Supporting Information

Stereoselective synthesis of conformationally restricted KOR agonists based on the 2,5-diazabicyclo[2.2.2]octane scaffold

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Content

1. X-ray crystallography

For the determination of the X-ray structures of (*R*,*R*,*S*)-**15a** (WMS 53-09) and (*R*,*S*,*R*)-**18** (WMS 53-08), suitable single crystals had to be formed. For both compounds the method of vapour diffusion was chosen. The setup consists of an inner and an outer chamber. The compound was dissolved in the inner chamber in ca. 0.5 mL solvent, whereas the outer chamber contained 2.5 mL of an antisolvent. By closing the outer chamber the solvents start to equilibrate via vapour diffusion.

1.1. Molecular structure of (*R*,*R*,*S*)-15a

(*R*,*R*,*S*)-**15a** was crystallized using the following system: Inner chamber THF, outer chamber n-hexane.

(1*R*,4*R*,7*S*)-2,5-Dibenzyl-7-(pyrrolidin-1-yl)-2,5-diazabicyclo[2.2.2]octane-3,6,-dione ((*R*,*R*,*S*)-15a)

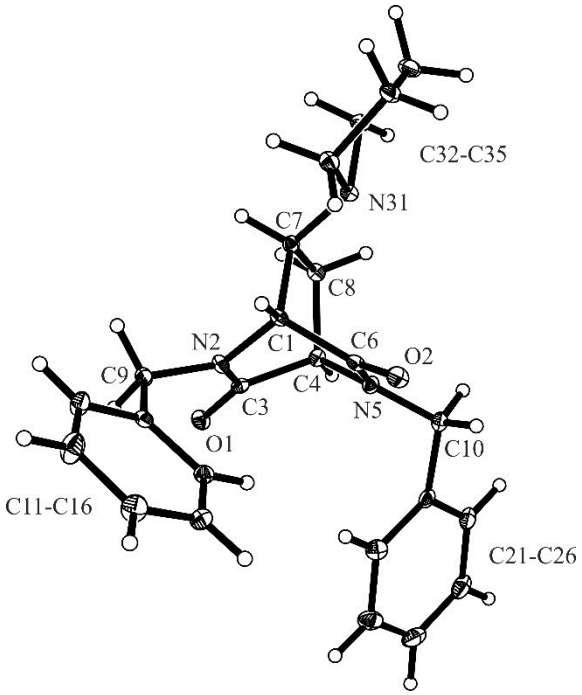


Table 1: Sample and crystal data for (*R*,*R*,*S*)-15a

Identification code	dan8114	
Chemical formula	$C_{24}H_{27}N_3O_2$	
Formula weight	389.48 g/mol	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal size	0.142 x 0.266 x 0.288 mm	
Crystal habit	colorless prism	
Crystal system	Tetragonal	
Space group	P 43	
Unit cell dimensions	a = 13.7270(3) Å	α = 90°
	b = 13.7270(3) Å	β= 90°
	c = 10.9453(3) Å	γ = 90°
Volume	2062.43(11) Å3	
Z	4	
Density (calculated)	1.254 g/cm^3	
Absorption coefficient	0.640 mm^{-1}	
F(000)	832	

Table 2: Data collection and structure refinement for (*R*,*R*,*S*)-15a

Theta range for data collection	3.22 to 68.39°
Index ranges	-15<=h<=16, -16<=k<=16, -11<=l<=13
Reflections collected	25621
Independent reflections	3636 [R(int) = 0.0259]
Coverage of independent reflections	99.4 %
Absorption correction	multi-scan
Max. and min. transmission	0.9150 and 0.8370
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	3636 / 1 / 262
Goodness-of-fit on F^2	1.103
Final R indices	3579 data; $I>2\sigma(I)$ R1 = 0.0260, wR2 = 0.0636
	all data R1 = 0.0267, wR2 = 0.0643
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0340P)^2+0.3333P]$ where $P=(F_o^2+2F_c^2)/3$
Absolute structure parameter	0.0(1)
Largest diff. peak and hole	0.107 and -0.156 eÅ^{-3}
R.M.S. deviation from mean	0.034 eÅ^{-3}

Table 3: Bond lengths (Å) for (*R*,*R*,*S*)-15a

C1-N2	1.470(2)	C1-C6	1.525(2)
C1-C7	1.549(2)	C1-H1	1.0
O1-C3	1.225(2)	N2-C3	1.354(2)
N2-C9	1.455(2)	O2-C6	1.231(2)
C3-C4	1.517(2)	C4-N5	1.476(2)
C4-C8	1.544(2)	C4-H4	1.0
N5-C6	1.352(2)	N5-C10	1.458(2)
C7-N31	1.461(2)	C7-C8	1.550(2)
C7-H7	1.0	C8-H8A	0.99
C8-H8B	0.99	C9-C11	1.514(2)
C9-H9A	0.99	C9-H9B	0.99
C10-C21	1.518(2)	C10-H10A	0.99
C10-H10B	0.99	C11-C12	1.388(3)
C11-C16	1.389(3)	C12-C13	1.391(2)
C12-H12	0.95	C13-C14	1.383(3)
C13-H13	0.95	C14-C15	1.386(3)
C14-H14	0.95	C15-C16	1.387(3)
C15-H15	0.95	C16-H16	0.95
C21-C26	1.392(3)	C21-C22	1.393(3)
C22-C23	1.389(3)	C22-H22	0.95
C23-C24	1.384(3)	C23-H23	0.95
C24-C25	1.385(3)	C24-H24	0.95
C25-C26	1.394(3)	C25-H25	0.95
C26-H26	0.95	N31-C32	1.470(2)
N31-C35	1.472(2)	C32-C33	1.531(2)
C32-H32A	0.99	C32-H32B	0.99
C33-C34	1.543(2)	C33-H33A	0.99
C33-H33B	0.99	C34-C35	1.528(2)
C34-H34A	0.99	C34-H34B	0.99
C35-H35A	0.99	C35-H35B	0.99

Table 4: Bond angles (°) for (*R*,*R*,*S*)-15a

N2-C1-C6	108.75(13)	N2-C1-C7	107.41(13)
C6-C1-C7	108.32(13)	N2-C1-H1	110.8
C6-C1-H1	110.8	C7-C1-H1	110.8
C3-N2-C9	123.70(14)	C3-N2-C1	115.70(13)
C9-N2-C1	120.30(13)	O1-C3-N2	125.45(16)
O1-C3-C4	125.43(15)	N2-C3-C4	109.09(13)
N5-C4-C3	108.03(13)	N5-C4-C8	107.75(13)
C3-C4-C8	108.12(14)	N5-C4-H4	110.9
C3-C4-H4	110.9	C8-C4-H4	110.9
C6-N5-C10	124.18(15)	C6-N5-C4	115.07(15)
C10-N5-C4	120.13(13)	O2-C6-N5	125.75(17)
O2-C6-C1	124.71(15)	N5-C6-C1	109.53(14)
N31-C7-C1	110.05(13)	N31-C7-C8	111.66(13)
C1-C7-C8	106.49(13)	N31-C7-H7	109.5
C1-C7-H7	109.5	C8-C7-H7	109.5
C4-C8-C7	108.91(13)	C4-C8-H8A	109.9
C7-C8-H8A	109.9	C4-C8-H8B	109.9
C7-C8-H8B	109.9	H8A-C8-H8B	108.3
N2-C9-C11	113.03(15)	N2-C9-H9A	109.0
C11-C9-H9A	109.0	N2-C9-H9B	109.0
C11-C9-H9B	109.0	H9A-C9-H9B	107.8
N5-C10-C21	113.96(14)	N5-C10-H10A	108.8
C21-C10-H10A	108.8	N5-C10-H10B	108.8
C21-C10-H10B	108.8	H10A-C10-H10B	107.7
C12-C11-C16	119.16(16)	C12-C11-C9	122.36(15)
C16-C11-C9	118.47(16)	C11-C12-C13	120.17(16)
C11-C12-H12	119.9	C13-C12-H12	119.9
C14-C13-C12	120.47(19)	C14-C13-H13	119.8
C12-C13-H13	119.8	C13-C14-C15	119.35(18)
C13-C14-H14	120.3	C15-C14-H14	120.3
C14-C15-C16	120.34(18)	C14-C15-H15	119.8
C16-C15-H15	119.8	C15-C16-C11	120.44(19)
C15-C16-H16	119.8	C11-C16-H16	119.8
C26-C21-C22	118.80(17)	C26-C21-C10	121.93(16)

C22-C21-C10	119.21(16)	C23-C22-C21	120.62(18)
C23-C22-H22	119.7	C21-C22-H22	119.7
C24-C23-C22	120.19(18)	C24-C23-H23	119.9
C22-C23-H23	119.9	C23-C24-C25	119.81(18)
C23-C24-H24	120.1	C25-C24-H24	120.1
C24-C25-C26	120.04(19)	C24-C25-H25	120.0
C26-C25-H25	120.0	C21-C26-C25	120.52(18)
C21-C26-H26	119.7	C25-C26-H26	119.7
C7-N31-C32	113.22(13)	C7-N31-C35	113.77(13)
C32-N31-C35	103.07(13)	N31-C32-C33	103.89(13)
N31-C32-H32A	111.0	C33-C32-H32A	111.0
N31-C32-H32B	111.0	C33-C32-H32B	111.0
H32A-C32-H32B	109.0	C32-C33-C34	104.12(13)
C32-C33-H33A	110.9	C34-C33-H33A	110.9
C32-C33-H33B	110.9	C34-C33-H33B	110.9
H33A-C33-H33B	109.0	C35-C34-C33	104.67(14)
C35-C34-H34A	110.8	C33-C34-H34A	110.8
C35-C34-H34B	110.8	C33-C34-H34B	110.8
H34A-C34-H34B	108.9	N31-C35-C34	103.54(13)
N31-C35-H35A	111.1	C34-C35-H35A	111.1
N31-C35-H35B	111.1	C34-C35-H35B	111.1
H35A-C35-H35B	109.0		

Table 5: Torsion angles (°) for (*R*,*R*,*S*)-15a

C6-C1-N2-C3	-55.54(18)	C7-C1-N2-C3	61.48(19)
C6-C1-N2-C9	130.52(15)	C7-C1-N2-C9	-112.47(16)
C9-N2-C3-O1	-3.6(3)	C1-N2-C3-O1	-177.30(16)
C9-N2-C3-C4	174.58(15)	C1-N2-C3-C4	0.87(19)
O1-C3-C4-N5	-126.90(17)	N2-C3-C4-N5	54.93(17)
O1-C3-C4-C8	116.75(18)	N2-C3-C4-C8	-61.41(17)
C3-C4-N5-C6	-58.37(17)	C8-C4-N5-C6	58.21(17)
C3-C4-N5-C10	130.24(15)	C8-C4-N5-C10	-113.18(15)
C10-N5-C6-O2	-5.7(3)	C4-N5-C6-O2	-176.74(15)
C10-N5-C6-C1	174.54(14)	C4-N5-C6-C1	3.54(18)
N2-C1-C6-O2	-127.54(16)	C7-C1-C6-O2	116.02(17)
N2-C1-C6-N5	52.18(16)	C7-C1-C6-N5	-64.26(16)
N2-C1-C7-N31	179.48(13)	C6-C1-C7-N31	-63.22(17)
N2-C1-C7-C8	-59.33(17)	C6-C1-C7-C8	57.97(17)
N5-C4-C8-C7	-58.88(17)	C3-C4-C8-C7	57.65(17)
N31-C7-C8-C4	122.14(15)	C1-C7-C8-C4	1.98(19)
C3-N2-C9-C11	127.14(16)	C1-N2-C9-C11	-59.42(19)
C6-N5-C10-C21	117.52(17)	C4-N5-C10-C21	-71.92(19)
N2-C9-C11-C12	-30.4(2)	N2-C9-C11-C16	150.37(16)
C16-C11-C12-C13	2.2(3)	C9-C11-C12-C13	-177.03(15)
C11-C12-C13-C14	0.5(3)	C12-C13-C14-C15	-2.1(3)
C13-C14-C15-C16	1.1(3)	C14-C15-C16-C11	1.5(3)
C12-C11-C16-C15	-3.1(3)	C9-C11-C16-C15	176.09(17)
N5-C10-C21-C26	-40.0(2)	N5-C10-C21-C22	143.02(16)
C26-C21-C22-C23	-1.8(3)	C10-C21-C22-C23	175.25(17)
C21-C22-C23-C24	1.0(3)	C22-C23-C24-C25	0.7(3)
C23-C24-C25-C26	-1.5(3)	C22-C21-C26-C25	1.0(3)
C10-C21-C26-C25	-175.94(17)	C24-C25-C26-C21	0.6(3)
C1-C7-N31-C32	-177.92(14)	C8-C7-N31-C32	64.03(18)
C1-C7-N31-C35	-60.67(18)	C8-C7-N31-C35	-178.71(14)
C7-N31-C32-C33	167.40(14)	C35-N31-C32-C33	44.04(18)
N31-C32-C33-C34	-26.33(19)	C32-C33-C34-C35	-0.3(2)
C7-N31-C35-C34	-167.09(14)	C32-N31-C35-C34	-44.10(17)
C33-C34-C35-N31	26.73(19)		

Table 6: Hydrogen bond distances (Å) and angles (°) for (R,R,S)-15a

	Donor-H	Acceptor-H	Donor-Acceptor	Angle
C4-H4...O1	1.00	2.39	3.121(2)	129.1
C9-H9B...O2	0.99	2.38	3.232(2)	144.3

1.2. Molecular structure of (*R*,*S*,*R*)-18

(*R*,*S*,*R*)-**18** (WMS 53-08) was crystallized using the following system; Inner chamber iPr_2O, outer chamber n-hexane. Due to partial racemization the formed crystals contained a racemic mixture of (*R*,*S*,*R*)-**18** and (*S*,*R*,*S*)-**18**.

1,1'-((1*R*,4*S*,7*R*)-7-(pyrrolidin-1-yl)-2,5-diazabicyclo[2.2.2]octane-2,5-diyl)bis(2-(3,4-dichlorophenyl)ethanone) ((*R*,*S*,*R*)-18)

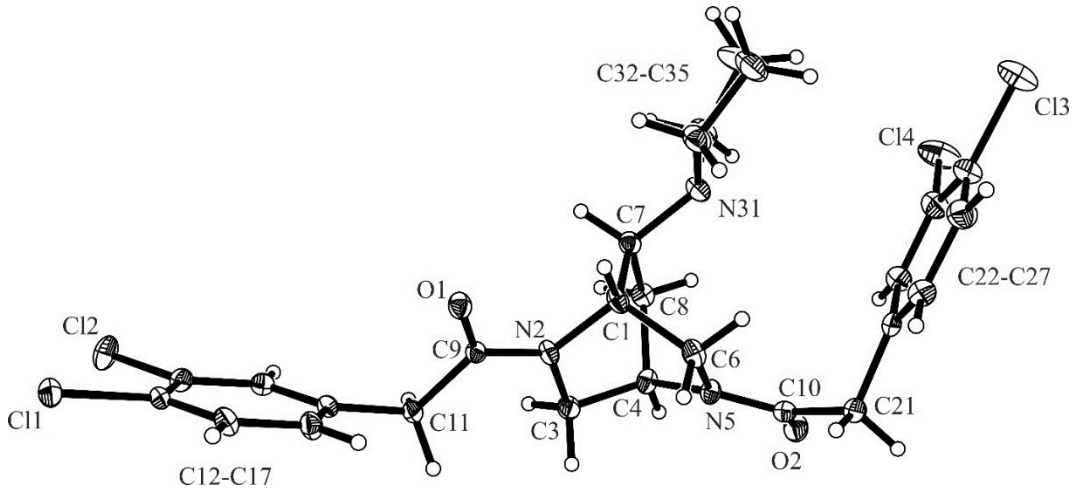


Table 7: Sample and crystal data for 18

Identification code	dan8093	
Chemical formula	$C_{26}H_{27}Cl_4N_3O_2$	
Formula weight	555.30 g/mol	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal size	0.015 x 0.051 x 0.228 mm	
Crystal habit	colorless needle	
Crystal system	Monoclinic	
Space group	P 1 2/c 1	
Unit cell dimensions	a = 24.6806(6) Å	α = 90°
	b = 6.2455(2) Å	β = 93.5410(10)°
	c = 16.1174(4) Å	γ = 90°
Volume	2479.64(12) $Å^3$	
Z	4	
Density (calculated)	1.487 g/cm^3	
Absorption coefficient	4.588 mm^{-1}	
F(000)	1152	

Table 8: Data collection and structure refinement for 18

Theta range for data collection	3.59 to 68.36°	
Index ranges	-29<=h<=29, -7<=k<=7, -19<=l<=19	
Reflections collected	31737	
Independent reflections	4563 [R(int) = 0.0860]	
Coverage of independent reflections	99.8%	
Absorption correction	multi-scan	
Max. and min. transmission	0.9340 and 0.4210	
Structure solution technique	direct methods	
Structure solution program	SHELXL-2014 (Sheldrick, 2014)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	4563 / 0 / 316	
Goodness-of-fit on F^2	1.055	
Δ/σmax	0.001	
Final R indices	3427 data; I>2σ(I)	R1 = 0.0551, wR2 = 0.1299
	all data	R1 = 0.0793, wR2 = 0.1425
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0644P)^2+3.0587P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.618 and -0.443 eÅ^{-3}	
R.M.S. deviation from mean	0.068 eÅ^{-3}	

Table 9: Bond lengths (Å) for 18

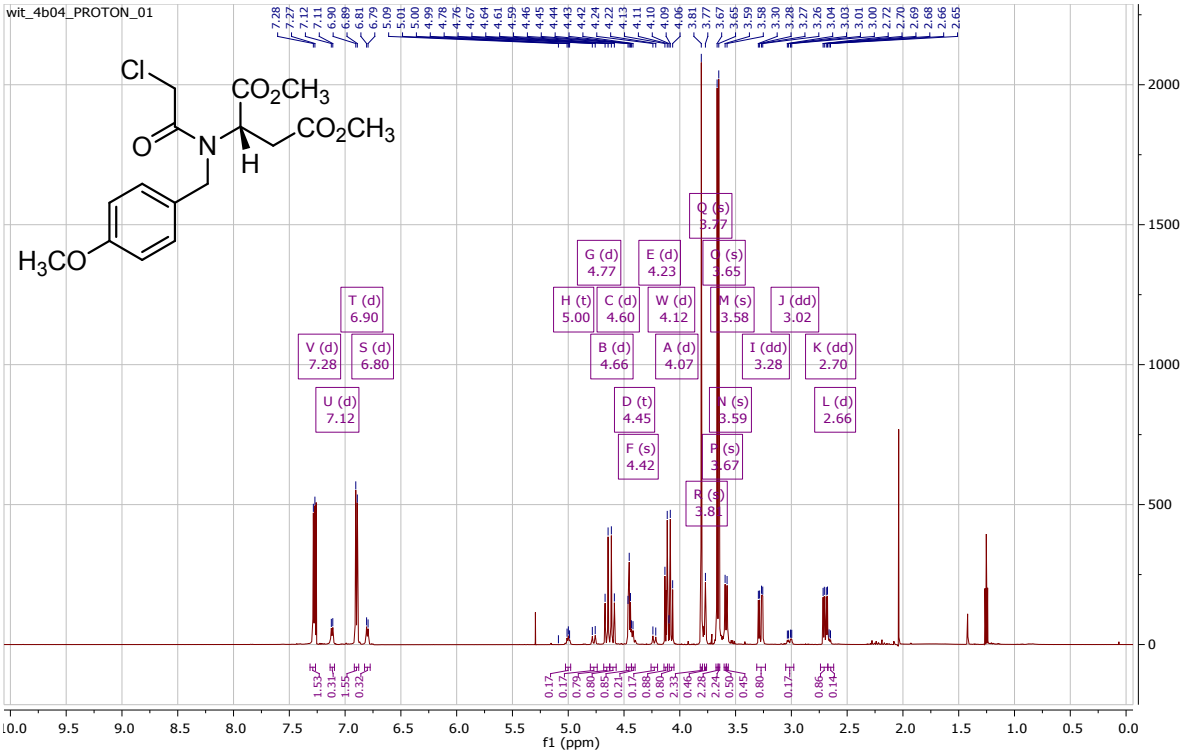
Cl1-C14	1.731(3)	Cl2-C15	1.731(3)
Cl3-C24	1.740(4)	Cl4-C25	1.735(4)
N2-C9	1.350(4)	N2-C1	1.472(4)
N2-C3	1.487(4)	N5-C10	1.362(4)
N5-C6	1.461(4)	N5-C4	1.468(4)
N31-C7	1.466(4)	N31-C35	1.471(5)
N31-C32	1.481(5)	O1-C9	1.225(4)
O2-C10	1.231(4)	C1-C6	1.515(5)
C1-C7	1.540(5)	C1-H1	1.0
C3-C4	1.515(5)	C3-H3A	0.99
C3-H3B	0.99	C4-C8	1.535(4)
C4-H4	1.0	C6-H6A	0.99
C6-H6B	0.99	C7-C8	1.550(5)
C7-H7	1.0----	C8-H8A	0.99
C8-H8B	0.99	C9-C11	1.530(4)
C10-C21	1.507(5)	C11-C12	1.501(4)
C11-H11A	0.99	C11-H11B	0.99
C12-C13	1.387(5)	C12-C17	1.398(5)
C13-C14	1.385(5)	C13-H13	0.95
C14-C15	1.388(5)	C15-C16	1.383(5)
C16-C17	1.380(5)	C16-H16	0.95
C17-H17	0.95	C21-C22	1.534(5)
C21-H21A	0.99	C21-H21B	0.99
C22-C23	1.379(5)	C22-C27	1.390(5)
C23-C24	1.374(5)	C23-H23	0.95
C24-C25	1.383(6)	C25-C26	1.376(6)
C26-C27	1.391(5)	C26-H26	0.95
C27-H27	0.95	C32-C33	1.497(6)
C32-H32A	0.99	C32-H32B	0.99
C33-C34	1.489(7)	C33-H33A	0.99
C33-H33B	0.99	C34-C35	1.516(5)
C34-H34A	0.99	C34-H34B	0.99
C35-H35A	0.99	C35-H35B	0.99

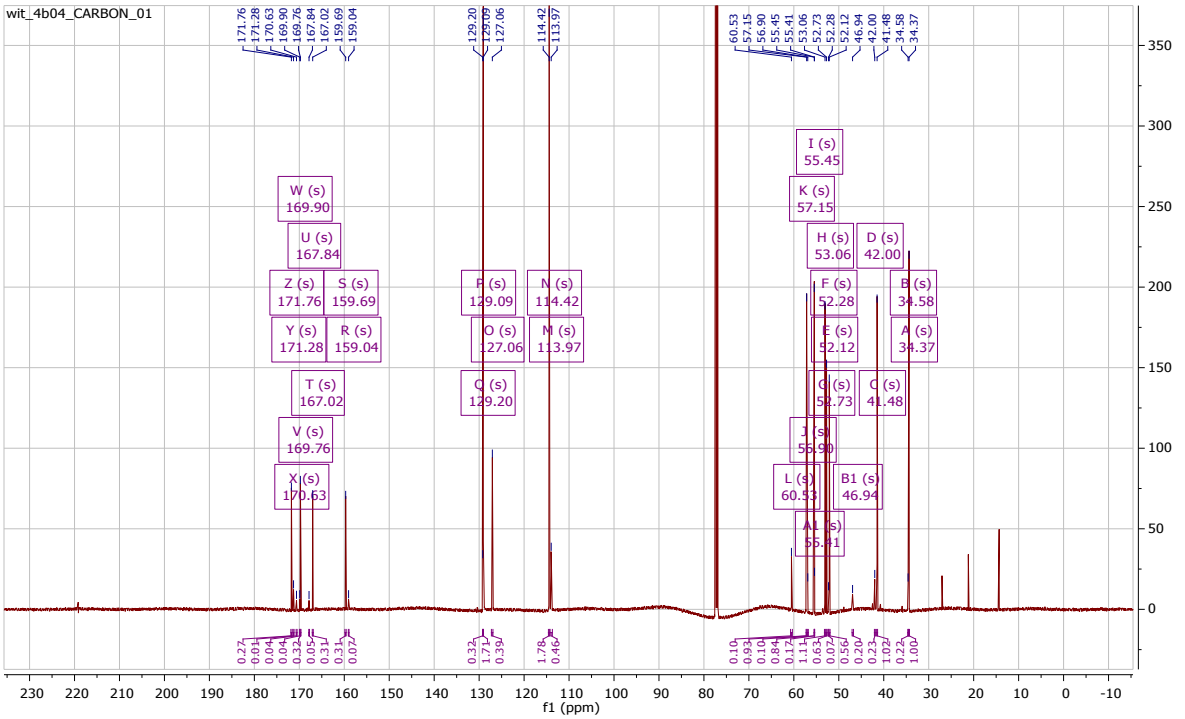
Table 10: Bond angles (°) for 18

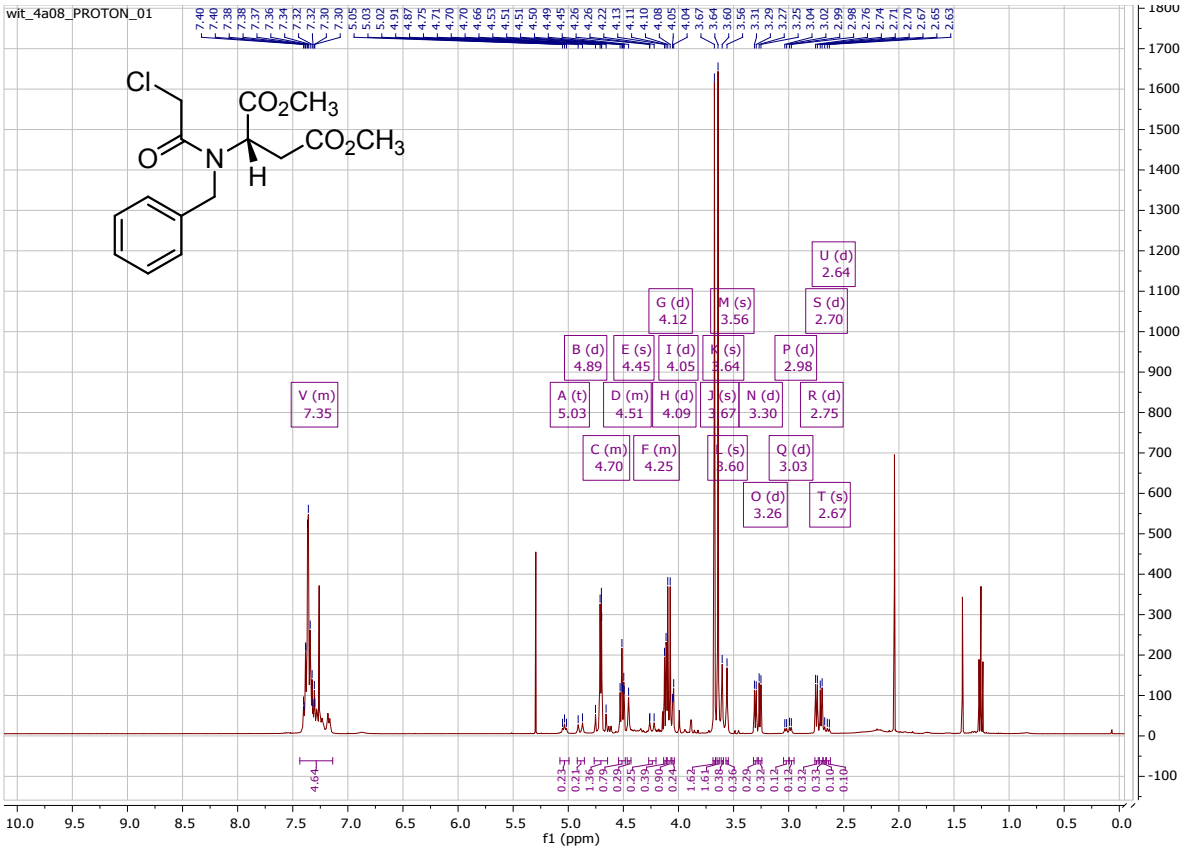
C9-N2-C1	121.8(3)	C9-N2-C3	124.5(3)
C1-N2-C3	113.5(3)	C10-N5-C6	124.2(3)
C10-N5-C4	119.4(3)	C6-N5-C4	113.4(3)
C7-N31-C35	114.0(3)	C7-N31-C32	111.8(3)
C35-N31-C32	105.8(3)	N2-C1-C6	109.1(3)
N2-C1-C7	106.2(3)	C6-C1-C7	111.5(3)
N2-C1-H1	110.0	C6-C1-H1	110.0
C7-C1-H1	110.0	N2-C3-C4	106.5(3)
N2-C3-H3A	110.4	C4-C3-H3A	110.4
N2-C3-H3B	110.4	C4-C3-H3B	110.4
H3A-C3-H3B	108.6	N5-C4-C3	109.5(3)
N5-C4-C8	107.8(3)	C3-C4-C8	109.8(3)
N5-C4-H4	109.9	C3-C4-H4	109.9
C8-C4-H4	109.9	N5-C6-C1	107.7(3)
N5-C6-H6A	110.2	C1-C6-H6A	110.2
N5-C6-H6B	110.2	C1-C6-H6B	110.2
H6A-C6-H6B	108.5	N31-C7-C1	111.4(3)
N31-C7-C8	110.4(3)	C1-C7-C8	107.5(3)
N31-C7-H7	109.2	C1-C7-H7	109.2
C8-C7-H7	109.2	C4-C8-C7	109.2(3)
C4-C8-H8A	109.8	C7-C8-H8A	109.8
C4-C8-H8B	109.8	C7-C8-H8B	109.8
H8A-C8-H8B	108.3	O1-C9-N2	122.9(3)
O1-C9-C11	122.1(3)	N2-C9-C11	115.0(3)
O2-C10-N5	122.6(3)	O2-C10-C21	121.0(3)
N5-C10-C21	116.4(3)	C12-C11-C9	113.5(3)
C12-C11-H11A	108.9	C9-C11-H11A	108.9
C12-C11-H11B	108.9	C9-C11-H11B	108.9
H11A-C11-H11B	107.7	C13-C12-C17	118.5(3)
C13-C12-C11	120.4(3)	C17-C12-C11	121.1(3)
C14-C13-C12	120.7(3)	C14-C13-H13	119.6
C12-C13-H13	119.6	C13-C14-C15	120.4(3)
C13-C14-Cl1	119.4(3)	C15-C14-Cl1	120.2(3)
C16-C15-C14	119.2(3)	C16-C15-Cl2	119.5(3)

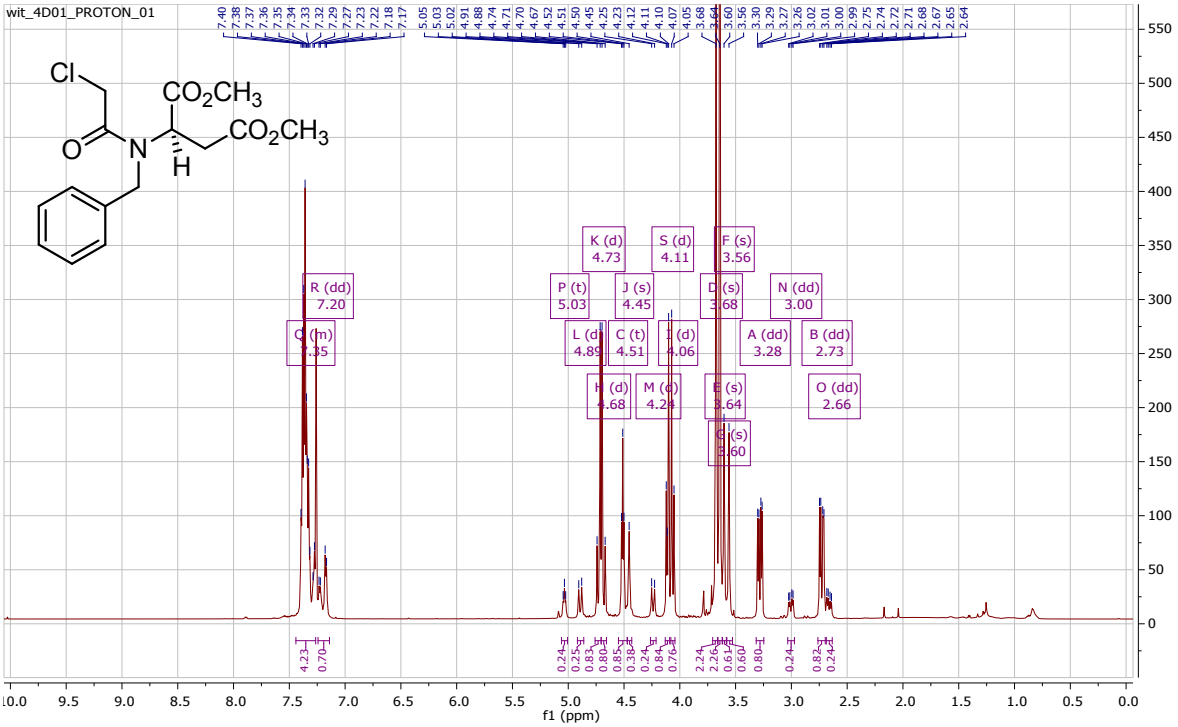
C14-C15-Cl2	121.4(3)	C17-C16-C15	120.6(3)
C17-C16-H16	119.7	C15-C16-H16	119.7
C16-C17-C12	120.6(3)	C16-C17-H17	119.7
C12-C17-H17	119.7	C10-C21-C22	112.2(3)
C10-C21-H21A	109.2	C22-C21-H21A	109.2
C10-C21-H21B	109.2	C22-C21-H21B	109.2
H21A-C21-H21B	107.9	C23-C22-C27	119.7(3)
C23-C22-C21	120.2(3)	C27-C22-C21	120.1(3)
C24-C23-C22	120.5(4)	C24-C23-H23	119.7
C22-C23-H23	119.7	C23-C24-C25	120.3(4)
C23-C24-Cl3	119.6(3)	C25-C24-Cl3	120.1(3)
C26-C25-C24	119.6(3)	C26-C25-Cl4	119.2(3)
C24-C25-Cl4	121.2(3)	C25-C26-C27	120.5(4)
C25-C26-H26	119.8	C27-C26-H26	119.8
C22-C27-C26	119.4(4)	C22-C27-H27	120.3
C26-C27-H27	120.3	N31-C32-C33	105.5(4)
N31-C32-H32A	110.6	C33-C32-H32A	110.6
N31-C32-H32B	110.6	C33-C32-H32B	110.6
H32A-C32-H32B	108.8	C34-C33-C32	107.8(4)
C34-C33-H33A	110.1	C32-C33-H33A	110.1
C34-C33-H33B	110.1	C32-C33-H33B	110.1
H33A-C33-H33B	108.5	C33-C34-C35	105.0(4)
C33-C34-H34A	110.8	C35-C34-H34A	110.8
C33-C34-H34B	110.8	C35-C34-H34B	110.8
H34A-C34-H34B	108.8	N31-C35-C34	104.4(3)
N31-C35-H35A	110.9	C34-C35-H35A	110.9
N31-C35-H35B	110.9	C34-C35-H35B	110.9
H35A-C35-H35B	108.9		

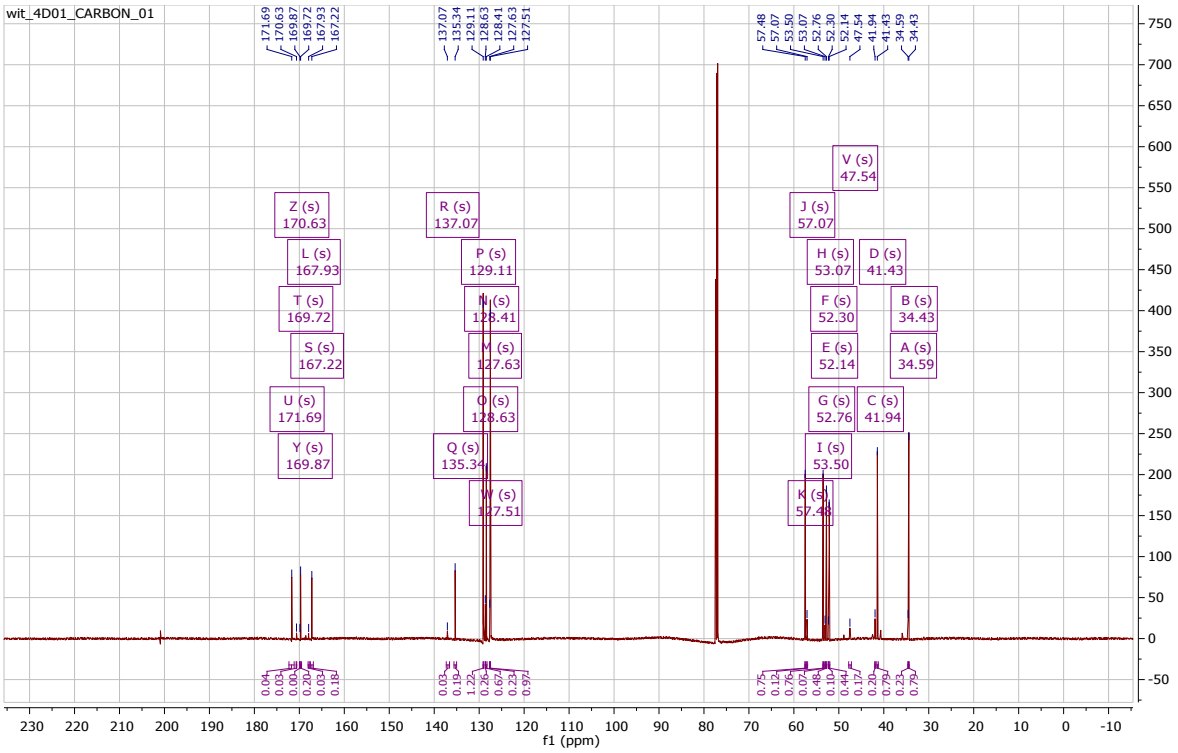
2. ^{1}H and ^{13}C NMR spectra

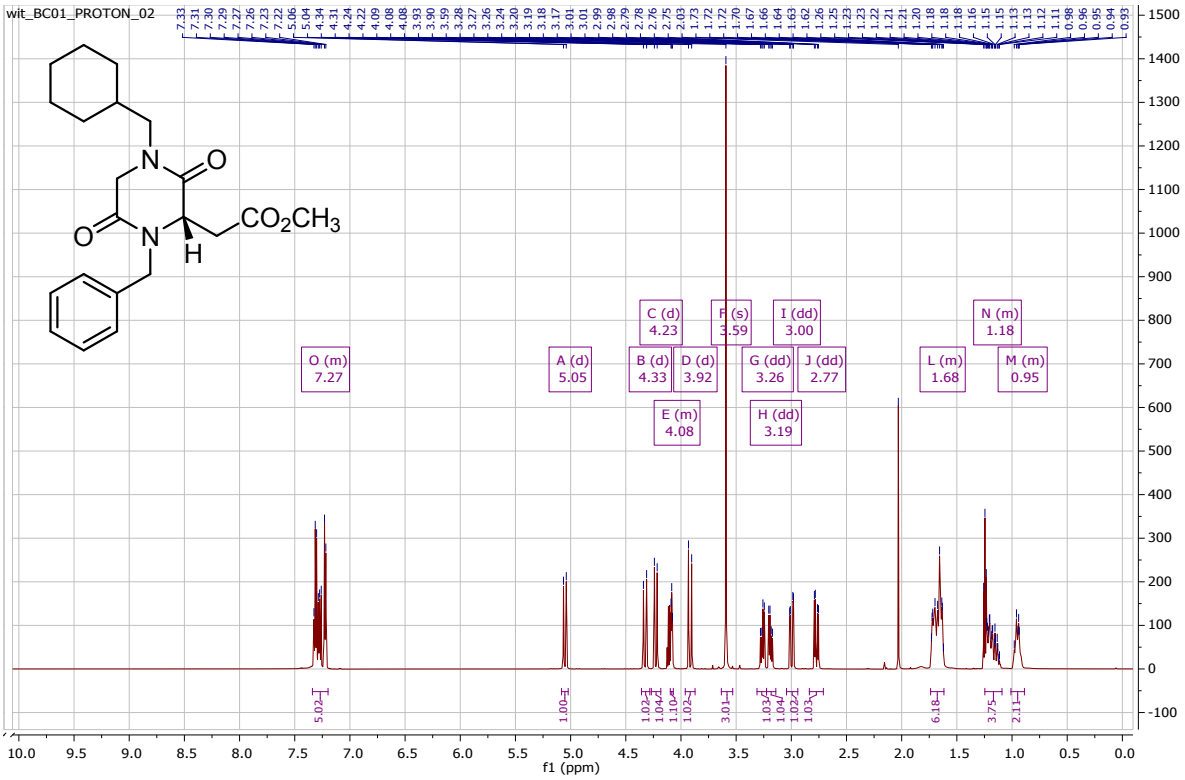


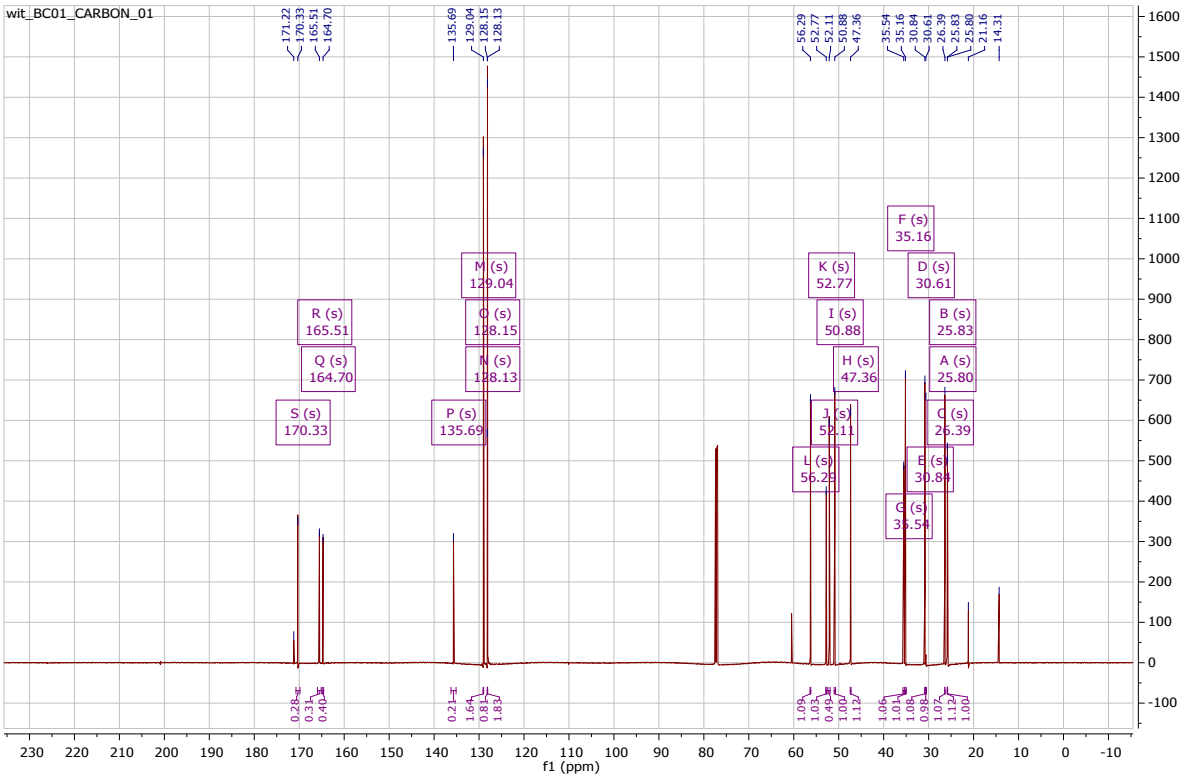


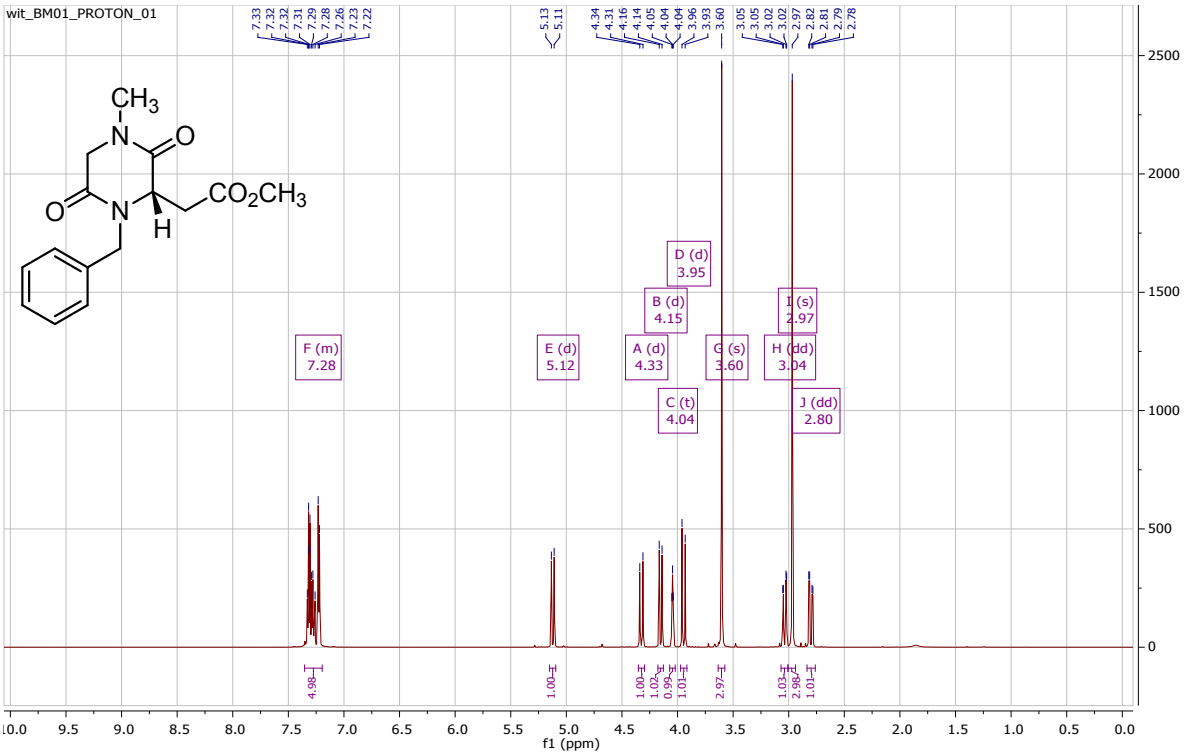

wit_4a08_PROTON_01
Cl
O
N
H
CO2CH3
CO2CH3
U (d) 2.64
G (d) 4.12
M (s) 3.56
S (d) 2.70
B (d) 4.89
E (s) 4.45
I (d) 4.05
K (s) 3.64
P (d) 2.98
V (m) 7.35
A (t) 5.03
D (m) 4.51
H (d) 4.09
J (s) 3.67
N (d) 3.30
R (d) 2.75
C (m) 4.70
F (m) 4.25
L (s) 3.60
Q (d) 3.03
O (d) 3.26
T (s) 2.67
f1 (ppm)


wit_4D01_PROTON_01
Cl
O
N
H
CO2CH3
CO2CH3
K (d) 4.73
S (d) 4.11
F (s) 3.56
R (dd) 7.20
P (t) 5.03
J (s) 4.45
N (dd) 3.00
A (dd) 3.28
B (dd) 2.73
O (dd) 2.66
f1 (ppm)

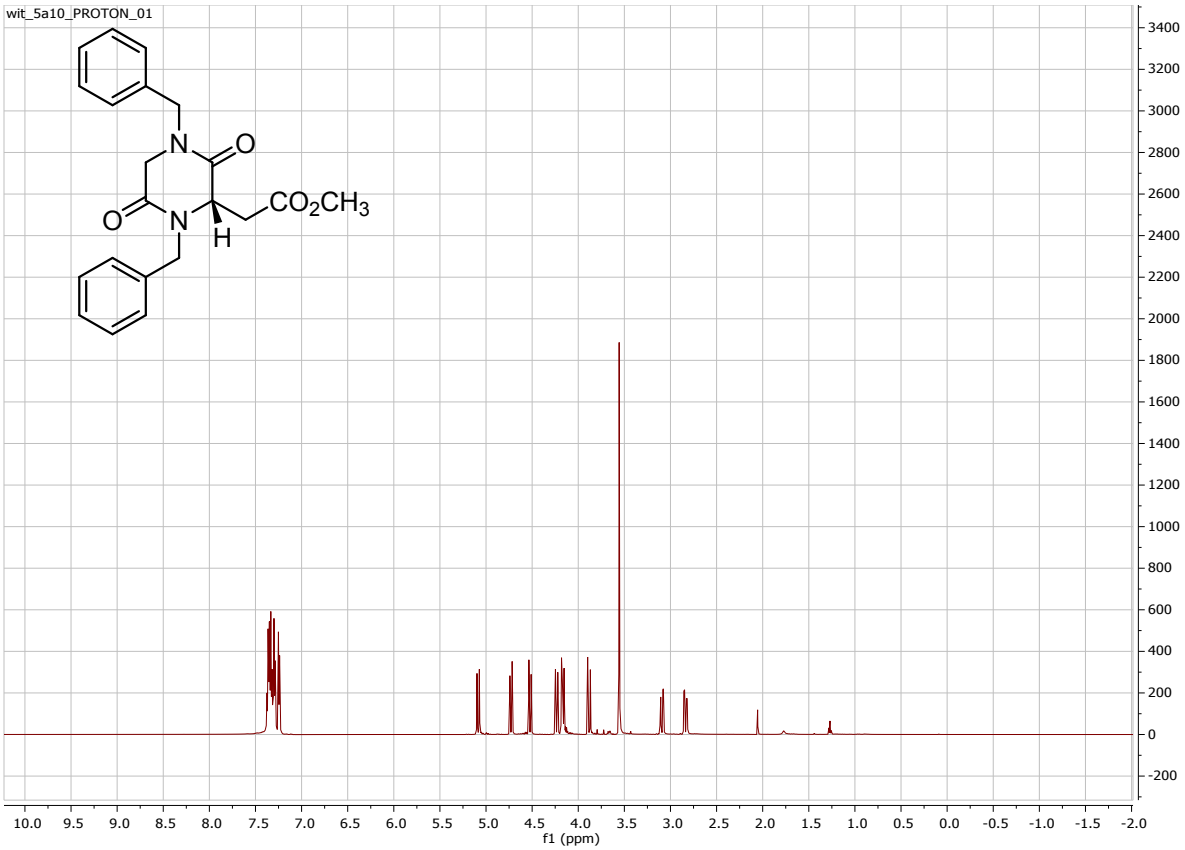

wit_4D01_CARBON_01
Z (s) 170.63
L (s) 167.93
T (s) 169.72
S (s) 167.22
U (s) 171.69
Y (s) 169.87
R (s) 137.07
P (s) 129.11
N (s) 128.41
M (s) 127.63
O (s) 128.63
Q (s) 135.34
W (s) 127.51
V (s) 47.54
J (s) 57.07
H (s) 53.07
D (s) 41.43
F (s) 52.30
B (s) 34.43
E (s) 52.14
A (s) 34.59
G (s) 52.76
C (s) 41.94
I (s) 53.50
K (s) 57.48
f1 (ppm)

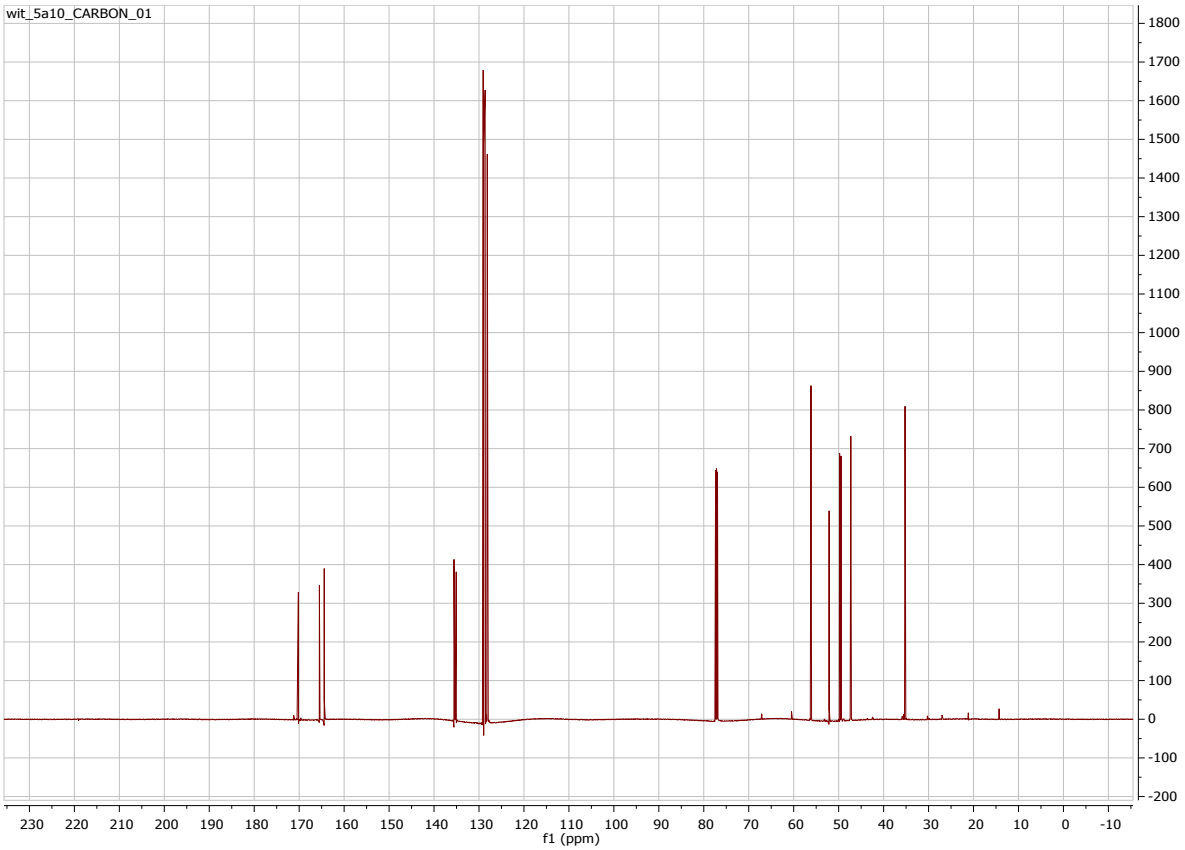

wit_BC01_PROTON_02
O (m) 7.27
A (d) 5.05
B (d) 4.33
C (d) 4.23
D (d) 3.92
E (m) 4.08
F (s) 3.59
G (dd) 3.26
H (dd) 3.19
I (dd) 3.00
J (dd) 2.77
L (m) 1.68
M (m) 0.95
N (m) 1.18
f1 (ppm)

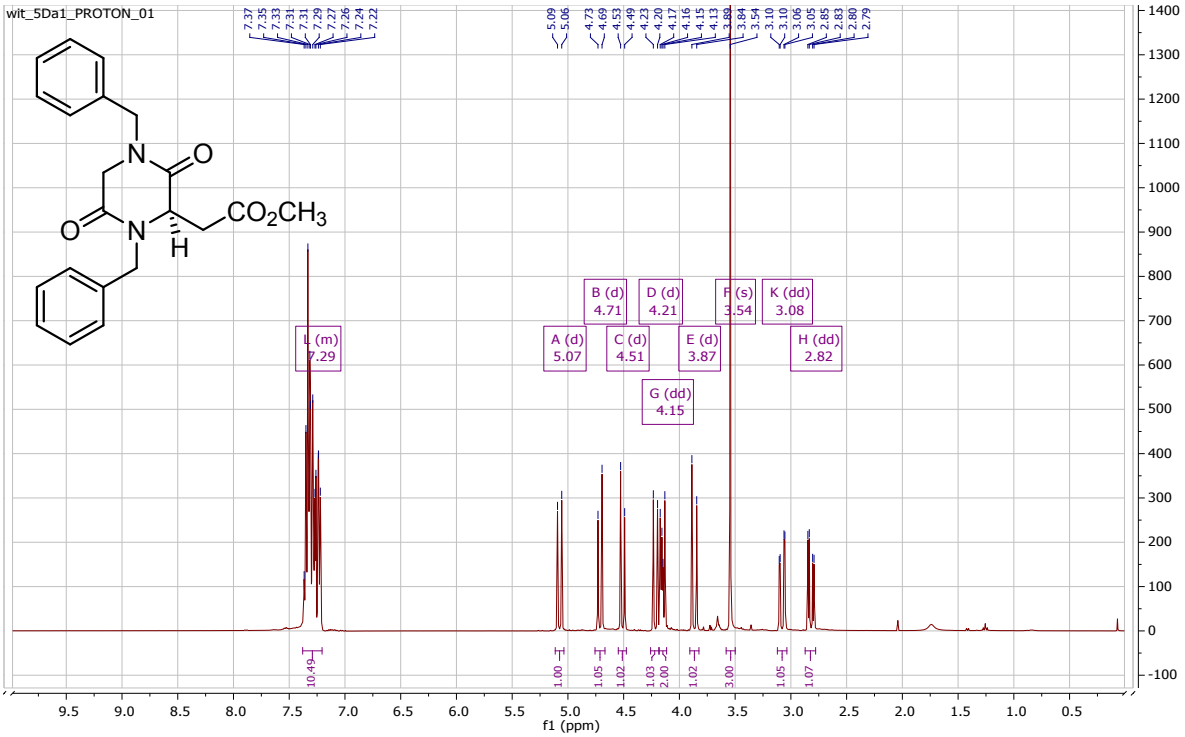

wit_BC01_CARBON_01
R (s) 165.51
Q (s) 164.70
S (s) 170.33
M (s) 129.04
O (s) 128.15
N (s) 128.13
P (s) 135.69
K (s) 52.77
I (s) 50.88
H (s) 47.36
J (s) 52.11
L (s) 56.29
F (s) 35.16
D (s) 30.61
B (s) 25.83
A (s) 25.80
C (s) 26.39
E (s) 30.84
G (s) 35.54
f1 (ppm)

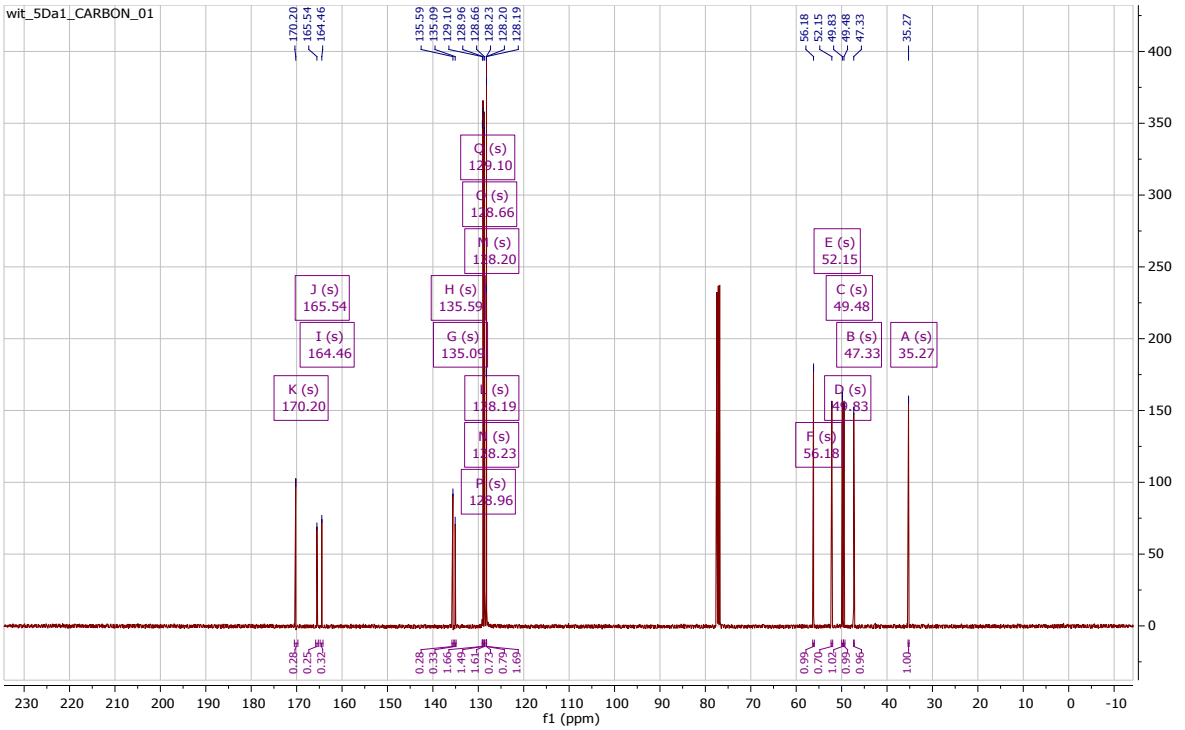

wit_BM01_PROTON_01
CH3
N
O
O
N
H
CO2CH3
F (m)
7.28
E (d)
5.12
A (d)
4.33
B (d)
4.15
C (t)
4.04
D (d)
3.95
G (s)
3.60
H (dd)
3.04
I (s)
2.97
J (dd)
2.80
f1 (ppm)

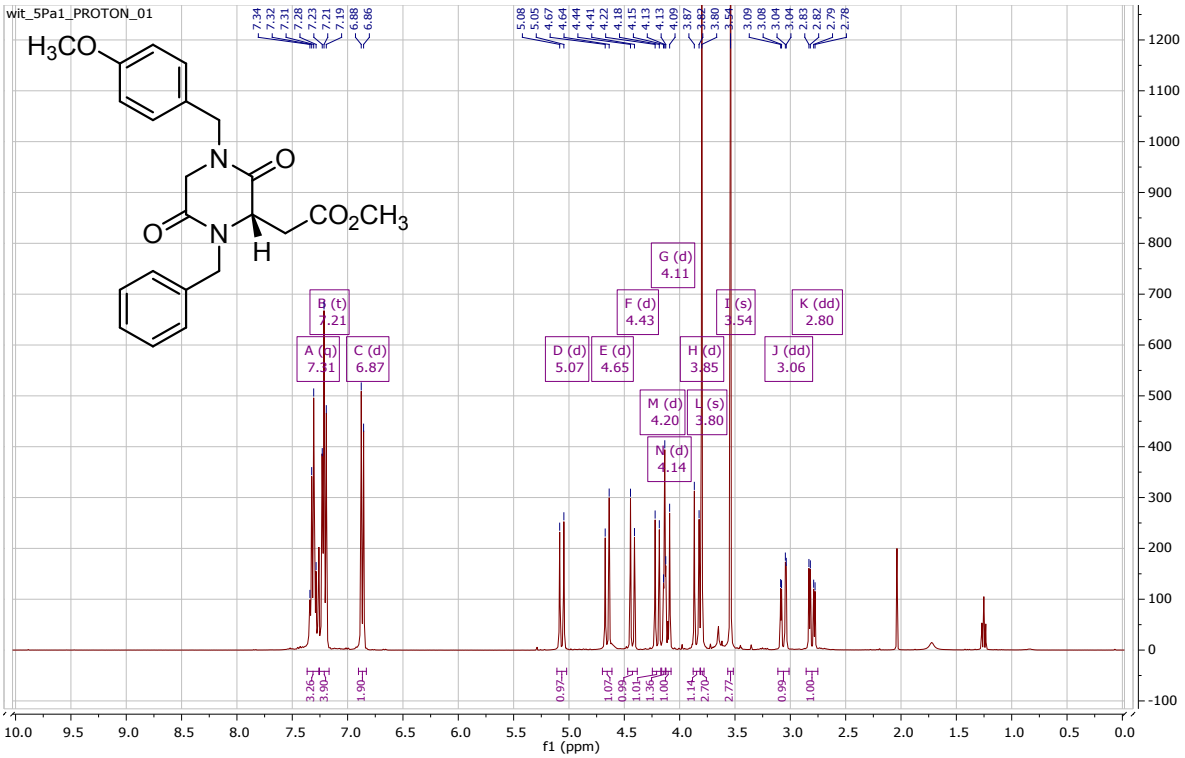

wit_BM01_CARBON_01
K (s)
165.63
J (s)
164.29
L (s)
170.43
H (s)
129.06
G (s)
128.21
I (s)
135.51
D (s)
52.16
B (s)
55.74
A (s)
47.12
C (s)
52.10
F (s)
34.91
E (s)
33.74
f1 (ppm)

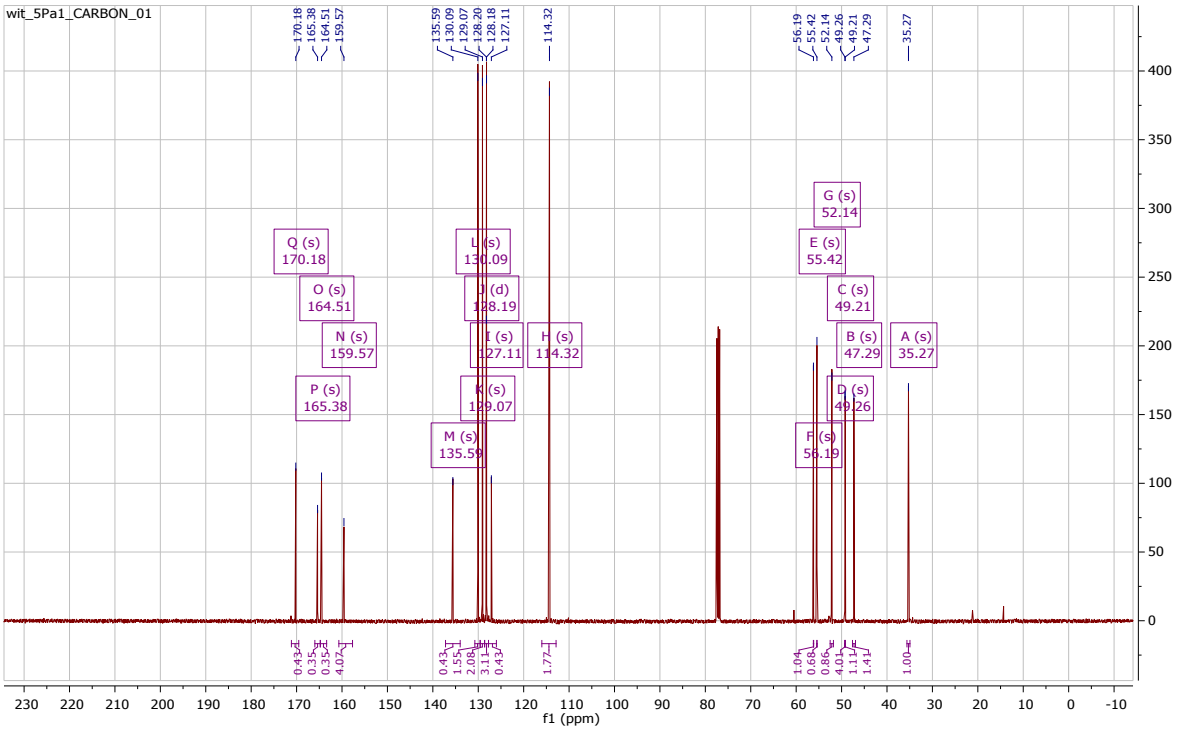

wit_5a10_PROTON_01
N
O
O
N
H
CO2CH3
f1 (ppm)

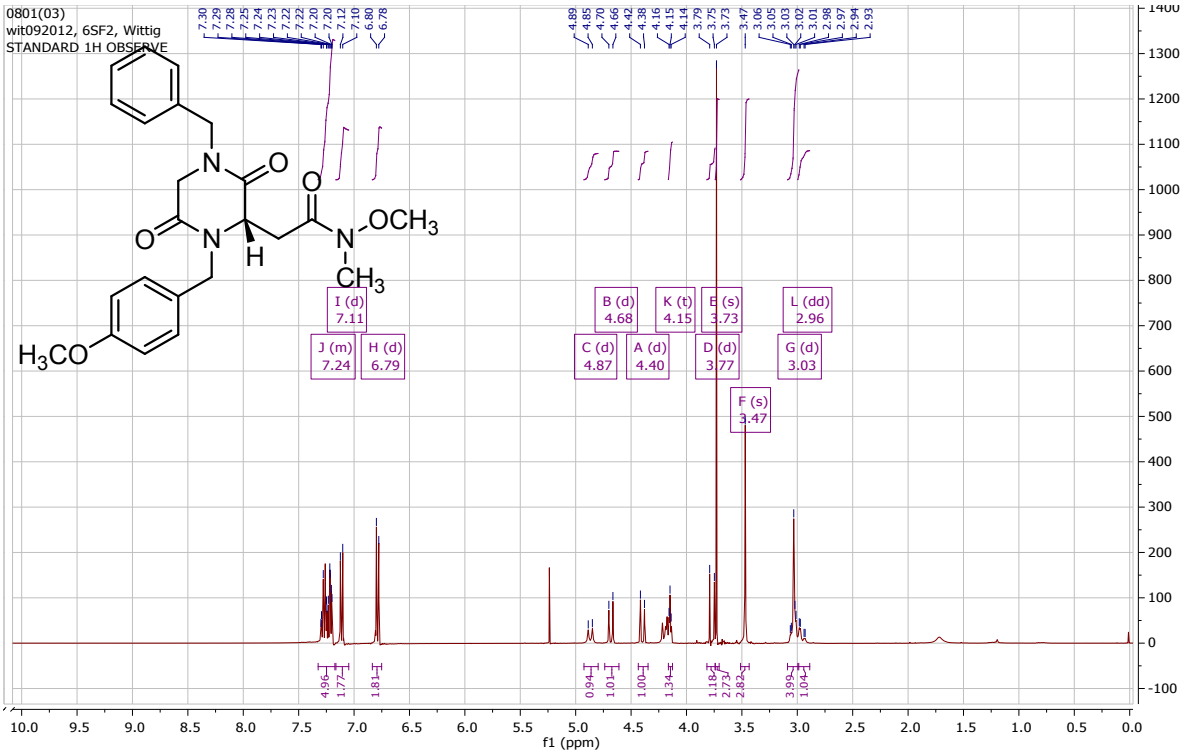

wit_5a10_CARBON_01
f1 (ppm)


wit_5Da1_PROTON_01
L (m) 7.29
A (d) 5.07
B (d) 4.71
C (d) 4.51
D (d) 4.21
E (d) 3.87
F (s) 3.54
G (dd) 4.15
H (dd) 2.82
K (dd) 3.08
f1 (ppm)

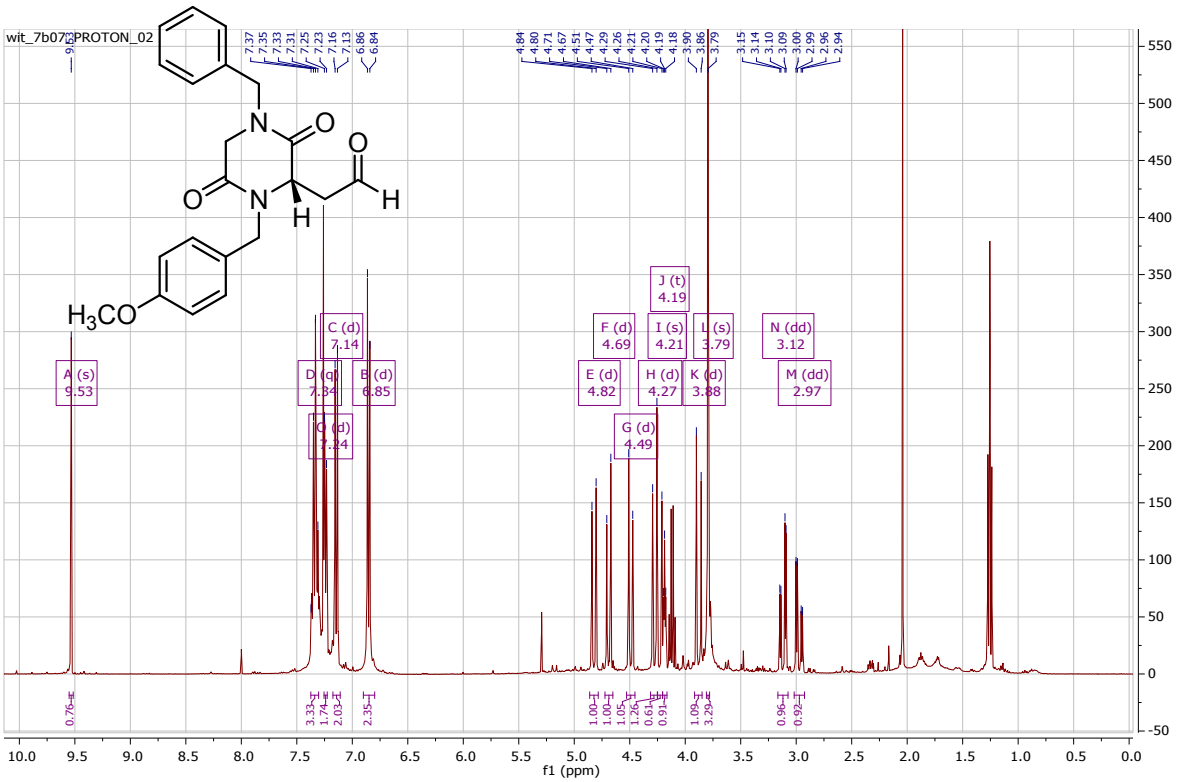

wit_5Da1_CARBON_01
K (s) 170.20
J (s) 165.54
I (s) 164.46
H (s) 135.59
G (s) 135.09
E (s) 52.15
C (s) 49.48
B (s) 47.33
A (s) 35.27
D (s) 49.83
F (s) 56.18
f1 (ppm)

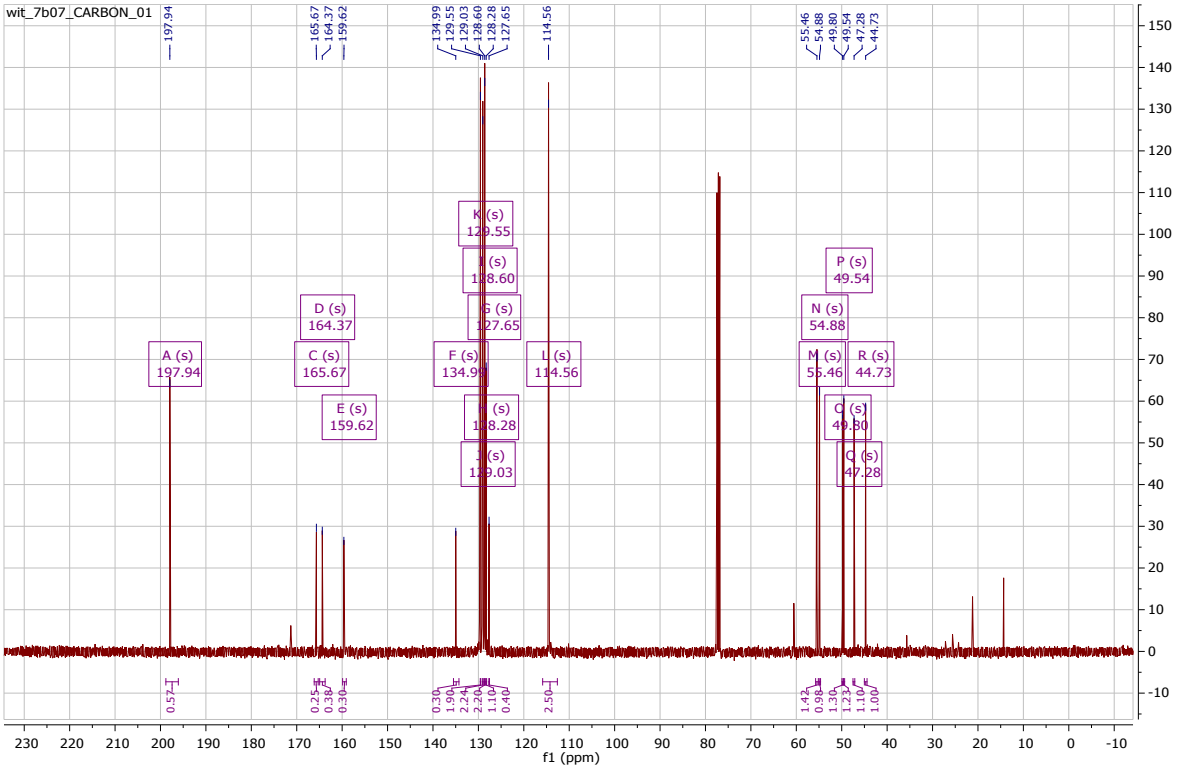

wit_5Pa1_PROTON_01
H3CO
N
O
O
N
H
CO2CH3
A (q) 7.31
B (t) 7.21
C (d) 6.87
D (d) 5.07
E (d) 4.65
F (d) 4.43
G (d) 4.11
H (d) 3.85
I (s) 3.54
J (dd) 3.06
K (dd) 2.80
L (s) 3.80
M (d) 4.20
N (d) 4.14
f1 (ppm)

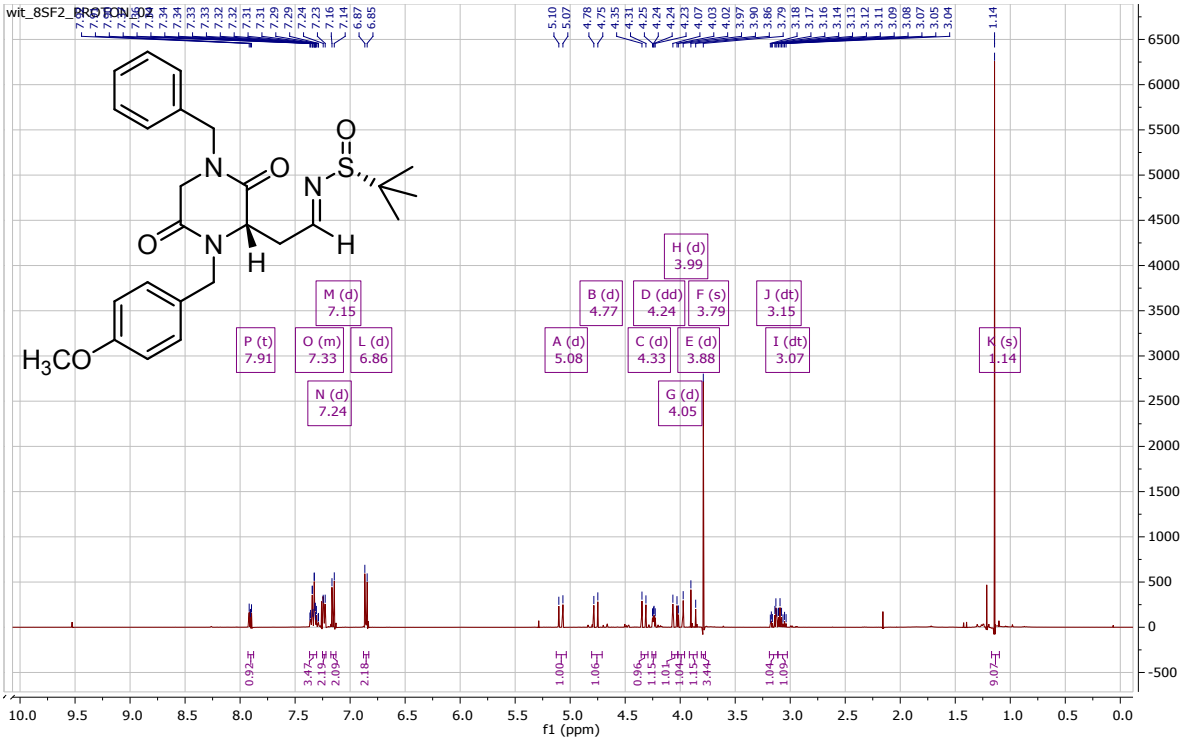

wit_5Pa1_CARBON_01
Q (s) 170.18
P (s) 165.38
O (s) 164.51
N (s) 159.57
M (s) 135.59
L (s) 130.09
K (s) 129.07
J (d) 128.19
I (s) 127.11
H (s) 114.32
G (s) 52.14
F (s) 56.19
E (s) 55.42
D (s) 49.26
C (s) 49.21
B (s) 47.29
A (s) 35.27
f1 (ppm)

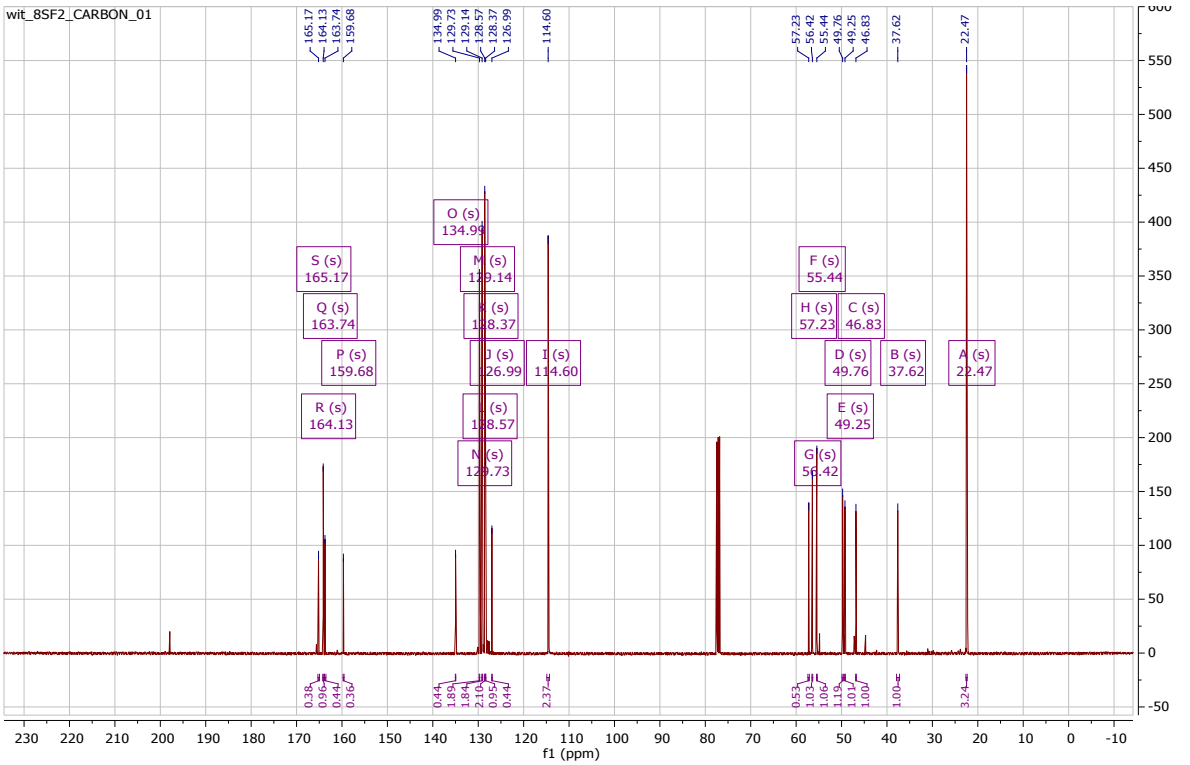

0801(03)
wit092012, 6SF2, Wittig
STANDARD 1H OBSERVE
I (d) 7.11
J (m) 7.24
H (d) 6.79
B (d) 4.68
K (t) 4.15
E (s) 3.73
L (dd) 2.96
C (d) 4.87
A (d) 4.40
D (d) 3.77
G (d) 3.03
F (s) 3.47
f1 (ppm)

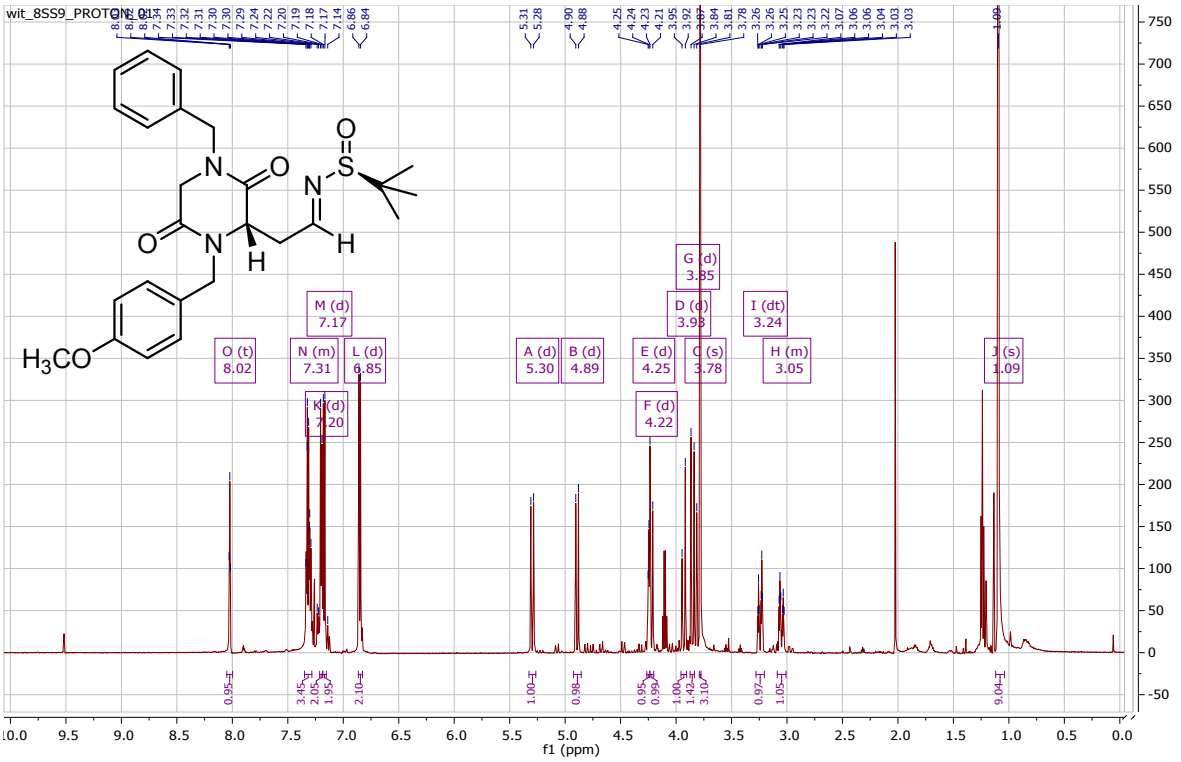

0803(03)
wit092012, 6SF2, Wittig
STANDARD 1H OBSERVE
R (s) 170.09
P (s) 164.88
O (s) 159.42
Q (s) 166.53
M (s) 129.46
K (s) 128.54
J (s) 128.01
L (s) 128.89
N (s) 135.34
I (s) 114.38
F (s) 55.47
D (s) 49.65
B (s) 32.92
H (s) 61.26
C (s) 46.94
A (s) 32.13
E (s) 49.80
G (s) 56.07
f1 (ppm)

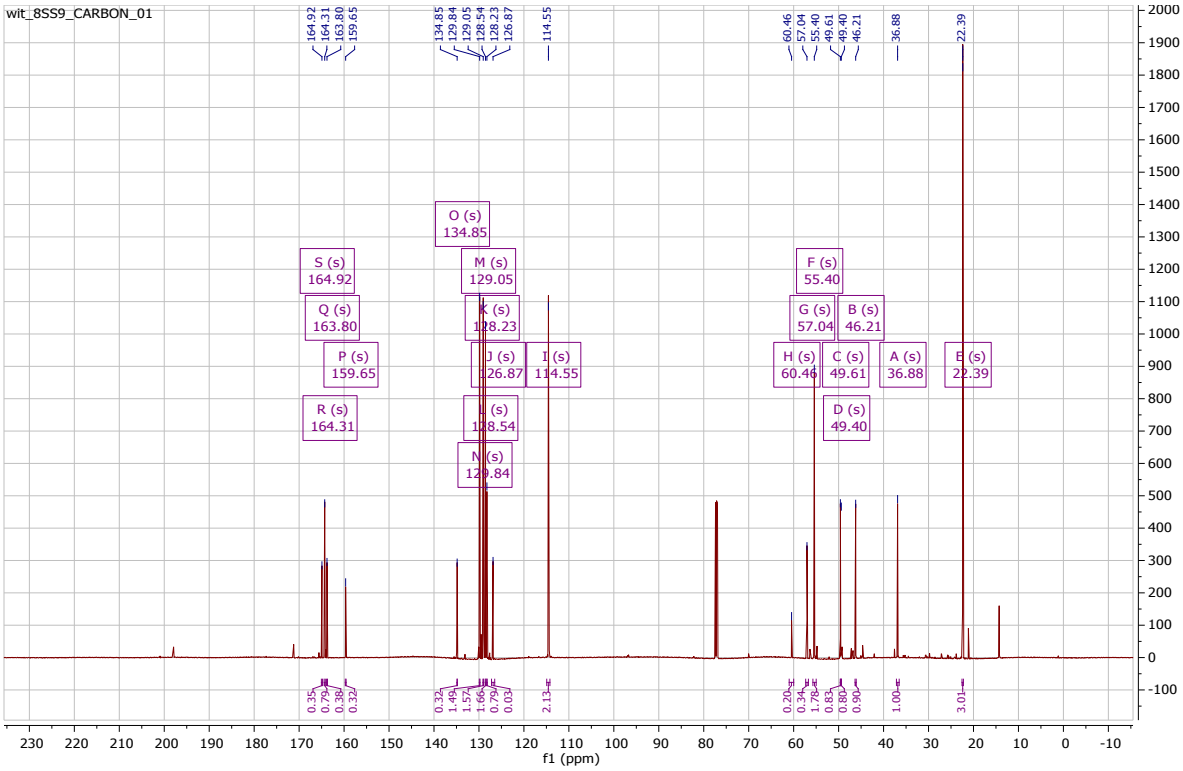

wit_7b07_PROTON_02
A (s) 9.53
B (d) 6.85
C (d) 7.14
D (qd) 7.34
F (d) 4.69
E (d) 4.82
G (d) 4.49
H (d) 4.27
I (s) 4.21
J (t) 4.19
K (d) 3.88
L (s) 3.79
M (dd) 2.97
N (dd) 3.12
f1 (ppm)

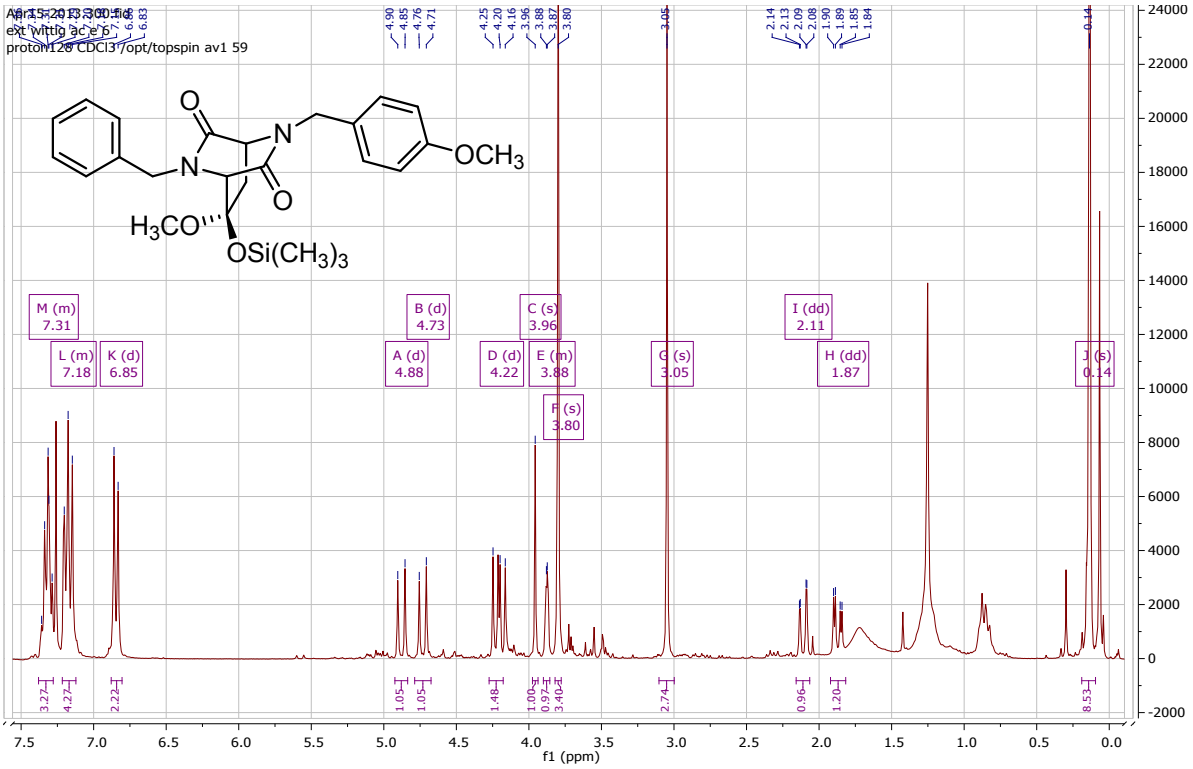

wit_7b07_CARBON_01
A (s) 197.94
C (s) 165.67
D (s) 164.37
E (s) 159.62
F (s) 134.99
I (s) 129.03
K (s) 129.55
L (s) 114.56
M (s) 55.46
N (s) 54.88
P (s) 49.54
Q (s) 49.80
R (s) 44.73
f1 (ppm)

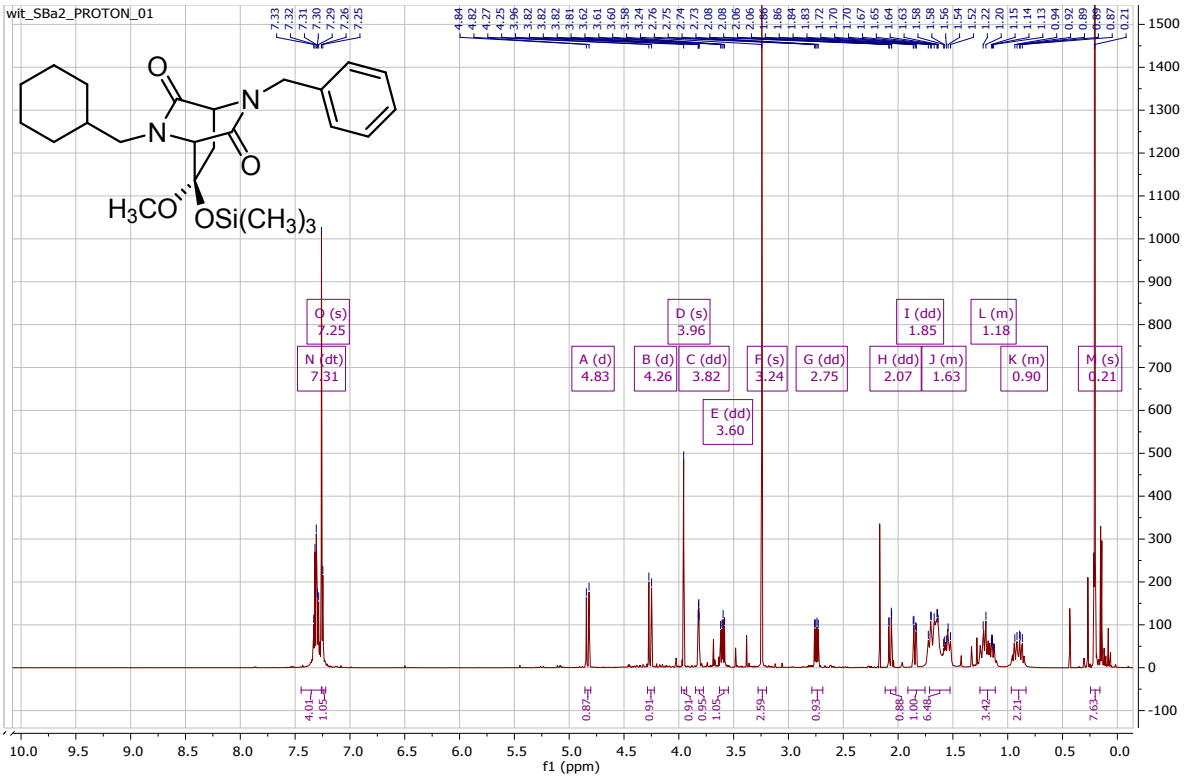

wit_8SF2_PROTON_02
H (d) 3.99
M (d) 7.15
B (d) 4.77
D (dd) 4.24
F (s) 3.79
J (dt) 3.15
P (t) 7.91
O (m) 7.33
L (d) 6.86
A (d) 5.08
C (d) 4.33
E (d) 3.88
I (dt) 3.07
K (s) 1.14
N (d) 7.24
G (d) 4.05
f1 (ppm)


wit_8SF2_CARBON_01
O (s) 134.99
M (s) 129.14
K (s) 128.37
J (s) 126.99
I (s) 114.60
S (s) 165.17
Q (s) 163.74
P (s) 159.68
R (s) 164.13
L (s) 128.57
N (s) 129.73
F (s) 55.44
H (s) 57.23
C (s) 46.83
D (s) 49.76
B (s) 37.62
A (s) 22.47
E (s) 49.25
G (s) 56.42
f1 (ppm)

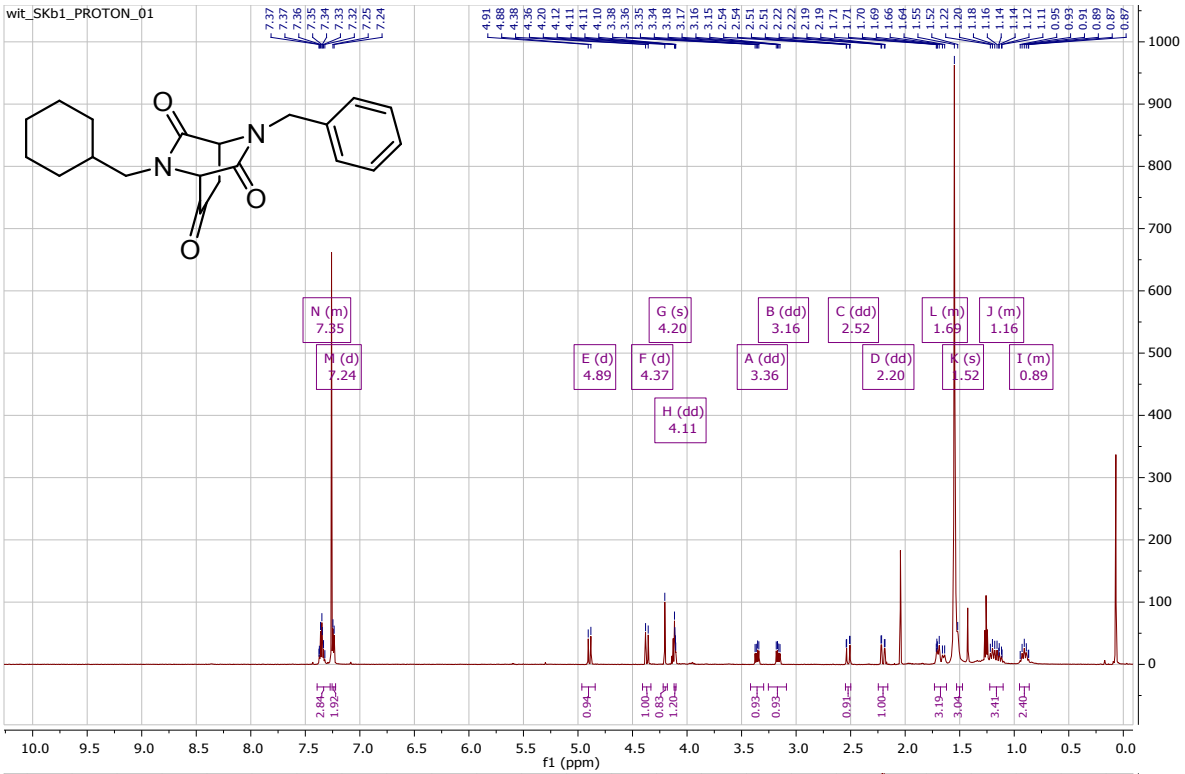

wit_8SS9_PROTON_01
O (t) 8.02
N (m) 7.31
L (d) 6.85
M (d) 7.17
K (d) 7.20
A (d) 5.30
B (d) 4.89
E (d) 4.25
F (d) 4.22
G (d) 3.85
D (d) 3.93
C (s) 3.78
I (dt) 3.24
H (m) 3.05
J (s) 1.09
f1 (ppm)

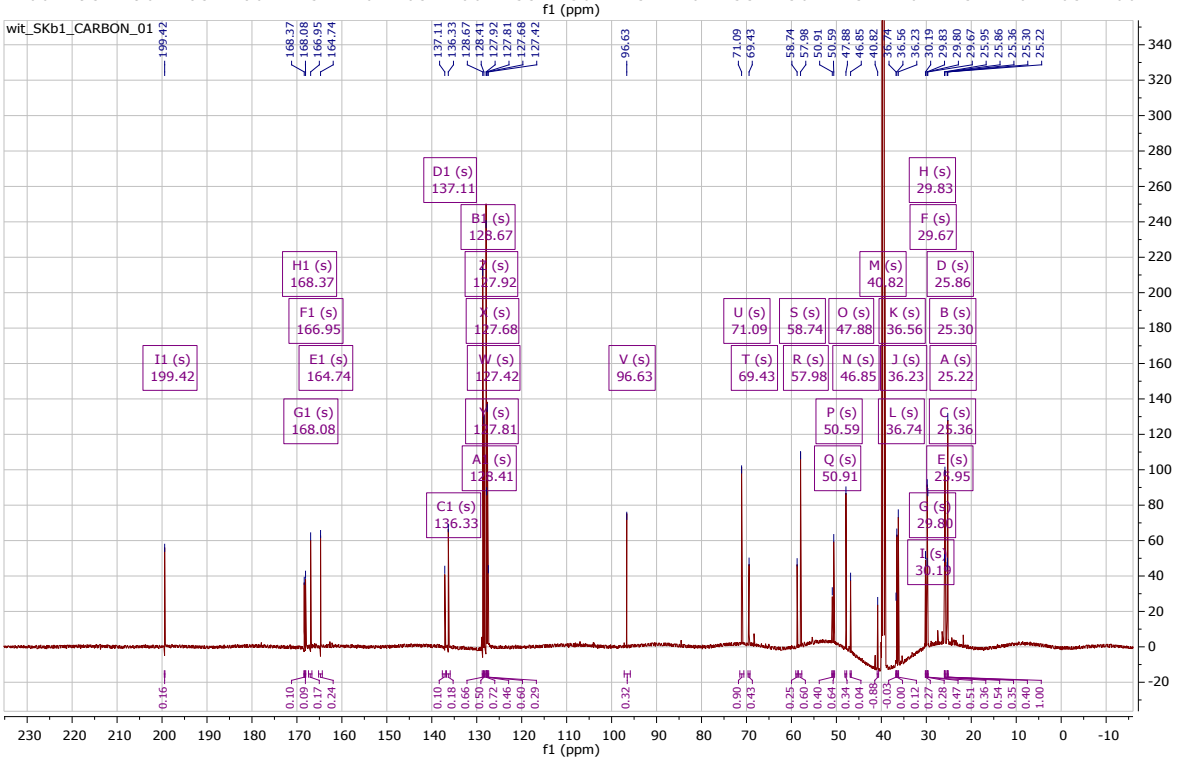

wit_8SS9_CARBON_01
S (s) 164.92
Q (s) 163.80
P (s) 159.65
R (s) 164.31
O (s) 134.85
M (s) 129.05
K (s) 128.23
J (s) 126.87
I (s) 114.55
L (s) 128.54
N (s) 129.84
F (s) 55.40
G (s) 57.04
B (s) 46.21
H (s) 60.46
C (s) 49.61
A (s) 36.88
E (s) 22.39
D (s) 49.40
f1 (ppm)

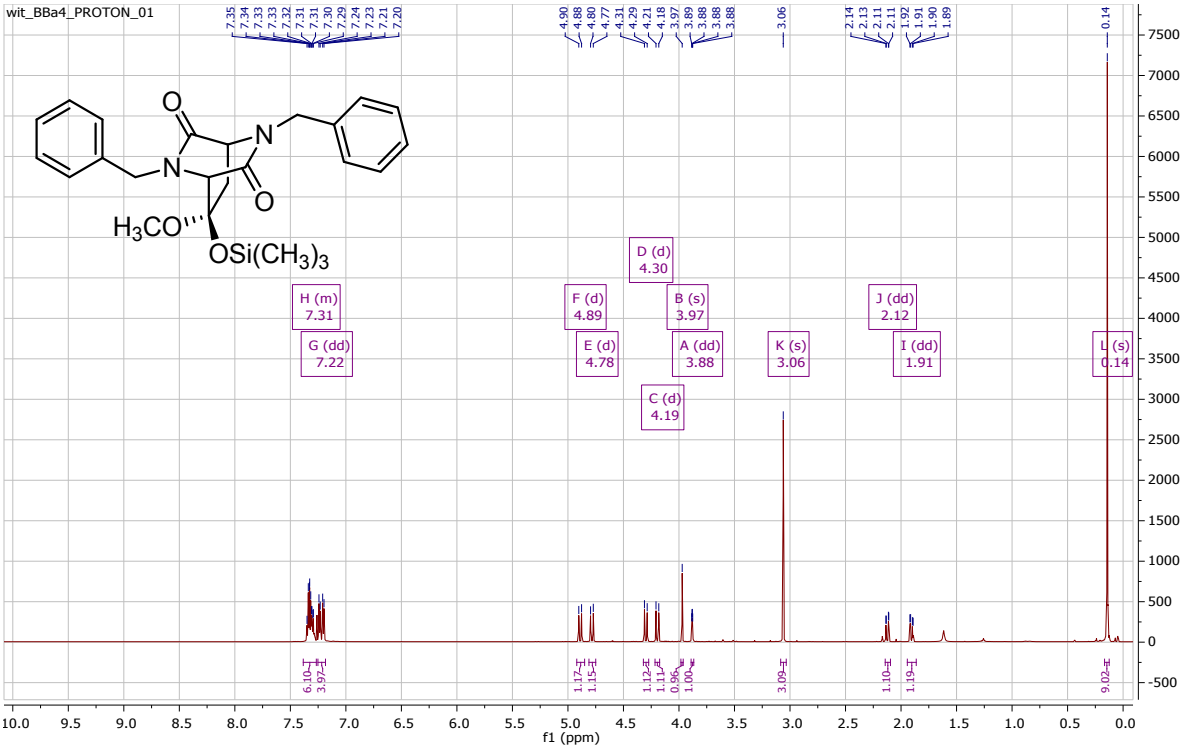

Apr15-2013 300.fid
ext wittig ac e 6
proton128 CDCl3 /opt/topspin av1 59
OCH3
H3CO'''
OSi(CH3)3
M (m) 7.31
L (m) 7.18
K (d) 6.85
B (d) 4.73
A (d) 4.88
C (s) 3.96
D (d) 4.22
E (m) 3.88
F (s) 3.80
G (s) 3.05
I (dd) 2.11
H (dd) 1.87
J (s) 0.14
f1 (ppm)

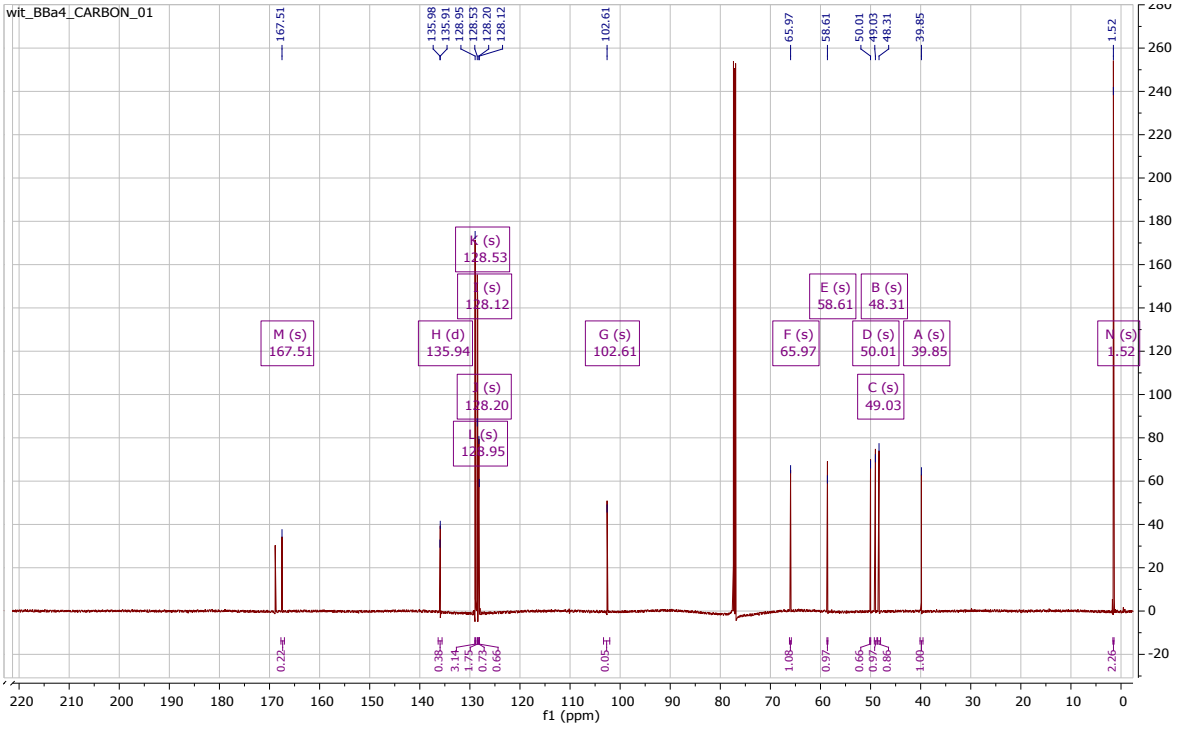

wit_SBa2_PROTON_01
O
N
N
O
H3CO
OSi(CH3)3
O (s) 7.25
N (dt) 7.31
A (d) 4.83
B (d) 4.26
C (dd) 3.82
D (s) 3.96
E (dd) 3.60
F (s) 3.24
G (dd) 2.75
H (dd) 2.07
I (dd) 1.85
J (m) 1.63
K (m) 0.90
L (m) 1.18
M (s) 0.21
f1 (ppm)

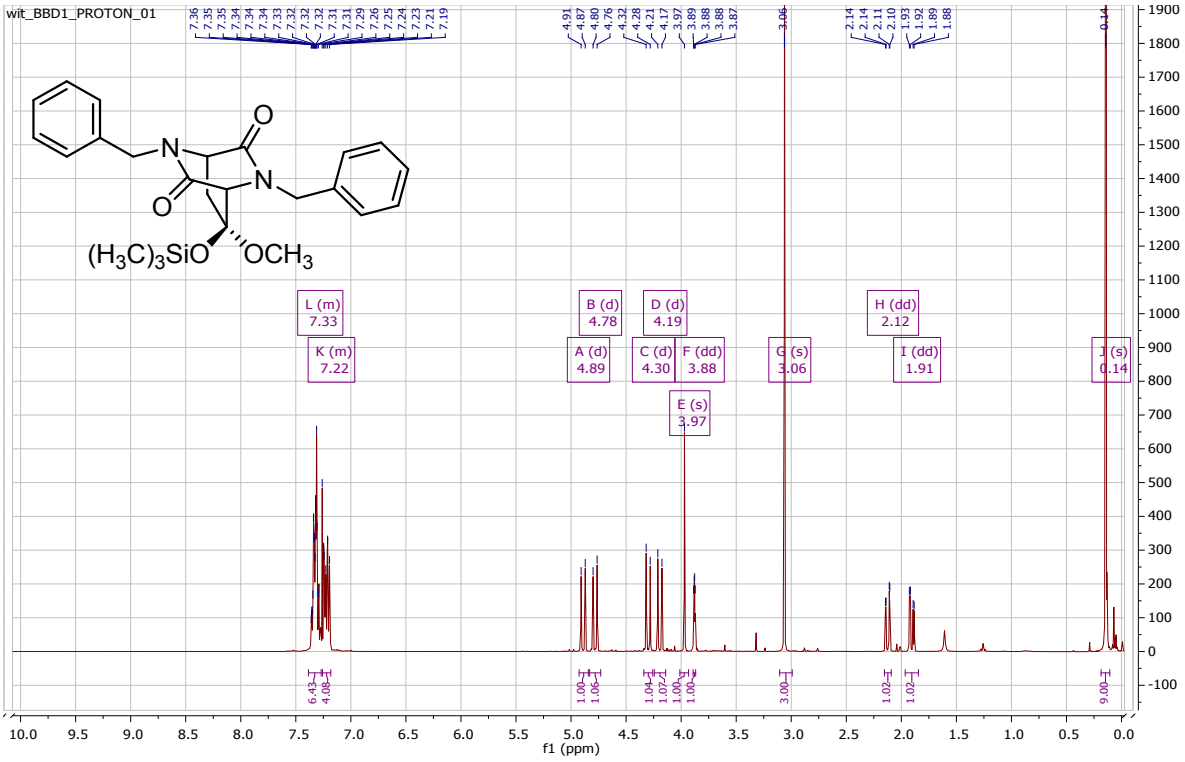

wit_SBa2_CARBON_01
F (s) 167.71
E (s) 168.92
A (s) 136.02
D (s) 128.53
B (s) 128.15
C (s) 128.90
G (s) 102.76
I (s) 67.67
T (s) 58.84
L (s) 48.29
J (s) 51.94
K (s) 50.40
M (s) 39.34
N (s) 37.13
P (s) 30.49
O (s) 30.89
Q (s) 26.45
R (s) 25.87
S (s) 25.78
H (s) 1.62
f1 (ppm)

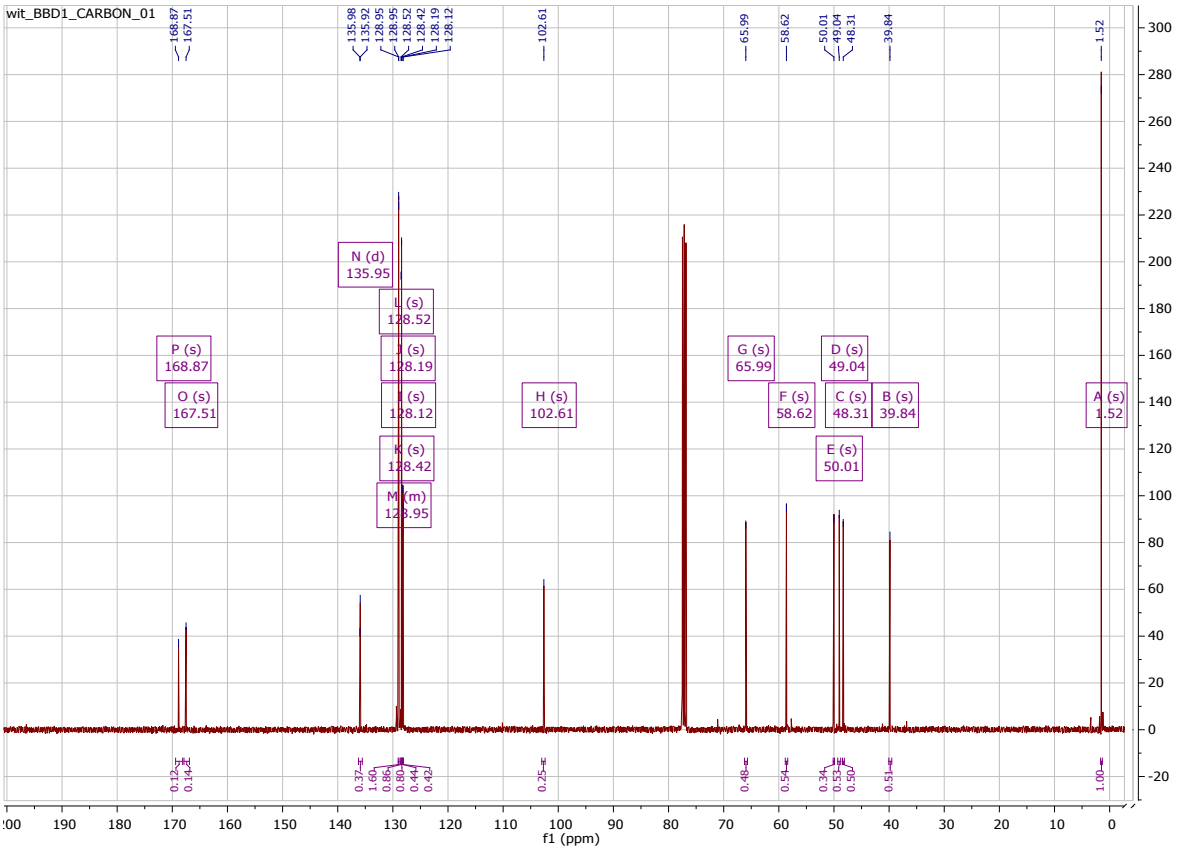

wit_SKb1_PROTON_01
O
N
N
O
O
N (m) 7.35
M (d) 7.24
E (d) 4.89
G (s) 4.20
F (d) 4.37
H (dd) 4.11
A (dd) 3.36
B (dd) 3.16
D (dd) 2.20
C (dd) 2.52
K (s) 1.52
L (m) 1.69
I (m) 0.89
J (m) 1.16
f1 (ppm)

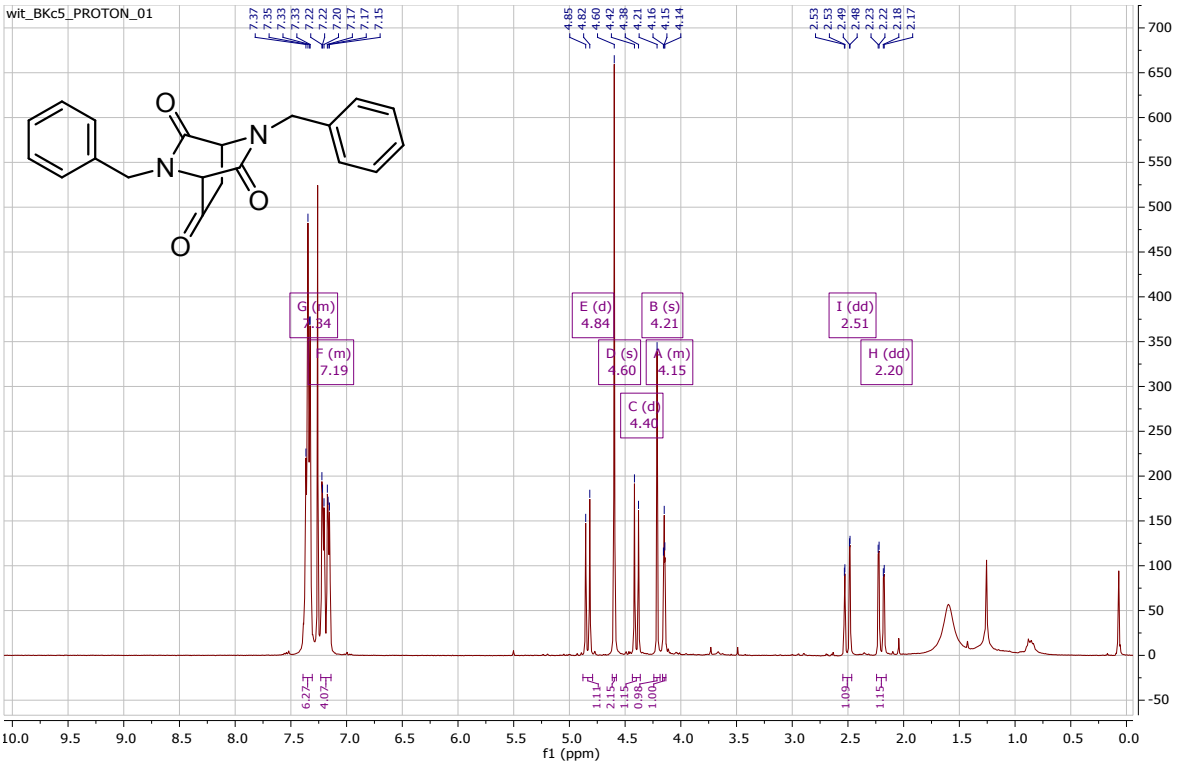

wit_SKb1_CARBON_01
I1 (s) 199.42
H1 (s) 168.37
F1 (s) 166.95
E1 (s) 164.74
G1 (s) 168.08
D1 (s) 137.11
C1 (s) 136.33
B1 (s) 128.67
A1 (s) 128.41
Z (s) 127.92
X (s) 127.68
W (s) 127.42
V (s) 127.81
V (s) 96.63
U (s) 71.09
T (s) 69.43
S (s) 58.74
R (s) 57.98
P (s) 50.59
Q (s) 50.91
O (s) 47.88
N (s) 46.85
M (s) 40.82
K (s) 36.56
J (s) 36.23
L (s) 36.74
H (s) 29.83
F (s) 29.67
D (s) 25.86
B (s) 25.30
A (s) 25.22
C (s) 25.36
E (s) 25.95
G (s) 29.80
I (s) 30.19
f1 (ppm)

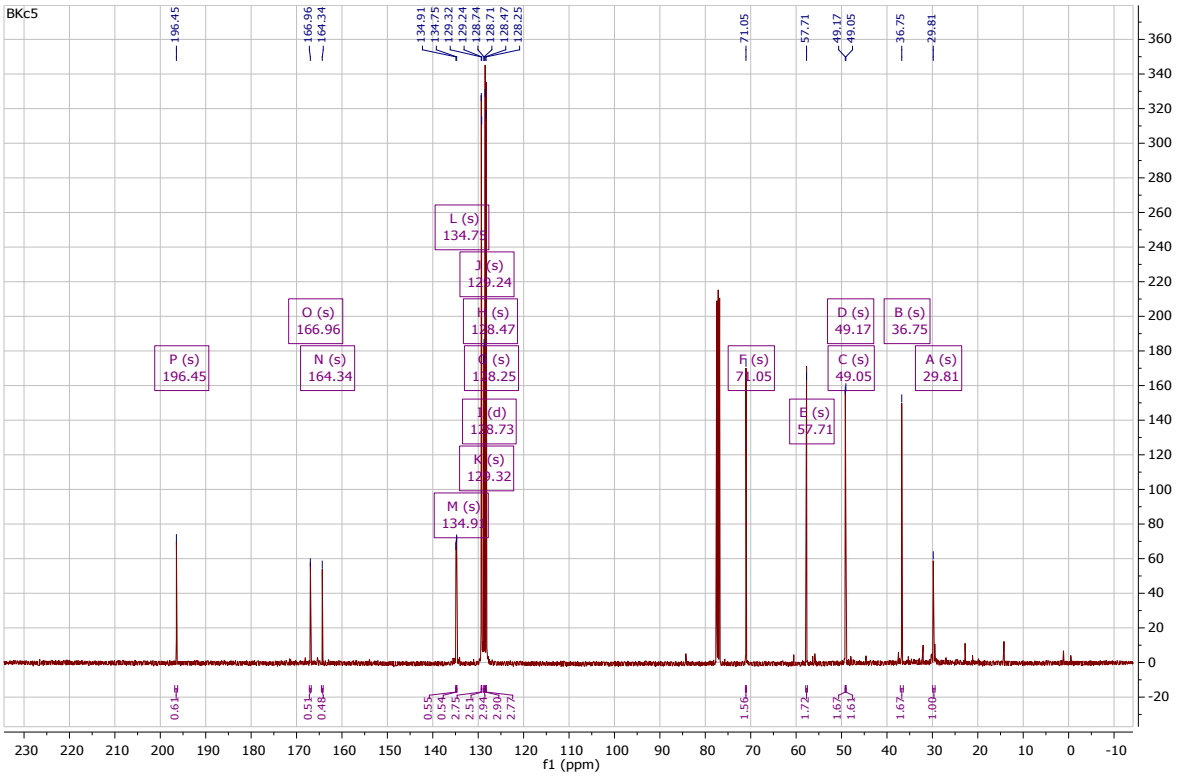

wit_BBa4_PROTON_01
H (m) 7.31
G (dd) 7.22
F (d) 4.89
E (d) 4.78
D (d) 4.30
B (s) 3.97
A (dd) 3.88
C (d) 4.19
K (s) 3.06
J (dd) 2.12
I (dd) 1.91
L (s) 0.14
f1 (ppm)

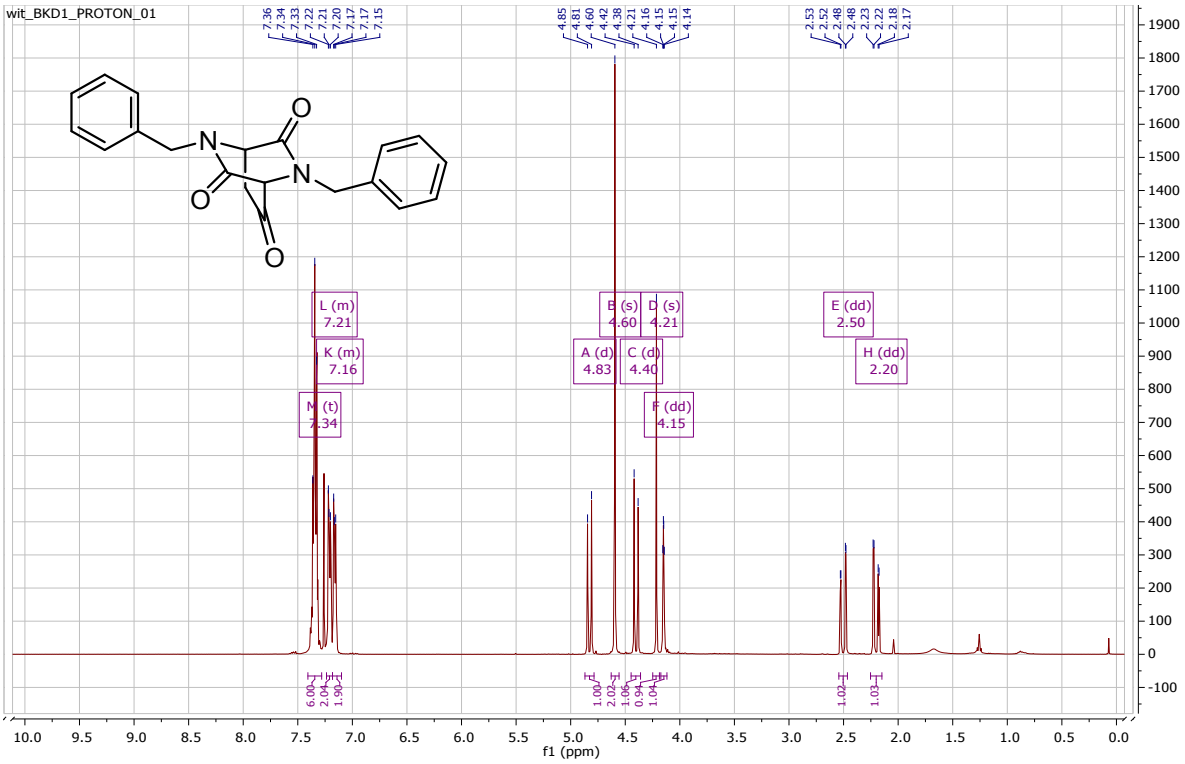

wit_BBa4_CARBON_01
M (s) 167.51
H (d) 135.94
K (s) 128.53
I (s) 128.12
J (s) 128.20
L (s) 128.95
G (s) 102.61
F (s) 65.97
E (s) 58.61
B (s) 48.31
D (s) 50.01
C (s) 49.03
A (s) 39.85
N (s) 1.52
f1 (ppm)

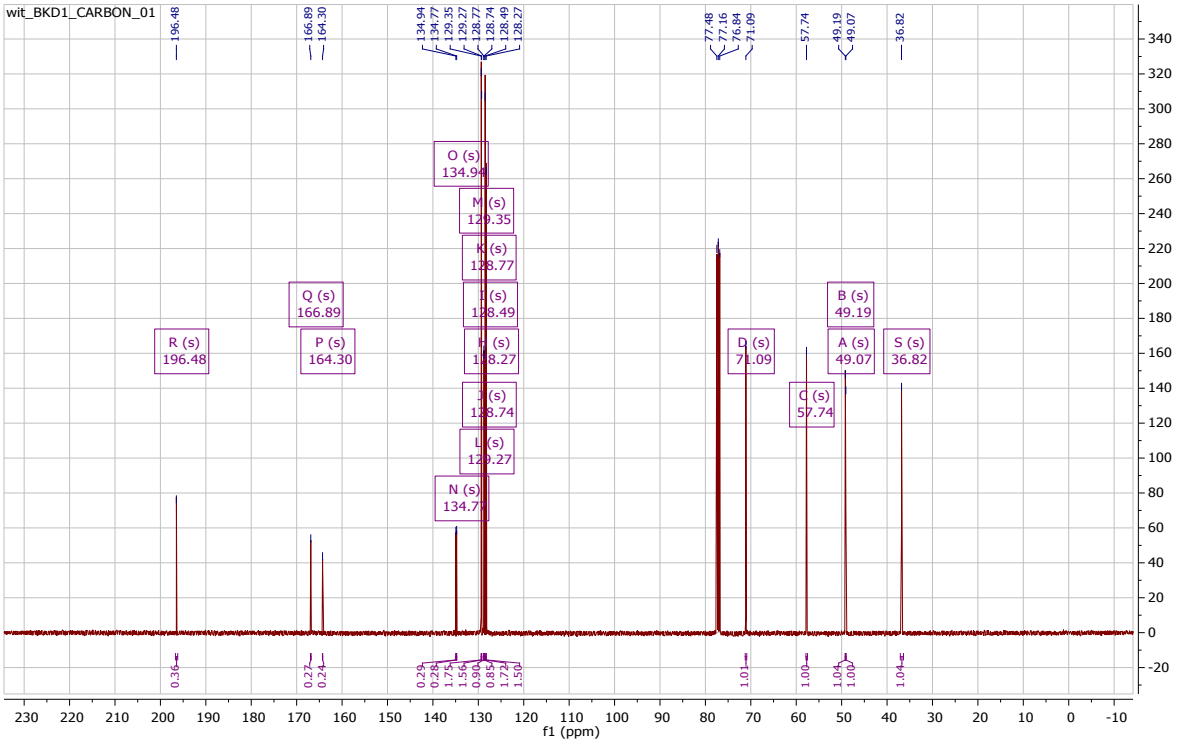

wit_BBD1_PROTON_01
L (m) 7.33
K (m) 7.22
B (d) 4.78
A (d) 4.89
D (d) 4.19
C (d) 4.30
F (dd) 3.88
E (s) 3.97
G (s) 3.06
H (dd) 2.12
I (dd) 1.91
J (s) 0.14
f1 (ppm)

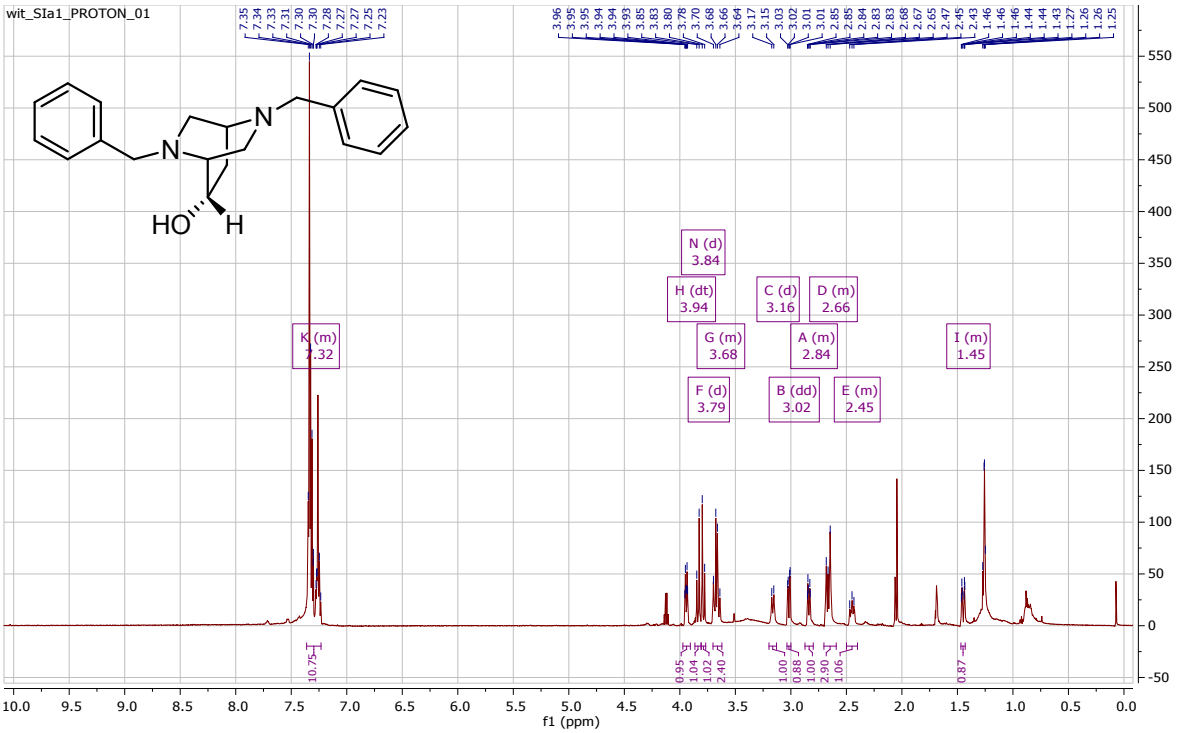

wit_BBD1_CARBON_01
N (d) 135.95
L (s) 128.52
J (s) 128.19
I (s) 128.12
K (s) 128.42
M (m) 128.95
P (s) 168.87
O (s) 167.51
H (s) 102.61
G (s) 65.99
F (s) 58.62
D (s) 49.04
C (s) 48.31
B (s) 39.84
E (s) 50.01
A (s) 1.52
f1 (ppm)

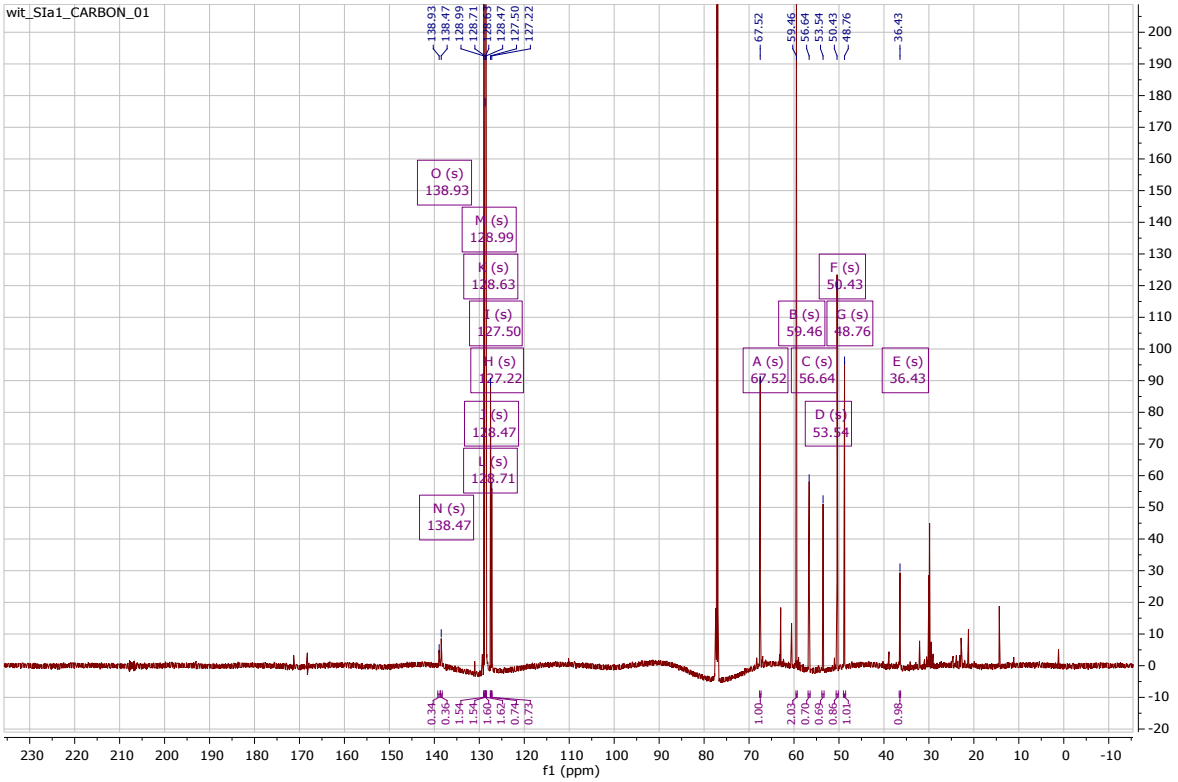

wit_BKc5_PROTON_01
G (m)
7.34
F (m)
7.19
E (d)
4.84
B (s)
4.21
D (s)
4.60
A (m)
4.15
C (d)
4.40
I (dd)
2.51
H (dd)
2.20
f1 (ppm)

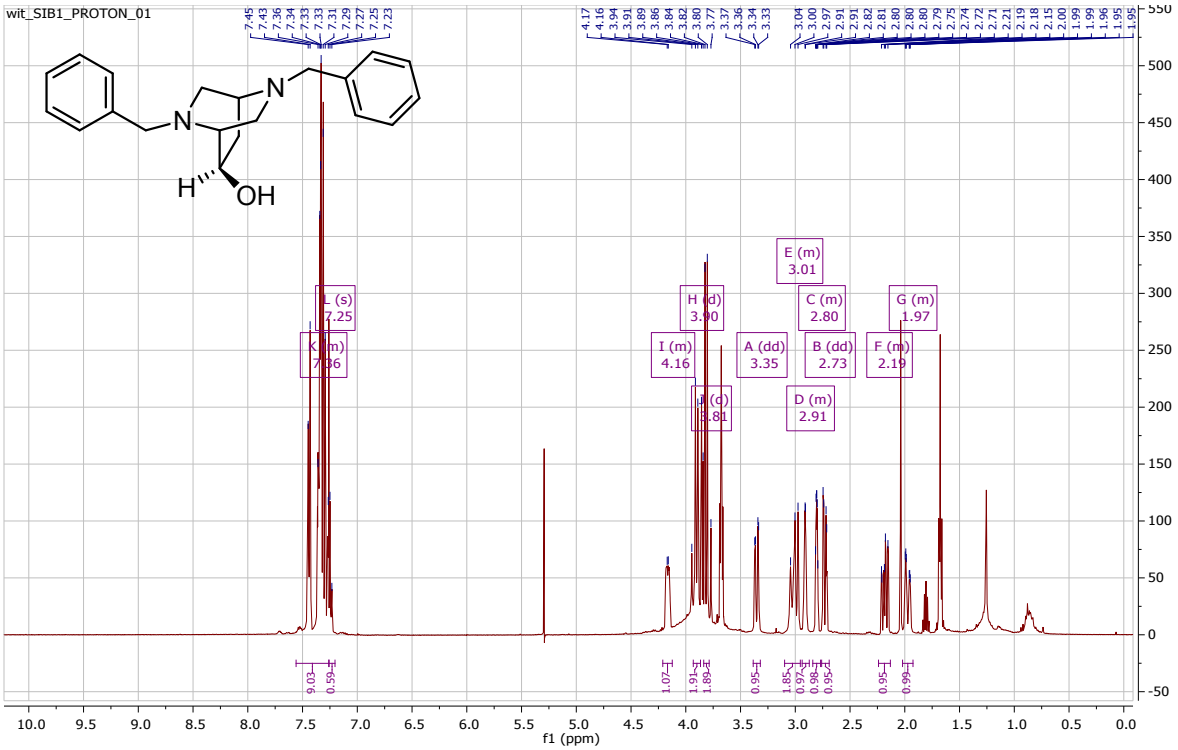

BKc5
P (s)
196.45
O (s)
166.96
N (s)
164.34
D (s)
49.17
B (s)
36.75
C (s)
49.05
A (s)
29.81
F (s)
71.05
E (s)
57.71
f1 (ppm)


wit_BKD1_PROTON_01
L (m) 7.21
K (m) 7.16
M (t) 7.34
B (s) 4.60
D (s) 4.21
A (d) 4.83
C (d) 4.40
F (dd) 4.15
E (dd) 2.50
H (dd) 2.20
f1 (ppm)

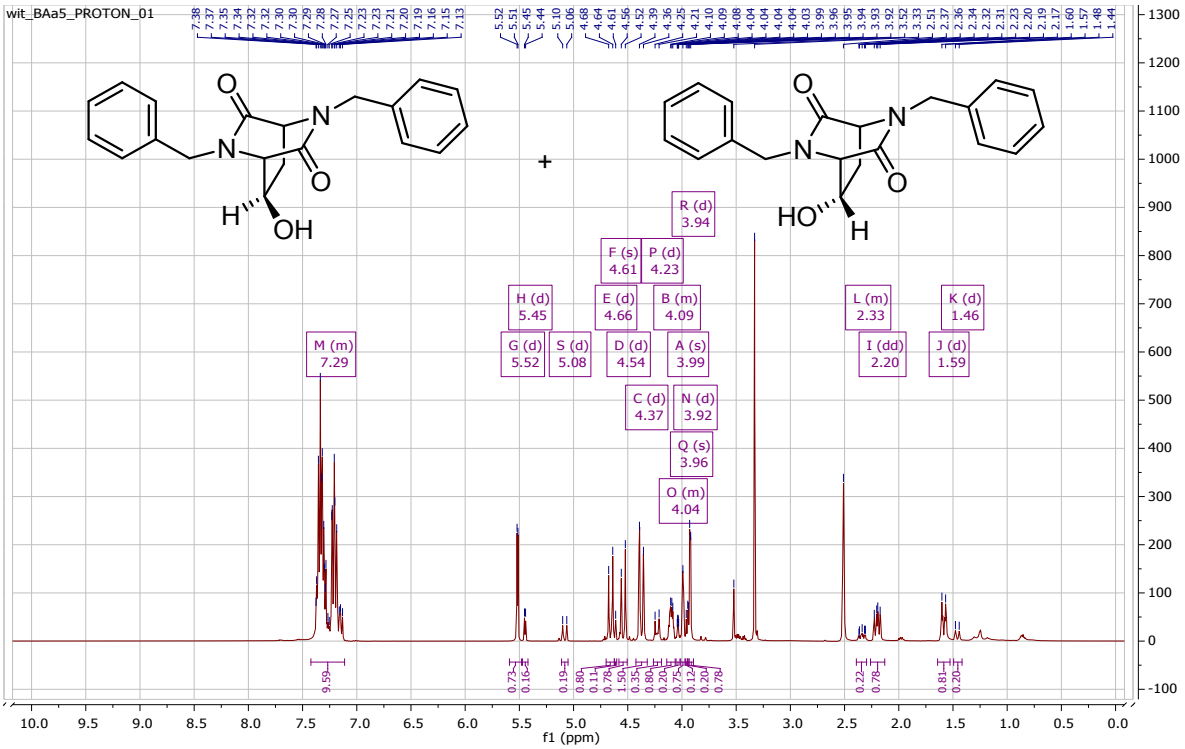

wit_BKD1_CARBON_01
O (s) 134.94
M (s) 129.35
K (s) 128.77
Q (s) 166.89
R (s) 196.48
P (s) 164.30
B (s) 49.19
D (s) 71.09
A (s) 49.07
S (s) 36.82
C (s) 57.74
f1 (ppm)

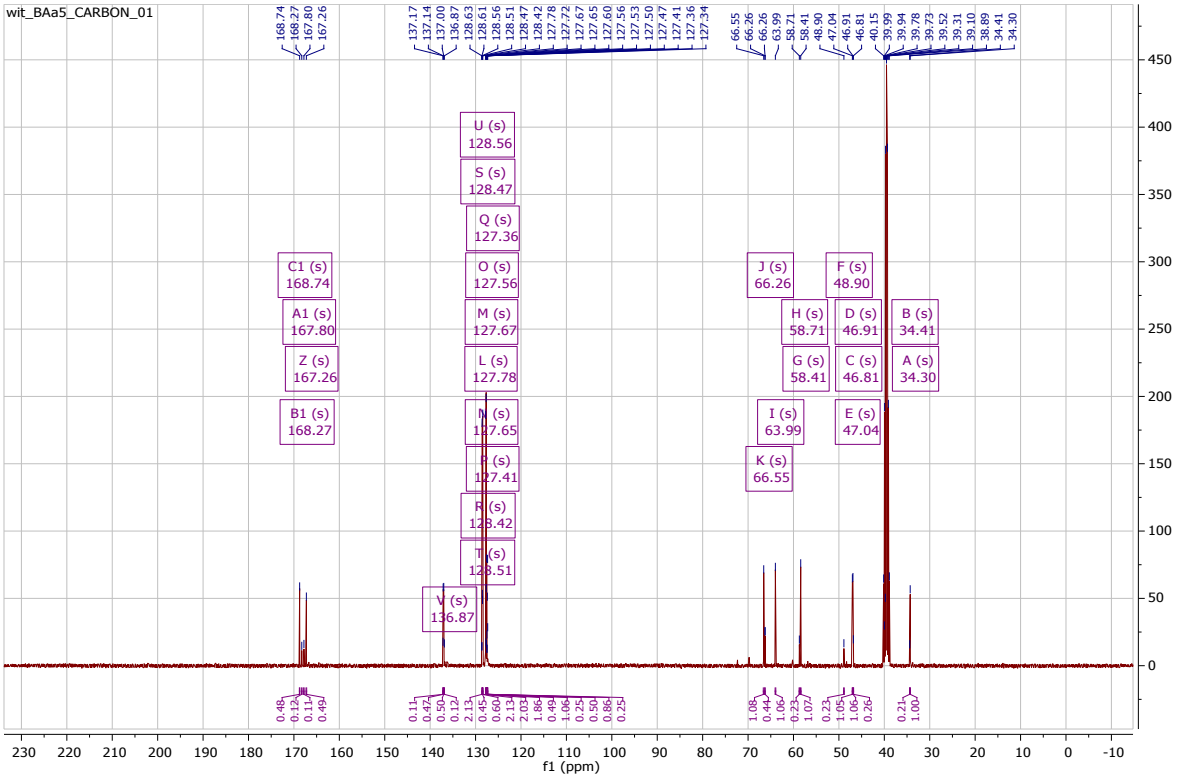

wit_SIa1_PROTON_01
HO
H
N
N
K (m)
7.32
N (d)
3.84
H (dt)
3.94
C (d)
3.16
D (m)
2.66
G (m)
3.68
A (m)
2.84
I (m)
1.45
F (d)
3.79
B (dd)
3.02
E (m)
2.45
f1 (ppm)

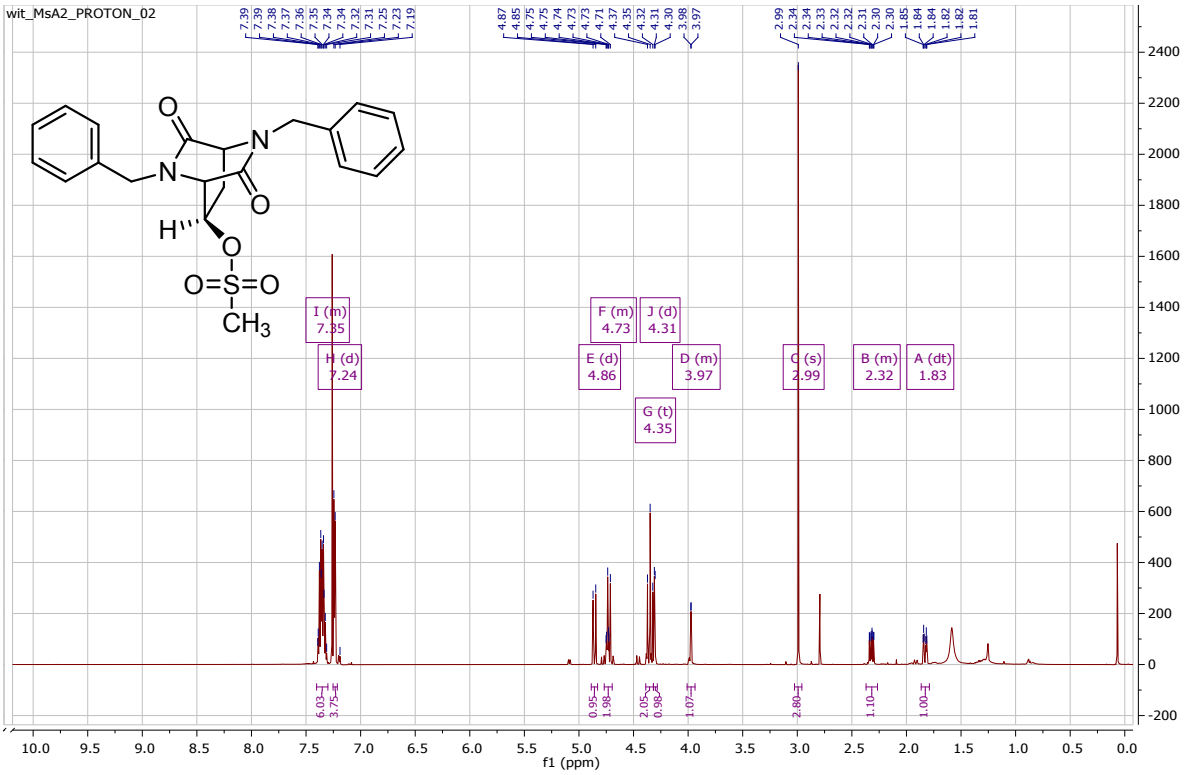

wit_SIa1_CARBON_01
O (s)
138.93
M (s)
128.99
K (s)
128.63
I (s)
127.50
H (s)
127.22
J (s)
128.47
L (s)
128.71
N (s)
138.47
F (s)
50.43
B (s)
59.46
G (s)
48.76
A (s)
67.52
C (s)
56.64
E (s)
36.43
D (s)
53.54
f1 (ppm)

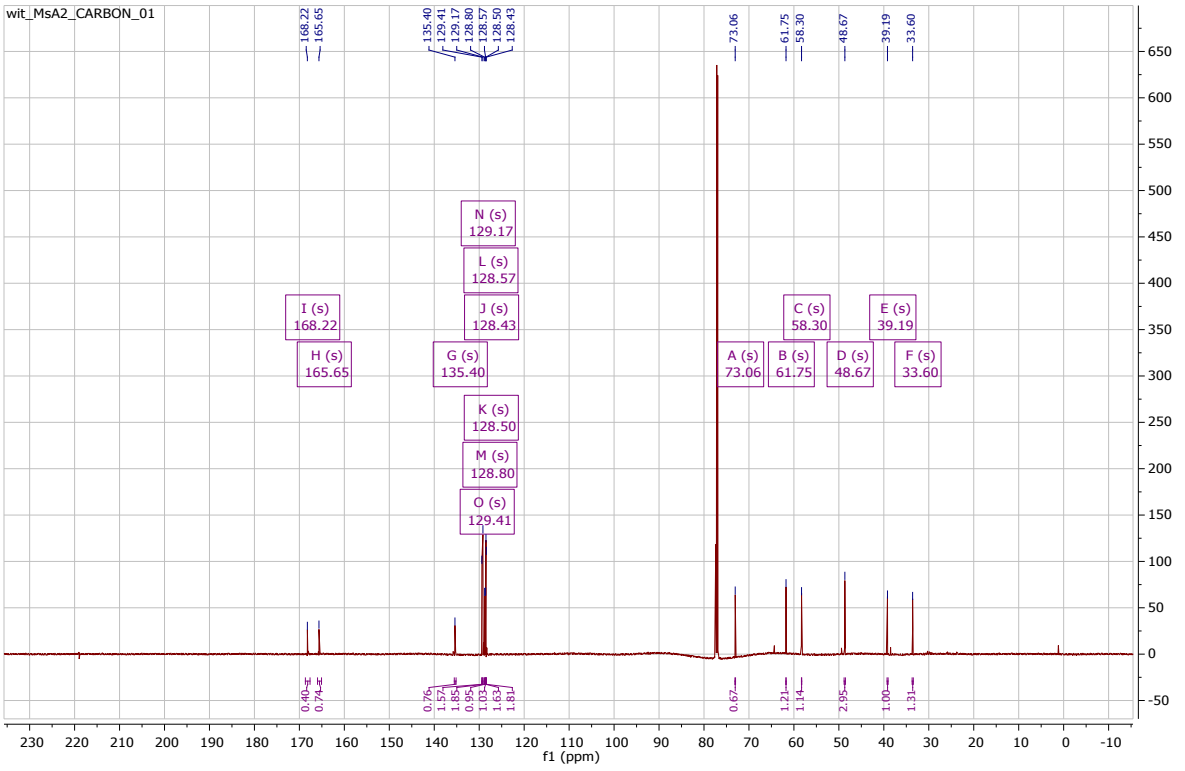

wit_SIB1_PROTON_01
L (s)
7.25
K (m)
7.36
H (dd)
3.90
E (m)
3.01
C (m)
2.80
G (m)
1.97
I (m)
4.16
A (dd)
3.35
B (dd)
2.73
F (m)
2.19
D (m)
2.91
f1 (ppm)

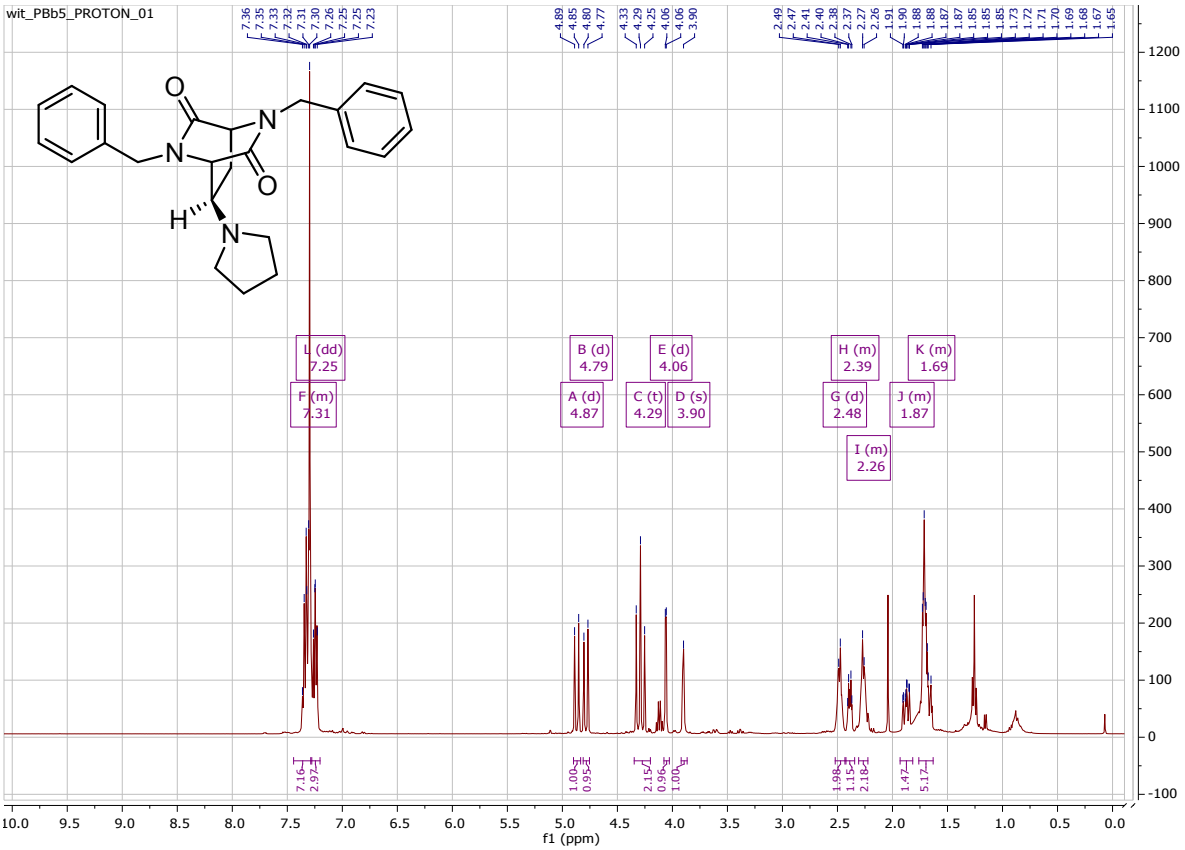

wit_SIB1_CARBON_01
P (s)
135.87
N (s)
129.41
E (s)
58.94
F (s)
66.42
B (s)
49.85
D (s)
58.75
A (s)
47.03
H (s)
35.80
C (s)
50.98
G (s)
54.57
O (s)
138.38
f1 (ppm)

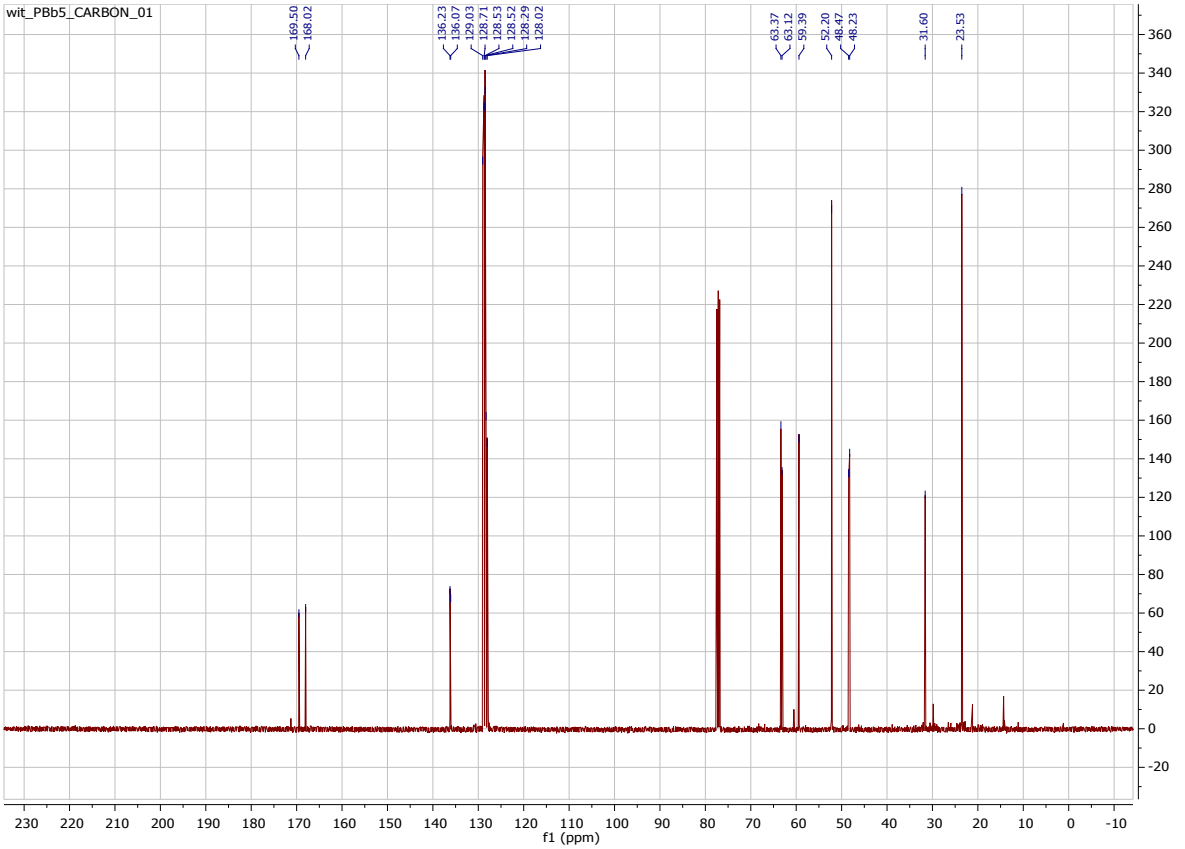

wit_BAa5_PROTON_01
M (m) 7.29
H (d) 5.45
G (d) 5.52
S (d) 5.08
F (s) 4.61
P (d) 4.23
E (d) 4.66
B (m) 4.09
D (d) 4.54
A (s) 3.99
R (d) 3.94
C (d) 4.37
N (d) 3.92
Q (s) 3.96
O (m) 4.04
L (m) 2.33
I (dd) 2.20
K (d) 1.46
J (d) 1.59
f1 (ppm)

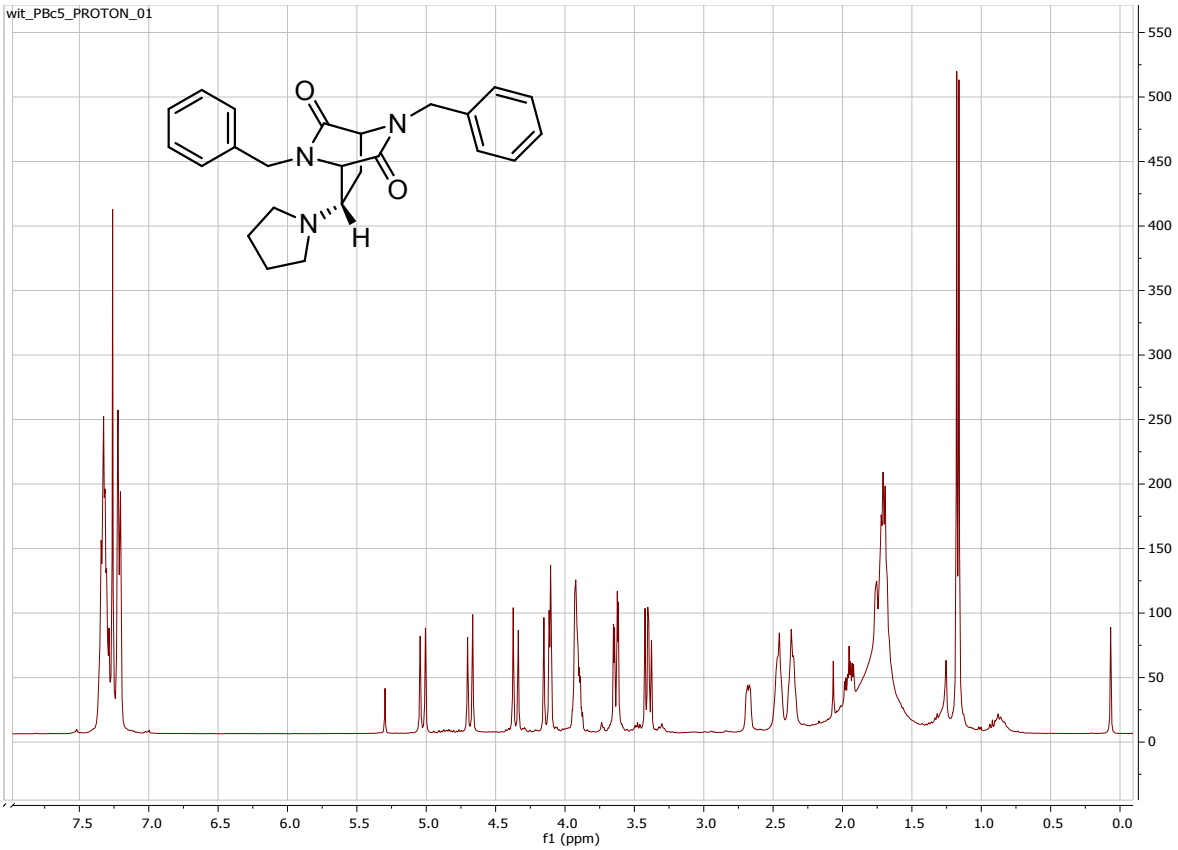

wit_BAa5_CARBON_01
U (s) 128.56
S (s) 128.47
Q (s) 127.36
C1 (s) 168.74
O (s) 127.56
A1 (s) 167.80
M (s) 127.67
Z (s) 167.26
L (s) 127.78
B1 (s) 168.27
J (s) 66.26
F (s) 48.90
H (s) 58.71
D (s) 46.91
B (s) 34.41
G (s) 58.41
C (s) 46.81
A (s) 34.30
I (s) 63.99
E (s) 47.04
K (s) 66.55
V (s) 136.87
f1 (ppm)

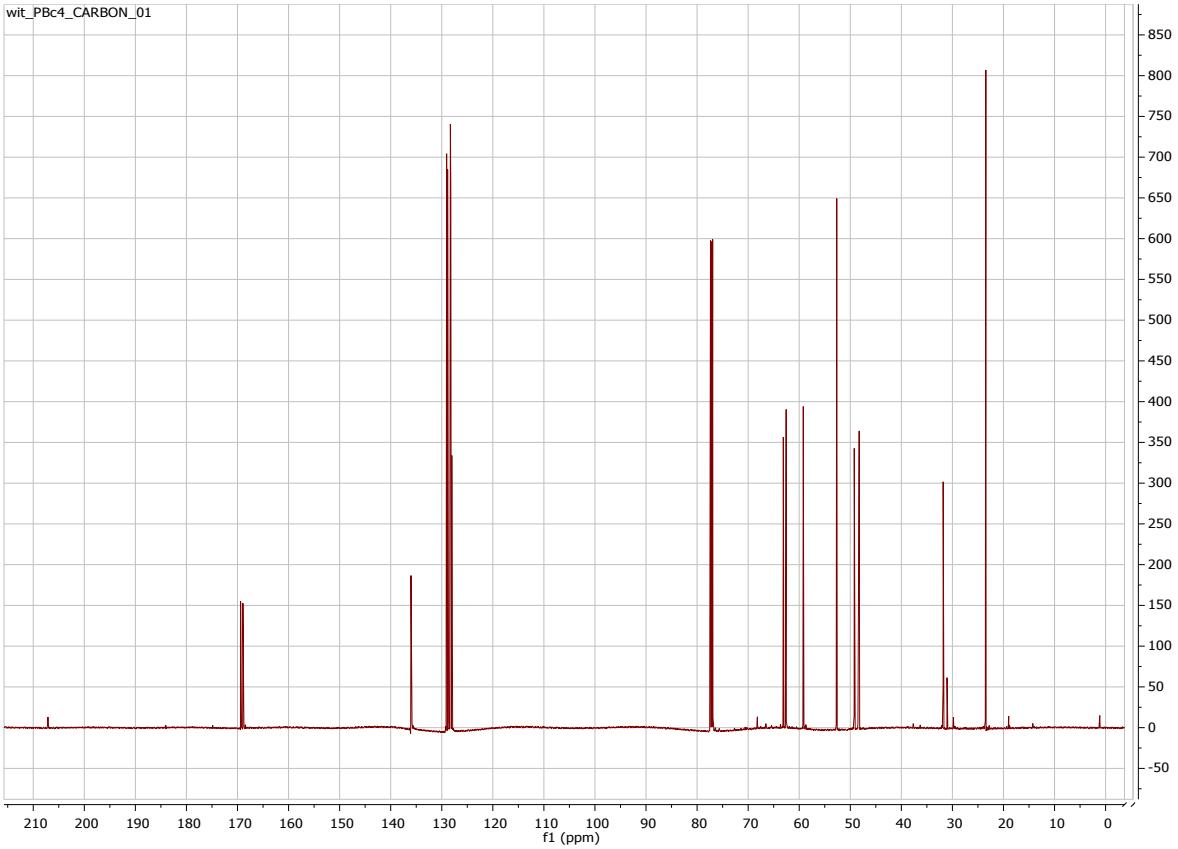

wit_MsA2_PROTON_02
I (m) 7.35
H (d) 7.24
F (m) 4.73
J (d) 4.31
E (d) 4.86
D (m) 3.97
G (t) 4.35
C (s) 2.99
B (m) 2.32
A (dt) 1.83
f1 (ppm)

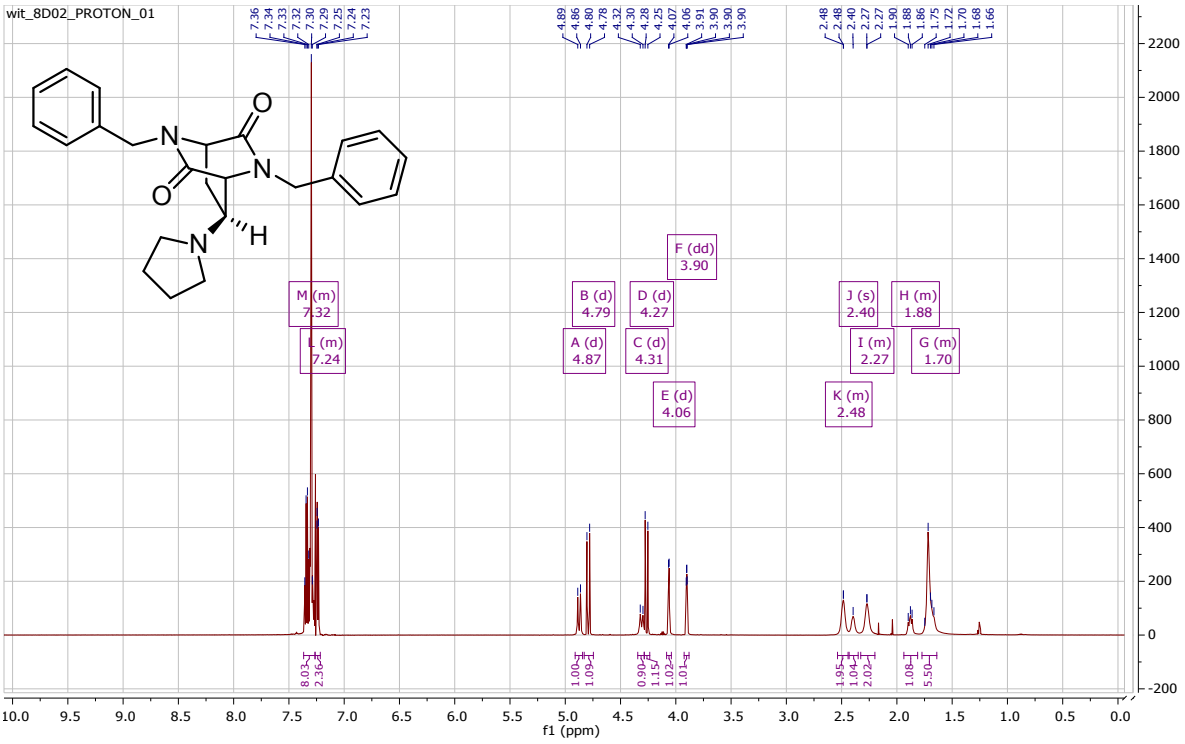

wit_MsA2_CARBON_01
N (s) 129.17
L (s) 128.57
J (s) 128.43
I (s) 168.22
H (s) 165.65
G (s) 135.40
K (s) 128.50
M (s) 128.80
O (s) 129.41
A (s) 73.06
B (s) 61.75
C (s) 58.30
D (s) 48.67
E (s) 39.19
F (s) 33.60
f1 (ppm)

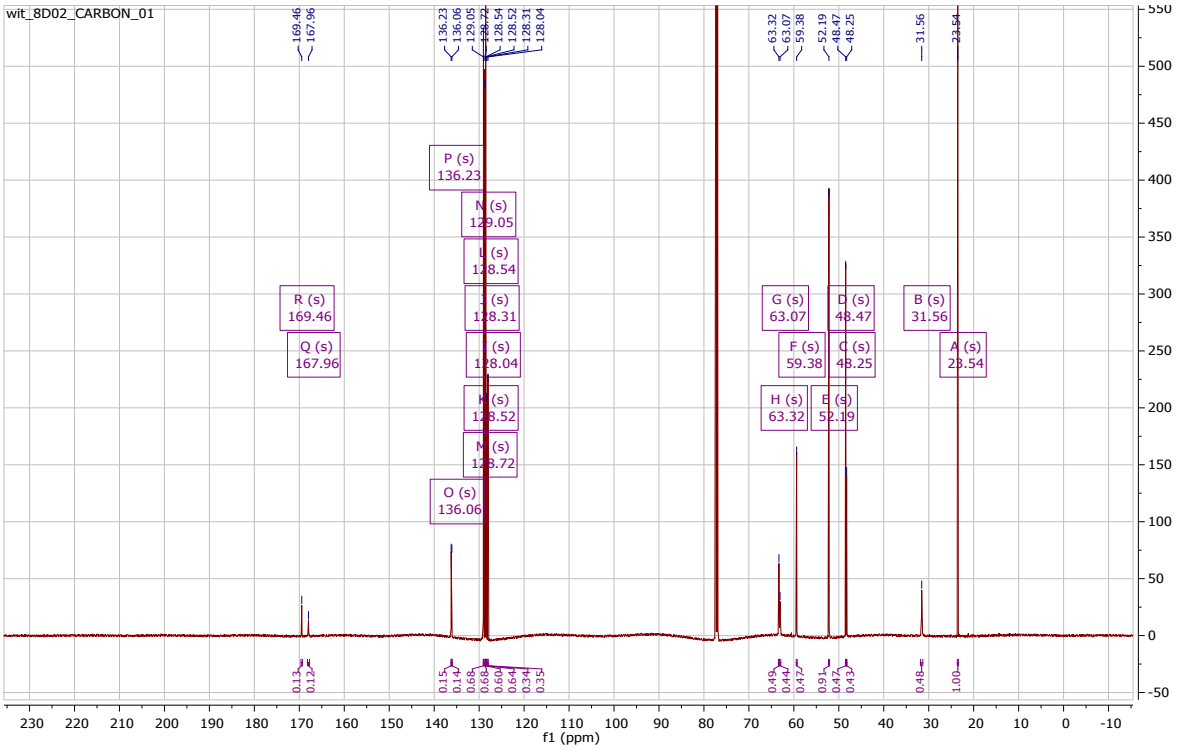

wit_PBb5_PROTON_01
L (dd) 7.25
F (m) 7.31
B (d) 4.79
A (d) 4.87
E (d) 4.06
C (t) 4.29
D (s) 3.90
H (m) 2.39
G (d) 2.48
I (m) 2.26
K (m) 1.69
J (m) 1.87
f1 (ppm)

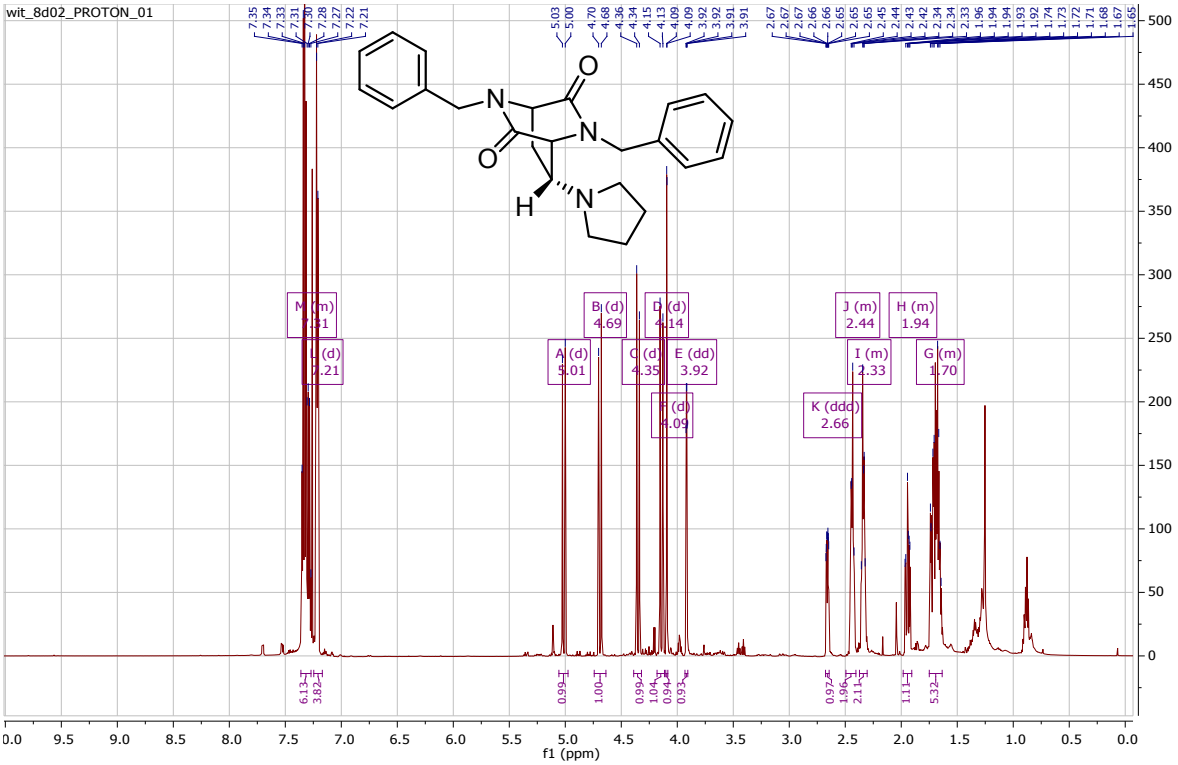

wit_PBb5_CARBON_01
f1 (ppm)

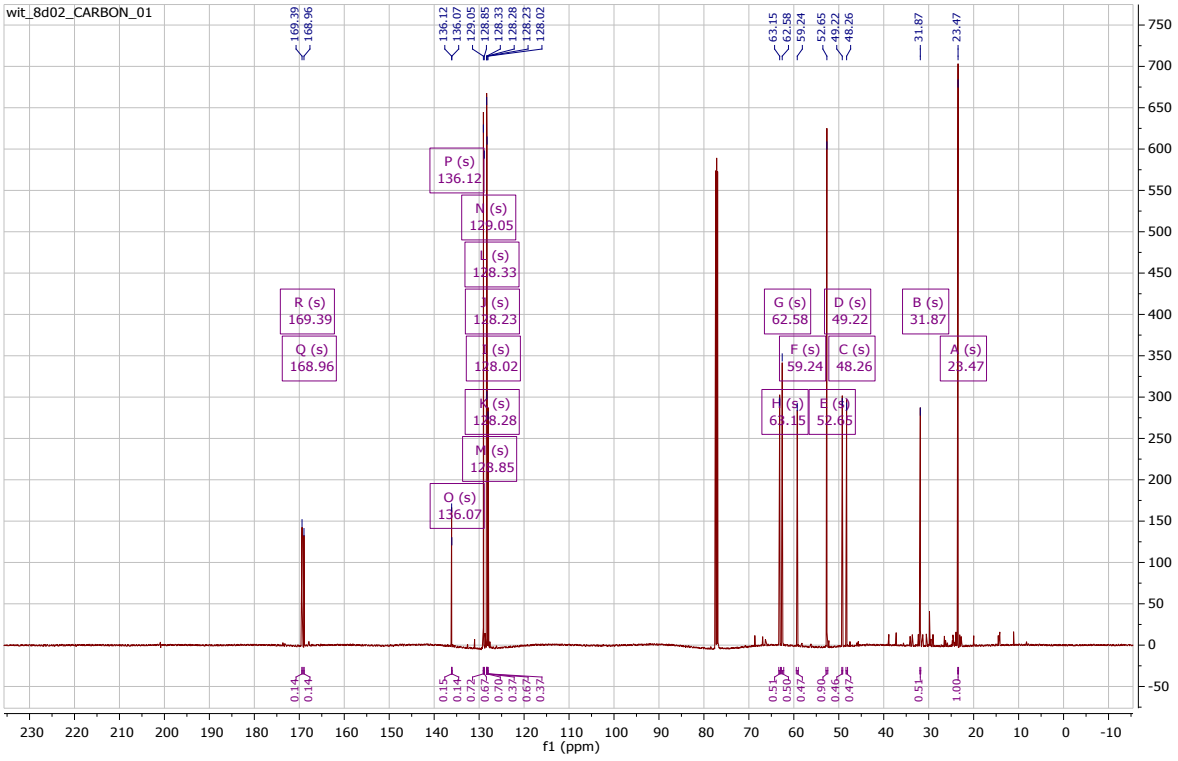

wit_PBc5_PROTON_01
O
N
N
O
N
H
f1 (ppm)

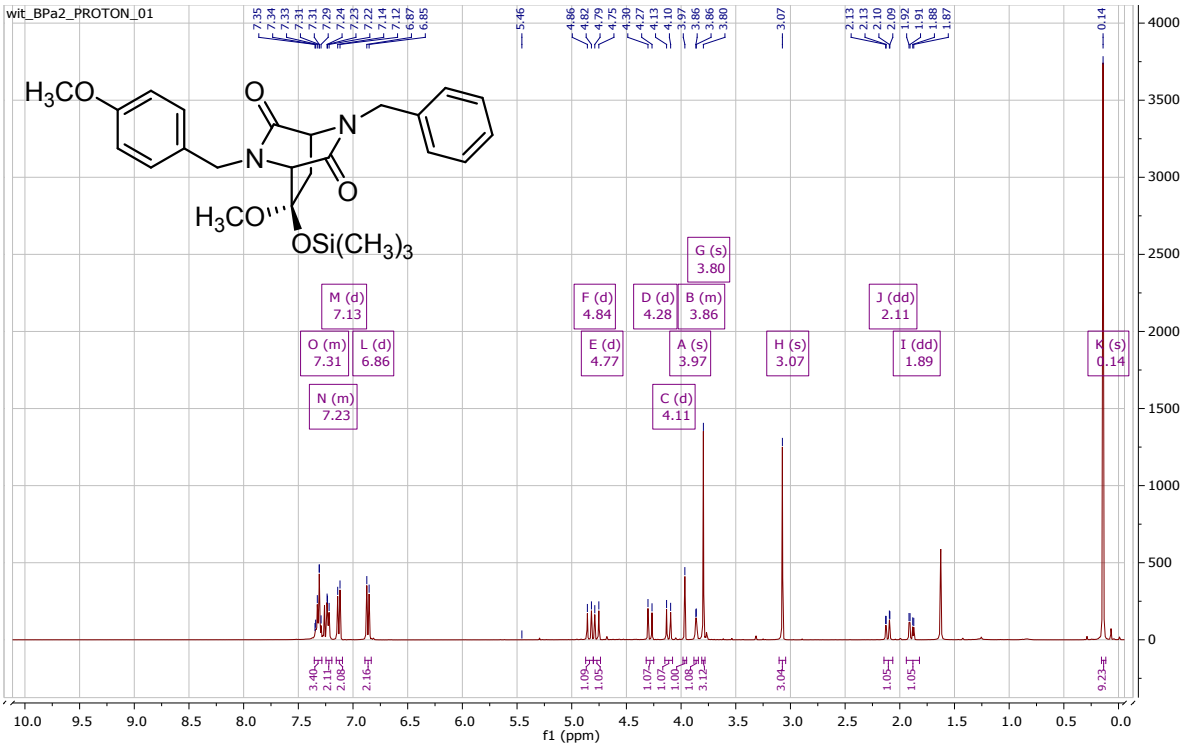

wit_PBc4_CARBON_01
f1 (ppm)

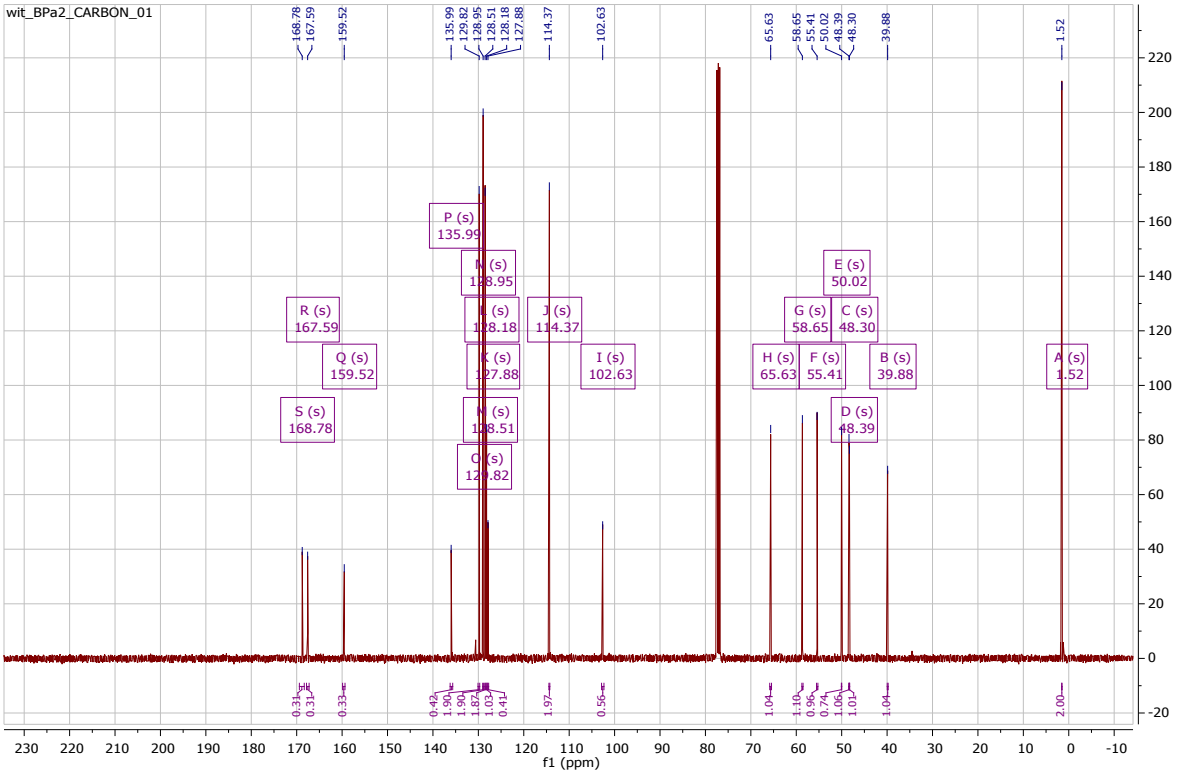

wit_8D02_PROTON_01
O
N
N
O
N
H
M (m) 7.32
L (m) 7.24
F (dd) 3.90
B (d) 4.79
D (d) 4.27
A (d) 4.87
C (d) 4.31
E (d) 4.06
J (s) 2.40
H (m) 1.88
I (m) 2.27
G (m) 1.70
K (m) 2.48
f1 (ppm)

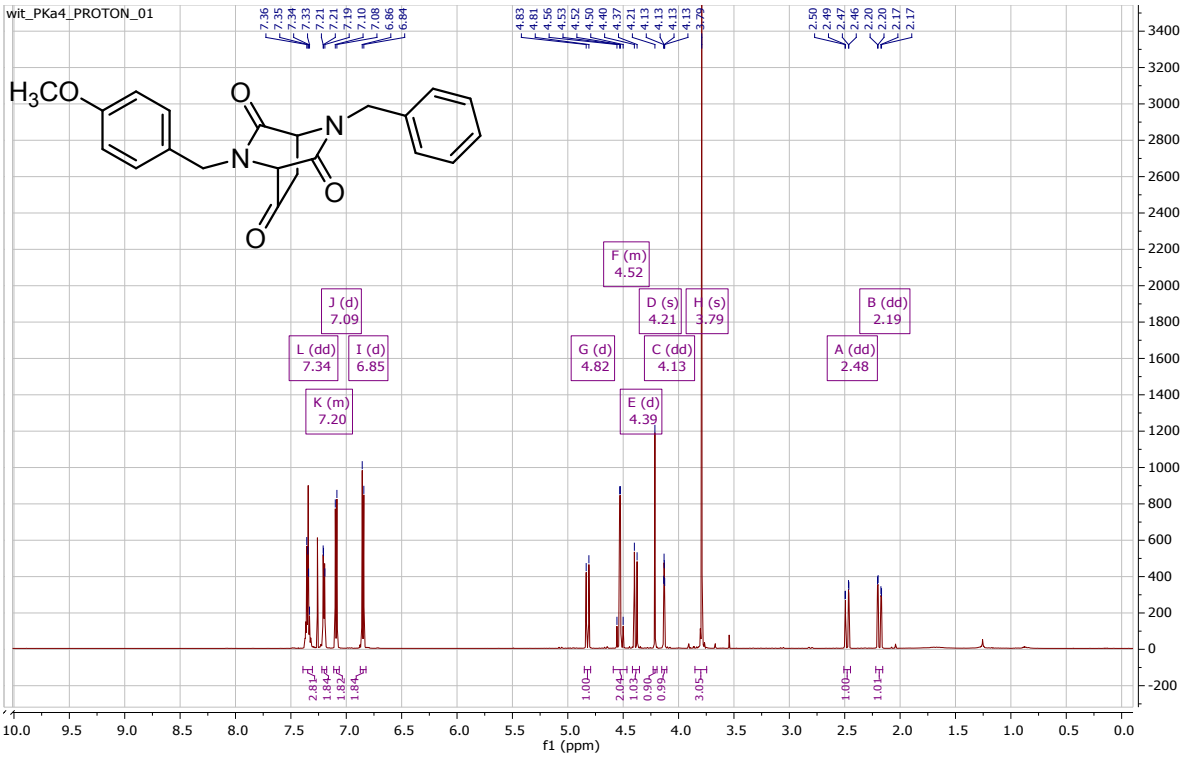

wit_8D02_CARBON_01
P (s) 136.23
N (s) 129.05
L (s) 128.54
J (s) 128.31
I (s) 128.04
K (s) 128.52
M (s) 128.72
O (s) 136.06
R (s) 169.46
Q (s) 167.96
G (s) 63.07
D (s) 48.47
F (s) 59.38
C (s) 48.25
H (s) 63.32
E (s) 52.19
B (s) 31.56
A (s) 23.54
f1 (ppm)

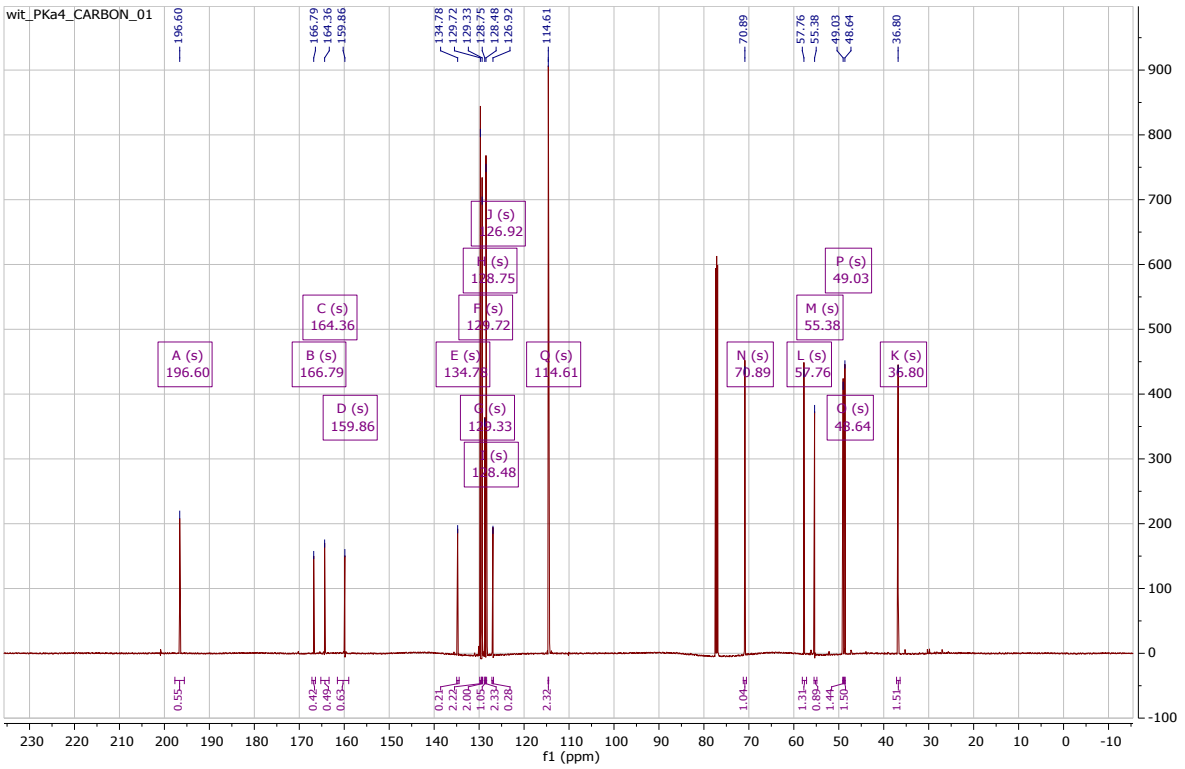

wit_8d02_PROTON_01
f1 (ppm)

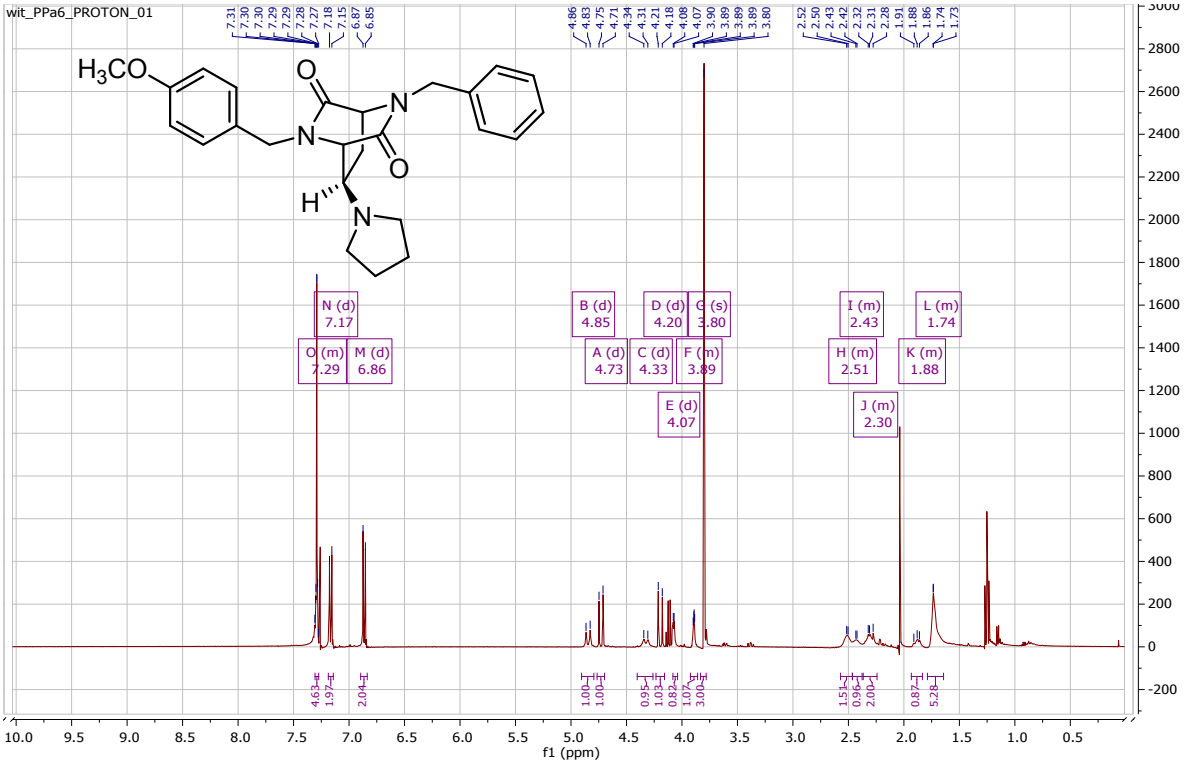

wit_8d02_CARBON_01
f1 (ppm)

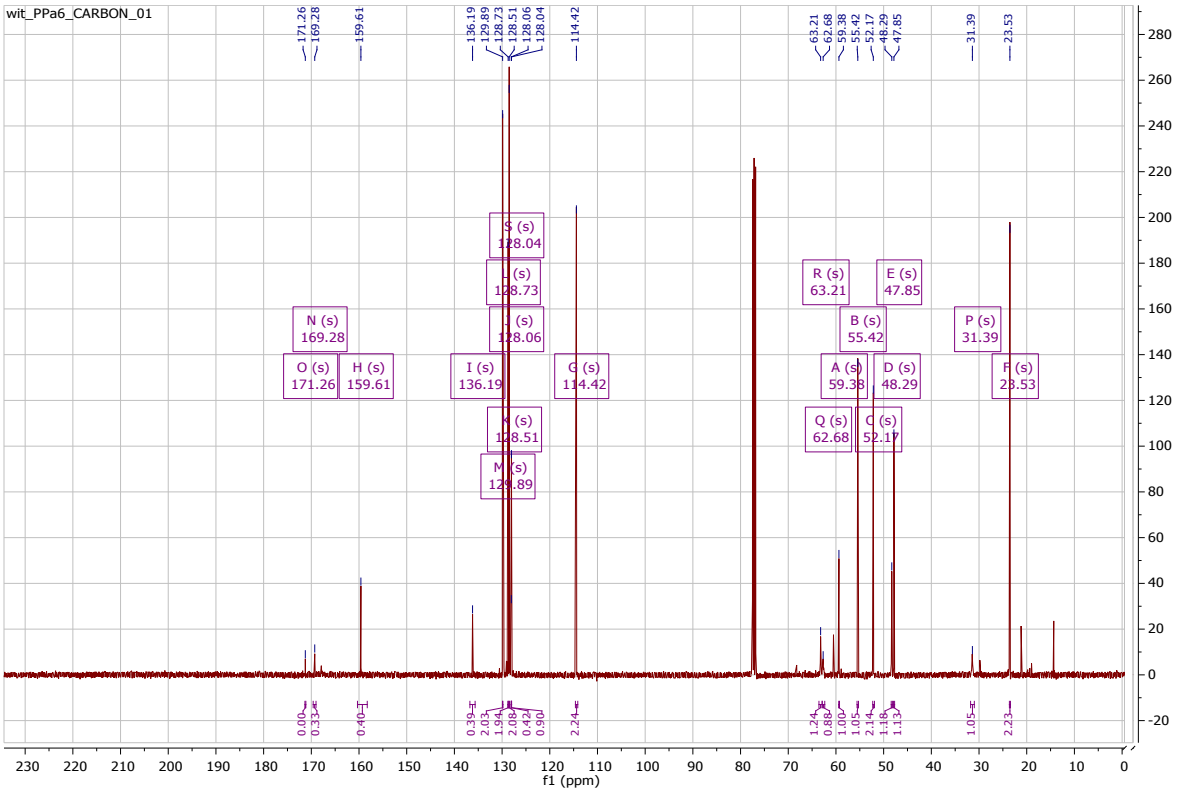

wit_BPa2_PROTON_01
H3CO
O
N
N
O
H3CO
OSi(CH3)3
M (d) 7.13
O (m) 7.31
L (d) 6.86
N (m) 7.23
F (d) 4.84
E (d) 4.77
D (d) 4.28
B (m) 3.86
G (s) 3.80
A (s) 3.97
C (d) 4.11
H (s) 3.07
J (dd) 2.11
I (dd) 1.89
K (s) 0.14
f1 (ppm)

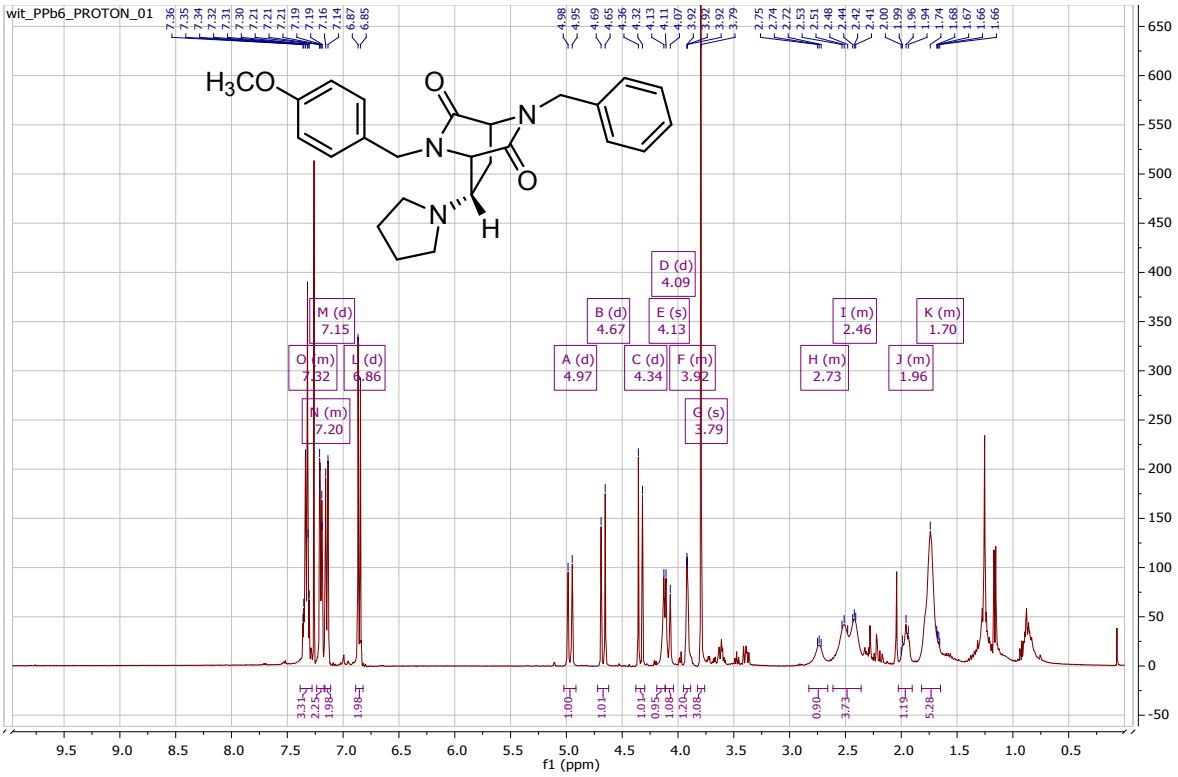

wit_BPa2_CARBON_01
P (s) 135.99
R (s) 167.59
Q (s) 159.52
S (s) 168.78
J (s) 114.37
I (s) 102.63
E (s) 50.02
G (s) 58.65
C (s) 48.30
H (s) 65.63
F (s) 55.41
B (s) 39.88
D (s) 48.39
A (s) 1.52
f1 (ppm)


wit_PKa4_PROTON_01
H3CO
O
N
N
O
O
F (m) 4.52
J (d) 7.09
D (s) 4.21
H (s) 3.79
B (dd) 2.19
L (dd) 7.34
I (d) 6.85
G (d) 4.82
C (dd) 4.13
A (dd) 2.48
K (m) 7.20
E (d) 4.39
f1 (ppm)

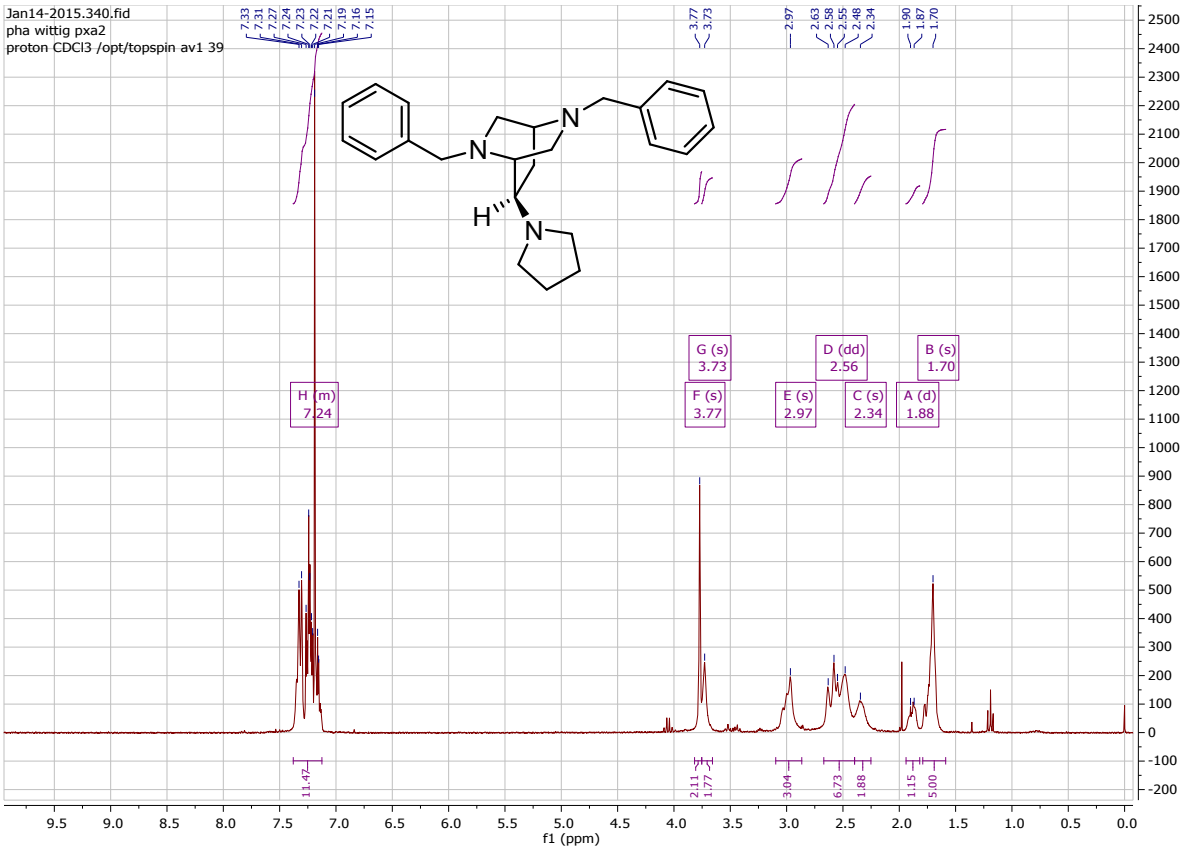

wit_PKa4_CARBON_01
A (s) 196.60
B (s) 166.79
C (s) 164.36
D (s) 159.86
E (s) 134.78
F (s) 129.72
G (s) 129.33
H (s) 128.75
I (s) 128.48
J (s) 126.92
Q (s) 114.61
N (s) 70.89
P (s) 49.03
M (s) 55.38
L (s) 57.76
O (s) 48.64
K (s) 36.80
f1 (ppm)

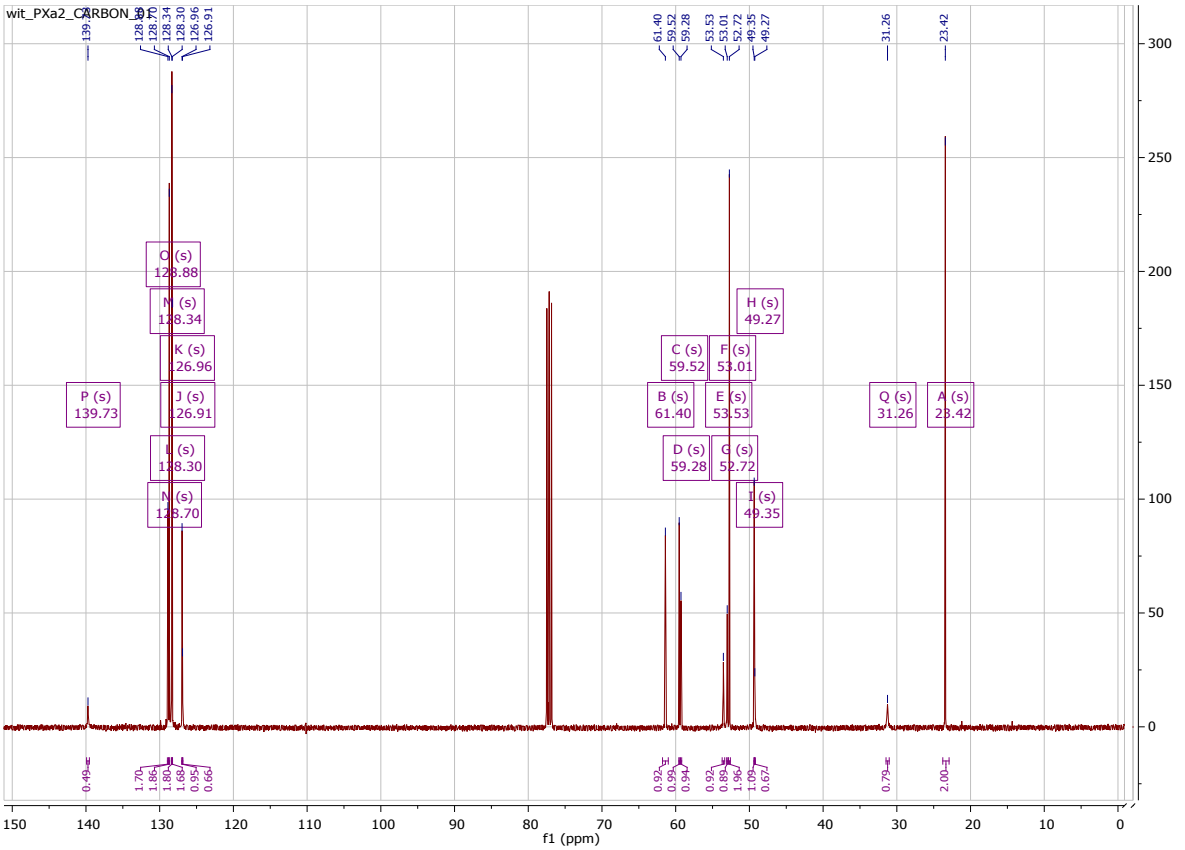

wit_PPa6_PROTON_01
H3CO
O
N
N
O
H
N
N (d) 7.17
O (m) 7.29
M (d) 6.86
B (d) 4.85
A (d) 4.73
D (d) 4.20
C (d) 4.33
G (s) 3.80
F (m) 3.89
E (d) 4.07
I (m) 2.43
H (m) 2.51
L (m) 1.74
K (m) 1.88
J (m) 2.30
f1 (ppm)

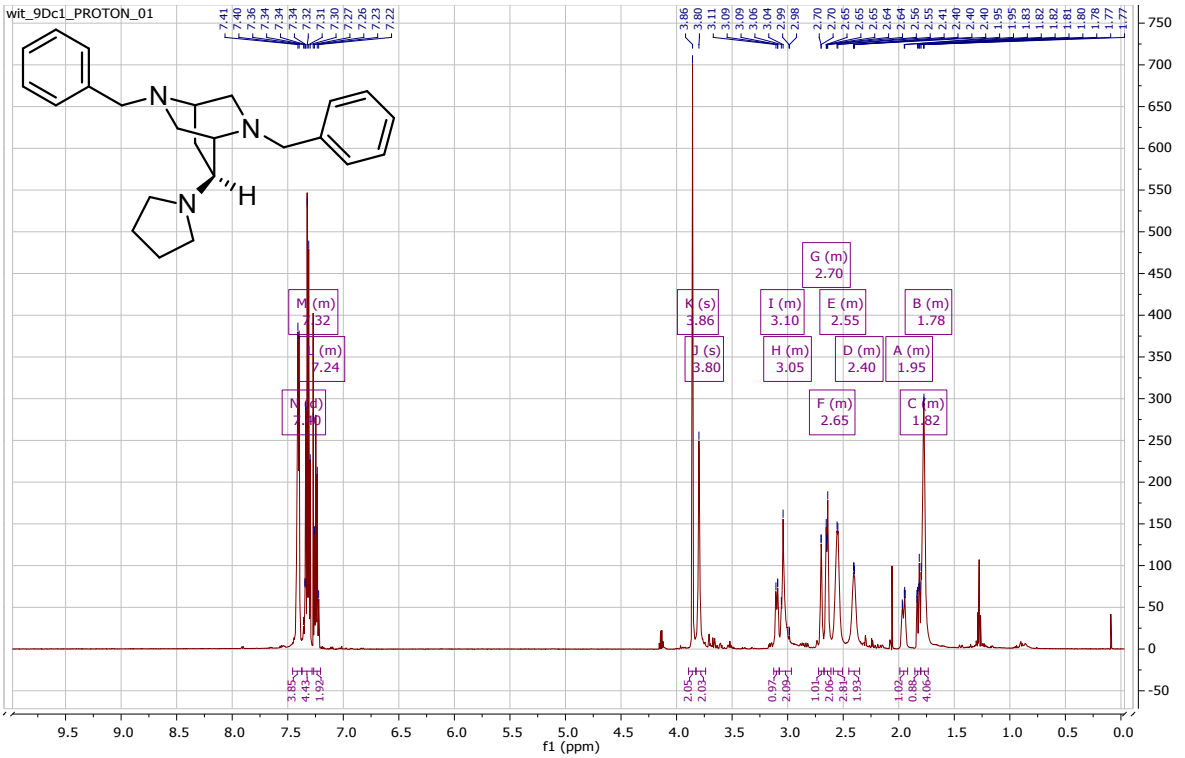

wit_PPa6_CARBON_01
S (s) 128.04
T (s) 128.73
J (s) 128.06
N (s) 169.28
O (s) 171.26
H (s) 159.61
I (s) 136.19
G (s) 114.42
K (s) 128.51
M (s) 129.89
R (s) 63.21
E (s) 47.85
B (s) 55.42
P (s) 31.39
A (s) 59.38
D (s) 48.29
F (s) 23.53
Q (s) 62.68
C (s) 52.17
f1 (ppm)


wit_PPb6_PROTON_01
H3CO
O
N
N
O
N
H
D (d) 4.09
M (d) 7.15
B (d) 4.67
E (s) 4.13
I (m) 2.46
K (m) 1.70
O (m) 7.32
L (d) 6.86
A (d) 4.97
C (d) 4.34
F (m) 3.92
H (m) 2.73
J (m) 1.96
N (m) 7.20
G (s) 3.79
f1 (ppm)

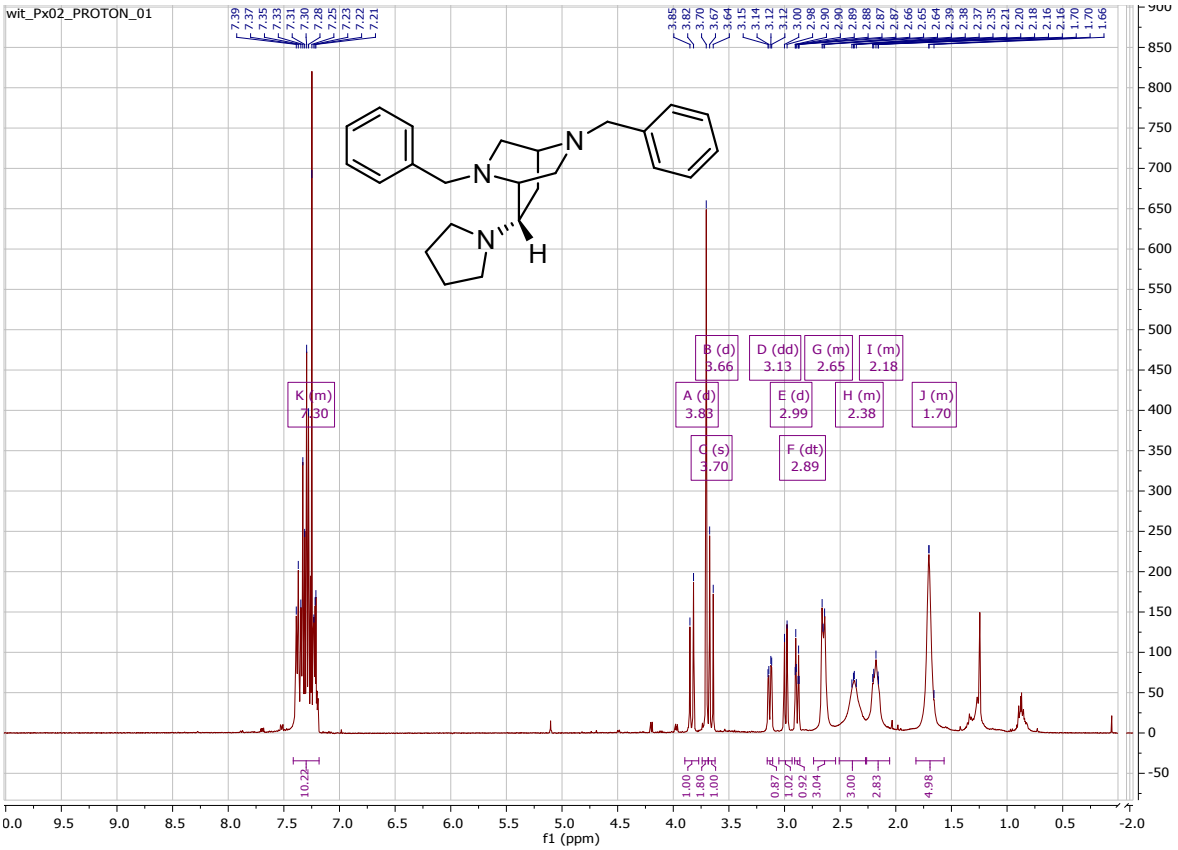

wit_PPb6_CARBON_01
S (s) 128.32
O (s) 136.00
F (s) 55.42
Q (s) 169.06
M (s) 129.07
H (s) 62.44
D (s) 48.63
B (s) 31.43
P (s) 159.49
K (s) 127.99
J (s) 114.32
G (s) 59.16
C (s) 48.31
A (s) 23.50
R (s) 168.73
N (s) 129.72
I (s) 62.61
E (s) 52.69
L (s) 128.33
f1 (ppm)

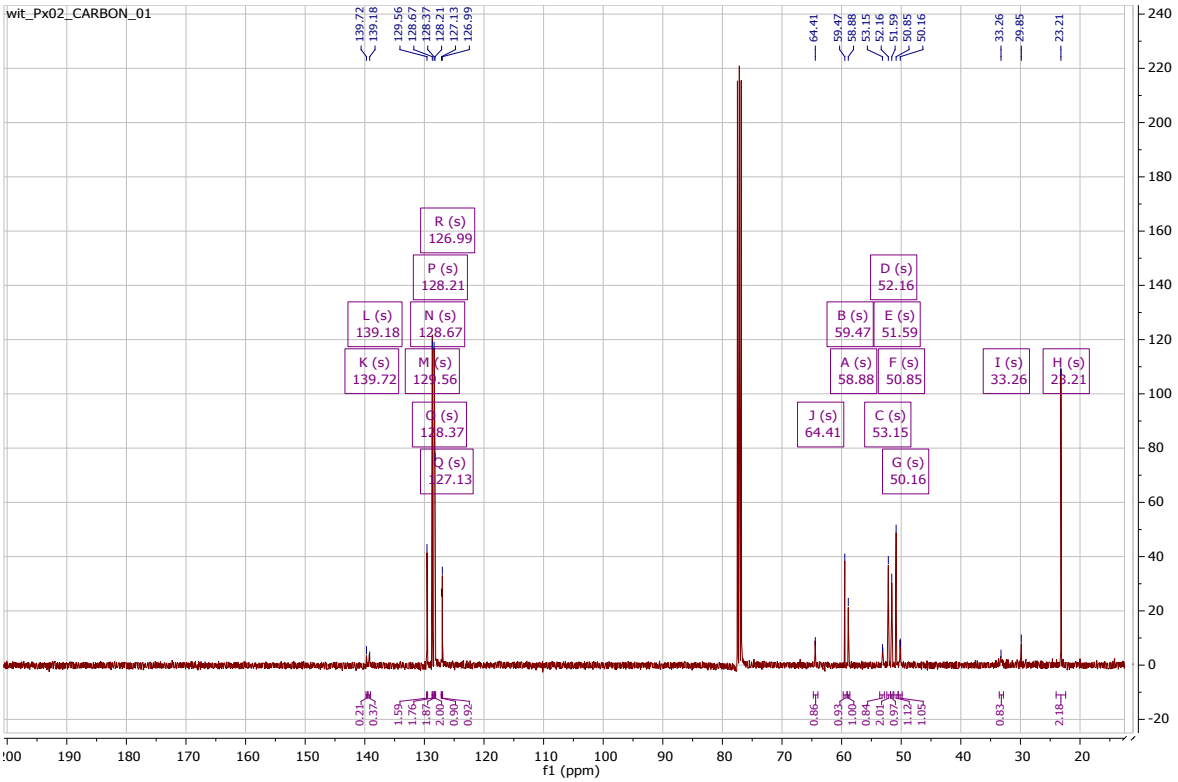

Jan14-2015.340.fid
pha wittig pxa2
proton CDCl3 /opt/topspin av1 39
H (m) 7.24
G (s) 3.73
F (s) 3.77
D (dd) 2.56
E (s) 2.97
C (s) 2.34
B (s) 1.70
A (d) 1.88
f1 (ppm)

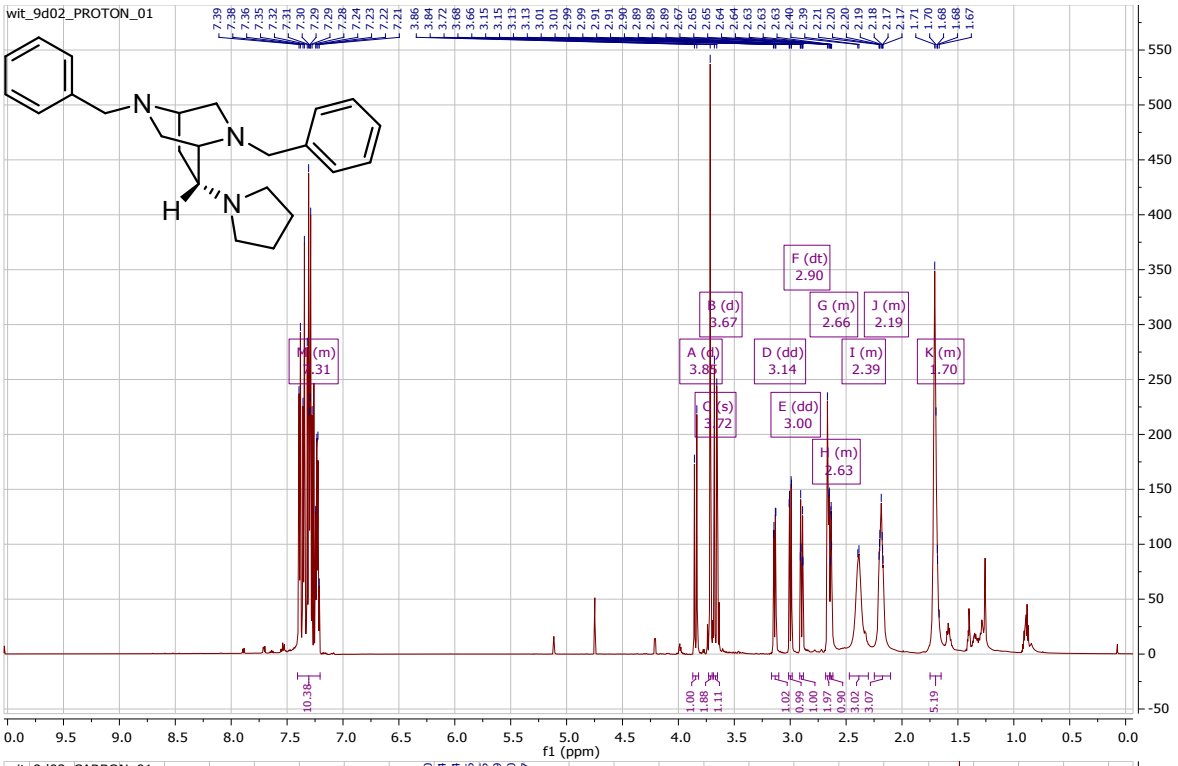

wit_PXa2_CARBON_01
O (s) 128.88
N (s) 128.34
K (s) 126.96
J (s) 126.91
L (s) 128.30
M (s) 128.70
P (s) 139.73
H (s) 49.27
C (s) 59.52
F (s) 53.01
B (s) 61.40
E (s) 53.53
D (s) 59.28
G (s) 52.72
I (s) 49.35
Q (s) 31.26
A (s) 23.42
f1 (ppm)

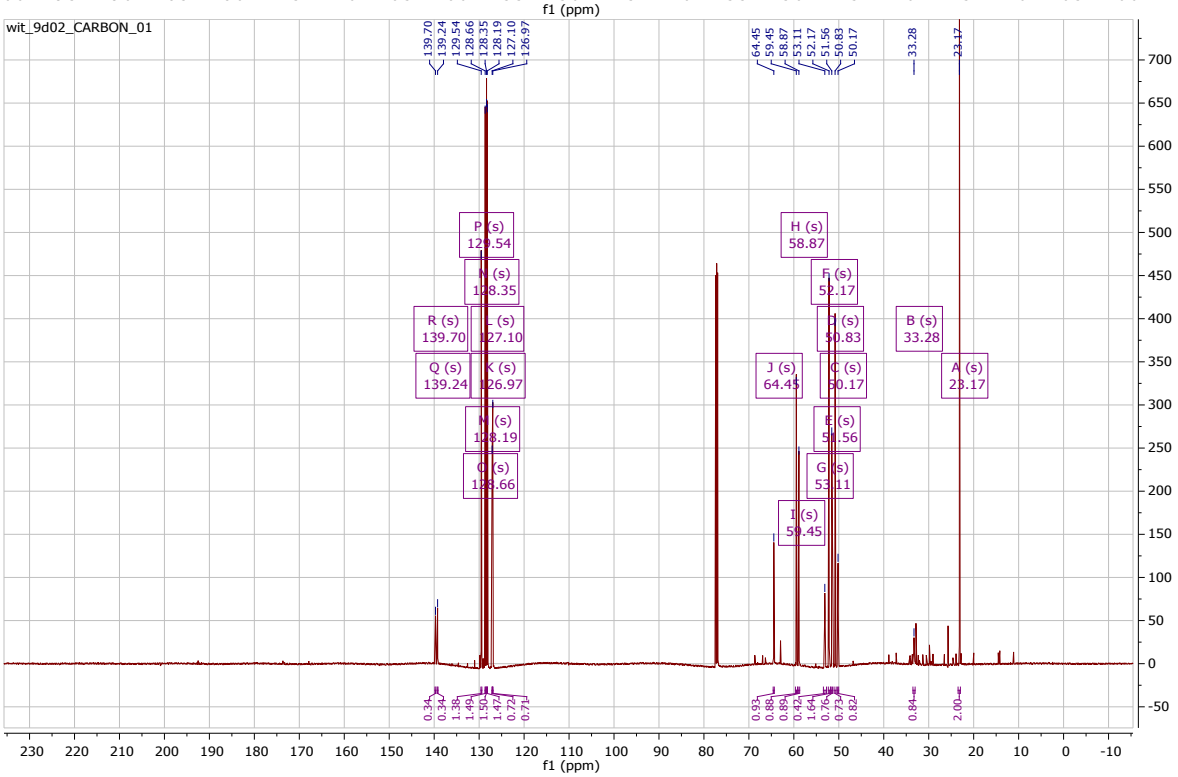

wit_9Dc1_PROTON_01
N
N
N
H
M (m)
7.32
L (m)
7.24
N (m)
7.30
K (s)
3.86
J (s)
3.80
G (m)
2.70
I (m)
3.10
E (m)
2.55
B (m)
1.78
H (m)
3.05
D (m)
2.40
A (m)
1.95
F (m)
2.65
C (m)
1.82
f1 (ppm)

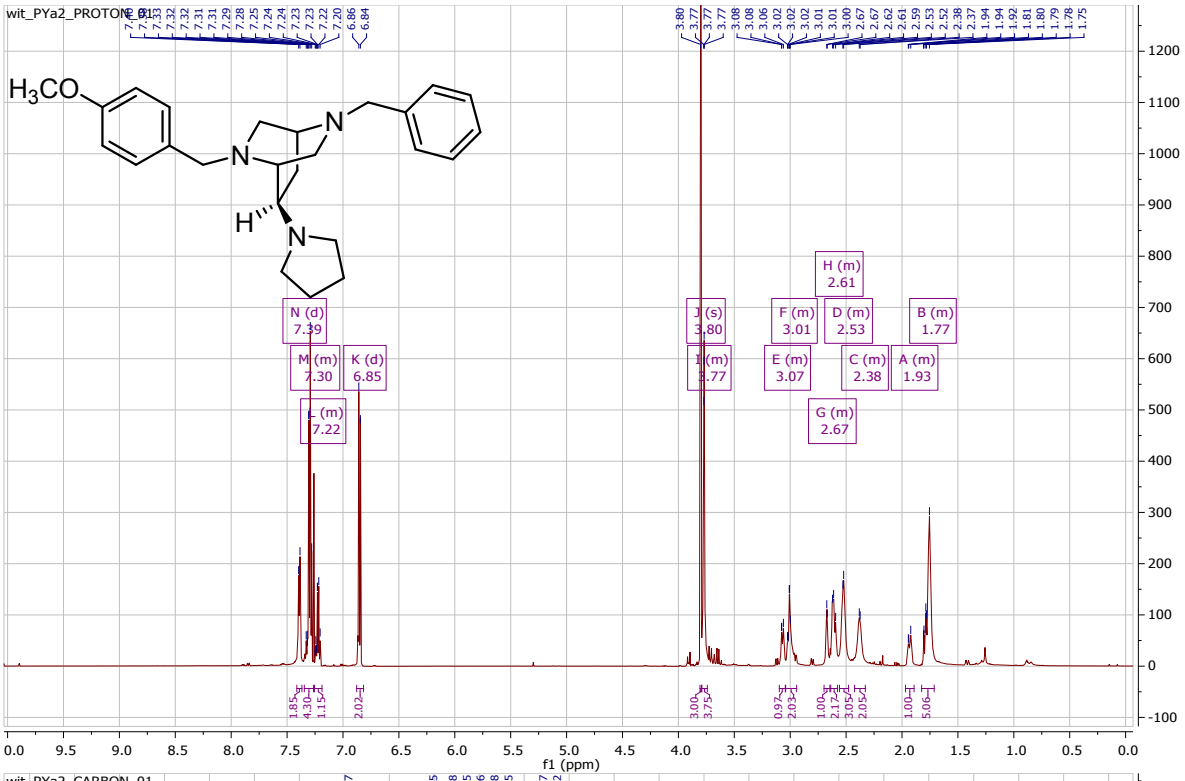

wit_9Dc1_CARBON_01
N (s)
128.85
L (s)
128.33
J (s)
126.87
P (s)
139.77
I (s)
126.95
K (s)
128.28
M (s)
128.69
G (s)
59.51
E (s)
53.58
C (s)
52.72
O (s)
31.30
H (s)
61.39
B (s)
49.31
A (s)
23.40
D (s)
53.01
F (s)
59.29
f1 (ppm)

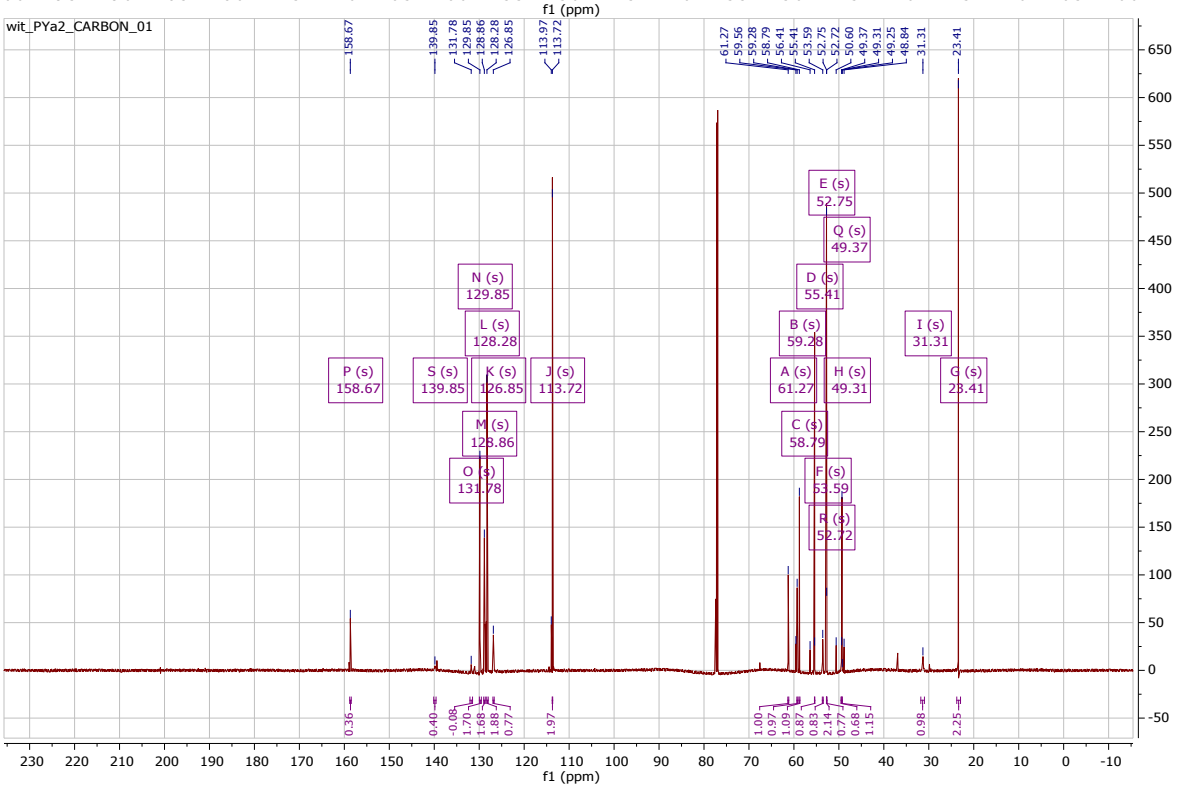

wit_Px02_PROTON_01
N
N
N
H
K (m) 7.30
B (d) 3.66
D (dd) 3.13
G (m) 2.65
I (m) 2.18
A (d) 3.83
E (d) 2.99
H (m) 2.38
J (m) 1.70
C (s) 3.70
F (dt) 2.89
f1 (ppm)

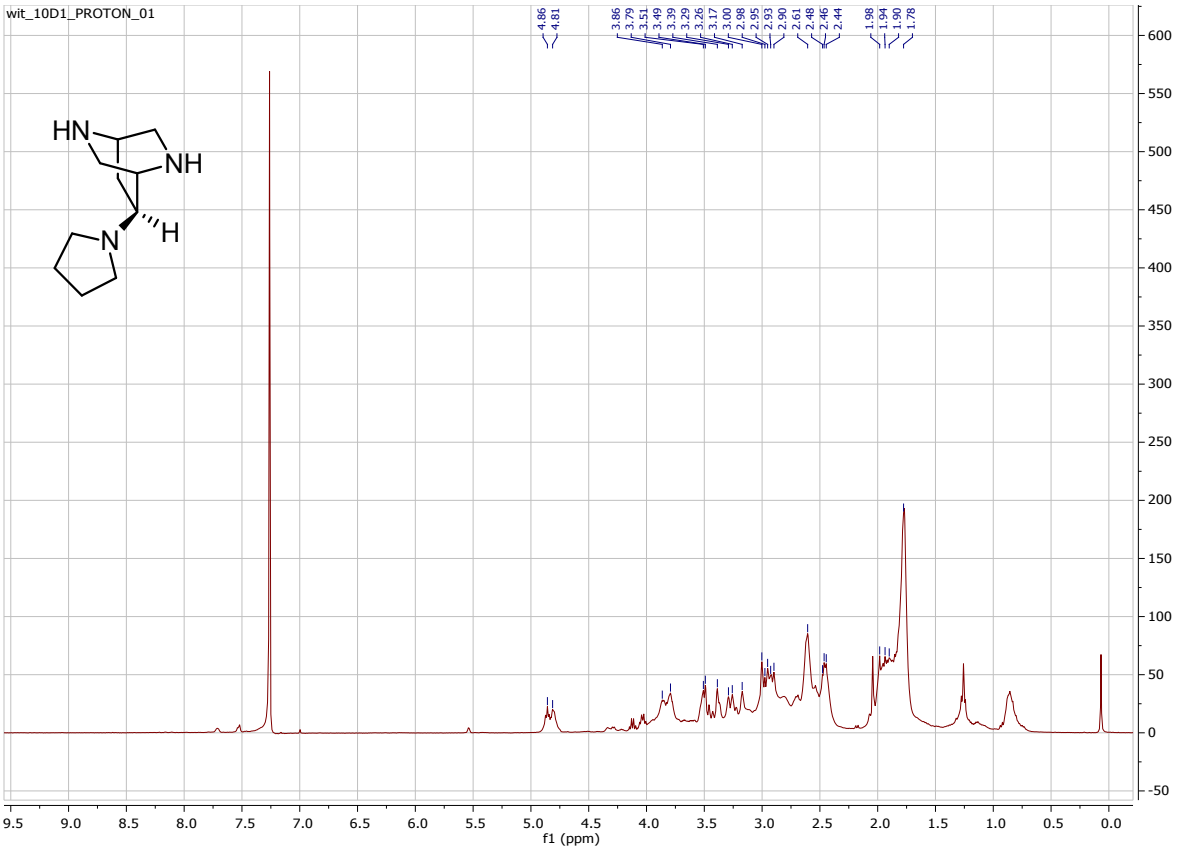

wit_Px02_CARBON_01
R (s) 126.99
P (s) 128.21
L (s) 139.18
N (s) 128.67
K (s) 139.72
M (s) 129.56
O (s) 128.37
Q (s) 127.13
D (s) 52.16
B (s) 59.47
E (s) 51.59
A (s) 58.88
F (s) 50.85
J (s) 64.41
C (s) 53.15
G (s) 50.16
I (s) 33.26
H (s) 23.21
f1 (ppm)

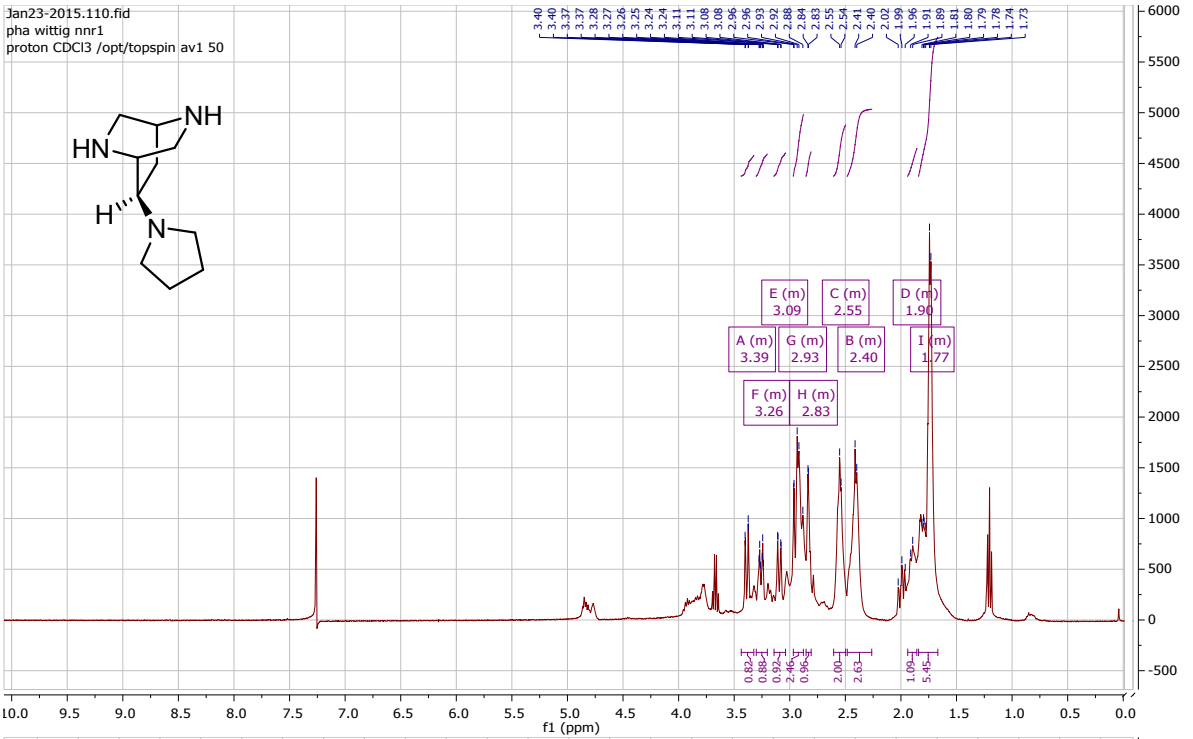

wit_9d02_PROTON_01
f1 (ppm)

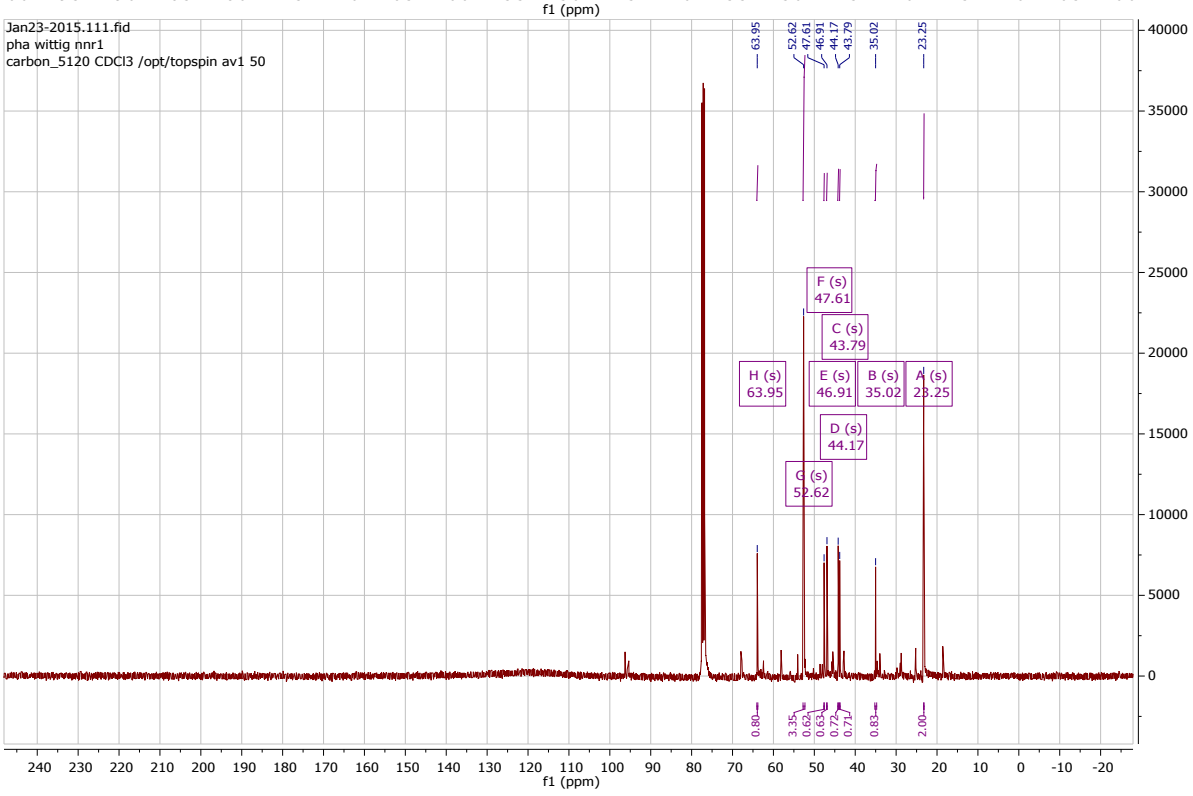

wit_9d02_CARBON_01
f1 (ppm)

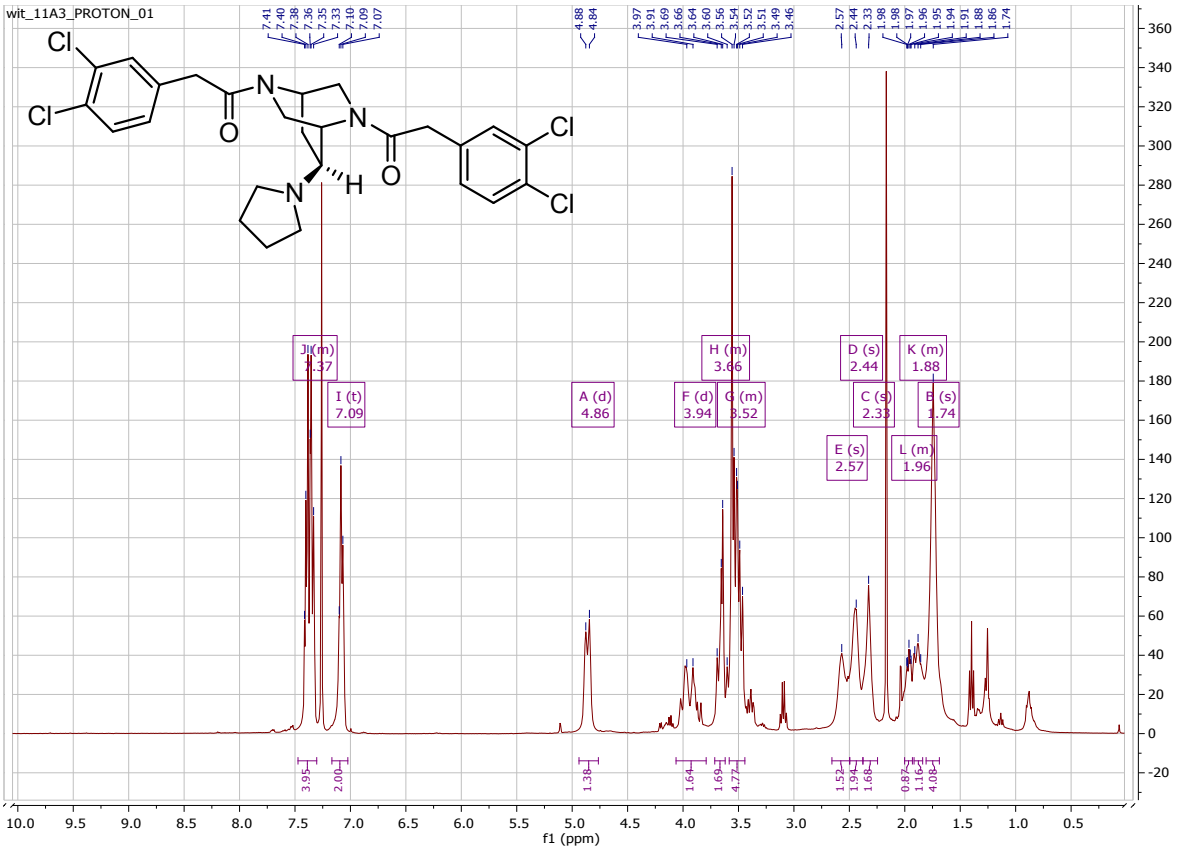

wit_PYa2_PROTON_01
H3CO
N
N
H
N
N (d) 7.39
M (m) 7.30
K (d) 6.85
L (m) 7.22
J (s) 3.80
I (m) 3.77
H (m) 2.61
F (m) 3.01
D (m) 2.53
B (m) 1.77
E (m) 3.07
C (m) 2.38
A (m) 1.93
G (m) 2.67
f1 (ppm)

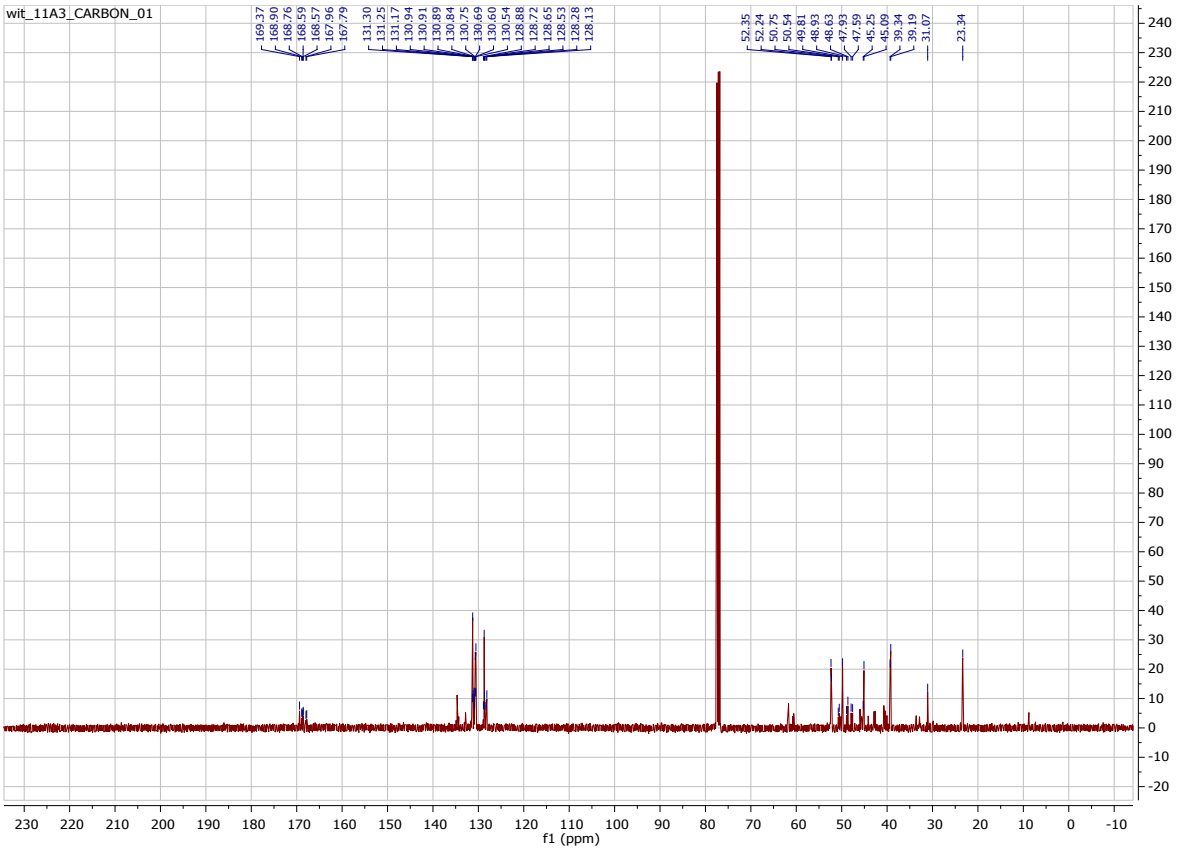

wit_PYa2_CARBON_01
P (s) 158.67
S (s) 139.85
N (s) 129.85
L (s) 128.28
K (s) 126.85
M (s) 128.86
O (s) 131.78
J (s) 113.72
E (s) 52.75
Q (s) 49.37
D (s) 55.41
B (s) 59.28
A (s) 61.27
H (s) 49.31
C (s) 58.79
F (s) 53.59
R (s) 52.72
I (s) 31.31
G (s) 23.41
f1 (ppm)

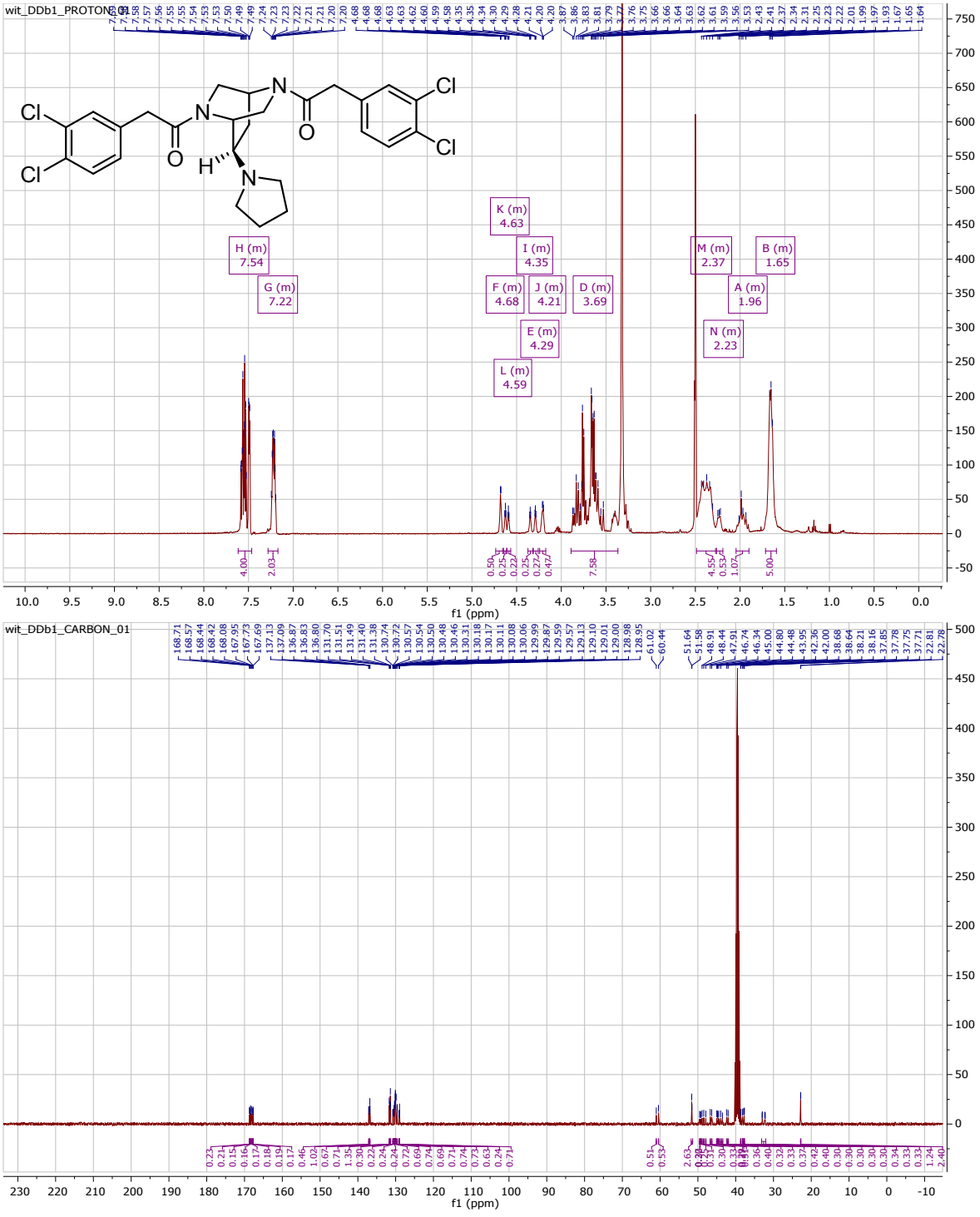

wit_10D1_PROTON_01
HN
NH
N
H
4.86
4.81
3.86
3.79
3.51
3.49
3.39
3.29
3.26
3.17
3.00
2.98
2.95
2.93
2.90
2.61
2.48
2.46
2.44
1.98
1.94
1.90
1.78
f1 (ppm)


Jan23-2015.110.fid
pha wittig nnr1
proton CDCl3 /opt/topspin av1 50
NH
HN
H
N
E (m) 3.09
C (m) 2.55
D (m) 1.90
A (m) 3.39
G (m) 2.93
B (m) 2.40
I (m) 1.77
F (m) 3.26
H (m) 2.83
f1 (ppm)


Jan23-2015.111.fid
pha wittig nnr1
carbon_5120 CDCl3 /opt/topspin av1 50
F (s) 47.61
C (s) 43.79
H (s) 63.95
E (s) 46.91
B (s) 35.02
A (s) 23.25
D (s) 44.17
G (s) 52.62
f1 (ppm)


wit_11A3_PROTON_01
Cl
Cl
O
N
N
O
H
N
Cl
Cl
J (m) 7.37
I (t) 7.09
A (d) 4.86
H (m) 3.66
F (d) 3.94
G (m) 3.52
D (s) 2.44
C (s) 2.33
E (s) 2.57
K (m) 1.88
L (m) 1.96
B (s) 1.74
f1 (ppm)


wit_11A3_CARBON_01
f1 (ppm)


wit_DDb1_PROTON_01
H (m) 7.54
G (m) 7.22
K (m) 4.63
I (m) 4.35
F (m) 4.68
J (m) 4.21
D (m) 3.69
E (m) 4.29
L (m) 4.59
M (m) 2.37
B (m) 1.65
A (m) 1.96
N (m) 2.23
f1 (ppm)
wit_DDb1_CARBON_01
f1 (ppm)