

SUPPORTING INFORMATION

Configurational and conformational assignments of quinolizidine and *beta*-carboline moieties in the Corynanthe-Tryptamine alkaloids

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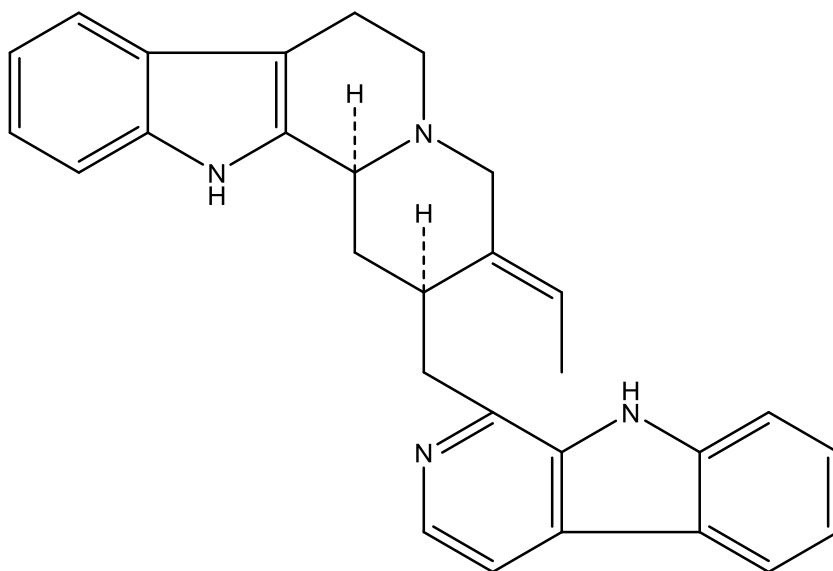
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TABLE OF CONTENTS

| | |
|--|----|
| Cartesian coordinates (Angstroms) of key configurations of compounds optimized at the M06-2X/pecG-2 level: | 3 |
| Compound: Usambarensine (1) | 3 |
| Compound: 4',17-tetrahydrousambarensine (2) | 5 |
| Compound: 19,20-dihydrousambarensine (3) | 7 |
| Compound: (3-4- <i>trans</i>)-5',6'-dihydrousambarensine (4)..... | 9 |
| Compound: (3-4- <i>cis</i>)-5',6'-dihydrousambarensine (4)..... | 11 |
| Compound: <i>N</i> -methylusambarensine (5)..... | 13 |
| Compound: 10'-hydroxy-4',17-tetrahydrousambarensine (6)..... | 15 |
| Compound: 10'-hydroxyusambarensine (7) | 17 |
| Compound: 10,10'-dimethoxy-3 <i>S</i> ,17 <i>S</i> - <i>Z</i> -tetrahydrousambarensine (8) | 19 |
| Compound: 10,10'-dimethoxy- <i>N</i> -4'-methyl-3 <i>S</i> ,17 <i>S</i> - <i>Z</i> -tetrahydrousambarensine (9)..... | 22 |
| Compound: strychnopentamine (10) | 25 |
| Compound: isostrychnopentamine (11)..... | 28 |
| Figure S1. Comparison of calculated ¹ H and ¹³ C NMR chemical shifts of <i>cis</i> - and <i>trans</i> - conformations of the C/D quinolizidine system of 5',6'-dihydrousambarensine (4)..... | 31 |

Cartesian coordinates (Angstroms) of key configurations of compounds optimized at the M06-2X/pecG-2 level:

Compound: Usambarensine (**1**)
Solvent: chloroform



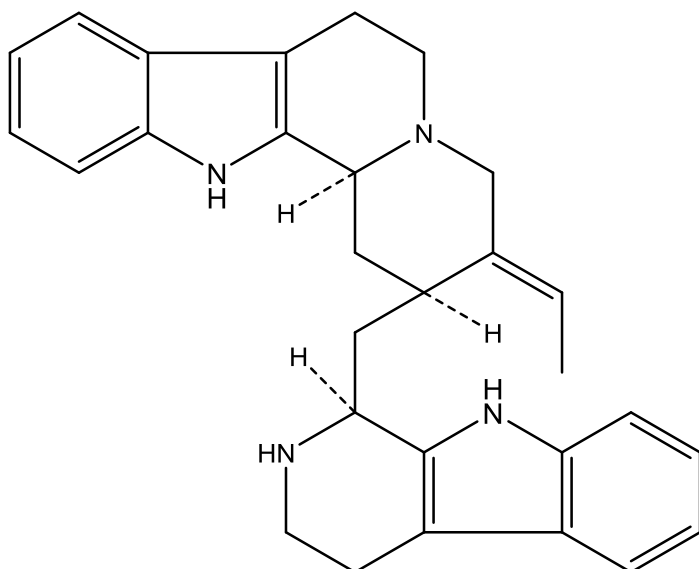
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| | | | |
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| N | 3.033031000 | -2.398375000 | -1.094921000 |
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Compound: 4',17-tetrahydrousambarensine (2)

Solvent: chloroform



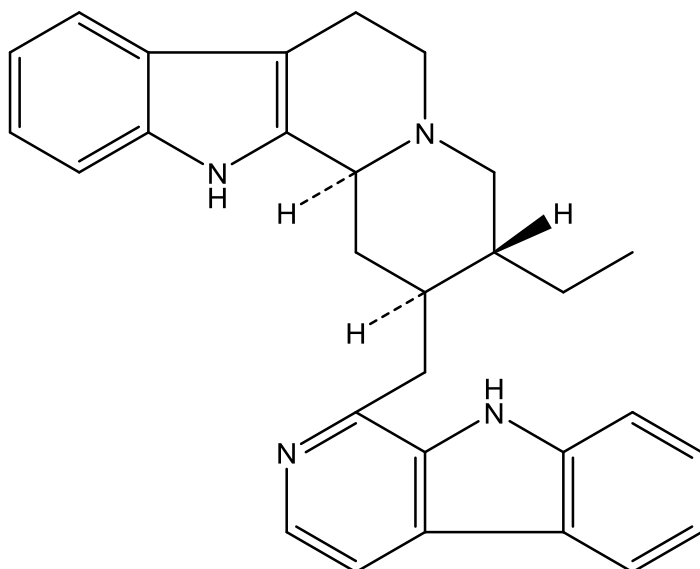
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| | | | |
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Compound: 19,20-dihydrousambarensine (3)

Solvent: chloroform



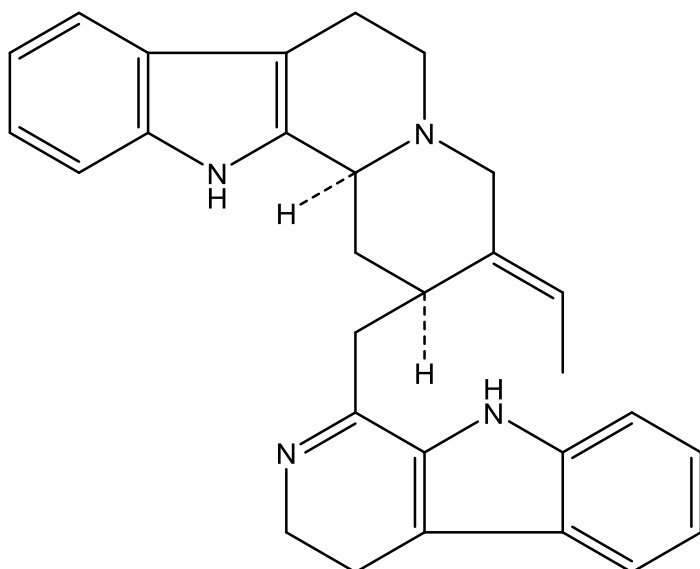
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| H | 8.745255000 | -1.395418000 | -1.429912000 |
| H | 6.763277000 | -0.428620000 | -2.539325000 |

Compound: (3-4-*trans*)-5',6'-dihydrousambarensine (**4**)

Solvent: chloroform



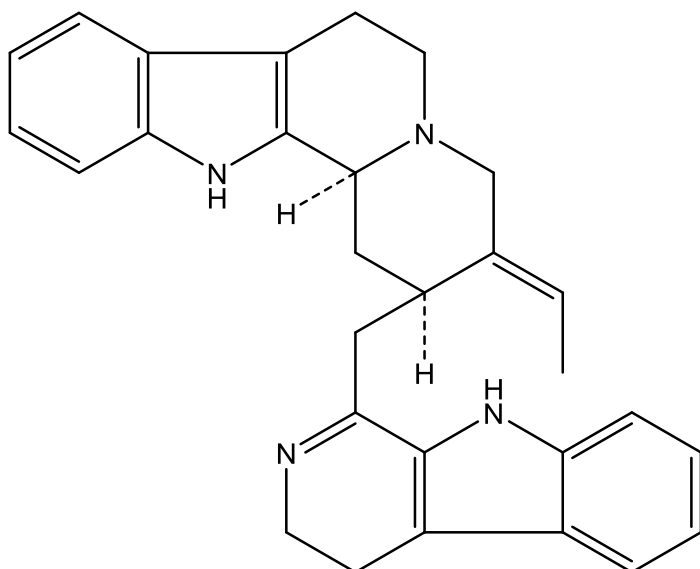
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| | | | |
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| H | -1.083515000 | 3.934007000 | -1.367432000 |
| H | -0.170674000 | 2.529229000 | -1.939903000 |

Compound: (3-4-*cis*)-5',6'-dihydrousambarensine (**4**)

Solvent: chloroform



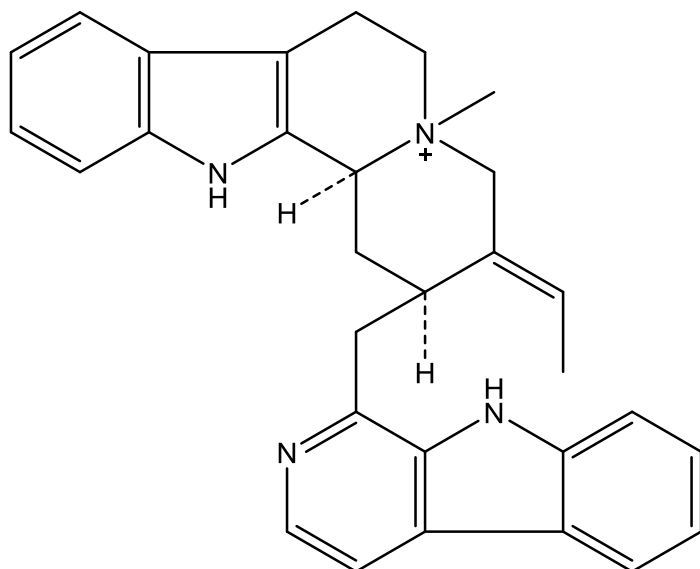
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| | | | |
|---|--------------|--------------|--------------|
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| C | 3.108624000 | -0.153153000 | 0.856388000 |
| C | 2.083564000 | 0.297208000 | 1.797336000 |
| N | 1.720562000 | -0.451311000 | 2.763644000 |
| C | 2.430182000 | -1.720397000 | 2.954043000 |
| C | 2.822687000 | -2.455437000 | 1.670849000 |
| C | 3.468379000 | -1.466346000 | 0.757751000 |
| C | 4.398171000 | -1.564349000 | -0.321406000 |
| C | 5.110861000 | -2.620449000 | -0.905968000 |
| C | 5.961015000 | -2.349494000 | -1.955074000 |
| C | 6.121025000 | -1.037793000 | -2.438809000 |
| C | 5.434962000 | 0.022757000 | -1.886546000 |
| C | 4.568474000 | -0.252368000 | -0.828170000 |
| C | 1.420110000 | 1.627643000 | 1.572860000 |
| N | -2.733045000 | -1.586447000 | -0.343900000 |
| C | -2.717161000 | -0.235180000 | -0.605079000 |
| C | -1.478957000 | 0.568915000 | -0.813712000 |
| N | -1.873281000 | 1.867591000 | -1.370961000 |
| C | -2.979089000 | 2.495553000 | -0.647052000 |
| C | -4.268419000 | 1.702795000 | -0.853000000 |
| C | -3.985590000 | 0.255532000 | -0.612164000 |
| C | -4.859387000 | -0.852533000 | -0.351744000 |
| C | -6.246128000 | -0.995267000 | -0.238158000 |
| C | -6.771865000 | -2.244055000 | 0.029842000 |
| C | -5.937403000 | -3.361433000 | 0.188802000 |
| C | -4.563810000 | -3.251722000 | 0.083543000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -4.037327000 | -1.991895000 | -0.187134000 |
| C | -0.654695000 | 0.676801000 | 0.481791000 |
| C | 0.548397000 | 1.616522000 | 0.311032000 |
| C | 0.748991000 | 4.688124000 | 1.571078000 |
| C | 0.129924000 | 4.171796000 | 0.302837000 |
| C | 0.044202000 | 2.944903000 | -0.209102000 |
| C | -0.706493000 | 2.735657000 | -1.510108000 |
| H | 3.703669000 | 1.584762000 | -0.224316000 |
| H | 3.339413000 | -1.492438000 | 3.519930000 |
| H | 1.811389000 | -2.354709000 | 3.583234000 |
| H | 3.491799000 | -3.278120000 | 1.918152000 |
| H | 1.941529000 | -2.893617000 | 1.192608000 |
| H | 4.994245000 | -3.629382000 | -0.534899000 |
| H | 6.517871000 | -3.151920000 | -2.416630000 |
| H | 6.797206000 | -0.858335000 | -3.262242000 |
| H | 5.560258000 | 1.028634000 | -2.260977000 |
| H | 2.189032000 | 2.398427000 | 1.483668000 |
| H | 0.819989000 | 1.847677000 | 2.452786000 |
| H | -1.926936000 | -2.184356000 | -0.298386000 |
| H | -0.850516000 | 0.081536000 | -1.567588000 |
| H | -2.774624000 | 2.583536000 | 0.427869000 |
| H | -3.091043000 | 3.507530000 | -1.034146000 |
| H | -5.035506000 | 2.069211000 | -0.169511000 |
| H | -4.639064000 | 1.859972000 | -1.868126000 |
| H | -6.895750000 | -0.138979000 | -0.360094000 |
| H | -7.841614000 | -2.367764000 | 0.119263000 |
| H | -6.377177000 | -4.325989000 | 0.398264000 |
| H | -3.921281000 | -4.111877000 | 0.208083000 |
| H | -1.285966000 | 1.046038000 | 1.292919000 |
| H | -0.313032000 | -0.317433000 | 0.774239000 |
| H | 1.155619000 | 1.199857000 | -0.503301000 |
| H | 1.750020000 | 5.081606000 | 1.383948000 |
| H | 0.154014000 | 5.517605000 | 1.949145000 |
| H | 0.820371000 | 3.948689000 | 2.358510000 |
| H | -0.321622000 | 4.952577000 | -0.303056000 |
| H | -1.032938000 | 3.688270000 | -1.923325000 |
| H | -0.039973000 | 2.265213000 | -2.239688000 |

Compound: *N*-methylusambarensine (5)

Solvent: chloroform



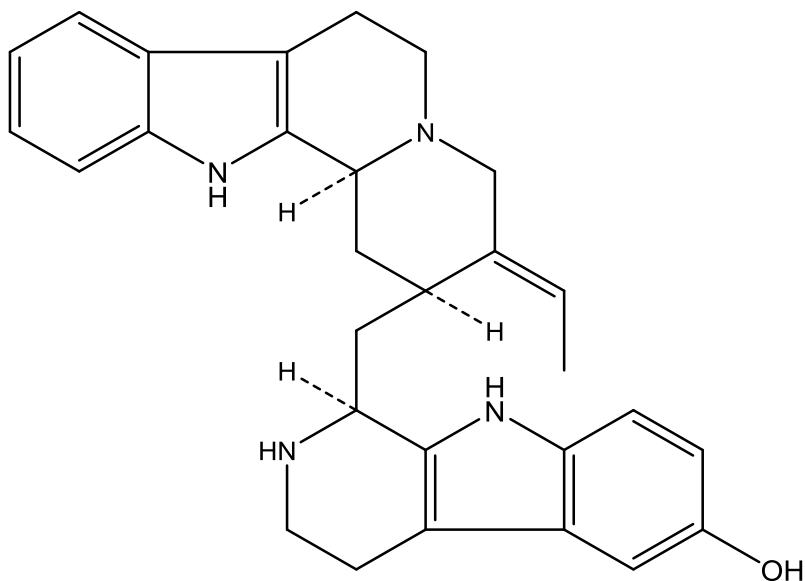
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| | | | |
|---|--------------|--------------|--------------|
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| C | 2.134803000 | 0.058265000 | 1.589051000 |
| N | 1.641808000 | -0.885934000 | 2.380631000 |
| C | 2.193309000 | -2.110208000 | 2.384685000 |
| C | 3.267875000 | -2.477023000 | 1.598677000 |
| C | 3.806988000 | -1.505846000 | 0.761009000 |
| C | 4.898991000 | -1.461307000 | -0.182430000 |
| C | 5.837799000 | -2.397513000 | -0.615157000 |
| C | 6.777377000 | -2.012631000 | -1.550347000 |
| C | 6.789460000 | -0.704616000 | -2.056117000 |
| C | 5.870561000 | 0.241116000 | -1.644729000 |
| C | 4.924489000 | -0.152368000 | -0.701880000 |
| C | 1.466137000 | 1.404531000 | 1.576271000 |
| N | -2.670522000 | -1.717871000 | -0.609214000 |
| C | -2.710880000 | -0.347416000 | -0.569459000 |
| C | -1.518580000 | 0.522817000 | -0.784062000 |
| N | -2.026391000 | 1.911444000 | -1.149752000 |
| C | -3.061736000 | 2.382901000 | -0.153045000 |
| C | -4.321925000 | 1.527901000 | -0.177180000 |
| C | -3.963007000 | 0.081846000 | -0.256685000 |
| C | -4.772633000 | -1.091937000 | -0.099308000 |
| C | -6.120421000 | -1.308049000 | 0.207591000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -6.582326000 | -2.605006000 | 0.283339000 |
| C | -5.724300000 | -3.694669000 | 0.058680000 |
| C | -4.391030000 | -3.511263000 | -0.245370000 |
| C | -3.927830000 | -2.199789000 | -0.321968000 |
| C | -0.612619000 | 0.535967000 | 0.446799000 |
| C | 0.533325000 | 1.551373000 | 0.368609000 |
| C | 0.618173000 | 4.433119000 | 2.073381000 |
| C | -0.056562000 | 4.048124000 | 0.795990000 |
| C | -0.085113000 | 2.905981000 | 0.108986000 |
| C | -0.860984000 | 2.883528000 | -1.176667000 |
| C | -2.616388000 | 1.894537000 | -2.522344000 |
| H | 3.749262000 | 1.559853000 | -0.273692000 |
| H | 1.741271000 | -2.825811000 | 3.057638000 |
| H | 3.668933000 | -3.478616000 | 1.644602000 |
| H | 5.829213000 | -3.404324000 | -0.221726000 |
| H | 7.514026000 | -2.721702000 | -1.897349000 |
| H | 7.537261000 | -0.428615000 | -2.785541000 |
| H | 5.886755000 | 1.247226000 | -2.037466000 |
| H | 2.220554000 | 2.191403000 | 1.549625000 |
| H | 0.903025000 | 1.504723000 | 2.501880000 |
| H | -1.862380000 | -2.281078000 | -0.811643000 |
| H | -0.944165000 | 0.199930000 | -1.654692000 |
| H | -2.585217000 | 2.354463000 | 0.821278000 |
| H | -3.270725000 | 3.420392000 | -0.401013000 |
| H | -4.879121000 | 1.747288000 | 0.732988000 |
| H | -4.966836000 | 1.818095000 | -1.008709000 |
| H | -6.784604000 | -0.472992000 | 0.382858000 |
| H | -7.619578000 | -2.791799000 | 0.519726000 |
| H | -6.117425000 | -4.698589000 | 0.125936000 |
| H | -3.732243000 | -4.350169000 | -0.417461000 |
| H | -1.205381000 | 0.719526000 | 1.343664000 |
| H | -0.216697000 | -0.473842000 | 0.546600000 |
| H | 1.118717000 | 1.308954000 | -0.527166000 |
| H | 1.424361000 | 5.137319000 | 1.862945000 |
| H | -0.094982000 | 4.961347000 | 2.704787000 |
| H | 1.023584000 | 3.606484000 | 2.638725000 |
| H | -0.614177000 | 4.866822000 | 0.350835000 |
| H | -1.282052000 | 3.853604000 | -1.424773000 |
| H | -0.232513000 | 2.552286000 | -2.003593000 |
| H | -1.837211000 | 1.625863000 | -3.228208000 |
| H | -3.418743000 | 1.168812000 | -2.565056000 |
| H | -2.990413000 | 2.890168000 | -2.740782000 |

Compound: 10'-hydroxy-4',17-tetrahydrousambarensine (**6**)

Solvent: methanol



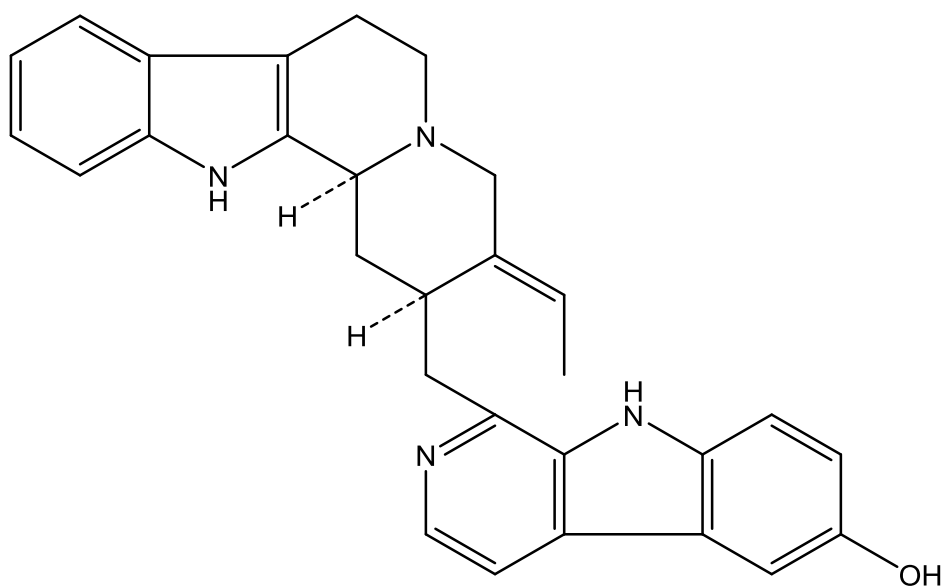
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| | | | |
|---|--------------|--------------|--------------|
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| C | -2.478555000 | 0.152080000 | 0.741506000 |
| N | -1.843211000 | -1.172385000 | 0.891989000 |
| C | -2.181385000 | -2.129619000 | -0.161057000 |
| C | -3.665166000 | -2.472806000 | -0.169704000 |
| C | -4.438542000 | -1.197809000 | -0.157408000 |
| C | -5.796054000 | -0.900725000 | -0.515157000 |
| C | -6.867741000 | -1.662359000 | -0.991896000 |
| C | -8.073892000 | -1.038087000 | -1.242750000 |
| C | -8.233792000 | 0.339575000 | -1.026873000 |
| C | -7.192812000 | 1.118401000 | -0.558245000 |
| C | -5.978630000 | 0.485874000 | -0.305925000 |
| C | -1.627026000 | 1.090737000 | -0.122002000 |
| C | -0.303174000 | 1.417746000 | 0.603458000 |
| C | 0.801242000 | 1.663491000 | -0.436317000 |
| C | 2.169231000 | 2.105152000 | 0.148877000 |
| C | 0.913161000 | 1.648846000 | 3.506338000 |
| C | 0.521795000 | 0.398923000 | 2.780838000 |
| C | 0.017072000 | 0.282765000 | 1.553163000 |
| C | -0.378526000 | -1.058059000 | 1.000113000 |
| N | 3.157408000 | -0.151743000 | 0.758611000 |
| C | 3.195765000 | 1.021483000 | 0.048043000 |

| | | | |
|---|--------------|--------------|--------------|
| N | 2.750573000 | 3.290148000 | -0.493206000 |
| C | 3.290976000 | 3.021026000 | -1.827595000 |
| C | 4.556867000 | 2.176397000 | -1.706386000 |
| C | 4.273563000 | 1.031952000 | -0.787646000 |
| C | 4.967114000 | -0.205683000 | -0.582597000 |
| C | 6.123405000 | -0.767680000 | -1.133450000 |
| C | 6.521323000 | -2.016228000 | -0.700347000 |
| C | 5.791560000 | -2.718536000 | 0.271353000 |
| C | 4.645425000 | -2.179822000 | 0.826350000 |
| C | 4.239682000 | -0.924186000 | 0.393482000 |
| H | -4.626947000 | 1.950192000 | 0.420383000 |
| H | -2.536811000 | 0.592365000 | 1.742548000 |
| H | -1.893455000 | -1.746313000 | -1.152331000 |
| H | -1.586993000 | -3.024698000 | 0.019479000 |
| H | -3.909528000 | -3.087183000 | 0.699116000 |
| H | -3.894888000 | -3.063471000 | -1.057273000 |
| H | -6.752185000 | -2.724717000 | -1.159390000 |
| H | -8.910285000 | -1.615024000 | -1.610348000 |
| H | -9.189465000 | 0.800561000 | -1.231303000 |
| H | -7.317198000 | 2.179320000 | -0.393266000 |
| H | -1.425753000 | 0.595377000 | -1.075115000 |
| H | -2.164250000 | 2.009544000 | -0.355350000 |
| H | -0.438807000 | 2.334620000 | 1.178179000 |
| H | 0.920815000 | 0.764232000 | -1.043585000 |
| H | 0.449199000 | 2.445310000 | -1.113928000 |
| H | 2.025659000 | 2.356249000 | 1.201445000 |
| H | 0.596451000 | 2.552677000 | 2.993059000 |
| H | 0.477334000 | 1.652750000 | 4.504879000 |
| H | 1.996046000 | 1.698665000 | 3.635796000 |
| H | 0.665789000 | -0.521445000 | 3.339973000 |
| H | -0.002437000 | -1.871227000 | 1.621673000 |
| H | 0.081190000 | -1.171970000 | 0.005413000 |
| H | 2.461353000 | -0.377297000 | 1.449773000 |
| H | 2.044331000 | 4.011814000 | -0.547392000 |
| H | 3.512140000 | 3.974993000 | -2.300804000 |
| H | 2.570096000 | 2.491931000 | -2.465282000 |
| H | 5.372695000 | 2.791286000 | -1.320009000 |
| H | 4.859559000 | 1.820078000 | -2.691922000 |
| H | 6.707442000 | -0.249984000 | -1.881562000 |
| O | 7.656919000 | -2.548161000 | -1.252902000 |
| H | 6.134994000 | -3.695056000 | 0.586560000 |
| H | 4.087700000 | -2.725912000 | 1.573985000 |
| H | 7.829146000 | -3.410959000 | -0.868561000 |

Compound: 10'-hydroxyusambarensine (7)

Solvent: methanol



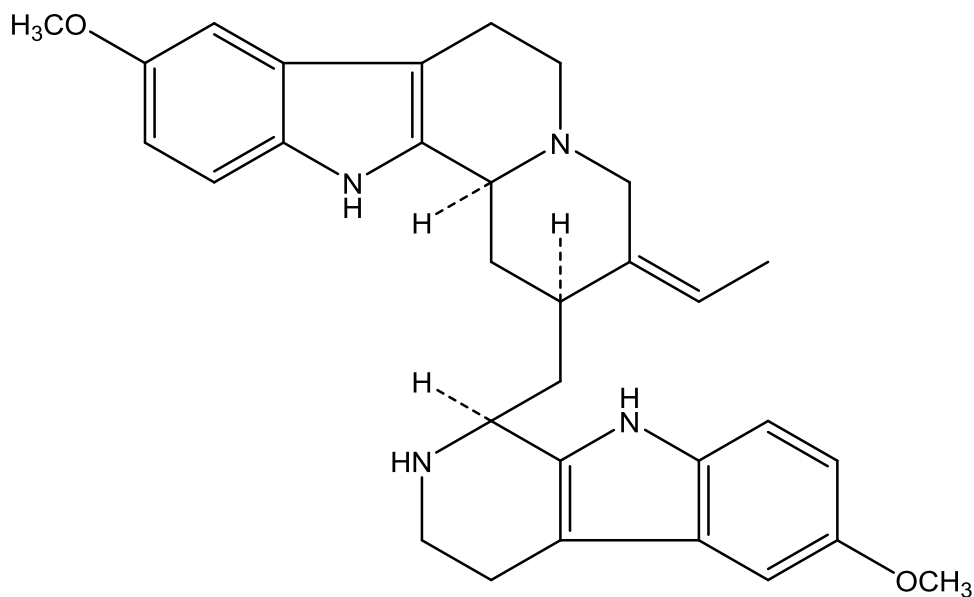
E^0 : -1416.1480314 a.u.

| | | | |
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| C | -3.918085000 | 0.001832000 | 0.268176000 |
| C | -2.447585000 | 0.058790000 | 0.495617000 |
| N | -1.917358000 | -1.315701000 | 0.600851000 |
| C | -2.547374000 | -2.280022000 | -0.299604000 |
| C | -4.028647000 | -2.466478000 | 0.001140000 |
| C | -4.661973000 | -1.117946000 | 0.065227000 |
| C | -6.027088000 | -0.694954000 | -0.063060000 |
| C | -7.237700000 | -1.359937000 | -0.282342000 |
| C | -8.402843000 | -0.622325000 | -0.358632000 |
| C | -8.384981000 | 0.774331000 | -0.220174000 |
| C | -7.204350000 | 1.459392000 | -0.004293000 |
| C | -6.031853000 | 0.712747000 | 0.072995000 |
| C | -1.686053000 | 0.875468000 | -0.554646000 |
| C | -0.248368000 | 1.119188000 | -0.061808000 |
| C | 0.690133000 | 1.333183000 | -1.265508000 |
| C | 1.734997000 | 1.233487000 | 2.352870000 |
| C | 1.026377000 | 0.022575000 | 1.833191000 |
| C | 0.183425000 | -0.045928000 | 0.806024000 |
| C | -0.458849000 | -1.344456000 | 0.406419000 |
| N | 3.131171000 | -0.530265000 | -0.929445000 |
| C | 3.113777000 | 0.828887000 | -0.715214000 |
| C | 2.072926000 | 1.748807000 | -0.861300000 |
| N | 2.285212000 | 3.029987000 | -0.593028000 |
| C | 3.497180000 | 3.436100000 | -0.179981000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 4.579278000 | 2.595759000 | -0.010258000 |
| C | 4.386856000 | 1.244559000 | -0.286543000 |
| C | 5.207178000 | 0.059283000 | -0.219431000 |
| C | 6.539081000 | -0.167713000 | 0.135702000 |
| C | 7.015442000 | -1.462016000 | 0.102481000 |
| C | 6.184525000 | -2.528303000 | -0.277170000 |
| C | 4.870305000 | -2.318951000 | -0.635432000 |
| C | 4.385294000 | -1.013498000 | -0.607127000 |
| H | -4.431418000 | 2.059363000 | 0.427142000 |
| H | -2.277508000 | 0.539749000 | 1.465083000 |
| H | -2.429658000 | -1.974638000 | -1.351433000 |
| H | -2.015021000 | -3.223156000 | -0.179205000 |
| H | -4.482682000 | -3.077092000 | -0.780172000 |
| H | -4.151245000 | -3.003751000 | 0.943608000 |
| H | -7.259284000 | -2.436170000 | -0.388824000 |
| H | -9.345193000 | -1.123663000 | -0.526560000 |
| H | -9.312523000 | 1.324966000 | -0.284085000 |
| H | -7.191849000 | 2.535111000 | 0.101088000 |
| H | -1.683109000 | 0.318150000 | -1.495212000 |
| H | -2.180273000 | 1.825374000 | -0.755675000 |
| H | -0.235097000 | 2.034176000 | 0.530968000 |
| H | 0.268150000 | 2.114517000 | -1.897443000 |
| H | 0.722925000 | 0.417295000 | -1.861013000 |
| H | 1.407505000 | 2.151726000 | 1.872777000 |
| H | 1.584416000 | 1.326754000 | 3.428451000 |
| H | 2.811284000 | 1.145380000 | 2.188545000 |
| H | 1.237235000 | -0.902639000 | 2.360845000 |
| H | -0.040570000 | -2.179654000 | 0.967685000 |
| H | -0.235097000 | -1.528651000 | -0.659401000 |
| H | 2.317579000 | -1.100453000 | -1.079049000 |
| H | 3.594673000 | 4.494553000 | 0.020362000 |
| H | 5.529981000 | 2.982327000 | 0.326520000 |
| H | 7.183966000 | 0.649438000 | 0.432195000 |
| H | 6.604766000 | -3.523437000 | -0.283868000 |
| H | 4.240148000 | -3.145581000 | -0.929423000 |
| H | 8.786512000 | -0.990714000 | 0.668269000 |
| O | 8.300887000 | -1.785054000 | 0.431526000 |

Compound: 10,10'-dimethoxy-3*S*,17*S*-*Z*-tetrahydrousambarensine (**8**)

Solvent: chloroform



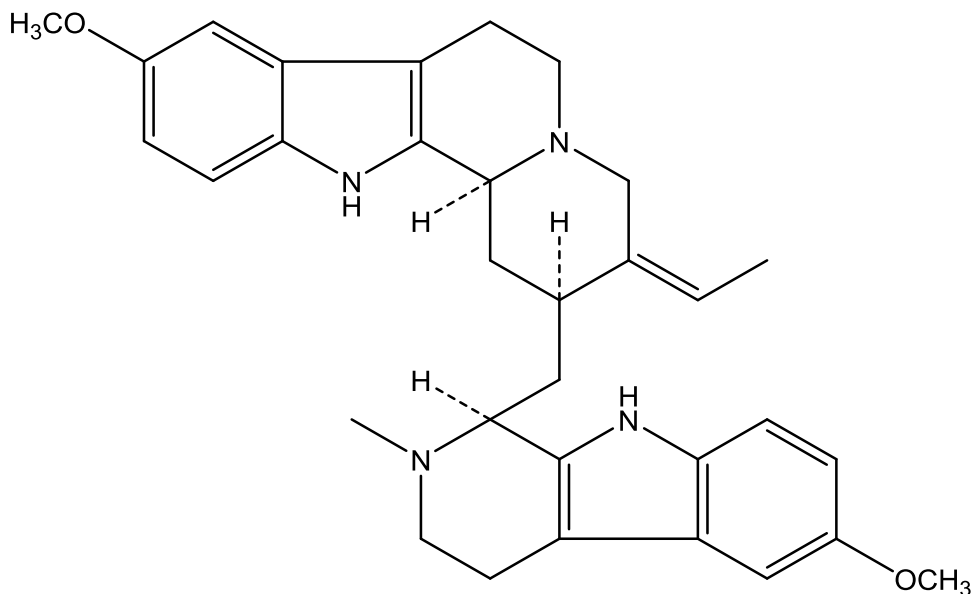
E^0 : -1572.3536574 a.u.

| | | | |
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| C | 3.676350000 | -0.017792000 | 0.482474000 |
| C | 2.473602000 | 0.813666000 | 0.787489000 |
| N | 2.653230000 | 2.120237000 | 0.154750000 |
| C | 3.952410000 | 2.703356000 | 0.481227000 |
| C | 5.085398000 | 1.928118000 | -0.187287000 |
| C | 4.870510000 | 0.468159000 | 0.041504000 |
| C | 5.746173000 | -0.654680000 | -0.109467000 |
| C | 7.081010000 | -0.787327000 | -0.526019000 |
| C | 7.635460000 | -2.052168000 | -0.551667000 |
| C | 6.886610000 | -3.183605000 | -0.170289000 |
| C | 5.577928000 | -3.068680000 | 0.240460000 |
| C | 5.012257000 | -1.795928000 | 0.268481000 |
| C | 1.166151000 | 0.178953000 | 0.327014000 |
| C | -0.030405000 | 1.083670000 | 0.652554000 |
| C | -1.344703000 | 0.416766000 | 0.264194000 |
| C | -2.590183000 | 1.032464000 | 0.935226000 |
| C | -0.354949000 | 4.363066000 | -1.521771000 |
| C | -0.552129000 | 3.047300000 | -0.833915000 |
| C | 0.239759000 | 2.447627000 | 0.050750000 |
| C | 1.555439000 | 3.014102000 | 0.518576000 |
| N | -4.255752000 | 0.761560000 | -0.960094000 |
| C | -3.848677000 | 0.503858000 | 0.326449000 |
| N | -2.687583000 | 0.790578000 | 2.379108000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -3.105661000 | -0.563835000 | 2.742761000 |
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| C | -4.751799000 | -0.309184000 | 0.946100000 |
| C | -5.795281000 | -0.568725000 | -0.000967000 |
| C | -6.978950000 | -1.322425000 | 0.053314000 |
| C | -7.780731000 | -1.363550000 | -1.071039000 |
| C | -7.424446000 | -0.670146000 | -2.244836000 |
| C | -6.266213000 | 0.070954000 | -2.312967000 |
| C | -5.453473000 | 0.116580000 | -1.182738000 |
| C | 9.713321000 | -1.224134000 | -1.332186000 |
| C | -9.361740000 | -2.768493000 | -0.003608000 |
| H | 2.999238000 | -1.983732000 | 0.919514000 |
| H | 2.409835000 | 0.944454000 | 1.885173000 |
| H | 3.952979000 | 3.736992000 | 0.139946000 |
| H | 4.106435000 | 2.715113000 | 1.572079000 |
| H | 6.040910000 | 2.253591000 | 0.226586000 |
| H | 5.103838000 | 2.155012000 | -1.255163000 |
| H | 7.644766000 | 0.085769000 | -0.816893000 |
| H | 7.371846000 | -4.147799000 | -0.209934000 |
| H | 5.012660000 | -3.942438000 | 0.531883000 |
| H | 1.213371000 | -0.001723000 | -0.748848000 |
| H | 1.031923000 | -0.782458000 | 0.825848000 |
| H | -0.017521000 | 1.215677000 | 1.742496000 |
| H | -1.458596000 | 0.431893000 | -0.821646000 |
| H | -1.302691000 | -0.637967000 | 0.542858000 |
| H | -2.557125000 | 2.115573000 | 0.798616000 |
| H | 0.573599000 | 4.856821000 | -1.255141000 |
| H | -0.362414000 | 4.224261000 | -2.603233000 |
| H | -1.176970000 | 5.040227000 | -1.287030000 |
| H | -1.466904000 | 2.540694000 | -1.118359000 |
| H | 1.519870000 | 3.155318000 | 1.613467000 |
| H | 1.753343000 | 3.984713000 | 0.076026000 |
| H | -3.789209000 | 1.362131000 | -1.616181000 |
| H | -1.814171000 | 1.023938000 | 2.829120000 |
| H | -2.976079000 | -0.674979000 | 3.817003000 |
| H | -2.498825000 | -1.337560000 | 2.256003000 |
| H | -5.214103000 | -0.216738000 | 3.034435000 |
| H | -4.825838000 | -1.829763000 | 2.453841000 |
| H | -7.243028000 | -1.847918000 | 0.958249000 |
| H | -8.089400000 | -0.737271000 | -3.093409000 |
| H | -6.001286000 | 0.598046000 | -3.218548000 |
| H | 10.683341000 | -1.629703000 | -1.598865000 |
| H | 9.281765000 | -0.715766000 | -2.196591000 |
| H | 9.830974000 | -0.506750000 | -0.517670000 |

| | | | |
|---|---------------|--------------|--------------|
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| H | -8.628555000 | -3.530562000 | 0.267794000 |
| H | -9.511405000 | -2.098313000 | 0.845130000 |
| O | 8.917337000 | -2.318495000 | -0.935721000 |
| O | -8.954349000 | -2.055415000 | -1.149736000 |

Compound: 10,10'-dimethoxy-*N*-4'-methyl-3*S*,17*S*-*Z*-tetrahydrousambarensine (**9**)
Solvent: chloroform



E^0 : -1611.6513851 a.u.

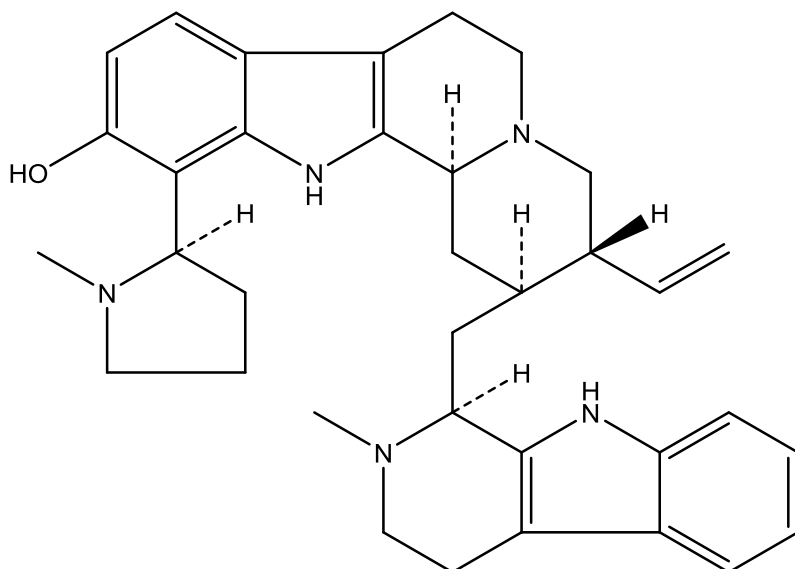
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| N | 2.501465000 | 1.888100000 | 0.677471000 |
| C | 3.732863000 | 2.546913000 | 1.106565000 |
| C | 4.911949000 | 2.130980000 | 0.230001000 |
| C | 4.901785000 | 0.644901000 | 0.083381000 |
| C | 5.902577000 | -0.270365000 | -0.376267000 |
| C | 7.214068000 | -0.106142000 | -0.851614000 |
| C | 7.922360000 | -1.233559000 | -1.219369000 |
| C | 7.349513000 | -2.517563000 | -1.121824000 |
| C | 6.065829000 | -2.693778000 | -0.657343000 |
| C | 5.345736000 | -1.560996000 | -0.284387000 |
| C | 1.290614000 | -0.224567000 | 0.381007000 |
| C | 0.010783000 | 0.399914000 | 0.951111000 |
| C | -1.240109000 | -0.319805000 | 0.451121000 |
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| C | -0.832877000 | 2.573824000 | 0.009463000 |
| C | 0.070032000 | 1.892888000 | 0.709316000 |
| C | 1.322050000 | 2.501334000 | 1.285484000 |
| N | -4.127671000 | 1.094505000 | -0.087340000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -3.754080000 | -0.029037000 | 0.612746000 |
| N | -2.673436000 | -1.279697000 | 2.320844000 |
| C | -3.165529000 | -2.495557000 | 1.676700000 |
| C | -4.593081000 | -2.316208000 | 1.165921000 |
| C | -4.707331000 | -0.993624000 | 0.485260000 |
| C | -5.753491000 | -0.443467000 | -0.325578000 |
| C | -6.977974000 | -0.949179000 | -0.790163000 |
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| C | -7.371600000 | 1.186338000 | -1.881032000 |
| C | -6.170736000 | 1.692800000 | -1.436436000 |
| C | -5.363564000 | 0.867437000 | -0.657653000 |
| C | 9.823441000 | 0.045913000 | -1.820453000 |
| C | -9.441839000 | -1.793857000 | -1.784635000 |
| C | -1.511380000 | -1.539928000 | 3.145965000 |
| H | 3.418199000 | -2.184616000 | 0.355710000 |
| H | 2.515002000 | 0.292690000 | 2.052579000 |
| H | 3.579036000 | 3.622580000 | 1.042192000 |
| H | 3.952269000 | 2.306397000 | 2.159072000 |
| H | 5.841678000 | 2.473847000 | 0.686367000 |
| H | 4.833459000 | 2.617819000 | -0.744232000 |
| H | 7.642039000 | 0.881992000 | -0.923579000 |
| H | 7.949793000 | -3.363104000 | -1.424257000 |
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| H | 1.308636000 | -1.287910000 | 0.629503000 |
| H | 0.066049000 | 0.269677000 | 2.037593000 |
| H | -1.477659000 | 0.003915000 | -0.561911000 |
| H | -1.016676000 | -1.384606000 | 0.367517000 |
| H | -2.332952000 | 0.736637000 | 1.986111000 |
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| H | -0.823211000 | 4.173558000 | -1.403880000 |
| H | -1.777923000 | 4.492294000 | 0.027642000 |
| H | -1.659461000 | 2.013959000 | -0.409862000 |
| H | 1.329976000 | 2.354210000 | 2.379930000 |
| H | 1.369270000 | 3.569841000 | 1.102735000 |
| H | -3.681292000 | 1.991828000 | -0.021590000 |
| H | -3.133369000 | -3.294156000 | 2.415616000 |
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| H | -5.291171000 | -2.367844000 | 2.004452000 |
| H | -4.844424000 | -3.135031000 | 0.490130000 |
| H | -7.276867000 | -1.955265000 | -0.538547000 |
| H | -8.034550000 | 1.785428000 | -2.487883000 |
| H | -5.870268000 | 2.700132000 | -1.688306000 |
| H | 10.817685000 | -0.139899000 | -2.212260000 |

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|---|---------------|--------------|--------------|
| H | 9.275611000 | 0.690628000 | -2.510438000 |
| H | 9.901903000 | 0.543766000 | -0.852002000 |
| H | -10.406623000 | -1.896699000 | -2.269558000 |
| H | -8.756468000 | -2.548224000 | -2.175887000 |
| H | -9.558325000 | -1.940272000 | -0.709048000 |
| H | -1.212445000 | -0.626029000 | 3.658289000 |
| H | -1.769279000 | -2.281921000 | 3.899178000 |
| H | -0.645314000 | -1.919927000 | 2.583816000 |
| O | 9.200386000 | -1.212993000 | -1.696721000 |
| O | -8.985097000 | -0.491679000 | -2.074455000 |

Compound: strychnopentamine (10)

Solvent: chloroform



E^0 : -1708.5341227 a.u.

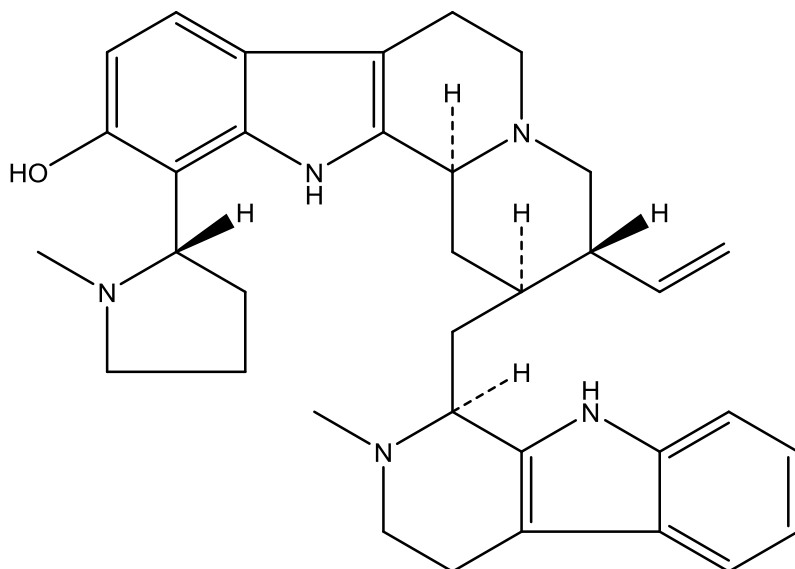
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| C | -1.484634000 | 2.051922000 | 0.364041000 |
| N | -2.199411000 | 3.137127000 | -0.308710000 |
| C | -1.631388000 | 4.444289000 | 0.015218000 |
| C | -0.239693000 | 4.611991000 | -0.589545000 |
| C | 0.563056000 | 3.387932000 | -0.294731000 |
| C | 1.977214000 | 3.139840000 | -0.350349000 |
| C | 3.092567000 | 3.907236000 | -0.694769000 |
| C | 4.348459000 | 3.344501000 | -0.613252000 |
| C | 4.520010000 | 2.013369000 | -0.199339000 |
| C | 3.435844000 | 1.208992000 | 0.143306000 |
| C | 2.174647000 | 1.804118000 | 0.064477000 |
| C | -2.003516000 | 0.703768000 | -0.118787000 |
| C | -3.499616000 | 0.562943000 | 0.148857000 |
| C | -4.076326000 | -0.744490000 | -0.388962000 |
| C | -3.503756000 | -2.038442000 | 0.212860000 |
| C | -6.725378000 | 1.789268000 | -0.876642000 |
| C | -5.700421000 | 1.767238000 | -0.038335000 |
| C | -4.255308000 | 1.769093000 | -0.437420000 |
| C | -3.612368000 | 3.078895000 | 0.023847000 |
| N | -1.836267000 | -2.371536000 | -1.676487000 |
| C | -2.170054000 | -2.433990000 | -0.343652000 |
| N | -3.395694000 | -1.966597000 | 1.674045000 |
| C | -4.710809000 | -1.827835000 | 2.278807000 |
| C | -2.712281000 | -3.135030000 | 2.231623000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -1.239227000 | -3.170975000 | 1.841272000 |
| C | -1.137883000 | -2.963772000 | 0.367383000 |
| C | -0.092167000 | -3.261531000 | -0.568530000 |
| C | 1.171388000 | -3.856040000 | -0.469556000 |
| C | 1.912303000 | -4.046917000 | -1.619874000 |
| C | 1.428782000 | -3.636385000 | -2.871581000 |
| C | 0.187093000 | -3.043948000 | -3.000475000 |
| C | -0.567813000 | -2.874265000 | -1.843574000 |
| C | 3.617689000 | -0.232078000 | 0.528060000 |
| O | 5.792045000 | 1.533163000 | -0.144204000 |
| N | 4.788884000 | -0.447746000 | 1.392067000 |
| C | 4.641478000 | 0.120645000 | 2.720090000 |
| C | 3.894144000 | -1.172609000 | -0.657874000 |
| C | 4.750036000 | -2.310166000 | -0.060276000 |
| C | 4.966726000 | -1.897202000 | 1.398381000 |
| H | 0.751174000 | 0.317329000 | 0.596666000 |
| H | -1.673180000 | 2.110625000 | 1.453523000 |
| H | -2.304220000 | 5.207604000 | -0.371835000 |
| H | -1.574674000 | 4.576951000 | 1.107502000 |
| H | -0.323110000 | 4.770639000 | -1.666750000 |
| H | 0.232550000 | 5.501680000 | -0.170525000 |
| H | 2.975875000 | 4.933418000 | -1.016069000 |
| H | 5.233799000 | 3.911934000 | -0.861462000 |
| H | -1.796252000 | 0.608058000 | -1.188111000 |
| H | -1.471154000 | -0.096505000 | 0.396495000 |
| H | -3.640305000 | 0.581786000 | 1.234560000 |
| H | -3.942235000 | -0.772244000 | -1.473660000 |
| H | -5.154689000 | -0.744941000 | -0.237604000 |
| H | -4.210743000 | -2.844236000 | -0.057778000 |
| H | -7.746884000 | 1.803597000 | -0.523554000 |
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| H | -4.184733000 | 1.727950000 | -1.528377000 |
| H | -4.116852000 | 3.914027000 | -0.461150000 |
| H | -3.767255000 | 3.190626000 | 1.111956000 |
| H | -2.421278000 | -2.023756000 | -2.415201000 |
| H | -5.370849000 | -2.672191000 | 2.029635000 |
| H | -4.606380000 | -1.781772000 | 3.360307000 |
| H | -5.193791000 | -0.910716000 | 1.949338000 |
| H | -3.201514000 | -4.062627000 | 1.893641000 |
| H | -2.811844000 | -3.090404000 | 3.314468000 |
| H | -0.809775000 | -4.129963000 | 2.133673000 |
| H | -0.695221000 | -2.395840000 | 2.386863000 |
| H | 1.554786000 | -4.173471000 | 0.491565000 |

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|---|--------------|--------------|--------------|
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| H | -0.189625000 | -2.735226000 | -3.965274000 |
| H | 2.722415000 | -0.586186000 | 1.063852000 |
| H | 4.448408000 | -0.631210000 | -1.421957000 |
| H | 2.966469000 | -1.525967000 | -1.102190000 |
| H | 5.699652000 | -2.389914000 | -0.583300000 |
| H | 4.254296000 | -3.274689000 | -0.122696000 |
| H | 5.946837000 | -2.159778000 | 1.790746000 |
| H | 4.206192000 | -2.359314000 | 2.044227000 |
| H | 5.760736000 | 0.702254000 | 0.384117000 |
| H | 4.517186000 | 1.199707000 | 2.648225000 |
| H | 5.532573000 | -0.088713000 | 3.307858000 |
| H | 3.770306000 | -0.299554000 | 3.240264000 |

Compound: isostrychnopentamine (**11**)

Solvent: chloroform



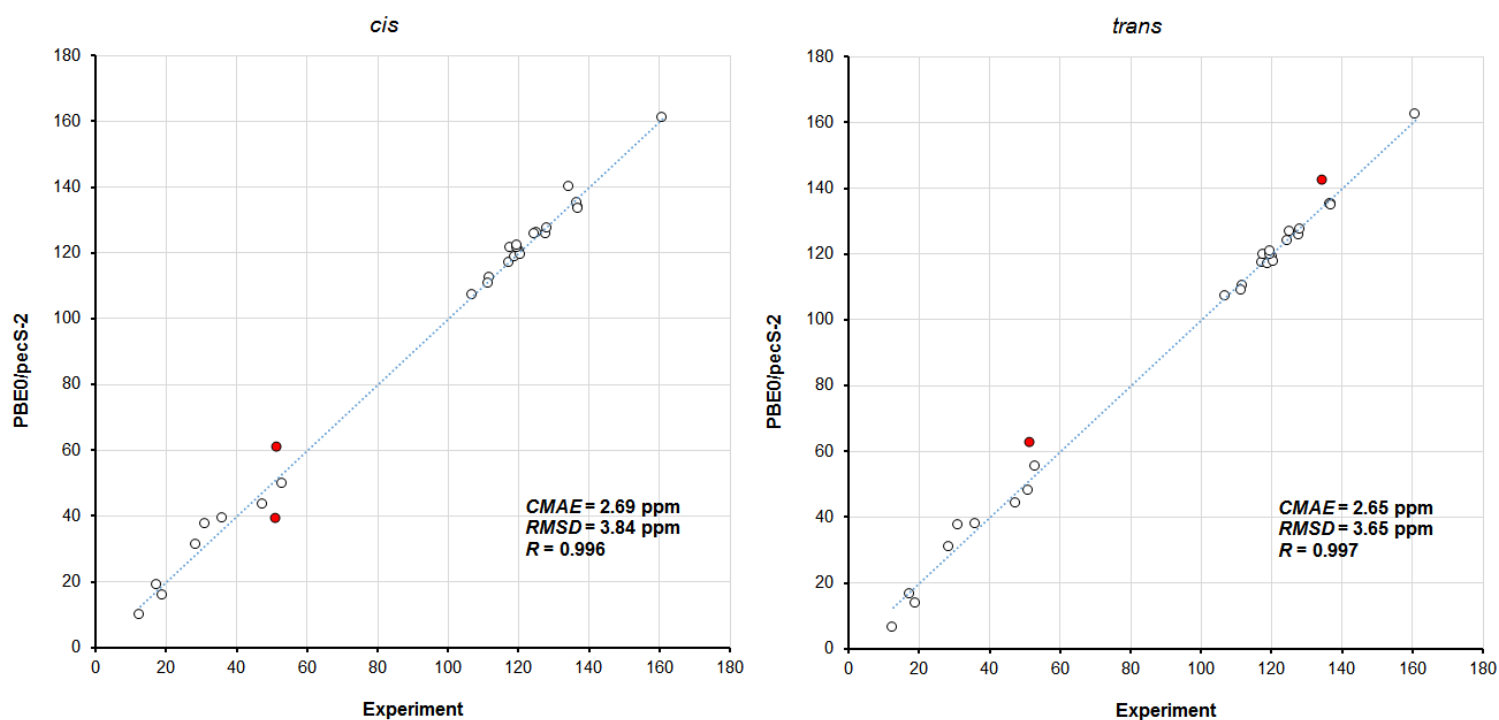
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| C | -0.820786000 | 2.193389000 | 0.320419000 |
| N | -1.317441000 | 3.433661000 | -0.276556000 |
| C | -0.482489000 | 4.583225000 | 0.065370000 |
| C | 0.887303000 | 4.488871000 | -0.602151000 |
| C | 1.433519000 | 3.119089000 | -0.370100000 |
| C | 2.764525000 | 2.593022000 | -0.475452000 |
| C | 3.987169000 | 3.145119000 | -0.852897000 |
| C | 5.109413000 | 2.346522000 | -0.836291000 |
| C | 5.029403000 | 1.002716000 | -0.440840000 |
| C | 3.838526000 | 0.396373000 | -0.051992000 |
| C | 2.710672000 | 1.230620000 | -0.087104000 |
| C | -1.608680000 | 1.006597000 | -0.223204000 |
| C | -3.101598000 | 1.148430000 | 0.067845000 |
| C | -3.930978000 | 0.037655000 | -0.573379000 |
| C | -3.723692000 | -1.383468000 | -0.030436000 |
| C | -6.043234000 | 3.048286000 | -0.722345000 |
| C | -5.010780000 | 2.785788000 | 0.064436000 |
| C | -3.609692000 | 2.525018000 | -0.401834000 |
| C | -2.701023000 | 3.644029000 | 0.109681000 |
| N | -1.984257000 | -1.975211000 | -1.792051000 |
| C | -2.475419000 | -2.059478000 | -0.509655000 |

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|---|--------------|--------------|--------------|
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| C | -5.019303000 | -0.972987000 | 1.951822000 |
| C | -3.463653000 | -2.783357000 | 1.929744000 |
| C | -2.028559000 | -3.215104000 | 1.649281000 |
| C | -1.711801000 | -2.915631000 | 0.222503000 |
| C | -0.686219000 | -3.412863000 | -0.648406000 |
| C | 0.343324000 | -4.349516000 | -0.509353000 |
| C | 1.151140000 | -4.622551000 | -1.595158000 |
| C | 0.959544000 | -3.969231000 | -2.822631000 |
| C | -0.056803000 | -3.048602000 | -2.994341000 |
| C | -0.882055000 | -2.790497000 | -1.902856000 |
| C | 3.857965000 | -1.056806000 | 0.402899000 |
| O | 6.165531000 | 0.234782000 | -0.425450000 |
| N | 3.980428000 | -1.242487000 | 1.859816000 |
| C | 4.934299000 | -0.388722000 | 2.533588000 |
| C | 2.592387000 | -1.871676000 | 0.073232000 |
| C | 1.815875000 | -1.996115000 | 1.407946000 |
| C | 2.633264000 | -1.170352000 | 2.402366000 |
| H | 1.032674000 | 0.071447000 | 0.513234000 |
| H | -0.972721000 | 2.226062000 | 1.416415000 |
| H | -1.000733000 | 5.482540000 | -0.262856000 |
| H | -0.353656000 | 4.655067000 | 1.157027000 |
| H | 0.791819000 | 4.696896000 | -1.669838000 |
| H | 1.547761000 | 5.250110000 | -0.184501000 |
| H | 4.056671000 | 4.180977000 | -1.155357000 |
| H | 6.071745000 | 2.748908000 | -1.125684000 |
| H | -1.437508000 | 0.942084000 | -1.301114000 |
| H | -1.239801000 | 0.081659000 | 0.225263000 |
| H | -3.232087000 | 1.099750000 | 1.153793000 |
| H | -3.741858000 | 0.031460000 | -1.650484000 |
| H | -4.987102000 | 0.283691000 | -0.475662000 |
| H | -4.571033000 | -1.980572000 | -0.416153000 |
| H | -7.027479000 | 3.243752000 | -0.320584000 |
| H | -5.934012000 | 3.076239000 | -1.799495000 |
| H | -5.155318000 | 2.766180000 | 1.142343000 |
| H | -3.585713000 | 2.549201000 | -1.495340000 |
| H | -3.037466000 | 4.593244000 | -0.306116000 |
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| H | -2.356289000 | -1.402681000 | -2.528461000 |
| H | -5.858284000 | -1.571846000 | 1.566448000 |
| H | -5.015917000 | -1.046587000 | 3.036741000 |
| H | -5.194713000 | 0.067254000 | 1.686892000 |
| H | -4.157812000 | -3.504128000 | 1.468302000 |
| H | -3.652891000 | -2.789854000 | 3.001389000 |

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| H | -1.346285000 | -2.688370000 | 2.320878000 |
| H | 0.500998000 | -4.853055000 | 0.435120000 |
| H | 1.950231000 | -5.344102000 | -1.500897000 |
| H | 1.614695000 | -4.195350000 | -3.651572000 |
| H | -0.212333000 | -2.556004000 | -3.943738000 |
| H | 4.729312000 | -1.509947000 | -0.061827000 |
| H | 2.881494000 | -2.857648000 | -0.275523000 |
| H | 2.005590000 | -1.424102000 | -0.727482000 |
| H | 1.788249000 | -3.036424000 | 1.723349000 |
| H | 0.774736000 | -1.675586000 | 1.337758000 |
| H | 2.613244000 | -1.577573000 | 3.412691000 |
| H | 2.275115000 | -0.131150000 | 2.458996000 |
| H | 6.905742000 | 0.758919000 | -0.740172000 |
| H | 5.911064000 | -0.486231000 | 2.064724000 |
| H | 5.014756000 | -0.694412000 | 3.575941000 |
| H | 4.646422000 | 0.671879000 | 2.507712000 |

Figure S1. Comparison of calculated ^1H and ^{13}C NMR chemical shifts of *cis*- and *trans*-conformations of the C/D quinolizidine system of 5',6'-dihydrousambarensine (**4**).



| Nuclei | Experiment | Calculated | | | |
|--------|------------|------------|-----------|--------------|-----------|
| | | <i>cis</i> | | <i>trans</i> | |
| | | CS | Deviation | CS | Deviation |
| 2 | 136.7 | 135.0 | 1.7 | 135.2 | 1.5 |
| 3 | 53.1 | 49.6 | 3.5 | 55.5 | -2.4 |
| 5 | 51.1 | 39.1 | 12.0 | 48.1 | 3.0 |
| 6 | 17.5 | 19.0 | -1.5 | 16.6 | 0.9 |
| 7 | 107.0 | 107.0 | 0.0 | 107.0 | 0.0 |
| 8 | 128.3 | 127.3 | 1.0 | 127.4 | 0.9 |
| 9 | 118.9 | 118.9 | 0.0 | 116.9 | 2.0 |
| 10 | 120.8 | 119.4 | 1.4 | 117.8 | 3.0 |
| 11 | 119.8 | 121.7 | -1.9 | 119.7 | 0.1 |
| 12 | 111.5 | 110.7 | 0.8 | 108.9 | 2.6 |
| 13 | 137.1 | 133.4 | 3.7 | 134.7 | 2.4 |
| 14 | 28.5 | 31.1 | -2.6 | 30.9 | -2.4 |
| 15 | 31.2 | 37.6 | -6.4 | 37.6 | -6.4 |
| 16 | 36.2 | 39.4 | -3.2 | 38.0 | -1.8 |
| 17 | 160.9 | 161.0 | -0.1 | 162.5 | -1.6 |
| 18 | 12.6 | 10.0 | 2.6 | 6.4 | 6.2 |
| 19 | 119.8 | 122.2 | -2.4 | 120.9 | -1.1 |
| 20 | 134.5 | 140.1 | -5.6 | 142.4 | -7.9 |
| 21 | 51.4 | 60.8 | -9.4 | 62.8 | -11.4 |
| 2' | 125.4 | 125.9 | -0.5 | 126.9 | -1.5 |
| 5' | 47.4 | 43.6 | 3.8 | 44.2 | 3.2 |
| 6' | 19.2 | 15.8 | 3.4 | 13.6 | 5.6 |
| 7' | 117.5 | 117.0 | 0.5 | 117.2 | 0.3 |
| 8' | 127.8 | 125.7 | 2.1 | 125.7 | 2.1 |
| 9' | 117.6 | 121.4 | -3.8 | 119.7 | -2.1 |
| 10' | 120.3 | 120.6 | -0.3 | 119.2 | 1.1 |
| 11' | 124.7 | 125.7 | -1.0 | 124.0 | 0.7 |
| 12' | 112.0 | 112.4 | -0.4 | 110.3 | 1.7 |
| 13' | 137.0 | 133.7 | 3.3 | 135.2 | 1.8 |