

Acetophenone

6	-1.675860000	2.185656000	0.000000000
6	-0.244647000	1.695580000	0.000000000
8	0.682268000	2.469322000	0.000000000
6	0.000000000	0.211092000	0.000000000
6	1.327354000	-0.234025000	0.000000000
6	1.610637000	-1.595409000	0.000000000
6	0.567804000	-2.524543000	0.000000000
6	-0.756411000	-2.088856000	0.000000000
6	-1.040696000	-0.723991000	0.000000000
1	-2.080455000	-0.393543000	0.000000000
1	-1.571237000	-2.814075000	0.000000000
1	0.789089000	-3.593080000	0.000000000
1	2.646514000	-1.937621000	0.000000000
1	2.119564000	0.515865000	0.000000000
1	-1.670056000	3.280648000	0.000000000
1	-2.210325000	1.817106000	0.887481000
1	-2.210325000	1.817106000	-0.887481000

CO₂

6	0.000000000	0.000000000	0.000000000
8	0.000000000	0.000000000	1.156065000
8	0.000000000	0.000000000	-1.156065000

CS₂

6	0.000000000	0.000000000	0.000000000
16	0.000000000	0.000000000	1.554000000
16	0.000000000	0.000000000	-1.554000000

MeNCS

16	-1.780966000	0.001135000	0.000718000
7	0.987790000	-0.005656000	-0.003278000
6	2.396856000	0.002676000	0.001608000
6	-0.189290000	-0.001534000	-0.001146000
1	2.785025000	-0.644125000	-0.797719000
1	2.777388000	-0.364134000	0.965290000
1	2.773118000	1.022843000	-0.158886000

PhNCS

16	3.689593000	0.000130000	0.000014000
7	0.922410000	-0.000288000	-0.000001000
6	2.104841000	-0.000279000	0.000004000
6	-0.452003000	-0.000128000	-0.000003000
6	-1.150045000	-1.215807000	-0.000004000
6	-1.149764000	1.215710000	-0.000004000
6	-2.541022000	-1.206862000	-0.000007000
6	-2.540744000	1.207087000	-0.000007000
6	-3.240523000	0.000193000	-0.000008000
1	-0.589616000	-2.150548000	-0.000003000
1	-0.589120000	2.150322000	-0.000003000
1	-3.082824000	-2.153450000	-0.000008000
1	-3.082327000	2.153800000	-0.000008000
1	-4.330901000	0.000319000	-0.000010000

Compound 1

7	-2.694302000	0.047819000	-0.292452000
6	-3.135048000	-1.253388000	-0.037641000
5	-1.238750000	0.191622000	-0.140766000
7	-2.040404000	-1.987492000	0.258939000
6	-4.485797000	-1.619107000	-0.114843000

1	-4.772337000	-2.649203000	0.098942000
7	0.152150000	-2.097378000	0.517809000
6	-5.412245000	-0.664118000	-0.462542000
1	-6.469396000	-0.916208000	-0.531235000
6	-4.964165000	0.661788000	-0.745069000
1	-5.672698000	1.434195000	-1.041974000
6	-3.641691000	0.980956000	-0.661817000
1	-3.247511000	1.971453000	-0.892460000
6	-0.879106000	-1.221146000	0.207017000
6	-0.377859000	-3.348209000	0.745869000
1	0.257727000	-4.187675000	1.013490000
6	-1.728967000	-3.306638000	0.598926000
1	-2.476331000	-4.082548000	0.717572000
6	-0.450190000	1.552511000	-0.221826000
6	0.598215000	1.761285000	-1.141795000
6	1.292757000	2.977409000	-1.150463000
1	2.100809000	3.120113000	-1.874182000
6	0.984941000	4.007636000	-0.264827000
6	-0.040506000	3.790191000	0.660628000
1	-0.282350000	4.575700000	1.382774000
6	-0.750767000	2.589453000	0.698896000
6	1.530875000	-1.762596000	0.406376000
6	2.079604000	-0.812289000	1.280854000
6	3.416914000	-0.449722000	1.097546000
1	3.851915000	0.298165000	1.765325000
6	4.207564000	-1.016157000	0.096302000
6	3.627197000	-1.964608000	-0.751600000
1	4.224203000	-2.400586000	-1.556827000
6	2.289950000	-2.341626000	-0.625171000
6	1.028030000	0.689689000	-2.113190000

1	0.225417000	-0.039170000	-2.290774000
1	1.896273000	0.138729000	-1.715934000
1	1.327848000	1.128014000	-3.075825000
6	1.718439000	5.323003000	-0.306667000
1	2.680663000	5.227022000	-0.827319000
1	1.910256000	5.704190000	0.706327000
1	1.126976000	6.085825000	-0.836812000
6	-1.799283000	2.394698000	1.768526000
1	-2.819418000	2.379297000	1.354231000
1	-1.755686000	3.200023000	2.513677000
1	-1.657608000	1.432097000	2.283969000
6	1.259272000	-0.186789000	2.375245000
1	0.704825000	0.682530000	1.988488000
1	1.907162000	0.157450000	3.191534000
1	0.522471000	-0.896330000	2.775472000
6	5.655843000	-0.631088000	-0.054675000
1	5.984234000	-0.719696000	-1.098930000
1	6.298973000	-1.287239000	0.552209000
1	5.828669000	0.401454000	0.276440000
6	1.659419000	-3.291087000	-1.610262000
1	1.508867000	-4.293547000	-1.181966000
1	2.294880000	-3.400283000	-2.498077000
1	0.672428000	-2.922835000	-1.927155000

Compound 2

8	-0.258924000	-0.984071000	-1.136617000
8	-0.842102000	-2.574684000	-2.618551000
7	1.075742000	-1.018173000	1.661016000
7	-0.990400000	-1.344465000	2.378222000
7	-2.357151000	-0.785620000	-0.076361000

6	3.551613000	-1.657963000	-1.026958000
1	3.793925000	-2.450358000	-1.740064000
6	3.983936000	0.504133000	-0.088375000
1	4.574983000	1.423165000	-0.055956000
6	-1.080230000	-1.822910000	-1.713960000
6	2.171089000	-0.827427000	0.754185000
6	-0.784284000	3.378217000	-1.553510000
1	-0.782281000	3.812521000	-2.557319000
6	-2.429738000	-1.694948000	-1.049181000
6	2.921623000	0.359519000	0.803365000
6	-0.804152000	3.640530000	0.810842000
1	-0.815636000	4.283707000	1.695001000
6	1.176777000	-1.592415000	2.908054000
1	2.141721000	-1.828392000	3.347589000
6	-0.259730000	-0.881457000	1.379973000
6	-0.757689000	4.228559000	-0.448976000
6	2.479888000	-1.853228000	-0.150243000
6	4.310062000	-0.489154000	-1.016690000
6	-0.824374000	1.987585000	-1.422753000
6	-0.816782000	1.385848000	-0.135786000
6	-3.409149000	-0.496491000	0.688013000
1	-3.261206000	0.253670000	1.463960000
6	-0.838662000	2.250046000	0.989091000
6	1.696688000	-3.137567000	-0.219610000
1	0.926533000	-3.200179000	0.559972000
1	2.369718000	-4.000378000	-0.109942000
1	1.203571000	-3.219451000	-1.199878000
6	-4.619871000	-1.142743000	0.463436000
1	-5.478468000	-0.902877000	1.088836000
6	5.440462000	-0.283569000	-1.990696000

1	6.309508000	0.176074000	-1.499595000
1	5.131161000	0.386763000	-2.807293000
1	5.758473000	-1.233417000	-2.439862000
6	-0.115236000	-1.778247000	3.334514000
1	-0.451737000	-2.207825000	4.275648000
6	-3.596299000	-2.381876000	-1.338012000
1	-3.597451000	-3.112173000	-2.146688000
6	2.590489000	1.460872000	1.773273000
1	2.335217000	1.064648000	2.765940000
1	1.728460000	2.043523000	1.412512000
1	3.440225000	2.147211000	1.878612000
6	-0.899610000	1.774199000	2.427436000
1	-1.704806000	1.053667000	2.614891000
1	-1.044682000	2.632683000	3.096344000
1	0.023820000	1.262412000	2.734848000
6	-0.902438000	1.197316000	-2.712036000
1	-0.007523000	0.583883000	-2.876297000
1	-1.019660000	1.880368000	-3.562998000
1	-1.767806000	0.516057000	-2.723769000
5	-0.834663000	-0.228862000	0.026294000
6	-4.714334000	-2.091441000	-0.557247000
1	-5.660473000	-2.603048000	-0.739030000
6	-0.683898000	5.722478000	-0.622604000
1	-0.893689000	6.245062000	0.319985000
1	-1.402906000	6.070273000	-1.378104000
1	0.318288000	6.027394000	-0.960870000

Compound 2 TS 1

8	-2.025466000	-1.154430000	-1.912481000
8	-4.223011000	-1.679506000	-1.596949000

7	-0.078029000	-1.801513000	0.959296000
7	-2.149029000	-1.155978000	0.841709000
7	-2.286926000	0.901590000	-0.052568000
6	3.117301000	-2.612409000	-0.710534000
1	3.469525000	-3.191850000	-1.567360000
6	3.563928000	-1.129828000	1.127850000
1	4.269763000	-0.549470000	1.727149000
6	-3.136109000	-1.197495000	-1.423747000
6	1.327631000	-1.844772000	0.677806000
6	2.296574000	2.327786000	-1.402275000
1	3.003222000	2.151302000	-2.218557000
6	-3.070026000	-0.282441000	0.179942000
6	2.209979000	-1.093291000	1.464376000
6	1.583945000	3.609096000	0.494554000
1	1.734042000	4.445139000	1.183564000
6	-0.871295000	-2.862479000	1.344317000
1	-0.439433000	-3.808991000	1.654827000
6	-0.877878000	-0.757649000	0.647156000
6	2.503470000	3.403154000	-0.541381000
6	1.749615000	-2.598562000	-0.426899000
6	4.035631000	-1.883242000	0.049315000
6	1.205541000	1.462230000	-1.252955000
6	0.289857000	1.678648000	-0.207813000
6	-2.958192000	2.056549000	-0.436512000
1	-2.328434000	2.841605000	-0.858352000
6	0.484929000	2.769910000	0.671769000
6	0.760009000	-3.315089000	-1.308444000
1	0.376562000	-4.229445000	-0.830437000
1	1.236949000	-3.609451000	-2.251528000
1	-0.108804000	-2.677082000	-1.540187000

6	-4.285936000	2.183682000	-0.232366000
1	-4.788883000	3.102627000	-0.529119000
6	5.498713000	-1.870454000	-0.306978000
1	6.127077000	-1.894772000	0.593687000
1	5.751237000	-0.952699000	-0.860064000
1	5.764314000	-2.727041000	-0.939624000
6	-2.176785000	-2.467634000	1.260745000
1	-3.096864000	-3.007886000	1.456752000
6	-4.424462000	-0.059379000	0.687912000
1	-4.960507000	-0.894621000	1.139603000
6	1.716931000	-0.245104000	2.604515000
1	1.354790000	0.723408000	2.223654000
1	2.528368000	-0.042888000	3.314662000
1	0.888490000	-0.726698000	3.142029000
6	-0.471307000	3.017346000	1.815025000
1	-0.609739000	2.111814000	2.426975000
1	-1.470297000	3.305244000	1.453014000
1	-0.106493000	3.819213000	2.469875000
6	1.044492000	0.314382000	-2.219456000
1	1.831693000	-0.437708000	-2.051509000
1	1.149547000	0.668579000	-3.255397000
1	0.064124000	-0.177652000	-2.133426000
5	-0.885277000	0.677132000	0.049264000
6	-5.025443000	1.117646000	0.424309000
1	-6.070494000	1.276367000	0.690336000
6	3.666014000	4.342201000	-0.730675000
1	3.350549000	5.248977000	-1.269856000
1	4.468856000	3.871346000	-1.313299000
1	4.080159000	4.662953000	0.235302000

Compound 2 Int 1

8	1.682147000	0.641106000	1.694748000
8	3.578989000	-0.178159000	2.606182000
7	0.035016000	-2.018641000	0.181623000
7	2.116780000	-1.510933000	0.020077000
7	2.472632000	0.721937000	-0.493786000
6	-3.380825000	-1.138303000	1.327734000
1	-3.859279000	-0.611290000	2.156788000
6	-3.540322000	-2.370719000	-0.724253000
1	-4.143786000	-2.807725000	-1.523630000
6	2.869608000	0.053235000	1.672354000
6	-1.395490000	-1.919274000	0.246150000
6	-1.353151000	3.708646000	0.481979000
1	-1.545987000	4.558983000	1.142486000
6	3.163202000	-0.308336000	0.195850000
6	-2.152383000	-2.499370000	-0.784376000
6	-1.856956000	2.468856000	-1.492238000
1	-2.447822000	2.325648000	-2.401515000
6	0.757053000	-3.205575000	0.236417000
1	0.262002000	-4.167485000	0.327022000
6	0.891686000	-0.987009000	0.064144000
6	-2.152896000	3.535599000	-0.650508000
6	-1.987170000	-1.239591000	1.320128000
6	-4.172337000	-1.687651000	0.318203000
6	-0.303229000	2.842217000	0.791587000
6	-0.034390000	1.729255000	-0.046154000
6	2.813118000	1.025214000	-1.769792000
1	2.136154000	1.712080000	-2.284672000
6	-0.817769000	1.572096000	-1.209919000
6	-1.176516000	-0.624850000	2.427926000

1	-0.255021000	-1.185351000	2.631751000
1	-1.771070000	-0.575642000	3.348665000
1	-0.875841000	0.400592000	2.164768000
6	3.967617000	0.562506000	-2.331541000
1	4.249329000	0.865413000	-3.337160000
6	-5.668247000	-1.518370000	0.336329000
1	-6.168688000	-2.317647000	-0.225777000
1	-5.950917000	-0.558564000	-0.122829000
1	-6.056128000	-1.519645000	1.363676000
6	2.078742000	-2.874209000	0.153068000
1	2.969213000	-3.495443000	0.155947000
6	4.533197000	-0.587527000	-0.250861000
1	5.218495000	-1.080800000	0.438040000
6	-1.501432000	-3.216323000	-1.939872000
1	-0.578265000	-2.712161000	-2.259723000
1	-2.187666000	-3.259479000	-2.794978000
1	-1.234451000	-4.251492000	-1.677634000
6	-0.605651000	0.448287000	-2.201719000
1	0.434612000	0.101820000	-2.254774000
1	-0.900552000	0.770421000	-3.210069000
1	-1.236059000	-0.416168000	-1.943366000
6	0.522922000	3.153384000	2.018695000
1	0.404366000	2.389355000	2.798955000
1	0.231908000	4.127062000	2.433879000
1	1.595090000	3.179283000	1.782557000
5	1.121499000	0.682487000	0.282884000
6	4.870900000	-0.197370000	-1.504166000
1	5.873804000	-0.410907000	-1.880991000
6	-3.283821000	4.485898000	-0.944724000
1	-2.932570000	5.528053000	-0.953412000

1	-4.067582000	4.413036000	-0.175541000
1	-3.743628000	4.271200000	-1.918377000

Compound 2 TS 2

8	-1.721289000	1.202911000	-1.463466000
8	-3.718837000	0.841017000	-2.452134000
7	-0.324924000	-1.894465000	-0.572844000
7	-2.373444000	-1.269850000	-0.322009000
7	-2.450836000	0.862612000	0.718812000
6	3.129676000	-0.829771000	-1.357068000
1	3.647616000	-0.192177000	-2.077902000
6	3.177260000	-2.251782000	0.577413000
1	3.732528000	-2.735136000	1.385349000
6	-2.973519000	0.774009000	-1.520167000
6	1.109370000	-1.820902000	-0.546594000
6	2.137302000	2.977555000	-0.220503000
1	2.557756000	3.786898000	-0.824899000
6	-3.301569000	0.154811000	-0.147662000
6	1.799914000	-2.467877000	0.485429000
6	2.350899000	1.395551000	1.549316000
1	2.936511000	0.933273000	2.350034000
6	-1.122833000	-3.000820000	-0.826992000
1	-0.695787000	-3.968773000	-1.072924000
6	-1.117638000	-0.847754000	-0.282400000
6	2.933100000	2.382681000	0.761379000
6	1.755049000	-1.017810000	-1.498412000
6	3.853013000	-1.419264000	-0.316819000
6	0.819497000	2.579666000	-0.456874000
6	0.251719000	1.522543000	0.301256000
6	-2.720343000	0.911627000	2.044654000

1	-1.941715000	1.356284000	2.667222000
6	1.030968000	0.973172000	1.344687000
6	0.994843000	-0.370068000	-2.623019000
1	0.247569000	-1.054472000	-3.049392000
1	1.683716000	-0.061460000	-3.418941000
1	0.453198000	0.522375000	-2.278627000
6	-3.925126000	0.504680000	2.543990000
1	-4.142387000	0.605706000	3.604840000
6	5.320333000	-1.128626000	-0.148291000
1	5.813268000	-1.889943000	0.470168000
1	5.457285000	-0.152882000	0.343680000
1	5.831888000	-1.082715000	-1.119317000
6	-2.421241000	-2.591697000	-0.683729000
1	-3.348635000	-3.147098000	-0.787529000
6	-4.676096000	-0.040518000	0.288480000
1	-5.432170000	-0.278116000	-0.459312000
6	1.092856000	-3.358919000	1.473940000
1	0.112527000	-2.953050000	1.759395000
1	1.697009000	-3.478832000	2.382461000
1	0.922392000	-4.362695000	1.054375000
6	0.493724000	-0.037443000	2.333930000
1	-0.364603000	-0.610987000	1.959988000
1	0.159505000	0.474564000	3.251008000
1	1.279631000	-0.745724000	2.631957000
6	0.052276000	3.325110000	-1.526622000
1	-0.072212000	2.726635000	-2.439896000
1	0.580742000	4.251363000	-1.788171000
1	-0.960786000	3.579878000	-1.192219000
5	-1.126606000	0.827614000	-0.120046000
6	-4.937772000	0.086113000	1.615665000

1	-5.953049000	-0.080866000	1.982293000
6	4.359863000	2.821608000	0.965070000
1	4.412156000	3.889702000	1.224016000
1	4.950221000	2.681965000	0.046749000
1	4.841147000	2.253469000	1.772532000

Compound 4

8	0.134542000	0.197159000	-0.803988000
7	0.017488000	0.295545000	1.527753000
7	0.200640000	-3.068336000	1.135889000
7	1.897444000	-2.084079000	0.116071000
6	-1.160925000	2.255461000	-0.781357000
6	-1.442466000	3.540806000	-0.304535000
1	-0.722688000	4.065037000	0.328285000
6	-2.646791000	4.167376000	-0.617364000
1	-2.854652000	5.166458000	-0.231130000
6	-3.584651000	3.514647000	-1.417574000
1	-4.532984000	3.998665000	-1.655681000
6	-3.302041000	2.242737000	-1.910798000
1	-4.029175000	1.721496000	-2.535206000
6	-2.094794000	1.617102000	-1.599542000
1	-1.876487000	0.615989000	-1.968537000
6	0.163182000	1.544694000	-0.443312000
6	0.348178000	1.506881000	1.074576000
6	1.331888000	2.242102000	-1.135211000
1	1.349487000	3.316300000	-0.900543000
1	1.204352000	2.128135000	-2.220354000
1	2.280577000	1.777692000	-0.834458000
6	0.788635000	2.487607000	1.960367000
1	1.094774000	3.466235000	1.592815000

6	0.835069000	2.177110000	3.317743000
1	1.169280000	2.927811000	4.035616000
6	0.475014000	0.901040000	3.759172000
1	0.519101000	0.631706000	4.813257000
6	0.080591000	-0.038152000	2.818078000
1	-0.183789000	-1.073918000	3.051218000
6	0.575397000	-1.972779000	0.498340000
6	1.276856000	-3.909512000	1.156195000
1	1.230770000	-4.896693000	1.611605000
6	2.344367000	-3.321503000	0.527263000
1	3.364036000	-3.645655000	0.339069000
6	-1.958103000	-1.035192000	0.175281000
6	-2.307551000	-1.962572000	-0.841753000
6	-3.641395000	-2.292092000	-1.090219000
1	-3.869000000	-3.003434000	-1.889823000
6	-4.688016000	-1.735111000	-0.357211000
6	-4.351678000	-0.808717000	0.623509000
1	-5.153154000	-0.330826000	1.193885000
6	-3.024202000	-0.446334000	0.895976000
6	2.796585000	-1.077195000	-0.362931000
6	3.547696000	-0.352847000	0.572682000
6	4.498655000	0.563269000	0.103180000
1	5.089446000	1.126467000	0.830969000
6	4.719556000	0.758944000	-1.258027000
6	3.949382000	0.020821000	-2.164560000
1	4.104364000	0.163404000	-3.237569000
6	2.983761000	-0.891954000	-1.744283000
6	-1.270284000	-2.612628000	-1.728529000
1	-1.734983000	-2.991763000	-2.648861000
1	-0.788698000	-3.456094000	-1.211477000

1	-0.480350000	-1.905703000	-2.007632000
6	-6.118706000	-2.128498000	-0.615688000
1	-6.817083000	-1.383190000	-0.211460000
1	-6.351487000	-3.095142000	-0.142280000
1	-6.313822000	-2.236907000	-1.692079000
6	-2.859255000	0.620835000	1.960264000
1	-3.842673000	1.024315000	2.234119000
1	-2.252453000	1.471091000	1.616974000
1	-2.409236000	0.227720000	2.883860000
6	3.366549000	-0.530748000	2.058692000
1	4.326473000	-0.773429000	2.537423000
1	2.654339000	-1.329984000	2.299647000
1	3.006286000	0.406238000	2.511557000
6	5.740721000	1.748468000	-1.754691000
1	6.422558000	1.281424000	-2.479680000
1	6.341347000	2.152229000	-0.929391000
1	5.251460000	2.592826000	-2.263623000
6	2.134098000	-1.618199000	-2.745957000
1	2.648222000	-1.699234000	-3.712202000
1	1.200511000	-1.053236000	-2.892685000
1	1.859753000	-2.621932000	-2.395915000
5	-0.364338000	-0.679697000	0.277510000

Compound 4 TS 1

8	1.033187000	-0.987376000	-1.179856000
7	1.589067000	0.443369000	0.965191000
7	0.943519000	-1.655296000	1.424504000
7	-1.160984000	-1.958459000	0.968728000
6	3.337718000	-0.420108000	-1.242075000
6	3.011327000	0.764391000	-1.916295000

1	1.958280000	0.967368000	-2.118282000
6	4.004294000	1.659504000	-2.302074000
1	3.733141000	2.580682000	-2.821219000
6	5.344712000	1.380520000	-2.028840000
1	6.124887000	2.082749000	-2.327684000
6	5.682678000	0.188633000	-1.390159000
1	6.729732000	-0.045624000	-1.189201000
6	4.686398000	-0.709533000	-1.006926000
1	4.966822000	-1.635233000	-0.502355000
6	2.212400000	-1.326378000	-0.790233000
6	2.101592000	-0.880161000	1.128162000
6	2.542078000	-2.814752000	-0.816015000
1	3.334267000	-3.095199000	-0.104591000
1	2.882863000	-3.090105000	-1.825840000
1	1.636350000	-3.394906000	-0.596525000
6	3.324968000	-1.020224000	1.905243000
1	3.610787000	-2.007248000	2.273799000
6	4.117652000	0.062478000	2.077501000
1	5.074919000	-0.035776000	2.591428000
6	3.697607000	1.363128000	1.598200000
1	4.357785000	2.224757000	1.672275000
6	2.460658000	1.506163000	1.067630000
1	2.067975000	2.461610000	0.714203000
6	-0.162998000	-1.048988000	0.947485000
6	0.664716000	-2.973311000	1.729288000
1	1.400644000	-3.659169000	2.134853000
6	-0.658649000	-3.154034000	1.450662000
1	-1.294917000	-4.024289000	1.579443000
6	-0.695785000	1.628069000	0.172761000
6	-0.905286000	2.571257000	1.210686000

6	-1.737261000	3.672641000	0.994153000
1	-1.893764000	4.387489000	1.807120000
6	-2.382627000	3.877319000	-0.227236000
6	-2.199268000	2.925400000	-1.228641000
1	-2.716610000	3.049308000	-2.184375000
6	-1.381700000	1.804322000	-1.047570000
6	-2.448609000	-1.750397000	0.374400000
6	-2.694214000	-2.333657000	-0.880296000
6	-3.939330000	-2.105415000	-1.464009000
1	-4.149116000	-2.543338000	-2.443257000
6	-4.907926000	-1.304283000	-0.847569000
6	-4.608706000	-0.723103000	0.384593000
1	-5.347936000	-0.081685000	0.870077000
6	-3.380997000	-0.933329000	1.020949000
6	-0.290550000	2.401148000	2.583151000
1	0.768127000	2.700961000	2.606114000
1	-0.324586000	1.353808000	2.918703000
1	-0.822592000	3.016261000	3.321020000
6	-3.238561000	5.095430000	-0.456153000
1	-2.628824000	5.937912000	-0.818576000
1	-3.728093000	5.419473000	0.472555000
1	-4.014811000	4.901924000	-1.208760000
6	-1.309526000	0.781952000	-2.153699000
1	-1.463195000	1.254437000	-3.133902000
1	-2.114198000	0.039522000	-2.018688000
1	-0.358163000	0.235987000	-2.153587000
6	-1.616848000	-3.106776000	-1.593548000
1	-1.923363000	-3.326702000	-2.623700000
1	-1.402300000	-4.064124000	-1.094004000
1	-0.680328000	-2.523072000	-1.612578000

6	-6.241819000	-1.081881000	-1.510252000
1	-6.845785000	-2.001599000	-1.489539000
1	-6.114291000	-0.796868000	-2.564056000
1	-6.811442000	-0.291114000	-1.005802000
6	-3.065062000	-0.262508000	2.329335000
1	-2.513407000	0.673749000	2.147038000
1	-2.442501000	-0.898846000	2.973213000
1	-3.987422000	-0.009423000	2.867149000
5	0.225178000	0.385390000	0.476354000

Compound 4 Int 1

8	1.336489000	0.583931000	-0.976211000
7	1.589568000	-0.219381000	1.184987000
7	1.066631000	-2.055992000	-0.103115000
7	-0.998939000	-2.049203000	-0.699811000
6	3.740386000	0.592888000	-0.755374000
6	3.672024000	1.766985000	0.002611000
1	2.706733000	2.083434000	0.396969000
6	4.816818000	2.520252000	0.252256000
1	4.742326000	3.433936000	0.844107000
6	6.051783000	2.112370000	-0.250938000
1	6.947981000	2.703615000	-0.056620000
6	6.130909000	0.945186000	-1.006933000
1	7.090494000	0.616734000	-1.409632000
6	4.983374000	0.192793000	-1.256855000
1	5.069169000	-0.715707000	-1.854656000
6	2.480514000	-0.241845000	-0.973466000
6	2.264646000	-1.142021000	0.317184000
6	2.534101000	-1.042934000	-2.272716000
1	3.242305000	-1.883294000	-2.216456000

1	2.839263000	-0.384533000	-3.096946000
1	1.538103000	-1.441494000	-2.505993000
6	3.398615000	-1.865562000	0.928632000
1	4.101295000	-2.392544000	0.280903000
6	3.545869000	-1.836756000	2.274619000
1	4.377647000	-2.381522000	2.727473000
6	2.678593000	-1.063438000	3.124511000
1	2.816464000	-1.040900000	4.202432000
6	1.747259000	-0.266147000	2.524211000
1	1.109893000	0.417804000	3.089963000
6	-0.018481000	-1.291818000	-0.181325000
6	0.817256000	-3.312542000	-0.596439000
1	1.564910000	-4.099342000	-0.628783000
6	-0.500759000	-3.319011000	-0.963824000
1	-1.126786000	-4.109050000	-1.367271000
6	-0.700220000	1.305964000	0.550789000
6	-1.698236000	0.929311000	1.478691000
6	-2.869661000	1.684878000	1.620106000
1	-3.630696000	1.353687000	2.333690000
6	-3.090758000	2.836881000	0.873428000
6	-2.084998000	3.235411000	-0.009498000
1	-2.224043000	4.152084000	-0.590484000
6	-0.905234000	2.505751000	-0.180641000
6	-2.348121000	-1.564143000	-0.794911000
6	-2.613217000	-0.509592000	-1.681320000
6	-3.873068000	0.084082000	-1.617575000
1	-4.090385000	0.924484000	-2.281338000
6	-4.849106000	-0.350782000	-0.716346000
6	-4.558243000	-1.436362000	0.111526000
1	-5.316120000	-1.795772000	0.812203000

6	-3.306802000	-2.058014000	0.097114000
6	-1.567331000	-0.268838000	2.393538000
1	-1.215819000	0.046539000	3.389143000
1	-0.856885000	-1.023255000	2.032378000
1	-2.544289000	-0.752946000	2.537399000
6	-4.355440000	3.643935000	1.013469000
1	-4.137725000	4.662510000	1.368483000
1	-5.049364000	3.179207000	1.727249000
1	-4.871619000	3.742571000	0.046263000
6	0.099950000	3.057243000	-1.167872000
1	-0.184643000	4.076196000	-1.462593000
1	0.166738000	2.437237000	-2.072135000
1	1.113970000	3.080168000	-0.752507000
6	-1.575742000	-0.039127000	-2.663917000
1	-1.986171000	0.752242000	-3.303307000
1	-1.247149000	-0.869868000	-3.308019000
1	-0.678642000	0.354048000	-2.163046000
6	-6.164329000	0.372832000	-0.610632000
1	-6.935996000	-0.257435000	-0.149654000
1	-6.522295000	0.698566000	-1.596754000
1	-6.046427000	1.273292000	0.012626000
6	-3.000783000	-3.201023000	1.029871000
1	-3.744372000	-3.248817000	1.835612000
1	-2.004965000	-3.096301000	1.483488000
1	-3.019840000	-4.166761000	0.501552000
5	0.484961000	0.282185000	0.195537000

Compound 4 TS 2

8	1.348297000	0.542493000	-0.942023000
7	1.597514000	-0.273699000	1.216111000

7	1.039691000	-2.178025000	-0.105809000
7	-1.023685000	-2.047859000	-0.736992000
6	3.749345000	0.611314000	-0.755634000
6	3.668530000	1.771597000	0.022520000
1	2.708467000	2.047008000	0.459445000
6	4.794119000	2.562255000	0.239698000
1	4.710158000	3.465176000	0.846589000
6	6.023086000	2.204339000	-0.314791000
1	6.904737000	2.824478000	-0.145749000
6	6.114794000	1.049954000	-1.088298000
1	7.069639000	0.760736000	-1.530403000
6	4.985417000	0.260272000	-1.306963000
1	5.080091000	-0.636850000	-1.920289000
6	2.504446000	-0.263552000	-0.934575000
6	2.353730000	-1.101690000	0.383663000
6	2.571124000	-1.097335000	-2.212375000
1	3.278672000	-1.935576000	-2.124975000
1	2.886041000	-0.458745000	-3.048322000
1	1.579079000	-1.502510000	-2.445137000
6	3.462655000	-1.813880000	0.995631000
1	4.210901000	-2.285685000	0.357455000
6	3.532606000	-1.867603000	2.352689000
1	4.350060000	-2.416130000	2.825676000
6	2.592483000	-1.171400000	3.177556000
1	2.660514000	-1.200944000	4.262452000
6	1.665262000	-0.378300000	2.560724000
1	0.966997000	0.251820000	3.114657000
6	-0.003672000	-1.365322000	-0.174976000
6	0.724897000	-3.394007000	-0.656277000
1	1.427063000	-4.220838000	-0.714870000

6	-0.586664000	-3.327196000	-1.044450000
1	-1.247434000	-4.067097000	-1.486786000
6	-0.697340000	1.236039000	0.569710000
6	-1.703721000	0.865803000	1.491499000
6	-2.854967000	1.648184000	1.654512000
1	-3.621979000	1.319654000	2.362976000
6	-3.049418000	2.821454000	0.935352000
6	-2.037385000	3.211452000	0.055943000
1	-2.155936000	4.142961000	-0.505586000
6	-0.876792000	2.457000000	-0.136036000
6	-2.351577000	-1.512561000	-0.835938000
6	-2.580215000	-0.439557000	-1.709912000
6	-3.823881000	0.188589000	-1.651051000
1	-4.010063000	1.044592000	-2.304306000
6	-4.822914000	-0.233855000	-0.769817000
6	-4.573316000	-1.343123000	0.040063000
1	-5.351185000	-1.696303000	0.721962000
6	-3.339305000	-1.998159000	0.029839000
6	-1.611820000	-0.356922000	2.378730000
1	-1.290291000	-0.070918000	3.393333000
1	-0.902570000	-1.112302000	2.017558000
1	-2.598410000	-0.831574000	2.480772000
6	-4.290699000	3.659417000	1.099833000
1	-4.998276000	3.193195000	1.799104000
1	-4.802725000	3.802060000	0.136033000
1	-4.044122000	4.660065000	1.485820000
6	0.133008000	3.011978000	-1.117244000
1	-0.148502000	4.034091000	-1.403841000
1	0.200326000	2.399574000	-2.026076000
1	1.146231000	3.030233000	-0.700039000

6	-1.523922000	0.008788000	-2.682449000
1	-1.890592000	0.849236000	-3.285045000
1	-1.254244000	-0.813781000	-3.363598000
1	-0.599416000	0.323872000	-2.177267000
6	-6.119114000	0.523385000	-0.664131000
1	-6.424821000	0.932289000	-1.636646000
1	-6.001904000	1.370906000	0.029678000
1	-6.928421000	-0.113189000	-0.282788000
6	-3.083494000	-3.174711000	0.935858000
1	-3.828053000	-3.208528000	1.741681000
1	-2.082820000	-3.127752000	1.387796000
1	-3.147040000	-4.125190000	0.383735000
5	0.479420000	0.202641000	0.200919000

Compound 5

16	-0.163607000	-0.565472000	-0.892652000
7	-2.084897000	-1.806759000	0.686160000
7	0.288851000	2.519899000	0.531010000
7	2.355497000	2.167984000	1.221992000
7	1.160954000	-0.690081000	1.500113000
6	-3.113644000	-1.912010000	-0.248413000
6	1.980792000	3.429889000	1.582929000
1	2.648468000	4.101570000	2.118284000
6	-0.925367000	-1.304886000	0.503717000
6	-2.952443000	-1.932755000	-1.645599000
1	-1.962520000	-1.847757000	-2.088814000
6	2.072062000	-0.605266000	2.482222000
1	2.964180000	-0.021026000	2.245566000
6	3.254355000	-1.721597000	-0.507562000
6	-0.000656000	-1.328369000	1.674789000

6	-4.060096000	-2.113470000	-2.473115000
1	-3.916294000	-2.144106000	-3.554412000
6	4.489857000	-2.077606000	-1.057875000
1	4.831874000	-3.111804000	-0.958051000
6	5.282514000	-1.166957000	-1.752902000
6	2.459529000	-2.850149000	0.120369000
1	1.400995000	-2.804297000	-0.169854000
1	2.854000000	-3.814652000	-0.224709000
1	2.511265000	-2.860705000	1.220603000
6	-3.706476000	1.675481000	-0.553191000
6	-5.108802000	1.315494000	-0.962008000
1	-5.588906000	2.145492000	-1.500295000
1	-5.098001000	0.442022000	-1.631812000
1	-5.727223000	1.059838000	-0.091539000
6	-1.499892000	2.529973000	-1.151856000
6	4.768290000	0.113712000	-1.935310000
1	5.334915000	0.833112000	-2.533617000
6	6.630248000	-1.556782000	-2.299837000
1	6.864518000	-0.999351000	-3.217086000
1	7.425887000	-1.339627000	-1.569898000
1	6.674098000	-2.630883000	-2.526446000
6	1.842020000	-1.212529000	3.705514000
1	2.594734000	-1.142775000	4.489245000
6	-0.296344000	-1.958973000	2.882539000
1	-1.256491000	-2.465508000	2.968474000
6	-4.407747000	-2.071482000	0.281282000
1	-4.513094000	-2.073774000	1.367098000
6	2.776893000	-0.387603000	-0.610898000
6	3.540660000	0.512522000	-1.395114000
6	-0.544613000	3.028336000	-2.199484000

1	-1.081070000	3.560992000	-2.995232000
1	0.220830000	3.692303000	-1.776931000
1	-0.024497000	2.173849000	-2.663468000
6	3.086390000	1.911629000	-1.747354000
1	1.997248000	1.979869000	-1.848671000
1	3.383593000	2.633330000	-0.974045000
1	3.535405000	2.218462000	-2.701895000
6	-1.938995000	1.749680000	1.126139000
6	-5.338277000	-2.262085000	-1.936330000
1	-6.197350000	-2.403022000	-2.593782000
6	-5.508353000	-2.234912000	-0.550281000
1	-6.502817000	-2.354247000	-0.117269000
6	0.641924000	-1.904683000	3.903778000
1	0.443173000	-2.394108000	4.858348000
6	-1.071088000	2.270952000	0.156937000
6	0.697028000	3.671828000	1.164488000
1	0.035808000	4.528493000	1.258053000
6	1.335434000	1.626273000	0.576781000
6	-3.249157000	1.448729000	0.745026000
1	-3.928160000	1.013007000	1.483001000
6	-1.489448000	1.514255000	2.545703000
1	-2.025446000	0.657804000	2.978172000
1	-0.408047000	1.328788000	2.614916000
1	-1.701626000	2.395821000	3.171083000
6	-2.820075000	2.229486000	-1.481819000
1	-3.163633000	2.415111000	-2.503065000
5	1.397983000	0.076257000	0.103193000

Compound 5 TS 1

16	1.570400000	-0.269869000	1.420498000
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7	0.524734000	1.998986000	-0.369717000
7	-0.581588000	-1.282636000	-1.522050000
7	0.980228000	0.237870000	-1.651678000
7	3.840625000	0.253629000	-0.107815000
6	-1.978786000	1.503412000	0.527507000
6	-2.744639000	2.567476000	-0.004996000
6	-3.996871000	2.867442000	0.540770000
1	-4.581099000	3.686157000	0.111292000
6	-4.528495000	2.136039000	1.603422000
6	-3.774379000	1.076382000	2.110833000
1	-4.178856000	0.479821000	2.933440000
6	-2.516888000	0.752142000	1.595871000
6	1.540850000	1.394034000	-1.125347000
6	2.694244000	0.215530000	0.364100000
6	-0.230273000	-0.035458000	-1.092551000
6	0.426676000	-1.773601000	-2.324880000
1	0.351762000	-2.751124000	-2.791493000
6	1.413698000	-0.836182000	-2.410124000
1	2.365863000	-0.849088000	-2.928450000
6	-2.263787000	3.364959000	-1.195714000
1	-1.437472000	4.042987000	-0.932825000
1	-3.076189000	3.976635000	-1.609342000
1	-1.885873000	2.706744000	-1.993271000
6	-5.867675000	2.486389000	2.197205000
1	-6.403960000	1.586492000	2.528559000
1	-6.498654000	3.019543000	1.473424000
1	-5.746043000	3.138943000	3.075883000
6	-1.747121000	-0.386010000	2.216099000
1	-0.926796000	-0.001754000	2.842205000
1	-1.287256000	-1.029654000	1.453312000

1	-2.399193000	-1.006793000	2.845209000
6	0.779971000	3.246486000	0.166976000
1	0.045276000	3.598233000	0.892714000
6	1.854118000	3.973420000	-0.228472000
1	2.019431000	4.957957000	0.206386000
6	2.744275000	3.460005000	-1.239303000
1	3.562271000	4.078434000	-1.607531000
6	2.563849000	2.200707000	-1.715921000
1	3.231254000	1.756684000	-2.453013000
6	-1.753396000	-1.980132000	-1.091182000
6	-3.012600000	-1.498543000	-1.476153000
6	-4.139987000	-2.159978000	-0.983658000
1	-5.128755000	-1.793951000	-1.271103000
6	-4.036772000	-3.268669000	-0.141838000
6	-2.762146000	-3.726275000	0.204075000
1	-2.663681000	-4.591041000	0.864937000
6	-1.603509000	-3.094744000	-0.249867000
6	-3.159632000	-0.302250000	-2.376550000
1	-3.134572000	0.625786000	-1.784595000
1	-4.120280000	-0.337488000	-2.905851000
1	-2.349101000	-0.250330000	-3.116370000
6	-5.270788000	-3.932888000	0.409284000
1	-5.594650000	-3.433498000	1.335594000
1	-5.084495000	-4.988268000	0.647790000
1	-6.104444000	-3.878930000	-0.303531000
6	-0.242063000	-3.568519000	0.187123000
1	0.396912000	-2.723723000	0.488482000
1	0.283662000	-4.100810000	-0.620238000
1	-0.333108000	-4.258731000	1.035058000
5	-0.617557000	1.127874000	-0.165592000

6	4.985332000	-0.355942000	0.436734000
6	6.196606000	-0.170061000	-0.243068000
6	4.966336000	-1.131064000	1.605373000
6	7.368841000	-0.748641000	0.232400000
6	6.144333000	-1.707532000	2.074473000
6	7.348133000	-1.521535000	1.394295000
1	6.187700000	0.441103000	-1.146416000
1	4.026293000	-1.275641000	2.139006000
1	8.305622000	-0.594836000	-0.305889000
1	6.120577000	-2.309168000	2.984886000
1	8.266522000	-1.975509000	1.769062000

Compound 5 Int 1

16	1.330213000	-0.001781000	1.131556000
7	0.656381000	2.223793000	-0.241899000
7	-0.501214000	-0.856017000	-1.879692000
7	0.980669000	0.710328000	-1.904616000
7	3.687408000	0.382836000	-0.280439000
6	-1.624545000	1.237043000	0.858579000
6	-2.494696000	2.196712000	0.280965000
6	-3.775436000	2.397693000	0.811803000
1	-4.427223000	3.143472000	0.347427000
6	-4.250923000	1.662344000	1.894448000
6	-3.412168000	0.681442000	2.423223000
1	-3.774776000	0.060768000	3.247345000
6	-2.125459000	0.454643000	1.927042000
6	1.734157000	1.661469000	-1.010113000
6	2.471864000	0.650340000	-0.055594000
6	-0.083331000	0.245204000	-1.240876000
6	0.340962000	-1.096199000	-2.959684000

1	0.167970000	-1.923597000	-3.641031000
6	1.294283000	-0.119202000	-2.955738000
1	2.131602000	0.057225000	-3.623174000
6	-2.140586000	3.003952000	-0.952037000
1	-1.527543000	3.885553000	-0.714854000
1	-3.057369000	3.363914000	-1.438702000
1	-1.570205000	2.418772000	-1.686384000
6	-5.617099000	1.914349000	2.475552000
1	-6.080244000	0.980904000	2.824262000
1	-6.285598000	2.379177000	1.738330000
1	-5.553958000	2.592906000	3.340524000
6	-1.331453000	-0.667797000	2.551523000
1	-0.449028000	-0.292681000	3.089482000
1	-0.974684000	-1.380016000	1.791889000
1	-1.952423000	-1.223262000	3.266604000
6	0.751813000	3.478242000	0.268174000
1	-0.004049000	3.729355000	1.017006000
6	1.689263000	4.363995000	-0.163146000
1	1.726619000	5.372965000	0.239303000
6	2.589528000	3.936995000	-1.209463000
1	3.282606000	4.662782000	-1.639999000
6	2.604235000	2.667212000	-1.668732000
1	3.316807000	2.323515000	-2.417861000
6	-1.539706000	-1.721986000	-1.389125000
6	-2.878711000	-1.356085000	-1.556860000
6	-3.851560000	-2.190773000	-0.996904000
1	-4.903190000	-1.916558000	-1.110023000
6	-3.515667000	-3.349541000	-0.298692000
6	-2.163208000	-3.689571000	-0.178055000
1	-1.884249000	-4.599475000	0.358995000

6	-1.152778000	-2.891516000	-0.711687000
6	-3.284010000	-0.103361000	-2.283403000
1	-3.433363000	0.715337000	-1.563217000
1	-4.232670000	-0.260322000	-2.813216000
1	-2.526400000	0.218259000	-3.010236000
6	-4.576910000	-4.207012000	0.337803000
1	-4.654060000	-3.985062000	1.413295000
1	-4.339417000	-5.274801000	0.237539000
1	-5.561304000	-4.025198000	-0.112342000
6	0.298530000	-3.259491000	-0.550230000
1	0.869906000	-2.433259000	-0.098647000
1	0.766787000	-3.492333000	-1.518463000
1	0.399536000	-4.141528000	0.093842000
5	-0.187848000	1.024922000	0.185694000
6	4.441935000	-0.505579000	0.498788000
6	5.259485000	-1.430502000	-0.164800000
6	4.451609000	-0.466346000	1.900773000
6	6.043536000	-2.324243000	0.558545000
6	5.255382000	-1.349586000	2.617041000
6	6.046899000	-2.287061000	1.953327000
1	5.261355000	-1.429218000	-1.255547000
1	3.833017000	0.267221000	2.419214000
1	6.666066000	-3.047688000	0.029255000
1	5.260976000	-1.304813000	3.707462000
1	6.670225000	-2.979690000	2.520408000

Compound 5 TS 2

16	1.069329000	0.139603000	1.273070000
7	0.170088000	2.465918000	0.285008000
7	-0.102901000	-0.498118000	-1.961840000

7	0.905186000	1.410911000	-1.721832000
7	3.413045000	1.030777000	0.097679000
6	-1.991819000	0.869888000	0.740085000
6	-2.969095000	1.660464000	0.087273000
6	-4.320530000	1.566974000	0.452265000
1	-5.048534000	2.201245000	-0.062857000
6	-4.764538000	0.670023000	1.416095000
6	-3.810546000	-0.169212000	1.997573000
1	-4.136398000	-0.919037000	2.723864000
6	-2.453633000	-0.086743000	1.682038000
6	1.416305000	2.327078000	-0.332198000
6	2.176230000	1.163495000	0.336577000
6	-0.023859000	0.612943000	-1.204085000
6	0.825877000	-0.390813000	-2.989201000
1	0.926377000	-1.162174000	-3.747102000
6	1.472500000	0.800062000	-2.815501000
1	2.260046000	1.259186000	-3.405439000
6	-2.682742000	2.590637000	-1.076787000
1	-2.781372000	3.647726000	-0.787119000
1	-3.420059000	2.411540000	-1.873433000
1	-1.684192000	2.465938000	-1.510196000
6	-6.213090000	0.594003000	1.819980000
1	-6.537099000	-0.448843000	1.944717000
1	-6.862258000	1.071922000	1.074247000
1	-6.376489000	1.104306000	2.781808000
6	-1.531892000	-1.084615000	2.340719000
1	-0.801238000	-0.595486000	3.000668000
1	-0.967575000	-1.660313000	1.590101000
1	-2.109963000	-1.795767000	2.945599000
6	-0.380795000	3.678060000	0.524428000

1	-1.357334000	3.649757000	1.010769000
6	0.262920000	4.841300000	0.214199000
1	-0.187871000	5.801675000	0.452095000
6	1.568531000	4.748572000	-0.364236000
1	2.129006000	5.664566000	-0.563242000
6	2.152136000	3.547435000	-0.618217000
1	3.174389000	3.442975000	-0.979214000
6	-0.755240000	-1.698146000	-1.511077000
6	-2.150626000	-1.785659000	-1.522006000
6	-2.737078000	-2.919833000	-0.946768000
1	-3.827727000	-2.989404000	-0.930746000
6	-1.975202000	-3.945405000	-0.393711000
6	-0.579936000	-3.835528000	-0.437148000
1	0.034079000	-4.634210000	-0.013546000
6	0.057111000	-2.722426000	-0.981253000
6	-3.034711000	-0.737836000	-2.141583000
1	-3.818622000	-0.436633000	-1.432568000
1	-3.524808000	-1.147409000	-3.038174000
1	-2.477723000	0.159129000	-2.435203000
6	-2.625575000	-5.132516000	0.265585000
1	-2.578073000	-5.036953000	1.361322000
1	-2.114977000	-6.066949000	-0.005263000
1	-3.682307000	-5.218626000	-0.018260000
6	1.562069000	-2.639817000	-0.997434000
1	1.917629000	-1.644742000	-0.699210000
1	1.962612000	-2.853910000	-2.000382000
1	1.991171000	-3.370610000	-0.300512000
5	-0.451849000	1.039036000	0.312745000
6	4.176837000	-0.025347000	0.614573000
6	5.012998000	-0.720052000	-0.270711000

6	4.159265000	-0.389025000	1.968376000
6	5.786564000	-1.784866000	0.181291000
6	4.953242000	-1.441838000	2.417166000
6	5.761446000	-2.150049000	1.528068000
1	5.031673000	-0.408325000	-1.315985000
1	3.525718000	0.164024000	2.662909000
1	6.422503000	-2.326872000	-0.520688000
1	4.936433000	-1.712798000	3.474138000
1	6.376283000	-2.977445000	1.884711000

Compound 6

16	-0.322683000	0.139869000	-1.537269000
7	0.695457000	1.497076000	0.625683000
7	-1.006999000	-1.418432000	1.437990000
7	0.971110000	-1.066046000	2.351832000
7	-1.920311000	2.364157000	-1.588055000
6	2.371979000	-0.325336000	-0.389249000
6	2.908495000	-1.631713000	-0.272260000
6	4.255321000	-1.872477000	-0.565429000
1	4.639188000	-2.891643000	-0.462533000
6	5.115089000	-0.867040000	-0.999017000
6	4.565026000	0.396878000	-1.200835000
1	5.195565000	1.191572000	-1.610120000
6	3.222491000	0.677272000	-0.926662000
6	-0.226907000	2.296142000	0.081001000
6	-0.967325000	1.707510000	-1.066900000
6	0.248543000	-0.879205000	1.259439000
6	-1.044098000	-1.977471000	2.696472000
1	-1.939724000	-2.465621000	3.069917000
6	0.192545000	-1.747221000	3.241982000

1	0.556833000	-2.041826000	4.223873000
6	2.086902000	-2.842608000	0.110916000
1	2.530116000	-3.746625000	-0.328765000
1	1.052023000	-2.767438000	-0.242548000
1	2.047071000	-2.969008000	1.201673000
6	6.573406000	-1.138828000	-1.257959000
1	6.975104000	-0.464615000	-2.026789000
1	6.733487000	-2.174476000	-1.587834000
1	7.167743000	-0.988825000	-0.342905000
6	2.743828000	2.065043000	-1.306955000
1	2.668097000	2.751046000	-0.448389000
1	1.763320000	2.027984000	-1.801012000
1	3.451959000	2.518022000	-2.012990000
6	1.419727000	1.884929000	1.687362000
1	2.113856000	1.138712000	2.080304000
6	1.246011000	3.147497000	2.229789000
1	1.846740000	3.450583000	3.085931000
6	0.299011000	4.007488000	1.661276000
1	0.151799000	5.007663000	2.071491000
6	-0.454444000	3.578075000	0.577615000
1	-1.217441000	4.183075000	0.089074000
6	-2.614870000	1.764736000	-2.699425000
1	-1.943448000	1.672583000	-3.571729000
1	-3.477758000	2.379185000	-2.985105000
1	-2.954029000	0.742965000	-2.448560000
6	-2.188035000	-1.244660000	0.645929000
6	-2.537358000	-2.199960000	-0.315166000
6	-3.703441000	-1.994455000	-1.056384000
1	-3.980611000	-2.730344000	-1.815428000
6	-4.508611000	-0.870201000	-0.866775000

6	-4.129263000	0.061758000	0.103492000
1	-4.740774000	0.955306000	0.257938000
6	-2.981930000	-0.110041000	0.878322000
6	-1.641577000	-3.370022000	-0.607450000
1	-0.852448000	-3.062330000	-1.313535000
1	-2.205090000	-4.188515000	-1.073229000
1	-1.146960000	-3.744666000	0.298376000
6	-5.754469000	-0.651212000	-1.684757000
1	-5.734793000	0.335300000	-2.171258000
1	-6.652899000	-0.685072000	-1.050585000
1	-5.860569000	-1.415861000	-2.464921000
6	-2.625616000	0.903002000	1.936342000
1	-1.555051000	0.888383000	2.183707000
1	-3.173001000	0.696363000	2.869426000
1	-2.899311000	1.913595000	1.601967000
5	0.841310000	0.000415000	0.032083000

Compound 6 TS 1

16	1.973502000	-0.829222000	1.969900000
7	1.871118000	1.342784000	-0.229005000
7	-0.002825000	-1.648530000	-1.154670000
7	1.942566000	-0.655542000	-1.203679000
7	4.474078000	-1.159432000	0.801301000
6	-0.755412000	1.708209000	0.293763000
6	-1.097581000	2.837767000	-0.486414000
6	-2.260593000	3.559548000	-0.198102000
1	-2.516454000	4.424145000	-0.817068000
6	-3.112124000	3.192487000	0.843988000
6	-2.776130000	2.066477000	1.598244000
1	-3.437519000	1.752080000	2.410647000

6	-1.619552000	1.325555000	1.343856000
6	2.749520000	0.370498000	-0.733310000
6	3.316201000	-0.818535000	1.055798000
6	0.646187000	-0.494371000	-0.819145000
6	0.905751000	-2.516904000	-1.722179000
1	0.602869000	-3.496103000	-2.080423000
6	2.127895000	-1.912652000	-1.753897000
1	3.088727000	-2.266329000	-2.110182000
6	-0.258625000	3.261104000	-1.670453000
1	0.691998000	3.721132000	-1.359930000
1	-0.796008000	3.993255000	-2.287302000
1	0.003788000	2.400025000	-2.304303000
6	-4.348908000	3.992395000	1.159448000
1	-5.175340000	3.339992000	1.473927000
1	-4.679800000	4.576449000	0.290210000
1	-4.157451000	4.699171000	1.981935000
6	-1.304881000	0.139050000	2.218701000
1	-0.469937000	0.370454000	2.897994000
1	-0.993926000	-0.732303000	1.625324000
1	-2.175601000	-0.146742000	2.824097000
6	2.413077000	2.542776000	0.189852000
1	1.730666000	3.192830000	0.739328000
6	3.692425000	2.877353000	-0.109871000
1	4.083264000	3.837106000	0.224854000
6	4.511281000	1.984403000	-0.890933000
1	5.514407000	2.287706000	-1.189117000
6	4.030186000	0.761361000	-1.235457000
1	4.626939000	0.036698000	-1.787463000
6	5.246283000	-1.962382000	1.729379000
1	4.665303000	-2.232063000	2.627394000

1	6.145142000	-1.407104000	2.034490000
1	5.583999000	-2.881070000	1.227782000
6	-1.369435000	-1.922001000	-0.835998000
6	-2.377940000	-1.179512000	-1.466712000
6	-3.699283000	-1.419912000	-1.082960000
1	-4.496099000	-0.845309000	-1.561794000
6	-4.025533000	-2.368749000	-0.112440000
6	-2.991306000	-3.099648000	0.478766000
1	-3.229164000	-3.844026000	1.242697000
6	-1.653455000	-2.889547000	0.141725000
6	-2.061617000	-0.145824000	-2.513084000
1	-1.844407000	0.823358000	-2.038048000
1	-2.918461000	-0.006534000	-3.184511000
1	-1.184996000	-0.430249000	-3.110997000
6	-5.455960000	-2.573219000	0.311754000
1	-5.730609000	-1.852900000	1.097898000
1	-5.613602000	-3.582215000	0.714835000
1	-6.146176000	-2.422648000	-0.529145000
6	-0.551991000	-3.644749000	0.838384000
1	0.265870000	-2.970553000	1.137934000
1	-0.114872000	-4.418816000	0.189169000
1	-0.941023000	-4.144239000	1.734475000
5	0.507402000	0.862307000	-0.113388000

Compound 6 Int 1

16	1.575087000	-0.560371000	1.841503000
7	2.108451000	1.209132000	-0.133030000
7	-0.022339000	-1.553133000	-1.279344000
7	1.983612000	-0.763362000	-1.255747000
7	4.089314000	-1.426632000	1.122916000

6	-0.511978000	1.519410000	0.539416000
6	-0.824940000	2.459837000	-0.475225000
6	-1.981481000	3.244642000	-0.378400000
1	-2.200619000	3.961058000	-1.175649000
6	-2.867617000	3.127247000	0.688960000
6	-2.577948000	2.171414000	1.662317000
1	-3.273489000	2.034240000	2.495019000
6	-1.433238000	1.371657000	1.604627000
6	2.943739000	0.077960000	-0.448074000
6	3.056824000	-0.748399000	0.877656000
6	0.742870000	-0.561646000	-0.802634000
6	0.772237000	-2.412813000	-2.029325000
1	0.352051000	-3.273891000	-2.539960000
6	2.046882000	-1.923827000	-1.989302000
1	2.961516000	-2.292205000	-2.442622000
6	0.014185000	2.646228000	-1.723401000
1	0.889099000	3.288055000	-1.545151000
1	-0.585658000	3.122463000	-2.511088000
1	0.402880000	1.696457000	-2.115193000
6	-4.089195000	4.001425000	0.796171000
1	-4.937339000	3.449814000	1.225054000
1	-4.389548000	4.390749000	-0.185986000
1	-3.894768000	4.865382000	1.450661000
6	-1.254351000	0.343664000	2.696331000
1	-0.362016000	0.547665000	3.304852000
1	-1.141601000	-0.669393000	2.280963000
1	-2.126996000	0.338484000	3.362590000
6	2.646539000	2.442444000	0.041541000
1	1.973485000	3.178613000	0.489041000
6	3.911456000	2.743391000	-0.357431000

1	4.309548000	3.746847000	-0.231224000
6	4.682796000	1.701523000	-0.995768000
1	5.664955000	1.946454000	-1.405679000
6	4.232684000	0.432438000	-1.093240000
1	4.834952000	-0.370794000	-1.516893000
6	4.144125000	-2.172371000	2.359396000
1	3.915843000	-1.527545000	3.225431000
1	5.139725000	-2.613556000	2.493455000
1	3.396003000	-2.984100000	2.357613000
6	-1.404935000	-1.738063000	-0.927798000
6	-2.387941000	-0.979391000	-1.571295000
6	-3.709315000	-1.134269000	-1.140148000
1	-4.489799000	-0.542886000	-1.625274000
6	-4.051747000	-2.009417000	-0.110472000
6	-3.039253000	-2.770629000	0.484108000
1	-3.293008000	-3.470953000	1.283589000
6	-1.705925000	-2.653510000	0.094816000
6	-2.066327000	-0.007865000	-2.673624000
1	-2.034402000	1.015977000	-2.272026000
1	-2.845568000	-0.039981000	-3.446814000
1	-1.097790000	-0.217944000	-3.145503000
6	-5.473175000	-2.113093000	0.374704000
1	-5.637268000	-1.429443000	1.222009000
1	-5.704840000	-3.129736000	0.719216000
1	-6.185911000	-1.840996000	-0.414688000
6	-0.625058000	-3.467328000	0.755221000
1	0.170109000	-2.818547000	1.155488000
1	-0.154433000	-4.162633000	0.043525000
1	-1.041527000	-4.058021000	1.580422000
5	0.786456000	0.604063000	0.336488000

Compound 6 TS 2

16	1.607018000	-0.874382000	1.778969000
7	2.149977000	1.307420000	0.317145000
7	0.138459000	-1.226579000	-1.531624000
7	2.139496000	-0.402183000	-1.370630000
7	4.135011000	-1.545543000	0.936055000
6	-0.582912000	1.230098000	0.774908000
6	-1.030318000	2.188317000	-0.170647000
6	-2.330787000	2.708655000	-0.096736000
1	-2.644638000	3.446104000	-0.842236000
6	-3.236323000	2.304121000	0.876313000
6	-2.795740000	1.362104000	1.806760000
1	-3.484001000	1.026798000	2.588282000
6	-1.506412000	0.826310000	1.775524000
6	3.109295000	0.386294000	-0.113758000
6	3.122123000	-0.798497000	0.856221000
6	0.915707000	-0.350656000	-0.864412000
6	0.922971000	-1.874788000	-2.473381000
1	0.506156000	-2.613718000	-3.151770000
6	2.188104000	-1.364820000	-2.347762000
1	3.090401000	-1.599013000	-2.904753000
6	-0.190387000	2.715881000	-1.318274000
1	0.303796000	3.661724000	-1.051139000
1	-0.830000000	2.932767000	-2.184087000
1	0.597537000	2.025193000	-1.643498000
6	-4.647860000	2.827456000	0.914348000
1	-4.771450000	3.695313000	0.253083000
1	-4.933869000	3.126913000	1.932729000
1	-5.360505000	2.052590000	0.589793000

6	-1.173758000	-0.199623000	2.832904000
1	-0.279749000	0.078778000	3.406978000
1	-0.983824000	-1.188572000	2.387837000
1	-2.011208000	-0.306956000	3.534743000
6	2.367823000	2.642669000	0.275026000
1	1.550879000	3.250705000	0.665949000
6	3.538855000	3.173120000	-0.182750000
1	3.699713000	4.248448000	-0.170802000
6	4.561527000	2.266451000	-0.607152000
1	5.527855000	2.664606000	-0.924096000
6	4.382678000	0.919630000	-0.561702000
1	5.173322000	0.204024000	-0.782554000
6	4.105021000	-2.638612000	1.879653000
1	3.908275000	-2.275139000	2.903071000
1	5.062653000	-3.173521000	1.871486000
1	3.297807000	-3.350003000	1.631876000
6	-1.239951000	-1.459328000	-1.191754000
6	-2.226090000	-0.614200000	-1.715366000
6	-3.520656000	-0.728324000	-1.203444000
1	-4.293258000	-0.050942000	-1.577029000
6	-3.843444000	-1.664786000	-0.221183000
6	-2.849292000	-2.548818000	0.208616000
1	-3.094986000	-3.315790000	0.947361000
6	-1.538190000	-2.468589000	-0.262831000
6	-1.940051000	0.358957000	-2.826011000
1	-2.508052000	1.286996000	-2.677800000
1	-2.248100000	-0.074910000	-3.790524000
1	-0.875321000	0.609484000	-2.897456000
6	-5.221428000	-1.700468000	0.382981000
1	-5.272633000	-1.013888000	1.243011000

1	-5.477228000	-2.705554000	0.743666000
1	-5.984807000	-1.383896000	-0.340395000
6	-0.483568000	-3.438579000	0.197948000
1	0.372401000	-2.914953000	0.648596000
1	-0.100954000	-4.031967000	-0.646608000
1	-0.897871000	-4.131332000	0.941229000
5	0.833429000	0.503634000	0.526139000

Compound 7

7	-0.935947000	1.637085000	0.736688000
7	1.219807000	-1.098541000	1.650507000
7	-0.677474000	-0.627530000	2.675096000
6	-0.045498000	-0.574772000	1.515226000
6	-3.077331000	0.250162000	-1.047122000
6	-0.171370000	2.477035000	0.026100000
6	-2.798980000	1.663535000	-1.521289000
1	-1.810696000	1.763963000	-1.990905000
1	-2.861534000	2.405591000	-0.710166000
1	-3.543364000	1.954208000	-2.273266000
6	0.174802000	-1.204243000	3.572981000
1	-0.103477000	-1.373232000	4.610980000
6	4.364835000	-0.936738000	-1.175769000
6	-3.756088000	-2.371554000	-0.442551000
1	-3.998722000	-3.415730000	-0.226224000
6	-1.695806000	2.055570000	1.752873000
1	-2.245715000	1.278925000	2.287183000
6	-2.517385000	-1.870559000	-0.022935000
6	3.980203000	0.198523000	-0.454447000
1	4.478505000	1.152264000	-0.646451000
6	1.364055000	-1.504064000	2.959570000

1	2.291680000	-1.942234000	3.316528000
6	-2.162021000	-0.522976000	-0.281421000
6	-4.679416000	-1.593893000	-1.133784000
6	2.972659000	0.151858000	0.507253000
6	2.674197000	-2.230196000	0.024304000
6	2.663559000	1.383608000	1.318168000
1	2.660271000	2.270546000	0.668702000
1	3.439460000	1.530826000	2.085478000
1	1.698806000	1.315752000	1.838054000
6	3.717238000	-2.141046000	-0.905160000
1	4.016894000	-3.043711000	-1.444156000
6	-0.940459000	4.302139000	1.341642000
1	-0.955932000	5.365221000	1.586285000
6	2.296500000	-1.066217000	0.707317000
6	5.439859000	-0.839178000	-2.225090000
1	5.709911000	-1.828348000	-2.616483000
1	6.346614000	-0.367829000	-1.819973000
1	5.096515000	-0.219317000	-3.066994000
6	-1.609601000	-2.860754000	0.672007000
1	-0.568017000	-2.761089000	0.346916000
1	-1.935764000	-3.886233000	0.452281000
1	-1.618067000	-2.718571000	1.761400000
6	-1.722027000	3.405353000	2.078141000
1	-2.349183000	3.747160000	2.900153000
6	-0.143938000	3.837762000	0.299217000
1	0.488543000	4.475411000	-0.318809000
6	-4.305741000	-0.287957000	-1.443306000
1	-4.988020000	0.333834000	-2.029852000
6	-6.024176000	-2.138936000	-1.536023000
1	-5.995932000	-3.231745000	-1.642689000

1	-6.361545000	-1.706163000	-2.487929000
1	-6.785222000	-1.899624000	-0.776810000
6	1.983949000	-3.552988000	0.235656000
1	1.445759000	-3.593288000	1.190074000
1	2.715864000	-4.371616000	0.209985000
1	1.254829000	-3.743981000	-0.567577000
5	-0.751014000	0.120878000	0.224970000
16	1.517378000	2.484853000	-2.178080000
6	0.544894000	1.743198000	-1.053457000
7	0.215930000	0.462667000	-0.946228000
6	0.635329000	-0.487645000	-1.948678000
1	0.277599000	-1.487355000	-1.671006000
1	1.732008000	-0.485987000	-2.040772000
1	0.215286000	-0.205612000	-2.928509000

Compound 7 TS 1

7	-1.971190000	0.854487000	-0.949488000
7	0.174539000	-1.986294000	-0.143012000
7	-1.838200000	-1.352232000	-0.687318000
6	-0.577429000	-0.895312000	-0.474520000
6	0.409804000	2.820627000	0.430213000
6	-2.756096000	-0.312222000	-0.830320000
6	-0.851625000	3.071505000	1.223218000
1	-1.444672000	3.882358000	0.770158000
1	-0.604086000	3.396006000	2.244513000
1	-1.489655000	2.180532000	1.282427000
6	-1.908233000	-2.713437000	-0.460350000
1	-2.837224000	-3.270735000	-0.510853000
6	4.339114000	-1.833579000	0.505056000
6	2.806027000	2.495994000	-0.954165000

1	3.742531000	2.362040000	-1.504046000
6	-2.591415000	2.022457000	-1.358927000
1	-1.964587000	2.913638000	-1.328354000
6	1.767863000	1.582687000	-1.159327000
6	3.455936000	-1.196952000	1.381017000
1	3.854112000	-0.639913000	2.232935000
6	-0.641423000	-3.098714000	-0.130238000
1	-0.252655000	-4.081362000	0.118646000
6	0.547502000	1.722911000	-0.457545000
6	2.680645000	3.568740000	-0.073149000
6	2.071722000	-1.255577000	1.210100000
6	2.433312000	-2.616079000	-0.802852000
6	1.143624000	-0.583583000	2.183836000
1	0.863910000	0.421115000	1.828114000
1	1.628508000	-0.477136000	3.162697000
1	0.211552000	-1.151982000	2.302280000
6	3.809025000	-2.545275000	-0.573809000
1	4.485908000	-3.040094000	-1.274621000
6	-4.575801000	0.768963000	-1.965567000
1	-5.568158000	0.759775000	-2.415561000
6	1.582452000	-1.963485000	0.101121000
6	5.825495000	-1.757918000	0.735016000
1	6.146172000	-0.717969000	0.888983000
1	6.383615000	-2.168658000	-0.116020000
1	6.110657000	-2.325875000	1.633299000
6	2.013053000	0.485322000	-2.168238000
1	2.243499000	0.921428000	-3.152097000
1	1.145518000	-0.174802000	-2.292281000
1	2.874812000	-0.130559000	-1.869038000
6	-3.857959000	2.015375000	-1.835684000

1	-4.307824000	2.950328000	-2.165955000
6	-4.010439000	-0.383161000	-1.529848000
1	-4.527423000	-1.340285000	-1.585174000
6	1.470741000	3.712501000	0.607205000
1	1.349156000	4.542778000	1.309245000
6	3.800375000	4.558054000	0.115875000
1	4.777918000	4.096143000	-0.077751000
1	3.804501000	4.965139000	1.136198000
1	3.691850000	5.406850000	-0.577324000
6	1.889610000	-3.326964000	-2.014384000
1	1.092013000	-2.739630000	-2.492709000
1	1.459912000	-4.306938000	-1.757245000
1	2.686680000	-3.496504000	-2.748983000
5	-0.585927000	0.642064000	-0.598196000
16	-4.676179000	-1.258129000	1.425142000
6	-3.264711000	-0.454639000	1.241713000
7	-2.272331000	0.067495000	1.746682000
6	-2.074766000	0.188504000	3.174174000
1	-1.229166000	0.856118000	3.386952000
1	-1.864494000	-0.799765000	3.615854000
1	-2.982528000	0.583051000	3.658655000

Compound 7 Int 1'

7	-1.924895000	1.019514000	-0.901452000
7	-0.030282000	-1.975083000	-0.098087000
7	-1.997466000	-1.239251000	-0.606076000
6	-0.718528000	-0.888310000	-0.471020000
6	0.964284000	2.427515000	0.481830000
6	-2.879091000	-0.050813000	-0.601126000
6	-0.164334000	2.918742000	1.355040000

1	-0.568700000	3.862141000	0.952577000
1	0.196027000	3.135172000	2.370688000
1	-0.995015000	2.198713000	1.421505000
6	-2.166778000	-2.558178000	-0.269825000
1	-3.148443000	-3.019965000	-0.218915000
6	4.083047000	-1.432494000	0.583064000
6	3.110389000	1.652197000	-1.137609000
1	3.942698000	1.356546000	-1.782913000
6	-2.420371000	2.248147000	-1.326858000
1	-1.731011000	3.088024000	-1.230080000
6	1.840590000	1.126393000	-1.382757000
6	3.137477000	-0.972026000	1.504822000
1	3.469589000	-0.405719000	2.378361000
6	-0.915316000	-3.032224000	0.028120000
1	-0.583165000	-4.022210000	0.324203000
6	0.755380000	1.484348000	-0.550537000
6	3.340093000	2.539693000	-0.084806000
6	1.772270000	-1.197377000	1.334117000
6	2.287791000	-2.431843000	-0.733701000
6	0.763902000	-0.698821000	2.333985000
1	0.158761000	0.133284000	1.940578000
1	1.269818000	-0.352264000	3.243423000
1	0.050153000	-1.489626000	2.609824000
6	3.644439000	-2.180314000	-0.511601000
1	4.375150000	-2.564985000	-1.227438000
6	-4.409484000	1.115968000	-2.103967000
1	-5.306072000	1.158577000	-2.723628000
6	1.377108000	-1.907467000	0.188634000
6	5.538282000	-1.089236000	0.753009000
1	5.725449000	-0.063979000	0.396029000

1	6.183159000	-1.768193000	0.180359000
1	5.837614000	-1.130411000	1.809020000
6	1.644725000	0.237547000	-2.585496000
1	1.340294000	0.839244000	-3.456501000
1	0.856395000	-0.512248000	-2.429662000
1	2.571878000	-0.290983000	-2.847014000
6	-3.640289000	2.334605000	-1.888610000
1	-4.012962000	3.296181000	-2.236555000
6	-4.028743000	-0.050378000	-1.558420000
1	-4.598163000	-0.970021000	-1.675980000
6	2.251917000	2.926440000	0.699886000
1	2.409118000	3.637414000	1.516270000
6	4.720321000	3.066753000	0.208625000
1	5.091163000	2.676210000	1.168948000
1	4.718016000	4.163597000	0.284223000
1	5.434397000	2.778590000	-0.574253000
6	1.829309000	-3.232507000	-1.923836000
1	0.915667000	-2.816099000	-2.371054000
1	1.606153000	-4.271908000	-1.636650000
1	2.609827000	-3.261530000	-2.694596000
5	-0.577242000	0.671096000	-0.640271000
16	-4.752502000	-0.905270000	1.270301000
6	-3.331679000	-0.036001000	0.927382000
7	-2.452763000	0.492395000	1.692311000
6	-2.683678000	0.424060000	3.112800000
1	-1.858675000	0.911535000	3.654472000
1	-2.777563000	-0.625214000	3.448864000
1	-3.635676000	0.909431000	3.388705000

Compound 7 TS 1'

7	-1.998351000	0.884423000	-0.845288000
7	0.199988000	-1.985688000	-0.252653000
7	-1.807483000	-1.370486000	-0.748399000
6	-0.576247000	-0.913323000	-0.487911000
6	0.467636000	2.750347000	0.718047000
6	-2.809655000	-0.293046000	-0.593087000
6	-0.642360000	2.856860000	1.733773000
1	-0.521857000	2.102956000	2.525790000
1	-1.631035000	2.669264000	1.294760000
1	-0.639301000	3.848280000	2.205438000
6	-1.863166000	-2.731077000	-0.600606000
1	-2.789678000	-3.291493000	-0.675862000
6	4.344847000	-1.845990000	0.514081000
6	2.565202000	2.661034000	-1.126282000
1	3.367653000	2.640436000	-1.868935000
6	-2.599655000	2.058725000	-1.259601000
1	-1.974968000	2.950479000	-1.183255000
6	1.532570000	1.726556000	-1.216461000
6	3.431722000	-1.334638000	1.438599000
1	3.799174000	-0.888909000	2.365443000
6	-0.586838000	-3.126350000	-0.316276000
1	-0.165612000	-4.113233000	-0.153295000
6	0.479305000	1.745512000	-0.274530000
6	2.586433000	3.632171000	-0.123137000
6	2.052488000	-1.379341000	1.221581000
6	2.486230000	-2.496716000	-0.926791000
6	1.088367000	-0.832796000	2.237019000
1	0.746168000	0.175116000	1.953627000
1	1.567535000	-0.765993000	3.221724000
1	0.186847000	-1.455395000	2.318971000

6	3.853607000	-2.430100000	-0.657123000
1	4.554532000	-2.837558000	-1.389141000
6	-4.526492000	0.780470000	-1.955985000
1	-5.467072000	0.757289000	-2.510564000
6	1.608061000	-1.957091000	0.024704000
6	5.826277000	-1.742843000	0.761692000
1	6.377203000	-2.526160000	0.224148000
1	6.057104000	-1.826513000	1.831901000
1	6.206174000	-0.769476000	0.416413000
6	1.545447000	0.728497000	-2.349795000
1	0.547873000	0.610847000	-2.799268000
1	1.877702000	-0.260095000	-1.998435000
1	2.237421000	1.044078000	-3.141322000
6	-3.842256000	2.052058000	-1.783736000
1	-4.295384000	2.979876000	-2.126386000
6	-4.025851000	-0.360005000	-1.450717000
1	-4.540021000	-1.315928000	-1.538415000
6	1.522058000	3.667276000	0.778207000
1	1.503697000	4.441244000	1.550622000
6	3.727814000	4.608409000	-0.015289000
1	4.141679000	4.849015000	-1.004280000
1	4.543841000	4.186109000	0.591137000
1	3.409454000	5.543680000	0.464653000
6	1.978817000	-3.104674000	-2.208824000
1	1.166216000	-2.504209000	-2.644150000
1	1.582403000	-4.118614000	-2.047786000
1	2.788988000	-3.178169000	-2.944611000
5	-0.657239000	0.674363000	-0.394064000
16	-4.470219000	-1.257032000	1.447469000
6	-3.086559000	-0.409379000	0.979285000

7	-2.092028000	0.047338000	1.648458000
6	-2.122261000	-0.105893000	3.080013000
1	-1.205303000	0.296358000	3.536332000
1	-2.233801000	-1.169450000	3.361323000
1	-2.996059000	0.409847000	3.514310000

Compound 7 Int 1

7	-2.201573000	0.223450000	-0.963506000
7	0.575647000	-2.017590000	0.138144000
7	-1.523132000	-1.842352000	-0.236857000
6	-0.407958000	-1.118828000	-0.107291000
6	-0.777272000	3.098053000	0.083114000
6	-2.774849000	-0.891210000	-0.285740000
6	-2.227478000	3.199148000	0.508696000
1	-2.353912000	3.069737000	1.593025000
1	-2.852682000	2.448036000	0.011592000
1	-2.614361000	4.195520000	0.256524000
6	-1.305056000	-3.174414000	-0.030680000
1	-2.098977000	-3.914027000	-0.070080000
6	4.718673000	-1.263546000	0.444545000
6	1.806987000	3.157789000	-0.935051000
1	2.803375000	3.175395000	-1.386952000
6	-2.265263000	0.262153000	-2.322142000
1	-1.613549000	0.999574000	-2.799002000
6	1.115083000	1.939070000	-0.881770000
6	3.831884000	-0.758984000	1.397359000
1	4.216291000	-0.153569000	2.221732000
6	0.033963000	-3.297574000	0.192176000
1	0.657155000	-4.166097000	0.381270000
6	-0.164365000	1.866842000	-0.289292000

6	1.253697000	4.342659000	-0.464898000
6	2.457101000	-0.998403000	1.327801000
6	2.834931000	-2.283378000	-0.727924000
6	1.518476000	-0.394288000	2.331553000
1	1.092267000	0.537137000	1.927361000
1	2.045781000	-0.148283000	3.261712000
1	0.682642000	-1.068221000	2.563421000
6	4.199792000	-2.019766000	-0.611100000
1	4.876067000	-2.399338000	-1.381039000
6	-4.071259000	-1.330670000	-2.272535000
1	-4.913485000	-1.784907000	-2.799505000
6	1.982221000	-1.768371000	0.260982000
6	6.199343000	-1.016085000	0.558950000
1	6.672861000	-0.971758000	-0.430761000
1	6.684372000	-1.827695000	1.122964000
1	6.406207000	-0.075533000	1.085910000
6	1.792306000	0.777909000	-1.573406000
1	1.133572000	-0.089697000	-1.690914000
1	2.702589000	0.460040000	-1.043331000
1	2.099967000	1.091706000	-2.582131000
6	-3.142412000	-0.512394000	-3.019164000
1	-3.222153000	-0.417850000	-4.099739000
6	-3.958361000	-1.487958000	-0.933766000
1	-4.674777000	-2.020974000	-0.309075000
6	-0.061130000	4.293189000	0.004581000
1	-0.555448000	5.223245000	0.300335000
6	2.018818000	5.639159000	-0.490782000
1	2.371383000	5.904377000	0.517996000
1	1.386750000	6.466414000	-0.843371000
1	2.897726000	5.571926000	-1.145616000

6	2.299679000	-3.039392000	-1.916287000
1	1.372642000	-2.583477000	-2.294113000
1	2.066763000	-4.085459000	-1.667506000
1	3.039429000	-3.047034000	-2.726288000
5	-0.998896000	0.521452000	-0.037480000
16	-3.881402000	-1.002317000	2.312469000
6	-2.819988000	-0.432392000	1.185116000
7	-1.792825000	0.403012000	1.332412000
6	-1.483318000	0.947324000	2.631830000
1	-0.710164000	1.720047000	2.532698000
1	-1.141892000	0.159766000	3.323656000
1	-2.391809000	1.381315000	3.076500000

Compound 7 TS 2

7	2.211737000	0.048629000	0.931300000
7	-0.831258000	-1.930422000	-0.059843000
7	1.282052000	-2.026098000	0.328792000
6	0.278287000	-1.166937000	0.165290000
6	1.145298000	2.977577000	-0.262005000
6	2.756379000	-1.080808000	0.323120000
6	2.569961000	2.876631000	-0.751319000
1	2.633515000	2.652895000	-1.826794000
1	3.136228000	2.097879000	-0.225177000
1	3.084446000	3.835958000	-0.596309000
6	0.879682000	-3.314060000	0.165090000
1	1.558813000	-4.160631000	0.234668000
6	-4.930811000	-0.913413000	-0.337486000
6	-1.354313000	3.441244000	0.856597000
1	-2.317987000	3.614050000	1.347494000
6	2.366999000	0.258100000	2.257499000

1	1.776526000	1.077368000	2.676901000
6	-0.848363000	2.134283000	0.814282000
6	-4.055419000	-0.628658000	-1.386002000
1	-4.440154000	-0.146404000	-2.289263000
6	-0.463944000	-3.269254000	-0.064164000
1	-1.198675000	-4.054768000	-0.222840000
6	0.383054000	1.853686000	0.178305000
6	-0.661416000	4.522739000	0.325071000
6	-2.694268000	-0.944877000	-1.327915000
6	-3.060262000	-1.866122000	0.914486000
6	-1.792766000	-0.609168000	-2.474960000
1	-1.279393000	0.347448000	-2.294193000
1	-2.365560000	-0.506985000	-3.406765000
1	-1.016931000	-1.372999000	-2.624021000
6	-4.410399000	-1.533047000	0.802999000
1	-5.075720000	-1.755698000	1.642423000
6	4.067394000	-1.436070000	2.310805000
1	4.884794000	-1.922785000	2.850829000
6	-2.210759000	-1.556434000	-0.164216000
6	-6.393950000	-0.592164000	-0.437877000
1	-6.970481000	-1.481265000	-0.743465000
1	-6.585262000	0.195143000	-1.180568000
1	-6.800420000	-0.258875000	0.528397000
6	-1.662394000	1.098605000	1.540892000
1	-1.100443000	0.175681000	1.723148000
1	-2.580379000	0.839046000	0.992722000
1	-1.976374000	1.490401000	2.520998000
6	3.264078000	-0.469066000	2.991668000
1	3.419809000	-0.246788000	4.047096000
6	3.868767000	-1.721465000	0.993665000

1	4.495607000	-2.399720000	0.412816000
6	0.607730000	4.265388000	-0.196465000
1	1.217645000	5.104617000	-0.546811000
6	-1.232095000	5.911228000	0.336651000
1	-2.050304000	6.007270000	1.065123000
1	-1.639090000	6.178782000	-0.653118000
1	-0.464887000	6.661440000	0.581824000
6	-2.543523000	-2.508737000	2.169874000
1	-1.571420000	-2.092411000	2.473044000
1	-2.397622000	-3.593584000	2.044337000
1	-3.252417000	-2.365566000	2.996711000
5	1.021661000	0.387093000	-0.010253000
16	3.744499000	-1.513932000	-2.274564000
6	2.754974000	-0.784673000	-1.171042000
7	1.786239000	0.111186000	-1.367670000
6	1.463390000	0.549012000	-2.696628000
1	0.755373000	1.387057000	-2.649802000
1	1.031624000	-0.268480000	-3.299155000
1	2.379599000	0.865065000	-3.221298000

Compound 8

16	1.454235000	-0.696710000	-0.450903000
16	-1.451727000	-0.657316000	0.451242000
7	-4.956900000	0.315178000	-1.768391000
7	1.788962000	1.332434000	1.337685000
7	-1.746413000	1.324489000	-1.394339000
7	-3.598564000	-1.371413000	-2.197066000
6	3.796886000	-0.255106000	1.447488000
7	3.565525000	-1.355119000	2.248576000
6	-0.425290000	1.214886000	-1.187255000

6	-0.021400000	2.693464000	-3.037734000
1	0.674981000	3.229841000	-3.684363000
6	-4.174035000	3.482238000	1.861744000
1	-4.057099000	4.562101000	1.990200000
6	5.124698000	2.613663000	-2.794839000
6	-2.436501000	-2.204743000	-2.235979000
6	-5.532090000	-0.485772000	-2.710514000
1	-6.508559000	-0.266848000	-3.137481000
6	-3.788978000	-0.225526000	-1.451553000
6	-2.408541000	-3.364860000	-1.449189000
6	2.369015000	-2.135085000	2.327824000
6	-5.034000000	2.798265000	2.710742000
6	-1.400033000	2.782389000	-3.239827000
1	-1.825539000	3.382774000	-4.042525000
6	-4.441915000	0.750028000	1.520495000
6	3.613881000	1.355674000	-0.696291000
6	-0.088791000	-3.703663000	-2.115373000
6	-3.565783000	1.447149000	0.639984000
6	4.274702000	3.340563000	-1.972133000
1	4.182626000	4.418572000	-2.132398000
6	1.474636000	2.865421000	3.127227000
1	1.913427000	3.489418000	3.904361000
6	-3.448476000	2.845588000	0.840281000
6	5.532523000	-0.519525000	2.715423000
1	6.518177000	-0.317550000	3.129485000
6	3.528330000	2.749832000	-0.938018000
6	2.275952000	-3.311635000	1.571061000
6	-4.653155000	-0.743210000	1.436738000
1	-5.276398000	-1.089324000	2.271423000
1	-3.701032000	-1.292904000	1.487553000

1	-5.155067000	-1.018407000	0.498231000
6	4.666983000	-1.531553000	3.050071000
1	4.719261000	-2.344955000	3.768555000
6	-1.352064000	-1.834808000	-3.038818000
6	0.465388000	1.238740000	1.138126000
6	-5.821503000	3.503002000	3.783321000
1	-5.742931000	2.976651000	4.745578000
1	-6.889744000	3.544935000	3.521010000
1	-5.470586000	4.533999000	3.924821000
6	5.935559000	3.269754000	-3.880754000
1	5.848601000	2.720613000	-4.829473000
1	7.003121000	3.291289000	-3.613307000
1	5.611862000	4.305288000	-4.051090000
6	2.661809000	3.727137000	-0.163357000
1	2.604243000	4.678765000	-0.708060000
1	3.085945000	3.955108000	0.825207000
1	1.628594000	3.385462000	-0.010177000
6	0.471141000	1.883740000	-2.021915000
1	1.541315000	1.733946000	-1.880981000
6	1.313572000	-1.693583000	3.132746000
6	-2.236259000	2.062885000	-2.405603000
1	-3.324851000	2.047660000	-2.506895000
6	2.295053000	2.098954000	2.319571000
1	3.383510000	2.067813000	2.418688000
6	-1.398408000	-4.171063000	2.145936000
1	-2.021367000	-3.588873000	1.448243000
1	-1.916903000	-4.199584000	3.114416000
1	-1.321329000	-5.197202000	1.760620000
6	4.646413000	-0.882653000	-1.431476000
1	5.279324000	-1.263294000	-2.243498000

1	3.680024000	-1.405500000	-1.495387000
1	5.116931000	-1.152975000	-0.475730000
6	-0.051864000	-3.515437000	2.262212000
6	0.093878000	2.791121000	2.934076000
1	-0.590828000	3.363771000	3.561836000
6	1.218847000	-4.432372000	-1.985390000
1	1.091621000	-5.419291000	-1.519443000
1	1.901913000	-3.840683000	-1.356291000
1	1.700647000	-4.569379000	-2.963704000
6	3.462426000	-3.793050000	0.782356000
1	3.264893000	-4.775076000	0.334742000
1	4.358832000	-3.869389000	1.414479000
1	3.705206000	-3.083041000	-0.023267000
6	-0.181228000	-2.589187000	-2.946711000
1	0.688628000	-2.286467000	-3.536181000
6	-3.625435000	-3.775186000	-0.665913000
1	-3.450864000	-4.719638000	-0.135445000
1	-4.499167000	-3.899985000	-1.322204000
1	-3.893487000	-3.002667000	0.070374000
6	-5.146304000	1.421439000	2.519725000
1	-5.804836000	0.845523000	3.176192000
6	-4.705285000	-1.545006000	-2.992144000
1	-4.787257000	-2.389558000	-3.670782000
6	-2.567149000	3.779781000	0.030256000
1	-1.539031000	3.416742000	-0.108217000
1	-2.495632000	4.750518000	0.538293000
1	-2.987145000	3.975875000	-0.966813000
6	1.055941000	-3.984712000	1.548713000
1	0.961869000	-4.891569000	0.945782000
6	0.105108000	-2.389763000	3.068290000

1	-0.743137000	-2.029463000	3.656841000
6	1.447964000	-0.525686000	4.073087000
1	0.685707000	0.237483000	3.858633000
1	2.441933000	-0.063939000	4.024273000
1	1.283105000	-0.860059000	5.108289000
6	-0.416438000	1.950793000	1.952335000
1	-1.489483000	1.814628000	1.819745000
6	0.011139000	0.342596000	-0.011912000
6	-1.416256000	-0.680263000	-4.002934000
1	-0.642781000	0.066169000	-3.769023000
1	-2.398552000	-0.191664000	-4.001638000
1	-1.217444000	-1.036134000	-5.024701000
6	-1.223801000	-4.097553000	-1.399703000
1	-1.181279000	-4.993925000	-0.775488000
6	5.203131000	1.240331000	-2.565224000
1	5.851357000	0.631120000	-3.201581000
6	4.477181000	0.613471000	-1.552744000
7	4.985176000	0.256008000	1.736188000
5	-2.763070000	0.516053000	-0.439227000
5	2.789673000	0.474996000	0.408252000

Compound 8 TS 1

16	-1.830475000	-0.783572000	-2.036512000
7	-1.961740000	1.221181000	0.174716000
7	0.027682000	-1.710199000	1.059609000
7	-1.954621000	-0.810005000	1.096937000
16	-4.682748000	-1.526656000	-1.123625000
6	0.659382000	1.703406000	-0.284604000
6	0.919223000	2.813786000	0.553842000
6	2.058200000	3.597431000	0.340591000

1	2.249933000	4.445792000	1.003463000
6	2.965079000	3.312810000	-0.680042000
6	2.713090000	2.201966000	-1.487467000
1	3.421081000	1.948400000	-2.281480000
6	1.584367000	1.399057000	-1.308463000
6	-2.808360000	0.178988000	0.592451000
6	-3.202004000	-0.900155000	-1.199955000
6	-0.664566000	-0.583163000	0.748241000
6	-0.851927000	-2.640231000	1.577771000
1	-0.511025000	-3.614503000	1.914263000
6	-2.100692000	-2.090538000	1.595155000
1	-3.056117000	-2.499272000	1.905086000
6	0.022503000	3.154589000	1.722909000
1	-0.919450000	3.623152000	1.399499000
1	0.523375000	3.854963000	2.403929000
1	-0.255924000	2.256531000	2.295260000
6	4.173522000	4.180332000	-0.915177000
1	4.436005000	4.752872000	-0.015590000
1	3.983554000	4.901399000	-1.725390000
1	5.044222000	3.578343000	-1.209976000
6	1.373623000	0.228620000	-2.234793000
1	0.572202000	0.443647000	-2.958239000
1	1.072451000	-0.674771000	-1.686112000
1	2.290457000	0.001177000	-2.794888000
6	-2.544460000	2.409783000	-0.214442000
1	-1.880582000	3.106931000	-0.728097000
6	-3.840734000	2.680228000	0.075167000
1	-4.271013000	3.631718000	-0.232604000
6	-4.620362000	1.730559000	0.831126000
1	-5.629129000	1.991833000	1.150552000

6	-4.098264000	0.517004000	1.136311000
1	-4.663305000	-0.237819000	1.681259000
6	1.418142000	-1.904242000	0.779133000
6	2.364926000	-1.139791000	1.475384000
6	3.708786000	-1.302527000	1.132360000
1	4.459684000	-0.711092000	1.662057000
6	4.114434000	-2.195291000	0.138373000
6	3.138594000	-2.948906000	-0.519595000
1	3.439120000	-3.649567000	-1.302396000
6	1.780867000	-2.816726000	-0.224263000
6	1.959848000	-0.162831000	2.545456000
1	1.688368000	0.804696000	2.095568000
1	2.791949000	0.011601000	3.239142000
1	1.093290000	-0.522904000	3.117002000
6	5.567650000	-2.316262000	-0.237105000
1	6.216628000	-2.198273000	0.641051000
1	5.844136000	-1.533344000	-0.960067000
1	5.781786000	-3.288473000	-0.699774000
6	0.743104000	-3.595002000	-0.989921000
1	-0.091461000	-2.948243000	-1.302685000
1	0.313667000	-4.408219000	-0.385326000
1	1.188959000	-4.046272000	-1.884875000
5	-0.580875000	0.791829000	0.042414000

Compound 8 Int 1

16	1.497130000	-0.481886000	1.917848000
7	2.096641000	1.178855000	-0.114012000
7	-0.022250000	-1.622055000	-1.182971000
7	1.987302000	-0.843846000	-1.135225000
16	4.226364000	-1.701709000	1.457078000
6	-0.535066000	1.565072000	0.460937000

6	-0.783955000	2.502026000	-0.573995000
6	-1.919182000	3.320879000	-0.524666000
1	-2.089883000	4.034761000	-1.335708000
6	-2.845890000	3.238445000	0.511679000
6	-2.622401000	2.280286000	1.500308000
1	-3.353230000	2.167694000	2.305947000
6	-1.499392000	1.448530000	1.490433000
6	2.921531000	0.022866000	-0.339464000
6	2.966081000	-0.762787000	1.045565000
6	0.731150000	-0.605777000	-0.744306000
6	0.793030000	-2.531239000	-1.848663000
1	0.385524000	-3.421544000	-2.317631000
6	2.068954000	-2.048858000	-1.792019000
1	2.997754000	-2.452810000	-2.181843000
6	0.099147000	2.639442000	-1.797732000
1	0.991345000	3.252202000	-1.603383000
1	-0.459848000	3.122645000	-2.610614000
1	0.463901000	1.669030000	-2.162040000
6	-4.042902000	4.150319000	0.568478000
1	-4.915655000	3.636165000	0.994208000
1	-4.311025000	4.520886000	-0.430115000
1	-3.835693000	5.026190000	1.202882000
6	-1.387626000	0.420085000	2.590398000
1	-0.535548000	0.624787000	3.254786000
1	-1.251122000	-0.593427000	2.182979000
1	-2.298552000	0.414238000	3.203158000
6	2.661700000	2.397979000	0.089726000
1	1.988016000	3.157077000	0.495612000
6	3.955114000	2.655011000	-0.241445000
1	4.377492000	3.646487000	-0.099783000

6	4.721457000	1.589603000	-0.843124000
1	5.721700000	1.806023000	-1.223844000
6	4.238639000	0.332628000	-0.949915000
1	4.826660000	-0.486687000	-1.362188000
6	-1.409409000	-1.795597000	-0.843580000
6	-2.382843000	-1.051908000	-1.518078000
6	-3.709933000	-1.198768000	-1.102323000
1	-4.484332000	-0.620593000	-1.612207000
6	-4.065879000	-2.051315000	-0.057954000
6	-3.060632000	-2.793731000	0.571805000
1	-3.324676000	-3.472714000	1.386221000
6	-1.721612000	-2.682928000	0.200312000
6	-2.038673000	-0.101785000	-2.631788000
1	-1.922109000	0.916998000	-2.231999000
1	-2.845547000	-0.078774000	-3.375832000
1	-1.103854000	-0.376715000	-3.137993000
6	-5.494405000	-2.151254000	0.406623000
1	-5.664999000	-1.480645000	1.262961000
1	-5.737847000	-3.171587000	0.731837000
1	-6.194502000	-1.861758000	-0.387702000
6	-0.648857000	-3.471237000	0.904401000
1	0.155798000	-2.813803000	1.269420000
1	-0.186838000	-4.211888000	0.234275000
1	-1.070735000	-4.009377000	1.761962000
5	0.748238000	0.621611000	0.324719000

Compound 8 TS 2

16	1.540597000	-0.767794000	1.880289000
7	2.130571000	1.286911000	0.288474000
7	0.142639000	-1.361260000	-1.414475000

7	2.150749000	-0.554012000	-1.261109000
16	4.290082000	-1.827125000	1.261997000
6	-0.612006000	1.275260000	0.679555000
6	-1.029739000	2.168155000	-0.339570000
6	-2.324725000	2.706796000	-0.326107000
1	-2.616977000	3.392524000	-1.127553000
6	-3.251157000	2.382896000	0.657754000
6	-2.838564000	1.504806000	1.660956000
1	-3.544078000	1.234432000	2.452099000
6	-1.556283000	0.953098000	1.690047000
6	3.092606000	0.326152000	-0.031980000
6	3.050820000	-0.799545000	1.026570000
6	0.912711000	-0.440940000	-0.803633000
6	0.945667000	-2.102932000	-2.267910000
1	0.539322000	-2.896711000	-2.888110000
6	2.214405000	-1.601354000	-2.146331000
1	3.130604000	-1.899439000	-2.647321000
6	-0.159946000	2.601055000	-1.503943000
1	0.338488000	3.559790000	-1.296533000
1	-0.777826000	2.758004000	-2.398100000
1	0.627380000	1.880624000	-1.759054000
6	-4.656091000	2.924343000	0.634223000
1	-5.373818000	2.135348000	0.358808000
1	-4.758875000	3.740571000	-0.092954000
1	-4.952640000	3.303859000	1.622407000
6	-1.251777000	0.000758000	2.821988000
1	-0.370999000	0.316203000	3.398096000
1	-1.057407000	-1.017540000	2.450819000
1	-2.104670000	-0.056642000	3.510786000
6	2.364986000	2.615161000	0.172716000

1	1.540914000	3.253377000	0.494416000
6	3.558369000	3.102681000	-0.274443000
1	3.733657000	4.174557000	-0.325378000
6	4.577116000	2.158854000	-0.611927000
1	5.555061000	2.522023000	-0.934599000
6	4.379507000	0.818864000	-0.485008000
1	5.167165000	0.086008000	-0.654548000
6	-1.240779000	-1.559059000	-1.073436000
6	-2.215799000	-0.750016000	-1.670281000
6	-3.514797000	-0.815401000	-1.162042000
1	-4.279794000	-0.164500000	-1.593862000
6	-3.851335000	-1.668550000	-0.110347000
6	-2.866826000	-2.520706000	0.398085000
1	-3.123205000	-3.222381000	1.195706000
6	-1.551179000	-2.487415000	-0.067479000
6	-1.911993000	0.132492000	-2.850005000
1	-2.474114000	1.073221000	-2.780022000
1	-2.214135000	-0.372556000	-3.781124000
1	-0.844586000	0.368827000	-2.930387000
6	-5.234580000	-1.645947000	0.482252000
1	-5.489707000	-2.607513000	0.946714000
1	-5.992497000	-1.412709000	-0.277678000
1	-5.296474000	-0.870685000	1.262505000
6	-0.510565000	-3.431862000	0.473262000
1	0.404736000	-2.904897000	0.777078000
1	-0.226655000	-4.174041000	-0.289085000
1	-0.899051000	-3.974595000	1.344189000
5	0.798664000	0.521239000	0.511617000

Compound 8 Int 2

16	-0.173901000	0.136920000	-1.659691000
7	0.348711000	1.227179000	0.774412000
7	-0.868658000	-1.833925000	1.148483000
7	1.161393000	-1.664072000	1.998404000
16	-2.239861000	2.289187000	-1.973720000
6	2.430996000	-0.077575000	-0.344189000
6	3.118605000	-1.300542000	-0.541663000
6	4.499446000	-1.304657000	-0.760767000
1	5.004471000	-2.264306000	-0.904650000
6	5.246605000	-0.130578000	-0.821934000
6	4.550235000	1.072908000	-0.737168000
1	5.095349000	2.012308000	-0.866610000
6	3.167719000	1.120114000	-0.527957000
6	-0.636566000	1.952281000	0.223856000
6	-1.076277000	1.499375000	-1.130777000
6	0.377133000	-1.259092000	1.013403000
6	-0.835982000	-2.647389000	2.256924000
1	-1.706622000	-3.219719000	2.564566000
6	0.432338000	-2.526296000	2.765868000
1	0.854406000	-3.022007000	3.637415000
6	2.426803000	-2.645098000	-0.596910000
1	2.983762000	-3.321104000	-1.260032000
1	1.399918000	-2.570687000	-0.979145000
1	2.367935000	-3.102355000	0.400165000
6	6.741322000	-0.161881000	-1.001021000
1	7.104880000	0.753523000	-1.487456000
1	7.052083000	-1.023487000	-1.607795000
1	7.249415000	-0.244578000	-0.027408000
6	2.527135000	2.492266000	-0.609364000
1	2.270247000	2.921184000	0.371623000

1	1.613473000	2.470923000	-1.220930000
1	3.221861000	3.193608000	-1.089175000
6	0.850498000	1.517114000	1.984106000
1	1.625199000	0.835217000	2.345691000
6	0.376044000	2.603936000	2.700176000
1	0.800816000	2.831707000	3.676619000
6	-0.645957000	3.381696000	2.146447000
1	-1.037754000	4.241546000	2.691664000
6	-1.164104000	3.052292000	0.900735000
1	-1.963206000	3.612602000	0.415521000
6	-2.064895000	-1.472900000	0.451539000
6	-2.377825000	-2.079885000	-0.769583000
6	-3.496411000	-1.613649000	-1.464398000
1	-3.736747000	-2.058955000	-2.433168000
6	-4.296075000	-0.581801000	-0.968825000
6	-3.987565000	-0.043693000	0.283388000
1	-4.614297000	0.752418000	0.693868000
6	-2.879720000	-0.475694000	1.012441000
6	-1.495366000	-3.145028000	-1.357356000
1	-0.707072000	-2.681811000	-1.973636000
1	-2.073641000	-3.813384000	-2.008283000
1	-1.001989000	-3.741394000	-0.578634000
6	-5.425731000	-0.019873000	-1.787380000
1	-5.051248000	0.810133000	-2.408326000
1	-6.228867000	0.373362000	-1.149917000
1	-5.850493000	-0.776018000	-2.460816000
6	-2.577808000	0.098181000	2.372584000
1	-1.500761000	0.267645000	2.518263000
1	-2.889624000	-0.597555000	3.166976000
1	-3.112787000	1.045210000	2.523188000

5	0.850758000	-0.086643000	-0.003427000
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