

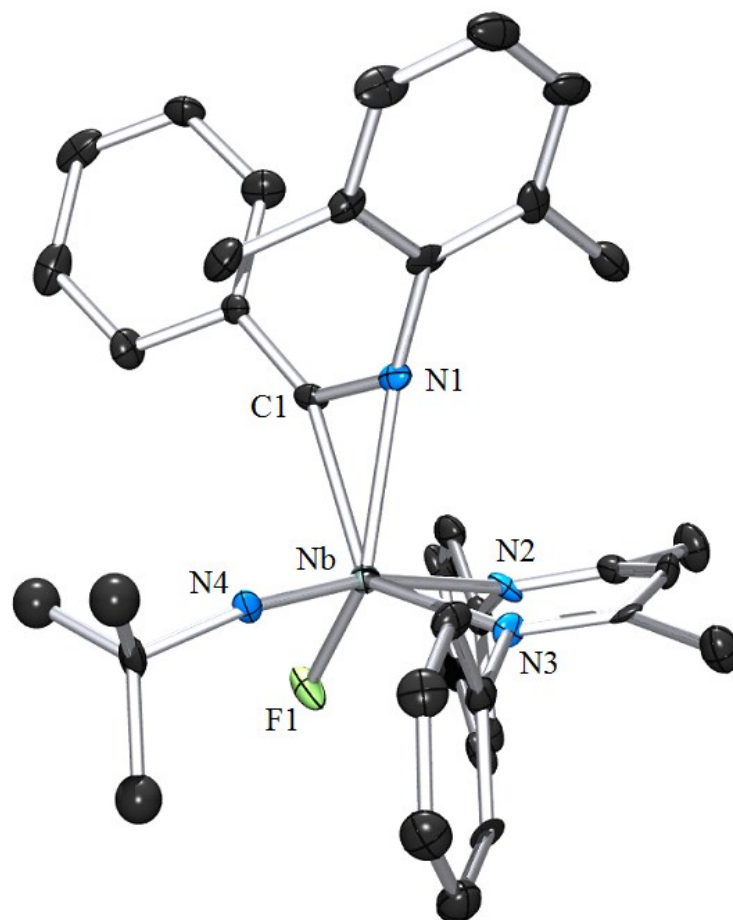
# **C-F $sp^2$ bond functionalization mediated by niobium complexes**

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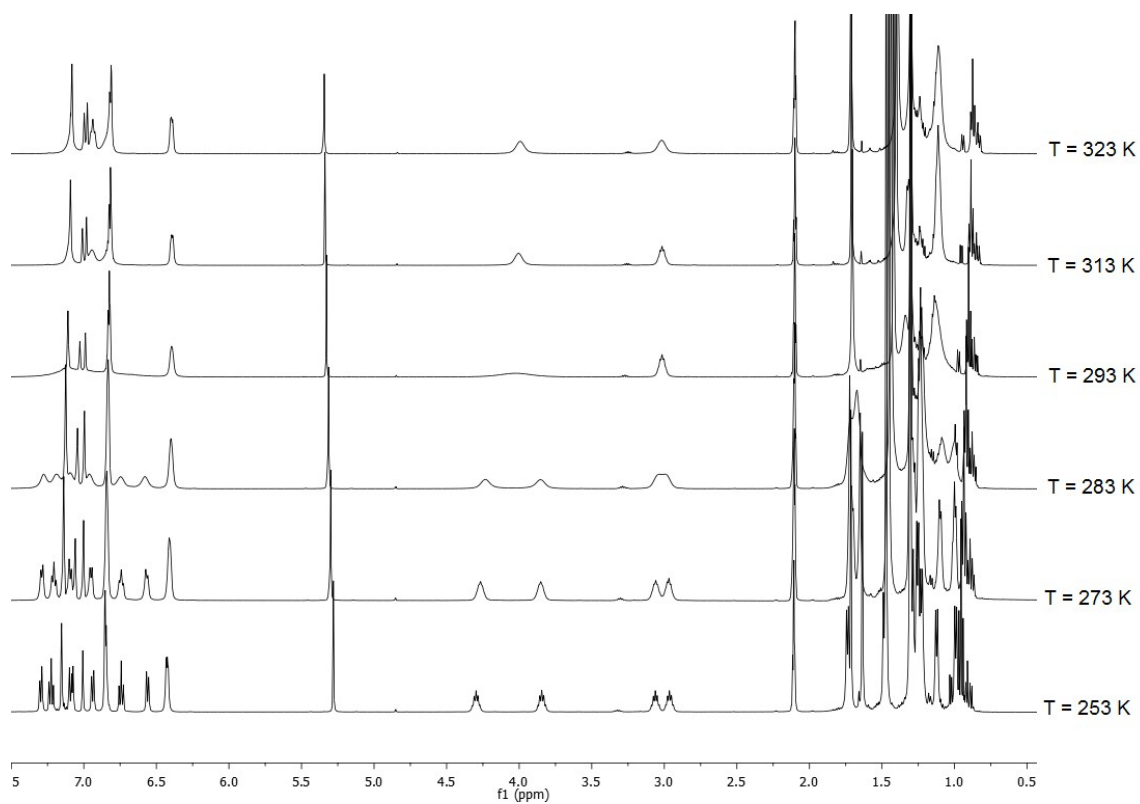
## A. X-ray crystallography of **3b**



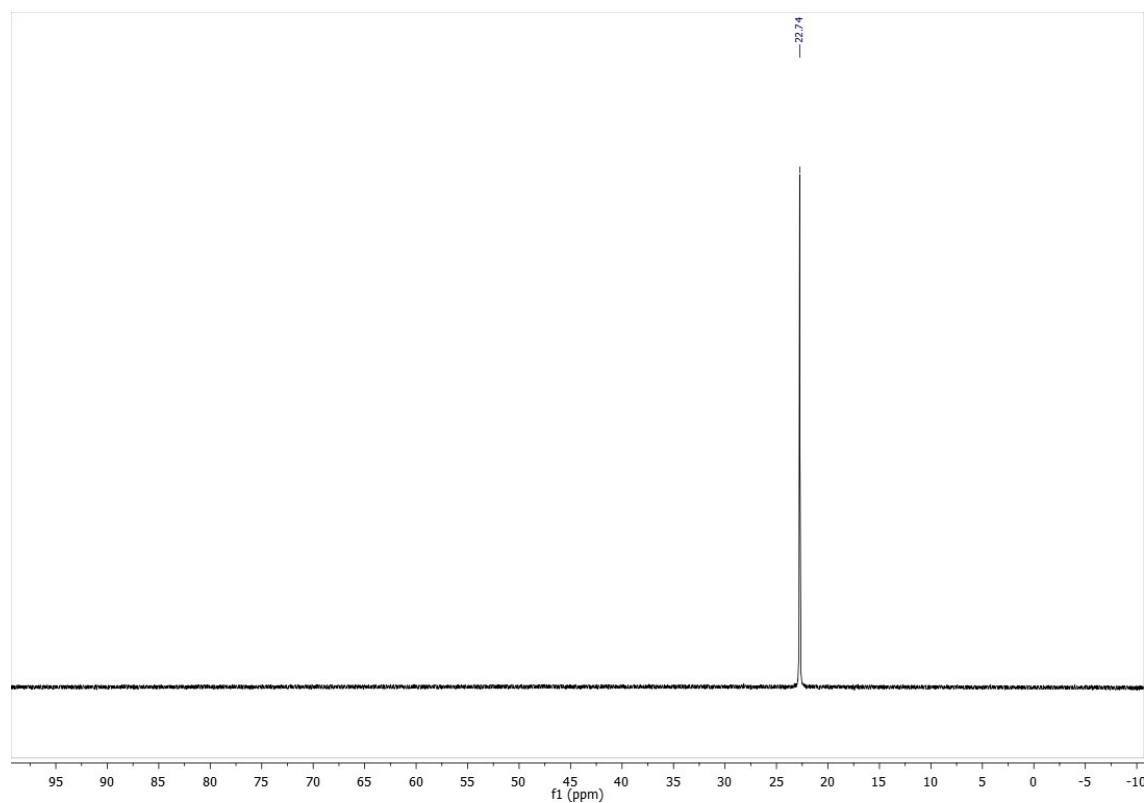
**Figure S.1** ORTEP diagram of **3b**, hydrogens have been removed for clarity. Thermal ellipsoids are represented at 50 %.

## B. NMR Spectroscopic analysis of 3a-b, 4a and 5

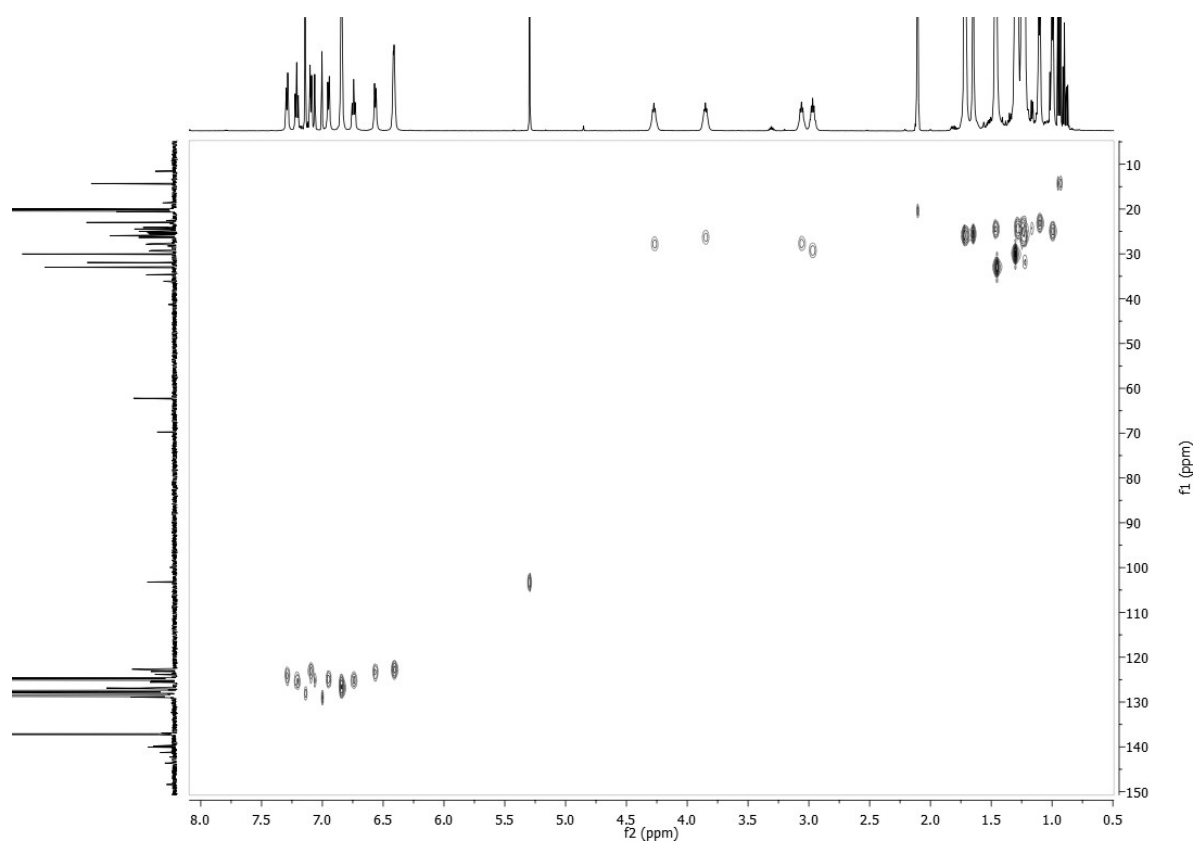
### B.1 NMR spectroscopy of 3a



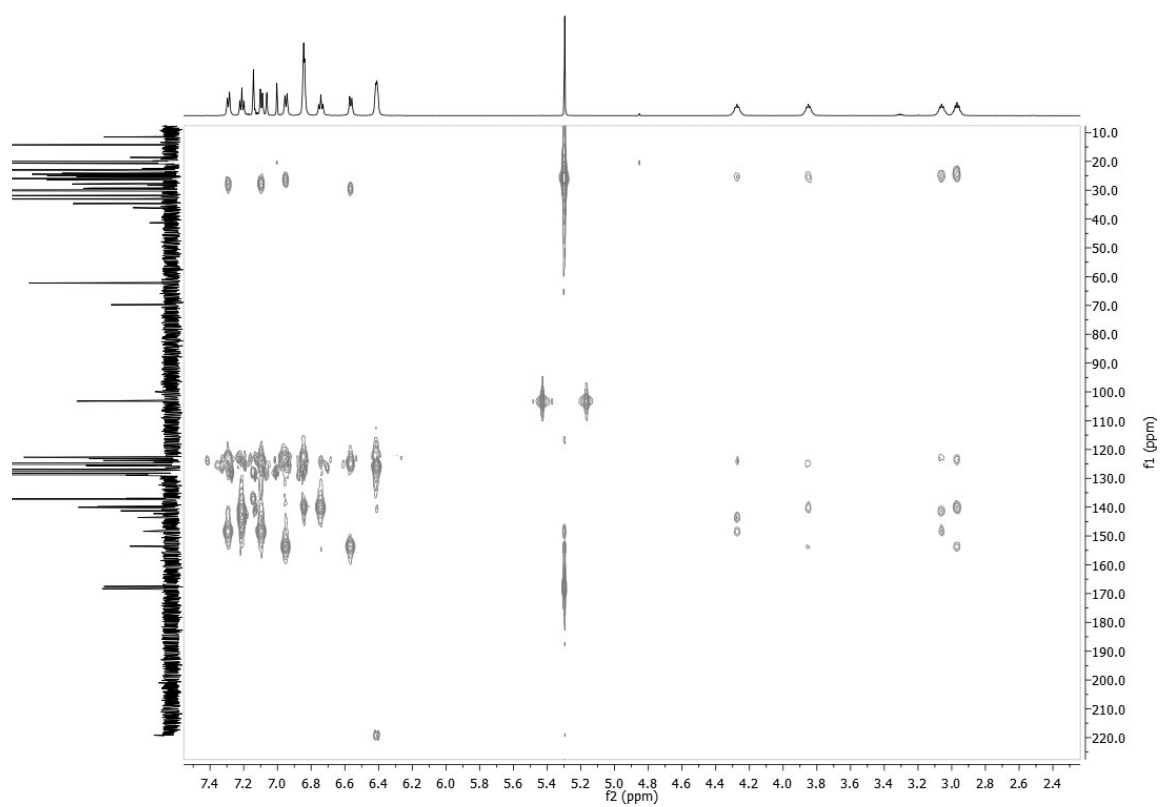
**Figure S.2** Variable temperature  $^1\text{H}$  NMR spectroscopy of 3a



**Figure S.3**  $^{19}\text{F}$  NMR spectrum of **3a** at 253 K.

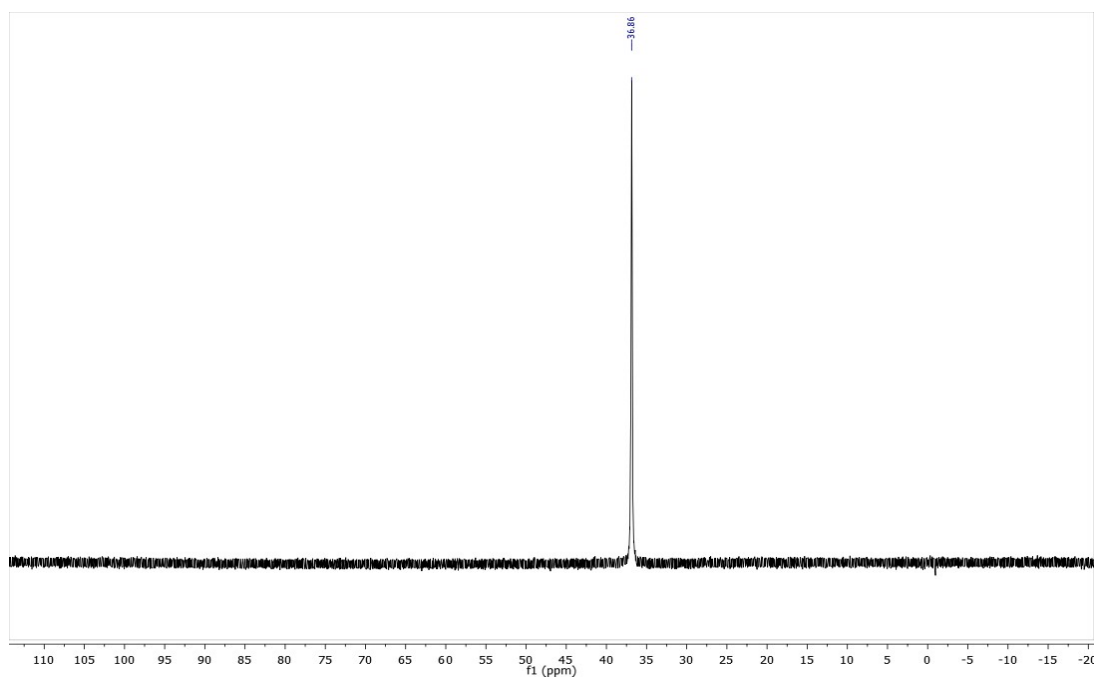


**Figure S.4**  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of **3a** at 253 K.

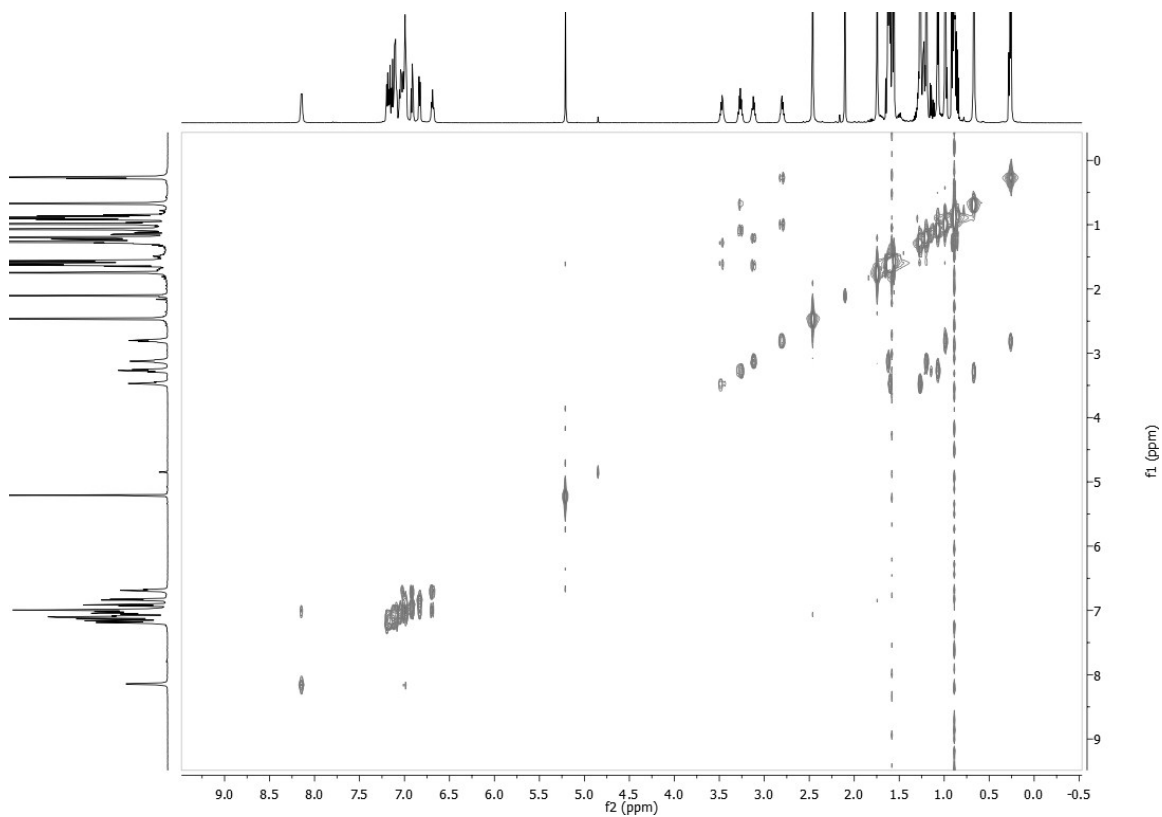


**Figure S.5**  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of **3a** at 253 K.

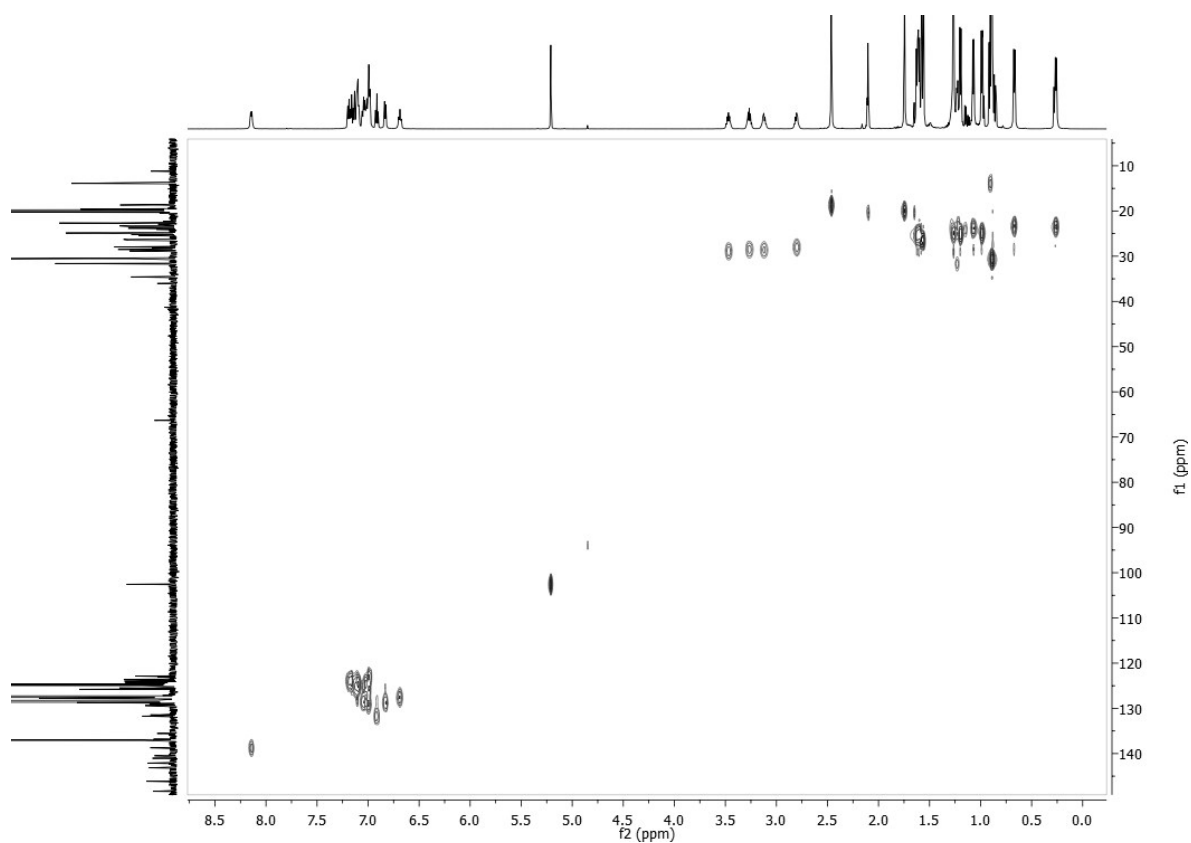
## B.2 NMR spectroscopy of **3b**



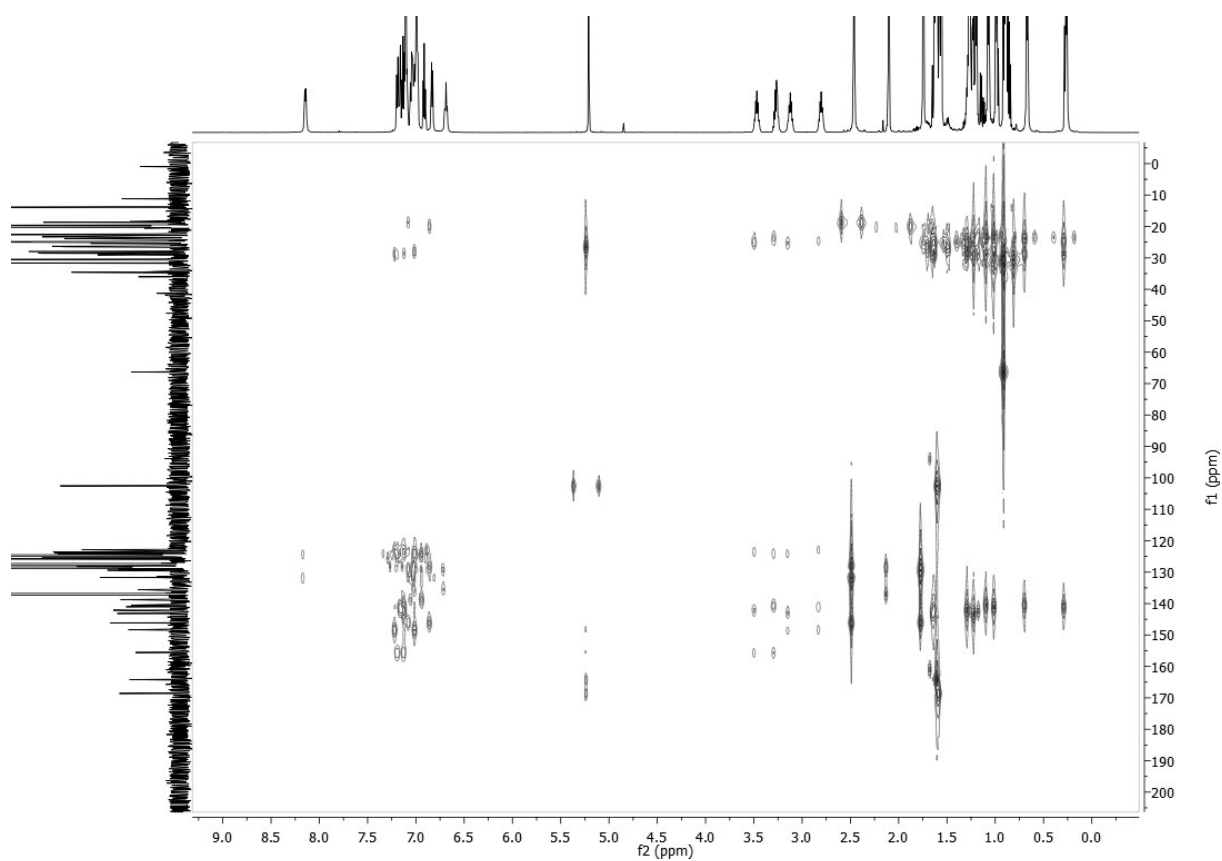
**Figure S.6**  $^{19}\text{F}$  NMR spectrum of **3b** at 298K.



**Figure S.7**  $^1\text{H}$ - $^1\text{H}$  COSY NMR spectrum of **3b** at 298K.



**Figure S.8**  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of **3b** at 298K.



**Figure S.9**  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of **3b** at 298K.

### B.3 NMR spectroscopy of 4a

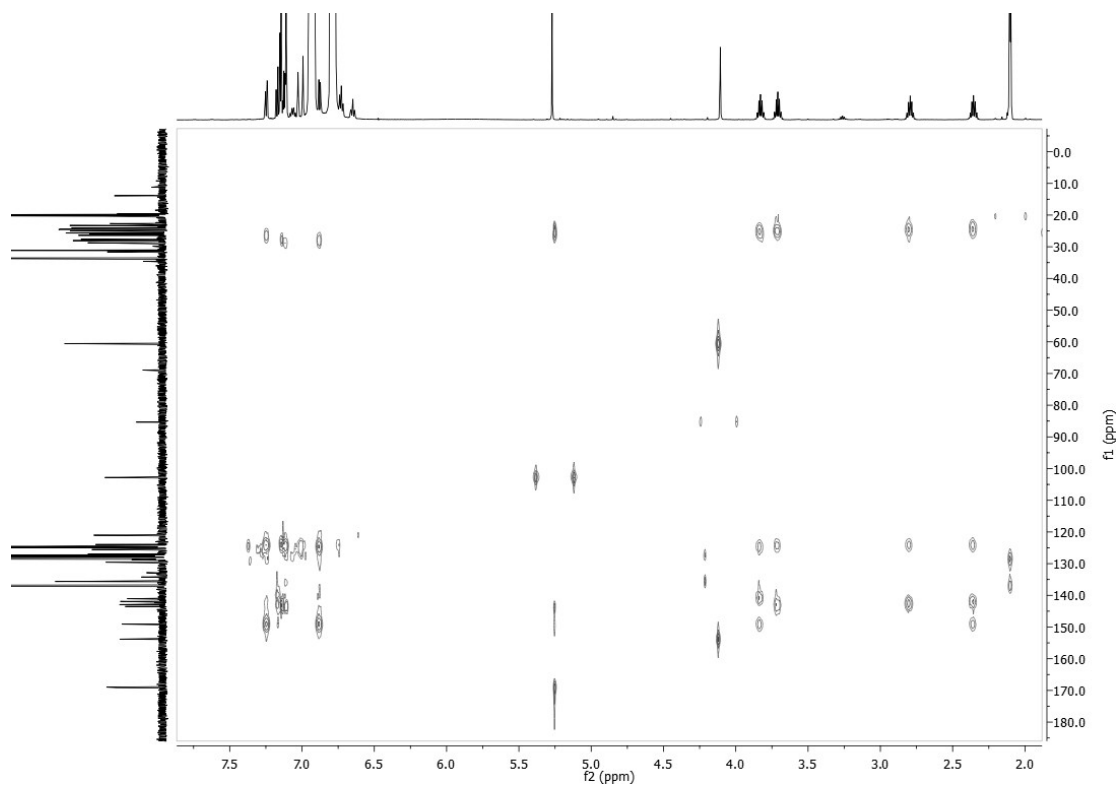


Figure S.10  $^1\text{H}$ - $^1\text{H}$  COSY NMR spectrum of **4a** at 298K.

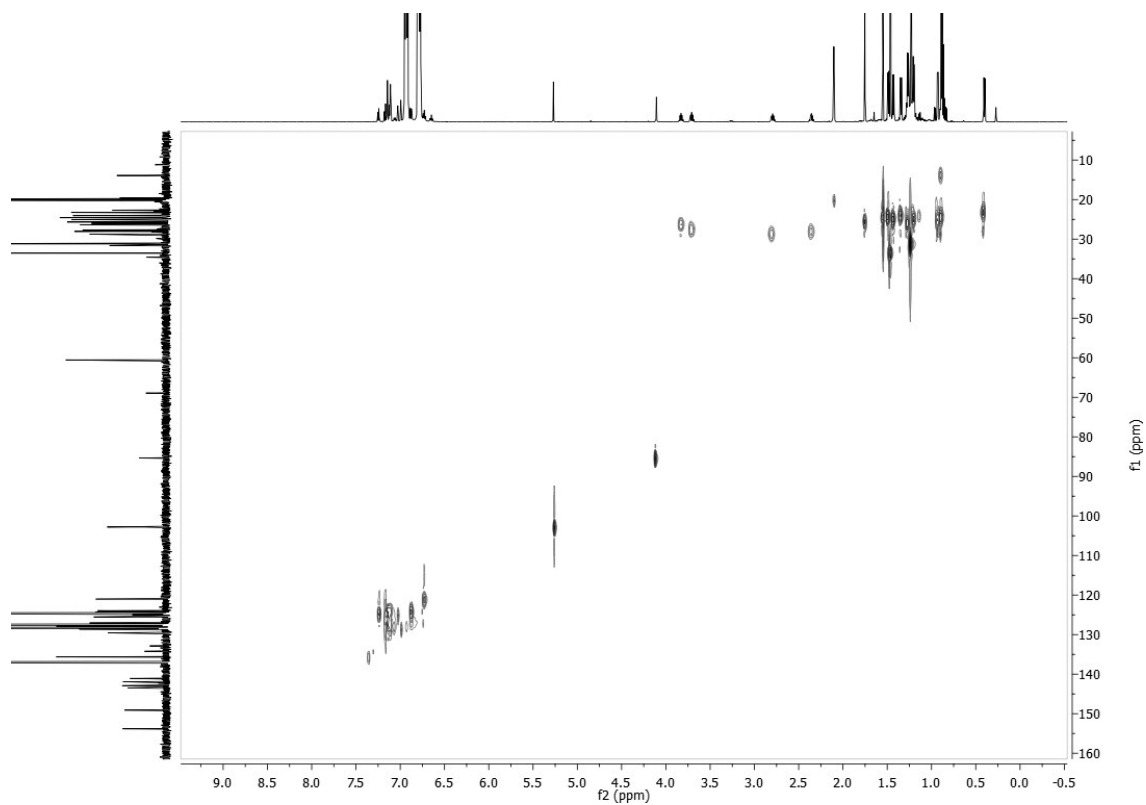
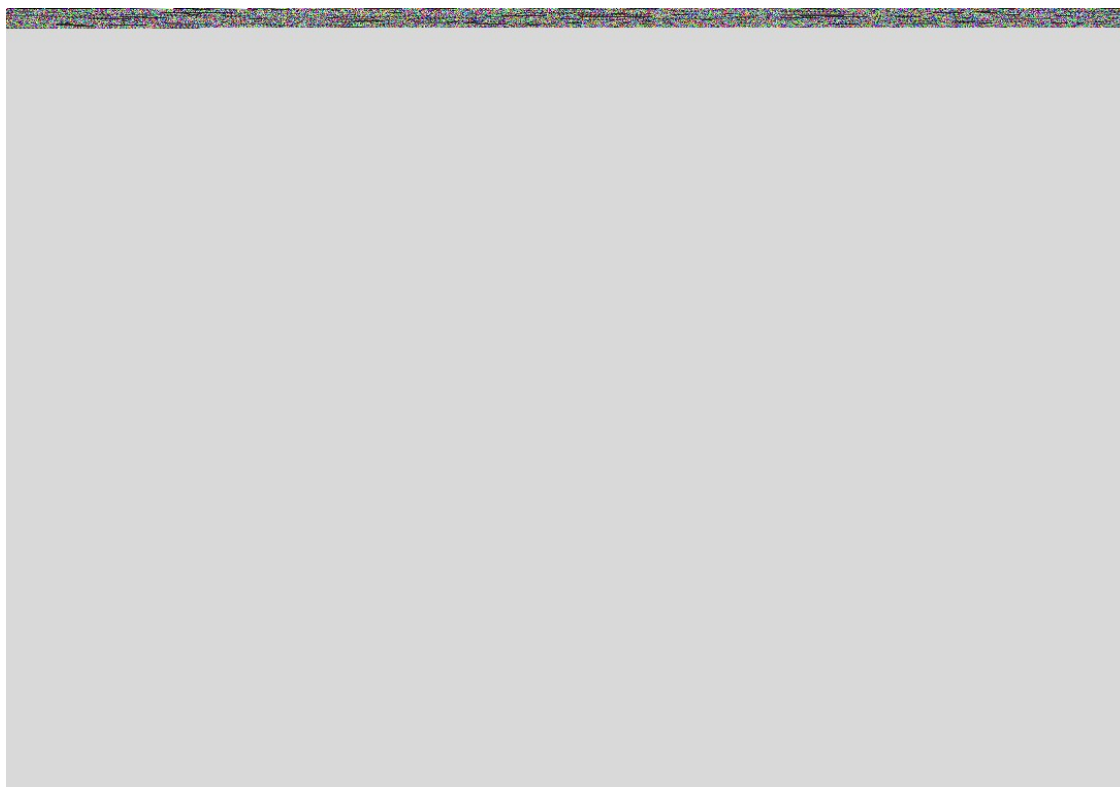
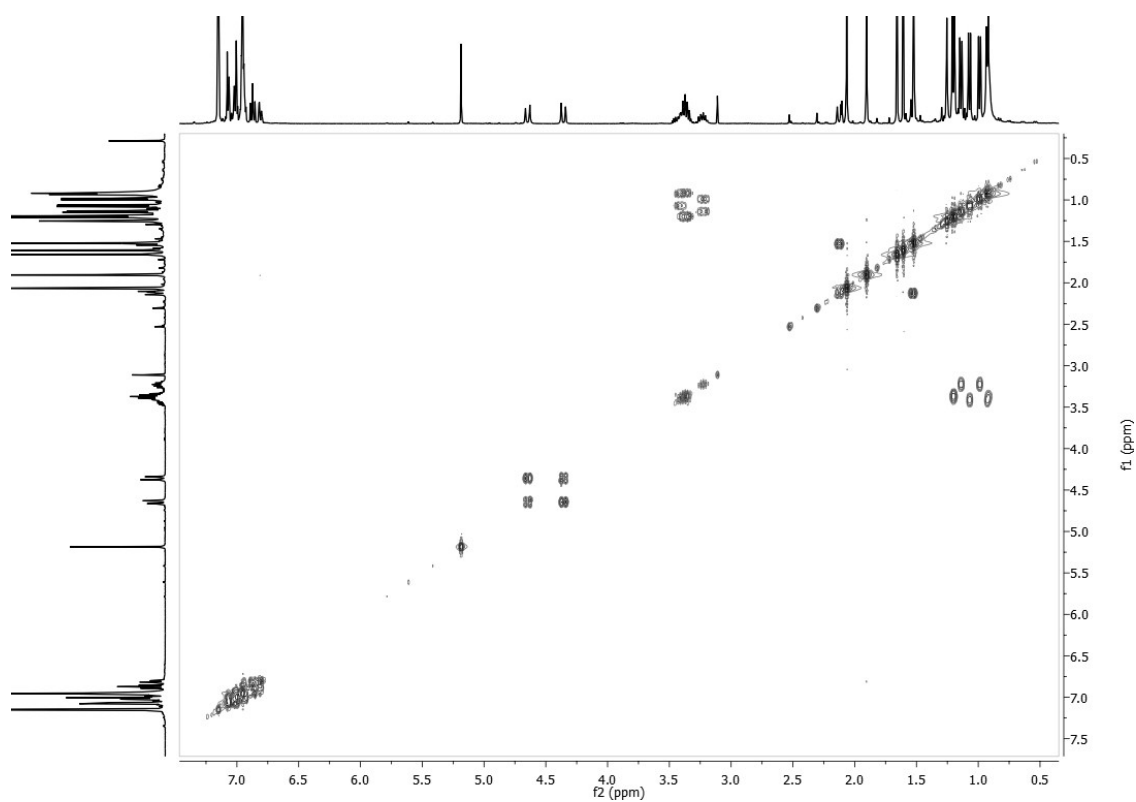


Figure S.11  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR spectrum of **4a** at 298K.



**Figure S.12**  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of **4a** at 298K.

#### B.4 NMR spectroscopy of **5**



**Figure S.13**  $^1\text{H}$ - $^1\text{H}$  COSY NMR spectrum of **5** at 298K.

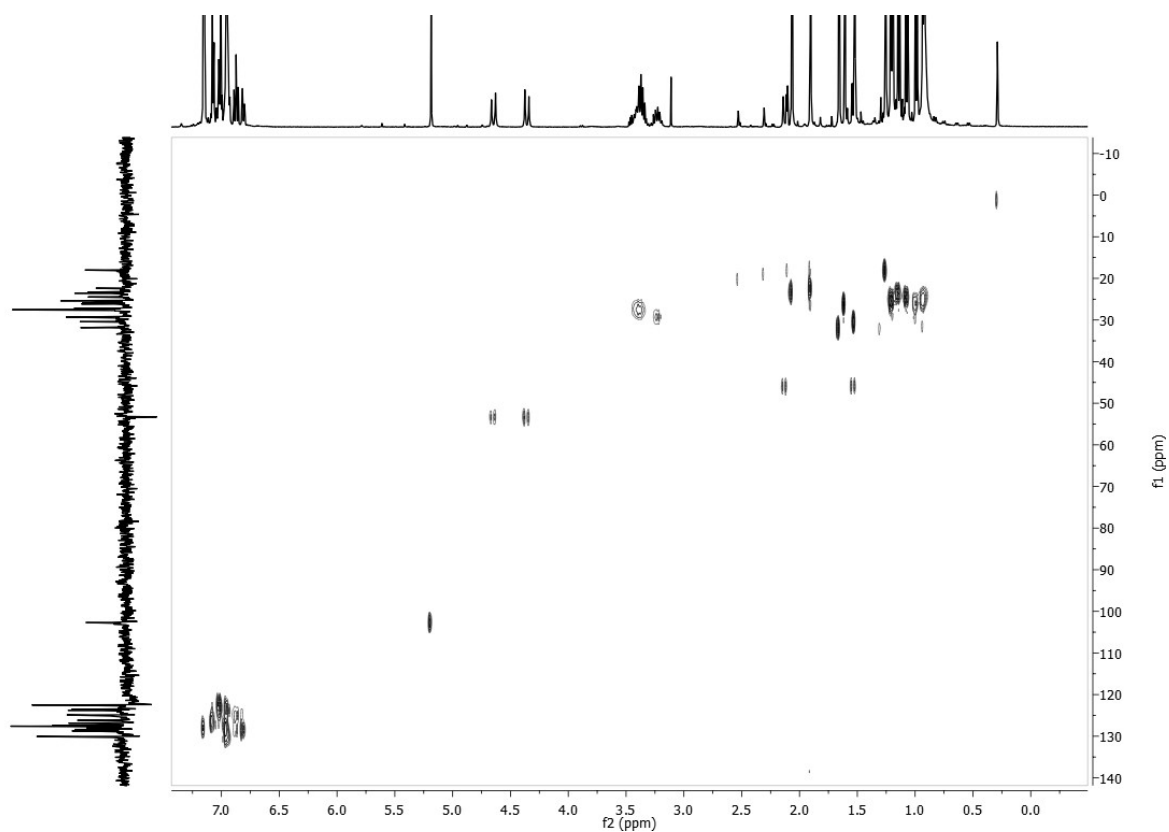


Figure S.14  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of **5** at 298K.

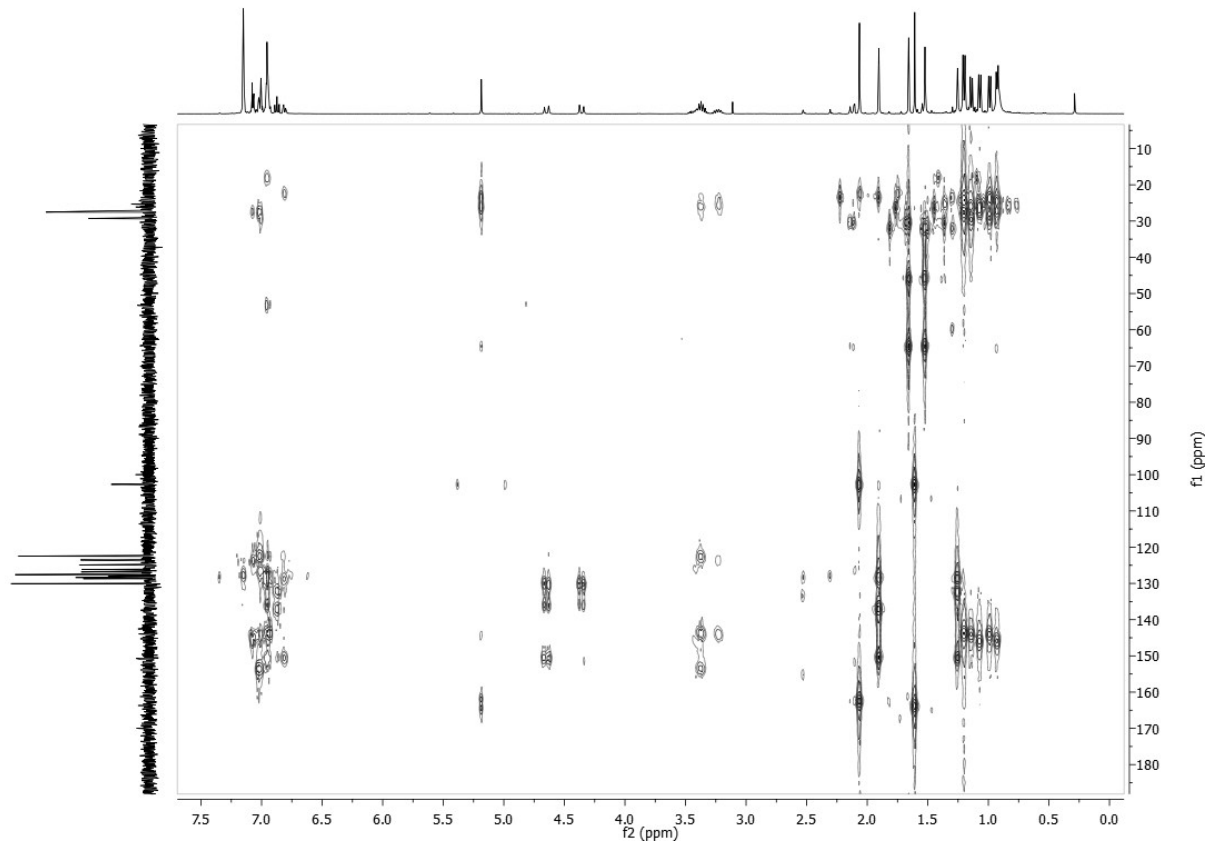


Figure S.15  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of **5** at 298K.