

# **Synthesis of Benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole Derivatives via C-H Bond Functionalization of Disulfide Intermediates**

Luis G. Ardón-Muñoz, Jeanne L. Bolliger\*

Department of Chemistry, 107 Physical Sciences, Oklahoma State University, Stillwater, OK,  
74078, United States.

Corresponding Author: [jeanne.bolliger@okstate.edu](mailto:jeanne.bolliger@okstate.edu)

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## 1. NMR Spectra of Isolated Compounds

### 1.1 NMR Spectra of 2-Fluoronitrobenzene Starting Materials

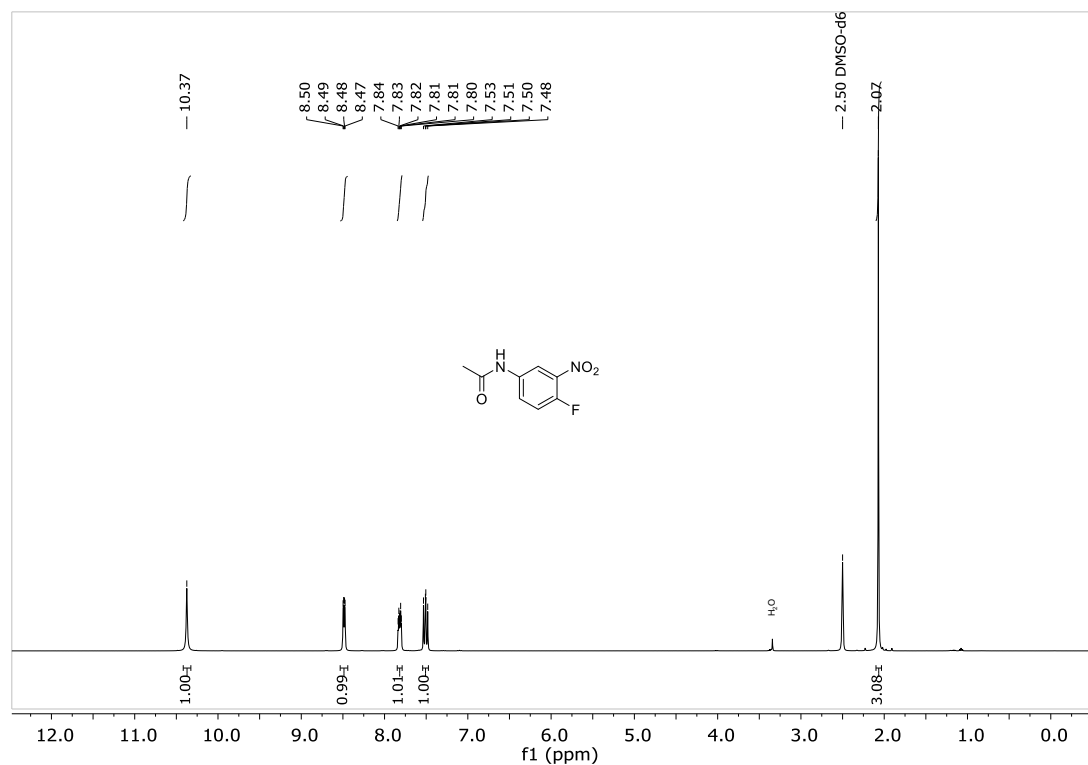


Figure S001: <sup>1</sup>H NMR spectrum of *N*-(4-Fluoro-3-nitrophenyl)acetamide (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).

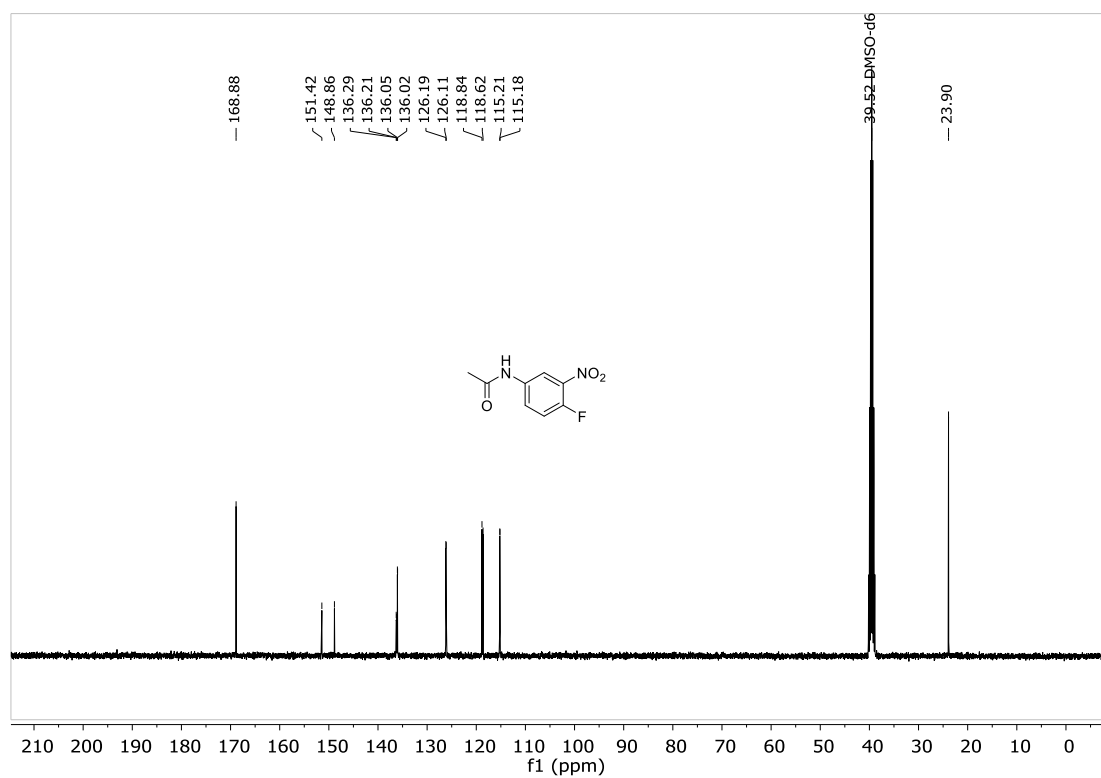
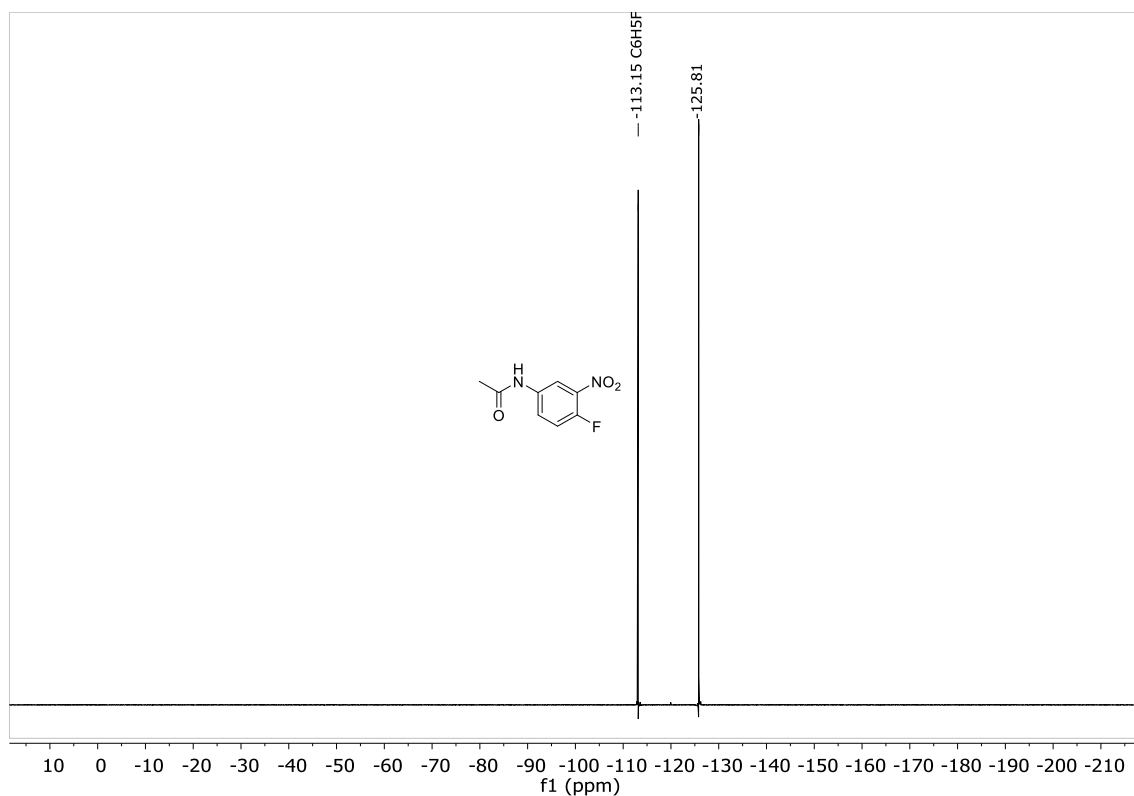
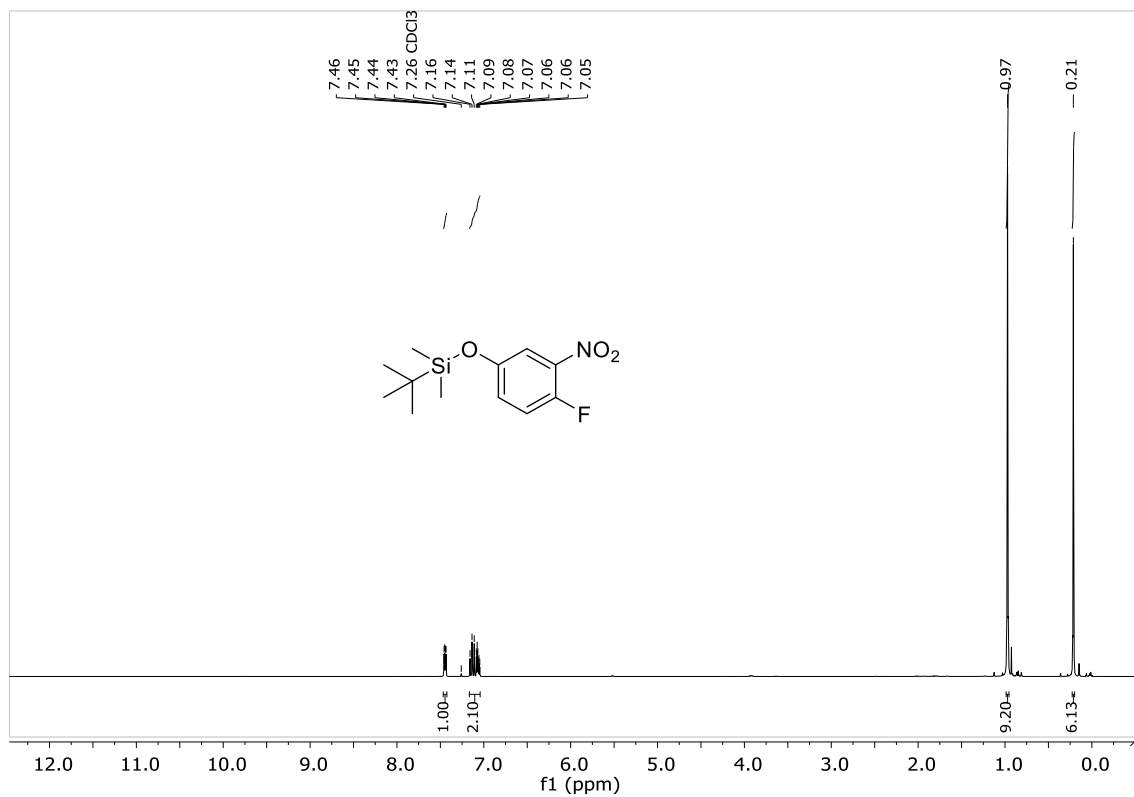


Figure S002: <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of *N*-(4-Fluoro-3-nitrophenyl)acetamide (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).

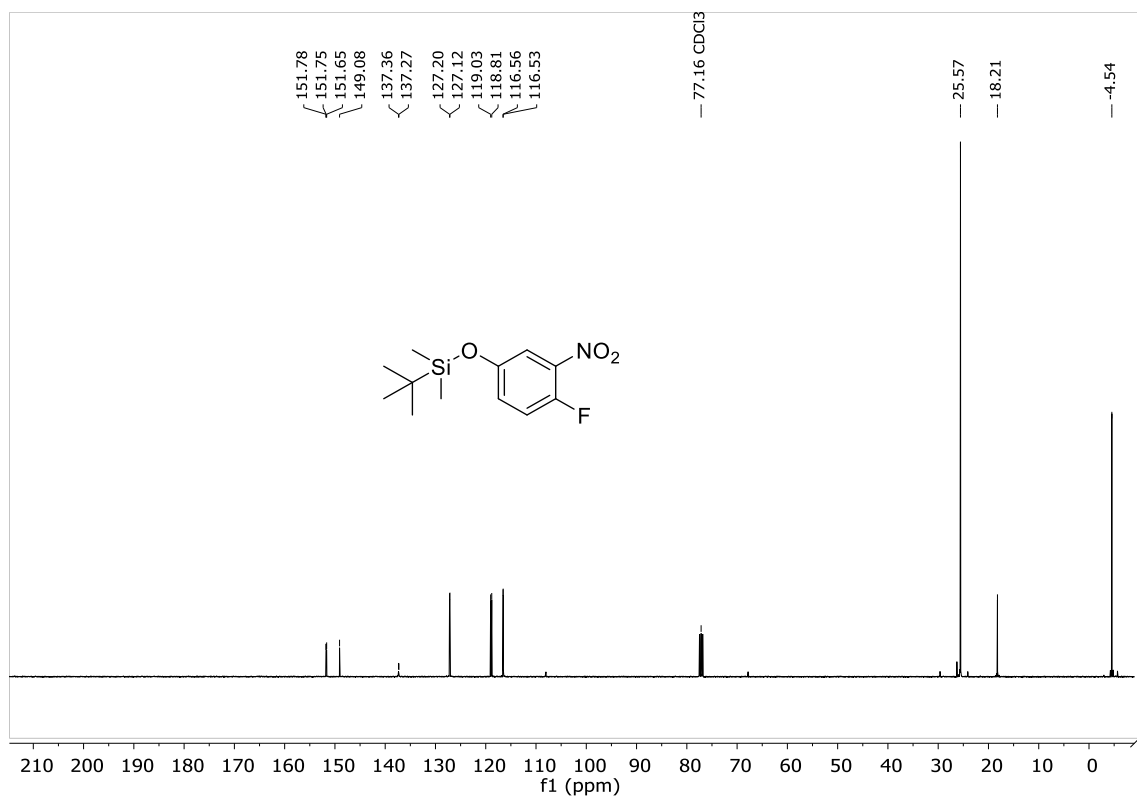


**Figure S003:**  $^{19}\text{F}\{^1\text{H}\}$  NMR spectrum of *N*-(4-fluoro-3-nitrophenyl)acetamide (376 MHz,  $\text{DMSO}-d_6$ , 298 K, referenced to fluorobenzene).

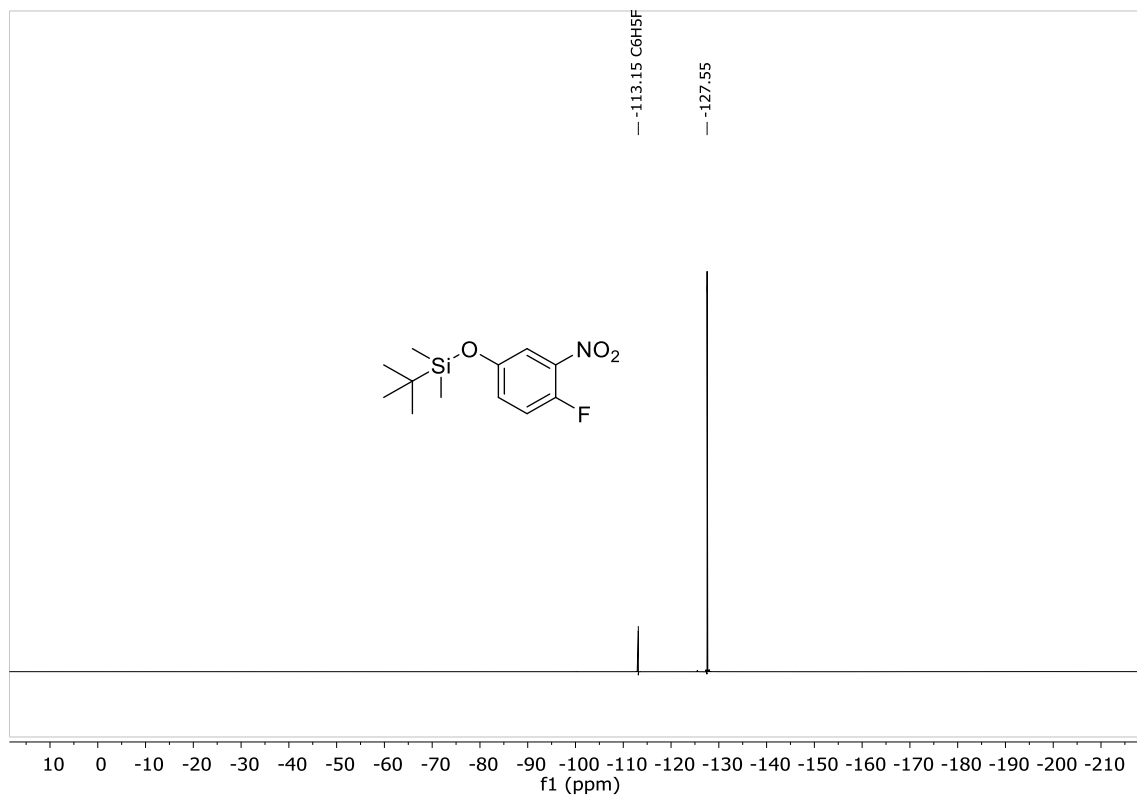


**Figure S004:**  $^1\text{H}$  NMR spectrum of *tert*-butyl(4-fluoro-3-nitrophenoxy)dimethylsilane (400 MHz,  $\text{CDCl}_3$ , 298 K).



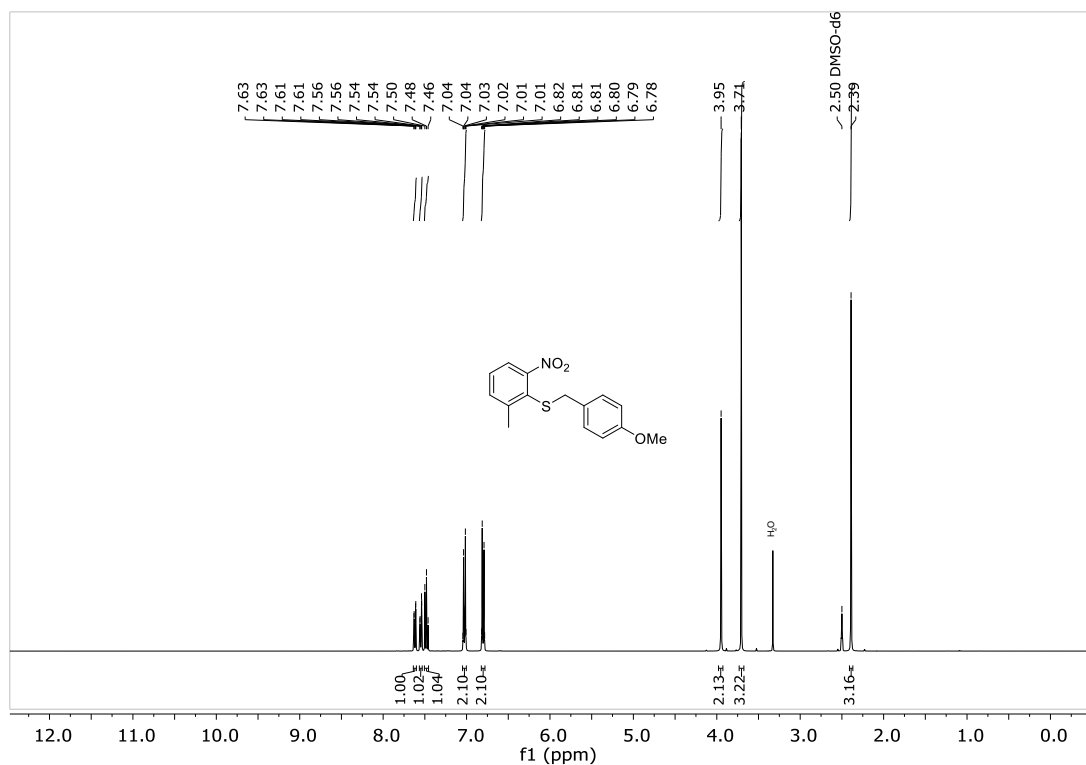


**Figure S005:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of *tert*-butyl(4-fluoro-3-nitrophenoxy)dimethylsilane (100 MHz,  $\text{CDCl}_3$ , 298 K).

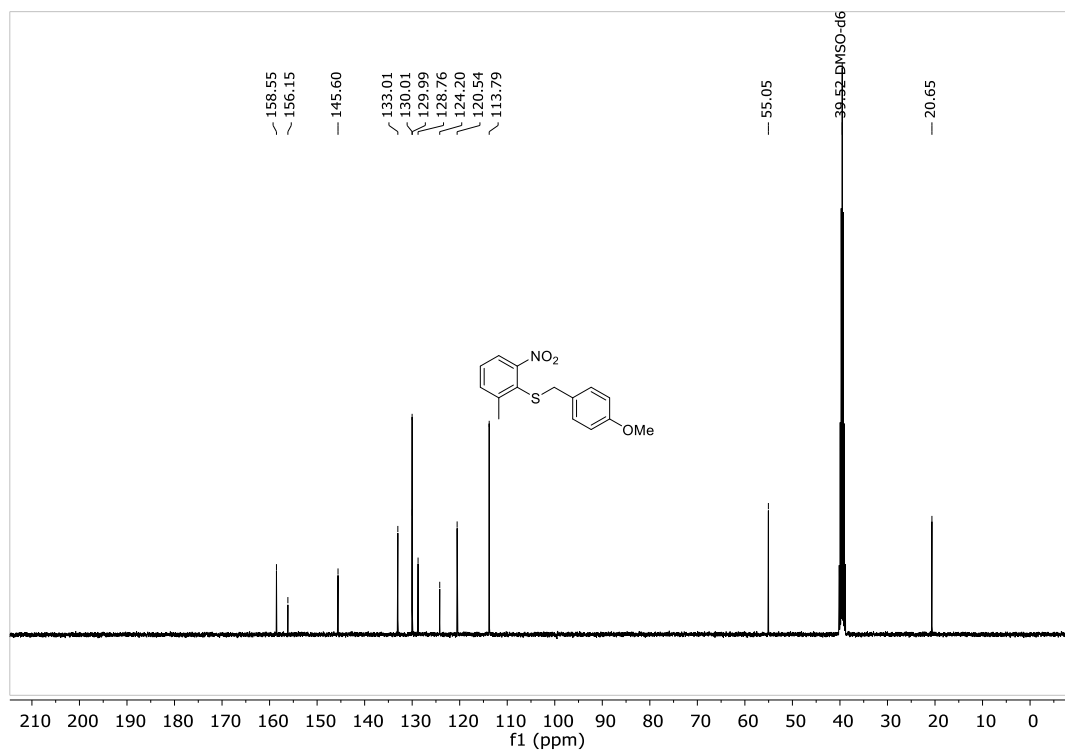


**Figure S006:**  $^{19}\text{F}\{^1\text{H}\}$  NMR spectrum of *tert*-butyl(4-fluoro-3-nitrophenoxy)dimethylsilane (376 MHz,  $\text{CDCl}_3$ , 298 K, referenced to fluorobenzene).

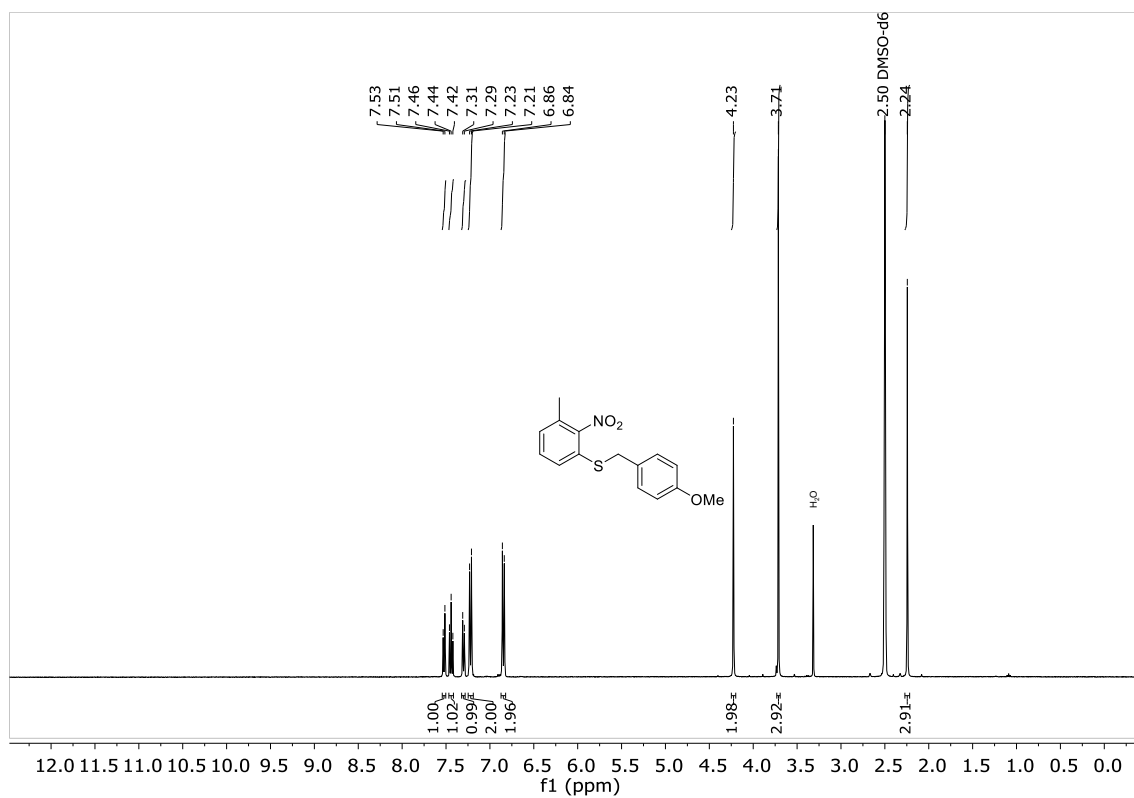
**1.2 NMR Spectra of Substituted (4-Methoxybenzyl)(2-nitrophenyl)sulfanes (1b-1r)**



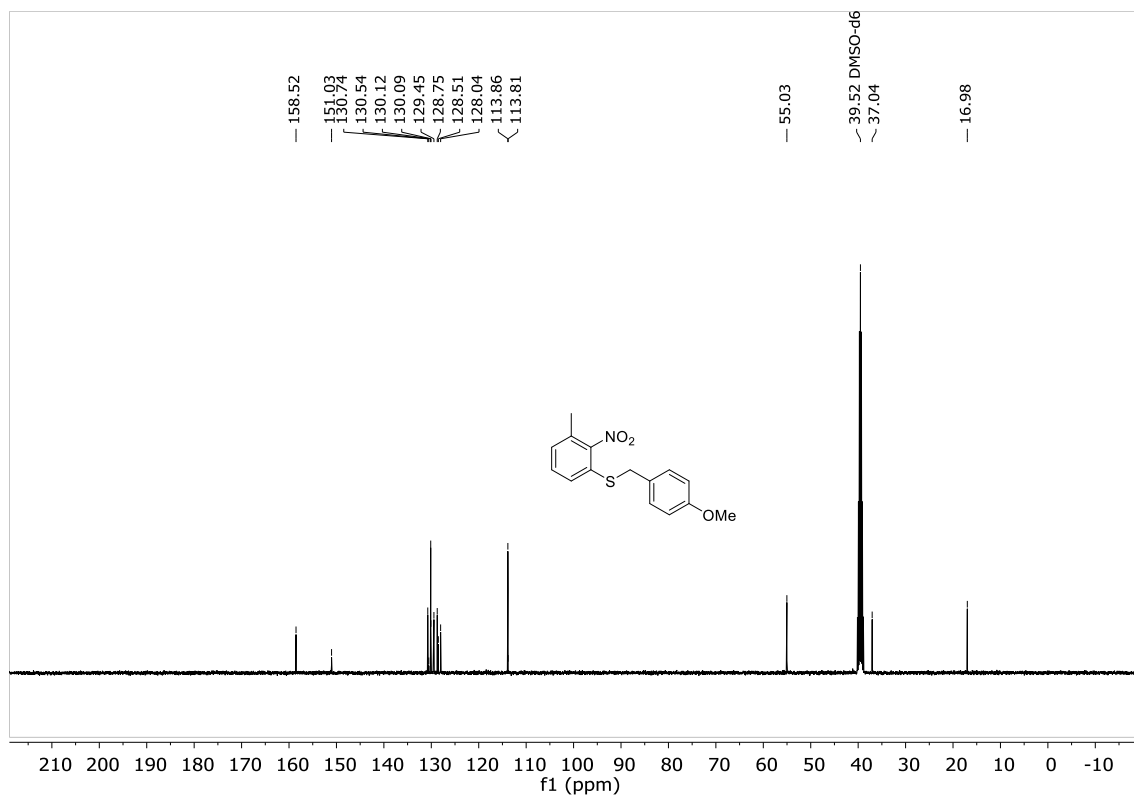
**Figure S007:** <sup>1</sup>H NMR spectrum of (4-methoxybenzyl)(2-methyl-6-nitrophenyl)sulfane (**1b**) (400 MHz, DMSO-d<sub>6</sub>, 298 K).



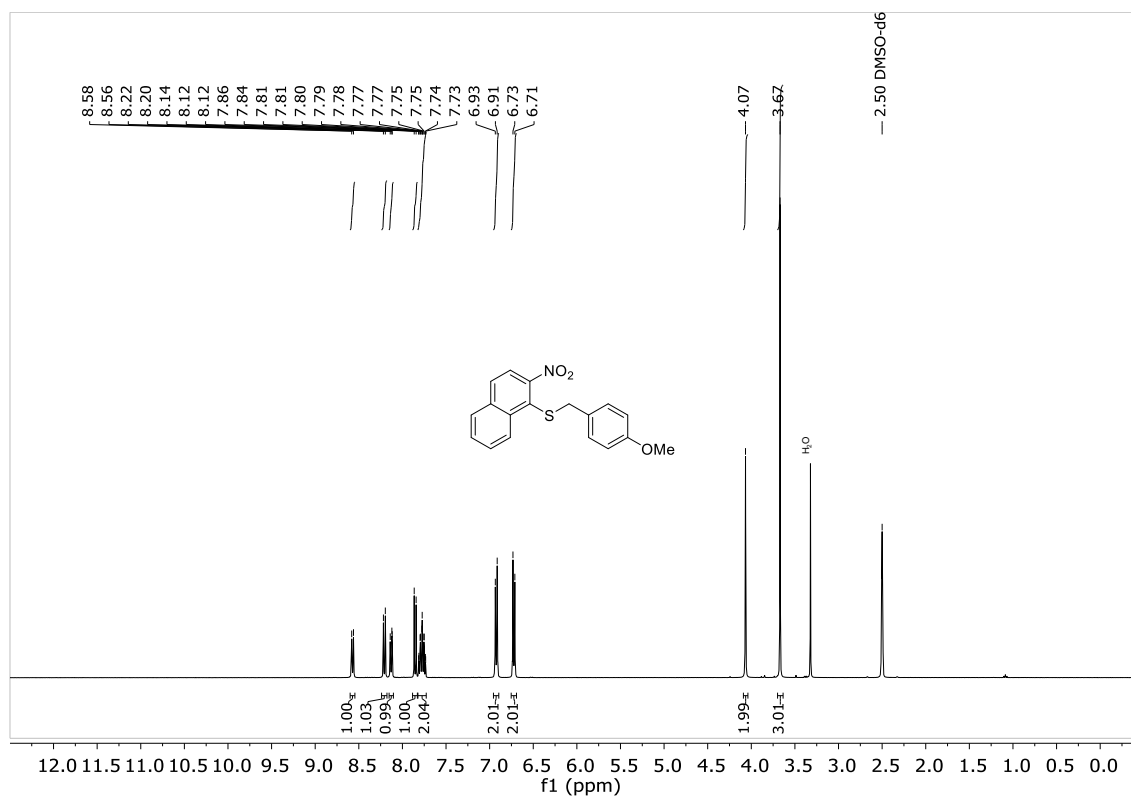
**Figure S008:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of (4-methoxybenzyl)(2-methyl-6-nitrophenyl)sulfane (**1b**) (100 MHz, DMSO-d<sub>6</sub>, 298 K).



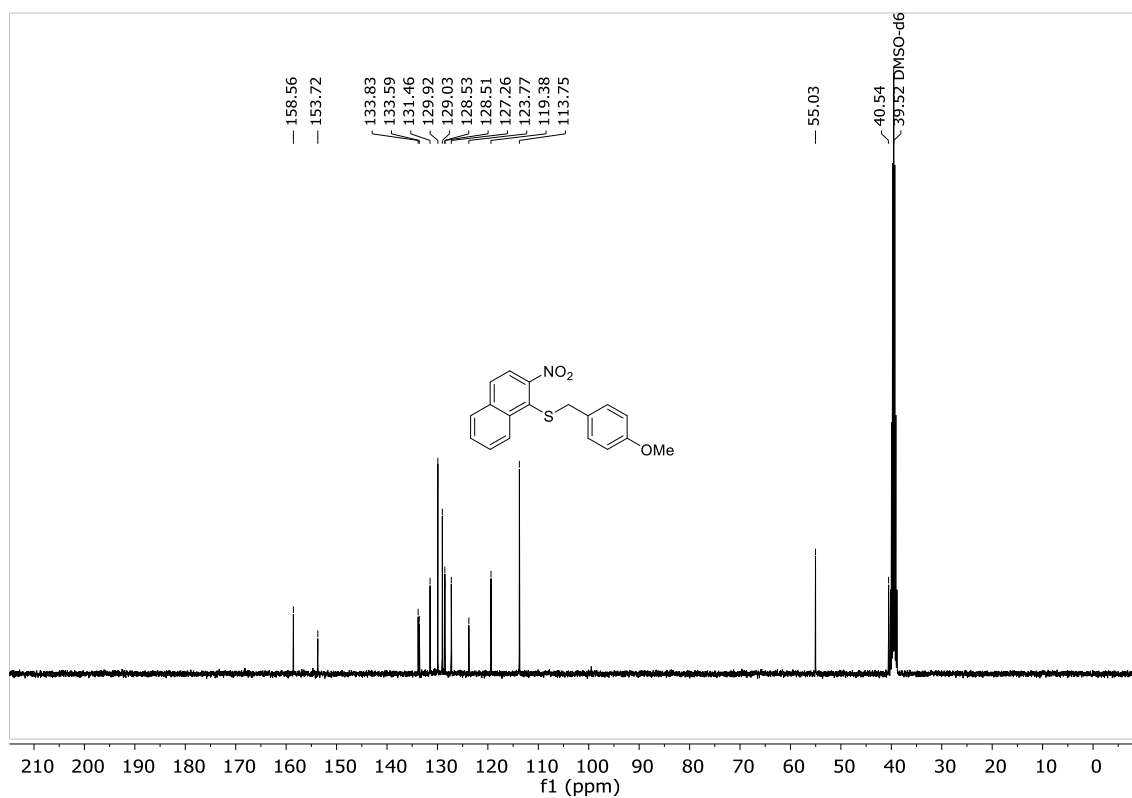
**Figure S009:** <sup>1</sup>H NMR spectrum of (4-methoxybenzyl)(3-methyl-2-nitrophenyl)sulfane (**1c**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



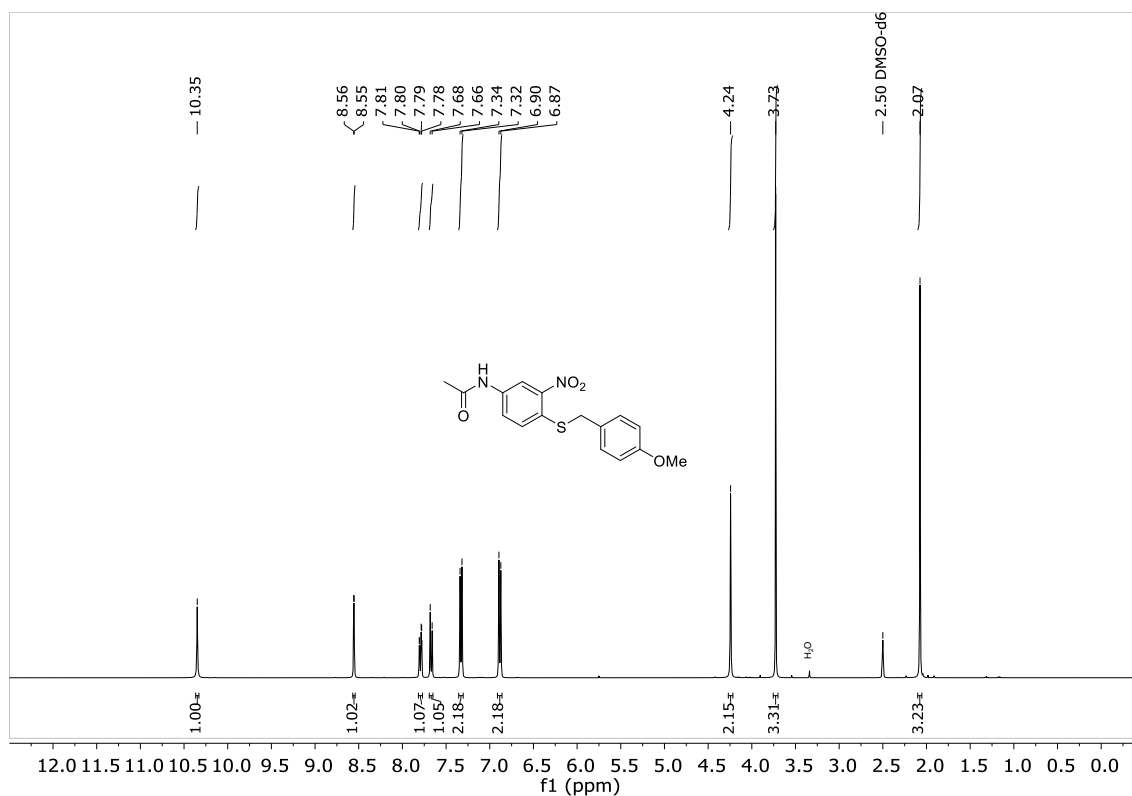
**Figure S010:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of (4-methoxybenzyl)(3-methyl-2-nitrophenyl)sulfane (**1c**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



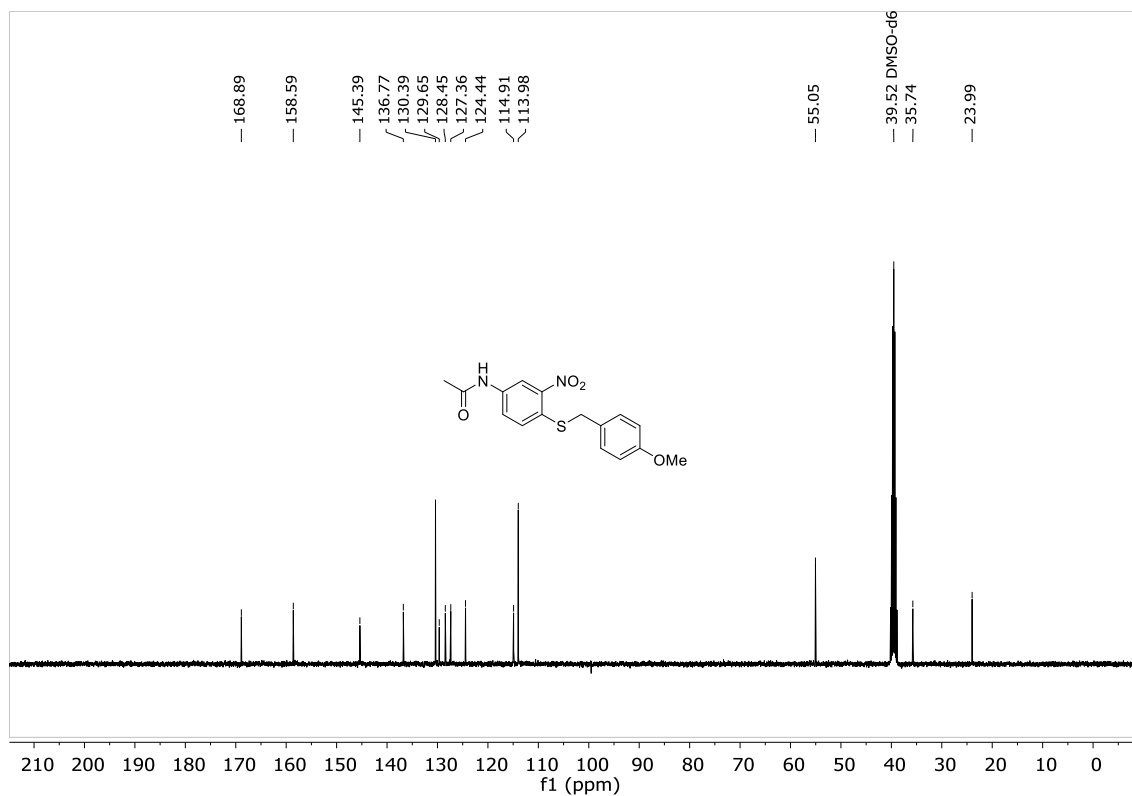
**Figure S011:** <sup>1</sup>H NMR spectrum of (4-methoxybenzyl)(2-nitronaphthalen-1-yl)sulfane (**1d**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



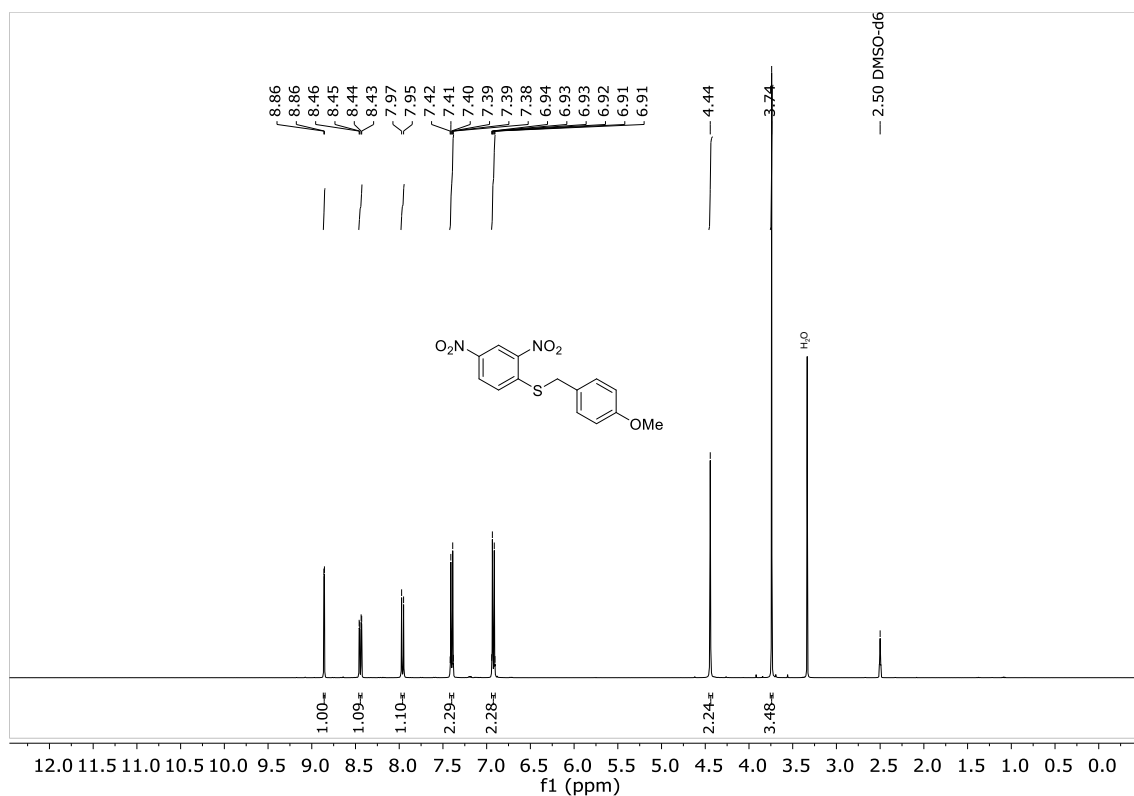
**Figure S012:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of (4-methoxybenzyl)(2-nitronaphthalen-1-yl)sulfane (**1d**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



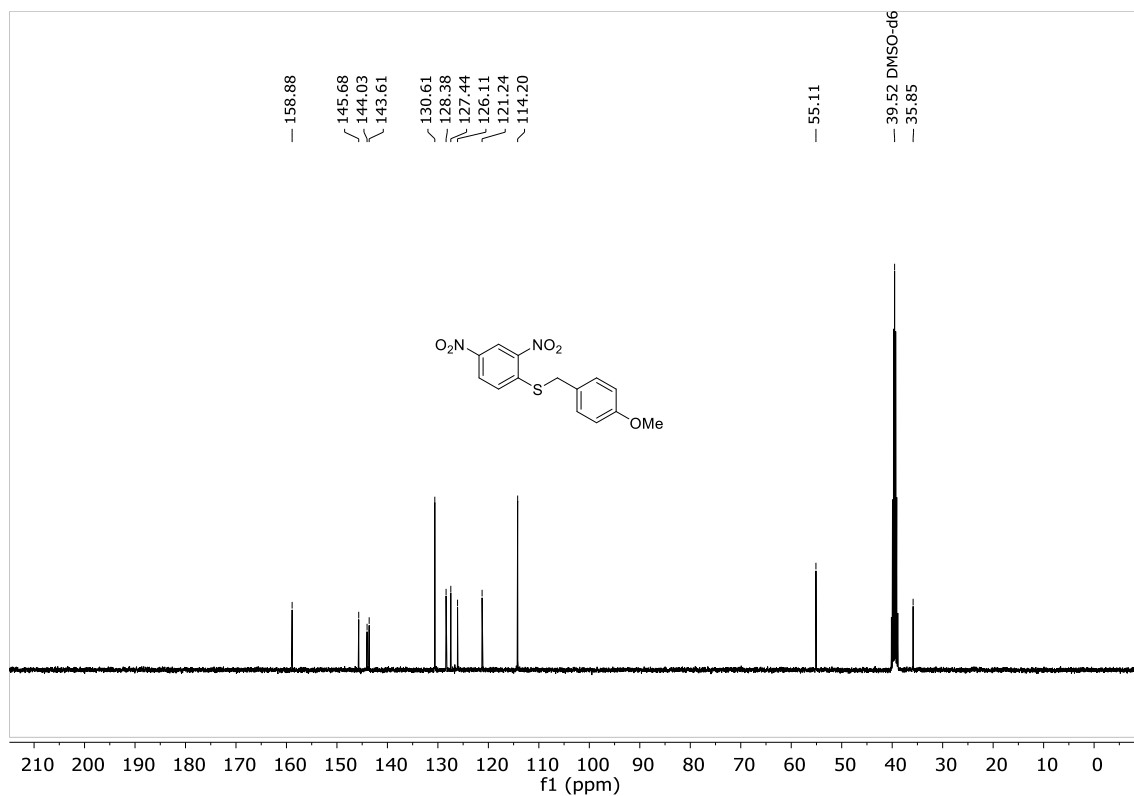
**Figure S013:**  $^1\text{H}$  NMR spectrum of *N*-(4-((4-methoxybenzyl)thio)-3-nitrophenyl)acetamide (**1f**) (400 MHz,  $\text{DMSO-}d_6$ , 298 K).



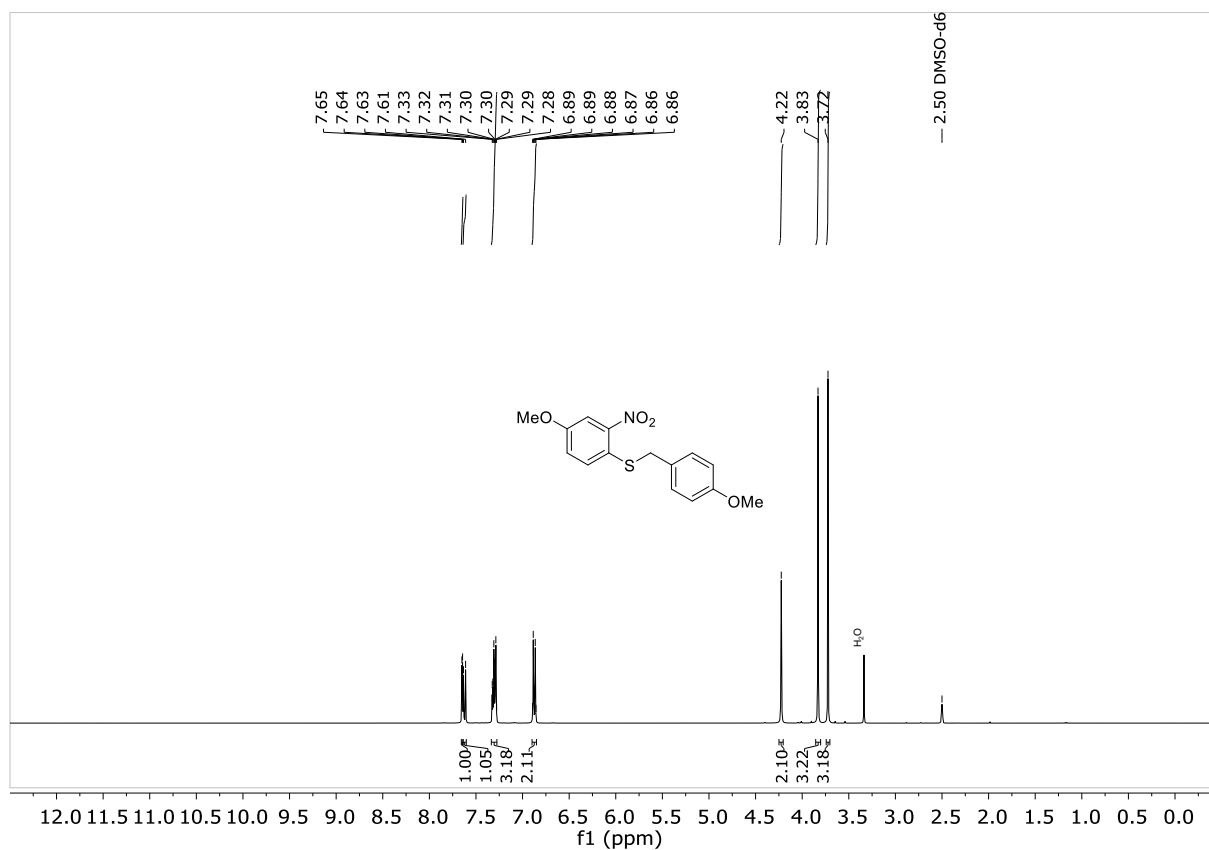
**Figure S014:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of *N*-(4-((4-methoxybenzyl)thio)-3-nitrophenyl)acetamide (**1f**) (100 MHz,  $\text{DMSO-}d_6$ , 298 K).



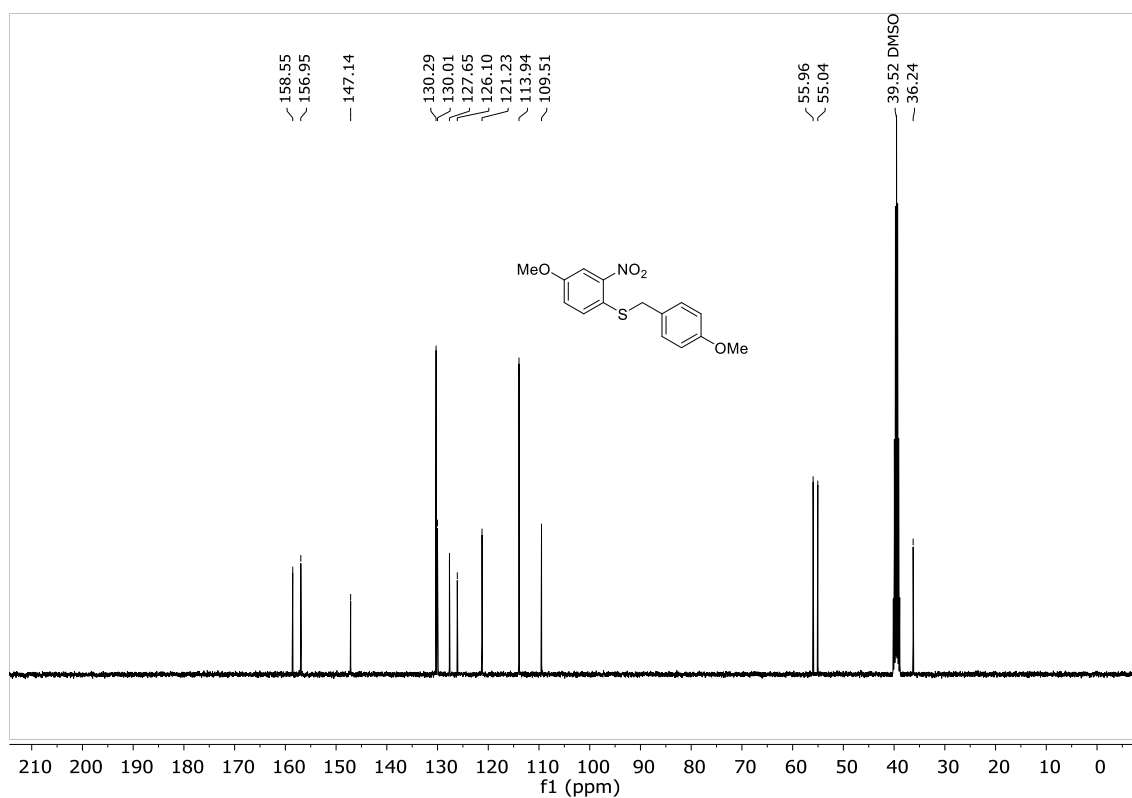
**Figure S0015:** <sup>1</sup>H NMR spectrum of (2,4-dinitrophenyl)(4-methoxybenzyl)sulfane (**1e**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



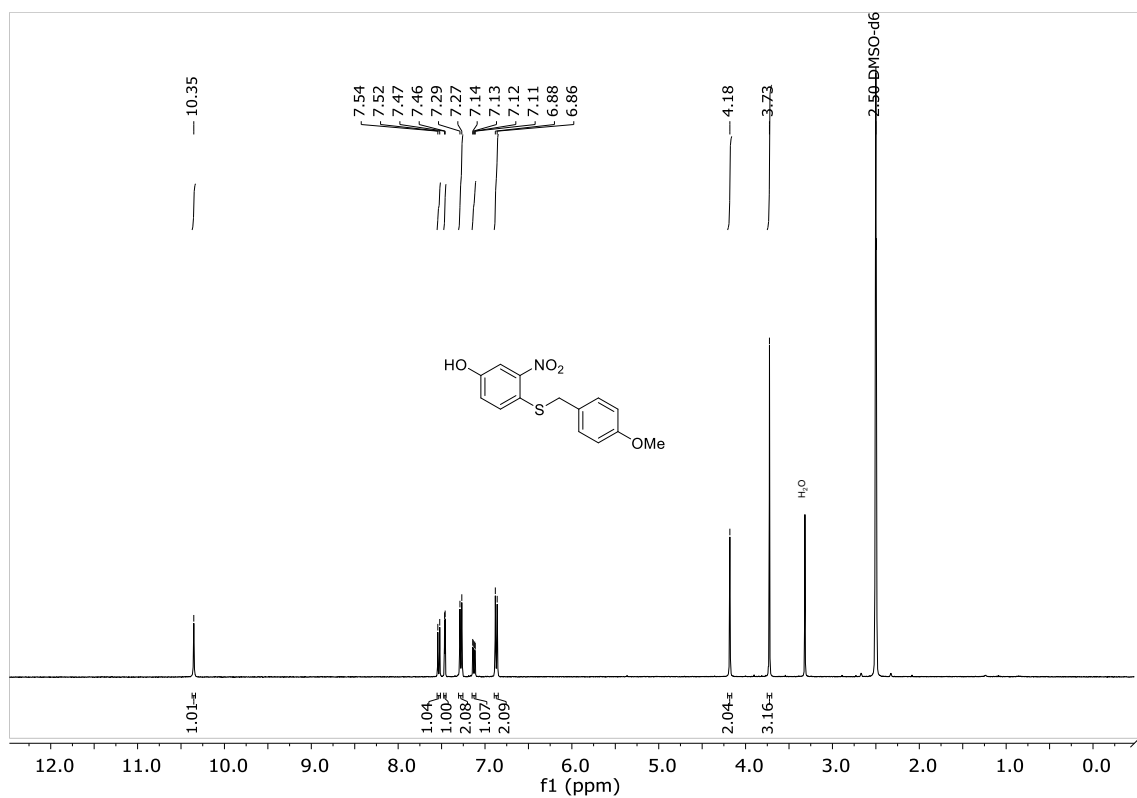
**Figure S016:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of (2,4-dinitrophenyl)(4-methoxybenzyl)sulfane (**1e**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



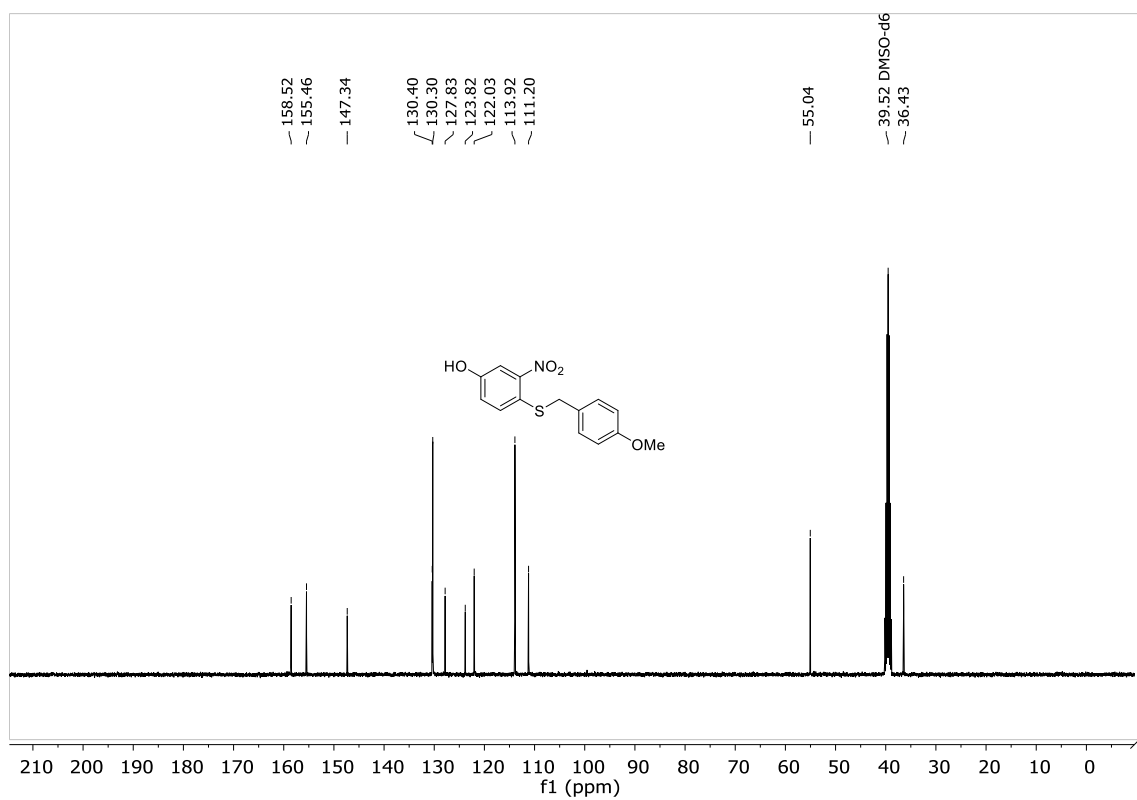
**Figure S017:** <sup>1</sup>H NMR spectrum of (4-methoxy-2-nitrophenyl)(4-methoxybenzyl)sulfane (**1g**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



**Figure S018:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of (4-methoxy-2-nitrophenyl)(4-methoxybenzyl)sulfane (**1g**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).

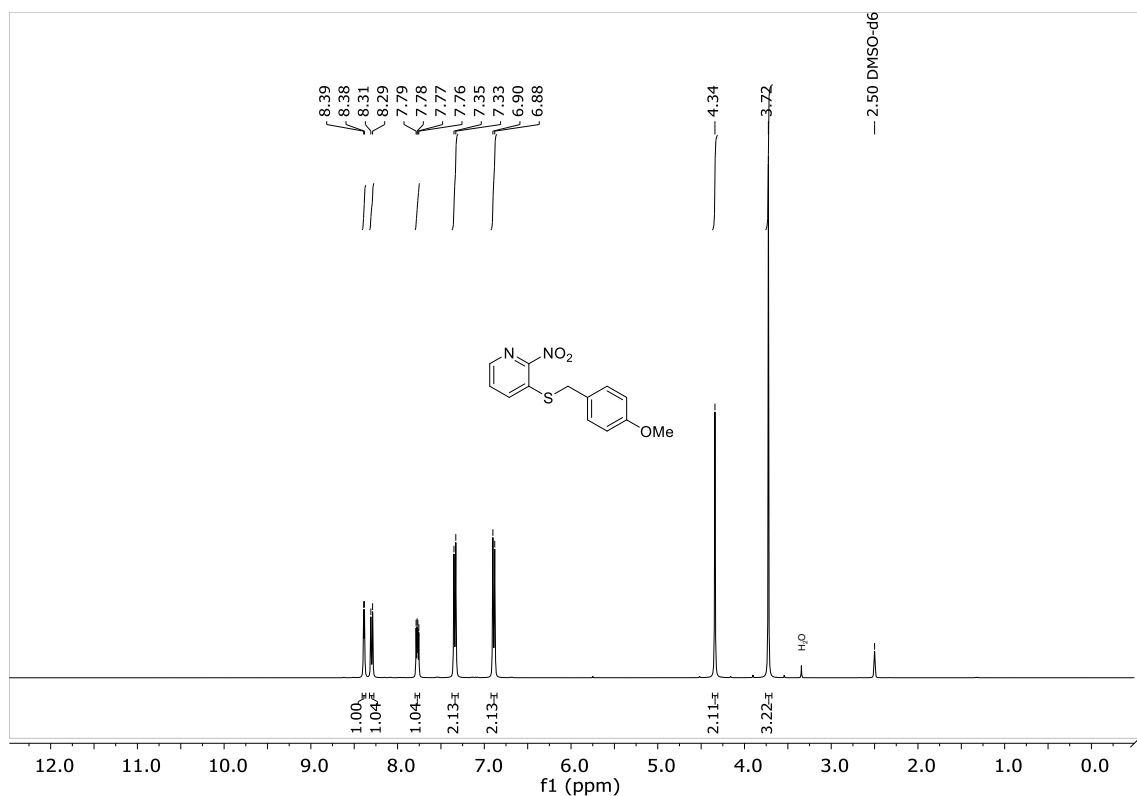


**Figure S019:** <sup>1</sup>H NMR spectrum of 4-((4-methoxybenzyl)thio)-3-nitrophenol (**1h**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).

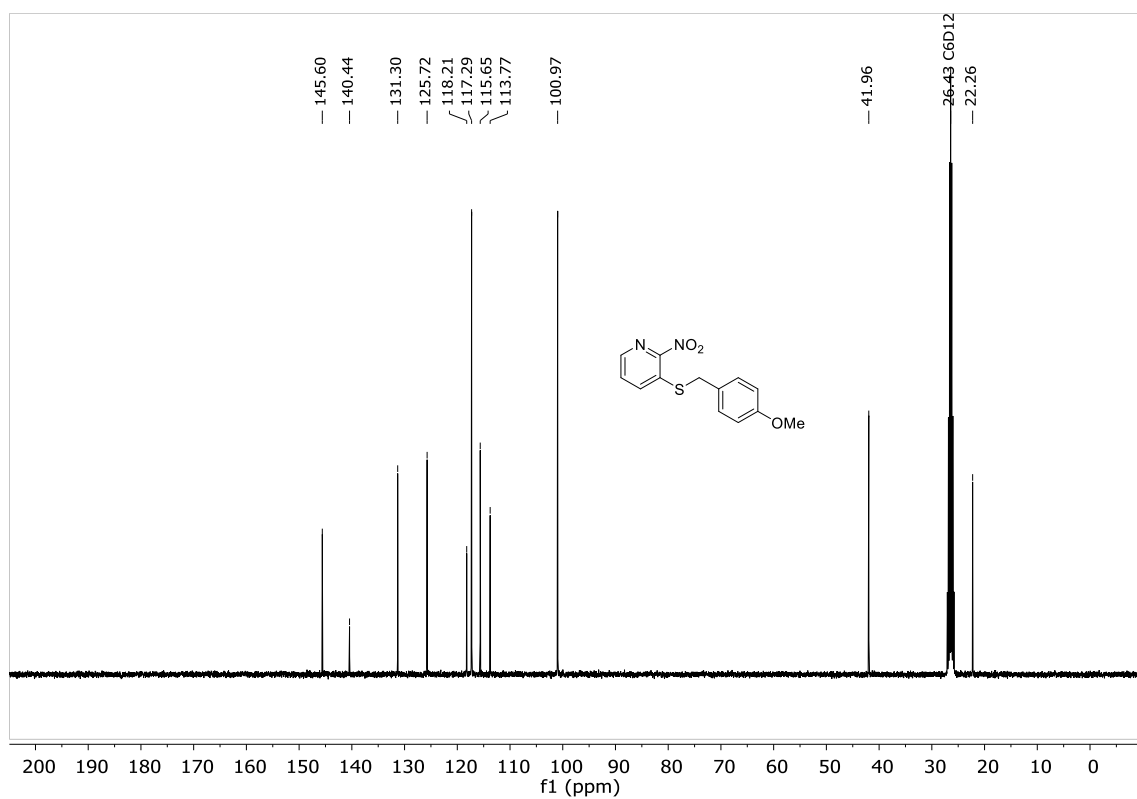


**Figure S020:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 4-((4-methoxybenzyl)thio)-3-nitrophenol (**1h**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).

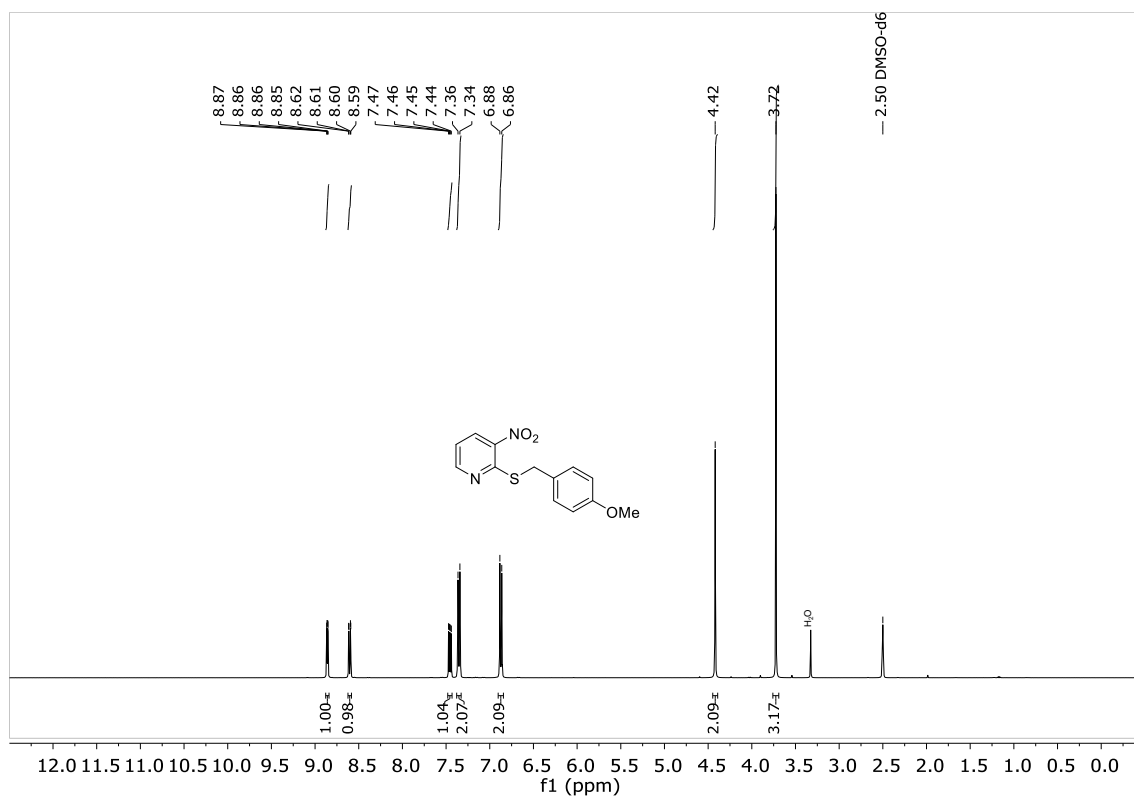




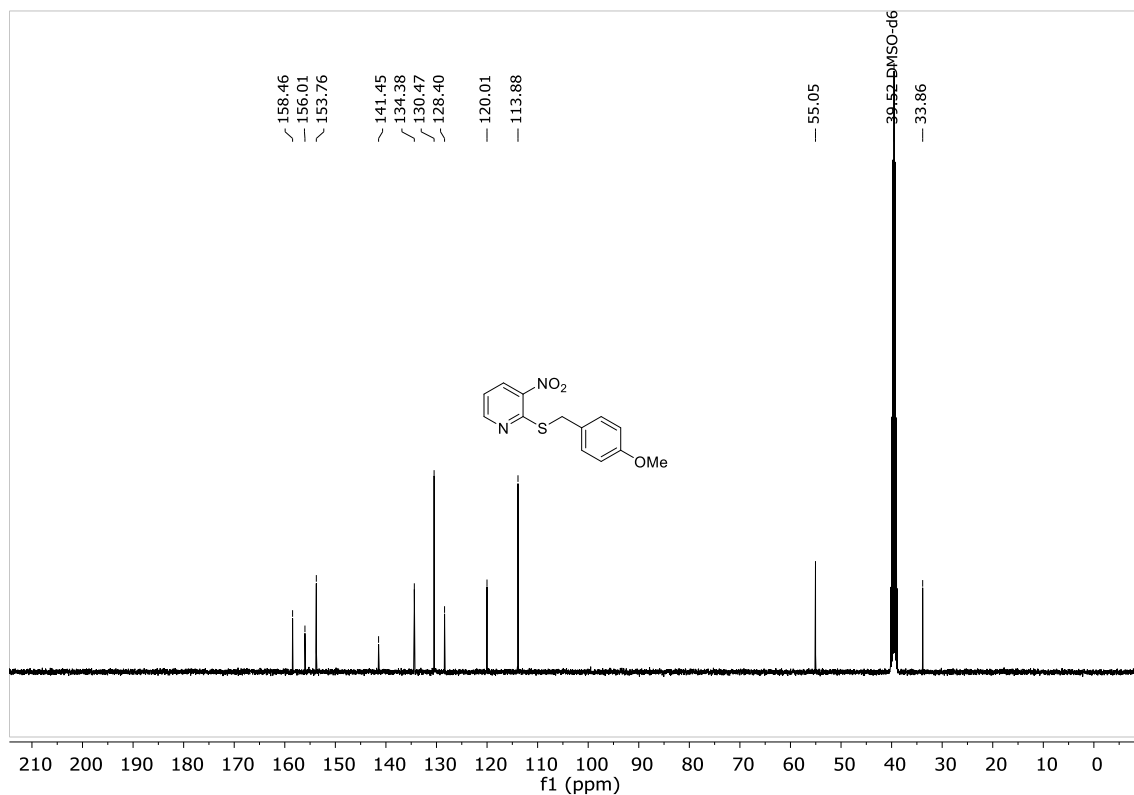
**Figure S021:** <sup>1</sup>H NMR spectrum of 3-((4-methoxybenzyl)thio)-2-nitropyridine (**1i**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



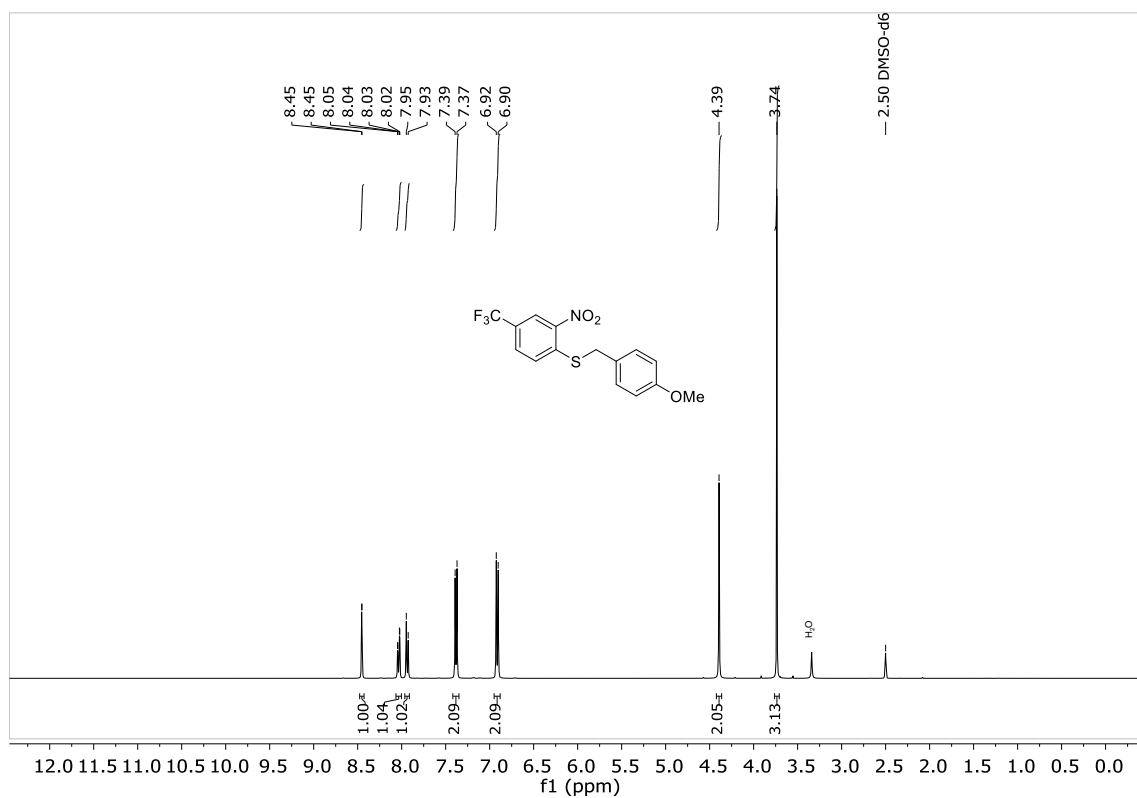
**Figure S022:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 3-((4-methoxybenzyl)thio)-2-nitropyridine (**1i**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



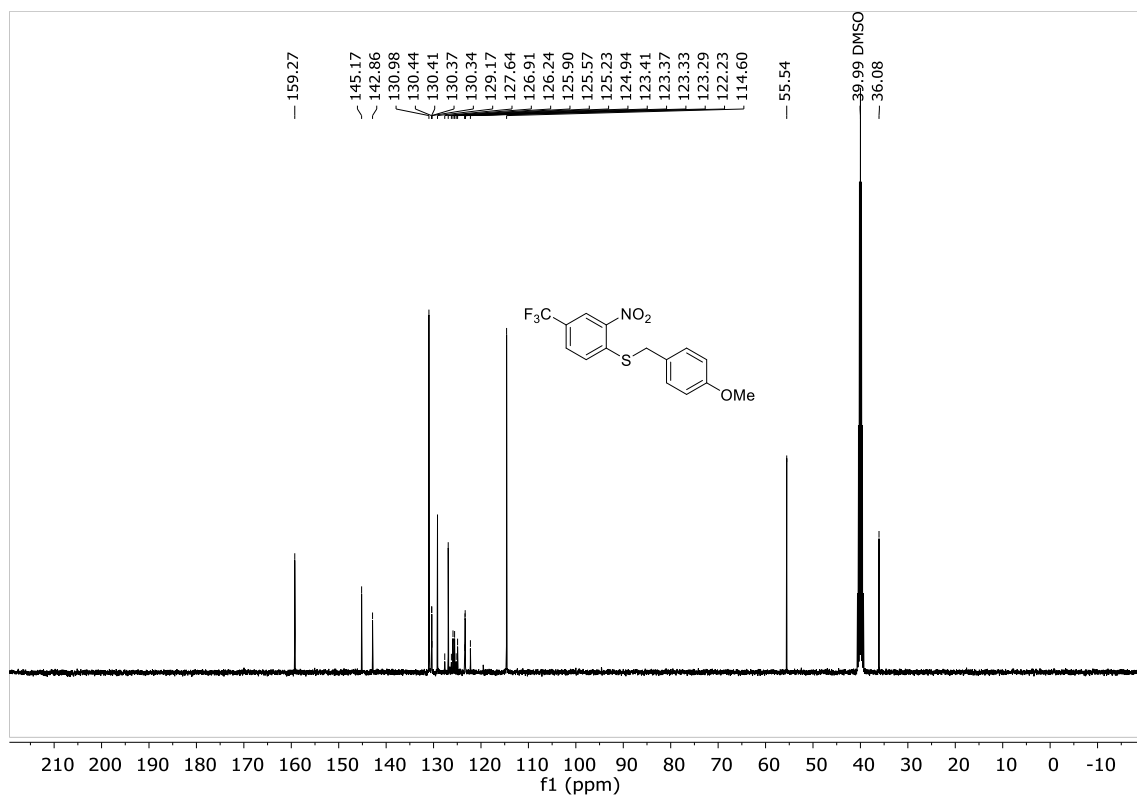
**Figure S023:** <sup>1</sup>H NMR spectrum of 2-((4-methoxybenzyl)thio)-3-nitropyridine (**1j**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



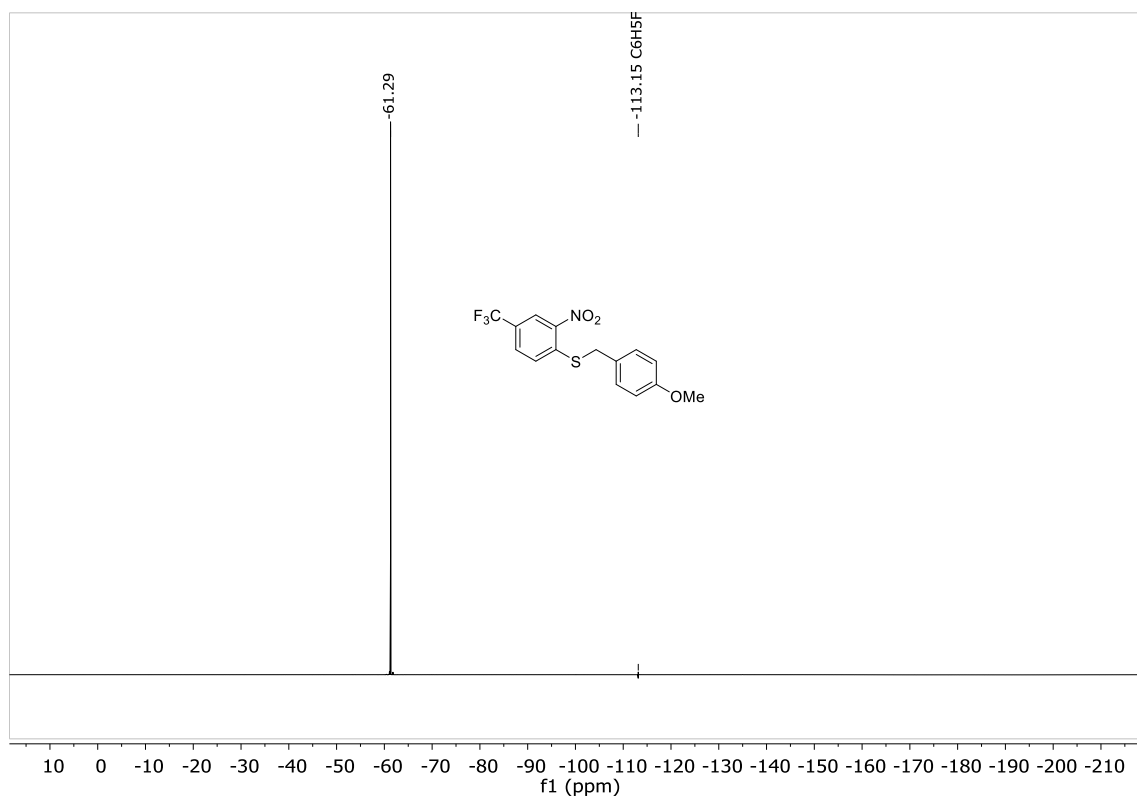
**Figure S024:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 2-((4-methoxybenzyl)thio)-3-nitropyridine (**1j**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



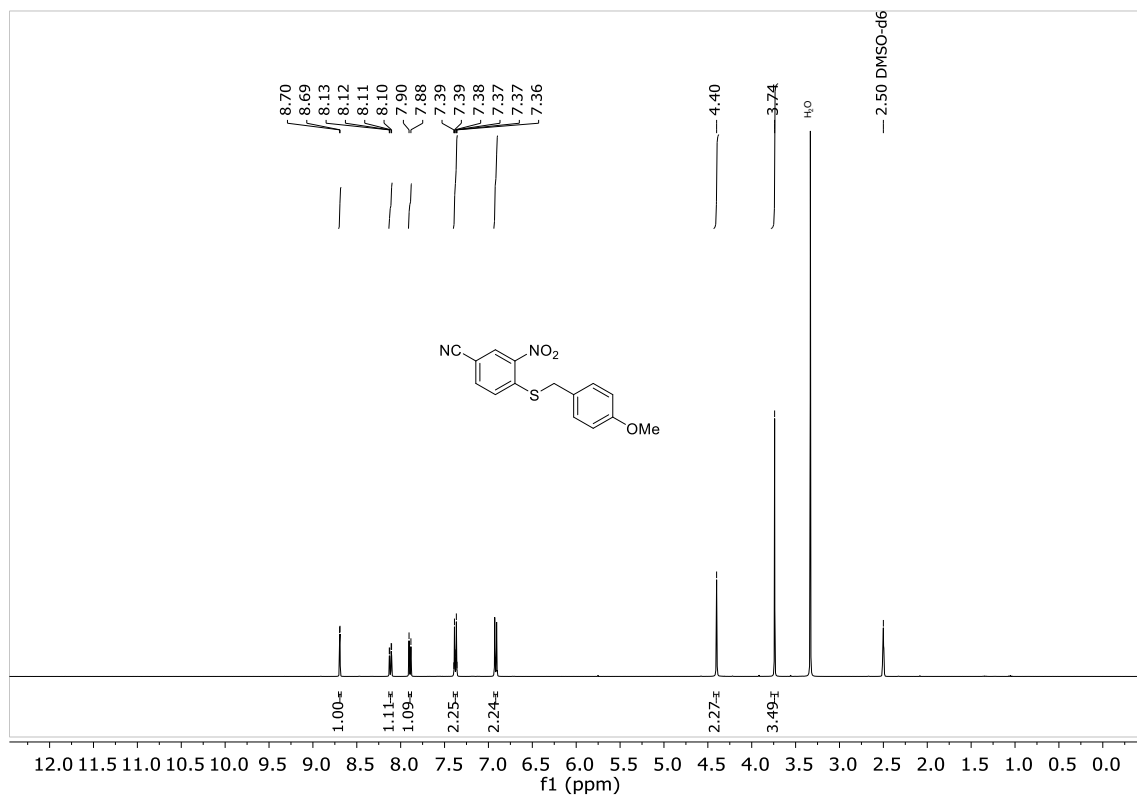
**Figure S025:** <sup>1</sup>H NMR spectrum of (4-methoxybenzyl)(2-nitro-4-(trifluoromethyl)phenyl)sulfane (**1k**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



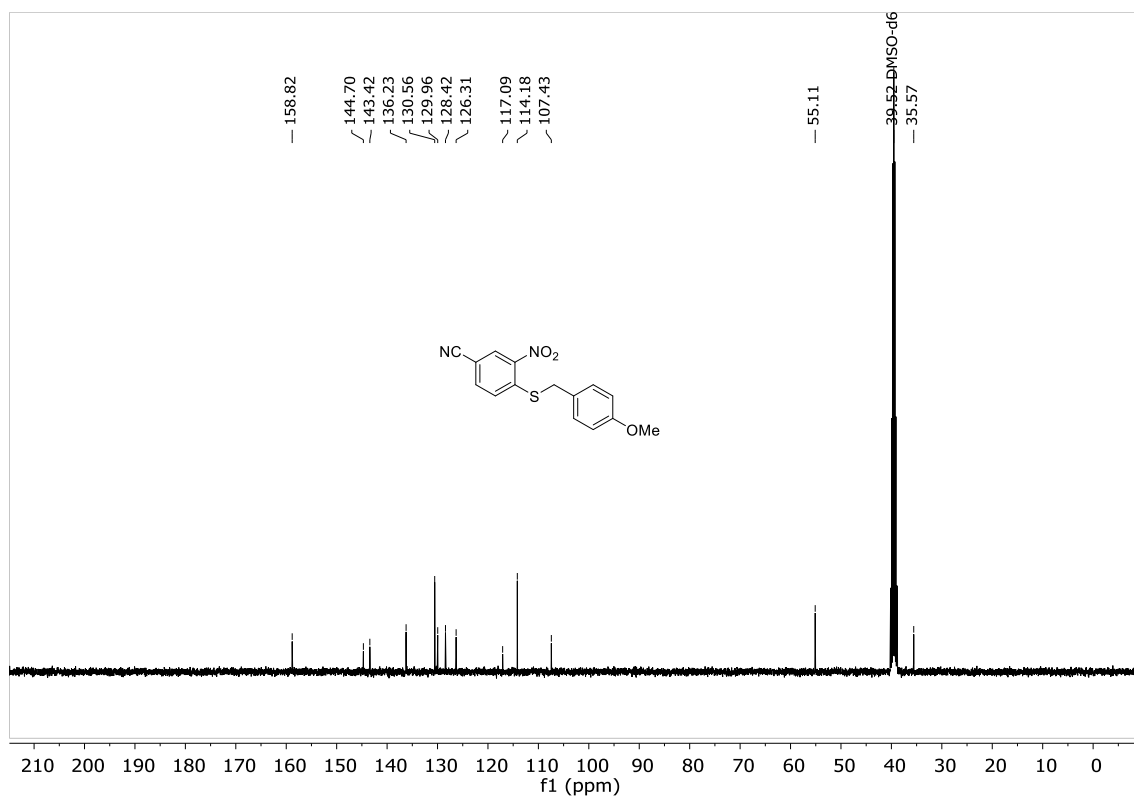
**Figure S026:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of (4-methoxybenzyl)(2-nitro-4-(trifluoromethyl)phenyl)sulfane (**1k**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



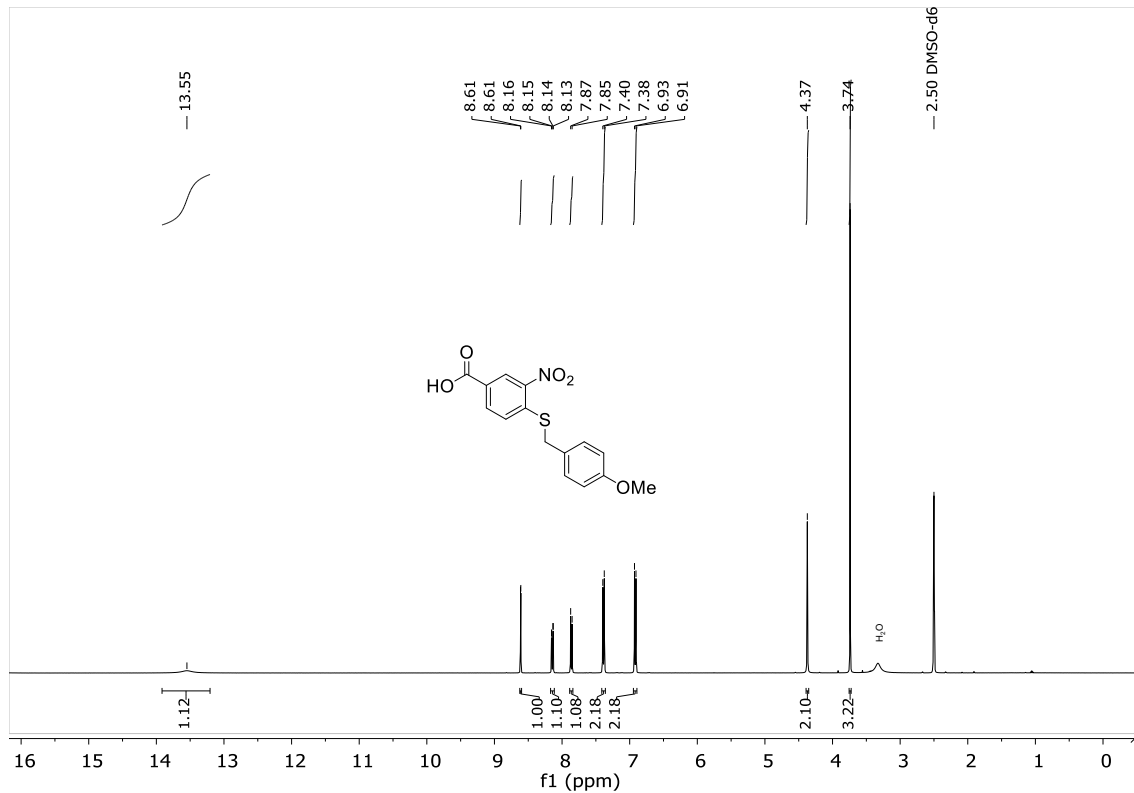
**Figure S027:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of (4-methoxybenzyl)(2-nitro-4-(trifluoromethyl)phenyl)sulfane (**1k**) (376 MHz, DMSO- $d_6$ , 298 K, referenced to fluorobenzene).



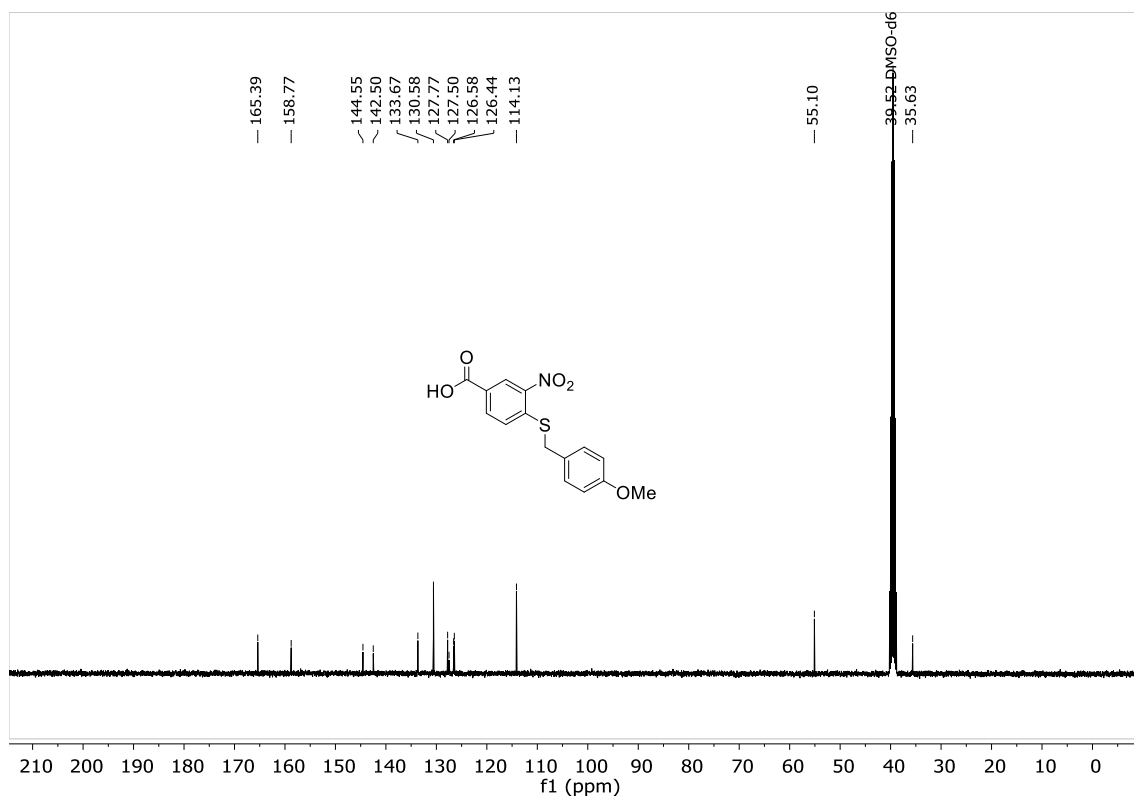
**Figure S028:**  $^1\text{H}$  NMR spectrum of 4-((4-methoxybenzyl)thio)-3-nitrobenzonitrile (**1l**) (400 MHz, DMSO- $d_6$ , 298 K).



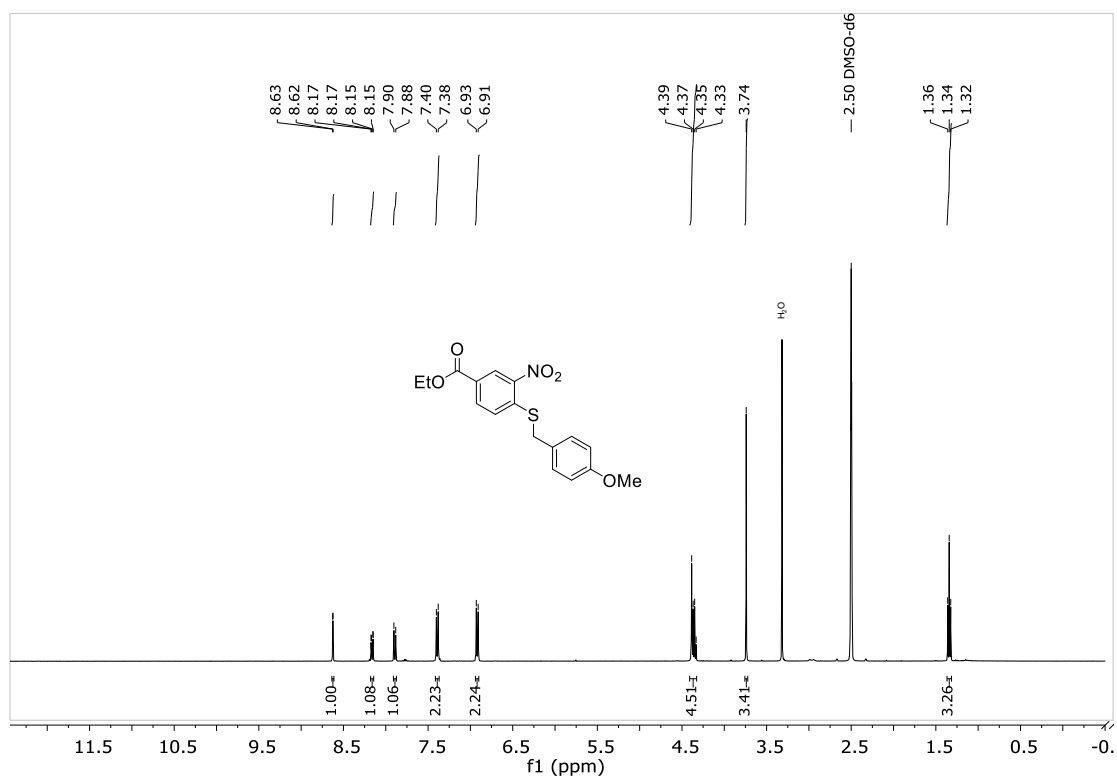
**Figure S029:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of 4-((4-methoxybenzyl)thio)-3-nitrobenzonitrile (**II**) (100 MHz, DMSO- $d_6$ , 298 K).



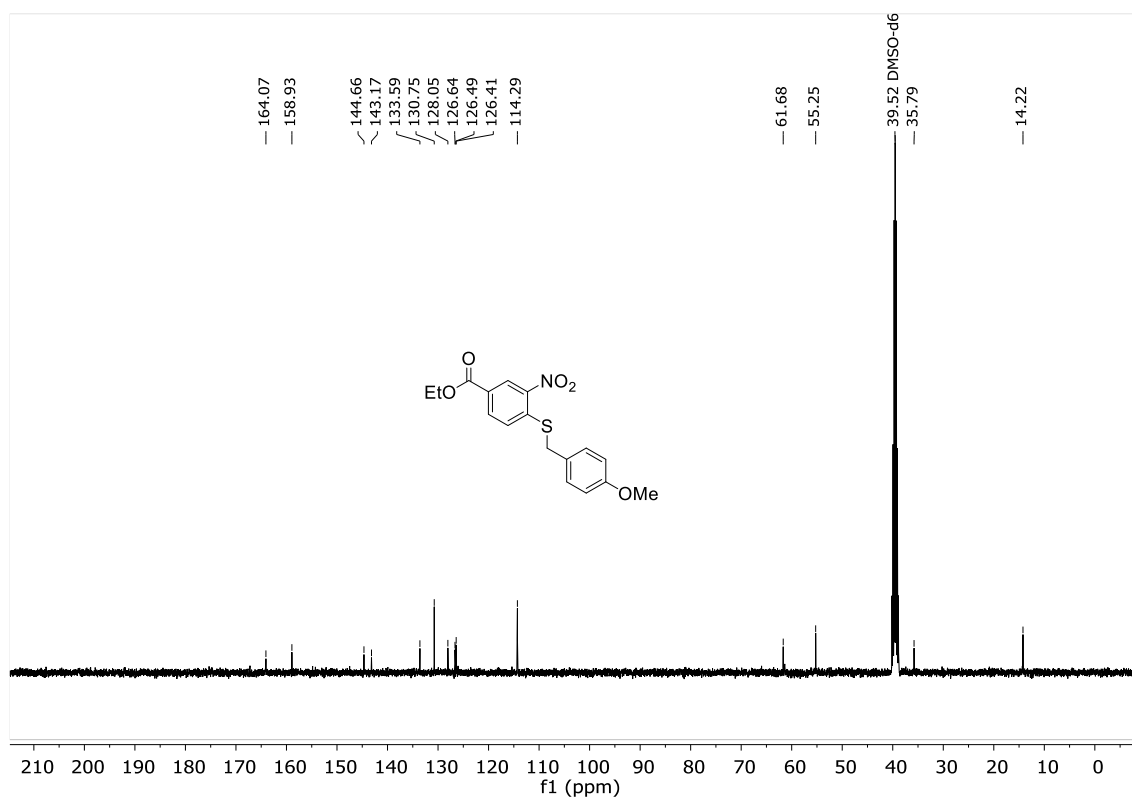
**Figure S030:**  $^1\text{H}$  NMR spectrum of 4-((4-methoxybenzyl)thio)-3-nitrobenzoic acid (**1m**) (400 MHz, DMSO- $d_6$ , 298 K).



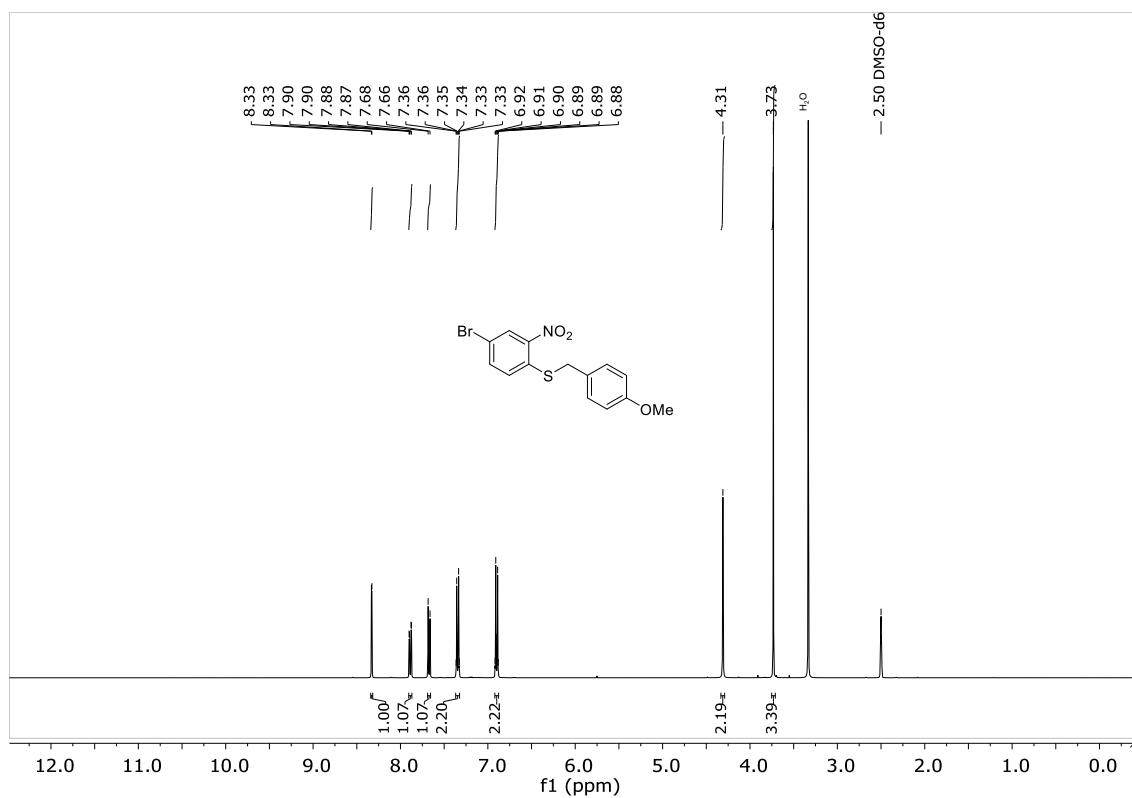
**Figure S031:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of 4-((4-methoxybenzyl)thio)-3-nitrobenzoic acid (**1m**) (400 MHz, DMSO- $d_6$ , 298 K).



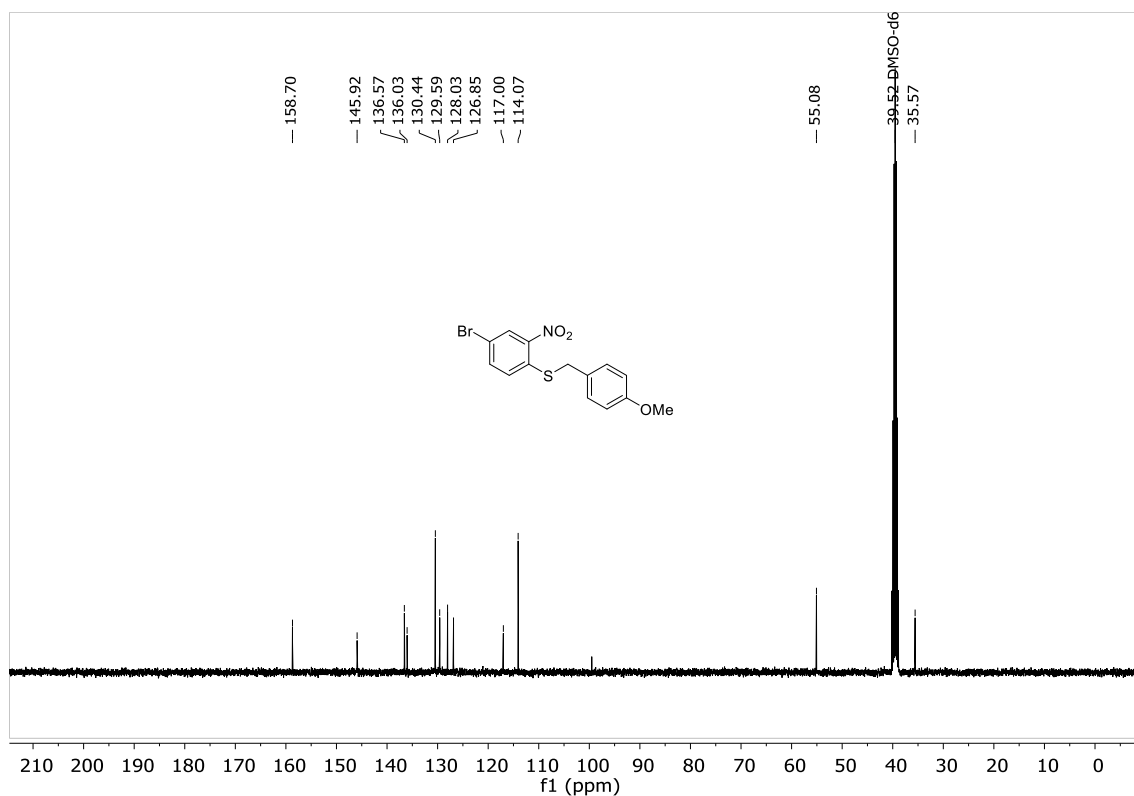
**Figure S032:**  $^1\text{H}$  NMR spectrum of ethyl 4-((4-methoxybenzyl)thio)-3-nitrobenzoate (**1m'**) (400 MHz, DMSO- $d_6$ , 298 K).



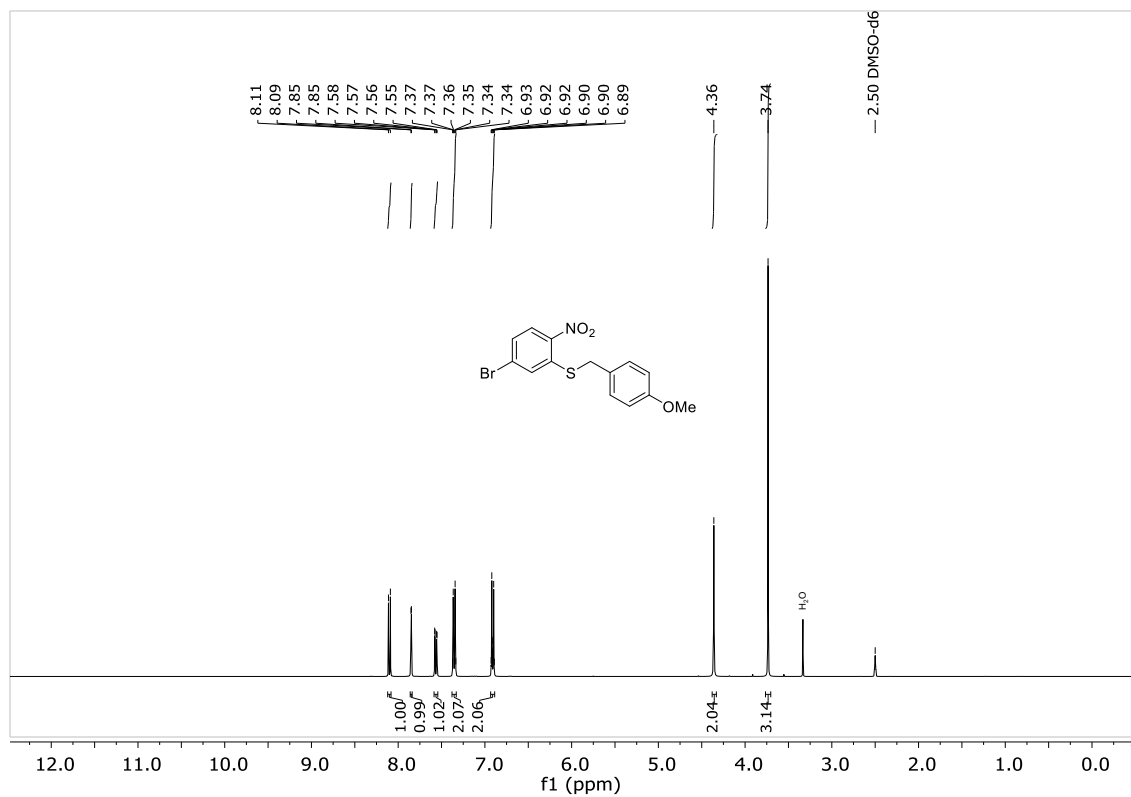
**Figure S033:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of ethyl 4-((4-methoxybenzyl)thio)-3-nitrobenzoate (**1m'**) (100 MHz, DMSO- $d_6$ , 298 K).



**Figure S034:**  $^1\text{H}$  NMR spectrum of (4-bromo-2-nitrophenyl)(4-methoxybenzyl)sulfane (**1n**) (400 MHz, DMSO- $d_6$ , 298 K).

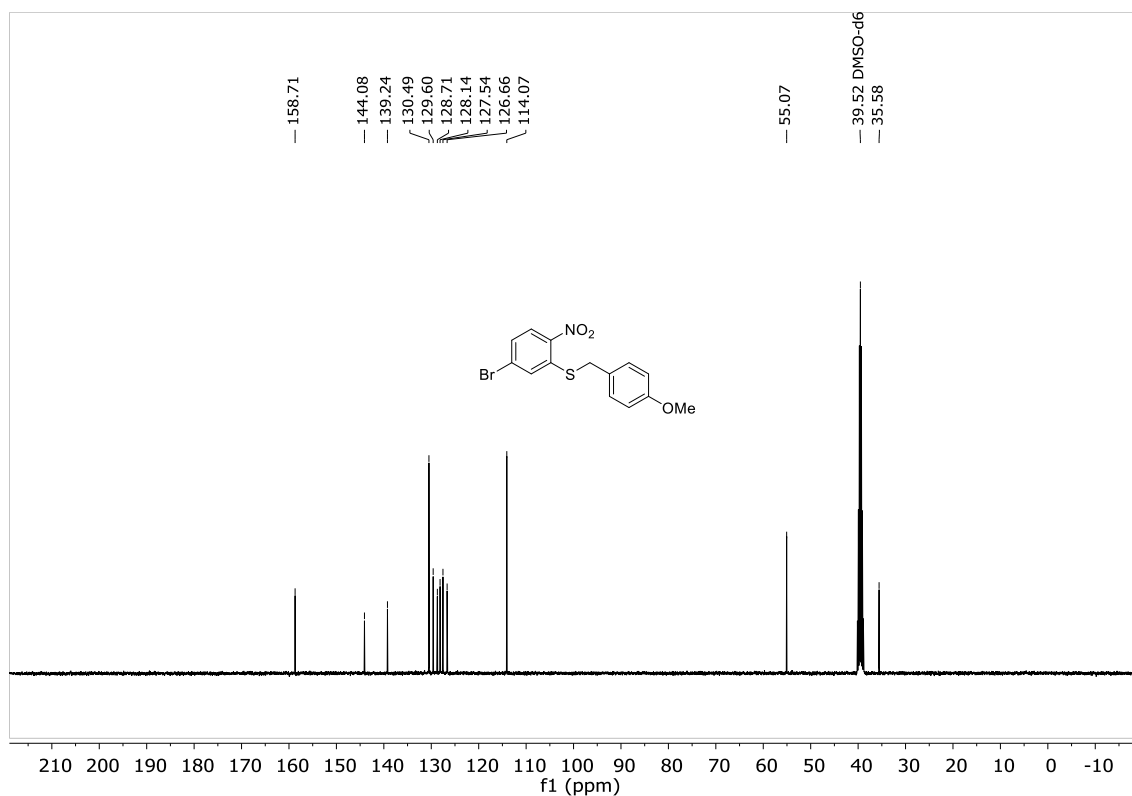


**Figure S035:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of (4-bromo-2-nitrophenyl)(4-methoxybenzyl)sulfane (**1n**) (100 MHz,  $\text{DMSO-}d_6$ , 298 K).

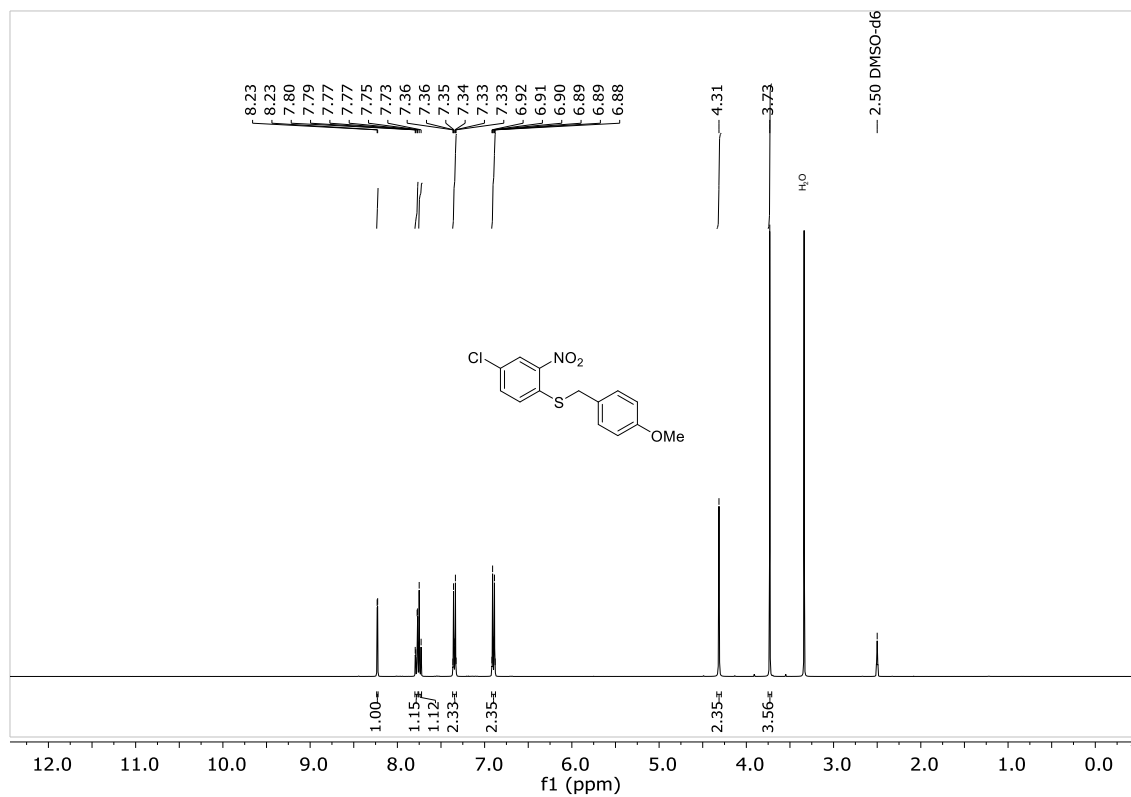


**Figure S036:**  $^1\text{H}$  NMR spectrum of (5-bromo-2-nitrophenyl)(4-methoxybenzyl)sulfane (**1o**) (400 MHz,  $\text{DMSO-}d_6$ , 298 K).

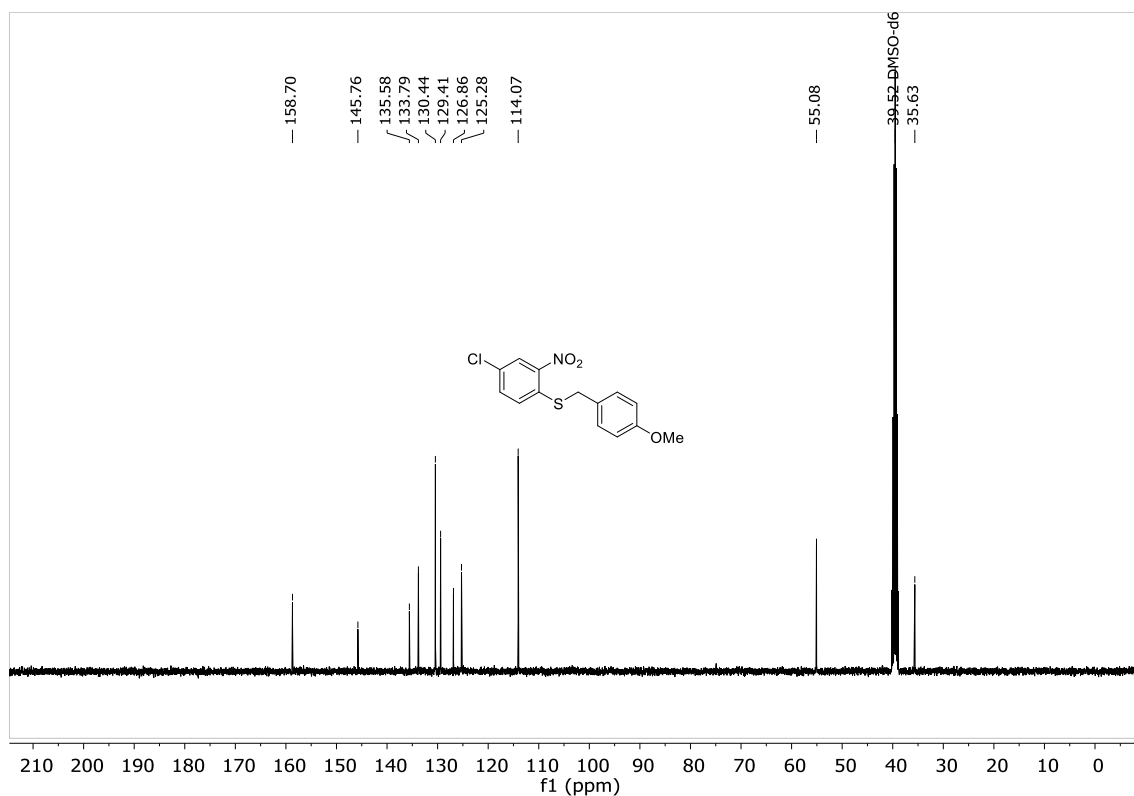




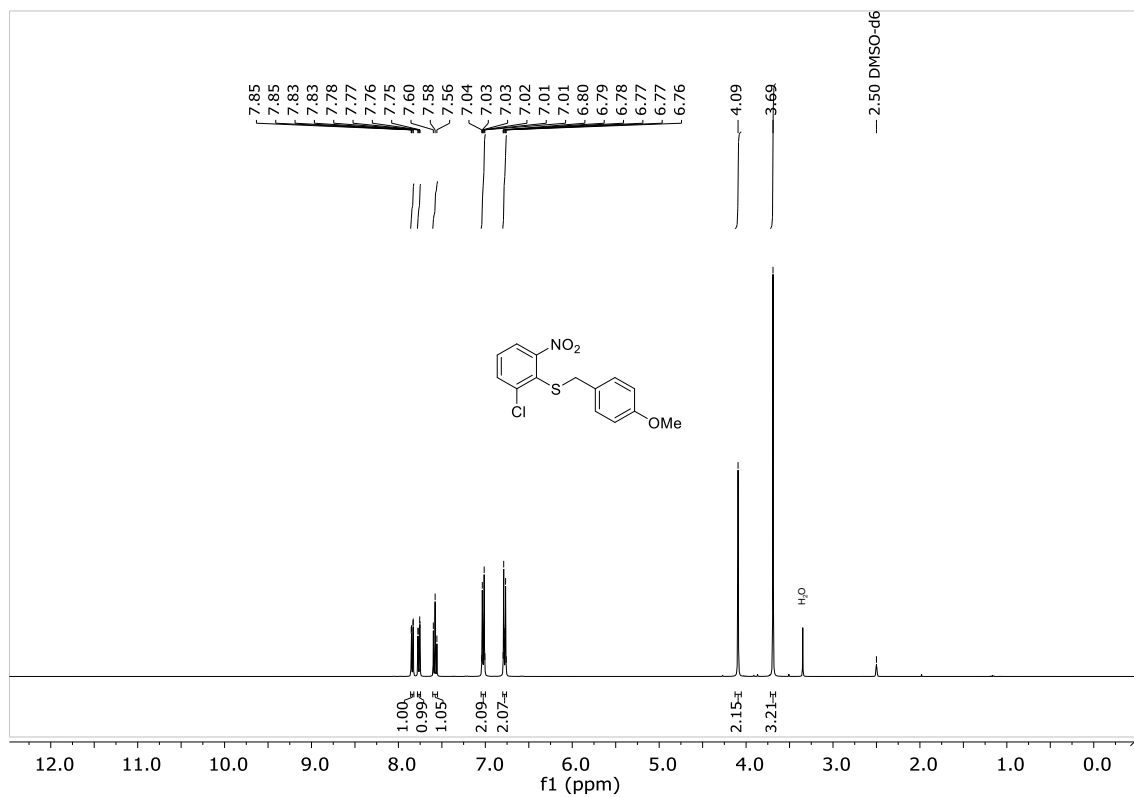
**Figure S037:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of (5-bromo-2-nitrophenyl)(4-methoxybenzyl)sulfane (**1o**) (100 MHz, DMSO- $d_6$ , 298 K).



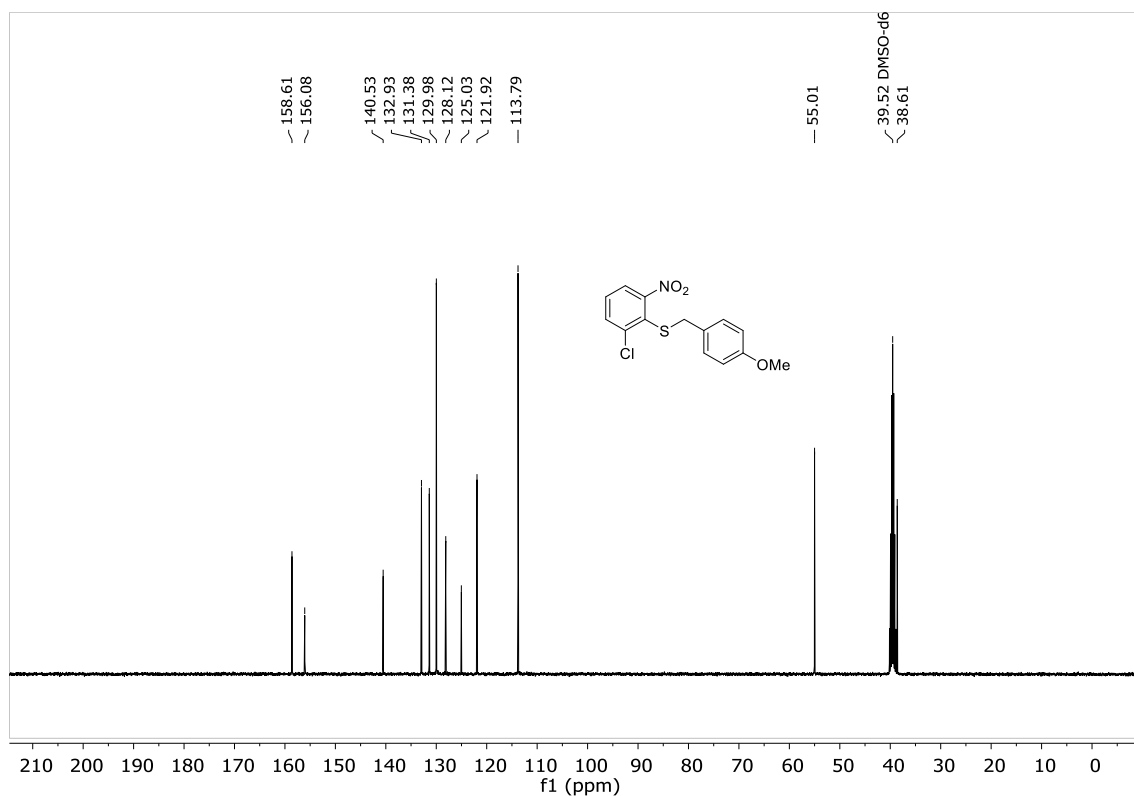
**Figure S038:**  $^1\text{H}$  NMR spectrum of (4-chloro-2-nitrophenyl)(4-methoxybenzyl)sulfane (**1p**) (400 MHz, DMSO- $d_6$ , 298 K).



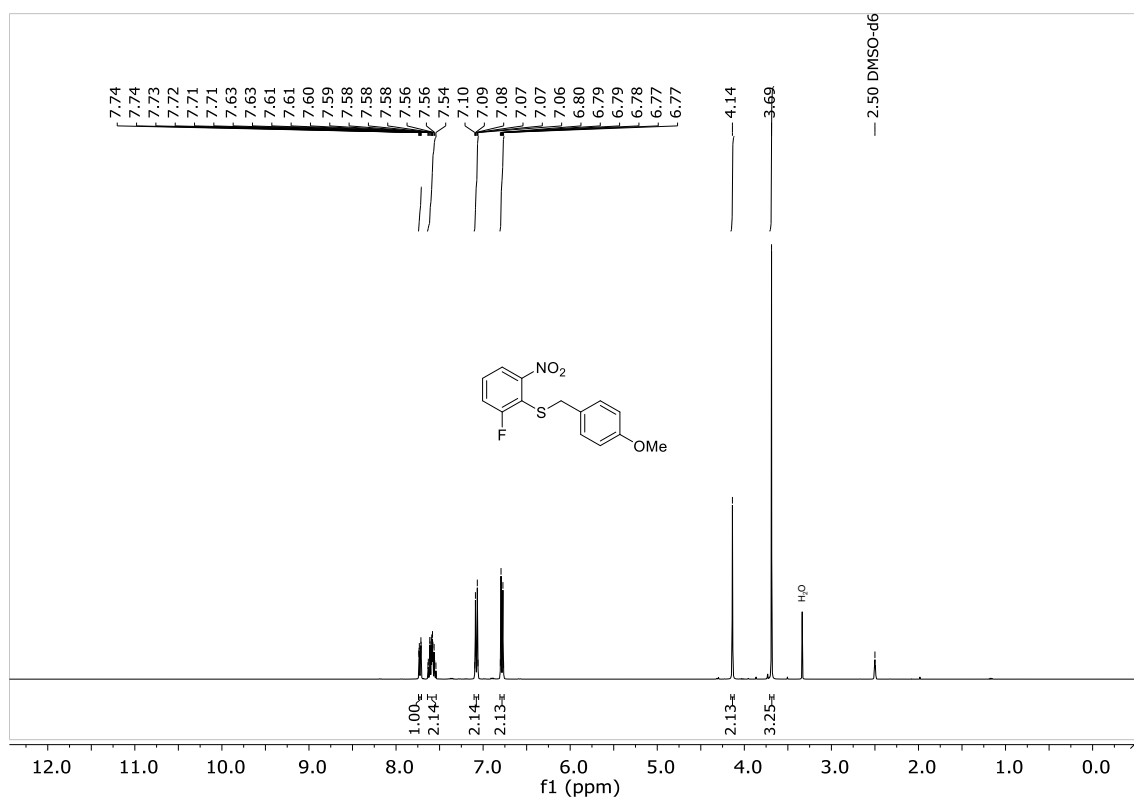
**Figure S039:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of (4-chloro-2-nitrophenyl)(4-methoxybenzyl)sulfane (**1p**) (100 MHz, DMSO- $d_6$ , 298 K).



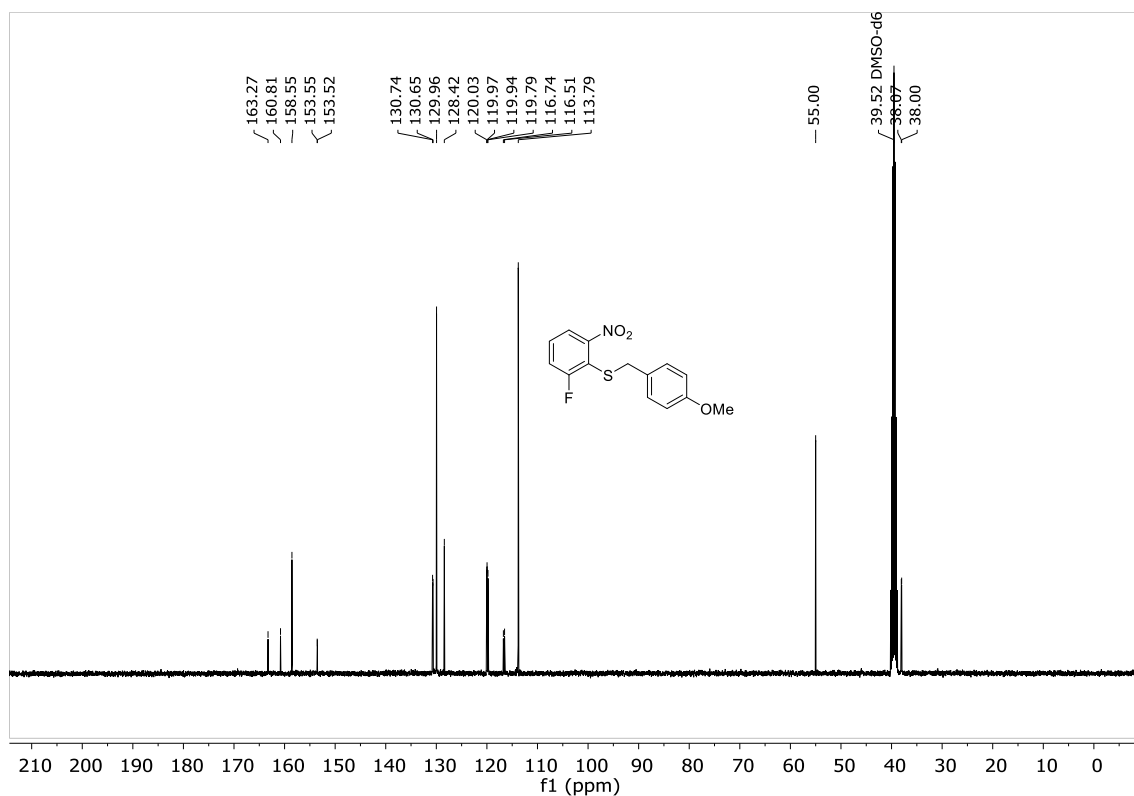
**Figure S040:**  $^1\text{H}$  NMR spectrum of (2-chloro-6-nitrophenyl)(4-methoxybenzyl)sulfane (**1q**) (400 MHz, DMSO- $d_6$ , 298 K).



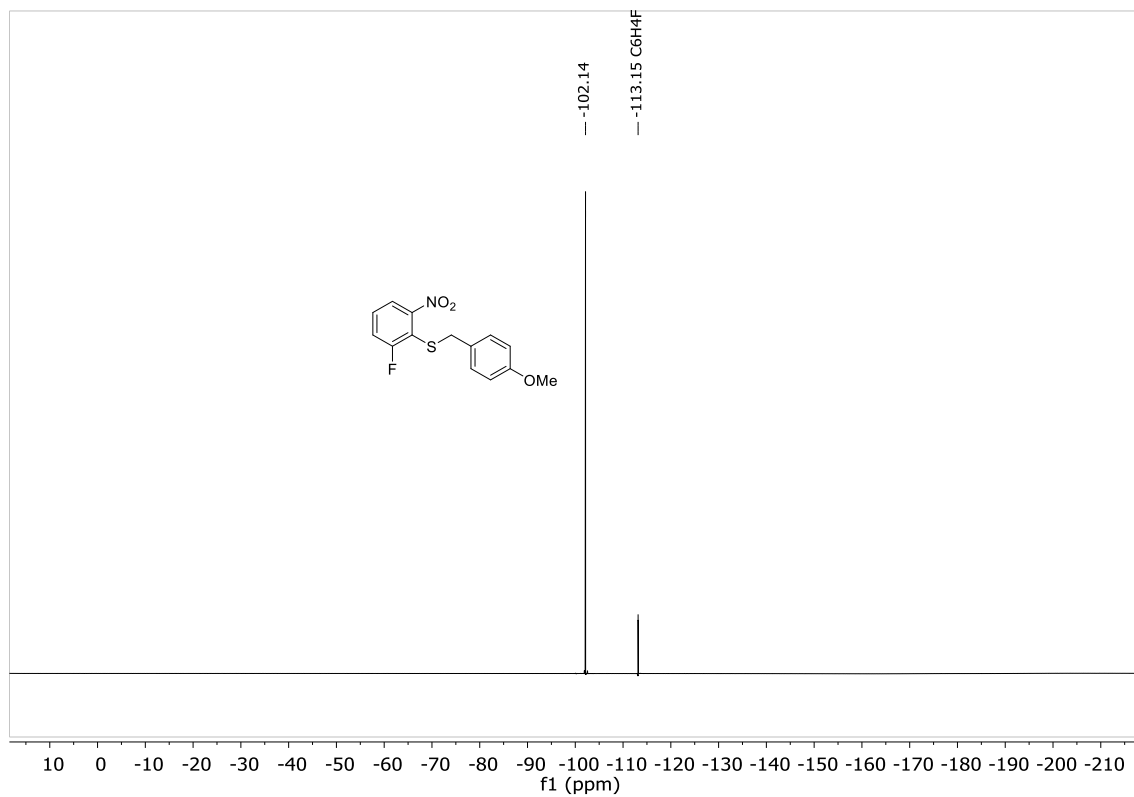
**Figure S041:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of (2-chloro-6-nitrophenyl)(4-methoxybenzyl)sulfane (**1q**) (100 MHz, DMSO- $d_6$ , 298 K).



**Figure S042:**  $^1\text{H}$  NMR spectrum of (2-fluoro-6-nitrophenyl)(4-methoxybenzyl)sulfane (**1r**) (400 MHz, DMSO- $d_6$ , 298 K).

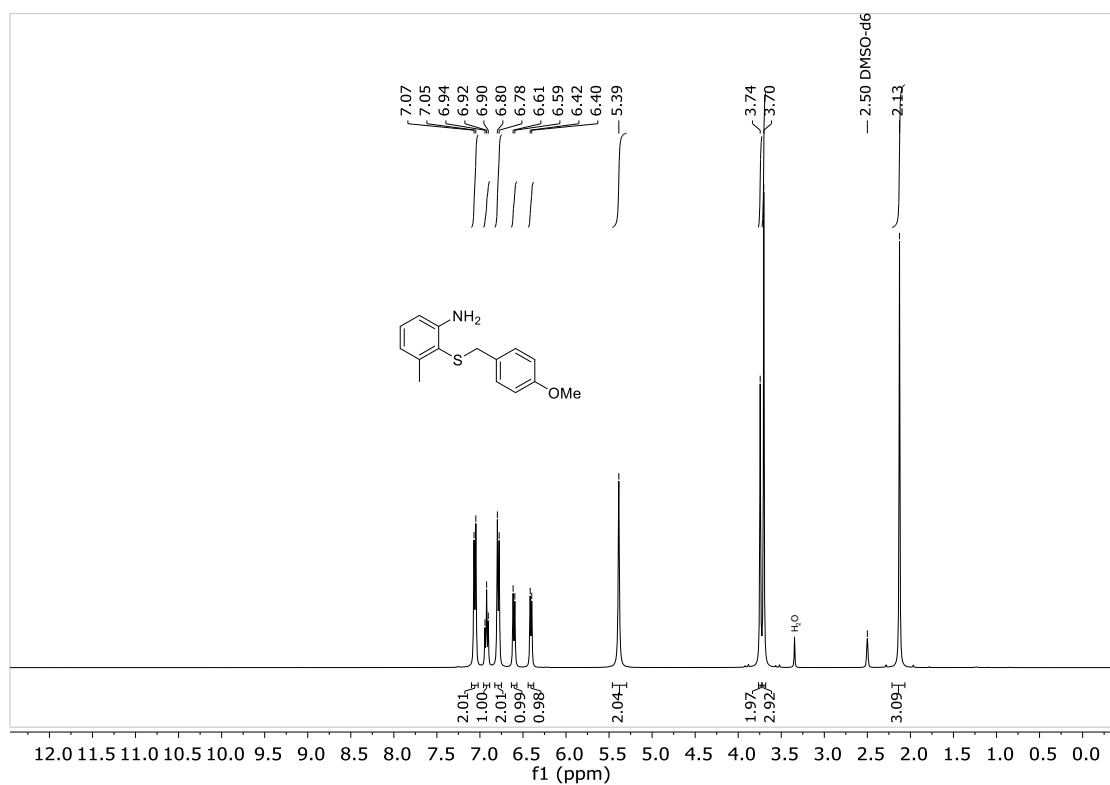


**Figure S043:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of (2-fluoro-6-nitrophenyl)(4-methoxybenzyl)sulfane (**1r**) (100 MHz, DMSO- $d_6$ , 298 K).

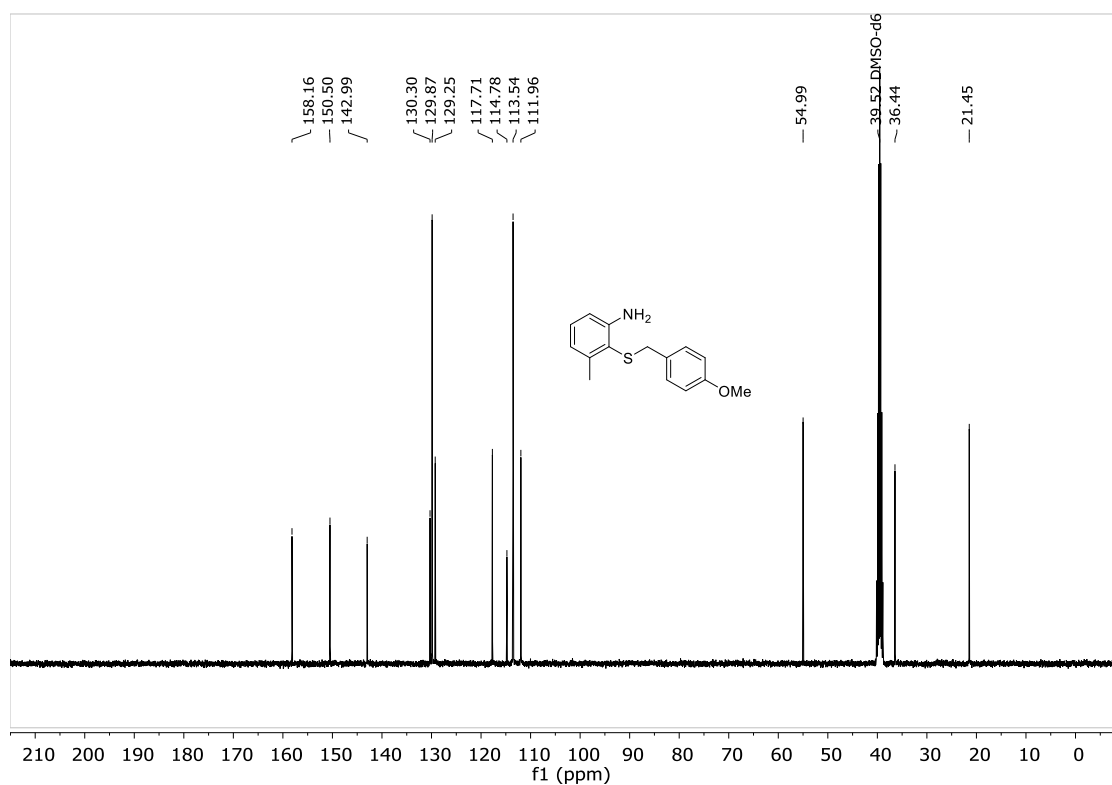


**Figure S044:**  $^{19}\text{F}\{^1\text{H}\}$  NMR spectrum of (2-fluoro-6-nitrophenyl)(4-methoxybenzyl)sulfane (**1r**) (376 MHz, DMSO- $d_6$ , 298 K, referenced to fluorobenzene).

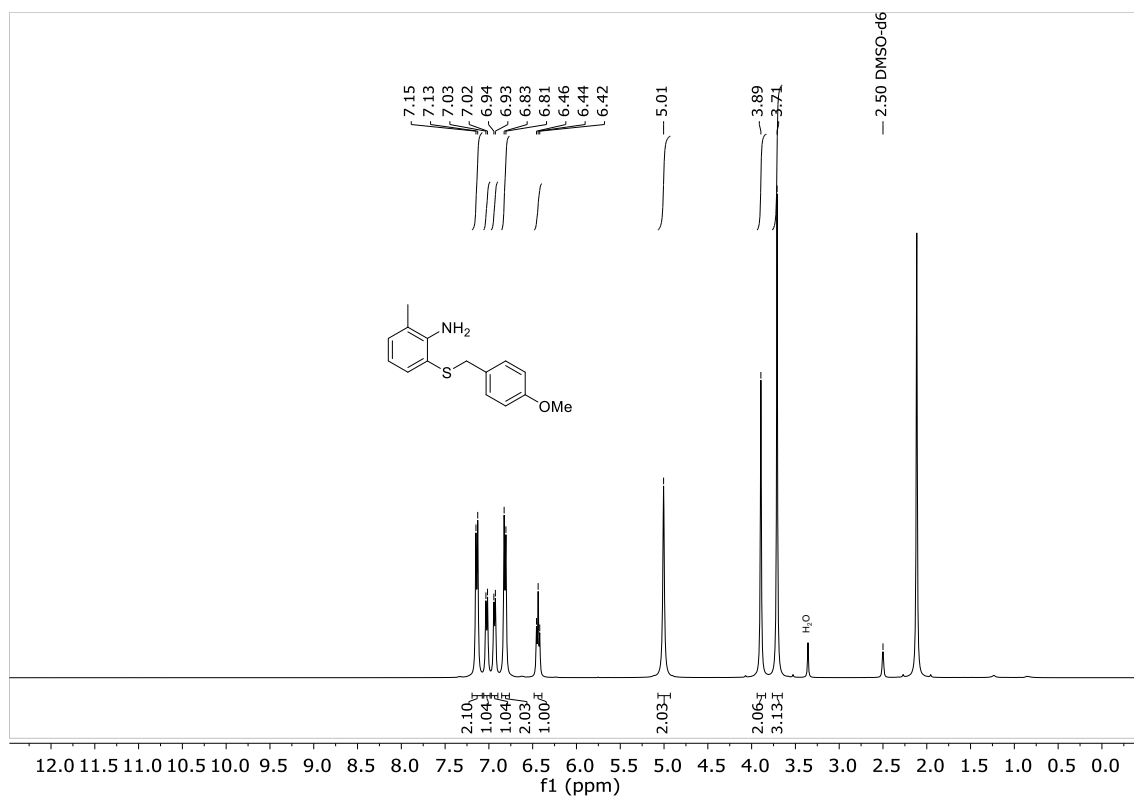
### 1.3 NMR Spectra of Substituted 2-((4-Methoxybenzyl)thio)anilines (2b-2s)



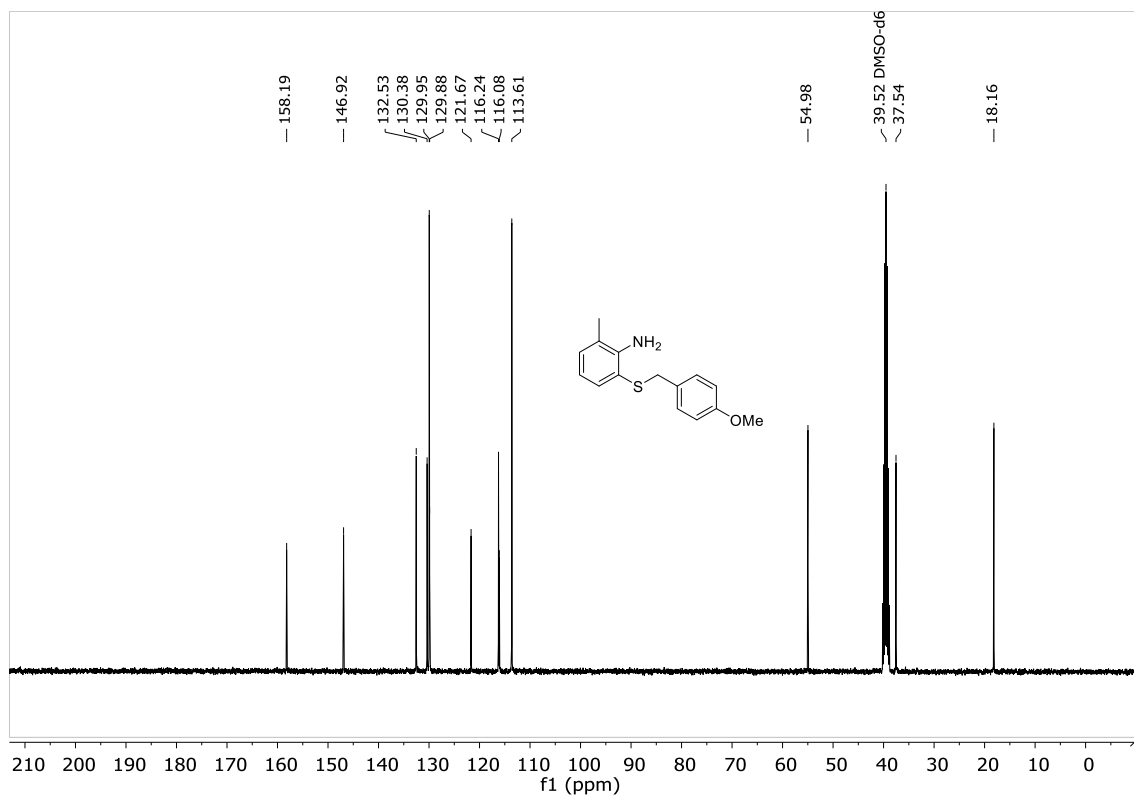
**Figure S045:** <sup>1</sup>H NMR spectrum of 2-((4-methoxybenzyl)thio)-3-methylaniline (**2b**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



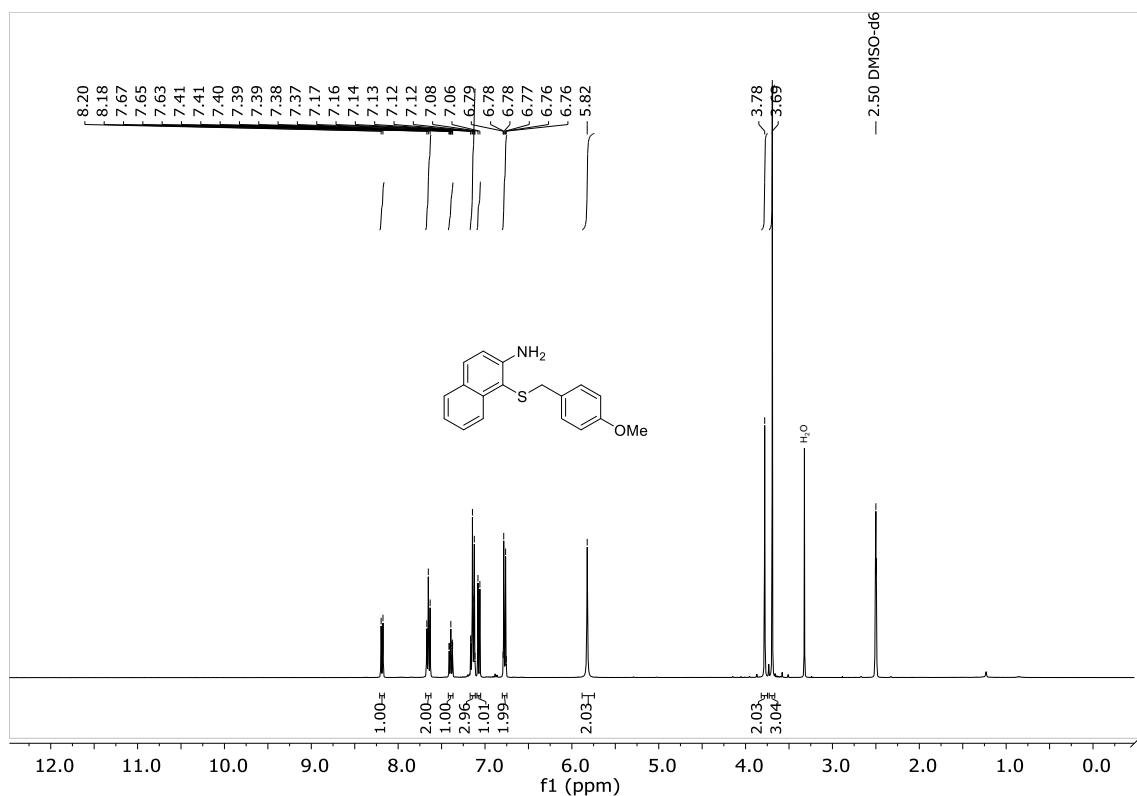
**Figure S046:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 2-((4-methoxybenzyl)thio)-3-methylaniline (**2b**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



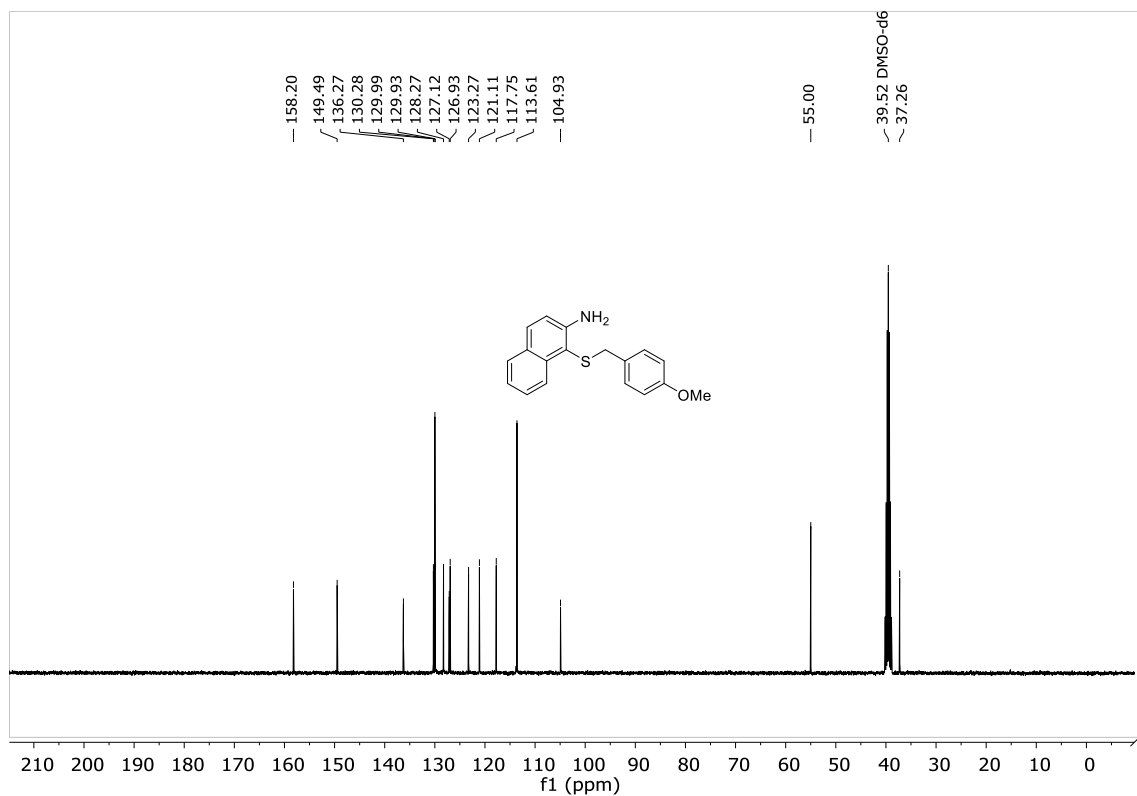
**Figure S047:** <sup>1</sup>H NMR spectrum of 2-((4-methoxybenzyl)thio)-6-methylaniline (**2c**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



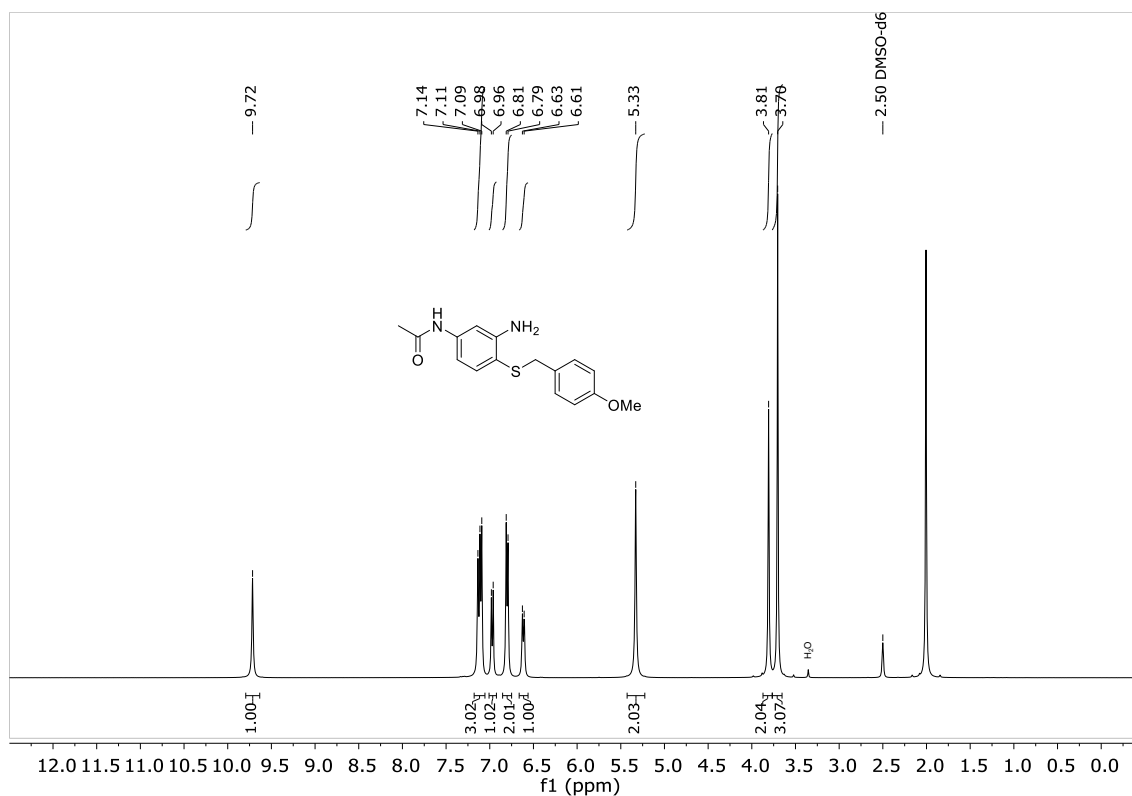
**Figure S048:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 2-((4-methoxybenzyl)thio)-6-methylaniline (**2c**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



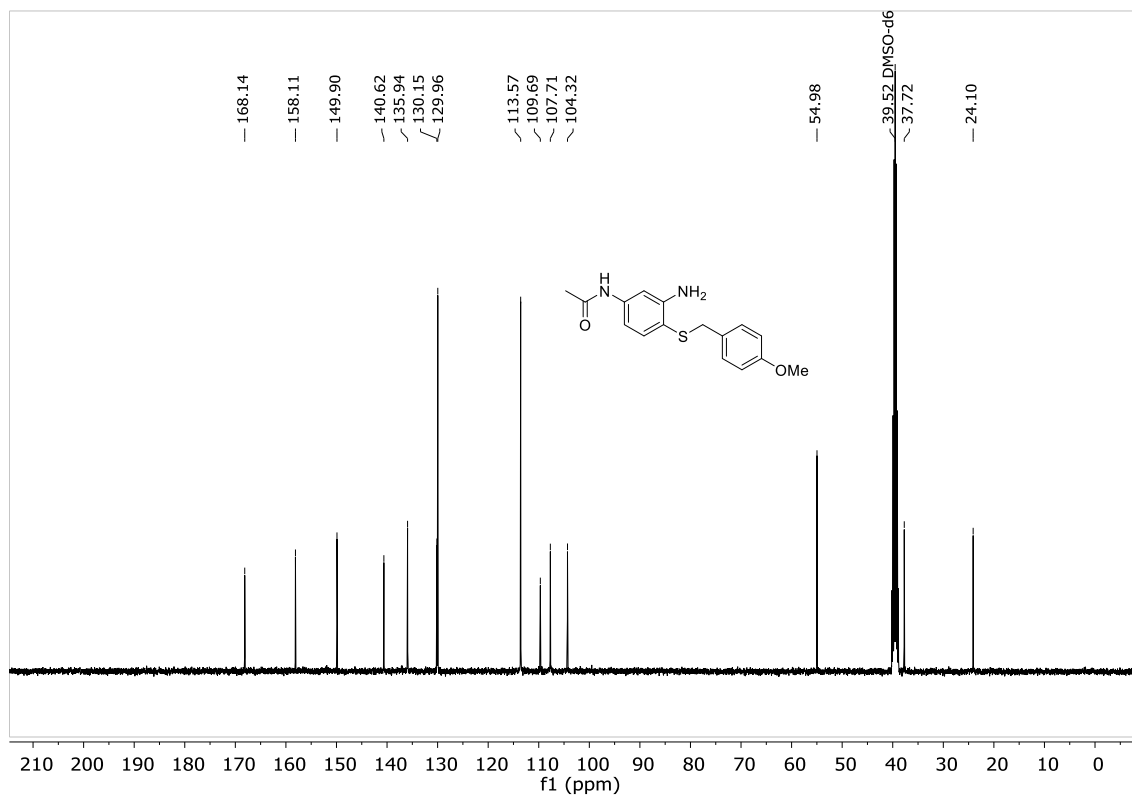
**Figure S049:** <sup>1</sup>H NMR spectrum of 1-((4-methoxybenzyl)thio)naphthalen-2-amine (**2d**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



**Figure S050:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 1-((4-methoxybenzyl)thio)naphthalen-2-amine (**2d**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).

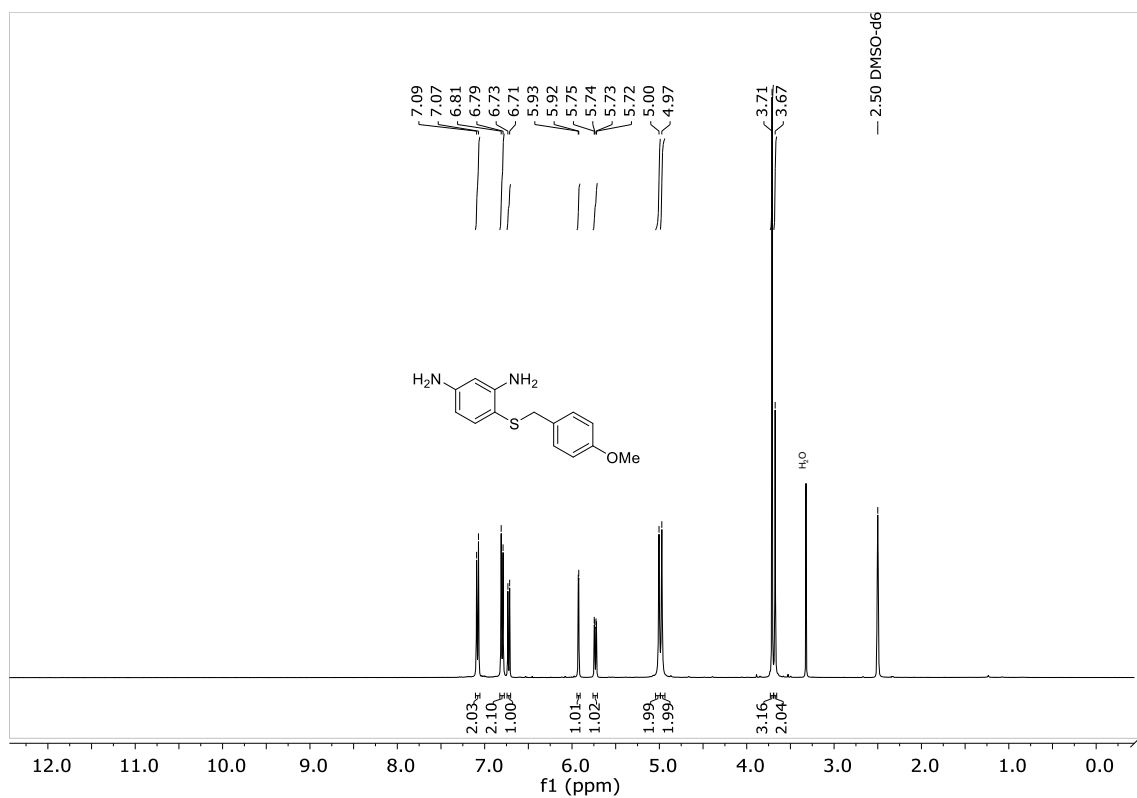


**Figure S051:**  $^1\text{H}$  NMR spectrum of *N*-(3-amino-4-((4-methoxybenzyl)thio)phenyl)acetamide (**2f**) (400 MHz,  $\text{DMSO-}d_6$ , 298 K).

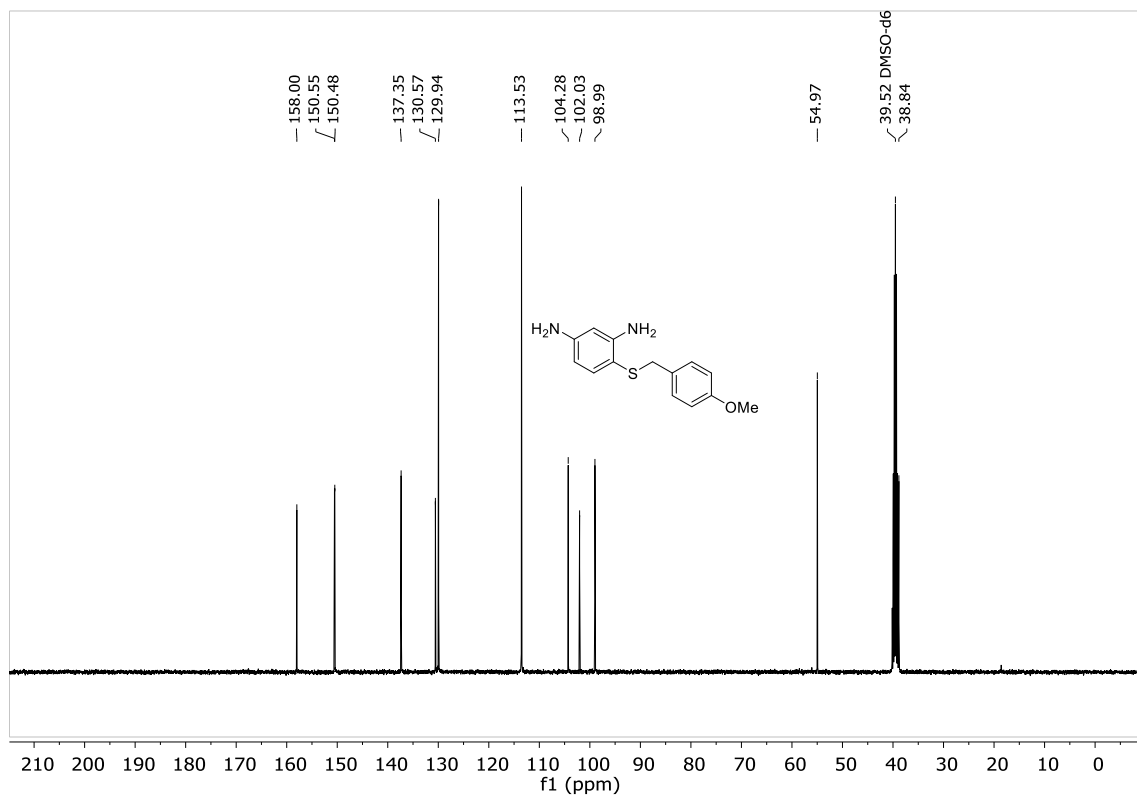


**Figure S052:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of *N*-(3-amino-4-((4-methoxybenzyl)thio)phenyl)acetamide (**2f**) (100 MHz,  $\text{DMSO-}d_6$ , 298 K).

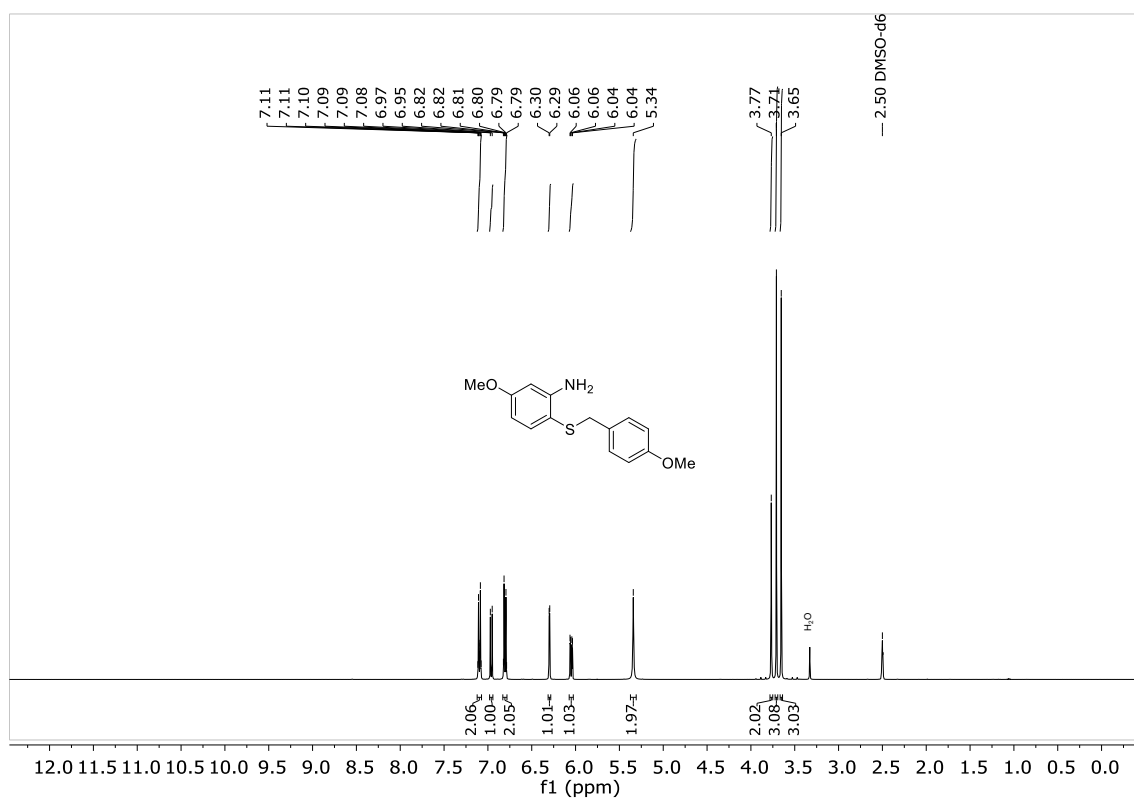




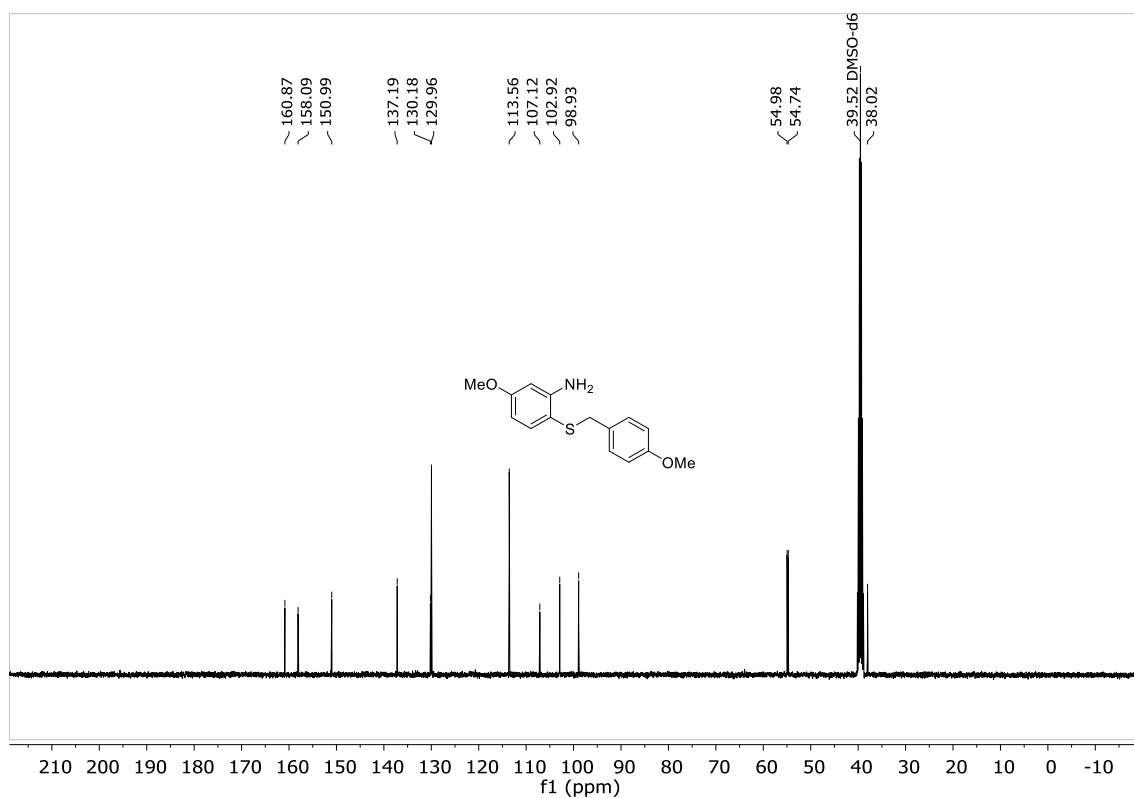
**Figure S053:** <sup>1</sup>H NMR spectrum of 4-((4-methoxybenzyl)thio)benzene-1,3-diamine (**2e**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



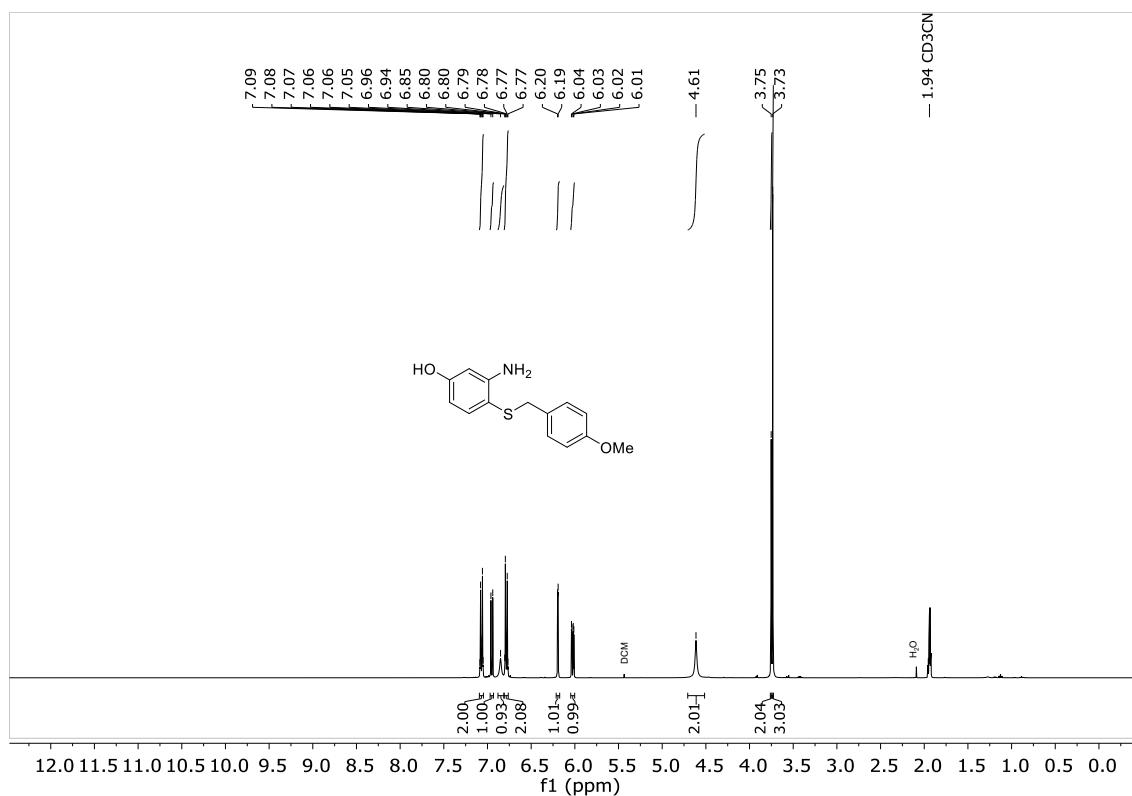
**Figure S054:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 4-((4-methoxybenzyl)thio)benzene-1,3-diamine (**2e**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



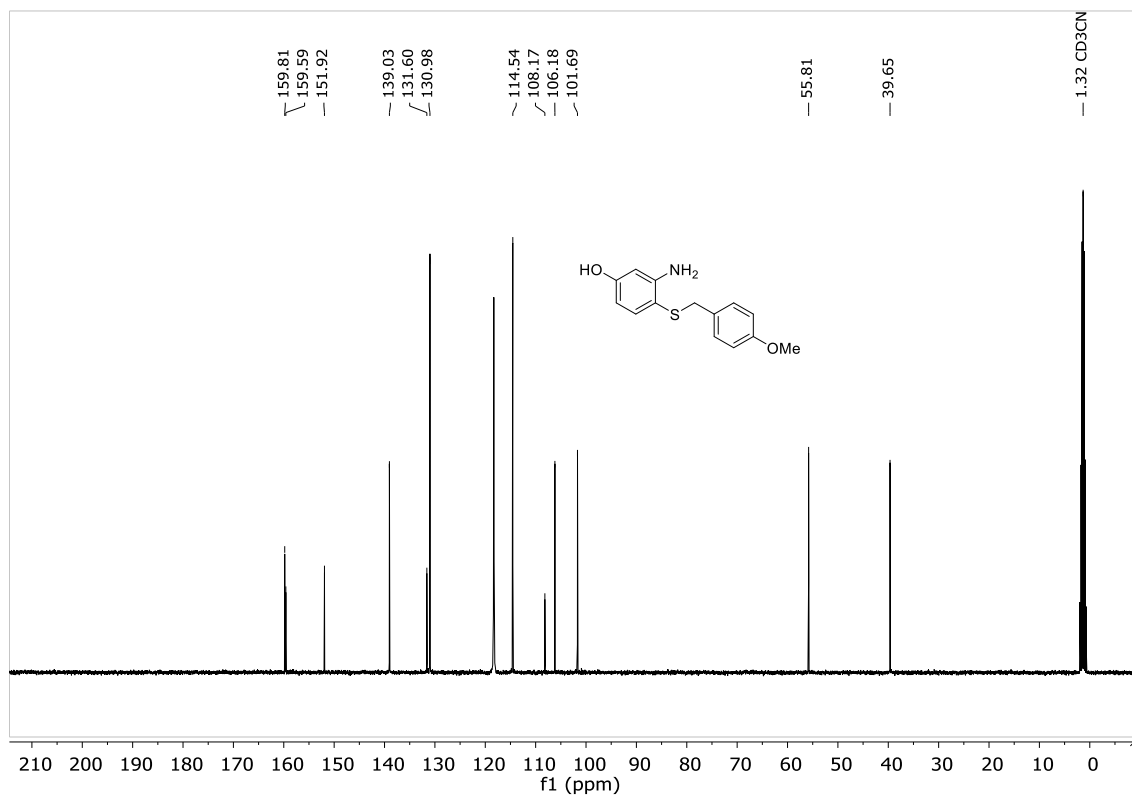
**Figure S055:** <sup>1</sup>H NMR spectrum of 5-methoxy-2-((4-methoxybenzyl)thio)aniline (**2h**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



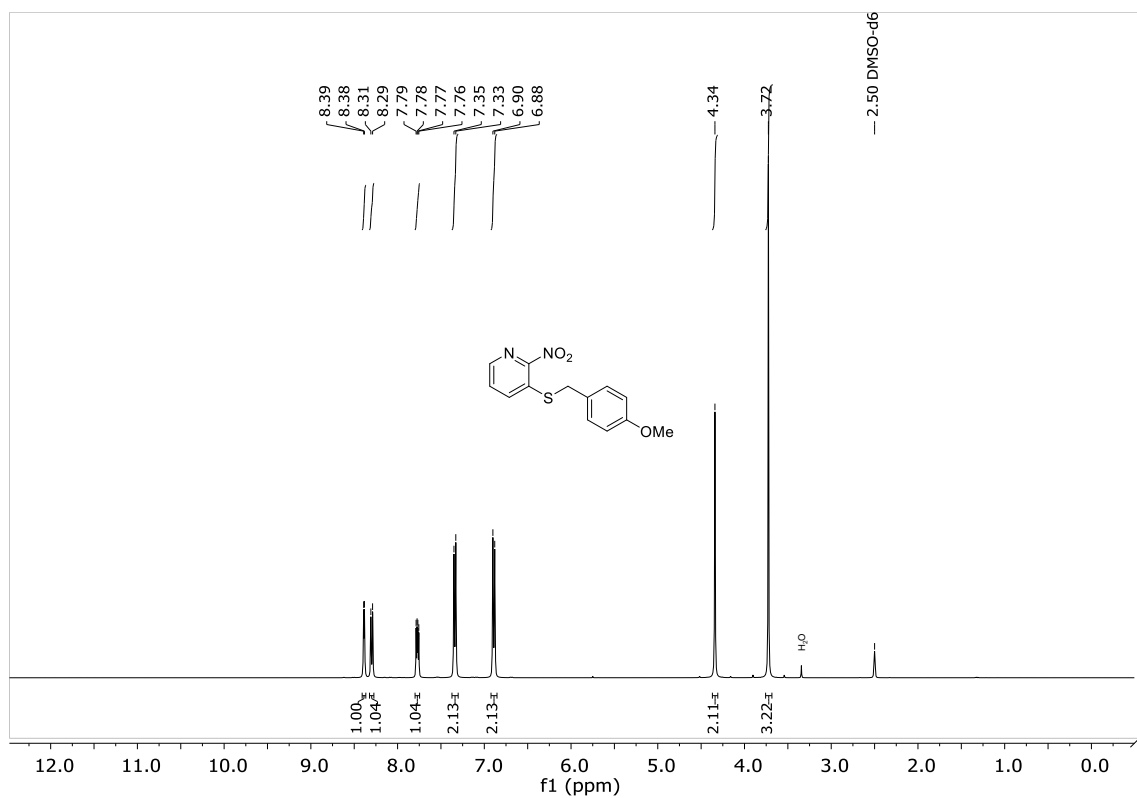
**Figure S056:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 5-methoxy-2-((4-methoxybenzyl)thio)aniline (**2h**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



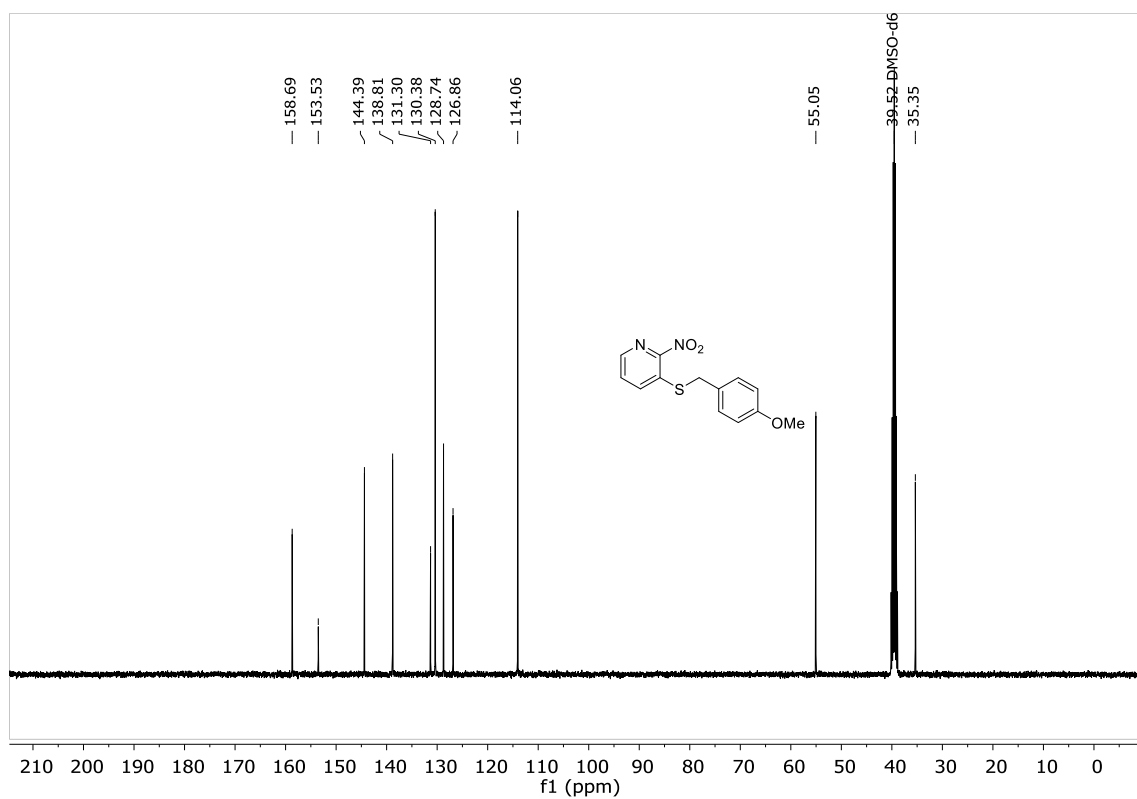
**Figure S057:**  $^1\text{H}$  NMR spectrum of 3-amino-4-((4-methoxybenzyl)thio)phenol (**2H**) (400 MHz,  $\text{DMSO-}d_6$ , 298 K).



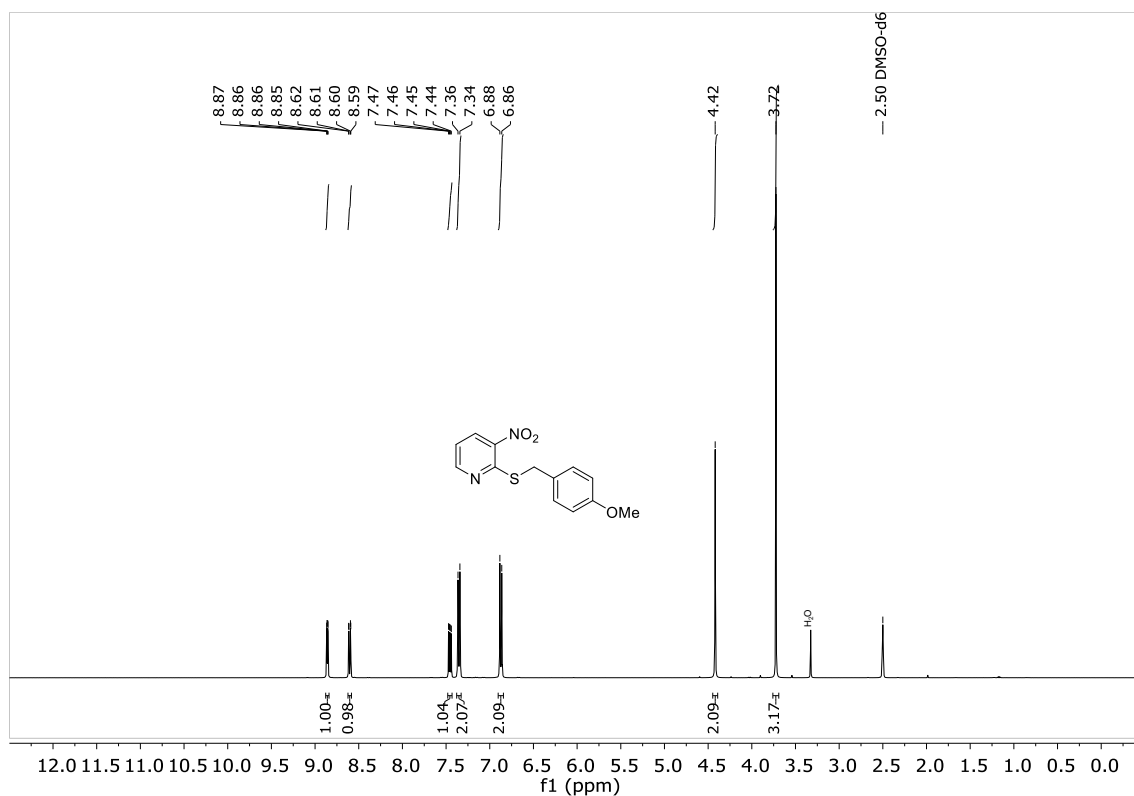
**Figure S058:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of 3-amino-4-((4-methoxybenzyl)thio)phenol (**2h**) (100 MHz,  $\text{DMSO-}d_6$ , 298 K).



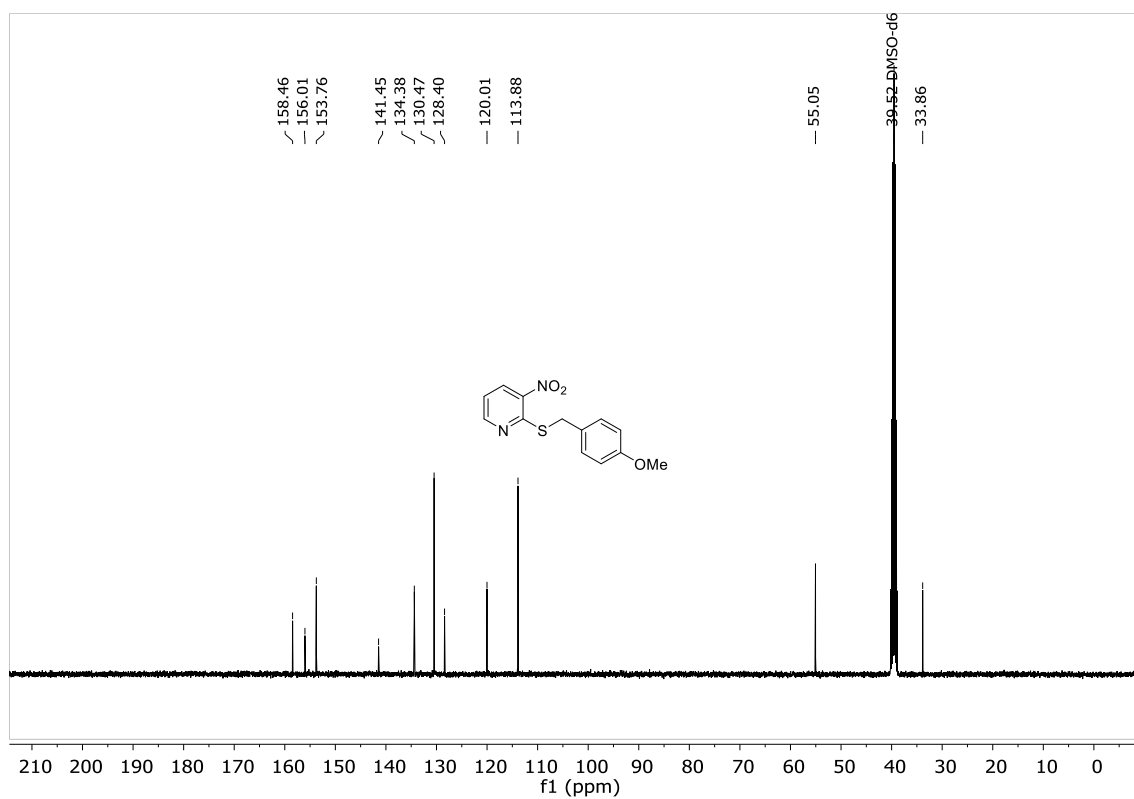
**Figure S059:** <sup>1</sup>H NMR spectrum of 3-((4-methoxybenzyl)thio)pyridin-2-amine (**2i**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



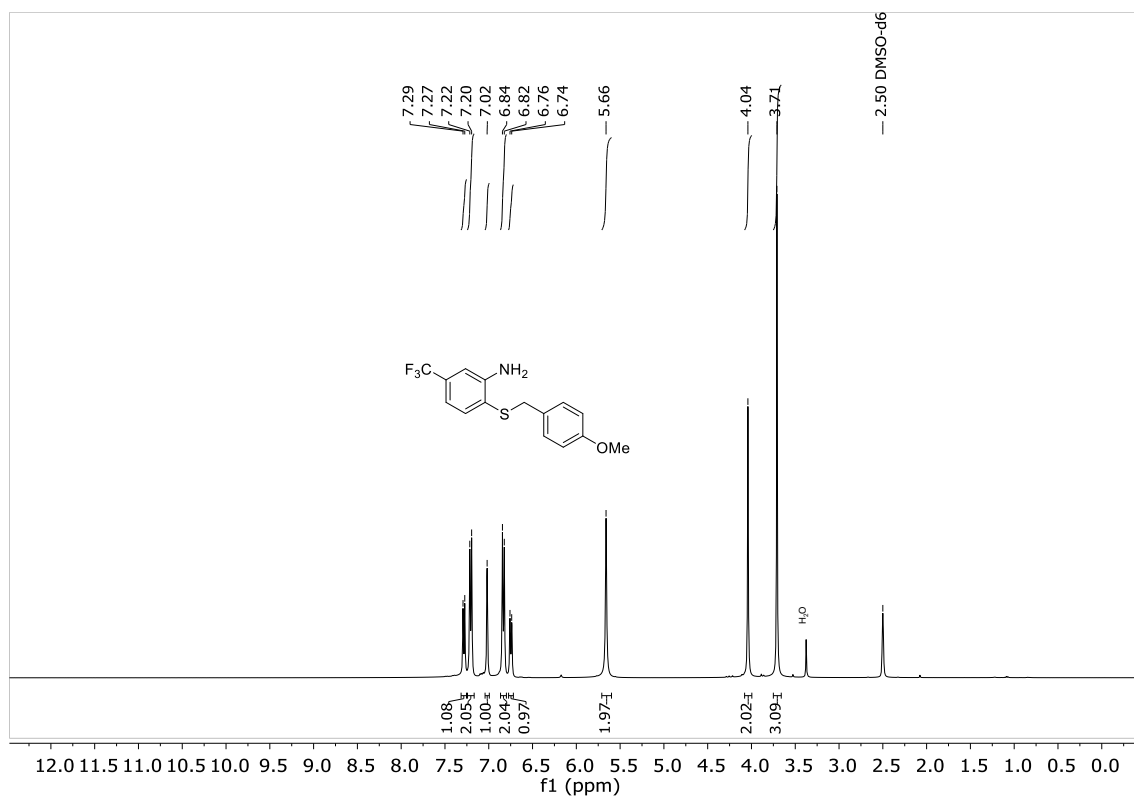
**Figure S060:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 3-((4-methoxybenzyl)thio)pyridin-2-amine (**2i**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



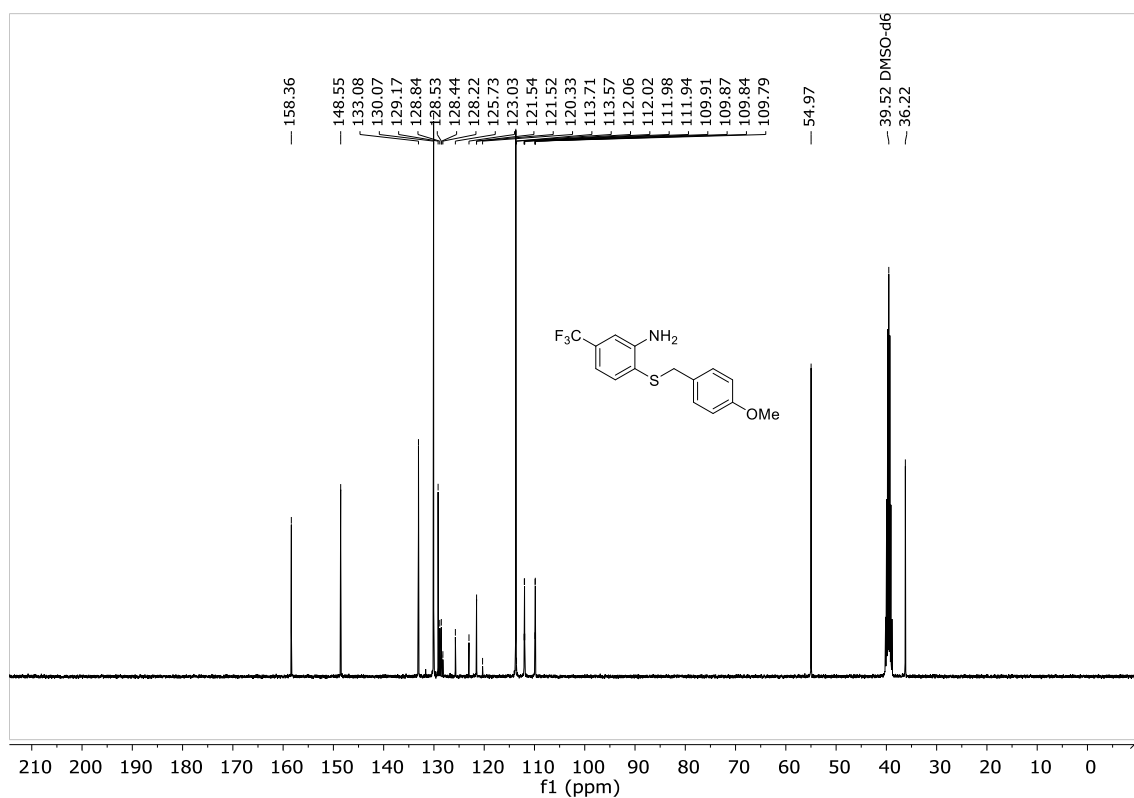
**Figure S061:** <sup>1</sup>H NMR spectrum of 2-((4-methoxybenzyl)thio)pyridin-3-amine (**2j**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



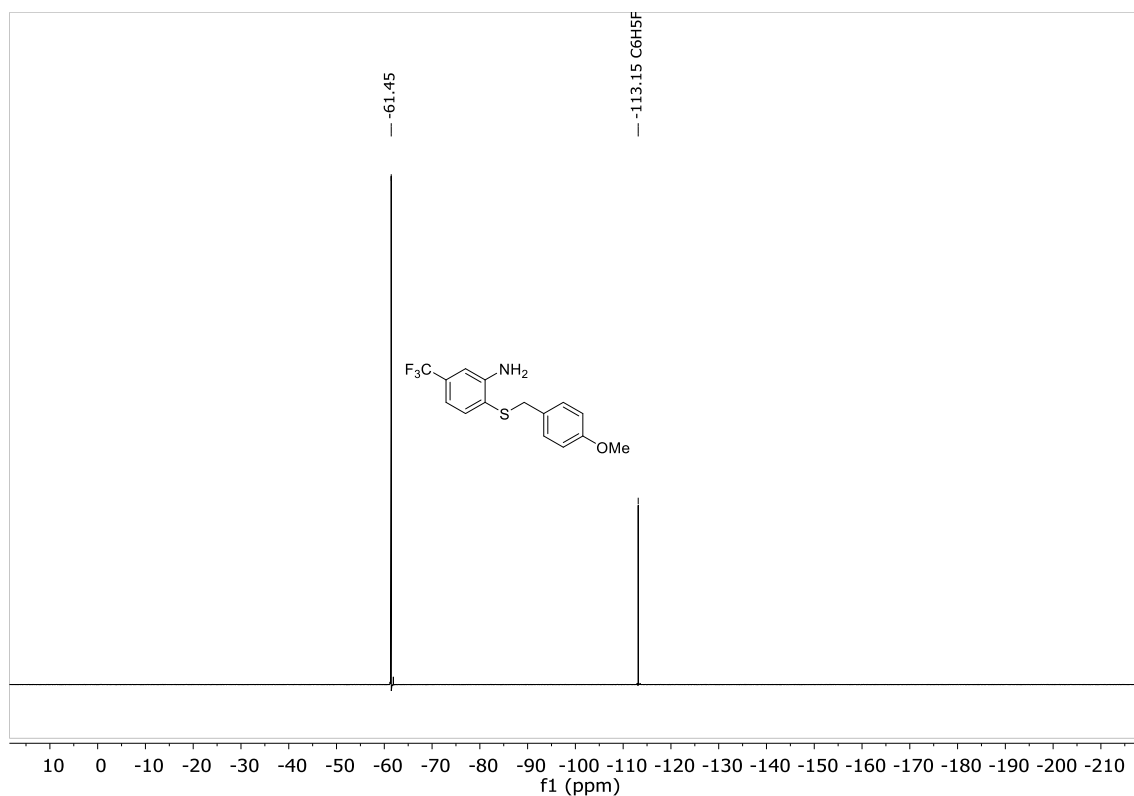
**Figure S062:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 2-((4-methoxybenzyl)thio)pyridin-3-amine (**2j**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



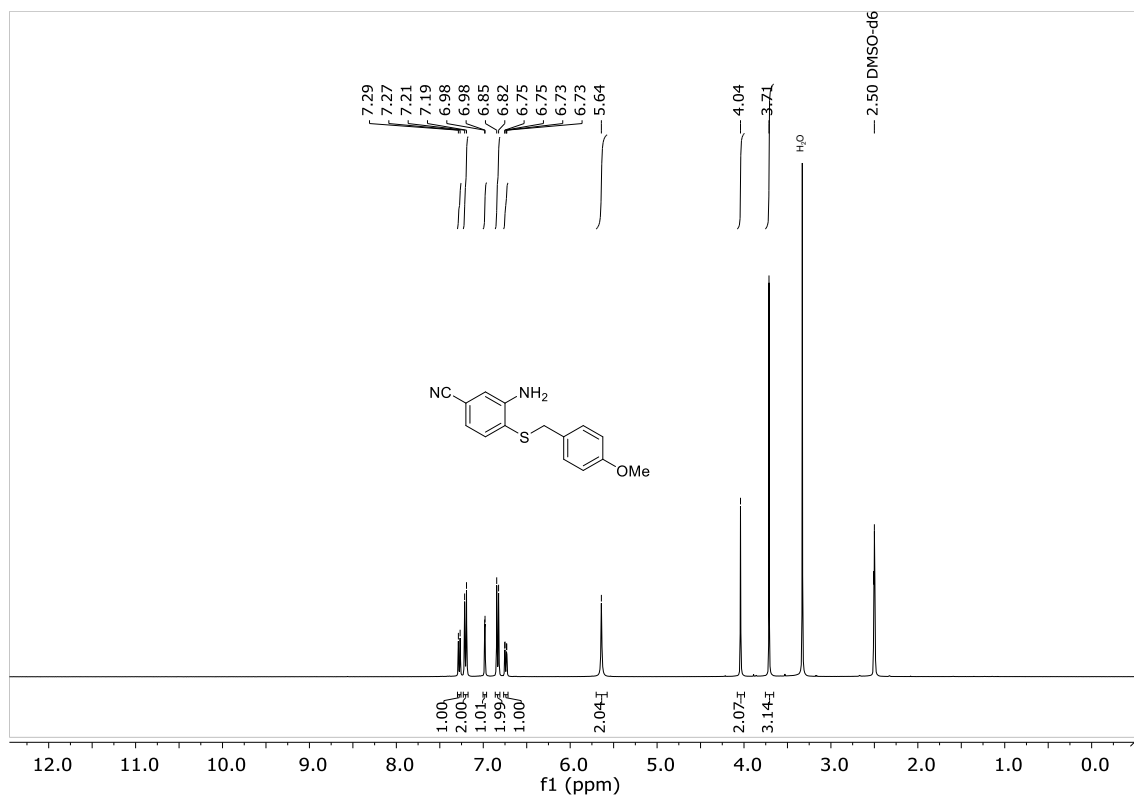
**Figure S063:** <sup>1</sup>H NMR spectrum of 2-((4-methoxybenzyl)thio)-5-(trifluoromethyl)aniline (**2k**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



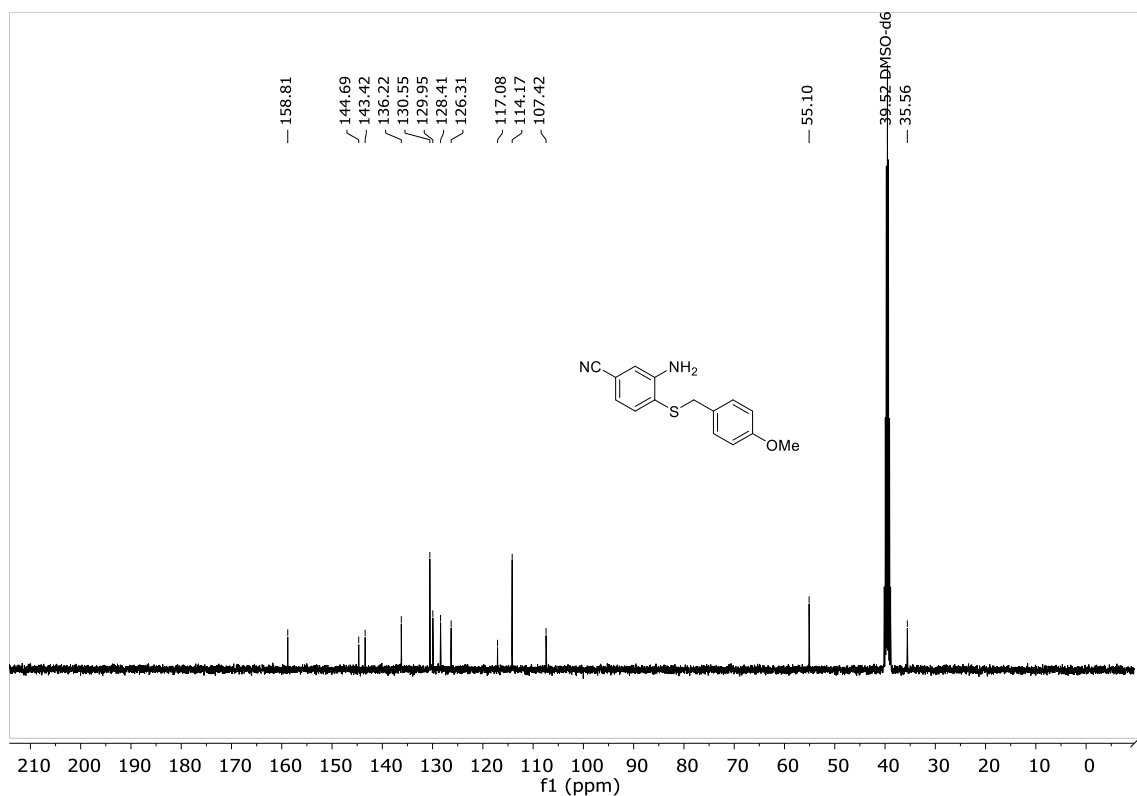
**Figure S064:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 2-((4-methoxybenzyl)thio)-5-(trifluoromethyl)aniline (**2k**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



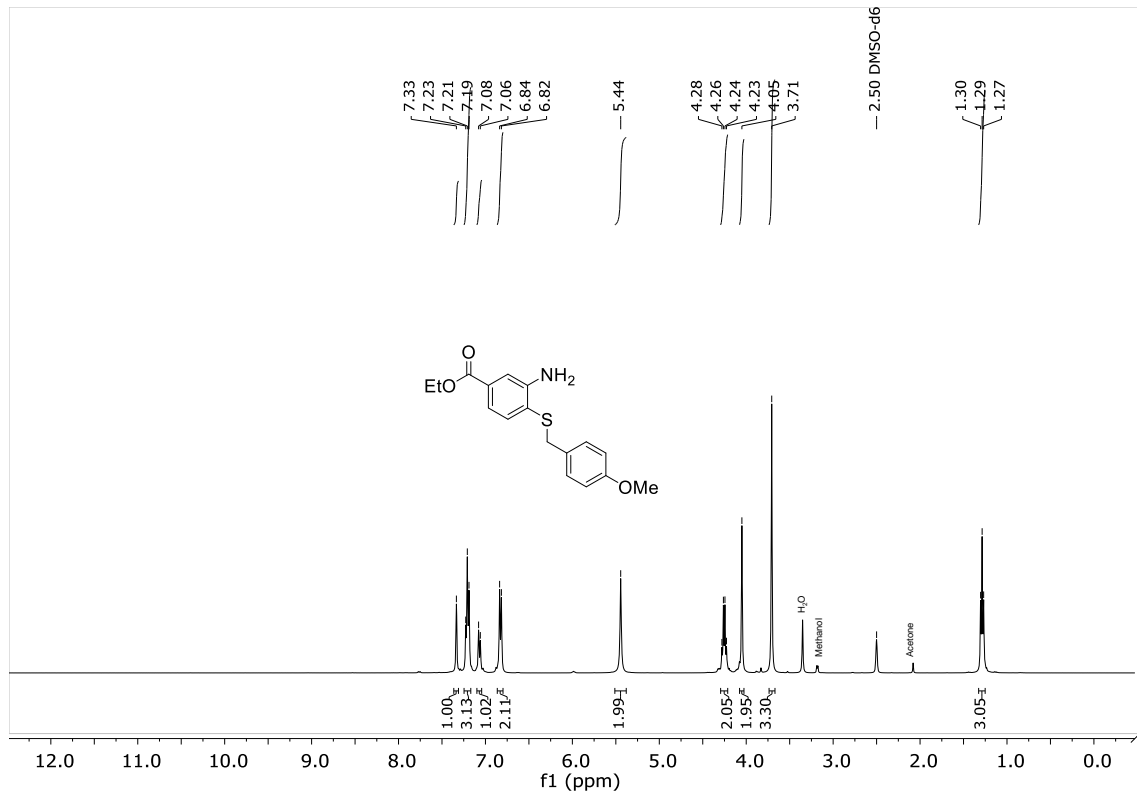
**Figure S065:**  $^{19}\text{F}\{^1\text{H}\}$  NMR spectrum of 2-((4-methoxybenzyl)thio)-5-(trifluoromethyl)aniline (**2k**) (3760 MHz, DMSO- $d_6$ , 298 K, referenced to fluorobenzene).



**Figure S066:**  $^1\text{H}$  NMR spectrum of 3-amino-4-((4-methoxybenzyl)thio)benzonitrile (**2l**) (400 MHz, DMSO- $d_6$ , 298 K).

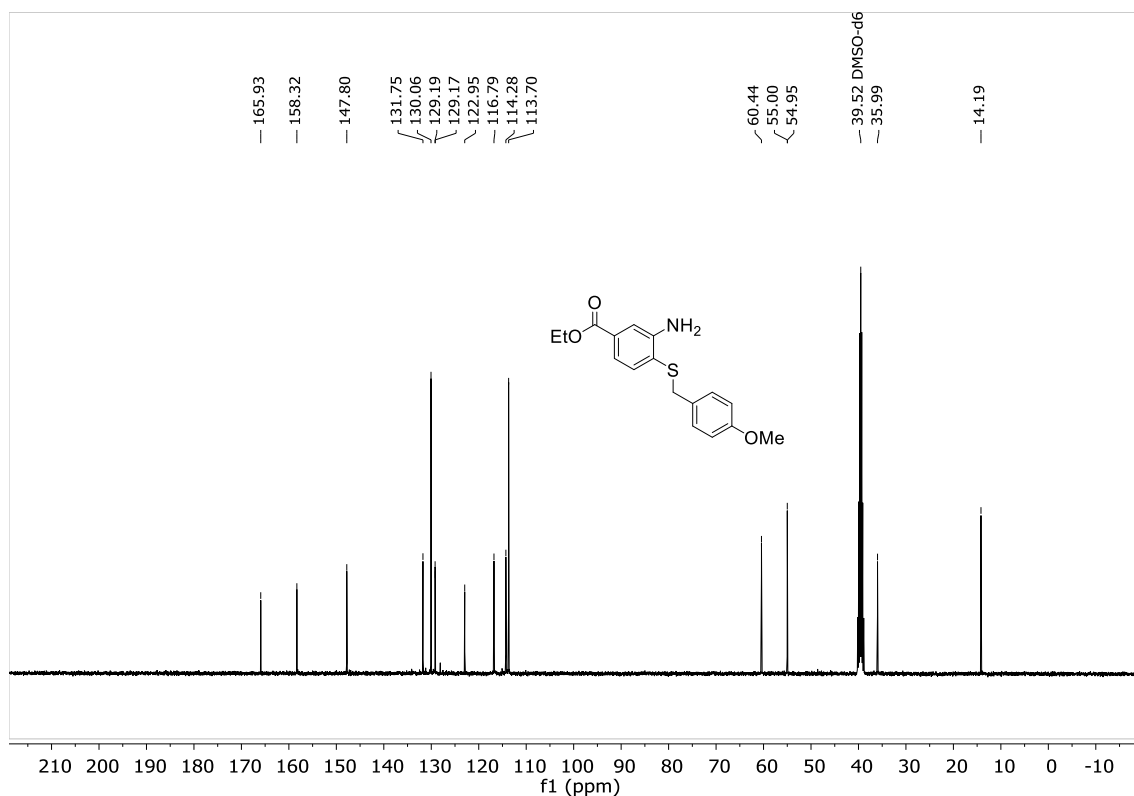


**Figure S067:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 3-amino-4-((4-methoxybenzyl)thio)benzonitrile (**2l**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).

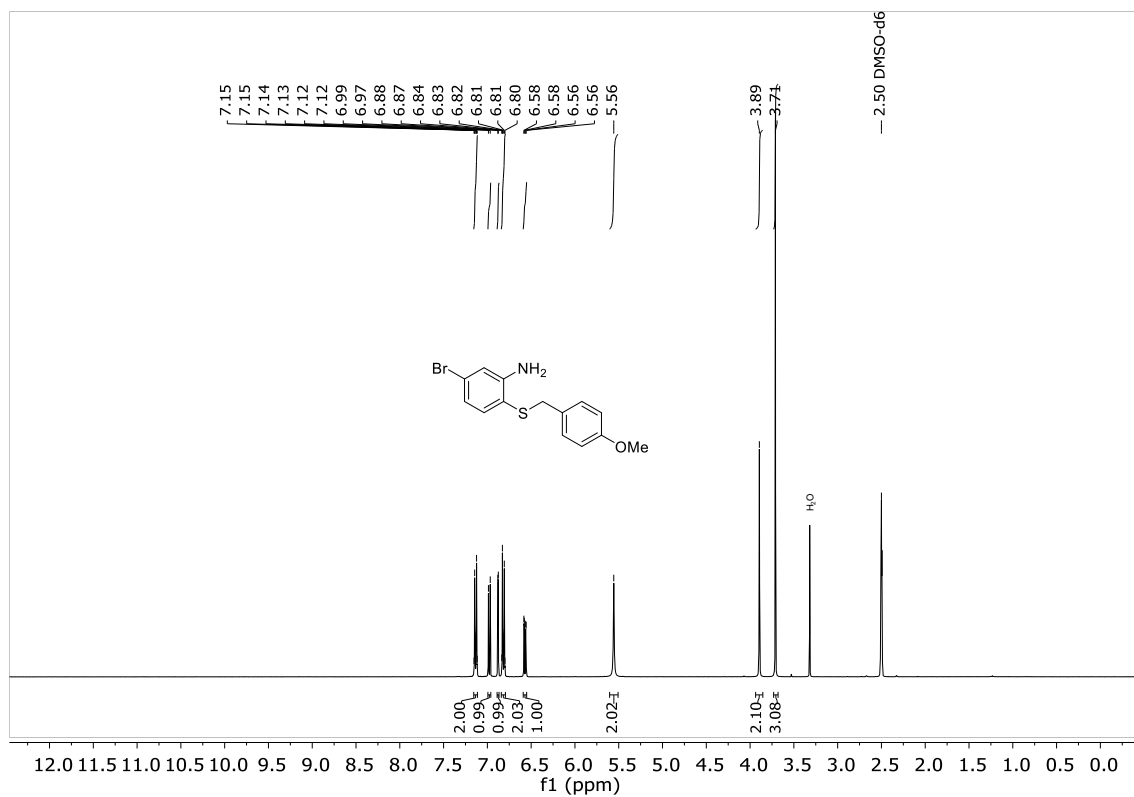


**Figure S068:** <sup>1</sup>H NMR spectrum of ethyl 3-amino-4-((4-methoxybenzyl)thio)benzoate (**2m**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).

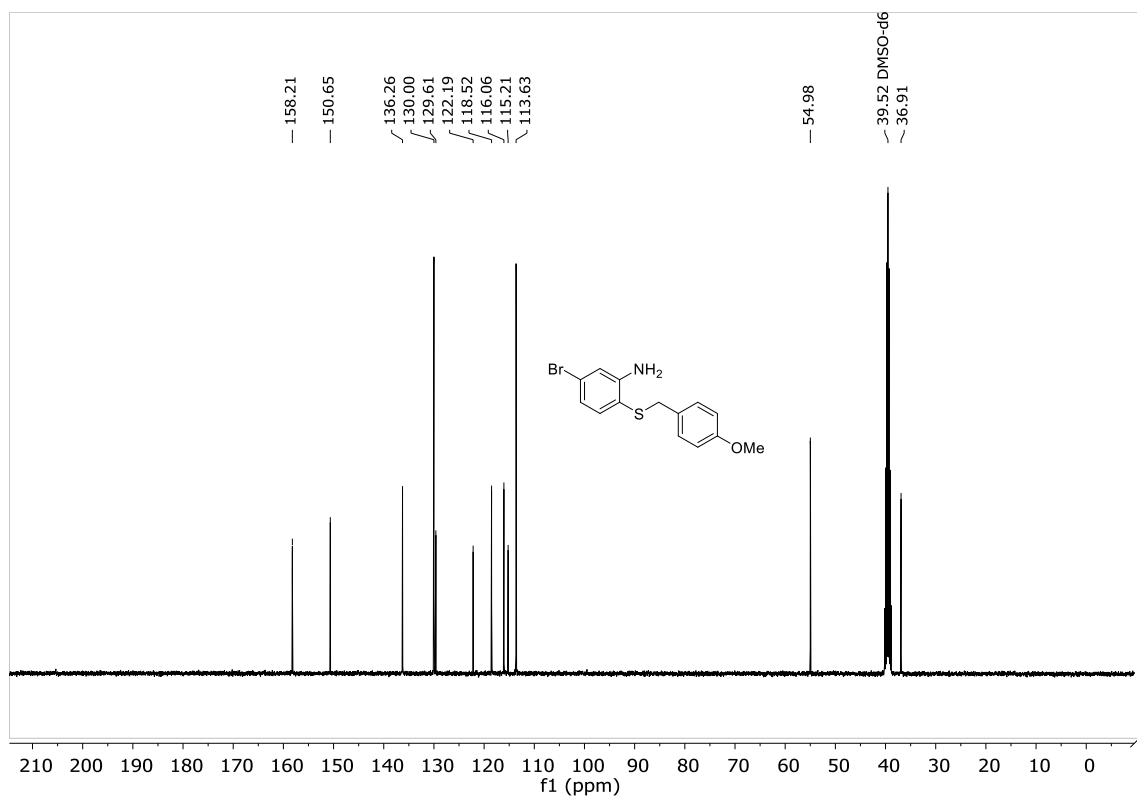




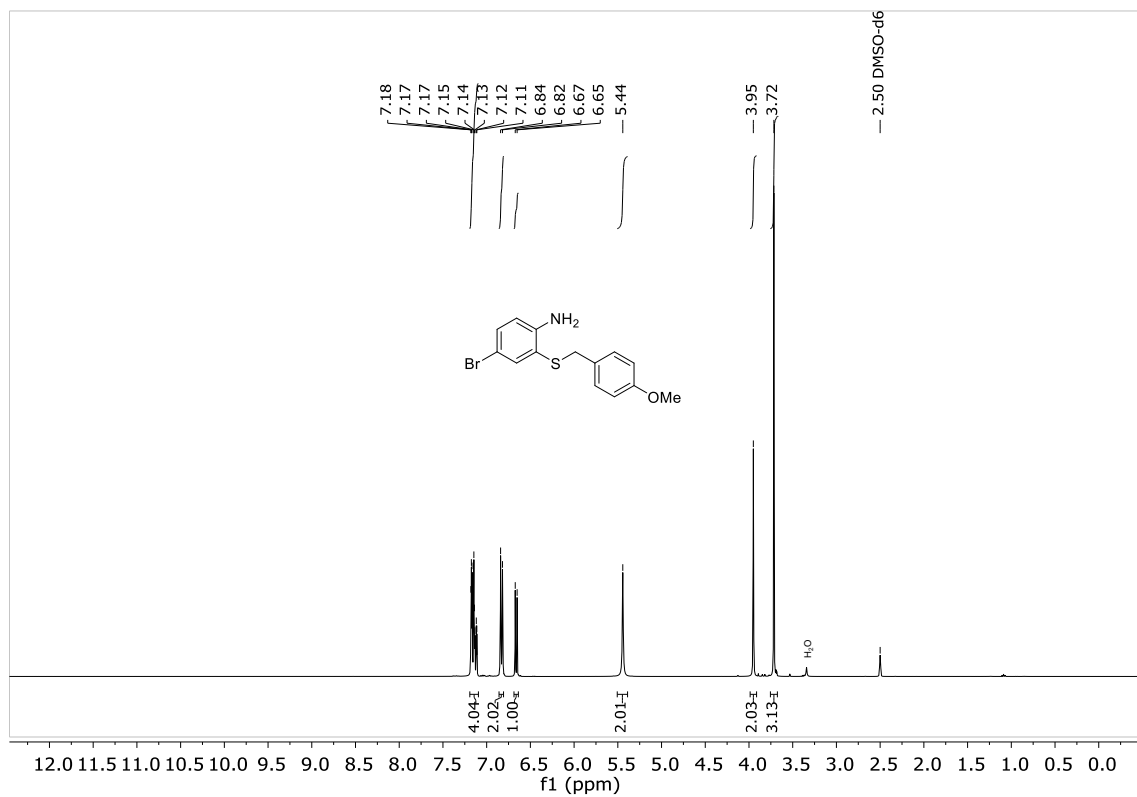
**Figure S069:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of ethyl 3-amino-4-((4-methoxybenzyl)thio)benzoate (**2m**) (100 MHz, DMSO- $d_6$ , 298 K).



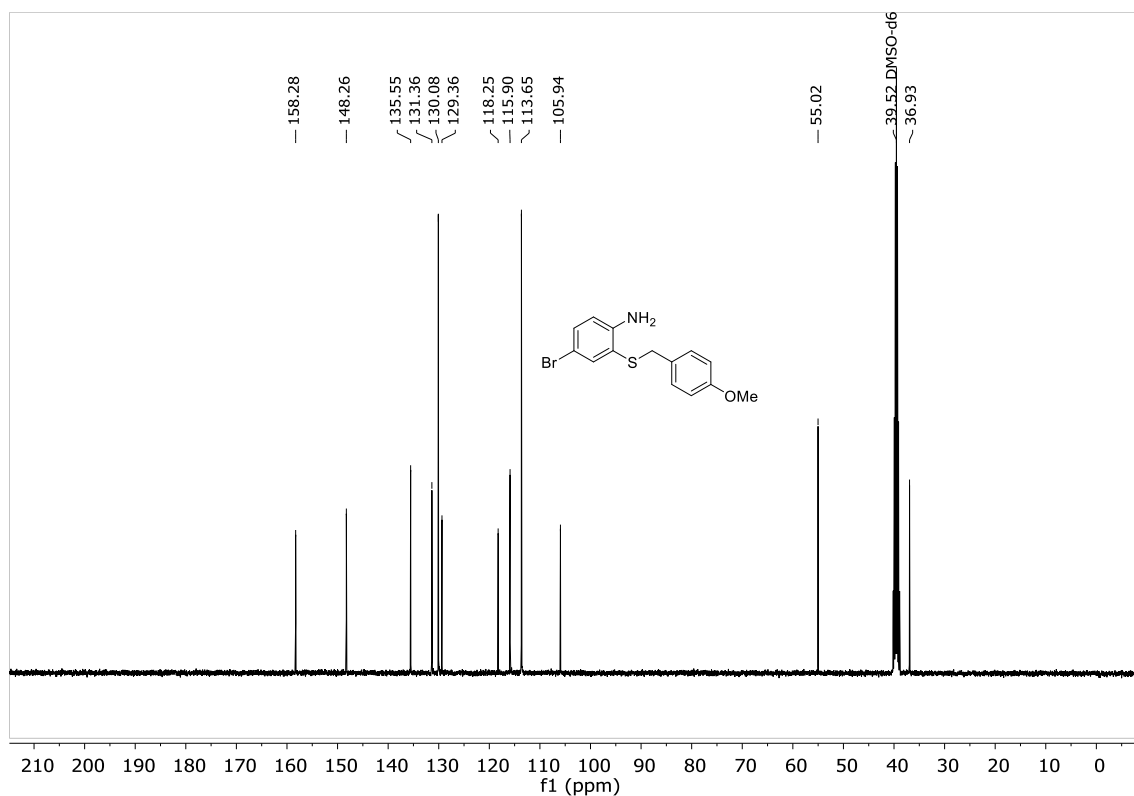
**Figure S070:**  $^1\text{H}$  NMR spectrum of 5-bromo-2-((4-methoxybenzyl)thio)aniline (**2n**) (400 MHz, DMSO- $d_6$ , 298 K).



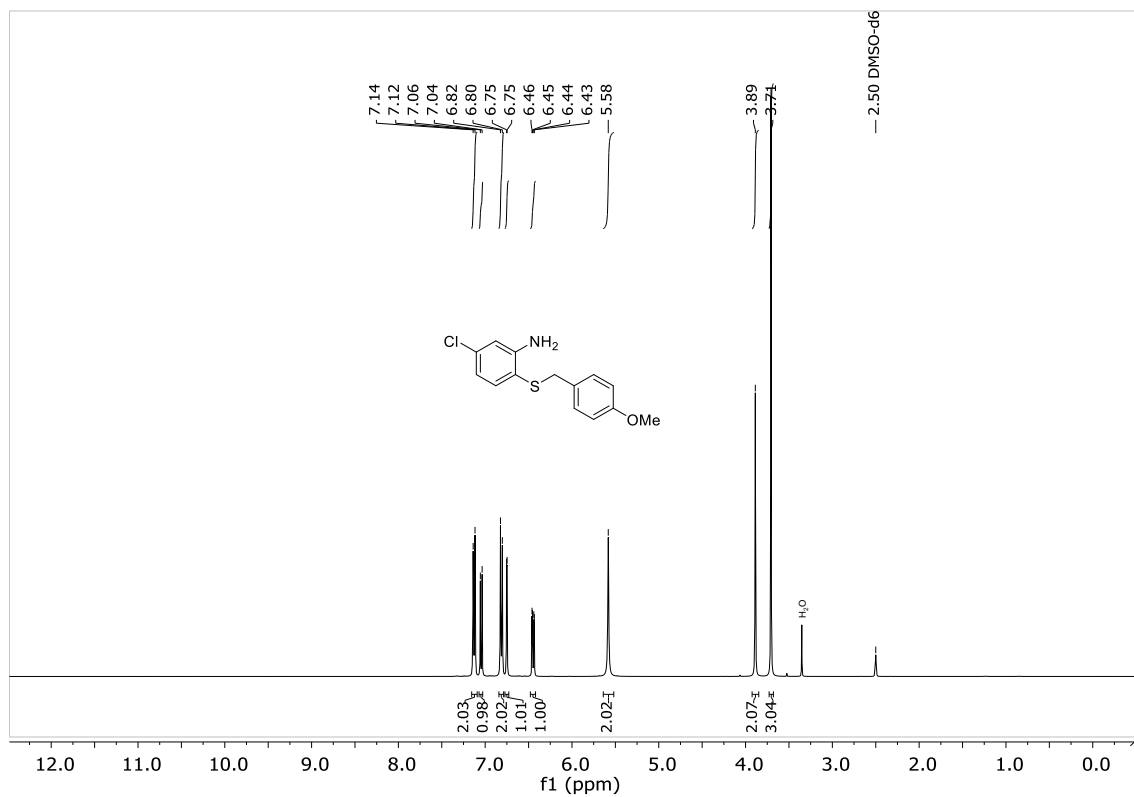
**Figure S071:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of 5-bromo-2-((4-methoxybenzyl)thio)aniline (**2n**) (100 MHz, DMSO- $d_6$ , 298 K).



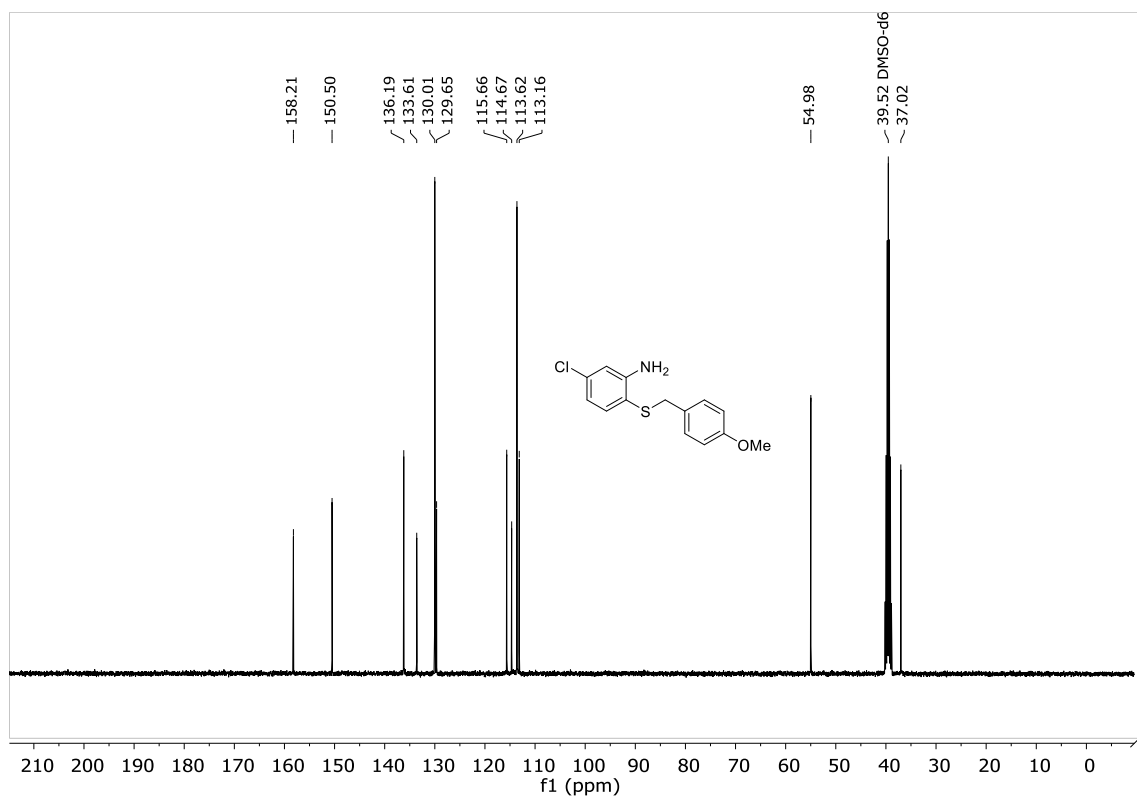
**Figure S072:**  $^1\text{H}$  NMR spectrum of 4-bromo-2-((4-methoxybenzyl)thio)aniline (**2o**) (400 MHz, DMSO- $d_6$ , 298 K).



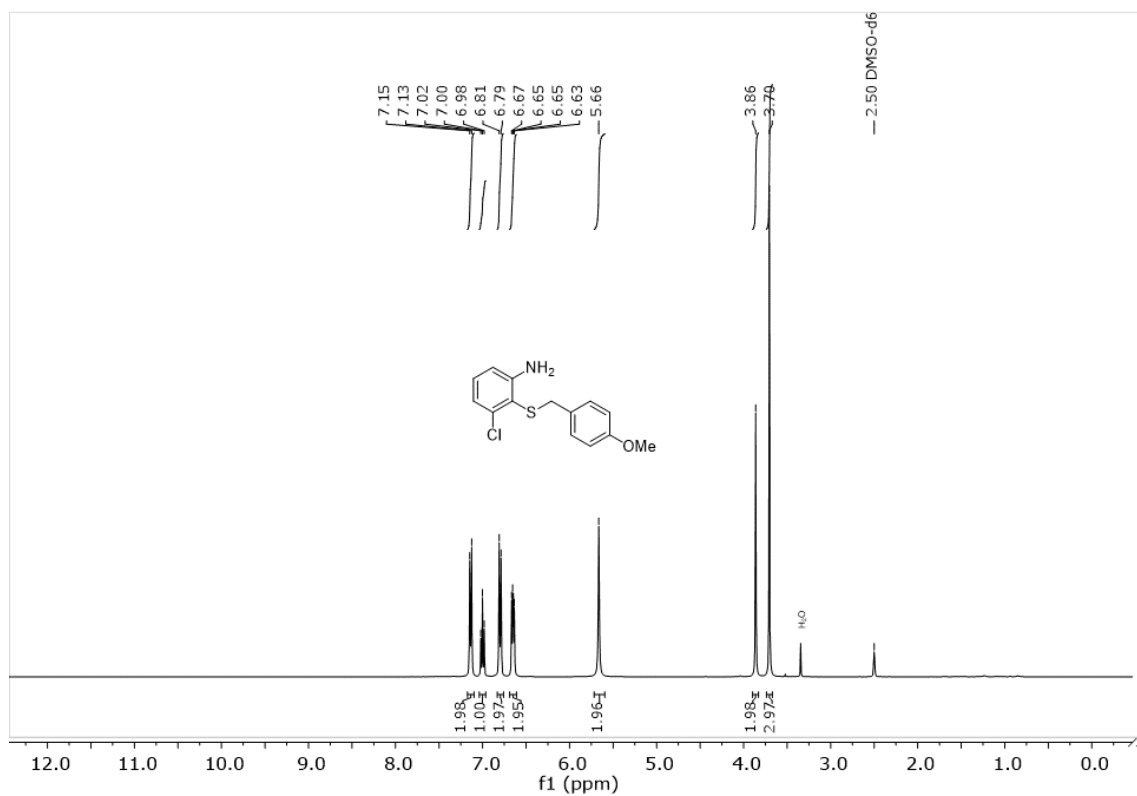
**Figure S073:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of 4-bromo-2-((4-methoxybenzyl)thio)aniline (**2o**) (100 MHz, DMSO- $d_6$ , 298 K).



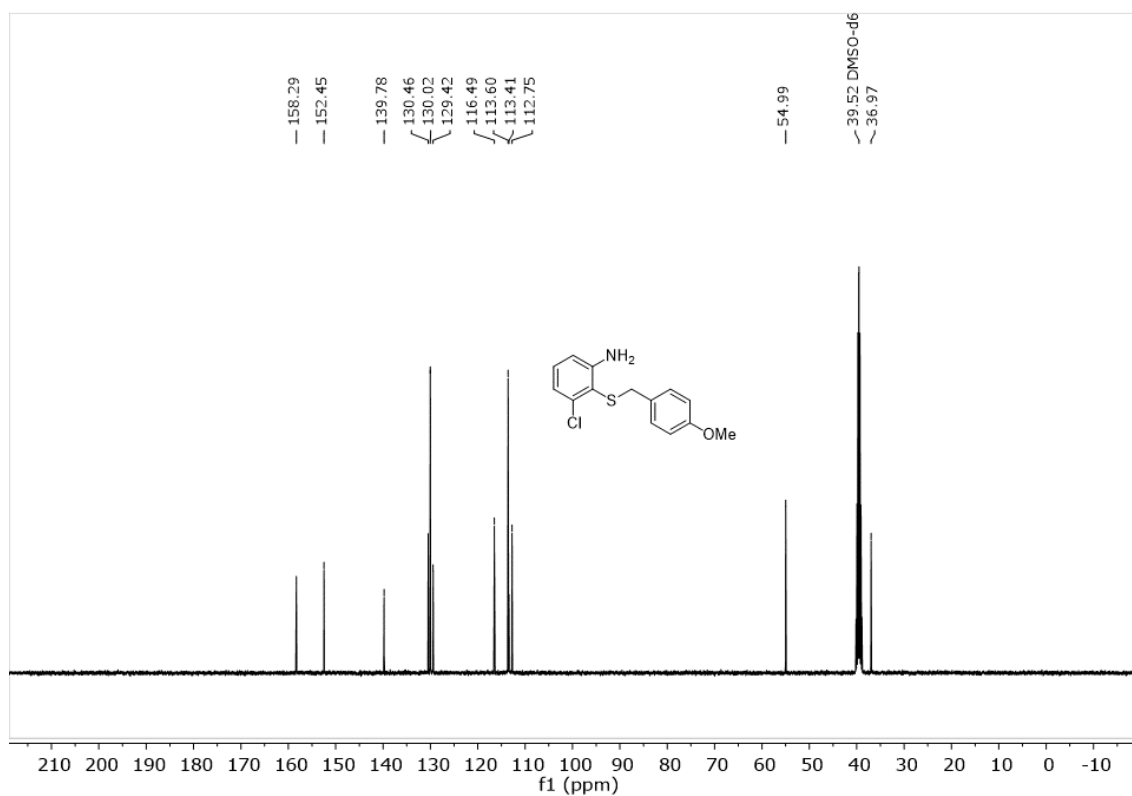
**Figure S074:**  $^1\text{H}$  NMR spectrum of 5-chloro-2-((4-methoxybenzyl)thio)aniline (**2p**) (400 MHz, DMSO- $d_6$ , 298 K).



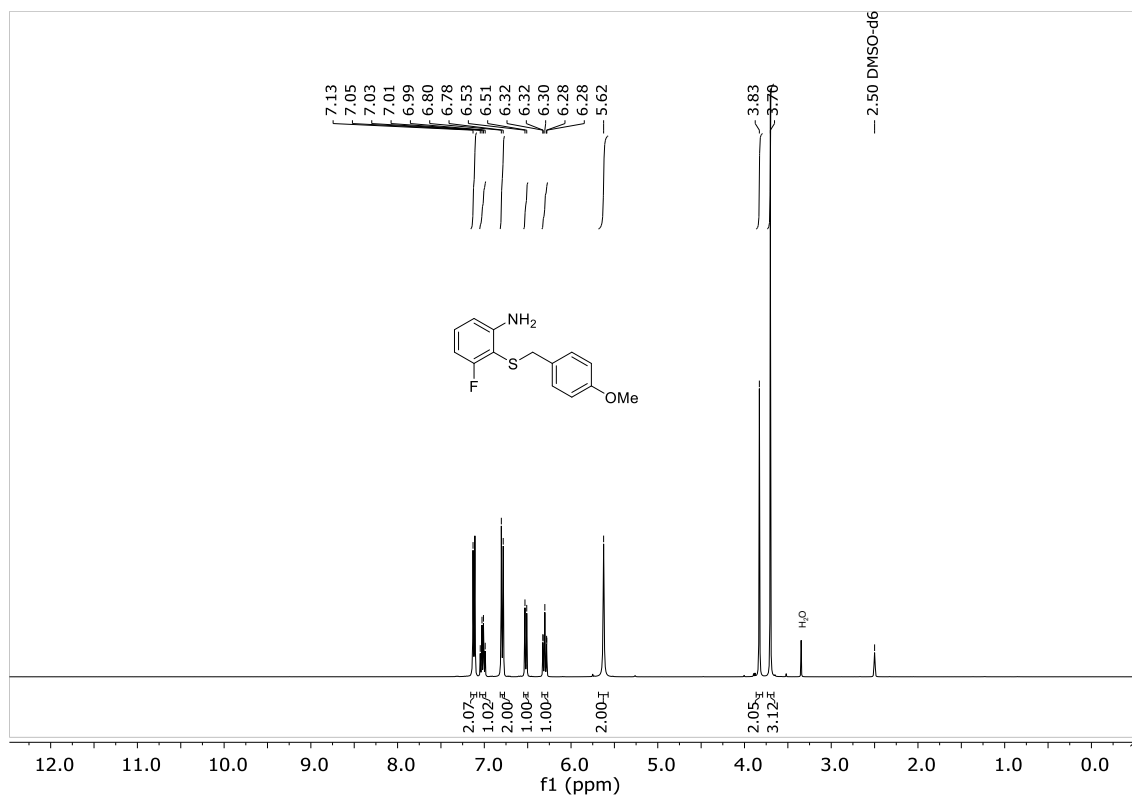
**Figure S075:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of 5-chloro-2-((4-methoxybenzyl)thio)aniline (**2p**) (100 MHz, DMSO- $d_6$ , 298 K).



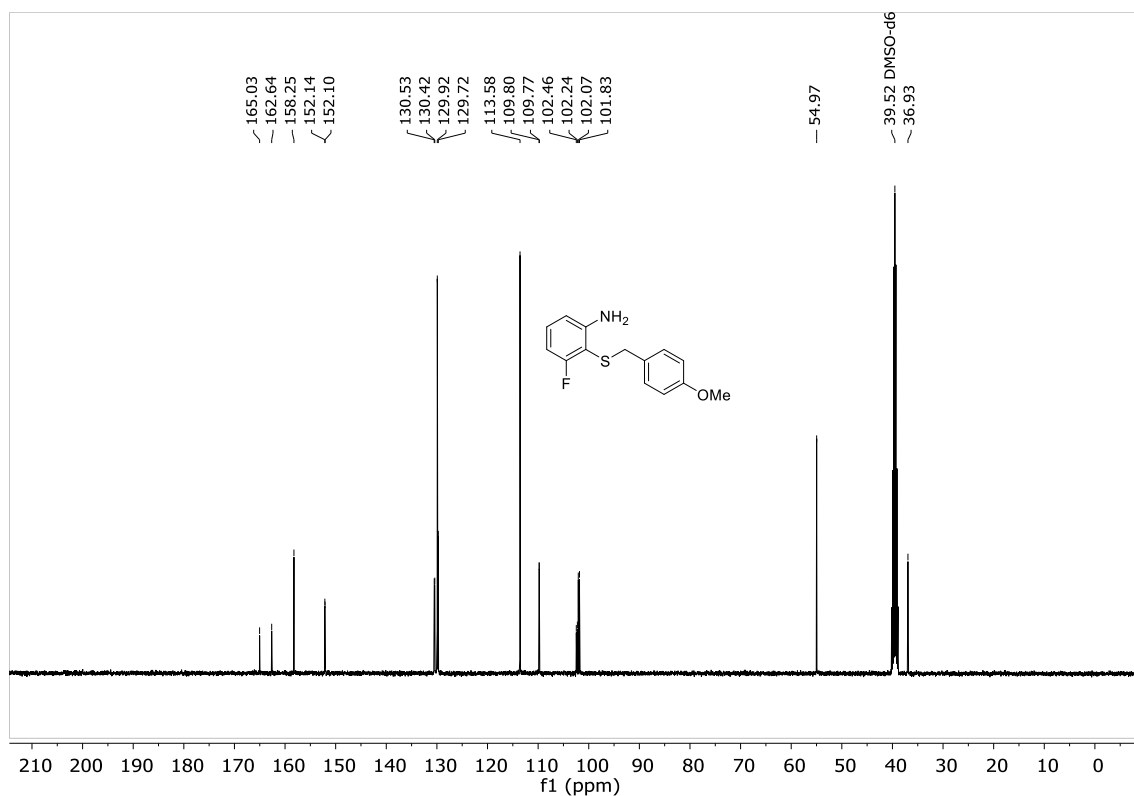
**Figure S076:**  $^1\text{H}$  NMR spectrum of 3-chloro-2-((4-methoxybenzyl)thio)aniline (**2q**) (400 MHz, DMSO- $d_6$ , 298 K).



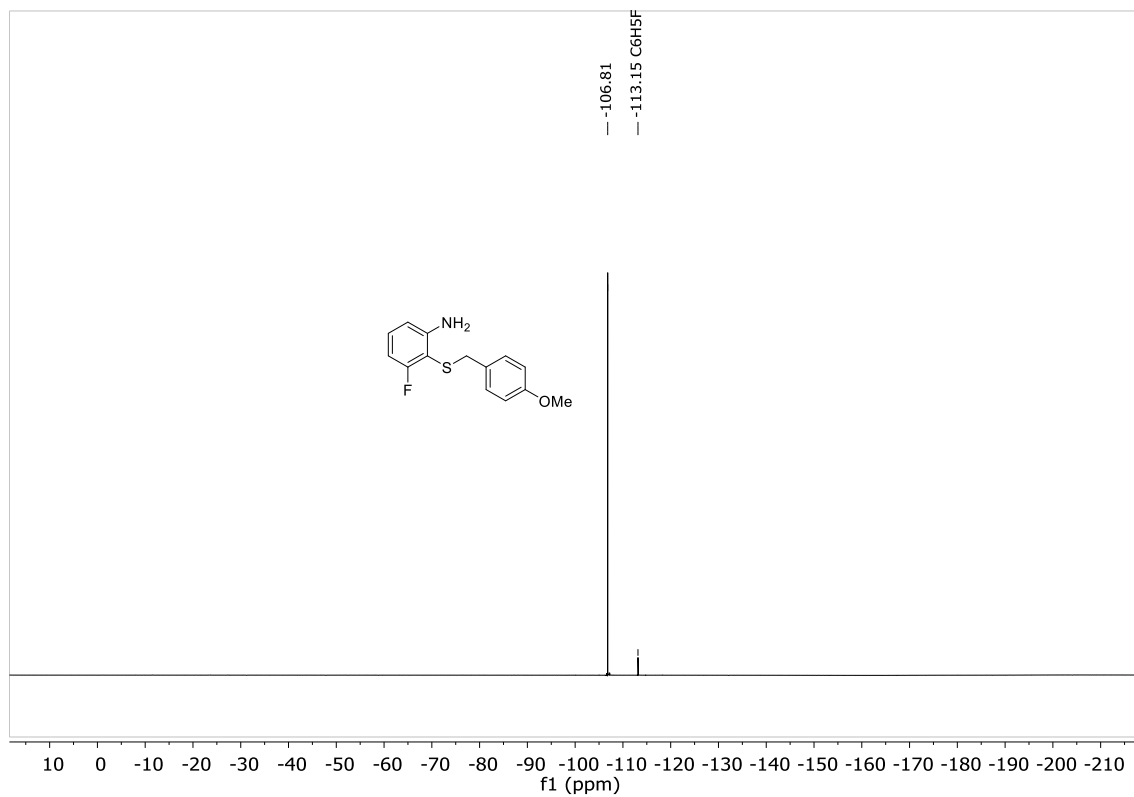
**Figure S077:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of 3-chloro-2-((4-methoxybenzyl)thio)aniline (**2q**) (100 MHz, DMSO- $d_6$ , 298 K).



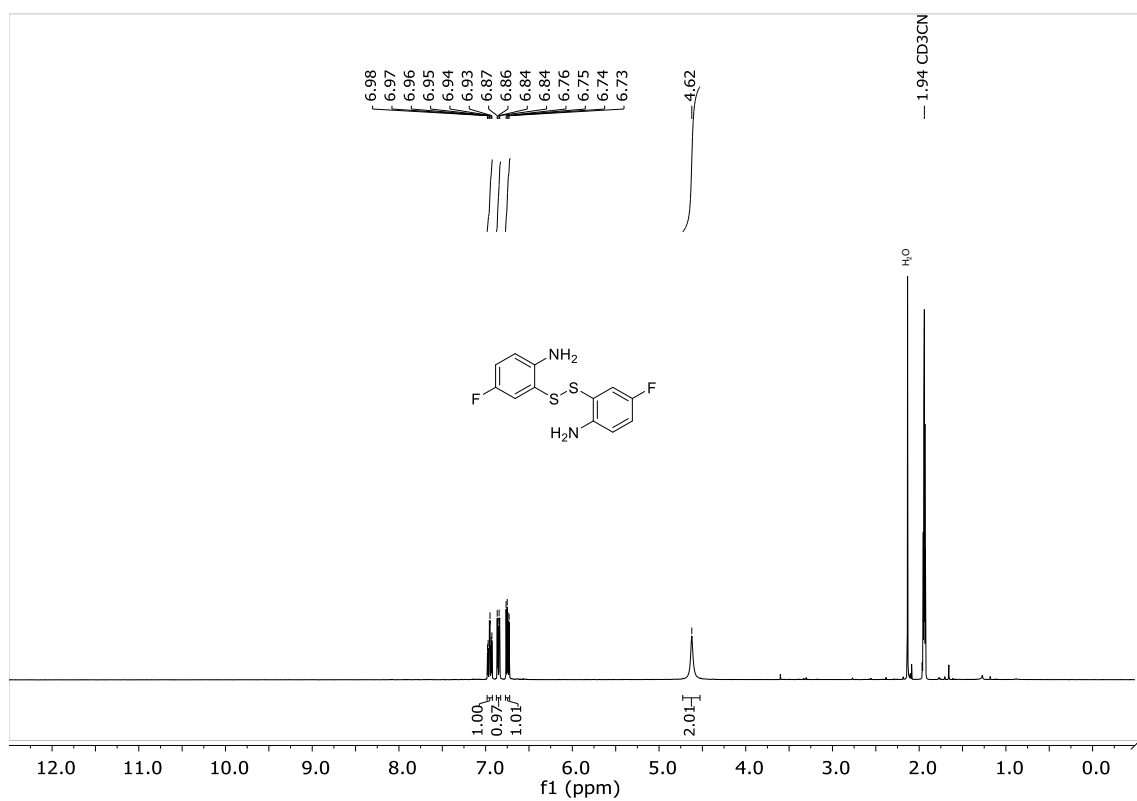
**Figure S078:**  $^1\text{H}$  NMR spectrum of 3-fluoro-2-((4-methoxybenzyl)thio)aniline (**2r**) (400 MHz, DMSO- $d_6$ , 298 K).



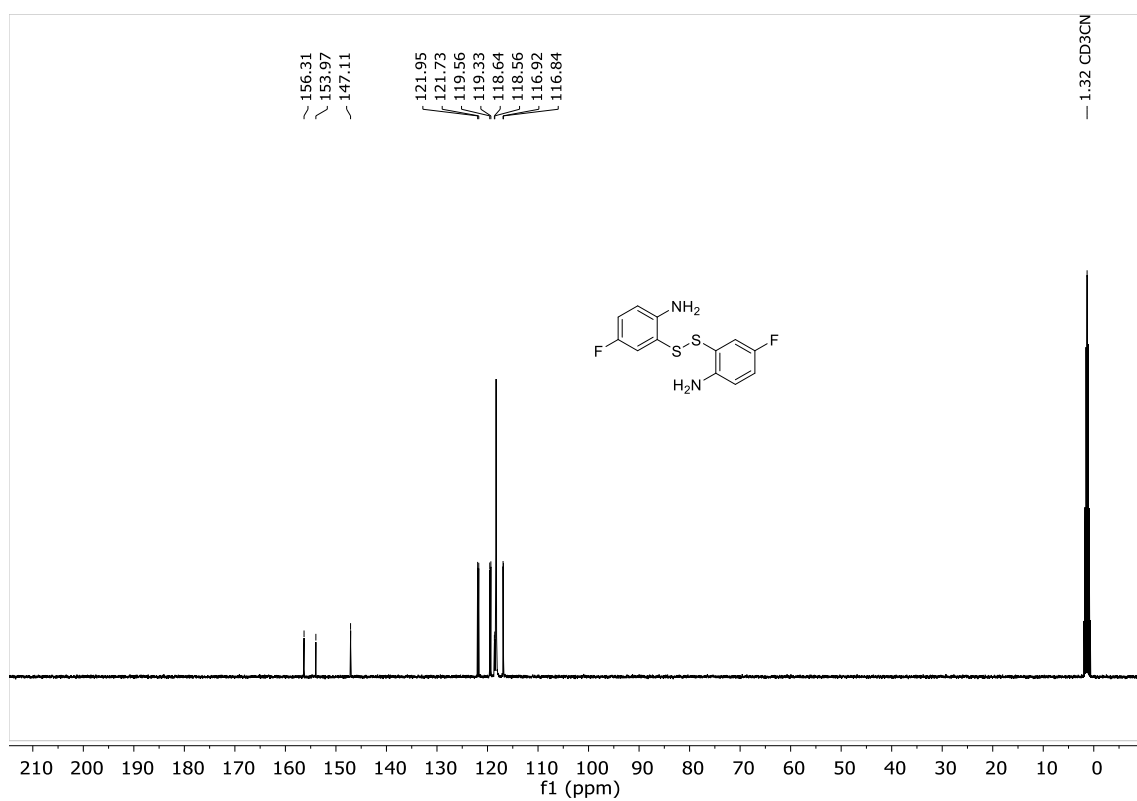
**Figure S079:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of 3-fluoro-2-((4-methoxybenzyl)thio)aniline (**2r**) (100 MHz, DMSO- $d_6$ , 298 K).



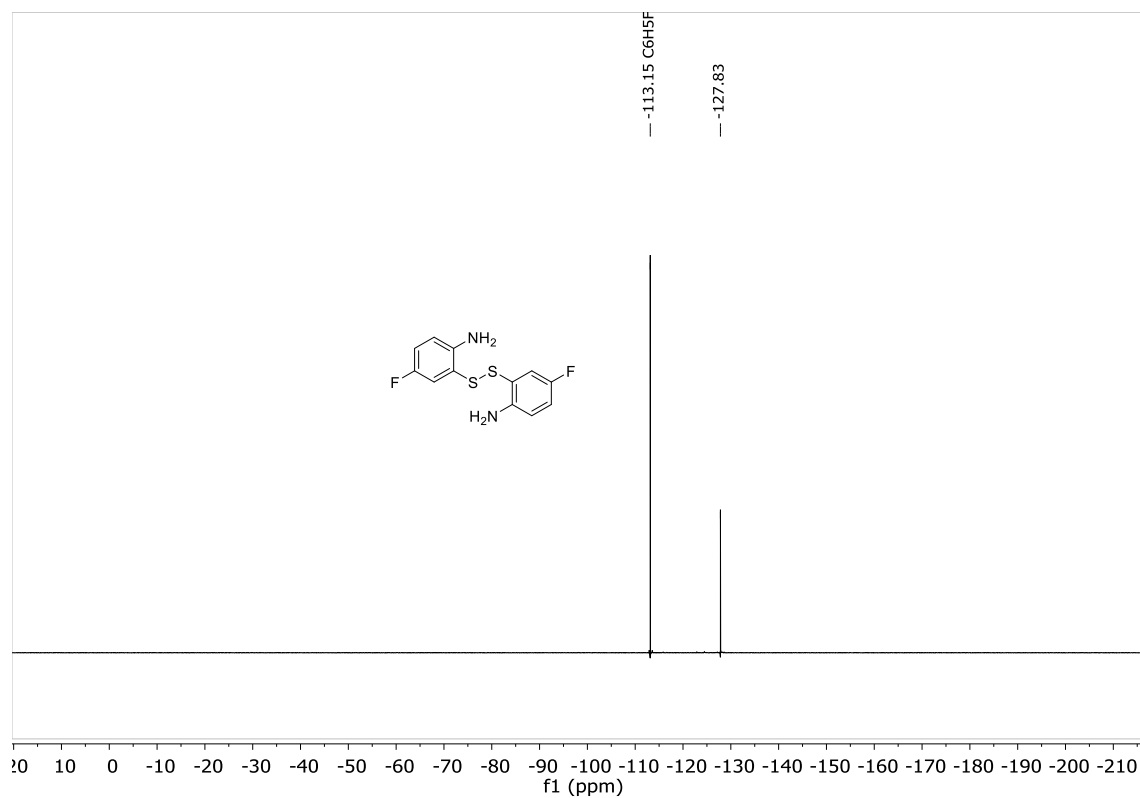
**Figure S080:**  $^{19}\text{F}\{^1\text{H}\}$  NMR spectrum of 3-fluoro-2-((4-methoxybenzyl)thio)aniline (**2r**) (376 MHz, DMSO- $d_6$ , 298 K, referenced to fluorobenzene).



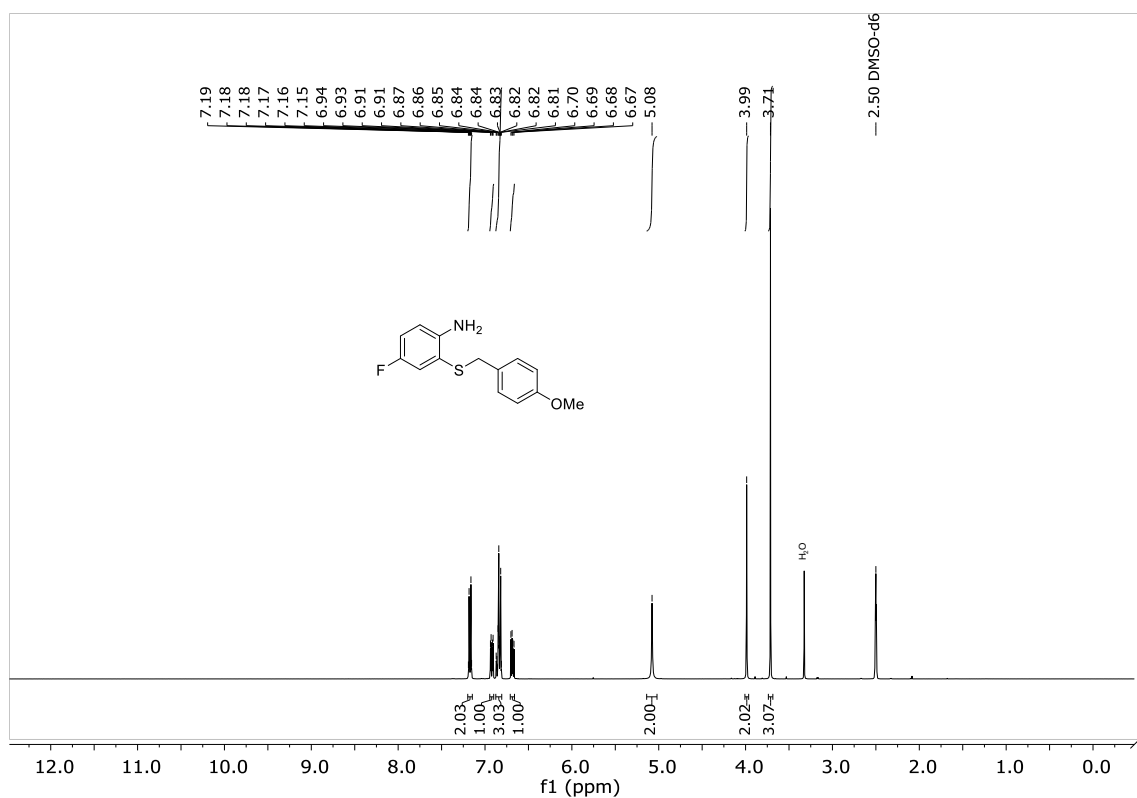
**Figure S081:** <sup>1</sup>H NMR spectrum of 2,2'-disulfanedibis(4-fluoroaniline) (400 MHz, CD<sub>3</sub>CN, 298 K).



**Figure S082:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 2,2'-disulfanedibis(4-fluoroaniline) (100 MHz, CD<sub>3</sub>CN, 298 K).

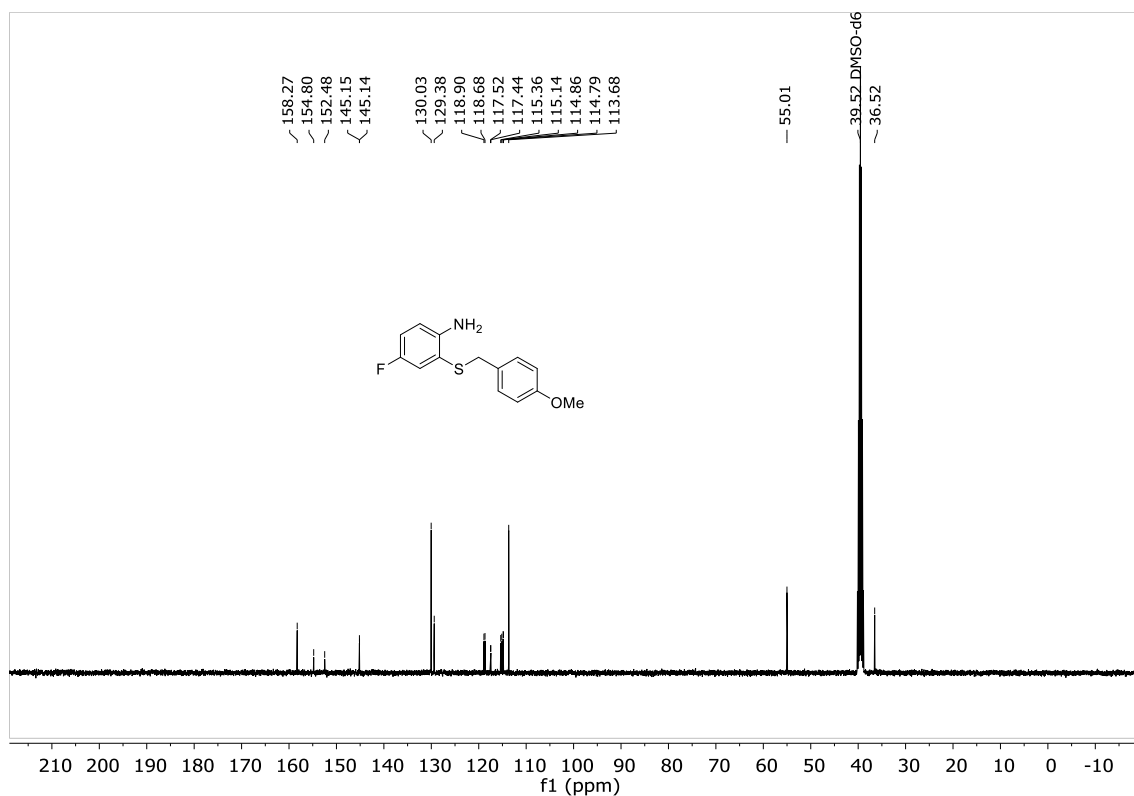


**Figure S083:**  $^{19}\text{F}\{^1\text{H}\}$  NMR spectrum of 2,2'-disulfanediylbis(4-fluoroaniline) (376 MHz,  $\text{CD}_3\text{CN}$ , 298 K, referenced to fluorobenzene).

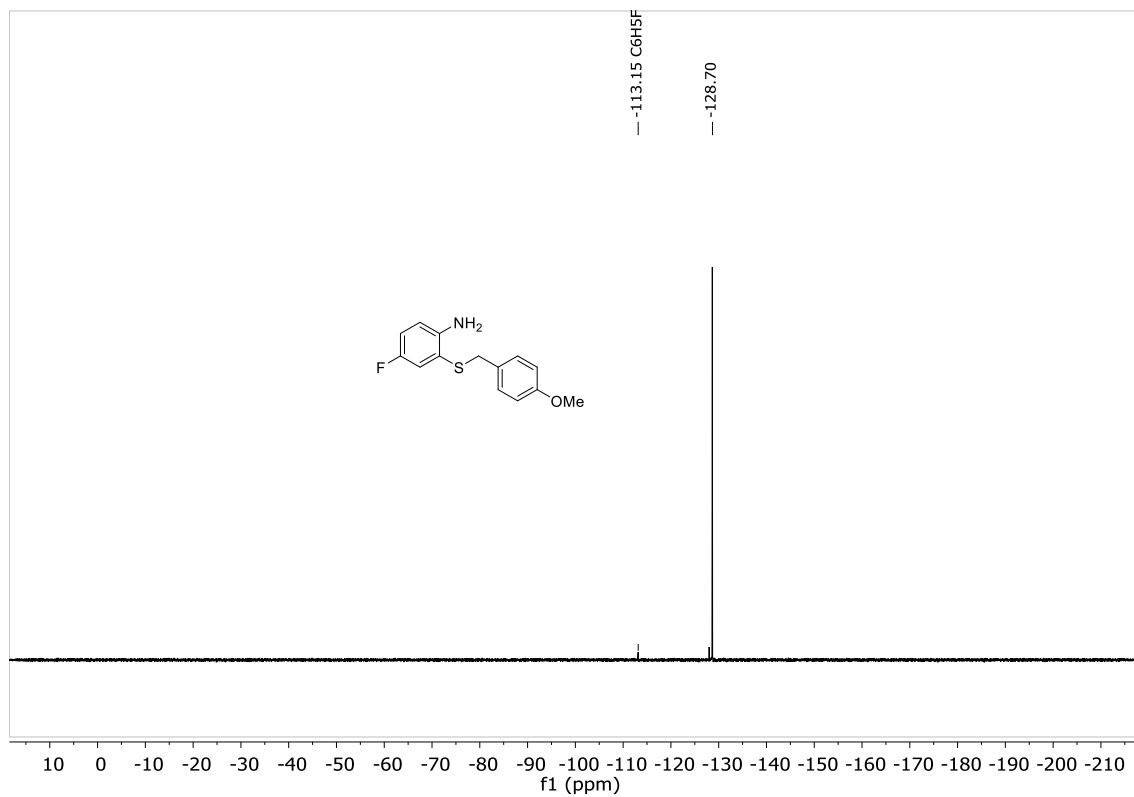


**Figure S084:**  $^1\text{H}$  NMR spectrum of 4-fluoro-2-((4-methoxybenzyl)thio)aniline (**2s**) (400 MHz,  $\text{DMSO}-d_6$ , 298 K).



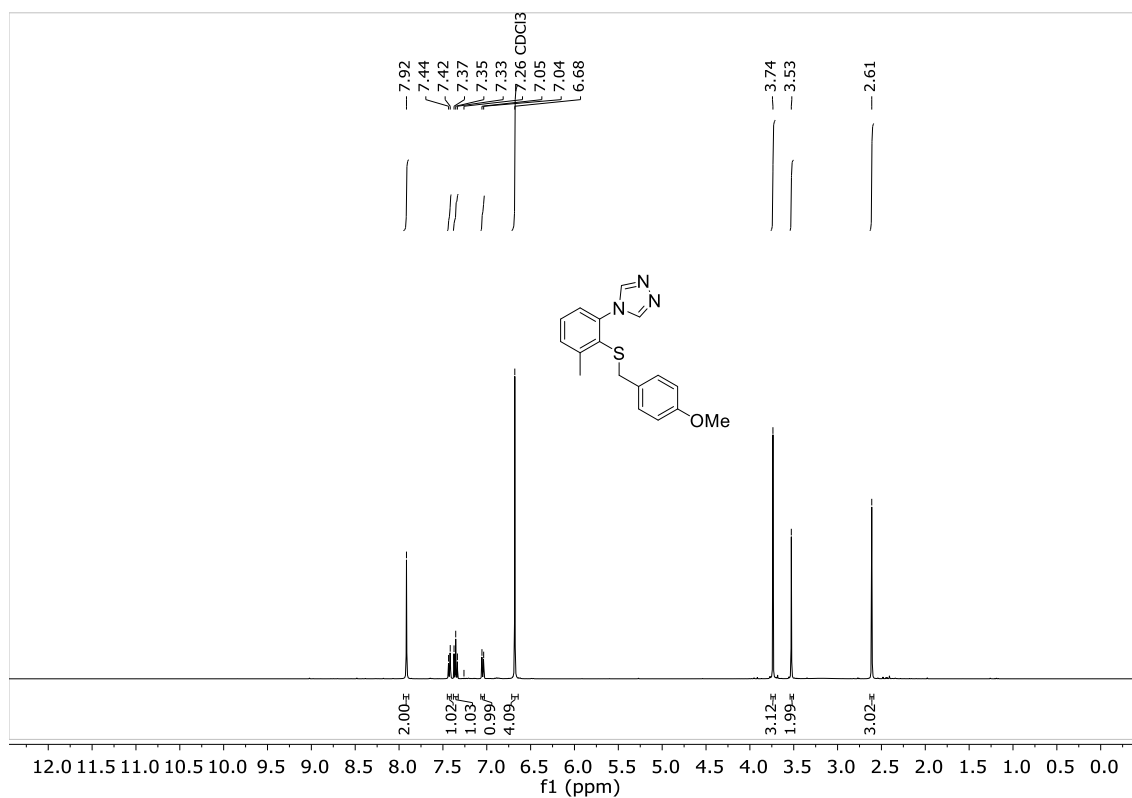


**Figure S085:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of 4-fluoro-2-((4-methoxybenzyl)thio)aniline (**2s**) (100 MHz, DMSO- $d_6$ , 298 K).

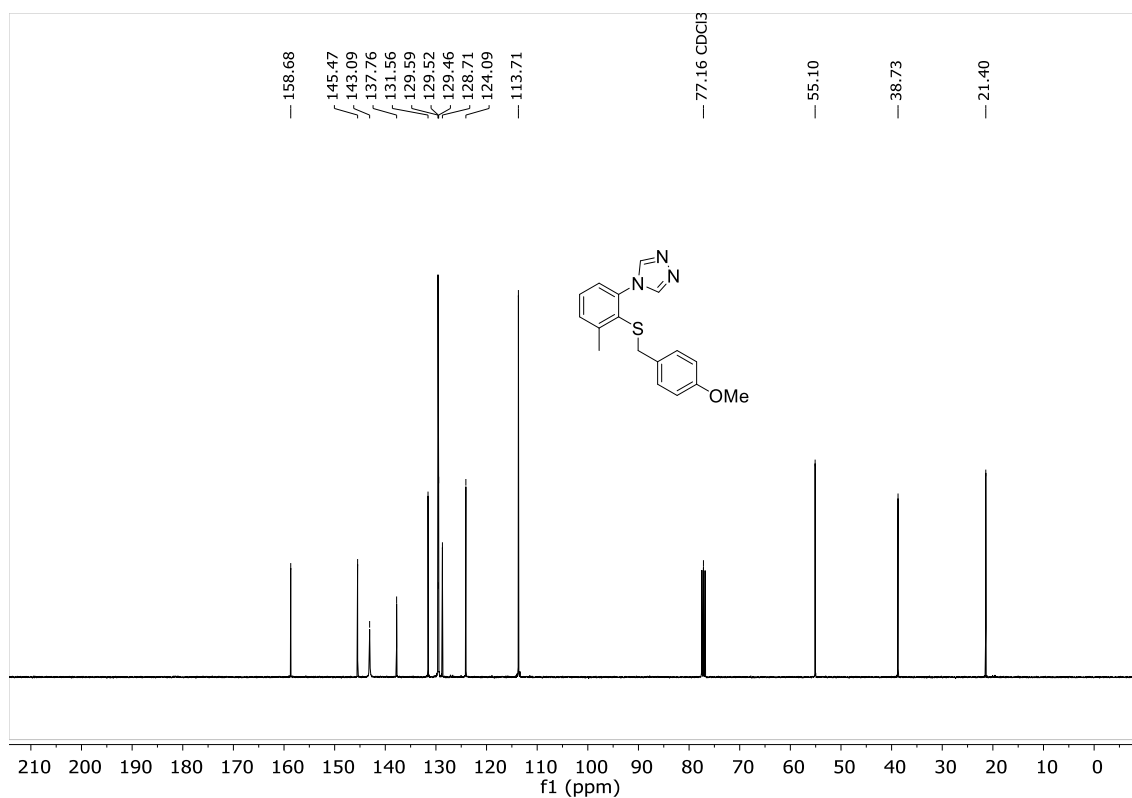


**Figure S086:**  $^{19}\text{F}\{^1\text{H}\}$  NMR spectrum of 4-fluoro-2-((4-methoxybenzyl)thio)aniline (**2s**) (376 MHz, DMSO- $d_6$ , 298 K, referenced to fluorobenzene).

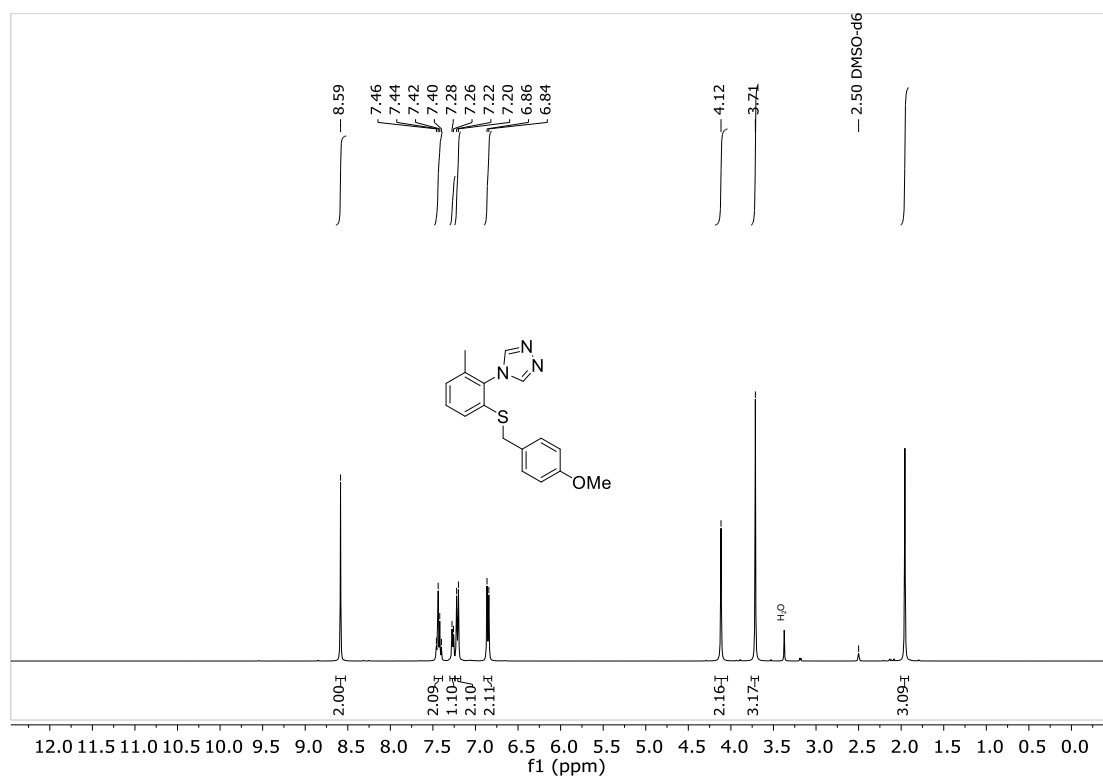
**1.4 NMR Spectra of Substituted 4-(2-((4-Methoxybenzyl)thio)phenyl)-4H-1,2,4-triazoles (3b-3s)**



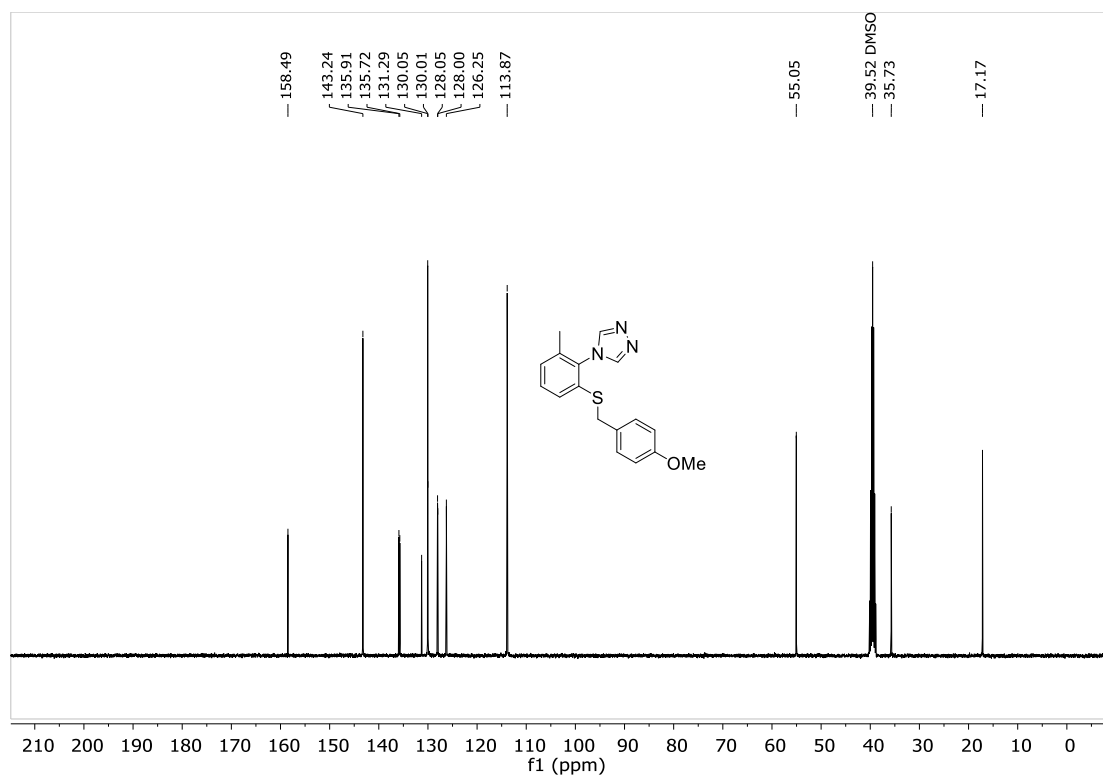
**Figure S087:** <sup>1</sup>H NMR spectrum of 4-(2-((4-methoxybenzyl)thio)-3-methylphenyl)-4H-1,2,4-triazole (**3b**) (400 MHz, CDCl<sub>3</sub>, 298 K).



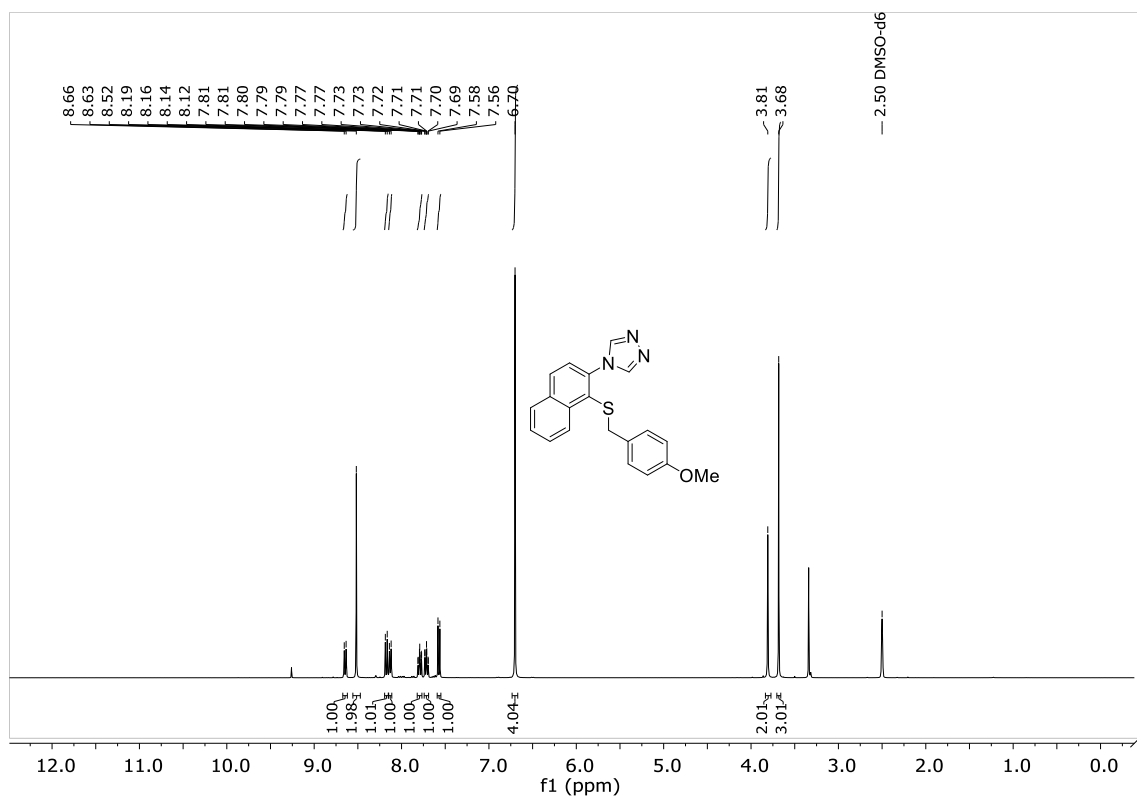
**Figure S088:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 4-(2-((4-methoxybenzyl)thio)-3-methylphenyl)-4H-1,2,4-triazole (**3b**) (100 MHz, CDCl<sub>3</sub>, 298 K).



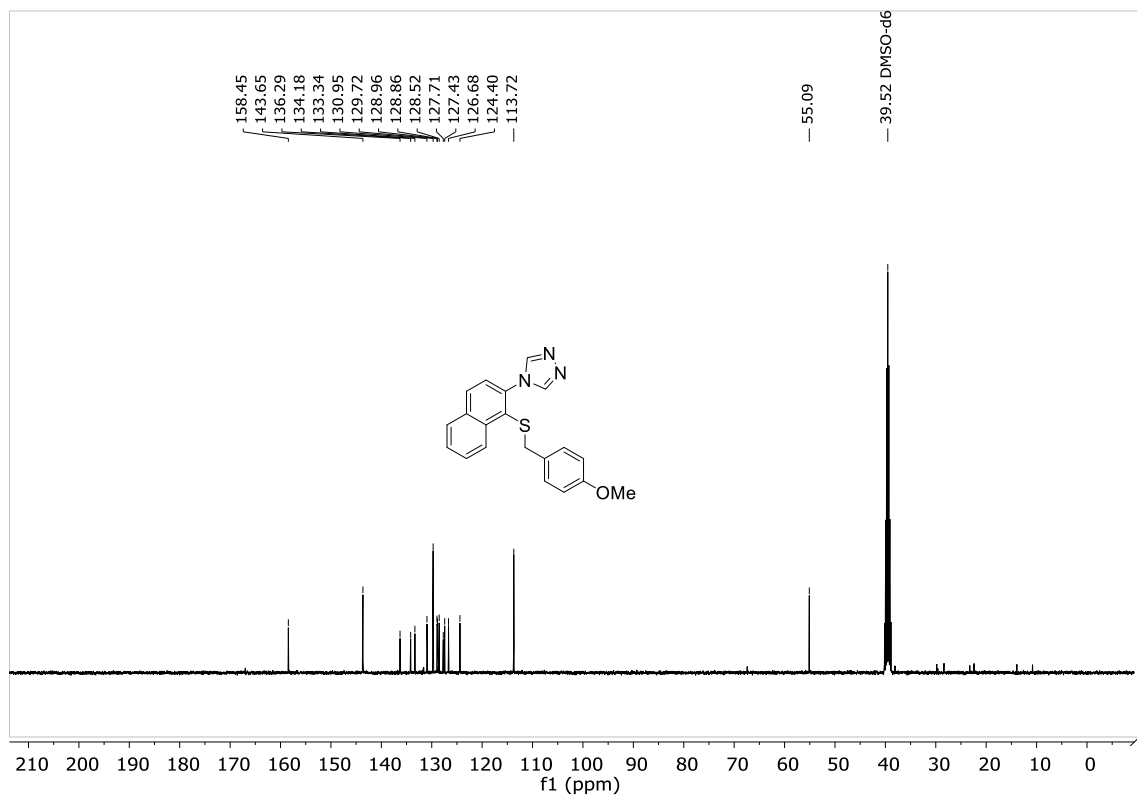
**Figure S089:** <sup>1</sup>H NMR spectrum of 4-(2-((4-methoxybenzyl)thio)-6-methylphenyl)-4H-1,2,4-triazole (**3c**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



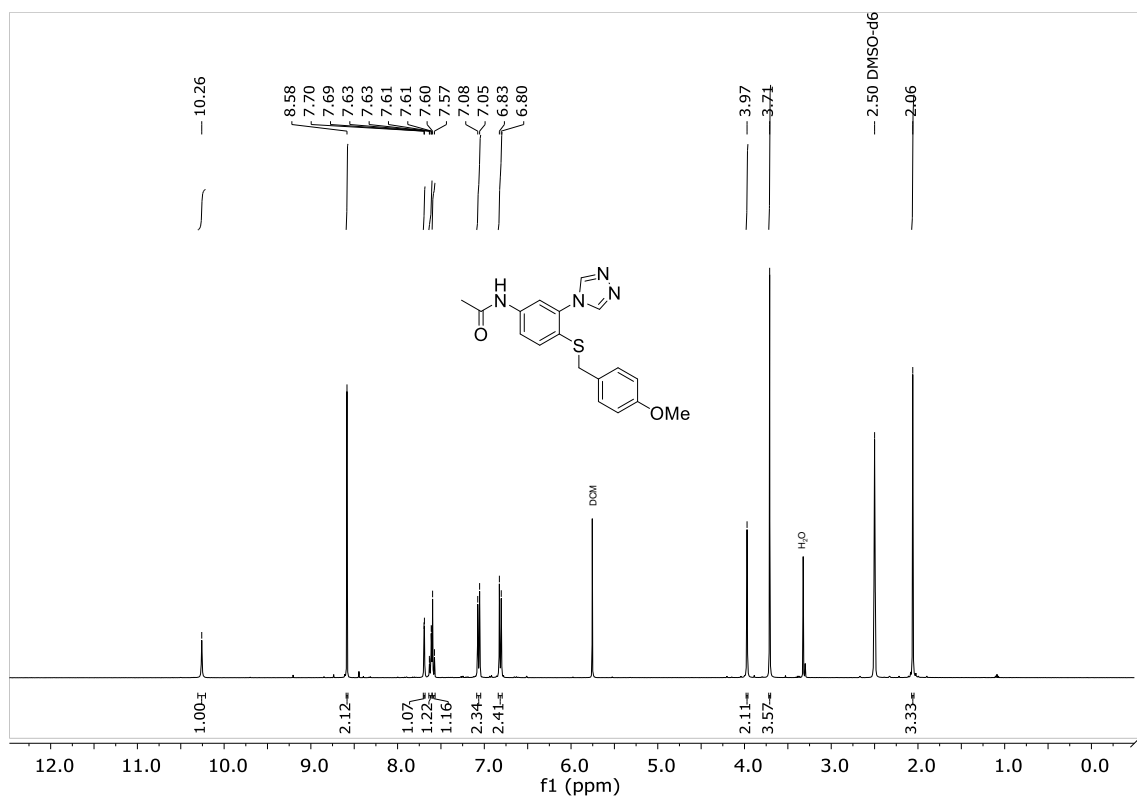
**Figure S090:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 4-(2-((4-methoxybenzyl)thio)-6-methylphenyl)-4H-1,2,4-triazole (**3c**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



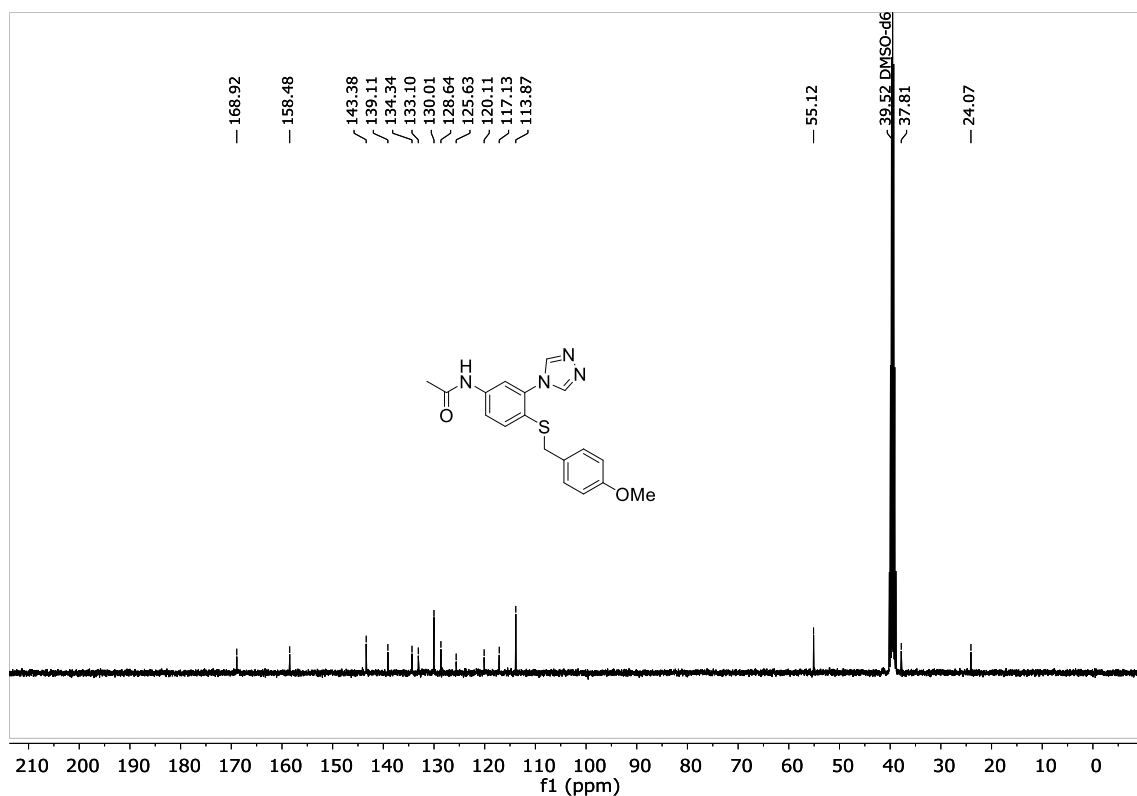
**Figure S091:** <sup>1</sup>H NMR spectrum of 4-(1-((4-methoxybenzyl)thio)naphthalen-2-yl)-4H-1,2,4-triazole (**3d**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



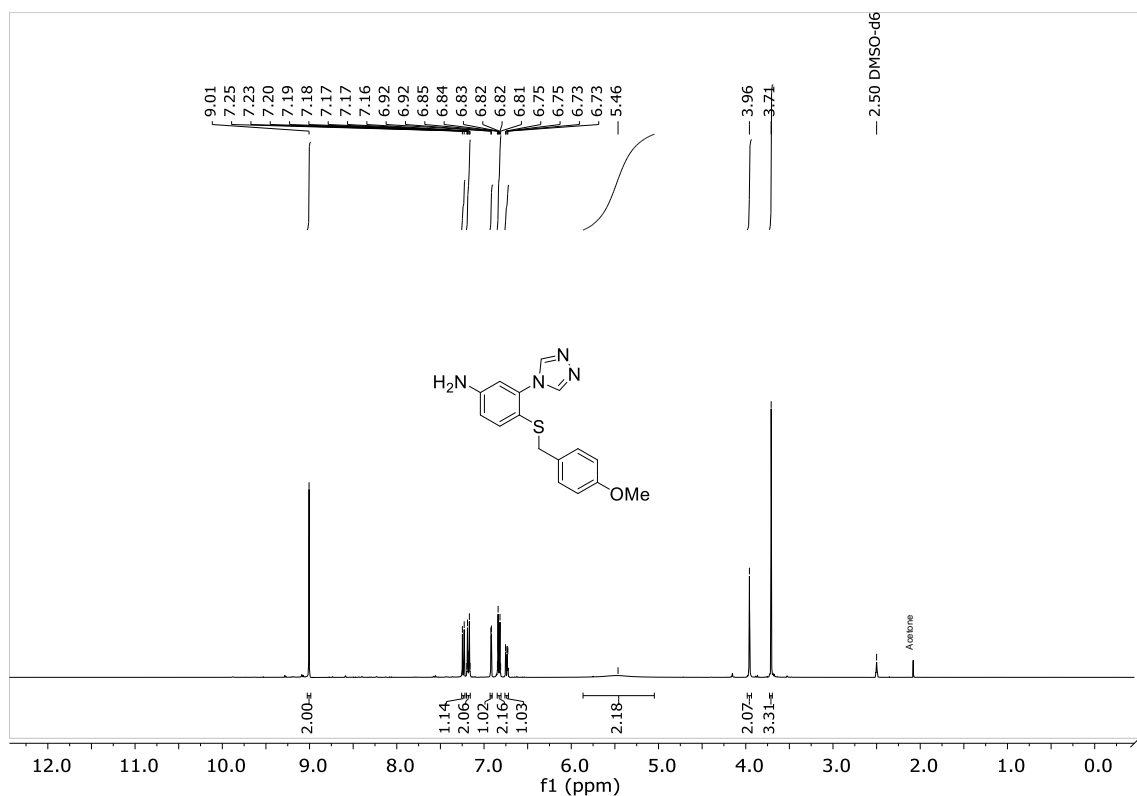
**Figure S092:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 4-(1-((4-methoxybenzyl)thio)naphthalen-2-yl)-4H-1,2,4-triazole (**3d**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



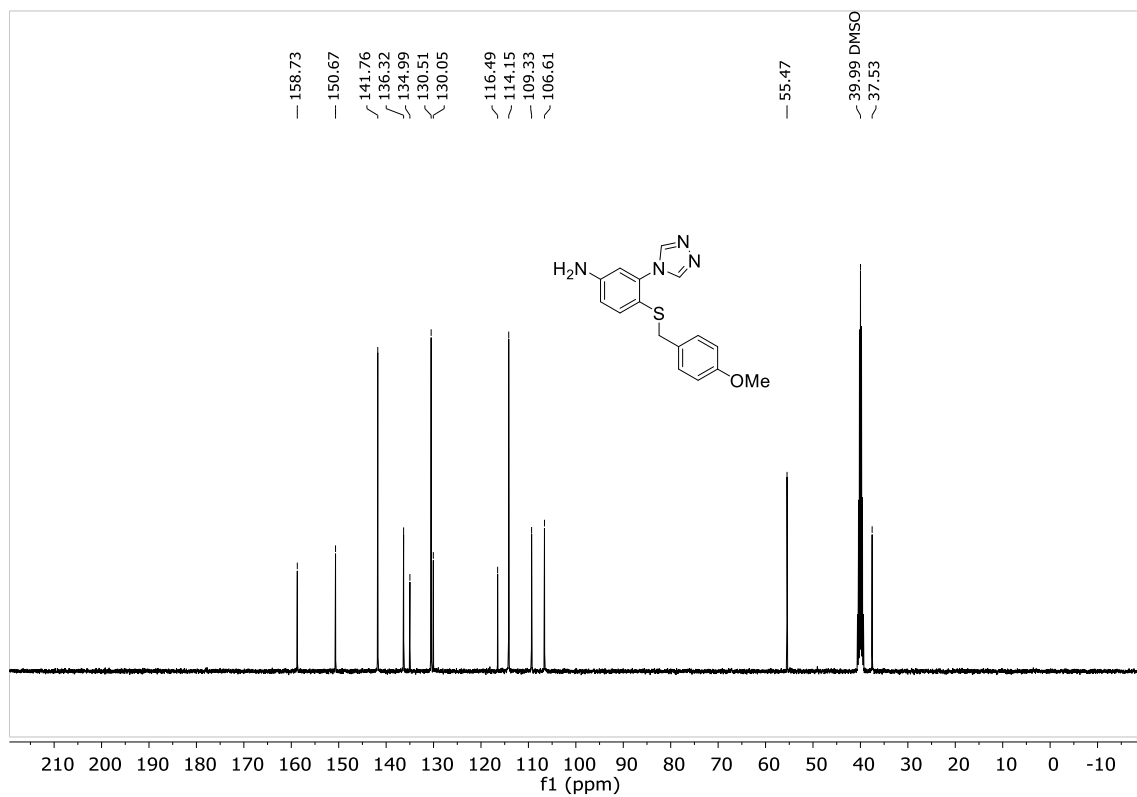
**Figure S093:** <sup>1</sup>H NMR spectrum of *N*-(4-((4-methoxybenzyl)thio)-3-(4*H*-1,2,4-triazol-4-yl)phenyl)acetamide (**3f**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



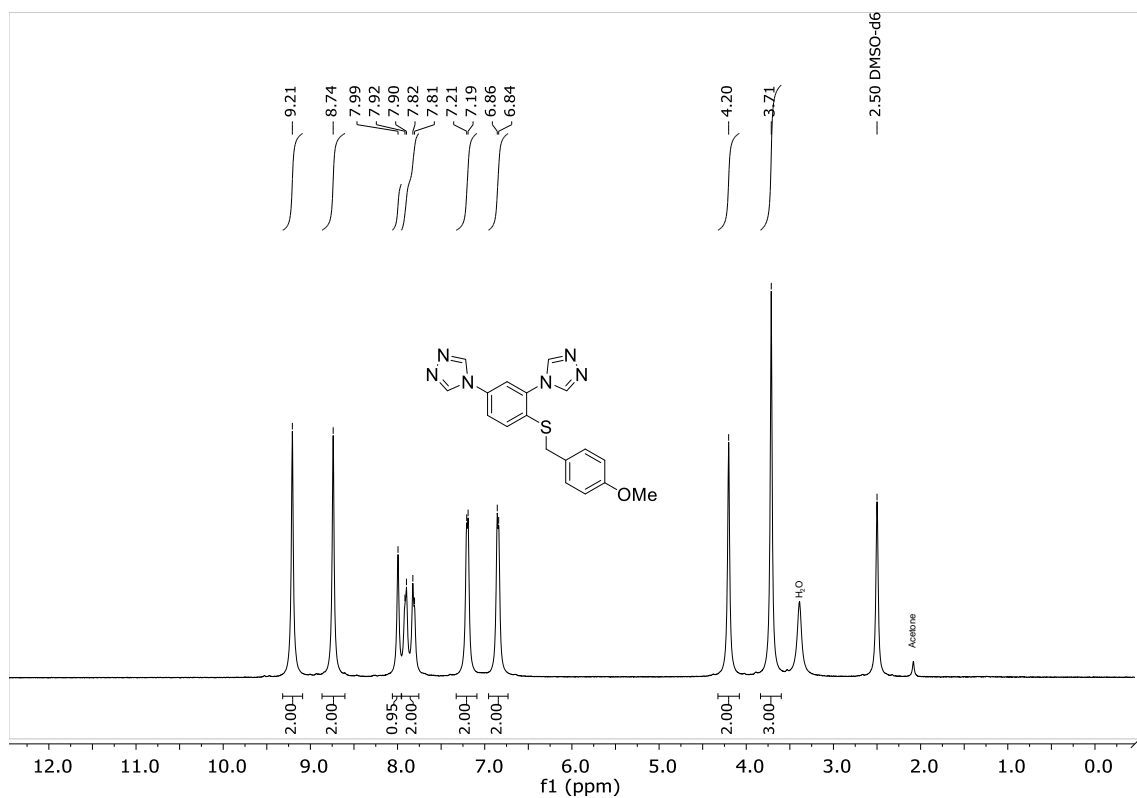
**Figure S094:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of *N*-(4-((4-methoxybenzyl)thio)-3-(4*H*-1,2,4-triazol-4-yl)phenyl)acetamide (**3f**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



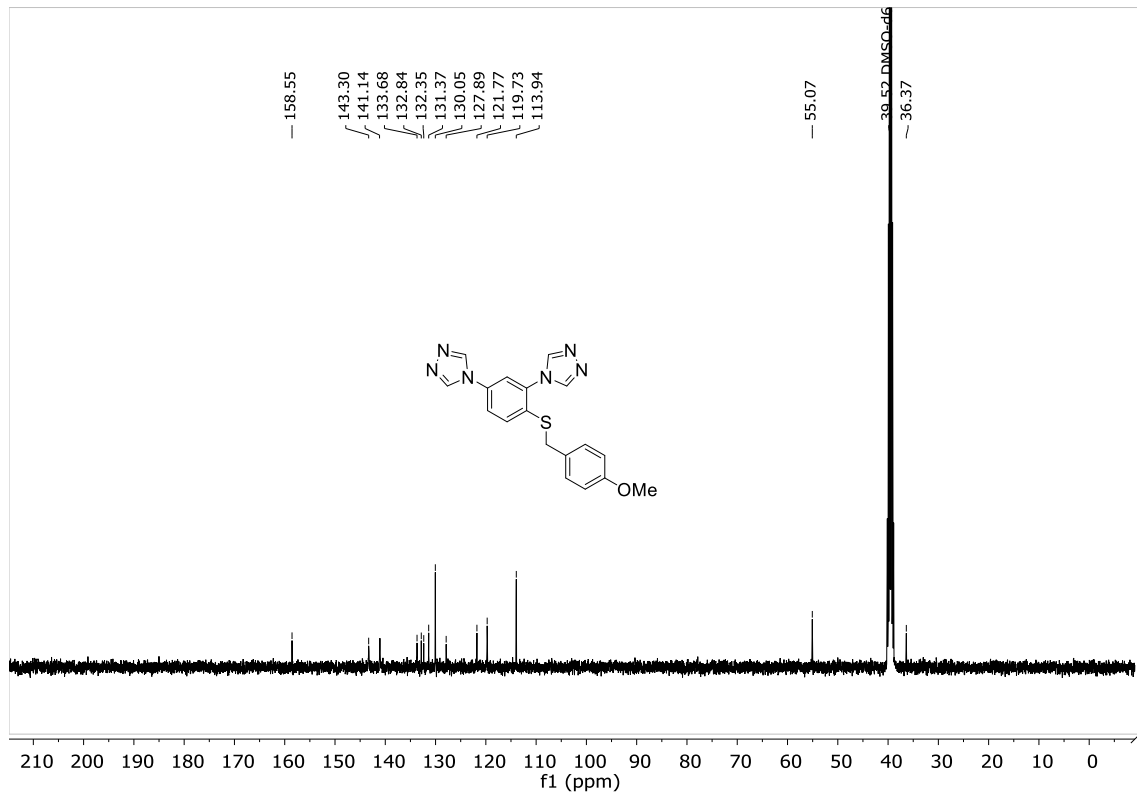
**Figure S095:** <sup>1</sup>H NMR spectrum of 4-((4-methoxybenzyl)thio)-3-(4*H*-1,2,4-triazol-4-yl)aniline (**3e**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



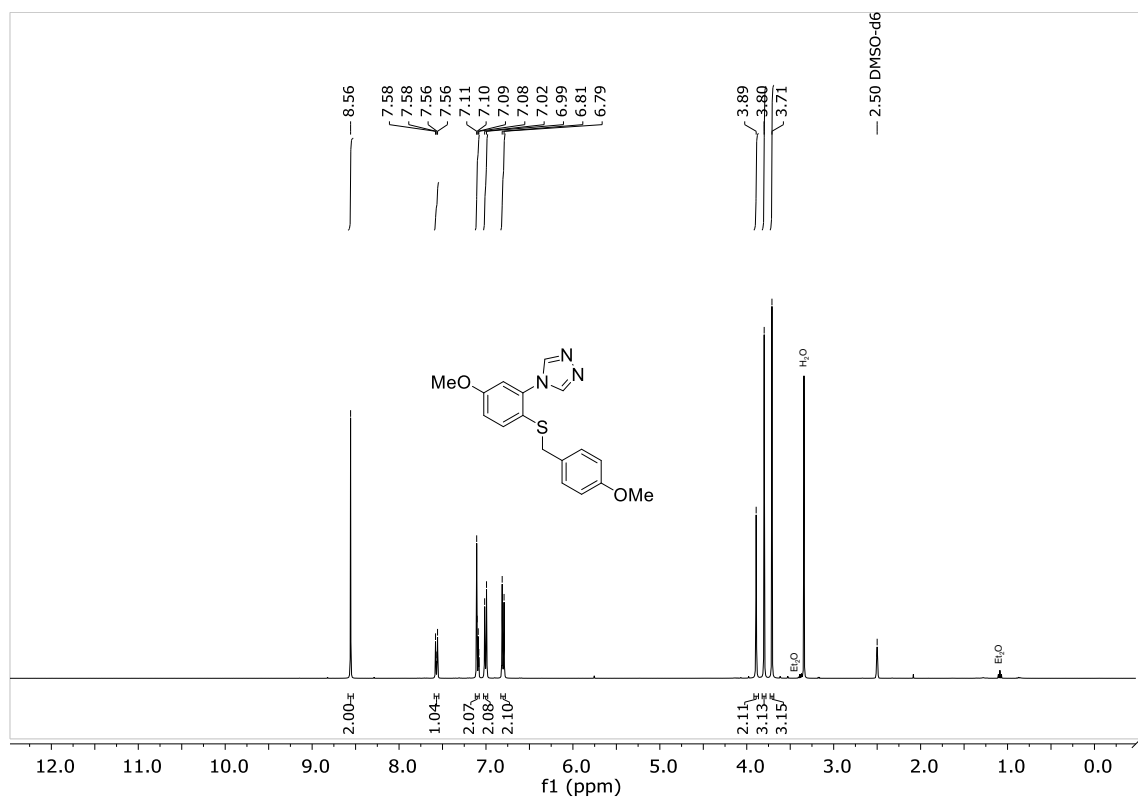
**Figure S096:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 4-((4-methoxybenzyl)thio)-3-(4*H*-1,2,4-triazol-4-yl)aniline (**3e**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



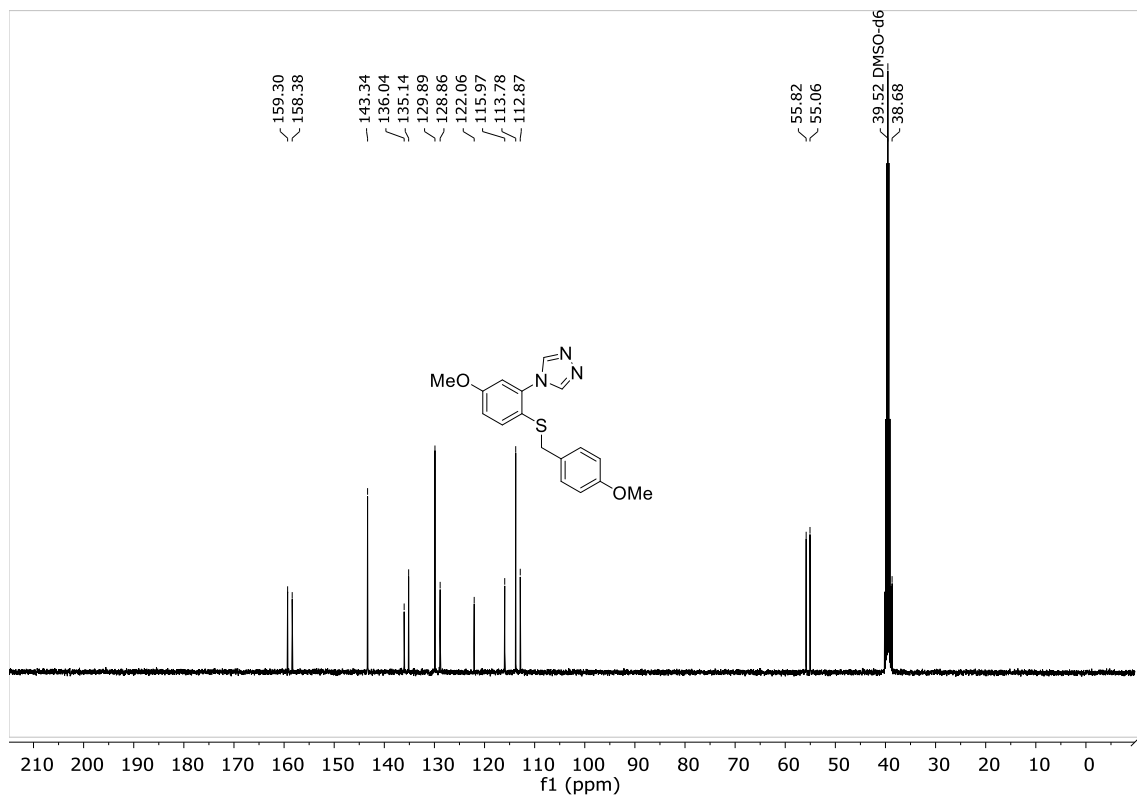
**Figure S097:** <sup>1</sup>H NMR 4,4'-((4-methoxybenzyl)thio)-1,3-phenylenebis(4*H*-1,2,4-triazole) (**3e**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



**Figure S098:** <sup>13</sup>C{<sup>1</sup>H} NMR 4,4'-((4-methoxybenzyl)thio)-1,3-phenylenebis(4*H*-1,2,4-triazole) (**3e**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).

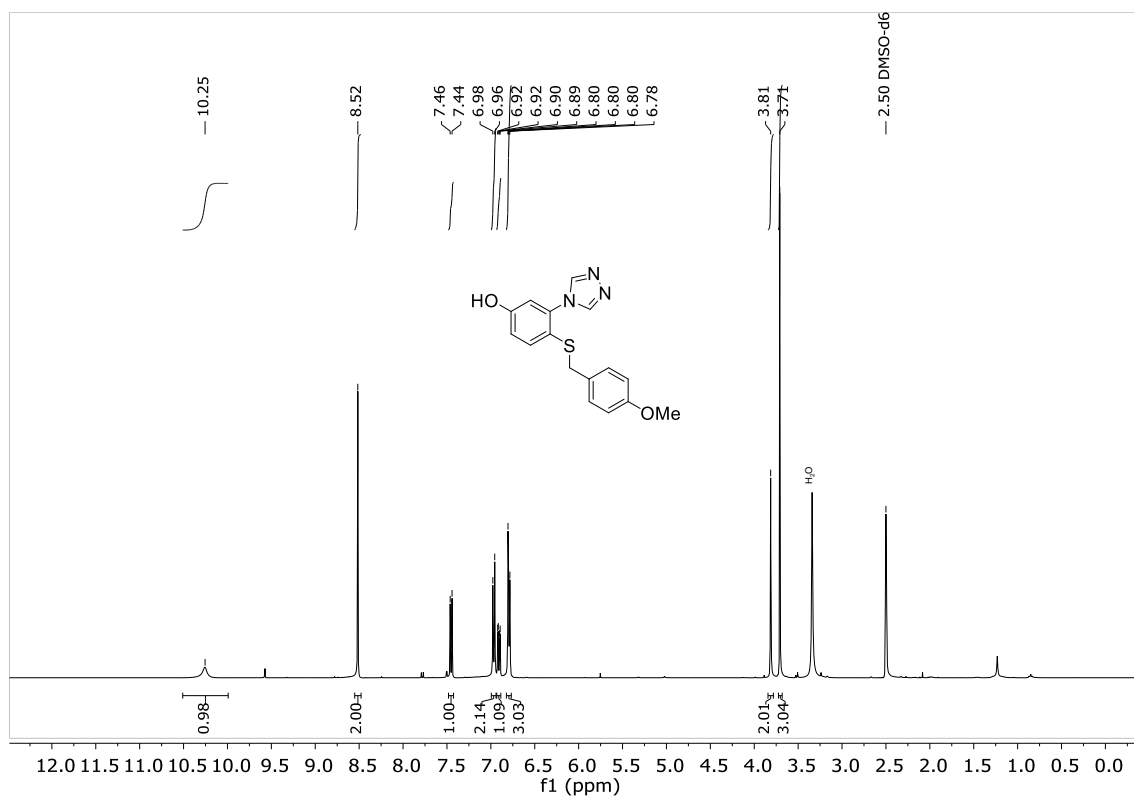


**Figure S099:** <sup>1</sup>H NMR 4-(5-methoxy-2-((4-methoxybenzyl)thio)phenyl)-4*H*-1,2,4-triazole (**3g**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).

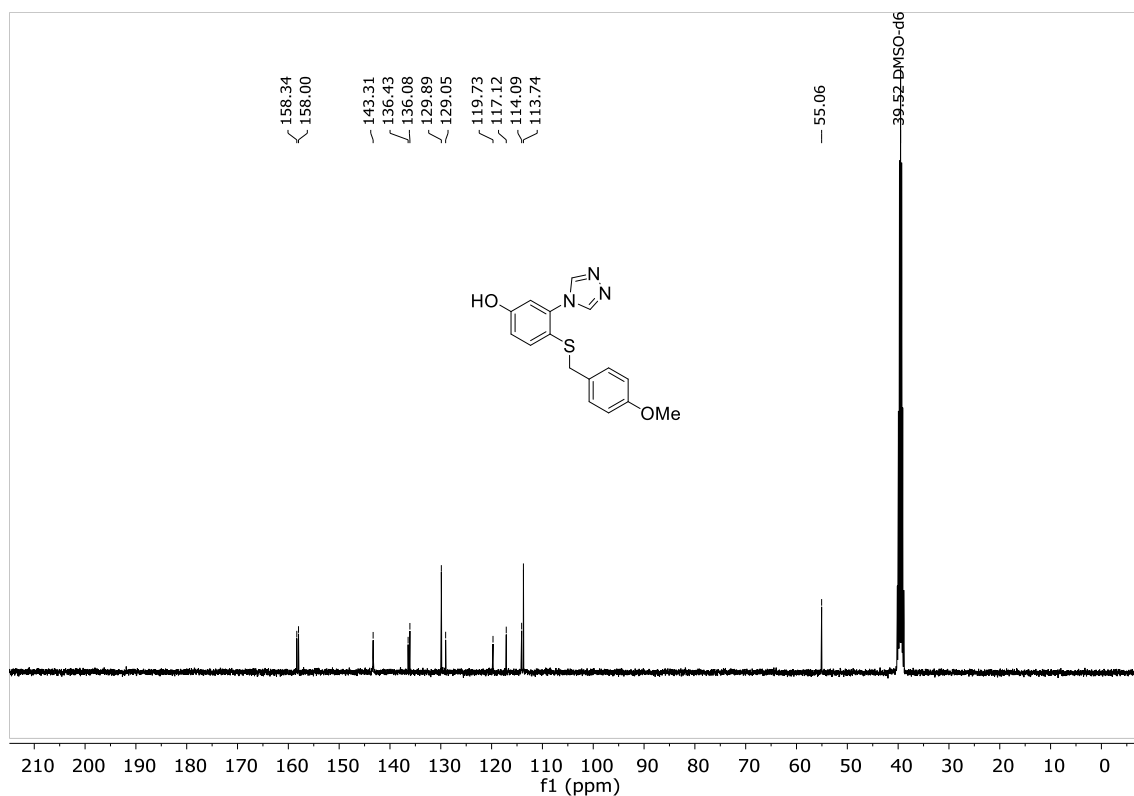


**Figure S100:** <sup>13</sup>C{<sup>1</sup>H} NMR 4-(5-methoxy-2-((4-methoxybenzyl)thio)phenyl)-4*H*-1,2,4-triazole (**3g**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).

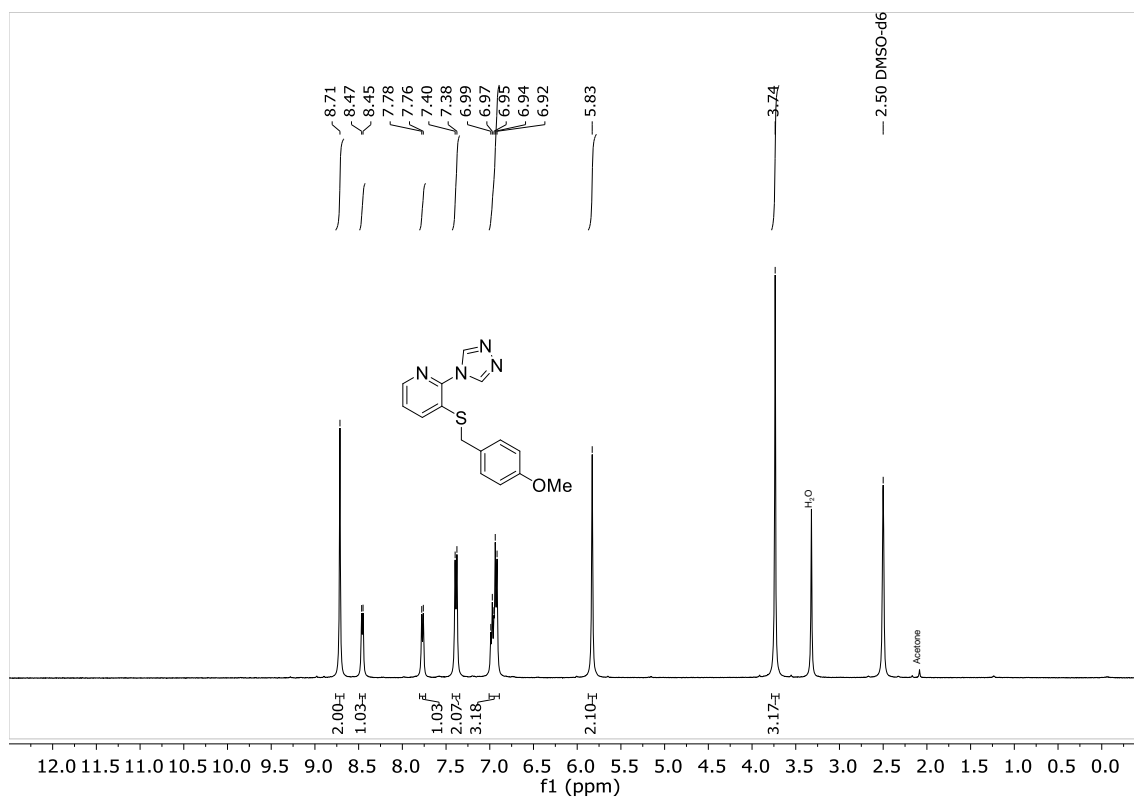




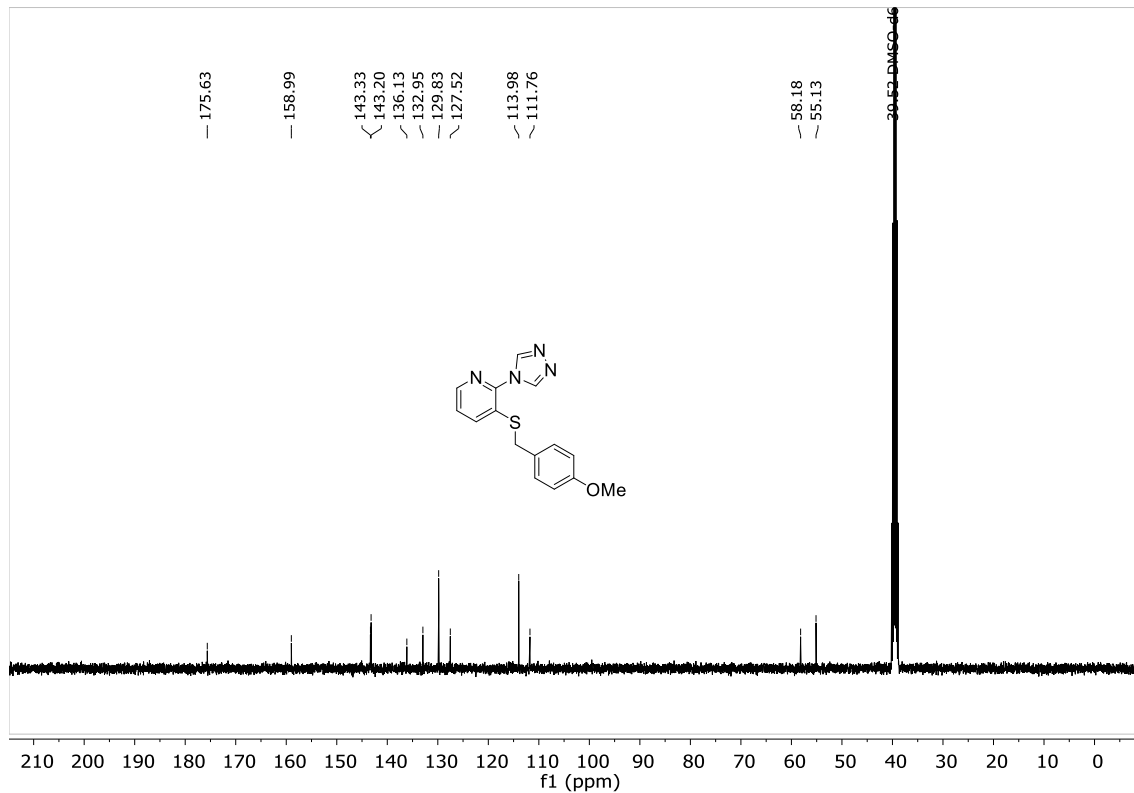
**Figure S101:** <sup>1</sup>H NMR spectrum of 4-((4-methoxybenzyl)thio)-3-(4*H*-1,2,4-triazol-4-yl)phenol (**3h**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



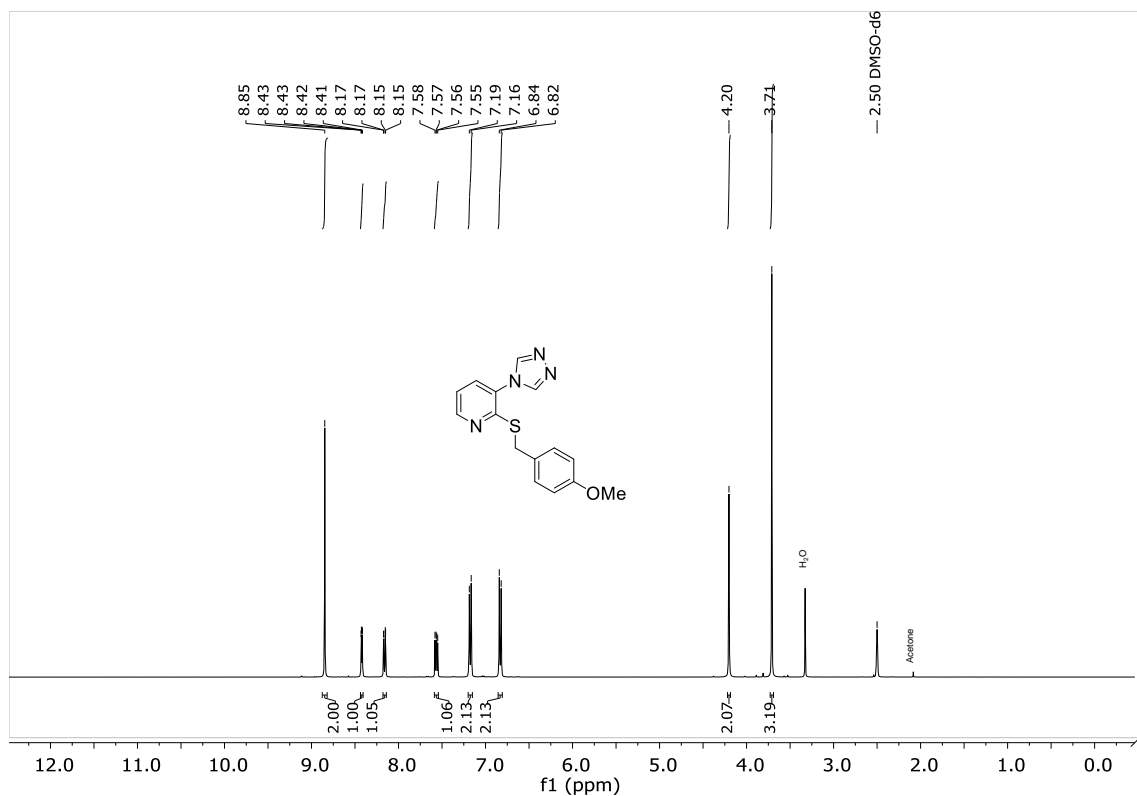
**Figure S102:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 4-((4-methoxybenzyl)thio)-3-(4*H*-1,2,4-triazol-4-yl)phenol (**3h**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



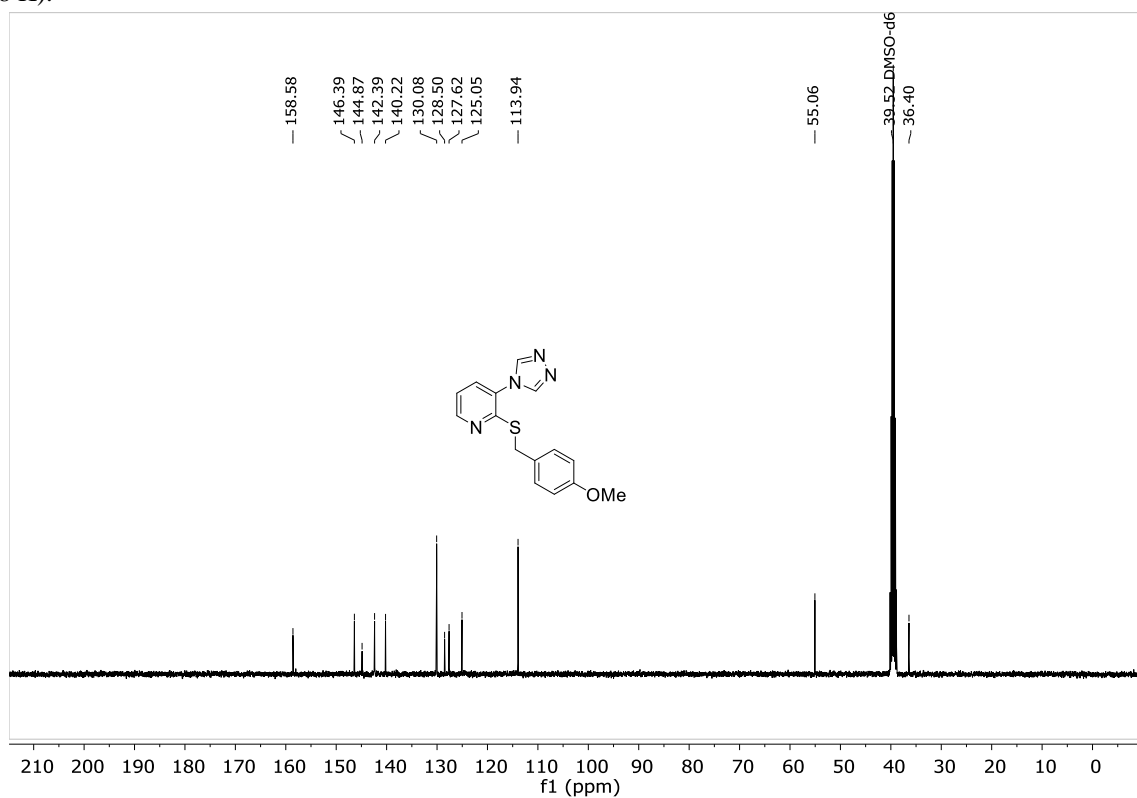
**Figure S103:** <sup>1</sup>H NMR 3-((4-methoxybenzyl)thio)-2-(4H-1,2,4-triazol-4-yl)pyridine (**3i**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



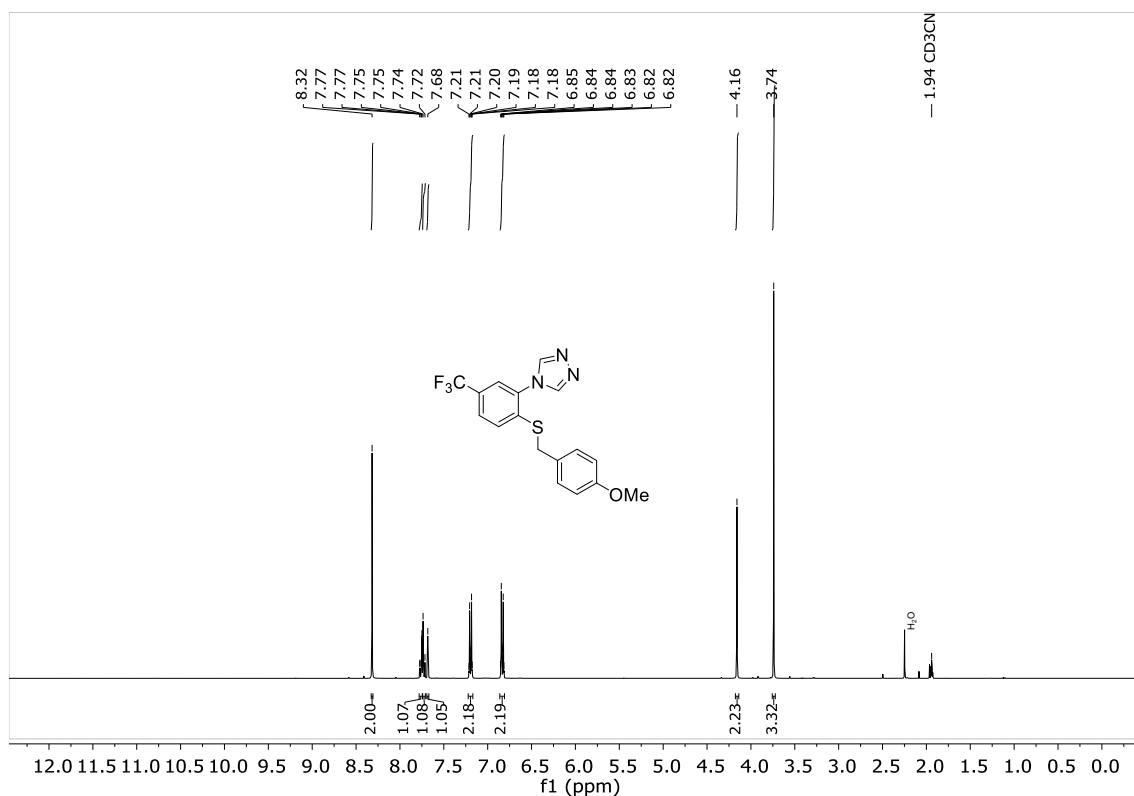
**Figure S104:** <sup>13</sup>C{<sup>1</sup>H} NMR 3-((4-methoxybenzyl)thio)-2-(4H-1,2,4-triazol-4-yl)pyridine (**3i**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



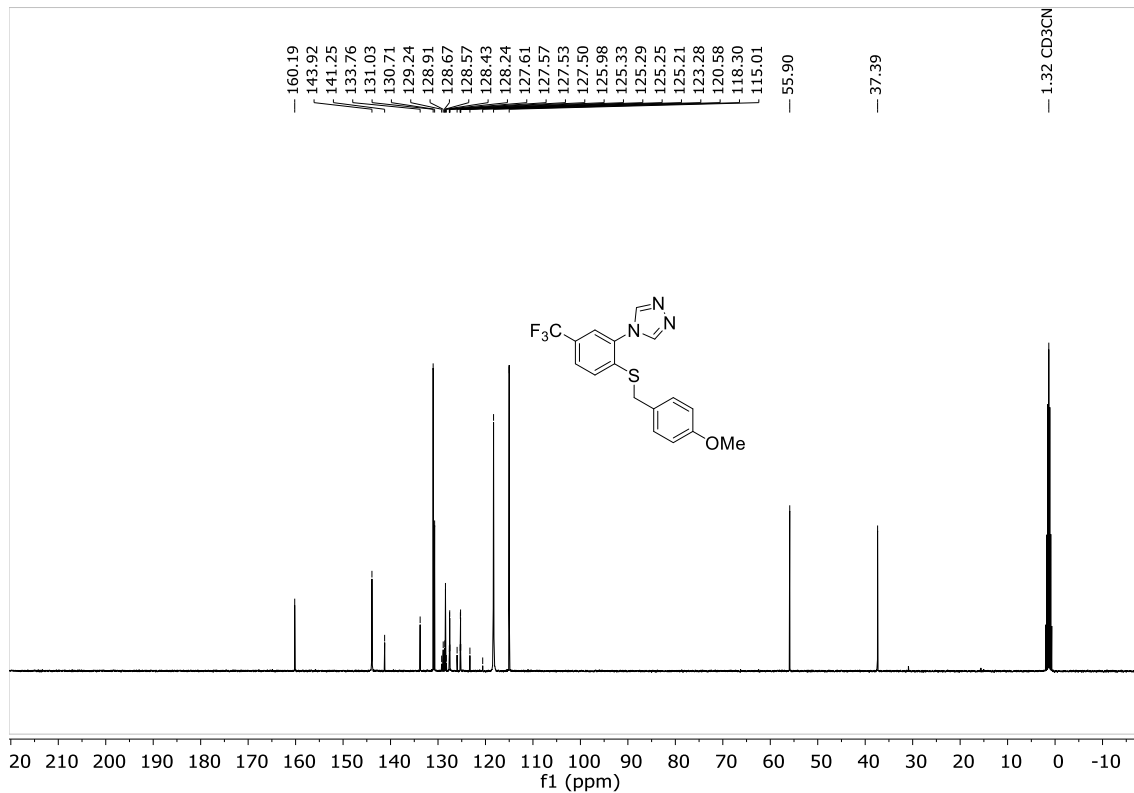
**Figure S105:** <sup>1</sup>H NMR 2-((4-methoxybenzyl)thio)-3-(4H-1,2,4-triazol-4-yl)pyridine (**3j**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



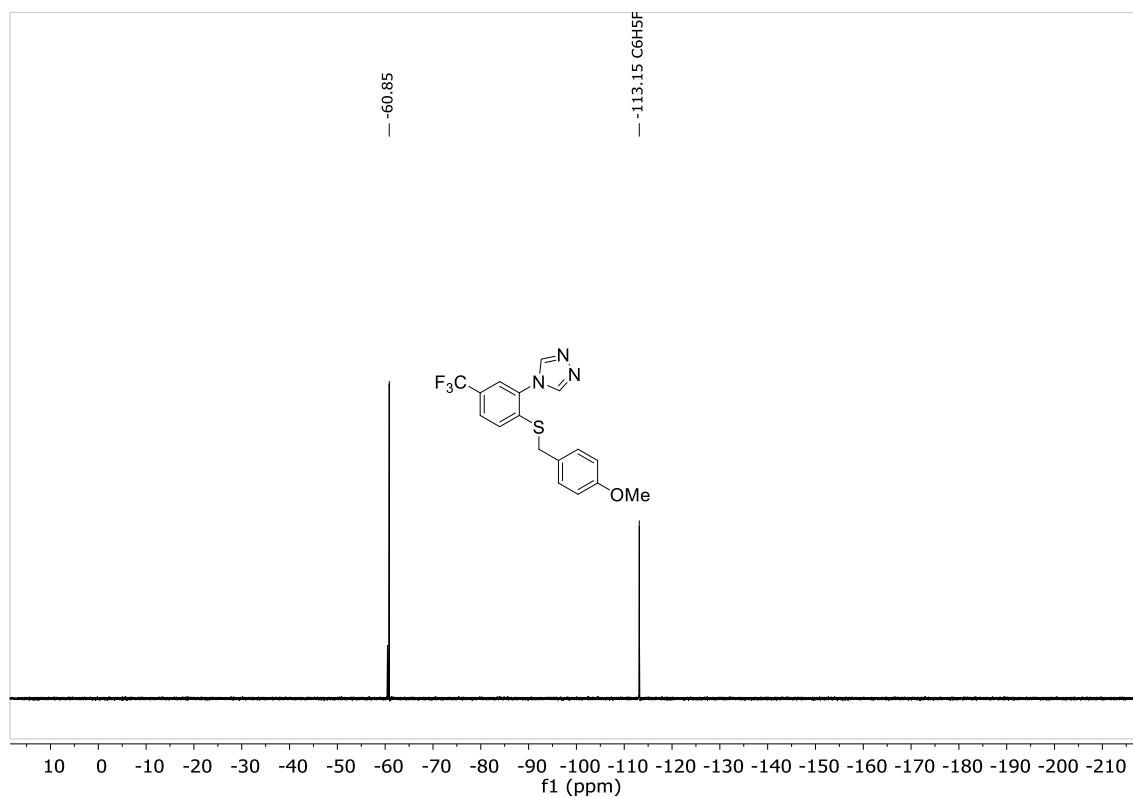
**Figure S106:** <sup>13</sup>C{<sup>1</sup>H} NMR 2-((4-methoxybenzyl)thio)-3-(4H-1,2,4-triazol-4-yl)pyridine (**3j**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



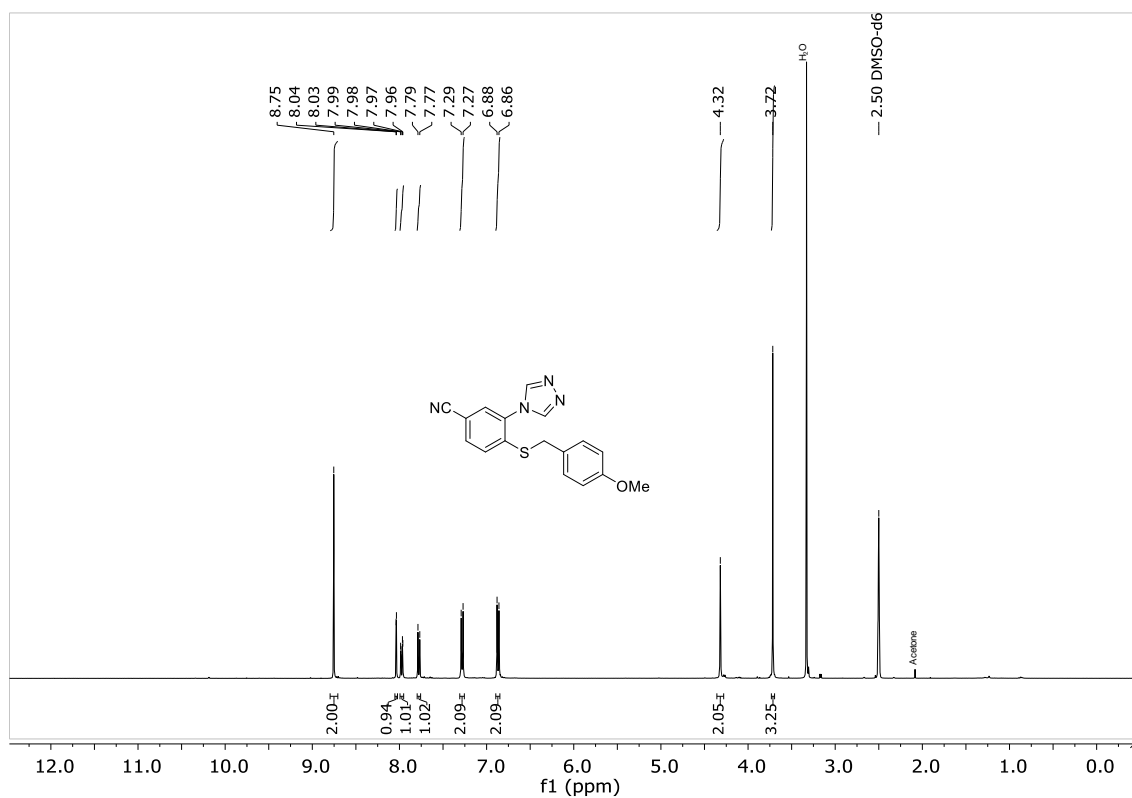
**Figure S107:** <sup>1</sup>H NMR 4-(2-((4-methoxybenzyl)thio)-5-(trifluoromethyl)phenyl)-4H-1,2,4-triazole (**3k**) (400 MHz, CD<sub>3</sub>CN, 298 K).



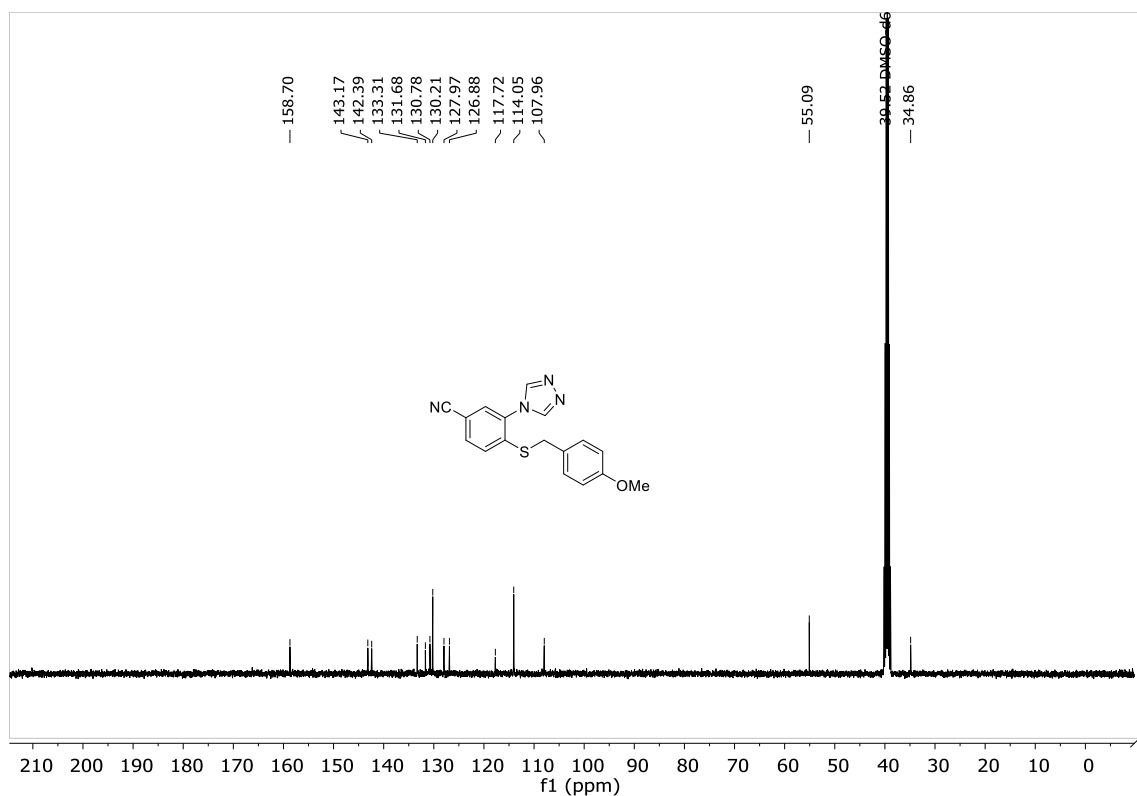
**Figure S108:** <sup>13</sup>C{<sup>1</sup>H} NMR 4-(2-((4-methoxybenzyl)thio)-5-(trifluoromethyl)phenyl)-4H-1,2,4-triazole (**3k**) (100 MHz, CD<sub>3</sub>CN, 298 K).



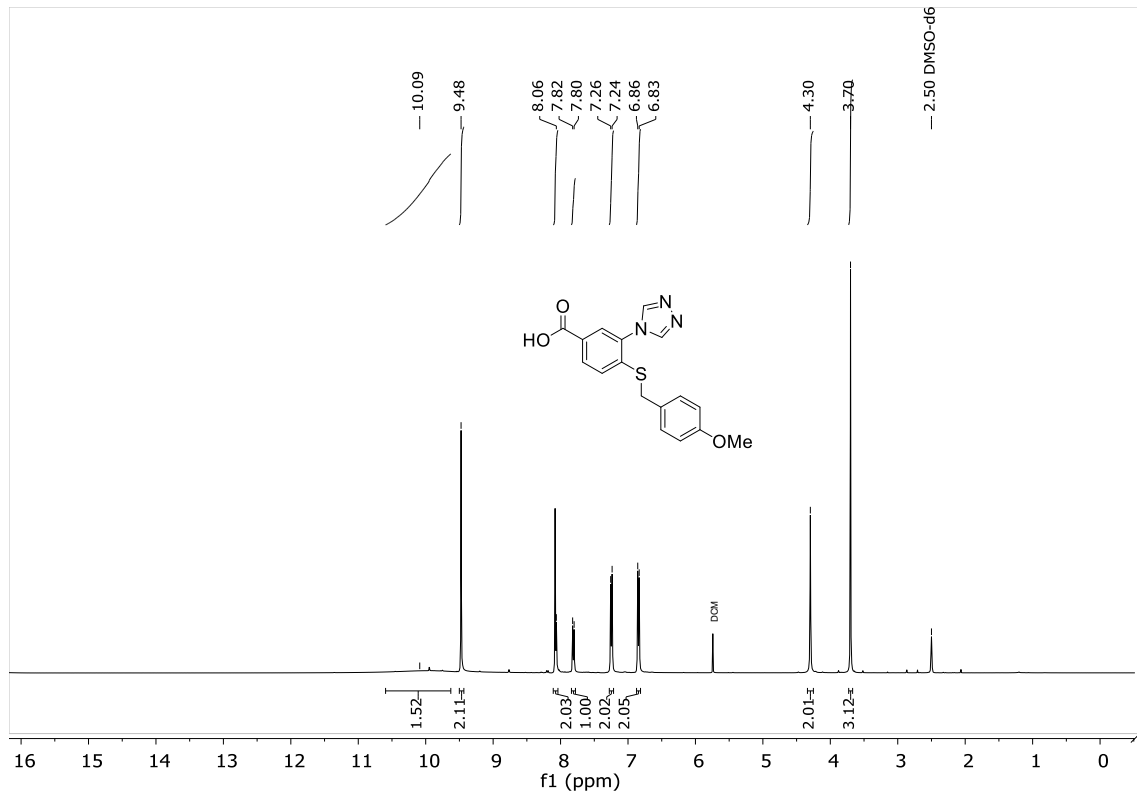
**Figure S109:** <sup>19</sup>F{<sup>1</sup>H} NMR 4-(2-((4-methoxybenzyl)thio)-5-(trifluoromethyl)phenyl)-4H-1,2,4-triazole (**3k**) (376 MHz, CD<sub>3</sub>CN, 298 K, referenced to fluorobenzene).



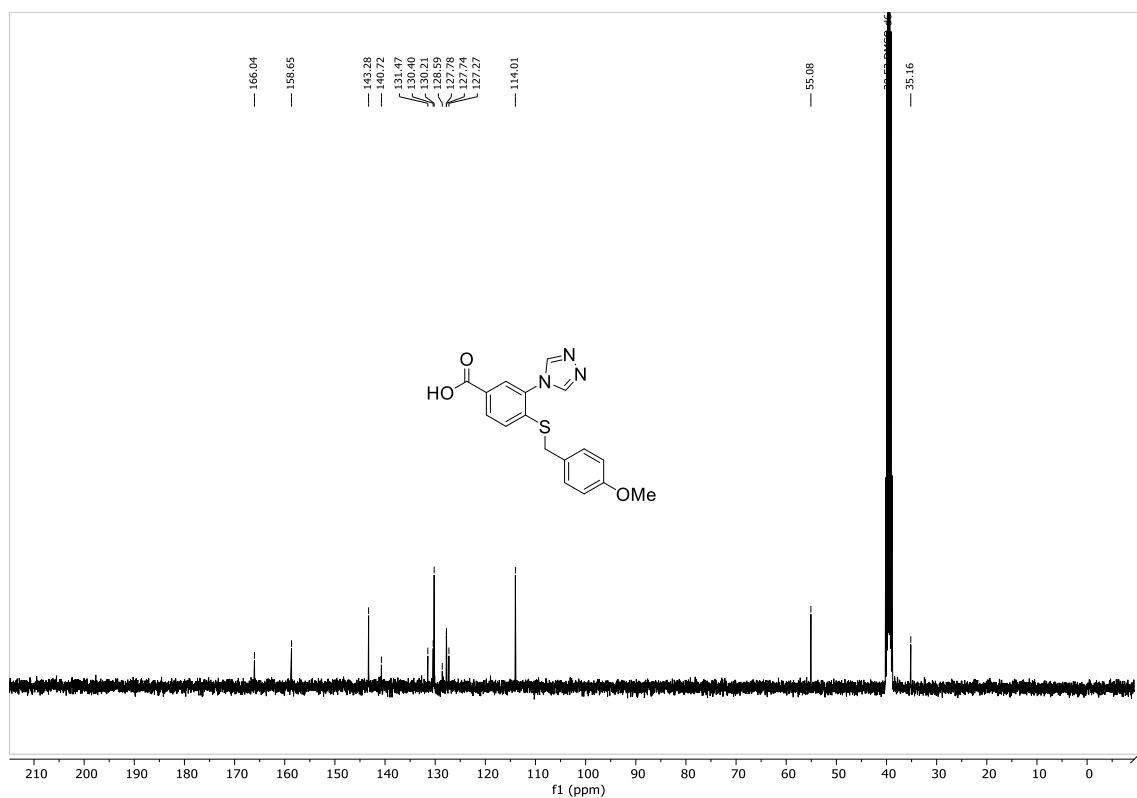
**Figure S110:** <sup>1</sup>H NMR spectrum of 4-((4-methoxybenzyl)thio)-3-(4H-1,2,4-triazol-4-yl)benzonitrile (**3l**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



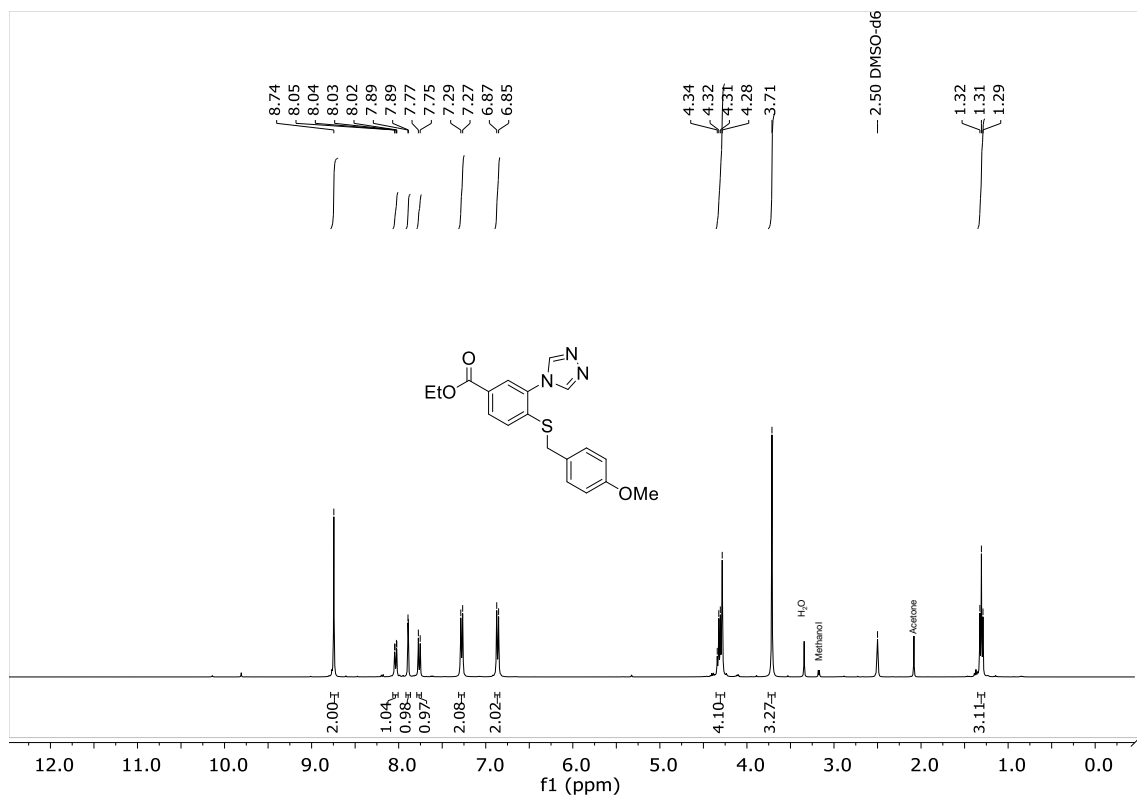
**Figure S111:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of 4-((4-methoxybenzyl)thio)-3-(4H-1,2,4-triazol-4-yl)benzonitrile (**3l**) (100 MHz, DMSO- $d_6$ , 298 K).



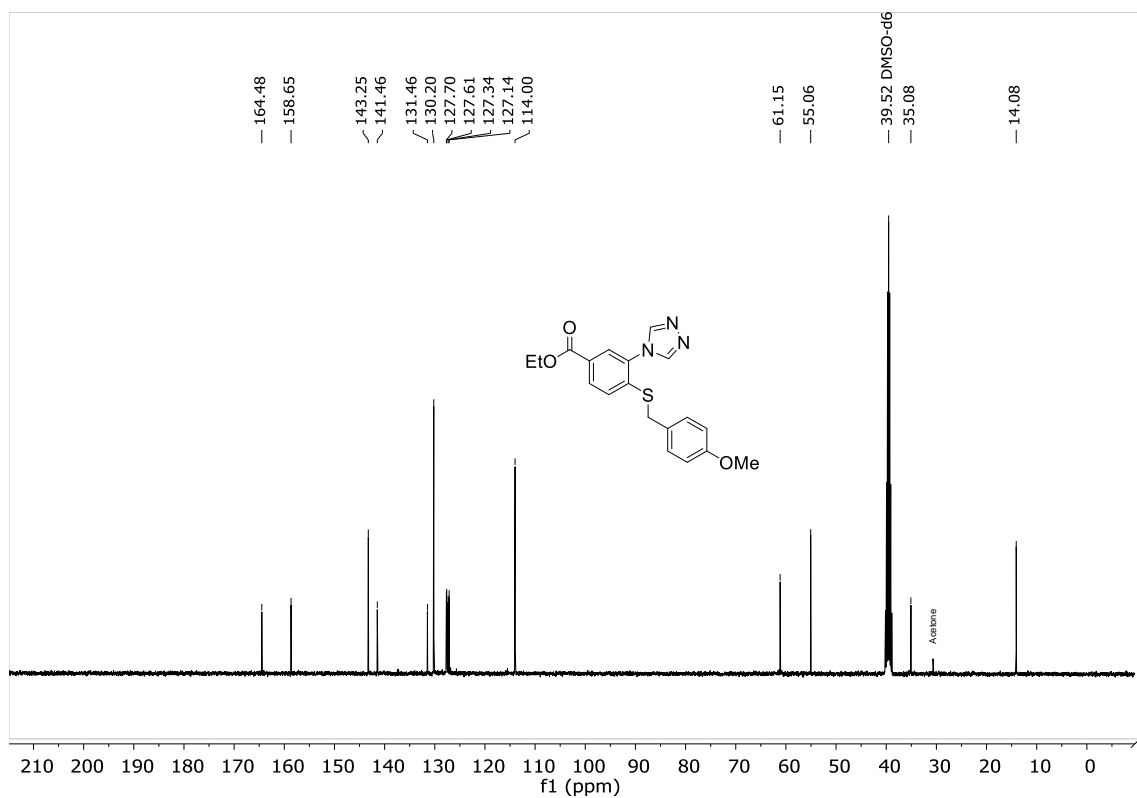
**Figure S112:**  $^1\text{H}$  NMR spectrum of 4-((4-methoxybenzyl)thio)-3-(4H-1,2,4-triazol-4-yl)benzoic acid (**3m**) (400 MHz, DMSO- $d_6$ , 298 K).



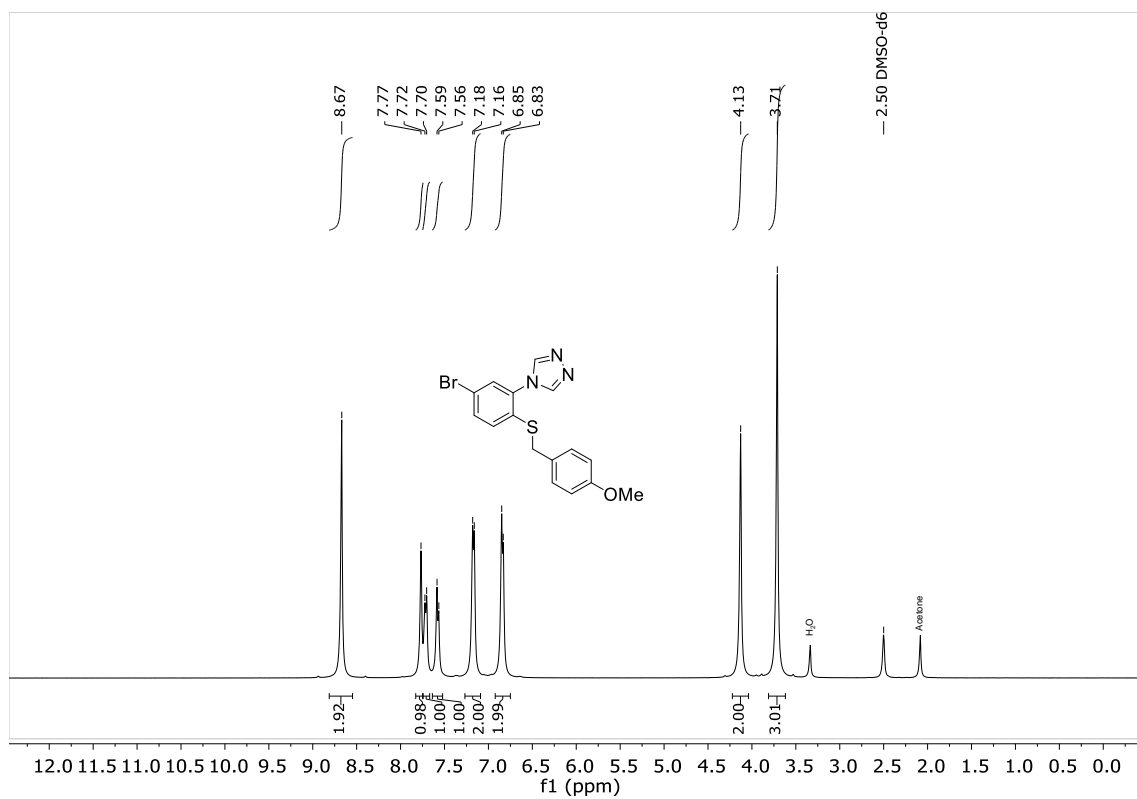
**Figure S113:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 4-((4-methoxybenzyl)thio)-3-(4H-1,2,4-triazol-4-yl)benzoic acid (**3m**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



**Figure S114:** <sup>1</sup>H NMR spectrum of ethyl 4-((4-methoxybenzyl)thio)-3-(4H-1,2,4-triazol-4-yl)benzoate (**3m**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).

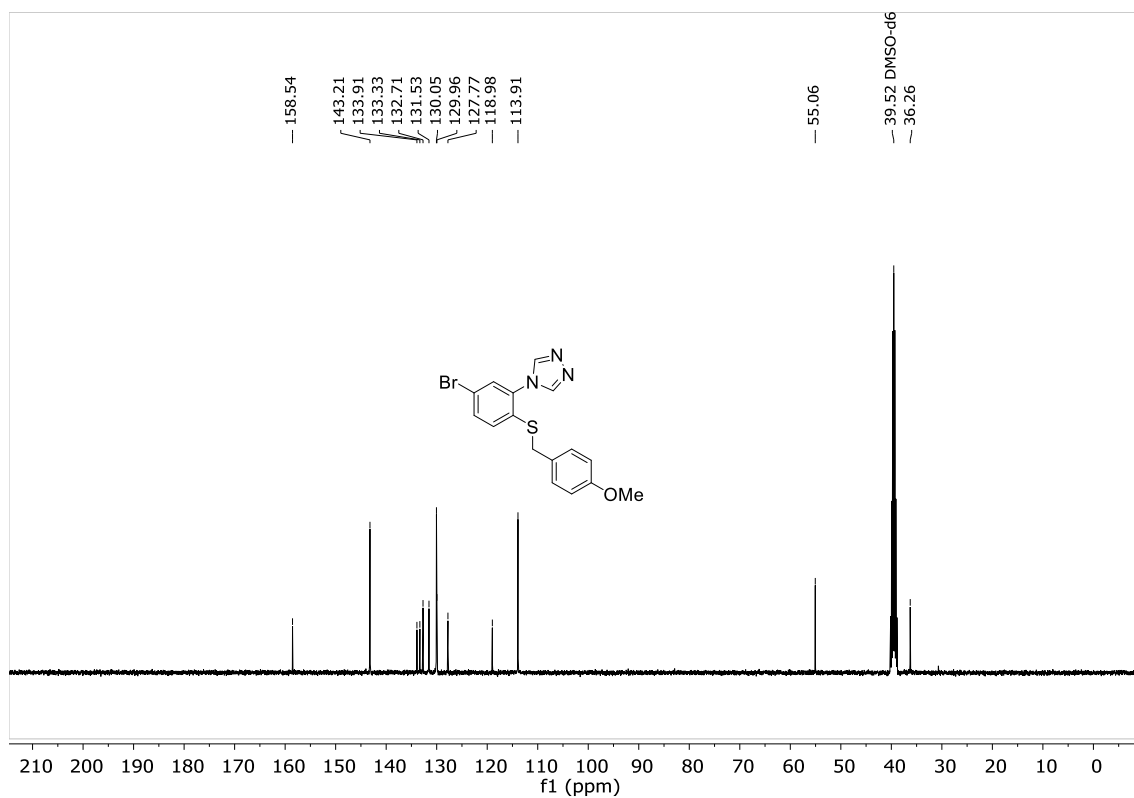


**Figure S115:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of ethyl 4-((4-methoxybenzyl)thio)-3-(4H-1,2,4-triazol-4-yl)benzoate (**3m**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).

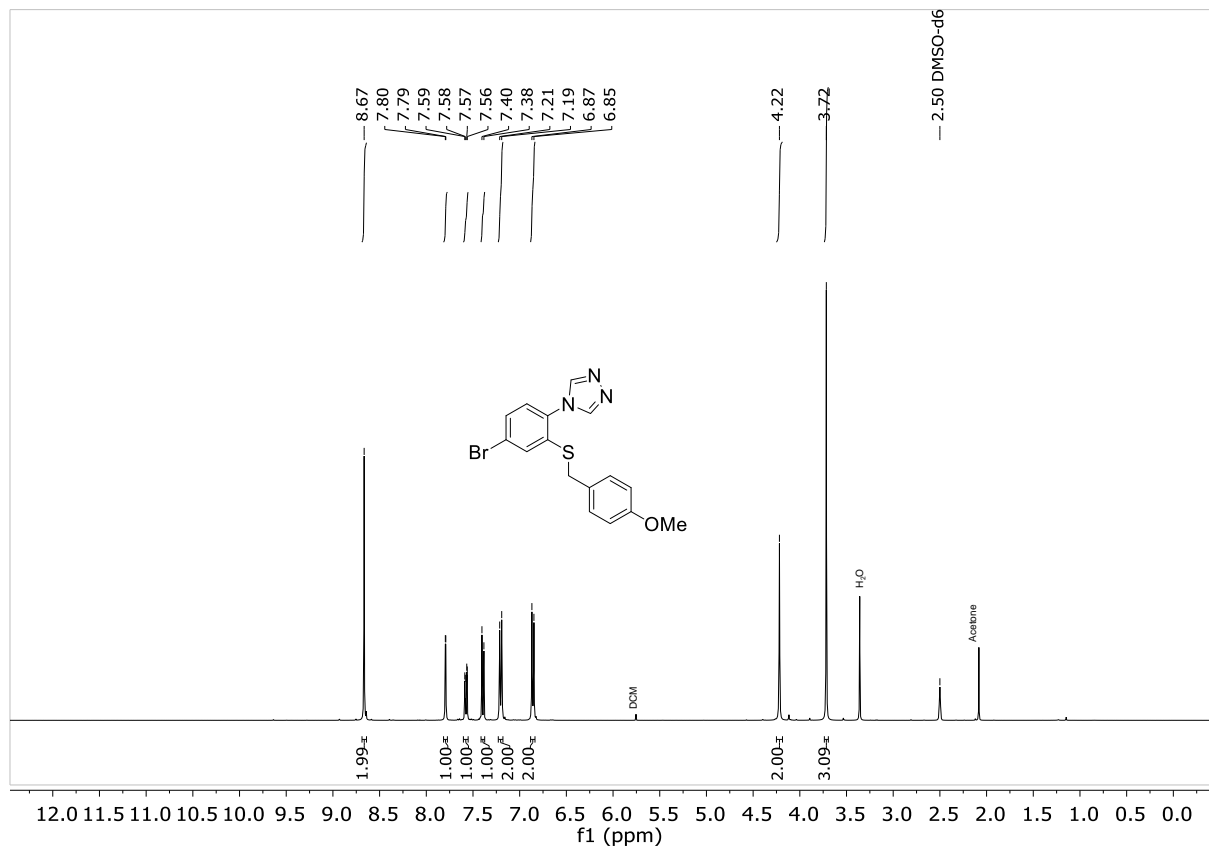


**Figure S116:** <sup>1</sup>H NMR spectrum of 4-(5-bromo-2-((4-methoxybenzyl)thio)phenyl)-4H-1,2,4-triazole (**3n**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).

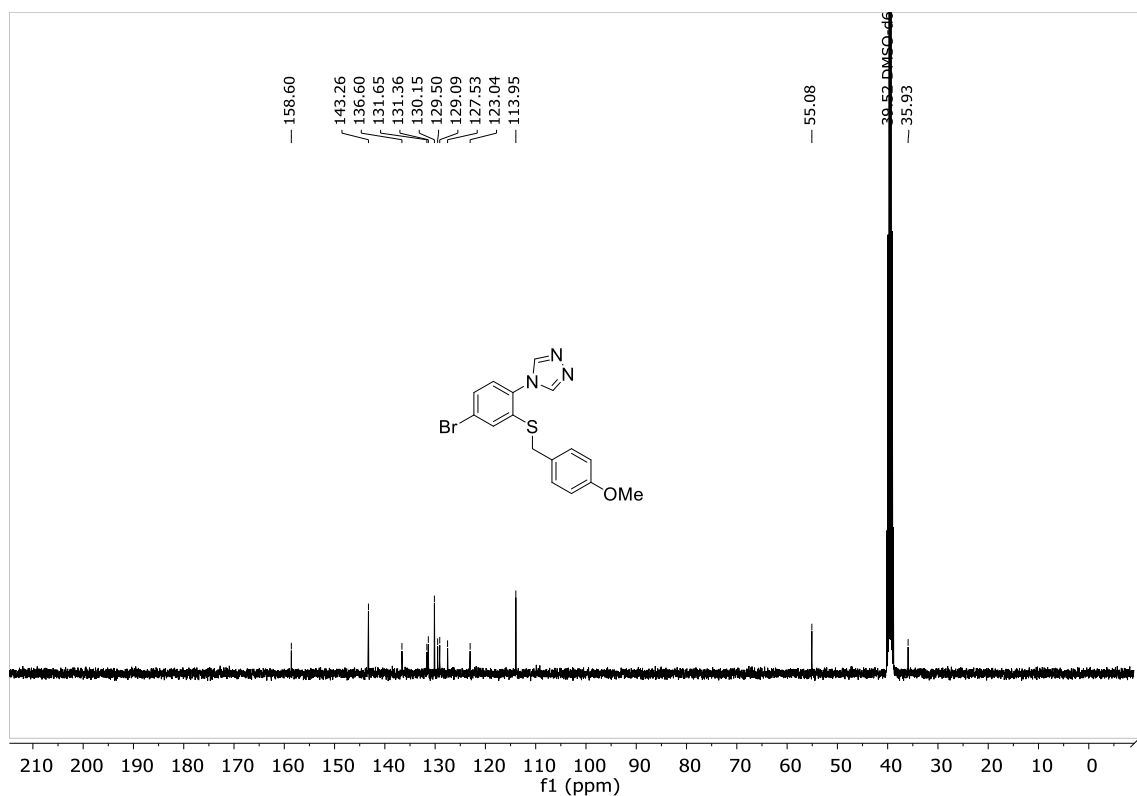




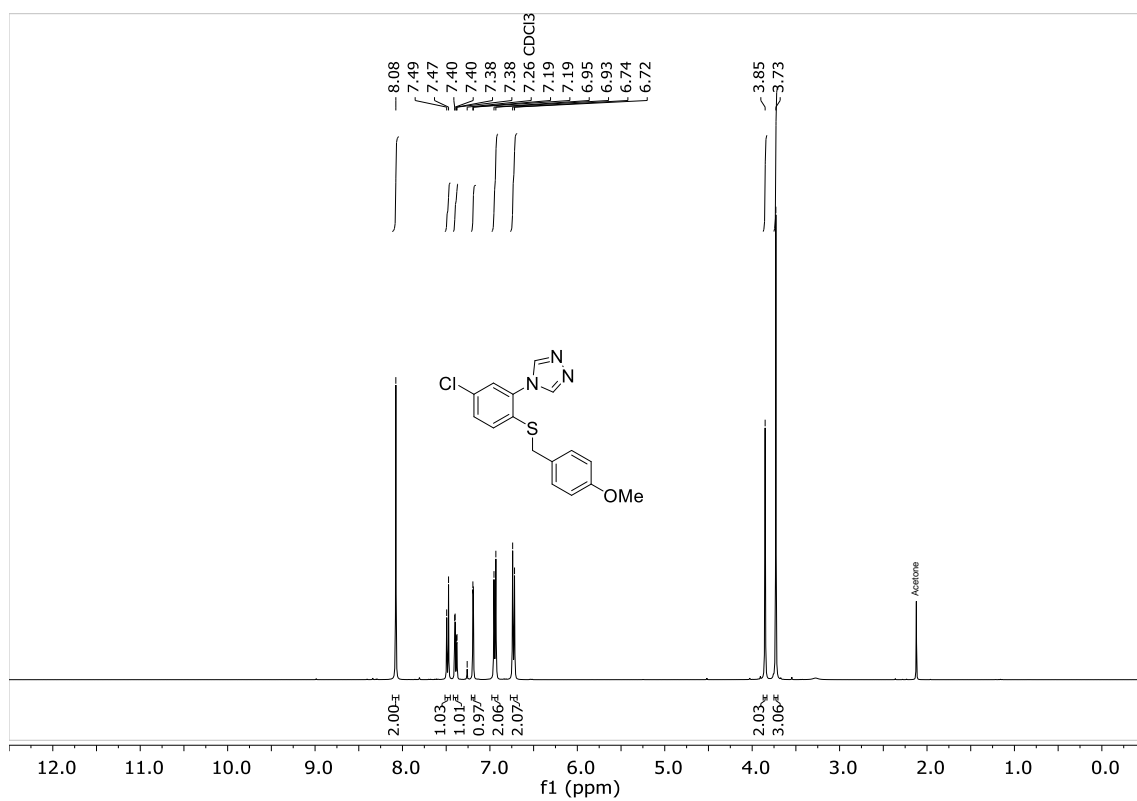
**Figure S117:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of 4-(5-bromo-2-((4-methoxybenzyl)thio)phenyl)-4H-1,2,4-triazole (**3n**) (100 MHz, DMSO- $d_6$ , 298 K).



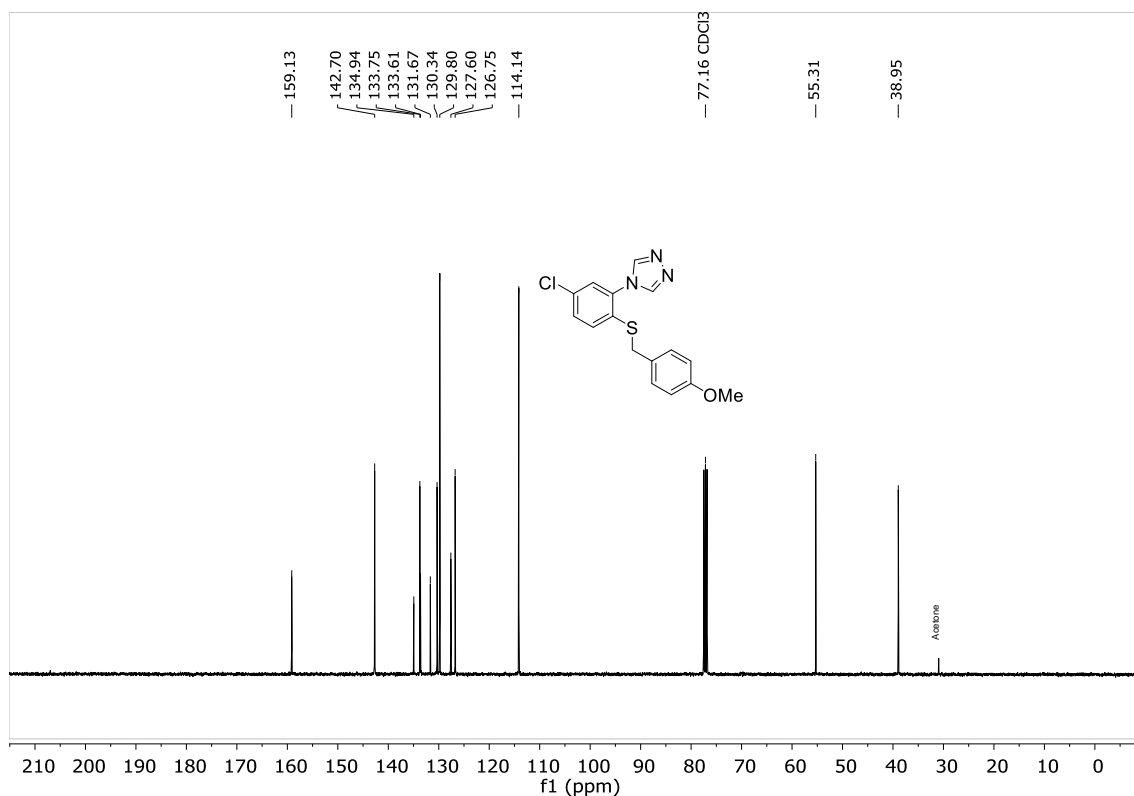
**Figure S118:**  $^1\text{H}$  NMR spectrum of 4-(4-bromo-2-((4-methoxybenzyl)thio)phenyl)-4H-1,2,4-triazole (**3o**) (400 MHz, DMSO- $d_6$ , 298 K).



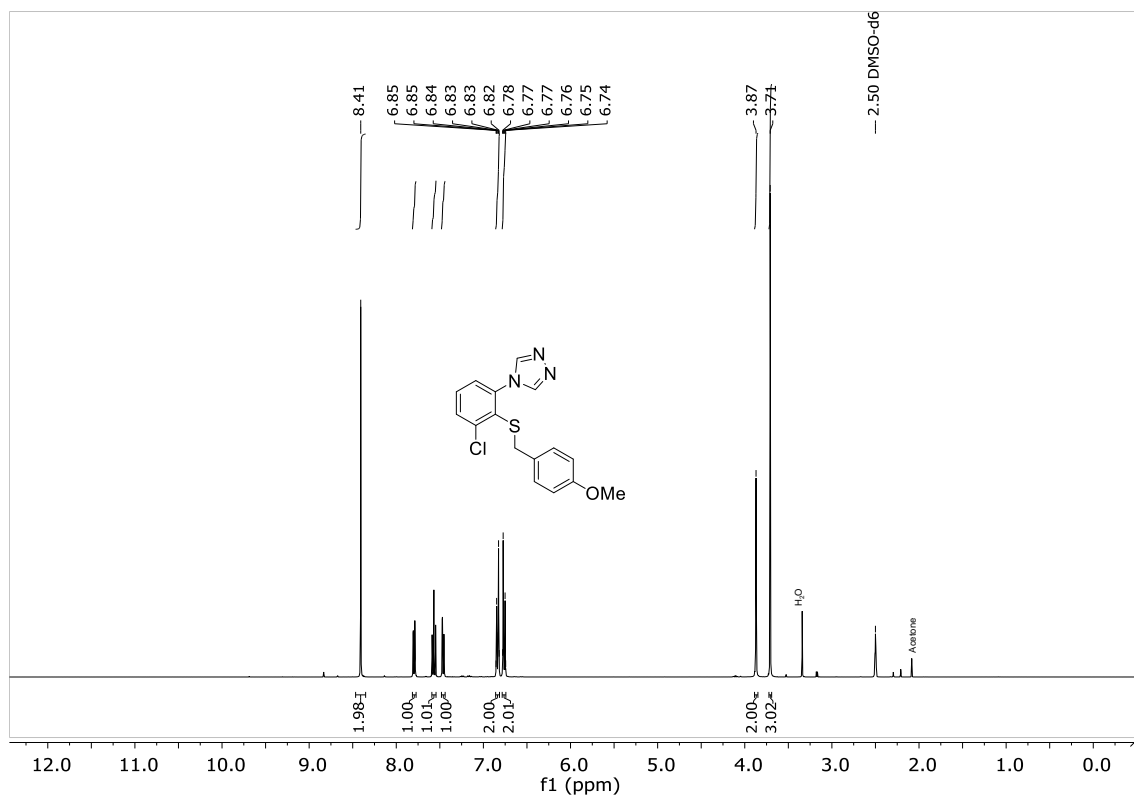
**Figure S119:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 4-(4-bromo-2-((4-methoxybenzyl)thio)phenyl)-4H-1,2,4-triazole (**3o**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



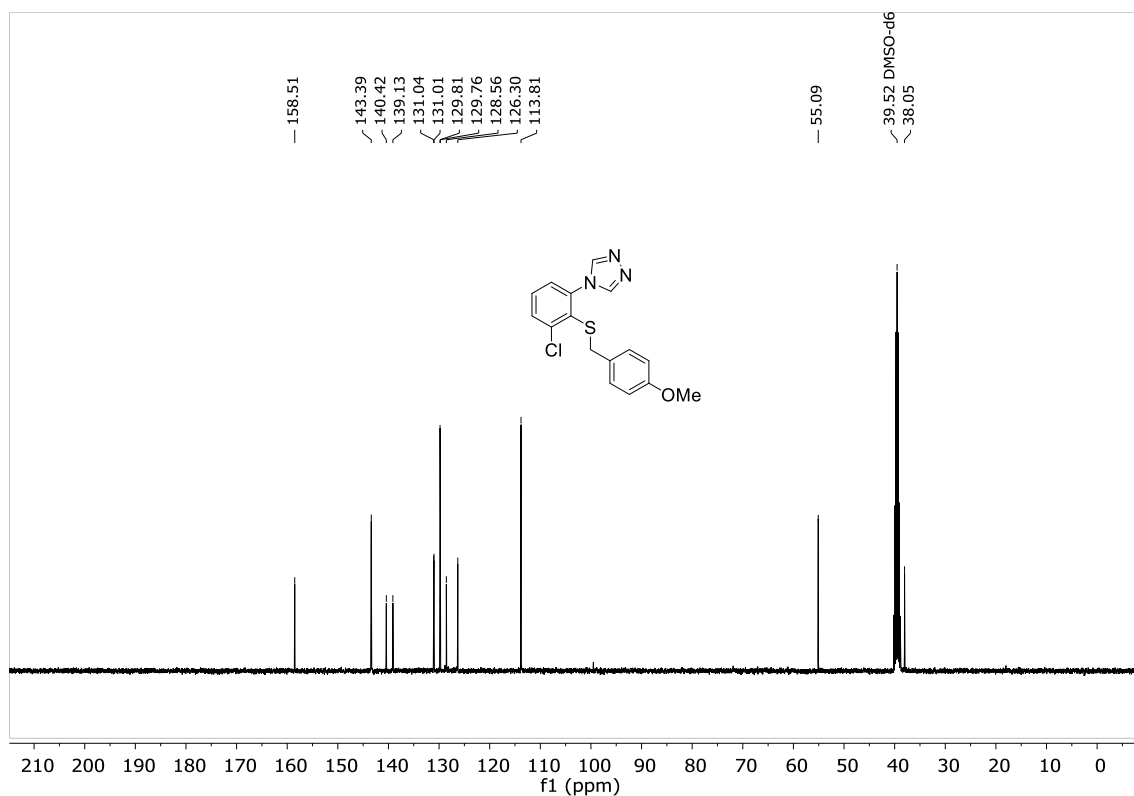
**Figure S120:** <sup>1</sup>H NMR 4-(5-chloro-2-((4-methoxybenzyl)thio)phenyl)-4H-1,2,4-triazole (**3p**) (400 MHz, CDCl<sub>3</sub>, 298 K).



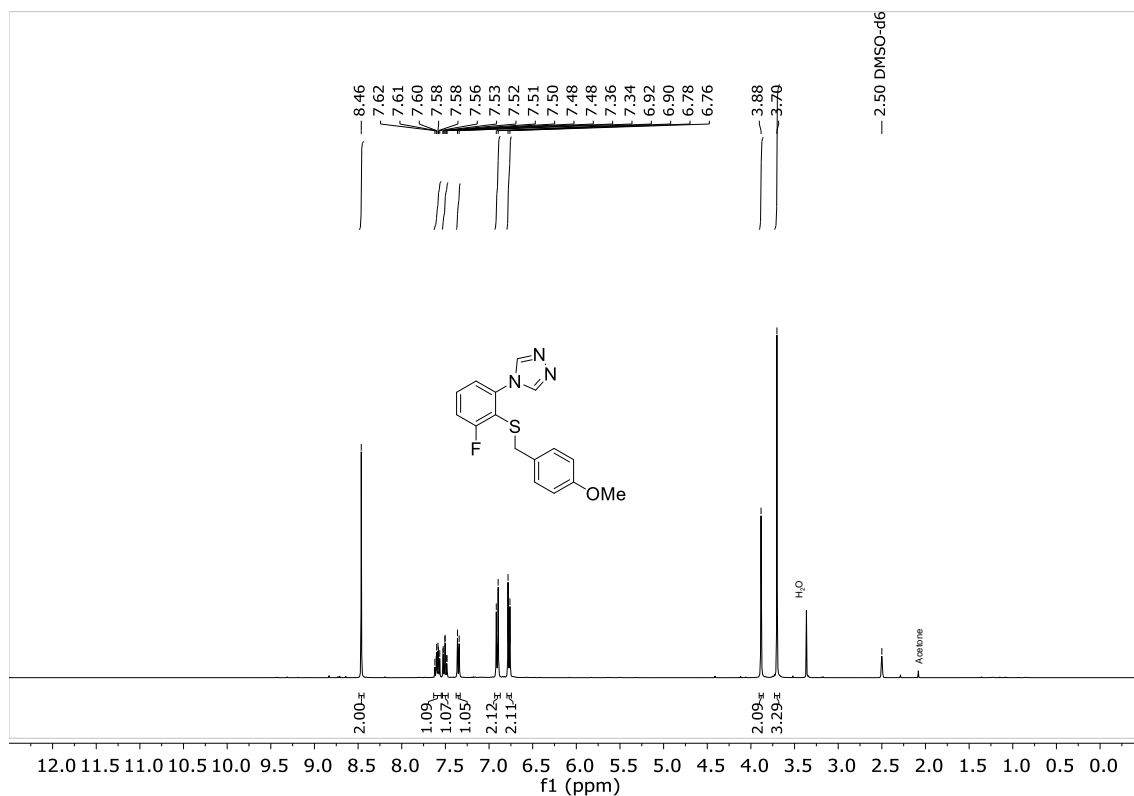
**Figure S121:** <sup>13</sup>C{<sup>1</sup>H} NMR 4-(5-chloro-2-((4-methoxybenzyl)thio)phenyl)-4H-1,2,4-triazole (**3p**) (100 MHz, CDCl<sub>3</sub>, 298 K).



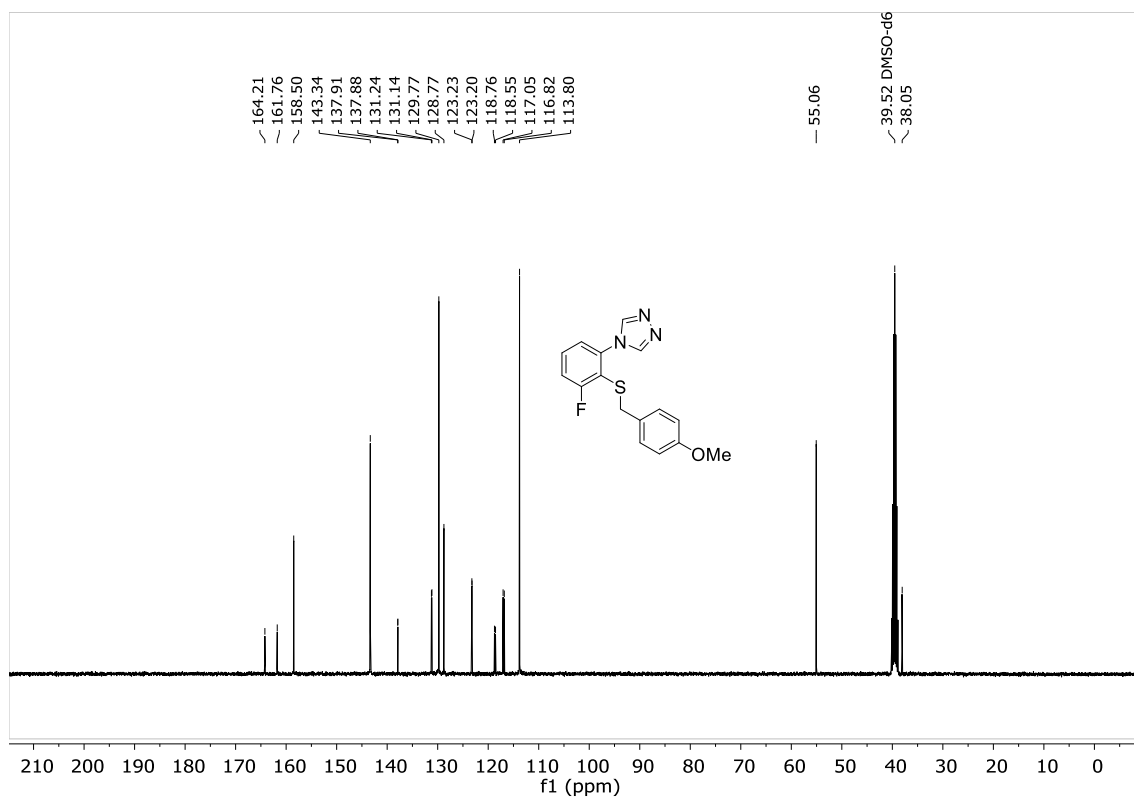
**Figure S122:** <sup>1</sup>H NMR spectrum of 4-(3-chloro-2-((4-methoxybenzyl)thio)phenyl)-4H-1,2,4-triazole (**3q**) (400 MHz, DMSO-d<sub>6</sub>, 298 K, 298 K).



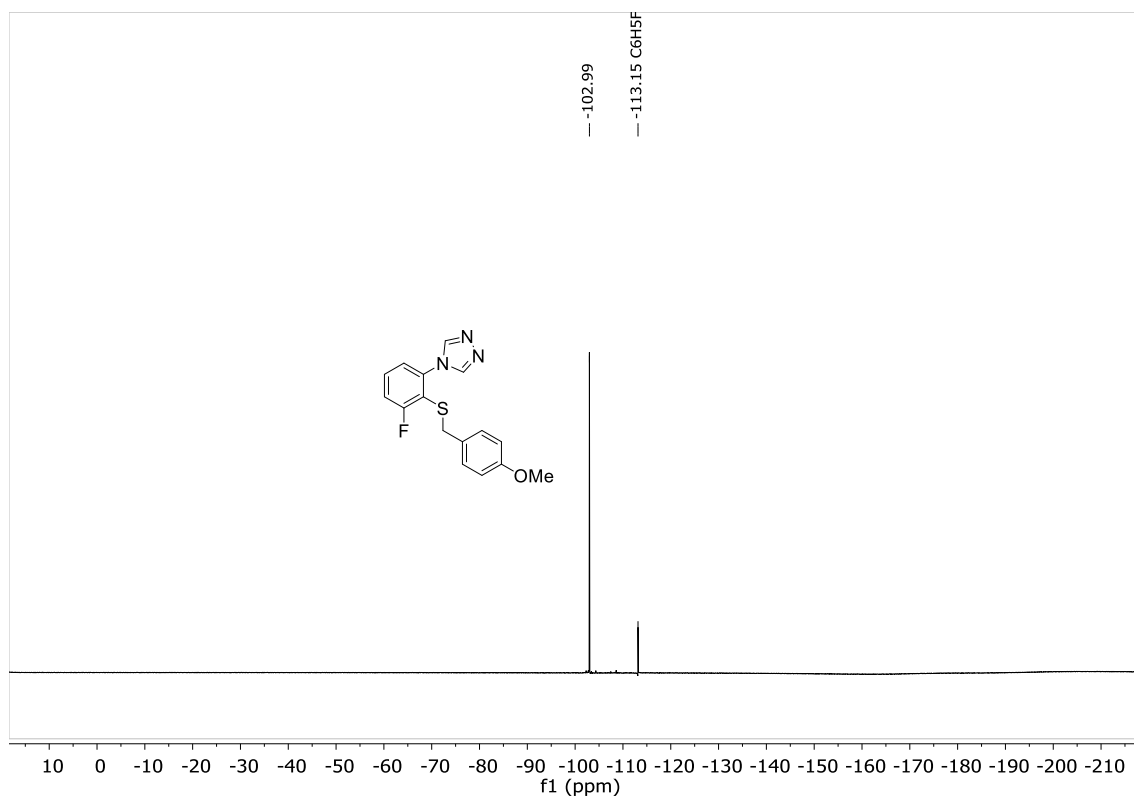
**Figure S123:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of 4-(3-chloro-2-((4-methoxybenzyl)thio)phenyl)-4H-1,2,4-triazole (**3q**) (100 MHz, DMSO- $d_6$ , 298 K, 298 K).



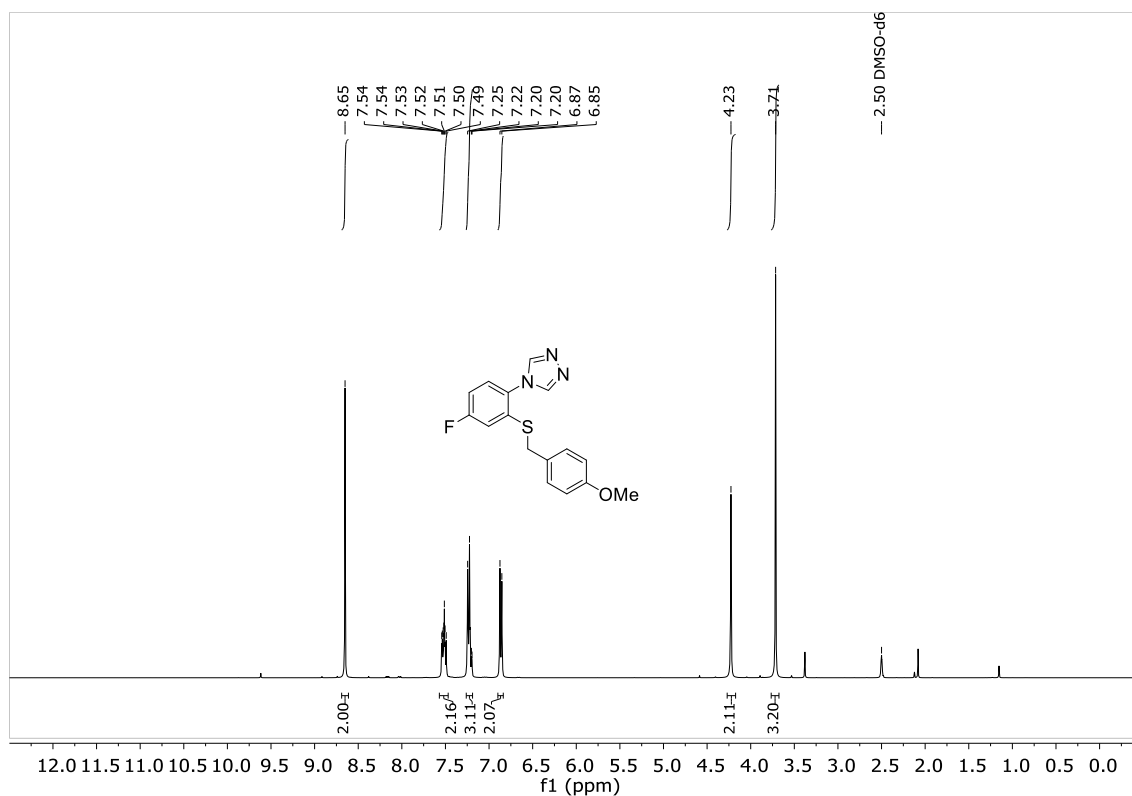
**Figure S124:**  $^1\text{H}$  NMR spectrum of 4-(3-fluoro-2-((4-methoxybenzyl)thio)phenyl)-4H-1,2,4-triazole (**3r**) (400 MHz, DMSO- $d_6$ , 298 K).



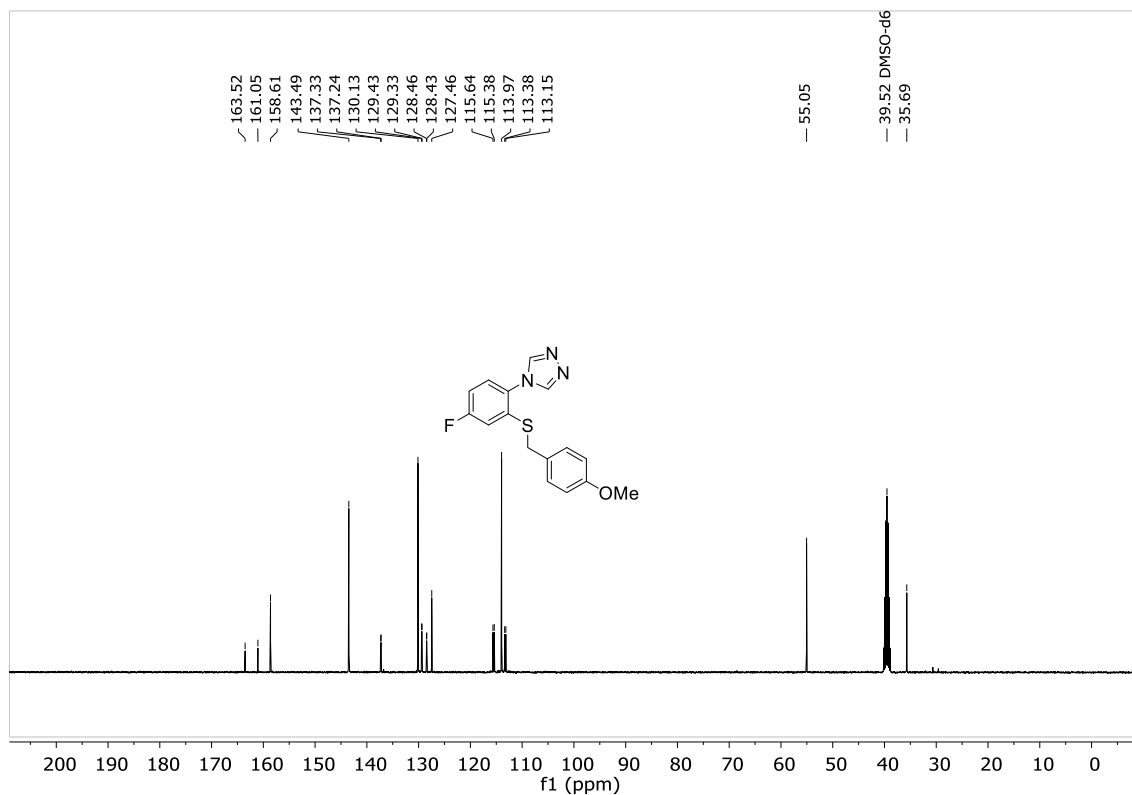
**Figure S125:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of 4-(3-fluoro-2-((4-methoxybenzyl)thio)phenyl)-4H-1,2,4-triazole (**3r**) (100 MHz, DMSO- $d_6$ , 298 K).



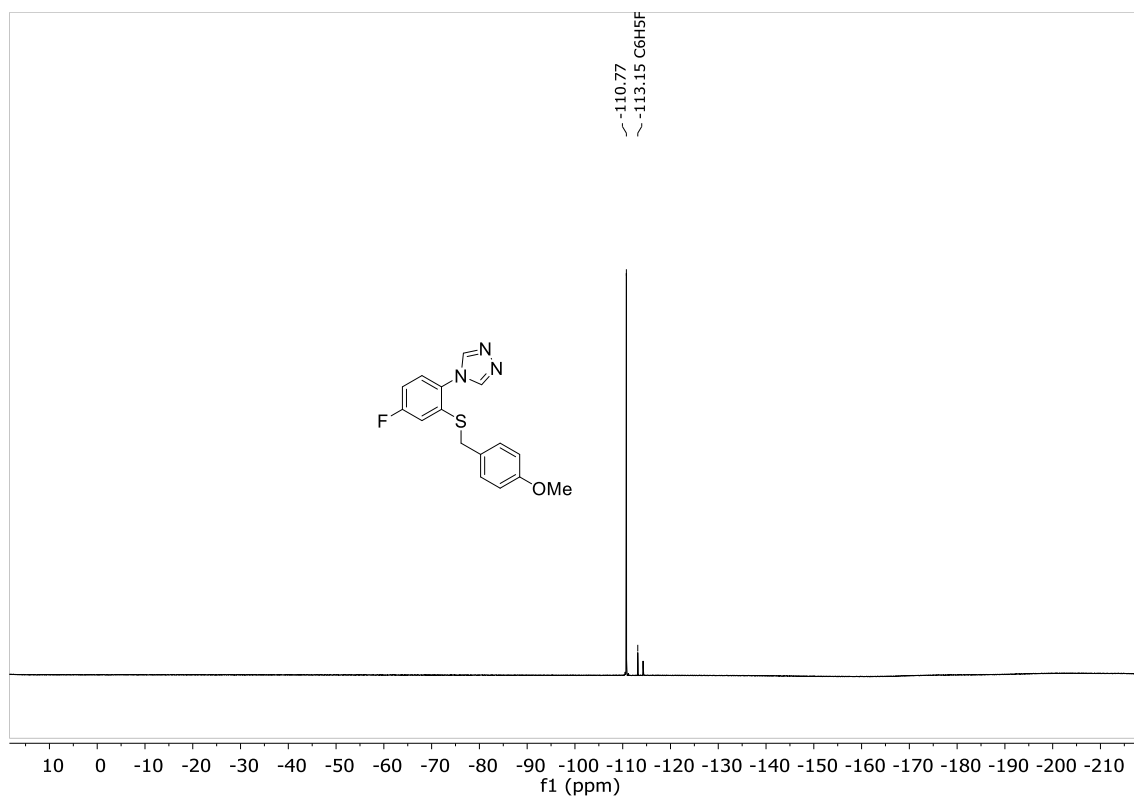
**Figure S126:**  $^{19}\text{F}\{^1\text{H}\}$  NMR spectrum of 4-(3-fluoro-2-((4-methoxybenzyl)thio)phenyl)-4H-1,2,4-triazole (**3r**) (376 MHz, DMSO- $d_6$ , 298 K, referenced to fluorobenzene).



**Figure S127:** <sup>1</sup>H NMR spectrum of 4-(4-fluoro-2-((4-methoxybenzyl)thio)phenyl)-4H-1,2,4-triazole (**3s**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).

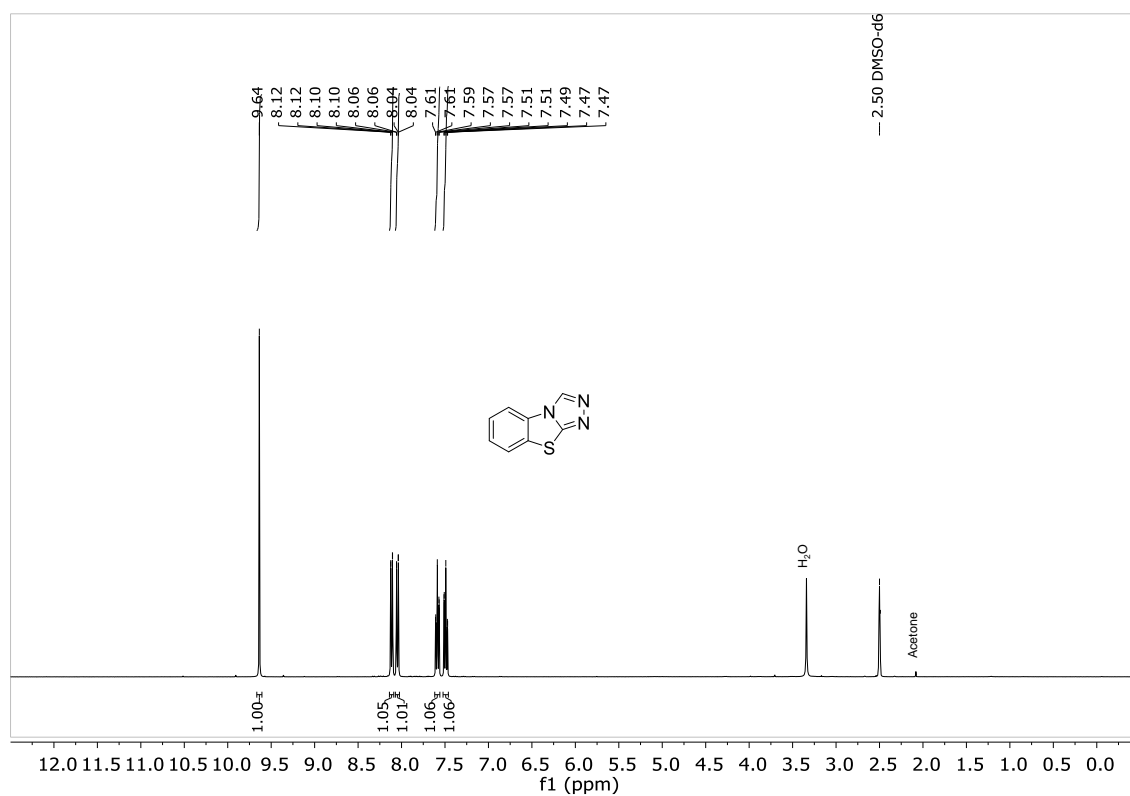


**Figure S128:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 4-(4-fluoro-2-((4-methoxybenzyl)thio)phenyl)-4H-1,2,4- (**3s**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).

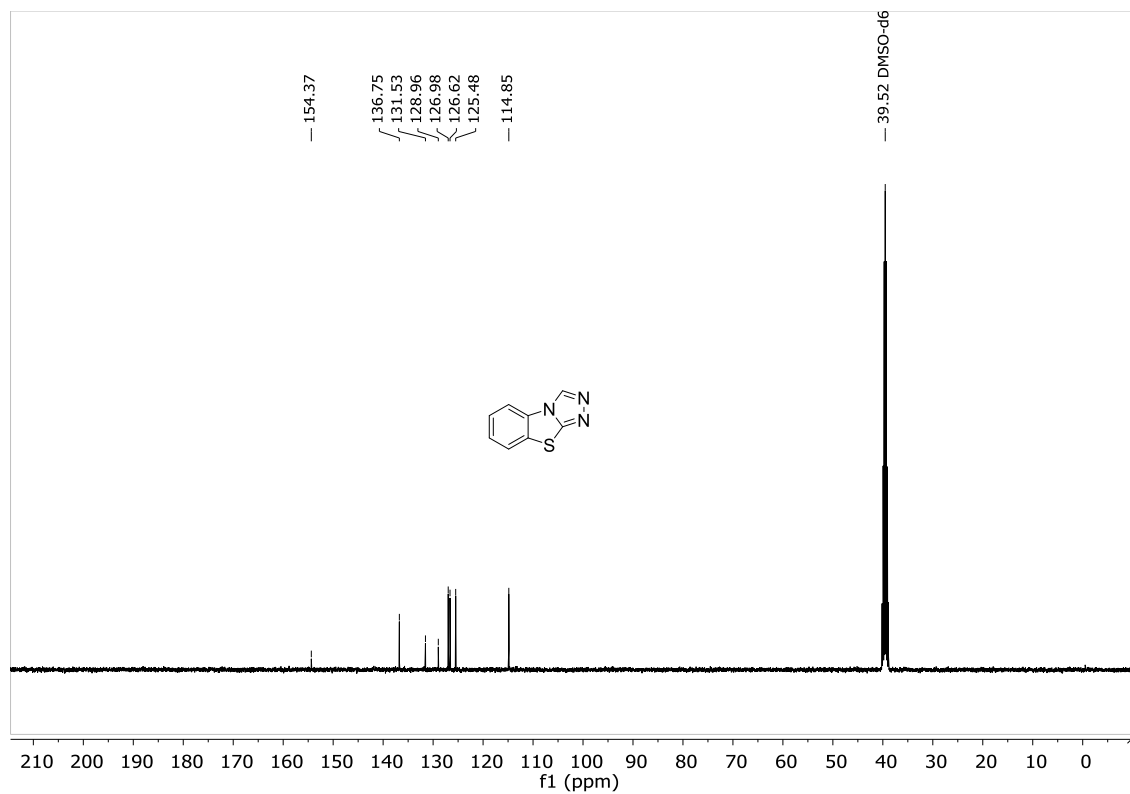


**Figure S129:** <sup>19</sup>F{<sup>1</sup>H} NMR spectrum of 4-(4-fluoro-2-((4-methoxybenzyl)thio)phenyl)-4*H*-1,2,4-triazole (**3s**) (376 MHz, DMSO-*d*<sub>6</sub>, 298 K, referenced to fluorobenzene).

**1.5 NMR Spectra of Benzo[4,5]thiazolo[2,3-c][1,2,4]triazoles (6a-6s)**

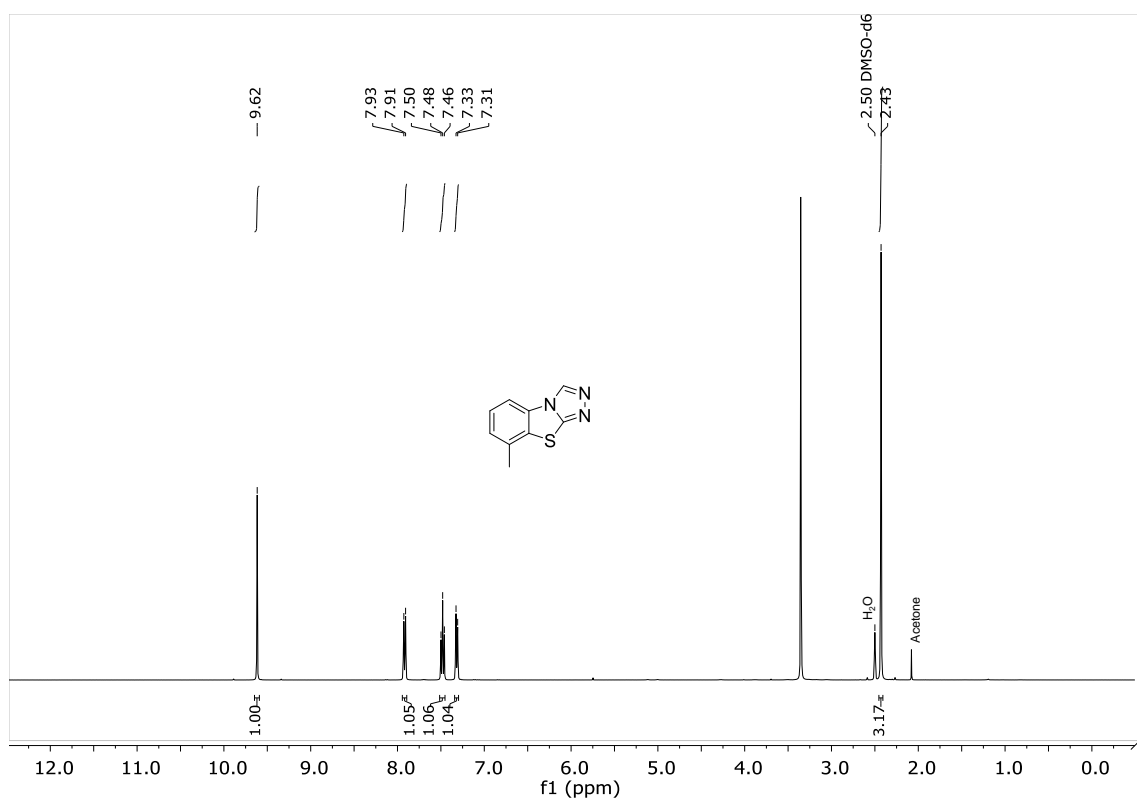


**Figure S130:** <sup>1</sup>H NMR spectrum of benzo[4,5]thiazolo[2,3-c][1,2,4]triazole (**6a**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).

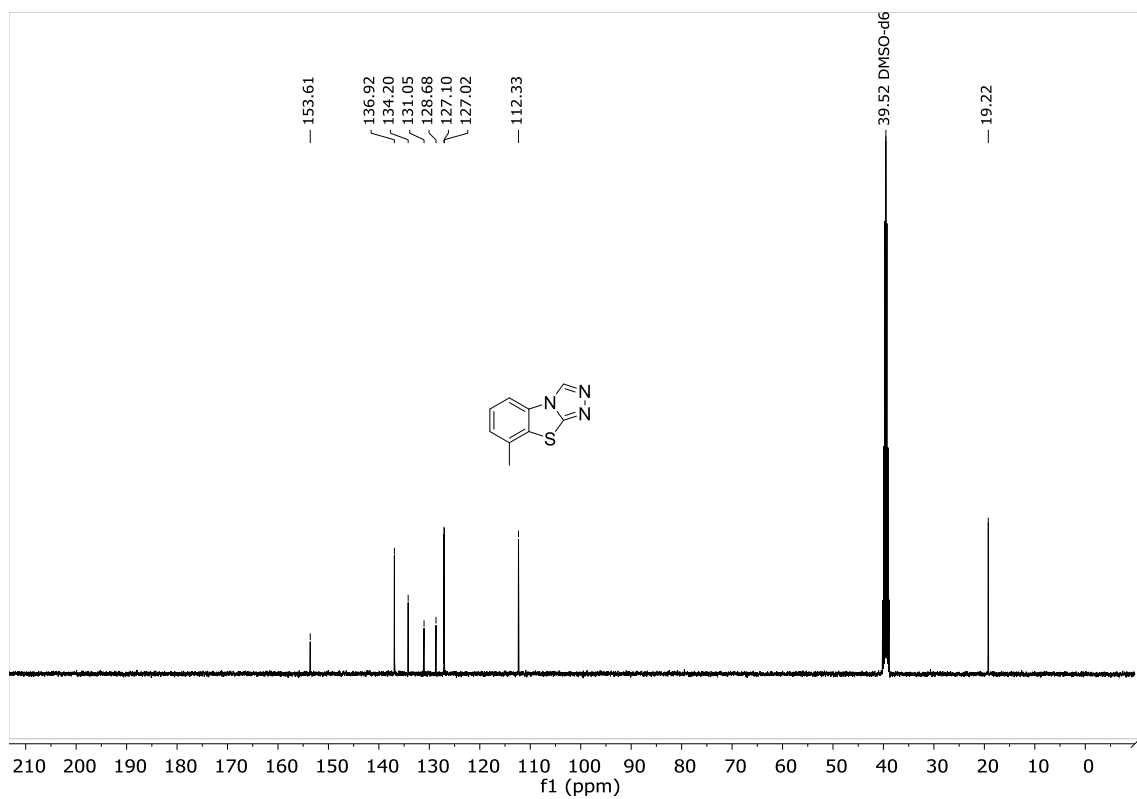


**Figure S131:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of benzo[4,5]thiazolo[2,3-c][1,2,4]triazole (**6a**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).

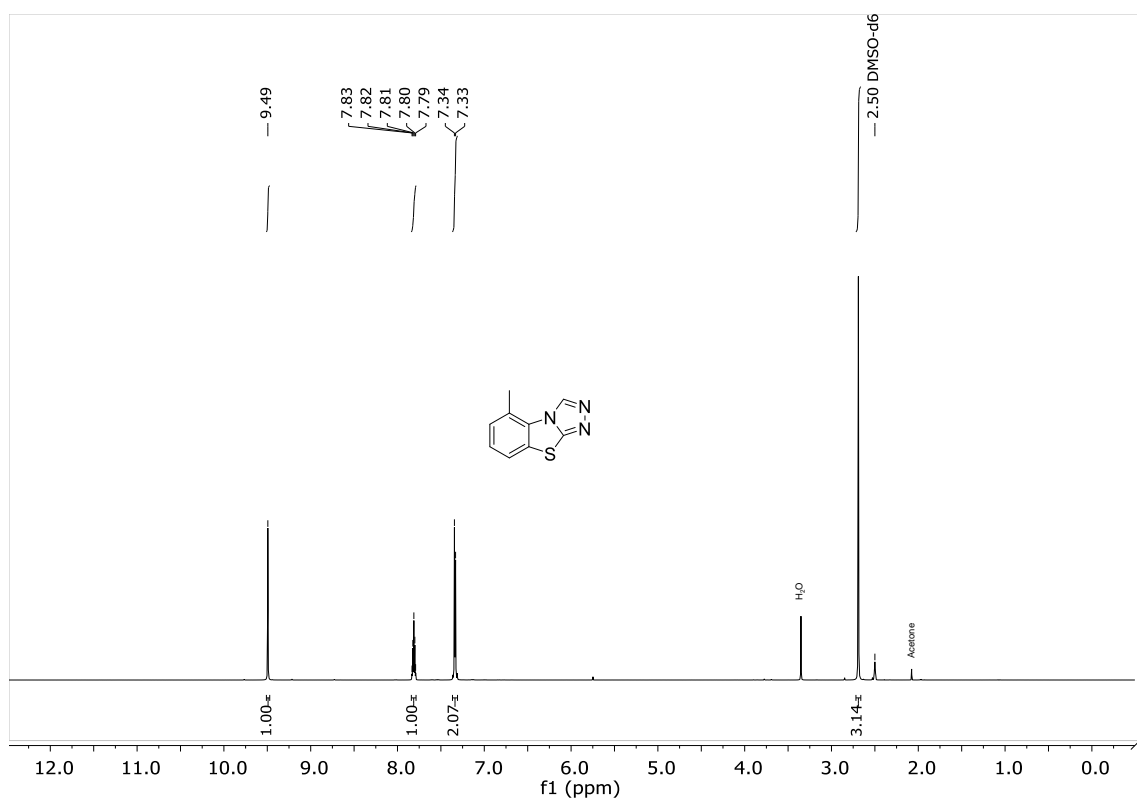




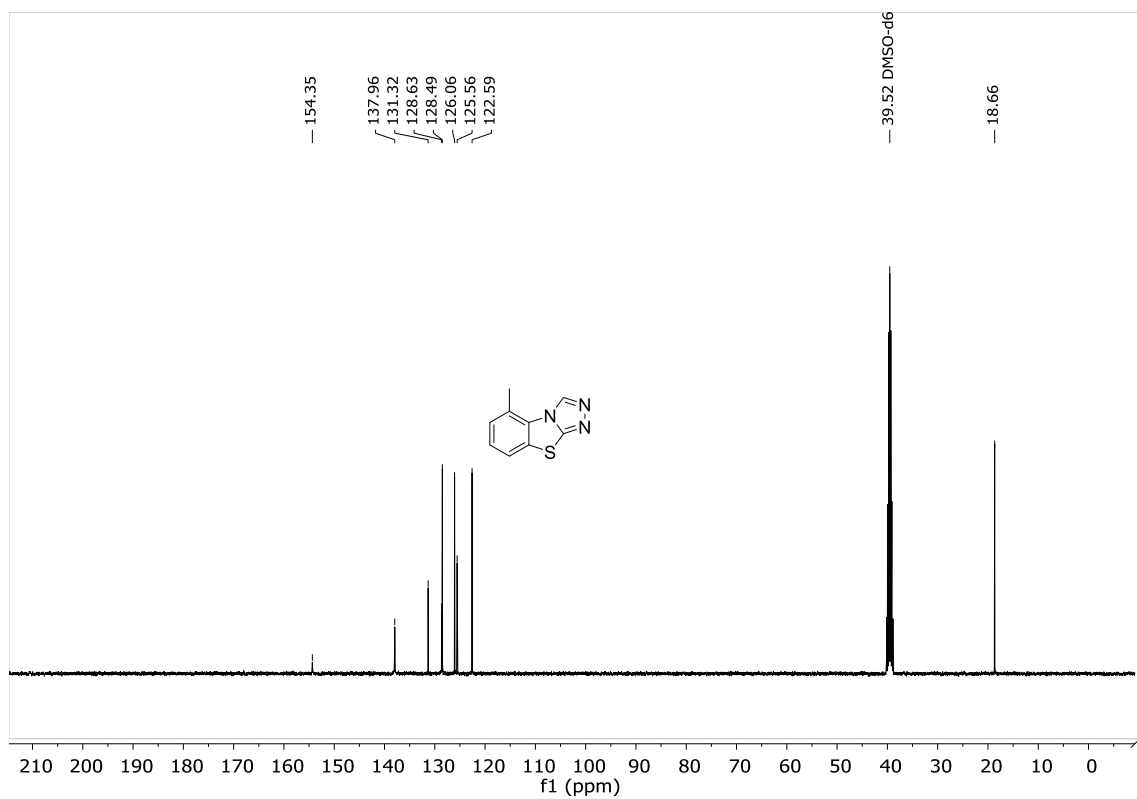
**Figure S132:** <sup>1</sup>H NMR spectrum of 5-methylbenzo[4,5]thiazolo[2,3-c][1,2,4]triazole (**6b**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



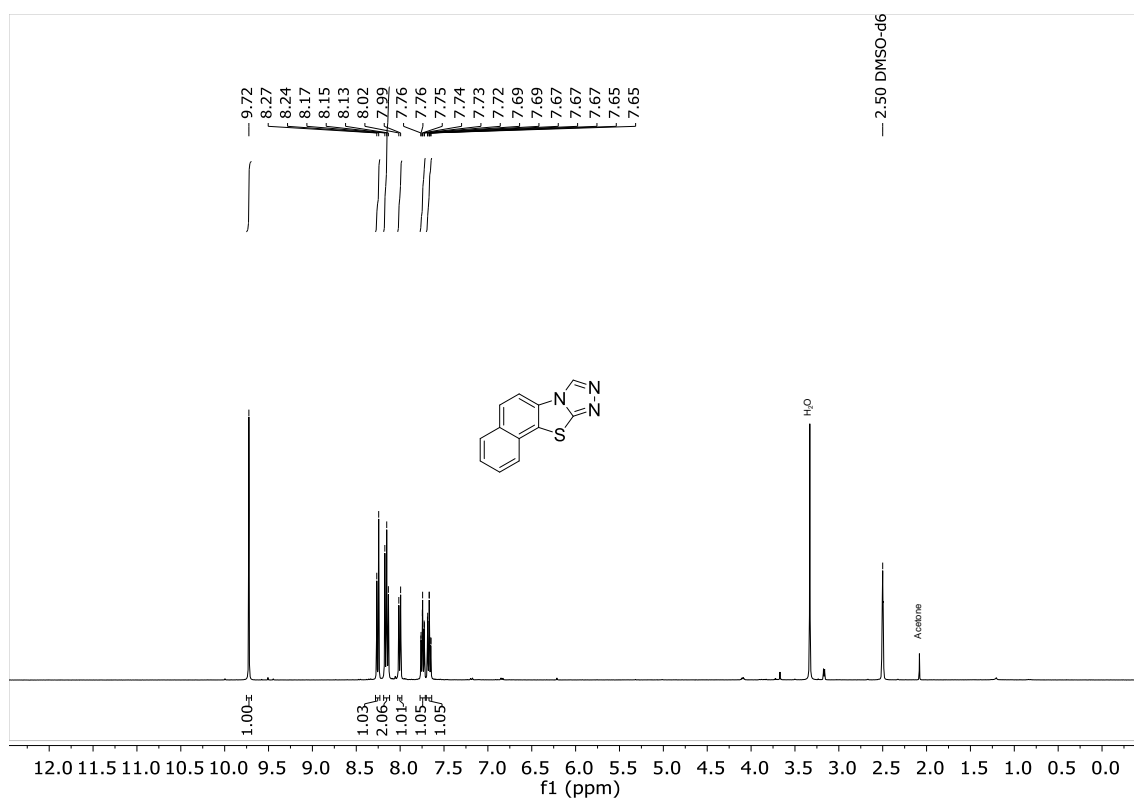
**Figure S133:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 5-methylbenzo[4,5]thiazolo[2,3-c][1,2,4]triazole (**6b**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



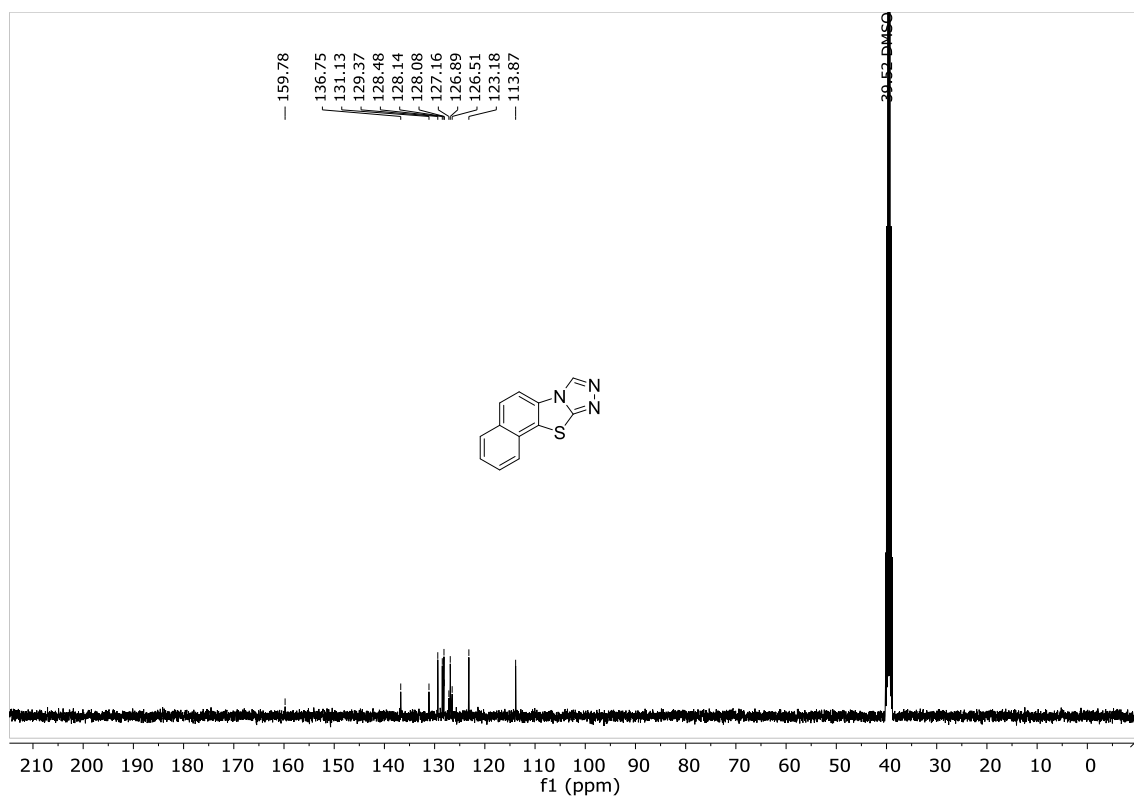
**Figure S134:** <sup>1</sup>H NMR spectrum of 5-methylbenzo[4,5]thiazolo[2,3-c][1,2,4]triazole (**6c**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



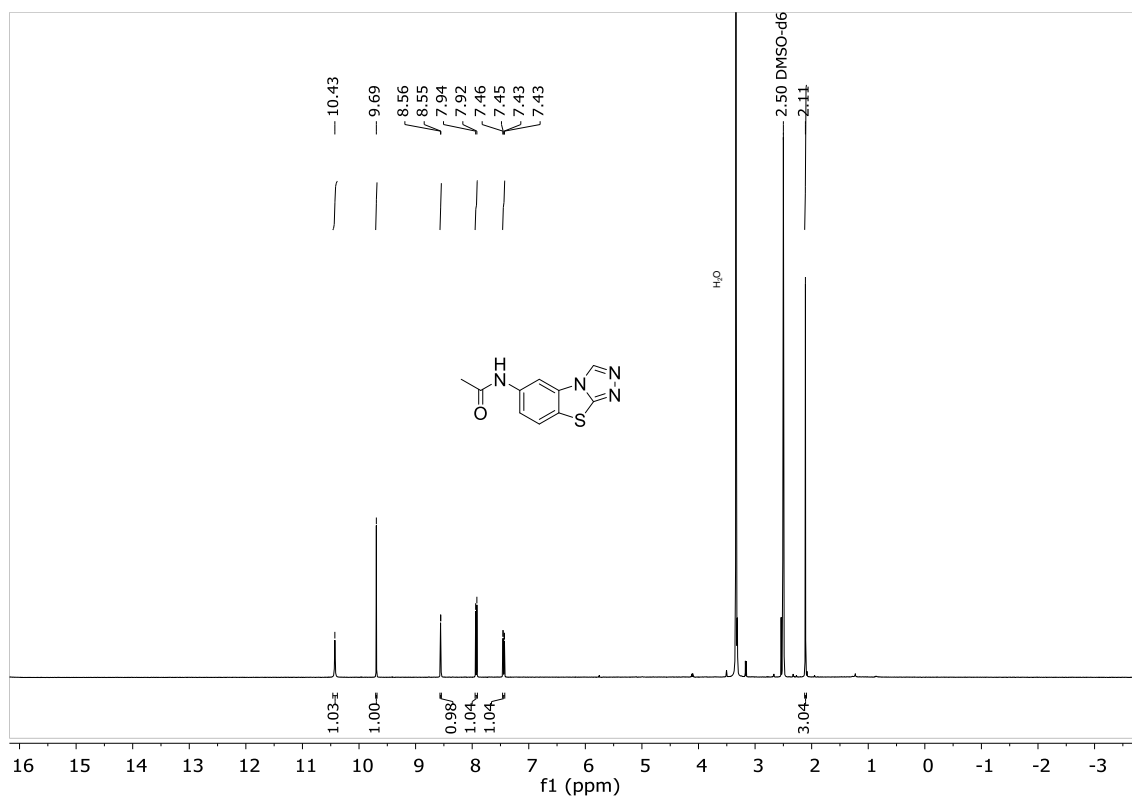
**Figure S135:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 5-methylbenzo[4,5]thiazolo[2,3-c][1,2,4]triazole (**6c**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



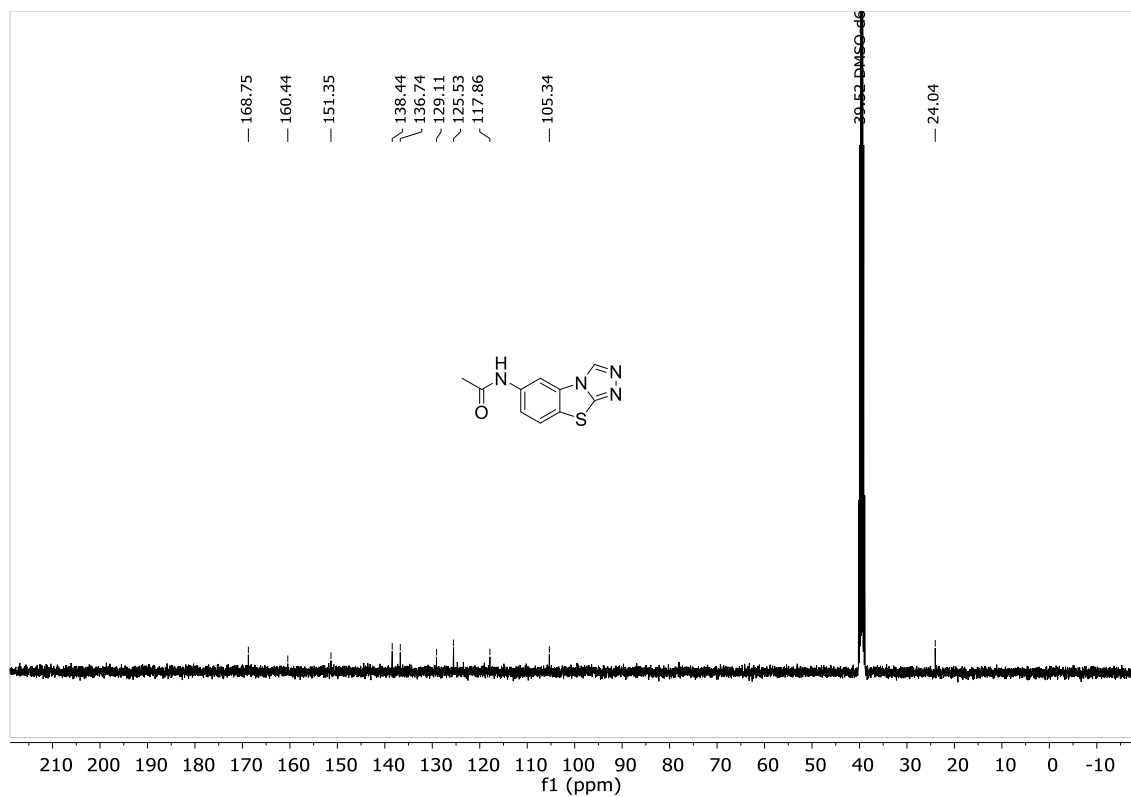
**Figure S136:** <sup>1</sup>H NMR spectrum of naphtho[2',1':4,5]thiazolo[2,3-c][1,2,4]triazole (**6d**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



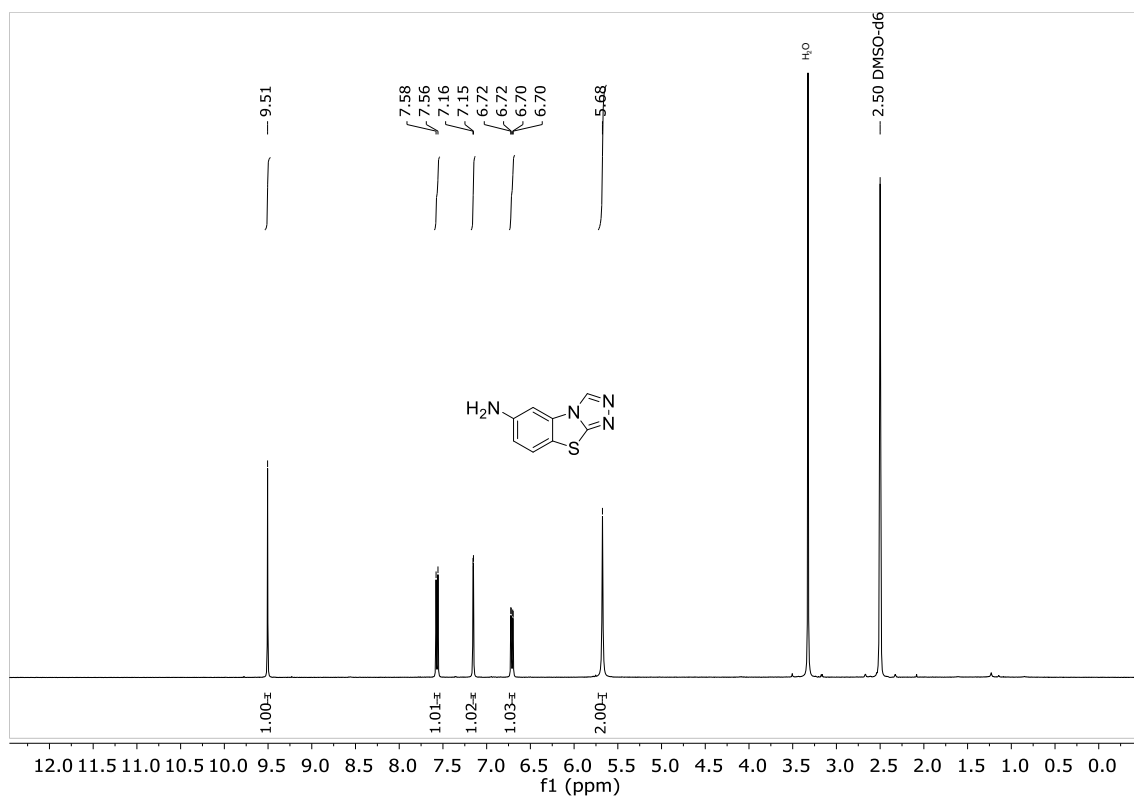
**Figure S137:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of naphtho[2',1':4,5]thiazolo[2,3-c][1,2,4]triazole (**6d**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



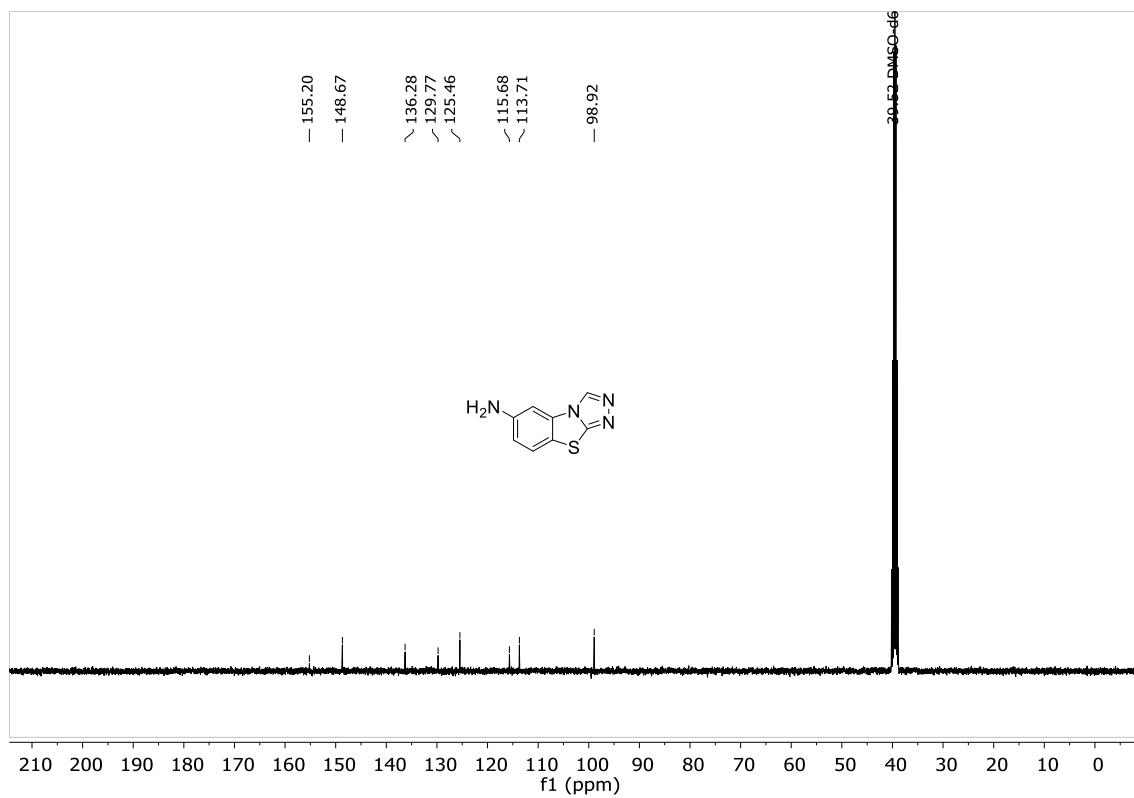
**Figure S138:** <sup>1</sup>H NMR spectrum of *N*-(benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazol-6-yl)acetamide (**6e**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



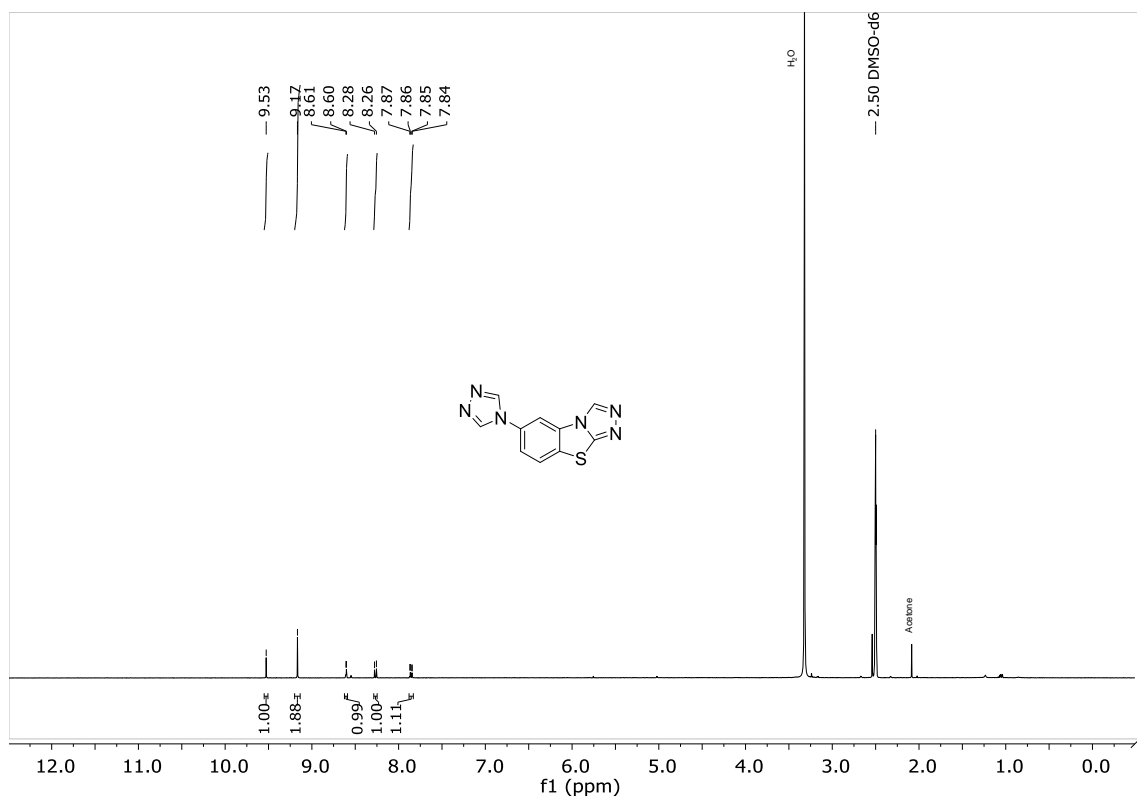
**Figure S139:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of *N*-(benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazol-6-yl)acetamide (**6e**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



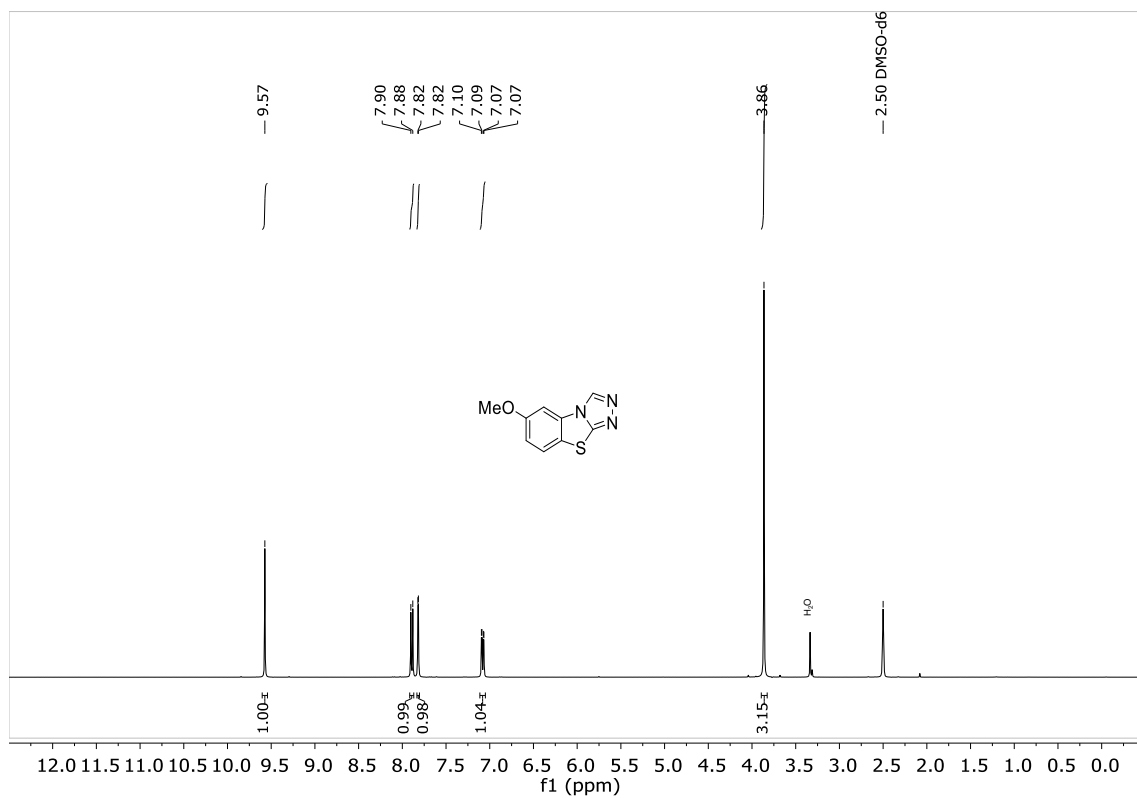
**Figure S140:** <sup>1</sup>H NMR spectrum of benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazol-6-amine (**6f**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



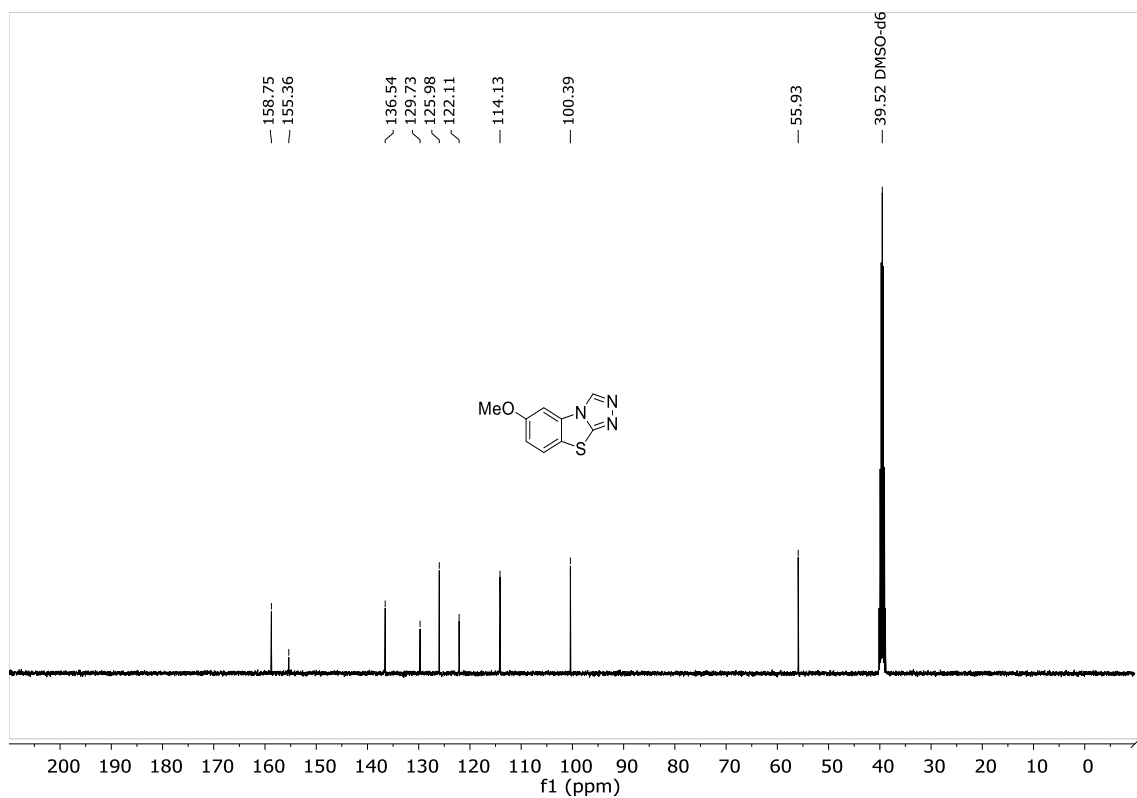
**Figure S141:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazol-6-amine (**6f**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



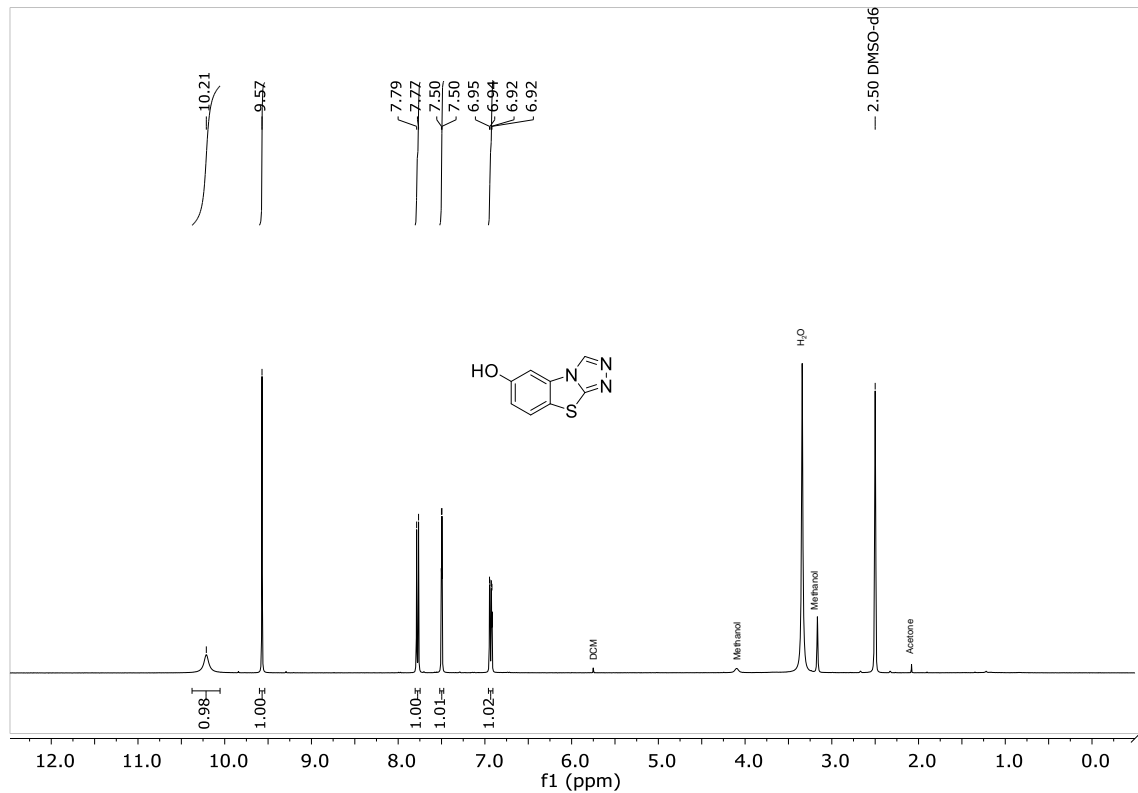
**Figure S142:** <sup>1</sup>H NMR spectrum of 6-(4H-1,2,4-triazol-4-yl)benzo[4,5]thiazolo[2,3-c][1,2,4]triazole (**6f**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



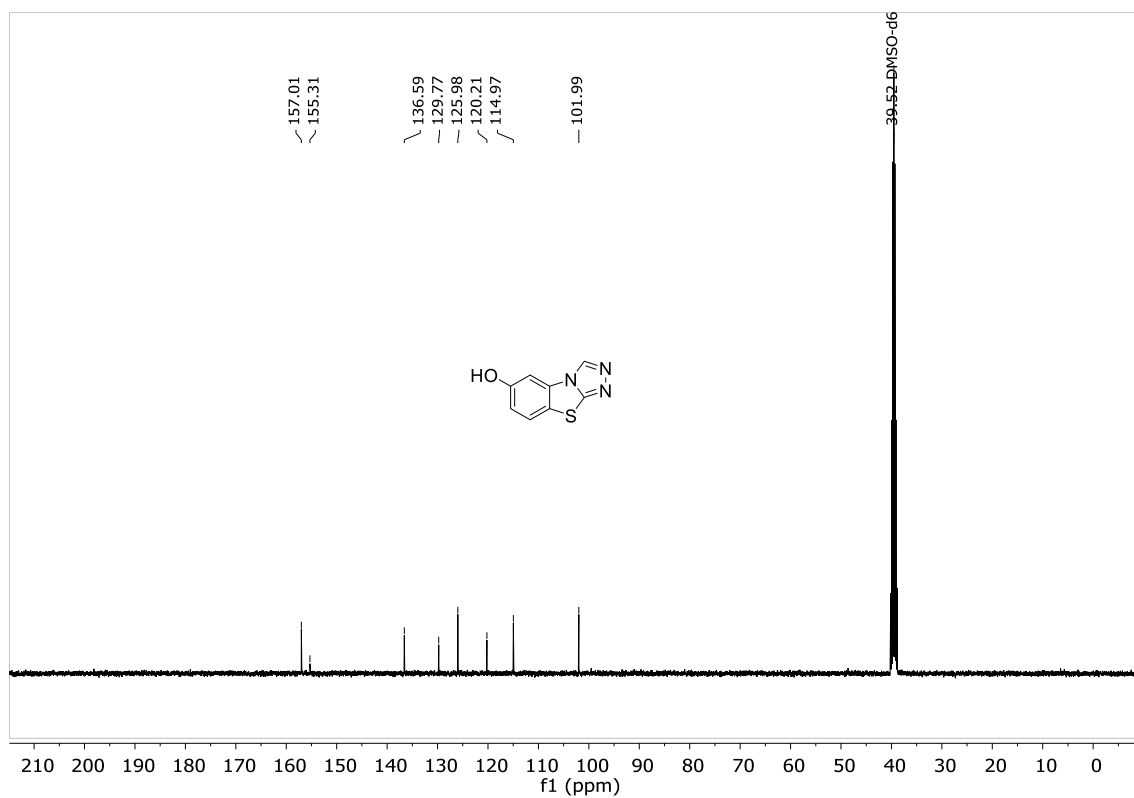
**Figure S143:** <sup>1</sup>H NMR spectrum of 6-methoxybenzo[4,5]thiazolo[2,3-c][1,2,4]triazole (**6g**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



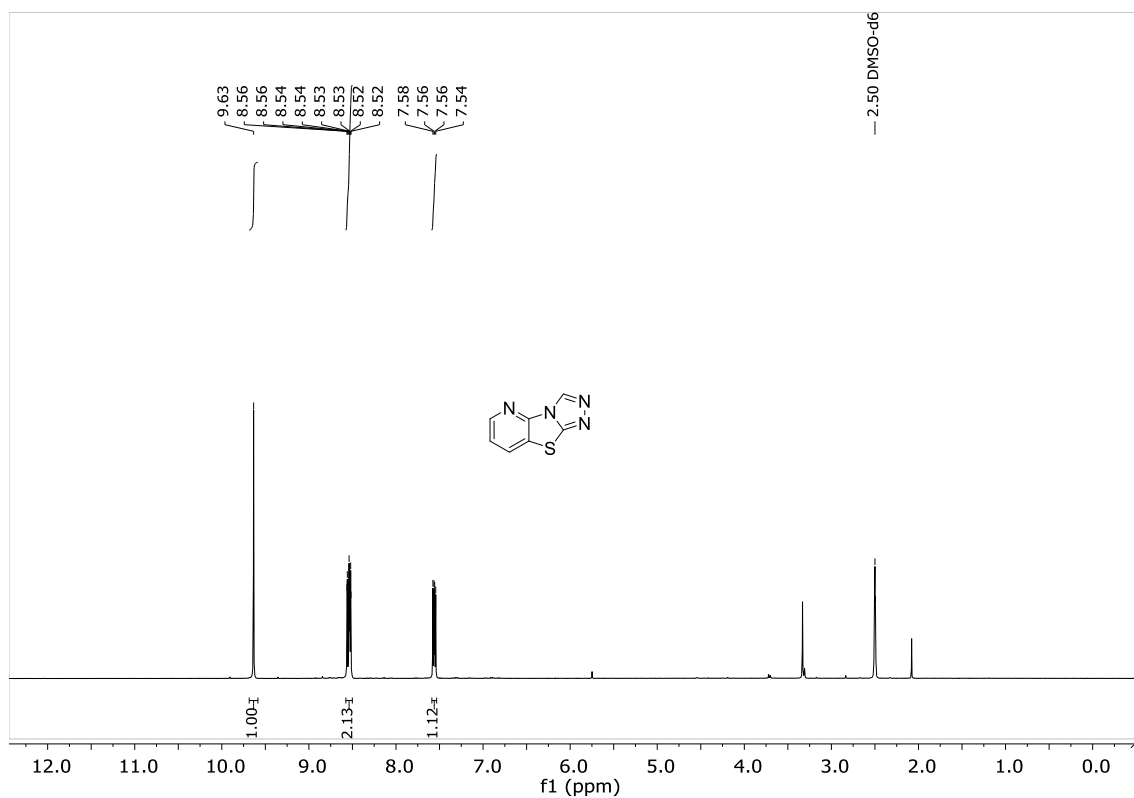
**Figure S144:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 6-methoxybenzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (**6g**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



**Figure S145:** <sup>1</sup>H NMR spectrum of benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazol-6-ol (**6h**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).

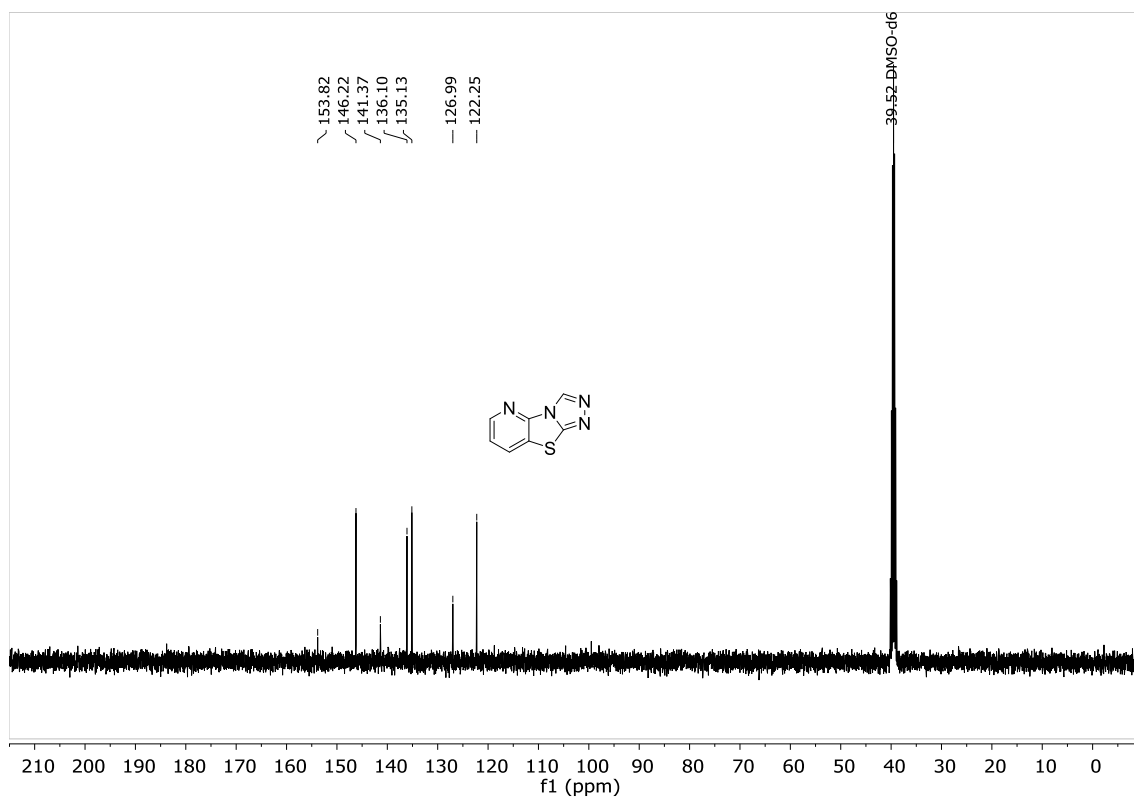


**Figure S146:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of benzo[4,5]thiazolo[2,3-c][1,2,4]triazol-6-ol (**6h**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).

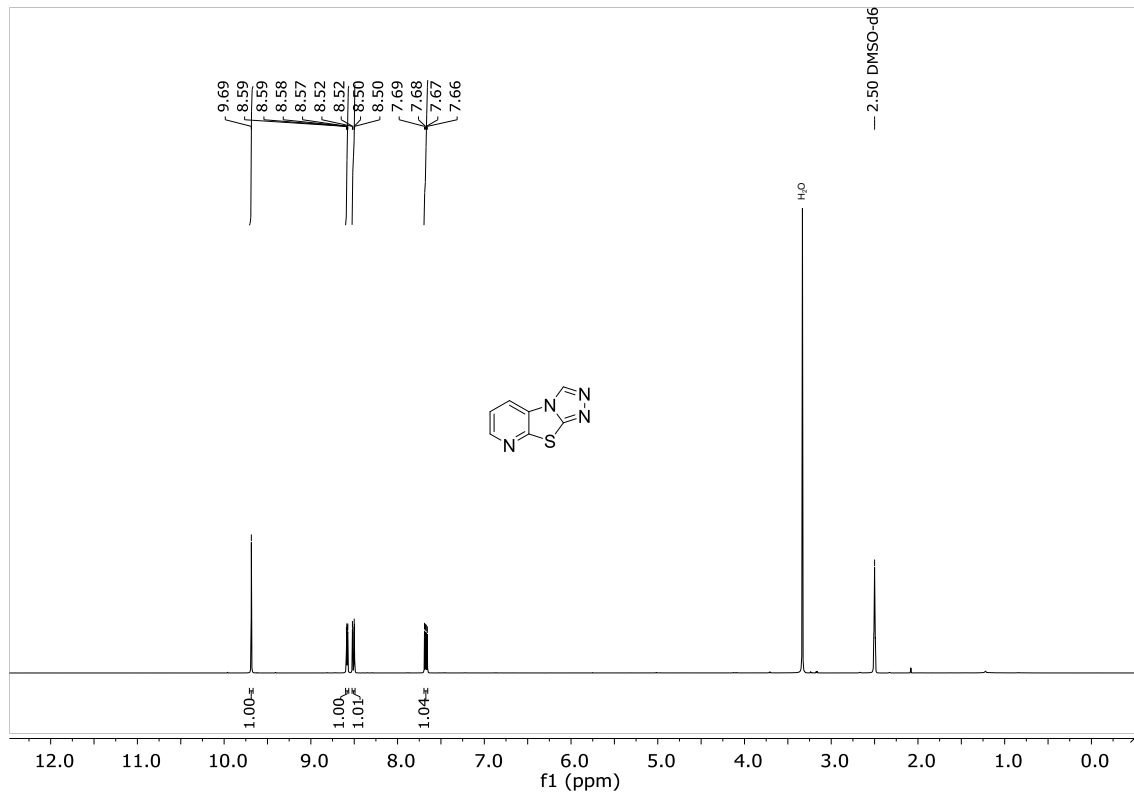


**Figure S147:** <sup>1</sup>H NMR spectrum of [1,2,4]triazolo[3',4':2,3]thiazolo[4,5-*b*]pyridine (**6i**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).

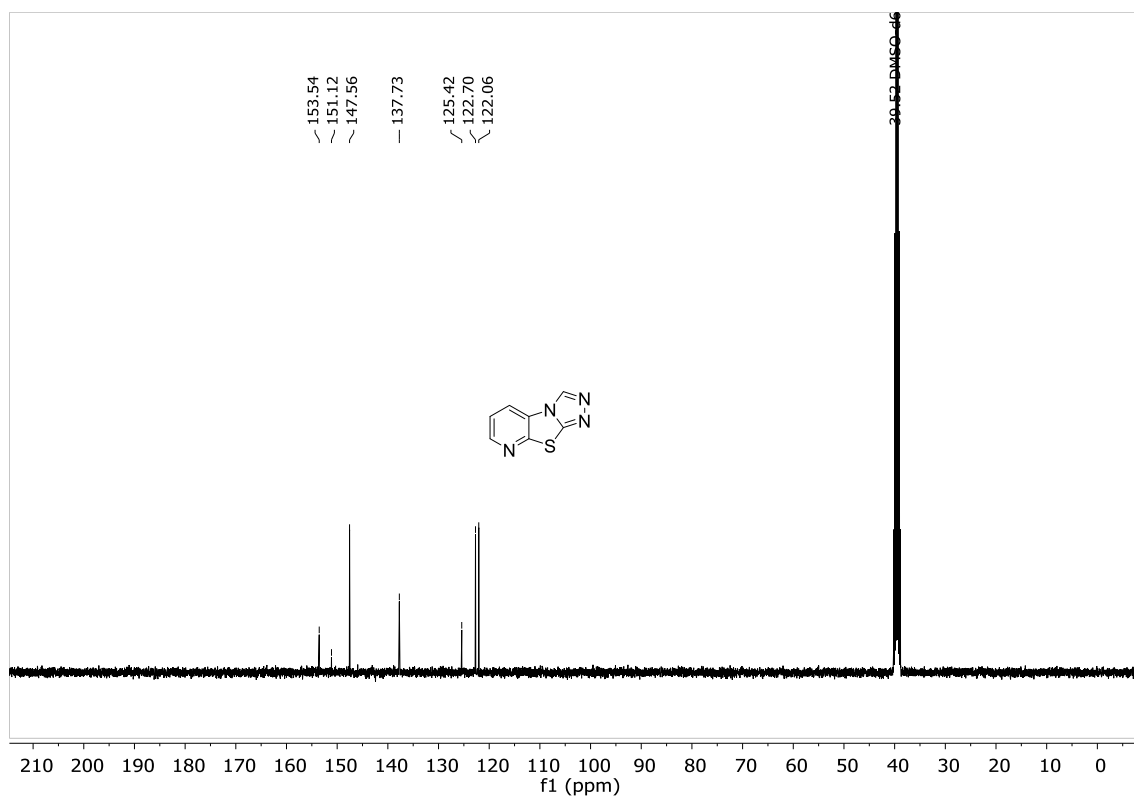




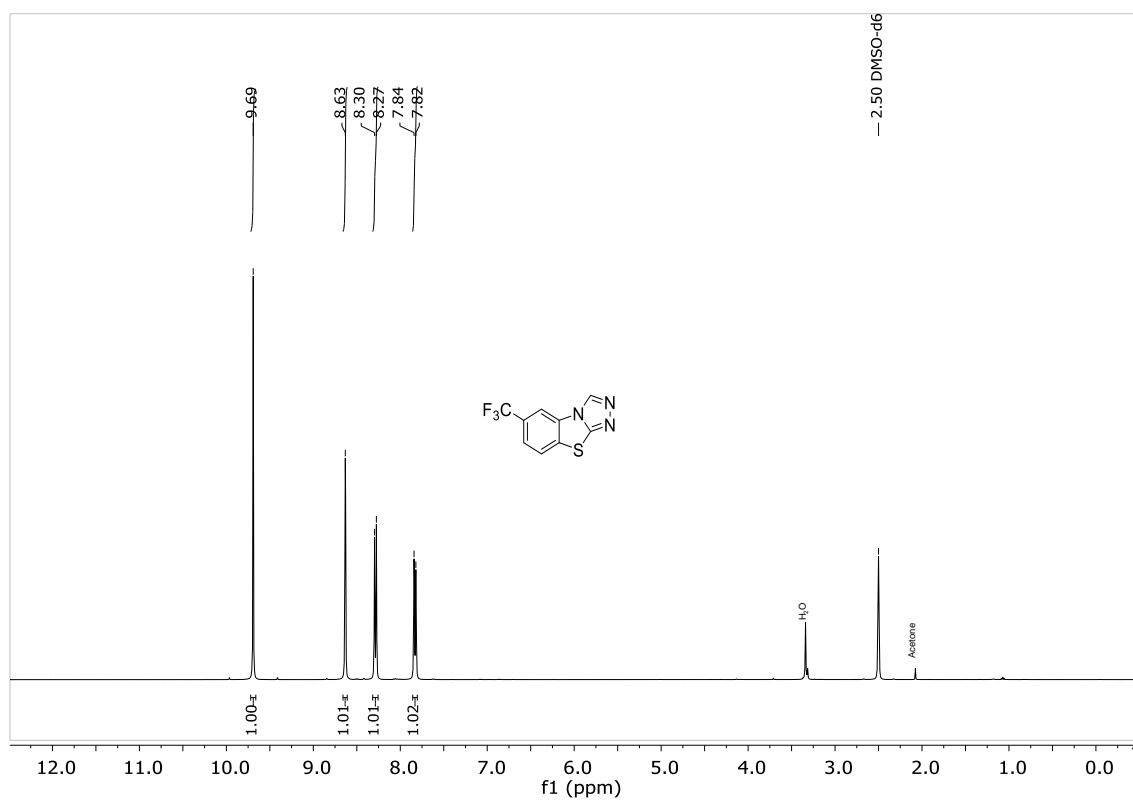
**Figure S148:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of [1,2,4]triazolo[3',4':2,3]thiazolo[4,5-*b*]pyridine (**6i**) (100 MHz, DMSO- $d_6$ , 298 K).



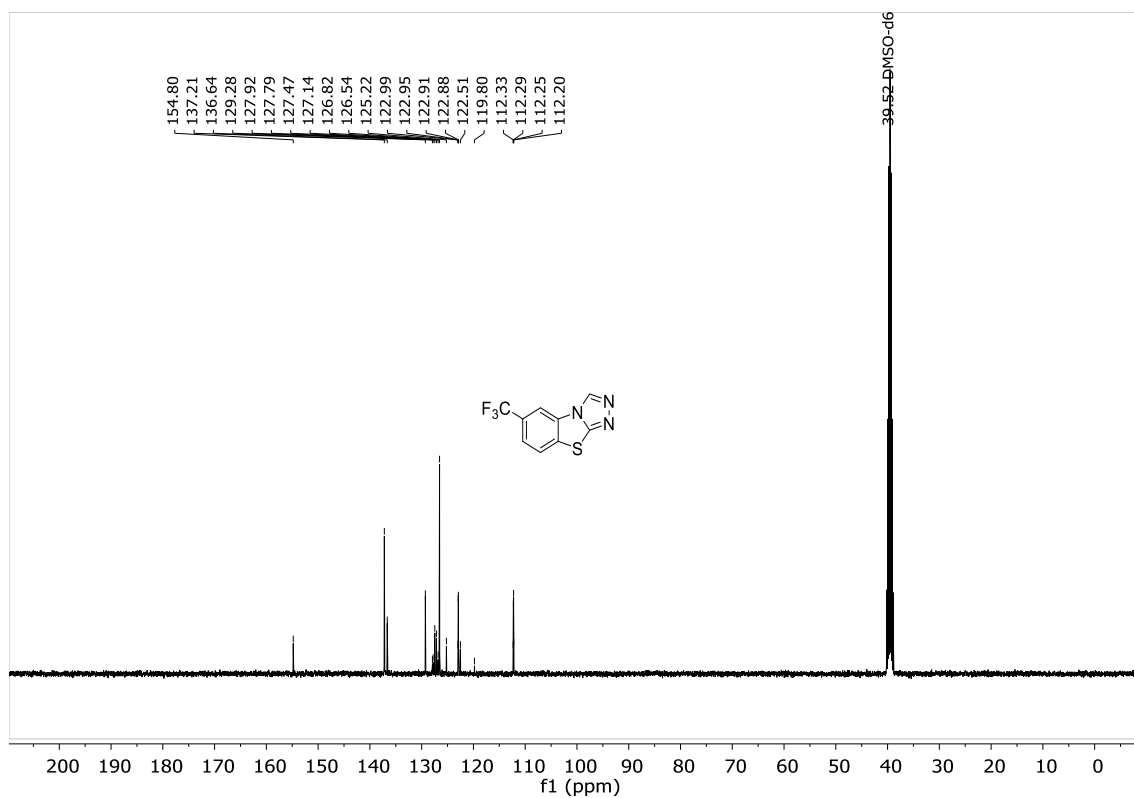
**Figure S149:**  $^1\text{H}$  NMR spectrum of [1,2,4]triazolo[3',4':2,3]thiazolo[5,4-*b*]pyridine (**6j**) (400 MHz, DMSO- $d_6$ , 298 K).



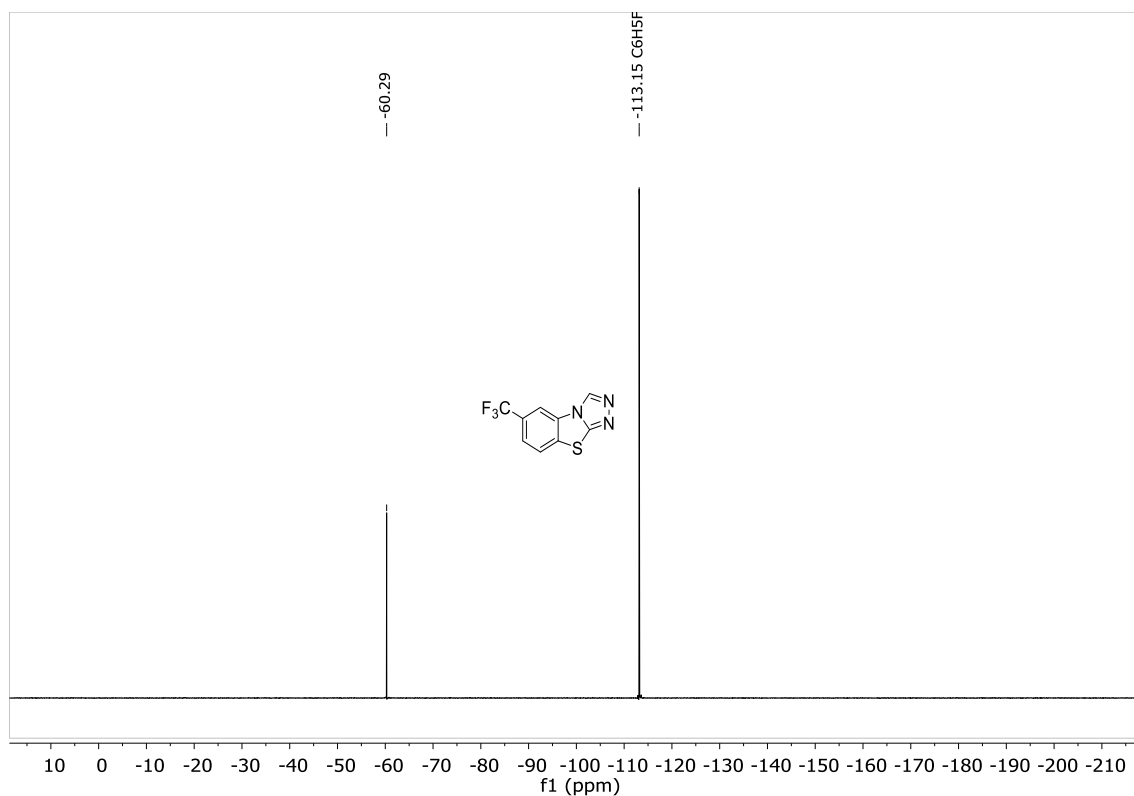
**Figure S150:**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of [1,2,4]triazolo[3',4':2,3]thiazolo[5,4-*b*]pyridine (**6j**) (100 MHz, DMSO- $d_6$ , 298 K).



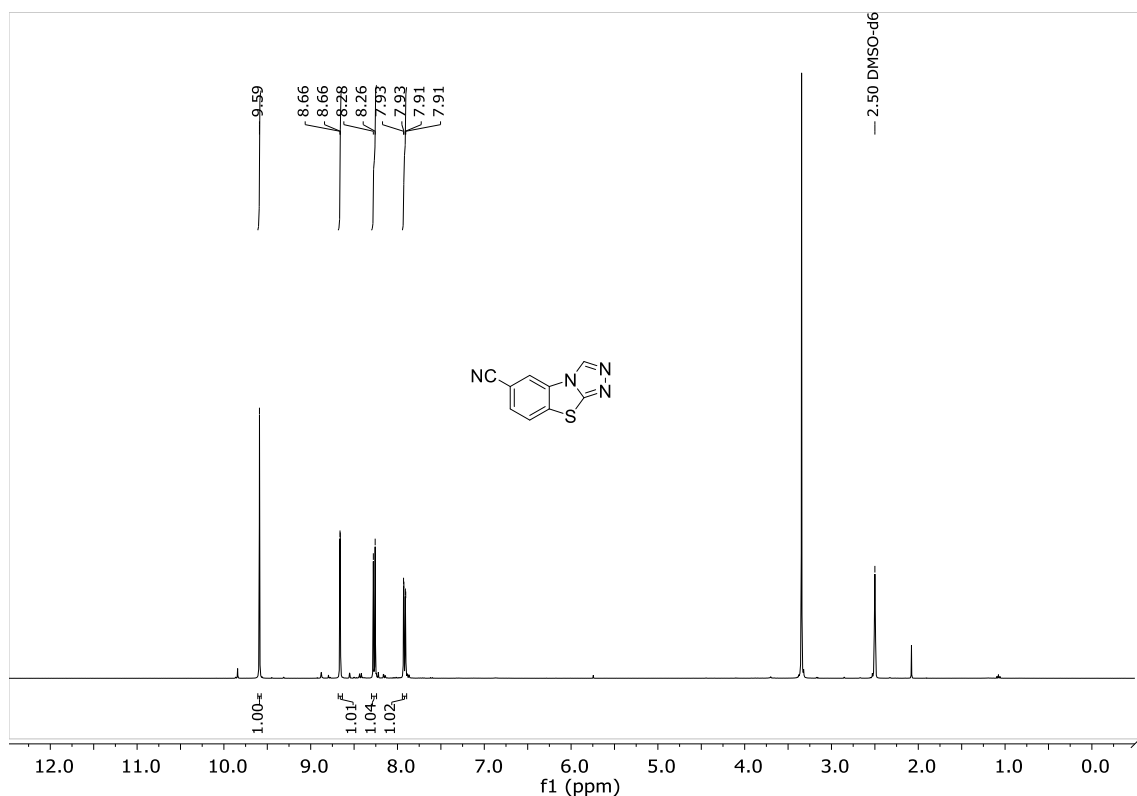
**Figure S151:**  $^1\text{H}$  NMR spectrum of 6-(trifluoromethyl)benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (**6k**) (400 MHz, DMSO- $d_6$ , 298 K).



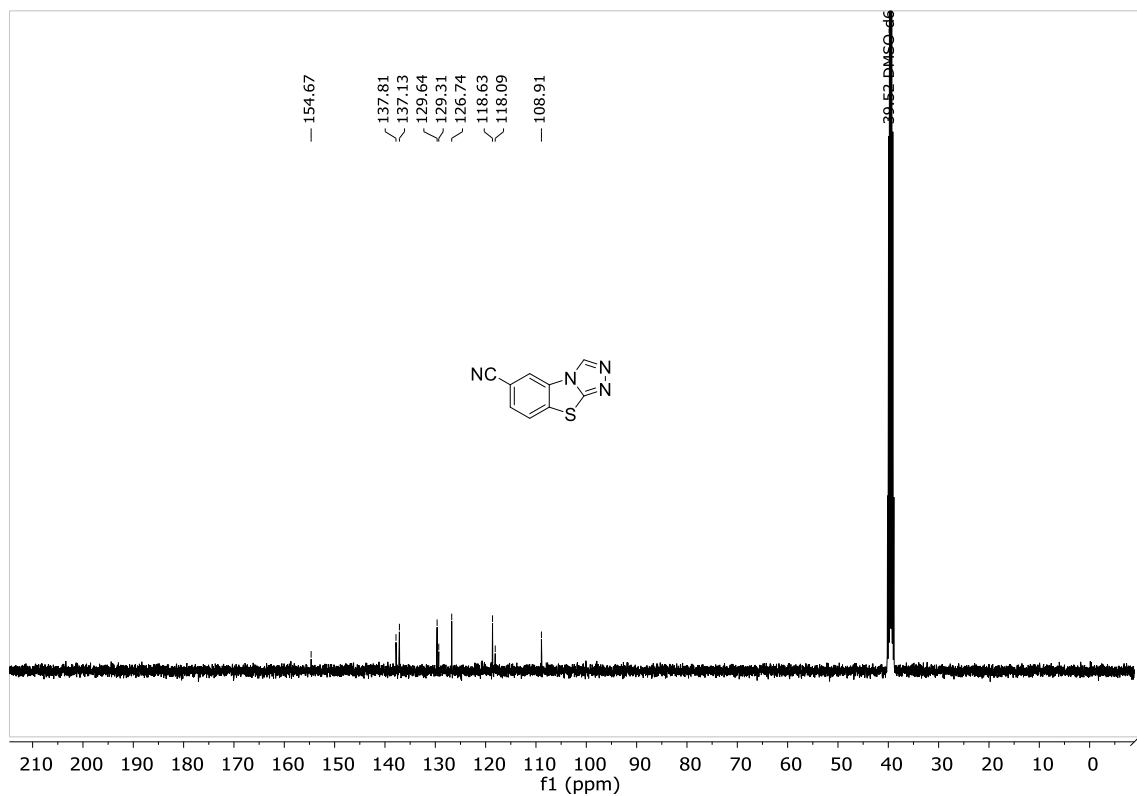
**Figure S152:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 6-(trifluoromethyl)benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (**6k**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



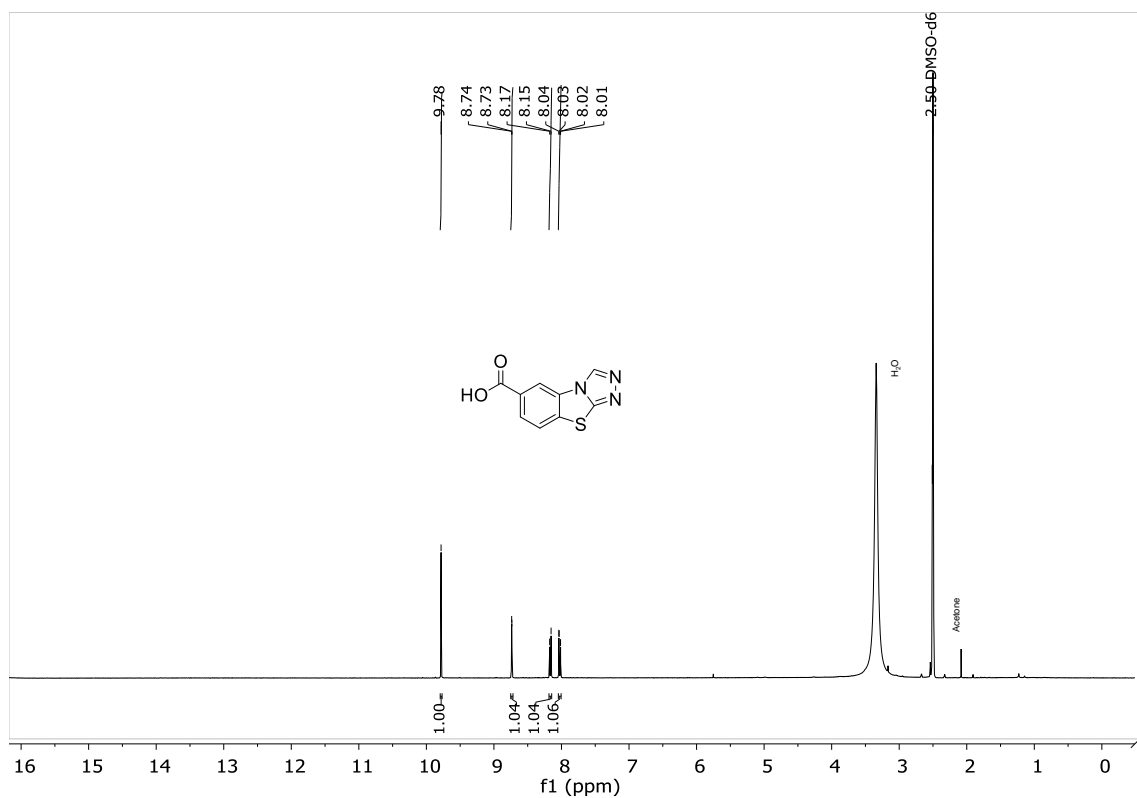
**Figure S153:** <sup>19</sup>F{<sup>1</sup>H} NMR spectrum of 6-(trifluoromethyl)benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (**6k**) (376 MHz, DMSO-*d*<sub>6</sub>, 298 K).



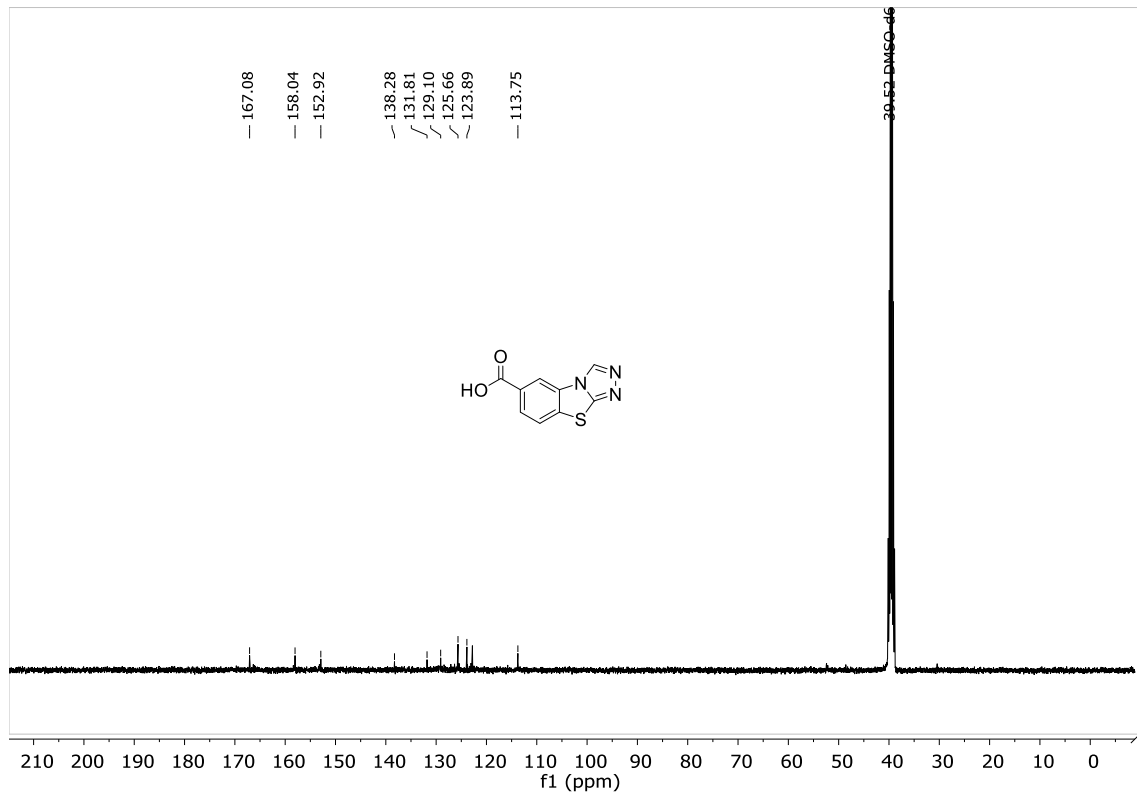
**Figure S154:** <sup>1</sup>H NMR spectrum of benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole-6-carbonitrile (**6I**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



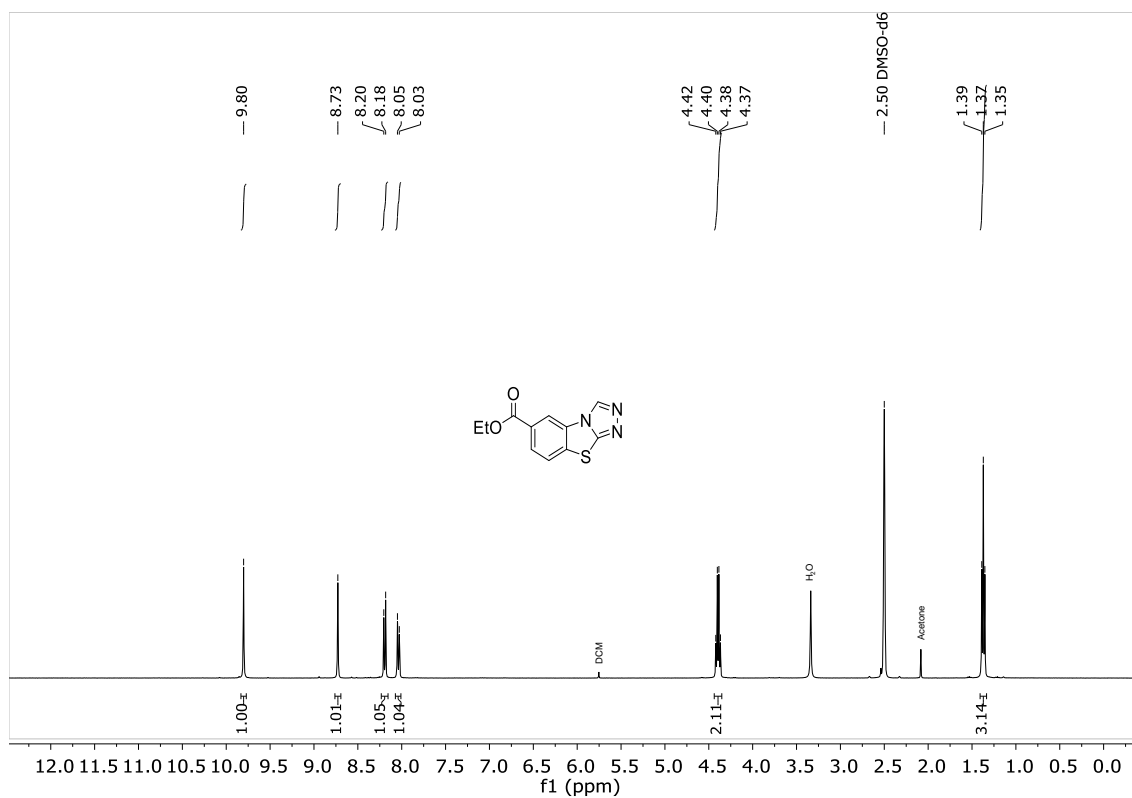
**Figure S155:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole-6-carbonitrile (**6I**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



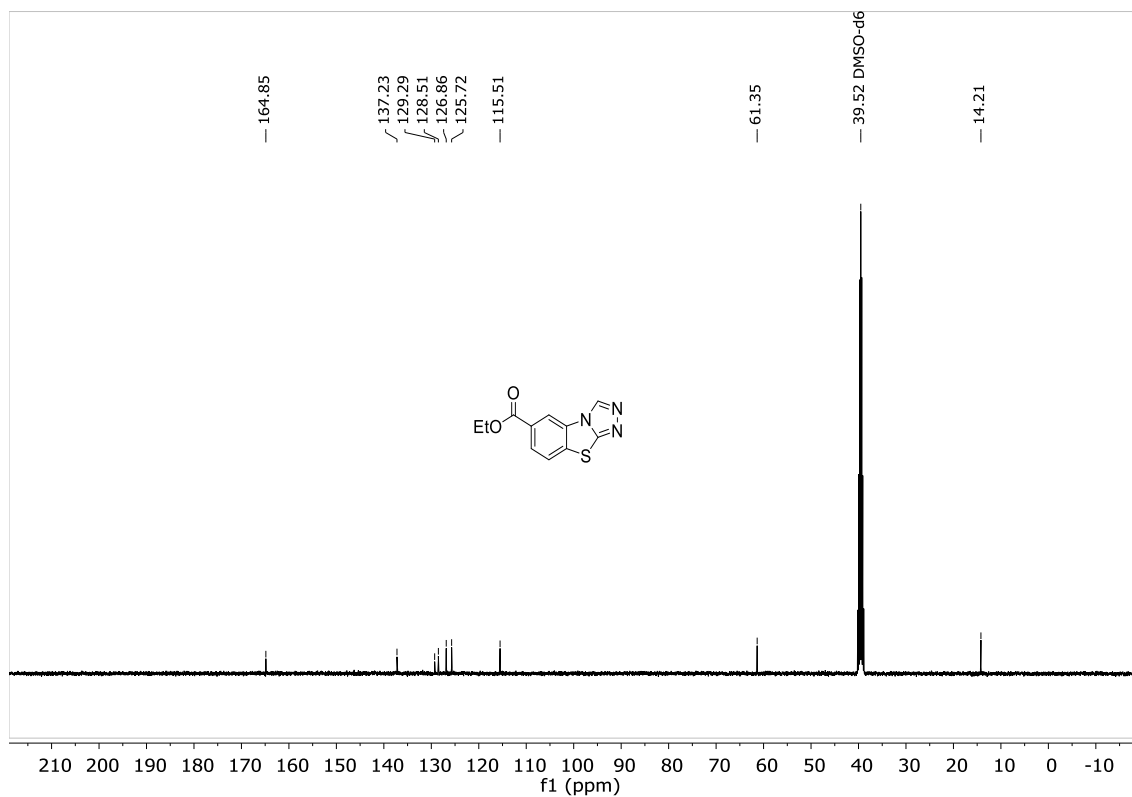
**Figure S156:** <sup>1</sup>H NMR spectrum of benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole-6-carboxylic acid (**6m**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



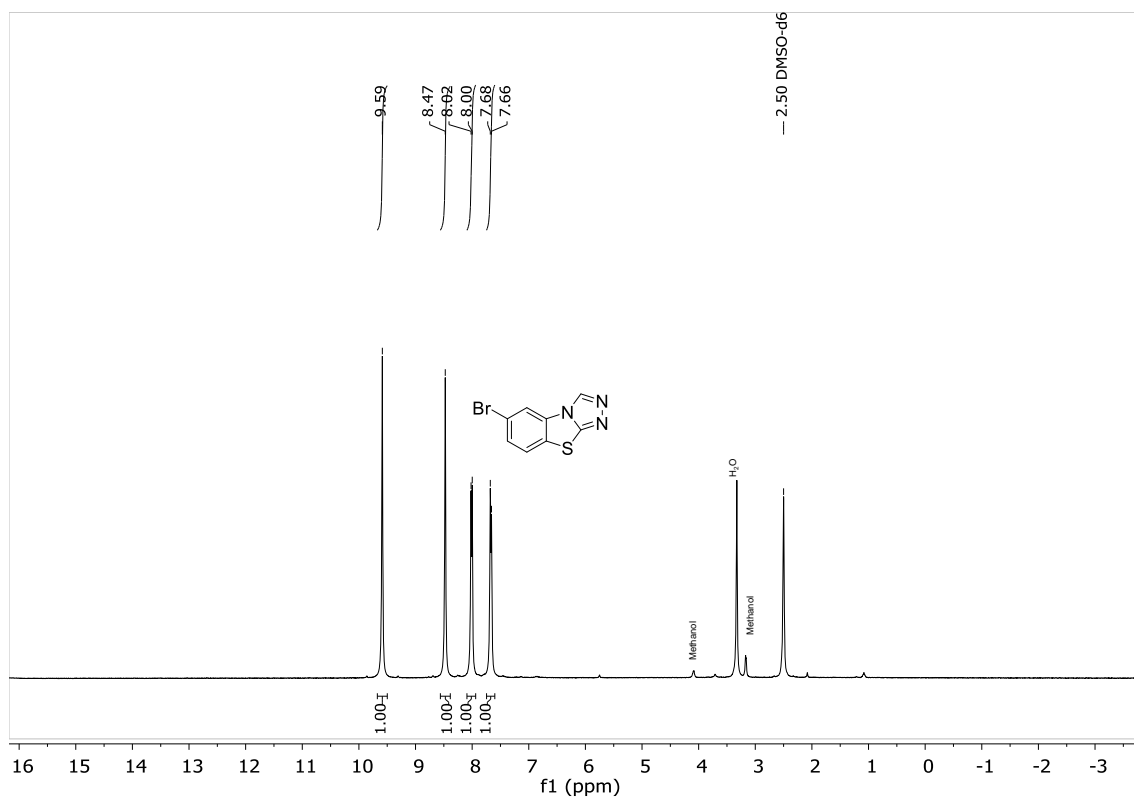
**Figure S157:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole-6-carboxylic acid (**6m**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



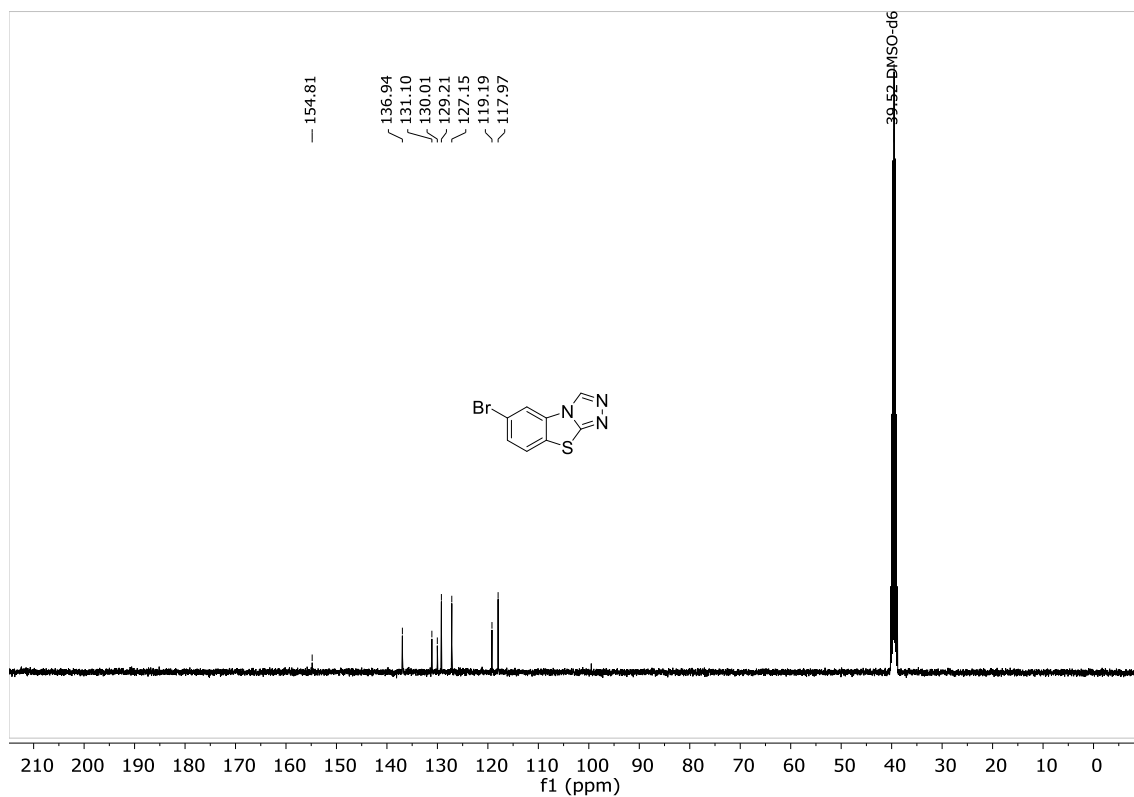
**Figure S158:** <sup>1</sup>H NMR spectrum of ethyl benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole-6-carboxylate (**6m'**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



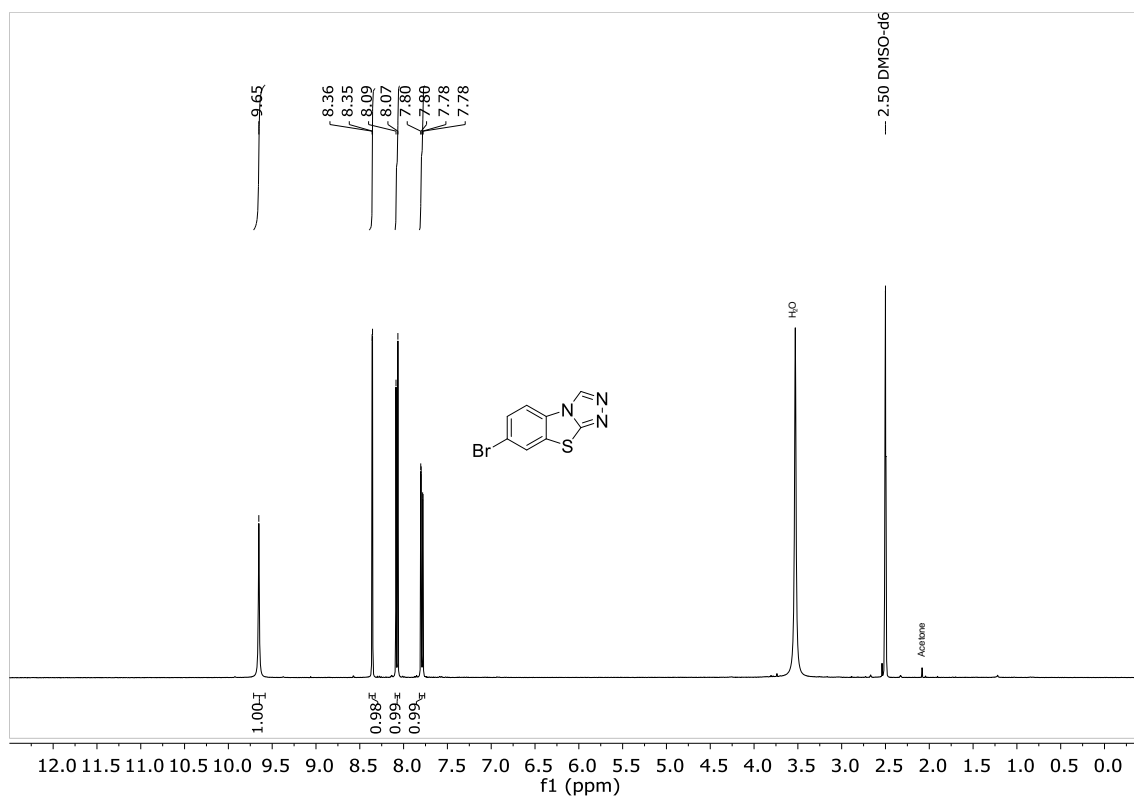
**Figure S159:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of ethyl benzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole-6-carboxylate (**6m**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



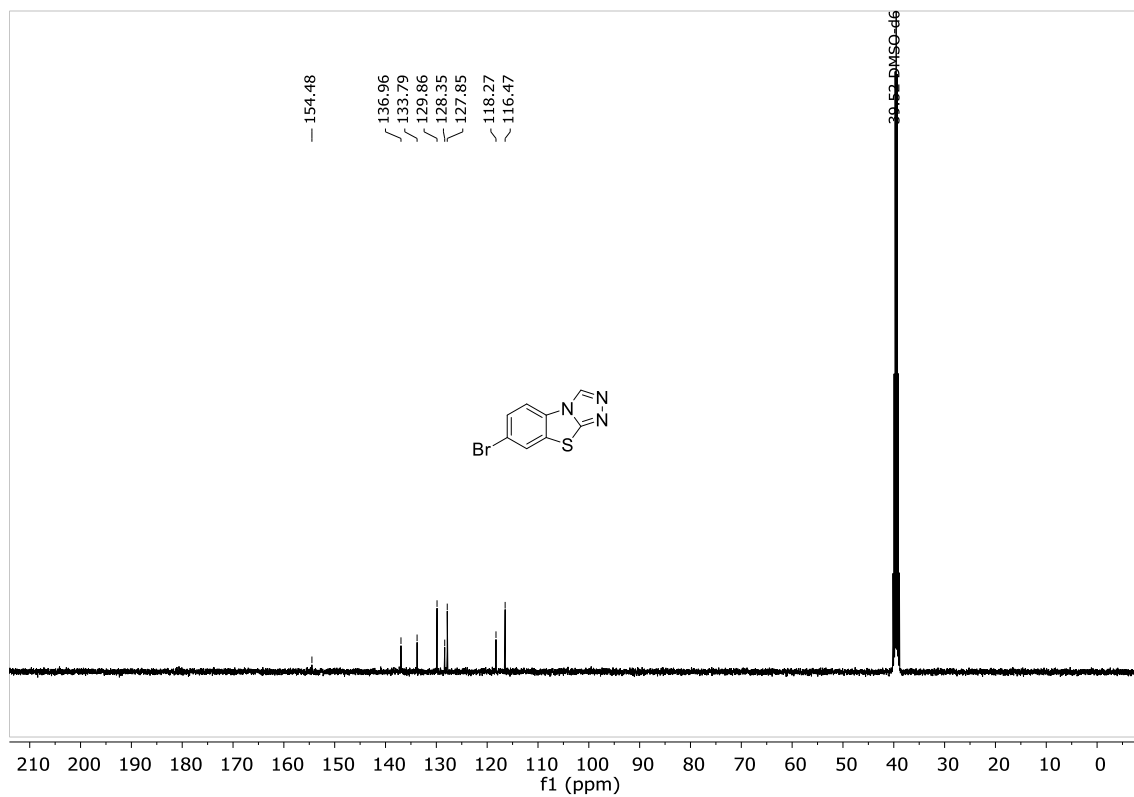
**Figure S160:** <sup>1</sup>H NMR spectrum of 6-bromobenzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (**6n**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



**Figure S161:** <sup>13</sup>C NMR spectrum of 6-bromobenzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (**6n**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).

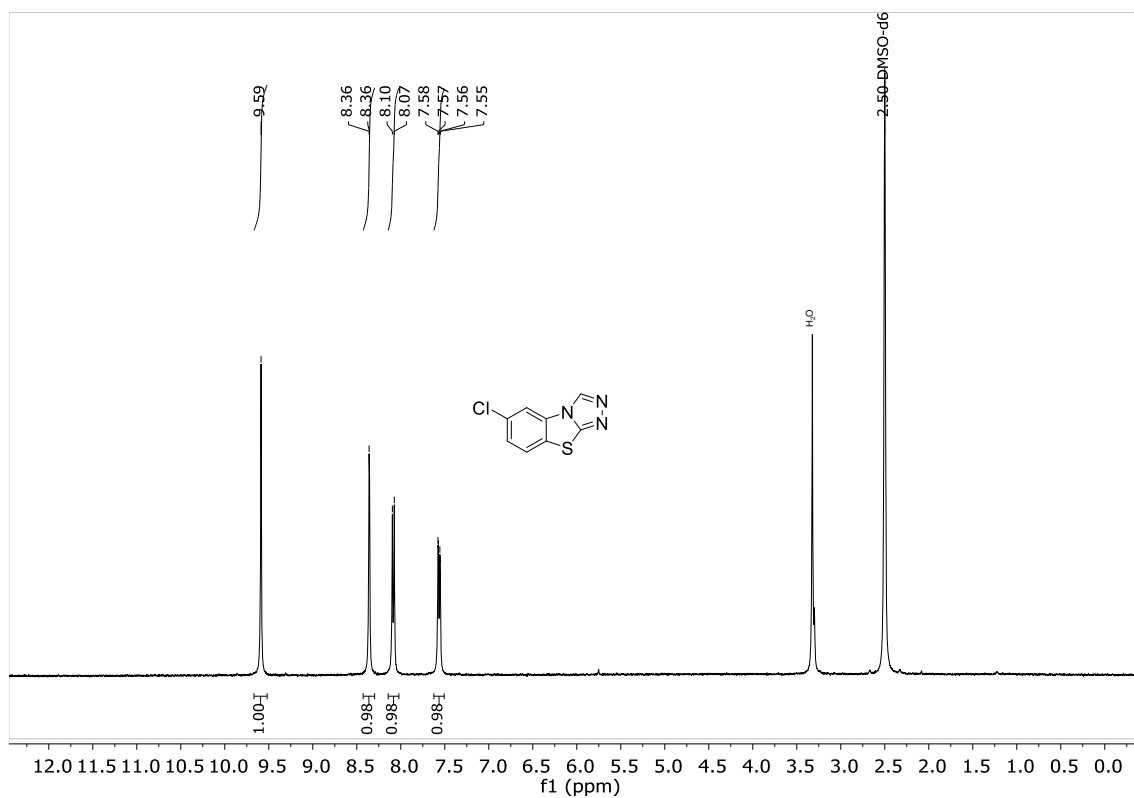


**Figure S162:** <sup>1</sup>H NMR spectrum of 7-bromobenzo[4,5]thiazolo[2,3-c][1,2,4]triazole (**6o**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).

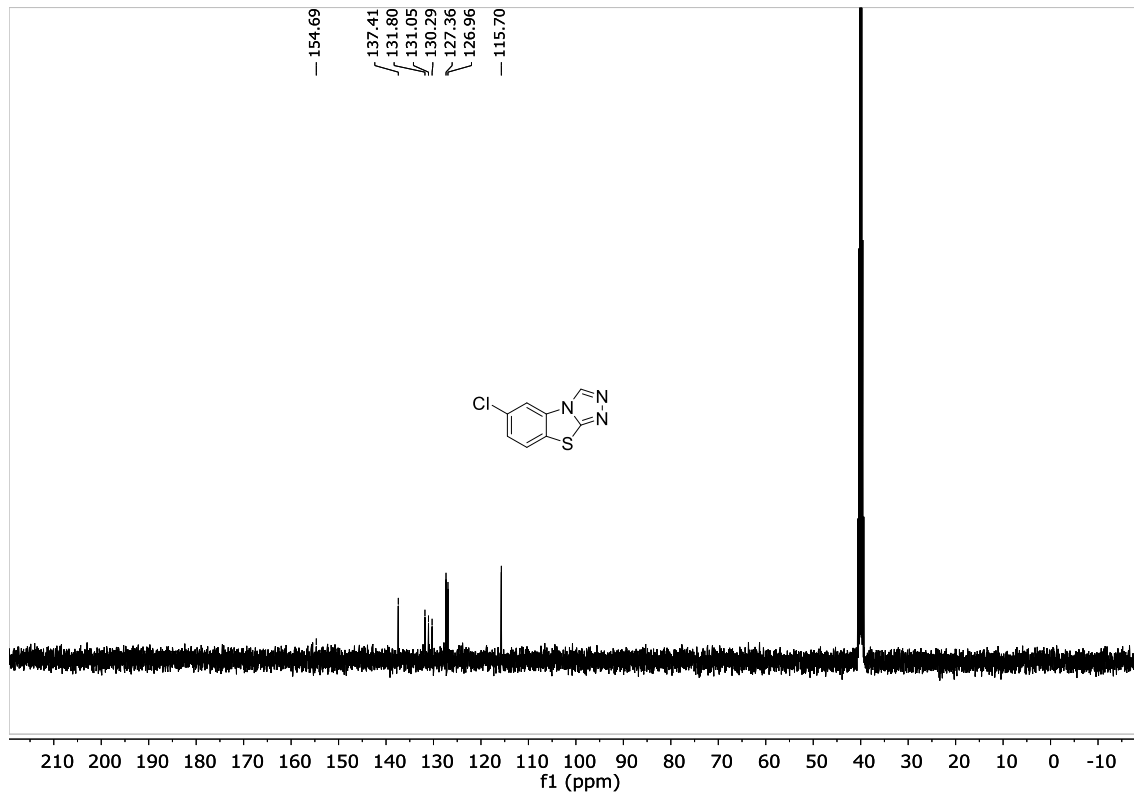


**Figure S163:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 7-bromobenzo[4,5]thiazolo[2,3-c][1,2,4]triazole (**6o**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).

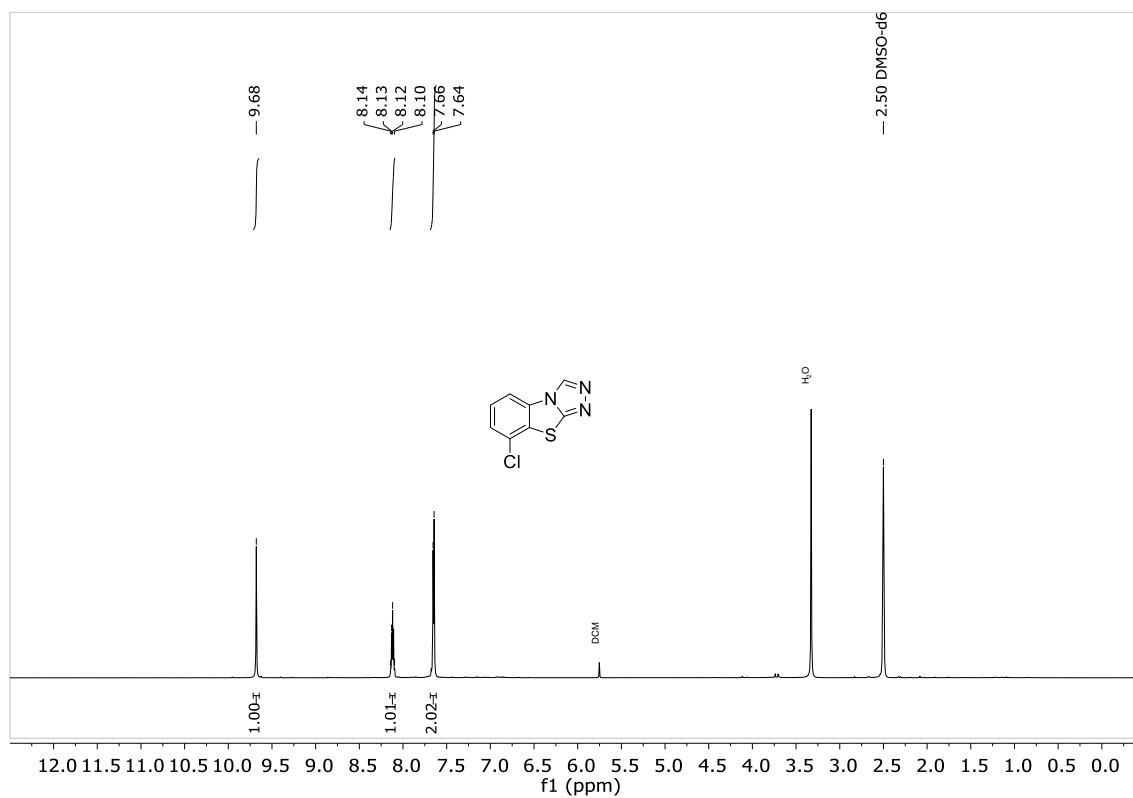




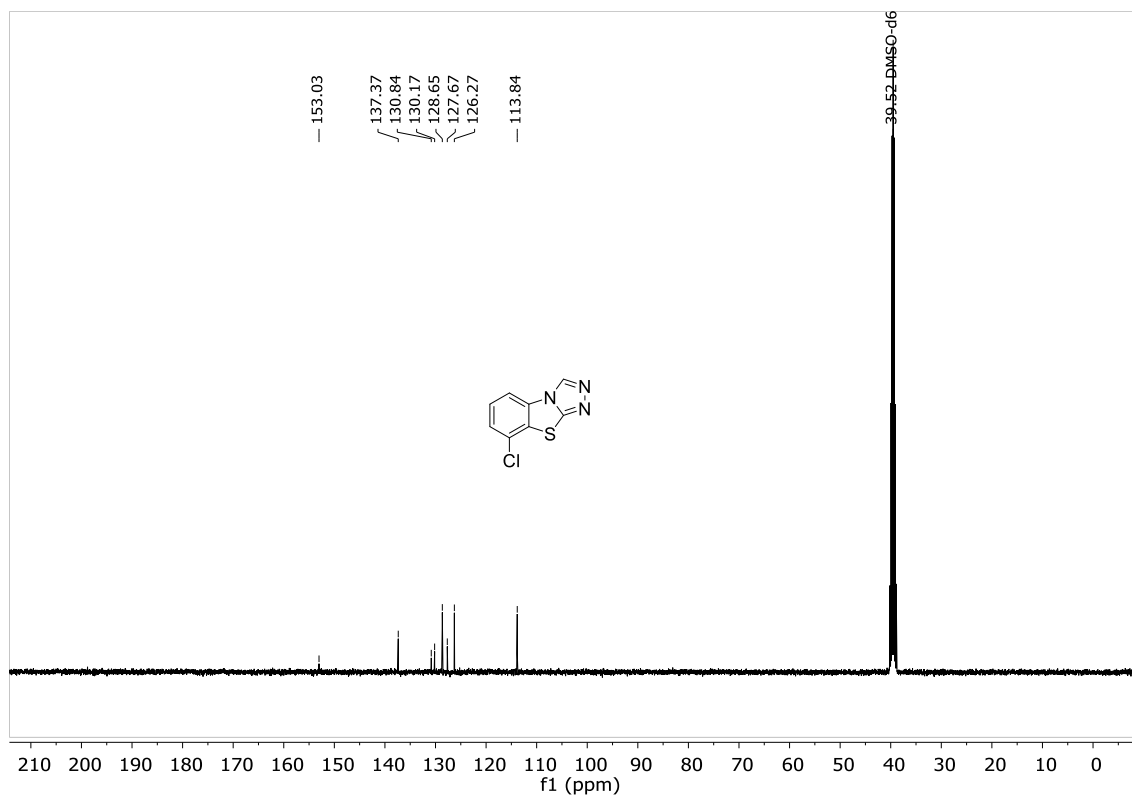
**Figure S164:** <sup>1</sup>H NMR spectrum of 6-chlorobenzo[4,5]thiazolo[2,3-c][1,2,4]triazole (**6p**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



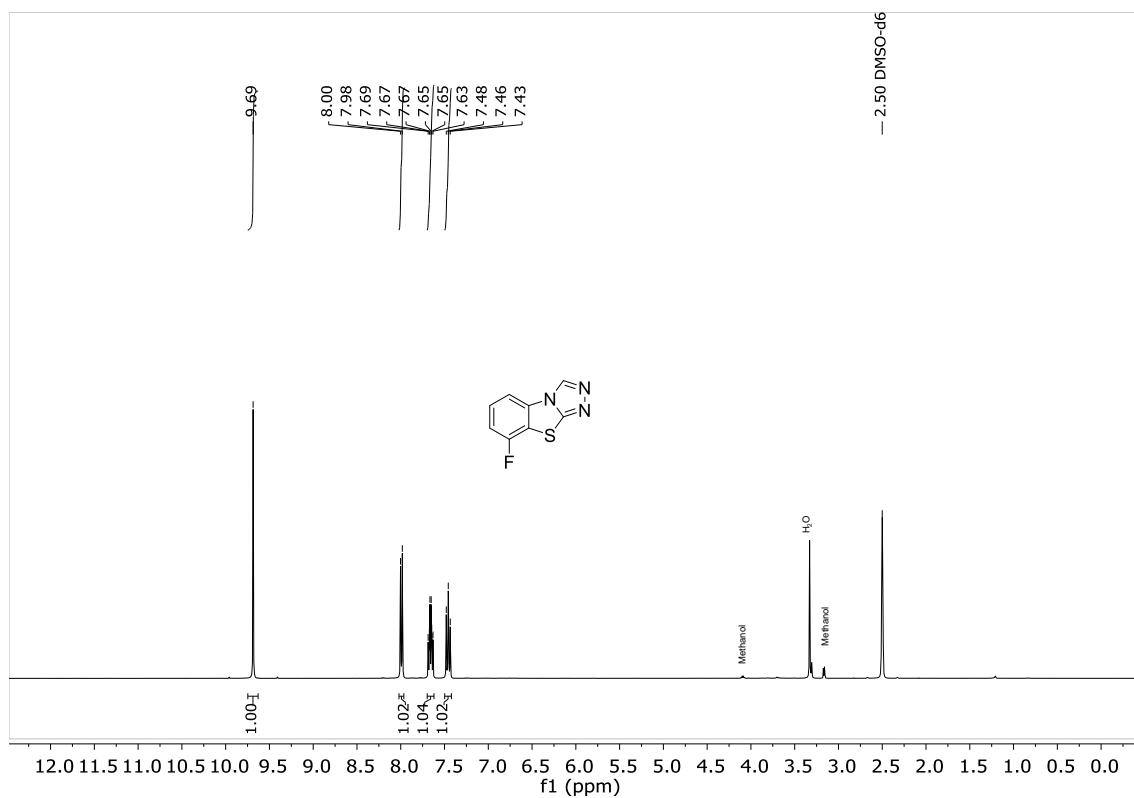
**Figure S165:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 6-chlorobenzo[4,5]thiazolo[2,3-c][1,2,4]triazole (**6p**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



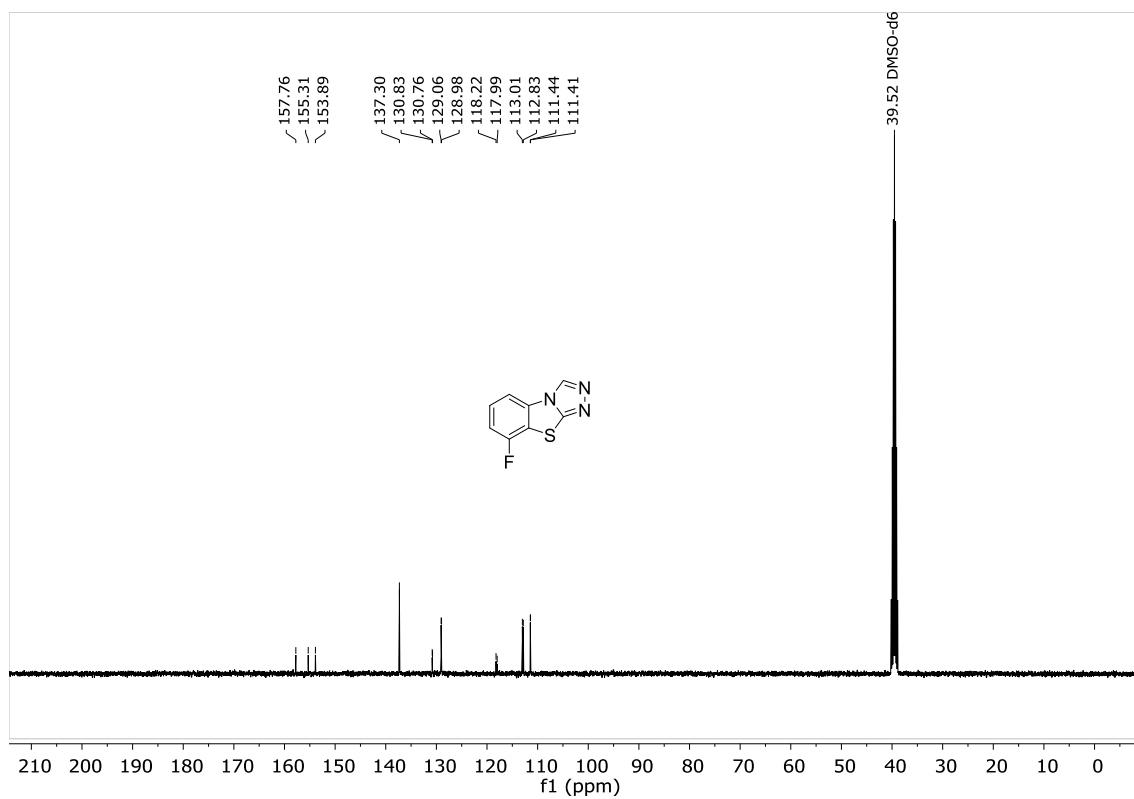
**Figure S166:** <sup>1</sup>H NMR spectrum of 8-chlorobenzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (**6q**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



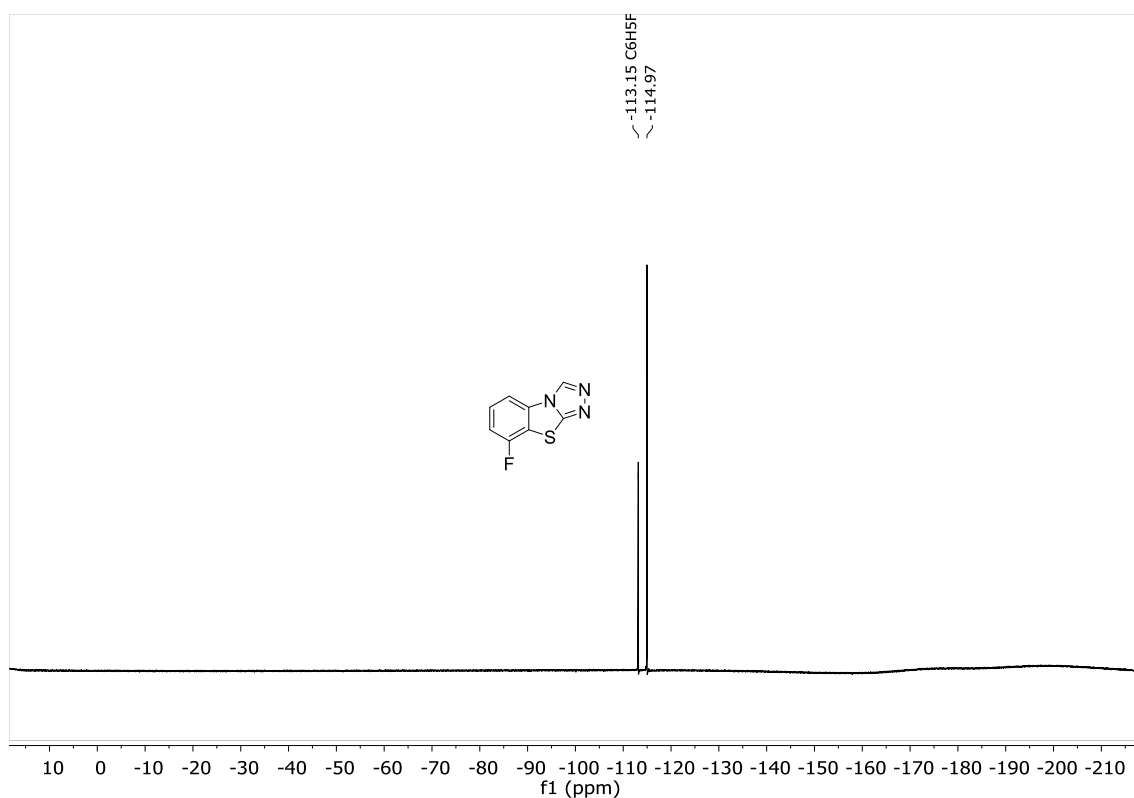
**Figure S167:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 8-chlorobenzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (**6q**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



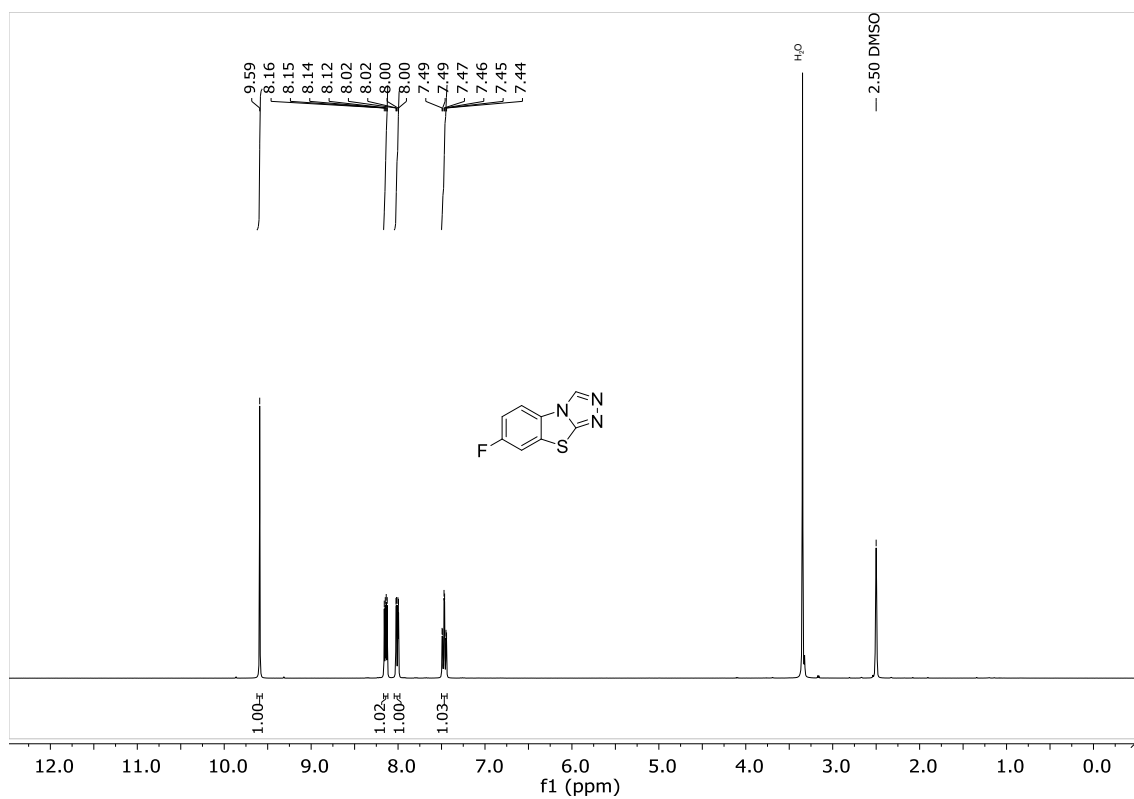
**Figure S168:** <sup>1</sup>H NMR spectrum of 8-fluorobenzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (**6r**) (400 MHz, DMSO-*d*<sub>6</sub>, 298 K).



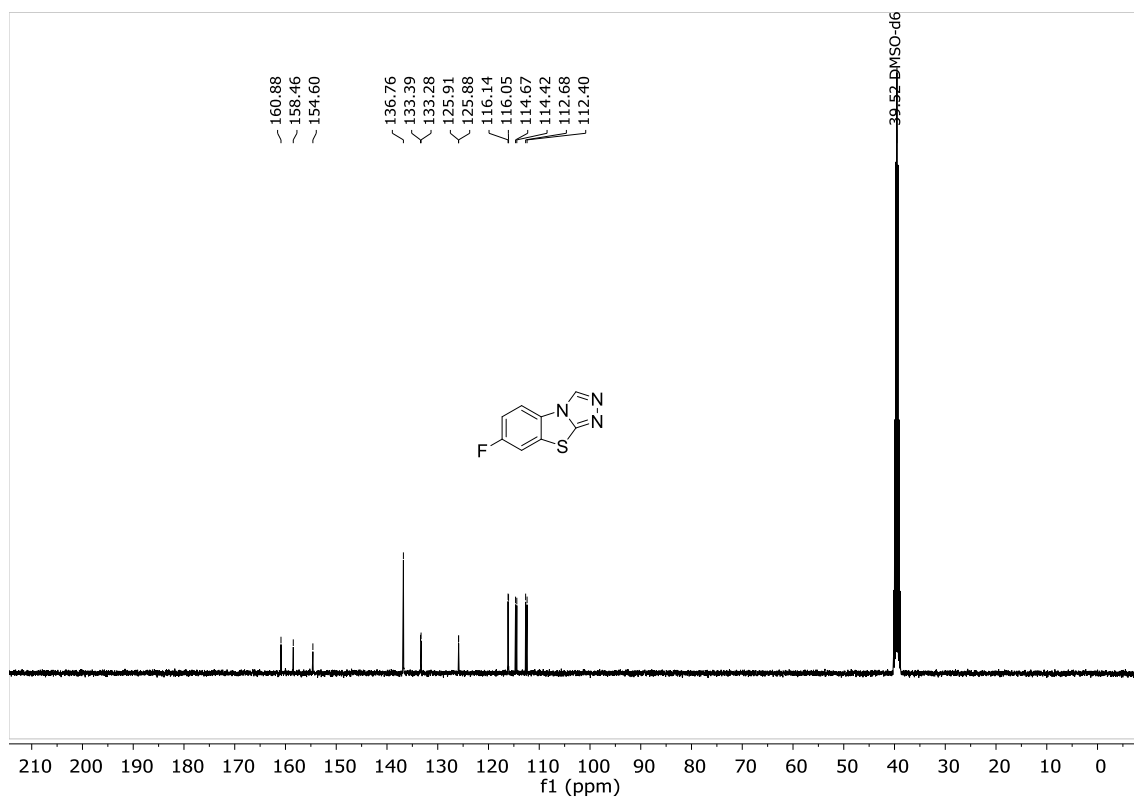
**Figure S169:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 8-fluorobenzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (**6r**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



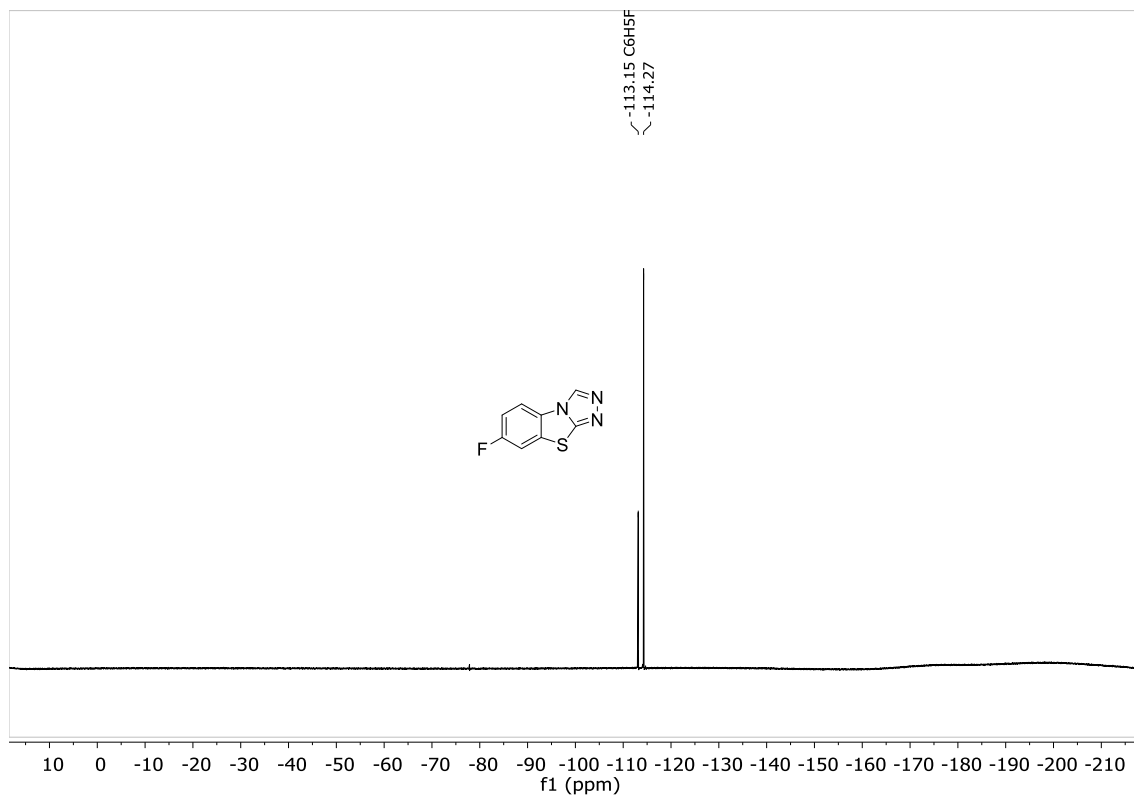
**Figure S170:**  $^{19}\text{F}\{^1\text{H}\}$  NMR spectrum of 8-fluorobenzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (**6r**) (376 MHz, DMSO- $d_6$  298 K, referenced to fluorobenzene).



**Figure S171:**  $^1\text{H}$  NMR spectrum of 7-fluorobenzo[4,5]thiazolo[2,3-*c*][1,2,4]triazole (**6s**) (400 MHz, DMSO- $d_6$ , 298 K).



**Figure S172:** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 7-fluorobenzo[4,5]thiazolo[2,3-c][1,2,4]triazole (**6s**) (100 MHz, DMSO-*d*<sub>6</sub>, 298 K).



**Figure S173:** <sup>19</sup>F{<sup>1</sup>H} NMR spectrum of 7-fluorobenzo[4,5]thiazolo[2,3-c][1,2,4]triazole (**6s**) (376 MHz, DMSO-*d*<sub>6</sub>, 298 K).