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Supporting Information

A structural study of *N,N'-bis*-arylacylguanidines

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TOTAL ENERGY RESULTS

Total energy and Gibbs energy (a.u.) calculated at the B3LYP/6-31+G(d,p) computational level for the experimentally observed tautomers of guanidines **1**, **2** and **3**.

Compound	Isomer	E_{Total} (a.u.)	Gibbs E (a.u.)
1	**ar1.*Z***	-1013.3812779	-1013.0705969
	ac.*Z*	-1013.3782468	-1013.0676218
2	**ar1.*Z***	-1029.4332883	-1029.1329853
	ac.*Z*	-1029.4313848	-1029.1303748
3[a]	**ac.*E***	-1711.5099586	-1711.2561226
	ar2.*Z*	-1711.2533452	-1711.2533452
	ar1.*Z*	-1711.5086628	-1711.2531378
	ac.*Z*	-1711.5041794	-1711.2497424

[a]A simplified model of compound **3** was used for the computational studies (see Figure 5)

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GENERAL INFORMATION

All the commercial chemicals were obtained from usual suppliers and were used without further purification. Dry solvents were prepared using standard procedures, according to Vogel, with distillation prior to use. Chromatographic columns were run using a flash purification system with silica cartridges. Solvents for synthesis purposes were used at GPR grade. Analytical TLC was performed using silica gel plates or aluminium oxide plates. Visualisation was by UV light (254 nm). NMR spectra were recorded in a spectrometer operating at 400.13 MHz and 600.1 MHz for 1H-NMR; 100.6 MHz and 150.9 MHz for 13C NMR. Shifts are referenced to the internal solvent signals. HRMS spectra were measured using methanol as carrier solvent. Melting points are uncorrected.

CARTESIAN COORDINATES OF THE OPTIMISED STRUCTURES AT B3LYP/6-31+G** LEVEL

N,N'-bis-phenyl-*N''*-(*tert*-butoxycarbonyl)-guanidine (1)

1.ar1.*Z*

0,1
C,-0.89635800,5.03024400,0.09060600
C,-0.89856400,4.17786900,1.19788200
C,-0.22652500,2.95362200,1.15226000
C,0.46015100,2.55595500,-0.01305900
C,0.46939800,3.42843300,-1.11801400
C,-0.20686000,4.64759300,-1.06514900
N,1.21021600,1.37036800,-0.06469800
C,0.66432400,0.20567000,-0.02765400
N,1.36712700,-0.96546700,-0.00910400
N,-0.74519800,0.04403100,-0.03241400
C,-1.49645500,-1.11053900,-0.02355400
O,-2.79792200,-0.78265500,-0.05007000
O,-1.03854200,-2.24788400,0.00415400
C,2.75816100,-1.18216900,0.01248600
C,-3.86887500,-1.81426700,-0.05345200
C,3.17551400,-2.52722600,0.01411900
C,4.52948700,-2.84920000,0.03801500
C,5.49643000,-1.83839200,0.06014700
C,5.08164600,-0.50585800,0.05818700
C,3.72595800,-0.16458800,0.03444000
H,0.78154600,-1.79797700,-0.00639300
H,-1.41605500,5.98277200,0.12991500
H,-1.41705800,4.46829200,2.10767800
H,-0.20469700,2.30782700,2.02585700
H,1.01746800,3.13411400,-2.00786900
H,-0.19015300,5.30517400,-1.93008300
H,2.43031900,-3.31888500,-0.00354100

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H,4.82831800,-3.89360300,0.03887700
H,6.55294200,-2.08785200,0.07853300
H,5.81958300,0.29146200,0.07527500
H,3.41199400,0.86910900,0.03116700
H,-1.26792000,0.91098700,-0.05728400
C,-3.74986700,-2.67926000,-1.31128500
H,-2.84496700,-3.28803600,-1.29475300
H,-4.61697000,-3.34517900,-1.37193800
H,-3.74175600,-2.05159500,-2.20805600
C,-5.13773200,-0.96051100,-0.09305100
H,-6.01942000,-1.60836100,-0.09695700
H,-5.19217300,-0.30580500,0.78169800
H,-5.15952500,-0.33930100,-0.99327600
C,-3.79923600,-2.63559400,1.23682900
H-2.89064500,-3.23768200,1.27928400
H,-3.83385100,-1.97845500,2.11163100
H-4.66386300,-3.30591900,1.28256100

1.ac.*Z*

0,1
C,-1.55989400,5.06056900,-0.05167400
C,-2.70155200,4.27312400,-0.22649300
C,-2.59727600,2.88467700,-0.26057200
C,-1.34635600,2.25573400,-0.12129400
C,-0.19641900,3.04232700,0.05079900
C,-0.31973100,4.43379600,0.08530600
N,-1.35907100,0.84234300,-0.15577600
C,-0.34601100,-0.07558300,-0.09582900
N,-0.72332200,-1.39239100,-0.09086600
N,0.90633500,0.33233200,-0.06632600
C,1.93281200,-0.57189600,-0.07265700
O,3.10381300,0.07802600,0.08443300
O,1.86104500,-1.80465800,-0.21469400
C,-2.02282400,-1.94708500,0.00950600
C,4.39794100,-0.62493000,0.09512000
C,-2.91793400,-1.56013800,1.02136000
C,-4.17763700,-2.15778700,1.10606600
C,-4.54840100,-3.16175400,0.20773000
C,-3.64832600,-3.56533700,-0.78303500
C,-2.39694100,-2.95731900,-0.89033000
H,0.08947300,-2.00879700,-0.20681600
H,-1.63721300,6.14314900,-0.02539800
H,-3.67731600,4.73703800,-0.33792800
H,-3.49188600,2.28086400,-0.39867200
H,0.76609500,2.56153500,0.14676500
H,0.57743500,5.03168800,0.21909200
H,-2.28147900,0.44398600,-0.26587300
H,-2.61620900,-0.81807100,1.75418600

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H,-4.86075900,-1.85082100,1.89269700
H,-5.52472300,-3.63031800,0.28385500
H,-3.92355800,-4.34880300,-1.48295400
H,-1.70193500,-3.25577700,-1.66953700
C,5.39063300,0.52418800,0.29828500
H,6.41393100,0.13631300,0.32258500
H,5.31165300,1.24960200,-0.51702800
H,5.19151900,1.04316400,1.24076000
C,4.46268400,-1.60639100,1.27146900
H,4.23031600,-1.09055100,2.20898200
H,3.76289100,-2.43227400,1.13838100
H,5.47678200,-2.01309400,1.35005800
C,4.64054700,-1.31336500,-1.25335100
H,3.94064500,-2.13484900,-1.41109800
H,4.53491900,-0.59331300,-2.07145600
H,5.66106000,-1.71058500,-1.28017500

***N-(Pyridin-2-yl)-N'-(phenyl)-N''-(tert-butoxycarbonyl)-guanidine* (2)**

2.ar1.*Z*

0,1
C,1.6497098603,-3.3386681071,-0.0185634466
C,0.4436327715,-4.0235297125,0.0725606006
N,-0.7537687247,-3.418299671,0.107035951
C,-0.8140297773,-2.0656098262,0.0511916651
C,0.3726212001,-1.2983403614,-0.0424985042
C,1.6007112183,-1.9377627388,-0.077062227
N,-2.0045933749,-1.3646693809,0.0810575952
C,-3.1914955307,-1.8976030213,0.1653710459
N,-4.323615159,-1.1394022208,0.1899381546
N,-3.3966486886,-3.2830004267,0.2367226188
C,-4.5814021857,-3.9752097323,0.3298144112
O,-4.3180312137,-5.2904298707,0.3755282194
O,-5.6998464296,-3.466937338,0.3650554448
C,-5.3962148673,-6.305222303,0.4757426671
C,-4.6050812047,-7.6151306694,0.4940343888
C,-6.169811722,-6.115219132,1.7838868145
C,-6.2990658307,-6.2286686156,-0.7590502646
C,-4.5037254178,0.2566444731,0.1378590948
C,-5.8378282589,0.7058855393,0.1873170949
C,-6.1310538424,2.0658994035,0.1425530336
C,-5.1013647715,3.0078918271,0.0475353754
C,-3.7795924254,2.5619636605,-0.0014338859
C,-3.4679197421,1.2002075143,0.0424607111
H,2.590400481,-3.8781194332,-0.0428866902
H,0.4240204907,-5.1103583266,0.1208979267
H,0.2886661593,-0.2184243984,-0.0852432168
H,2.5160544179,-1.3568499766,-0.1488626698

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H,-5.1762201966,-1.6946993932,0.258438452
H,-2.5031249881,-3.8026912757,0.2136178009
H,-5.2933186885,-8.4627840283,0.5665416559
H,-4.0148914943,-7.7238714172,-0.4207014934
H,-3.9253409893,-7.6450585951,1.3507358659
H,-6.8705671512,-6.9470598055,1.9110609451
H,-6.7342983945,-5.1818169568,1.7825993409
H,-5.4841456329,-6.1165323039,2.6372752195
H,-5.7035147514,-6.3098821236,-1.6739905849
H,-7.0061270621,-7.064662728,-0.7397183353
H,-6.8640340186,-5.2958695483,-0.783870273
H,-6.644322589,-0.0196463101,0.2612021449
H,-7.1675204733,2.3885241283,0.1821488251
H,-5.3275928345,4.0692074294,0.0124652306
H,-2.9680498997,3.2807940283,-0.0752883876
H,-2.4446582681,0.8587117446,0.004421685

2.ac.*Z*

0,1
C,3.8110057901,-3.3045214356,-0.1740253628
C,3.6669525254,-1.9243446983,-0.2261564659
N,2.4787224157,-1.2981284651,-0.1763299114
C,1.3679422609,-2.0427989895,-0.0705424284
C,1.4119349523,-3.4537370574,-0.0105372481
C,2.6465327025,-4.079218449,-0.0633533168
N,0.12523734,-1.4257415299,-0.0165647459
C,-0.2486338175,-0.0918543583,-0.0536495895
N,-1.5101821064,0.2888426144,0.0106560031
N,0.7509797449,0.8176621678,-0.1599089457
C,0.7133708015,2.2280038941,-0.2224197007
C,-2.5244151338,-0.6200417954,0.1173472679
O,-3.7046375241,0.0279334891,0.1644055288
O,-2.4387784712,-1.8616883837,0.1679423463
C,-4.9906372331,-0.6807532751,0.2795434752
C,-5.9972578494,0.4740678886,0.2919392021
C,-5.2173723524,-1.577270456,-0.9436539635
C,-5.0533775571,-1.461666662,1.5977235208
C,1.9636366629,2.8658369052,-0.3323530199
C,2.0487749189,4.2538188071,-0.4018117874
C,0.8886437945,5.033575352,-0.3630164914
C,-0.3504609693,4.3996206806,-0.2539392522
C,-0.4539930537,3.0077581361,-0.1831054142
H,4.7943183822,-3.7592365401,-0.2180427279
H,4.5353256021,-1.2757490702,-0.3118719016
H,0.4919155323,-4.0230731089,0.0749404857
H,2.7066514064,-5.1626663452,-0.018995862
H,-0.7123228664,-2.0193872105,0.0641167135
H,1.6797940384,0.3872801976,-0.2004533001

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H,-7.0160591143,0.0828730828,0.3756400654
H,-5.807775823,1.1398155839,1.139156008
H,-5.9221218695,1.0591865409,-0.6294139918
H,-6.2330361507,-1.9863913611,-0.9105522459
H,-4.5075766587,-2.4050568997,-0.9690347196
H,-5.1166801626,-0.9940840364,-1.8649369236
H,-4.8393048809,-0.7980878185,2.4420163626
H,-6.0622965965,-1.8667588513,1.7320466304
H,-4.3409618282,-2.2875488336,1.6067058335
H,2.8698430812,2.2659225099,-0.3630560918
H,3.0239946702,4.7247150161,-0.4863257225
H,0.951631958,6.1161915207,-0.416982691
H,-1.260975077,4.991600702,-0.2225490287
H,-1.4145514845,2.5212005418,-0.0986965931

***N*-(*tert*-butoxy)-*N'*-(4-chloro-3-trifluoromethyl)-*N''*-(4-methylaminophenyl)-guanidine (**Simplified model of compound **3)**.

3'.ac.*E*

0,1
N,-4.94315700,-3.33586100,0.32390100
C,-4.35197300,-2.09134400,0.23250400
C,-4.02573700,-1.38002500,1.41007400
C,-3.40097900,-0.14155700,1.34652600
C,-3.07513500,0.43432300,0.10728100
C,-3.40323200,-0.25943500,-1.06296100
C,-4.03208800,-1.50367700,-1.00952400
N,-2.45799200,1.72368200,0.04462700
C,-1.12271200,1.97082100,0.00556800
N,-0.31685900,0.85761500,0.02874000
N,-0.58086200,3.17843600,-0.05158700
C,1.08104800,0.71937100,0.00355700
C,1.57449300,-0.59491800,0.02972800
C,2.94331400,-0.86443500,0.01034700
C,3.84882900,0.20772100,-0.03650600
C,3.36295800,1.51380900,-0.06269700
C,1.99553200,1.78218100,-0.04356300
Cl,5.58490800,-0.03397800,-0.06349100
C,-1.37694600,4.29877100,-0.07478200
C,-0.59725900,5.59539700,-0.14247300
O,-2.62227300,4.32109100,-0.04484900
H,-3.00497600,2.59444000,0.02793500
C,-5.49462000,-4.03916400,-0.81913400
C,3.39967000,-2.30575700,0.03971500
F,2.34845400,-3.16574200,0.08365400
F,4.16607200,-2.58145100,1.12242300
F,4.12219200,-2.63904500,-1.05695700
H,-5.32680700,-3.57494400,1.22544200

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H,-4.26674400,-1.81137000,2.37855200
H,-3.16340800,0.39500700,2.26043900
H,-3.17074100,0.18600200,-2.02596000
H,-4.27660900,-2.01146500,-1.93537400
H,-0.82726800,-0.01567700,0.06989100
H,0.88255000,-1.42935400,0.06603400
H,4.06804500,2.33695500,-0.09880800
H,1.62643500,2.79713800,-0.06447100
H,0.03876300,5.60359200,-1.03393600
H,0.06466700,5.67856600,0.72616000
H,-1.28306600,6.44295900,-0.16769500
H,-5.94428600,-4.97107800,-0.47104200
H,-6.26451900,-3.45683800,-1.34733300
H,-4.70665800,-4.29845700,-1.53550400

3'.ar2.*Z*

0,1
C,4.28880700,0.26261900,-0.10046400
C,4.08631000,1.64394500,-0.12431100
C,2.80094000,2.16720300,-0.08001400
C,1.68157500,1.31887700,-0.01064100
C,1.88728000,-0.06866400,0.01306900
C,3.18310700,-0.59665300,-0.03213900
N,0.42467600,1.93511000,0.02921700
C,-0.82097400,1.36646800,0.09386400
N,-1.02988100,0.10079800,0.16097400
N,-1.88523500,2.31107900,0.11144000
C,-2.33440900,-0.43973000,0.16749200
C,-2.76658800,-1.19099100,1.27741200
C,-4.01588100,-1.79731100,1.29100700
C,-4.88978900,-1.70074100,0.18669300
C,-4.45044100,-0.97545600,-0.93472600
C,-3.19537300,-0.35685000,-0.93860700
C,-1.85069400,3.68591200,0.06834300
O,-0.80733500,4.33518100,-0.02117700
Cl,5.94008600,-0.32629100,-0.15686100
H,0.40635500,2.95515200,-0.00550100
C,-3.19934700,4.37065700,0.14618800
H,-3.23299400,4.96851700,1.06190900
H,-3.28777500,5.05889500,-0.69844500
H,-4.04512500,3.67877800,0.14051900
C,-6.95920000,-2.48664700,-0.94165000
C,3.34449200,-2.10128900,-0.00259300
F,3.97476700,-2.57126800,-1.10850700
F,4.06334700,-2.51821900,1.07046000
F,2.15163300,-2.73950000,0.06154800
N,-6.15053000,-2.29197500,0.24868700
H,4.94289800,2.30652200,-0.17725500

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H,2.66289900,3.24485600,-0.09893500
H,1.03404900,-0.72731500,0.06756100
H,-2.79374500,1.86836800,0.18117700
H,-2.10160600,-1.29477700,2.12942000
H,-4.32649500,-2.36101000,2.16793300
H,-5.07455400,-0.89801500,-1.81818200
H,-2.86460200,0.16521400,-1.83284600
H,-7.86043300,-3.03840000,-0.66531000
H,-7.27735500,-1.52235600,-1.35344300
H,-6.43672600,-3.04337100,-1.73595200
H,-6.22740100,-3.02786800,0.93613800

3'.ar1.*Z*

0,1
C,5.64925700,-0.98374400,0.34298600
C,5.66957500,0.42712100,0.33533200
C,4.50480800,1.15734600,0.15594400
C,3.26429400,0.51577100,-0.02013200
C,3.23163500,-0.88352600,-0.01622100
C,4.40909400,-1.61747200,0.15901900
N,2.14006400,1.35856800,-0.18490000
C,0.84140700,1.03890000,-0.40091700
N,0.41026300,-0.17240000,-0.54865500
N,-0.03310400,2.15867600,-0.50205400
C,0.24103900,3.50650600,-0.40583500
O,1.36798200,3.95222400,-0.19282100
C,-0.95084400,4.42392100,-0.58389200
N,6.82815000,-1.69131000,0.56702300
C,6.92214400,-3.11757100,0.31422000
H,6.61108800,0.95174800,0.47932300
H,4.55381300,2.24358700,0.15362100
H,2.29125600,-1.39685200,-0.15561300
H,4.34414900,-2.69977900,0.15314100
H,2.31113200,2.36233300,-0.12709000
H,-0.99265100,1.90085600,-0.68999800
H,-1.89594600,3.89698100,-0.73647700
H,-1.03323800,5.05964400,0.30187100
H,-0.76166800,5.07703500,-1.44062100
H,7.67020100,-1.16859500,0.37403400
H,7.95258300,-3.43602600,0.48732100
H,6.28405800,-3.67481300,1.00899200
H,6.63629000,-3.39669600,-0.71269400
C,-0.93947300,-0.49987600,-0.65366800
C,-1.87216500,-0.22109000,0.36559000
C,-1.38715000,-1.23682900,-1.76736800
C,-3.20735900,-0.63319900,0.27447800
H,-1.54181000,0.29528100,1.25927500
C,-2.71155400,-1.64900600,-1.86682100

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H,-0.67723400,-1.48236000,-2.55052600
C,-3.62869000,-1.34964500,-0.85614500
H,-3.04572100,-2.21064100,-2.73239700
Cl,-5.28205200,-1.90018900,-1.05463100
C,-4.15147600,-0.29551700,1.40705200
F,-3.52669700,0.39490600,2.39538900
F,-5.18665500,0.48039700,0.99554900
F,-4.68444100,-1.39792100,1.98434100

3'.ac.*Z*

0,1
N,-1.49403500,0.21597500,-0.00286100
C,-0.98133700,1.47125200,-0.12583800
N,0.38571400,1.57426400,-0.20154600
N,-1.78429000,2.52403600,-0.14457300
C,1.34699600,0.56513900,-0.40245700
C,2.54015600,0.62351400,0.33229400
C,3.56111800,-0.30937900,0.13555400
C,3.37882700,-1.33743500,-0.80470500
C,2.19553100,-1.40083100,-1.54171800
C,1.19113400,-0.45376400,-1.35600600
Cl,4.59753300,-2.55768800,-1.10213600
C,-1.27627100,3.79806500,-0.18983800
O,-0.06975400,4.11506700,-0.13746200
C,-2.33544900,4.87444400,-0.28707400
H,0.67114900,2.56607800,-0.13368200
C,4.82735700,-0.18849800,0.95770000
F,5.92469100,-0.02424200,0.18192500
F,5.03963400,-1.28224100,1.72879700
F,4.78007300,0.87487300,1.79622800
H,2.66989700,1.40883400,1.06734900
H,2.07391900,-2.18478000,-2.28088900
H,0.30006500,-0.49277100,-1.97382600
H,-1.86607200,5.85667000,-0.35222100
H,-2.96691500,4.70140600,-1.16481800
H,-2.98780300,4.83239900,0.59156500
C,-2.83432700,-0.25073400,0.05226400
C,-3.01805600,-1.59403800,0.40313600
C,-3.96652600,0.52412300,-0.24765800
C,-4.28865600,-2.16580400,0.45694000
H,-2.15656400,-2.21191800,0.64906700
C,-5.23216000,-0.04880800,-0.19798200
H,-3.84447500,1.56663700,-0.50278600
C,-5.42857700,-1.40032500,0.15069900
H,-4.38184300,-3.20808100,0.73959100
H,-6.09488000,0.56762900,-0.44018800
N,-6.71102600,-1.93976100,0.14987200
H,-7.45176300,-1.25654600,0.21100200

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C,-7.00426400,-3.22305900,0.76129200
H,-6.69525100,-3.28133600,1.81721400
H,-8.08058200,-3.39952900,0.70439700
H,-6.50888600,-4.03358300,0.21494600
H,-0.80713100,-0.51121700,0.14088000

Tetramethylsilane

0,1
Si,-1.384719048,-0.0002074412,-0.000534035
C,-3.2798935977,-0.0000267963,-0.0006646287
H,-3.6775851757,1.0215237138,0.0044778128
H,-3.6784930544,-0.5063173914,-0.88765022
H,-3.6782083059,-0.5149631897,0.8814232413
C,-0.7520926438,0.8934538434,1.5466476156
H,-1.0987530021,0.3991447839,2.4616889605
H,0.343692536,0.9120304658,1.5750286404
H,-1.1016809249,1.9320978329,1.5783763662
C,-0.752697508,-1.7867704959,0.0011642995
H,-1.102932937,-2.3337660947,-0.8819285098
H,0.3430953405,-1.821134593,-0.0004965386
H,-1.0997201177,-2.3309825844,0.8873728924
C,-0.7514986318,0.8930598074,-1.5475792636
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H,-1.1003720966,1.9319265503,-1.5774025981

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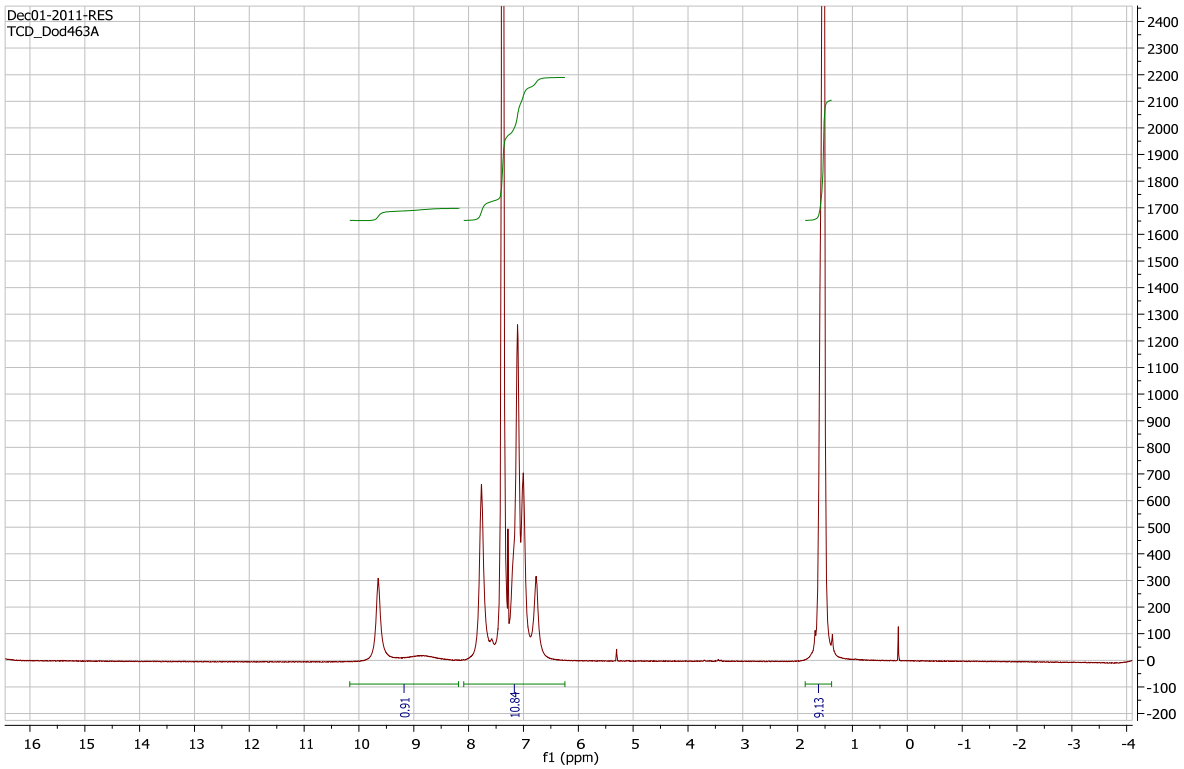
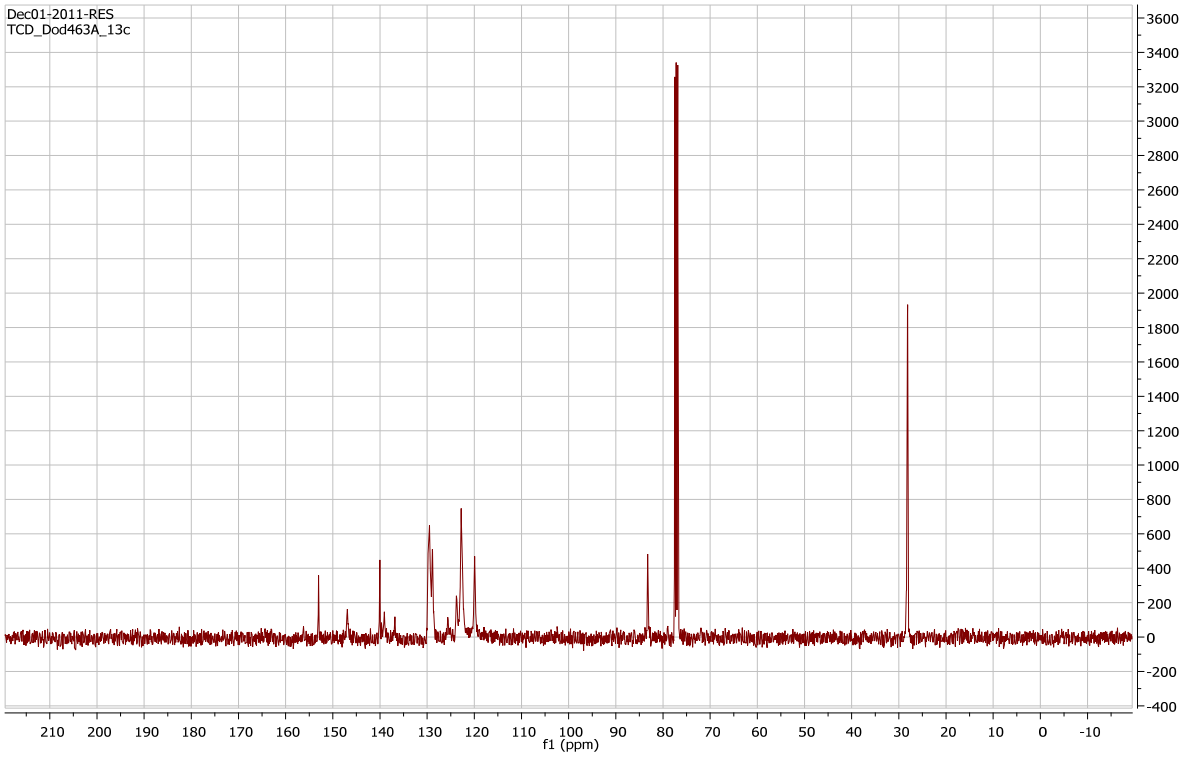
NMR SPECTRA

Compound 1: ^{1}H NMR, 20 °C, 400 MHz, $CDCl_3$



^{13}C NMR, 20 °C, 100 MHz, $CDCl_3$



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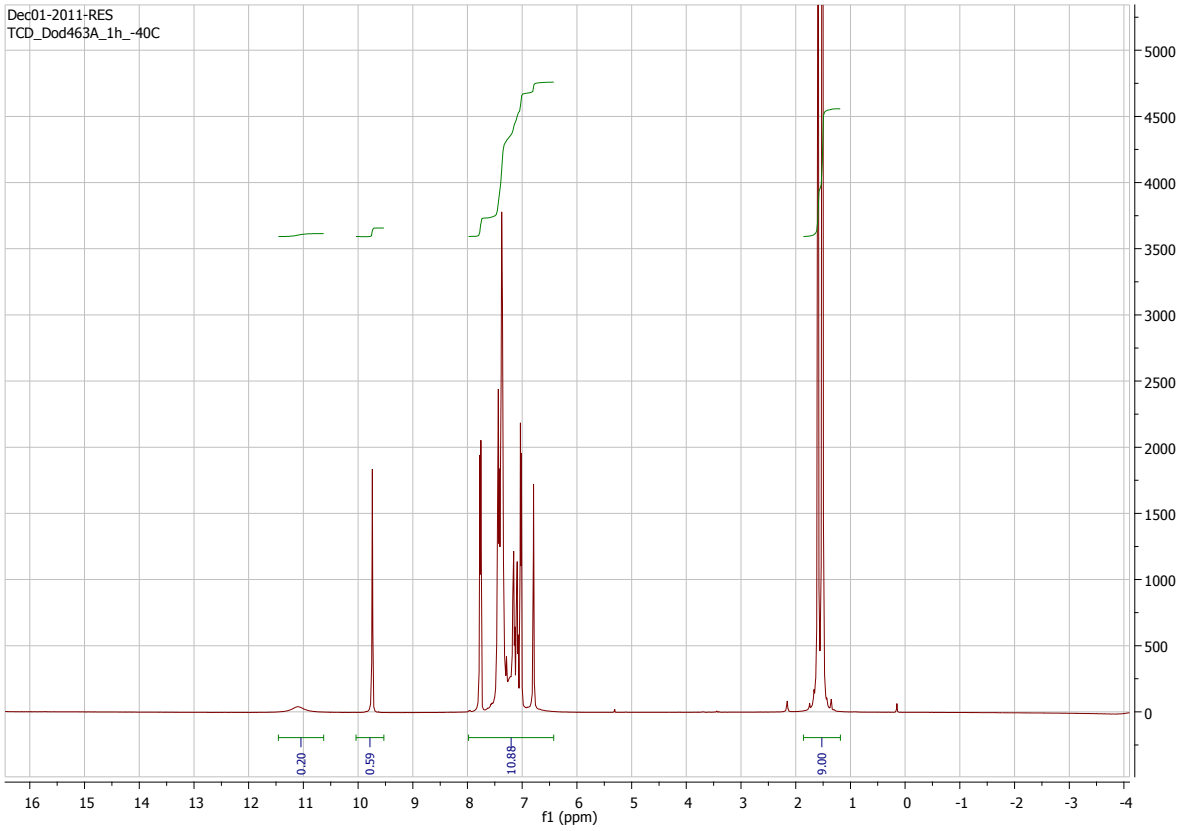
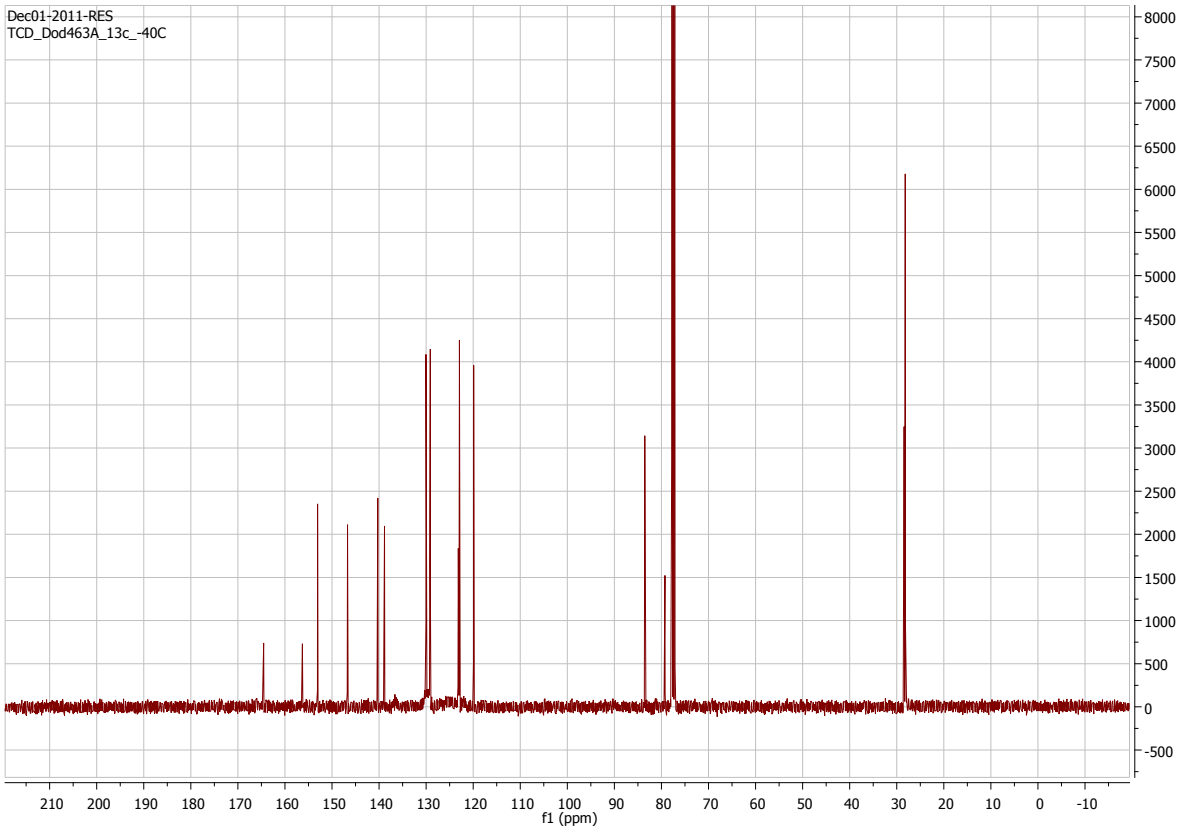
^{1}H NMR, -40 °C, 400 MHz, $CDCl_3$



^{13}C NMR, -40 °C, 100 MHz, $CDCl_3$



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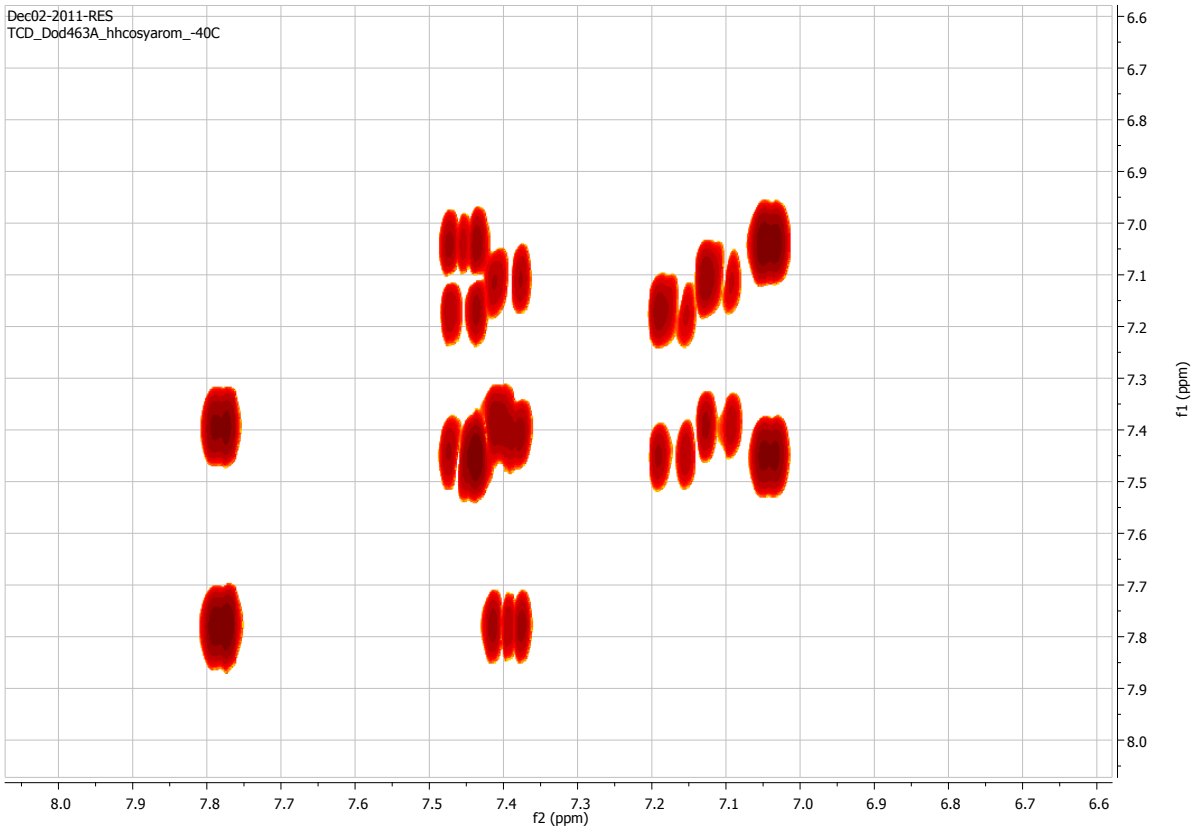
HH COSY, -40 °C, 400 MHz, $CDCl_3$

HH COSY, Aromatic region, -40 °C, 400 MHz, $CDCl_3$



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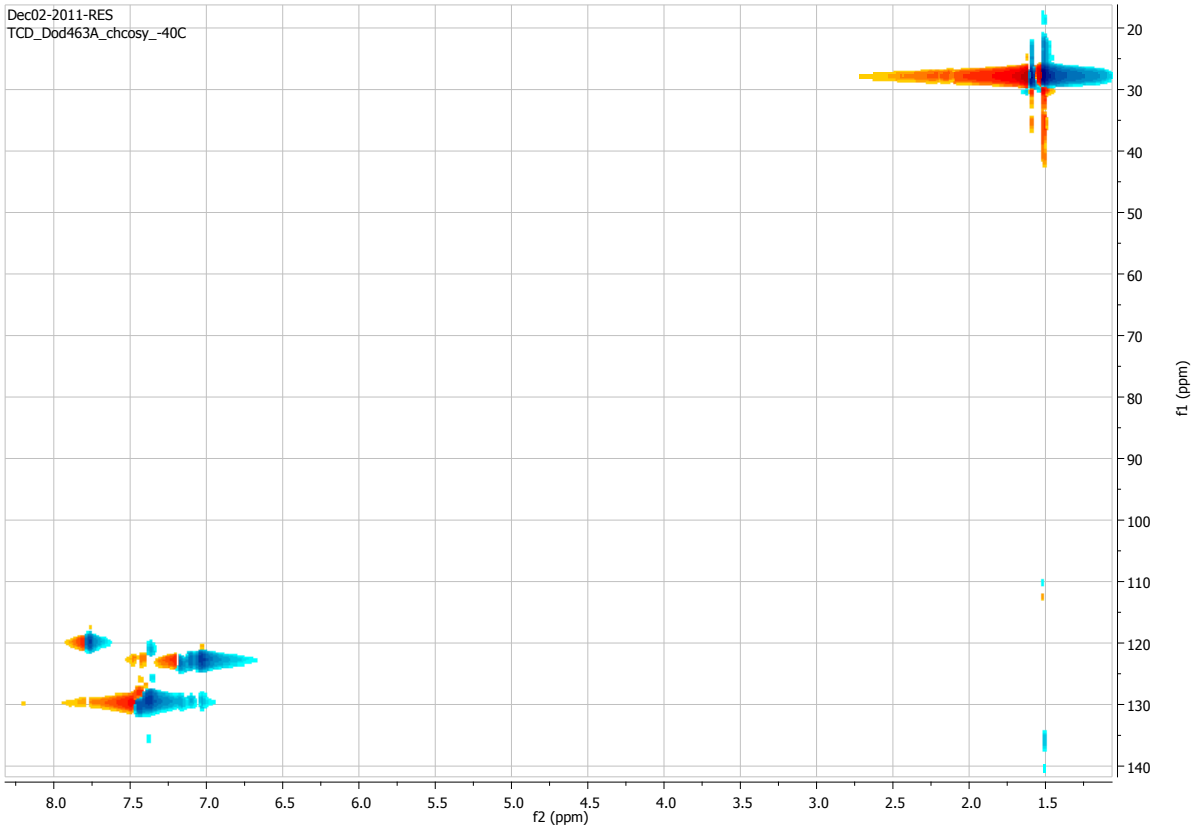
HSQC, -40 °C, 400 MHz, $CDCl_3$



HMBC, -40 °C, 400 MHz, $CDCl_3$

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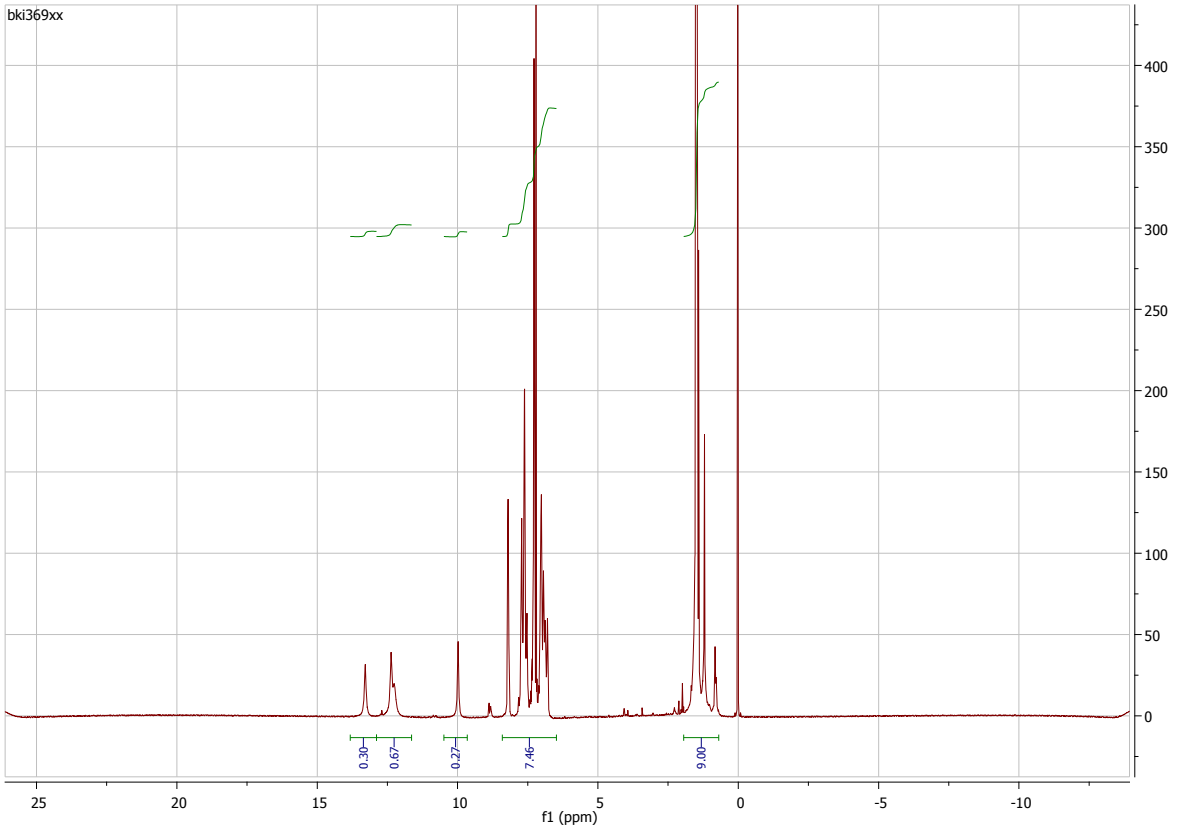
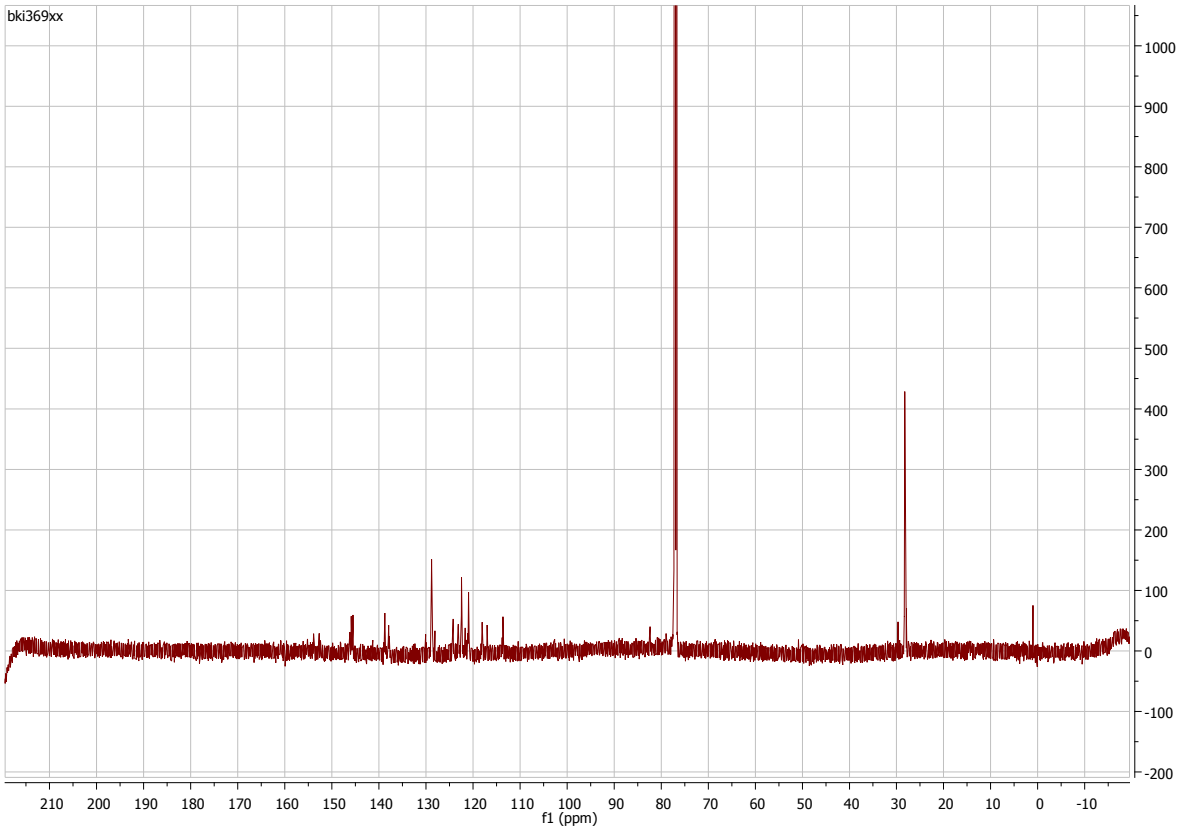
Compound 2: ^{1}H NMR, 20 °C, 400 MHz, $CDCl_3$



^{13}C NMR, 20 °C, 100 MHz, $CDCl_3$



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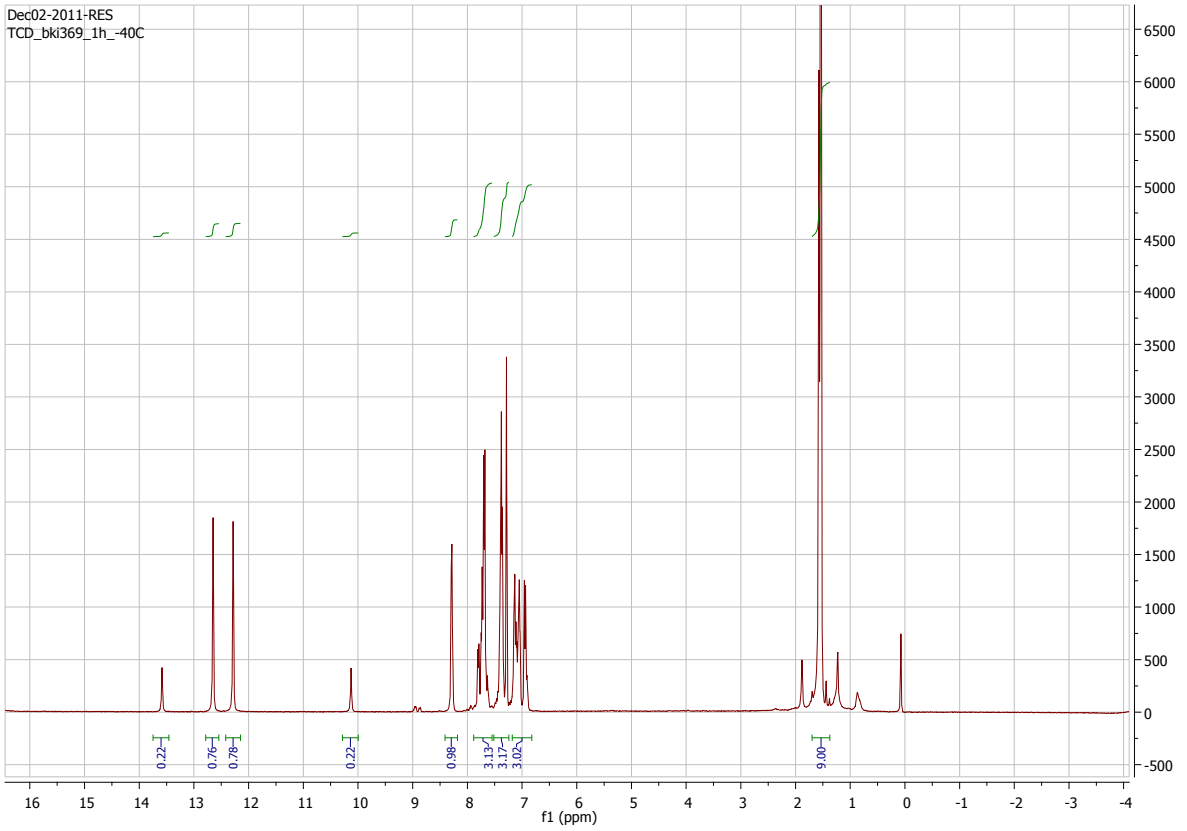
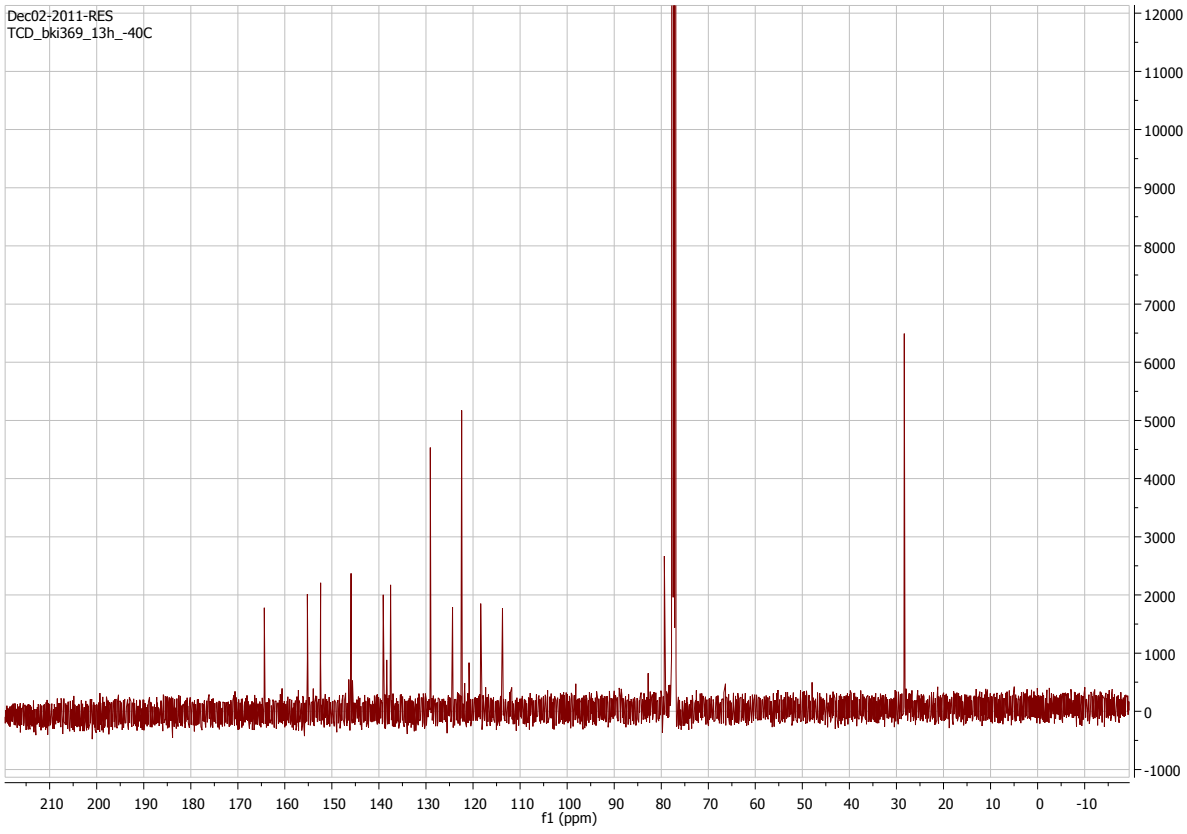
^{1}H NMR, -40 °C, 400 MHz, $CDCl_3$



^{13}C NMR, -40 °C, 100 MHz, $CDCl_3$



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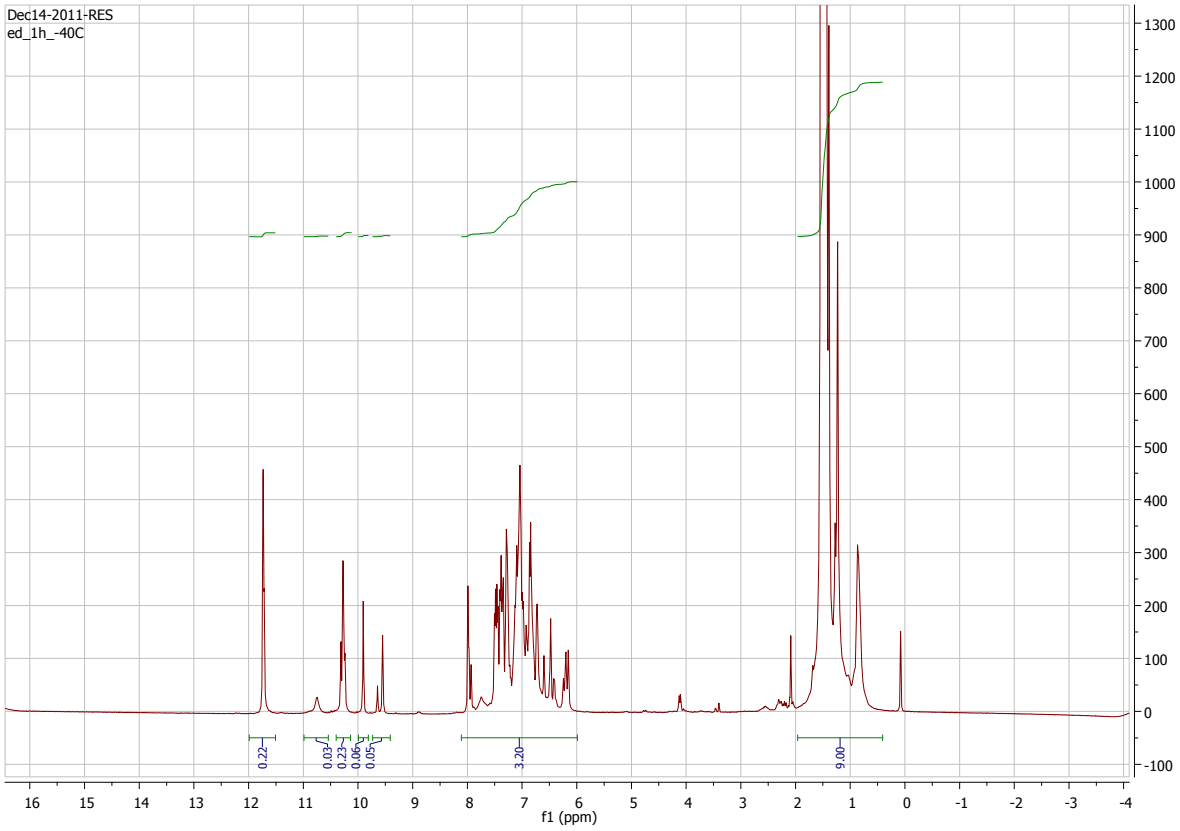
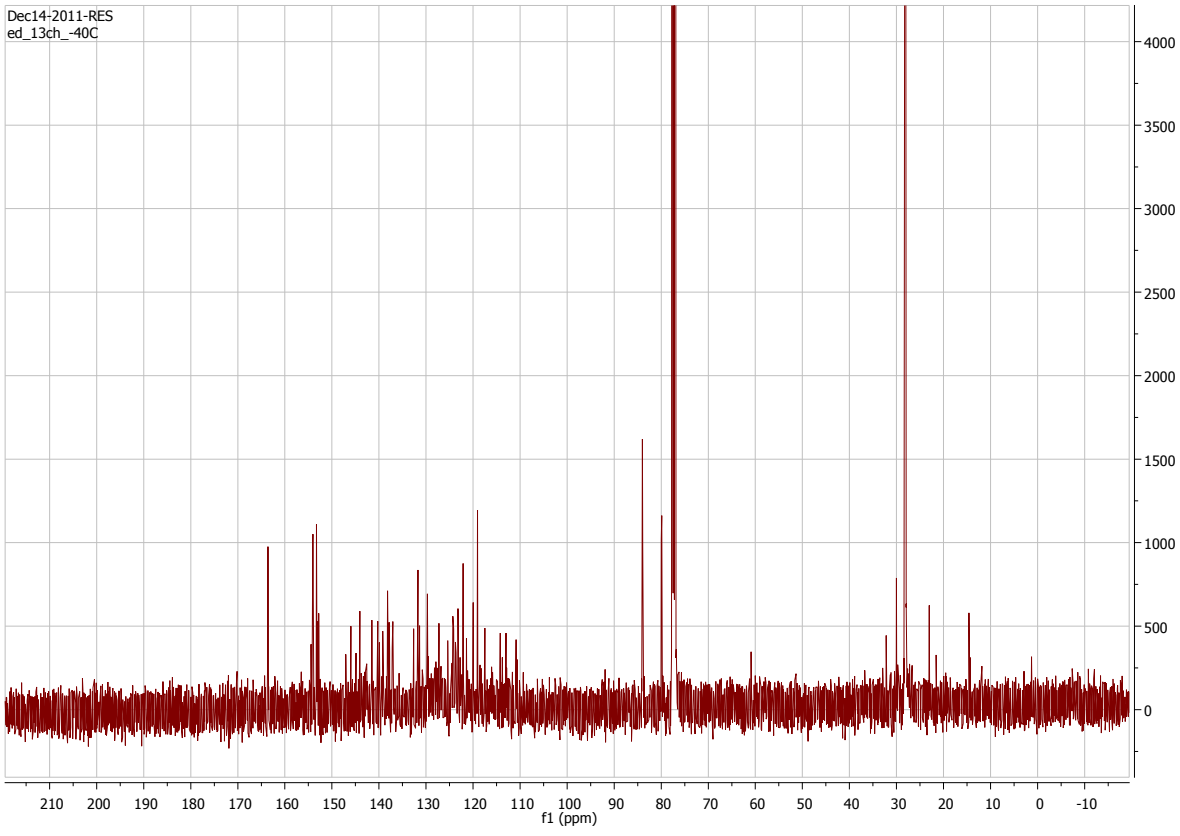
Compound 3: ^{1}H NMR, -40 °C, 400 MHz, $CDCl_3$



^{13}C NMR, -40 °C, 100 MHz, $CDCl_3$



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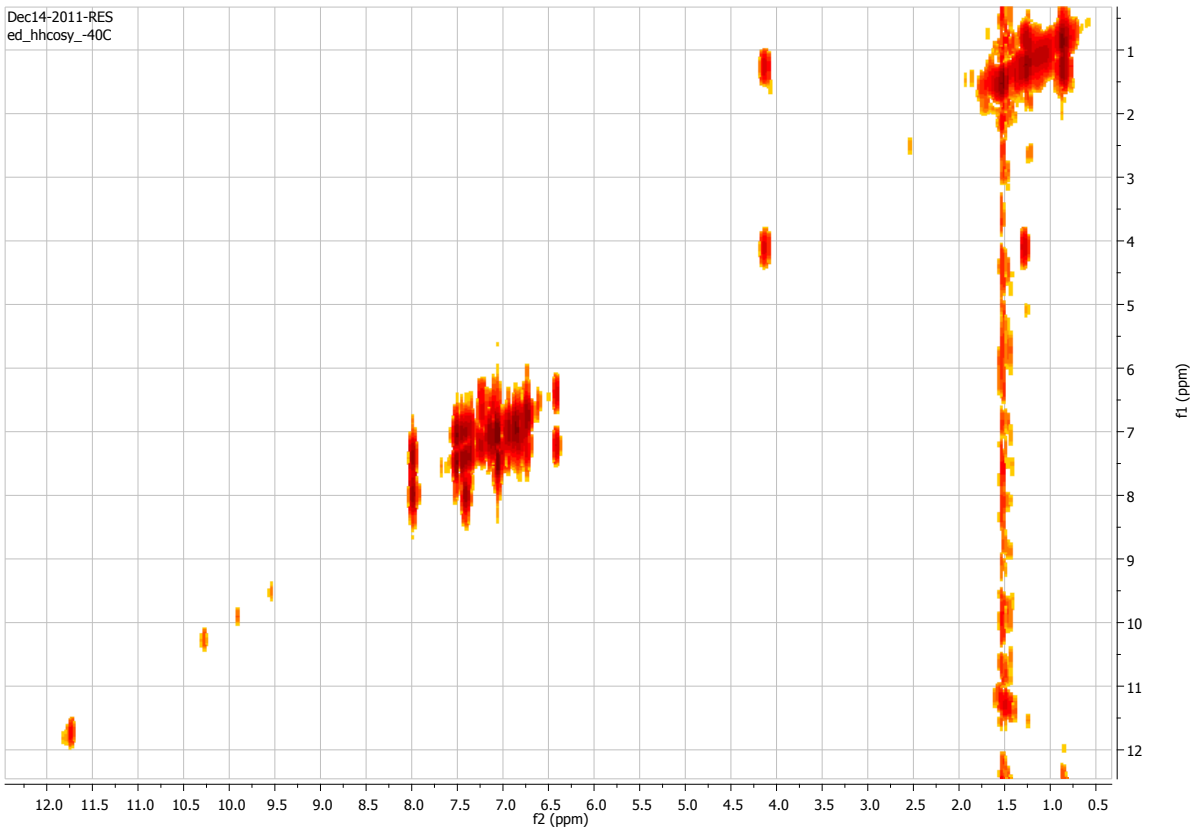
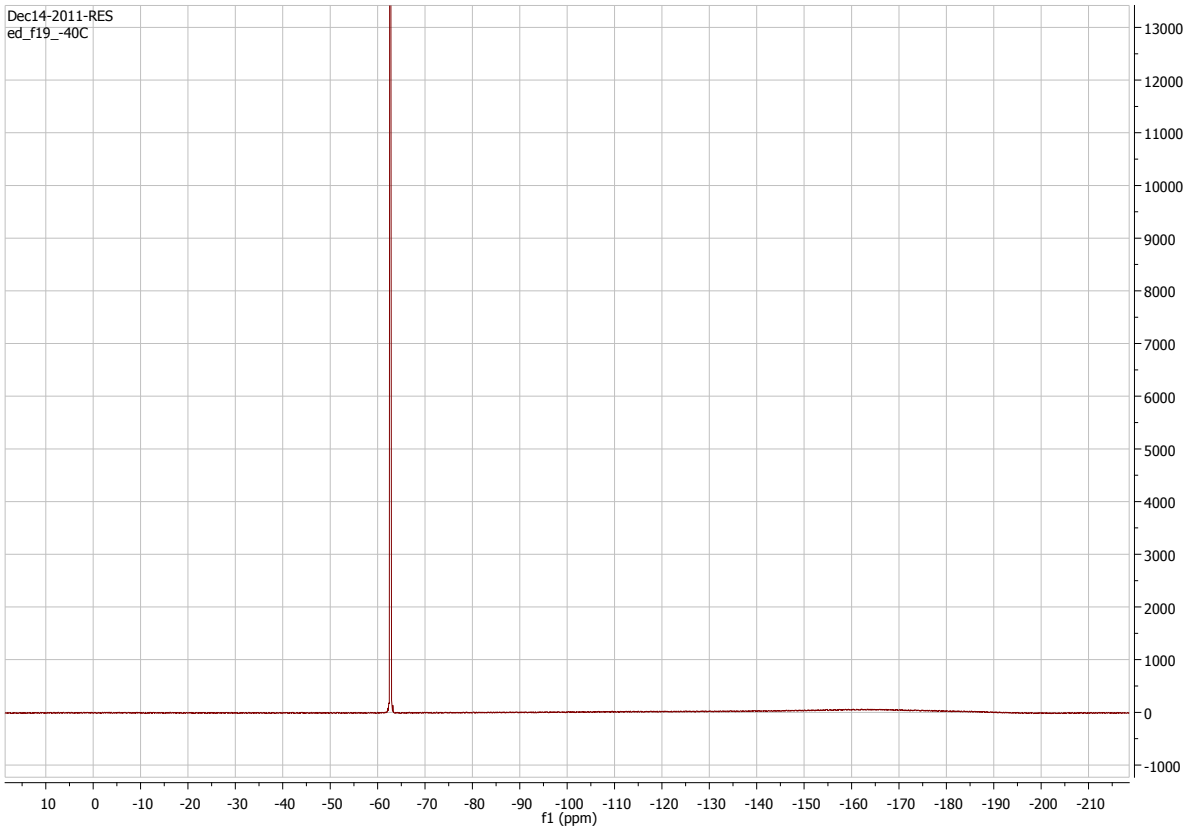
HH COSY, -40 °C, 400 MHz, $CDCl_3$



^{19}F NMR, -40 °C, 376 MHz, $CDCl_3$



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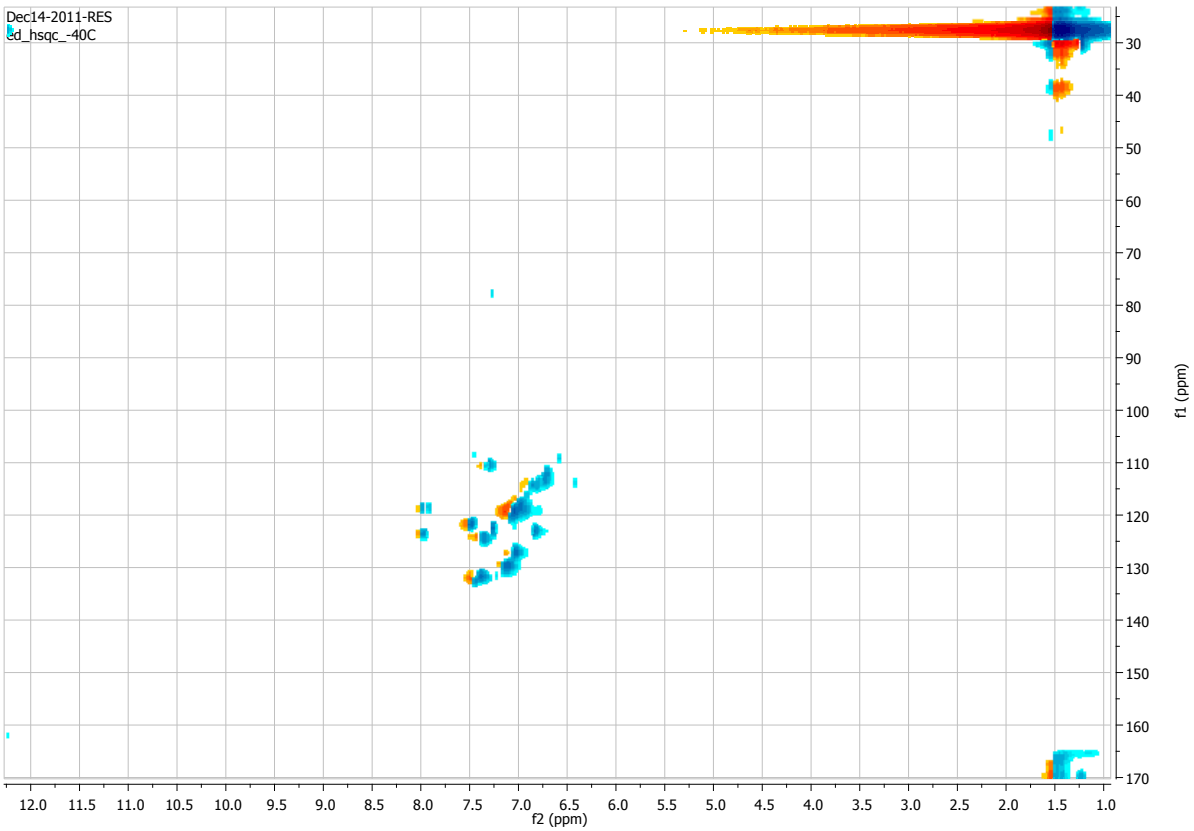
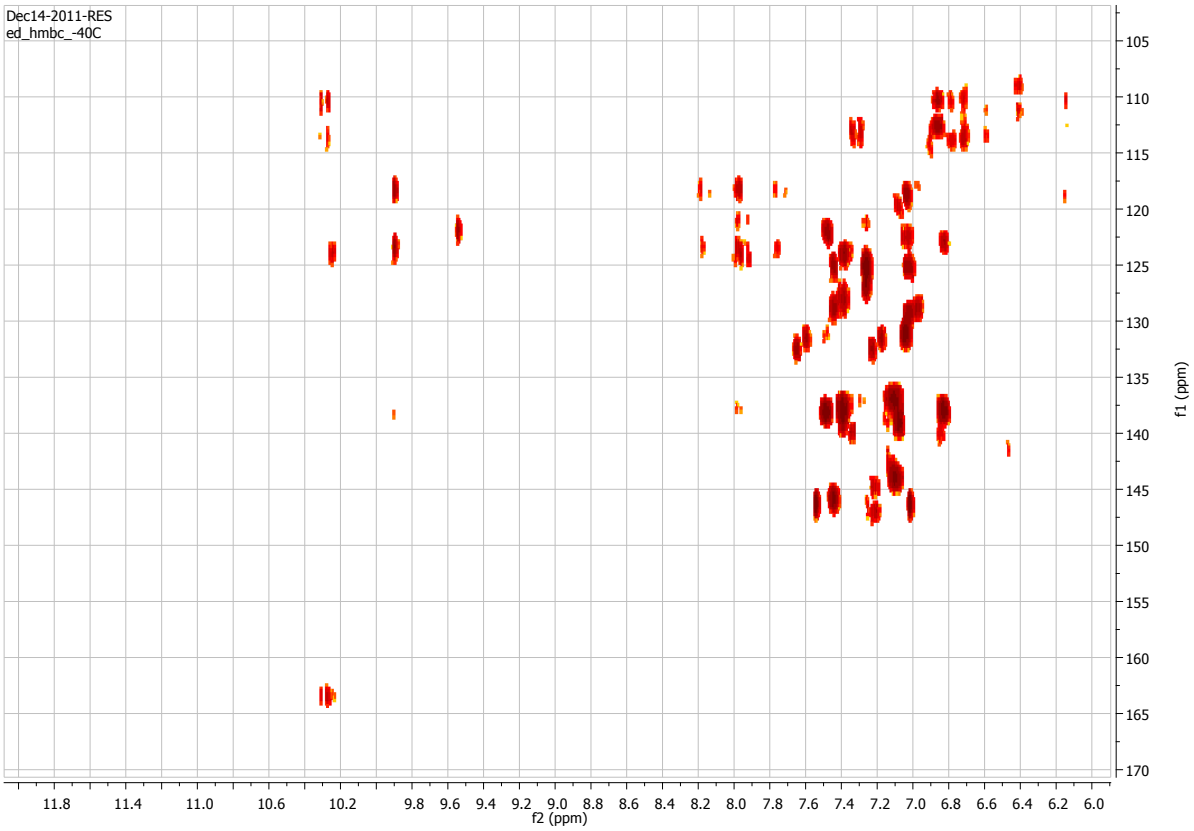
HSQC, -40 °C, 400 MHz, $CDCl_3$



HMBC, -40 °C, 400 MHz, $CDCl_3$