

**Table S1.** Internal coordinates of the optimized structures of the test compounds at B3LYP/6-31G in the gas-phase

<b>Phe</b>
C,0,-2.0146131067,0.755600187,-0.2153405328 C,0,-1.5232934102,-0.5105125795,0.1234803932 C,0,-2.4033679746,-1.5539294409,0.4302255526 C,0,-3.7857574695,-1.3226171178,0.3960224475 C,0,-4.2877464583,-0.063749848,0.0594563599 C,0,-3.3976010516,0.9724775415,-0.2455290193 O,0,-3.9592846739,2.20514627,-0.5736790719 H,0,-1.3280124828,1.5642558944,-0.4532140233 H,0,-0.4508924174,-0.6773814215,0.1465438618 H,0,-2.0187350017,-2.5336976911,0.6923159033 H,0,-4.4764345867,-2.1259032991,0.6324616884 H,0,-5.3521798454,0.1362431572,0.0271075562 H,0,-3.274241521,2.8720033476,-0.7717061157
<b>Anis</b>
C,0,-1.9697824623,0.0701696922,-0.0140212464 C,0,-1.5090433745,-1.2133897919,0.3126228672 C,0,-2.4073808158,-2.253387747,0.5643315406 C,0,-3.7865801029,-2.0054807836,0.4881134527 C,0,-4.2597561787,-0.7344739755,0.1645090013 C,0,-3.3494349772,0.3038670997,-0.0866612977 O,0,-3.9201477837,1.5352331183,-0.4013965867 C,0,-3.0470369325,2.6606309226,-0.6735618554 H,0,-1.2572329497,0.8631461363,-0.2057182617 H,0,-0.4396787519,-1.3932812952,0.3686142448 H,0,-2.0422381396,-3.2433393486,0.8163456279 H,0,-4.4942944462,-2.8056181074,0.6816086925 H,0,-5.3198634581,-0.518940511,0.0996813232 H,0,-3.7144982327,3.4942503213,-0.8885962877 H,0,-2.4226986831,2.9018091557,0.1953896814 H,0,-2.4049657109,2.4679341142,-1.5417008961
<b>Guai</b>
C,0,-2.654333941,-0.4598535828,0.1221298499 C,0,-1.8594151526,0.6562631817,-0.1744914112 C,0,-0.465455691,0.5576832736,-0.1467871794 C,0,0.1510001825,-0.6619037759,0.1788502052 C,0,-0.6433143946,-1.7682151193,0.4728684457 C,0,-2.0479330196,-1.6702120398,0.4453035552

O,0,-2.8237307903,-2.7801653508,0.7403058047  
O,0,-0.1841929282,-3.0472320725,0.8141535902  
C,0,1.2451680366,-3.2810747011,0.8784679686  
H,0,-3.7366536943,-0.4108693714,0.1079654725  
H,0,-2.3331256394,1.5991096668,-0.4262399036  
H,0,0.1491710899,1.4215244591,-0.3763619907  
H,0,1.2320523365,-0.7341363887,0.1991972716  
H,0,-2.232177081,-3.5358531132,0.9422829216  
H,0,1.3565123154,-4.3280254173,1.1578558737  
H,0,1.7163051502,-3.1036834001,-0.0953089494  
H,0,1.7139512209,-2.6419742483,1.6357464756

### Ver

C,0,-0.3462534161,-1.8635419127,0.4615117471  
C,0,0.3202790086,-0.6535783043,0.206199778  
C,0,-0.4109957453,0.5000907516,-0.0633351426  
C,0,-1.8149240051,0.4534521234,-0.0798197333  
C,0,-2.4848510398,-0.7444666388,0.172661808  
C,0,-1.7406437694,-1.91853061,0.4470043382  
O,0,-3.8653922682,-0.8877125165,0.17819769  
C,0,-4.6802090846,0.2787949099,-0.0991842141  
O,0,-2.4852641124,-3.0650438539,0.6867796657  
C,0,-1.7787113302,-4.2981903058,0.9726785008  
H,0,0.2306703501,-2.7560685499,0.6702818514  
H,0,1.4047698963,-0.6275147085,0.2211561311  
H,0,0.0947541517,1.4391901613,-0.2616603277  
H,0,-2.3757105294,1.3558191301,-0.2902533131  
H,0,-5.7087997328,-0.0755059345,-0.0424523333  
H,0,-4.5184995154,1.0669277028,0.6464884906  
H,0,-4.4807319532,0.6776464983,-1.1014004321  
H,0,-2.5597350338,-5.0427756071,1.1221471623  
H,0,-1.1382856115,-4.5967257714,0.1336005244  
H,0,-1.1718352593,-4.2105345642,1.8822608086

### Eug

C,0,-4.258017694,4.0694023726,-1.0287615187  
C,0,-3.048094911,4.2785060666,-1.7055344231  
C,0,-2.1407470638,3.2307477882,-1.908484211  
C,0,-2.4659424137,1.9467685238,-1.4247296541  
C,0,-3.6666649074,1.7410995024,-0.7534277779  
C,0,-4.5702443395,2.8023655156,-0.5506530645  
O,0,-5.7637771713,2.5790740153,0.1181068313  
C,0,-0.8127659924,3.4655575674,-2.6198726079

C,0,-0.53625979,2.4785842255,-3.7307790269  
C,0,0.5384643344,1.6835235823,-3.7982429078  
O,0,-4.114975141,0.5247181725,-0.222869887  
C,0,-3.277439034,-0.6502764596,-0.3686091416  
H,0,-4.9651658725,4.8746066224,-0.8686775097  
H,0,-2.8111381886,5.2711218754,-2.0764227473  
H,0,-1.7747602324,1.1283607707,-1.5910935618  
H,0,-5.8095376218,1.6344809711,0.3771724715  
H,0,-0.8186508649,4.4850289196,-3.0313047244  
H,0,0.0143609363,3.4299034481,-1.8957221258  
H,0,-1.2913203649,2.4335487561,-4.5161789074  
H,0,0.6934780629,0.9948145957,-4.6234100004  
H,0,1.310650274,1.6995874122,-3.0320506329  
H,0,-3.8244723919,-1.4590871907,0.1146012634  
H,0,-3.1170385851,-0.888581879,-1.4261938544  
H,0,-2.3105890272,-0.506333174,0.1270797183

## MEug

C,0,-1.0977010427,1.1596125287,1.0767812493  
C,0,-1.5971779226,1.6531548901,-0.1341697668  
C,0,-1.6030167662,0.8480925527,-1.2792922754  
C,0,-1.0932159311,-0.4601708297,-1.1891658746  
C,0,-0.5805915979,-0.9513174671,0.0142704667  
C,0,-0.5899883432,-0.1356039899,1.1682701858  
C,0,-2.1238596674,1.3763050682,-2.6114492585  
C,0,-3.1065336592,0.450629408,-3.2910084998  
C,0,-2.9544377712,-0.058323112,-4.5195679226  
O,0,-0.0401001261,-0.5296234059,2.3890530219  
C,0,-0.5419044595,-1.7563684467,3.0153132719  
O,0,-0.0354831763,-2.2262990673,0.1610298638  
C,0,0.0654639404,-3.0782804936,-1.00958588  
H,0,-1.0860963794,1.770129852,1.9724257304  
H,0,-1.9856559694,2.6658529366,-0.1832565366  
H,0,-1.1024742402,-1.0841175474,-2.0750767175  
H,0,-2.6030324848,2.3494735851,-2.4325793972  
H,0,-1.2821583136,1.567626386,-3.2930113351  
H,0,-3.9916665027,0.1961248472,-2.7072521228  
H,0,-3.6955036175,-0.7147857827,-4.965771464  
H,0,-2.0837153837,0.1713228615,-5.1299748285  
H,0,-0.0479039305,-1.7967283053,3.9864887582  
H,0,-1.6283703628,-1.698561993,3.1543985391  
H,0,-0.2871558967,-2.6317792292,2.4169456272  
H,0,0.5488660057,-3.9889330559,-0.6575509891

H,0,-0.9240777058,-3.3171625059,-1.4166035838  
H,0,0.6786163044,-2.6094556846,-1.7877252621

### **iEug**

C,0,-2.328890146,1.9577285987,-0.0282605587  
C,0,-2.2938941259,0.5615111031,-0.027603379  
C,0,-1.0715589898,-0.1393388853,-0.0188710326  
C,0,0.1268454427,0.6122199658,-0.0107308379  
C,0,0.0882703798,2.0019940319,-0.0114359504  
C,0,-1.1410323953,2.6850036044,-0.0202051673  
O,0,-1.1689121449,4.069851846,-0.0208404268  
O,0,1.1979201899,2.8571026239,-0.0038773494  
C,0,2.5264464432,2.277308908,0.004609106  
C,0,-0.9750176999,-1.6079411928,-0.0177593577  
C,0,-1.9812189095,-2.5017439739,-0.0246431609  
C,0,-1.7924984507,-3.9927291542,-0.0228650007  
H,0,-3.267008704,2.5000177956,-0.0349674566  
H,0,-3.230277045,0.0151534876,-0.0339596583  
H,0,1.0761332797,0.0879296174,-0.0039173516  
H,0,-0.2474612358,4.4054471558,-0.0145050442  
H,0,3.212898102,3.1232294748,0.0086955381  
H,0,2.6939106619,1.6665659759,-0.8901452427  
H,0,2.6826869787,1.6670525199,0.9017234494  
H,0,0.0452807621,-1.9948361626,-0.0104135937  
H,0,-3.0152372216,-2.1574570346,-0.0320897422  
H,0,-2.2527863131,-4.4567429633,-0.9067996037  
H,0,-2.2652927191,-4.4562244383,0.8547179357  
H,0,-0.7307331393,-4.2632349039,-0.0152461149

### **MiEug**

C,0,-2.2511750638,1.2242262549,-0.3202283973  
C,0,-2.3311786804,-0.1613428199,-0.1834868715  
C,0,-1.1616682836,-0.9379660684,-0.0781632514  
C,0,0.0820218919,-0.2723514264,-0.131102875  
C,0,0.1643411993,1.1134838899,-0.2828823438  
C,0,-1.0178399623,1.8796571319,-0.3674182338  
O,0,-1.0324586217,3.2569474748,-0.5808122785  
C,0,-0.2850361115,4.119621497,0.3393546768  
C,0,-1.1660431404,-2.4013741711,0.0803311  
C,0,-2.2339076843,-3.2157677718,0.1664992511  
C,0,-2.1539934355,-4.7076706519,0.3285970642  
O,0,1.367785805,1.8139850679,-0.369593881  
C,0,2.6115843477,1.0668171374,-0.3624509514

H,0,-3.1445433399,1.8328272748,-0.4011950852  
H,0,-3.3063870874,-0.6338080134,-0.1533964951  
H,0,0.9877169711,-0.863642463,-0.0607203802  
H,0,-0.5451723771,5.1357883919,0.0419212165  
H,0,0.7881338073,3.9519475181,0.2458870738  
H,0,-0.6039439386,3.9425748135,1.3736270497  
H,0,-0.1757593029,-2.856168175,0.132854624  
H,0,-3.2401629461,-2.7999161677,0.1197068499  
H,0,-2.6568176611,-5.0383271441,1.2483943672  
H,0,-1.1148713787,-5.0524725548,0.3698416589  
H,0,-2.6499954031,-5.2283030469,-0.5027665312  
H,0,3.3940552666,1.8162466459,-0.4766209273  
H,0,2.6522875511,0.358342378,-1.1978044553  
H,0,2.7496325785,0.5290379984,0.5831030258

#### Est

C,0,-1.1744036132,1.2072712749,1.04561661  
C,0,-1.5300476458,1.6937245153,-0.2110635108  
C,0,-1.6185410961,0.8412554336,-1.3269193719  
C,0,-1.3437160155,-0.5206677926,-1.1373978518  
C,0,-0.9845068281,-1.0270626831,0.1178905547  
C,0,-0.8995827578,-0.1572643005,1.2127452833  
C,0,-1.9856607336,1.383692872,-2.7036480734  
C,0,-3.1004955722,0.6182642583,-3.3790717963  
C,0,-3.0081455678,0.0283295552,-4.5768489631  
O,0,-0.5548995234,-0.5485844353,2.5051105866  
C,0,-0.259341599,-1.9463072796,2.7536449431  
H,0,-1.1059490496,1.8596779712,1.908410716  
H,0,-1.7422496755,2.7527250011,-0.3299346556  
H,0,-1.4170829042,-1.2003976524,-1.9812133693  
H,0,-0.7789828916,-2.0852527673,0.2259036004  
H,0,-2.2826348968,2.4368942583,-2.5934394187  
H,0,-1.1019740794,1.3806456992,-3.3583181976  
H,0,-4.0336721117,0.5574554997,-2.8182745675  
H,0,-3.8429724274,-0.5062887093,-5.0200292712  
H,0,-2.0922156261,0.0632062505,-5.1627851491  
H,0,-0.0238122416,-2.0044491065,3.8158329566  
H,0,-1.1241638347,-2.5834281018,2.5320854491  
H,0,0.6029116911,-2.2833097608,2.1655194963

#### Aneth

C,0,-1.9822312773,1.7356679606,-0.4204799486  
C,0,-1.5517135123,0.4456019886,-0.0905924113

C,0,-2.4565338101,-0.6031962714,0.1545761038 C,0,-3.8363243799,-0.3063492035,0.0552639562 C,0,-4.2795013869,0.9688664697,-0.2711594302 C,0,-3.3535615129,1.9980339899,-0.5111108357 C,0,-1.9346848661,-1.9353224977,0.4965852382 C,0,-2.6361945295,-3.0529081896,0.7620434851 C,0,-2.0213056677,-4.380927981,1.1049040946 O,0,-3.9022739302,3.236654448,-0.8302573456 C,0,-3.0081360404,4.3484440597,-1.0922040289 H,0,-1.2487481787,2.5120222854,-0.6007731322 H,0,-0.4851980508,0.249070982,-0.0219946628 H,0,-4.5707034662,-1.0840950821,0.2360229234 H,0,-5.3361714939,1.197779785,-0.3476157549 H,0,-0.8461145775,-1.9986734176,0.5328207249 H,0,-3.725625913,-3.0315335245,0.7361130576 H,0,-0.9270321861,-4.3268187101,1.111343269 H,0,-2.3479970164,-4.7310366606,2.094396768 H,0,-2.316880918,-5.1578153136,0.3855608659 H,0,-3.6593763888,5.1928152359,-1.3153996156 H,0,-2.3911589292,4.5792598358,-0.2154112031 H,0,-2.3594829681,4.1444598113,-1.9526331178
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<b>1,8-cineole</b>
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C,0,-1.0032386424,0.2131703135,-0.6083080726 C,0,-1.2099693674,-1.2952632815,-0.3564453419 C,0,-0.7576707411,-1.6565635269,1.0906682517 C,0,-0.1660576026,-0.3936536593,1.766277237 C,0,1.0012651752,0.1775172435,0.9098833725 O,0,0.4500709304,0.5072597256,-0.4477393794 C,0,2.1377525971,-0.8347351114,0.6934198411 C,0,1.5827075231,1.4808677885,1.4811179803 C,0,-1.3360636607,0.6203861853,-2.0402855243 C,0,-1.7715947521,1.0455051524,0.4397342851 C,0,-1.3099198601,0.6462449613,1.8738538549 H,0,-0.6253874993,-1.8518266688,-1.1024597986 H,0,-2.2683147385,-1.5460845303,-0.5180592899 H,0,-0.0303522004,-2.4750744333,1.0783291771 H,0,-1.6092461841,-2.0044573454,1.6891574602 H,0,0.2223969453,-0.641344476,2.768470726 H,0,2.9167994089,-0.3851006078,0.0652862754 H,0,1.7841011395,-1.7427468077,0.1956253564 H,0,2.5901834593,-1.1154983112,1.6537120952 H,0,2.3818657527,1.8465685466,0.8244249741 H,0,2.0095955635,1.3067437727,2.477678225
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H,0,0.8234680578,2.2649921652,1.5589311231
H,0,-1.1297797631,1.6866694867,-2.1947979235
H,0,-2.3973542742,0.4372848219,-2.2503822547
H,0,-0.7355051214,0.0429032158,-2.753888856
H,0,-2.851140811,0.8829013498,0.3083281852
H,0,-1.5759936925,2.1093441125,0.2447483202
H,0,-0.9901793584,1.5276980039,2.4394580019
H,0,-2.1369352835,0.1963739148,2.4378216984







