

Supplementary Material

Synthesis of a Novel Tetracyclic Isoxazole by Intramolecular Nitrile Oxide Cycloaddition

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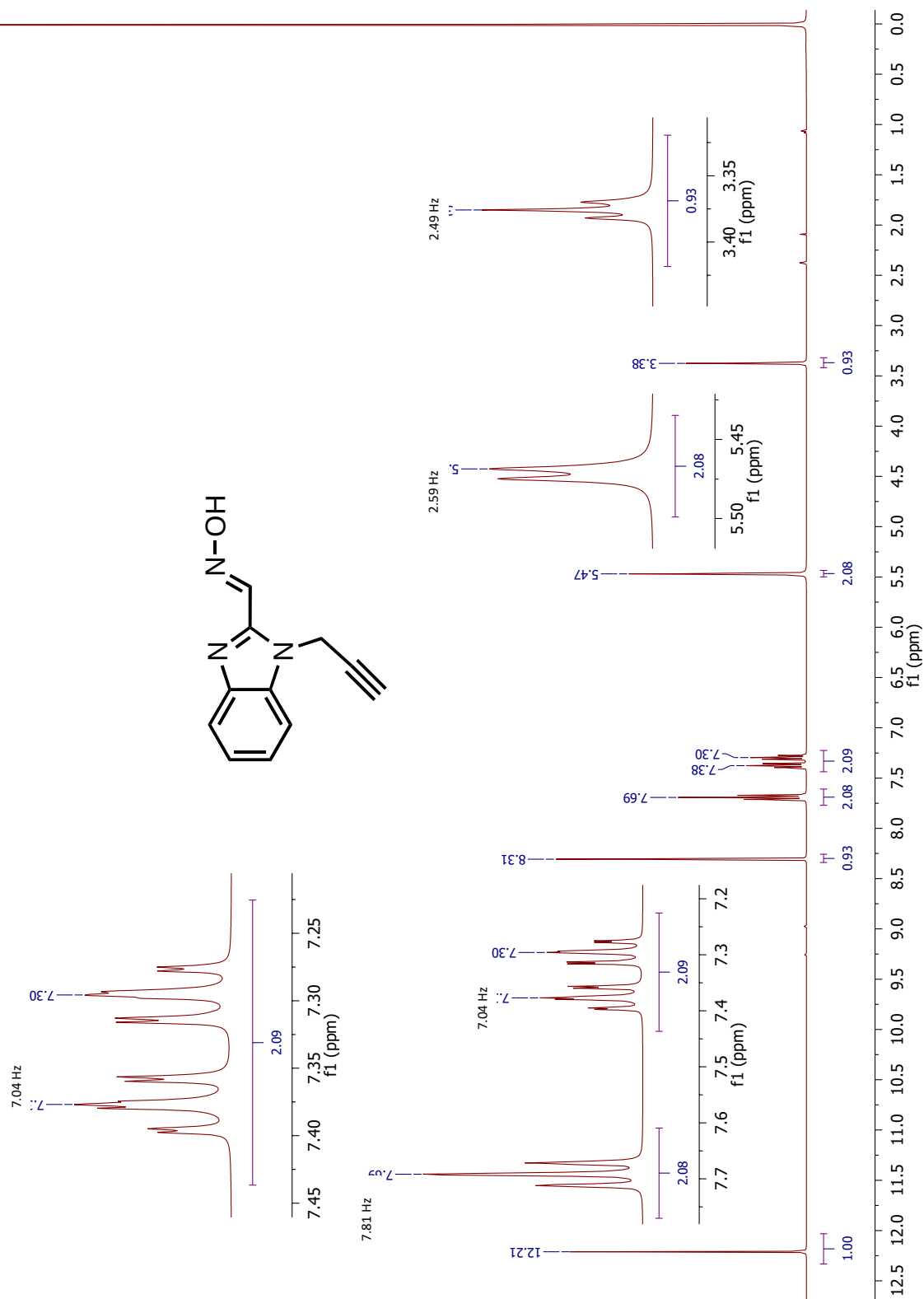
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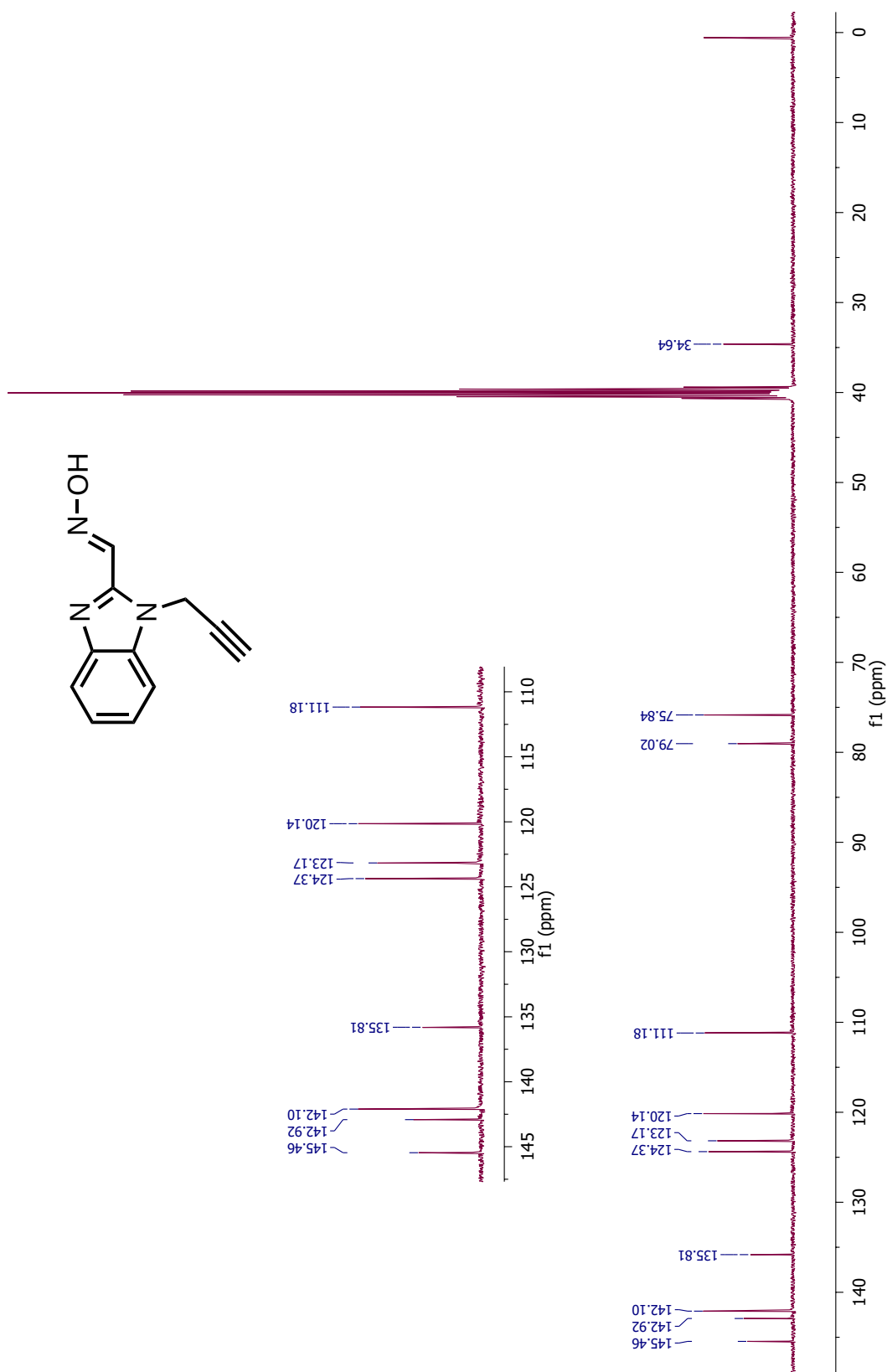
Spectral Data of Compounds **5** and **6**

Figure S1. Spectral data of 5 : 1-(2-propyn-1-yl)-1 <i>H</i> -benzimidazole-2-aldoxime	
S1.1 ¹ H-NMR of 1-(2-propyn-1-yl)-1 <i>H</i> -benzimidazole-2-aldoxime	1
S1.2 ¹³ C-NMR of 1-(2-propyn-1-yl)-1 <i>H</i> -benzimidazole-2-aldoxime	2
S1.3 HSQC of 1-(2-propyn-1-yl)-1 <i>H</i> -benzimidazole-2-aldoxime	3
S1.4 HMBC of 1-(2-propyn-1-yl)-1 <i>H</i> -benzimidazole-2-aldoxime	4
S1.5 FT-IR of 1-(2-propyn-1-yl)-1 <i>H</i> -benzimidazole-2-aldoxime	5
S1.6 HRMS of 1-(2-propyn-1-yl)-1 <i>H</i> -benzimidazole-2-aldoxime	6
Figure S2. Spectral data of 6 : isoxazolo-4 <i>H</i> -[3',4':3,4]pyrrolo[1,2- <i>a</i>]benzimidazole	
S2.1 ¹ H-NMR of isoxazolo-4 <i>H</i> -[3',4':3,4]pyrrolo[1,2- <i>a</i>]benzimidazole	7
S2.2 ¹³ C-NMR of isoxazolo-4 <i>H</i> -[3',4':3,4]pyrrolo[1,2- <i>a</i>]benzimidazole	8
S2.3 HSQC of isoxazolo-4 <i>H</i> -[3',4':3,4]pyrrolo[1,2- <i>a</i>]benzimidazole	9
S2.4 HMBC of isoxazolo-4 <i>H</i> -[3',4':3,4]pyrrolo[1,2- <i>a</i>]benzimidazole	10
S2.5 FT-IR of isoxazolo-4 <i>H</i> -[3',4':3,4]pyrrolo[1,2- <i>a</i>]benzimidazole	11
S2.6 HRMS of isoxazolo-4 <i>H</i> -[3',4':3,4]pyrrolo[1,2- <i>a</i>]benzimidazole	12

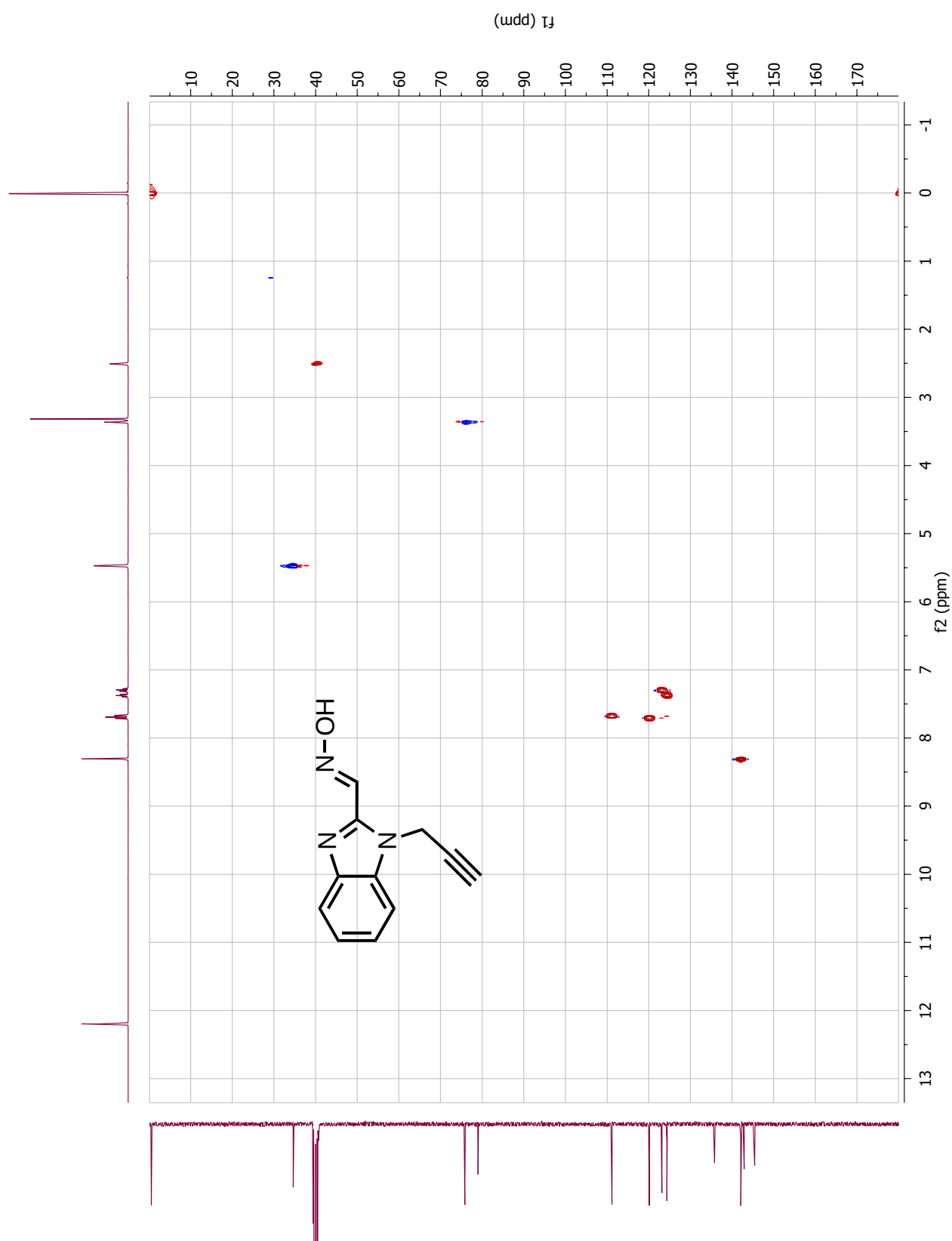
Figure S1. Spectral data of **5**: 1-(2-propyn-1-yl)-1*H*-benzimidazole-2-aldoxime
 S1.1 ^1H -NMR of 1-(2-propyn-1-yl)-1*H*-benzimidazole-2-aldoxime ($\text{DMSO}-d_6$) (**5**)



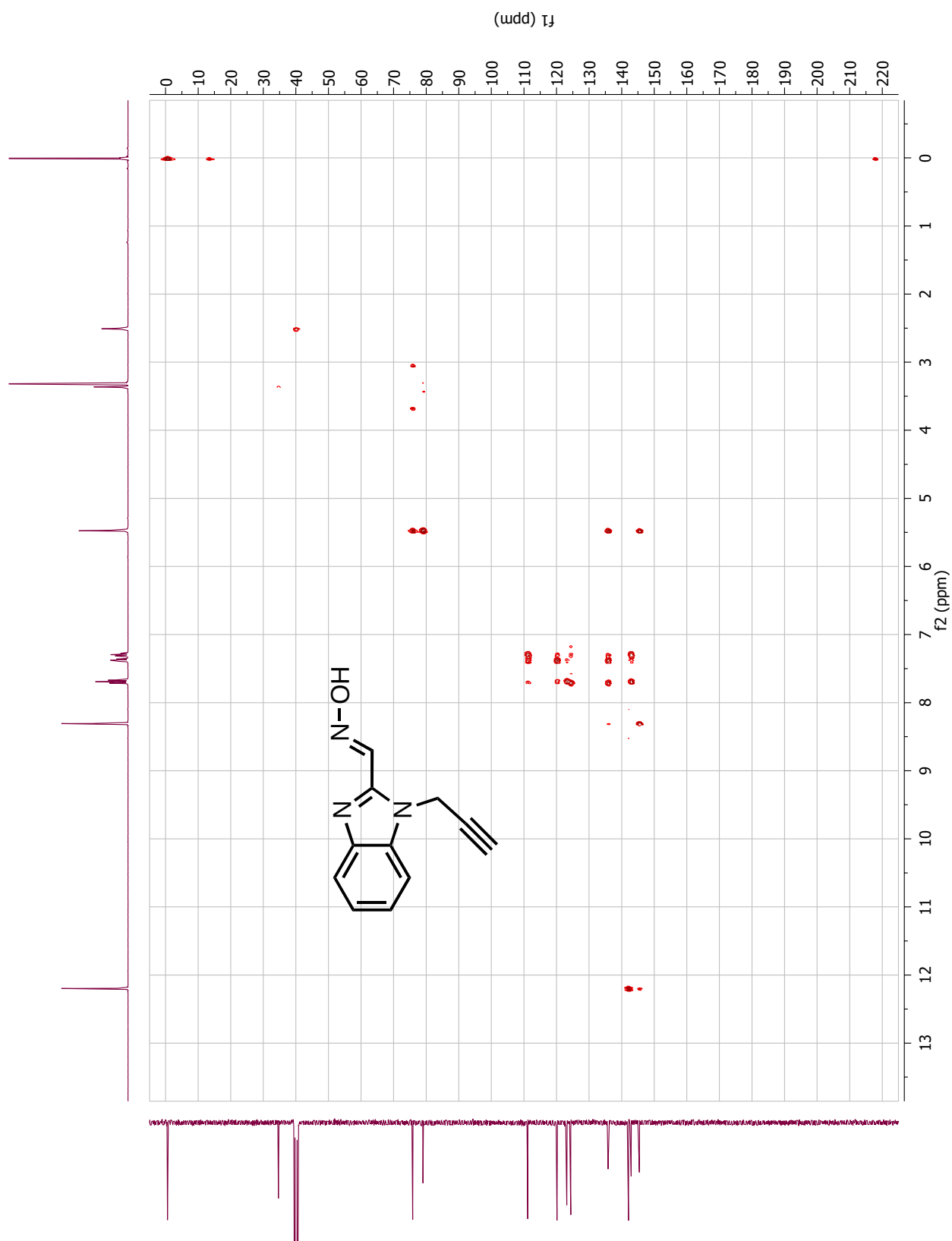
S1.2 ^{13}C -NMR of 1-(2-propyn-1-yl)-1*H*-benzimidazole-2-aldoxime (DMSO- d_6) (**5**)



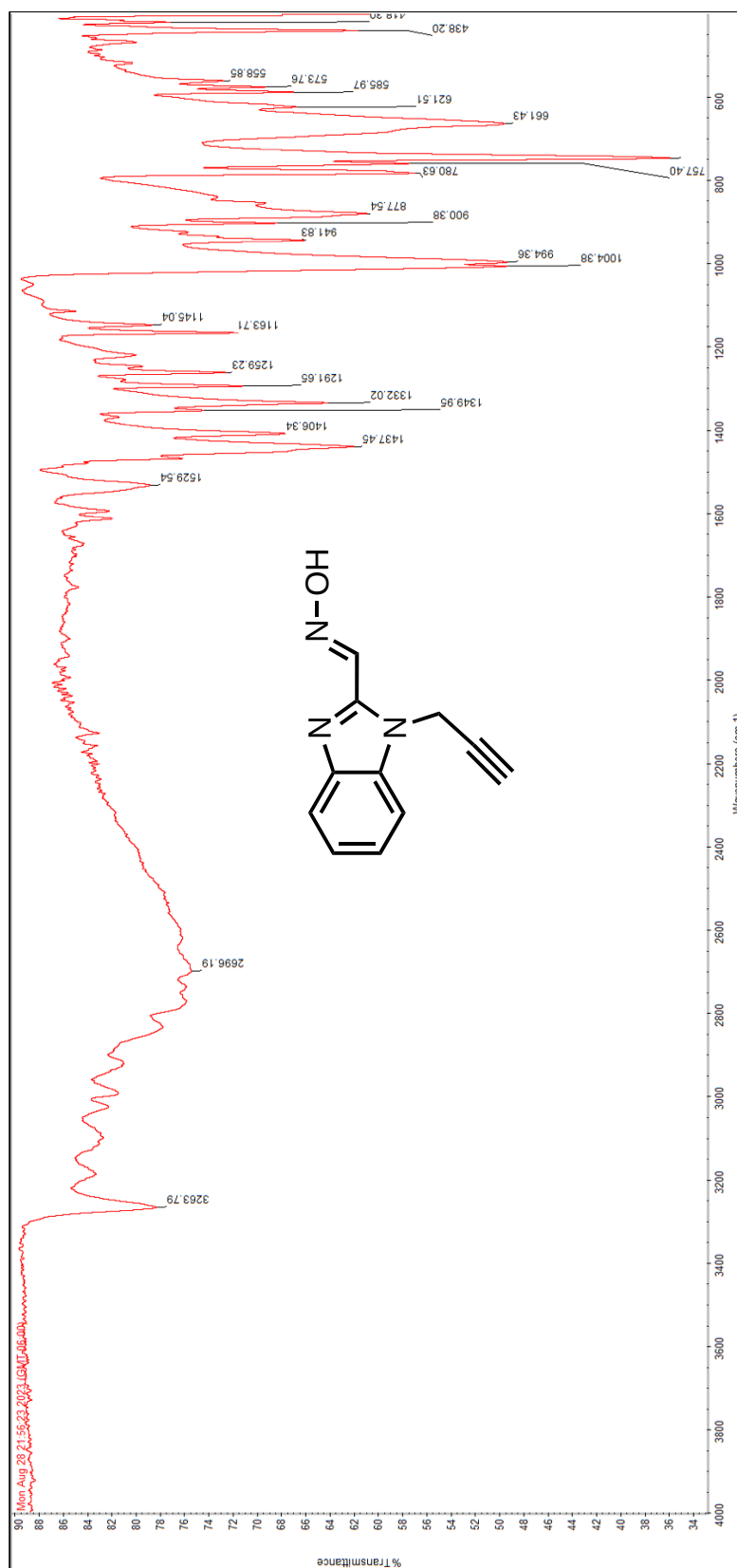
S1.3 HSQC of 1-(2-propyn-1-yl)-1*H*-benzimidazole-2-aldoxime (**5**)



S1.4 HMBC of 1-(2-propyn-1-yl)-1*H*-benzimidazole-2-aldoxime (**5**)



S1.5 FT-IR of 1-(2-propyn-1-yl)-1*H*-benzimidazole-2-aldoxime (5)



S1.6 HRMS of 1-(2-propyn-1-yl)-1*H*-benzimidazole-2-aldoxime (**5**)

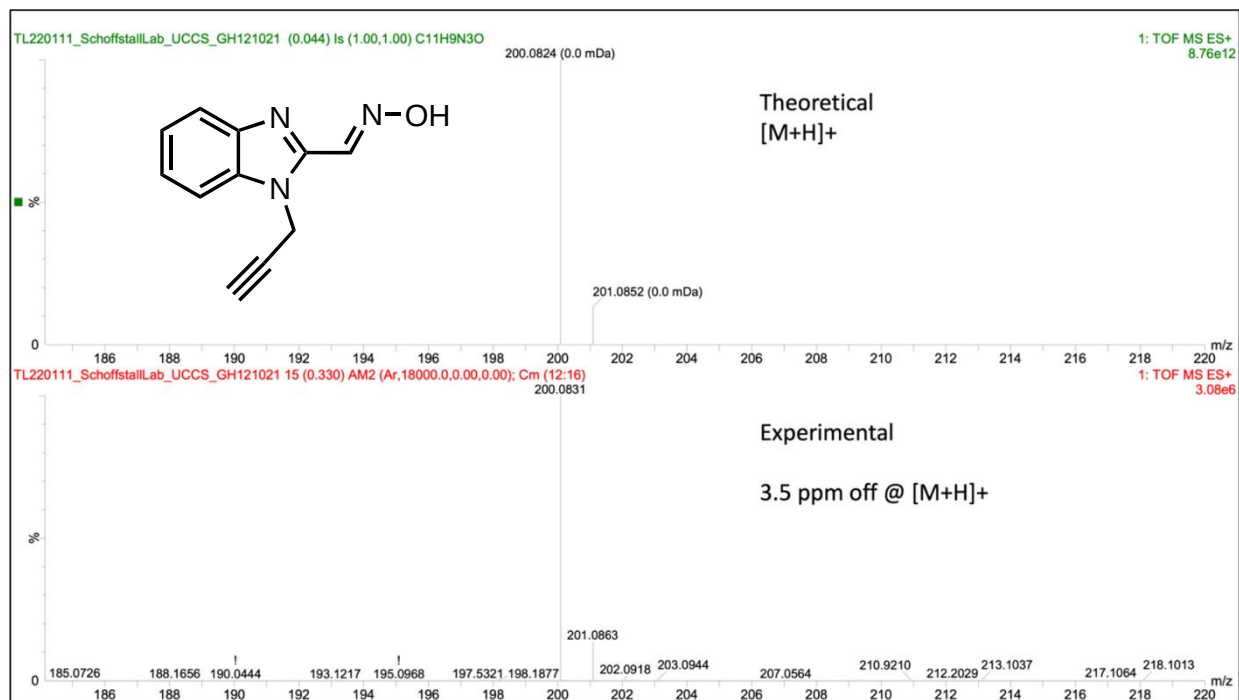
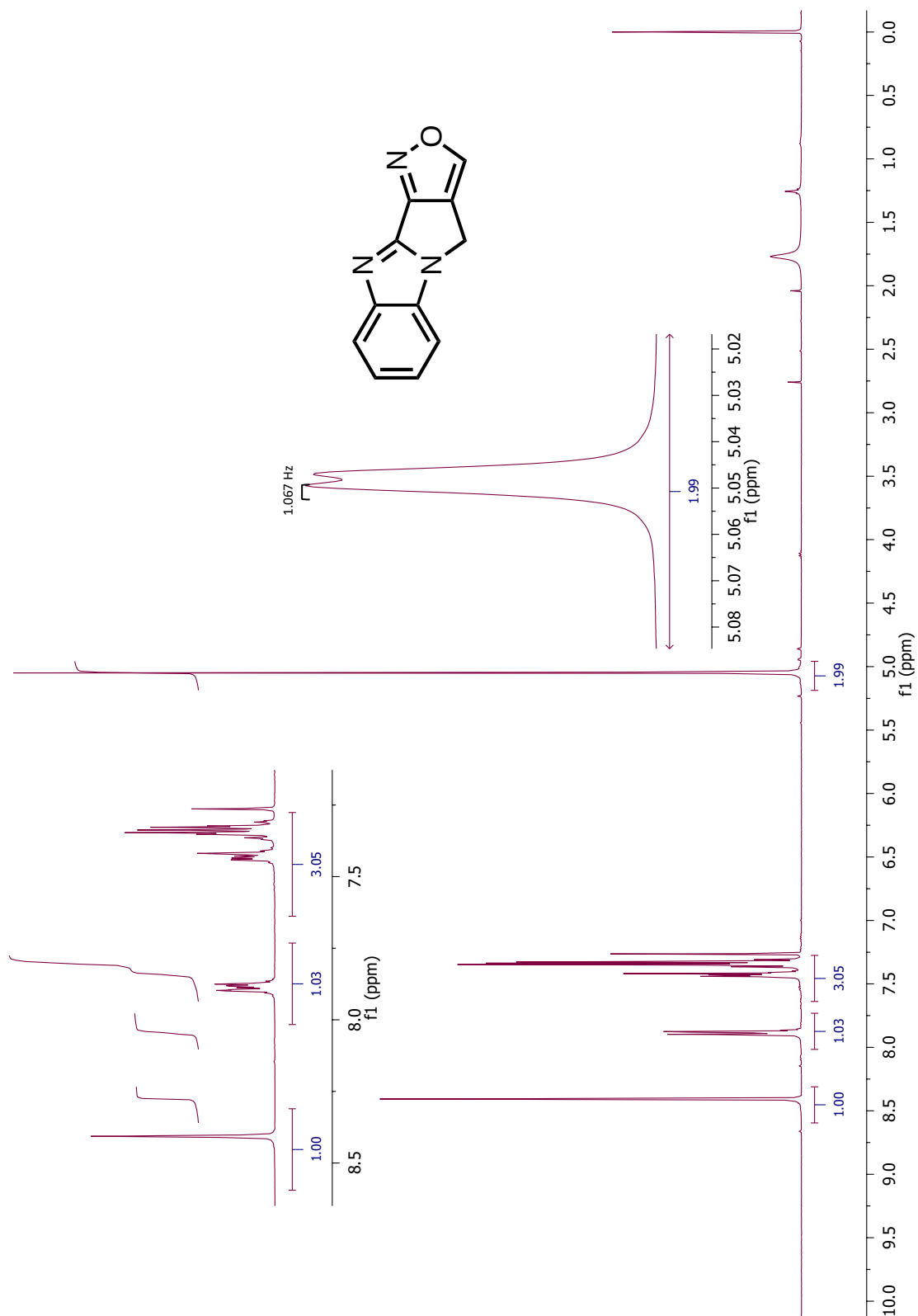
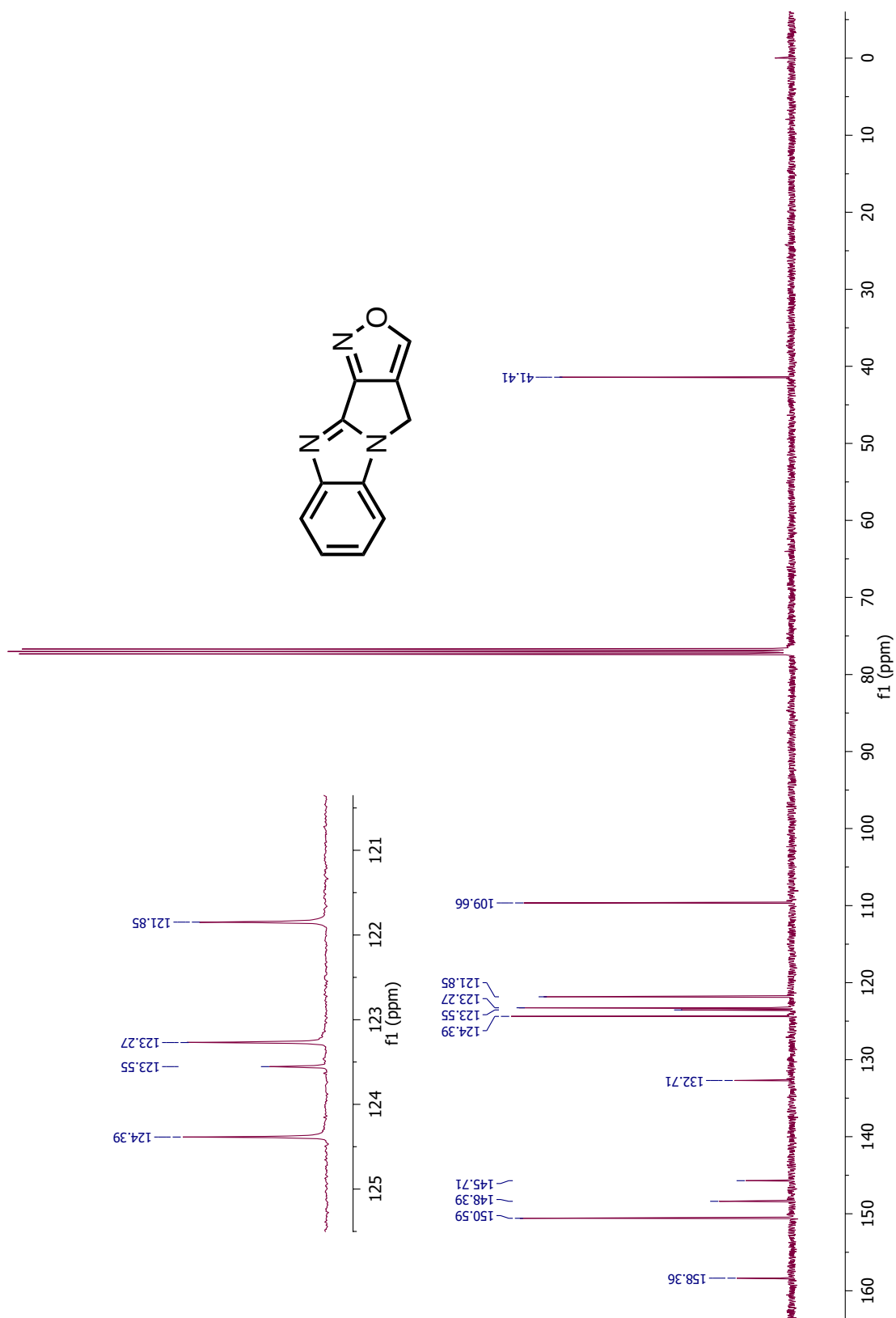


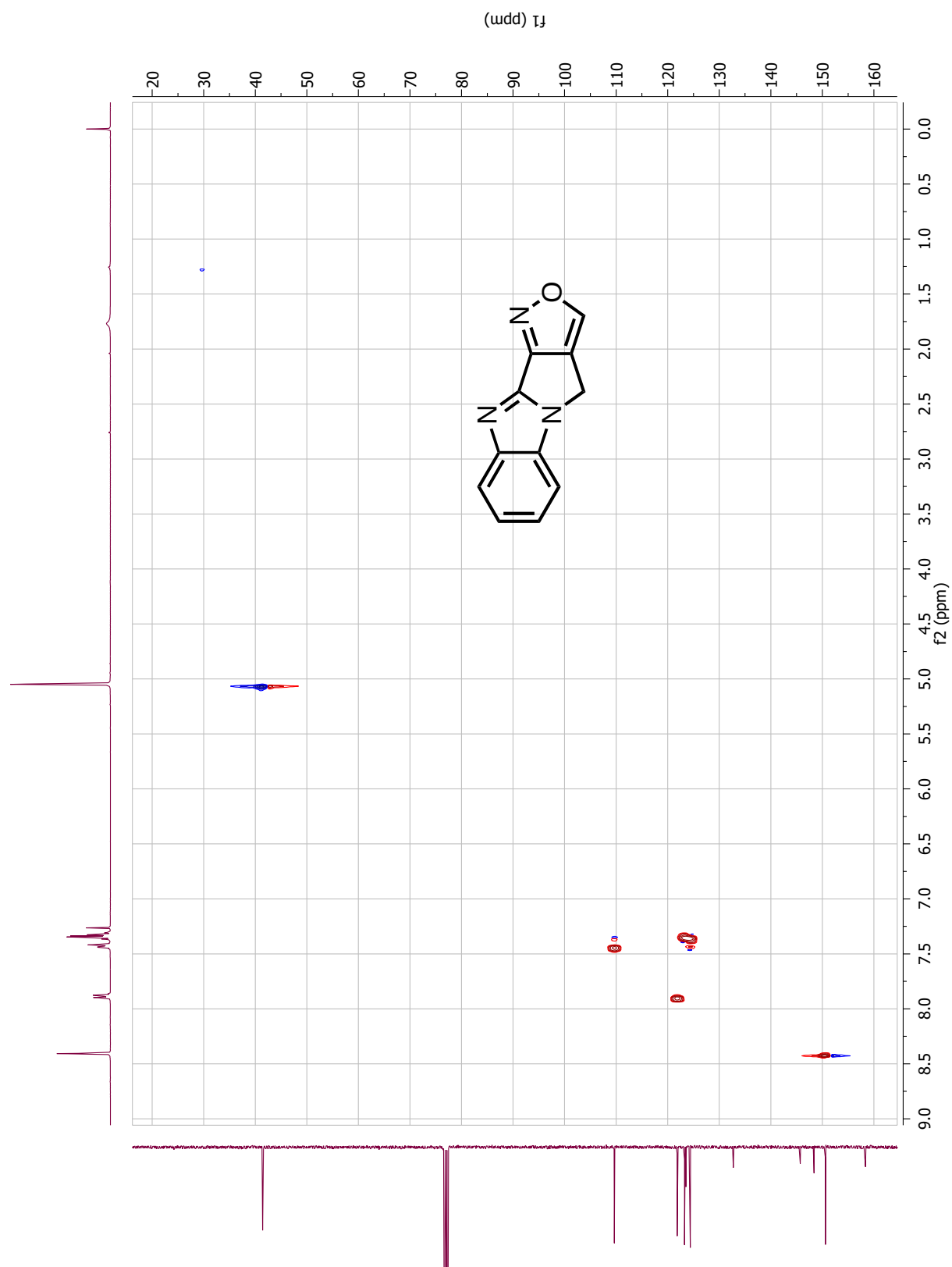
Figure S2. Spectral data of **6**: isoxazolo-4*H*-[3',4':3,4]pyrrolo[1,2-*a*]benzimidazole
 S2.1 ^1H -NMR of isoxazolo-4*H*-[3',4':3,4]pyrrolo[1,2-*a*]benzimidazole (CDCl_3) (**6**)



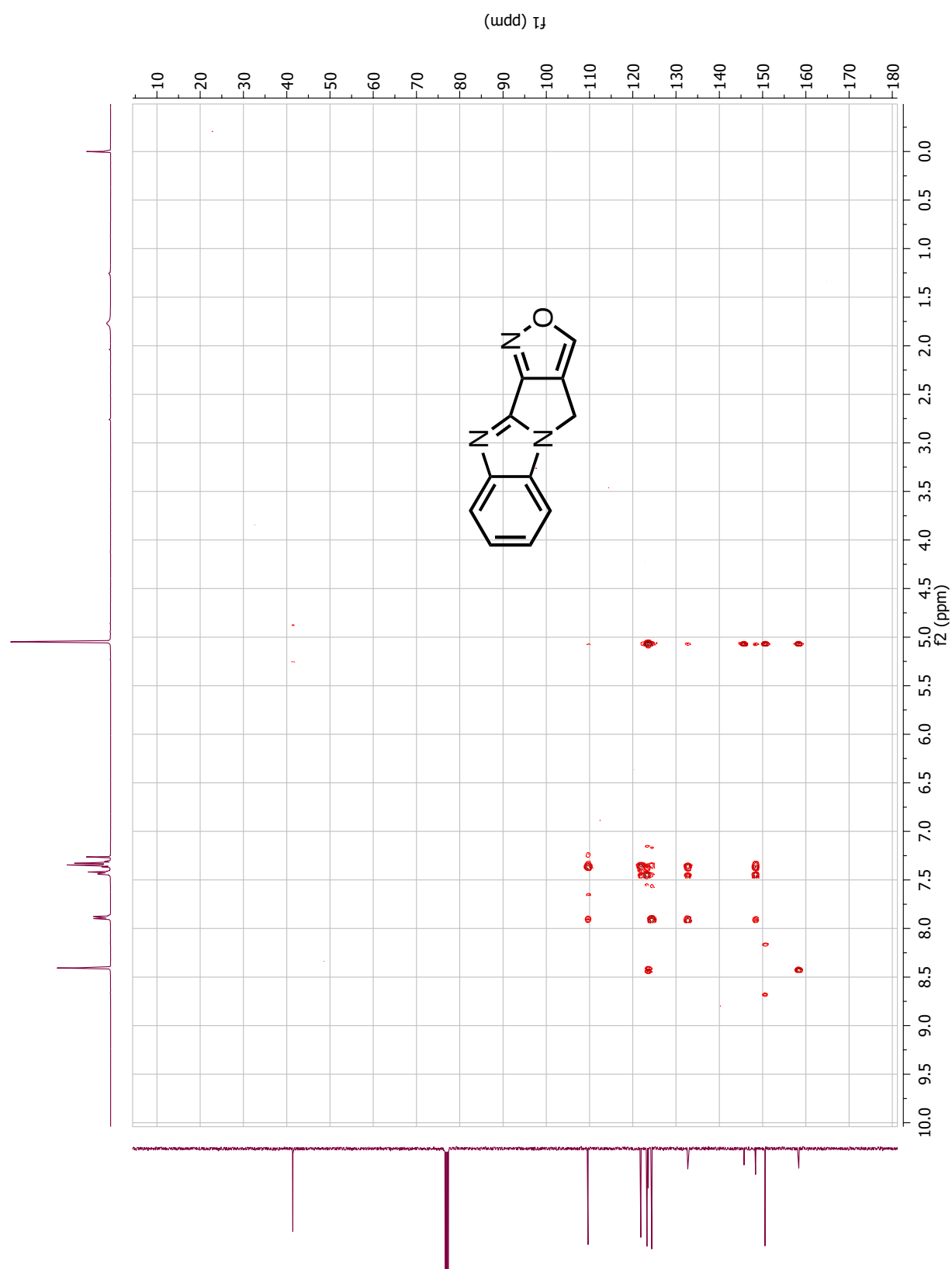
S2.2 ^{13}C -NMR of isoxazolo-4*H*-[3',4':3,4]pyrrolo[1,2-*a*]benzimidazole (CDCl_3) (**6**)



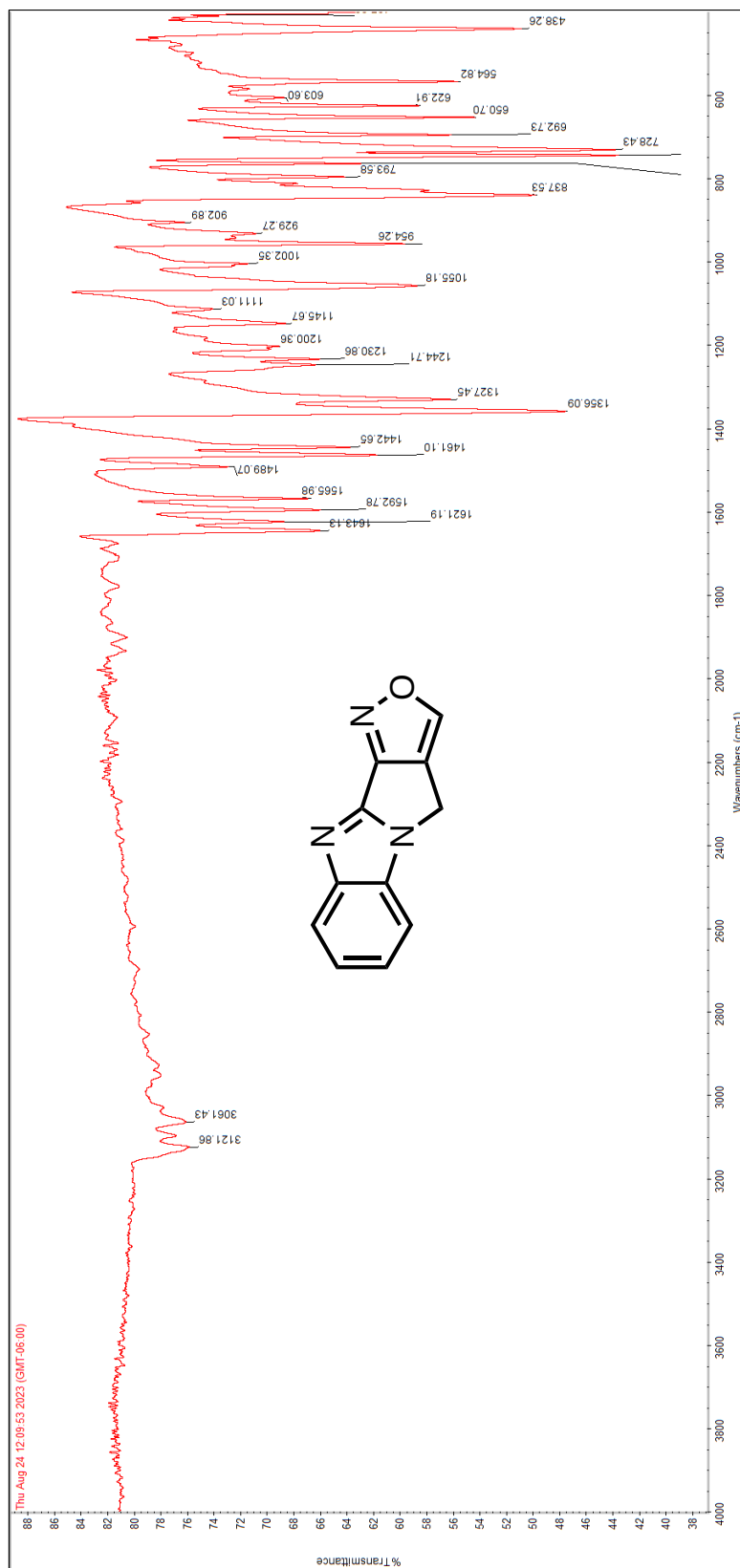
S2.3 HSQC of isoxazolo-4*H*-[3',4':3,4]pyrrolo[1,2-*a*]benzimidazole (CDCl₃) (**6**)



S2.4 HMBC of isoxazolo-4*H*-[3',4':3,4]pyrrolo[1,2-*a*]benzimidazole (CDCl₃) (**6**)



S2.5 FT-IR of isoxazolo-4*H*-[3',4':3,4]pyrrolo[1,2-*a*]benzimidazole (**6**)



S2.6 HRMS of isoxazolo-4*H*-[3',4':3,4]pyrrolo[1,2-*a*]benzimidazole (6)

