

*Supplementary Materials*

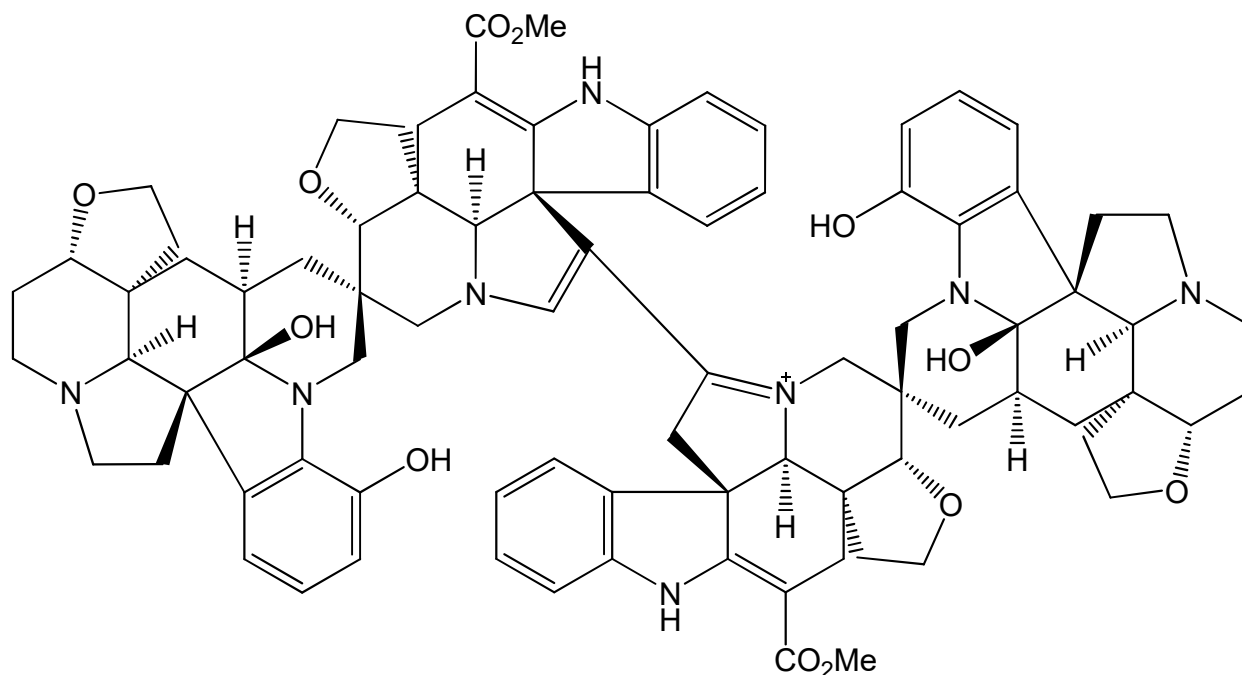
# **Stereochemical Study of the Super Large Tetrakis Alkaloid Alasmontamine A by Means of an Advanced Computational NMR**

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**Cartesian coordinates (Angstroms) of key configurations of alasmontamine A optimized at the M06-2X/aug-cc-pVDZ level in the liquid phase of methanol, modulated within the IEF-PCM scheme:**

Compound: diastereomer «0»



Imaginary frequencies: none

$E^0$ : -4595.1873024 a.u.

N	-6.469236000	-0.974674000	2.483841000
C	-5.993793000	-0.541149000	1.279537000
C	-1.767896000	1.264250000	-0.604795000
N	-2.648759000	0.327001000	0.094932000
C	-2.574431000	-0.993994000	-0.000847000
C	-3.817697000	-1.614627000	0.569250000
C	-4.478135000	-0.462855000	1.374619000
C	-4.239007000	-0.636317000	2.856495000
C	-3.077322000	-0.572441000	3.610159000
C	-3.155101000	-0.844527000	4.982488000
C	-4.377154000	-1.183550000	5.566640000
C	-5.552922000	-1.260039000	4.811748000
C	-5.456906000	-0.979425000	3.454591000
C	-2.510989000	2.534253000	-1.072824000

C	-3.950993000	2.125250000	-1.450755000
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C	-5.755026000	0.440004000	-0.938723000
C	-5.810148000	3.512329000	-1.038860000
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C	1.562594000	3.941604000	-1.427529000
C	2.885049000	3.584149000	-1.212455000
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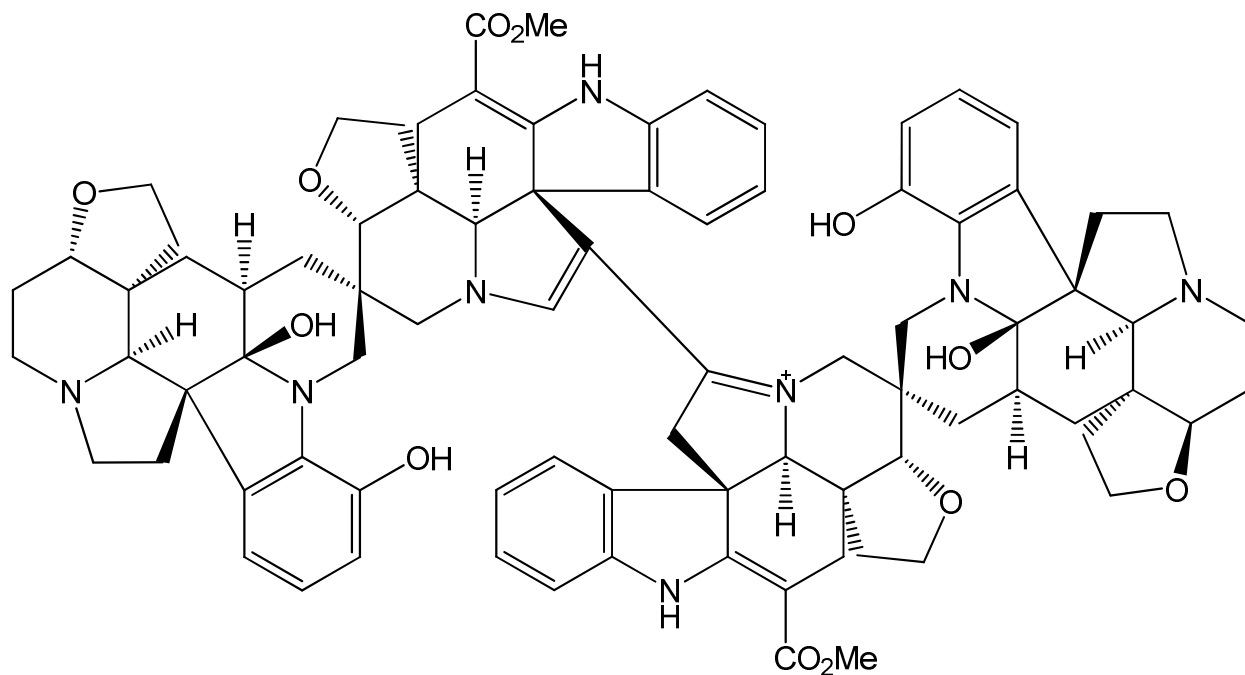
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O	-8.650081000	0.156418000	-1.064625000
O	-4.692911000	3.254161000	-1.898791000
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O	2.016509000	6.986108000	2.663244000
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Compound: diastereomer «15'»



Imaginary frequencies: none

$E^0$ : -4595.1785102 a.u.

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C	-2.461987000	-1.088791000	-0.047047000
C	-3.709996000	-1.722436000	0.500300000
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C	-2.950696000	-1.078055000	4.913740000
C	-4.161353000	-1.422851000	5.518256000
C	-5.355761000	-1.470135000	4.790499000
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C	-2.414596000	2.442271000	-1.076156000
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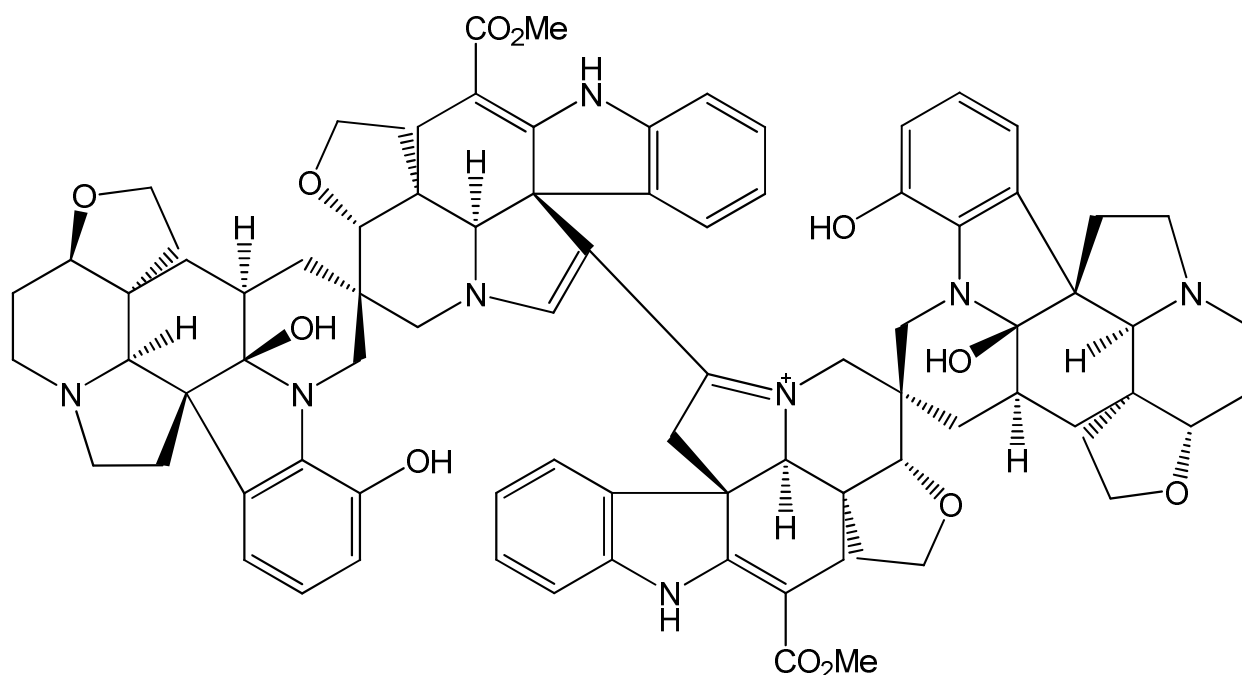
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H	3.603247000	4.597969000	-0.865183000
H	4.529427000	2.363579000	-1.518288000
H	3.049659000	0.660677000	-2.549312000
H	-0.050357000	9.244726000	2.232545000
H	-1.282301000	8.159269000	1.545714000
H	1.650049000	7.477573000	2.077583000
H	-0.272700000	3.546320000	0.303257000
H	-1.337067000	5.047297000	2.028224000
H	-1.669307000	6.219346000	0.749833000
H	0.159910000	4.741748000	3.963695000
H	1.761404000	5.510146000	4.154109000
H	2.356584000	5.150588000	1.898677000
H	1.067244000	3.923163000	1.895043000
H	2.108955000	6.557575000	-0.066391000
H	-2.651832000	3.240984000	0.951594000
H	-3.150582000	4.342752000	-0.348245000
H	-2.486652000	3.607034000	-2.876323000
H	-1.622782000	2.068952000	-3.079270000
H	-4.200288000	-5.102746000	-0.887173000
H	2.413815000	-2.406575000	-2.431469000
H	2.475390000	-1.335360000	-1.001680000
H	0.368606000	-0.483543000	-0.371245000
H	-1.428963000	-1.482634000	-3.792251000
H	-3.321184000	-1.309551000	-5.416752000
H	-5.404560000	-2.598569000	-5.048969000
H	-5.648091000	-4.100638000	-3.072003000
H	2.332725000	-5.555161000	-0.199499000
H	0.213874000	-5.552281000	1.137373000
H	-0.025522000	-3.798719000	1.041046000
H	1.044934000	-5.884471000	-3.685128000
H	1.787160000	-7.126859000	-2.638925000
H	-0.814078000	-6.000322000	-2.184404000
H	0.140762000	-6.883937000	-0.977692000
H	0.077366000	-3.688152000	-2.749008000
H	-4.269731000	-7.035684000	2.638435000
H	-3.887533000	-8.191852000	1.324987000
H	-5.372889000	-7.179546000	1.223182000
H	9.636961000	-0.586172000	1.608786000

H	9.917114000	-2.308193000	1.979909000
H	8.169690000	-0.688966000	3.436506000
H	7.866779000	-2.432053000	3.675162000
H	5.899096000	-0.295652000	3.585942000
H	5.492668000	-2.025121000	3.552853000
H	5.481045000	1.825714000	1.456934000
H	3.286853000	3.020958000	1.590991000
H	1.176463000	1.697537000	1.856655000
H	10.633232000	-1.667086000	-0.374269000
H	9.431975000	-2.969607000	-0.324165000
H	8.740669000	-1.478299000	-2.057681000
H	4.592689000	-1.510906000	-0.854426000
H	6.508059000	-2.532402000	-2.100022000
H	7.047181000	-3.294030000	-0.595409000
H	8.051607000	1.520134000	-2.348852000
H	7.765481000	1.864178000	-0.621051000
H	6.427915000	-0.189020000	-2.415043000
H	5.782441000	0.556160000	-0.932152000
H	7.393481000	0.175402000	1.118030000
H	4.297280000	-3.703957000	-2.085048000
H	4.631438000	-4.560066000	-0.568842000
H	1.687795000	-2.947756000	1.258135000
H	2.931959000	-4.191561000	1.449554000
H	-1.373699000	6.562036000	-1.446206000
H	0.990082000	0.259768000	-3.452458000
H	6.514724000	-3.475654000	1.577234000
H	1.010447000	-1.407714000	2.688682000
O	-3.656096000	-6.177064000	0.841925000
O	5.546423000	-3.574242000	1.599259000
O	9.023168000	0.279317000	-0.989903000
O	0.944719000	-0.861646000	1.893362000
O	-8.573516000	0.119683000	-0.977906000
O	-4.610248000	3.114968000	-1.919381000
O	-1.574860000	5.711956000	-1.880362000
O	0.247446000	6.714106000	3.377189000
O	-8.612058000	-0.866327000	1.044007000
O	0.452444000	0.956312000	-3.054981000
O	2.294218000	-5.150867000	-2.235083000
O	-1.771539000	-6.769887000	1.916659000

Compound: diastereomer «15'''»



Imaginary frequencies: none

$E^0$ : -4595.1801423 a.u.

N	-6.443495000	-1.159540000	2.418538000
C	-5.982738000	-0.695756000	1.219573000
C	-1.780904000	1.229930000	-0.606550000
N	-2.650953000	0.257099000	0.055397000
C	-2.543084000	-1.061376000	-0.058590000
C	-3.787490000	-1.716088000	0.472661000
C	-4.468412000	-0.596407000	1.305665000
C	-4.214994000	-0.800046000	2.781437000
C	-3.047651000	-0.738974000	3.526028000
C	-3.109019000	-1.046446000	4.891943000
C	-4.321386000	-1.416481000	5.477766000
C	-5.503033000	-1.489695000	4.731499000
C	-5.423545000	-1.173787000	3.380906000
C	-2.553225000	2.479678000	-1.086837000
C	-3.980726000	2.036087000	-1.477974000
C	-6.622388000	-0.319064000	0.079565000
C	-5.769465000	0.329401000	-0.981751000
C	-5.853362000	3.404306000	-1.054504000
C	-5.616593000	2.560982000	0.193780000
C	-4.811621000	1.372684000	-0.356770000
C	-3.900710000	0.707949000	0.694296000
C	-8.068222000	-0.374292000	-0.103383000
C	-10.139849000	-1.020137000	0.812350000
N	-0.645254000	3.705368000	-2.240676000

C	-0.716370000	4.828644000	-1.297129000
C	0.642185000	8.648531000	0.324483000
N	0.381995000	7.517660000	-0.557463000
C	0.977835000	7.679407000	-1.886729000
C	1.084802000	6.247721000	-2.438230000
C	0.746422000	5.324446000	-1.231344000
C	1.478707000	4.007444000	-1.374466000
C	2.805036000	3.688097000	-1.125880000
C	3.281708000	2.434392000	-1.522811000
C	2.435676000	1.543501000	-2.179916000
C	1.099973000	1.868620000	-2.446823000
C	0.608824000	3.108695000	-2.025577000
C	-0.009376000	8.411967000	1.679333000
C	0.394157000	7.074611000	2.274573000
C	-1.175844000	4.287864000	0.071962000
C	-1.121098000	5.389342000	1.120961000
C	2.284407000	5.782602000	2.698535000
C	1.223109000	4.884333000	2.042119000
C	0.314915000	5.882425000	1.307044000
C	0.961295000	6.270630000	-0.035057000
C	-2.545206000	3.620439000	-0.048468000
C	-1.906776000	2.996967000	-2.397489000
N	-3.508182000	-4.419181000	-1.097517000
C	-2.274567000	-4.235541000	-0.536055000
C	2.110186000	-2.175920000	-1.295224000
N	0.661984000	-2.235388000	-1.207085000
C	-0.142152000	-1.326017000	-0.692909000
C	-1.461216000	-1.762585000	-0.605432000
C	-1.557040000	-3.128926000	-1.316801000
C	-2.464654000	-2.971371000	-2.523945000
C	-2.349677000	-2.163685000	-3.645384000
C	-3.407417000	-2.135909000	-4.562861000
C	-4.560538000	-2.891365000	-4.333467000
C	-4.693924000	-3.693968000	-3.195660000
C	-3.625673000	-3.720456000	-2.305534000
C	2.767192000	-3.322075000	-0.501525000
C	2.029819000	-4.635913000	-0.804611000
C	-1.647655000	-4.902223000	0.468623000
C	-0.168243000	-4.640489000	0.621728000
C	1.415032000	-6.074170000	-2.501040000
C	0.214745000	-5.954807000	-1.545020000
C	0.484141000	-4.648382000	-0.772760000
C	-0.050101000	-3.461077000	-1.592983000
C	-2.265804000	-5.961724000	1.260314000

C	-4.236358000	-7.155050000	1.750370000
N	3.661136000	-2.090712000	1.535778000
C	5.051931000	-2.284479000	1.107279000
C	9.332437000	-1.936851000	1.259431000
N	7.919251000	-1.905716000	1.622056000
C	7.681213000	-1.745935000	3.059287000
C	6.219420000	-1.266406000	3.151870000
C	5.780661000	-1.041333000	1.677388000
C	4.676470000	-0.015279000	1.608367000
C	4.731332000	1.363854000	1.729096000
C	3.536338000	2.083219000	1.843307000
C	2.319919000	1.405185000	1.881616000
C	2.261076000	0.012262000	1.788349000
C	3.447354000	-0.709349000	1.607312000
C	9.517472000	-2.079193000	-0.256279000
C	8.714521000	-0.965263000	-0.884379000
C	5.085873000	-2.298393000	-0.433462000
C	6.516343000	-2.294101000	-0.962077000
C	7.678918000	0.005674000	-2.665113000
C	6.768591000	0.169240000	-1.420533000
C	7.222490000	-0.996665000	-0.529009000
C	7.132731000	-0.828157000	0.985029000
C	4.237208000	-3.459092000	-0.941271000
C	2.704613000	-3.065648000	1.024565000
H	-7.430770000	-1.258073000	2.615581000
H	-0.957561000	1.509724000	0.070146000
H	-1.347878000	0.714681000	-1.476152000
H	-3.558762000	-2.598196000	1.082170000
H	-4.417838000	-2.039259000	-0.369217000
H	-2.100417000	-0.453511000	3.061977000
H	-2.205802000	-0.996724000	5.499365000
H	-4.353369000	-1.653547000	6.541672000
H	-6.447836000	-1.777346000	5.192179000
H	-3.878495000	1.330523000	-2.322224000
H	-6.420196000	0.823140000	-1.715333000
H	-5.176398000	-0.407800000	-1.550695000
H	-5.883317000	4.481258000	-0.841399000
H	-6.787096000	3.120701000	-1.564587000
H	-5.033179000	3.118474000	0.937635000
H	-6.555853000	2.245326000	0.666318000
H	-3.651754000	1.416929000	1.494109000
H	-10.493452000	-1.503734000	1.727364000
H	-10.414379000	-1.614574000	-0.067296000
H	-10.564088000	-0.013104000	0.720248000



H	1.736611000	8.789945000	0.444808000
H	0.236805000	9.558994000	-0.139660000
H	1.984684000	8.131000000	-1.799252000
H	0.358098000	8.344819000	-2.503930000
H	2.105922000	6.039917000	-2.779372000
H	0.398373000	6.057877000	-3.271469000
H	3.465608000	4.403816000	-0.632344000
H	4.313679000	2.148364000	-1.320495000
H	2.816435000	0.580518000	-2.528630000
H	0.258451000	9.216687000	2.378407000
H	-1.103979000	8.424146000	1.566746000
H	-0.242312000	6.852473000	3.152119000
H	-0.436397000	3.523869000	0.367228000
H	-1.502502000	5.015141000	2.084042000
H	-1.776995000	6.222509000	0.818886000
H	3.232807000	5.787383000	2.139447000
H	2.492948000	5.477819000	3.734427000
H	1.669053000	4.144800000	1.363994000
H	0.639341000	4.348473000	2.805499000
H	2.054798000	6.408006000	0.119504000
H	-2.834527000	3.253048000	0.947528000
H	-3.285185000	4.377163000	-0.350509000
H	-2.609402000	3.715358000	-2.839303000
H	-1.773859000	2.171495000	-3.105576000
H	-4.139460000	-5.144028000	-0.782122000
H	2.394470000	-2.254845000	-2.356741000
H	2.425405000	-1.193679000	-0.917098000
H	0.274807000	-0.384155000	-0.339803000
H	-1.453569000	-1.560843000	-3.809634000
H	-3.332850000	-1.517842000	-5.457096000
H	-5.378764000	-2.854770000	-5.053290000
H	-5.595923000	-4.278421000	-3.015449000
H	2.393426000	-5.406446000	-0.096815000
H	0.274506000	-5.421476000	1.253447000
H	0.001880000	-3.675660000	1.123280000
H	1.144173000	-5.918740000	-3.553347000
H	1.908605000	-7.052296000	-2.403810000
H	-0.742080000	-5.936637000	-2.083533000
H	0.183288000	-6.795534000	-0.837810000
H	0.113160000	-3.632133000	-2.666951000
H	-4.178368000	-6.930887000	2.822190000
H	-3.769947000	-8.127815000	1.553925000
H	-5.276748000	-7.152497000	1.413311000
H	9.836665000	-1.007694000	1.602162000

H	9.803799000	-2.779038000	1.785281000
H	8.363594000	-0.983332000	3.480981000
H	7.865728000	-2.694556000	3.583492000
H	6.159648000	-0.312635000	3.690348000
H	5.561177000	-1.987290000	3.650352000
H	5.693839000	1.878455000	1.746668000
H	3.559099000	3.169918000	1.921124000
H	1.377050000	1.939551000	2.010767000
H	10.583122000	-1.981837000	-0.505200000
H	9.174147000	-3.064435000	-0.601748000
H	9.117915000	-0.008960000	-0.489359000
H	4.614896000	-1.354271000	-0.754686000
H	6.506523000	-2.365275000	-2.060084000
H	7.046779000	-3.182710000	-0.589684000
H	7.145644000	-0.427166000	-3.522223000
H	8.116764000	0.967249000	-2.970435000
H	5.705796000	0.134231000	-1.692294000
H	6.961393000	1.129647000	-0.920096000
H	7.537519000	0.169823000	1.266574000
H	4.285521000	-3.512190000	-2.037635000
H	4.641482000	-4.406004000	-0.550713000
H	1.704295000	-2.739412000	1.316066000
H	2.911036000	-4.017267000	1.536631000
H	-1.375794000	6.629163000	-1.365908000
H	0.785089000	0.303898000	-3.519189000
H	6.488173000	-3.462983000	1.559814000
H	0.975357000	-1.110942000	2.699913000
O	-3.581728000	-6.128214000	0.994480000
O	5.517754000	-3.505947000	1.634332000
O	8.730817000	-0.908103000	-2.301119000
O	1.020176000	-0.607058000	1.875779000
O	-8.665629000	0.047502000	-1.079042000
O	-4.748548000	3.145061000	-1.931012000
O	-1.622351000	5.787714000	-1.790985000
O	1.762345000	7.118039000	2.682070000
O	-8.714039000	-0.949247000	0.937313000
O	0.263117000	1.015808000	-3.128119000
O	2.330894000	-5.034907000	-2.136649000
O	-1.685497000	-6.640594000	2.089764000

**Figure S1.** Integration probability distribution (%) of alternate diastereomers based on CMAE data.

