632463000
C	4.564855000	-3.266776000	1.289369000
C	3.791360000	-2.289018000	0.681807000
C	4.272128000	1.558469000	-0.923715000
C	3.352941000	1.968064000	0.225917000
C	3.101825000	0.788758000	1.193448000
C	4.292152000	0.499036000	2.117471000
C	1.716517000	4.880575000	0.088635000
C	1.244009000	3.465962000	0.427198000
C	2.037461000	2.435493000	-0.354549000
C	1.605900000	1.918680000	-1.507106000
N	-4.243679000	2.143530000	-0.162569000
C	-4.188694000	0.708957000	0.178112000
C	-2.203659000	-0.723238000	1.102695000
N	-2.923521000	-1.597604000	2.030272000
C	-3.137841000	-0.717773000	3.183977000
C	-3.365765000	0.717669000	2.624282000

C	-2.951984000	0.628571000	1.130450000
C	-2.131850000	1.797148000	0.643527000
C	-0.806783000	2.102205000	0.840333000
C	-0.248273000	3.255543000	0.271068000
C	-1.073658000	4.090326000	-0.468005000
C	-2.426770000	3.800908000	-0.671714000
C	-2.942845000	2.643388000	-0.119316000
C	-2.040079000	-1.326847000	-0.271094000
C	-3.429245000	-1.546418000	-0.867938000
C	-4.088129000	-0.165692000	-1.086952000
C	-5.446246000	-0.280997000	-1.779137000
C	-4.882734000	-4.183745000	-1.717006000
C	-4.739246000	-3.635768000	-0.330301000
C	-4.164738000	-2.494569000	0.053434000
C	-4.211188000	-2.082672000	1.506038000
H	2.445429000	-1.698113000	2.123200000
H	1.415376000	-0.188889000	0.292034000
H	4.192679000	0.168450000	-2.568232000
H	0.504438000	0.032859000	-2.702842000
H	1.803036000	-0.339487000	-3.830930000
H	2.514924000	-2.104359000	-2.536494000
H	1.244050000	-1.816841000	-1.357438000
H	5.585773000	-1.762039000	-2.155243000
H	6.991386000	-3.500508000	-1.080128000
H	6.339706000	-4.444576000	1.096565000
H	4.289679000	-3.678282000	2.250232000
H	4.475720000	2.422964000	-1.555935000
H	5.217712000	1.170213000	-0.558572000
H	3.811155000	2.780092000	0.796215000
H	2.327120000	1.112148000	1.899237000
H	4.450653000	1.394486000	2.718160000
H	4.030116000	-0.304868000	2.811445000
H	1.199651000	5.627795000	0.690464000
H	2.785992000	4.972579000	0.272762000
H	1.545020000	5.099780000	-0.964468000
H	1.475896000	3.293322000	1.484157000
H	0.634864000	2.190518000	-1.905200000
H	-4.796229000	2.389048000	-0.970487000
H	-5.099841000	0.448021000	0.708386000
H	-1.218990000	-0.552992000	1.547301000
H	-2.241486000	-0.734527000	3.802669000
H	-3.966634000	-1.079069000	3.788448000
H	-4.399079000	1.044546000	2.722955000
H	-2.745305000	1.436775000	3.154371000

H	-0.169085000	1.443834000	1.421436000
H	-0.667486000	4.986625000	-0.915096000
H	-3.047106000	4.464315000	-1.258063000
H	-1.497670000	-2.269063000	-0.197040000
H	-1.459947000	-0.647633000	-0.899194000
H	-3.327782000	-2.004738000	-1.849446000
H	-3.426010000	0.357989000	-1.785328000
H	-5.336809000	-0.891088000	-2.681442000
H	-5.794043000	0.701528000	-2.098760000
H	-4.381544000	-5.148561000	-1.799226000
H	-5.935257000	-4.358195000	-1.944082000
H	-4.481211000	-3.527233000	-2.483075000
H	-5.176001000	-4.252718000	0.449059000
H	-4.525175000	-2.929745000	2.114355000
H	-4.990608000	-1.316464000	1.618908000
H	5.503975000	-0.623054000	1.071689000
H	-6.217861000	-1.688424000	-0.679154000
O	5.545136000	0.229248000	1.516230000
O	-6.470251000	-0.799334000	-0.948262000