Electronic Supplementary Material (ESI) for RSC Advances.

Convergent Synthesis, Kinetics Insight and Allosteric Computational Ascriptions of Thiazole-(5-aryl)oxadiazole Hybrids Embraced with Propanamides as Alkaline Phosphatase Inhibitors

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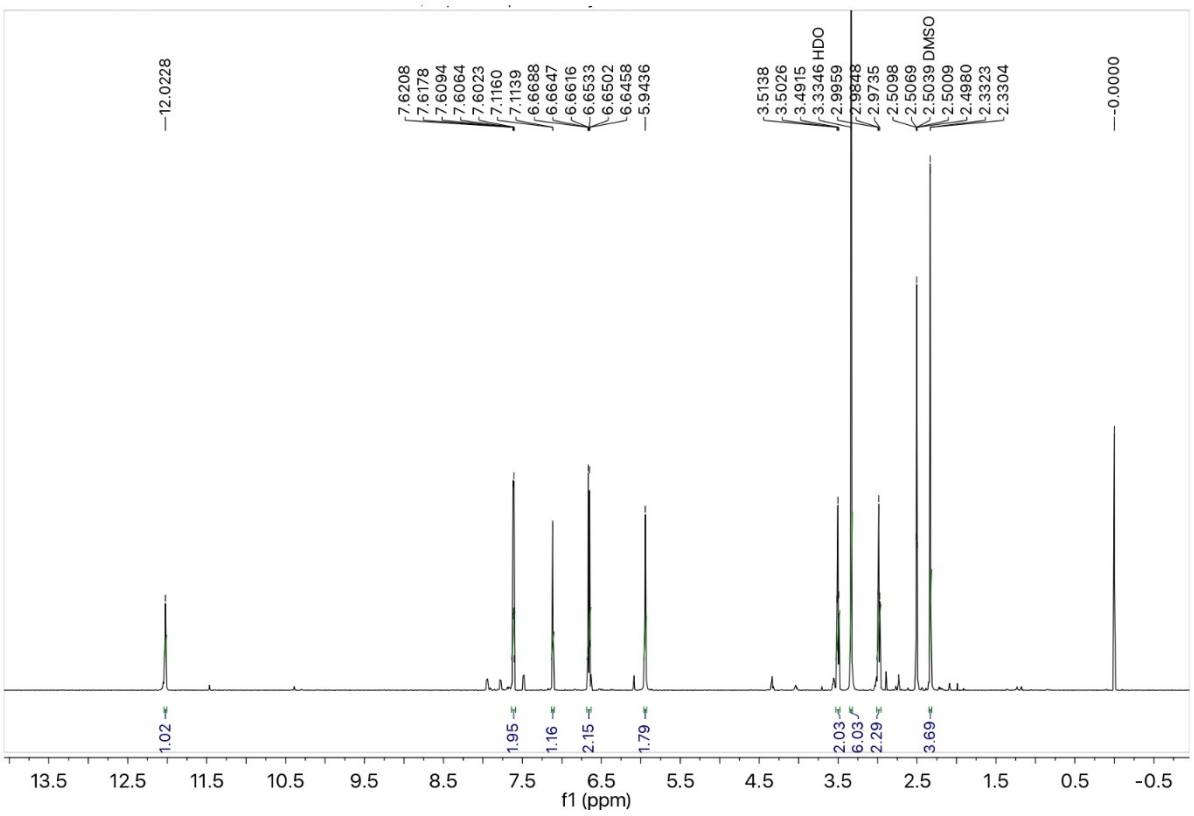
A)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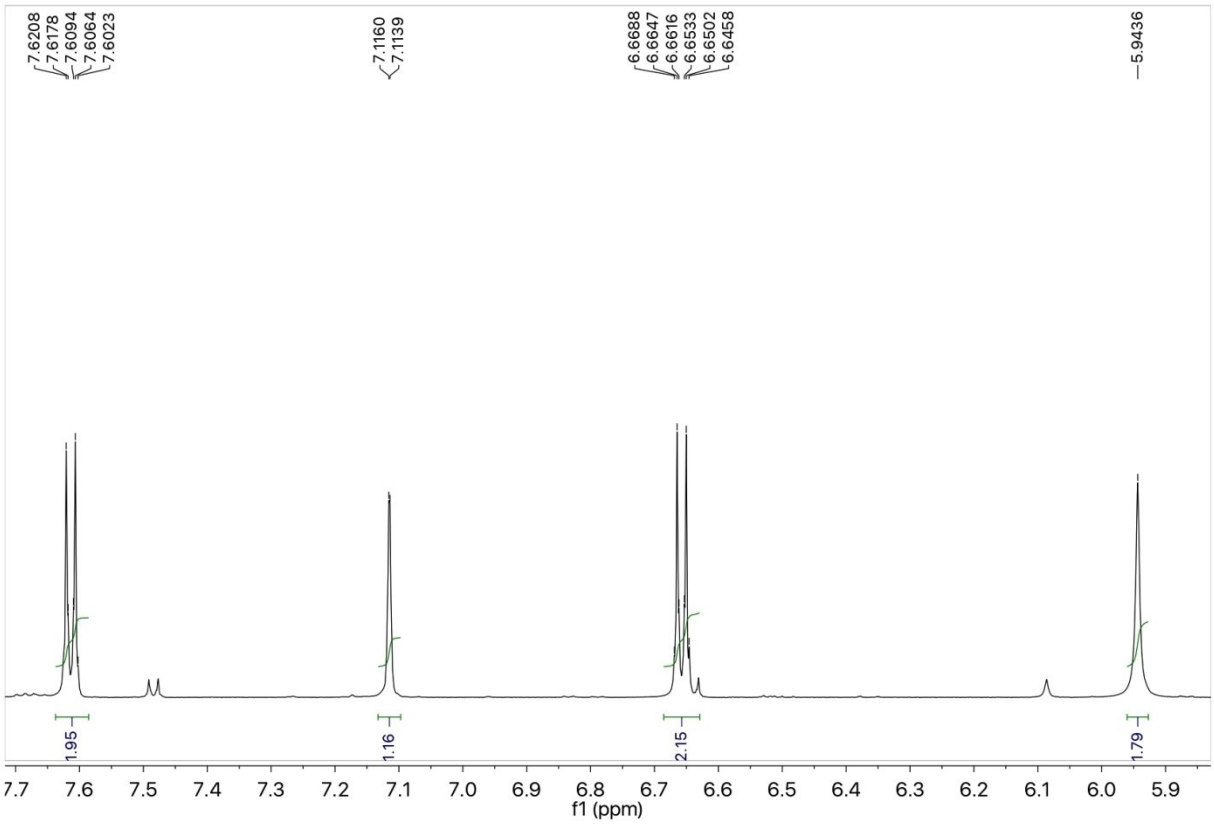
6.6533
6.6502
6.6458
5.9436
3.5138
3.5026
3.4915
3.3346 HDO
2.9959
2.9848
2.9735
2.5098
2.5069
2.5039 DMSO
2.5009
2.4980
2.3323
2.3304
0.0000
1.02
1.95
1.16
2.15
1.79
2.03
6.03
2.29
3.69
13.5
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

B)



C)

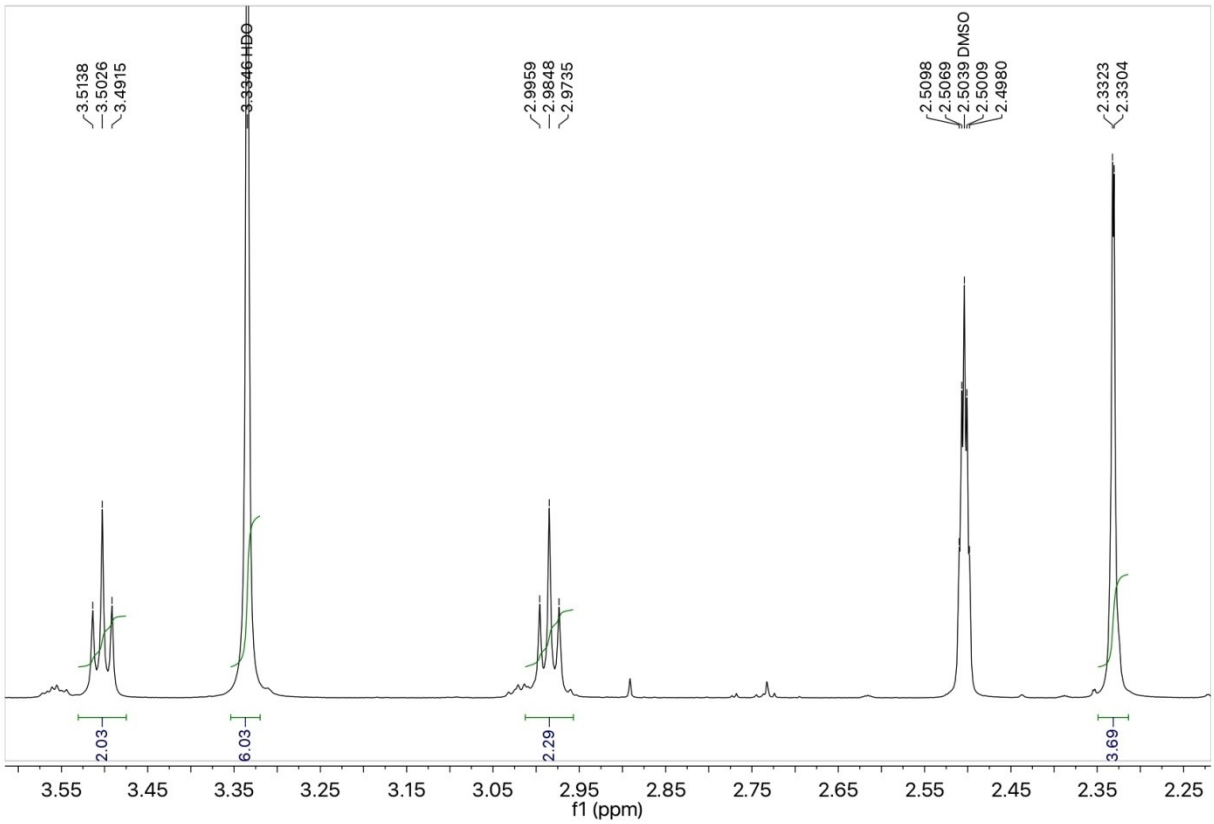


Fig. S1-A) ^{1}H-NMR spectrum of **8g**. B) Expanded aromatic region of ^{1}H-NMR spectrum of **8g**. C) Expanded aliphatic region of ^{1}H-NMR spectrum of **8g**.

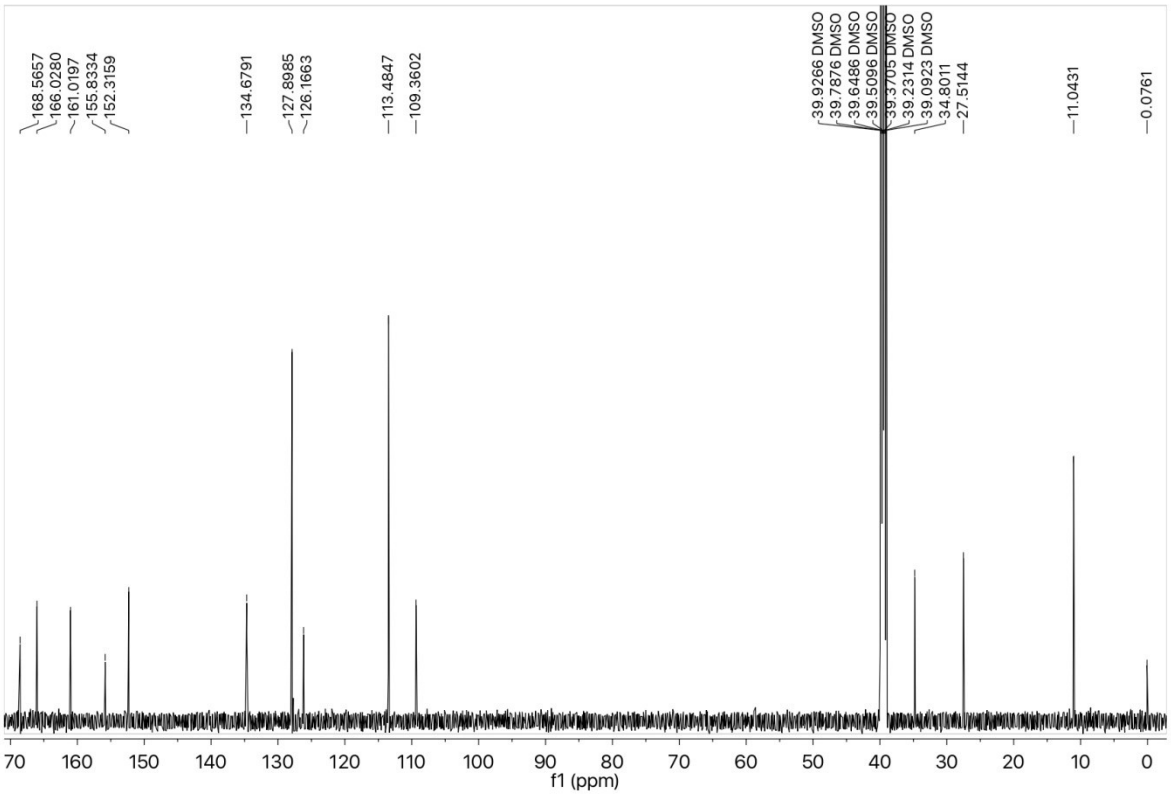


Fig. S2 ^{13}C-NMR spectrum of **8g**.

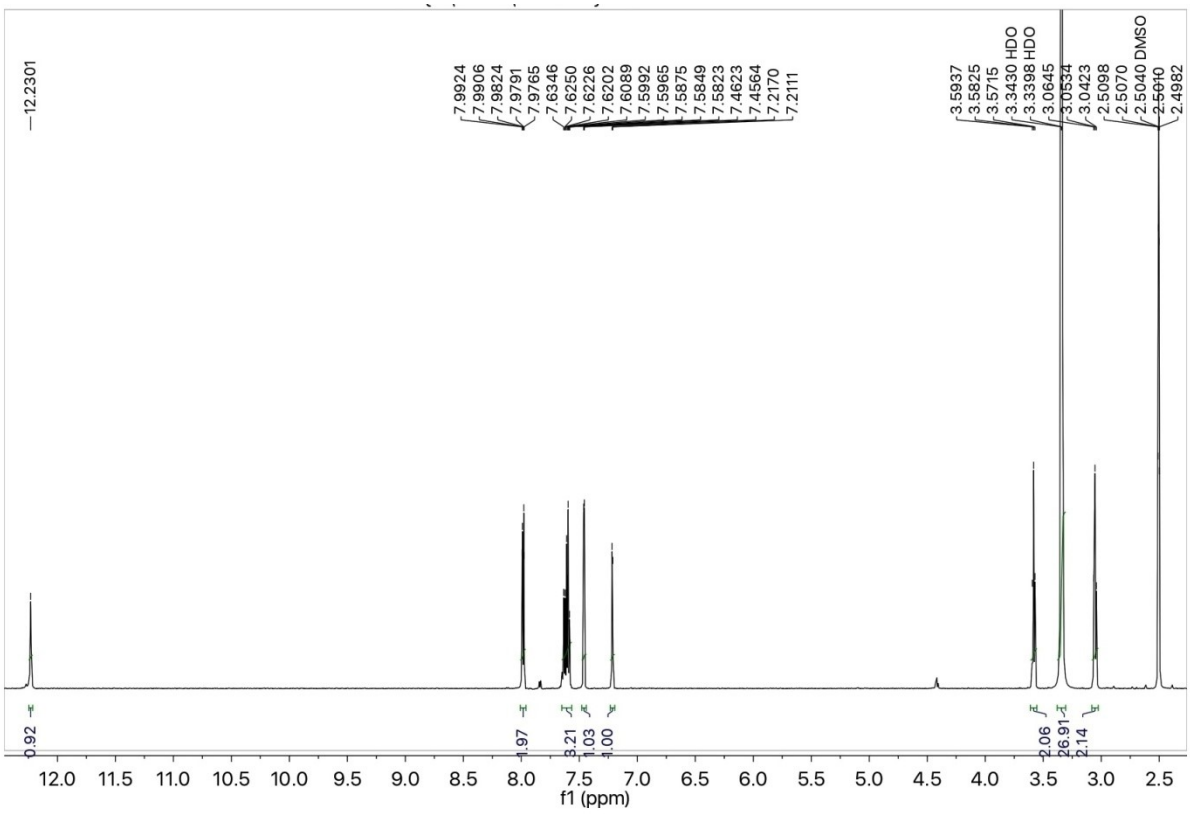


Fig. S3 ^{1}H-NMR spectrum of **8a**.

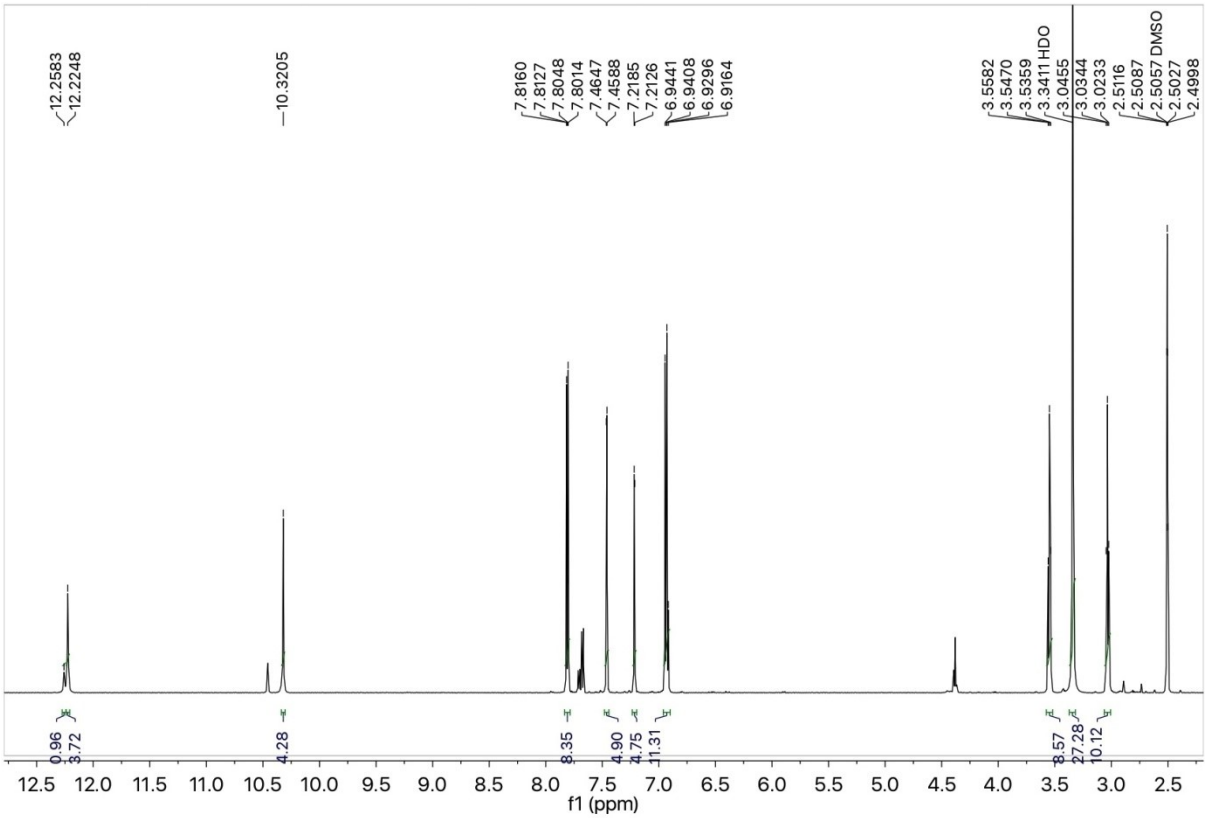


Fig. S4 ^{1}H-NMR spectrum of **8b**.

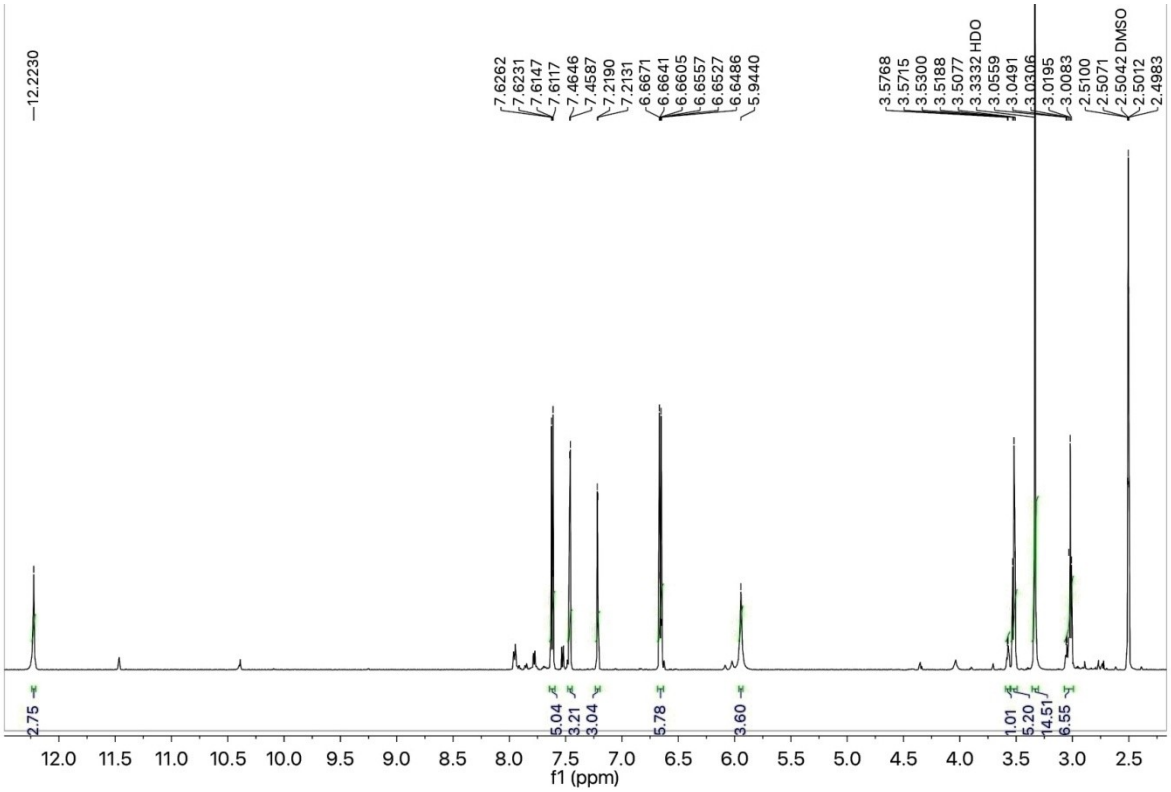


Fig. S5 ^{1}H-NMR spectrum of **8c**

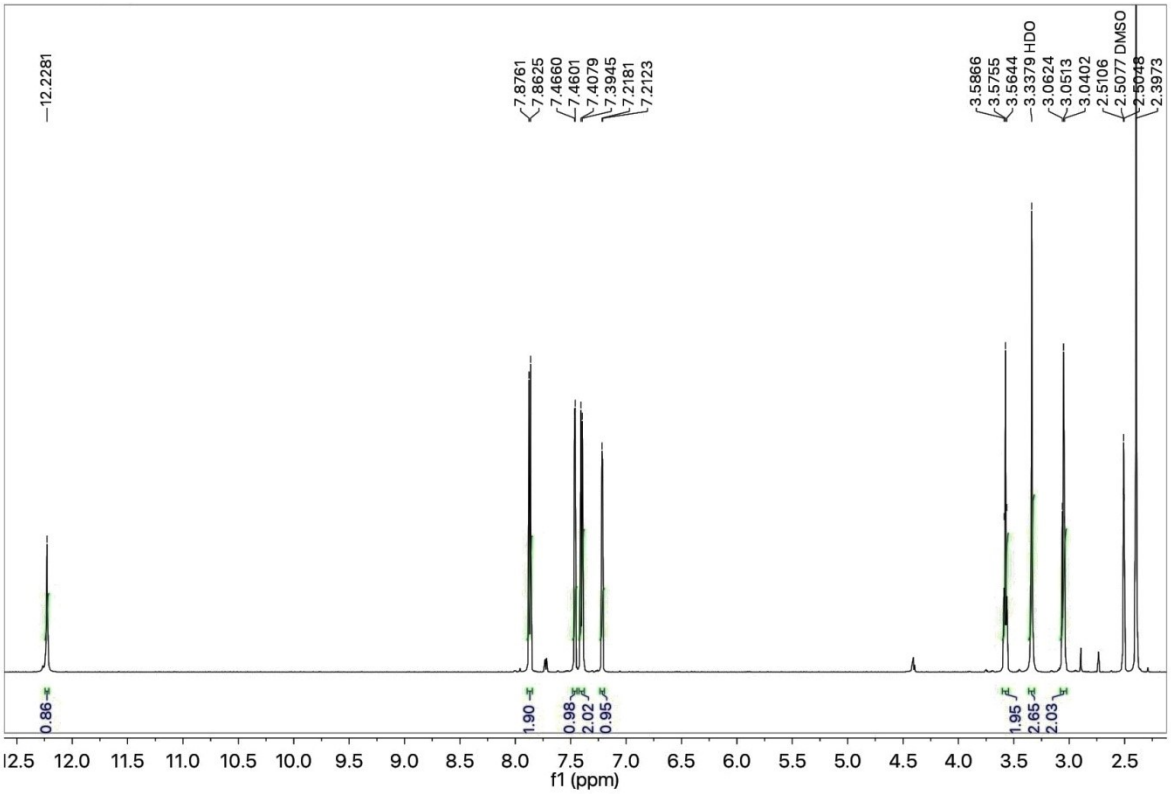


Fig. S6 ^{1}H-NMR spectrum of **8d**

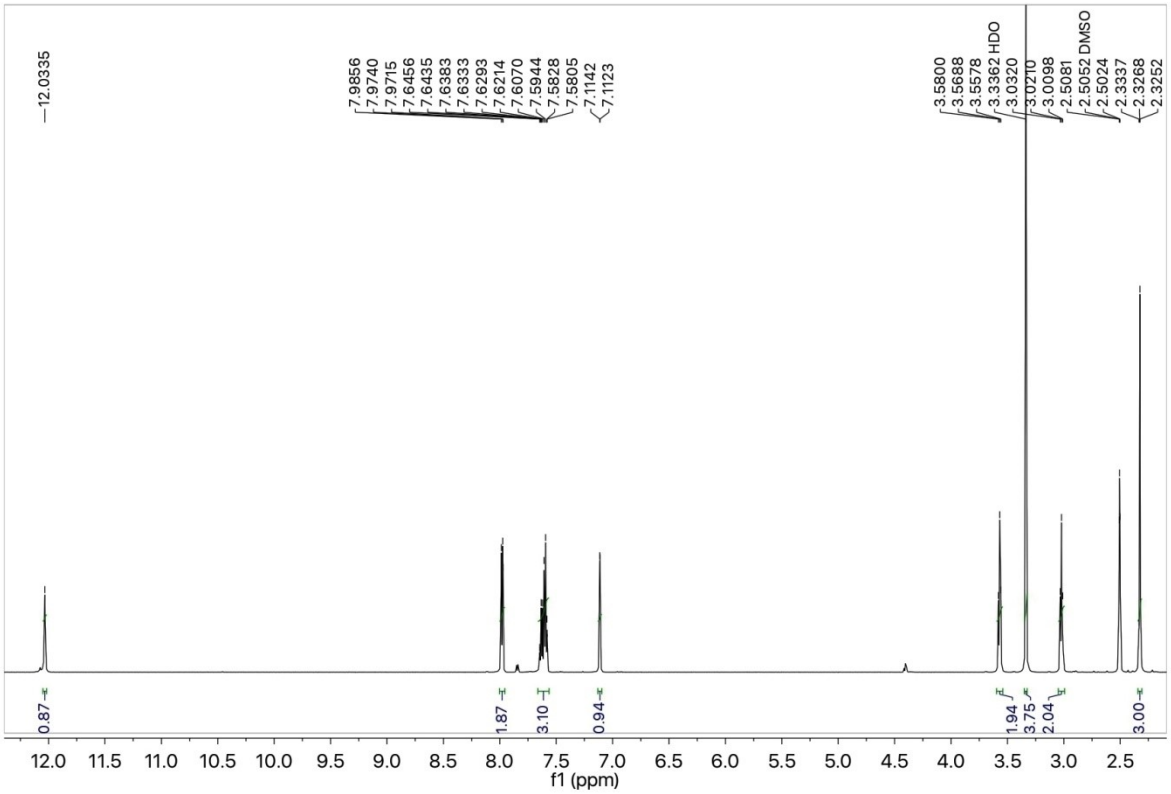


Fig. S7 ^{1}H-NMR spectrum of **8e**

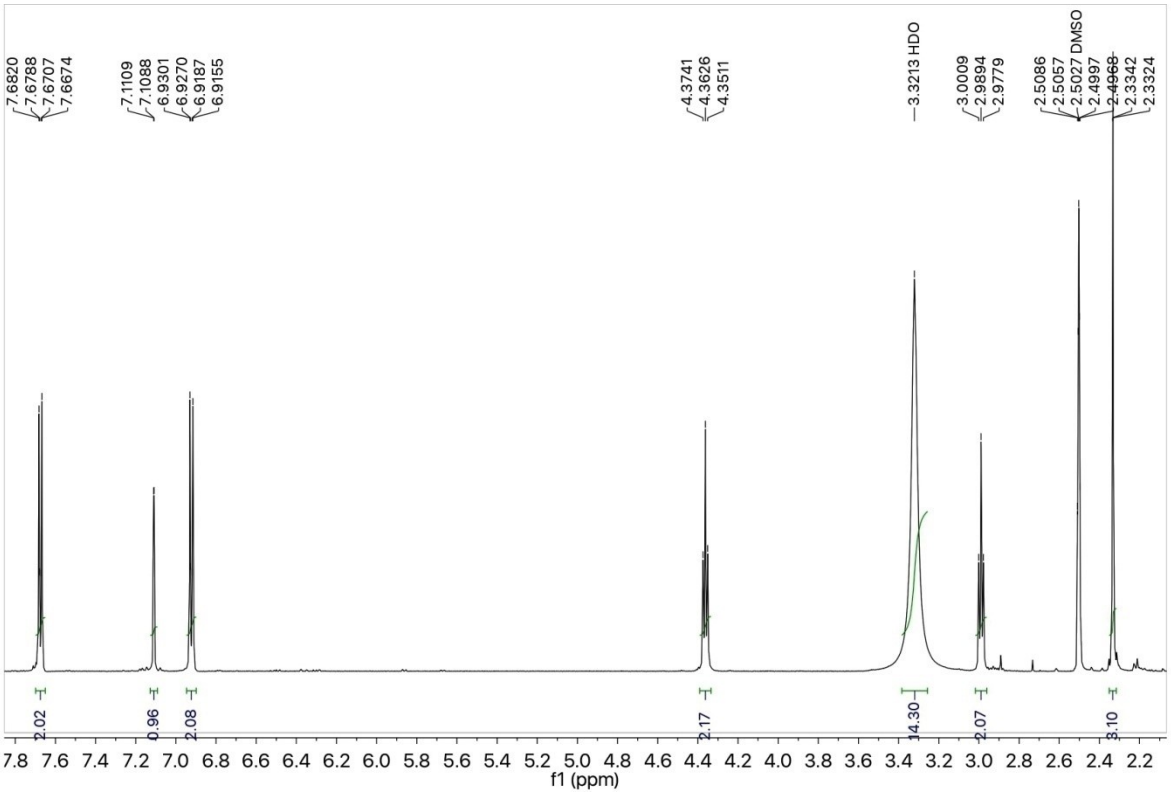


Fig. S8 ^{1}H-NMR spectrum of **8f**

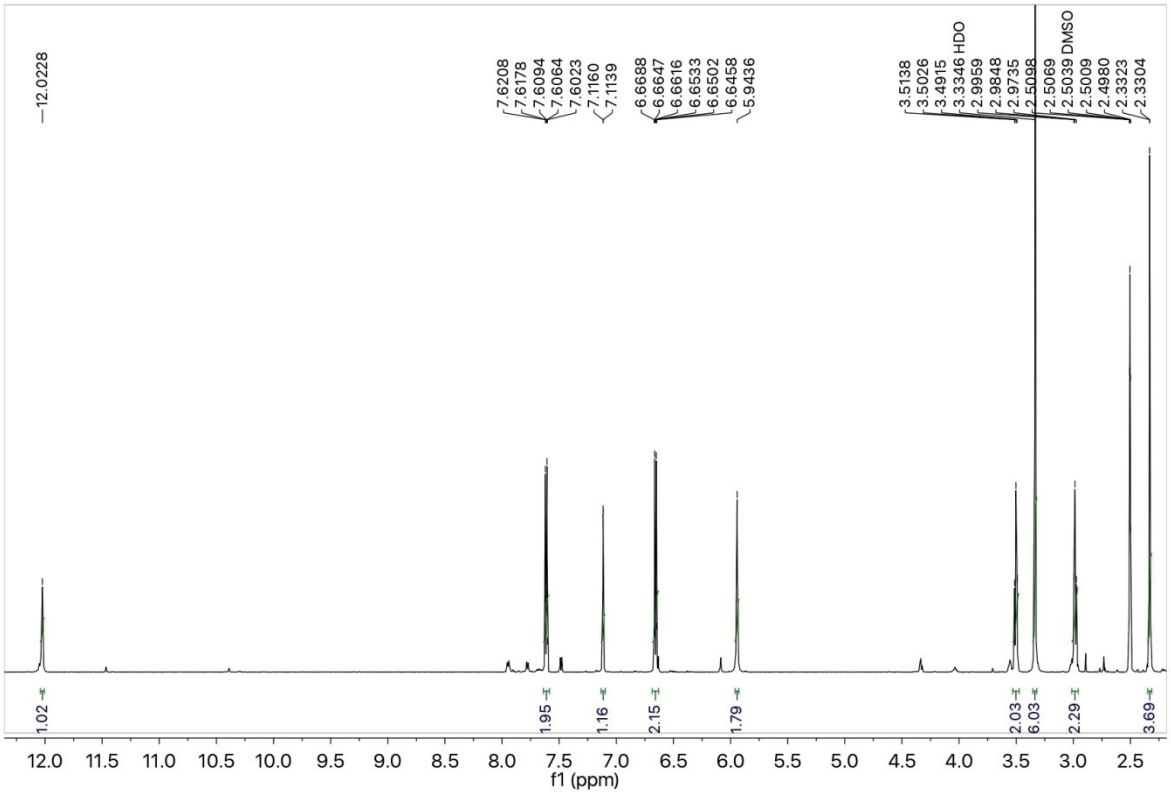


Fig. S9 ^{1}H-NMR spectrum of **8g**

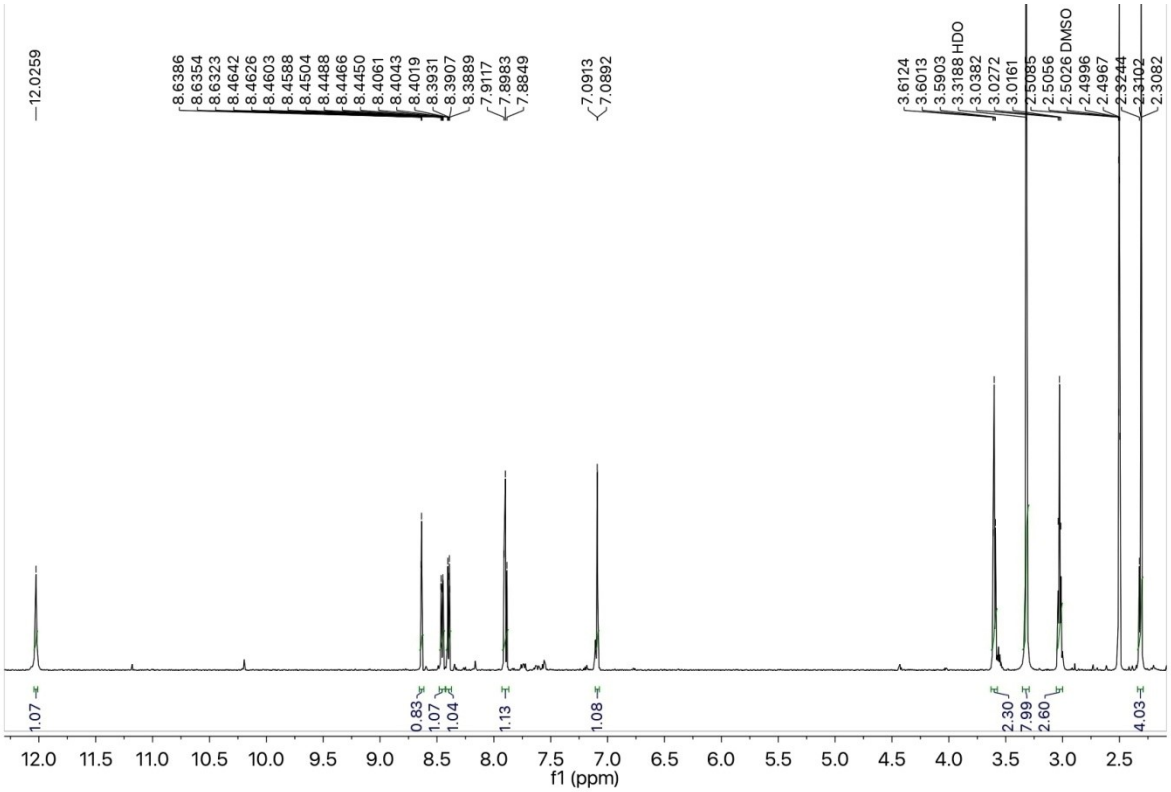


Fig. S10 ^{1}H-NMR spectrum of **8h**

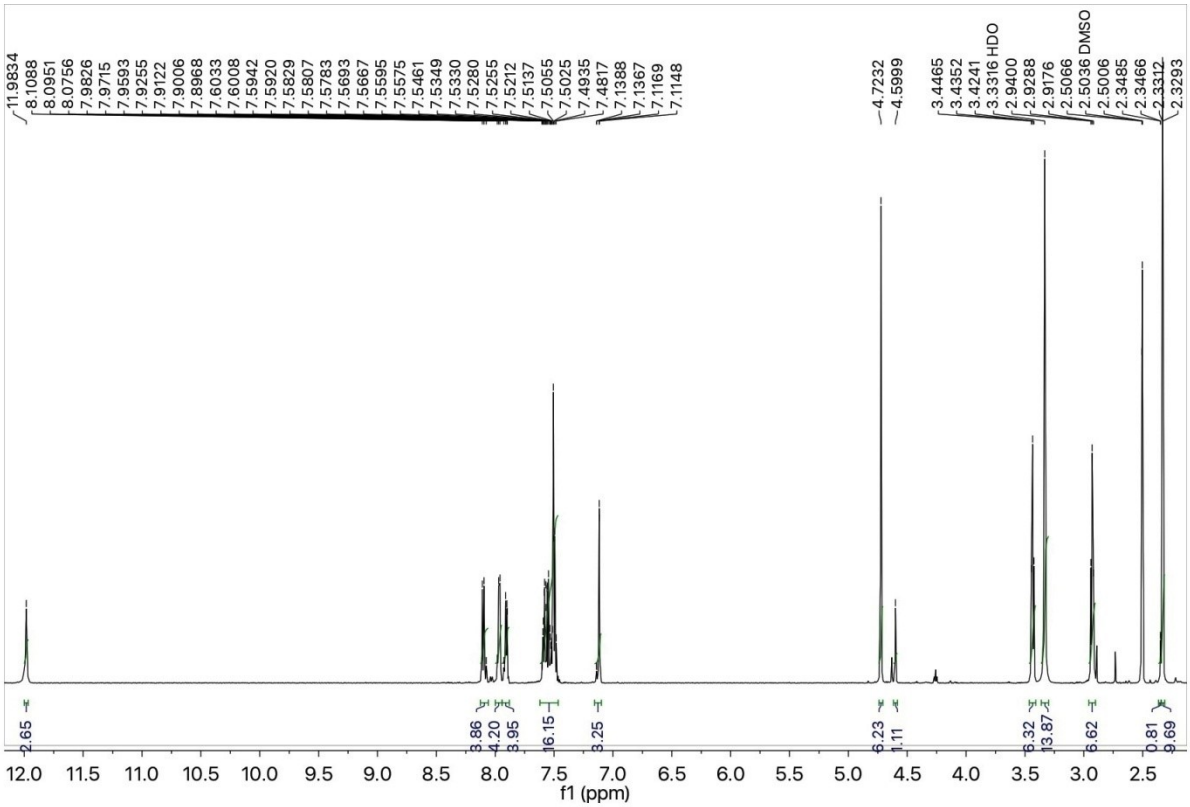


Fig. S11 ^{1}H-NMR spectrum of **8i**

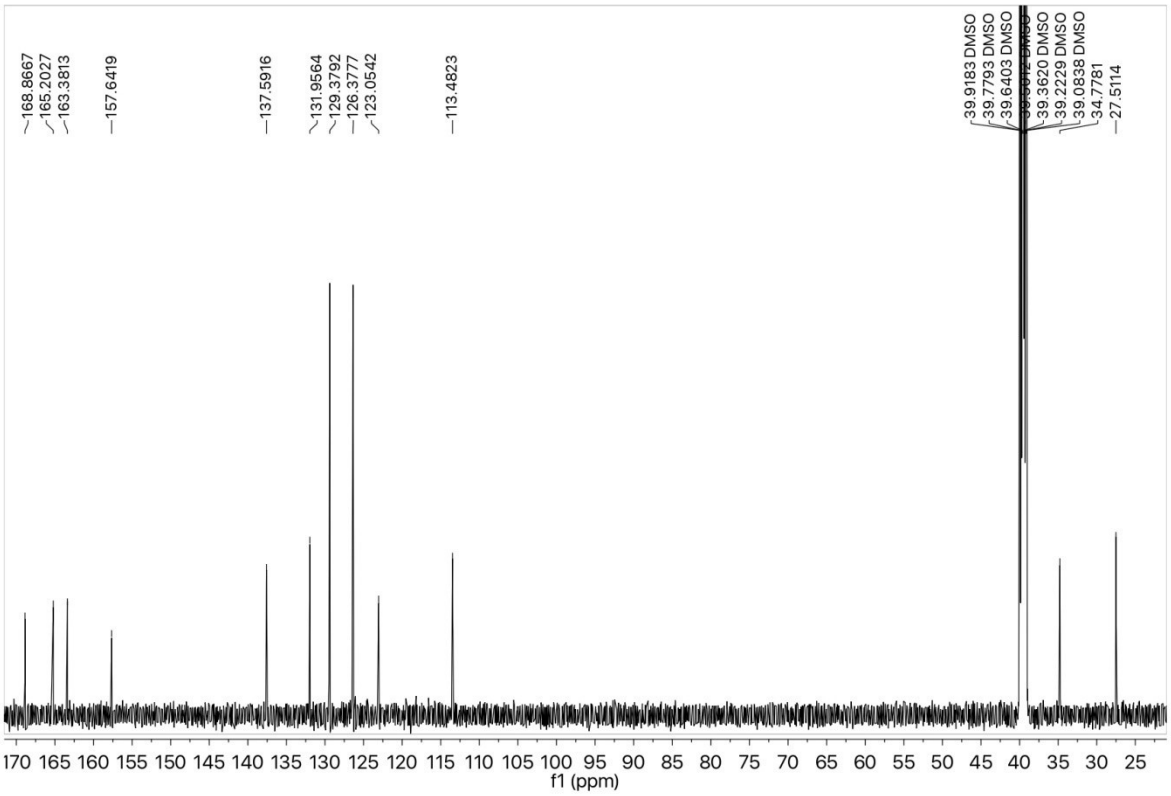


Fig. S12 ^{13}C-NMR spectrum of **8a**

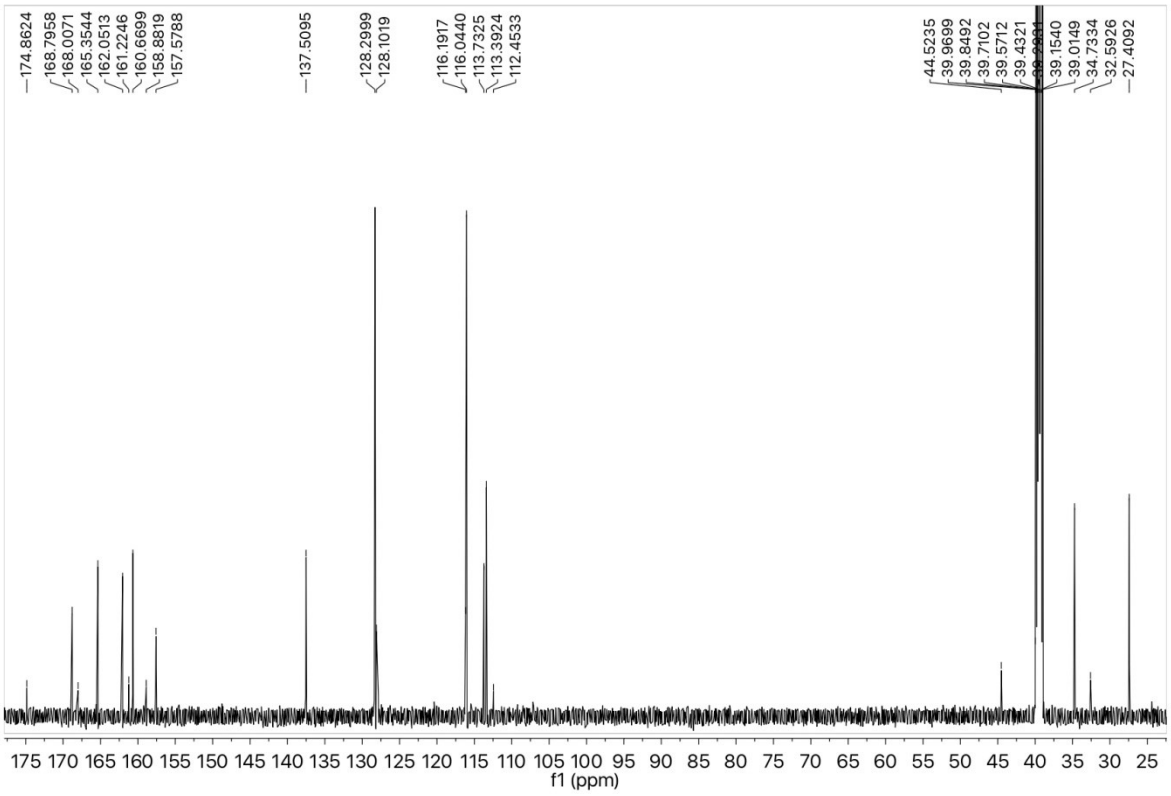


Fig. S13 ^{13}C-NMR spectrum of **8b**

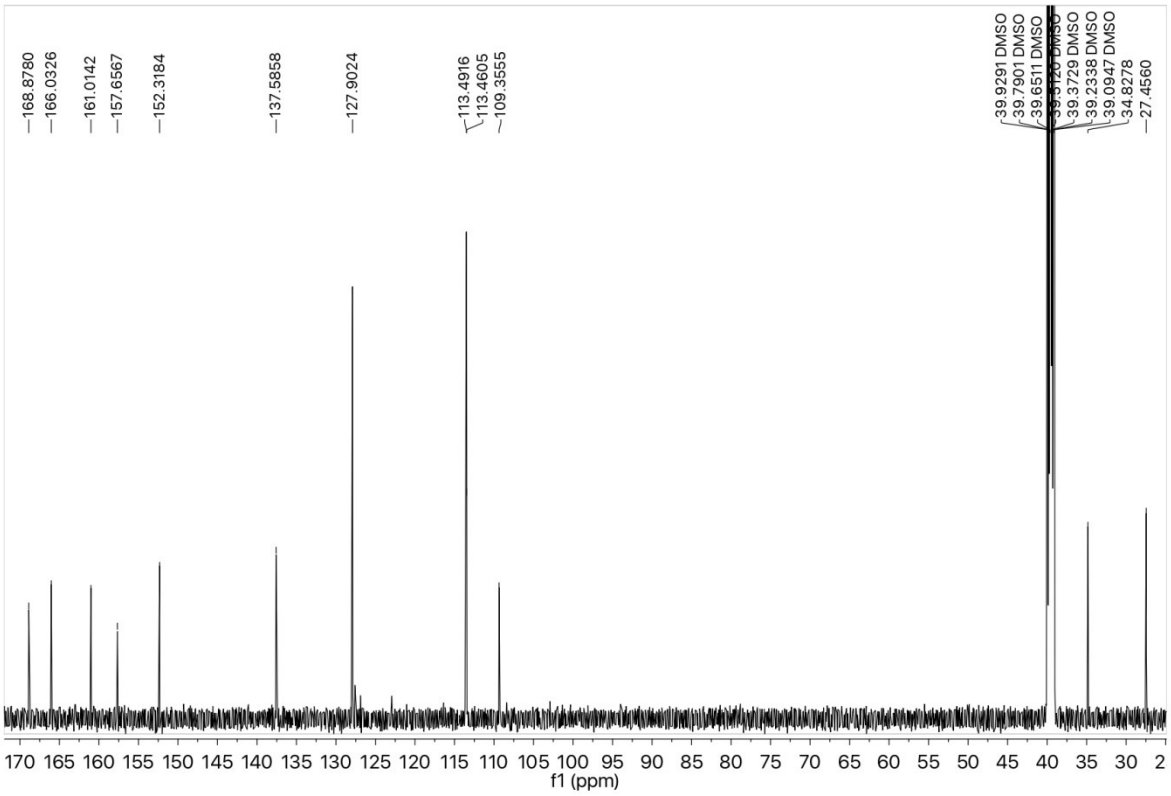


Fig. S14 ^{13}C -NMR spectrum of **8c**

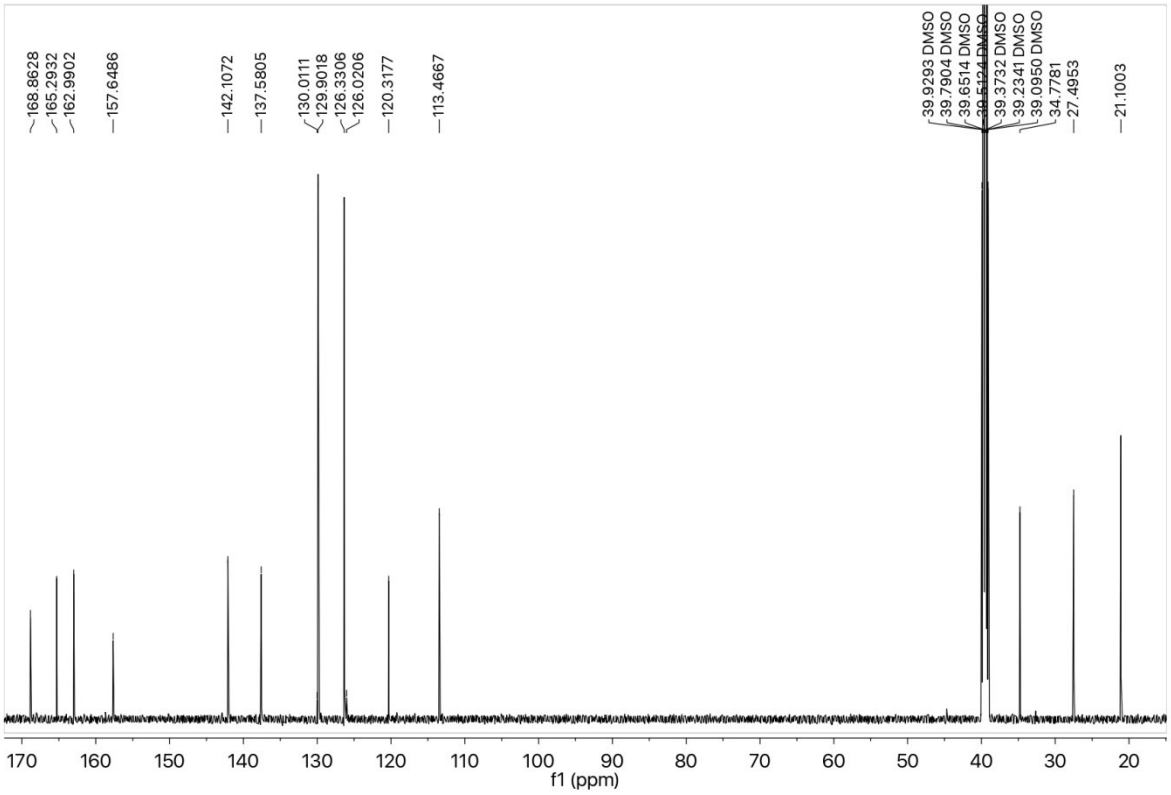


Fig. S15 ^{13}C -NMR spectrum of **8d**

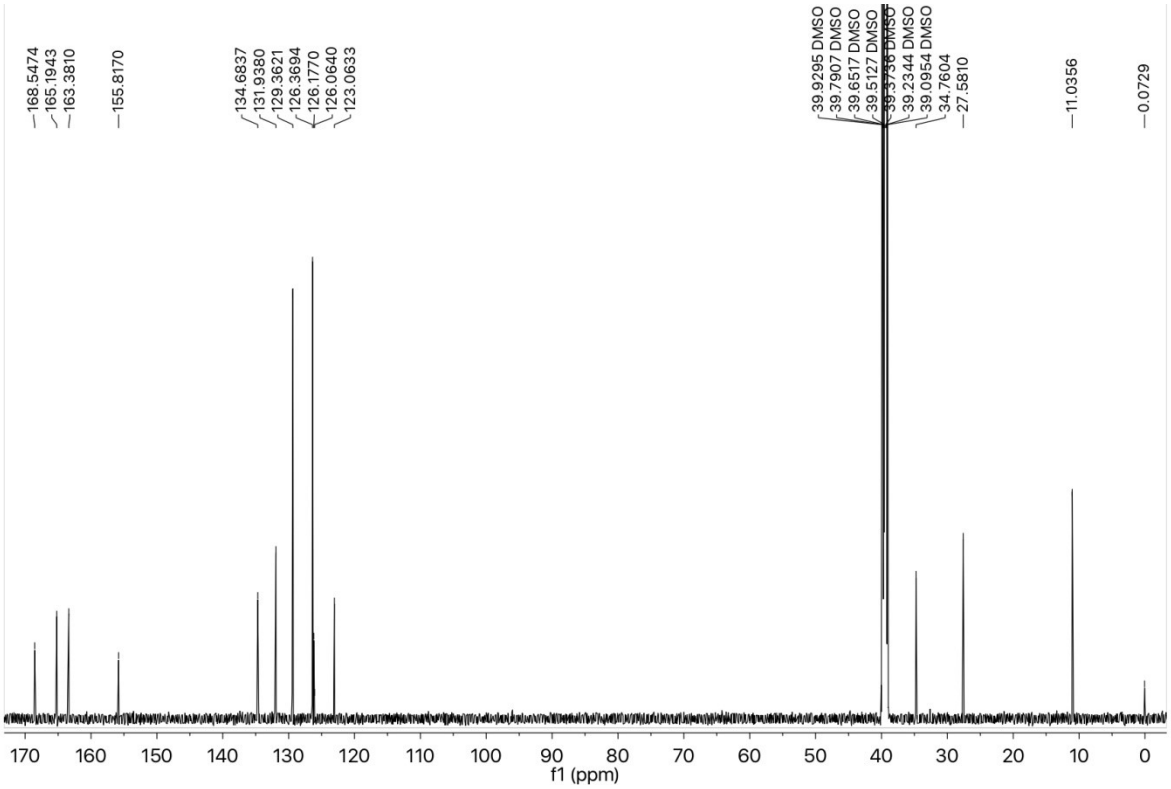


Fig. S16 ^{13}C -NMR spectrum of **8e**

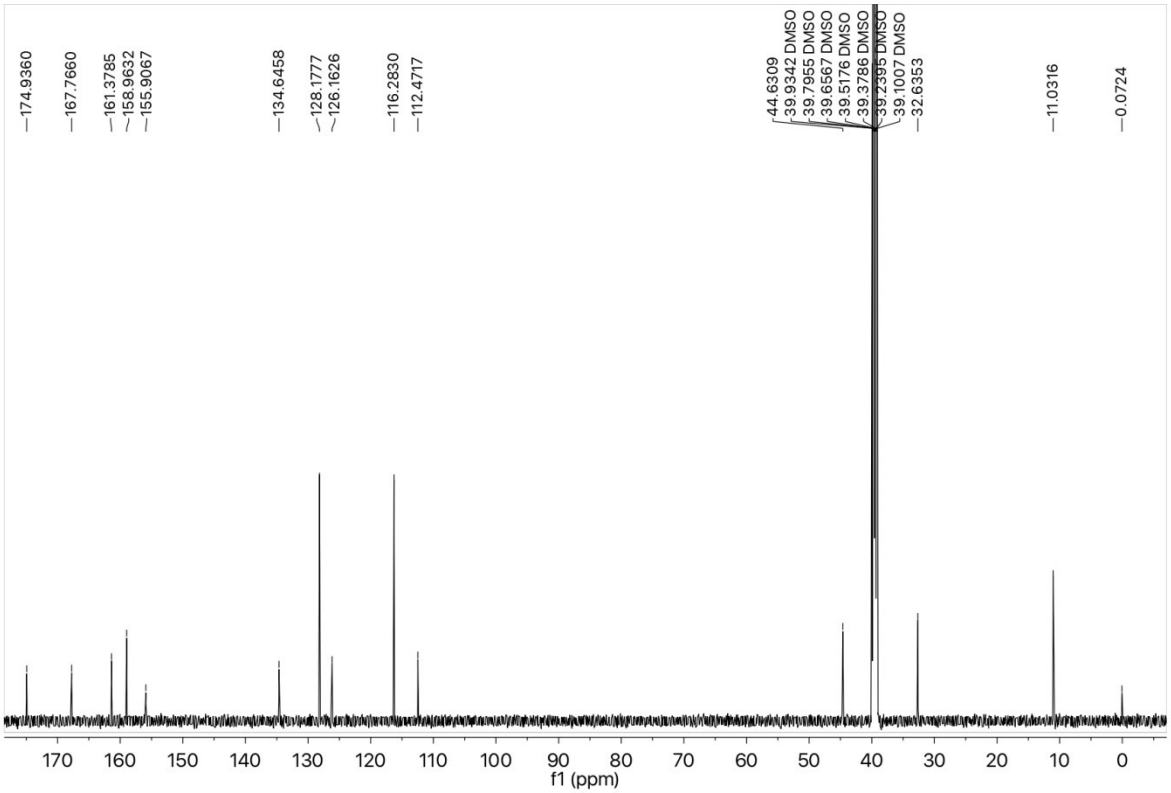


Fig. S17 ^{13}C -NMR spectrum of **8f**

Fig. S18 ^{13}C -NMR spectrum of **8g**

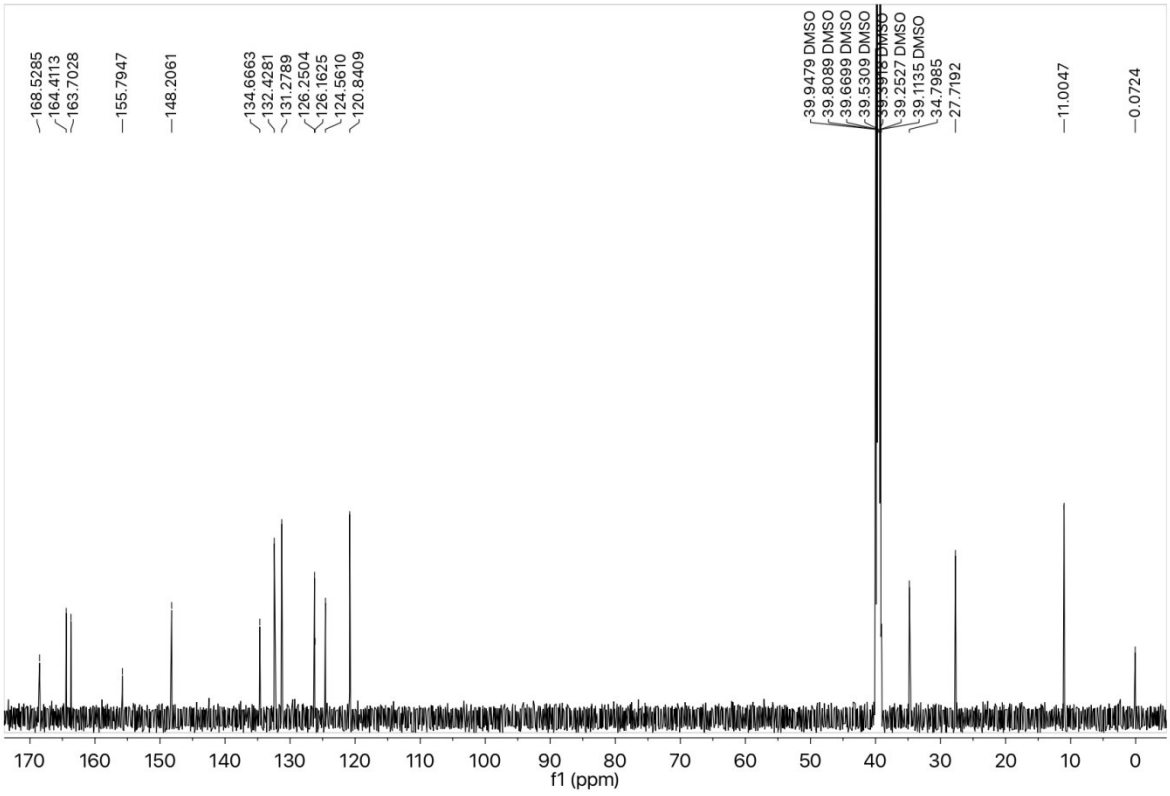


Fig. S19 ^{13}C -NMR spectrum of **8h**

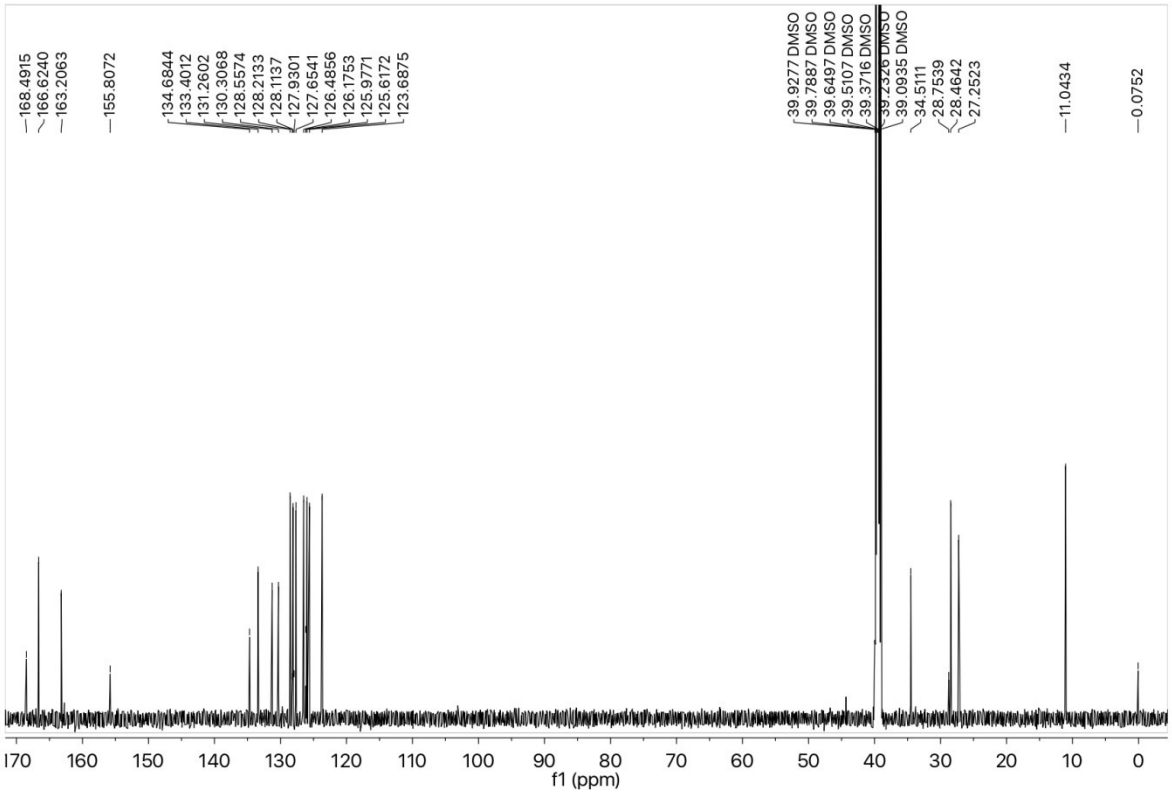


Fig. S20 ^{13}C -NMR spectrum of **8i**

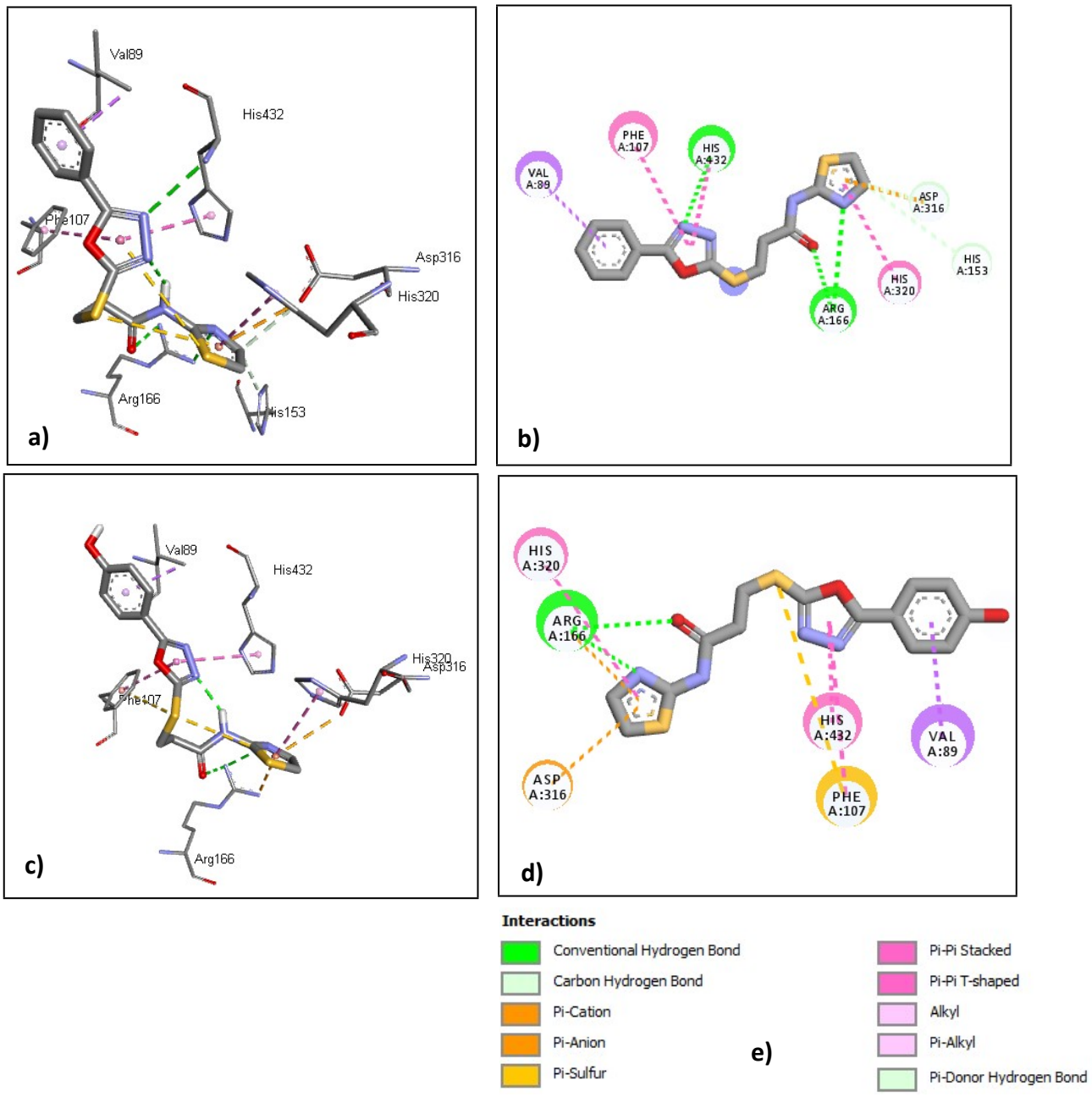


Fig. S21 The diagram shows 3D structure of **8a** and **8b** (a & c). 2D Binding interactions of compounds **8a** and **8b** (b and d). The types of interactions are shown below (e) with allosteric site of human alkaline phosphatase.

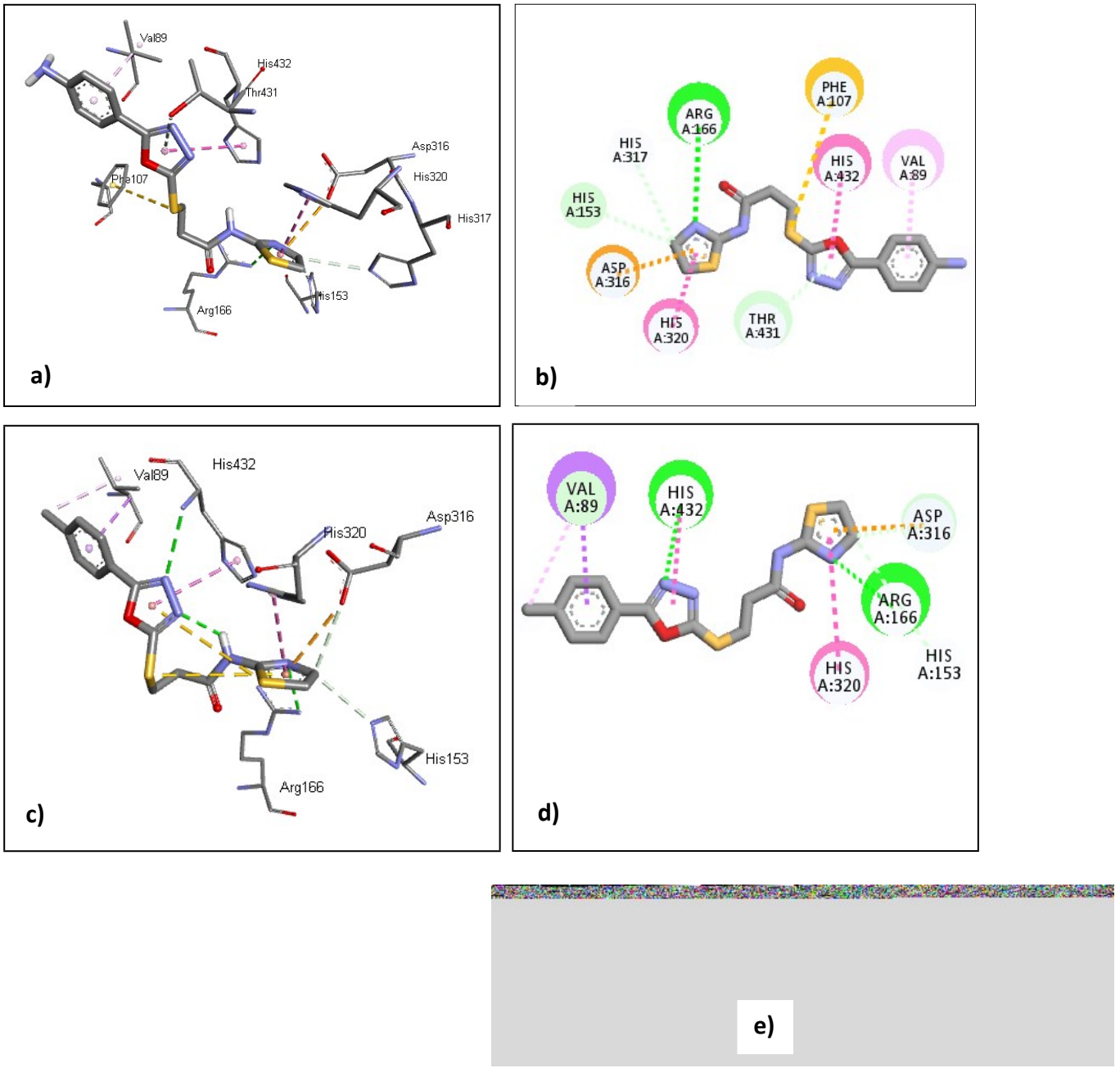


Fig. S22 The diagram shows the 3D structure of **8c** and **8d** (a & c). 2D Binding interactions of compounds **8c** and **8d** (b and d). The types of interactions are shown below (e) with allosteric site of human alkaline phosphatase.

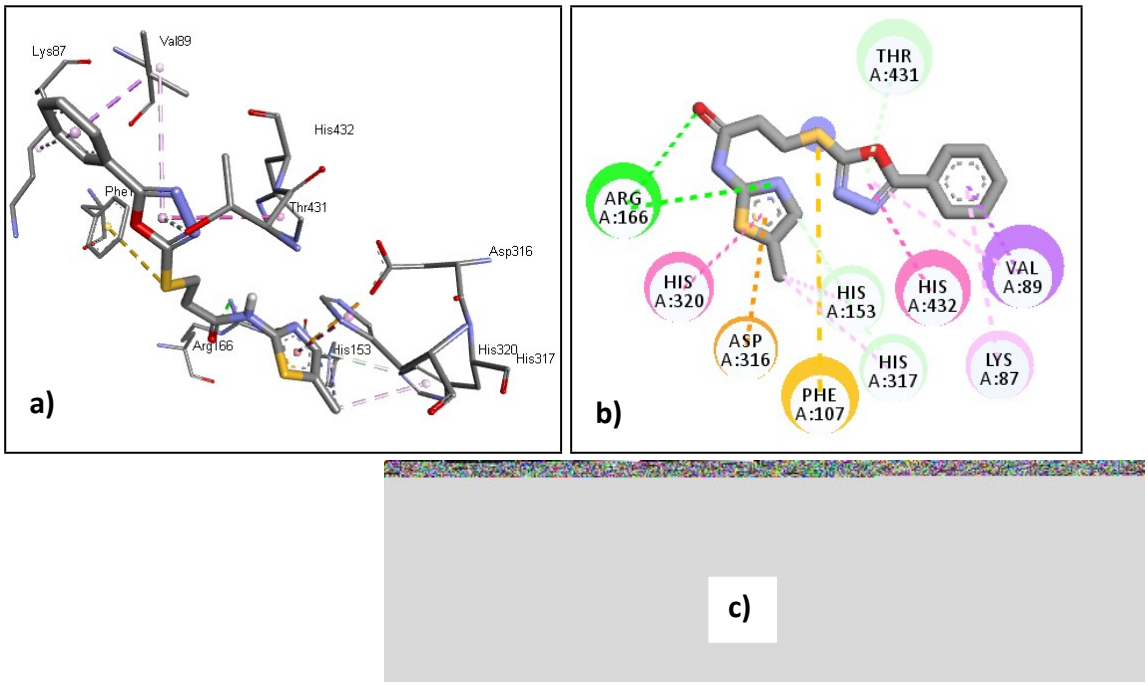


Fig. S23 The diagram shows the hydrogen donor (purple) and (green) hydrogen acceptor regions of compounds **8e** (a), and 2D binding interactions of compounds **8e** (b). The types of interactions are shown below (c) with allosteric site of human alkaline phosphatase.