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Supporting information for article:

The structure of the anti-aging agent J147 used for treating Alzheimer's disease

Guy J. Clarkson, M. Ángeles Farrán, Rosa M. Claramunt, Ibon Alkorta and José Elguero

SUPPLEMENTARY INFORMATION

The structure of an anti-aging agent used for treating Alzheimer's disease, **J147** [(*E*)-*N*-(3-methoxybenzylidene)-*N'*-(2,4-dimethylphenyl)-*N'*-(2,2,2-trifluoroaceto)hydrazide]

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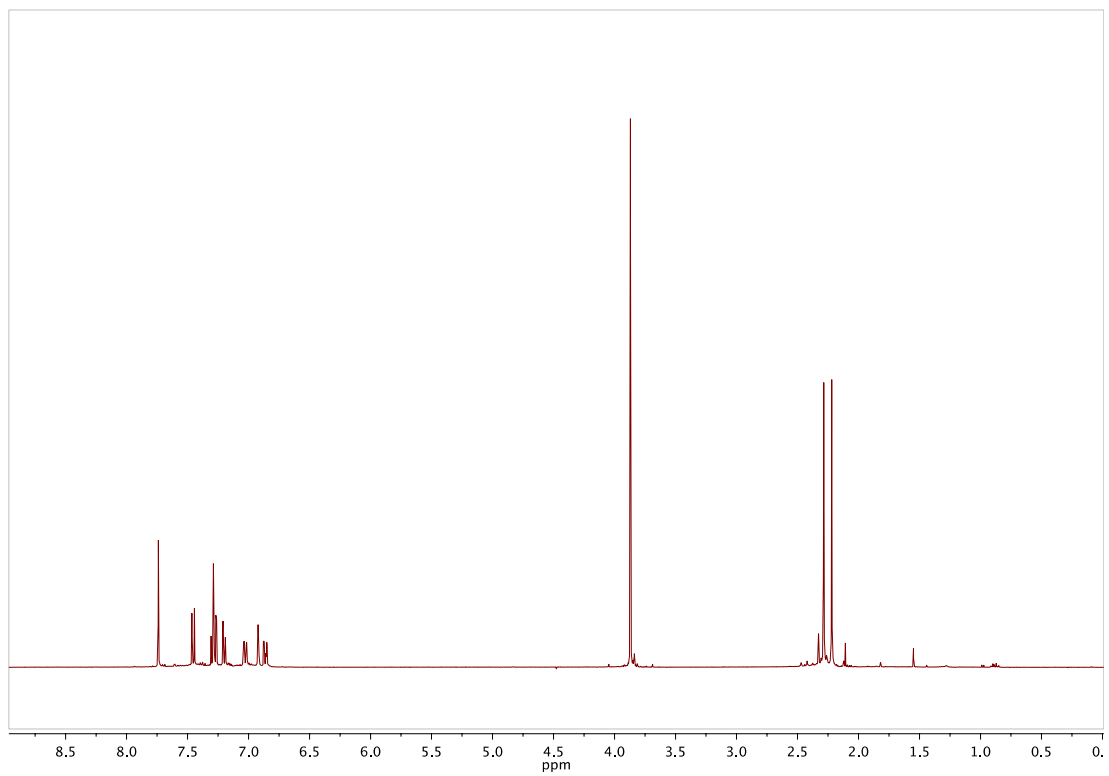


Figure S1. ¹H NMR spectrum of *N*-(3-methoxybenzylidene)-*N'*-(2,4-Dimethylphenyl)hydrazine

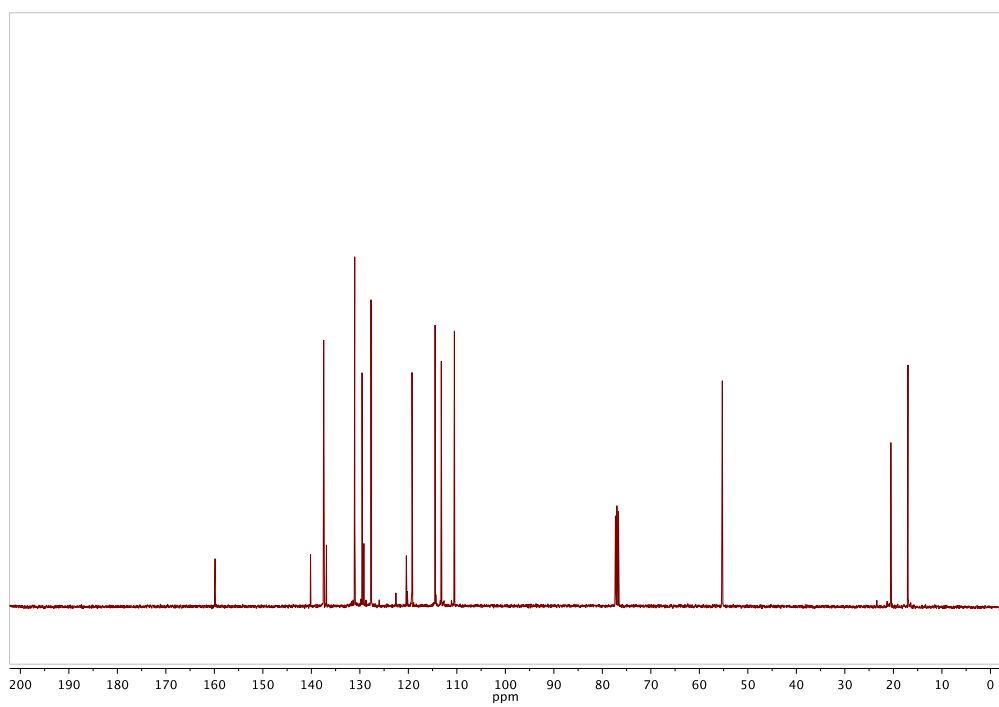


Figure S2. ¹³C NMR spectrum of *N*-(3-methoxybenzylidene)-*N'*-(2,4-Dimethylphenyl)hydrazine

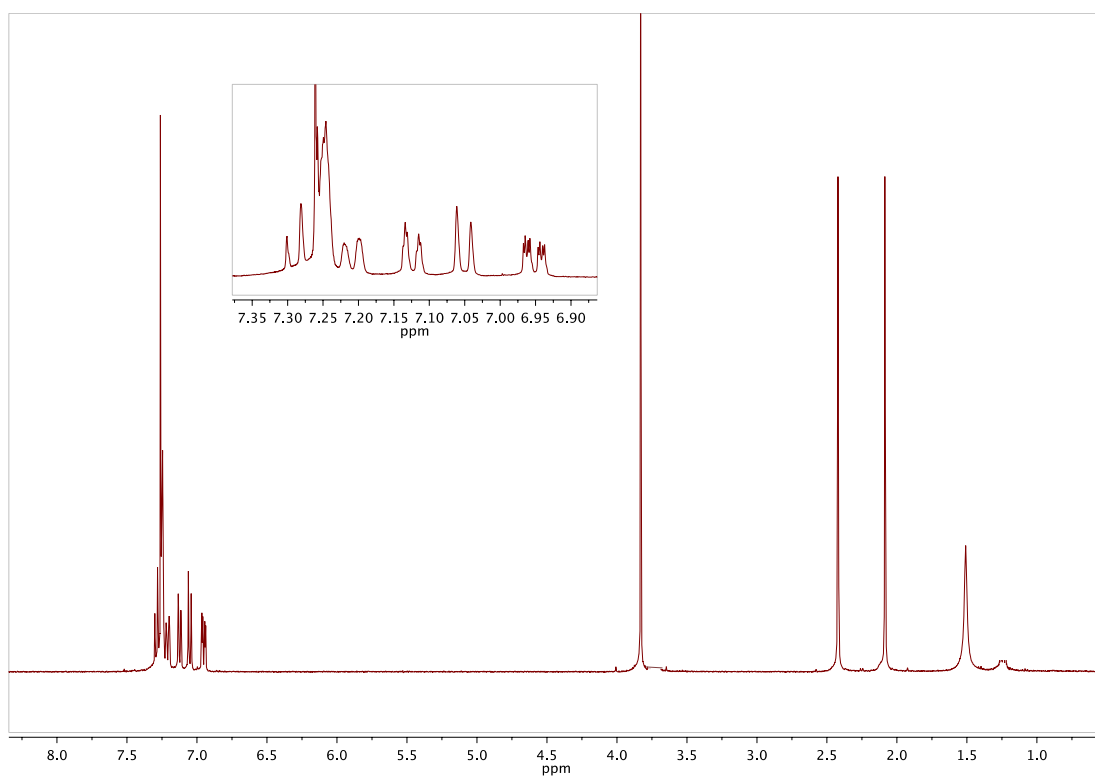


Figure S3. ^1H NMR spectrum of (*E*)-*N*-(3-methoxybenzylidene)-*N'*-(2,4-dimethylphenyl)-*N'*-(2,2,2-trifluoroaceto)hydrazide (**J147**)

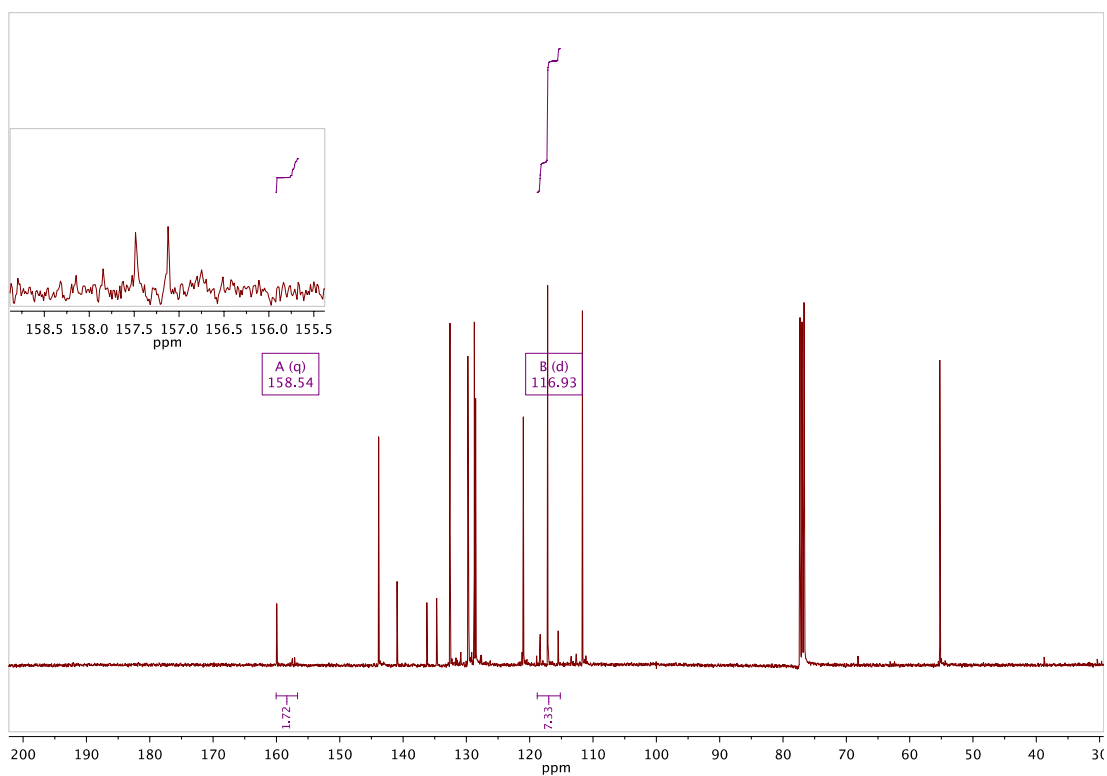


Figure S4. ^{13}C NMR spectrum of (*E*)-*N*-(3-methoxybenzylidene)-*N'*-(2,4-dimethylphenyl)-*N'*-(2,2,2-trifluoroaceto)hydrazide (**J147**)

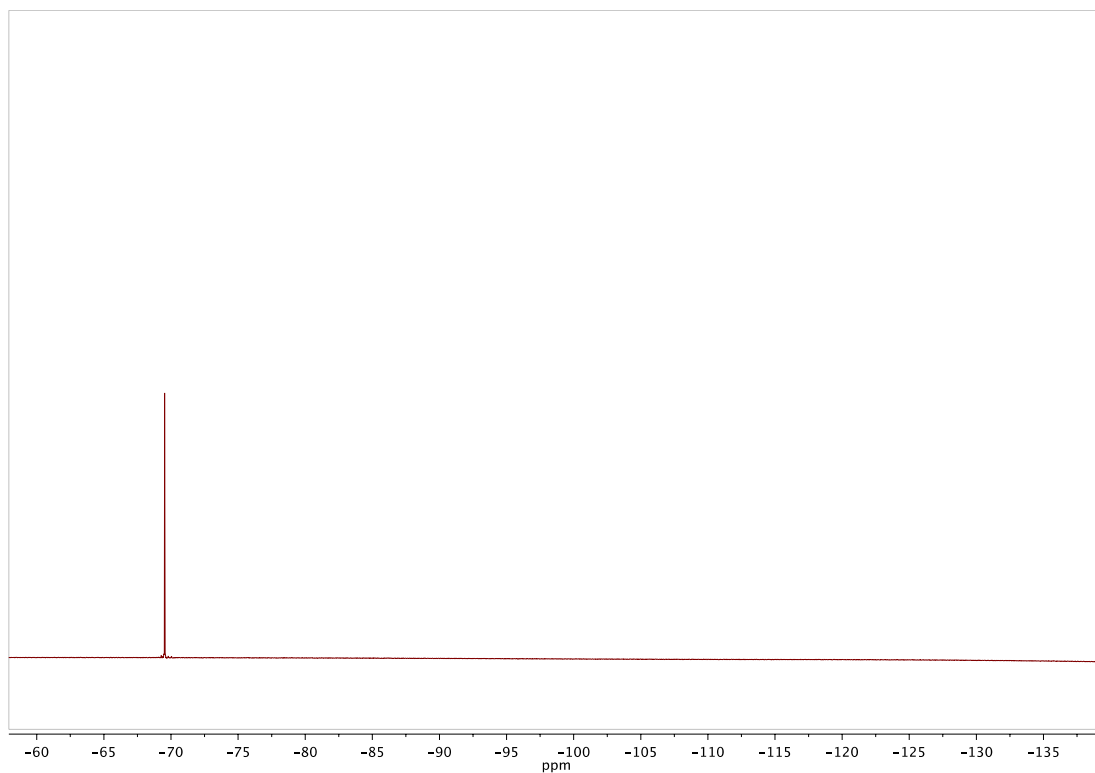


Figura S5. ^{19}F of spectrum of (*E*)-*N*-(3-methoxybenzylidene)-*N'*-(2,4-dimethylphenyl)-*N'*-(2,2,2-trifluoroaceto)hydrazide (**J147**)

Electronic energy and geometry of the J147 rotamers calculated at B3LYP/6-311++G(d,p) computational level.

1111, Total Energy= -1255.95650867 Hartree, NIMAG= 0

C,-3.7781820822,1.6543445456,0.9548035953
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1112, Total Energy= -1255.95463329 Hartree, NIMAG= 0

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1121, Total Energy= -1255.95456753 Hartree, NIMAG= 0

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1122, Total Energy= -1255.95510514 Hartree, NIMAG= 0

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1211, Total Energy= -1255.94361260 Hartree, NIMAG= 0

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1212, Total Energy= -1255.94209351 Hartree, NIMAG= 0

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1221, Total Energy= -1255.94210277 Hartree, NIMAG= 0

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H,0.452887443,5.3268095839,-4.3295041548
H,2.0721464804,5.5849414995,-3.6826828972
H,1.8129662458,4.377016766,-4.9428708389
C,-0.9925171547,3.4010377368,0.184969681
H,-1.2871049842,4.4515221544,0.1649990495
H,-1.8978830367,2.7969309909,0.0681952984
H,-0.5698611485,3.1784267845,1.1671306695
N,0.4930330502,0.8850960672,0.0567316534
C,-0.6320271408,0.1102595936,0.0413659059
O,-1.4148319895,0.0592035333,-0.8828918051
C,-0.8971443603,-0.7799570894,1.2976702039
F,-1.0187435872,-0.0485708172,2.4231462609
F,0.0980536791,-1.6814574056,1.4984077737
F,-2.0273872678,-1.4657432446,1.1349291718
N,1.2474820616,1.1536816905,1.2491448275
C,2.2021570391,0.326509836,1.4516222197
H,2.3764874959,-0.5079613424,0.7685319267
C,3.1026732275,0.4440960399,2.6014016594
C,2.9828780277,1.4795864825,3.5341777459
C,4.1094580102,-0.5253921953,2.7457816657
C,3.8732448385,1.538582555,4.6020785039
H,2.2008489746,2.2173442757,3.4143173092
C,4.9950573776,-0.456320734,3.8219735831
H,4.1818538382,-1.3209350085,2.0154983856
C,4.8723749496,0.58346448,4.7514854861
H,3.7891067949,2.3369097105,5.3305034486
H,5.5683727035,0.6202586978,5.5808627794
O,6.0016120337,-1.3447066325,4.0525750799

C,6.1709696371,-2.4349712096,3.1544918667
H,6.3995685466,-2.0860986257,2.1416812635
H,7.0151473094,-3.005445163,3.5373347425
H,5.2821412113,-3.0743868772,3.1313102347

1222, Total Energy= -1255.94233834 Hartree, NIMAG= 0

C,1.1851891814,3.759866134,-2.9123444436
C,0.2972874794,4.0323629003,-1.86582681
C,0.0185248416,3.1101066575,-0.8553132439
C,0.67282103,1.8708632464,-0.914622589
C,1.5581250033,1.5746500183,-1.9442034696
C,1.811311225,2.5119922052,-2.9412065107
H,-0.2019620278,4.9965237435,-1.8370196827
H,2.0365816427,0.6024111468,-1.9690521491
H,2.4958150264,2.2675815572,-3.7462874701
C,1.4693420911,4.800512676,-3.9681760148
H,0.558971244,5.3298148163,-4.2605874946
H,2.1777354659,5.549804065,-3.598567401
H,1.9026626207,4.3506482147,-4.8637599683
C,-0.9664247865,3.4298016257,0.2393462725
H,-1.2340256872,4.4875395256,0.2210871001
H,-1.8857994517,2.8492753047,0.1128361688
H,-0.5576309223,3.1926561047,1.2239386767
N,0.4572597314,0.8780251065,0.1142718252
C,-0.6858821965,0.130788414,0.0891111335
O,-1.4651801234,0.1025311655,-0.8390585702
C,-0.9745944483,-0.7604157916,1.3392819891
F,-1.1045295907,-0.0288168954,2.4643080025
F,0.009341341,-1.67017825,1.5512737047
F,-2.1092827008,-1.4353380937,1.1610422362
N,1.2030532812,1.1261415398,1.3182210632
C,2.1603516983,0.2993397775,1.5072013225
H,2.3449941892,-0.5196466163,0.8086103217
C,3.0527827086,0.4000968419,2.6652950757
C,2.9013332748,1.4036697466,3.6388131434
C,4.0780143251,-0.537856307,2.7858466289
C,3.7807096548,1.4448359911,4.7069941889
H,2.1008975792,2.1246296276,3.5413656369
C,4.9630600007,-0.4886210218,3.8688391461
H,4.2076496785,-1.3215930604,2.0481065082
C,4.8136520769,0.5079135431,4.8349538543
H,3.67312618,2.2129989741,5.4643809736
H,5.48288544,0.5672117222,5.6826002589
O,5.9263671395,-1.451621308,3.8869056718
C,6.8536361342,-1.468383189,4.9659460175
H,6.345900302,-1.6147856822,5.9251382171
H,7.5144875324,-2.3119117823,4.7751708943
H,7.443101896,-0.5459680342,4.9994229956

2111, Total Energy= -1255.95028497 Hartree, NIMAG= 0

C,-2.4184155131,-1.8118879031,-0.3126365049
C,-1.1099369696,-2.0464783118,-0.7477607418
C,-0.1035161663,-1.0811436517,-0.6638099138
C,-0.4484548569,0.1685831341,-0.1246485911
C,-1.7409375552,0.42023463,0.3303569596
C,-2.7218526444,-0.5599253806,0.2294458303
H,-0.8630215131,-3.0141559329,-1.1740563485
H,-1.9747188943,1.3909548148,0.7511318315
H,-3.7286973492,-0.3471506772,0.5718965932
C,-3.4656068787,-2.8947105256,-0.4016142015
H,-3.2960391616,-3.543530404,-1.2637051936
H,-3.4489370016,-3.5269794793,0.4928160212
H,-4.4688741574,-2.4717758851,-0.4851805346
C,1.2879274845,-1.3725411824,-1.1659203665
H,1.4157677365,-2.440708671,-1.3476888861
H,1.4787613689,-0.8475116899,-2.1063890135
H,2.0530705184,-1.0525564471,-0.4551769839
N,0.5652306224,1.1875813425,0.042143064
C,0.8276357516,2.2126579801,-0.8511996869
O,1.6762756558,3.0565425005,-0.7164002354
C,-0.0809129413,2.2734545674,-2.1240508031
F,-1.3668516067,2.5425384948,-1.8056429662
F,-0.0658355189,1.1233238977,-2.8353263357
F,0.3464332669,3.2449252308,-2.9286622676
N,1.3752045701,1.217367933,1.1651686677
C,1.2020422796,0.35110578,2.0917527648
H,0.4341652873,-0.4229653633,2.0424649305
C,2.0460808704,0.3639685835,3.2912979332
C,1.8264016001,-0.5984141383,4.2804541141
C,3.0610742997,1.3233852249,3.4550770041
C,2.618359942,-0.6025520026,5.4307550412
H,1.0428523434,-1.3372253351,4.1533153671
C,3.8428304981,1.309812051,4.60539047
H,3.2050100862,2.0547919329,2.6725072023
C,3.6198585118,0.3402956877,5.5983169485
H,2.4508078494,-1.3474128173,6.2003299197
H,4.2435939911,0.3526508842,6.4839220427
O,4.8477702532,2.1924131355,4.8623605491
C,5.1265332625,3.2037140499,3.8986966279
H,4.2617260901,3.8571765712,3.7458589212
H,5.9516585629,3.7829974891,4.3091761316
H,5.4270625753,2.7683612823,2.9403112492

2112, Total Energy= -1255.94807053 Hartree, NIMAG= 0

C,-2.388095174,-1.7932436576,-0.3027735736
C,-1.078229422,-2.025142688,-0.7351742502
C,-0.0727435789,-1.0594368236,-0.6445261691
C,-0.4199599087,0.1879366716,-0.1012510632
C,-1.713828223,0.4365952842,0.3513760577
C,-2.6938520686,-0.5438125531,0.243758926
H,-0.8294966834,-2.9908186953,-1.1649894599

H,-1.9492840754,1.4053811493,0.7756694571
H,-3.7018200767,-0.3330911116,0.5842337431
C,-3.4343914856,-2.8763322897,-0.3995455174
H,-3.2619518593,-3.5211588983,-1.2640811399
H,-3.4200579004,-3.5126823669,0.4920450845
H,-4.4376711462,-2.4536058332,-0.4842162786
C,1.3203048792,-1.3476193952,-1.1439783257
H,1.4497279383,-2.4150194508,-1.3292637767
H,1.5129142874,-0.818926132,-2.0820018132
H,2.0833227222,-1.0290897022,-0.430332089
N,0.5925687742,1.2068711943,0.0721156668
C,0.8567817256,2.2347690414,-0.8190684454
O,1.7038968134,3.0784733912,-0.681133494
C,-0.0494184524,2.2970176694,-2.0939024993
F,-1.3370691061,2.5617255284,-1.777991031
F,-0.0298508422,1.1489534749,-2.8088046053
F,0.3770661067,3.2718568391,-2.8946582889
N,1.4000288692,1.232424836,1.1968344414
C,1.2205316768,0.3635654664,2.1189296172
H,0.4489923338,-0.4065427058,2.0625715191
C,2.057490502,0.3621924895,3.325145486
C,1.8130747158,-0.6091188233,4.3103093136
C,3.0796902999,1.2954909355,3.512102815
C,2.5882658459,-0.6329028972,5.4621336686
H,1.0202632946,-1.3354333532,4.169446559
C,3.8539928456,1.2654071908,4.6724758648
H,3.2762183895,2.0485935031,2.7597204711
C,3.6104069348,0.2968358683,5.6555318773
H,2.4021243017,-1.3807482188,6.2246746697
H,4.2011704326,0.2589547158,6.5606420563
O,4.8246484464,2.2187509165,4.7597499162
C,5.6514183679,2.2514765207,5.9152695229
H,6.2238981592,1.3239196987,6.0247920819
H,6.3385079217,3.0822011563,5.7639180062
H,5.0643045979,2.4284377343,6.8230279491

2121, Total Energy= -1255.94807790 Hartree, NIMAG= 0

C,-2.3899825564,-1.82703036,-0.2585992156
C,-1.0848098325,-2.0533146341,-0.707861203
C,-0.0869822447,-1.0773015399,-0.6466729178
C,-0.4370710139,0.1744337235,-0.115343544
C,-1.726046179,0.417765157,0.3540185285
C,-2.6986095585,-0.5728395859,0.2753309644
H,-0.8340940395,-3.0223872174,-1.1288144354
H,-1.9640771001,1.39044227,0.7678500672
H,-3.7033108667,-0.3660667155,0.6277069485
C,-3.4282798692,-2.9200596385,-0.3257215544
H,-3.2629468067,-3.5747524509,-1.1841857226
H,-3.395874502,-3.5446108026,0.5737291416
H,-4.4362103435,-2.5068283239,-0.4013344594
C,1.3002429185,-1.3597290198,-1.1652969068

H,1.4375019435,-2.4286738092,-1.3354870731
H,1.4711784971,-0.8448911399,-2.1151695494
H,2.0721988083,-1.0215813557,-0.470553863
N,0.5685141152,1.2049693778,0.0269578407
C,0.8081535703,2.2229535028,-0.8824844572
O,1.6497854561,3.0759713616,-0.7699384666
C,-0.1202635994,2.2602445086,-2.1420238546
F,-1.4038721871,2.5209450882,-1.8070877131
F,-0.1053876941,1.1017321916,-2.8400124034
F,0.2854098427,3.2257952188,-2.9643262276
N,1.3941072015,1.2543990728,1.1374138719
C,1.239259694,0.3974923468,2.0753457911
H,0.4740434073,-0.3807385837,2.0411726176
C,2.0976285931,0.4247136427,3.2655551839
C,3.1157841682,1.3711526038,3.4268140523
C,1.8716933318,-0.5396277299,4.262758775
C,3.8947115626,1.3452216491,4.5798315507
H,3.2812739712,2.1100282644,2.6536868296
C,2.6602561651,-0.5544811065,5.4141449454
H,1.0795841576,-1.2641429864,4.1225807814
C,3.6768142534,0.3940986628,5.5707661311
H,4.6845228993,2.0762687959,4.7110640592
H,4.2785008758,0.3668883132,6.4711477623
O,2.5174588772,-1.4484822971,6.4357933401
C,1.501332156,-2.4369577224,6.3409092535
H,1.6579231175,-3.0906653717,5.4757513776
H,1.5736473383,-3.0257856585,7.2537637711
H,0.5057954317,-1.9835218521,6.2810589825

2122, Total Energy= -1255.94867247 Hartree, NIMAG= 0

C,-2.3648000039,-1.8034492028,-0.2509624255
C,-1.0588622671,-2.0304569284,-0.6974857181
C,-0.0601871643,-1.0556525585,-0.6324550888
C,-0.4104560776,0.1957048184,-0.1005450127
C,-1.7003922428,0.440049813,0.36552271
C,-2.6736637946,-0.5494446444,0.2832355362
H,-0.8077391637,-2.9997788738,-1.1175524087
H,-1.9382153685,1.4121757726,0.7807484782
H,-3.6787302662,-0.3425189692,0.6344131108
C,-3.4031822887,-2.8962205417,-0.3192984368
H,-3.2364326688,-3.5516262505,-1.1769615234
H,-3.3719859948,-3.5198022735,0.580819714
H,-4.4109393377,-2.4828780434,-0.3967842566
C,1.3285304895,-1.339596288,-1.1462584134
H,1.4644787749,-2.4085380171,-1.3173864299
H,1.5042980346,-0.8235293172,-2.0945938065
H,2.0983040596,-1.0043554105,-0.4476813846
N,0.5963244266,1.2243540537,0.0480875002
C,0.8411833181,2.2443055736,-0.8573153079
O,1.6837233503,3.0958647508,-0.7392644098
C,-0.0817479208,2.286246839,-2.120790155

F,-1.3662363833,2.548436907,-1.7907562528
F,-0.06574506,1.1297861288,-2.821880161
F,0.329182087,3.253469297,-2.9388792368
N,1.4165112301,1.2703265456,1.1627921208
C,1.2569740428,0.4099023083,2.0966323728
H,0.4936133709,-0.369444968,2.0583949153
C,2.1111529221,0.4365353126,3.289911277
C,3.1293579614,1.3926604444,3.4588671872
C,1.8943752985,-0.5231143901,4.2794178821
C,3.8999461604,1.3652169131,4.60857494
H,3.2933268061,2.1352594278,2.6890958114
C,2.678686046,-0.5433024399,5.4381654857
H,1.1153588996,-1.2696450173,4.1715698302
C,3.6883284416,0.4052511504,5.6063770233
H,4.685862009,2.0994857848,4.7461875615
H,4.3083293139,0.4117486368,6.4925580108
O,2.3770362374,-1.5255879126,6.3367549511
C,3.1348230047,-1.6039023027,7.5370080258
H,3.0312663411,-0.692119417,8.1351028332
H,2.726346052,-2.4469024085,8.0917420723
H,4.1947325847,-1.7861456927,7.3291794889

2211, Total Energy= -1255.94804528 Hartree, NIMAG= 0

C,1.2510435267,3.9257930895,-2.7030085424
C,0.4096488047,4.1690969944,-1.6116151714
C,0.0482349193,3.1723588605,-0.7035191347
C,0.5603802689,1.8856338428,-0.9209074413
C,1.4171337558,1.6219319151,-1.982433349
C,1.7559955858,2.6352452643,-2.8739315968
H,0.0192689182,5.171216403,-1.4611405717
H,1.8185872138,0.6236366605,-2.1079860221
H,2.4215052765,2.4185346365,-3.7024278999
C,1.5822154525,5.0277944872,-3.6794989935
H,0.7975339527,5.1241559519,-4.4376677243
H,1.6700998609,5.993936394,-3.1768312817
H,2.5203525115,4.8286521527,-4.201749068
C,-0.8554808636,3.4760614907,0.4629720894
H,-1.1290304545,4.5321588196,0.4742820009
H,-1.7779085102,2.8905692727,0.4129222421
H,-0.3683423417,3.2359549759,1.4115988321
N,0.2688681488,0.824452767,0.0270221108
C,-0.6819689751,-0.1441695878,-0.1698700012
O,-0.9189435434,-1.0644064001,0.5851321882
C,-1.5359132856,-0.0553388205,-1.4843152929
F,-0.795217813,-0.3277259212,-2.5799360337
F,-2.1092510193,1.1537571363,-1.6593601468
F,-2.5160935068,-0.9573798083,-1.4277583366
N,1.0821244816,0.9327454259,1.1497954276
C,1.0782378134,0.0782864587,2.1108946416
H,0.4407559325,-0.797165266,2.1302765445
C,1.9784705101,0.2784343553,3.2546234306

C,1.9293435777,-0.643653015,4.3036666146
C,2.8752189737,1.3604431066,3.3123869286
C,2.7701663855,-0.4849749154,5.4072842376
H,1.2385912625,-1.4779245369,4.2570998682
C,3.7090213313,1.5073810929,4.4155399713
H,2.8949361886,2.0549580243,2.4848484939
C,3.6548721553,0.5796112925,5.4694597422
H,2.7331540389,-1.1984473409,6.2225231222
H,4.315870744,0.718172477,6.3164580547
O,4.6138714758,2.5158780483,4.5691660123
C,4.7281228928,3.4884279259,3.5373572409
H,3.7881617013,4.0323217112,3.3960867809
H,5.5008811609,4.1806784906,3.8672085992
H,5.029441841,3.0305956385,2.5893500936

2212, Total Energy= -1255.94676013 Hartree, NIMAG= 0

C,1.295228479,3.9236621363,-2.6856865616
C,0.4720774241,4.1795475388,-1.5833551445
C,0.1043113222,3.1877119701,-0.6727051408
C,0.5905357952,1.8925858374,-0.8994387097
C,1.4290652864,1.6158042766,-1.9720419353
C,1.7745352645,2.6247759922,-2.8658693357
H,0.1028297735,5.1884181218,-1.4251134496
H,1.8121888026,0.6111548631,-2.103952984
H,2.4266436863,2.3983426072,-3.7023614506
C,1.6354449738,5.0224002986,-3.6627239484
H,0.8422236983,5.1386481005,-4.4091784276
H,1.7512416813,5.9841709202,-3.1573506462
H,2.5617283783,4.8056412115,-4.1989193195
C,-0.7764206146,3.5055611231,0.5072904346
H,-1.0460579135,4.5626770251,0.5135527561
H,-1.7012671066,2.9223128762,0.4810139276
H,-0.2708195916,3.2733681101,1.4482121267
N,0.2922688328,0.8336709671,0.0491226503
C,-0.6675228826,-0.12649136,-0.1456894577
O,-0.9036076184,-1.0510619239,0.6044560589
C,-1.5378474294,-0.0186013051,-1.4479909671
F,-0.8168172559,-0.2987973637,-2.5546792843
F,-2.0948283564,1.1994517049,-1.6107662943
F,-2.5313242047,-0.9058391649,-1.3811546566
N,1.1040187105,0.9376668269,1.1726482216
C,1.1125178368,0.0699868732,2.1205657186
H,0.4887704854,-0.8156160375,2.1263262598
C,2.0082774634,0.2667458186,3.2704275982
C,1.9744904764,-0.6827706037,4.3052276678
C,2.8799068578,1.3544940692,3.3603321829
C,2.8053247032,-0.53159214,5.4075752843
H,1.2999337284,-1.5288831067,4.2391425467
C,3.7119448553,1.499997711,4.4703292188
H,2.9191910439,2.0906654488,2.5680703508
C,3.677314004,0.553445745,5.5027858967

H,2.7811114073,-1.2625326738,6.2078407343
H,4.3154580481,0.6498218089,6.3706621816
O,4.5255862831,2.5955866351,4.4606748025
C,5.4055480719,2.8034441201,5.5572976974
H,6.1184753527,1.9782182538,5.6607563116
H,5.9474919246,3.7205502538,5.3326491197
H,4.8540690626,2.929908354,6.4953267559

2221, Total Energy= -1255.94693980 Hartree, NIMAG= 0

C,1.2077604485,3.9115694141,-2.750674886
C,0.3857567487,4.1647044575,-1.6468296891
C,0.0499249185,3.1791588644,-0.7171566646
C,0.5679132572,1.8933589791,-0.9258088156
C,1.406129089,1.6202139409,-1.9996109105
C,1.7193706583,2.6225749959,-2.912529125
H,-0.0086759332,5.1661714295,-1.5030018594
H,1.8142276249,0.623691101,-2.1175875601
H,2.3713429727,2.3989070557,-3.7498680226
C,1.5124614168,5.001877006,-3.7486388716
H,0.7137703689,5.0811011887,-4.4940921989
H,1.6014665063,5.9756914949,-3.2612698391
H,2.442931722,4.8026863228,-4.2844071189
C,-0.8309943127,3.4939157479,0.4635611922
H,-1.1254933081,4.5443583651,0.4559322025
H,-1.7420622195,2.8889132023,0.4515919718
H,-0.3146911093,3.2875383611,1.4047038597
N,0.3036573046,0.8433675263,0.0426555748
C,-0.6338070919,-0.1426834977,-0.1281537396
O,-0.8417486995,-1.0599804982,0.6396108989
C,-1.5164444118,-0.0785721151,-1.424983521
F,-0.7971497726,-0.3588401451,-2.5326618858
F,-2.1053998397,1.1221469573,-1.6030888767
F,-2.4865476528,-0.9893833108,-1.3353877192
N,1.121702773,0.986782173,1.1575080383
C,1.1564757527,0.1365753901,2.1209752649
H,0.5511596555,-0.7616664736,2.1444019102
C,2.0551943156,0.3735035034,3.2600721418
C,2.9084372946,1.4801659068,3.3339696599
C,2.0376335311,-0.5676015844,4.3037270551
C,3.7314879085,1.6359303147,4.4453909688
H,2.9198159724,2.1979888203,2.5245133373
C,2.8670138493,-0.4001745384,5.4137247554
H,1.3721025616,-1.4179444604,4.229533589
C,3.7175279251,0.7090821887,5.4820860723
H,4.3958863171,2.4905538655,4.5077790941
H,4.3547464504,0.82218775,6.3508112461
O,2.9196737008,-1.2571814085,6.4735575548
C,2.0816625886,-2.4060814367,6.4650150845
H,2.3099249029,-3.0612502591,5.6174729088
H,2.2918636302,-2.9330527095,7.3940873512
H,1.0224841051,-2.1284518755,6.4378001811

2222, Total Energy= -1255.94688049 Hartree, NIMAG= 0

C,1.2443939741,3.9249330335,-2.7326129168
C,0.4278851744,4.181698989,-1.6255369874
C,0.0878505954,3.196536414,-0.6969573781
C,0.5956492354,1.9073756991,-0.9099896071
C,1.4283306539,1.6305390596,-1.9871317939
C,1.7460669292,2.6325983563,-2.8988560607
H,0.0410966068,5.1856748825,-1.4783577299
H,1.8282781861,0.6311583601,-2.1087572998
H,2.3934722567,2.4059279608,-3.7389404124
C,1.5535435433,5.0150461693,-3.7294537412
H,0.751251775,5.103944977,-4.4699340355
H,1.6547088002,5.9866921654,-3.2400695928
H,2.4788931024,4.8084652674,-4.2712653866
C,-0.7870251053,3.5149667034,0.487276336
H,-1.0735416409,4.5676538744,0.4832644426
H,-1.7026573707,2.9169229136,0.4765826628
H,-0.2695709563,3.3021268811,1.4263486135
N,0.3263744162,0.8573664962,0.056878109
C,-0.6212000011,-0.1199655147,-0.1120071814
O,-0.8351275301,-1.0356539349,0.655181856
C,-1.5066854079,-0.0457615112,-1.4064834426
F,-0.7920402584,-0.3269140133,-2.517035225
F,-2.0876986392,1.1598653977,-1.5790863811
F,-2.4827111623,-0.9499962406,-1.3176447262
N,1.1517880799,0.9893677353,1.1675247647
C,1.1814942147,0.13856109,2.1304951556
H,0.5668916837,-0.75301485,2.1606111581
C,2.0922917418,0.3687783693,3.2616938019
C,2.9613035346,1.4735916701,3.3247132965
C,2.0808609283,-0.5582587705,4.3043962958
C,3.7911997406,1.6230682116,4.4224709805
H,2.9718303516,2.1886365105,2.5129433456
C,2.9227728014,-0.3995026958,5.4112192892
H,1.4204468795,-1.4176106383,4.2770888753
C,3.7838606932,0.6969723721,5.4733631136
H,4.4646849272,2.4712576575,4.476942834
H,4.44492,0.8425254682,6.3169275738
O,2.8254754385,-1.3662495655,6.3686630625
C,3.6533821479,-1.268931154,7.520130778
H,3.4470189727,-0.3529951418,8.0843715315
H,3.4093449983,-2.1334945076,8.1350054387
H,4.7151201789,-1.3022979169,7.2527873231