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Supporting information for article:

The structures of 1,4-diaryl-5-trifluoromethyl-1*H*-1,2,3-triazoles related to J147, a drug for treating Alzheimer's disease

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Supporting Information contains the ^1H , ^{13}C and ^{19}F NMR spectra of compounds **1-7** (Figures S1-S21), X-ray (Figure S22) and Theoretical Calculations data.

CCDC 1590416-1590422 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

S1. NMR Characterization of Compounds 1-7

1-(3,4-dimethylphenyl)-4-phenyl-5-(trifluoromethyl)-1*H*-1,2,3-triazole (**1**)

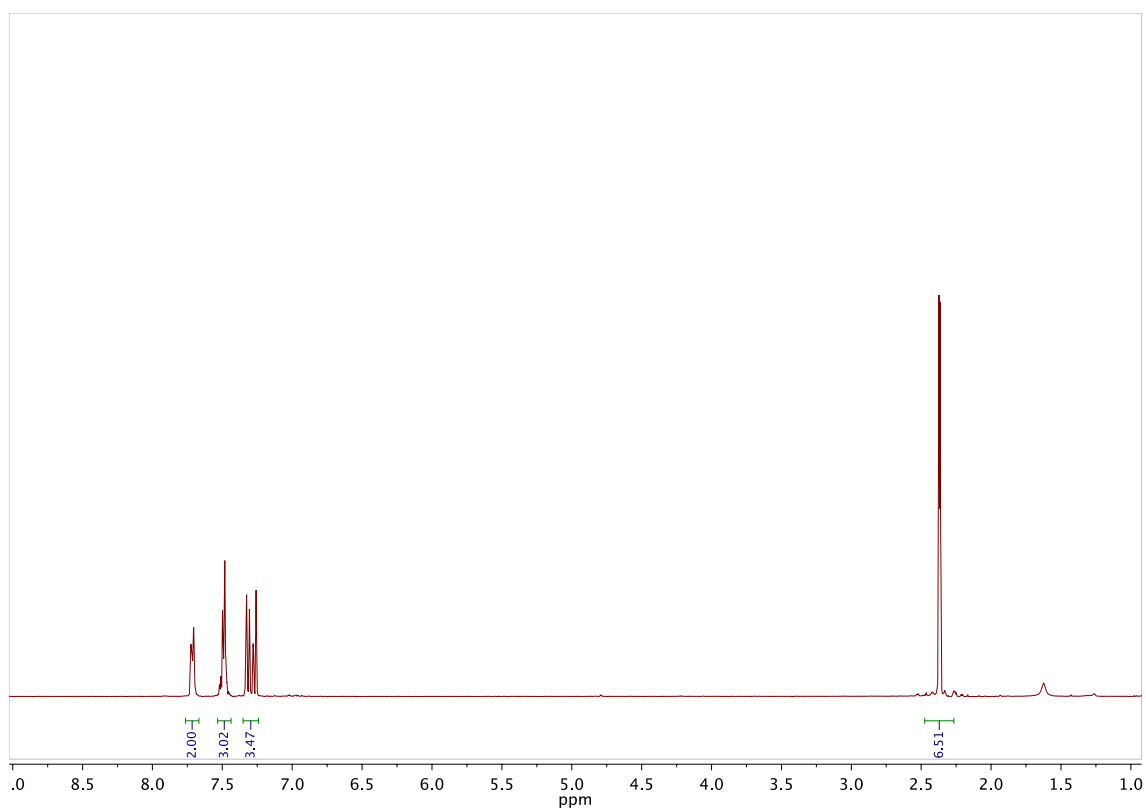


Figure S1 ^1H NMR spectrum of triazole **1**

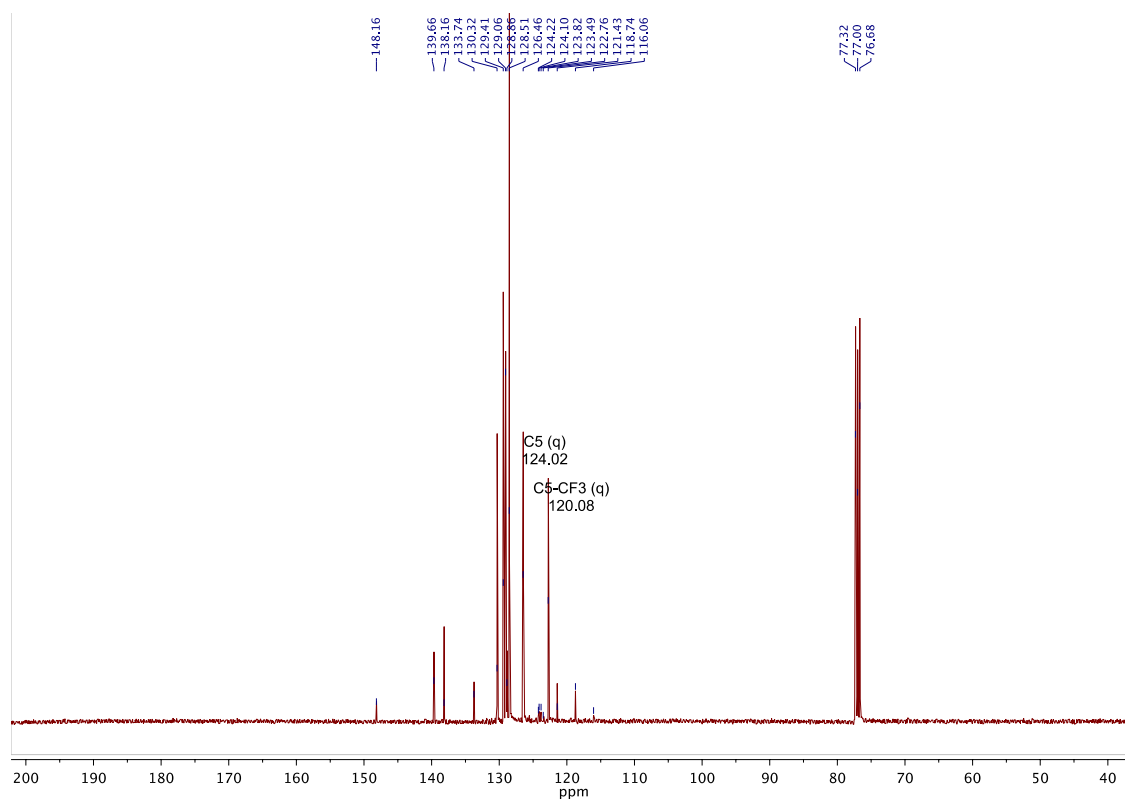


Figure S2 ¹³C NMR spectrum of triazole **1**

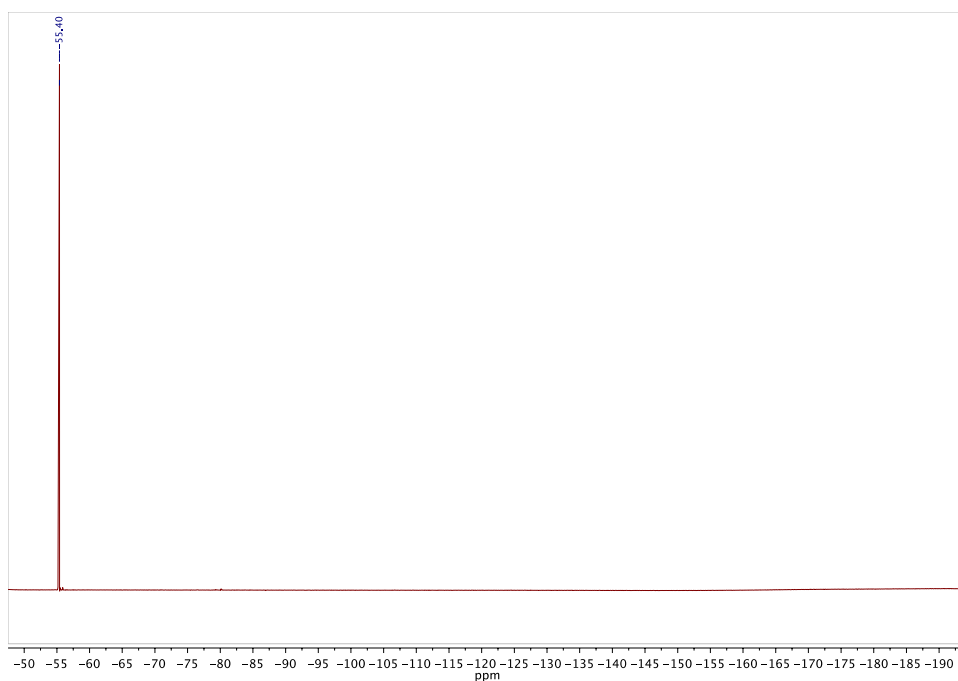
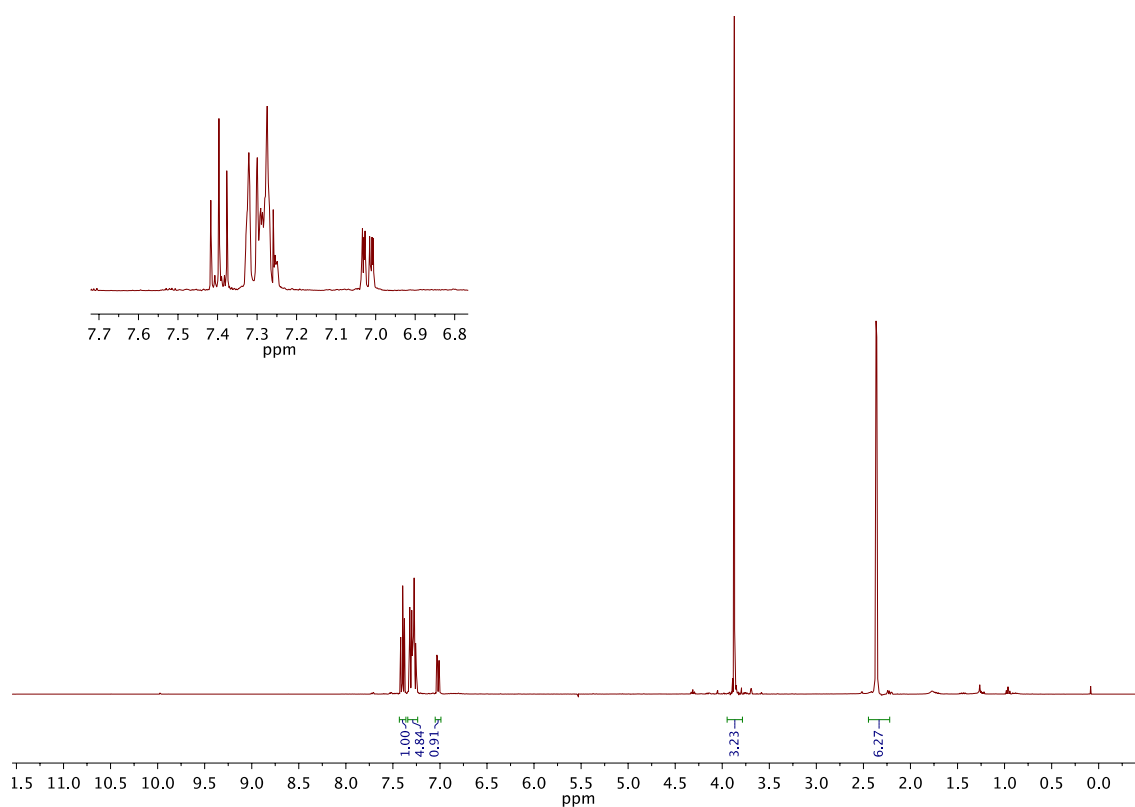
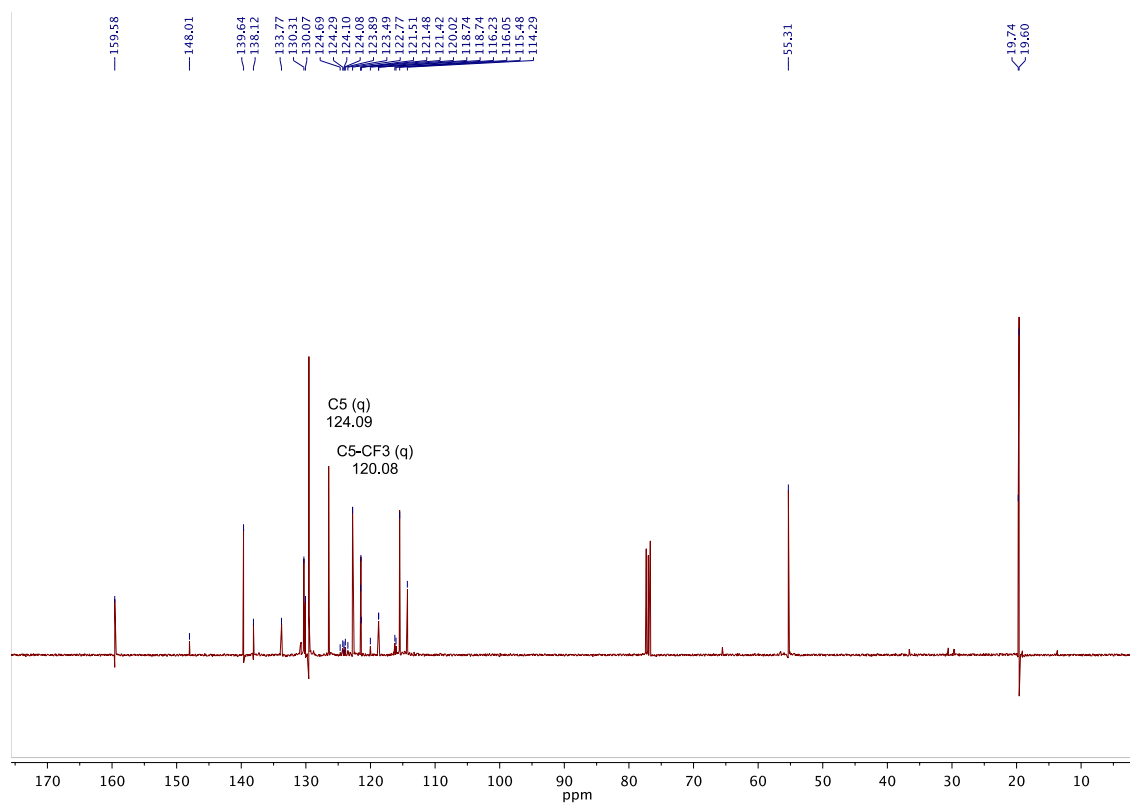


Figure S3 ¹⁹F NMR spectrum of triazole **1**

1-(3,4-dimethylphenyl)-4-(3-methoxyphenyl)-5-(trifluoromethyl)-1*H*-1,2,3-triazole (2)**Figure S4** ¹H NMR spectrum of triazole 2**Figure S5** ¹³C NMR spectrum of triazole 2

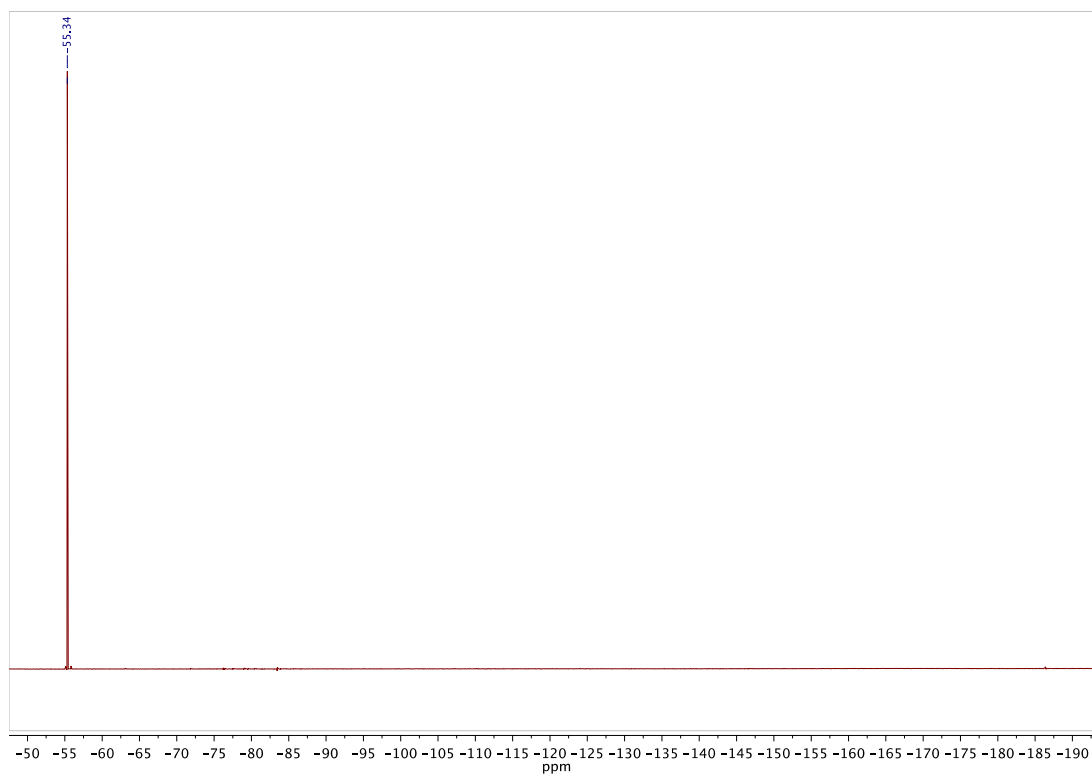


Figure S6 ^{19}F NMR spectrum of triazole **2**

1-(3,4-dimethylphenyl)-4-(4-methoxyphenyl)-5-(trifluoromethyl)-1*H*-1,2,3-triazole (3**)**

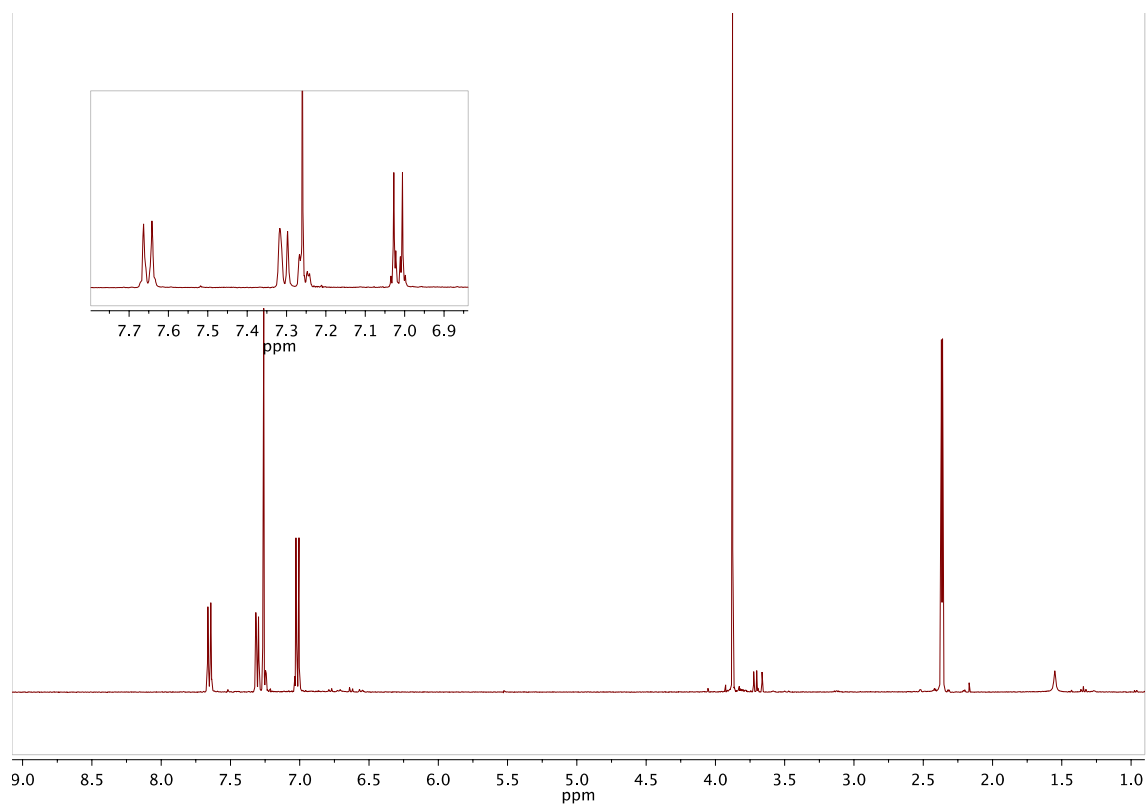
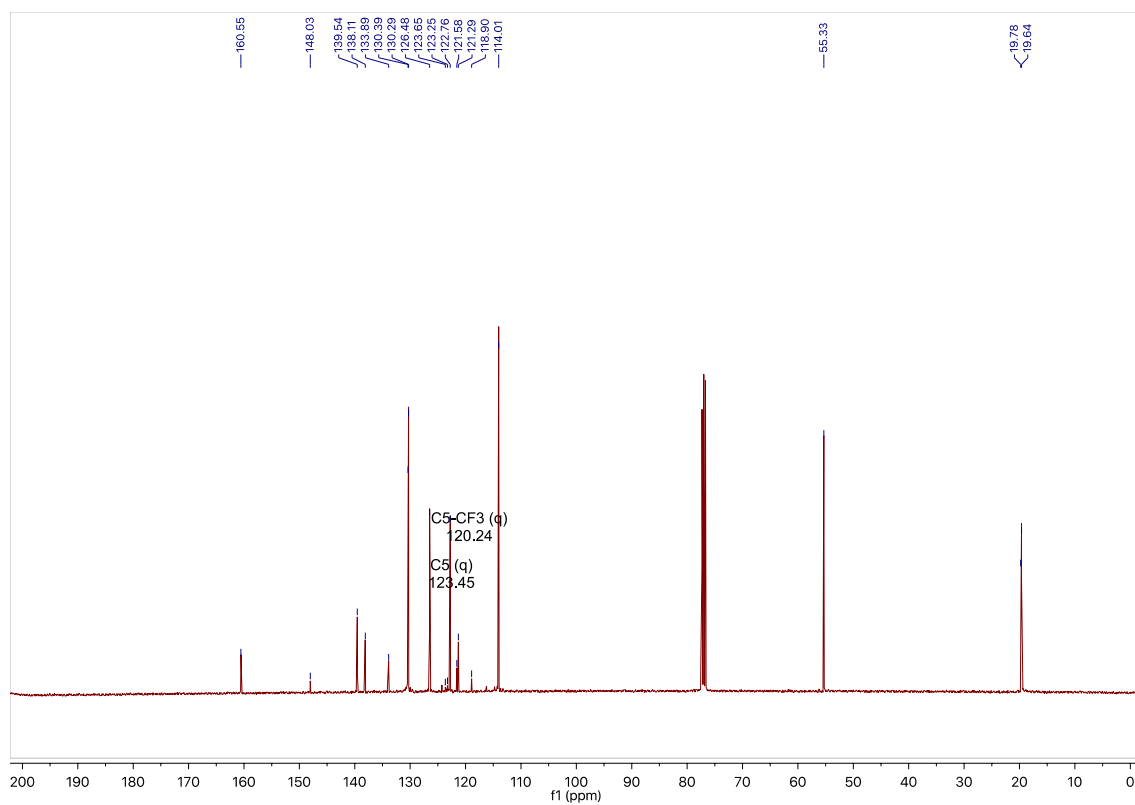
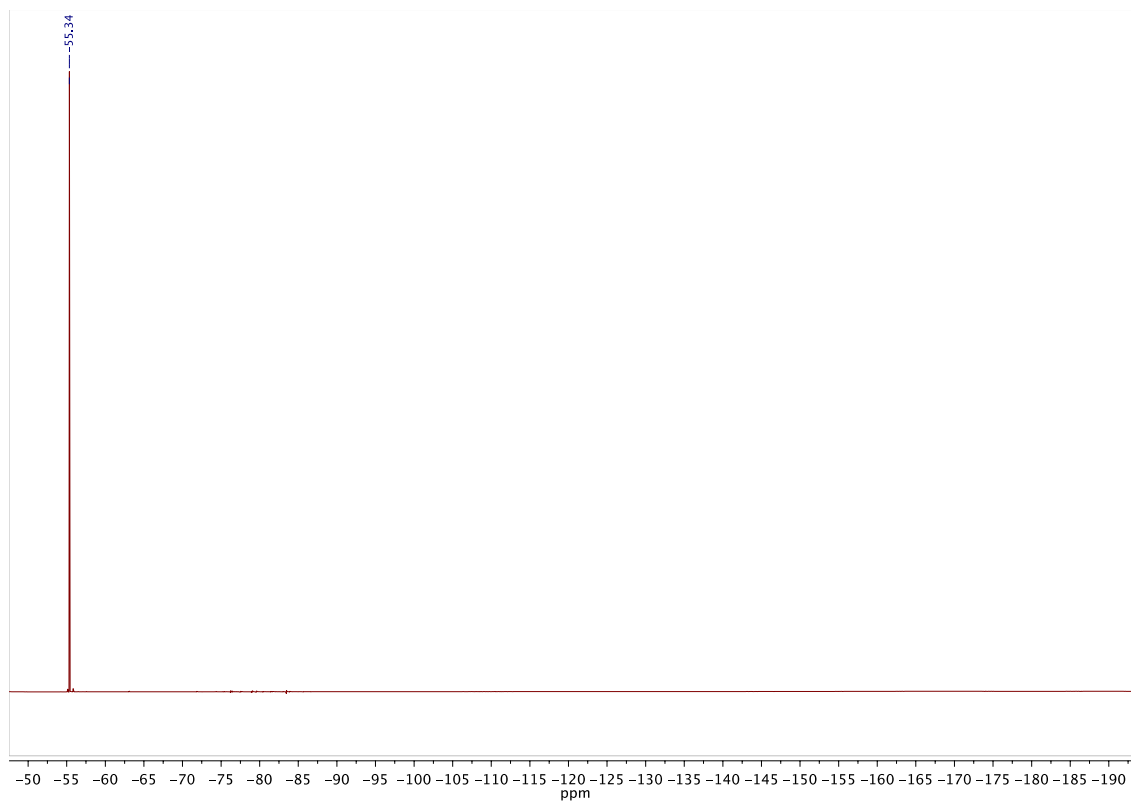
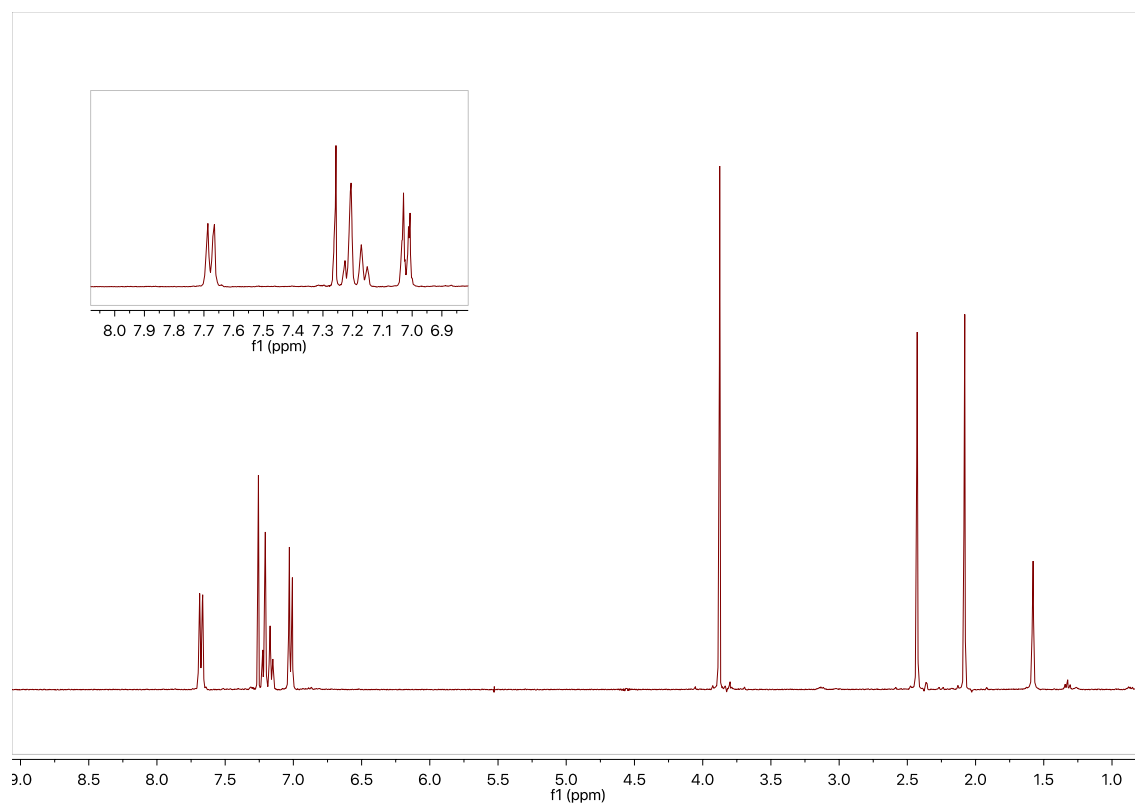
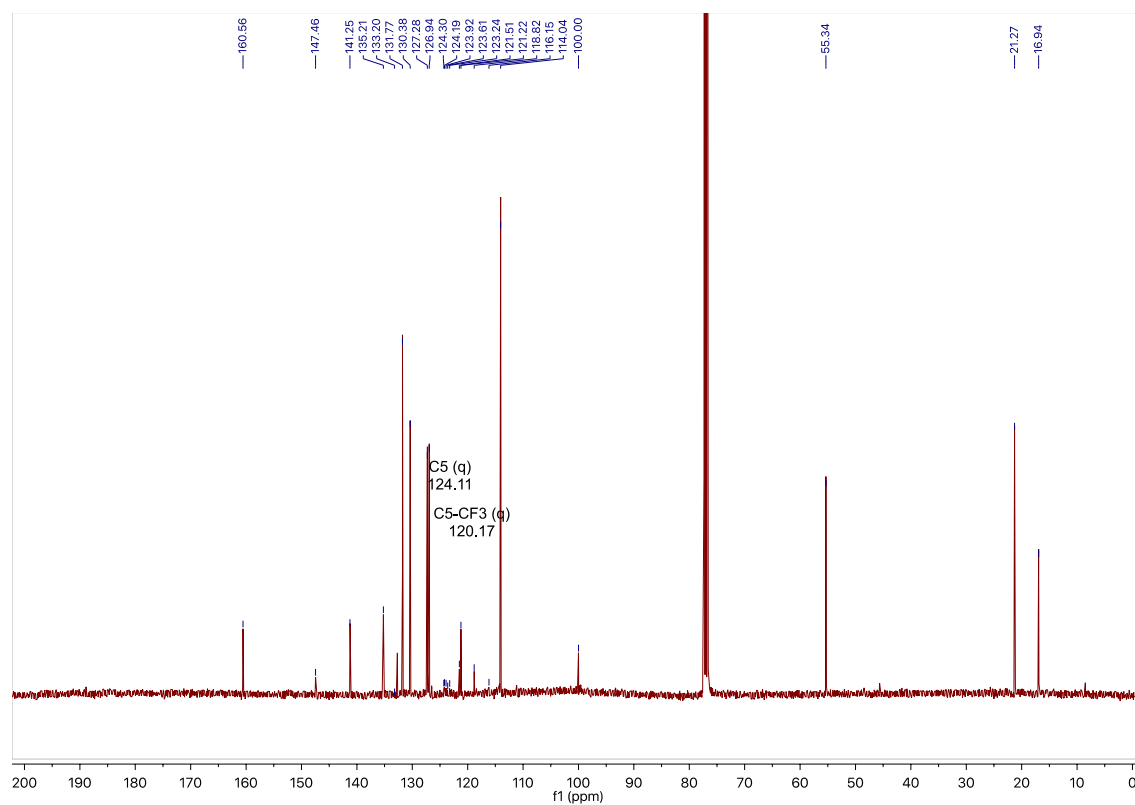


Figure S7 ^1H NMR spectrum of triazole **3**

**Figure S8** ¹³C NMR spectrum of triazole **3****Figure S9** ¹⁹F NMR spectrum of triazole **3**

1-(2,4-dimethylphenyl)-4-(4-methoxyphenyl)-5-(trifluoromethyl)-1*H*-1,2,3-triazole (4)**Figure S10** ¹H NMR spectrum of triazole **4****Figure S11** ¹³C NMR spectrum of triazole **4**

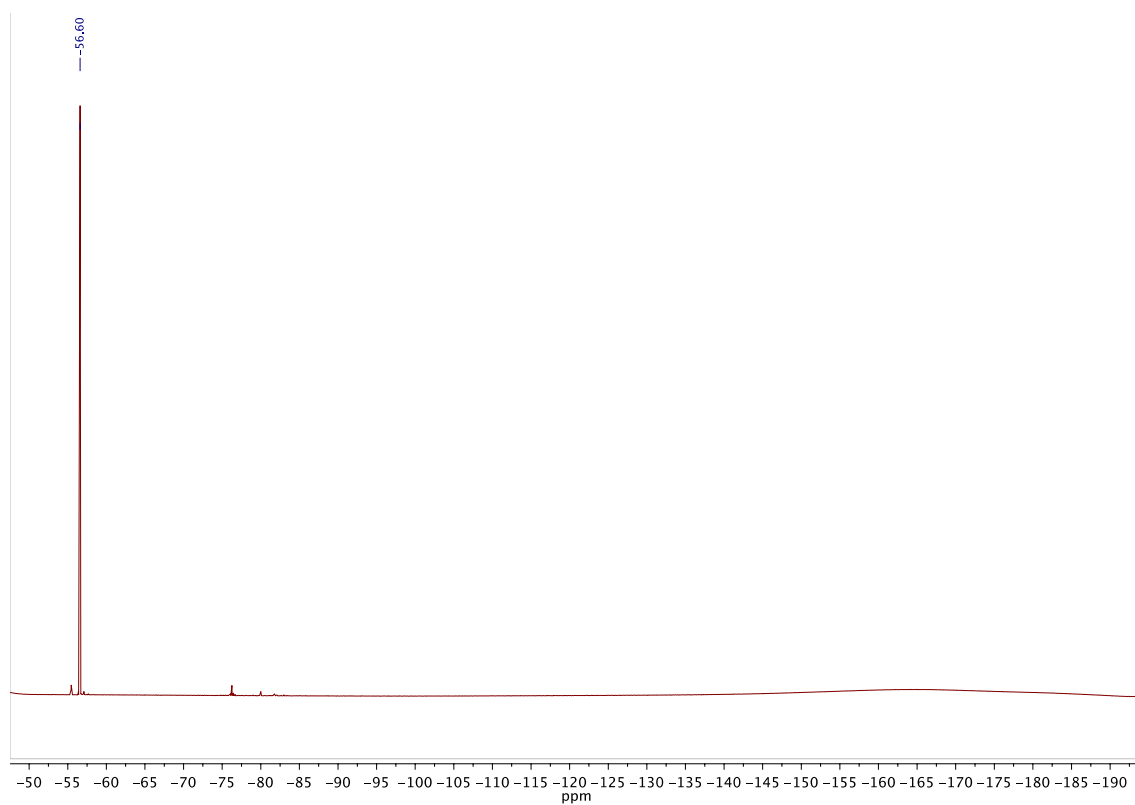


Figure S12 ^{19}F NMR spectrum of triazole **4**

1-(2,4-bis(trifluoromethyl)phenyl)-4-(3-methoxyphenyl)-5-(trifluoromethyl)-1*H*-1,2,3-triazole
(5)

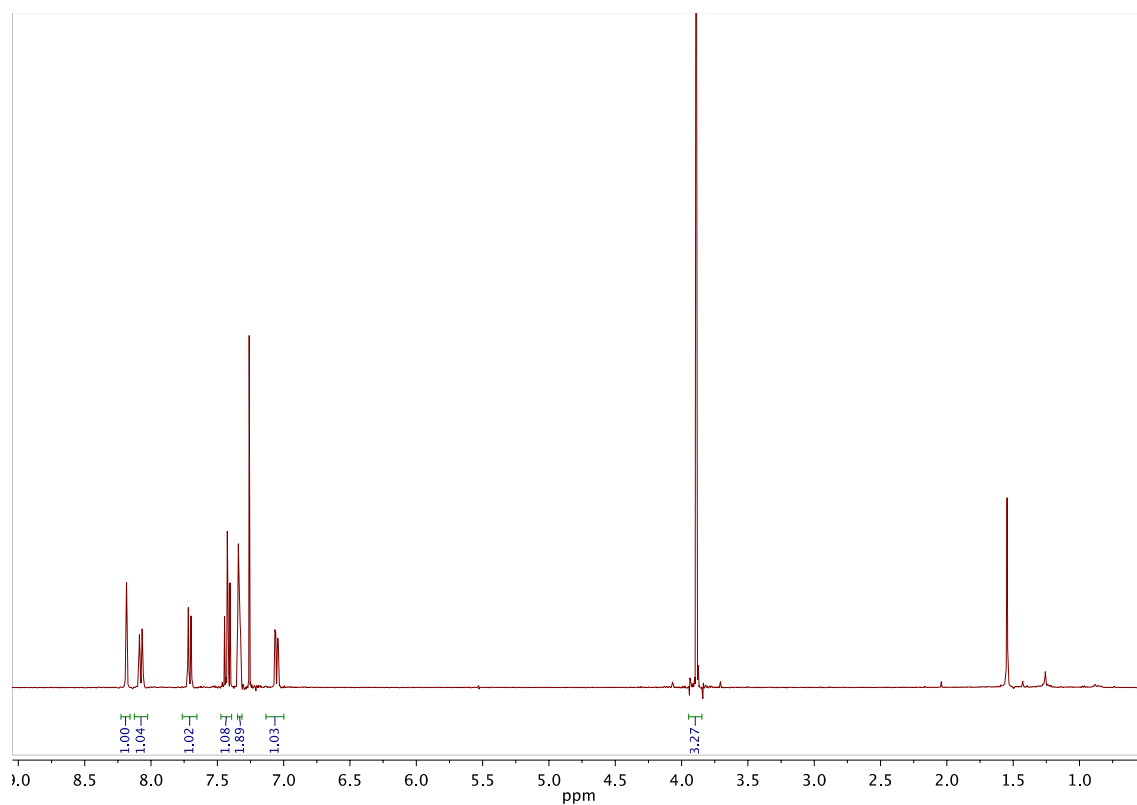
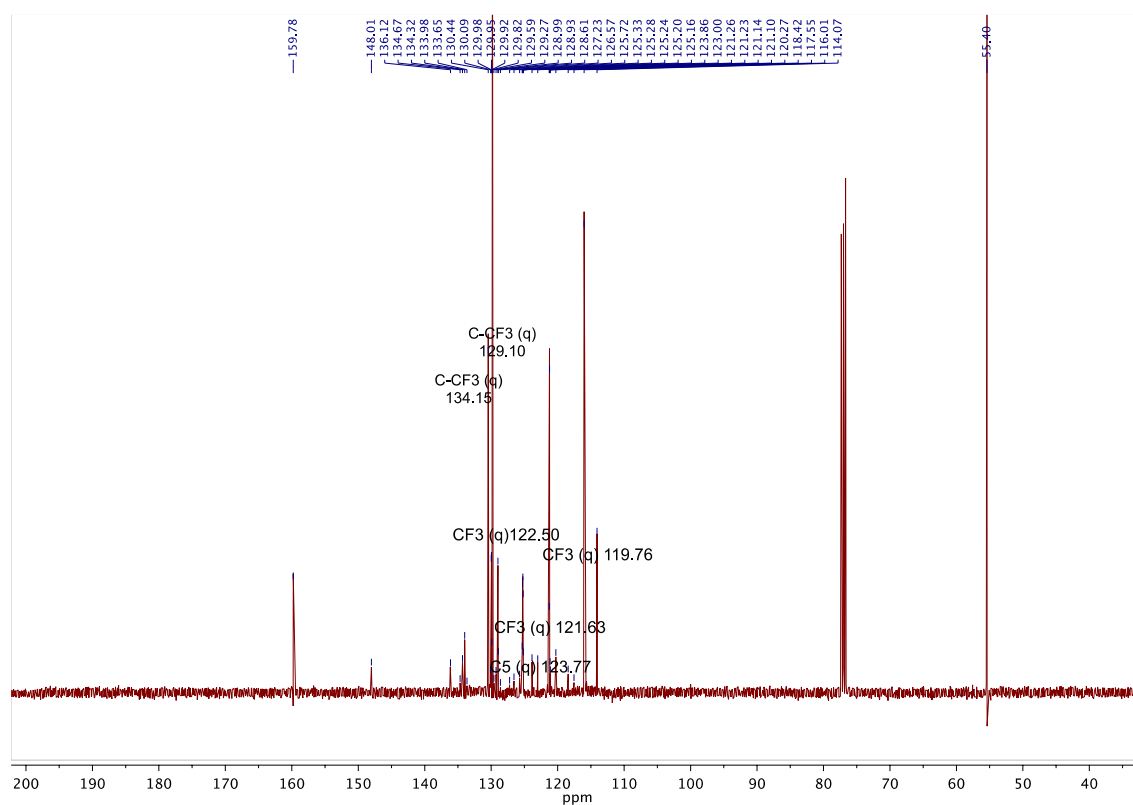
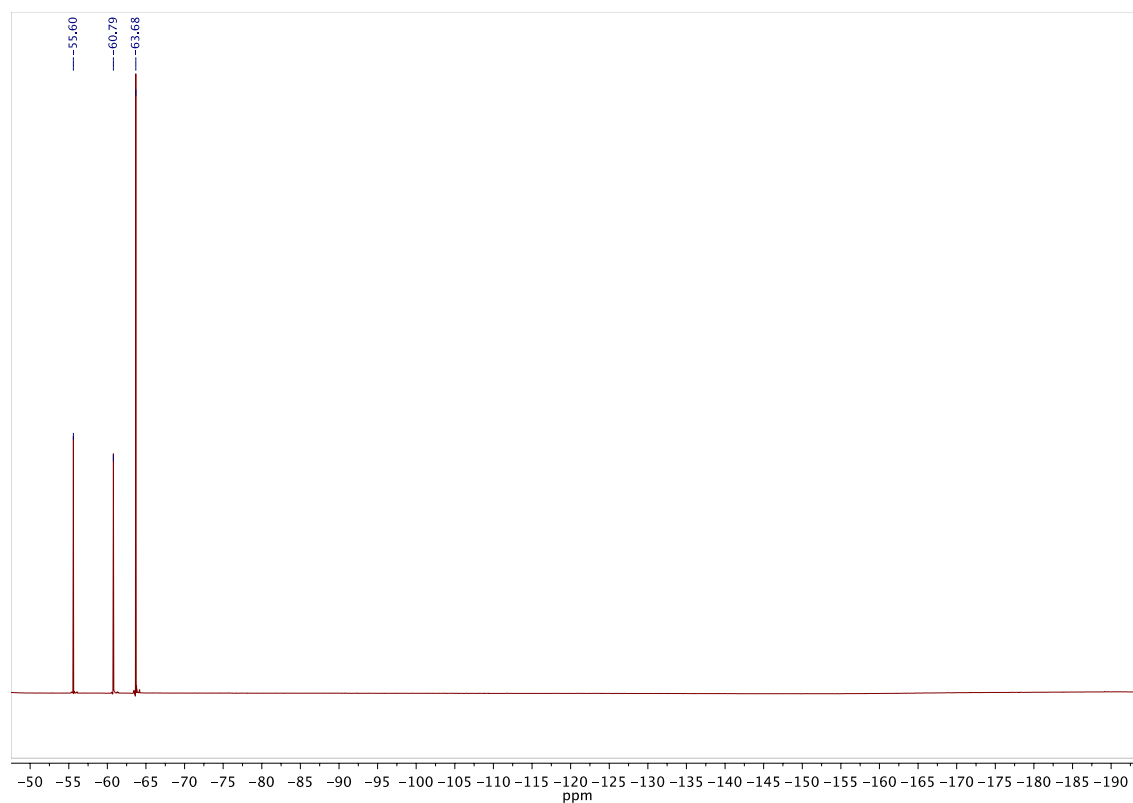
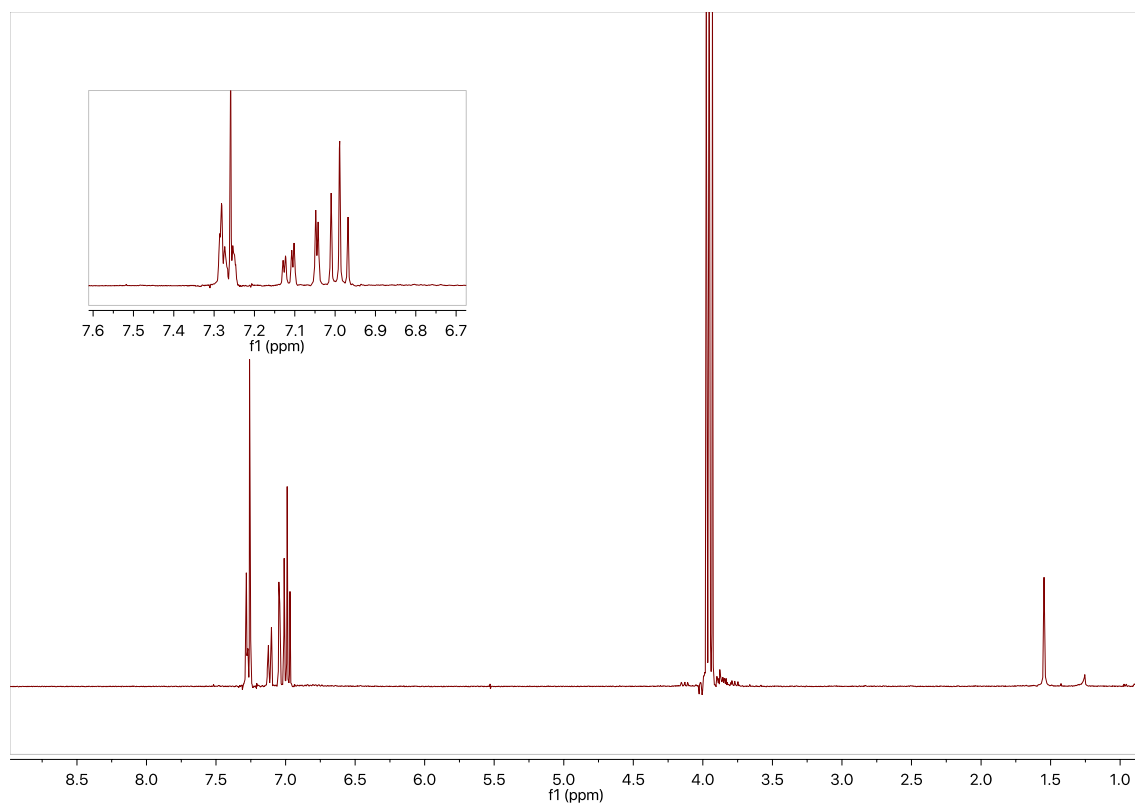
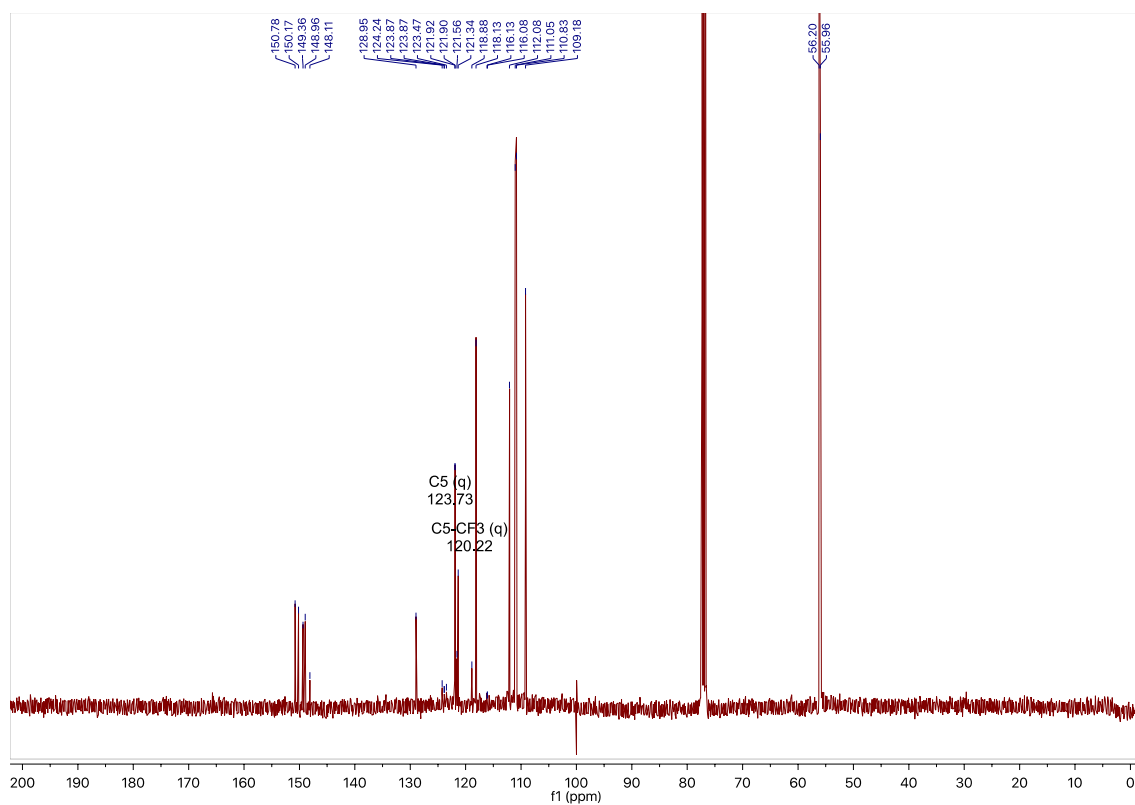


Figure S13 ^1H NMR spectrum of triazole **5**

**Figure S14** ¹³C NMR spectrum of triazole 5**Figure S15** ¹⁹F NMR spectrum of triazole 5

1,4-bis(3,4-dimethoxyphenyl)-5-(trifluoromethyl)-1*H*-1,2,3-triazole (6)**Figure S16** ^1H NMR spectrum of triazole **6****Figure S17** ^{13}C NMR spectrum of triazole **6**

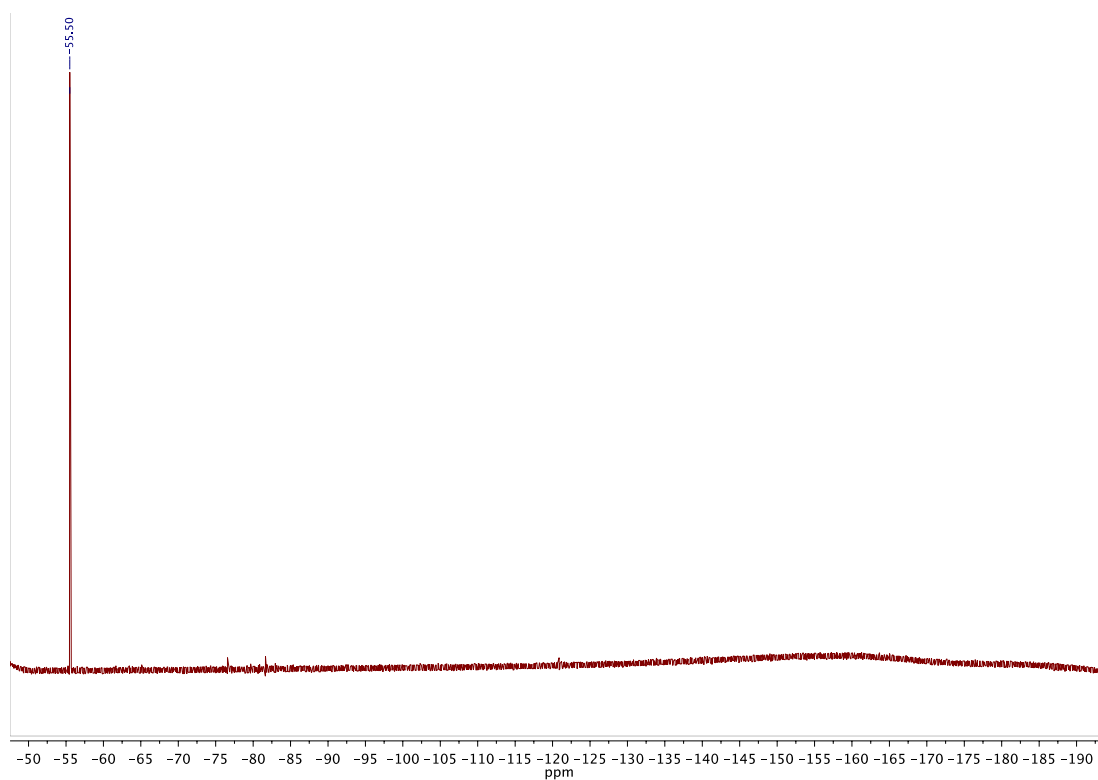


Figure S18 ^{19}F NMR spectrum of triazole **6**

1-(3-hydroxyphenyl)-4-(3,4-dimethoxyphenyl)-5-(trifluoromethyl)-1*H*-1,2,3-triazole (7**)**

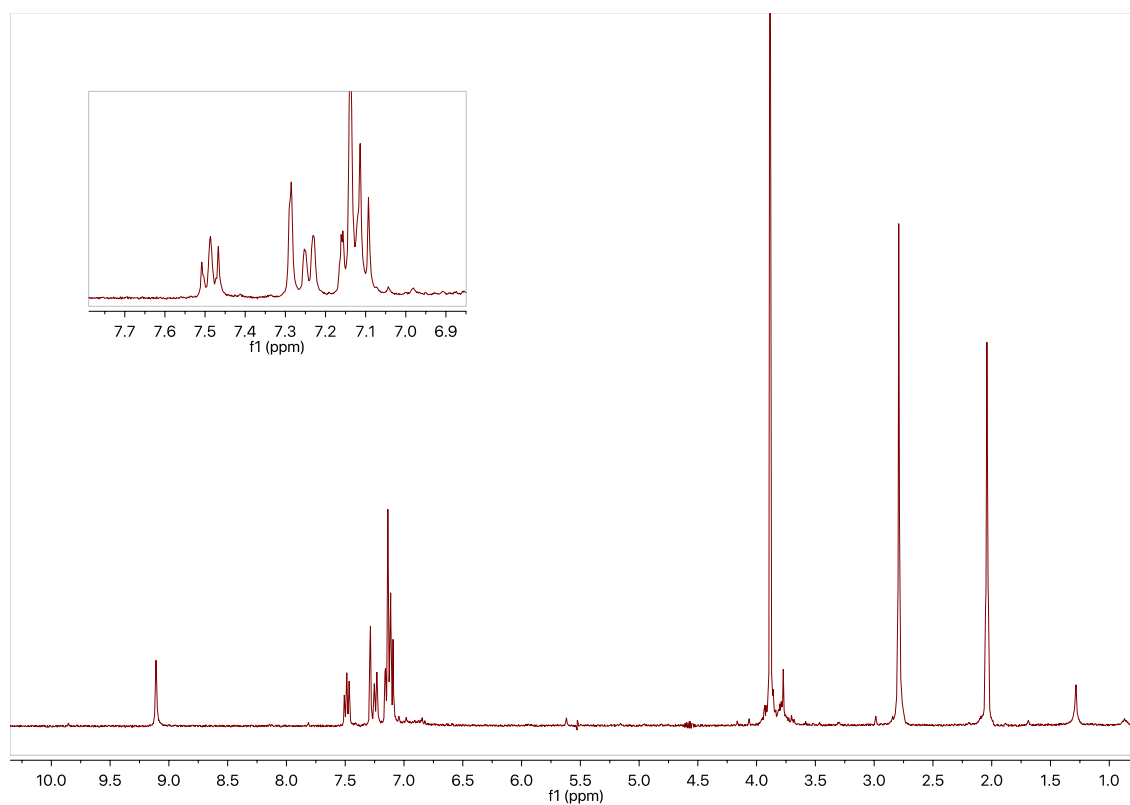


Figure S19 ^1H NMR spectrum of triazole **7**

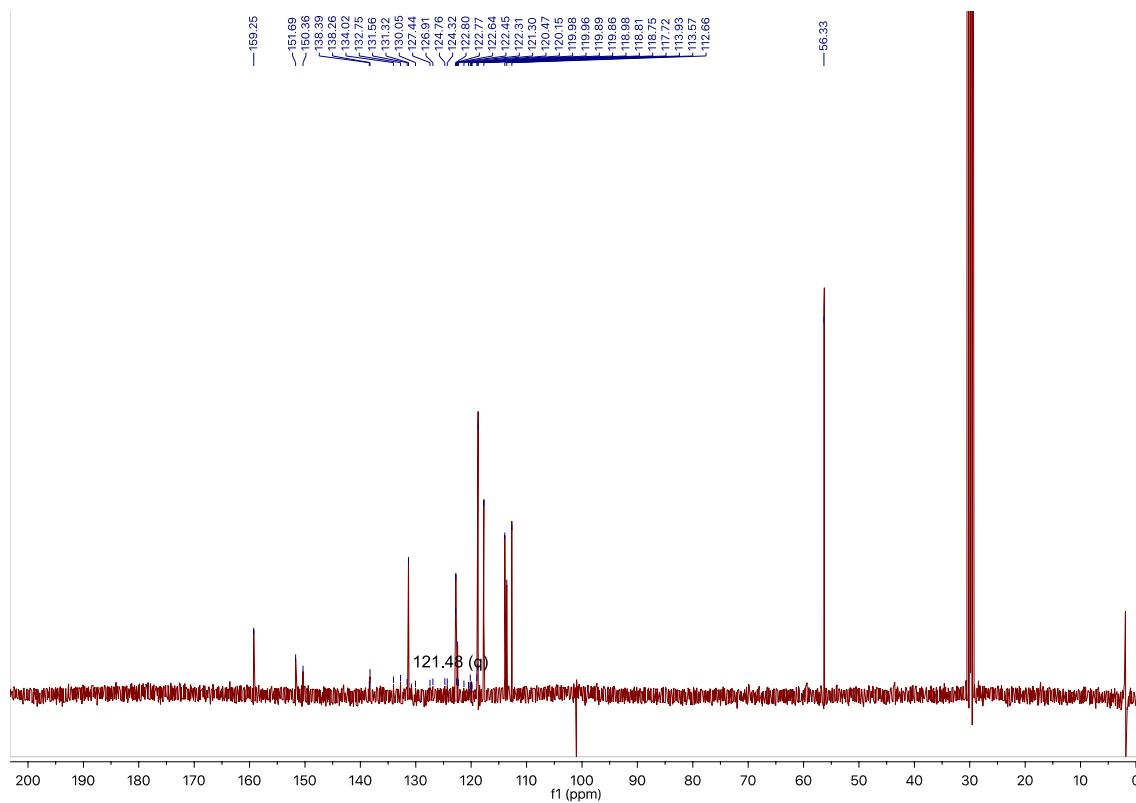


Figure S20 ¹³C NMR spectrum of triazole 7

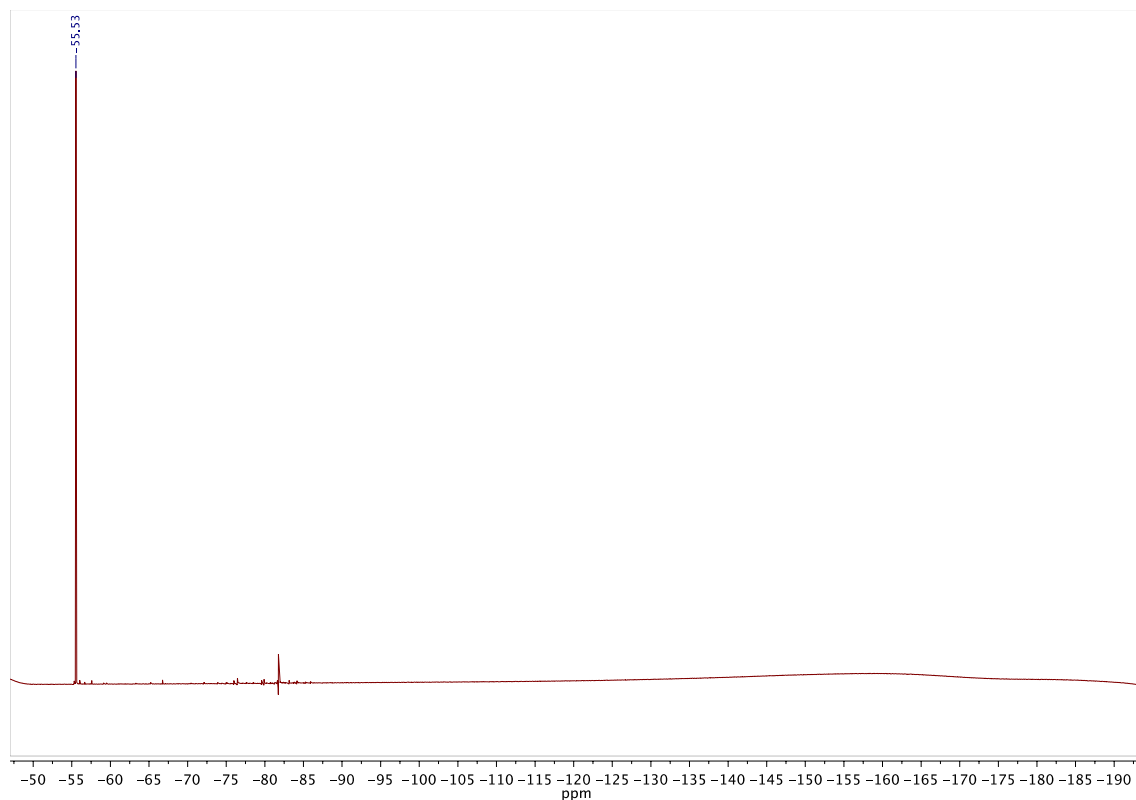


Figure S21 ¹⁹F NMR spectrum of triazole 7

S2. X-Ray Crystallography of Compound 7

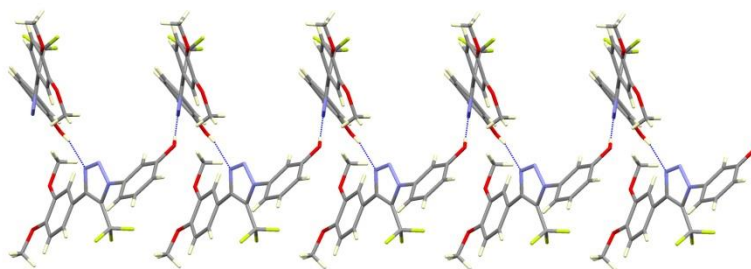


Figure S22 View of the chain formed by hydrogen bonds in 7

S3. Theoretical Calculations: electronic energy and optimized geometries at B3LYP/6-311++G(d,p) computational level

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J147_180_000_000, Electronic Energy= -1255.93491834 Hartree, NIMAG= 0

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C,-1.1637549313,1.2257499598,3.8390677606
C,-0.4441984251,1.718735494,2.743878121
C,0.4724256074,2.7493524164,2.9879347542
C,0.6168855475,3.2921262267,4.2629005433
C,-0.1221687088,2.7924608703,5.3245767115
H,-1.8802864855,0.4283401977,3.6657981426
H,1.3024436559,4.1167705109,4.4148735031
H,-0.0045072711,3.2294058773,6.3104193212
C,-1.8054560771,1.1651658085,6.2839449357
H,-2.6927439803,0.6312121627,5.937480392
H,-1.1982184637,0.4572649806,6.8586524244
H,-2.1284229134,1.9504826285,6.9718459568
C,-0.6845469898,1.1535174665,1.3671085985

H,-1.6699583855,0.6874226012,1.315019392
H,-0.6290789087,1.9234851225,0.5950303226
H,0.0575861889,0.3898855837,1.1127927396
N,1.2241328658,3.3302185109,1.8929010085
C,0.8340309575,4.5808671397,1.445446711
O,-0.0143240947,5.2548117181,1.9764353717
C,1.5795966225,5.1529059566,0.1910920356
F,1.2760829685,4.4752005755,-0.9311764817
F,2.9185251235,5.1678539169,0.3406666393
F,1.1897327822,6.4206837583,0.0061316921
N,2.0833515586,2.6404805663,1.0531840687
C,2.7275101332,1.5880040836,1.3949634414
H,3.2818324263,1.172882841,0.552859637
C,2.9147743965,0.8514037764,2.6673606989
C,2.8624094996,-0.552972445,2.6438381428
C,3.2822923119,1.5031894041,3.8419567015
C,3.1269776356,-1.2714943431,3.8005257078
H,2.6114656238,-1.0700715118,1.7246168816
C,3.5677945756,0.7726728012,5.000286721
H,3.3802323423,2.5797356453,3.8779373646
C,3.4804496108,-0.6215274057,4.985561526
H,3.0713107373,-2.3541535015,3.788264244
H,3.6937671533,-1.2048697119,5.8708979343
O,3.9250626821,1.5146899474,6.0866414119
C,4.2554284382,0.840491014,7.2945847237
H,5.1141956351,0.1746884897,7.1577062597
H,4.5143690613,1.6206417393,8.0082430131
H,3.4046301098,0.2669945159,7.6777791868

J147_180_000_180, Electronic Energy= -1255.94209351 Hartree, NIMAG= 0

C,1.1692543299,3.7760262617,-2.9066749725
C,0.3064407619,4.0492944047,-1.839580893
C,0.0341696701,3.1195997143,-0.8341000746
C,0.6688524379,1.8718064599,-0.9205904789
C,1.5289052784,1.5745453706,-1.9710187024
C,1.7760362241,2.519526222,-2.9623190016

H,-0.1776258333,5.020304749,-1.7897430289
H,1.9922948776,0.5957530393,-2.0162342321
H,2.4407306471,2.2745887247,-3.7836842908
C,1.4479740948,4.8247489687,-3.9559523931
H,0.5399026006,5.3704434689,-4.2244158394
H,2.1742081538,5.5594494278,-3.591720762
H,1.8572174492,4.3792329695,-4.8649483938
C,-0.9232971695,3.4410801104,0.2841183668
H,-1.1786873233,4.5019636467,0.2806369019
H,-1.8519593687,2.8723850579,0.1725573397
H,-0.4962530233,3.1908078492,1.2576403143
N,0.4592540372,0.8703806361,0.1012286557
C,-0.6937044553,0.1379540743,0.0883255211
O,-1.4891078598,0.1294642925,-0.8265089306
C,-0.9732950507,-0.7624284157,1.3340673789
F,-1.0665042951,-0.0428826441,2.4700683423
F,-0.0019977037,-1.6928673946,1.5146410712
F,-2.1235153085,-1.4146419864,1.1712749583
N,1.2313500077,1.095571183,1.2924370317
C,2.1730698985,0.2472025756,1.4621781939
H,2.3280243665,-0.5724246296,0.757257491
C,3.0889614802,0.3196267804,2.6044521931
C,4.102428119,-0.646364593,2.710589091
C,2.9726659142,1.3186269882,3.5731385445
C,4.9855393889,-0.5984963976,3.7808322959
H,4.1900751514,-1.4248191681,1.9612805724
C,3.8640274889,1.3608171442,4.6456319778
H,2.1913565794,2.0638022974,3.5013922945
C,4.8762743859,0.3972816173,4.7518245956
H,5.7697073631,-1.341347161,3.870365956
H,5.5747391627,0.4130910075,5.5774875313
O,3.669974573,2.3723095287,5.5365319544
C,4.5341922884,2.4712418627,6.6621003312
H,5.5736399019,2.6293382231,6.3552769942
H,4.1892197145,3.3372865714,7.2239543482
H,4.4693076145,1.5797737022,7.2949680069

J147_180_180_000, Electronic Energy= -1255.93598830 Hartree, NIMAG= 0

C,5.6697249521,3.1652287549,4.2444265776
C,4.4542388338,3.8384703865,4.3548972085
C,3.3720216675,3.5992165141,3.4980223652
C,3.5453976083,2.6357144204,2.4990693597
C,4.7565591958,1.9571339018,2.3580178943
C,5.8067884615,2.2139008066,3.225779595
H,4.3333835708,4.5817944665,5.1371125808
H,4.8699924899,1.2297056672,1.5628372563
H,6.743511192,1.6799298236,3.1047009558
C,6.8125540658,3.4524408648,5.1874783974
H,6.5387704842,4.2066026574,5.9276543119
H,7.1195147823,2.5492565733,5.7238040881
H,7.6885944337,3.8193974043,4.6437811254
C,2.099518387,4.3886096658,3.6585252938
H,1.9739031205,4.7120829172,4.6933023855
H,2.1220920795,5.2756455099,3.0188658678
H,1.2175407435,3.8118366485,3.3717062709
N,2.4880601272,2.3429031531,1.5506683005
C,2.186663787,3.3123368171,0.6101294619
O,2.651132181,4.4264754192,0.6160042766
C,1.1350741774,2.9369080556,-0.4888281126
F,-0.0049322254,2.437719466,0.0286647514
F,1.6257614095,2.0603454925,-1.3825308847
F,0.8080689503,4.0486366986,-1.1611785999
N,2.061372167,1.0627771449,1.2246101936
C,2.0742651041,0.0716241782,2.0364834141
H,1.7621250794,-0.8464384523,1.5381127143
C,2.3816751146,-0.1009522727,3.4739881088
C,3.0687959345,-1.2633285751,3.8657897451
C,1.9068867258,0.773650862,4.4484334227
C,3.30925242,-1.5022771596,5.2104583231
H,3.4157503928,-1.9643637095,3.1151673452
C,2.1355771361,0.5178774132,5.8046055774
H,1.3297617374,1.648841128,4.1846961603
C,2.848766965,-0.6196241256,6.1906301882

H,3.8531607939,-2.3901488421,5.5124848194
H,3.0392287267,-0.8336170496,7.2334789167
O,1.6174023447,1.4366692849,6.6685743572
C,1.7903952838,1.2326096844,8.0655082941
H,2.8505316835,1.2303525085,8.3406189377
H,1.2941989495,2.0709440757,8.5513445451
H,1.3248026464,0.296878712,8.3927954199

J147_180_180_180, Electronic Energy= -1255.95463329 Hartree, NIMAG= 0

C,-2.427879047,-1.7244664015,-0.3505769156
C,-1.1455504277,-1.9471370327,-0.8622943671
C,-0.1110760931,-1.0169379518,-0.7296209716
C,-0.3991299221,0.1743154255,-0.0512414622
C,-1.667908241,0.4245953704,0.4627188006
C,-2.6777008451,-0.5196669792,0.3131475591
H,-0.9435419666,-2.8731041352,-1.3923286597
H,-1.8600389733,1.3631918595,0.9700291941
H,-3.6667788871,-0.3139646696,0.7079148659
C,-3.5071480095,-2.7695313472,-0.494516011
H,-3.3901629689,-3.3390959421,-1.4191748639
H,-3.4730151406,-3.4827221077,0.3363254541
H,-4.5009375367,-2.3168101014,-0.497007196
C,1.2482890727,-1.2727220039,-1.328645967
H,1.3327332196,-2.3054299103,-1.6702591532
H,1.4189849013,-0.6183180016,-2.1890414426
H,2.0512391861,-1.0841989011,-0.6115929201
N,0.6364003667,1.1674365035,0.1372244238
C,0.8522276036,2.0963456096,-0.8537751376
O,0.2346597754,2.1247427292,-1.8924611965
C,1.9682521879,3.1623728029,-0.5953929121
F,3.1870726291,2.6025652017,-0.466655188
F,1.7204978537,3.9107466079,0.4962646668
F,2.0202612711,3.992002391,-1.6437373636
N,1.4379978466,1.2201363435,1.2576335571
C,1.278335461,0.3524593925,2.1850999885
H,0.5217232278,-0.4309775848,2.1216849734

C,2.1114614364,0.3669917398,3.3925759551
C,1.8907069854,-0.6185391458,4.3695036965
C,3.1076386109,1.3256599253,3.5914225767
C,2.663710605,-0.6317140618,5.5228062907
H,1.1182740227,-1.3648622726,4.220537146
C,3.8802745337,1.306049771,4.7532069515
H,3.2892870028,2.0914155603,2.84852713
C,3.6603983558,0.3229098155,5.7271103834
H,2.4955907023,-1.3910306265,6.2781339854
H,4.2497211958,0.2927537329,6.6334580151
O,4.8244555541,2.2844493379,4.8508352508
C,5.6495598482,2.3273643167,6.0074630874
H,6.2456048335,1.4138046763,6.1079538999
H,6.3148560872,3.1771310621,5.8649262428
H,5.0572086121,2.4798286117,6.9162221832

J147_180_180_180_rx, Electronic Energy= -1255.95456753 Hartree, NIMAG= 0

C,-2.424446529,-1.7199145679,-0.3489101061
C,-1.1498971582,-1.9371266272,-0.8818583607
C,-0.1152998912,-1.0052743298,-0.7609748949
C,-0.3956076734,0.1826329163,-0.0734658502
C,-1.6566425749,0.4272330615,0.4620958627
C,-2.6663733966,-0.5189403811,0.3247800771
H,-0.9544451477,-2.8599361598,-1.4198246062
H,-1.8434793015,1.3638013524,0.9750918357
H,-3.6497735245,-0.3169968689,0.7353561441
C,-3.50381758,-2.7663429765,-0.4823074534
H,-3.3982910129,-3.3316981679,-1.4108612005
H,-3.4572854031,-3.4831303915,0.3448555966
H,-4.498383848,-2.3155174479,-0.4694027418
C,1.2347791998,-1.2556235504,-1.3829289334
H,1.3202987269,-2.2898583379,-1.7196278603
H,1.3848801099,-0.6056472684,-2.2504877238
H,2.04934588,-1.0565655633,-0.6820330266
N,0.6386675542,1.1801321876,0.0983758366
C,0.8444113781,2.1006696865,-0.9024930567

O,0.2176852846,2.1197010629,-1.9358668661
C,1.9626424524,3.1690475293,-0.6636415795
F,3.182103108,2.6102741423,-0.5340388084
F,1.7217963384,3.9314010037,0.4200846156
F,2.00971475,3.9853069436,-1.7224235087
N,1.4442405539,1.2501264075,1.2149500672
C,1.2946181432,0.3916327278,2.1527866008
H,0.5428680824,-0.3976205663,2.0983983385
C,2.1320619343,0.4288277854,3.3563015926
C,3.1238266438,1.3974850496,3.5470999853
C,1.9126748177,-0.5522128672,4.3387935343
C,3.883864101,1.37617095,4.7129184279
H,3.2876015531,2.1506449189,2.7878458752
C,2.681693171,-0.5622228559,5.5033391404
H,1.1412039658,-1.2941082895,4.1765728602
C,3.6723026289,0.4085594479,5.6887276451
H,4.6533389049,2.1244389982,4.8658893324
H,4.2590595795,0.3849422264,6.5989668832
O,2.5432547923,-1.4713604943,6.5114660766
C,1.5539438125,-2.4839443052,6.3871853225
H,1.7420647996,-3.1227628423,5.517291114
H,1.6254831672,-3.081729236,7.2942061178
H,0.5485823379,-2.0547032828,6.3153074147