

## SUPPLEMENTARY MATERIAL

# N-Substituted 2-(benzenosulfonyl)-1-carbotioamide derivatives exert antimicrobial and cytotoxic effects via aldehyde dehydrogenase pathway; synthesis, *in silico* and *in vitro* studies

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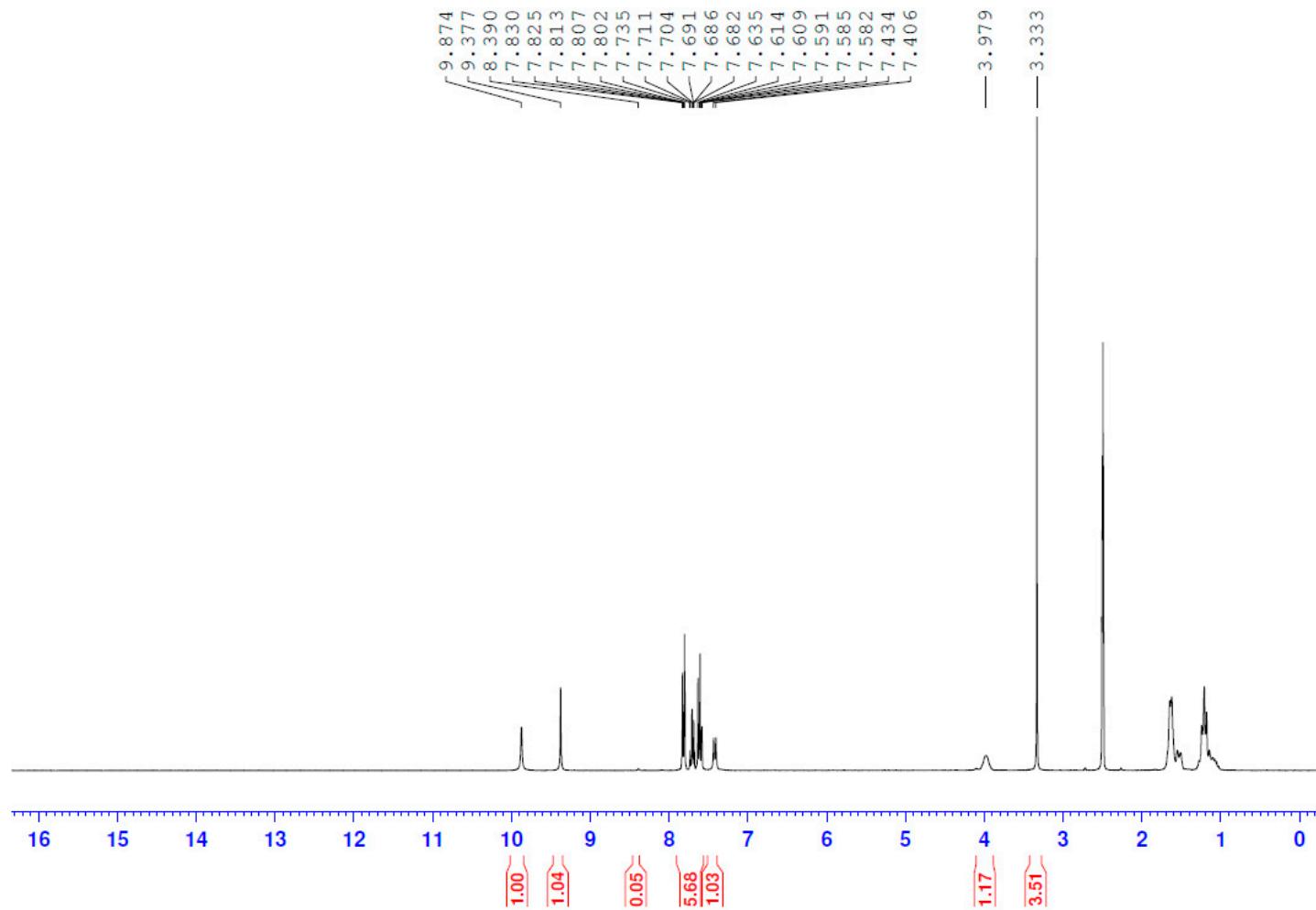
<sup>5</sup> Department of Molecular Biology, Faculty of Medicine, The John Paul II Catholic University of Lublin, Konstantynów 1J/4.03, 20-708 Lublin, Poland

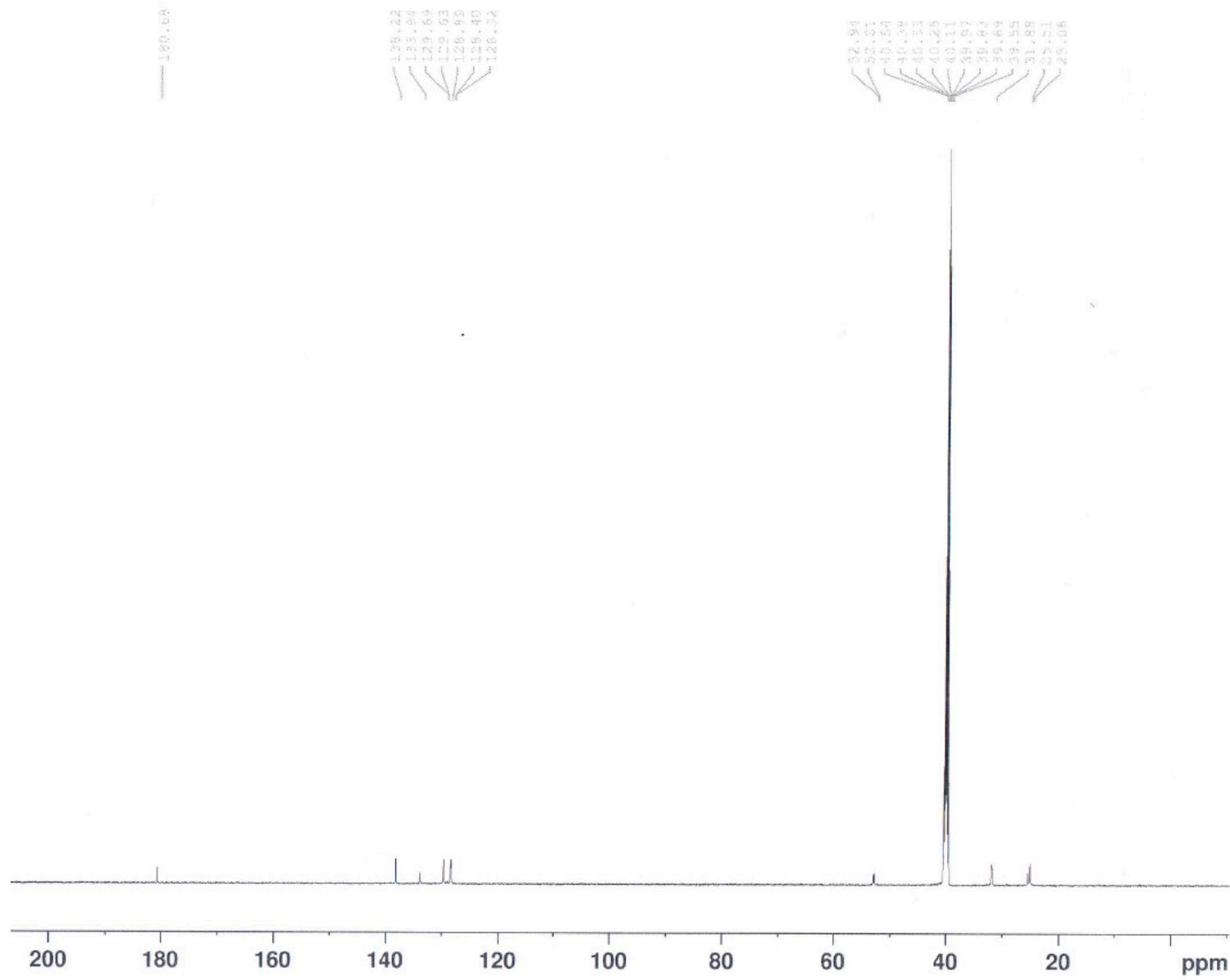
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<sup>7</sup> Department of Medicinal Chemistry, Faculty of Pharmacy, Medical University of Lublin, Jaczewskiego 4, 20-090, Lublin, PL, Poland

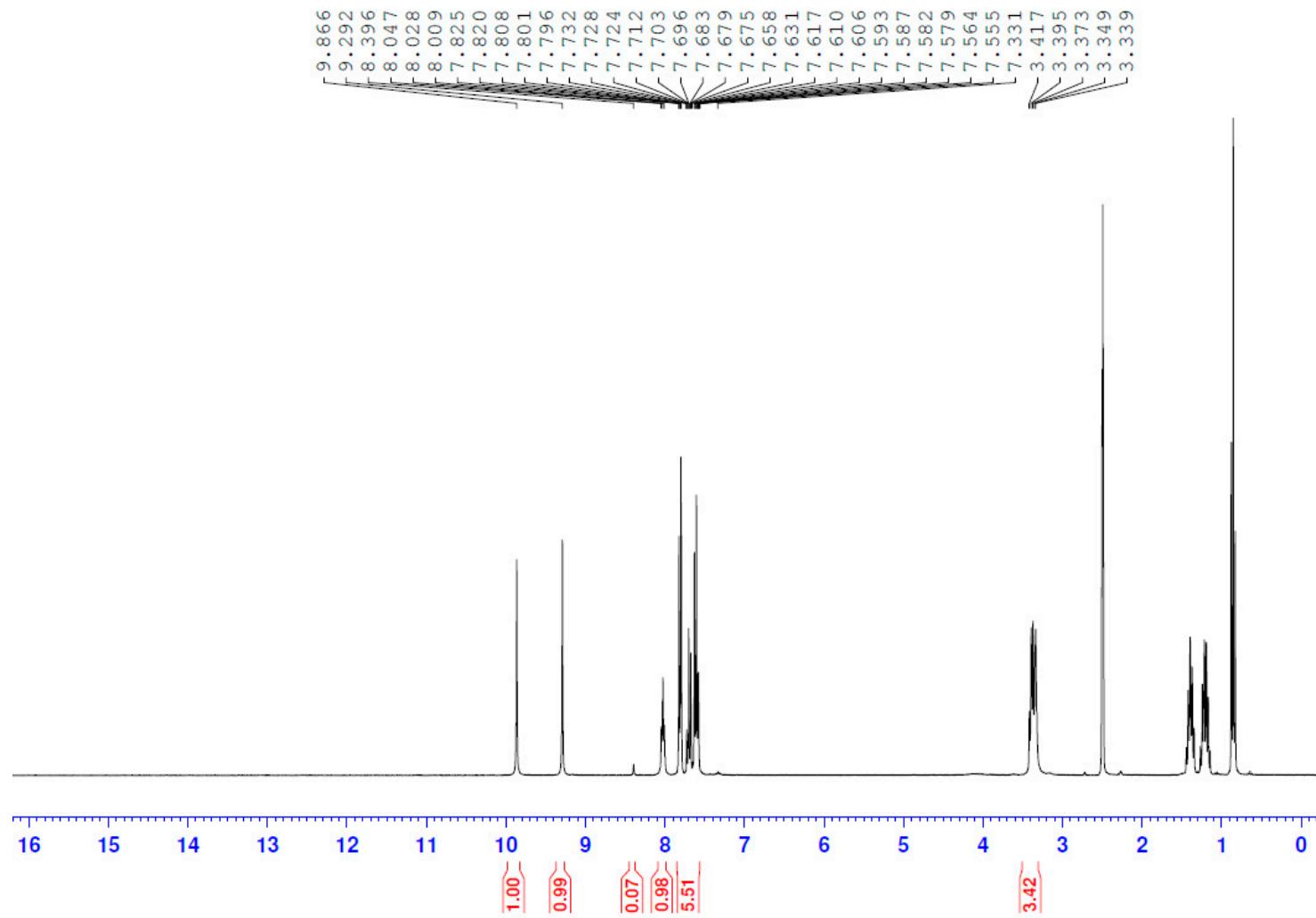
\* Correspondence: monika.pitucha@umlub.pl (MP);

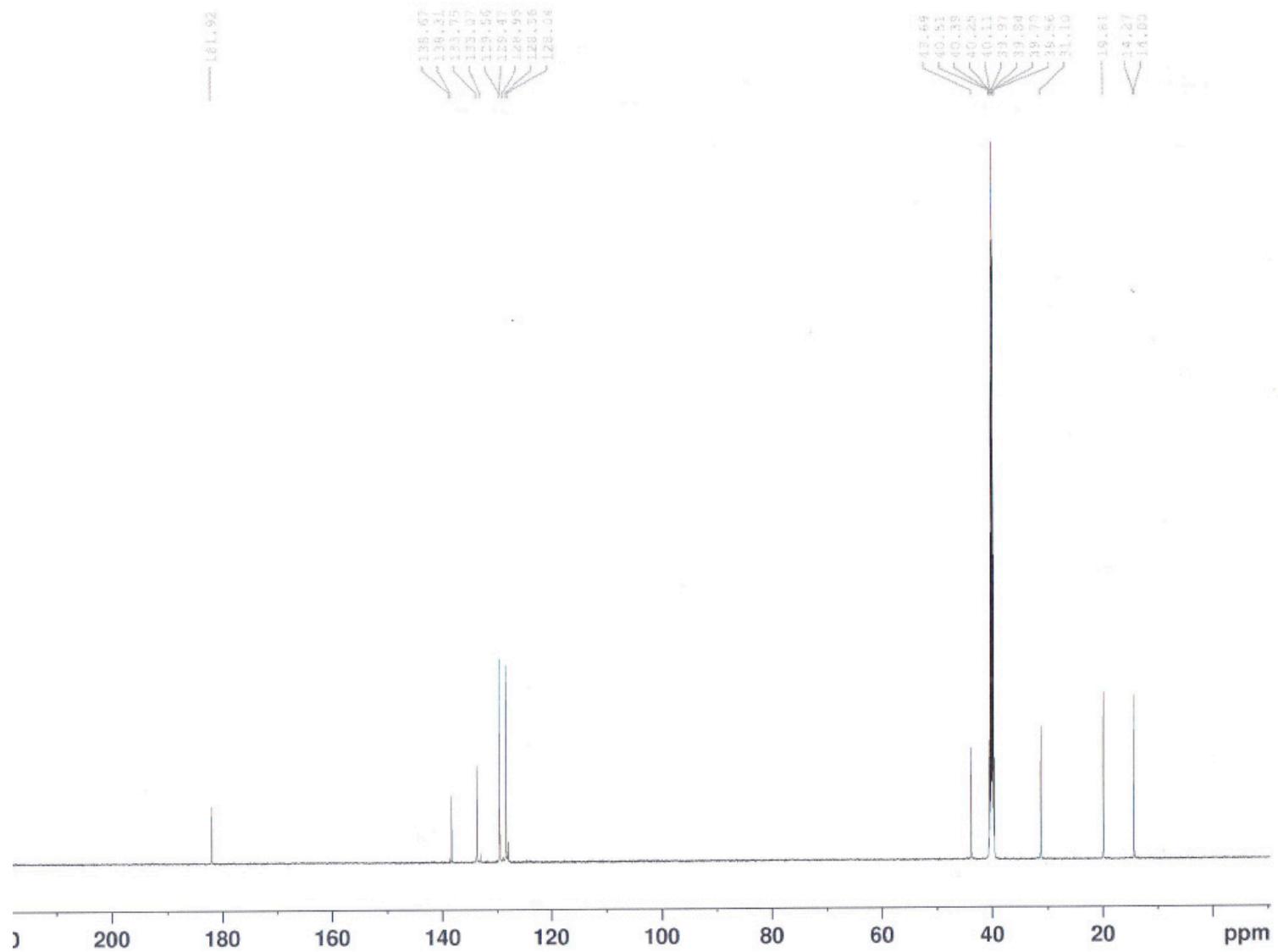
**Figure S1.** NMR spectra for WZ1



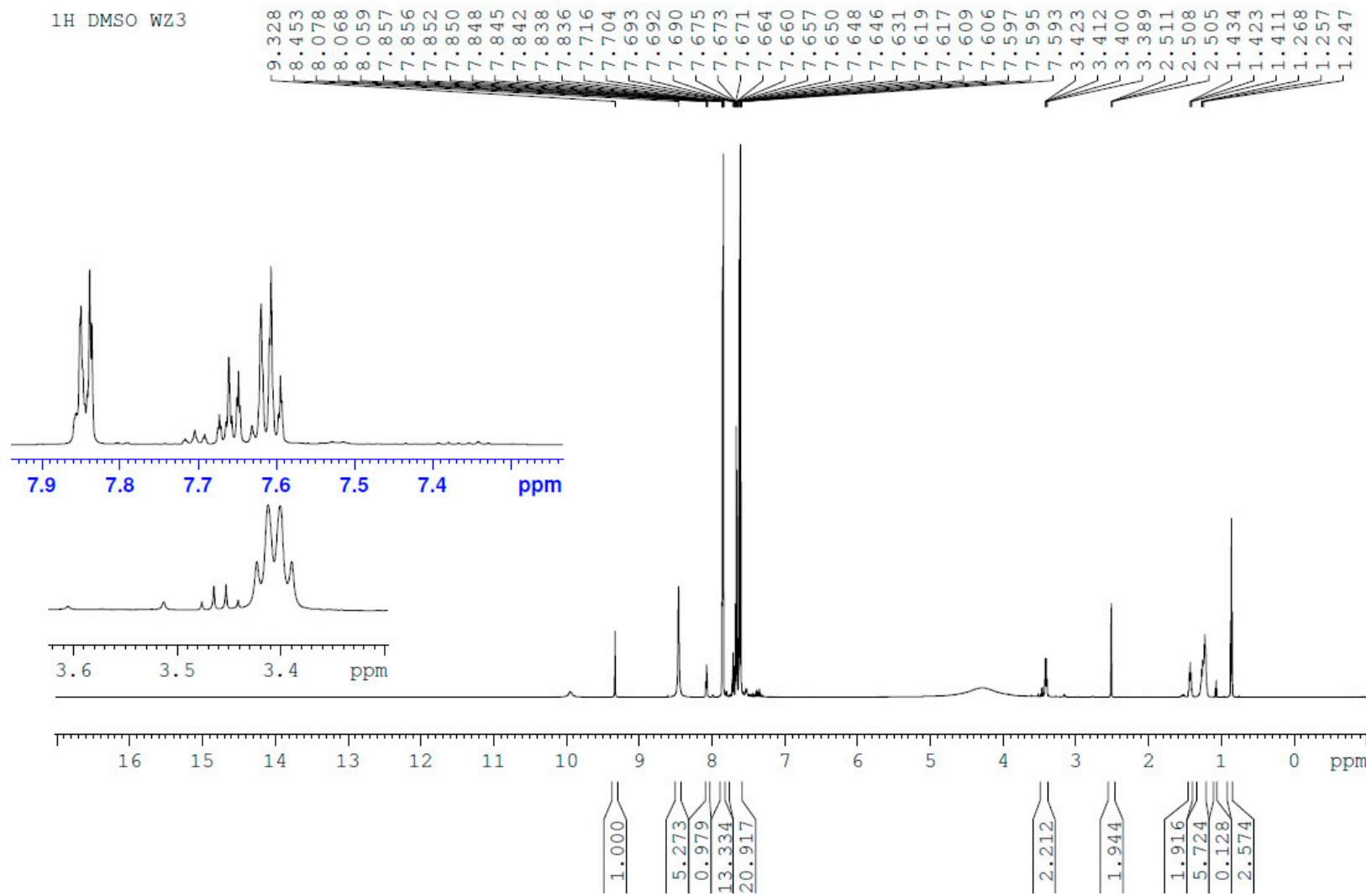


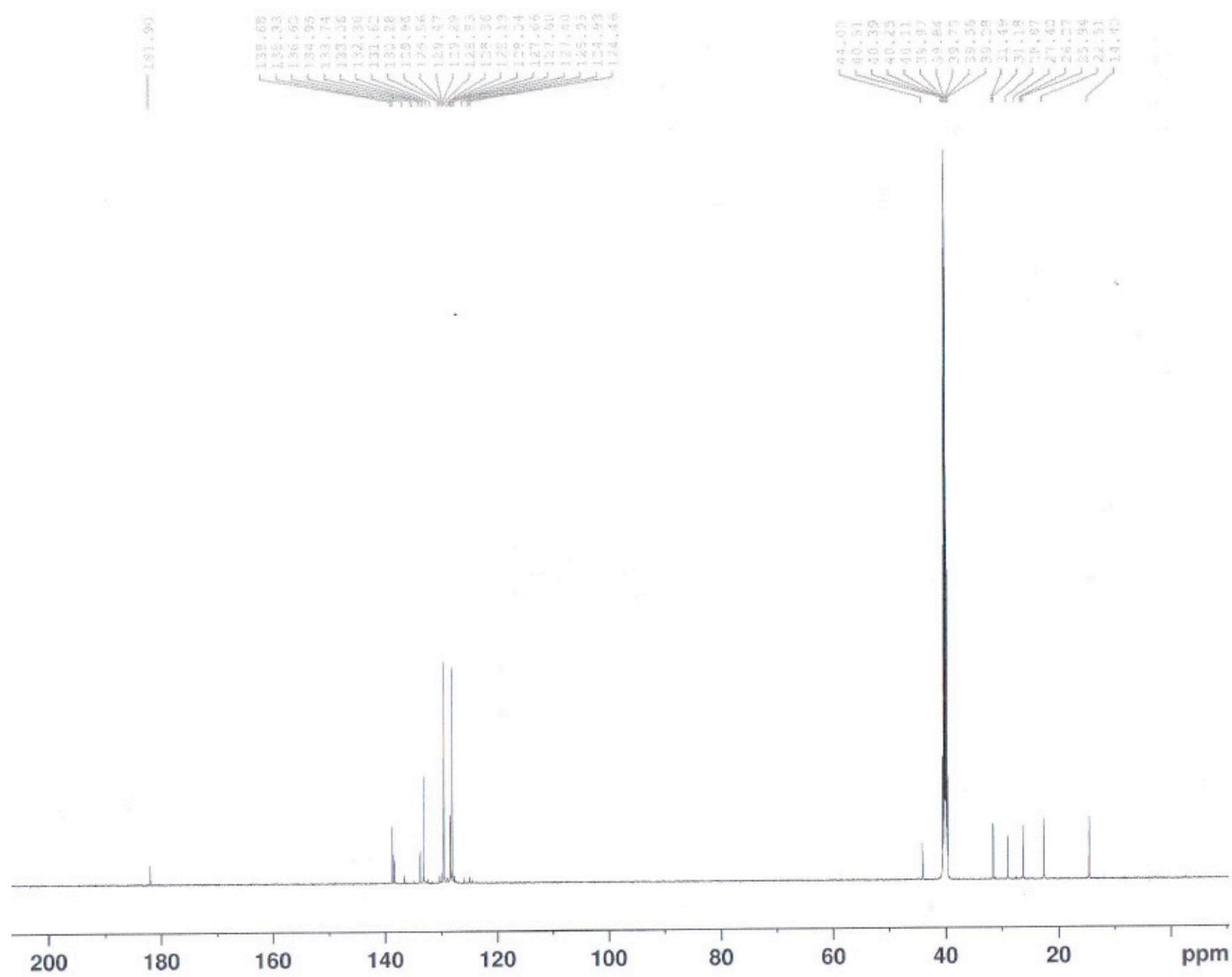
**Figure S2.** NMR spectra for WZ-2



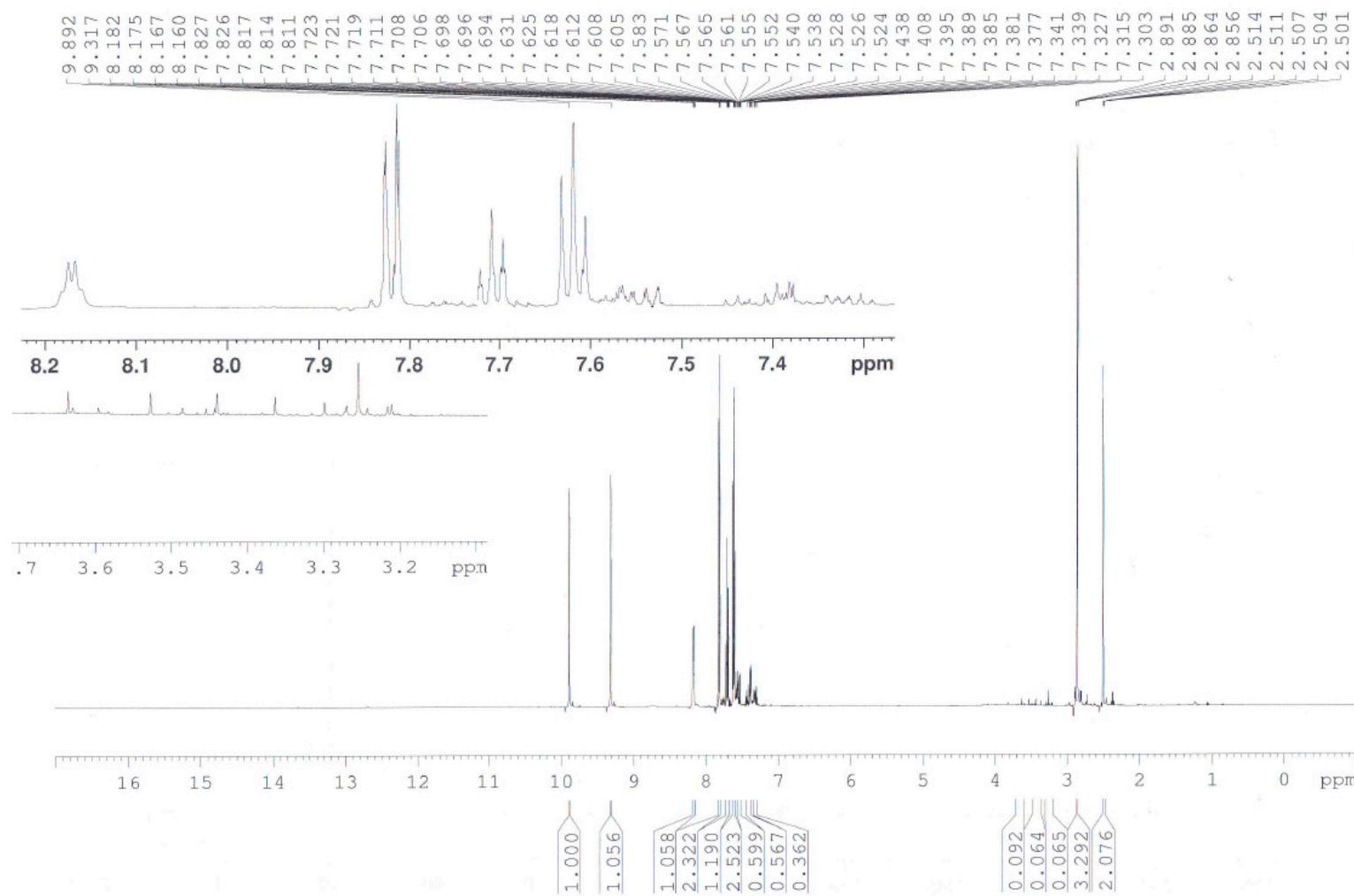


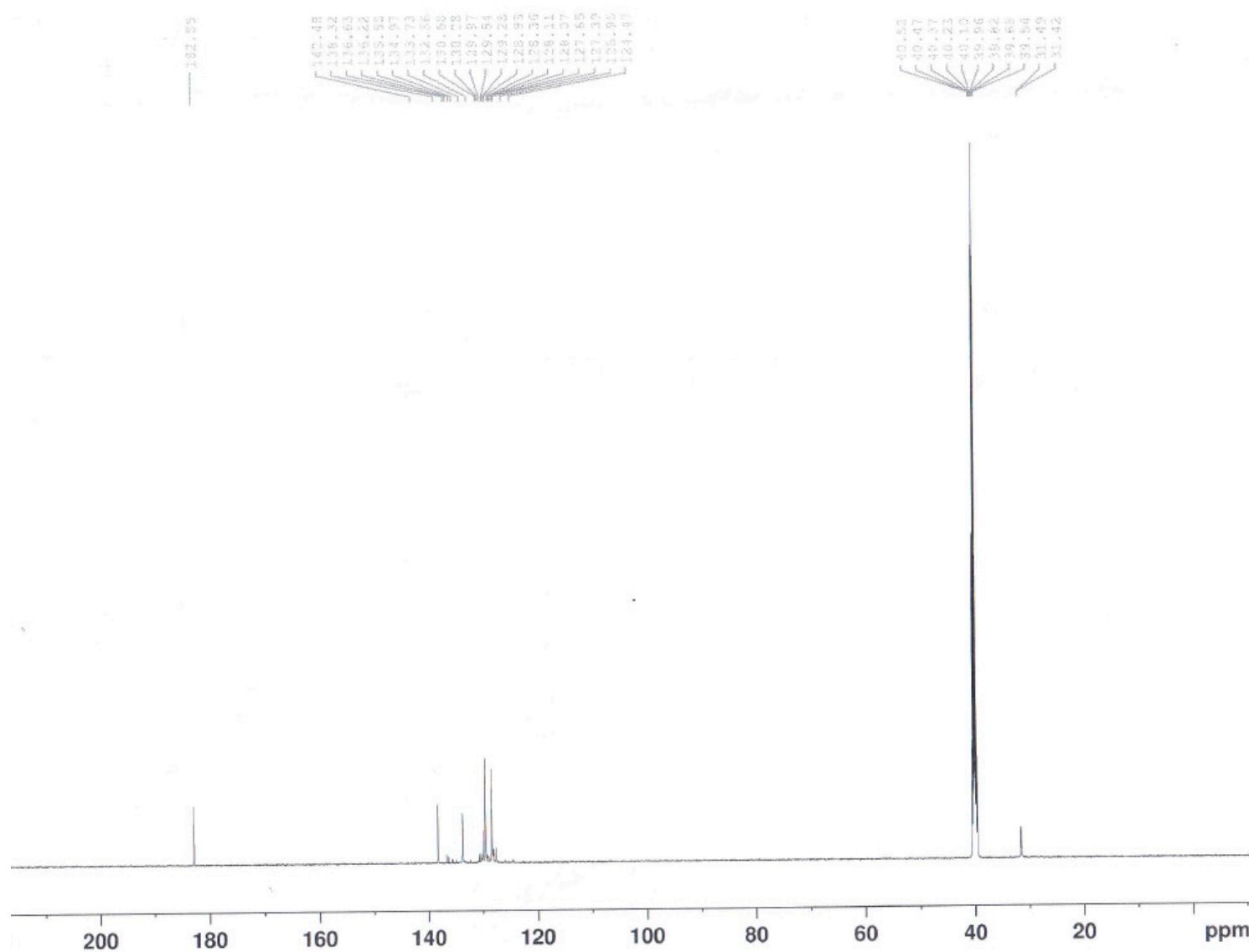
**Figure S3.** NMR spectra for WZ-3



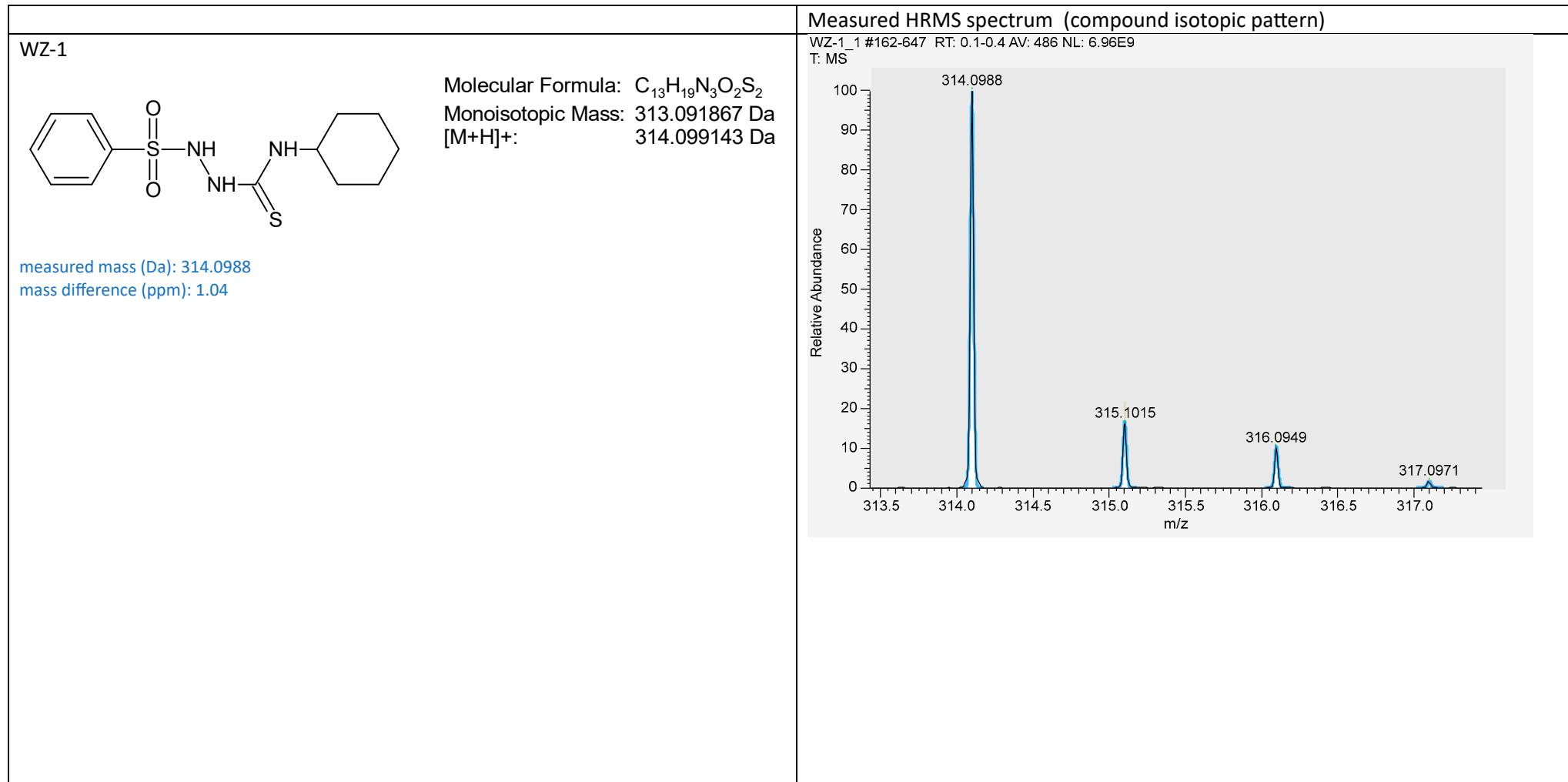


**Figure S4.** NMR spectra for WZ-4

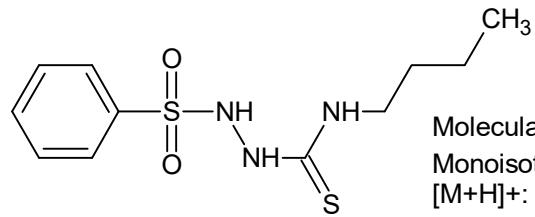




**Figure S5.** MS spectra for compounds WZ1-WZ-4



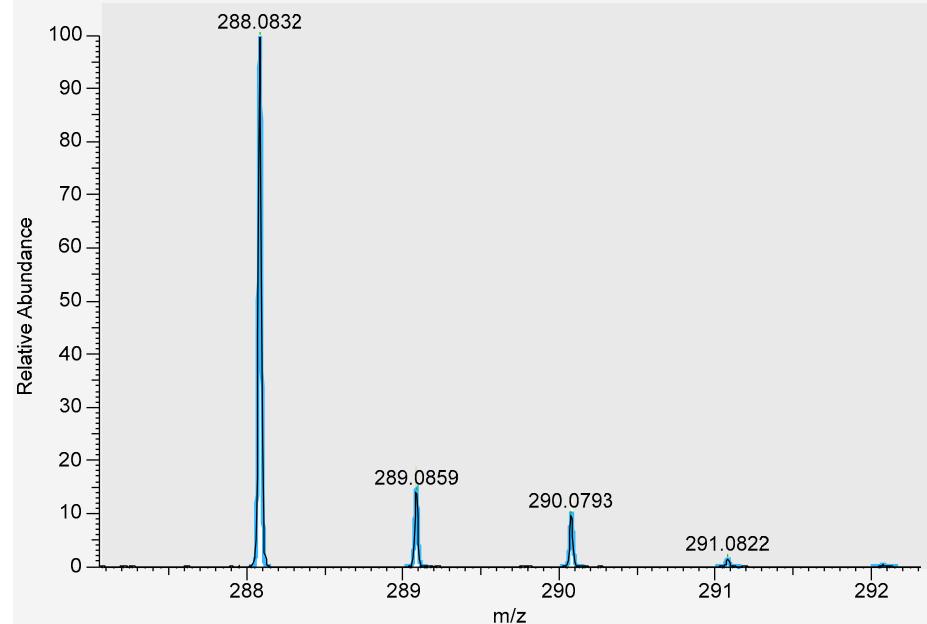
WZ-2



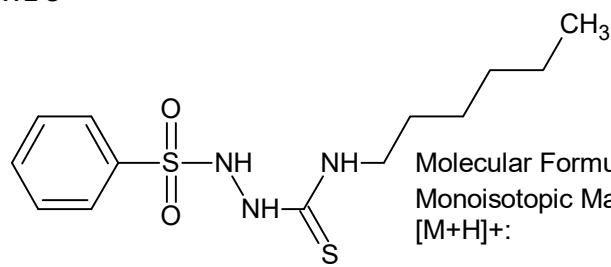
Molecular Formula: C<sub>11</sub>H<sub>17</sub>N<sub>3</sub>O<sub>2</sub>S<sub>2</sub>  
Monoisotopic Mass: 287.076217 Da  
[M+H]<sup>+</sup>: 288.083493 Da

measured mass (Da): 288.0832  
mass difference (ppm): 1.15

WZ-2\_1 #160-648 RT: 0.1-0.4 AV: 489 NL: 5.21E9  
T: MS



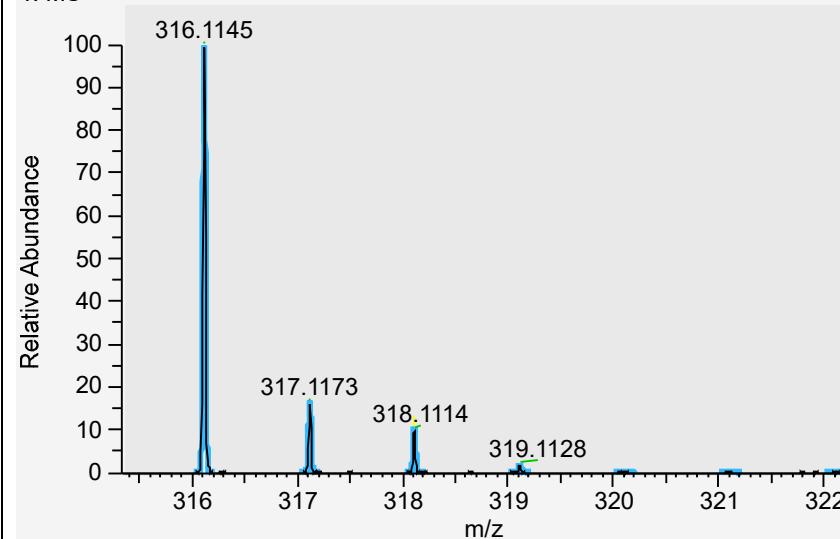
WZ-3



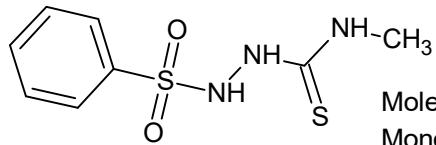
Molecular Formula: C<sub>13</sub>H<sub>21</sub>N<sub>3</sub>O<sub>2</sub>S<sub>2</sub>  
Monoisotopic Mass: 315.107517 Da  
[M+H]<sup>+</sup>: 316.114793 Da

measured mass (Da): 316.1145  
mass difference (ppm): 0.87

WZ-3\_1 #162-650 RT: 0.1-0.4 AV: 489 NL: 5.26E9  
T: MS



WZ-4



Molecular Formula: C<sub>8</sub>H<sub>11</sub>N<sub>3</sub>O<sub>2</sub>S<sub>2</sub>  
Monoisotopic Mass: 245.029267 Da  
[M+H]<sup>+</sup>: 246.036543 Da

measured mass (Da): 246.0365  
mass difference (ppm): 0.01

WZ-4\_1 #162-648 RT: 0.1-0.4 AV: 487 NL: 3.50E9  
T: MS

