Supporting Information for

A new ONO^{3-} trianionic pincer-type ligand for generating highly nucleophilic metal-carbon multiple bonds: an inorganic enamine.

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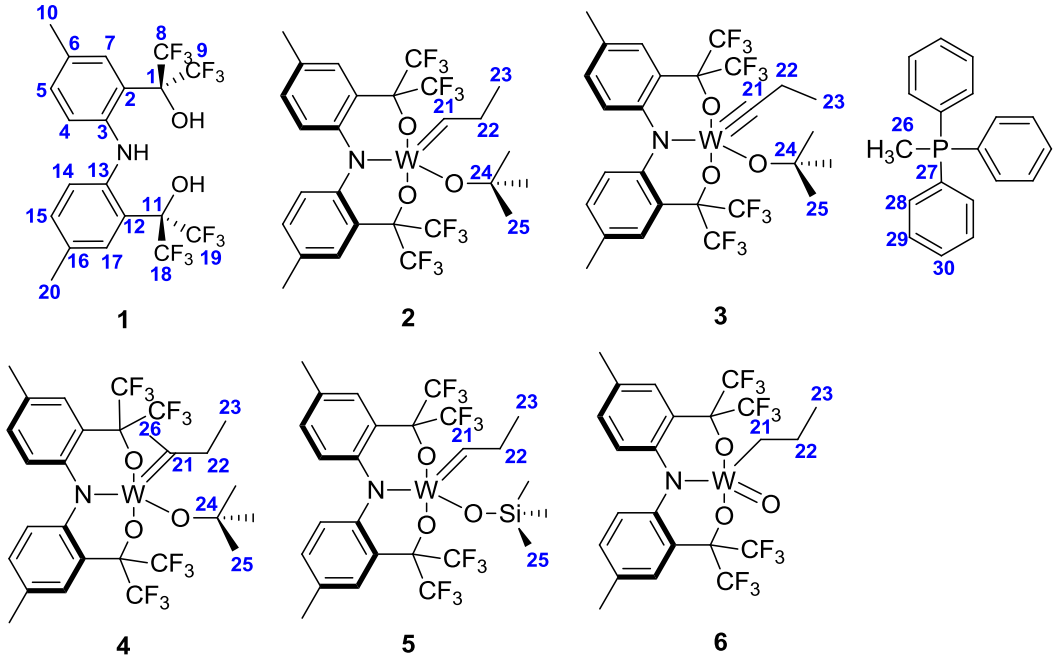

Figure S1. Labelling scheme for ^{1}H and ^{13}C NMR peaks.

Table S1. ^{1}H, ^{13}C, ^{19}F and ^{15}N chemical shifts in compounds **1-6** in C_6D_6.

Compd.	1	2	3 [a]	4 [c]	5	6
C1	80.6	82.9	83.6	83.8	83.1	84.1
C2	120.9	123.5	121.0	122.8	123.1	123.3
C3	143.0	146.1	154.2	145.3	145.8	145.8
C4	126.1	123.0	123.3	124.0	123.6	124.7
C5	132.1	131.1	130.3	131.6	131.0	132.6
C6	134.4	133.8	123.0	133.2	134.0	132.9
C7	128.3	126.3	127.2	126.9	126.4	126.9
C8	123.2	124.6	125.8	124.2	124.3	nm
C9	123.3	123.6	124.8	123.6	123.4	nm
C10	20.2	20.1	20.5	20.2	20.0	20.0
C11	80.6	83.8	85.6	83.6	84.0	84.6
C12	120.9	126.8	130.9	126.5	126.9	127.4
C13	143.0	145.2	156.3	142.8	145.0	144.8
C14	126.1	123.9	125.0	126.9	123.7	nm
C15	132.1	132.3	129.9	131.9	132.0	132.9
C16	134.4	134.5	127.1	134.2	134.5	134.7
C17	128.3	127.4	127.2	127.3	127.2	126.7
C18	123.2	124.4	125.3	124.0	124.3	nm
C19	123.3	123.8	125.1	123.7	123.5	nm

C20	20.2	20.3	20.7	20.4	20.2	20.2
C21	-	259.6	280.6	284.3	262.1	82.0
C22	-	32.9	38.6	34.0	31.3	26.2
C23	-	20.7	17.1	18.4	20.6	18.6
C24	-	89.5	77.8	89.9	-	-
C25	-	29.1	33.5	29.1	-0.1	-
N	66.2	232.1	148.3	217.8	234.2	232.5
H4	6.69	6.56	7.30	6.54	6.51	6.48
H5	6.63	6.63	6.90	6.61	6.61	6.65
H7	7.47	7.69	7.76	7.67	7.68	7.49
H10	1.83	1.97	2.21	1.93	1.97	1.90
H14	6.69	6.55	7.61	6.71	6.53	6.70
H15	6.63	6.78	7.04	6.76	6.76	6.59
H17	7.47	7.68	7.92	7.65	7.66	7.48
H20	1.83	1.93	2.28	1.93	1.93	1.87
H21	-	7.32	-	-	7.20	2.99, 2.95
H22	-	5.05, 4.76	4.42, 4.38	4.62, 4.50	5.28, 4.91	2.69, 2.58
H23	-	0.74	0.88	0.70	0.67	0.89
H25	-	1.18	1.76	1.19	0.12	-
F8 [e]	-74.16	-71.06	-70.99	-71.10	-71.30	-70.85
F9	-75.69	-73.44	-73.53	-75.63	-73.90	-73.70
F18	-74.16	-70.71	-68.97	-70.83	-70.50	-68.99
F19	-75.69	-76.73	-75.97	-76.28	-76.60	-75.96

[a] δH26=2.49 ppm, δH28=7.12 ppm, δH29=16 ppm, δH30=7.23 ppm, and δC26=8.5 ppm, δC27=118.5 ppm, δC28=132.5 ppm, δC29=130.0 ppm, δC30=134.6 ppm. [b] δH26=2.33 ppm, δH28=6.99 ppm, δH29=6.99 ppm, δH30=7.07 ppm, and δC26=8.5 ppm, δC27=118.7 ppm, δC28=132.5 ppm, δC29=129.9 ppm, δC30=134.6 ppm. [c] the methyl in position 26 has δH=4.87 ppm and δC=23.5 ppm. [d] Not measured, the sample was too dilute. [e] The fluorine signals in compounds **2**-**7** are quartets with a typical coupling constant of 9-10 Hz. In compound **1** the signals are broad due to a fluxional process in the ligand, as demonstrated by the spectrum at 70 °C.

Compounds **1**-**7** were characterized by ^{1}H, ^{13}C, ^{19}F and ^{15}N NMR. The chemical shifts are presented in Table 1. The assignments were made primarily based on the cross-peaks seen in the ^{1}H-^{13}C gHMBC spectra. The chemical shifts of the fluorinated carbons were measured in the ^{19}F-^{13}C gHSQC spectra, and their assignment to positions 8 and 9 *vs.* 18 and 19 was made based on the long-range coupling of the fluorines to the quaternary carbon two bonds away, coupling seen in the ^{19}F-^{13}C gHMBC spectra. The chemical shift of the ^{15}N was measured in the ^{1}H-^{15}N gHMBC spectrum, where it shows cross-peaks with H4 and H14. In the case of compounds **2** and **6**, it also shows cross-peaks with H21, which confirms the structural integrity of these compounds. No stereochemical assignments were made, *i.e.* H7 and H17 are interchangeable, as well as C8 and C9. In Table 1, C1 and C2 were assigned as the most shielded of the pairs C1, C11 and C2, C12; F8 and F9 were assigned as the most deshielded of the pairs F8, F18 and F9, F19.

In a typical assignment procedure, H7 displays cross-peaks with a carbon around 20 ppm, assigned as C10, with a carbon between 80-85 ppm, assigned as C1, with a carbon between 150-160 ppm, assigned as C3 and with a carbon at approx 130 ppm, assigned as C5. H10, H5 and C7 were then identified by one-bond correlations, or by the couplings H10-C5, H10-C7, H5-C7. H4 was identified as coupling with H5, or by its coupling with C6, the third carbon coupling with H10. One coupling of F8 or F9 with C1 was sufficient to identify these fluorines, since the pairs H8-F9 and F18-F19 are revealed by selective decoupling in the ^{19}F spectra. The assignments for the positions 11-20 was done in a similar way to the one for positions 1-10. The proton signals for positions 21-27 can be assigned based on their intensity and multiplicity. The carbons in these positions were assigned based on their one-bond and long-range couplings to protons.

The ^{13}C chemical shifts difference in positions 3/13and 6/16 as well as the ^{15}N chemical shifts difference between compounds **3** compared to **2**, **4**, **5** and **6** suggest that in **3** the nitrogen is more 'amino-like' while in **2**, **4**, **5** and **6** it is an amido.

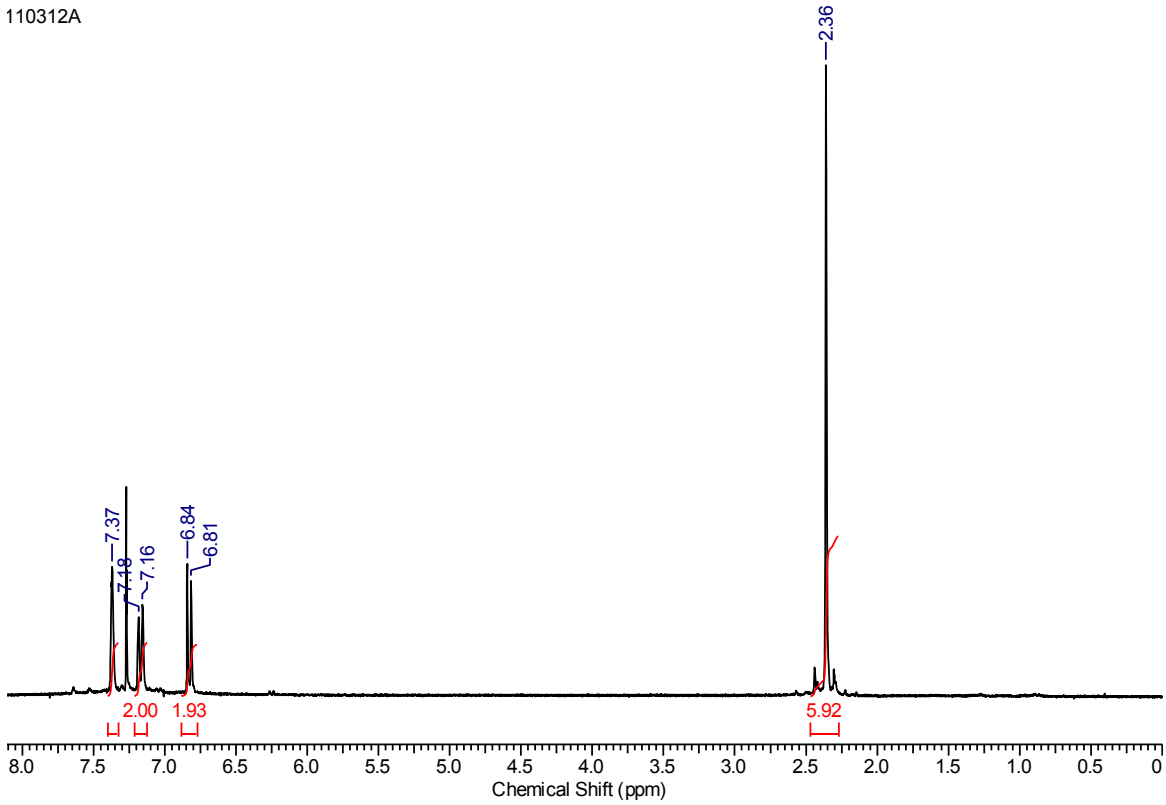

Figure S2. ^{1}H NMR ($CDCl_3$, 300 MHz) spectrum of **1**.

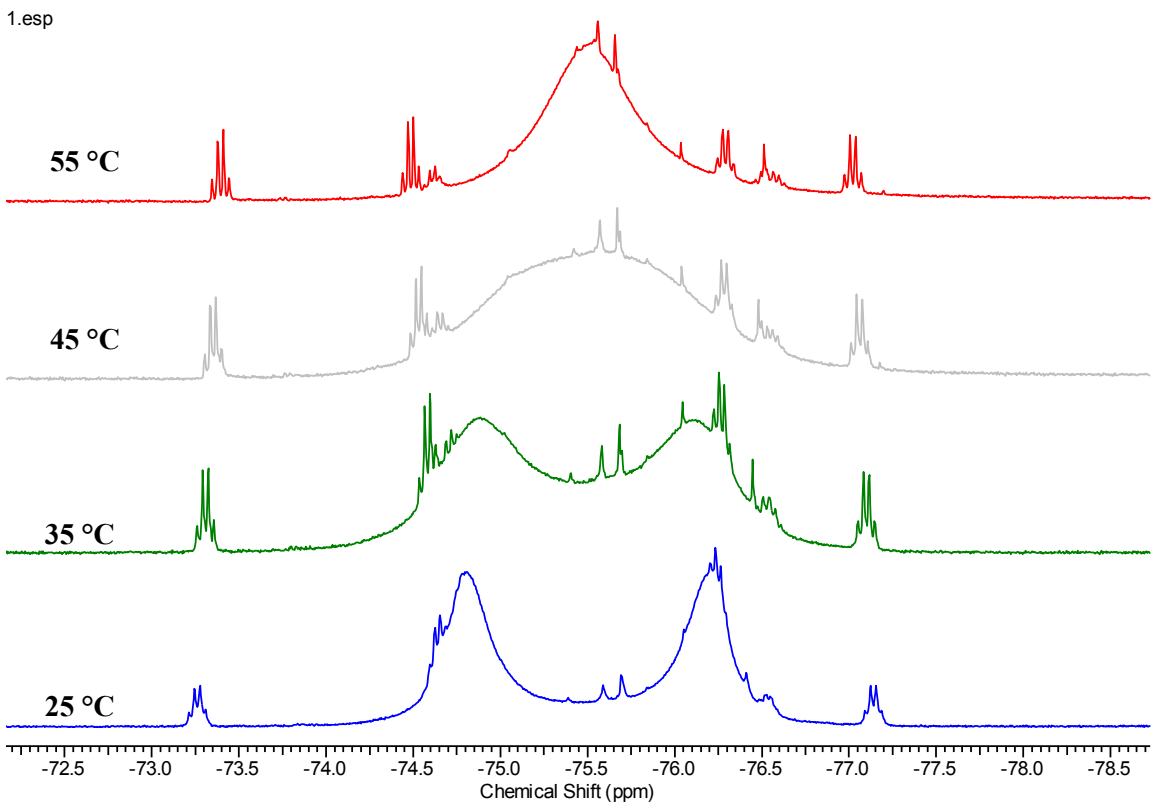

Figure S3. Variable Temperature $^{19}F\{^{1}H\}$ NMR ($CDCl_3$, 282 MHz) spectrum of **1**.

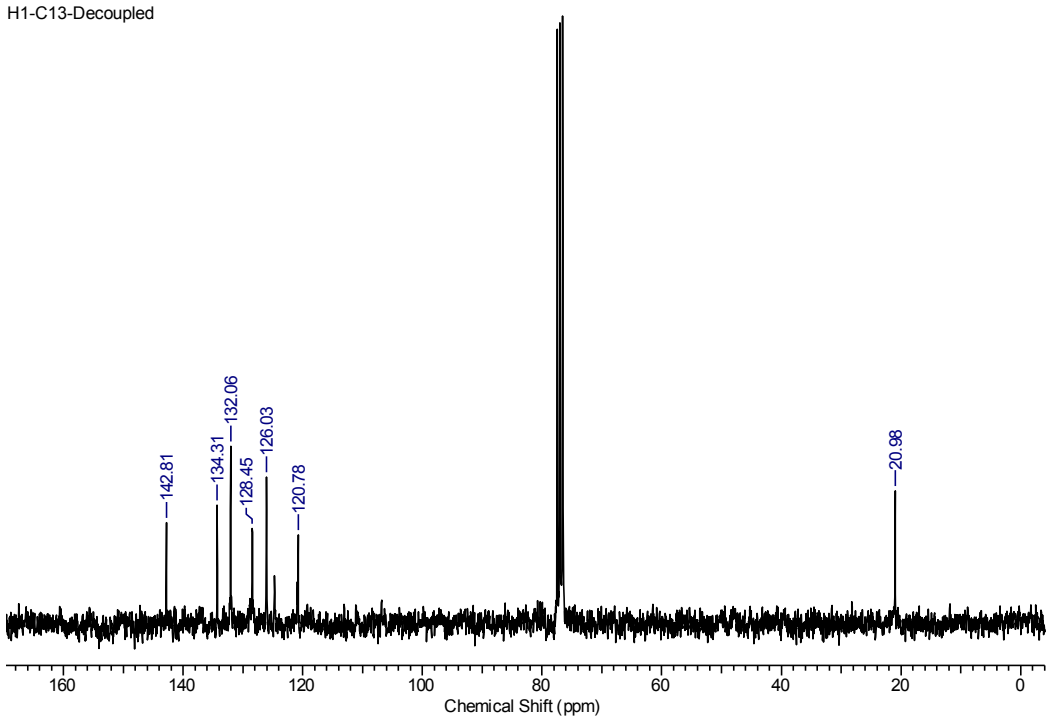

Figure S4. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 75 MHz) spectrum of **1**.

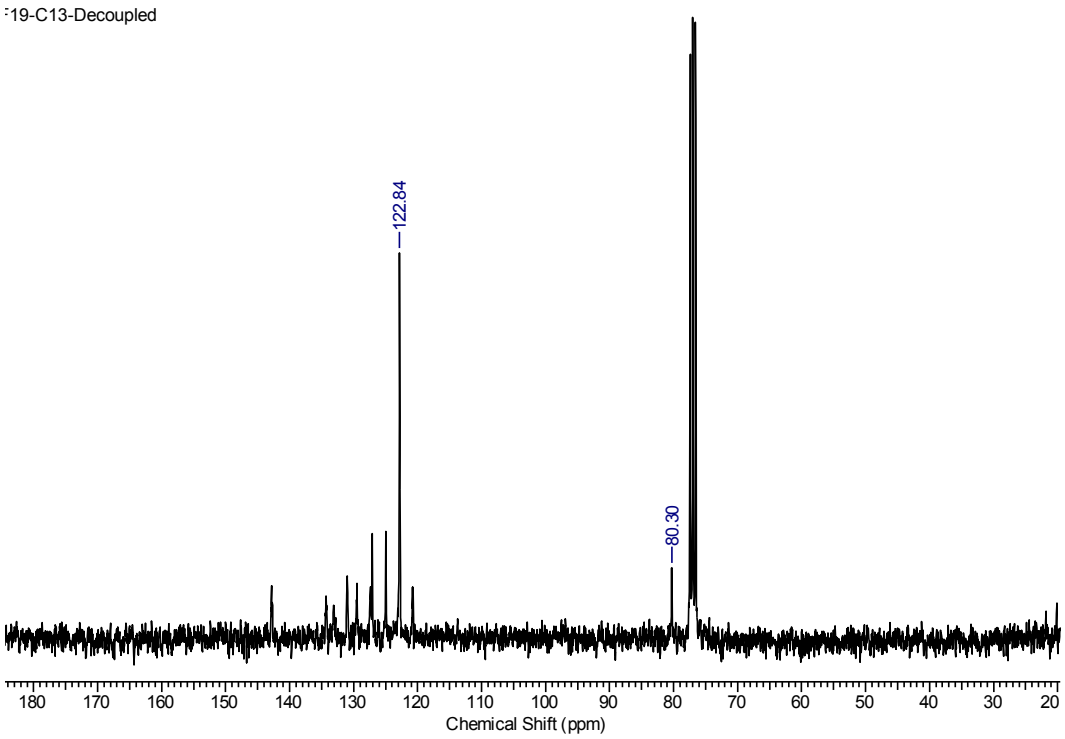

Figure S5. $^{13}C\{^{19}F\}$ NMR ($CDCl_3$, 75 MHz) spectrum of **1**.

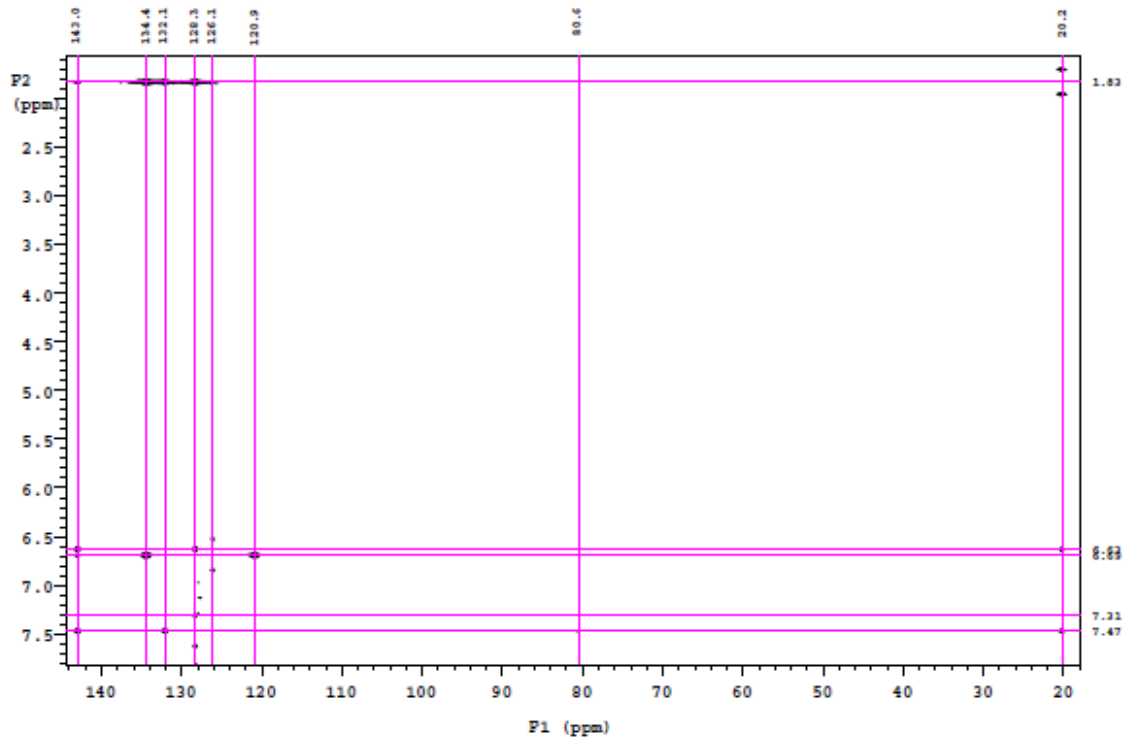

Figure S6. ^{1}H-^{13}C gHMBC (C_6D_6, 500 MHz) spectrum of **1**.

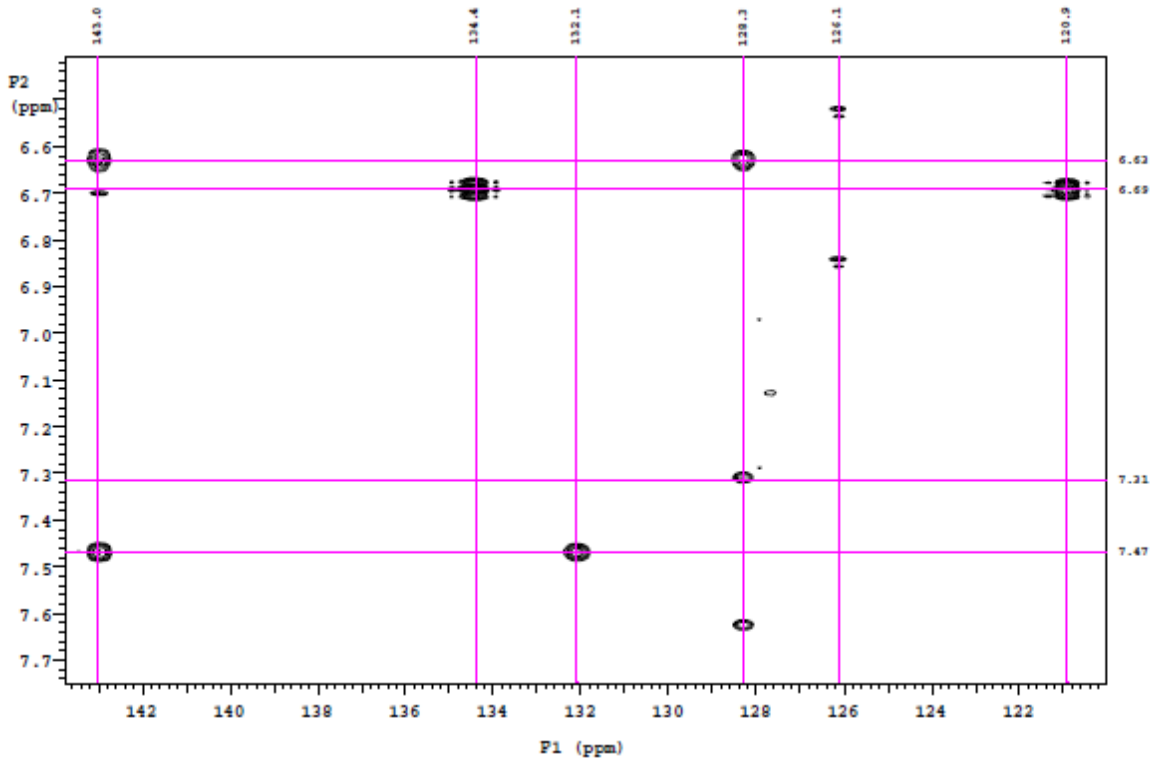

Figure S7. ^{1}H-^{13}C gHMBC (C_6D_6, 500 MHz) spectrum of **1**, expanded.

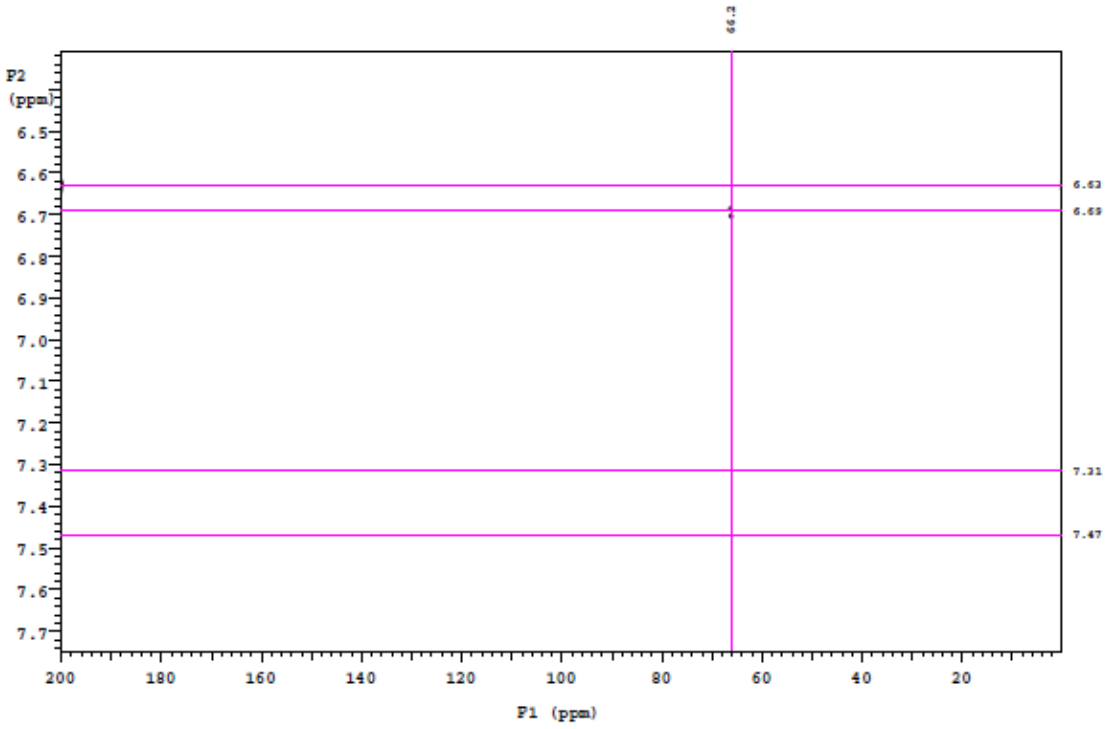

Figure S8. ^{1}H-^{15}N gHMBC (C_6D_6, 500 MHz) spectrum of **1**.

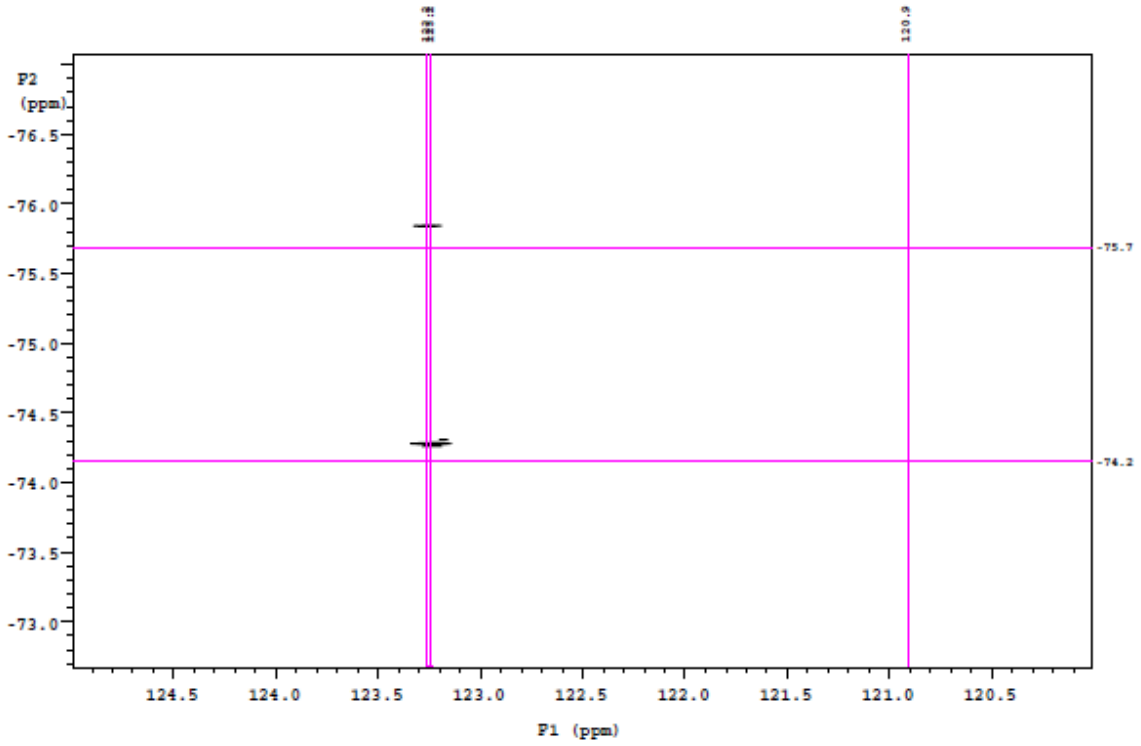

Figure S9. ^{19}F-^{13}C gHSQC (C_6D_6, 470 MHz) spectrum of **1**.

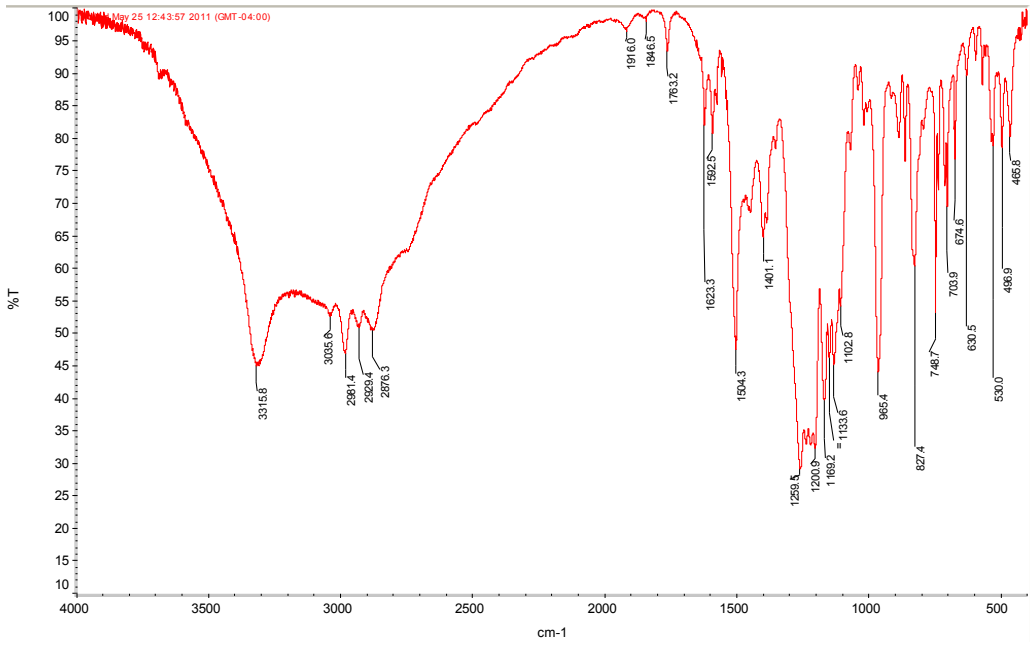

Figure S10. IR spectrum of **1** (neat film from diethyl ether solution).

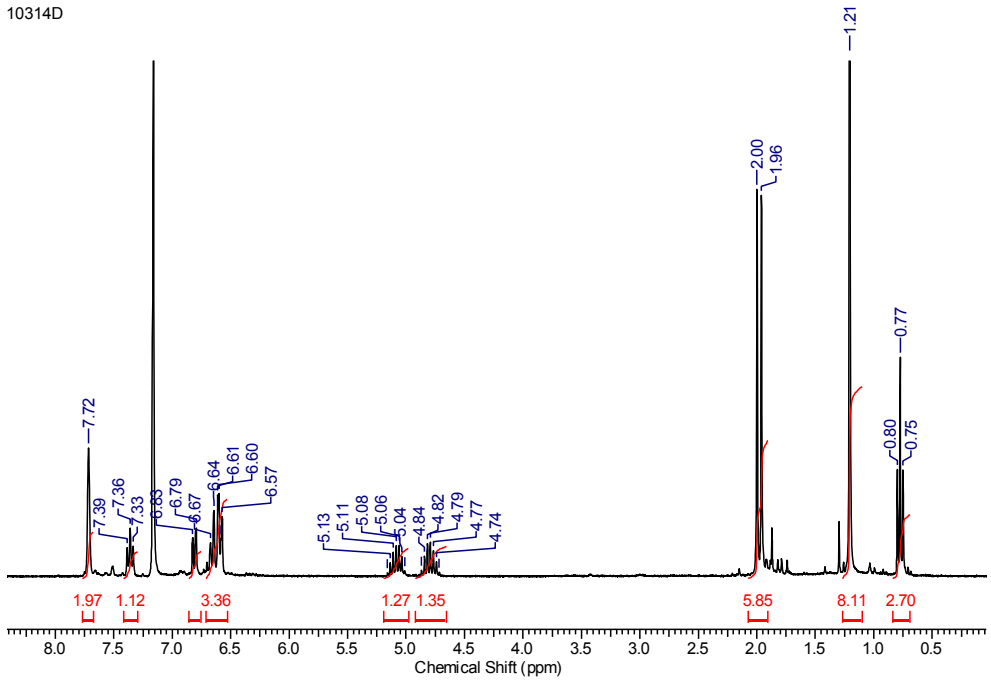

Figure S11. ^{1}H NMR (C_6D_6, 300 MHz) spectrum of **2**.

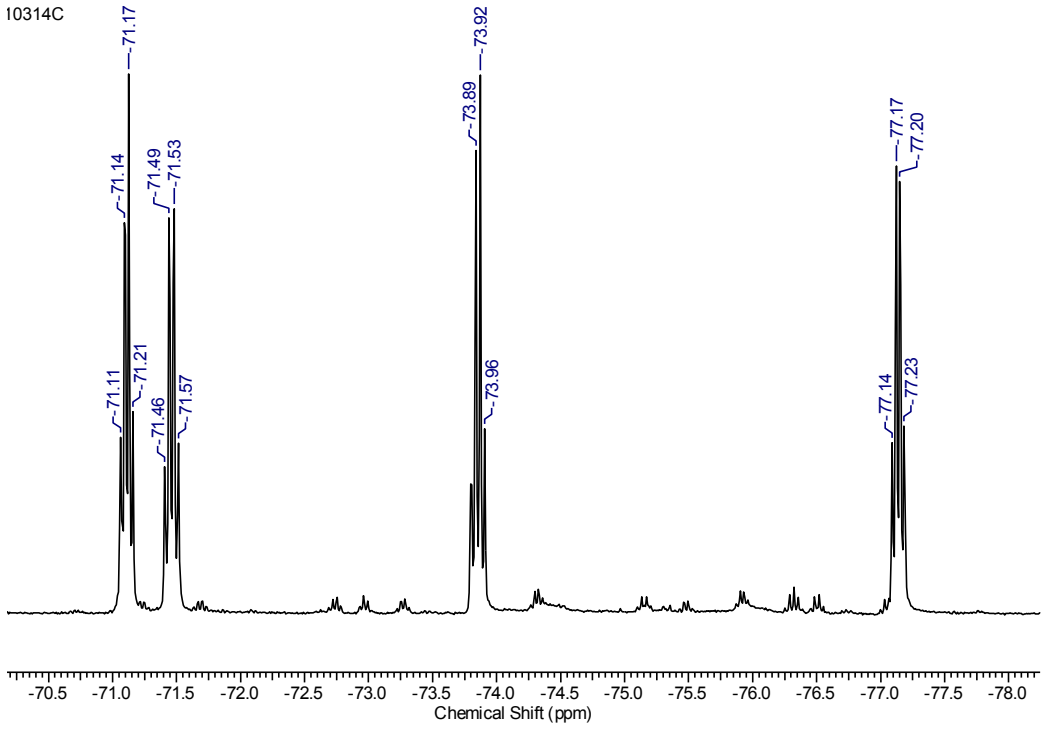

Figure S12. ^{19}F{^{1}H} NMR (C_6D_6, 282 MHz) spectrum of **2**.

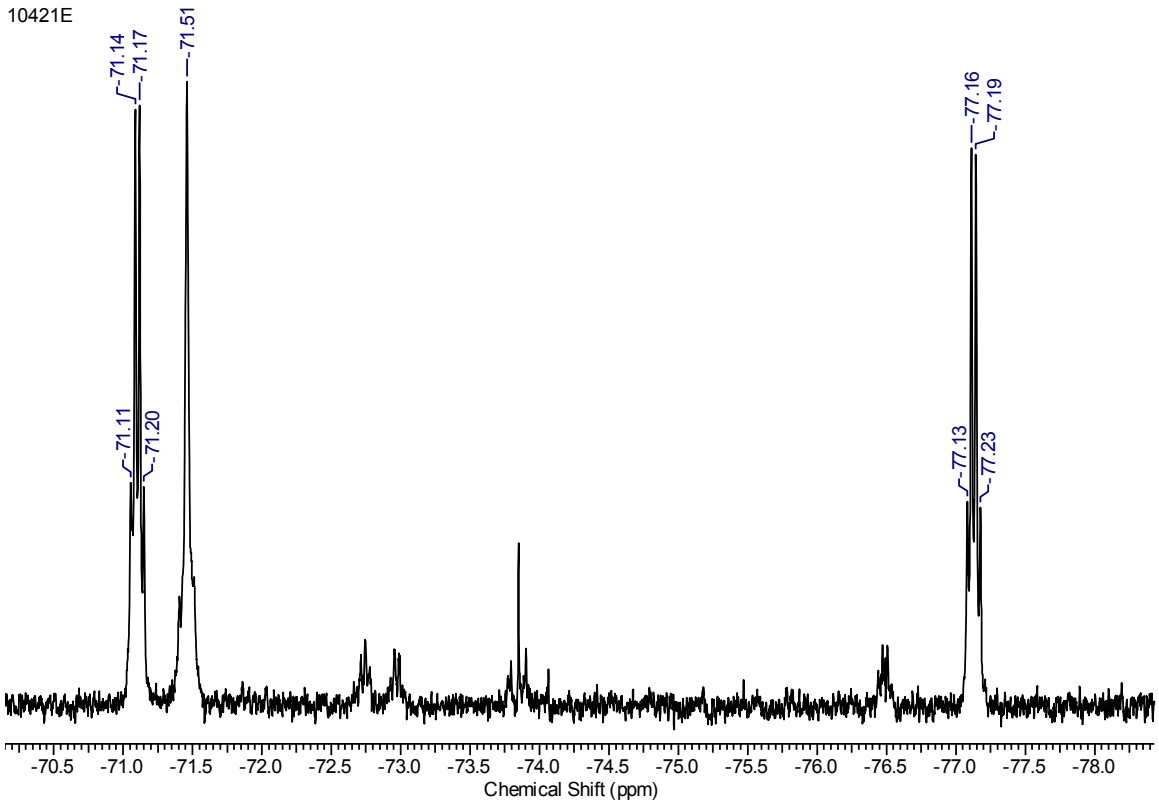

Figure S13. $^{19}F\{^{1}H\}$ NMR (C_6D_6, 282 MHz) spectrum of **2** with selective decoupling at 73.9 ppm.

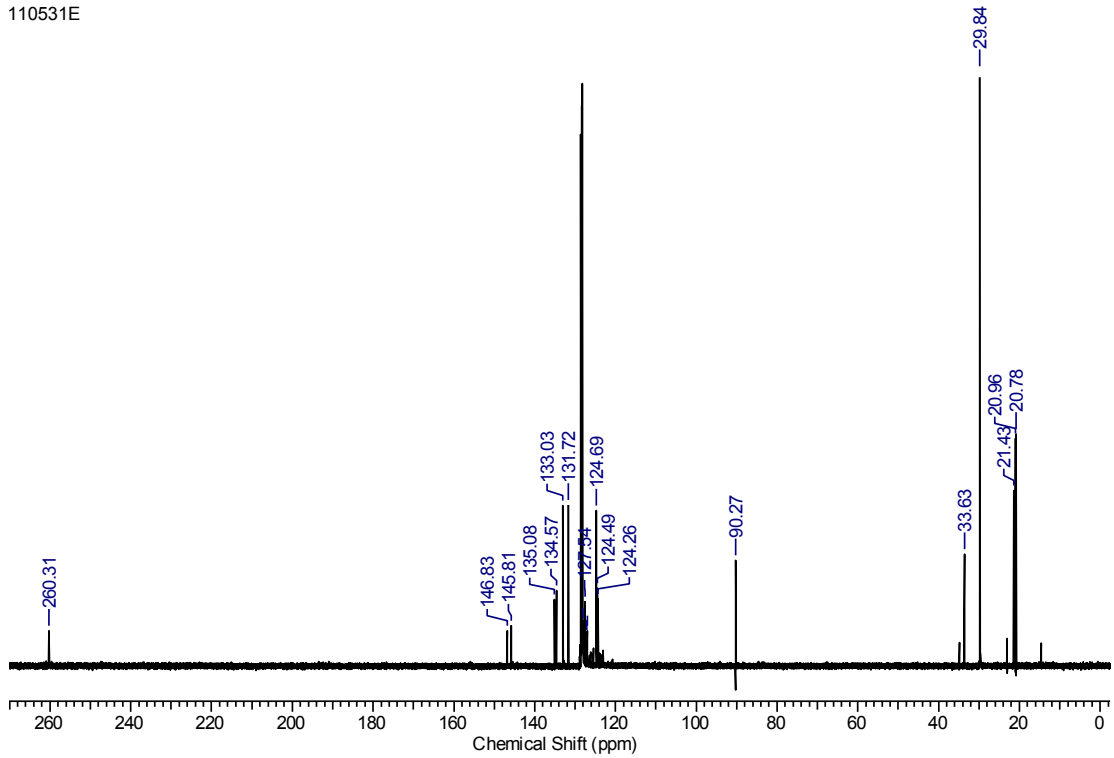

Figure S14. $^{13}C\{^{1}H\}$ NMR (C_6D_6, 126 MHz) spectrum of **2**.

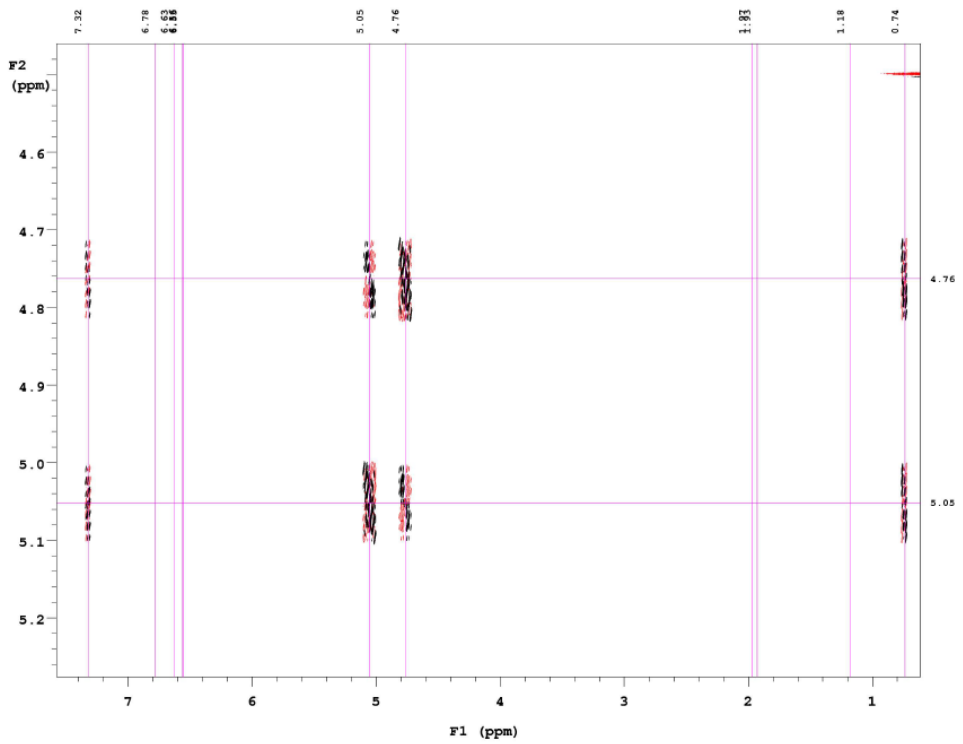

Figure S15. ^{1}H-^{1}H gDQFCOSY (C_6D_6, 500 MHz) spectrum of **2**, expanded.

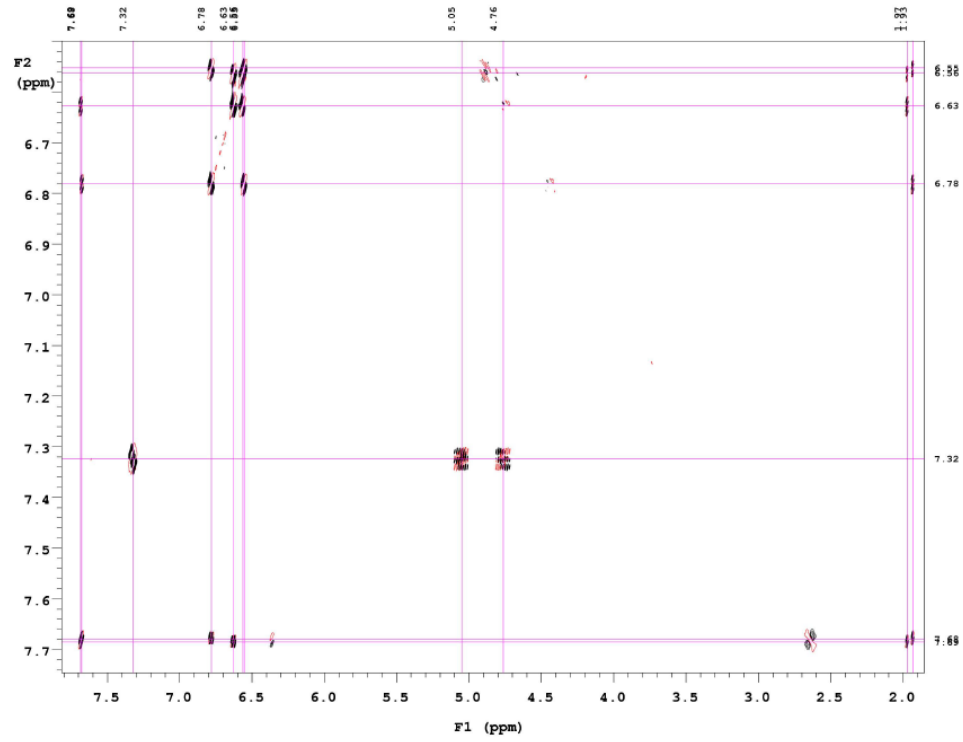

Figure S16. ^{1}H-^{1}H gDQFCOSY (C_6D_6, 500 MHz) spectrum of **2**, full.

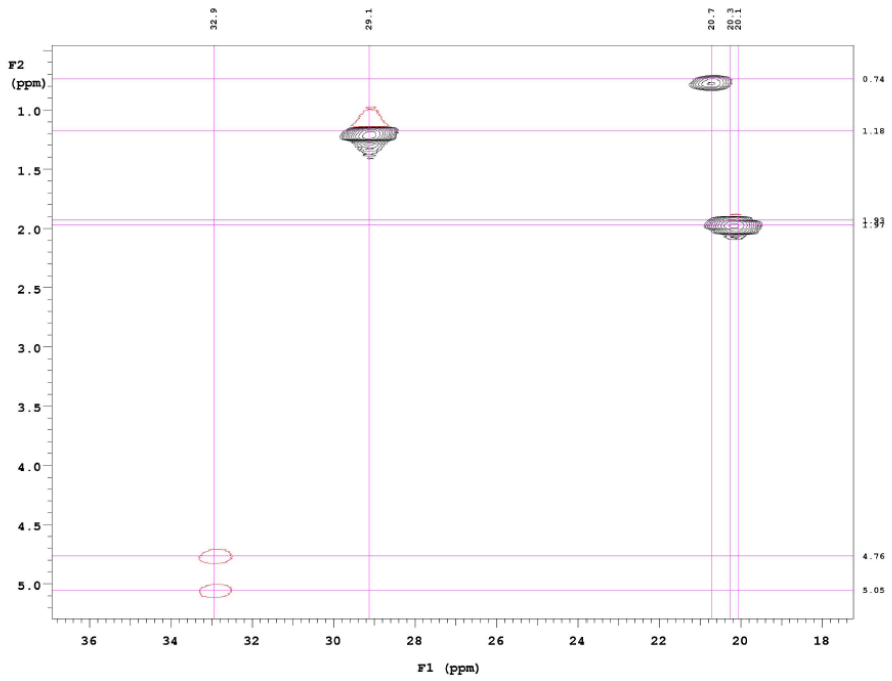

Figure S17. ^{1}H-^{13}C gHSQC (C_6D_6, 500 MHz) spectrum of **2**, expanded.

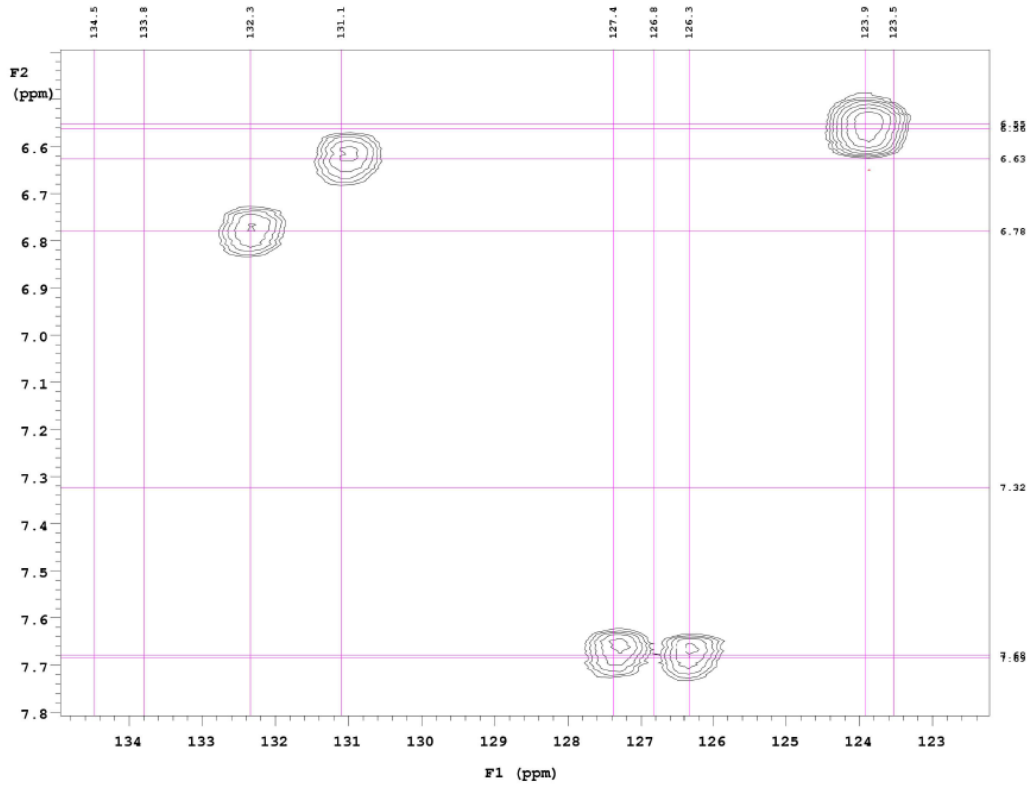

Figure S18. ^{1}H-^{13}C gHSQC (C_6D_6, 500 MHz) spectrum of **2**, expanded.

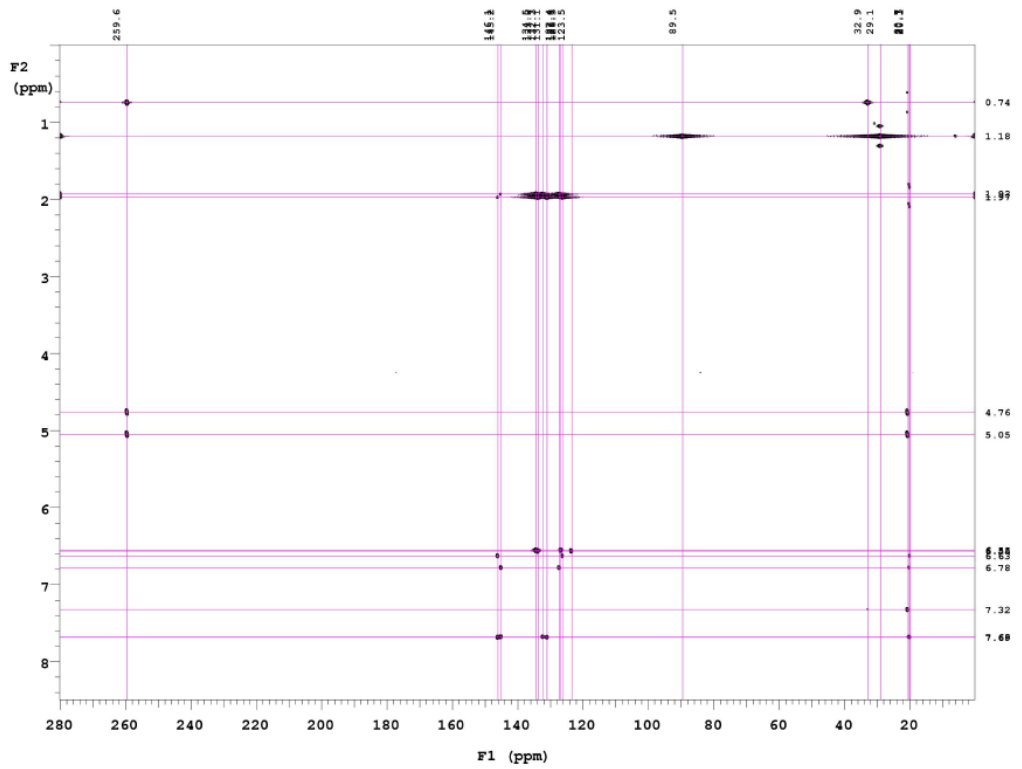

Figure S19. ^{1}H-^{13}C gHMBC (C_6D_6, 500 MHz) spectrum of **2**, full.

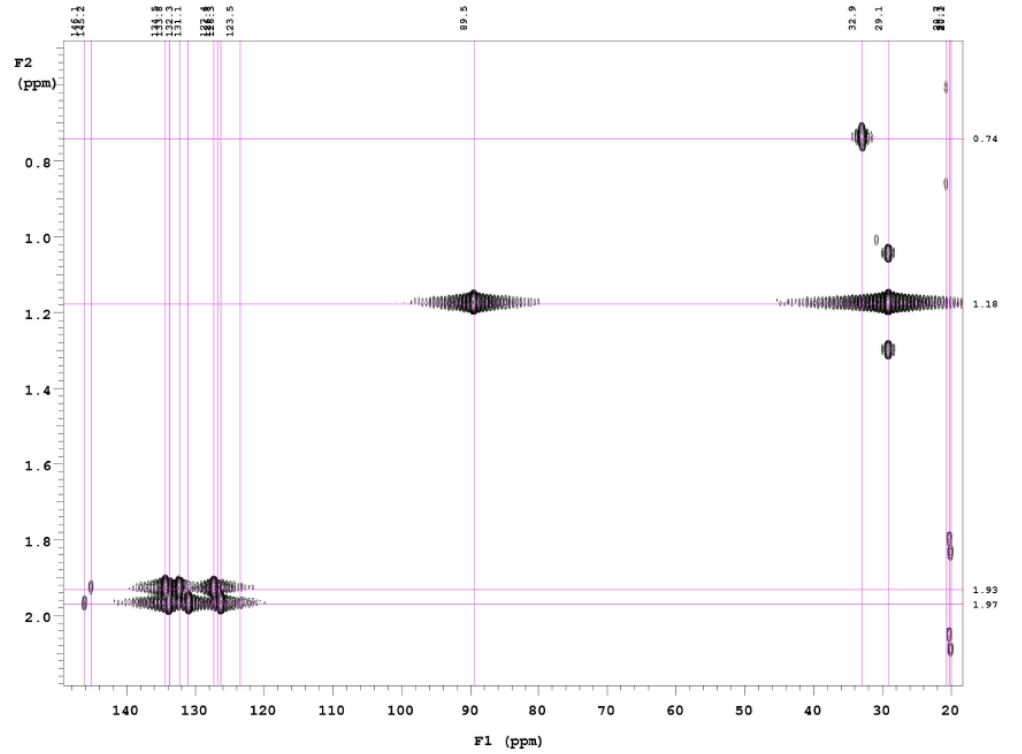

Figure S20. ^{1}H-^{13}C gHMBC (C_6D_6, 500 MHz) spectrum of **2**, expanded.

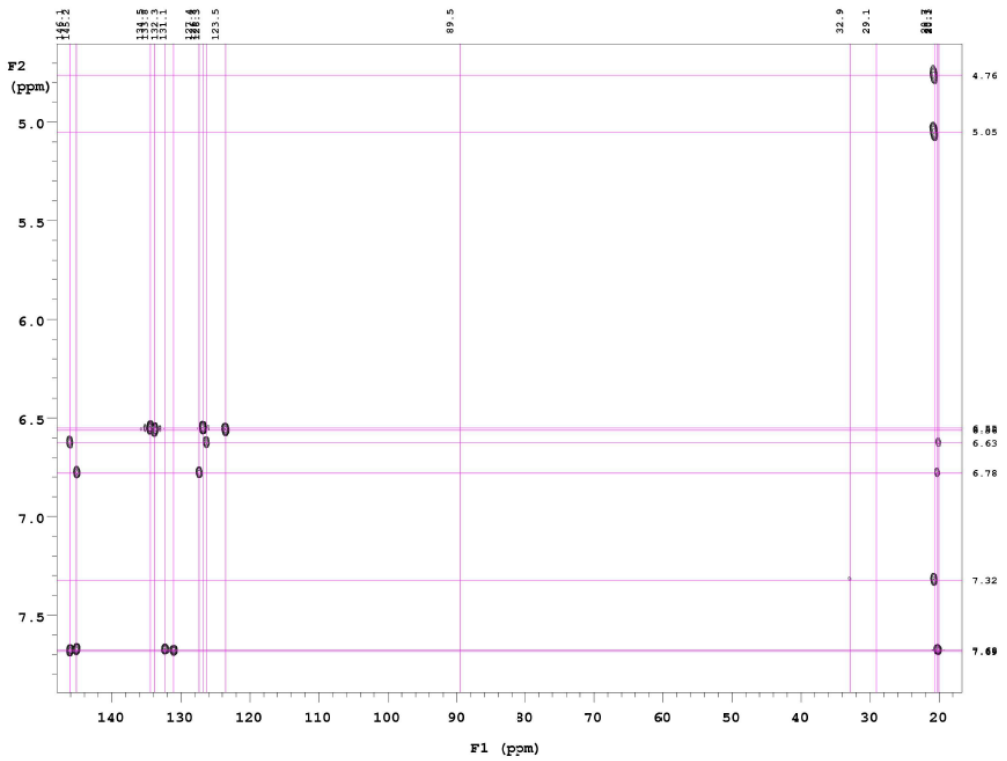

Figure S21. ^{1}H-^{13}C gHMBC (C_6D_6, 500 MHz) spectrum of **2**, expanded.

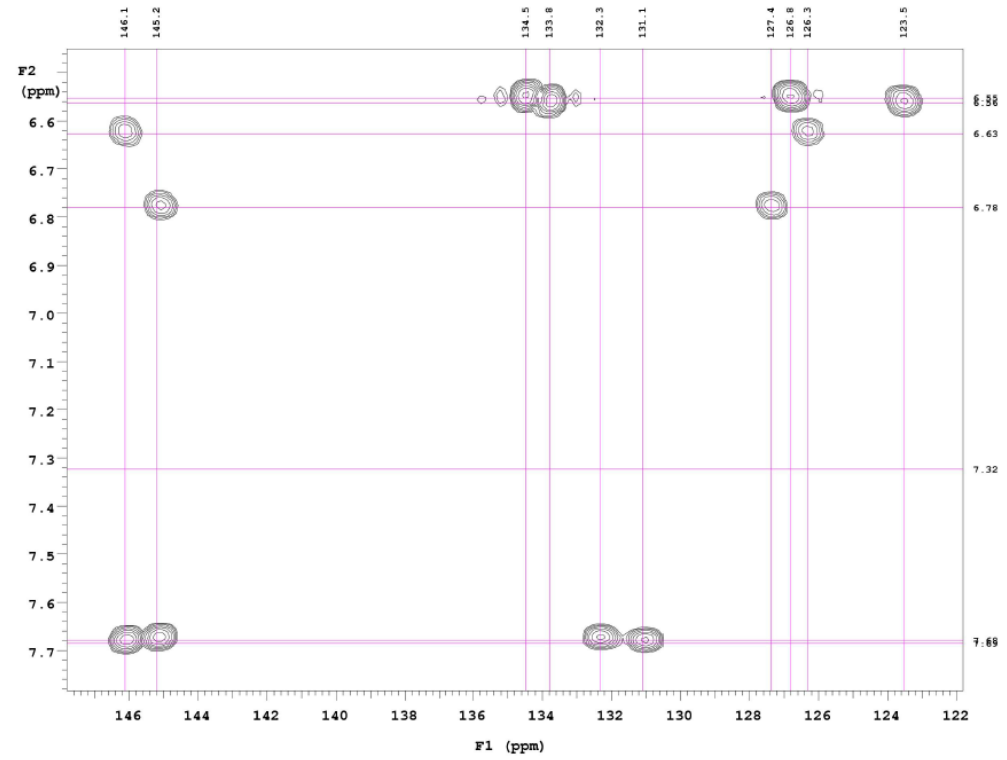

Figure S22. ^{1}H-^{13}C gHMBC (C_6D_6, 500 MHz) spectrum of **2**, expanded.

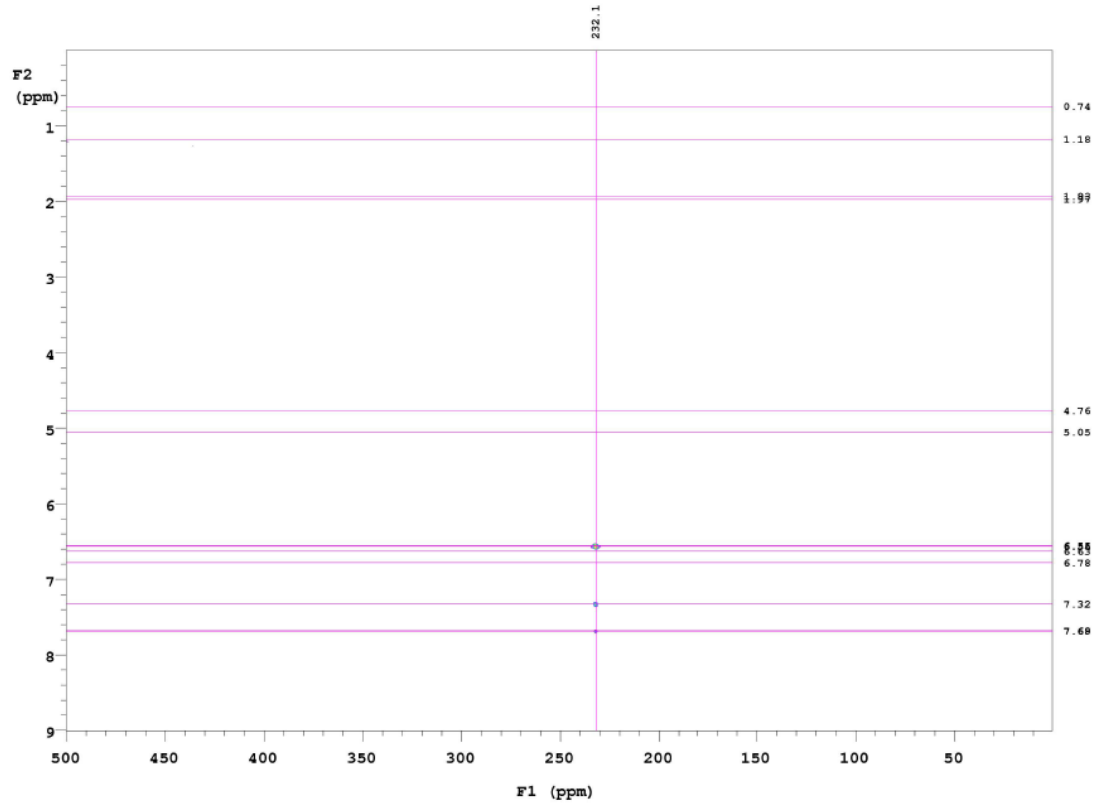

Figure S23. ^{1}H-^{15}N gHMBC (C_6D_6, 500 MHz) spectrum of **2**.

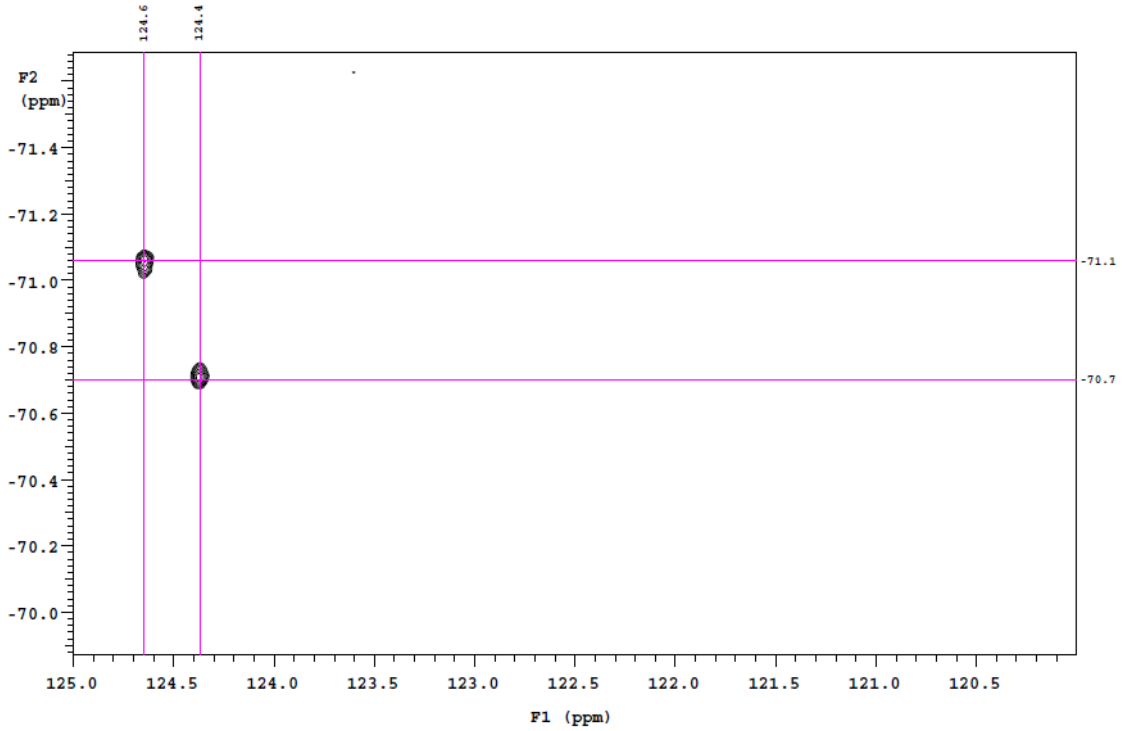

Figure S24. ^{19}F-^{13}C gHSQC (C_6D_6, 470 MHz) spectrum of **2**, expanded.

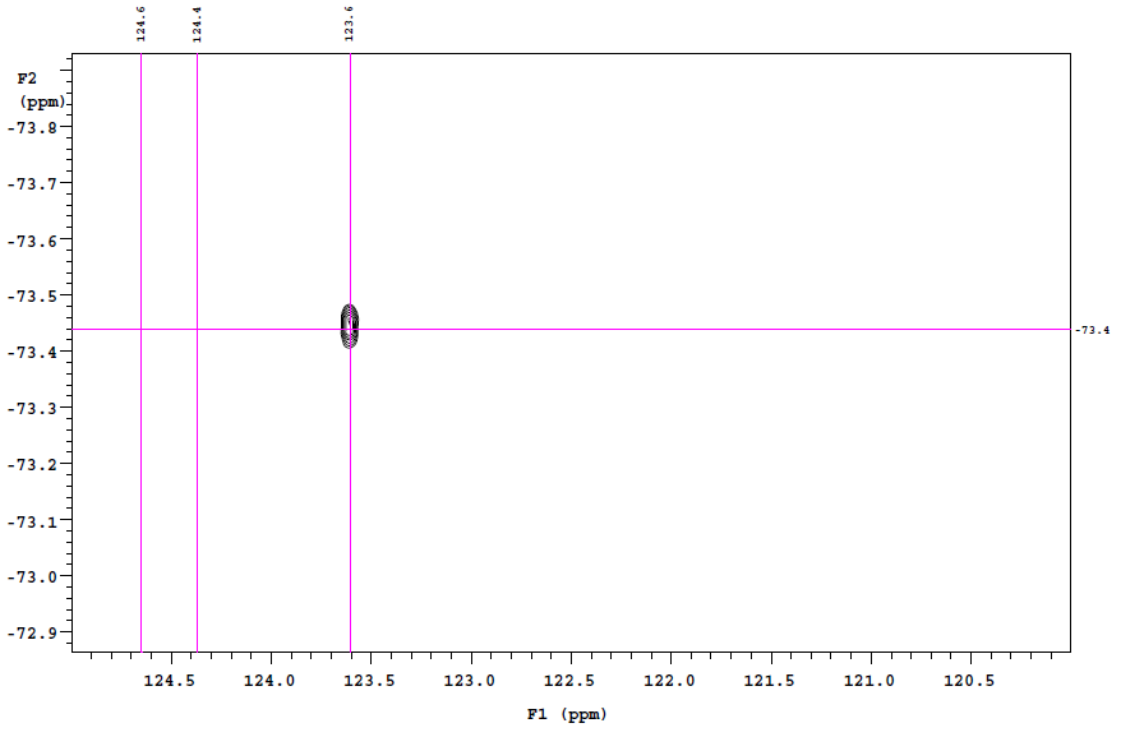

Figure S25. ^{19}F-^{13}C gHSQC (C_6D_6, 470 MHz) spectrum of **2**, expanded.

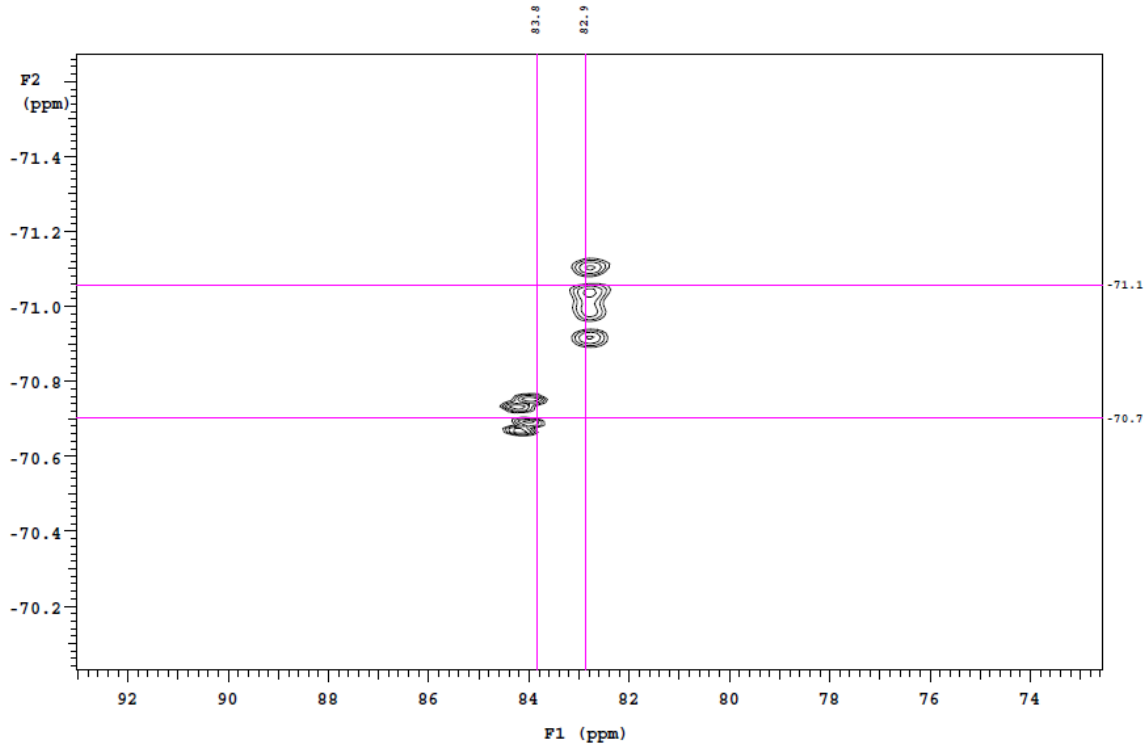

Figure S26. ^{19}F-^{13}C gHMBC (C_6D_6, 470 MHz) spectrum of **2**, expanded.

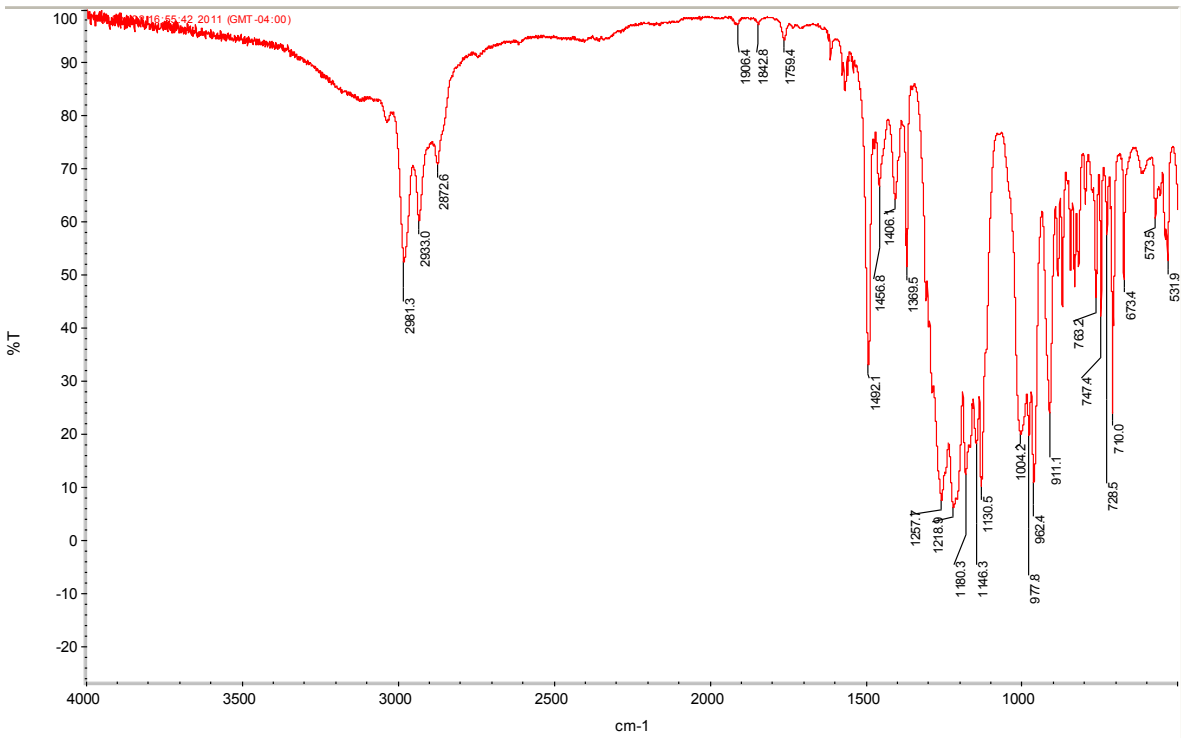

Figure S27. IR spectrum of **2** (neat film from Diethyl Ether solution).

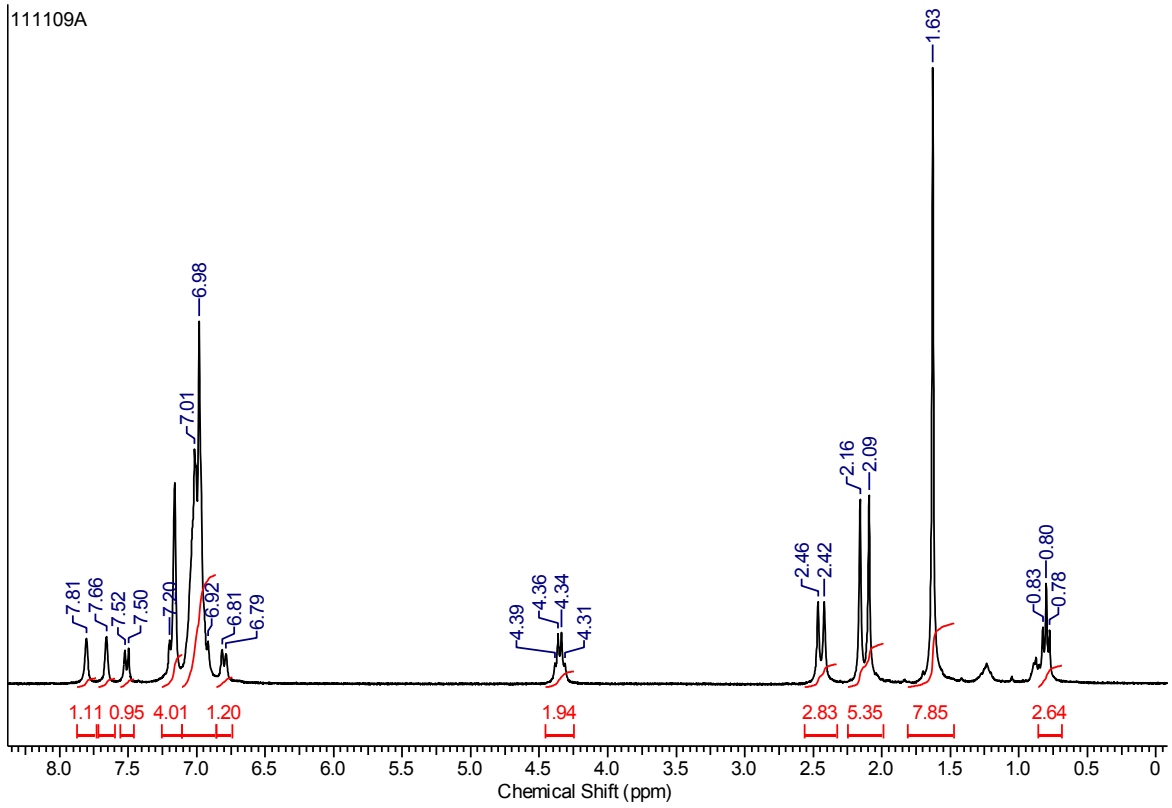

Figure S28. ^{1}H NMR (C_6D_6, 300 MHz) spectrum of **3**.

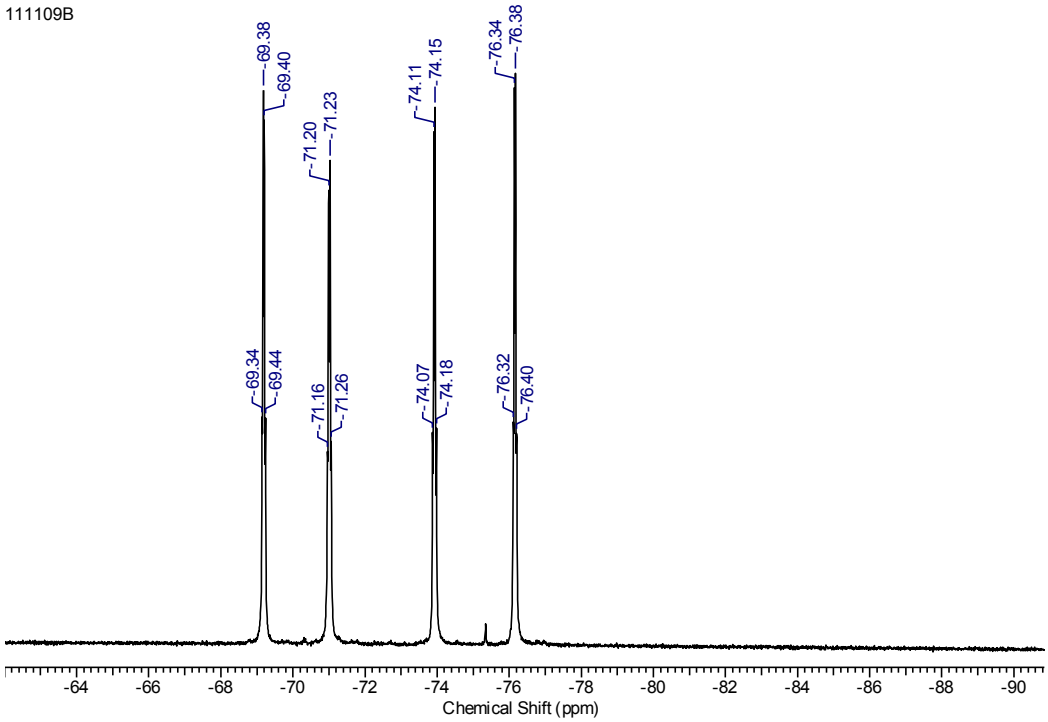

Figure S29. $^{19}F\{^{1}H\}$ NMR (C_6D_6, 282 MHz) spectrum of **3**.

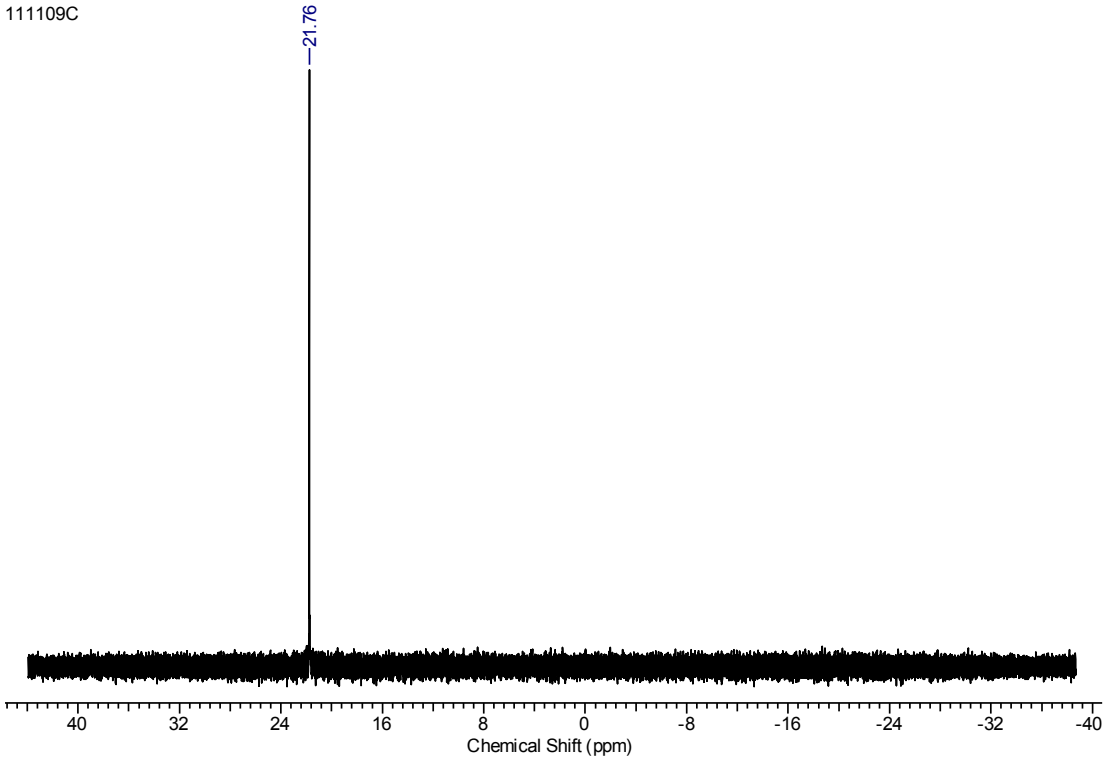

Figure S30. $^{31}P\{^{1}H\}$ NMR (C_6D_6, 121 MHz) spectrum of **3**.

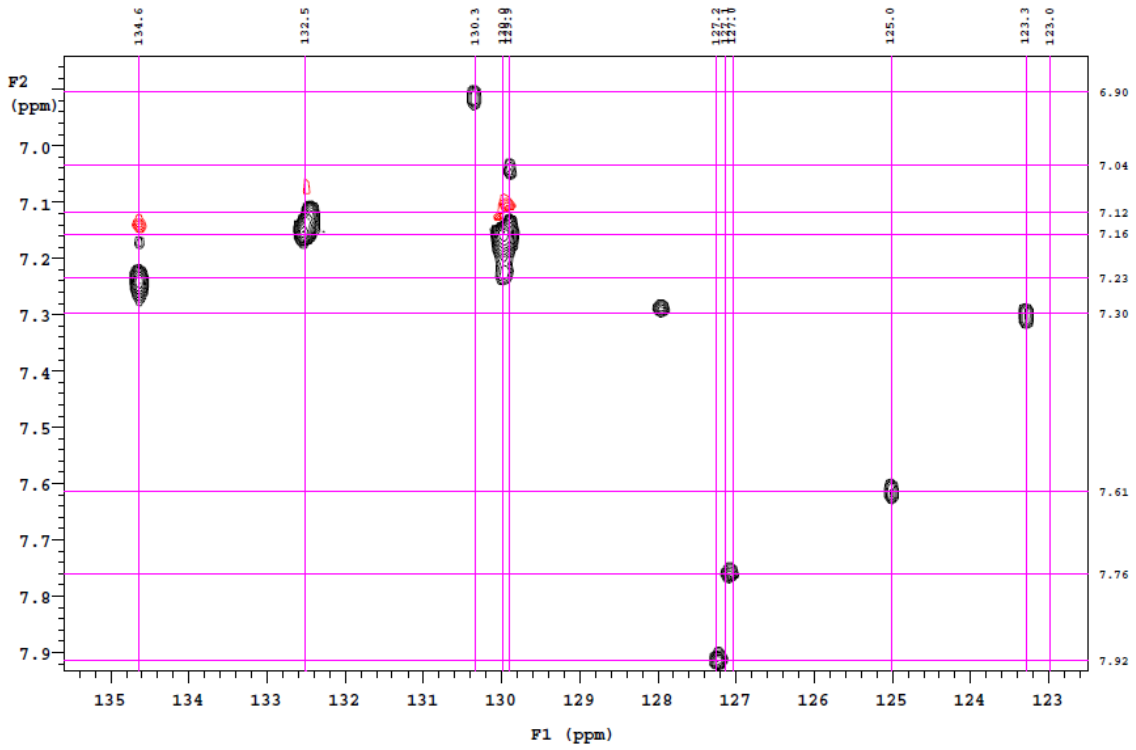

Figure S31. ^{1}H-^{13}C gHSQC (C_6D_6, 500 MHz) spectrum of **3**.

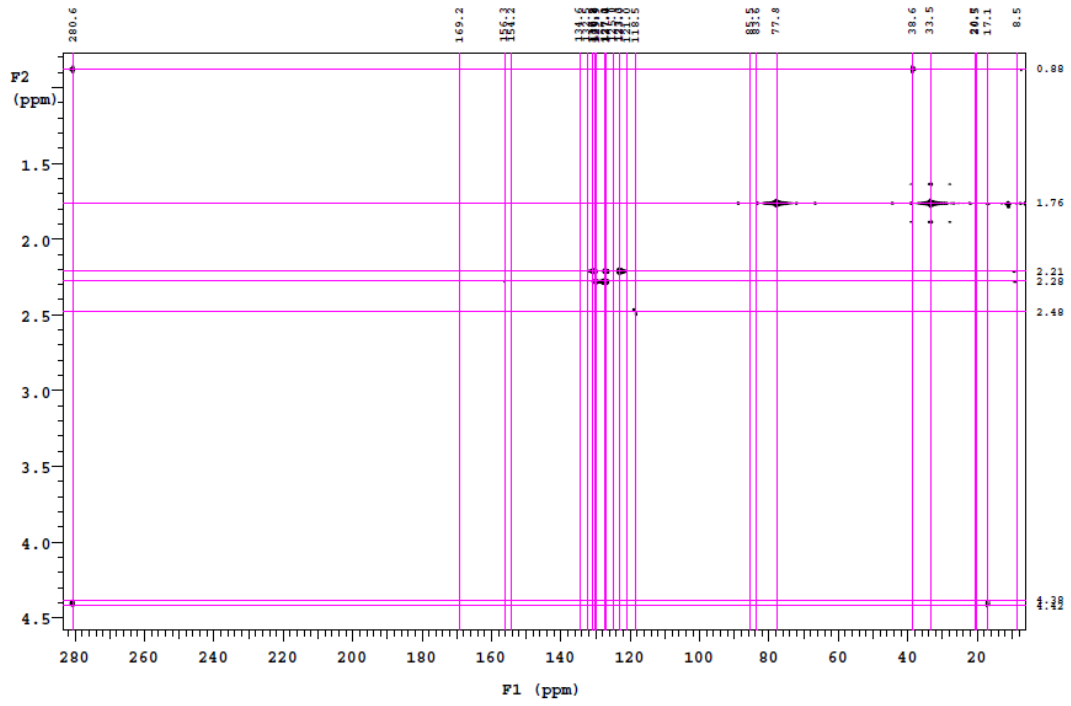

Figure S32. ^{1}H-^{13}C gHMBC (C_6D_6, 500 MHz) spectrum of **3**.

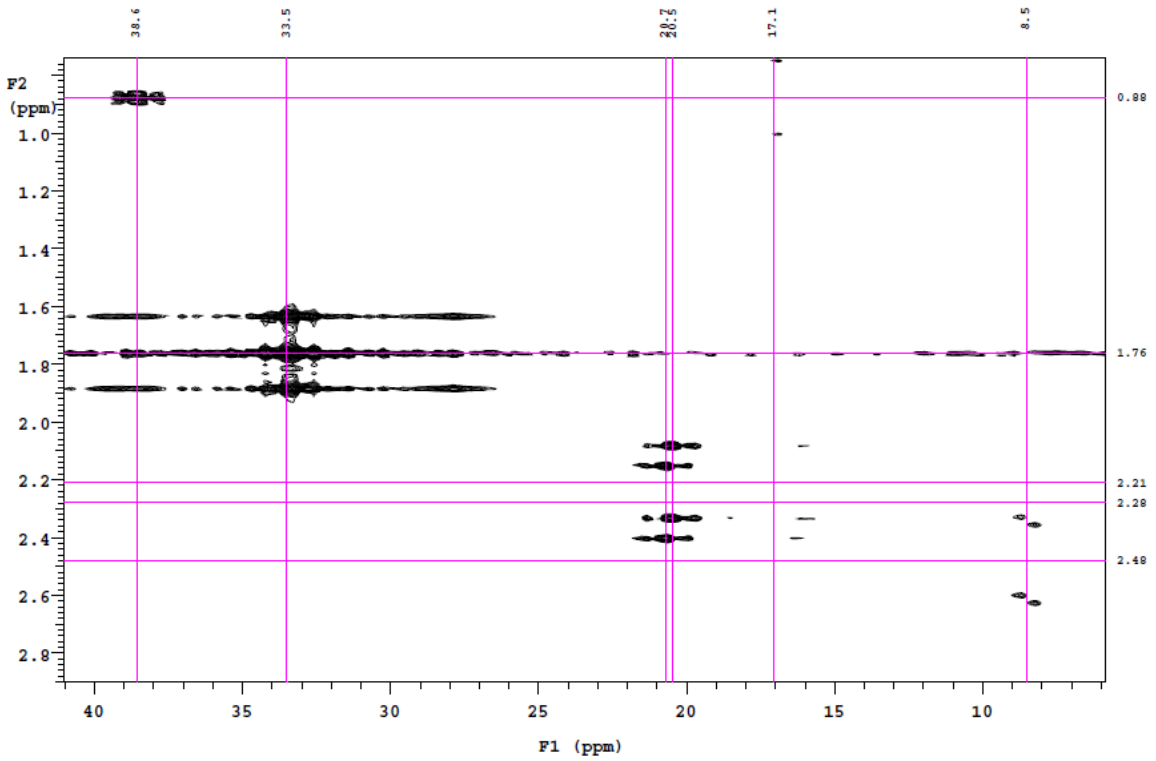

Figure S33. ^{1}H-^{13}C gHMBC (C_6D_6, 500 MHz) spectrum of **3**, expanded.

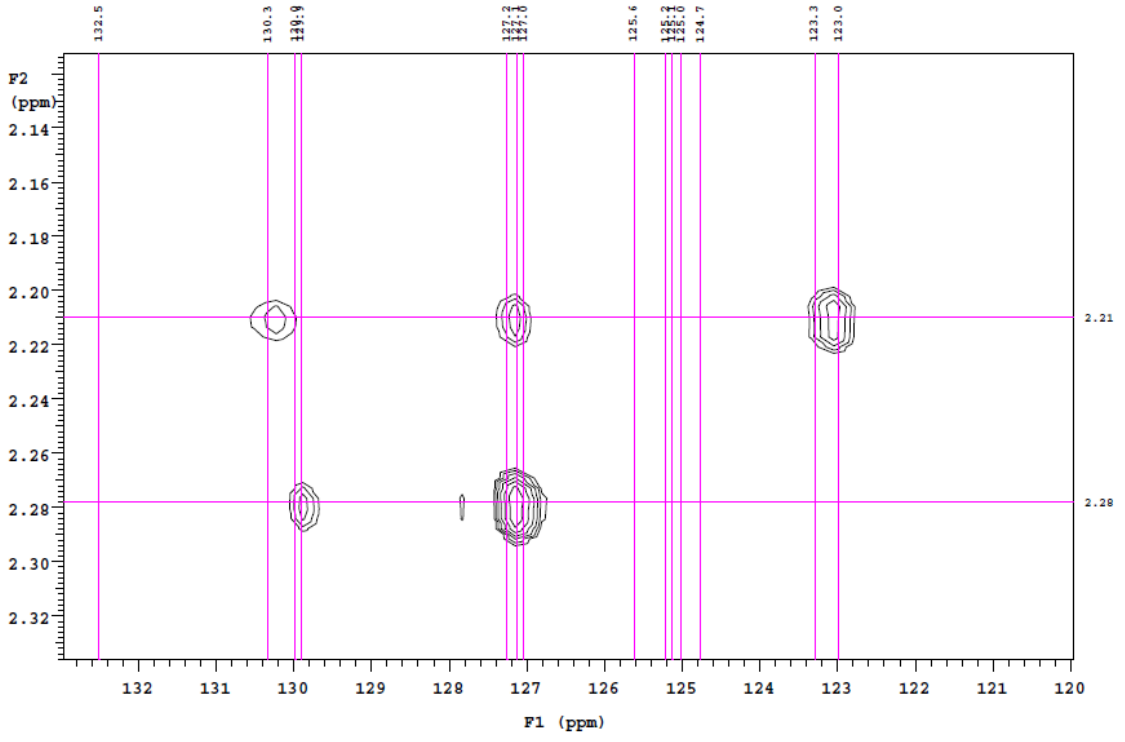

Figure S34. ^{1}H-^{13}C gHMBC (C_6D_6, 500 MHz) spectrum of **3**, expanded.

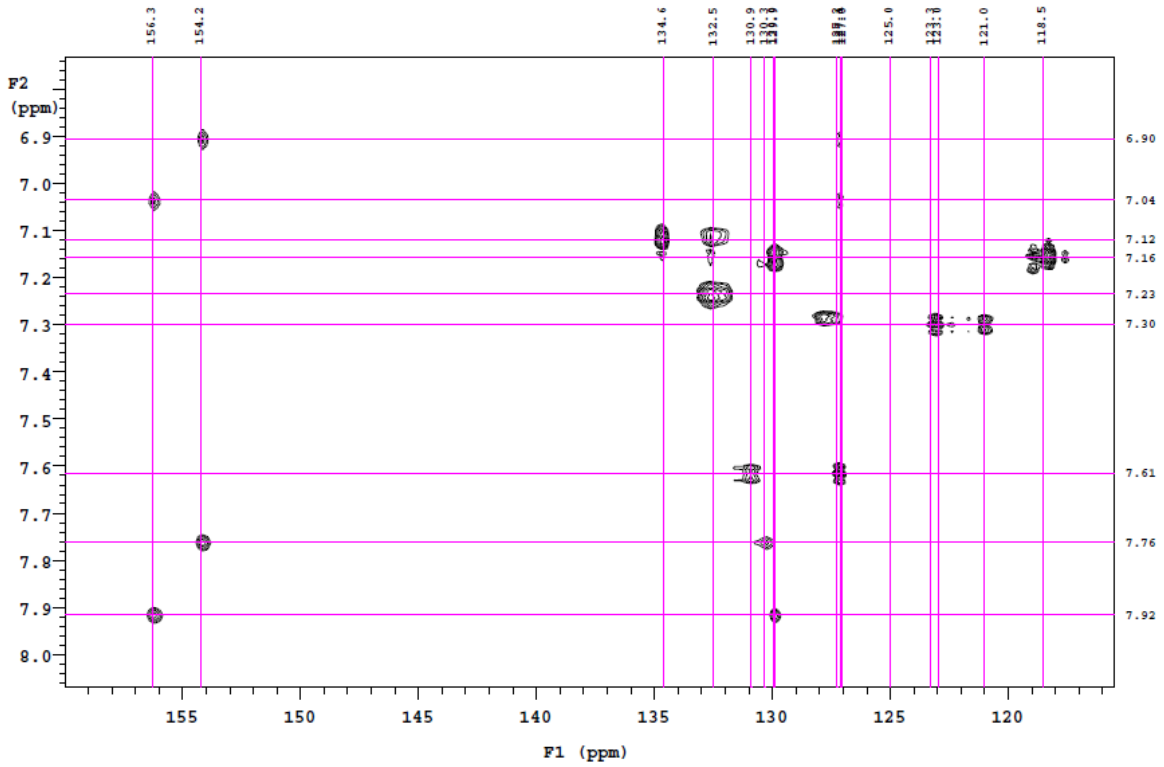

Figure S35. ^{1}H-^{13}C gHMBC (C_6D_6, 500 MHz) spectrum of **3**, expanded.

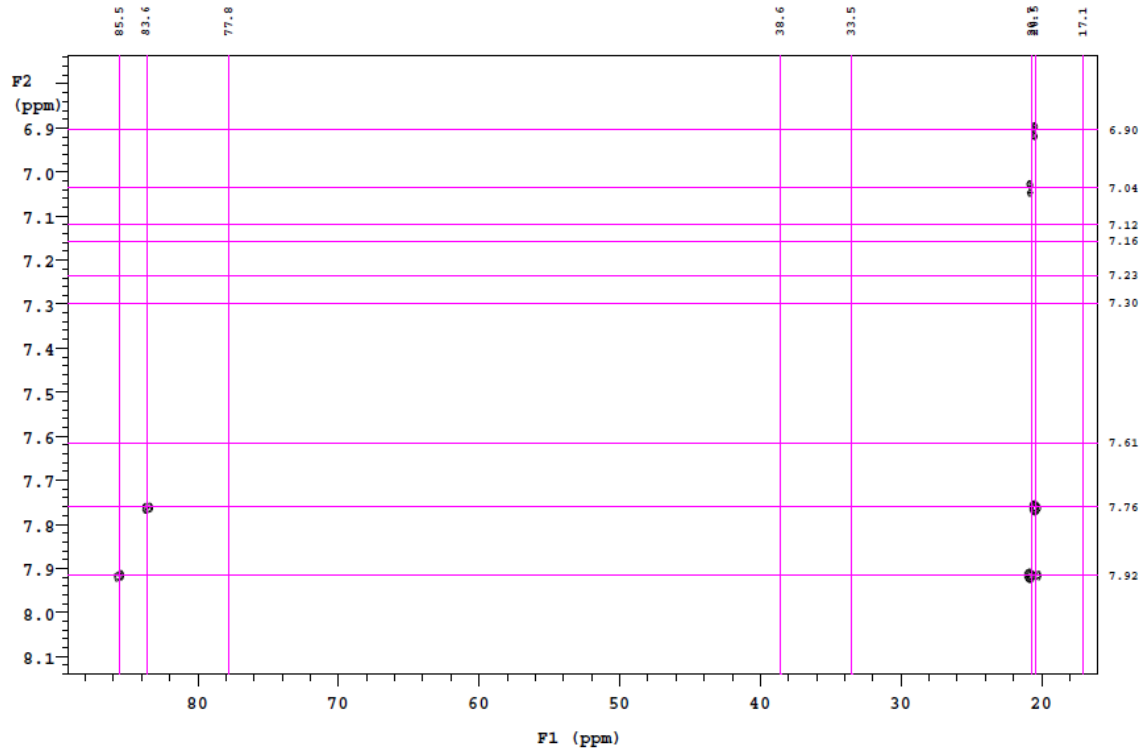

Figure S36. ^{1}H-^{13}C gHMBC (C_6D_6, 500 MHz) spectrum of **3**, expanded.

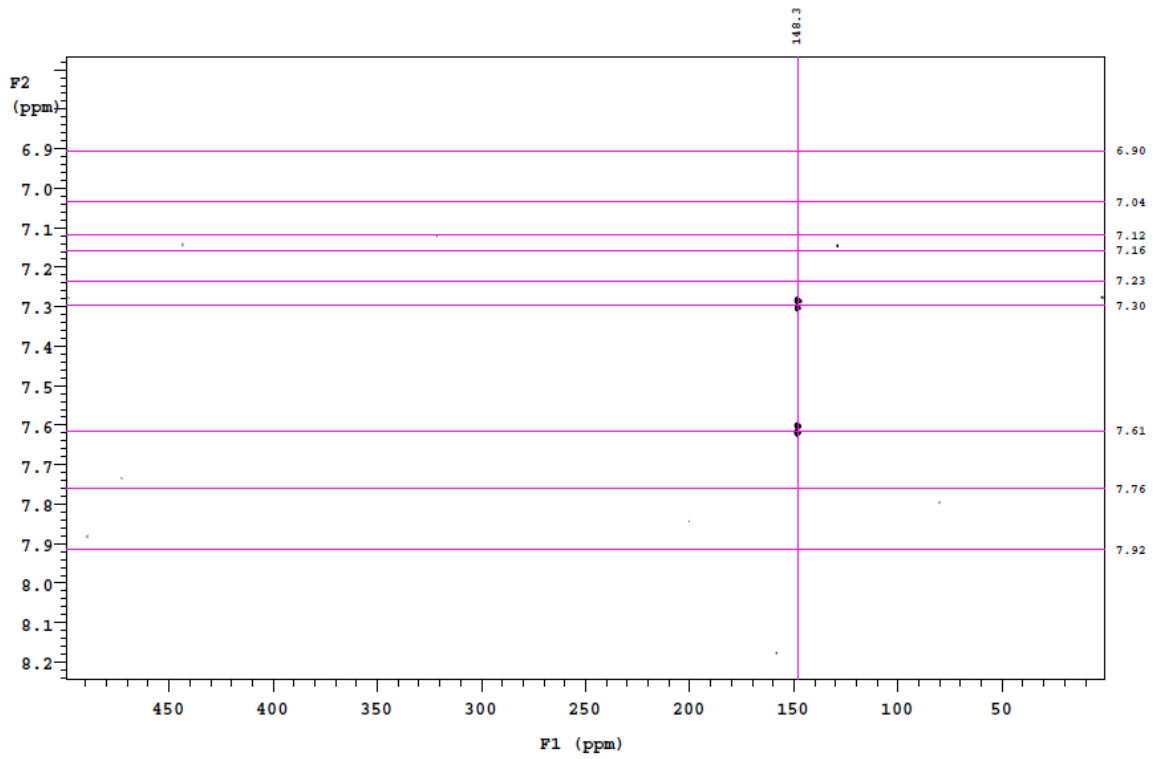

Figure S37. ^{1}H-^{15}N gHMBC (C_6D_6, 500 MHz) spectrum of **3**.

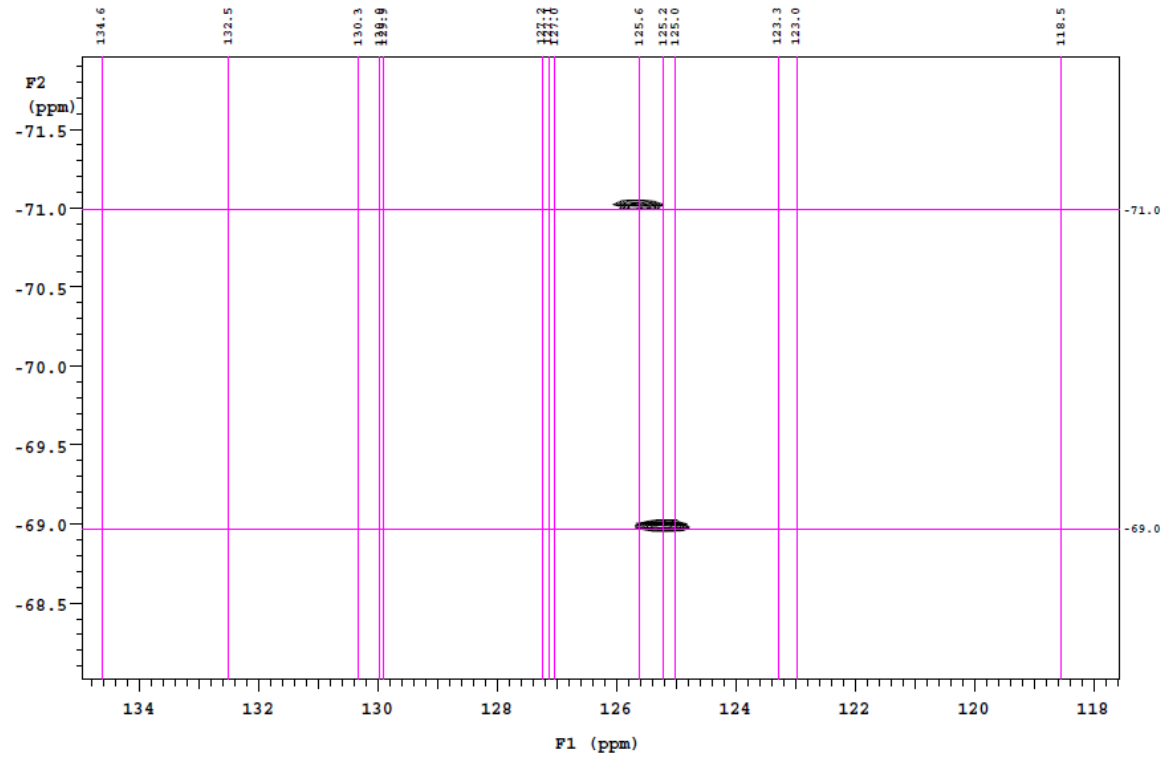

Figure S39. ^{19}F-^{13}C gHSQC (C_6D_6, 470 MHz) spectrum of **3**, expanded.

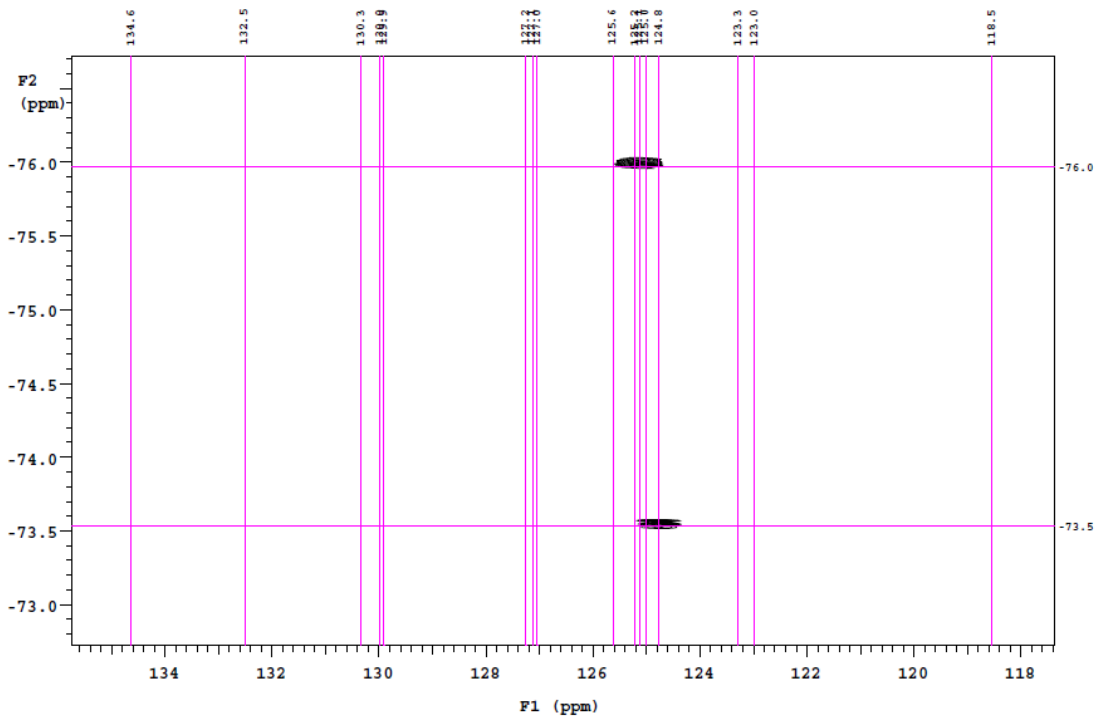

Figure S39. ^{19}F-^{13}C gHSQC (C_6D_6, 470 MHz) spectrum of **3**, expanded.

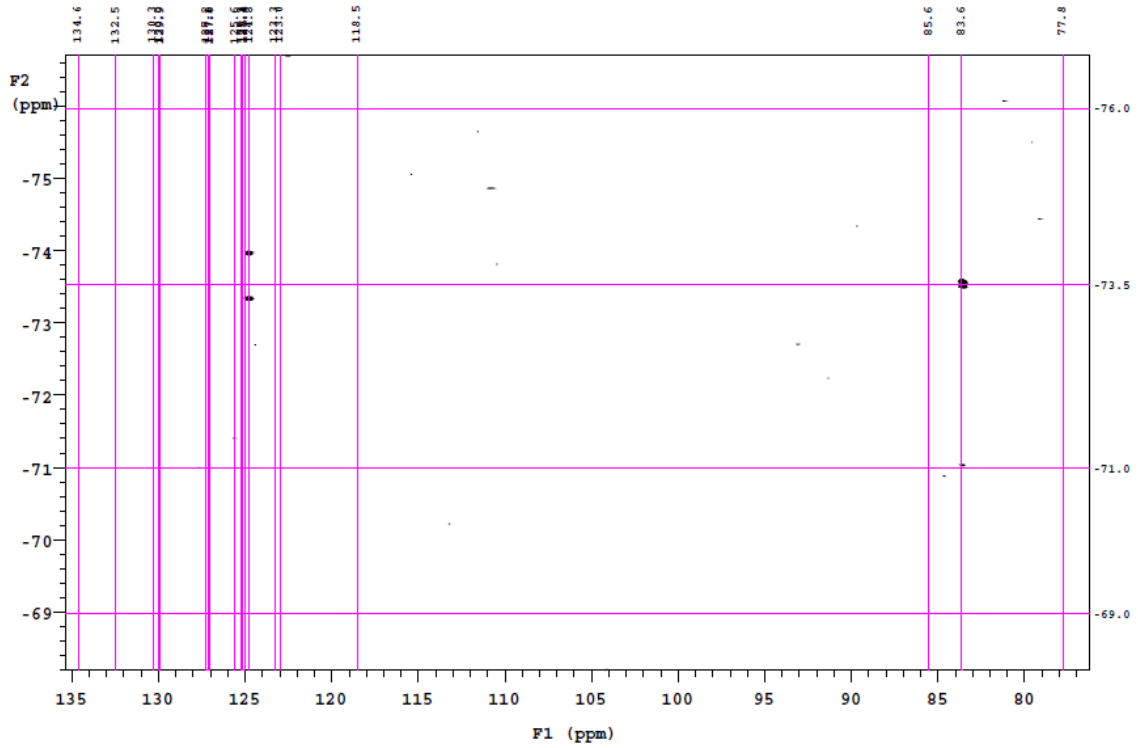

Figure S40. ^{19}F-^{13}C gHMBC (C_6D_6, 470 MHz) spectrum of **3**, expanded.

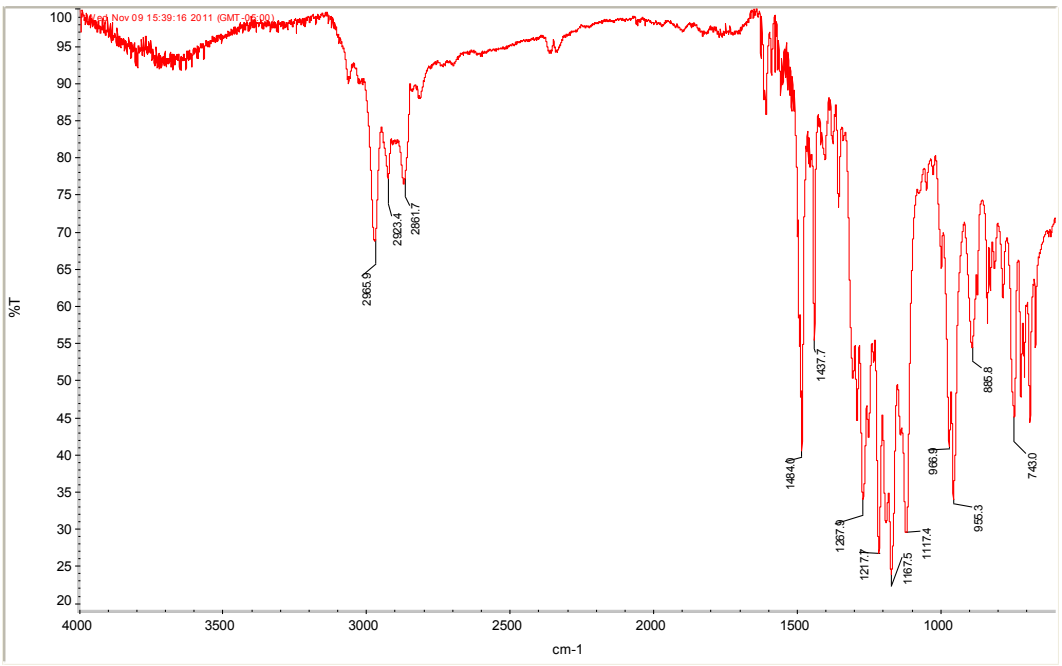

Figure S41. IR spectrum of **3** (neat film from diethyl ether solution).

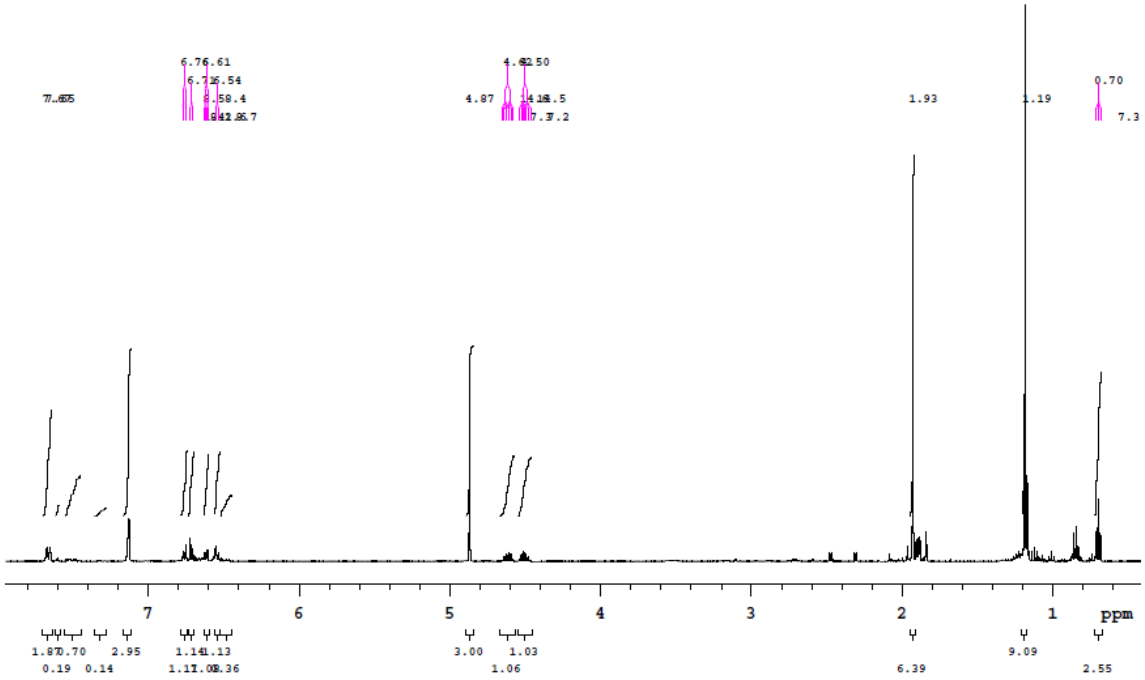

Figure S42. ^{1}H NMR (C_6D_6, 500 MHz) spectrum of **4**.

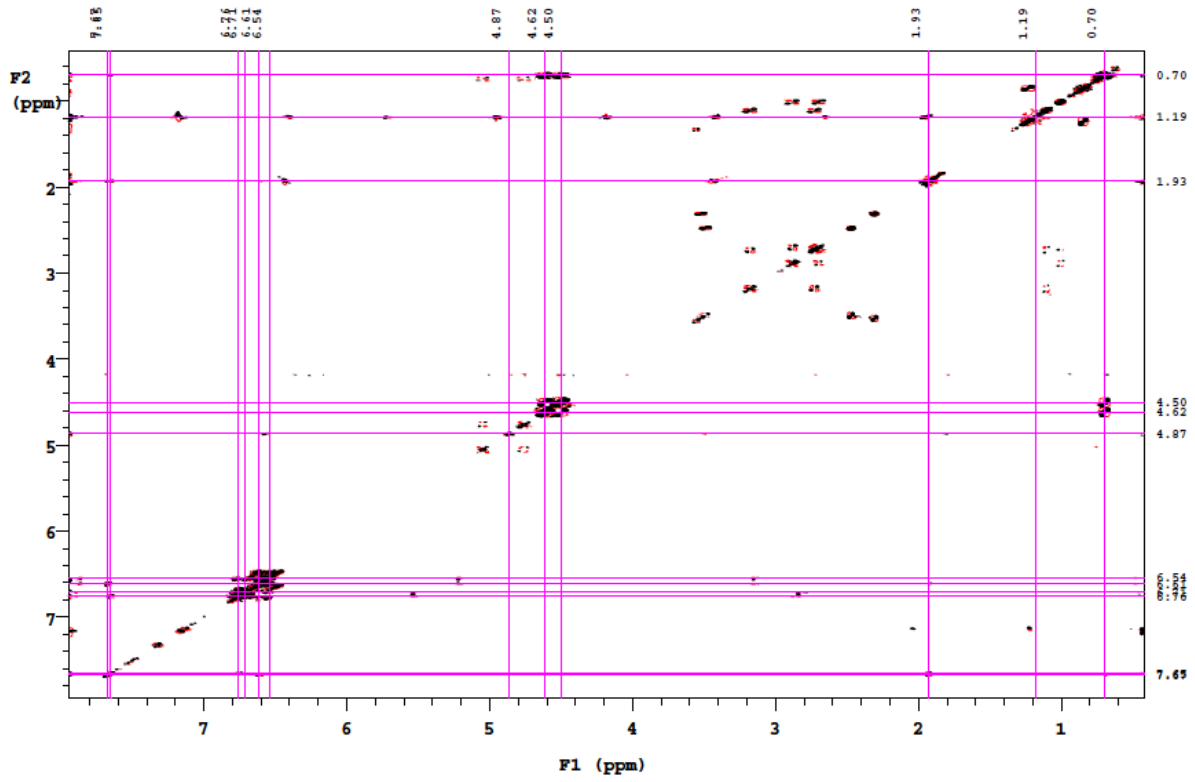

Figure S43. ^{1}H-^{1}H gDQFCOSY (C_6D_6, 500 MHz) spectrum of **4**.

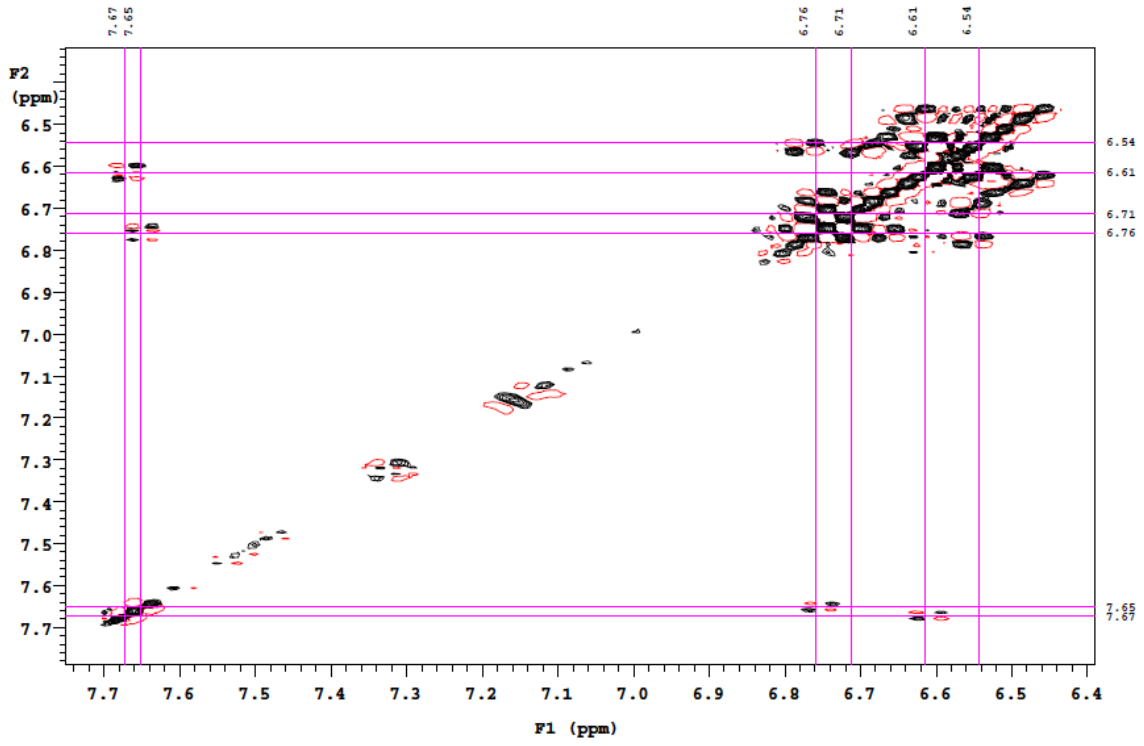

Figure S44. ^{1}H-^{1}H gDQFCOSY (C_6D_6, 500 MHz) spectrum of **4**, expanded.

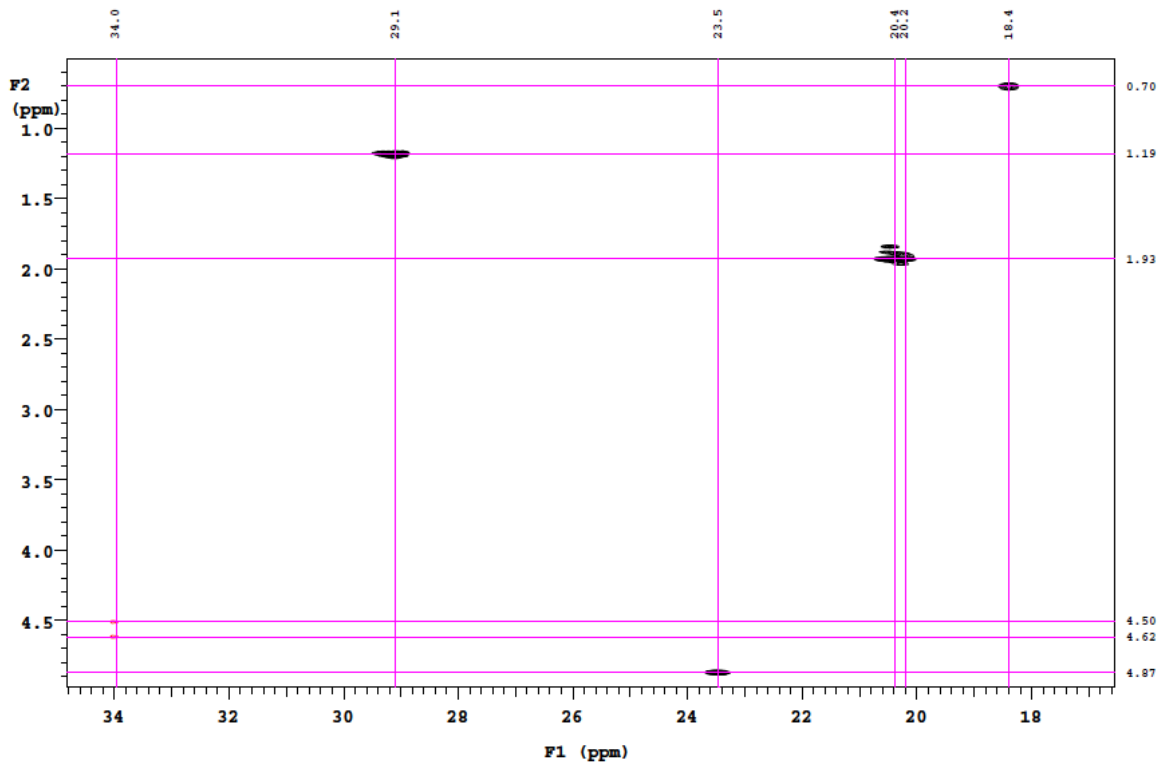

Figure S45. ^{1}H-^{13}C gHSQC (C_6D_6, 500 MHz) spectrum of **4**, expanded.

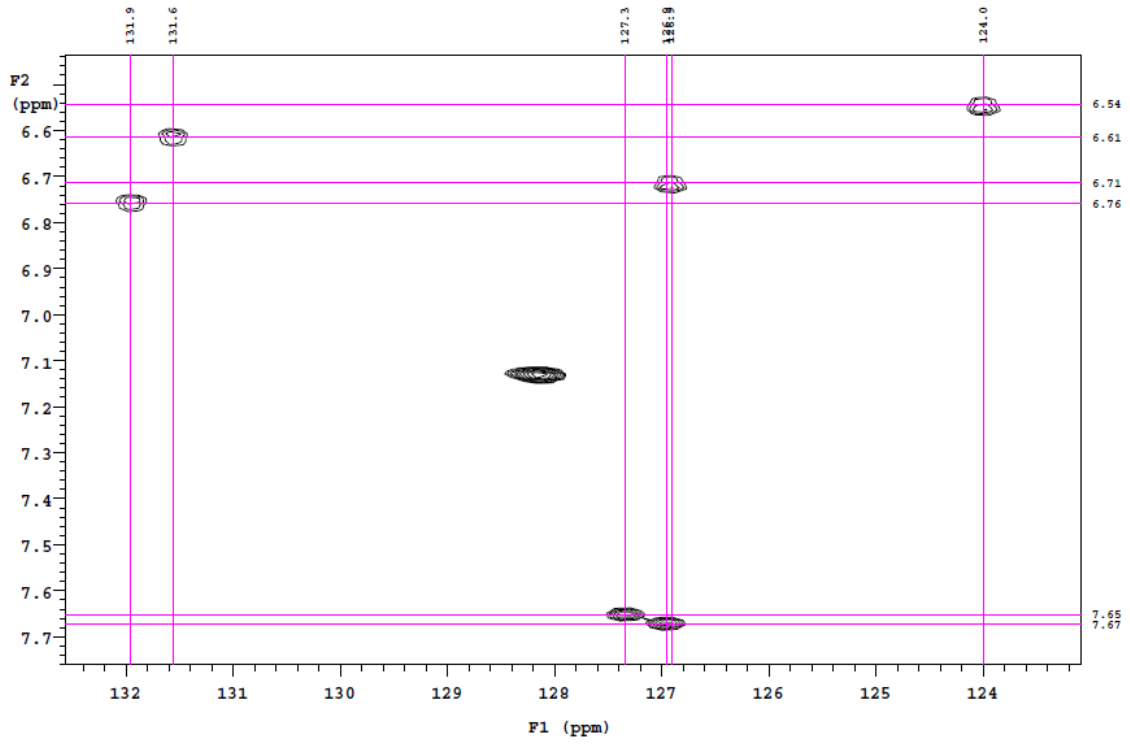

Figure S46. ^{1}H-^{13}C gHSQC (C_6D_6, 500 MHz) spectrum of **4**, expanded.

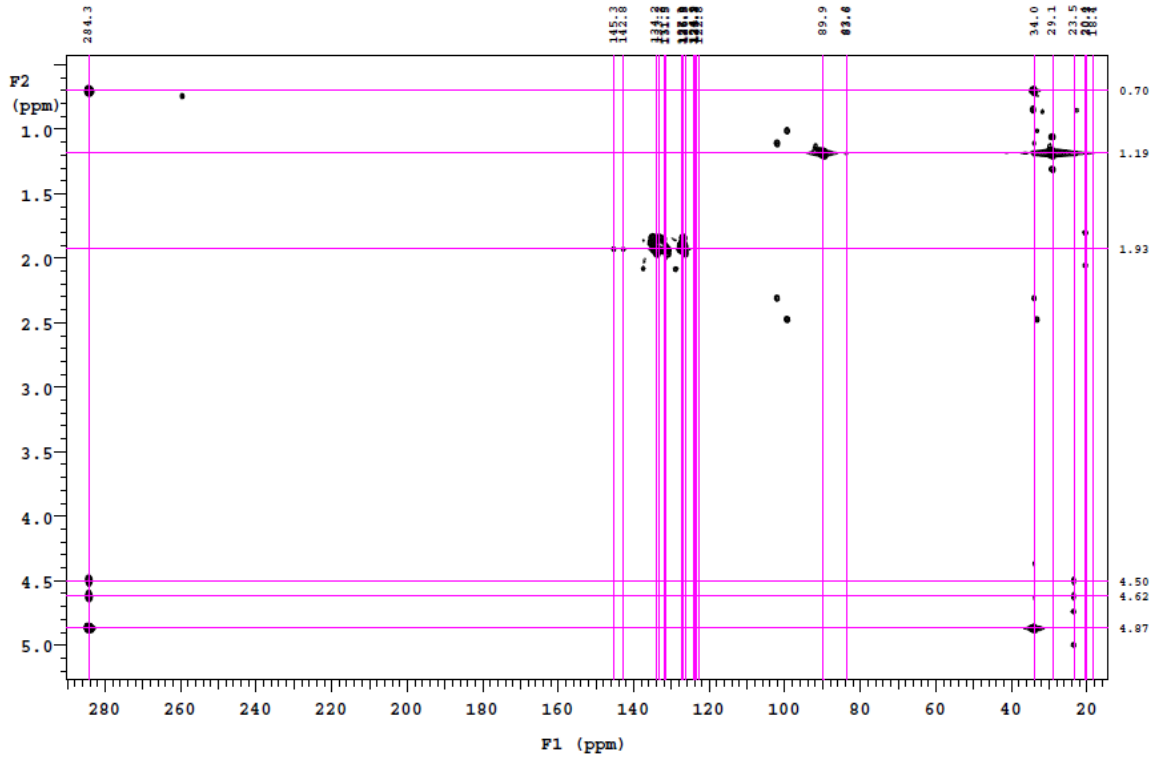

Figure S47. ^{1}H-^{13}C gHMBC (C_6D_6, 500 MHz) spectrum of **4**, expanded.

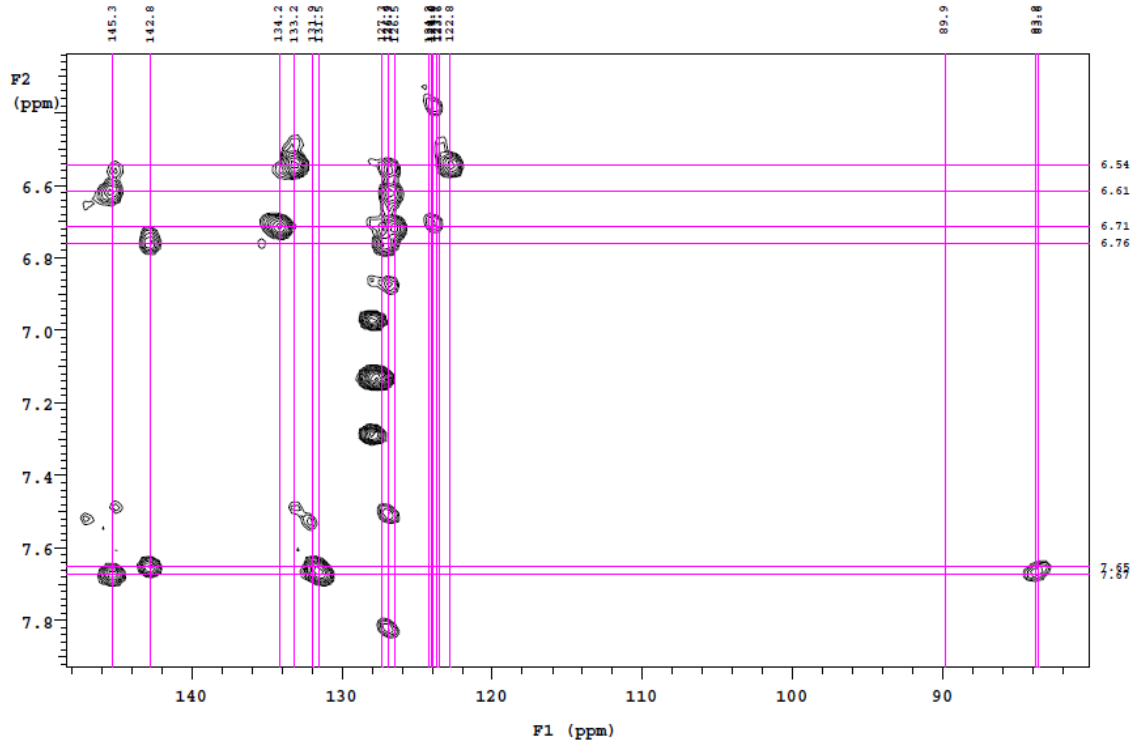

Figure S48. ^{1}H-^{13}C gHMBC (C_6D_6, 500 MHz) spectrum of **4**, expanded.

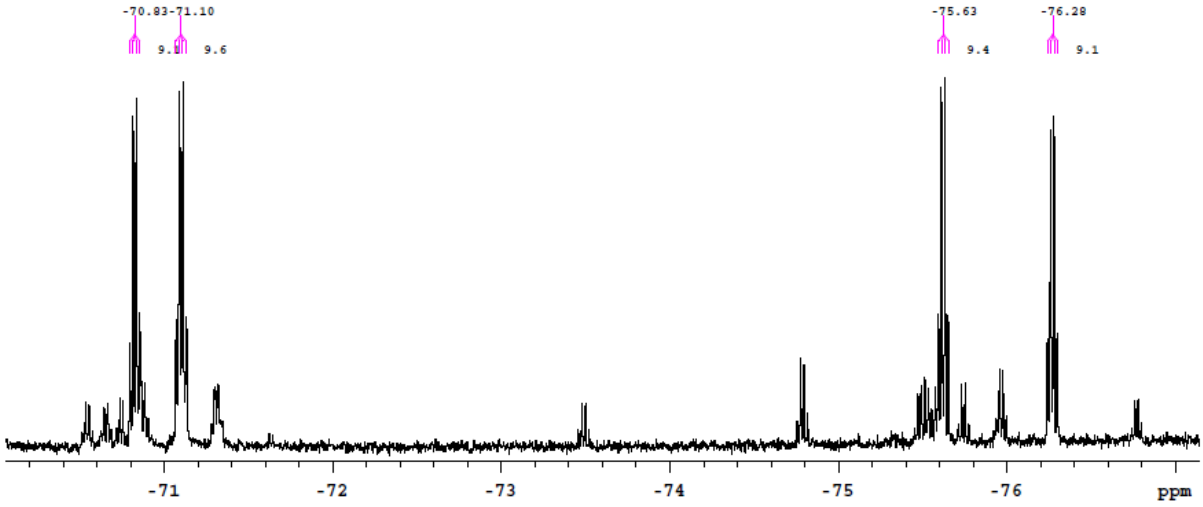

Figure S49. $^{19}F\{^{1}H\}$ NMR (C_6D_6, 470 MHz) spectrum of **4**.

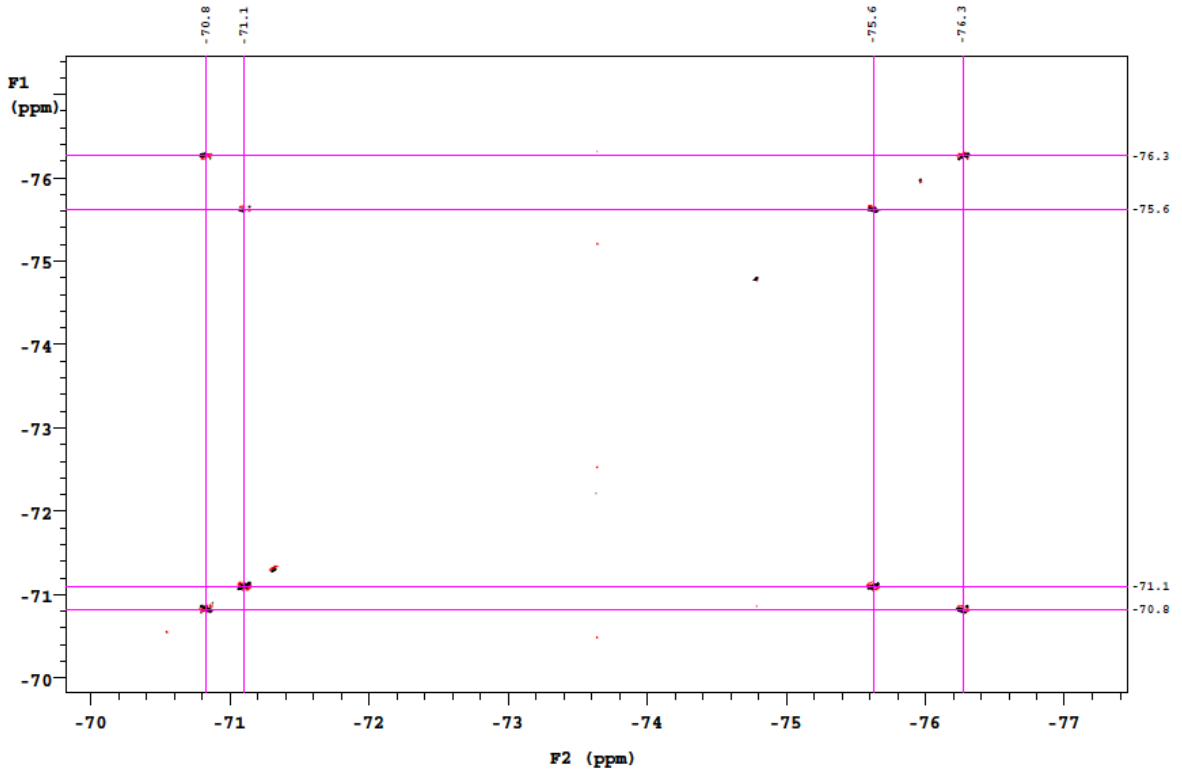

Figure S50. ^{19}F-^{19}F gDQFCOSY (C_6D_6, 470 MHz) spectrum of **4**.

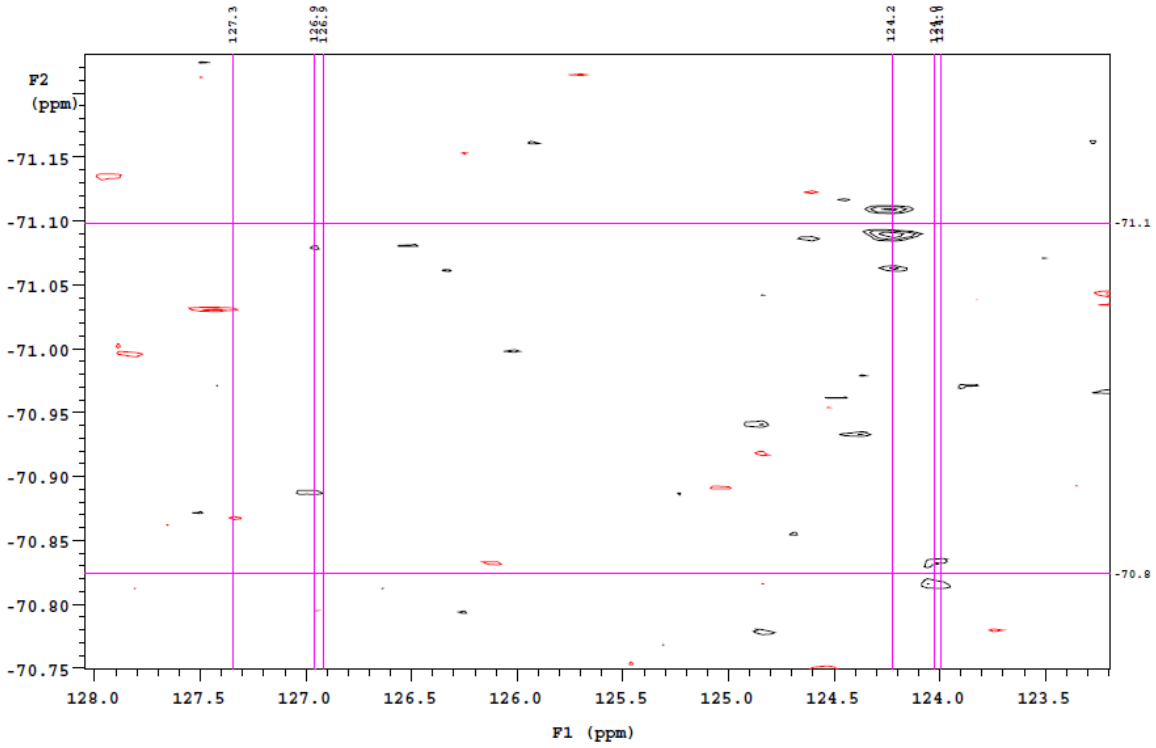

Figure S51. ^{19}F-^{13}C gHSQC (C_6D_6, 470 MHz) spectrum of **4**, expanded.

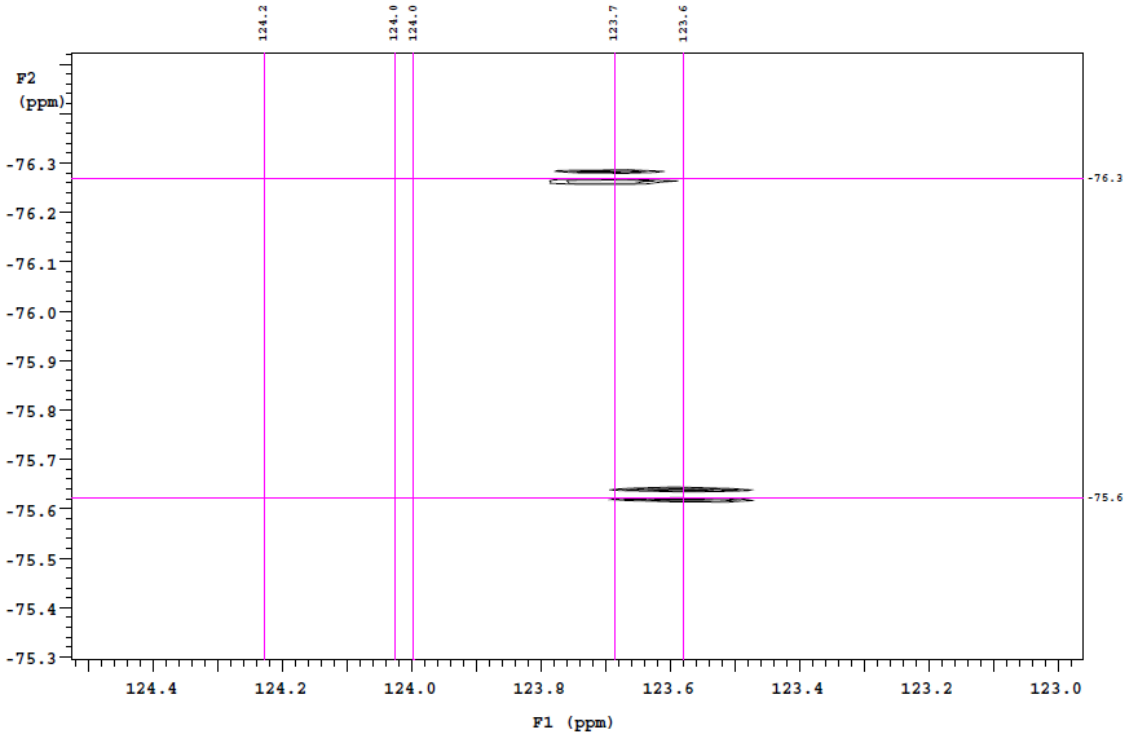

Figure S52. ^{19}F-^{13}C gHSQC (C_6D_6, 470 MHz) spectrum of **4**, expanded.

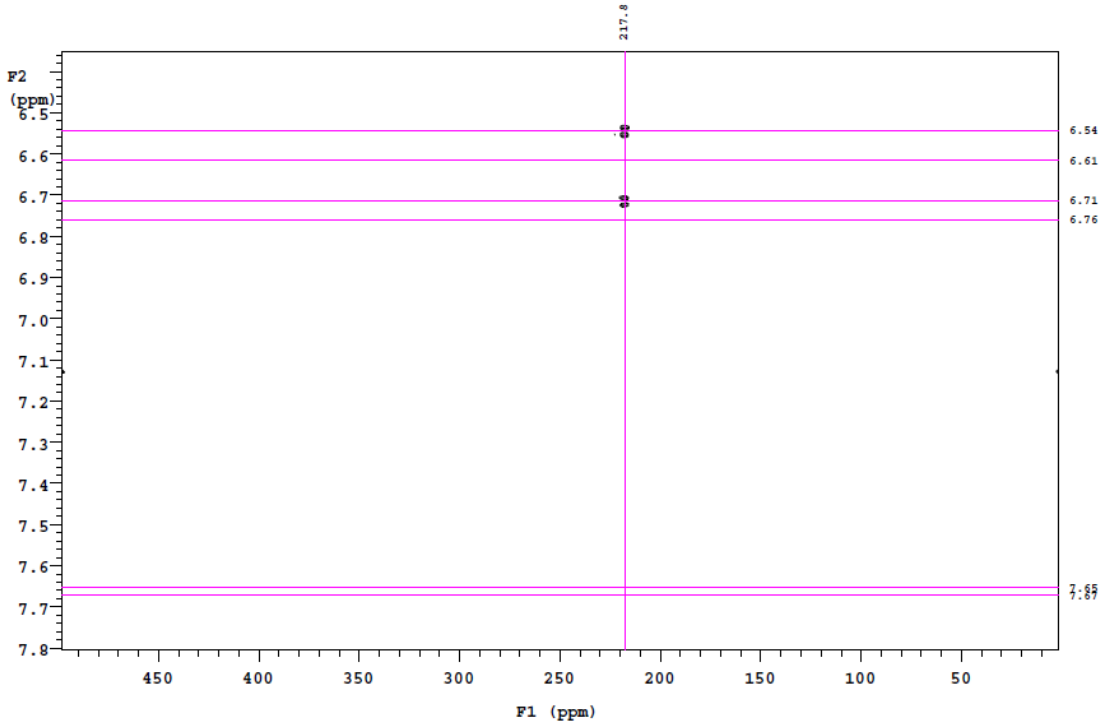

Figure S53. ^{1}H-^{15}N gHMBC (C_6D_6, 500 MHz) spectrum of **4**.

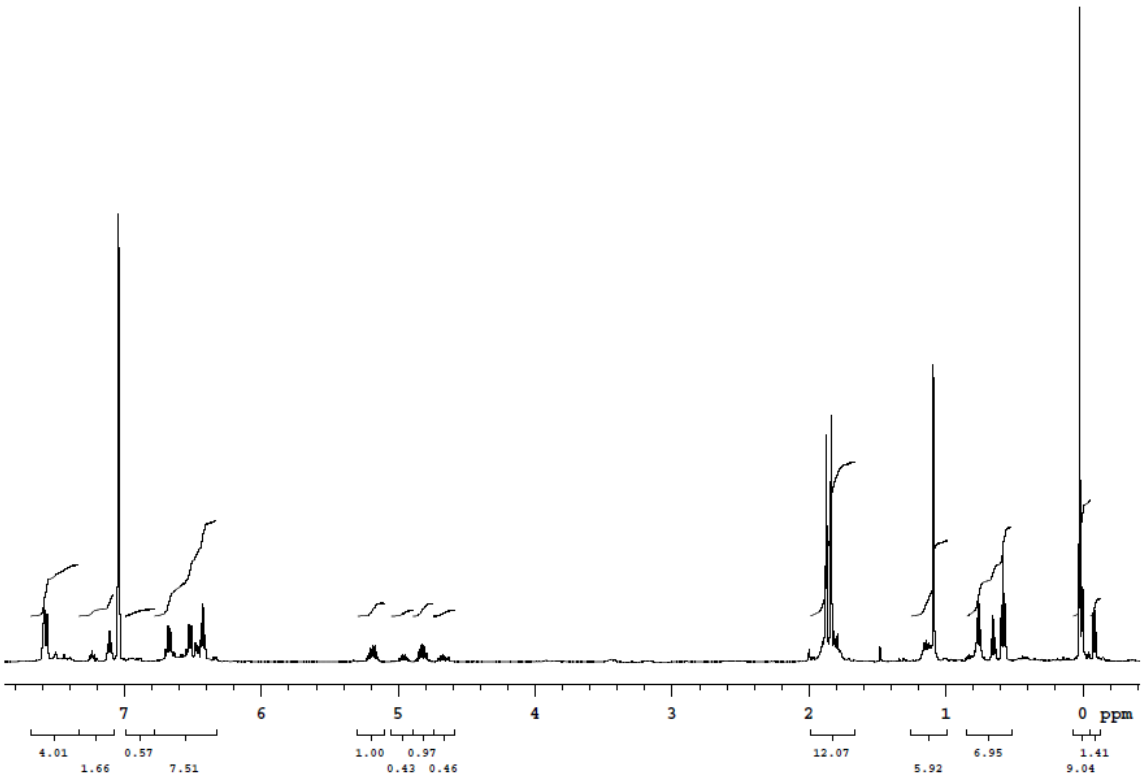

Figure S54. ^{1}H NMR (C_6D_6, 500 MHz) spectrum of **5**.

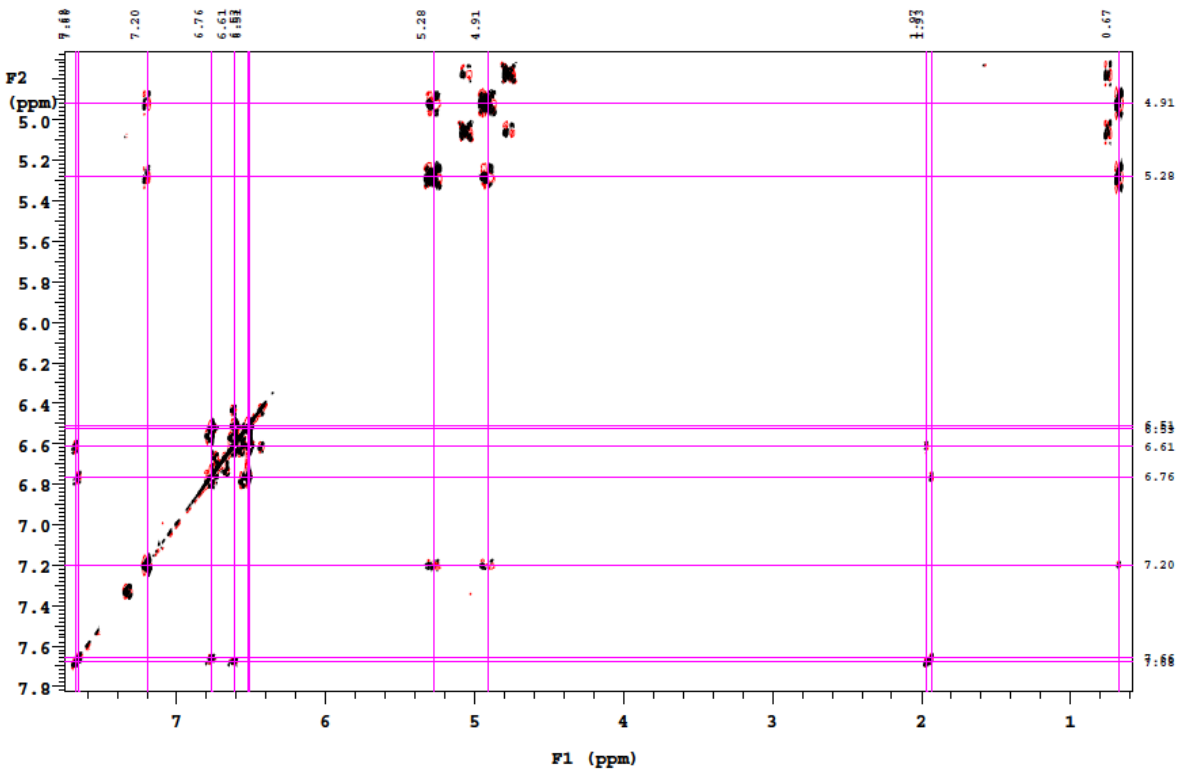

Figure S55. ^{1}H-^{1}H gDQCOSY (C_6D_6, 500 MHz) spectrum of **5**.

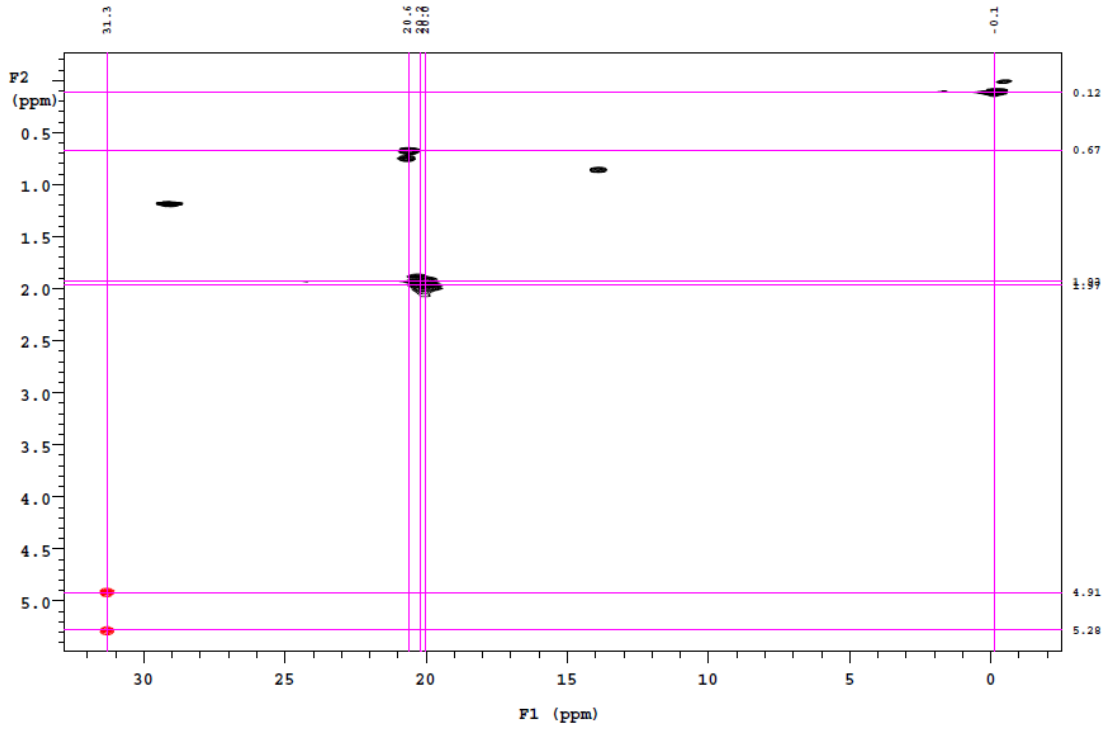

Figure S56. ^{1}H-^{13}C gHSQCAD (C_6D_6, 500 MHz) spectrum of **5**, expanded.

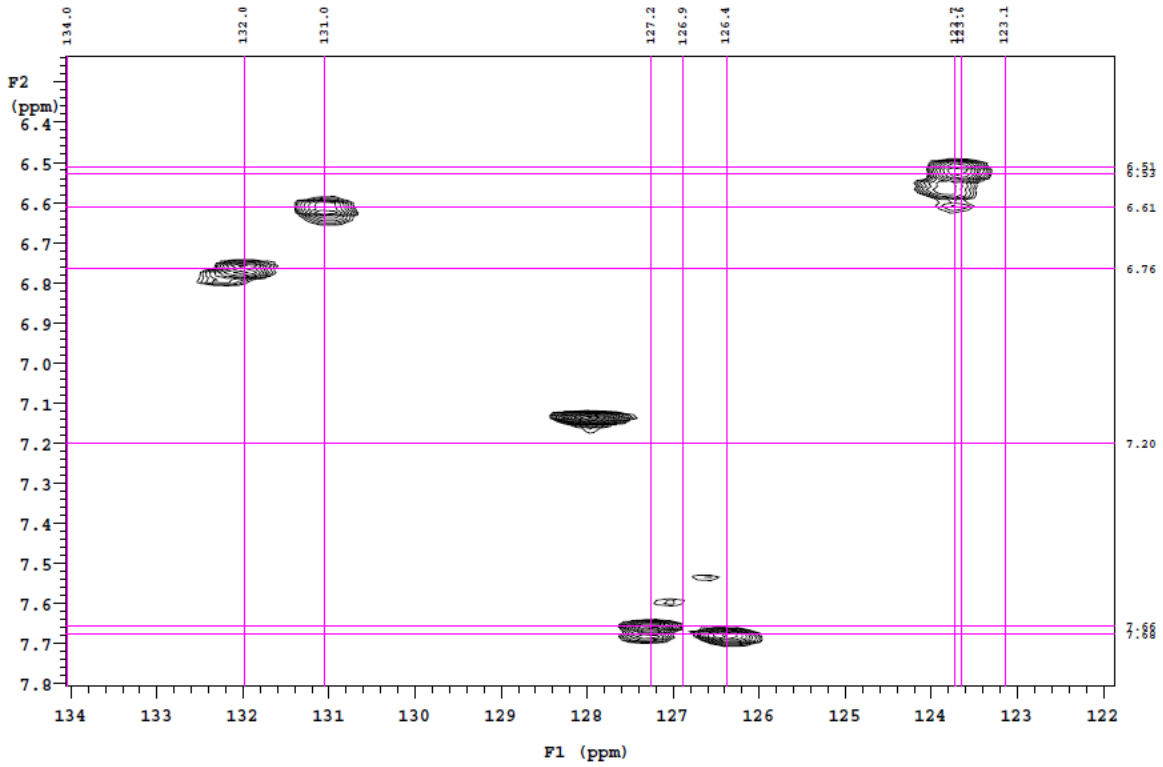

Figure S57. ^{1}H-^{13}C gHSQCAD (C_6D_6, 500 MHz) spectrum of **5**, expanded.

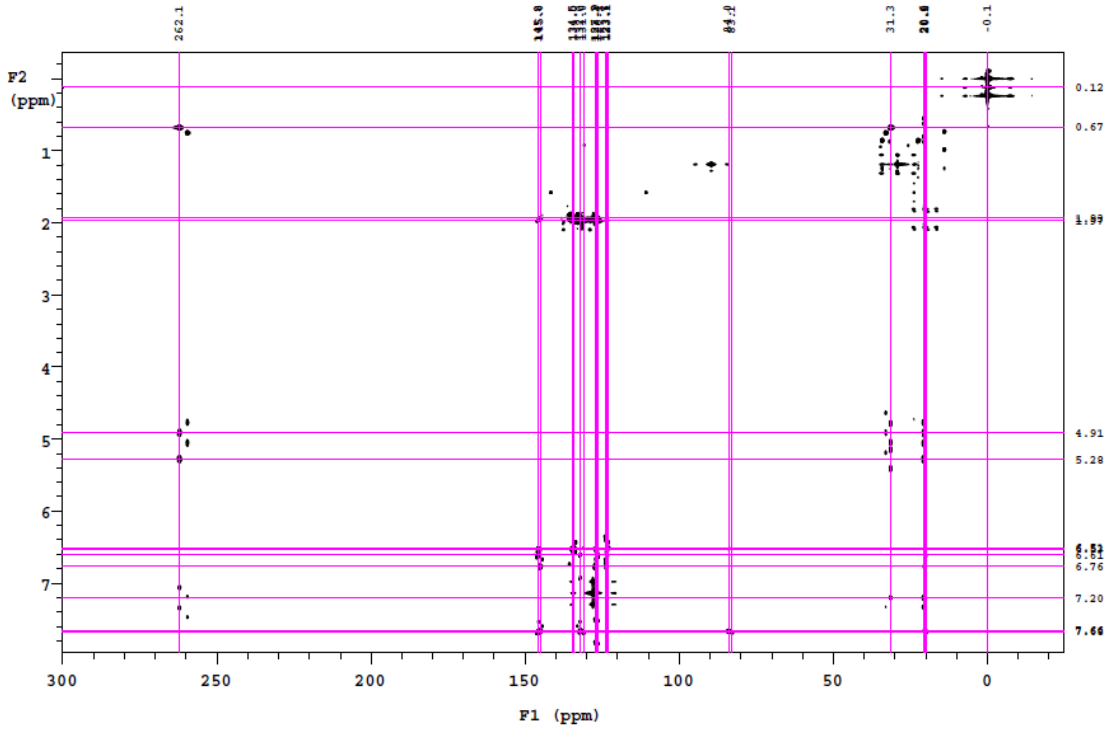

Figure S58. ^{1}H-^{13}C gHMBCAD (C_6D_6, 500 MHz) spectrum of **5**.

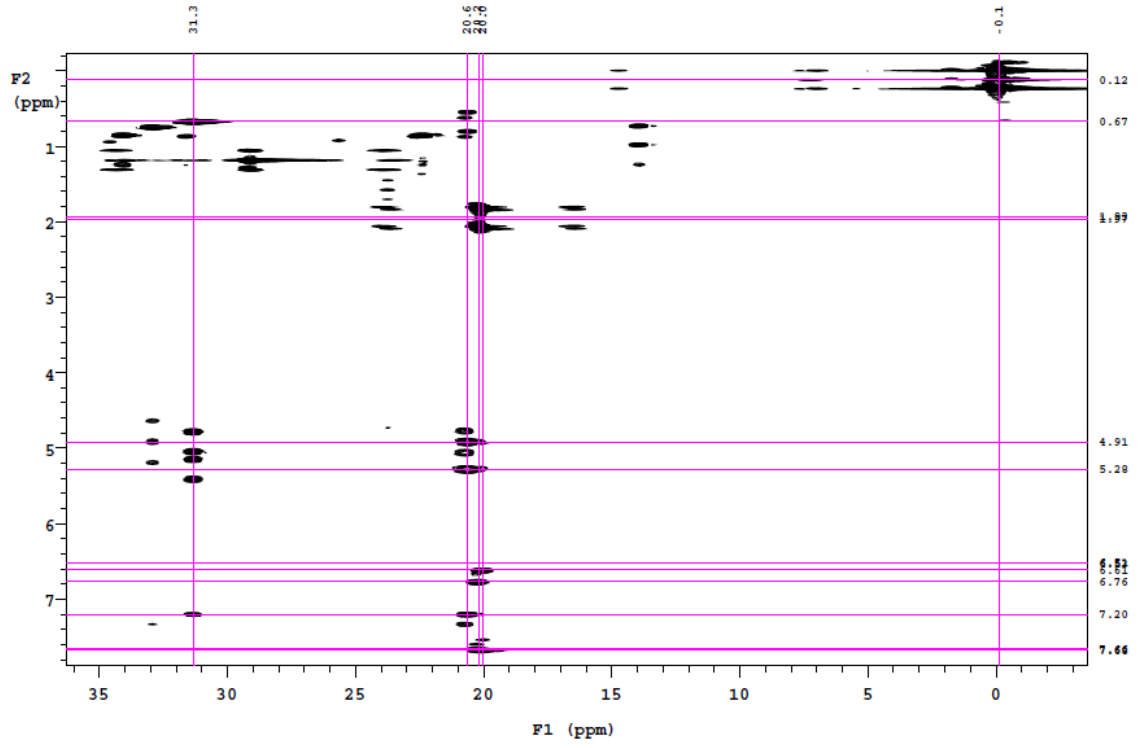

Figure S59. ^{1}H-^{13}C gHMBCAD (C_6D_6, 500 MHz) spectrum of **5**, expanded.

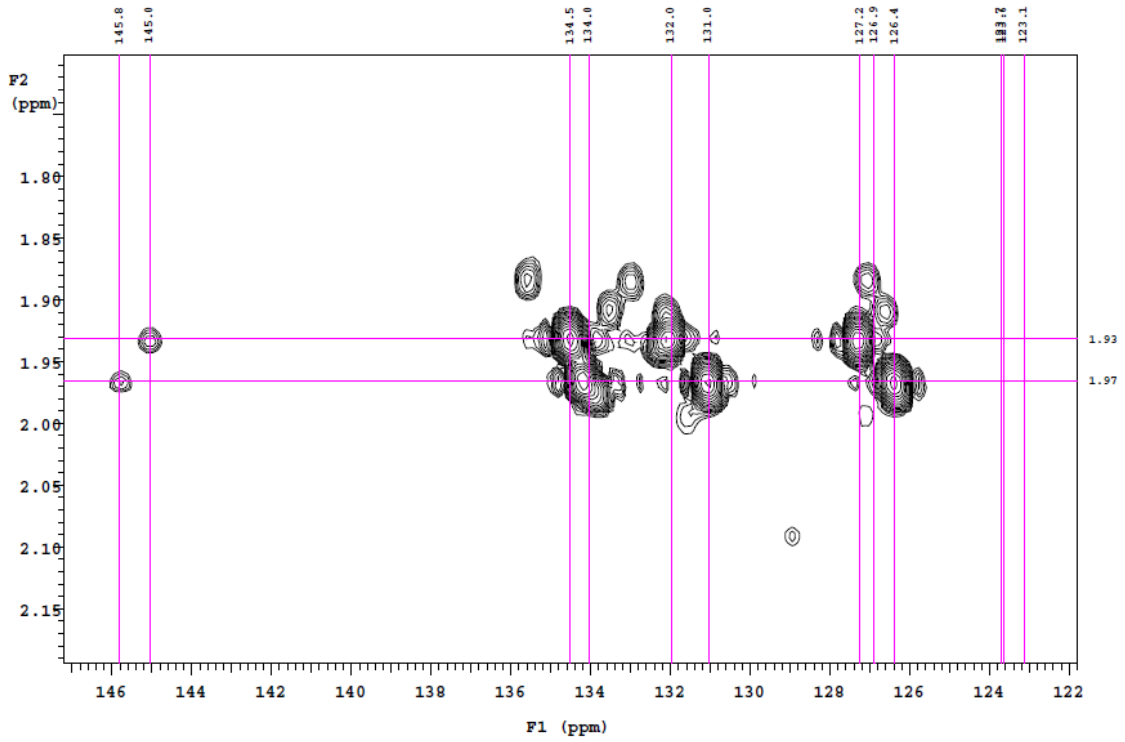

Figure S60. ^{1}H-^{13}C gHMBCAD (C_6D_6, 500 MHz) spectrum of **5**, expanded.

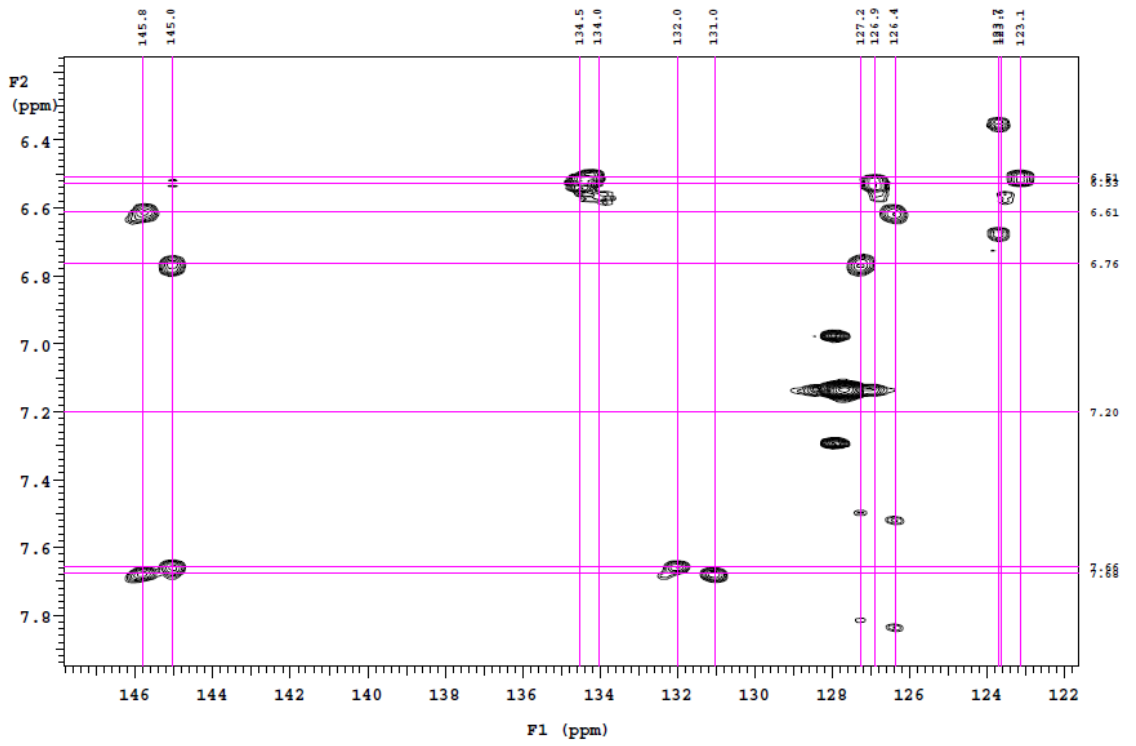

Figure S61. ^{1}H-^{13}C gHMBCAD (C_6D_6, 500 MHz) spectrum of **5**, expanded.

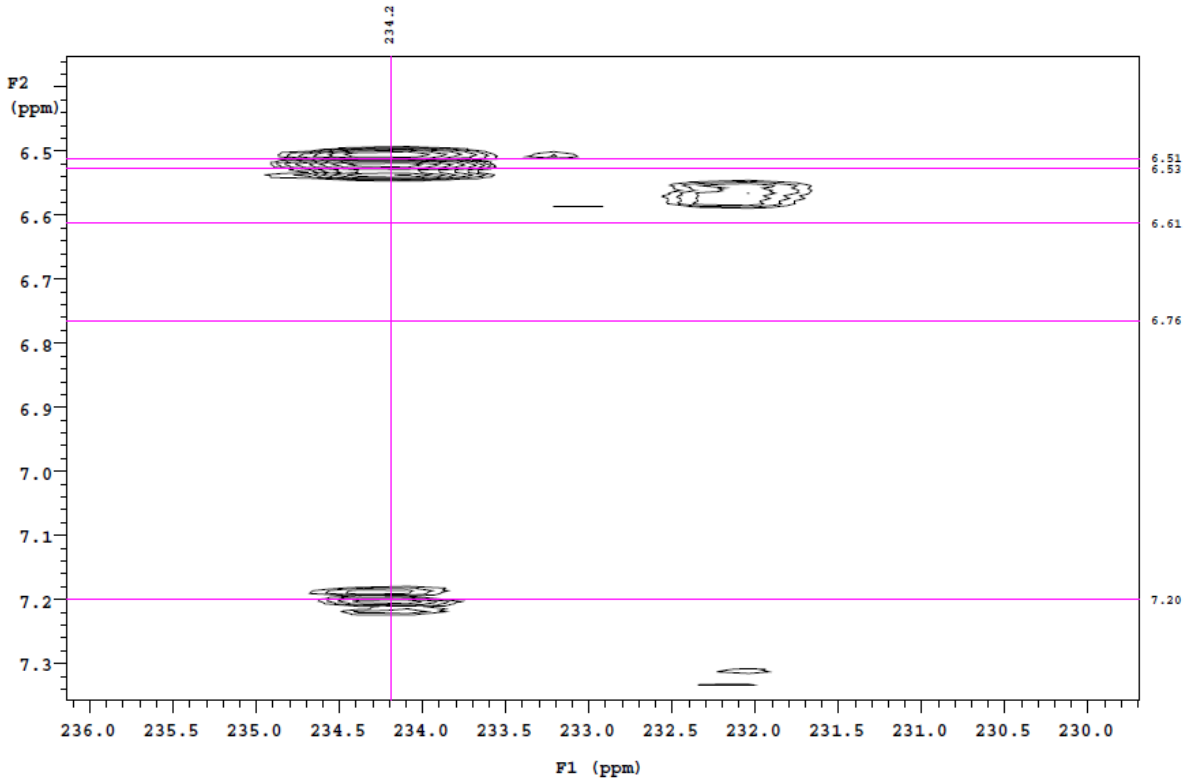

Figure S62. ^{1}H-^{15}N gHMBCAD (C_6D_6, 500 MHz) spectrum of **5**, expanded.

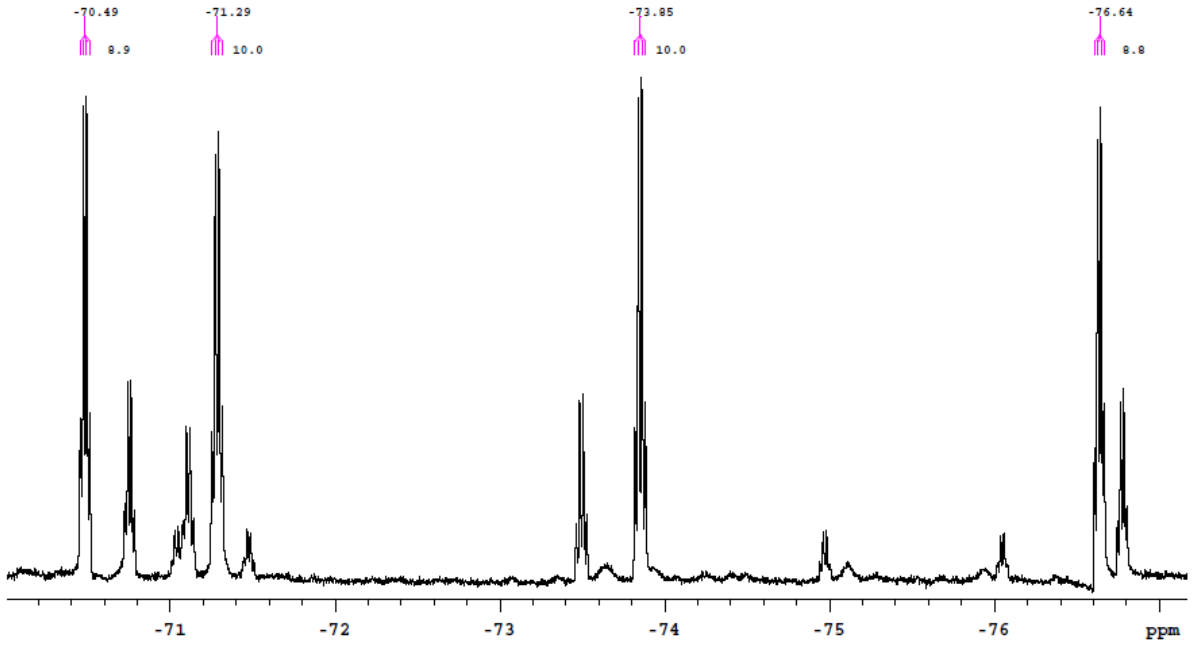

Figure S63. $^{19}F\{^{1}H\}$ NMR (C_6D_6, 470 MHz) spectrum of **5**.

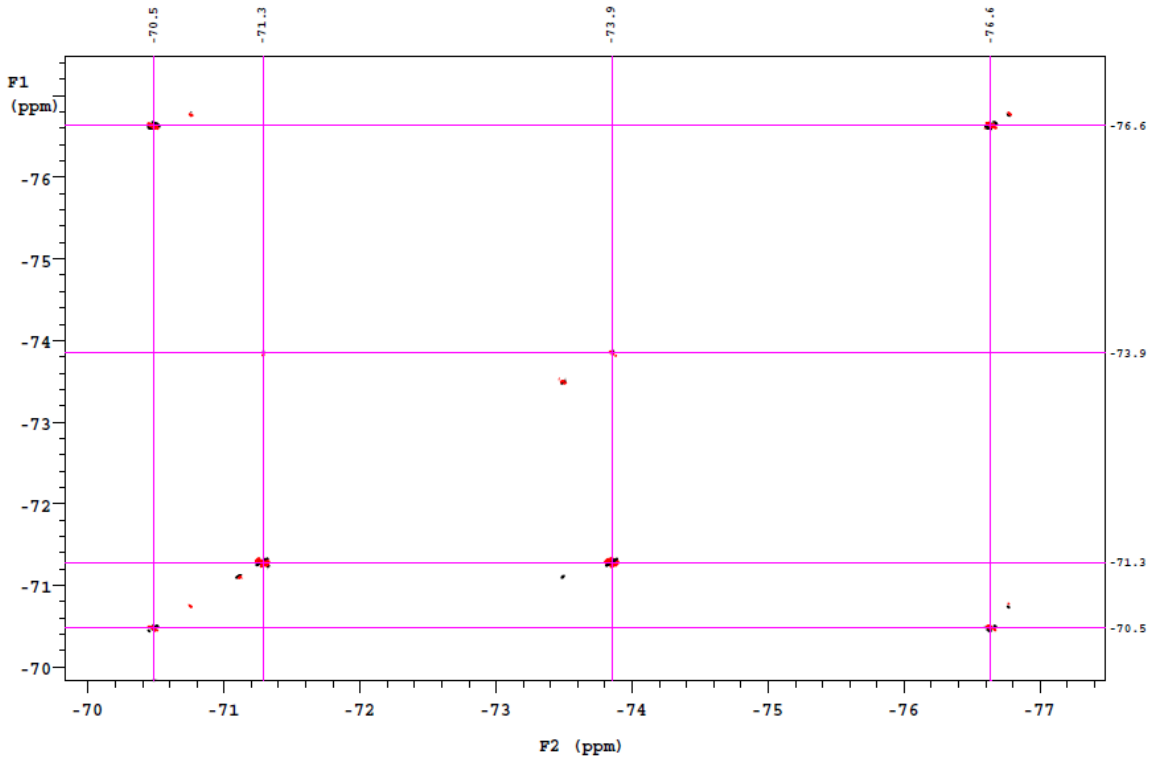

Figure S64. ^{19}F-^{19}F gDQCOSY (C_6D_6, 470 MHz) spectrum of **5**.

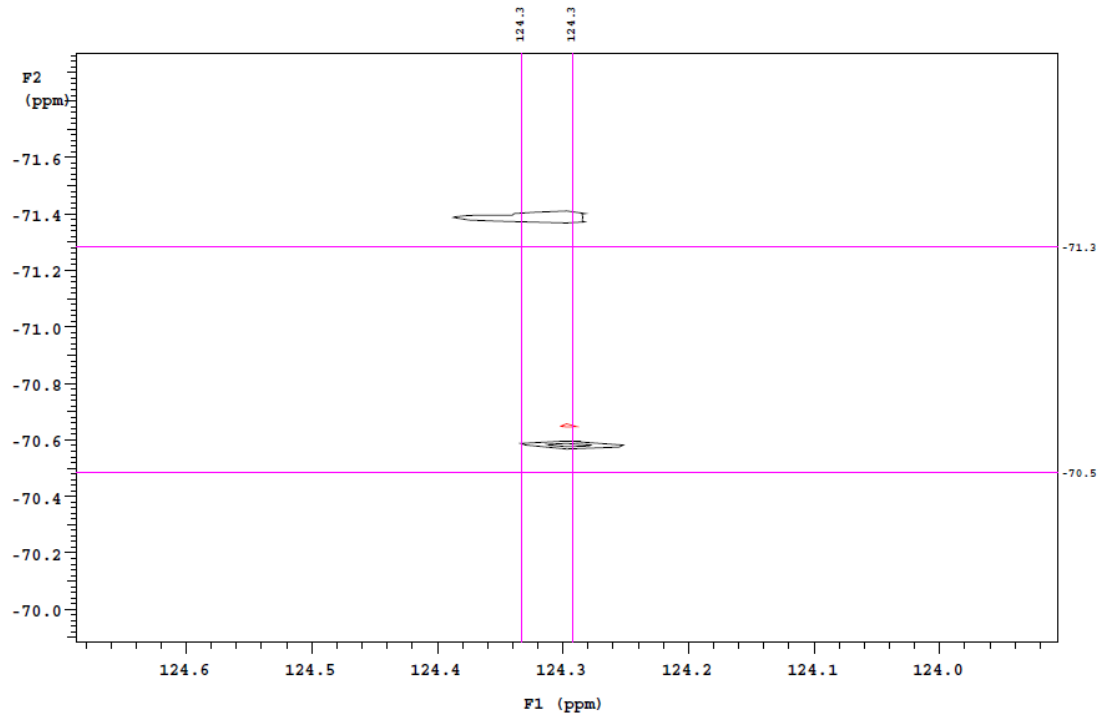

Figure S65. ^{19}F-^{13}C gHSQCAD (C_6D_6, 470 MHz) spectrum of **5**, expanded.

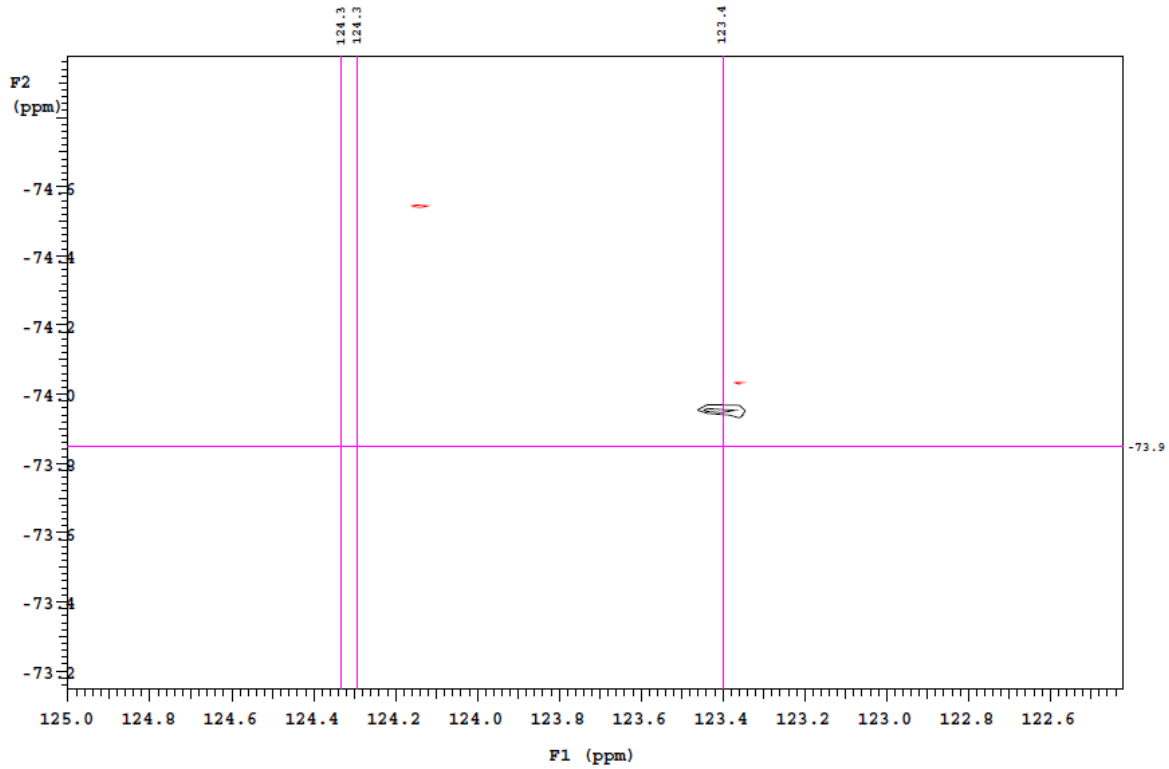

Figure S66. ^{19}F-^{13}C gHSQCAD (C_6D_6, 470 MHz) spectrum of **5**, expanded.

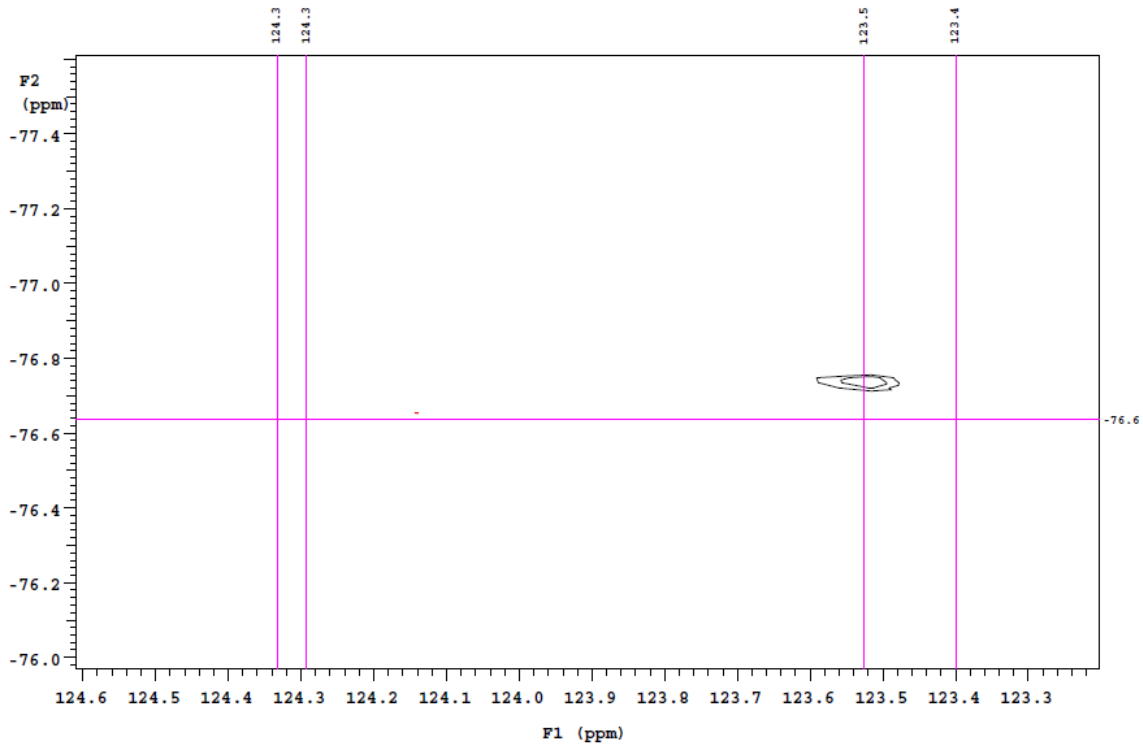

Figure S67. ^{19}F-^{13}C gHSQCAD (C_6D_6, 470 MHz) spectrum of **5**, expanded.

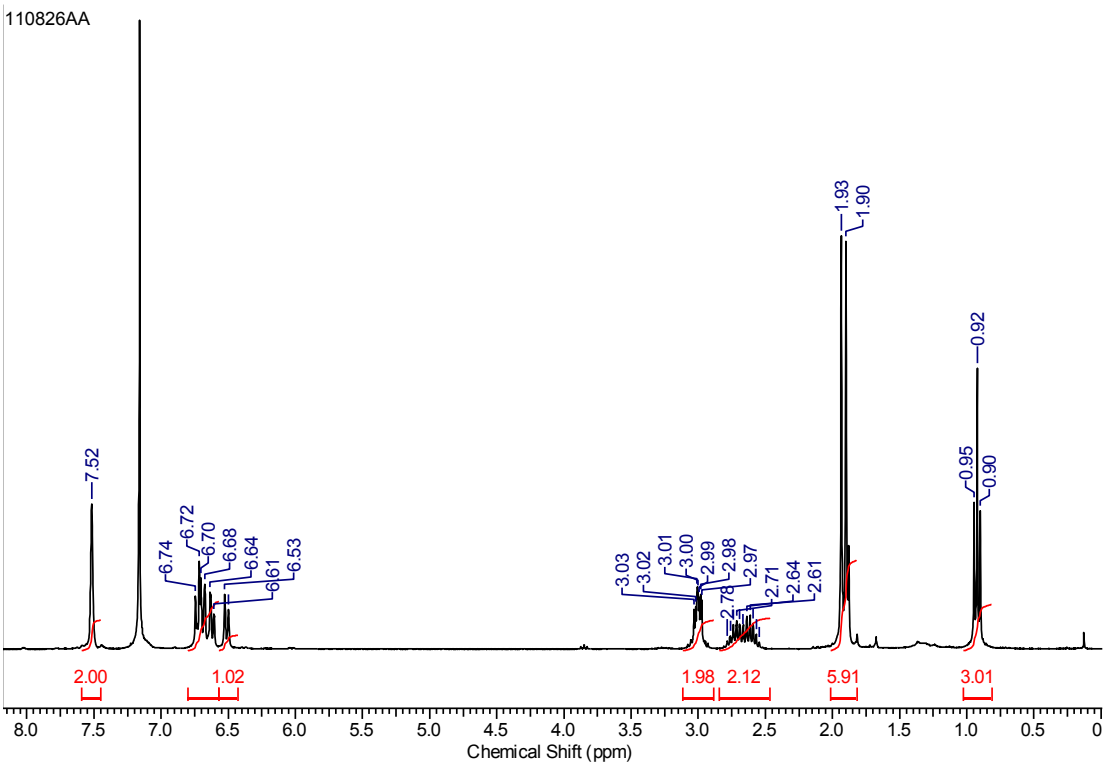

Figure S68. ^{1}H NMR (C_6D_6, 300 MHz) spectrum of **6**.

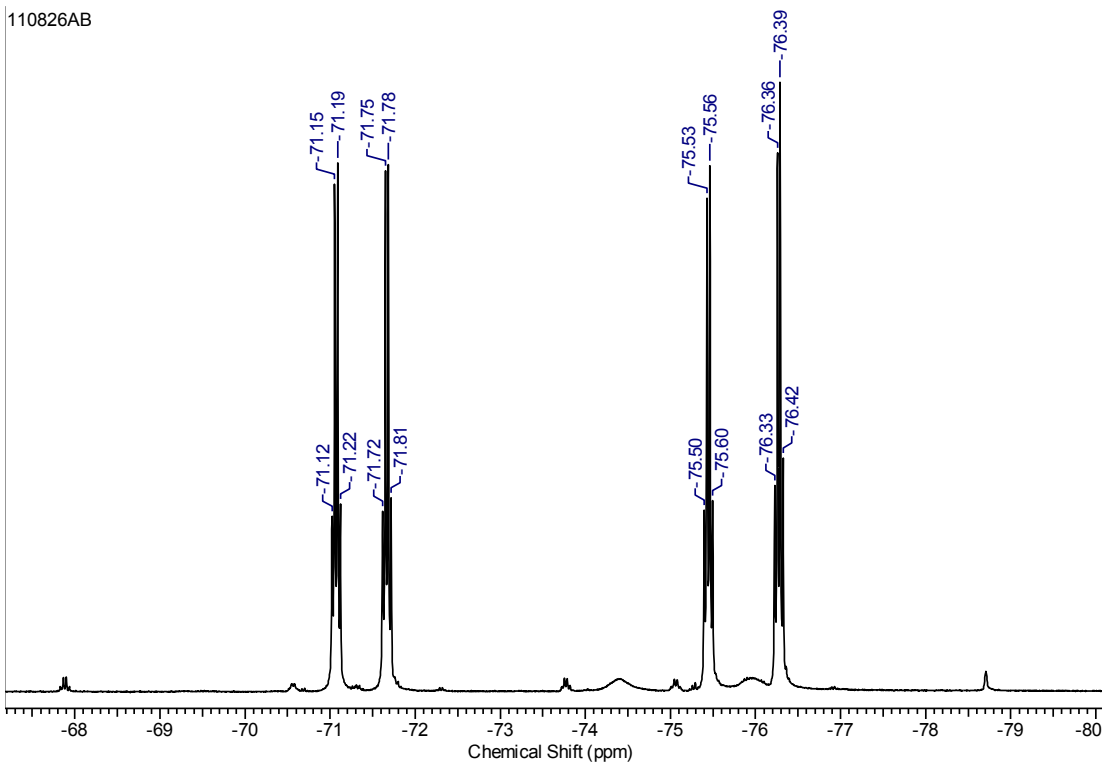

Figure S69. ^{19}F NMR (C_6D_6, 282 MHz) spectrum of **6**.

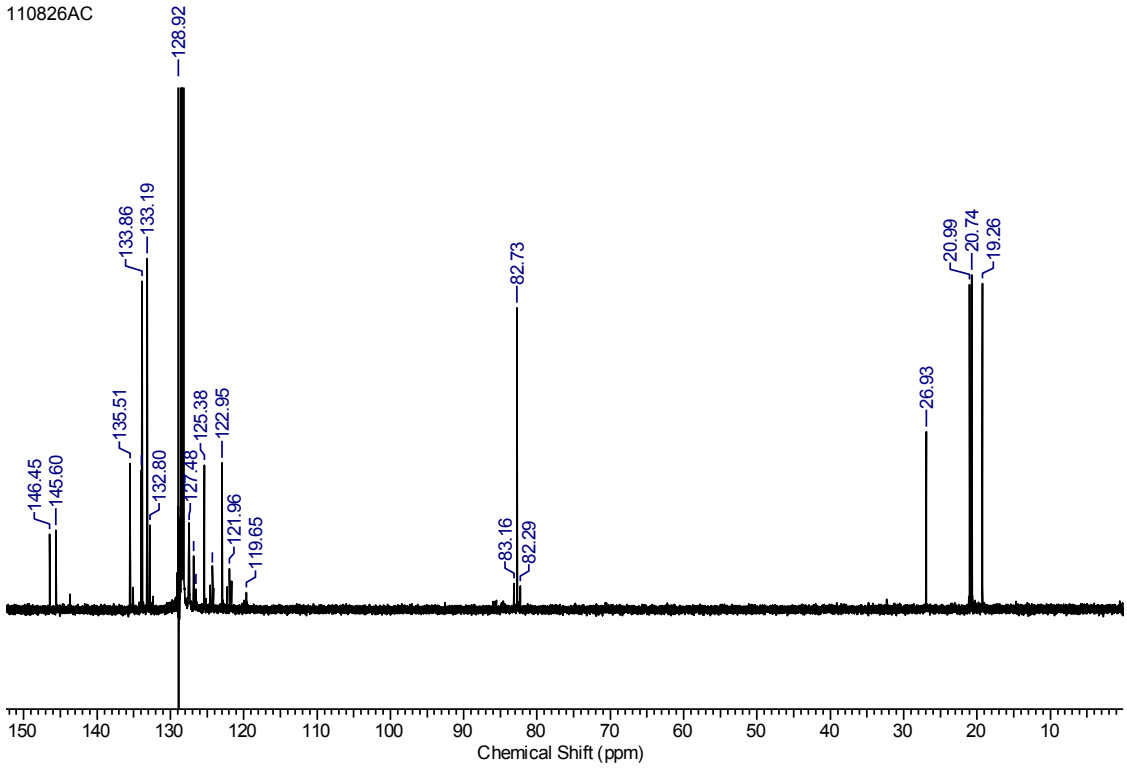

Figure S70. $^{13}C\{^1H\}$ NMR (C_6D_6, 126 MHz) spectrum of **6**.

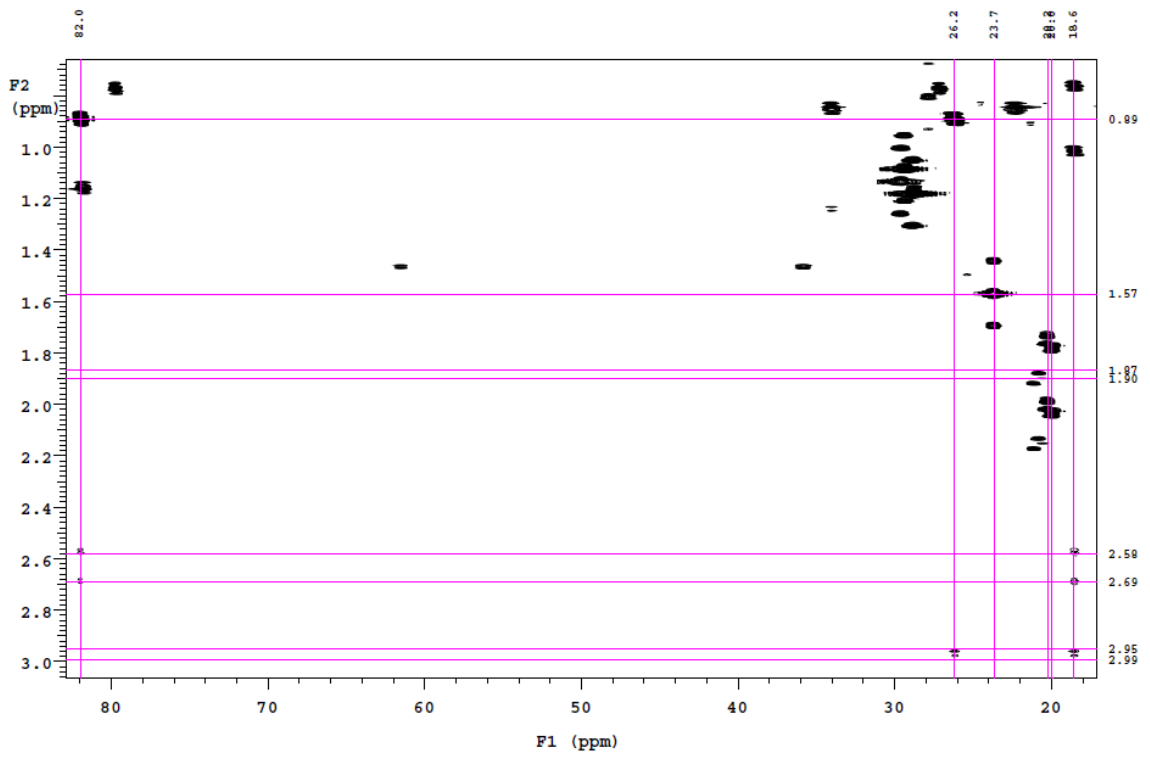

Figure S71. ^{1}H -^{13}C gHMBC (C_6D_6, 500 MHz) spectrum of **6**, expanded.

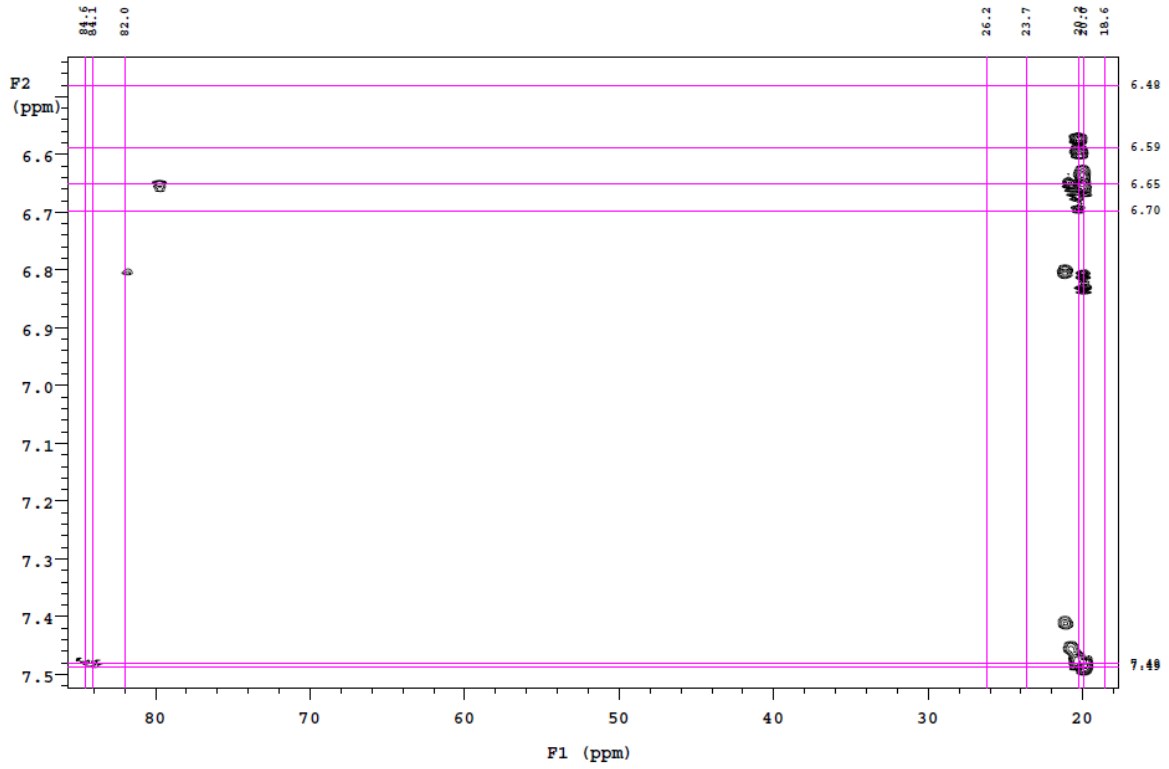

Figure S72. ^{1}H -^{13}C gHMBC (C_6D_6, 500 MHz) spectrum of **6**, expanded.

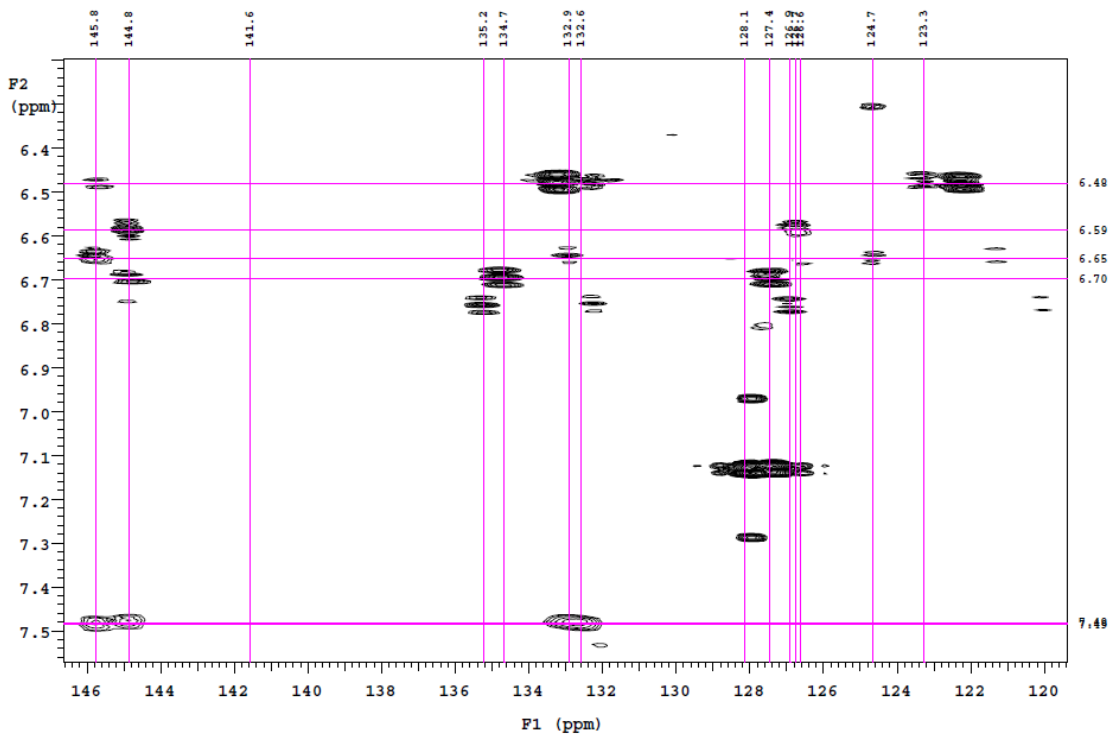

Figure S73. ^{1}H-^{13}C gHMBC (C_6D_6, 500 MHz) spectrum of **6**, expanded.

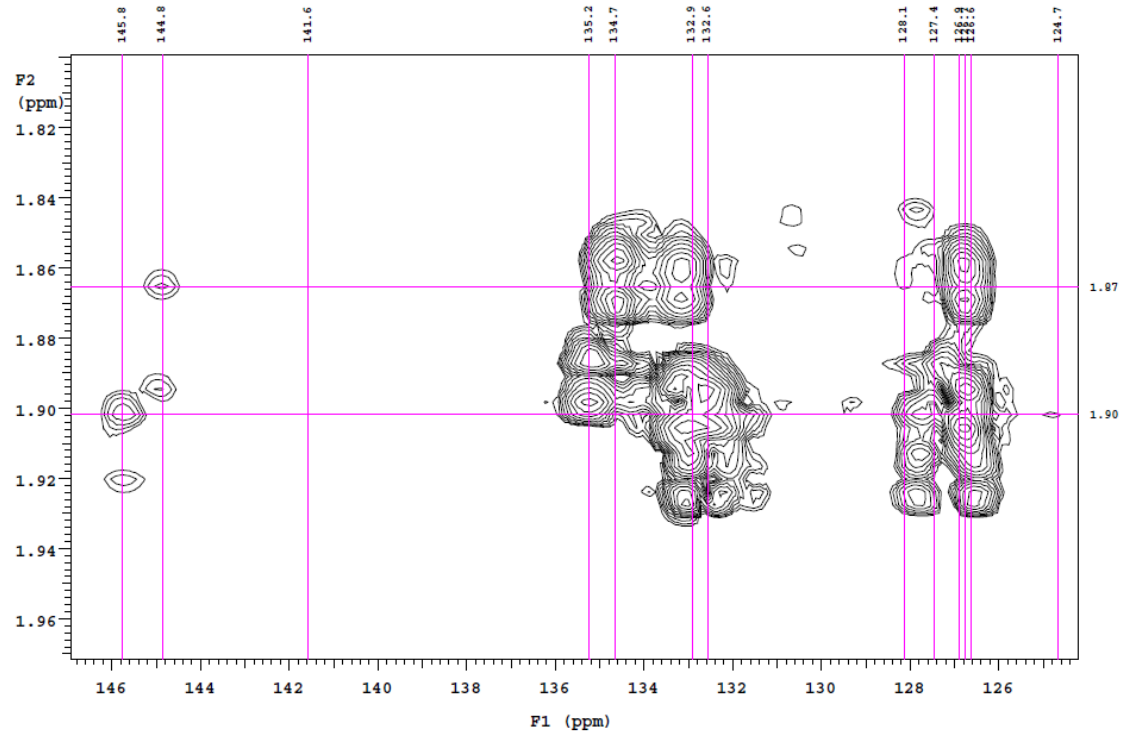

Figure S74. ^{1}H-^{13}C gHMBC (C_6D_6, 500 MHz) spectrum of **6**, expanded.

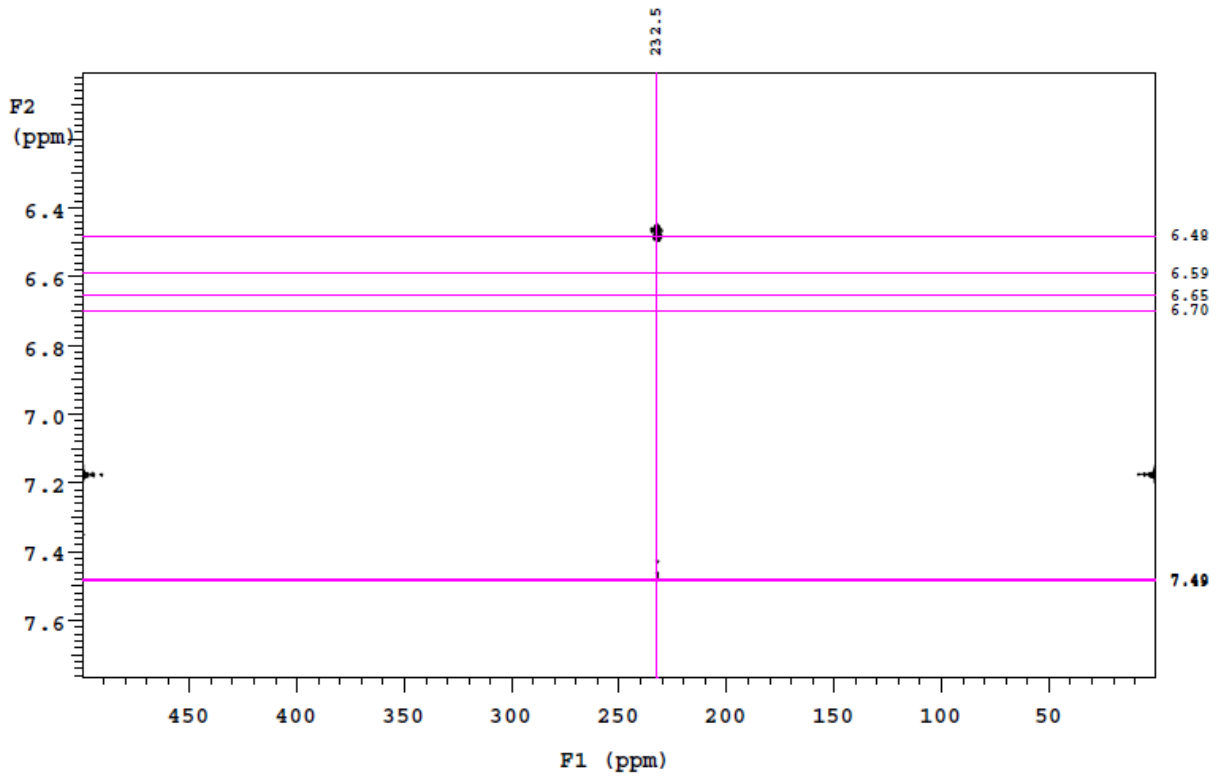

Figure S75. ^{1}H-^{15}N gHMBC (C_6D_6, 500 MHz) spectrum of **6**.

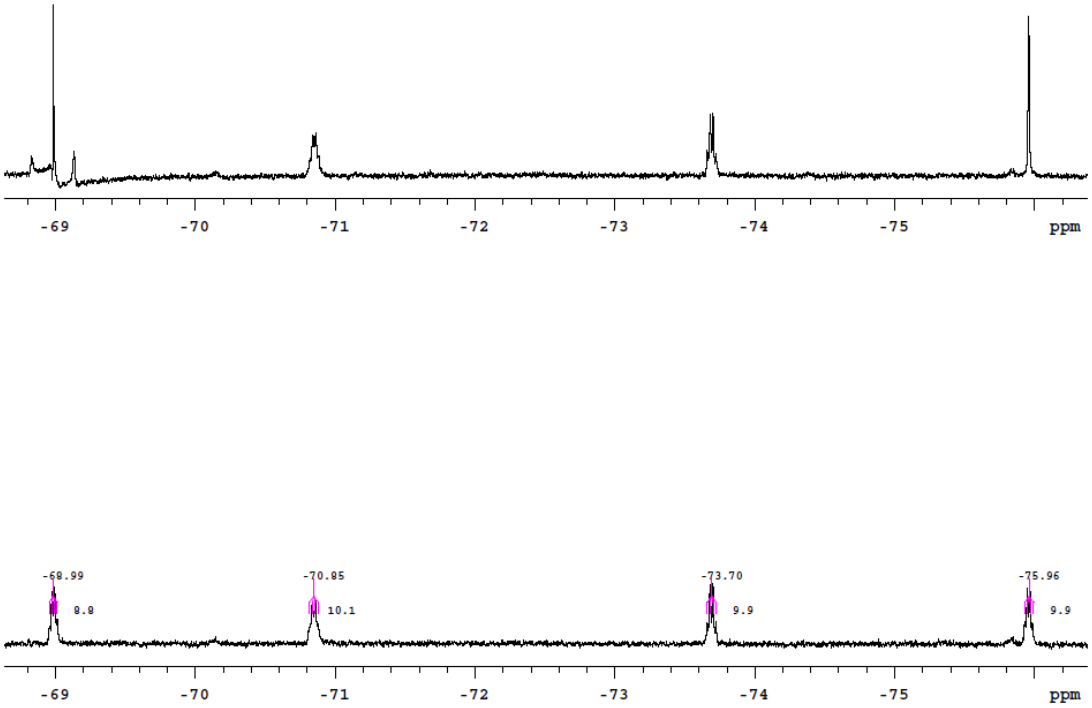

Figure S76. $^{19}F\{^{1}H\}$ NMR (C_6D_6, 470 MHz) spectrum of **6** (bottom) and spectra with selective homonuclear decoupling (top).

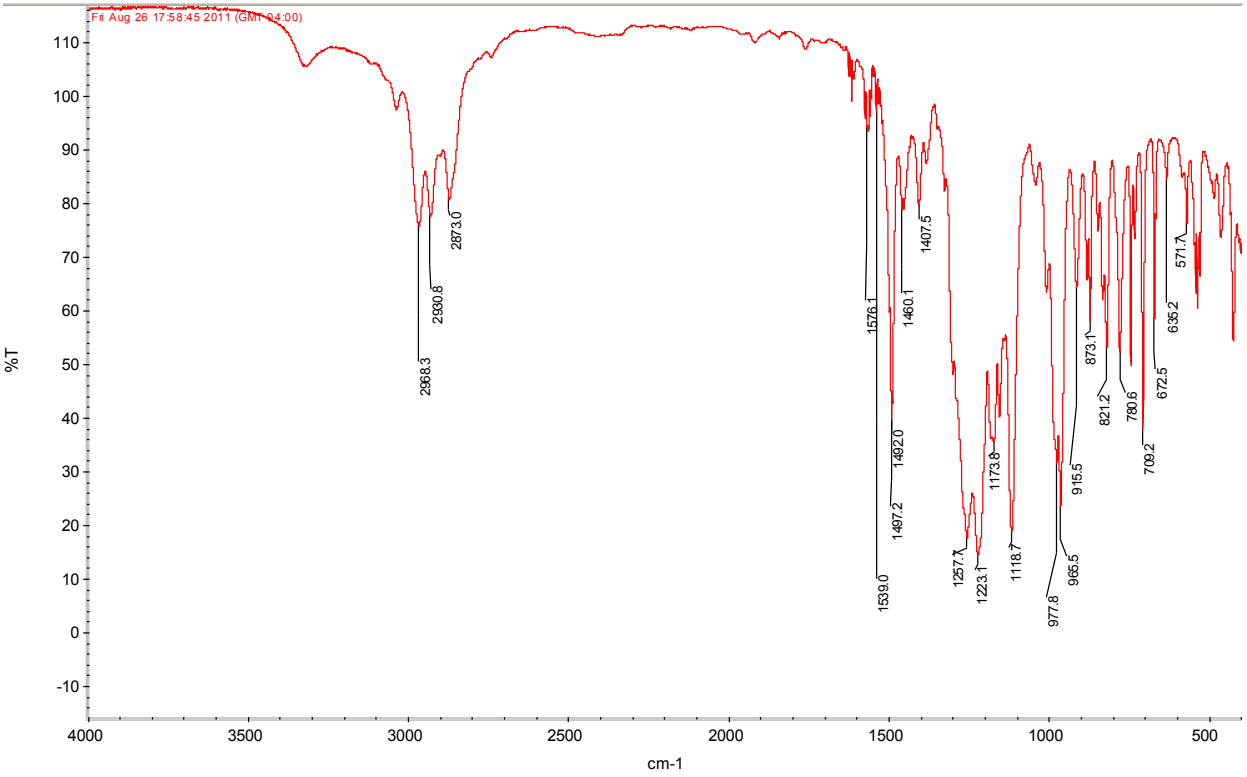

Figure S77. IR spectrum of **6** (neat film from diethyl ether solution).

X-Ray experimental for 2: X-Ray Intensity data were collected at 100 K on a Bruker **SMART** diffractometer using MoKα radiation (λ = 0.71073 Å) and an APEXII CCD area detector. Raw data frames were read by program SAINT[1] and integrated using 3D profiling algorithms. The resulting data were reduced to produce hkl reflections and their intensities and estimated standard deviations. The data were corrected for Lorentz and polarization effects and numerical absorption corrections were applied based on indexed and measured faces. The structure was solved and refined in SHELXTL6.1, using full-matrix least-squares refinement. The non-H atoms were refined with anisotropic thermal parameters and all of the H atoms were calculated in idealized positions and refined riding on their parent atoms. A disorder between H4a and a small percentage of Br on C4 was identified with the final refinement yielding 3% of Br and 97% of the proton. The Br atom was refined with several site occupation factors until an acceptable value was reached; which was 3%. The presence of the bromide is due to an unavoidable small amount of over-bromination during the synthesis of the ligand precursor bis(2-bromo-4-methylphenyl)amine. In the final cycle of refinement, 5441 reflections (of which 4758 are observed with $I > 2\sigma(I)$) were used to refine 403 parameters and the resulting R_1, wR_2 and S (goodness of fit) were 2.51%, 4.76% and 1.050, respectively. The refinement was carried out by minimizing the wR_2 function using F^2 rather than F values. R_1 is calculated to provide a reference to the conventional R value but its function is not minimized. SHELXTL6 (2000). Bruker-AXS, Madison, Wisconsin, USA.

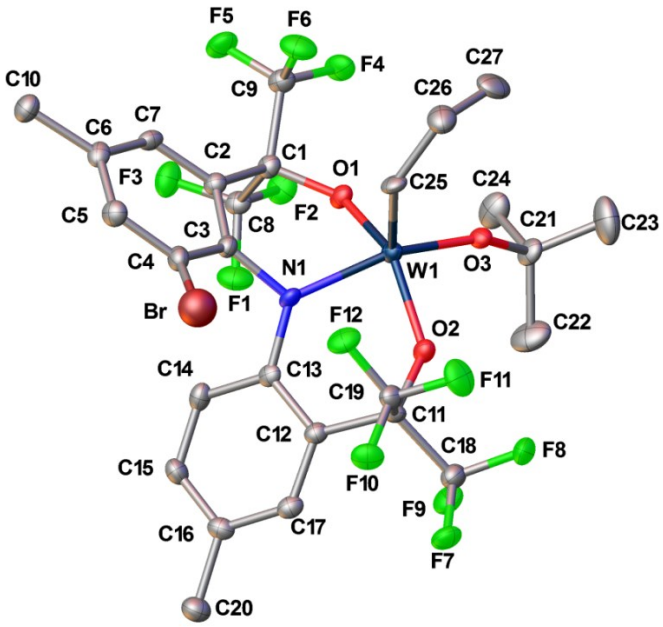

Figure S78. Molecular Structure of **2**.

Table S2. Crystal data and structure refinement for **2**.

Identification code	orei24	
Empirical formula	$C_{27}H_{26.94}Br_{0.03}F_{12}NO_3W$	
Formula weight	827.68	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.5483(3) Å	α= 86.891(2)°.
	b = 9.4574(3) Å	β= 82.183(2)°.
	c = 19.5076(6) Å	γ = 70.699(2)°.
Volume	1474.54(8) $Å^3$	
Z	2	
Density (calculated)	1.864 Mg/m^3	
Absorption coefficient	4.064 mm^{-1}	
F(000)	806	
Crystal size	0.14 x 0.12 x 0.08 mm^3	
Theta range for data collection	1.05 to 25.48°.	
Index ranges	-10≤h≤10, -11≤k≤11, -23≤l≤23	
Reflections collected	28207	
Independent reflections	5441 [R(int) = 0.0620]	
Completeness to theta = 25.48°	99.1 %	
Absorption correction	Numerical	
Max. and min. transmission	0.6607 and 0.5304	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5441 / 0 / 403	
Goodness-of-fit on F^2	1.050	
Final R indices [I>2sigma(I)]	R1 = 0.0251, wR2 = 0.0476 [4758]	
R indices (all data)	R1 = 0.0337, wR2 = 0.0503	

Largest diff. peak and hole	1.198 and -0.981 e.Å^{-3}

$R1 = \Sigma(||F_O| - |F_C||) / \Sigma|F_O|$ $\quad wR2 = [\Sigma[w(F_O^2 - F_C^2)^2] / \Sigma[w(F_O^2)^2]]^{1/2}$

$S = [\Sigma[w(F_O^2 - F_C^2)^2] / (n-p)]^{1/2}$ $\quad w= 1/[\sigma^2(F_O^2)+(m*p)^2+n*p]$, $p = [\max(F_O^2,0)+ 2* F_C^2]/3$, m & n are constants.

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	X	Y	Z	U(eq)
W1	3609(1)	1736(1)	2549(1)	16(1)
F1	5880(2)	4612(2)	2861(1)	30(1)
F2	7688(2)	2958(2)	3406(1)	27(1)
F3	6058(2)	4965(2)	3925(1)	30(1)
F4	6595(2)	982(2)	4222(1)	29(1)
F5	5490(2)	2925(2)	4863(1)	31(1)
F6	3976(2)	1660(2)	4595(1)	31(1)
F7	1602(3)	3244(2)	8(1)	28(1)
F8	2913(3)	1095(2)	423(1)	31(1)
F9	4092(2)	2785(2)	270(1)	29(1)
F10	-894(2)	4073(2)	1021(1)	27(1)
F11	17(3)	1759(2)	1329(1)	35(1)
F12	-415(2)	3500(2)	2066(1)	28(1)
O1	5040(3)	2101(3)	3171(1)	19(1)
O2	3011(3)	2015(3)	1620(1)	20(1)
O3	5245(3)	-24(3)	2314(1)	18(1)
N1	2585(3)	3959(3)	2559(2)	17(1)
Br	-970(20)	5834(19)	2883(9)	50(4)
C1	4814(4)	3133(4)	3689(2)	18(1)
C2	3058(4)	4308(4)	3776(2)	17(1)
C3	2080(4)	4656(4)	3227(2)	17(1)
C4	460(4)	5697(4)	3337(2)	20(1)
C5	-103(4)	6470(4)	3956(2)	22(1)
C6	889(4)	6213(4)	4487(2)	19(1)
C7	2446(4)	5116(4)	4387(2)	18(1)
C8	6117(4)	3925(4)	3474(2)	20(1)
C9	5219(4)	2179(4)	4348(2)	22(1)
C10	309(4)	7124(4)	5144(2)	24(1)
C11	1969(4)	3106(4)	1228(2)	17(1)
C12	2072(4)	4648(4)	1346(2)	17(1)
C13	2442(4)	4975(4)	1990(2)	16(1)
C14	2661(4)	6366(4)	2059(2)	21(1)
C15	2447(4)	7408(4)	1526(2)	21(1)
C16	2010(4)	7124(4)	898(2)	20(1)
C17	1849(4)	5732(4)	826(2)	19(1)
C18	2638(4)	2562(4)	475(2)	23(1)
C19	150(4)	3108(4)	1412(2)	21(1)
C20	1761(5)	8246(4)	318(2)	27(1)
C21	6921(4)	-850(4)	1986(2)	23(1)
C22	7123(5)	-172(5)	1275(2)	42(1)
C23	7040(5)	-2471(5)	1966(3)	48(1)
C24	8137(4)	-623(5)	2438(2)	35(1)
C25	1954(4)	1209(4)	3141(2)	20(1)
C26	1779(5)	-170(4)	3514(2)	30(1)
C27	3404(5)	-1428(4)	3571(2)	34(1)

Table S4. Bond lengths [Å] for **2**.

Bond	Length	Bond	Length
W1-O3	1.819(2)	C1-C2	1.539(4)
W1-C25	1.882(4)	C1-C9	1.541(5)
W1-O2	1.931(2)	C2-C7	1.395(5)
W1-O1	1.953(2)	C2-C3	1.404(5)
W1-N1	1.993(3)	C3-C4	1.405(4)
F1-C8	1.337(4)	C4-C5	1.388(5)
F2-C8	1.345(4)	C5-C6	1.389(5)
F3-C8	1.339(4)	C6-C7	1.387(5)
F4-C9	1.340(4)	C6-C10	1.514(5)
F5-C9	1.345(4)	C11-C12	1.522(5)
F6-C9	1.335(4)	C11-C19	1.547(5)
F7-C18	1.344(4)	C11-C18	1.552(5)
F8-C18	1.336(4)	C12-C17	1.387(5)
F9-C18	1.333(4)	C12-C13	1.411(5)
F10-C19	1.335(4)	C13-C14	1.404(5)
F11-C19	1.338(4)	C14-C15	1.381(5)
F12-C19	1.328(4)	C15-C16	1.392(5)
O1-C1	1.392(4)	C16-C17	1.384(5)
O2-C11	1.391(4)	C16-C20	1.496(5)
O3-C21	1.462(4)	C21-C23	1.505(6)
N1-C13	1.418(5)	C21-C22	1.509(6)
N1-C3	1.440(4)	C21-C24	1.523(5)
Br-C4	1.571(16)	C25-C26	1.499(5)
C1-C8	1.539(5)	C26-C27	1.515(5)

Symmetry transformations used to generate equivalent atoms:

Table S5. Bond angles [°] for **2**.

Bond	Angle	Bond	Angle
O2-C11-C12	111.2(3)	F9-C18-F7	107.1(3)
O2-C11-C19	109.6(3)	F8-C18-F7	106.3(3)
C12-C11-C19	110.3(3)	F9-C18-C11	110.8(3)
O2-C11-C18	103.1(3)	F8-C18-C11	111.3(3)
C12-C11-C18	112.4(3)	F7-C18-C11	114.1(3)
C19-C11-C18	110.1(3)	F12-C19-F10	106.9(3)
C17-C12-C13	119.1(3)	F12-C19-F11	107.5(3)
C17-C12-C11	121.4(3)	F10-C19-F11	107.0(3)
C13-C12-C11	119.5(3)	F12-C19-C11	110.9(3)
C14-C13-C12	117.7(3)	F10-C19-C11	112.2(3)
C14-C13-N1	120.0(3)	F11-C19-C11	112.0(3)
C12-C13-N1	122.3(3)	O3-C21-C23	107.3(3)
C15-C14-C13	121.3(3)	O3-C21-C22	107.0(3)
C14-C15-C16	121.5(3)	C23-C21-C22	112.9(3)
C17-C16-C15	116.8(3)	O3-C21-C24	106.4(3)
C17-C16-C20	121.1(3)	C23-C21-C24	111.6(3)
C15-C16-C20	122.1(3)	C22-C21-C24	111.3(4)
C16-C17-C12	123.5(3)	C26-C25-W1	137.2(3)
F9-C18-F8	106.8(3)	C25-C26-C27	115.1(3)

Symmetry transformations used to generate equivalent atoms:

Table S6. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
W1	15(1)	16(1)	15(1)	-1(1)	0(1)	-2(1)
F1	25(1)	39(1)	27(1)	10(1)	-1(1)	-13(1)
F2	13(1)	34(1)	32(1)	-5(1)	1(1)	-4(1)
F3	25(1)	32(1)	36(2)	-12(1)	0(1)	-13(1)
F4	24(1)	28(1)	26(1)	3(1)	-6(1)	4(1)
F5	32(1)	38(1)	20(1)	-2(1)	-11(1)	-4(1)
F6	25(1)	37(1)	31(1)	14(1)	0(1)	-12(1)
F7	34(1)	34(1)	16(1)	0(1)	-8(1)	-9(1)
F8	48(1)	22(1)	22(1)	-6(1)	-4(1)	-10(1)
F9	27(1)	36(1)	21(1)	-6(1)	6(1)	-9(1)
F10	20(1)	34(1)	26(1)	5(1)	-9(1)	-8(1)
F11	33(1)	28(1)	52(2)	0(1)	-6(1)	-19(1)
F12	20(1)	41(1)	19(1)	-1(1)	4(1)	-10(1)
O1	17(1)	20(1)	16(1)	-4(1)	-1(1)	0(1)
O2	20(1)	18(1)	18(1)	-3(1)	-3(1)	-2(1)
O3	18(1)	18(1)	14(1)	0(1)	2(1)	-3(1)
N1	18(1)	19(2)	11(2)	-3(1)	-4(1)	-2(1)
C1	15(2)	20(2)	18(2)	-2(2)	0(2)	-4(2)
C2	13(2)	19(2)	16(2)	-1(2)	0(2)	-4(1)
C3	18(2)	16(2)	16(2)	-2(2)	0(2)	-5(1)
C4	21(2)	17(2)	20(2)	-3(2)	3(2)	-4(2)
C5	16(2)	23(2)	23(2)	-2(2)	0(2)	-2(2)
C6	17(2)	20(2)	20(2)	-4(2)	5(2)	-8(2)
C7	19(2)	23(2)	14(2)	1(2)	-4(2)	-10(2)
C8	16(2)	24(2)	19(2)	0(2)	2(2)	-5(2)
C9	18(2)	26(2)	20(2)	0(2)	-2(2)	-4(2)
C10	22(2)	27(2)	22(2)	-6(2)	0(2)	-6(2)
C11	18(2)	17(2)	13(2)	3(2)	-2(2)	-4(2)
C12	14(2)	20(2)	15(2)	0(2)	0(2)	-6(1)
C13	9(2)	18(2)	16(2)	-2(2)	1(1)	0(1)
C14	17(2)	21(2)	23(2)	-7(2)	-3(2)	-4(2)
C15	20(2)	16(2)	26(2)	1(2)	-3(2)	-5(2)
C16	15(2)	22(2)	21(2)	4(2)	-2(2)	-5(2)
C17	14(2)	25(2)	16(2)	0(2)	-1(2)	-6(2)
C18	26(2)	24(2)	19(2)	-1(2)	-2(2)	-9(2)
C19	24(2)	20(2)	20(2)	0(2)	-4(2)	-10(2)
C20	30(2)	25(2)	26(2)	5(2)	-4(2)	-10(2)
C21	16(2)	26(2)	20(2)	-6(2)	4(2)	2(2)
C22	30(2)	60(3)	26(3)	-2(2)	9(2)	-5(2)
C23	31(2)	28(3)	77(4)	-17(2)	4(2)	-2(2)
C24	20(2)	39(3)	38(3)	-11(2)	-3(2)	3(2)
C25	21(2)	25(2)	10(2)	0(2)	3(2)	-6(2)
C26	31(2)	30(2)	27(3)	-1(2)	7(2)	-12(2)
C27	46(2)	30(2)	31(3)	12(2)	-5(2)	-23(2)

X-Ray experimental for 6: X-Ray Intensity data were collected at 100 K on a Bruker **DUO** diffractometer using MoKα radiation (λ = 0.71073 Å) and an APEXII CCD area detector. Raw data frames were read by program SAINT[1] and integrated using 3D profiling algorithms. The resulting data were reduced to produce hkl reflections and their intensities and estimated standard deviations. The data were corrected for Lorentz and polarization effects and numerical absorption corrections were applied based on indexed and measured faces. The structure was solved and refined in SHELXTL6.1, using full-matrix least-squares refinement. The non-H atoms were refined with anisotropic thermal parameters and all of the H atoms were calculated in idealized positions and refined riding on their parent atoms. In the final cycle of refinement, 5714 reflections (of which 4559 are observed with I > 2σ (I)) were used to refine 363 parameters and the resulting R_1, wR_2 and S (goodness of fit) were 1.87%, 3.38% and 0.901, respectively. The highest residual electron density peak is within 1 Å of W1 and thus attributed to its anisotropy. The refinement was carried out by minimizing the wR_2 function using F^2 rather than F values. R_1 is calculated to provide a reference to the conventional R value but its function is not minimized. *SHELXTL6* (2008). Bruker-AXS, Madison, Wisconsin, USA.

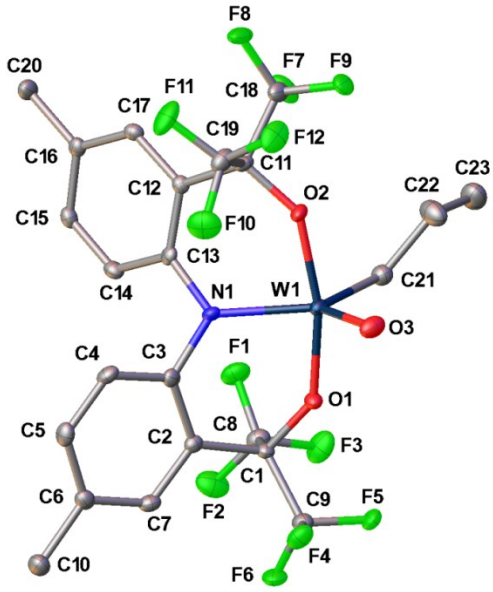

Figure S79. Molecular Structure of **6**.

Table S7. Crystal data and structure refinement for **6**.

Identification code	orei30	
Empirical formula	$C_{23}H_{19}F_{12}NO_3W$	
Formula weight	769.24	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 12.0588(6) Å	α= 90°.
	b = 16.9746(9) Å	β= 112.895(1)°.
	c = 13.2038(7) Å	γ = 90°.

Volume	2489.8(2) $Å^3$
Z	4
Density (calculated)	2.052 Mg/m^3
Absorption coefficient	4.757 mm^{-1}
F(000)	1480
Crystal size	0.09 x 0.04 x 0.02 mm^3
Theta range for data collection	1.83 to 27.50°.
Index ranges	$-14 \le h \le 15$, $-22 \le k \le 22$, $-17 \le l \le 17$
Reflections collected	45799
Independent reflections	5714 [R(int) = 0.0472]
Completeness to theta = 25.48°	100.0 %
Absorption correction	Numerical
Max. and min. transmission	0.9193 and 0.6660
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5714 / 0 / 363
Goodness-of-fit on F^2	0.901
Final R indices [I>2sigma(I)]	R1 = 0.0187, wR2 = 0.0338 [4559]
R indices (all data)	R1 = 0.0300, wR2 = 0.0352
Largest diff. peak and hole	1.581 and -0.643 $e.Å^{-3}$

$R1 = \sum(||F_O| - |F_C||) / \sum|F_O|$ $\quad wR2 = [\sum[w(F_O^2 - F_C^2)^2] / \sum[w(F_O^2)^2]]^{1/2}$

$S = [\sum[w(F_O^2 - F_C^2)^2] / (n-p)]^{1/2}$ $\quad w = 1/[\sigma^2(F_O^2)+(m*p)^2+n*p]$, $p = [\max(F_O^2,0)+ 2* F_C^2]/3$, m & n are constants.

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **6**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	X	Y	Z	U(eq)
W1	480(1)	3415(1)	5351(1)	13(1)
F1	-589(1)	2776(1)	7359(1)	24(1)
F2	-2463(1)	2603(1)	7013(1)	30(1)
F3	-1757(2)	3775(1)	7087(1)	30(1)
F4	-3435(1)	3292(1)	3771(1)	23(1)
F5	-3028(1)	4199(1)	4992(1)	20(1)
F6	-4058(1)	3193(1)	5091(1)	24(1)
F7	4190(1)	3026(1)	7507(1)	29(1)
F8	4996(1)	2374(1)	6565(1)	29(1)
F9	4234(1)	3521(1)	6027(1)	25(1)
F10	1699(2)	1921(1)	4099(1)	32(1)
F11	3487(2)	1470(1)	4926(1)	31(1)
F12	3223(2)	2618(1)	4189(1)	30(1)
O1	-1079(1)	3459(1)	5339(1)	15(1)
O2	2042(2)	3116(1)	5534(2)	16(1)
O3	132(2)	3908(1)	4142(2)	21(1)
N1	303(2)	2258(1)	5623(2)	14(1)
C1	-1942(2)	2999(2)	5524(2)	13(1)
C2	-1897(2)	2152(2)	5159(2)	13(1)
C3	-816(2)	1836(2)	5179(2)	13(1)
C4	-839(2)	1080(2)	4763(2)	16(1)
C5	-1874(2)	633(2)	4403(2)	17(1)
C6	-2942(2)	923(2)	4425(2)	16(1)
C7	-2935(2)	1690(2)	4796(2)	16(1)
C8	-1692(2)	3038(2)	6761(2)	19(1)
C9	-3139(2)	3419(2)	4833(2)	18(1)
C10	-4086(2)	445(2)	4046(2)	22(1)
C11	2834(2)	2479(2)	5827(2)	14(1)

C12	2473(2)	1868(1)	6485(2)	11(1)
C13	1275(2)	1804(1)	6384(2)	12(1)
C14	1031(2)	1279(2)	7091(2)	15(1)
C15	1904(2)	801(2)	7803(2)	14(1)
C16	3081(2)	821(2)	7858(2)	13(1)
C17	3344(2)	1364(1)	7202(2)	13(1)
C18	4085(2)	2853(2)	6494(2)	20(1)
C19	2818(3)	2122(2)	4746(2)	21(1)
C20	4035(2)	288(2)	8616(2)	20(1)
C21	1128(2)	4226(2)	6656(2)	19(1)
C22	2203(3)	4744(2)	6772(3)	30(1)
C23	2564(3)	5280(2)	7769(2)	32(1)

Table S9. Bond lengths [Å] for **6**.

Bond	Length	Bond	Length
W1-O3	1.7040(18)	C1-C8	1.543(3)
W1-O2	1.8737(16)	C1-C9	1.549(3)
W1-O1	1.8753(16)	C2-C7	1.395(3)
W1-N1	2.022(2)	C2-C3	1.400(3)
W1-C21	2.105(3)	C3-C4	1.393(4)
F1-C8	1.332(3)	C4-C5	1.378(4)
F2-C8	1.327(3)	C5-C6	1.390(4)
F3-C8	1.334(3)	C6-C7	1.390(4)
F4-C9	1.323(3)	C6-C10	1.508(3)
F5-C9	1.340(3)	C11-C12	1.521(3)
F6-C9	1.336(3)	C11-C19	1.543(4)
F7-C18	1.326(3)	C11-C18	1.556(4)
F8-C18	1.340(3)	C12-C17	1.399(3)
F9-C18	1.336(3)	C12-C13	1.402(3)
F10-C19	1.330(3)	C13-C14	1.402(3)
F11-C19	1.335(3)	C14-C15	1.371(3)
F12-C19	1.330(3)	C15-C16	1.394(3)
O1-C1	1.397(3)	C16-C17	1.383(3)
O2-C11	1.394(3)	C16-C20	1.499(3)
N1-C3	1.435(3)	C21-C22	1.523(4)
N1-C13	1.437(3)	C22-C23	1.518(4)
C1-C2	1.524(3)		

Symmetry transformations used to generate equivalent atoms:

Table S10. Bond angles [°] for **6**.

Bond	Angle	Bond	Angle
O3-W1-O2	97.06(8)	C1-O1-W1	142.07(16)
O3-W1-O1	95.23(8)	C11-O2-W1	142.37(16)
O2-W1-O1	165.07(8)	C3-N1-C13	113.55(19)
O3-W1-N1	129.69(9)	C3-N1-W1	124.01(15)
O2-W1-N1	83.37(8)	C13-N1-W1	122.11(15)
O1-W1-N1	82.27(8)	O1-C1-C2	110.6(2)
O3-W1-C21	108.82(10)	O1-C1-C8	108.0(2)
O2-W1-C21	92.15(9)	C2-C1-C8	111.1(2)
O1-W1-C21	91.87(9)	O1-C1-C9	103.1(2)
N1-W1-C21	121.46(9)	C2-C1-C9	112.8(2)

C8-C1-C9	110.9(2)	C12-C11-C18	112.6(2)
C7-C2-C3	119.8(2)	C19-C11-C18	110.2(2)
C7-C2-C1	120.1(2)	C17-C12-C13	119.4(2)
C3-C2-C1	120.2(2)	C17-C12-C11	119.8(2)
C4-C3-C2	118.0(2)	C13-C12-C11	120.8(2)
C4-C3-N1	119.5(2)	C14-C13-C12	117.5(2)
C2-C3-N1	122.5(2)	C14-C13-N1	118.8(2)
C5-C4-C3	121.3(2)	C12-C13-N1	123.7(2)
C4-C5-C6	121.3(2)	C15-C14-C13	121.9(2)
C7-C6-C5	117.5(2)	C14-C15-C16	121.1(2)
C7-C6-C10	120.0(2)	C17-C16-C15	117.4(2)
C5-C6-C10	122.5(2)	C17-C16-C20	121.1(2)
C6-C7-C2	121.9(2)	C15-C16-C20	121.4(2)
F2-C8-F1	107.5(2)	C16-C17-C12	122.5(2)
F2-C8-F3	107.9(2)	F7-C18-F9	107.5(2)
F1-C8-F3	107.0(2)	F7-C18-F8	108.1(2)
F2-C8-C1	111.9(2)	F9-C18-F8	107.0(2)
F1-C8-C1	110.5(2)	F7-C18-C11	110.7(2)
F3-C8-C1	111.7(2)	F9-C18-C11	111.1(2)
F4-C9-F6	108.4(2)	F8-C18-C11	112.3(2)
F4-C9-F5	107.2(2)	F10-C19-F12	107.8(2)
F6-C9-F5	106.6(2)	F10-C19-F11	107.1(2)
F4-C9-C1	110.8(2)	F12-C19-F11	107.2(2)
F6-C9-C1	113.1(2)	F10-C19-C11	109.9(2)
F5-C9-C1	110.5(2)	F12-C19-C11	112.8(2)
O2-C11-C12	111.7(2)	F11-C19-C11	111.8(2)
O2-C11-C19	106.7(2)	C22-C21-W1	119.37(19)
C12-C11-C19	110.9(2)	C23-C22-C21	112.2(2)
O2-C11-C18	104.4(2)		

Symmetry transformations used to generate equivalent atoms:

Table S11. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **6**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
W1	11(1)	13(1)	16(1)	3(1)	6(1)	2(1)
F1	20(1)	32(1)	16(1)	0(1)	2(1)	6(1)
F2	28(1)	45(1)	23(1)	3(1)	15(1)	-5(1)
F3	42(1)	26(1)	22(1)	-7(1)	10(1)	9(1)
F4	23(1)	26(1)	17(1)	1(1)	3(1)	7(1)
F5	18(1)	14(1)	29(1)	1(1)	9(1)	5(1)
F6	12(1)	25(1)	37(1)	4(1)	12(1)	2(1)
F7	30(1)	33(1)	22(1)	-4(1)	7(1)	-15(1)
F8	12(1)	30(1)	45(1)	17(1)	11(1)	4(1)
F9	18(1)	20(1)	38(1)	10(1)	13(1)	-3(1)
F10	30(1)	44(1)	18(1)	-8(1)	5(1)	-2(1)
F11	48(1)	24(1)	29(1)	6(1)	24(1)	19(1)
F12	42(1)	33(1)	27(1)	12(1)	25(1)	9(1)
O1	12(1)	13(1)	24(1)	-1(1)	9(1)	0(1)
O2	13(1)	12(1)	26(1)	4(1)	10(1)	4(1)
O3	20(1)	26(1)	20(1)	8(1)	11(1)	6(1)
N1	8(1)	14(1)	17(1)	1(1)	3(1)	2(1)
C1	10(1)	13(1)	16(1)	0(1)	6(1)	0(1)

C2	13(1)	14(1)	12(1)	2(1)	6(1)	2(1)
C3	14(1)	13(1)	12(1)	4(1)	4(1)	1(1)
C4	14(1)	18(2)	16(1)	0(1)	5(1)	6(1)
C5	23(1)	13(1)	15(1)	-3(1)	6(1)	0(1)
C6	15(1)	17(2)	14(1)	2(1)	3(1)	-1(1)
C7	12(1)	20(2)	17(1)	1(1)	5(1)	2(1)
C8	17(1)	22(2)	18(1)	-1(1)	7(1)	2(1)
C9	14(1)	18(1)	22(1)	-1(1)	8(1)	1(1)
C10	18(1)	18(2)	27(2)	-1(1)	4(1)	-2(1)
C11	10(1)	15(1)	15(1)	3(1)	5(1)	3(1)
C12	13(1)	12(1)	10(1)	-1(1)	6(1)	-1(1)
C13	14(1)	9(1)	12(1)	-3(1)	4(1)	2(1)
C14	13(1)	16(1)	18(1)	-3(1)	8(1)	-2(1)
C15	18(1)	12(1)	14(1)	-1(1)	6(1)	-3(1)
C16	15(1)	11(1)	12(1)	-2(1)	3(1)	-1(1)
C17	11(1)	15(2)	13(1)	-2(1)	4(1)	-1(1)
C18	17(1)	19(2)	24(2)	9(1)	9(1)	1(1)
C19	24(2)	21(2)	20(2)	6(1)	12(1)	7(1)
C20	16(1)	18(2)	21(1)	7(1)	3(1)	0(1)
C21	17(1)	18(2)	21(1)	0(1)	6(1)	1(1)
C22	27(2)	27(2)	39(2)	-12(2)	16(1)	-6(1)
C23	27(2)	26(2)	35(2)	-3(1)	3(1)	-4(1)

Density Functional Theory Geometry Optimization

Spin-restricted density functional theory calculations of complex **2'**, **2-Me'**, **3**, and **7'** were executed in the *Gaussian 03* program suite. Calculations employed geometry optimization and single point analysis using hybrid functional (the three-parameter exchange functional of Becke (B3) and the correlation functional of Lee, Yang, and Parr (LYP) (B3LYP). Full geometry optimization and single point analysis for the complexes were performed using the LANL2DZ basis set. The atomic coordinates were generated from Gabedit 2.3.0. Molecular orbital pictures were generated from Gabedit with isovalues of 0.051687au.

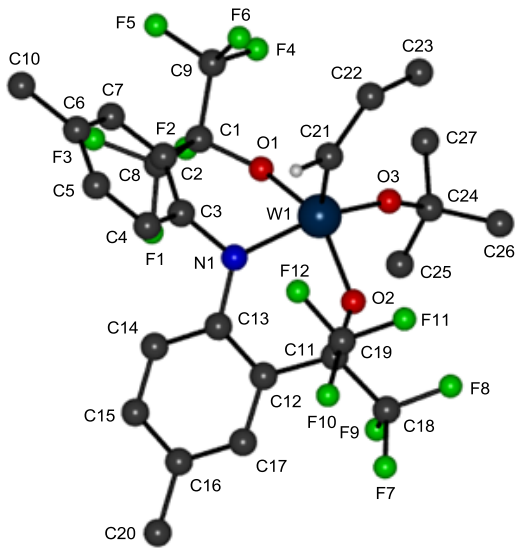

Figure S80. Labeling Scheme of the geometry optimization structure for **2'**.

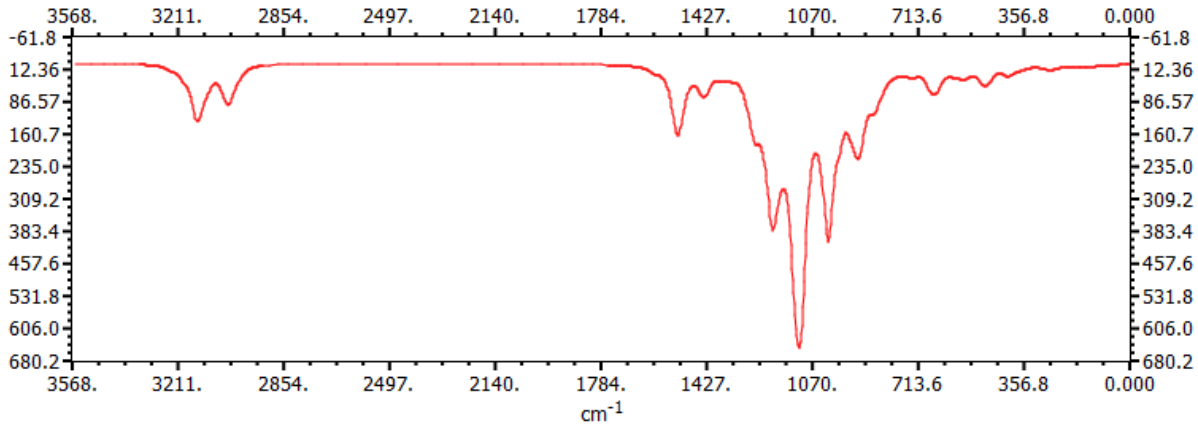

Figure S81. Guassian optimized IR spectrum for **2'**.

Table S12. Atomic coordinates of the geometry optimization calculation for **2'**.

Atom	x	y	z
W1	-0.0409	-1.0611	0.2816
O3	-0.0307	-2.8045	-0.2955
O2	-1.9879	-0.9337	0.1985
O1	1.6624	-0.7544	-0.6847
N1	-0.2099	0.9342	0.0761
F9	-4.118	-0.8952	-1.6468
F8	-4.4186	-2.0004	0.2741
F7	-5.4852	-0.067	-0.0667

F6	3.7799	-0.7689	1.3622
F5	5.1488	0.1355	-0.1766
F4	4.0975	-1.7899	-0.6015
F3	3.9524	1.6741	-2.1331
F2	3.3662	-0.3547	-2.8888
F12	-2.1509	0.9511	2.4232
F11	-3.5306	-0.8041	2.6137
F10	-4.3423	1.2102	2.0389
F1	1.807	1.2346	-2.6162
C9	3.9294	-0.5425	-0.0107
C8	2.9638	0.686	-2.0551
C7	3.2803	2.2873	0.7953
C6	2.9816	3.4071	1.5874
C5	1.6209	3.6704	1.8642
C4	0.6155	2.8509	1.3477
C3	0.9137	1.7334	0.5274
C27	1.2944	-4.5194	-1.369
C26	-1.1393	-4.9189	-0.6738
C25	-0.6006	-3.3298	-2.5999
C24	-0.1215	-3.9238	-1.2593
C23	1.3996	-3.5024	2.5443
C22	1.0725	-2.0968	3.0829
C21	0.4793	-1.095	2.1067
C20	-4.423	4.1175	-2.3745
C2	2.2782	1.4362	0.2743
C19	-3.2703	0.3318	1.8515
C18	-4.2645	-0.729	-0.2681
C17	-3.6455	2.1055	-1.0224
C16	-3.3323	3.2537	-1.7715
C15	-1.9676	3.5711	-1.9395
C14	-0.9691	2.7954	-1.3435
C13	-1.2804	1.6628	-0.5517
C12	-2.6516	1.3015	-0.4287
C11	-3.0139	0.0162	0.3299
C10	4.0785	4.2936	2.1447
C1	2.6736	0.2206	-0.5831

Table S13. Calculated geometry optimization bond lengths [Å] for **2'**.

Bond	Length	Bond	Length
W1-O3	1.8364	O3-C24	1.4799
W1-O2	1.9529	O2-C11	1.4044
W1-O1	1.9822	O1-C1	1.4083
W1-N1	2.013	N1-C3	1.4508
W1-C21	1.8981	N1-C12	1.4391

F9-C18	1.3964	C2-C3	1.4192
F8-C18	1.3907	C24-C27	1.54
F7-C18	1.4032	C24-C26	1.5391
F6-C9	1.3994	C24-C25	1.5427
F5-C9	1.4051	C22-C23	1.5403
F4-C9	1.3905	C21-C22	1.5194
F3-C8	1.4	C1-C2	1.5393
F2-C8	1.3928	C19-F10	1.3985
F12-C19	1.4012	C16-C20	1.5164
F11-C19	1.3925	C16-C17	1.4062
C9-C1	1.577	C15-C16	1.4111
C8-F1	1.3979	C14-C15	1.3978
C8-C1	1.5709	C13-C14	1.4166
C6-C7	1.4037	C12-C17	1.4095
C6-C5	1.4133	C12-C13	1.4233
C6-C10	1.5165	C11-C19	1.5749
C4-C5	1.3962	C11-C18	1.5738
C3-C4	1.4179	C11-C12	1.5359
C2-C7	1.4142		

Table S14. Calculated geometry optimization bond angles [°] for **2'**.

Bonds	Angle	Bonds	Angle
O1-W1-N1	82.47	F3-C8-F1	106.56
O1-W1-O3	89.37	F3-C8-C1	113.06
O1-W1-C21	103.65	F2-C8-F1	106.98
O1-W1-O2	145.68	F2-C8-C1	113.13
N1-W1-O3	155.42	F1-C8-C1	109.85
N1-W1-C21	97.98	C2-C7-C6	122.49
N1-W1-O2	81.22	C7-C6-C5	117.64
O3-W1-C21	106.48	C7-C6-C10	121.32
O3-W1-O2	93.1	C5-C6-C10	121.03
C21-W1-O2	108.38	C6-C5-C4	120.77
W1-O3-C24	157.27	C3-C4-C5	121.68
W1-O2-C11	140.22	C2-C3-C4	118.06
C1-O1-W1	133.54	C2-C3-N1	125.01
C3-N1-W1	116.7	C4-C3-N1	116.82
C3-N1-C13	115.66	C27-C24-O3	106.41
W1-N1-C13	127.5	C27-C24-C26	112.64
F5-C9-F4	106.13	C27-C24-C25	111.87
F5-C9-C1	114.5	O3-C24-C26	106.37
F5-C9-F6	106.66	O3-C24-C25	107.09
F4-C9-C1	112.09	C26-C24-C25	111.97
F4-C9-F6	106.53	C21-C22-C23	117.38
C1-C9-F6	110.44	W1-C21-C22	137.44
F3-C8-F2	106.86	C1-C2-C7	119.9

C1-C2-C3	120.78	C14-C13-N1	119.02
C7-C2-C3	119.31	C14-C13-C12	117.58
C11-C19-F12	110.65	N1-C13-C12	123.4
C11-C19-F10	112.34	C13-C12-C17	119.88
C11-C19-F11	113.31	V13-C12-C11	118.84
F12-C19-F10	106.27	C17-C12-C11	121.27
F12-C19-F11	106.65	C12-C11-O2	110.33
F10-C19-F11	107.2	C12-C11-C18	113.33
F9-C18-C11	110.38	C12-C11-C19	110.36
F9-C18-F8	106.72	O2-C11-C18	102.98
F9-C18-F7	106.81	O2-C11-C19	110.18
C11-C18-F8	111.89	C18-C11-C19	109.43
C11-C18-F7	114.41	C8-C1-C9	109.66
F8-C18-F7	106.2	C8-C1-C2	109.6
C16-C17-C12	122.21	C8-C1-O1	105.67
C15-C16-C17	117.55	C9-C1-C2	112.61
C15-C16-C20	121.34	C9-C1-O1	105.25
C17-C16-C20	121.12	C2-C1-O1	113.74
C24-C15-C16	121.01	O1-W1-N1	82.47
C15-C14-C13	121.67	O1-W1-O3	89.37

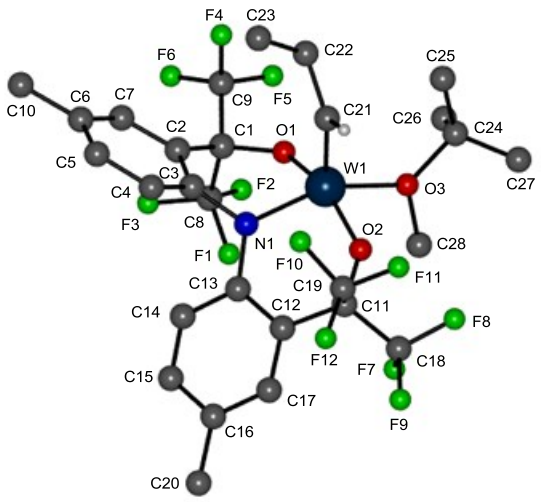

Figure S82. Labelling Scheme of the geometry optimization calculation for **2-Me'**.

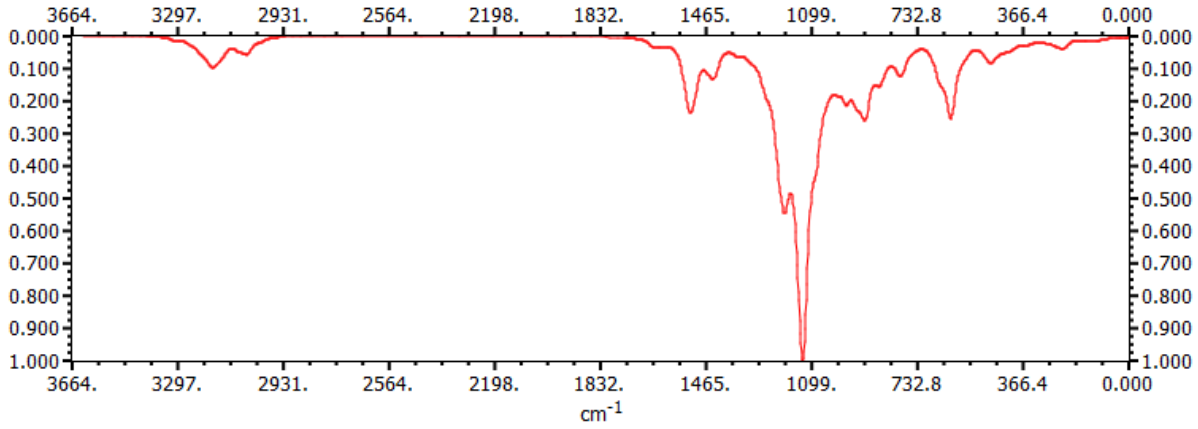

Figure S83. Guassian optimizated IR spectrum calculation for **2-Me'**.

Table S15. Atomic coordinates of the geometry optimization calculation for **2-Me'**.

Atom	x	y	z
W1	0.2132	0.94	0.191
O3	0.4645	2.8454	-0.7416
O2	2.0871	0.812	0.2758
O1	-1.4882	0.8203	-0.6099
N1	0.2258	-1.0408	0.1267
F9	5.5042	-0.0203	-0.5445
F8	4.4196	1.9084	-0.1519
F7	3.905	0.6952	-1.9653
F6	-4.8618	-0.1926	-1.3608
F5	-3.7903	1.7678	-1.313
F4	-4.1503	0.678	0.5982
F3	-2.9253	-1.7887	-2.7146
F2	-2.6108	0.3708	-3.2767
F12	4.601	-1.4049	1.6655
F11	4.0614	0.6939	2.2912
F10	2.5127	-0.9253	2.3824
F1	-0.8665	-0.8725	-2.6328
C9	-3.8191	0.5045	-0.7501
C8	-2.2244	-0.6304	-2.3968
C7	-3.3538	-2.2314	0.4212
C6	-3.2279	-3.3229	1.2963
C5	-1.9511	-3.604	1.8196
C4	-0.8344	-2.84	1.4423
C3	-0.957	-1.7622	0.5441
C28	1.2399	2.7338	-2.018
C27	1.1663	5.2423	-0.5001
C26	-1.1318	4.6159	-1.4807

C25	-0.6346	4.3089	0.9755
C24	-0.0559	4.3212	-0.4351
C23	-1.866	0.3669	3.7238
C22	-1.6371	1.4238	2.6793
C21	-0.3095	1.2522	1.9865
C20	4.3248	-4.4022	-2.3371
C2	-2.2495	-1.4299	0.0508
C19	3.6034	-0.4451	1.638
C18	4.263	0.605	-0.6183
C17	3.6208	-2.2774	-1.0806
C16	3.2808	-3.4847	-1.7271
C15	1.918	-3.8103	-1.7951
C14	0.9403	-2.9953	-1.2056
C13	1.2721	-1.8001	-0.5248
C12	2.6516	-1.4303	-0.5025
C11	3.1352	-0.1461	0.1743
C10	-4.4356	-4.1715	1.6573
C1	-2.4314	-0.222	-0.8944

Table S16. Calculated geometry optimization bond lengths [Å] for **2-Me'**.

Bond	Length	Bond	Length
W1-O3	2.1362	C9-C1	1.573
W1-O2	1.8801	C8-C1	1.5706
W1-O1	1.8843	C7-C6	1.4047
W1-N1	1.9819	C7-C2	1.4139
W1-C21	1.896	C6-C5	1.4082
O3-C28	1.4976	C6-C10	1.5195
O3-C24	1.5946	C5-C4	1.4046
O2-C11	1.4237	C3-C4	1.4084
O1-C1	1.4341	C2-C3	1.4228
N1-C3	1.4469	C24-C27	1.5318
N1-C13	1.4477	C24-C26	1.529
F9-C18	1.3918	C24-C25	1.5248
F8-C18	1.3932	C22-C23	1.5034
F7-C18	1.3967	C22-C21	1.5073
F6-C9	1.395	C1-C8	1.3994
F5-C9	1.3833	C1-C2	1.5446
F4-C9	1.3992	C16-C20	1.5179
F3-C8	1.3907	C16-C17	1.4112
F2-C8	1.3877	C15-C16	1.4028
F12-C19	1.3846	C14-C15	1.4027
F11-C19	1.3906	C14-C13	1.4149
F10-C19	1.4051	C13-C12	1.4284

C12-C17	1.4111	C11-C19	1.5656
C12-C11	1.53	C11-C18	1.5698

Table S17. Calculated geometry optimization bond angles [°] for **2-Me'**.

Bonds	Angle	Bonds	Angle
O1-W1-N1	85.9	C27-C24-O3	106.74
O1-W1-O3	88.7	C27-C24-C26	114.62
O1-W1-C21	99.44	C27-C24-C25	110.3
O1-W1-O2	156.17	O3-C24-C26	106.05
N1-W1-O3	151.23	O3-C24-C25	107.11
N1-W1-C21	101.36	C26-C24-C25	111.54
N1-W1-O2	85.82	C21-C22-C23	111.92
O3-W1-C21	107.4	W1-C21-C22	134.18
O3-W1-O2	87.89	C1-C2-C7	120.77
C21-W1-O2	104.08	C1-C2-C3	120.12
W1-O3-C24	134.68	C7-C2-C3	119.1
W1-O3-C28	111.5	C11-C19-F10	109.17
C24-O3-C28	113.69	C11-C19-F12	111.49
W1-O2-C11	140.93	C11-C19-F11	112.41
C1-O1-W1	136.41	F10-C19-C12	108.18
C3-N1-W1	118.93	F10-C19-F11	106.66
C3-N1-C13	117.33	F12-C19-F11	108.74
W1-N1-C13	122.92	F7-C18-C11	109.49
F6-C9-F5	107.08	F7-C18-F8	106.93
F6-C9-C1	112.86	F7-C18-F9	107.98
F6-C9-F4	107.87	C11-C18-F8	111.06
F5-C9-C1	111.48	C11-C18-F9	113.52
F5-C9-F4	106.48	F8-C18-F9	107.6
C1-C9-F4	110.76	C16-C17-V12	122.39
F3-C8-F2	108.4	C15-C16-V17	117.06
F3-C8-F1	107.84	C15-C16-C20	120.56
F3-C8-C1	111.64	C17-C16-C20	122.38
F2-C8-F1	106.74	C14-C15-C16	121.46
F2-C8-C1	112.47	C15-C14-C13	121.98
F1-C8-C1	109.52	C14-C13-N1	119.35
C2-C7-C6	122.25	C14-C13-C12	116.92
C7-C6-C5	117.9	N1-C13-C12	123.72
C7-C6-C10	120.71	C13-C12-C17	120.1
C5-C6-C10	121.39	C13-C12-C11	121.97
C6-C5-C4	120.83	C17-C12-C11	117.9
C3-C4-C5	121.22	C12-C11-O2	111.33
C2-C3-C4	118.61	C12-C11-C18	113.91
C2-C3-N1	121.75	C12-C11-C19	110.35
C4-C3-N1	119.62	O2-C11-C18	104.06

O2-C11-C19	106.39	C8-C1-O1	106.98
C18-C11-C19	110.4	C9-C1-C2	114.14
C8-C1-C9	108.91	C9-C1-O1	103.08
C8-C1-C2	111.5	C2-C1-O1	111.68

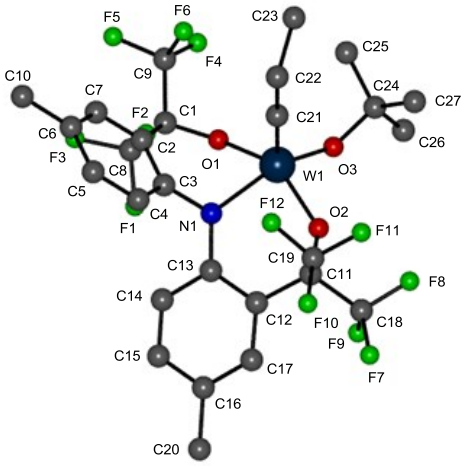

Figure S84. Labeling Scheme of the geometry optimization calculation for **3'**.

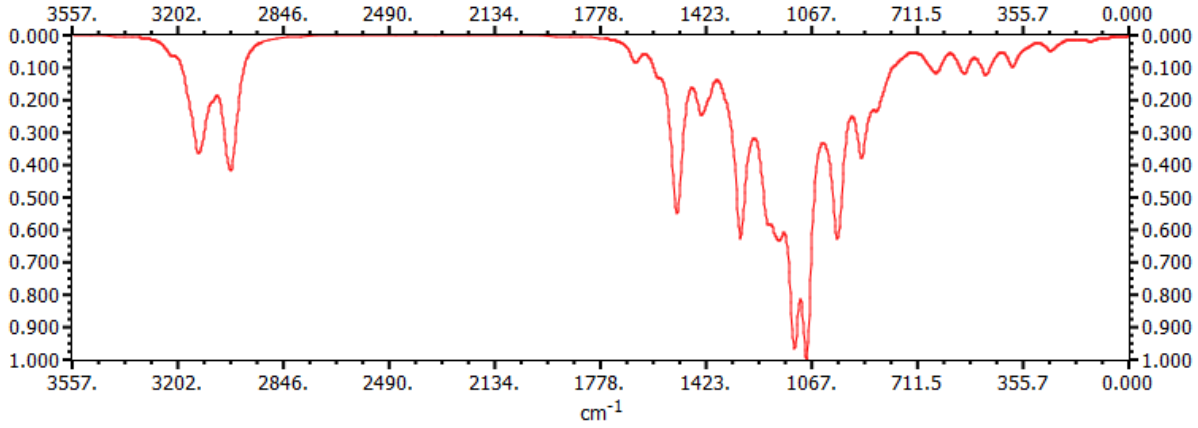

Figure S85. Guassian optimizated IR spectrum calculation for **3'**.

Table S18. Atomic coordinates of the geometry optimization calculation for **3'**.

Atom	x	y	z
W1	0.0531	1.1305	-0.2795
O3	0.0821	2.8351	-1.1551
O2	2.0414	1.0396	-0.2245

O1	-1.6124	0.5411	-1.2181
N1	0.2997	-0.9962	-0.2244
F9	4.3016	0.8284	-1.9721
F8	4.4452	2.1516	-0.1783
F7	5.5682	0.2261	-0.219
F6	-3.7794	0.7943	0.8809
F5	-5.0841	-0.3389	-0.552
F4	-4.069	1.5388	-1.2041
F3	-3.8482	-2.1839	-2.1446
F2	-3.4055	-0.286	-3.2481
F12	2.1401	-0.5929	2.1972
F11	3.5559	1.1408	2.2412
F10	4.3281	-0.9362	1.8895
F1	-1.7545	-1.7344	-2.7938
C9	-3.869	0.3845	-0.4527
C8	-2.9031	-1.1462	-2.2657
C7	-3.1266	-2.2282	0.8159
C6	-2.8042	-3.2469	1.7236
C5	-1.432	-3.5103	1.9461
C4	-0.4477	-2.781	1.2809
C3	-0.7605	-1.7432	0.3548
C27	0.5838	4.8224	0.1644
C26	0.2116	4.9109	-2.3521
C25	-1.7423	4.406	-0.7982
C24	-0.2222	4.2559	-1.0245
C23	-1.8541	2.6531	3.1181
C22	-0.8456	1.5094	2.8312
C21	-0.4785	1.3619	1.3917
C20	4.7628	-4.1589	-2.2048
C2	-2.1442	-1.4713	0.1335
C19	3.2684	-0.059	1.5782
C18	4.3349	0.8219	-0.5761
C17	3.8213	-2.0655	-1.0953
C16	3.6079	-3.3198	-1.6871
C15	2.2693	-3.7604	-1.8038
C14	1.2136	-2.983	-1.3309
C13	1.4144	-1.7159	-0.7017
C12	2.7674	-1.2547	-0.6165
C11	3.0538	0.1171	0.0219
C10	-3.883	-4.0309	2.45
C1	-2.5811	-0.4177	-0.9053

Table S19. Calculated geometry optimization bond lengths [Å] for {[F_6ONO]W(CCH_2CH_3)(O^tBu)} (**3'**).

Bond	Length	Bond	Length
W1-O3	1.9165	C6-C7	1.402
W1-O2	1.9911	C6-C5	1.4149
W1-O1	2.0005	C6-C10	1.5186
W1-N1	2.1417	C5-C4	1.394
W1-C21	1.7689	C4-C3	1.4257
O3-C24	1.4589	C2-C3	1.4274
O2-C11	1.3917	C2-C1	1.5427
O1-C1	1.3984	C24-C27	1.544
N1-C3	1.4204	C24-C26	1.5426
N1-C13	1.4101	C24-C25	1.5442
F9-C18	1.3964	C22-C23	1.5516
F8-C18	1.3923	C21-C22	1.4929
F7-C18	1.4154	C1-C9	1.5834
F5-C9	1.4176	C17-C12	1.4133
F3-C8	1.4087	C16-C20	1.5186
F1-C8	1.3943	C16-C17	1.4032
F12-C19	1.3933	C15-C16	1.4141
F11-C19	1.4007	C15-C14	1.3937
F10-C19	1.4104	C14-C13	1.4289
C9-F6	1.3981	C13-C12	1.432
C9-F4	1.3918	C12-C11	1.54
C8-F2	1.3991	C11-C19	1.5809
C8-C1	1.5764	C11-C18	1.5797
C7-C2	1.4155		

Table S20. Calculated geometry optimization bond angles [°] for **3'**.

Bonds	Angle	Bonds	Angle
N1-W1-O1	79.36	C3-N1-W1	116.53
N1-W1-C21	98.06	C13-N1-W1	126.1
N1-W1-O2	80.73	F5-C9-C1	114.75
N1-W1-O3	153.28	F5-C9-F4	105.21
O1-W1-C21	103.39	F5-C9-F6	105.75
O1-W1-O2	146.18	C1-C9-C4	112.5
O1-W1-O3	93.46	C1-C9-F6	111.65
C21-W1-O2	106.26	F4-C9-F6	106.32
C21-W1-O3	108.65	F3-C8-F1	105.93
O2-W1-O3	92.18	F3-C8-F2	105.81
W1-O3-C24	145.3	C3-C8-C1	113.78
W1-O2-C11	139.61	F1-C8-F2	106.81
C1-O1-W1	132.36	F1-C8-C1	110.7
C3-N1-C13	117.37	F2-C8-C1	113.27

C6-C7-C2	122.75	C11-C18-F8	112.47
C5-C6-C7	117.39	F9-C18-F7	105.96
C5-C6-C10	121.17	F9-C18-F8	106.44
C7-C6-C10	121.43	F7-C18-F8	105.13
C6-C5-C4	120.82	C16-C17-C12	122.84
C5-C4-C3	122.4	C15-C16-C17	117.21
C4-C3-C2	116.88	C15-C16-C20	121.31
C4-C3-N1	118.94	C17-C16-C20	121.47
C2-C3-N1	124.07	C14-C15-C16	121.01
O3-C24-C25	108.25	C15-C14-C13	122.52
O3-C24-C27	108.51	C14-C13-N1	119.38
O3-C24-C26	106.13	C14-C13-C12	116.4
C25-C24-C27	111.43	N1-C13-C12	124.22
C25-C24-C26	111.2	C13-C12-C17	119.98
C27-C24-C26	111.1	C13-C12-C11	119.16
C21-C22-C23	114.26	C17-C12-C11	120.85
W1-C21-C22	176.2	C12-C11-O2	112.44
C7-C2-C3	119.75	C12-C11-C19	109.52
C7-C2-C1	119.55	C12-C11-C18	113.04
C3-C2-C1	120.6	O1-C11-C19	110.3
C11-C19-F12	111.72	O1-C11-C18	103.14
C11-C19-F10	112.87	C19-C11-C18	108.2
C11-C19-C11	113.48	C8-C1-C2	108.87
F12-C19-F10	105.79	C8-C1-C9	108.34
F12-C19-F11	106.51	C8-C1-O1	105.39
F10-C19-F11	105.91	C2-C1-C9	112.57
C11-C18-F9	111.17	C2-C1-O1	115.01
C11-C18-F7	115.04	C9-C1-O1	106.27

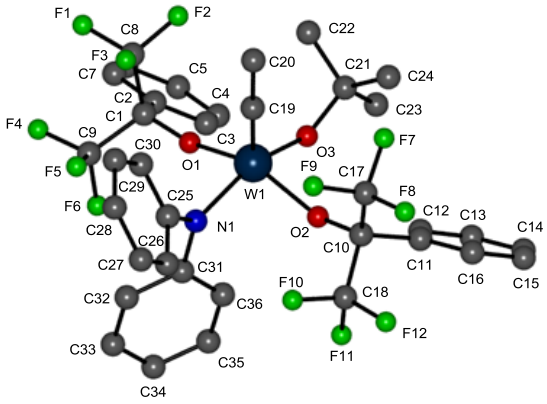

Figure S86. Labeling Scheme of the geometry optimization calculation for **7'**.

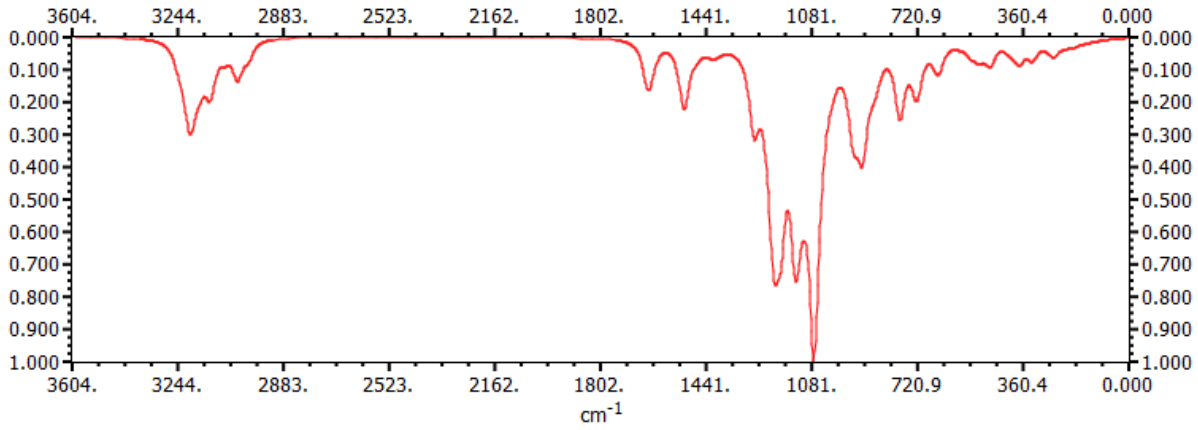

Figure S87. Guassian optimizated IR spectrum calculation for **7'**.

Table S21. Atomic coordinates of the geometry optimization calculation for **7'**.

Atom	x	y	z
W1	0.0187	0.1921	-0.431
O3	0.0207	-1.778	-0.2805
O2	1.9643	0.1041	0.1867
O1	-1.9629	0.0791	-0.0219
N1	-0.0383	2.1264	0.3166
F9	3.027	1.7553	-1.9033
F8	5.0498	0.8345	-1.7163
F7	3.3159	-0.4184	-2.3746
F6	-3.5951	1.2859	1.9272
F5	-3.2951	2.5854	0.1201
F4	-5.2639	1.5845	0.4668
F3	-3.0533	1.3346	-2.3643
F2	-3.3314	-0.8829	-2.4415
F12	5.2641	1.5091	0.9152
F11	3.5861	0.9737	2.2984
F10	3.3011	2.5656	0.7473
F1	-5.0688	0.4508	-1.9887
C9	-3.8658	1.3957	0.5684
C8	-3.6917	0.2647	-1.7345
C7	-5.4171	-1.3535	0.3341
C6	-5.9739	-2.5109	0.9077
C5	-5.1478	-3.4623	1.5354
C4	-3.7573	-3.2497	1.58
C36	0.2408	1.2472	2.6152
C35	-0.0184	1.3171	3.994

C34	-0.7361	2.3966	4.5405
C33	-1.1948	3.4097	3.6726
C32	-0.95	3.3417	2.294
C31	-0.2278	2.2542	1.7285
C30	-0.6608	3.5718	-1.6094
C3	-3.1946	-2.0963	1.0044
C29	-0.5173	4.7649	-2.3391
C28	0.3587	5.7776	-1.9013
C27	1.089	5.5737	-0.7127
C26	0.9484	4.3829	0.0177
C25	0.0754	3.3533	-0.4212
C24	0.1252	-4.1812	-0.1095
C23	1.3466	-2.9726	-1.9837
C22	-1.1728	-3.083	-1.9895
C21	0.0827	-2.9911	-1.0949
C20	0.23	0.7625	-3.6213
C2	-4.0219	-1.142	0.3818
C19	0.1333	0.5225	-2.1569
C18	3.8667	1.315	0.9743
C17	3.673	0.5987	-1.4852
C16	5.4364	-1.3509	0.2117
C15	6.0226	-2.5565	0.6382
C14	5.2385	-3.5526	1.2501
C13	3.8588	-3.337	1.4238
C12	3.2669	-2.1371	0.9909
C11	4.0515	-1.1372	0.3856
C10	3.3331	0.1896	-0.0018
C1	-3.329	0.1241	-0.2037

Table S22. Calculated geometry optimization bond lengths [Å] for **7'**.

Bond	Length	Bond	Length
W1-O3	1.9759	F2-C8	1.3952
W1-O2	2.0432	F1-C8	1.4127
W1-O1	2.0265	F12-C18	1.4121
W1-N1	2.0745	F11-C18	1.3958
W1-C19	1.761	C9-F6	1.3899
O3-C21	1.4624	C9-F5	1.3936
O1-C10	1.3844	C8-F3	1.396
O1-C1	1.3789	C8-C1	1.5794
N1-C31	1.4302	C7-C6	1.4067
N1-C25	1.4362	C7-C2	1.412
F7-C17	1.3975	C6-C5	1.4077
F4-C9	1.4144	C5-C4	1.4073

C3-C4	1.4065	C21-C23	1.5452
C35-C36	1.4047	C1-C9	1.5815
C34-C35	1.4068	C1-C2	1.5575
C33-C34	1.4107	C19-C20	1.4871
C33-C32	1.4018	C18-F10	1.3911
C32-C31	1.4227	C17-F9	1.3892
C31-C36	1.4212	C17-F8	1.4158
C30-C25	1.4147	C16-C15	1.4067
C2-C3	1.4081	C15-C14	1.4077
C29-C30	1.406	C13-C14	1.4072
C28-C29	1.4087	C12-C13	1.4063
C28-C27	1.4098	C11-C16	1.412
C27-C26	1.404	C11-C12	1.4077
C26-C25	1.4194	C10-C18	1.5825
C22-C21	1.5444	C10-C17	1.5759
C21-C24	1.5457	C10-C11	1.5577

Table S23. Calculated geometry optimization bond angles [°] for **7'**.

Bonds	Angle	Bonds	Angle
N1-W1-O1	87.27	F2-C8-F3	106.48
N1-W1-C19	100.38	F2-C8-C1	111.02
N1-W1-O2	87.56	F3-C8-C1	113.6
N1-W1-O3	154.46	C6-C7-C2	120.04
O1-W1-C19	105.78	C7-C6-C5	120.38
O1-W1-O2	150.19	C6-C5-C4	119.46
O1-W1-O3	85.99	C5-C4-C3	120.41
C19-W1-O2	104.03	C31-C36-C35	121.09
C19-W1-O3	105.17	C34-C35-C36	120.9
O1-W1-O3	86.16	C33-C34-C35	118.55
W1-O3-C21	141.7	C32-C33-C34	120.89
W1-O2-C10	153.86	C33-C32-C31	121.11
C1-O1-W1	160.1	C32-C21-N1	121.87
C25-N1-C31	116.18	C32-C21-C36	117.45
C25-C1-W1	127.53	N1-C31-C36	120.59
C31-N1-W1	116.28	C29-C30-C25	120.92
F4-C9-C1	114.07	C2-C3-C4	120.11
F4-C9-F5	105.53	C28-C29-C30	120.81
F4-C9-F6	105.86	C27-C28-C29	118.7
C1-C9-F5	112.98	C28-C27-C26	120.62
C1-C9-F6	110.34	C27-C26-C25	121.06
F5-C9-F6	107.59	C26-C25-C30	117.89
F1-C8-F2	105.6	C26-C25-N1	120.63
F1-C8-F3	105.28	C30-C25-N1	121.48
F1-C8-C1	114.2	O3-C21-C22	109.72

O3-C21-C23	110.19	C11-C16-C15	120.07
O3-C21-C24	106.55	C16-C15-C14	120.41
C22-C21-C23	109.42	C13-C14-C15	119.43
C22-C21-C24	110.23	C12-C13-C14	120.36
C23-C21-C24	110.69	C11-C12-C13	120.26
C1-C2-C7	123.27	C10-C11-C12	117.06
C1-C2-C3	117.11	C10-C11-C16	123.41
C7-C2-C3	119.6	C12-C11-C16	119.47
W1-C19-C20	178.47	O2-C10-C18	107.05
C10-C18-F11	110.09	O2-C10-C17	110.94
C10-C18-F12	113.93	O2-C10-C11	111.69
C10-C18-F10	113.68	C18-C10-C17	108.86
F11-C18-F12	105.8	C18-C10-C11	107.27
F11-C18-F10	107.03	C17-C10-C11	110.84
F12-C18-F10	105.78	C8-C1-C9	108.88
C10-C17-F7	110.79	C8-C1-O1	110.99
C10-C17-F8	113.99	C8-C1-C2	109.54
C10-C17-F9	113.52	C9-C1-O1	107.35
F7-C17-F8	105.42	C9-C1-C2	108.61
F7-C17-F9	107.19	O1-C1-C2	111.38
F8-C17-F9	105.34		

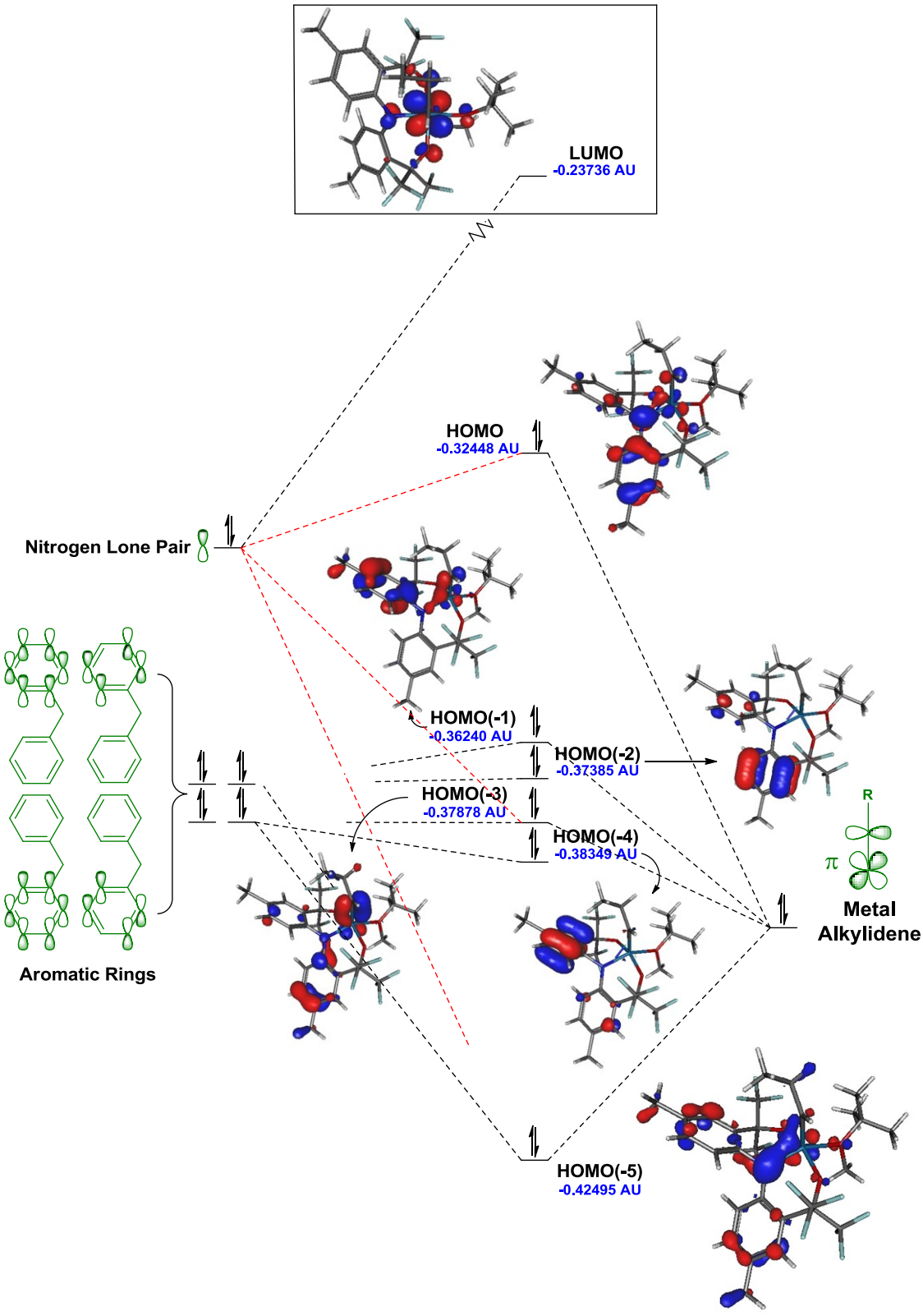

Figure S88. Molecular Orbital Diagram of **2-Me'** containing LUMO – HOMO(-5). (Isovalue = 0.051687) .

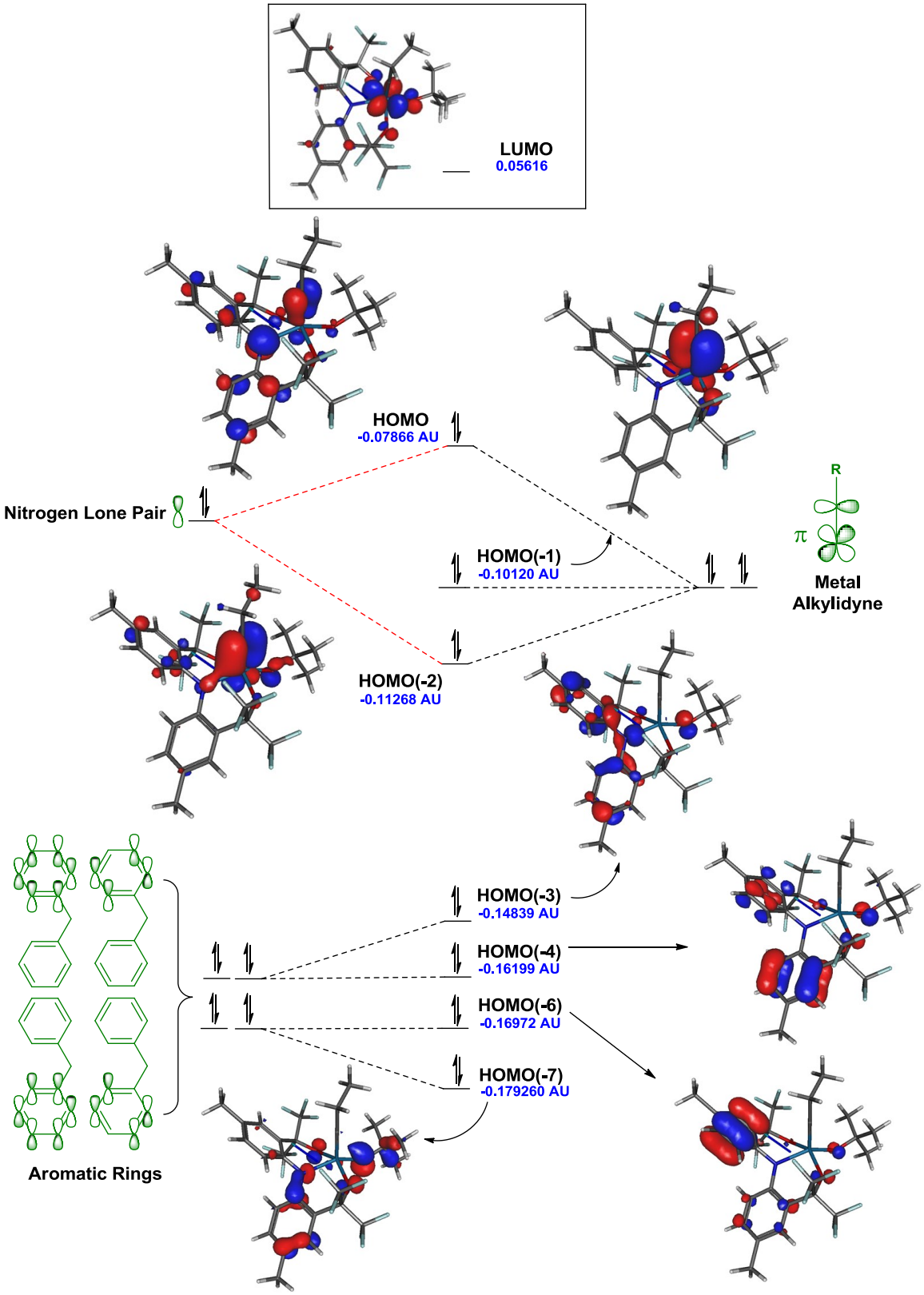

Figure S89. Molecular Orbital Diagram of **3'** containing LUMO – HOMO(-5). (Isovalue = 0.051687) .

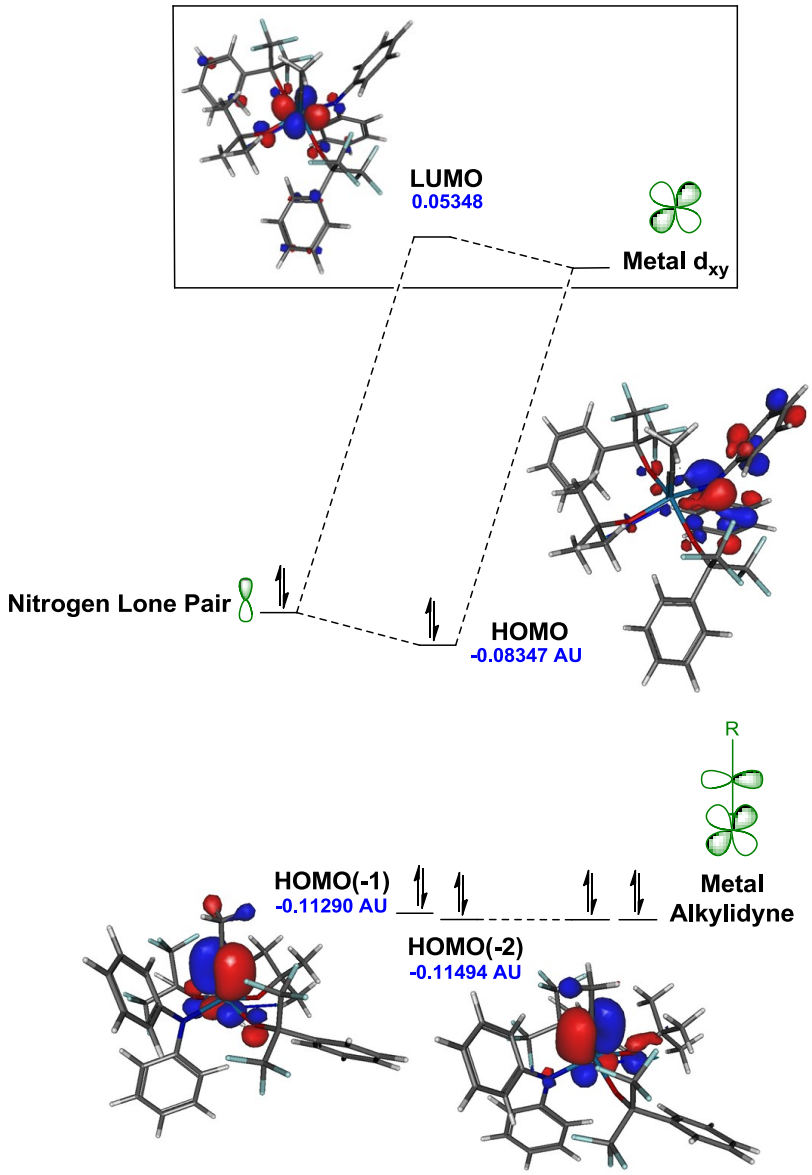

Figure S90. Molecular Orbital Diagram of **7'** containing LUMO – HOMO(-5). (Isovalue = 0.051687) .