

Supplementary Information for

Experimental and Theoretical Investigation of the Coordination of 8-hydroxquinoline Inhibitors to Biomimetic Zinc Complexes and Histone Deacetylase (HDAC) 8

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Enzyme Sequence and SDS-Pages Images

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1  MEEPEEPADSGQSLVPVYIYSPEYVSMCDLAKIPKRASMVHSLIEAYALHKQMRIVKPK 60
61  VASMEEMATFHTDAYLQHLQKVSQEGDDHPDSIEYGLGYDCPATEGIFDYAAAIGGATI 120
121 TAAQCLIDGMCKVAINWSGGWHHAKKDEASGFCYLNDAVLGILRLRRKFERILYVDLDLH 180
181 HGDGVEDAFSFTSKVMTVSLHKFSPGFFPGTGDVSDVGLGKGRYYSVNVPIQDGIQDEKY 240
241 YQICESVLKEVYQAFNPKAVVLQLGADTIAGDPMCSFNMTVPVGIGKCLKYILQWQLATLI 300
301 LGGGGYNLANTARCWTYLTGVILGKTLSSSEIPDHEFFTAYGPDYVLEITPSCRPRNEPH 360
361 RIQQILNYIKGNLKHVV 377
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Figure S1: Amino acid sequence of human histone deacetylase 8

Figure S1 shows the amino acid sequence of human HDAC8 and can be accessed from the Uniprot code: Q9BY41. The sequence is 277 amino acids long and was back translated to codons optimized for expression in *E. coli* using the online bioinformatics software Benchling.¹

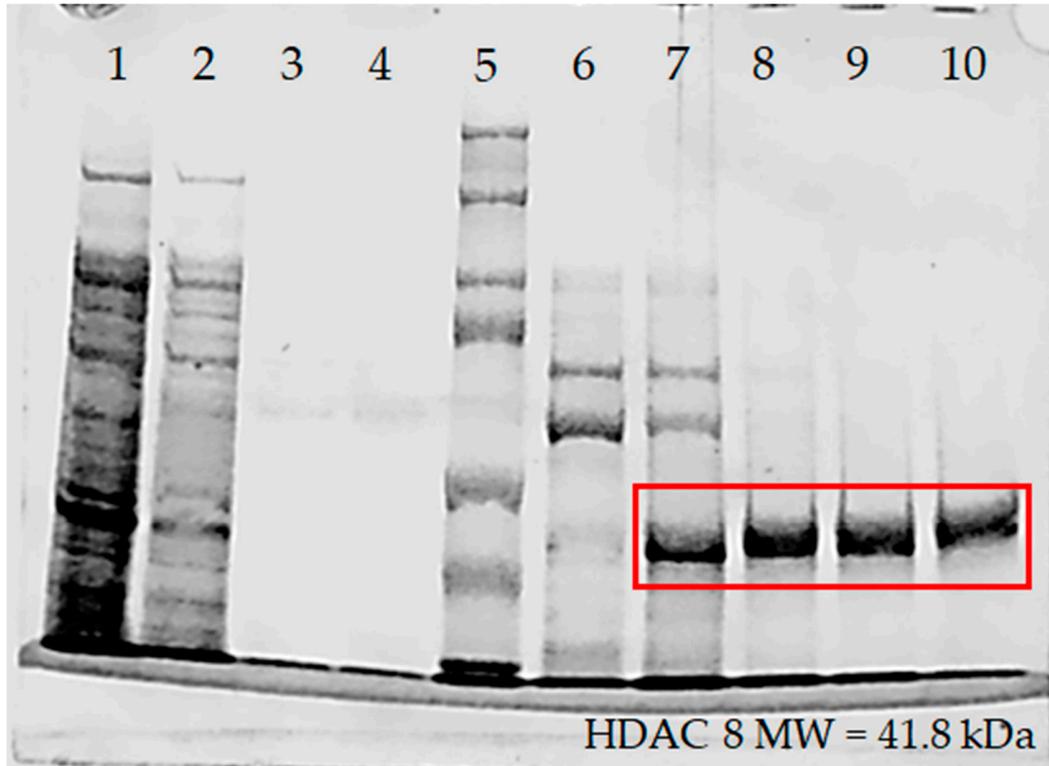


Figure S2: SDS-PAGE showing FPLC run from the original purification protocol

Figure S2 shows the SDS-PAGE corresponding to an FPLC run performed using the original expression and purification protocol. Lanes from left to right are as follows: 1) loaded sample, 2) loading and wash flowthrough, 3) 100 mM imidazole wash fraction 2, 4) fraction 3, 5) ladder, 6) 300 mM elution fraction 4, 7) fraction 5, 8) fraction 6, 9) fraction 7, and 10) fraction 8.

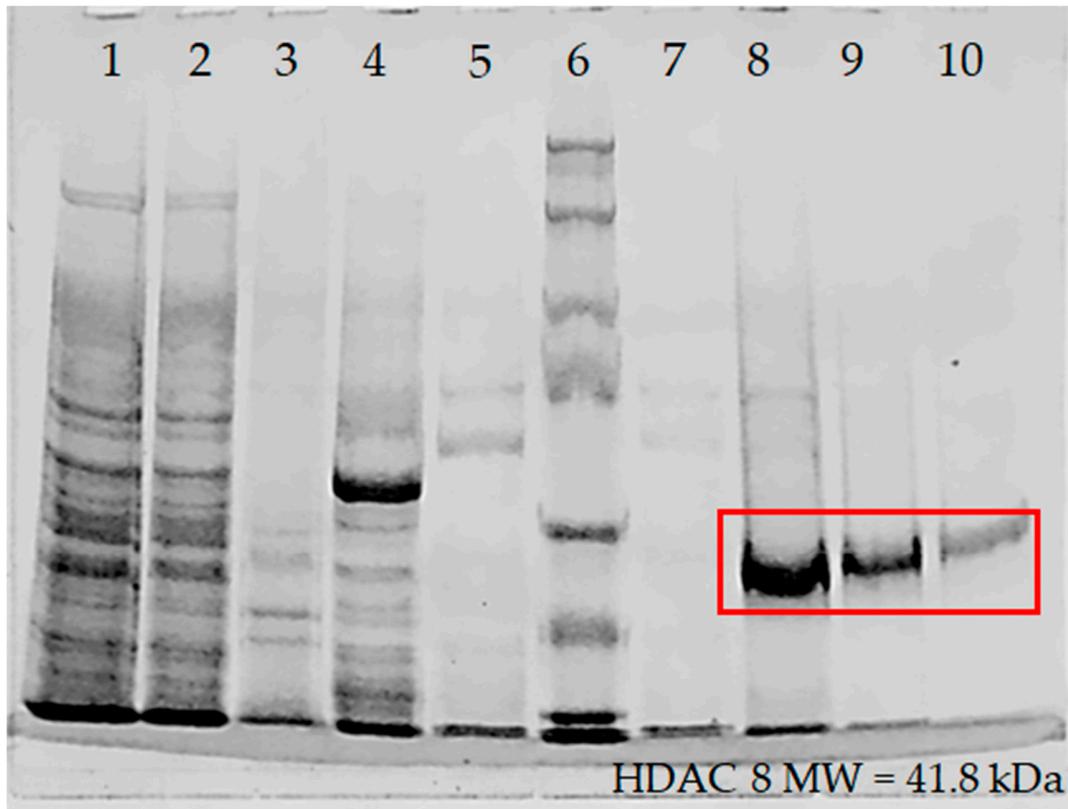


Figure S3: SDS-PAGE showing FPLC run from the modified purification protocol

Figure S3 shows the SDS-PAGE corresponding to an FPLC run performed using the modified expression and purification protocol. Lanes from left to right are as follows: 1) loaded sample, 2) loading and wash flowthrough, 3) insoluble fraction, 4) 100 mM imidazole wash fraction 2, 5) fraction 3, 6) ladder, 7) fraction 4, 8) 300 mM elution fraction 7, 9) fraction 8, and 10) fraction 9.

NMR Data for TpZn(X) species

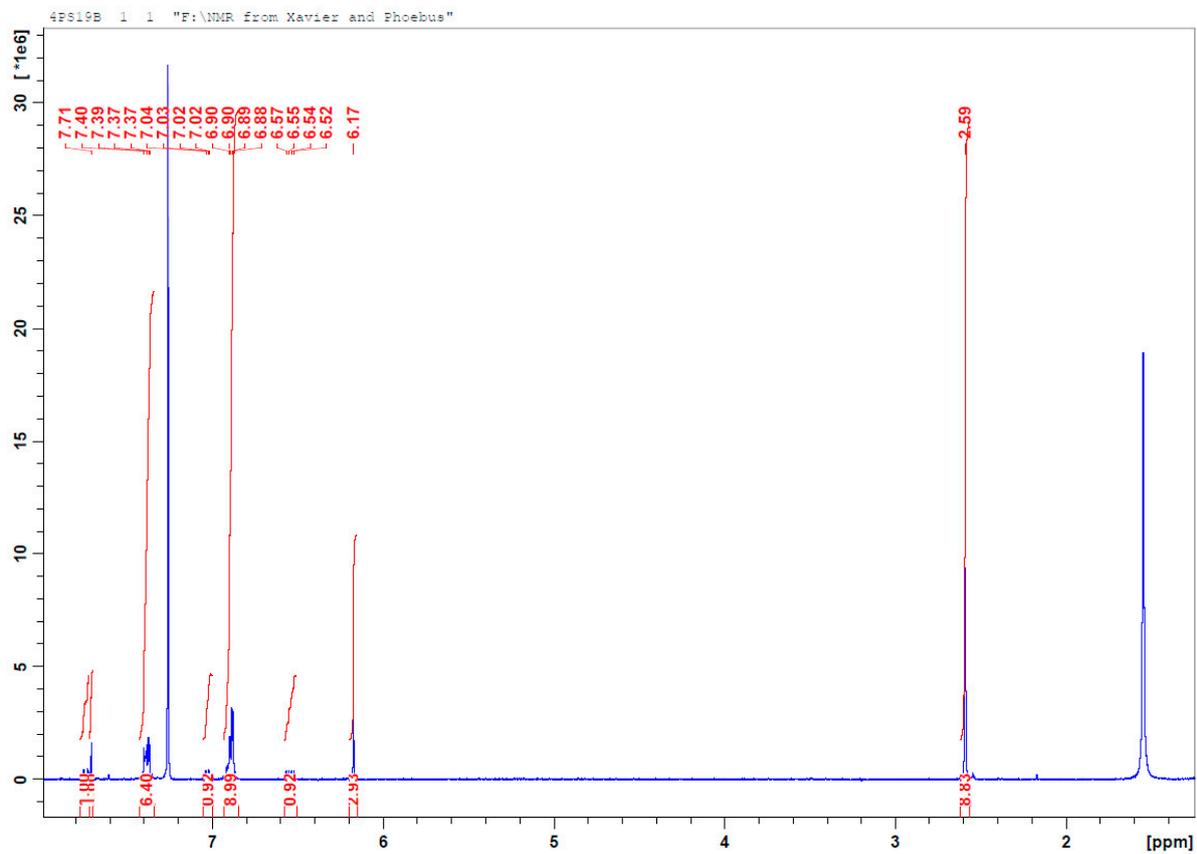


Figure S4. NMR spectrum of TpZn(B-H) in CDCl₃ at 300 MHz.

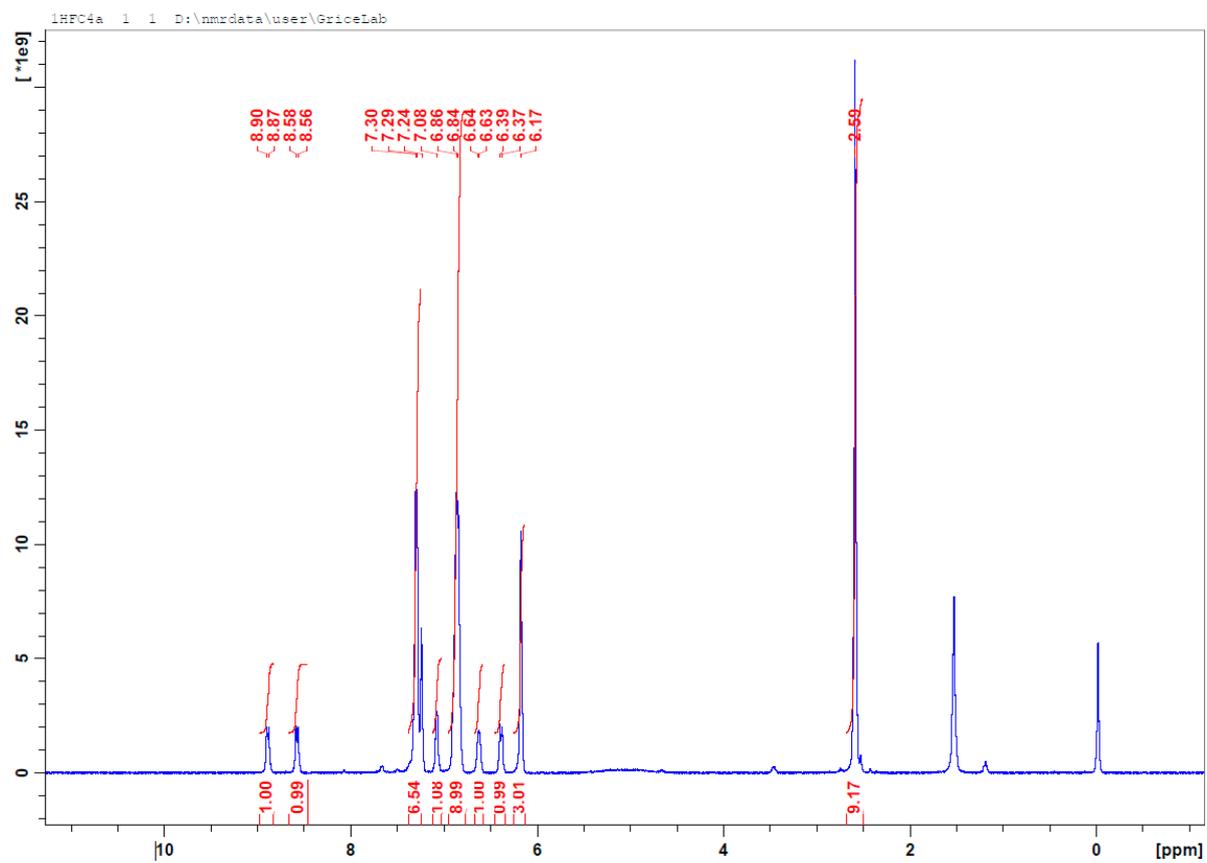


Figure S5. NMR spectrum of $\text{TpZn}(\text{C-H})$ in CDCl_3 at 400 MHz.

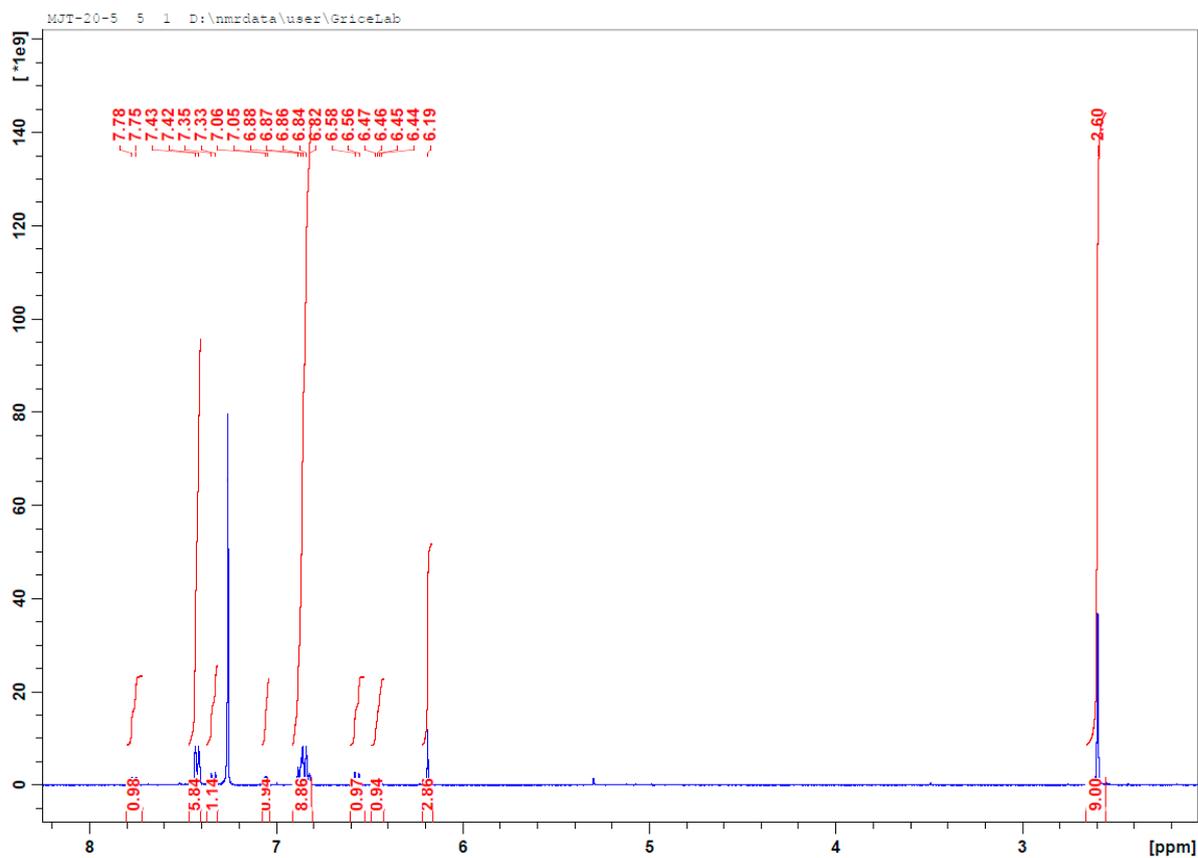


Figure S6. NMR spectrum of TpZn(D-H) in CDCl₃ at 400 MHz.

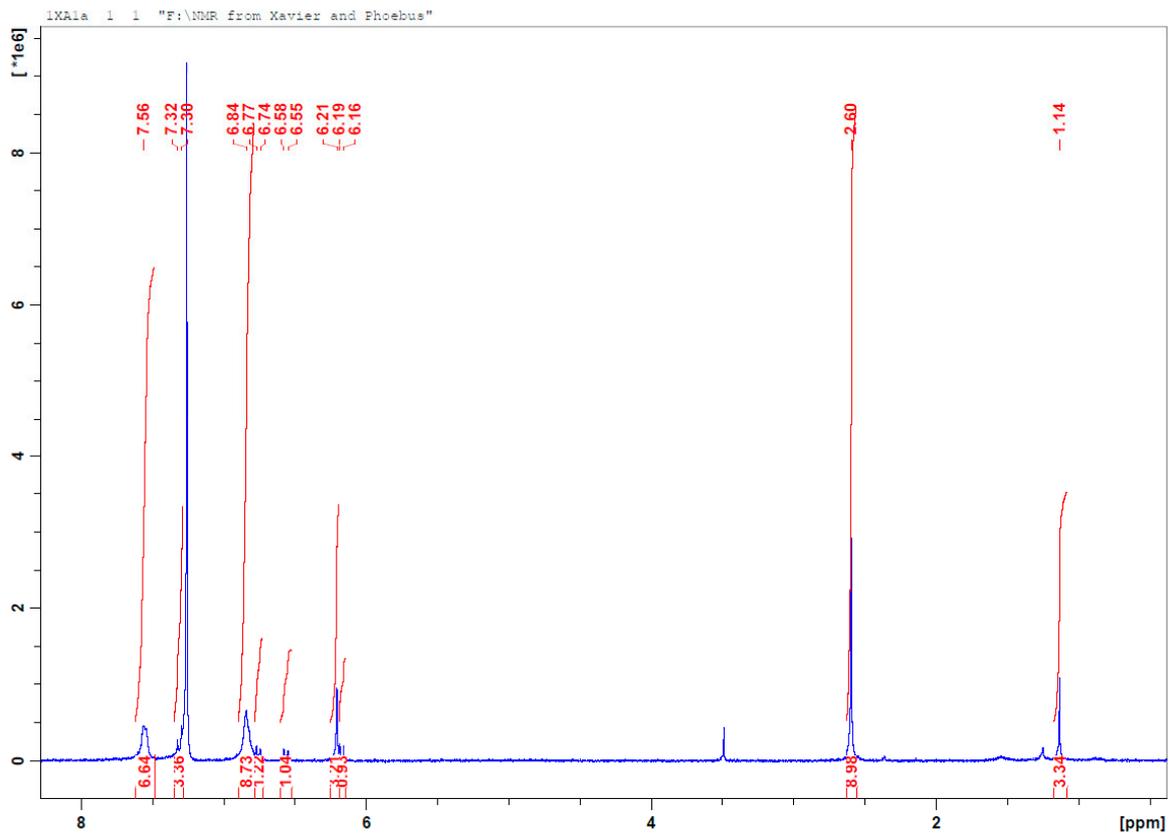


Figure S7. NMR spectrum of TpZn(E-H) in CDCl₃ at 300 MHz.

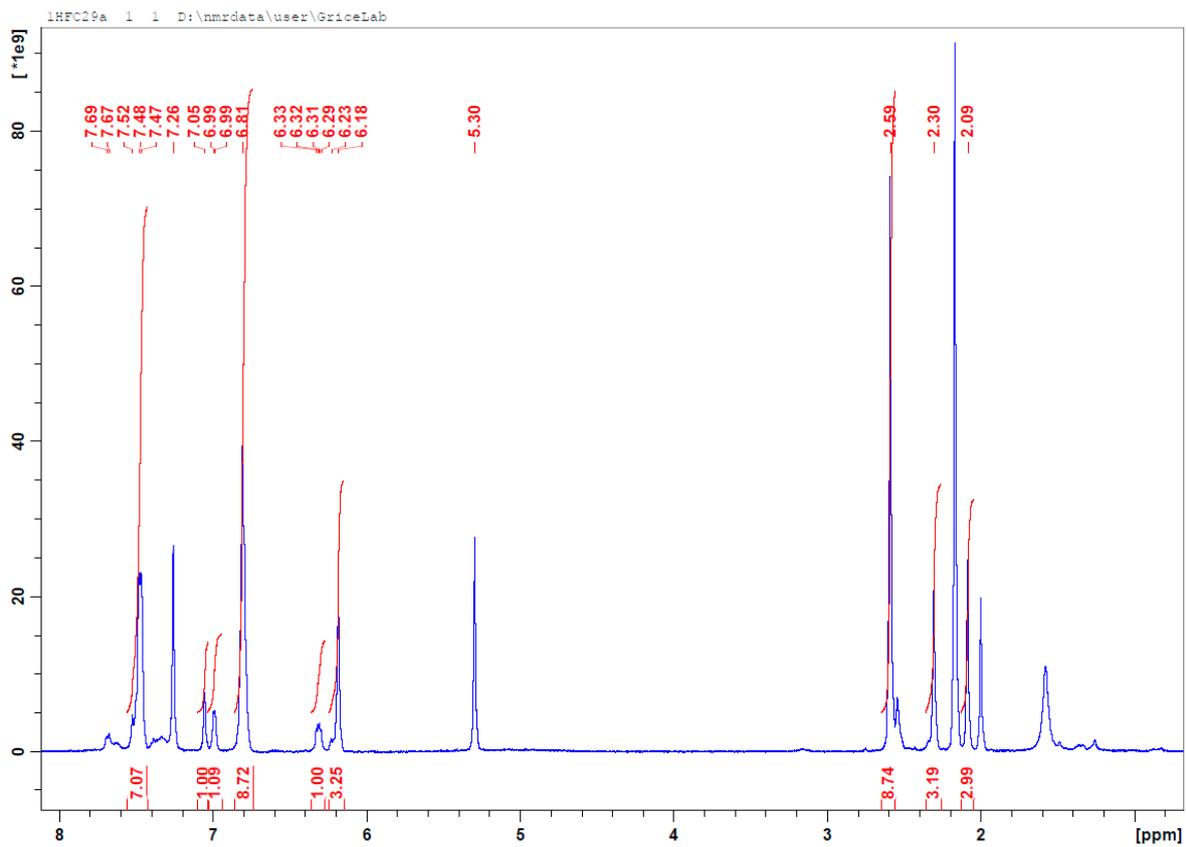


Figure S8. NMR spectrum of TpZn(F-H) in CDCl₃ at 400 MHz.

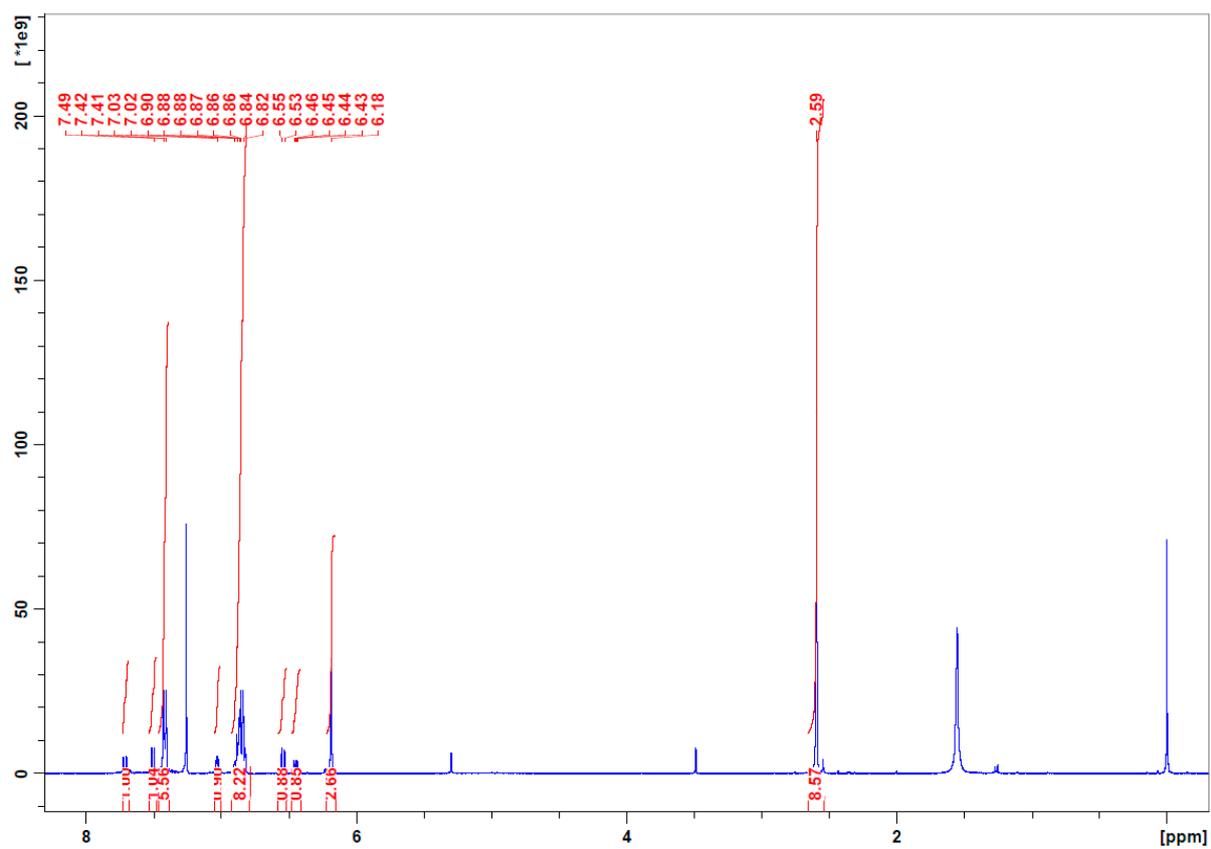


Figure S9. NMR spectrum of TpZn(G-H) in CDCl_3 at 400 MHz.

References

- (1) Benchling. <https://www.benchling.com/> (accessed 2023)