



UNIVERSITAT DE  
BARCELONA

***P*-Stereogenic ligands  
with the *tert*-butylmethylphosphine fragment.  
Coordination chemistry and catalysis  
of their organometallic complexes**

Guillem Vázquez Bigas

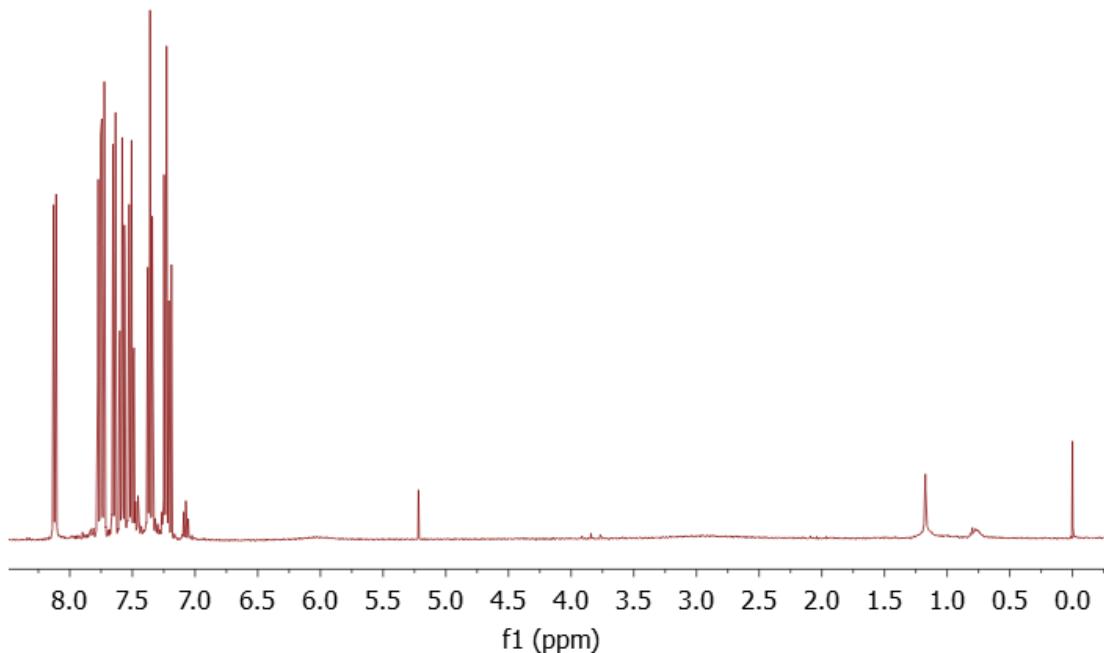
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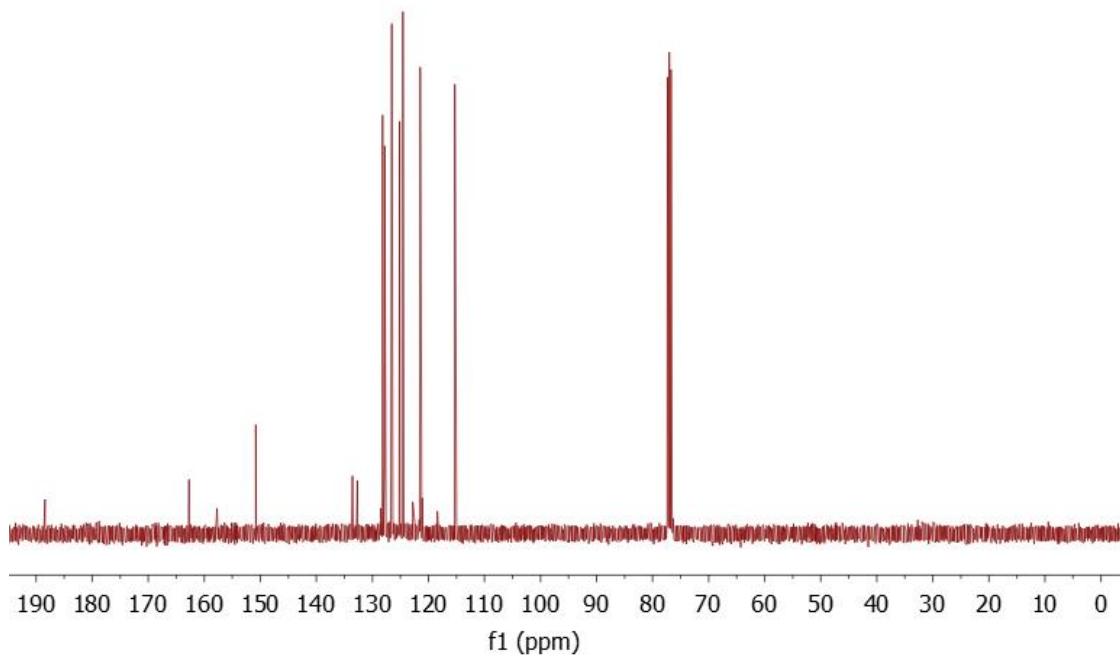
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## Chapter 6: Detection of aggregated A $\beta$ with fluorescent probes

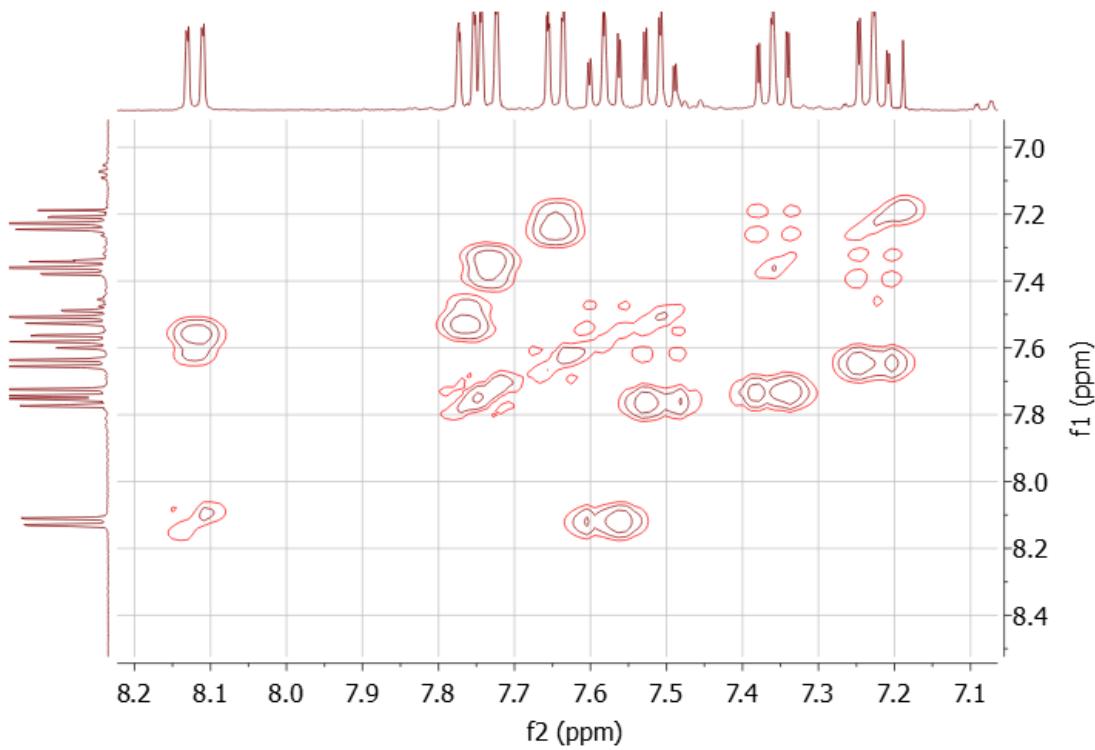
**2-azidobenzo[*d*]thiazole / benzo[4,5]thiazolo[3,2-*d*]tetrazole**



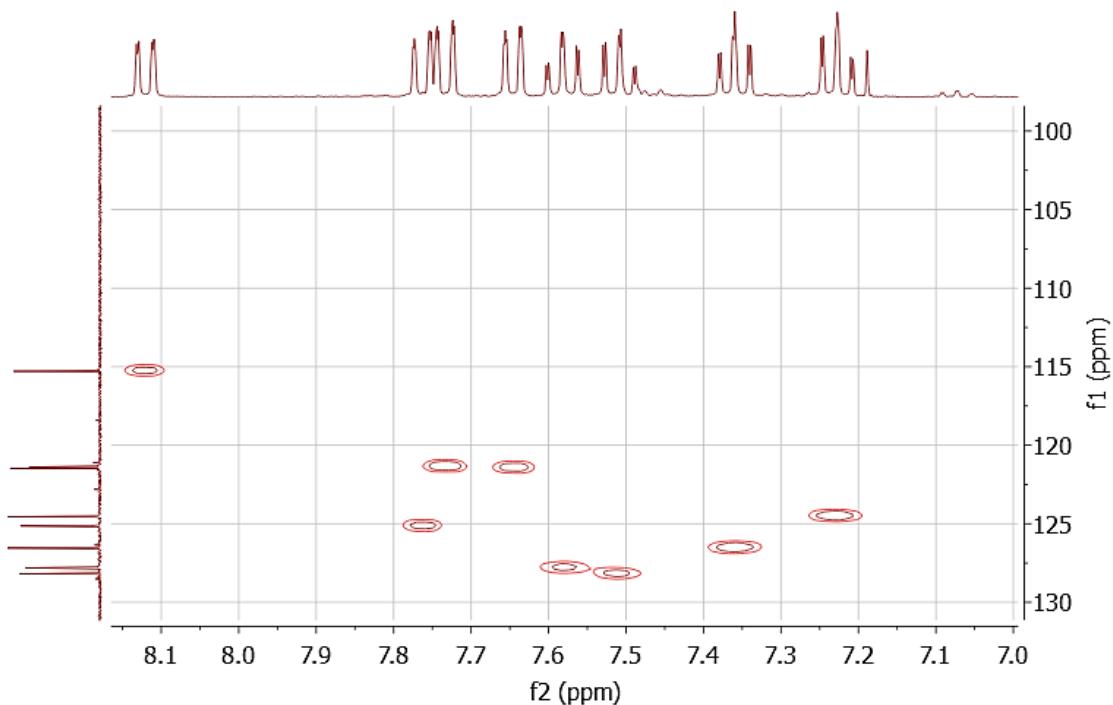
**Figure S6.1:**  $^1\text{H}$  NMR spectrum of 2-azidobenzo[*d*]thiazole / benzo[4,5]thiazolo[3,2-*d*]tetrazole in  $\text{CDCl}_3$ .



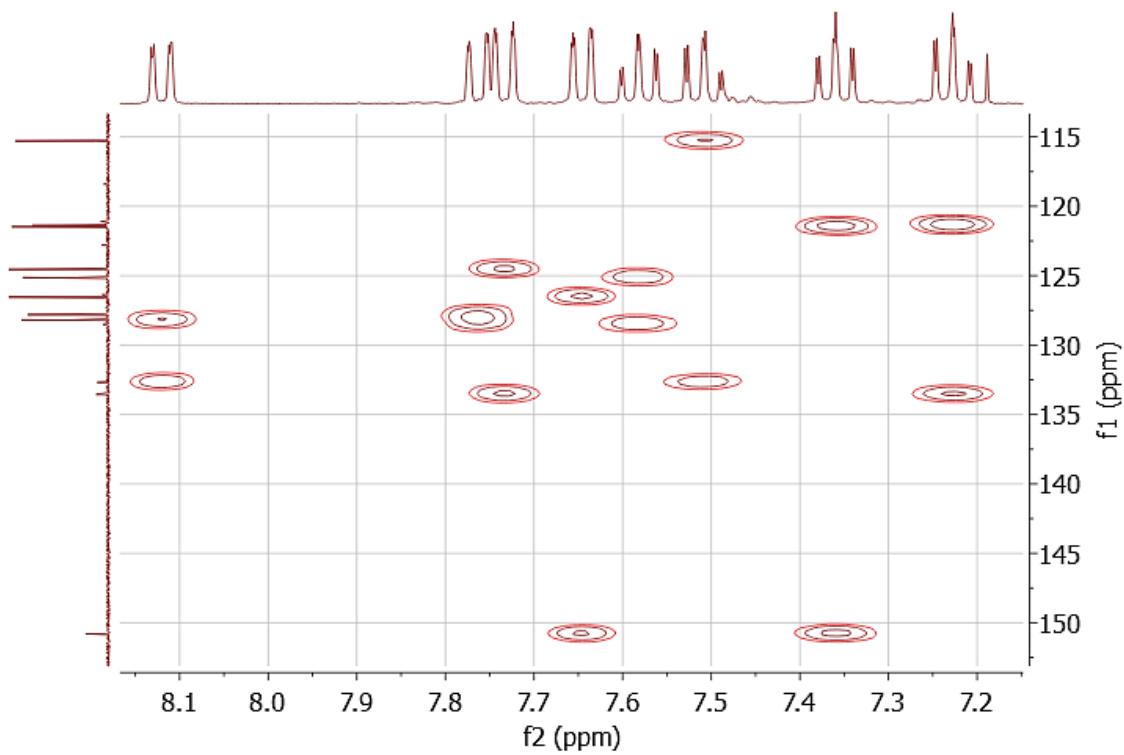
**Figure S6.2:**  $^{13}\text{C}$  NMR spectrum of 2-azidobenzo[*d*]thiazole / benzo[4,5]thiazolo[3,2-*d*]tetrazole in  $\text{CDCl}_3$ .



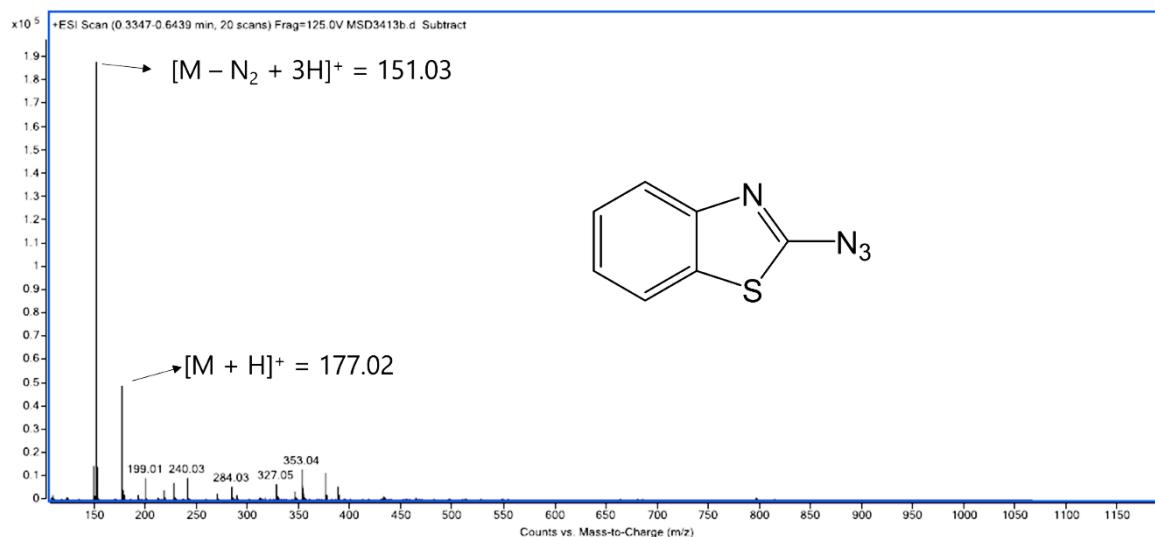
**Figure S6.3:** COSY NMR spectrum of 2-azidobenzo[*d*]thiazole / benzo[4,5]thiazolo[3,2-*d*]tetrazole in CDCl<sub>3</sub>.



**Figure S6.4:** HSQC NMR spectrum of 2-azidobenzo[*d*]thiazole / benzo[4,5]thiazolo[3,2-*d*]tetrazole in CDCl<sub>3</sub>.

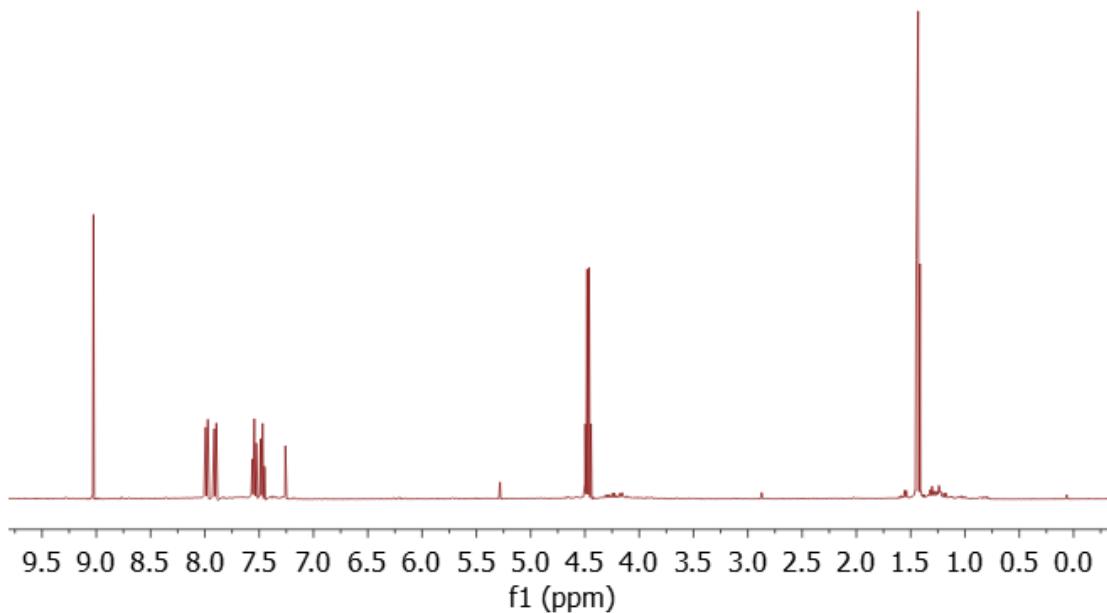


**Figure S6.5:** HMBC NMR spectrum of 2-azidobenzo[*d*]thiazole / benzo[4,5]thiazolo[3,2-*d*]tetrazole in  $\text{CDCl}_3$ .

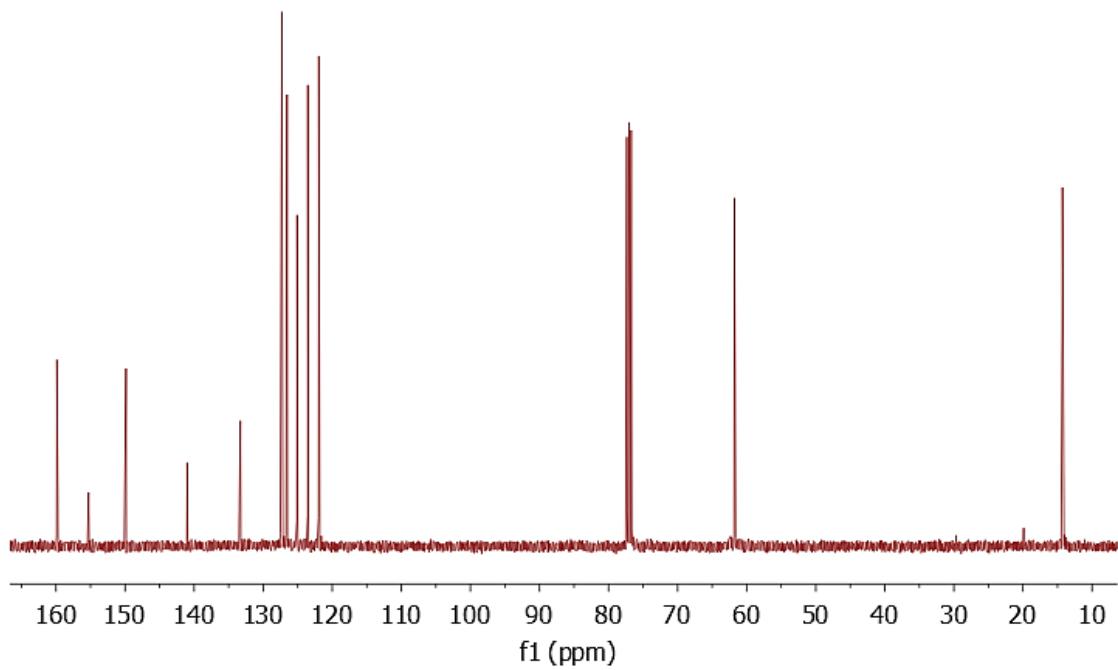


**Figure S6.6:** ESI mass spectrum of 2-azidobenzo[*d*]thiazole / benzo[4,5]thiazolo[3,2-*d*]tetrazole.

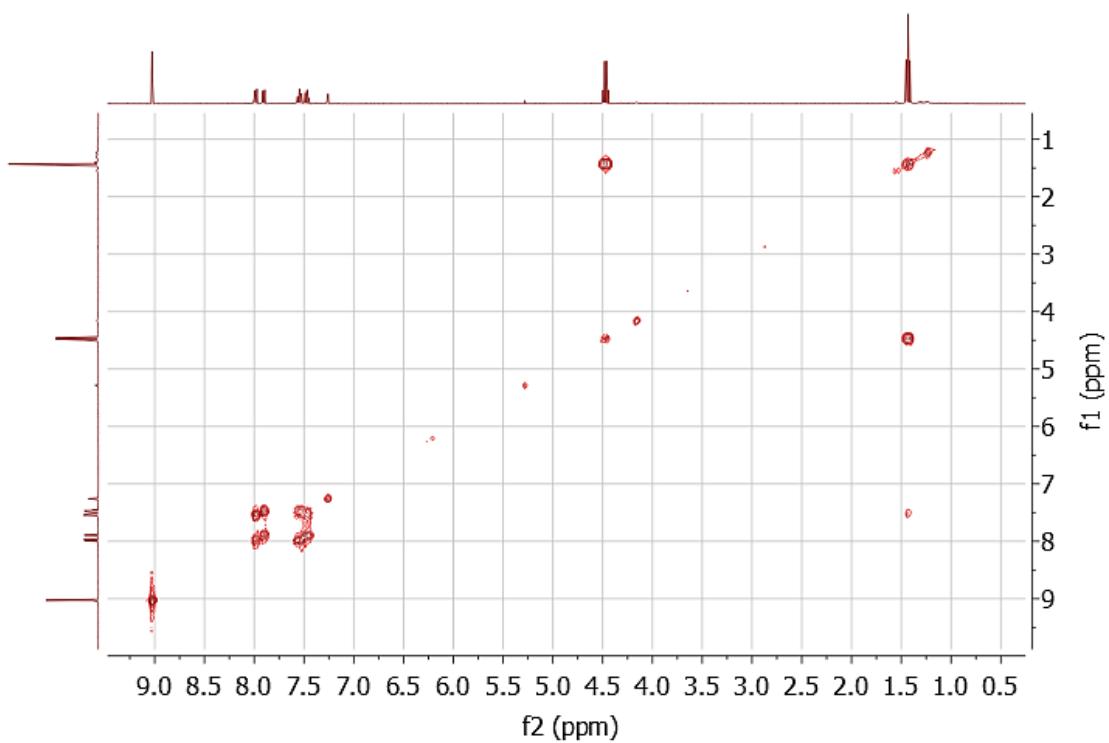
**Ethyl-1-(benzo[d]thiazol-2-yl)-1H-1,2,3-triazole-4-carboxylate**



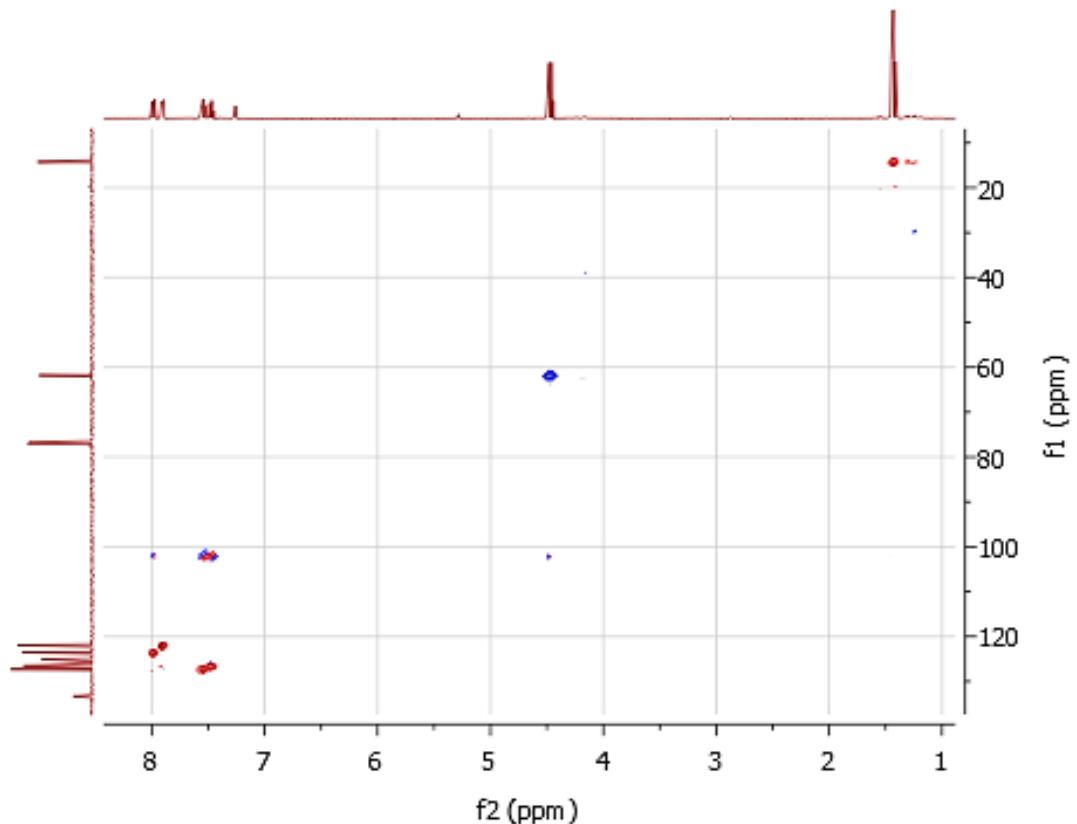
**Figure S6.7:** <sup>1</sup>H NMR spectrum of ethyl-1-(benzo[d]thiazol-2-yl)-1H-1,2,3-triazole-4-carboxylate in CDCl<sub>3</sub>.



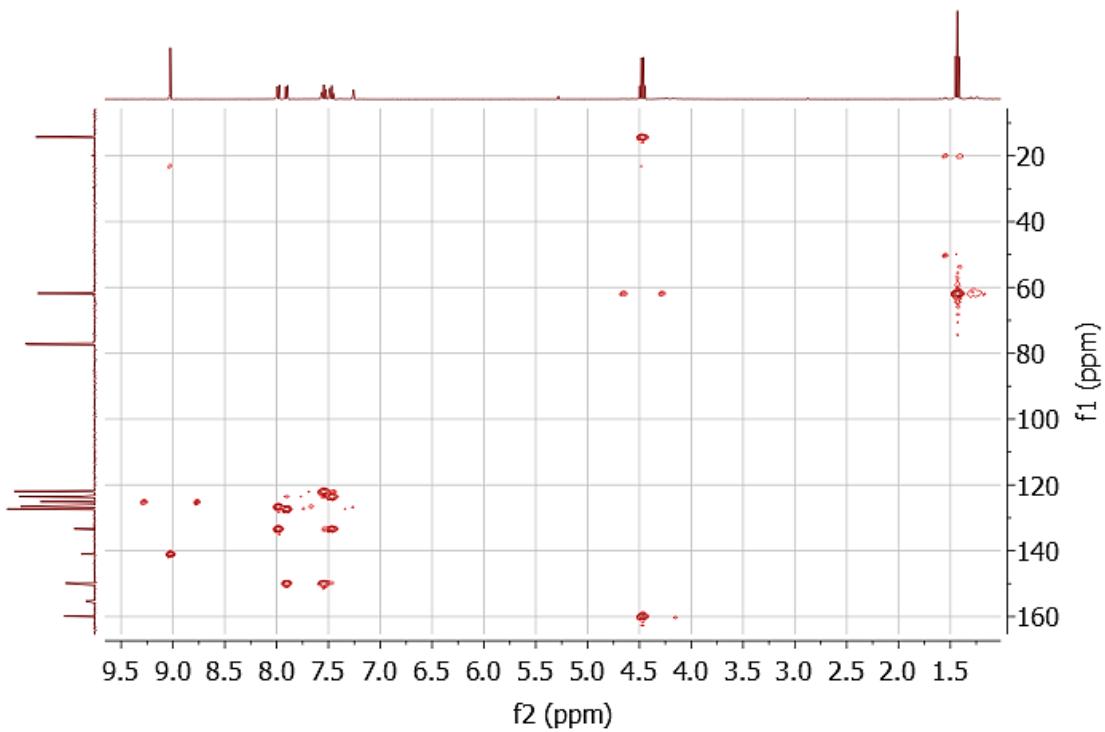
**Figure S6.8:** <sup>13</sup>C NMR spectrum of ethyl-1-(benzo[d]thiazol-2-yl)-1H-1,2,3-triazole-4-carboxylate in CDCl<sub>3</sub>.



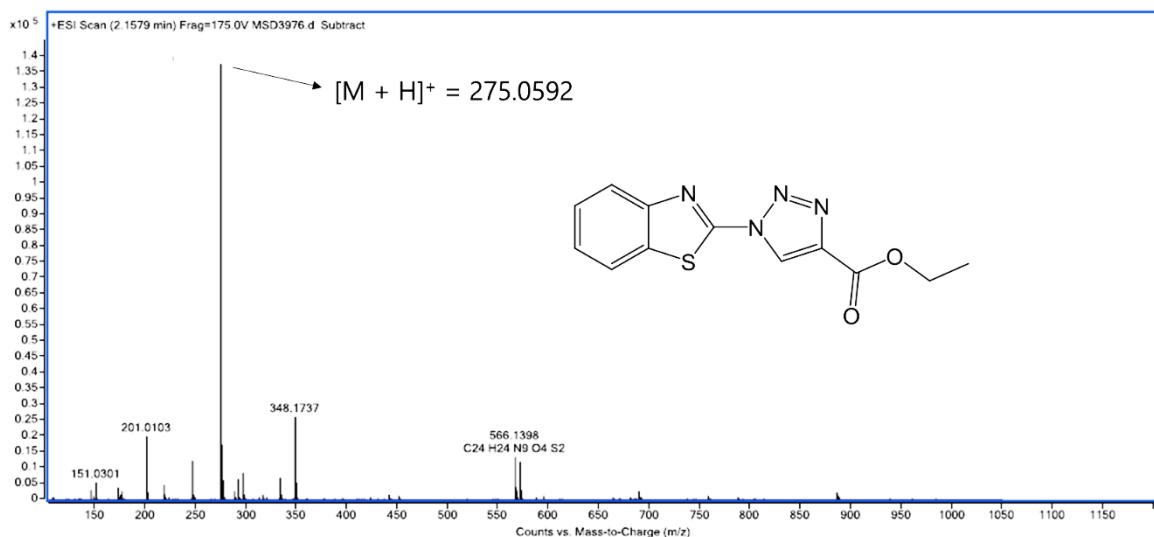
**Figure S6.9:** COSY NMR spectrum of ethyl-1-(benzo[d]thiazol-2-yl)-1H-1,2,3-triazole-4-carboxylate in  $\text{CDCl}_3$ .



**Figure S6.10:** HSQC NMR spectrum of ethyl-1-(benzo[d]thiazol-2-yl)-1H-1,2,3-triazole-4-carboxylate in  $\text{CDCl}_3$ .

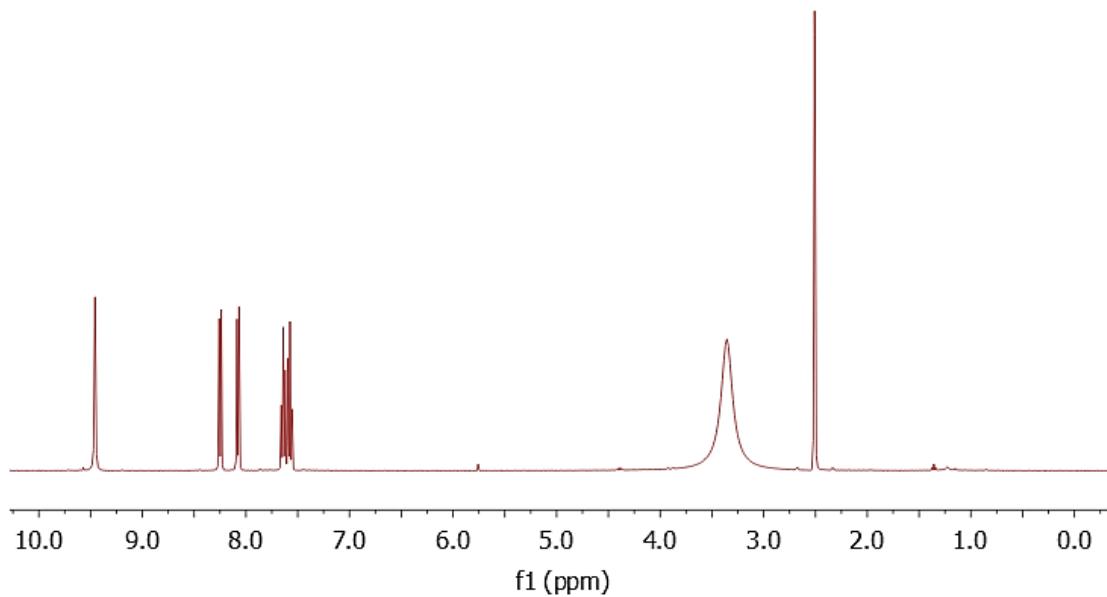


**Figure S6.11:** HMBC NMR spectrum of ethyl-1-(benzo[d]thiazol-2-yl)-1H-1,2,3-triazole-4-carboxylate in  $\text{CDCl}_3$ .

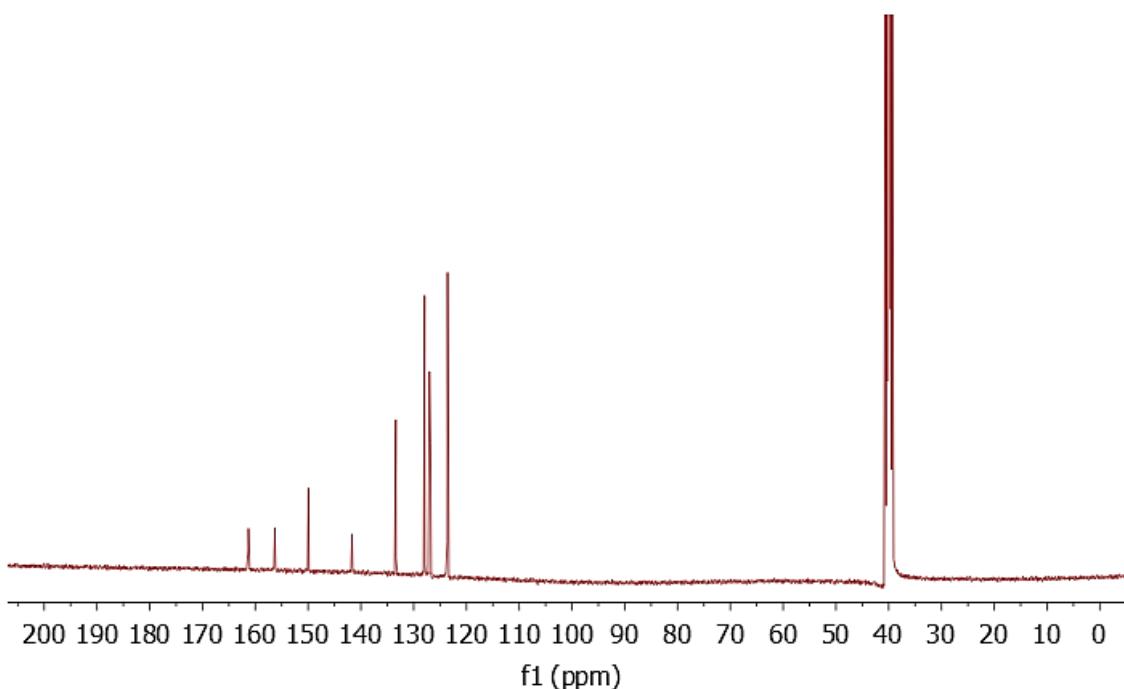


**Figure S6.12:** ESI mass spectrum of ethyl-1-(benzo[d]thiazol-2-yl)-1H-1,2,3-triazole-4-carboxylate.

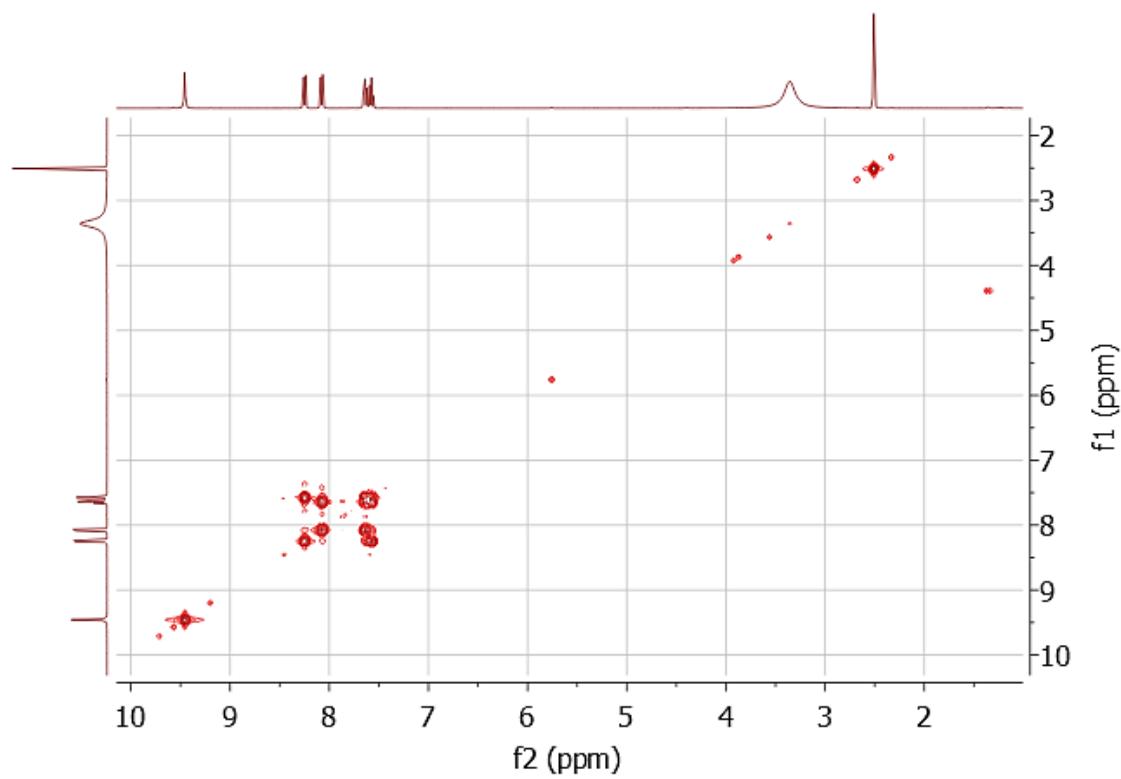
**1-(benzo[d]thiazol-2-yl)-1*H*-1,2,3-triazole-4-carboxylic acid (BzTz)**



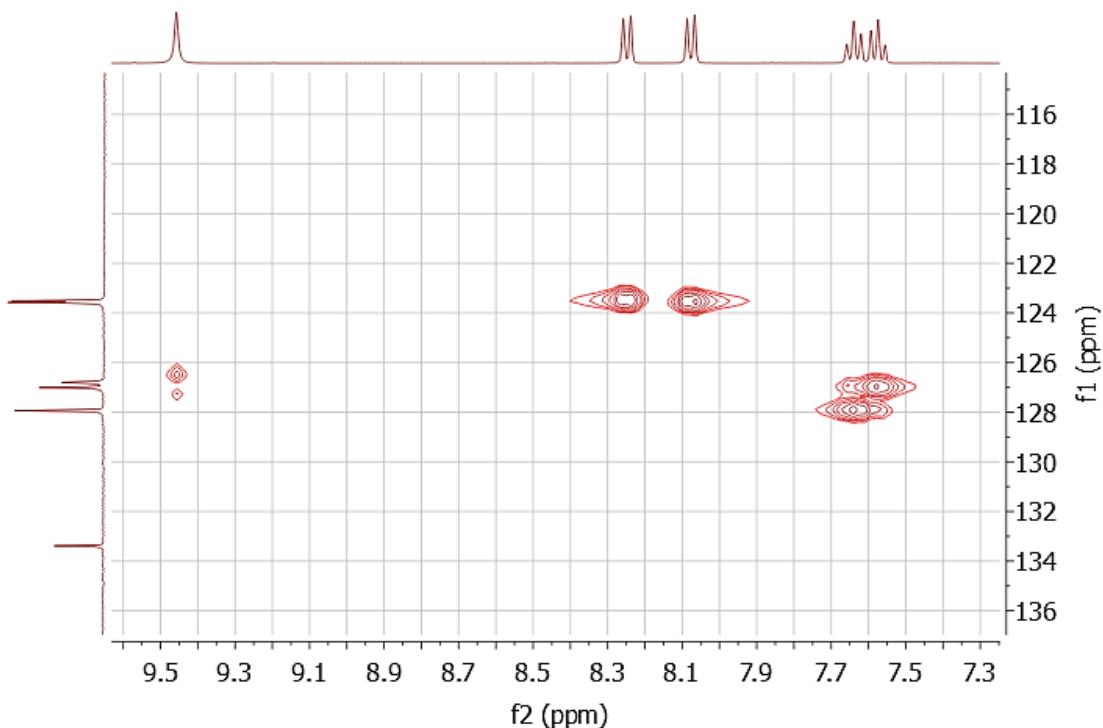
**Figure S6.13:** <sup>1</sup>H NMR spectrum of 1-(benzo[d]thiazol-2-yl)-1*H*-1,2,3-triazole-4-carboxylic acid (BzTz) in DMSO-d<sub>6</sub>.



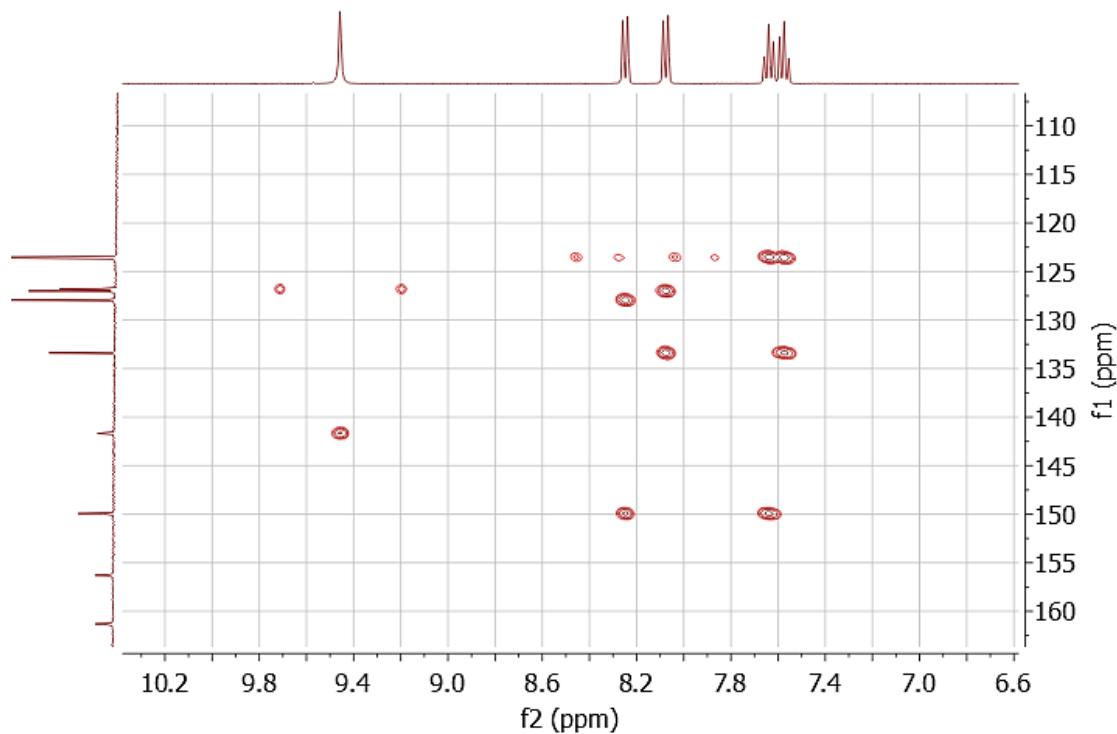
**Figure S6.14:** <sup>13</sup>C NMR spectrum of 1-(benzo[d]thiazol-2-yl)-1*H*-1,2,3-triazole-4-carboxylic acid (BzTz) in DMSO-d<sub>6</sub>.



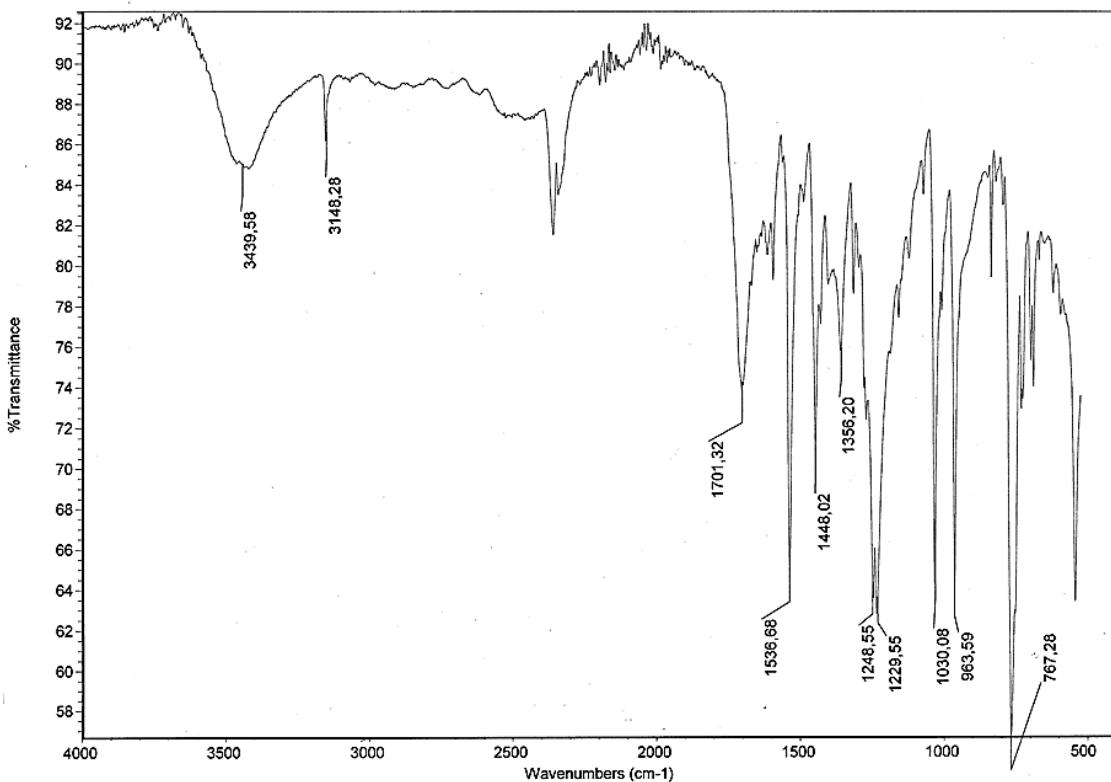
**Figure S6.15:** COSY NMR spectrum of 1-(benzo[*d*]thiazol-2-yl)-1*H*-1,2,3-triazole-4-carboxylic acid (BzTz) in DMSO-d<sub>6</sub>.



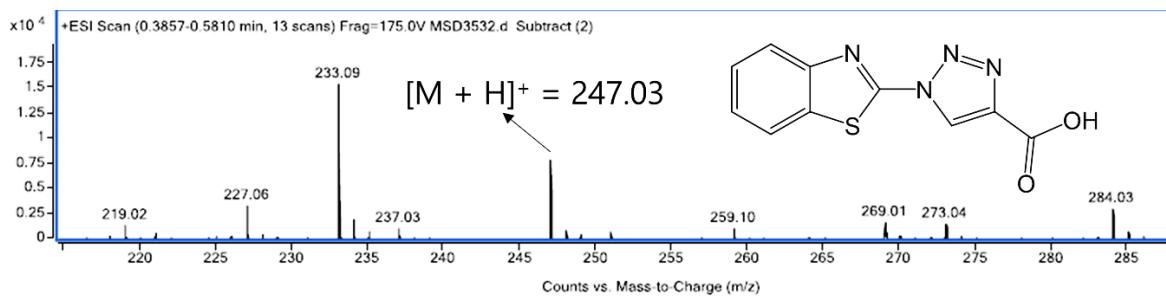
**Figure S6.16:** HSQC NMR spectrum of 1-(benzo[*d*]thiazol-2-yl)-1*H*-1,2,3-triazole-4-carboxylic acid (BzTz) in DMSO-d<sub>6</sub>.



**Figure S6.17:** HMBC NMR spectrum of 1-(benzo[*d*]thiazol-2-yl)-1*H*-1,2,3-triazole-4-carboxylic acid (BzTz) in DMSO-d<sub>6</sub>.

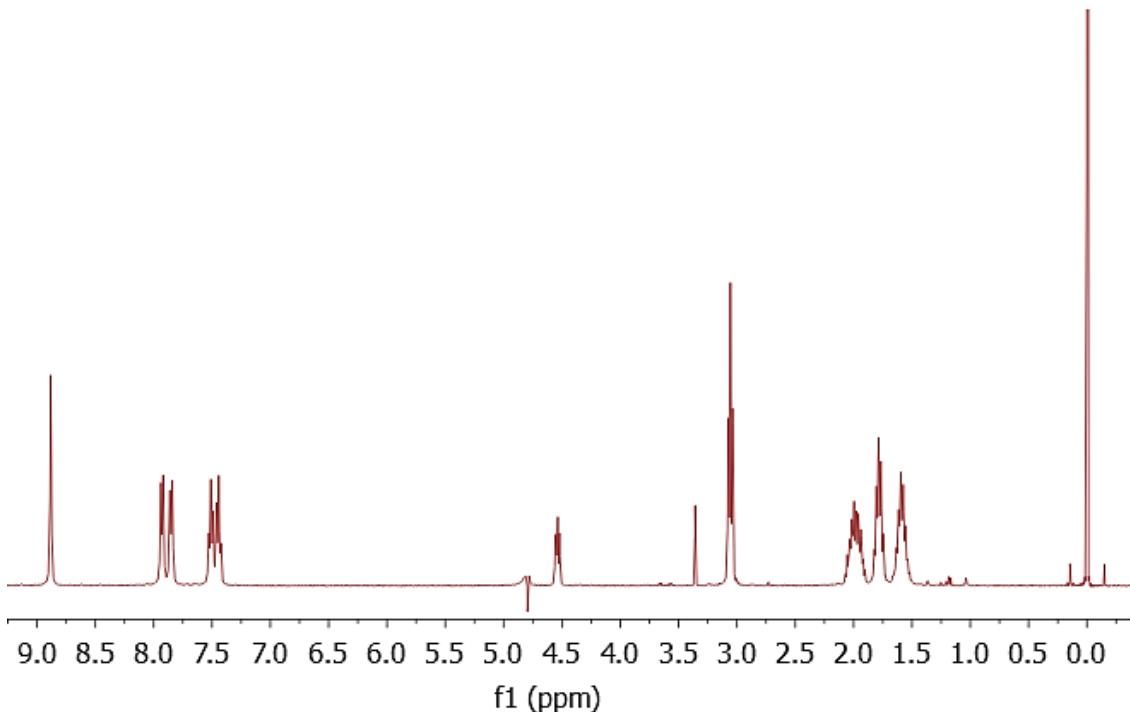


**Figure S6.18:** IR spectrum of 1-(benzo[*d*]thiazol-2-yl)-1*H*-1,2,3-triazole-4-carboxylic acid (BzTz).

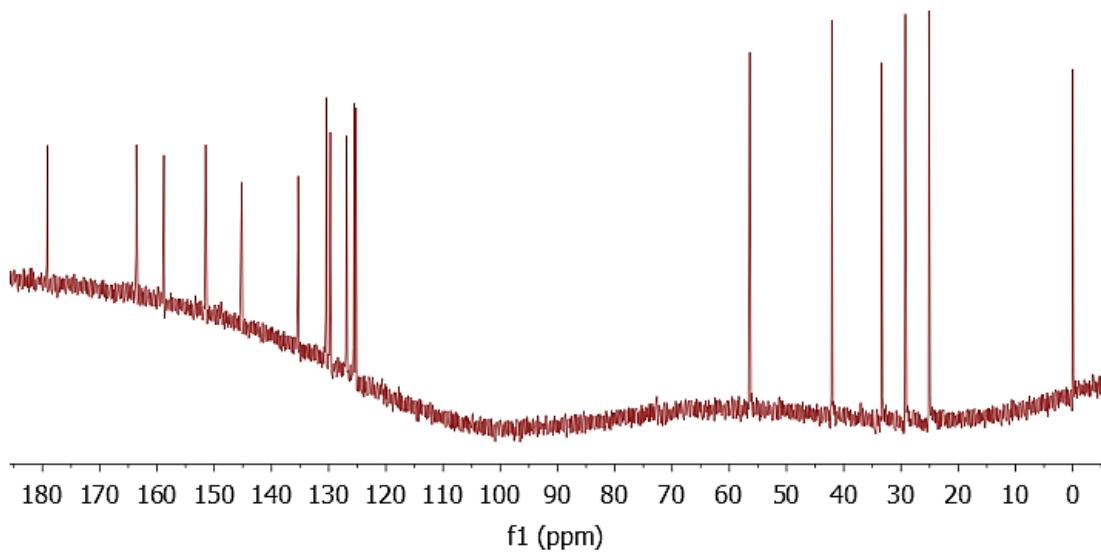


**Figure S6.19:** ESI mass spectrum of 1-(benzo[*d*]thiazol-2-yl)-1*H*-1,2,3-triazole-4-carboxylic acid (BzTz).

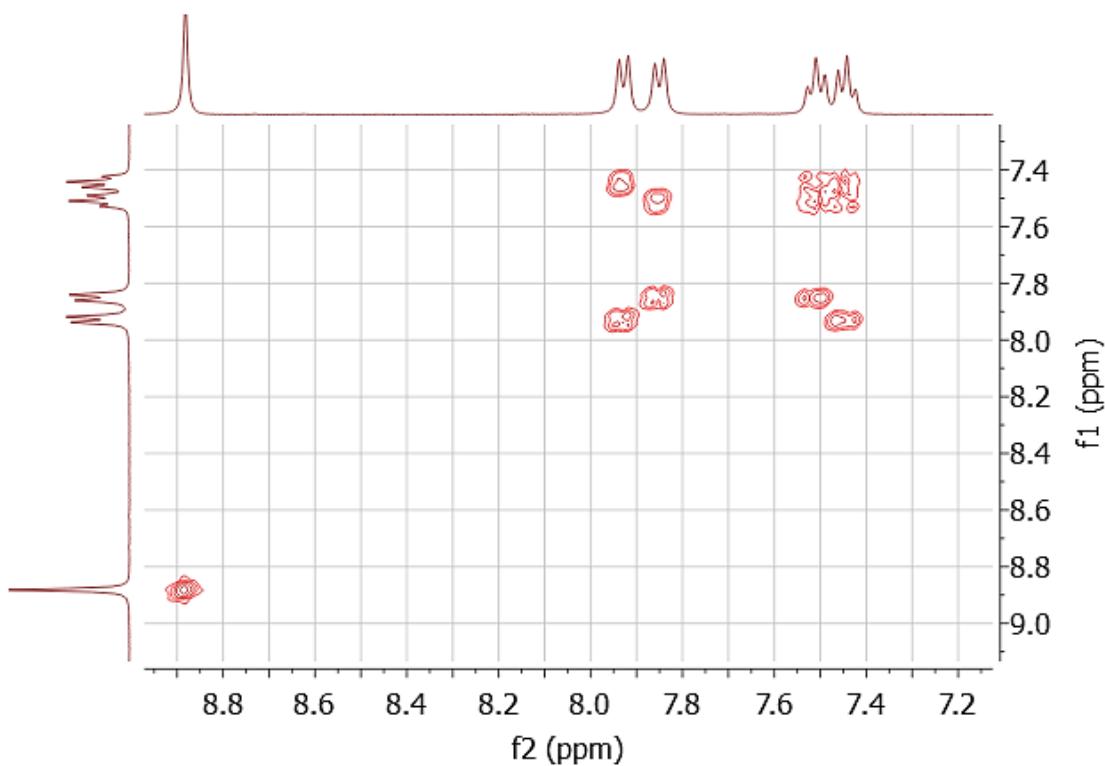
**BzTz-Lys-NH<sub>2</sub>**



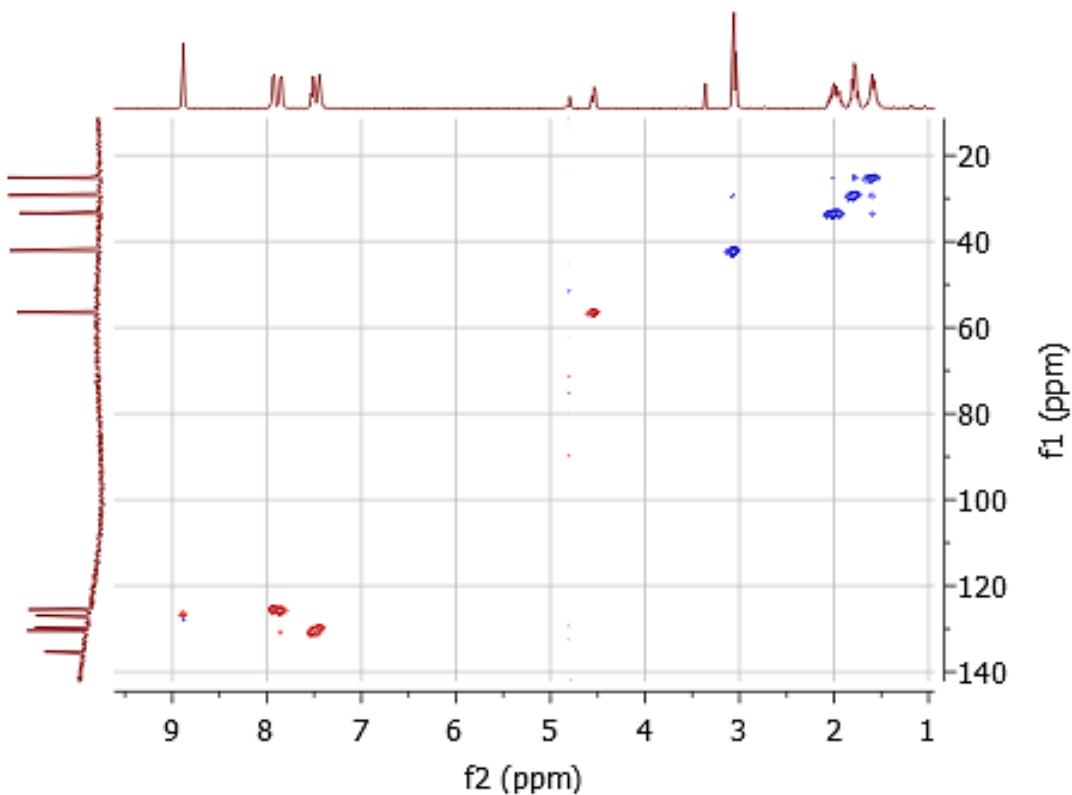
**Figure S6.20:**  $^1\text{H}$  NMR spectrum of BzTz-Lys-NH<sub>2</sub> in D<sub>2</sub>O (pH 7.4).



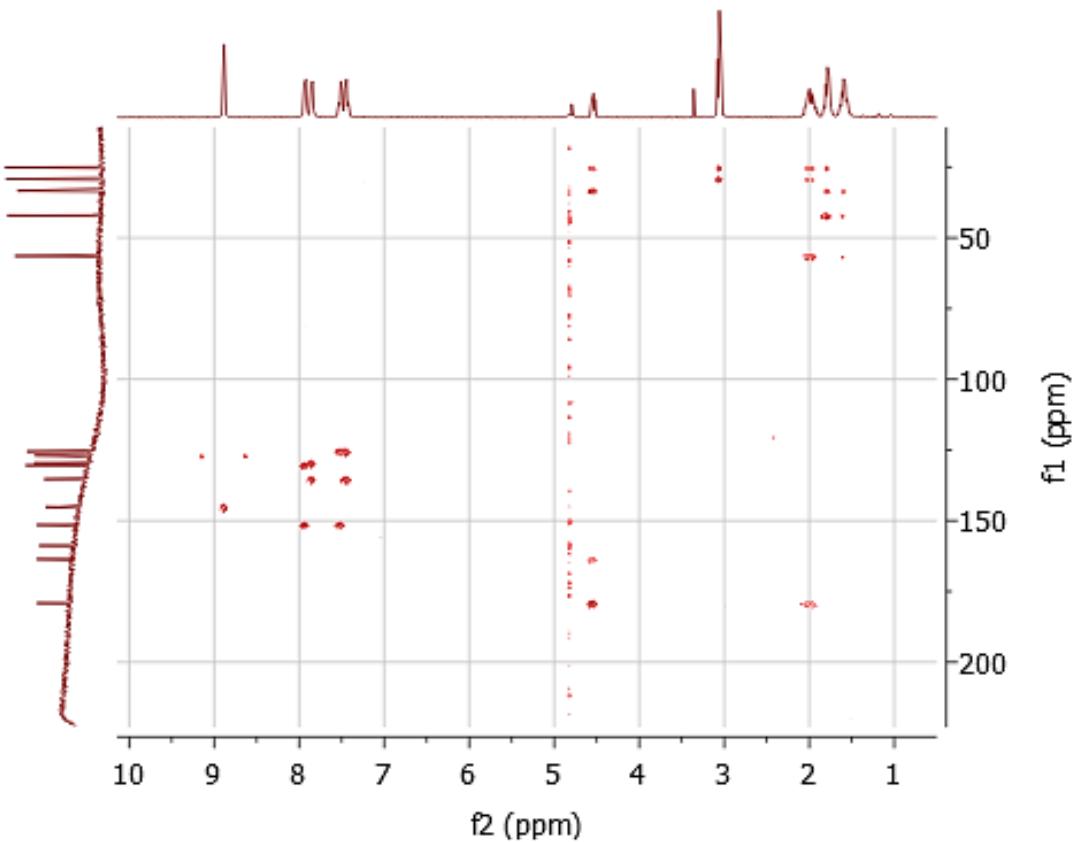
**Figure S6.21:**  $^{13}\text{C}$  NMR spectrum of BzTz-Lys-NH<sub>2</sub> in D<sub>2</sub>O (pH 7.4).



**Figure S6.22:** COSY NMR spectrum of BzTz-Lys-NH<sub>2</sub> in D<sub>2</sub>O (pH 7.4).



**Figure S6.23:** HSQC NMR spectrum of BzTz-Lys-NH<sub>2</sub> in D<sub>2</sub>O (pH 7.4).



**Figure S6.24:** HMBC NMR spectrum of BzTz-Lys-NH<sub>2</sub> in D<sub>2</sub>O (pH 7.4).