

Supporting Information

Design, synthesis, *in vitro*, and *in silico* studies of 1,3,4-thiadiazole-thiazolidinone hybrids as carbonic anhydrase inhibitors

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Supporting Figure Captions:

Fig. S1: IR Spectrum of 7a

Fig. S2: ^1H NMR Spectrum of 7a

Fig. S3: ^{13}C NMR Spectrum of 7a

Fig. S4: IR Spectrum of 7b

Fig. S5: ^1H NMR Spectrum of 7b

Fig. S6: ^{13}C NMR Spectrum of 7b

Fig. S7: IR Spectrum of 7c

Fig. S8: ^1H NMR Spectrum of 7c

Fig. S9: ^{13}C NMR Spectrum of 7c

Fig. S10: IR Spectrum of 7d

Fig. S11: ^1H NMR Spectrum of 7d

Fig. S12: ^{13}C NMR Spectrum of 7d

Fig. S13: IR Spectrum of 7e

Fig. S14: ^1H NMR Spectrum of 7e

Fig. S15: ^{13}C NMR Spectrum of 7e

Fig. S16: IR Spectrum of 7f

Fig. S17: ^1H NMR Spectrum of 7f

Fig. S18: ^{13}C NMR Spectrum of 7f

Fig. S19: IR Spectrum of 7g

Fig. S20: ^1H NMR Spectrum of 7g

Fig. S21: ^{13}C NMR Spectrum of 7g

Fig. S22: IR Spectrum of 7h

Fig. S23: ^1H NMR Spectrum of 7h

Fig. S24: ^{13}C NMR Spectrum of 7h

Fig. S25: IR Spectrum of 7i

Fig. S26: ^1H NMR Spectrum of 7i

Fig. S27: ^{13}C NMR Spectrum of 7i

Fig. S28: IR Spectrum of 7j

Fig. S29: ^1H NMR Spectrum of 7j

Fig. S30: ^{13}C NMR Spectrum of 7j

Fig. S31: COSY Spectrum of 7e

Fig. S32: HSQC Spectrum of 7e

Fig. S33: HMBC Spectrum of 7e

Fig. S34: Ramachandran graph of carbonic anhydrase

Fig. S35: 2D-docking depiction of 7a complex against carbonic anhydrase

Fig. S36: 2D-docking depiction of 7b complex against carbonic anhydrase

Fig. S37: 2D-docking depiction of 7c complex against carbonic anhydrase

Fig. S38: 2D-docking depiction of 7d complex against carbonic anhydrase

Fig. S39: 2D-docking depiction of 7e complex against carbonic anhydrase

Fig. S40: 2D-docking depiction of 7f complex against carbonic anhydrase

Fig. S41: 2D-docking depiction of 7g complex against carbonic anhydrase

Fig. S42: 2D-docking depiction of 7h complex against carbonic anhydrase

Fig. S43: 2D-docking depiction of 7j complex against carbonic anhydrase

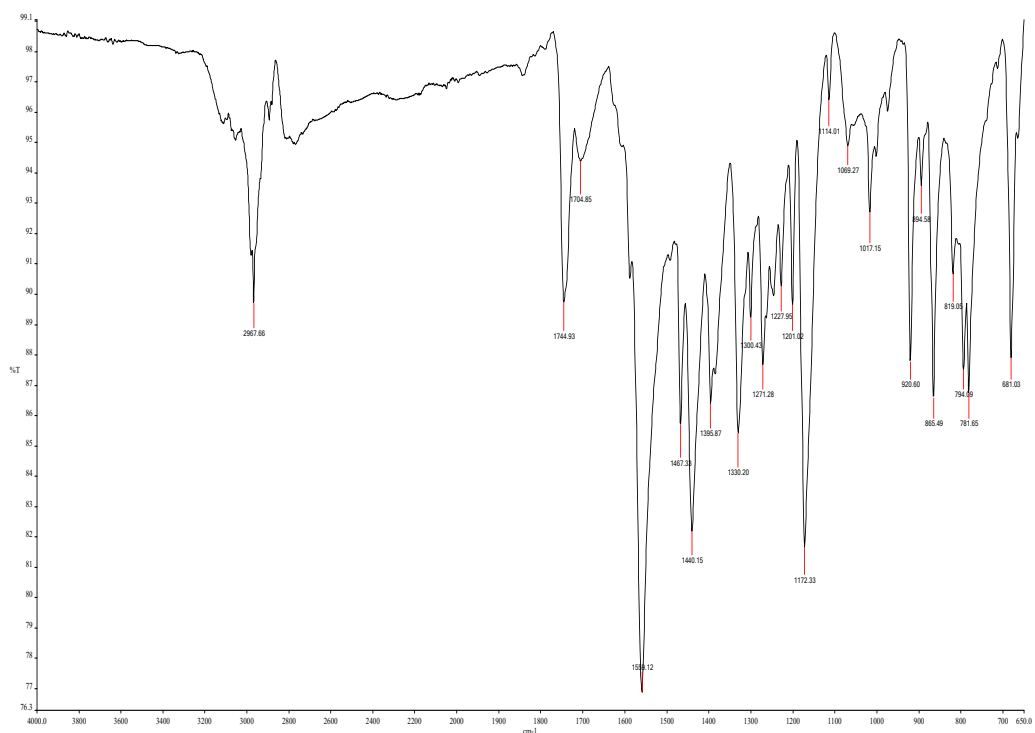


Fig. S1, ES‡

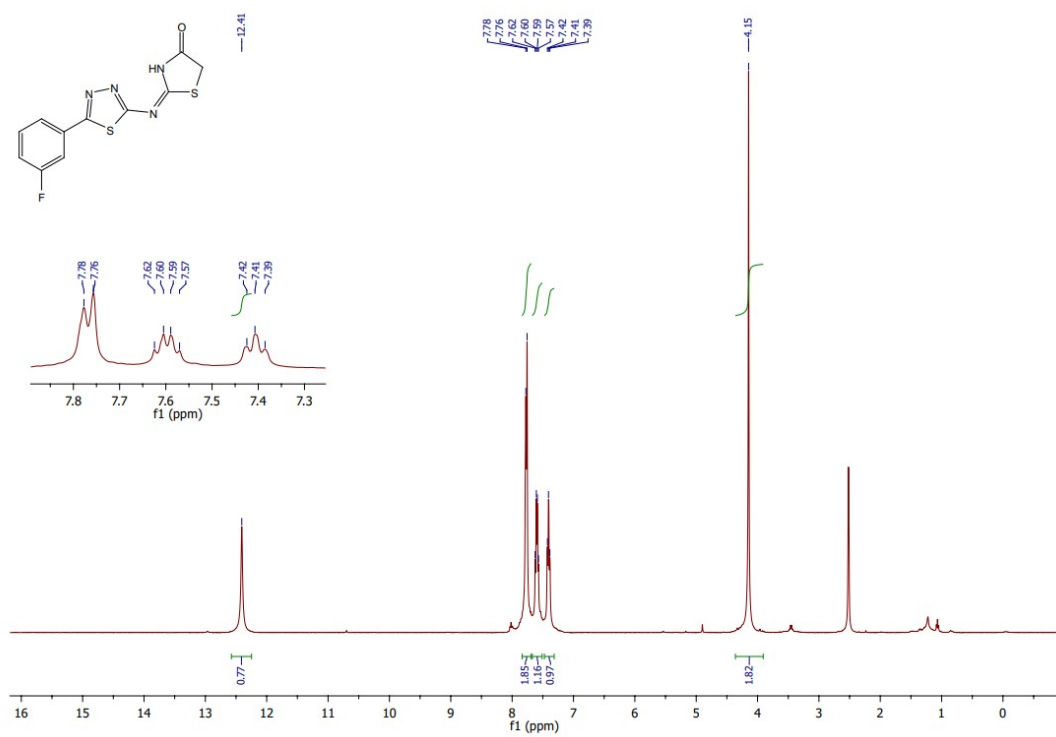


Fig. S2, ES‡

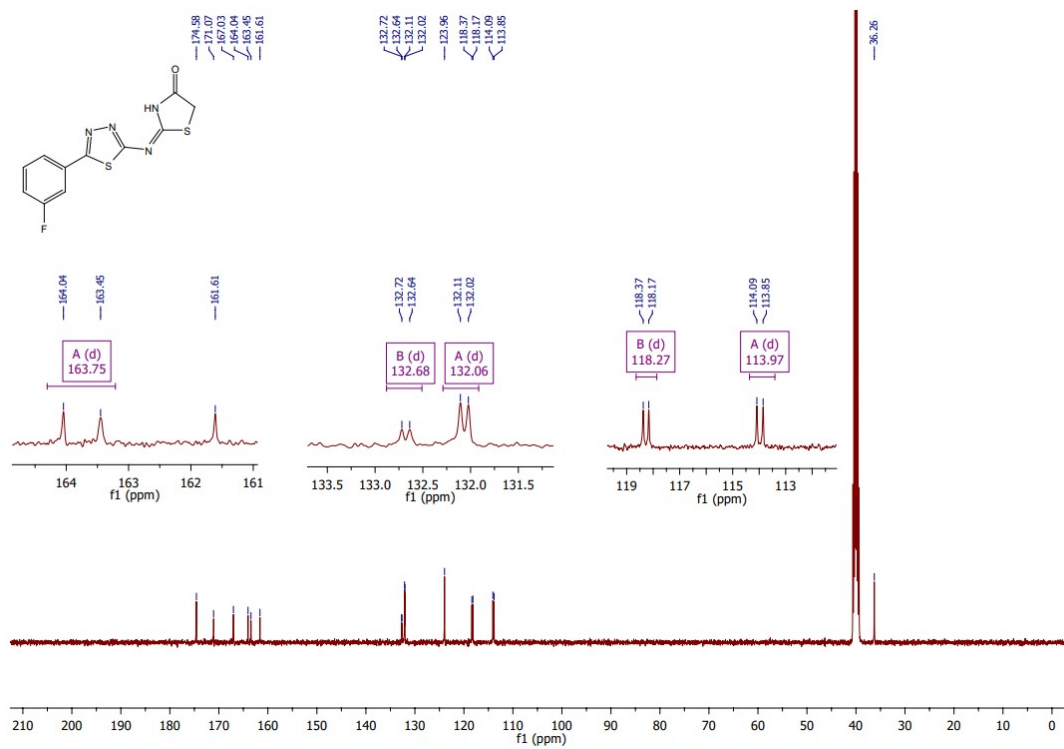


Fig. S3, ES†

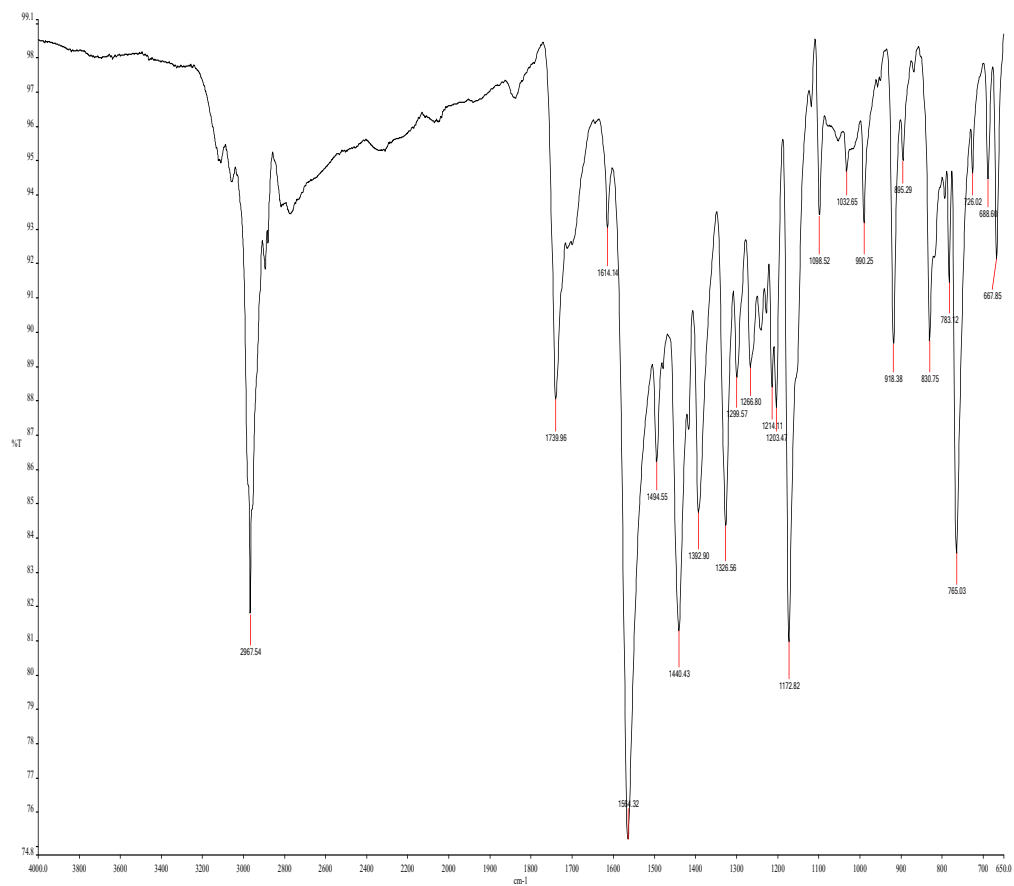


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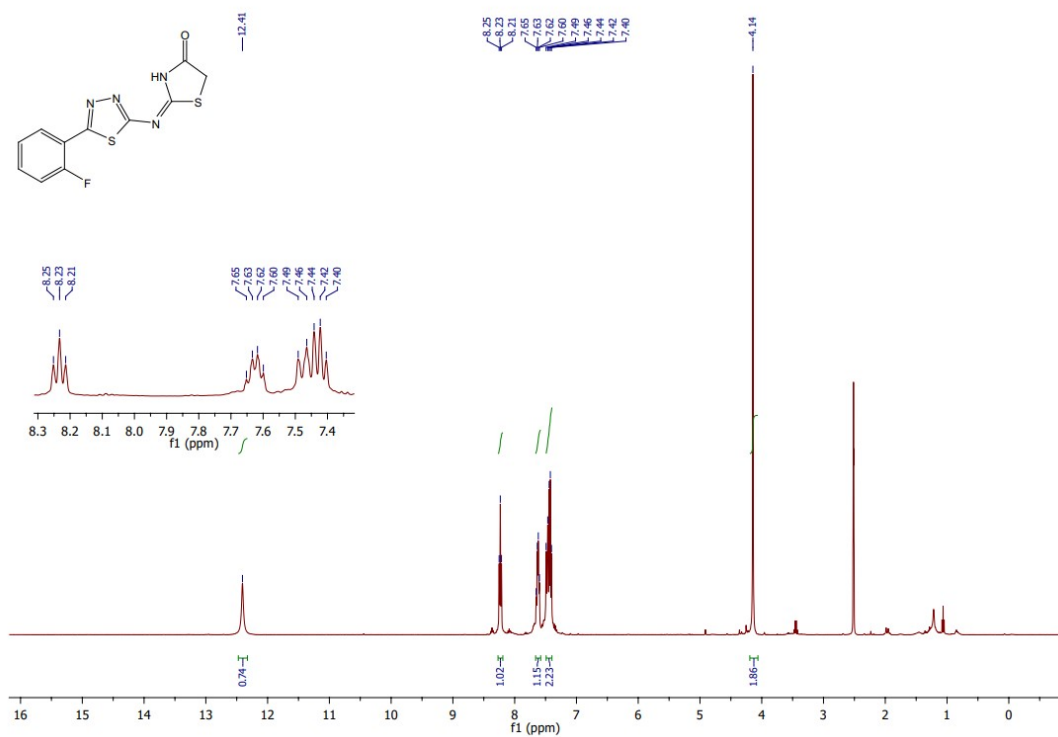


Fig. S5, ES†

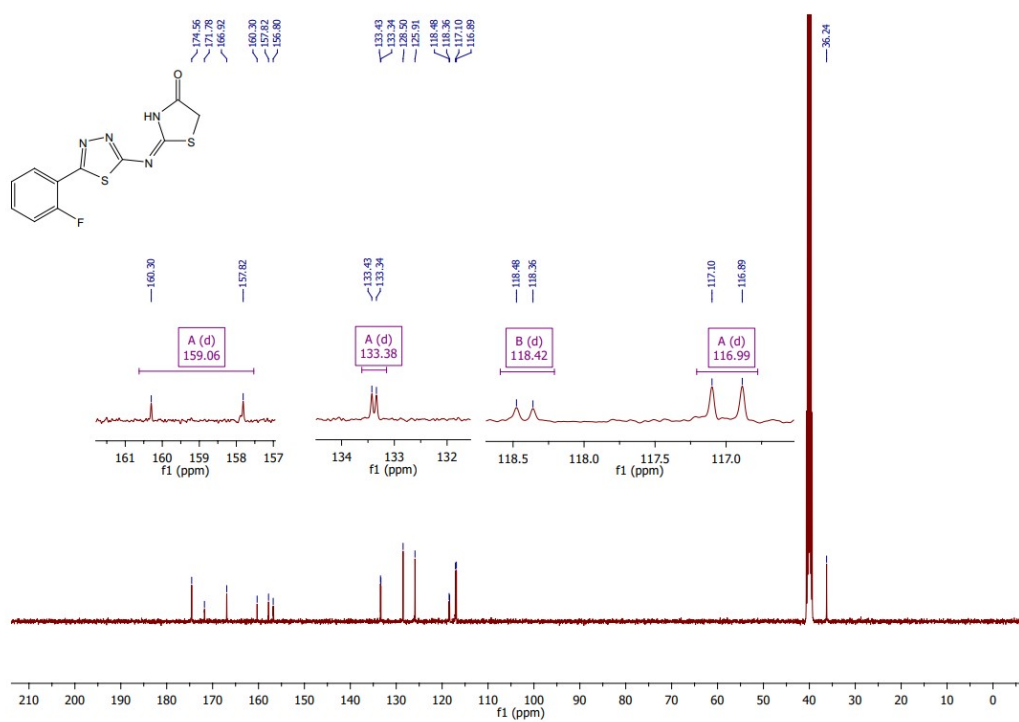


Fig. S6, ES†

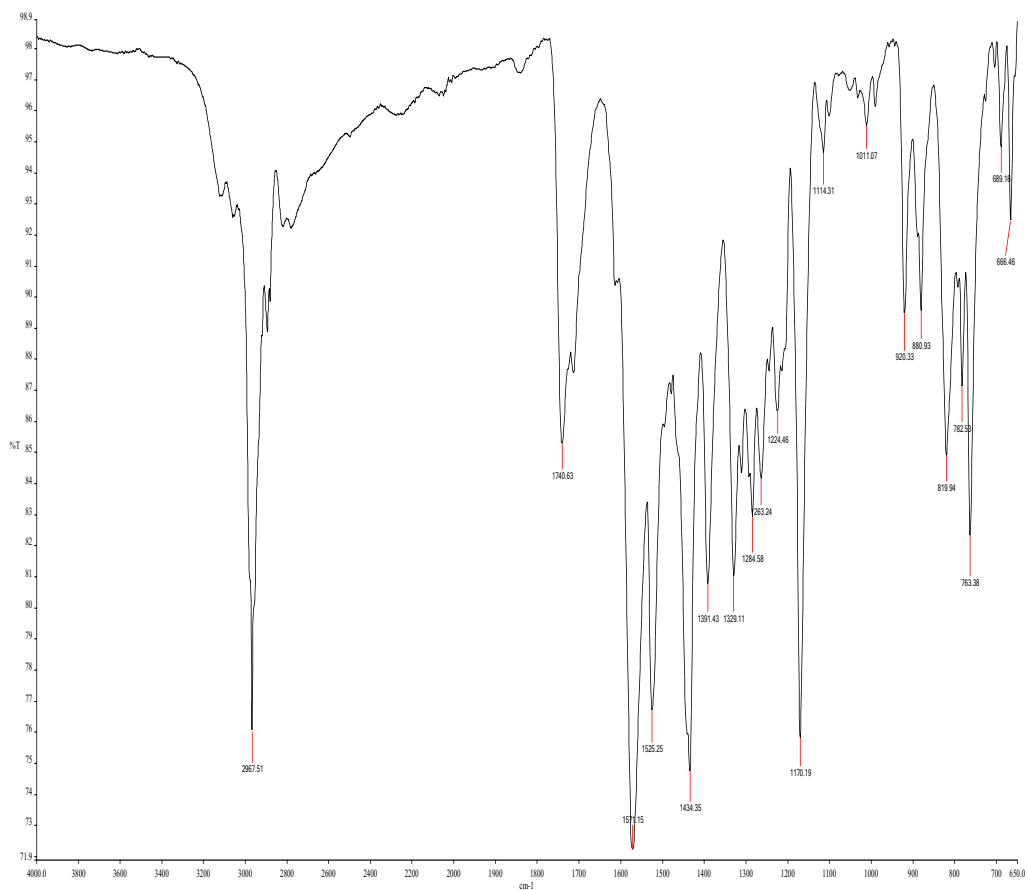


Fig. S7, ES†

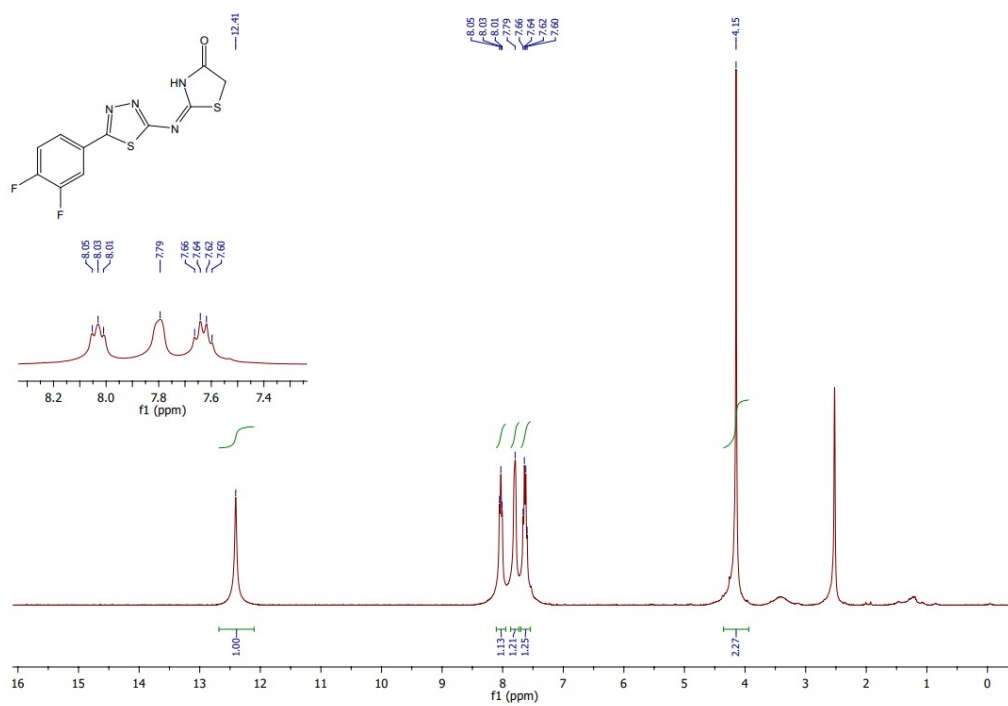


Fig. S8, ES†

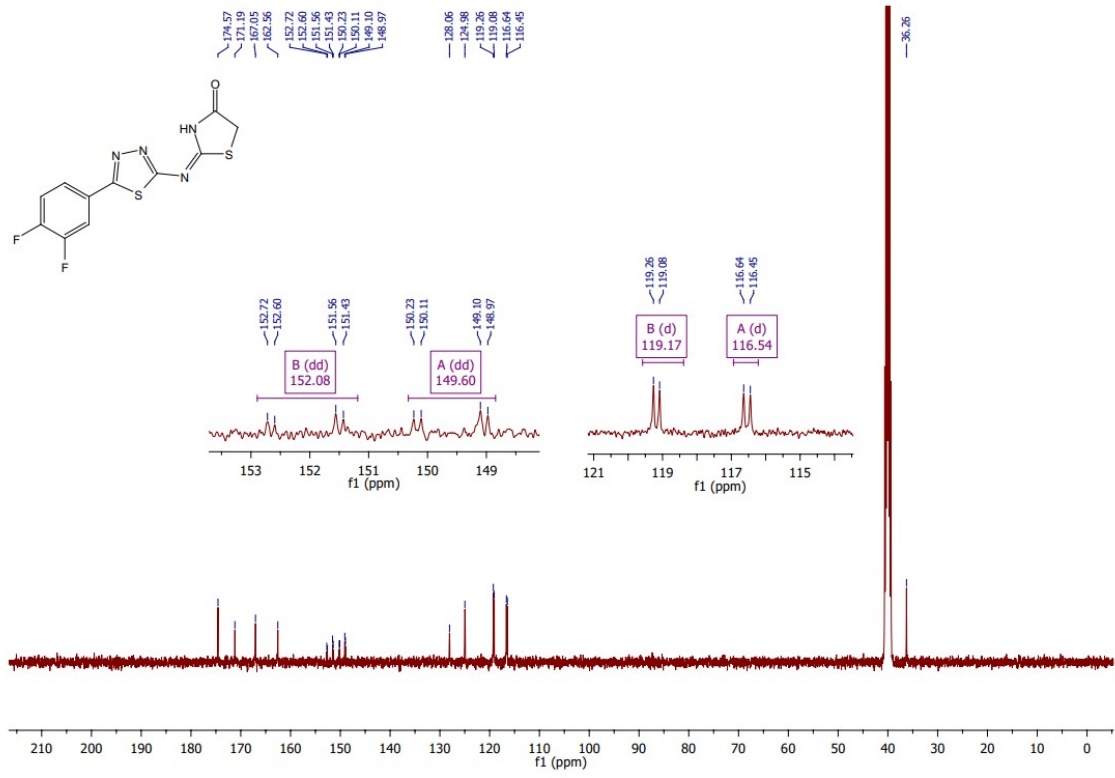


Fig. S9, ES†

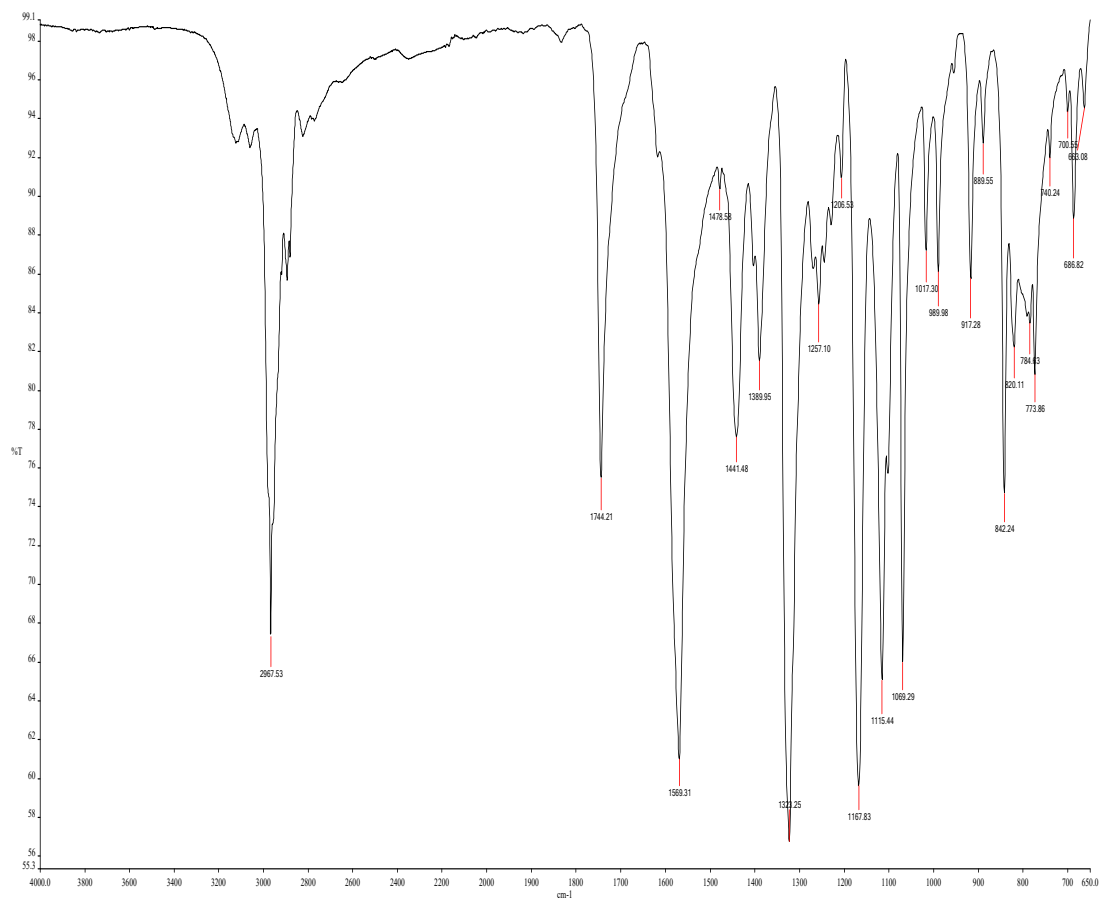


Fig. S10, ES†

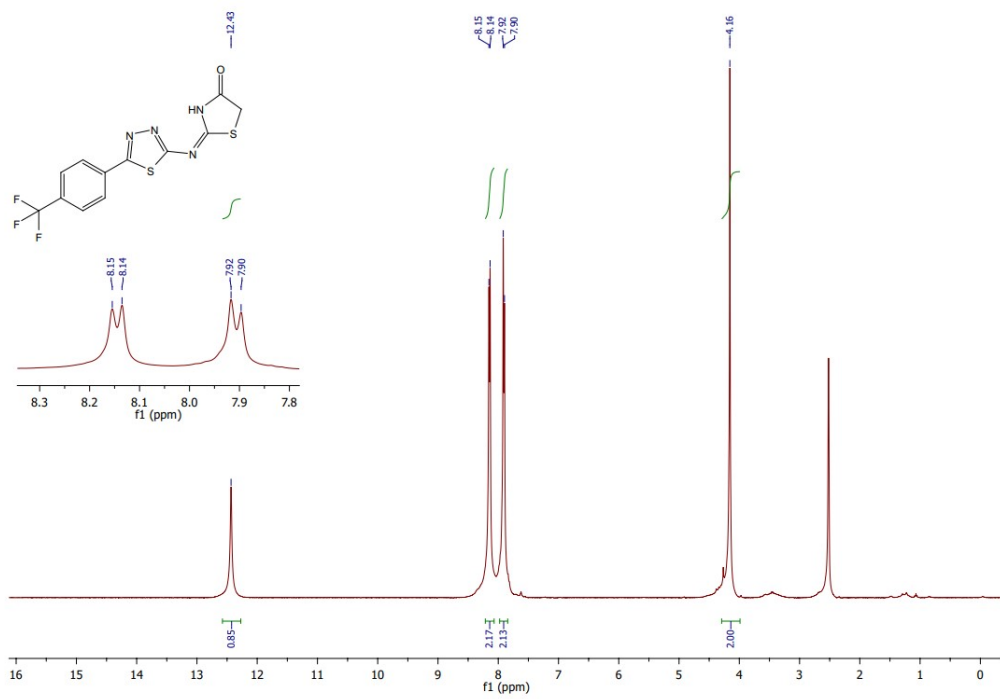


Fig. S11, ES†

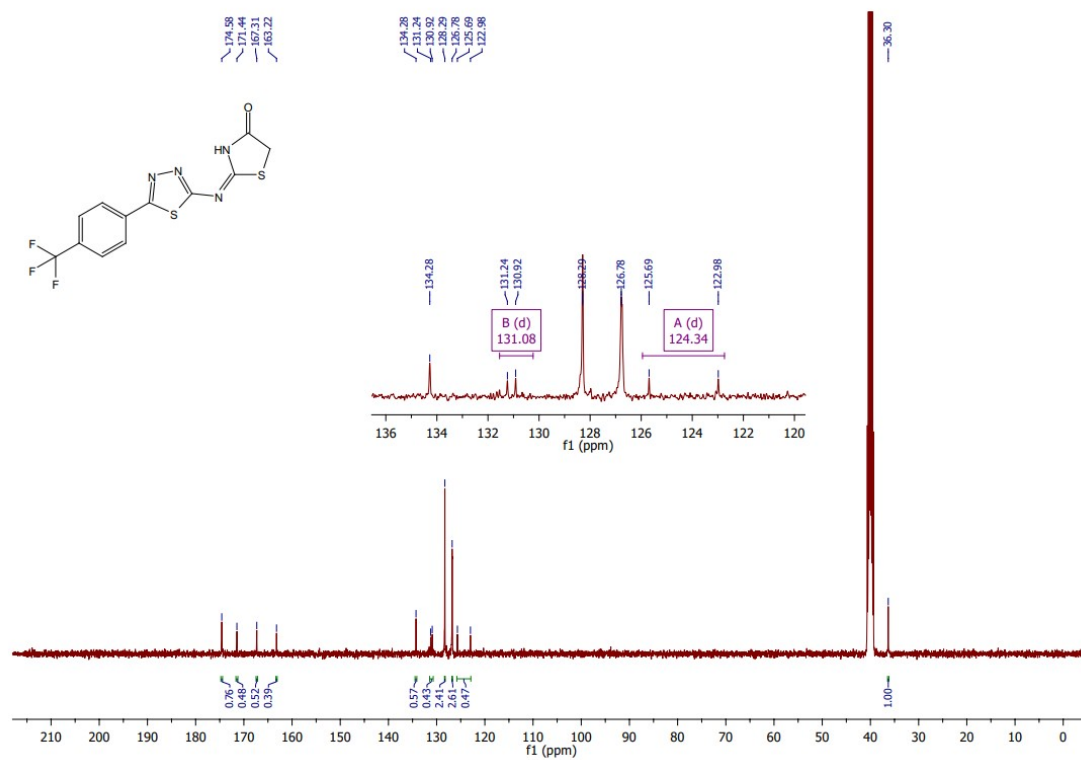


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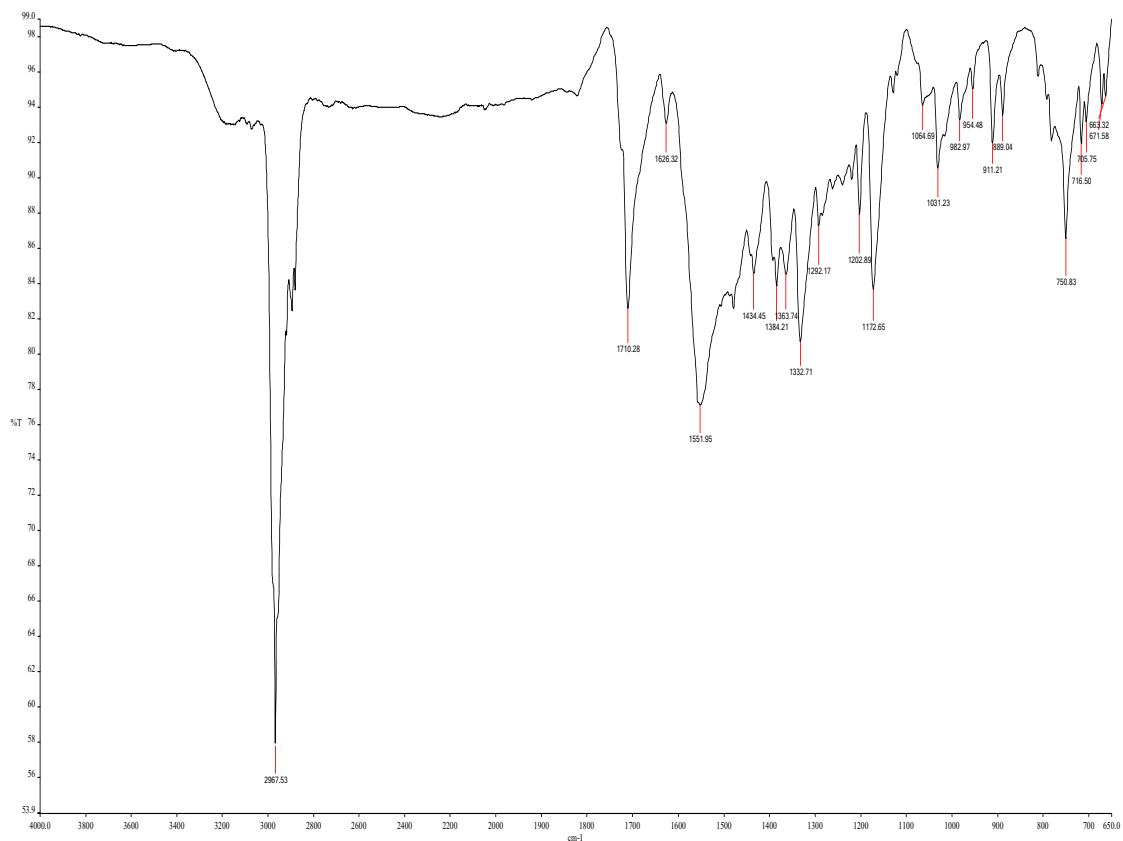


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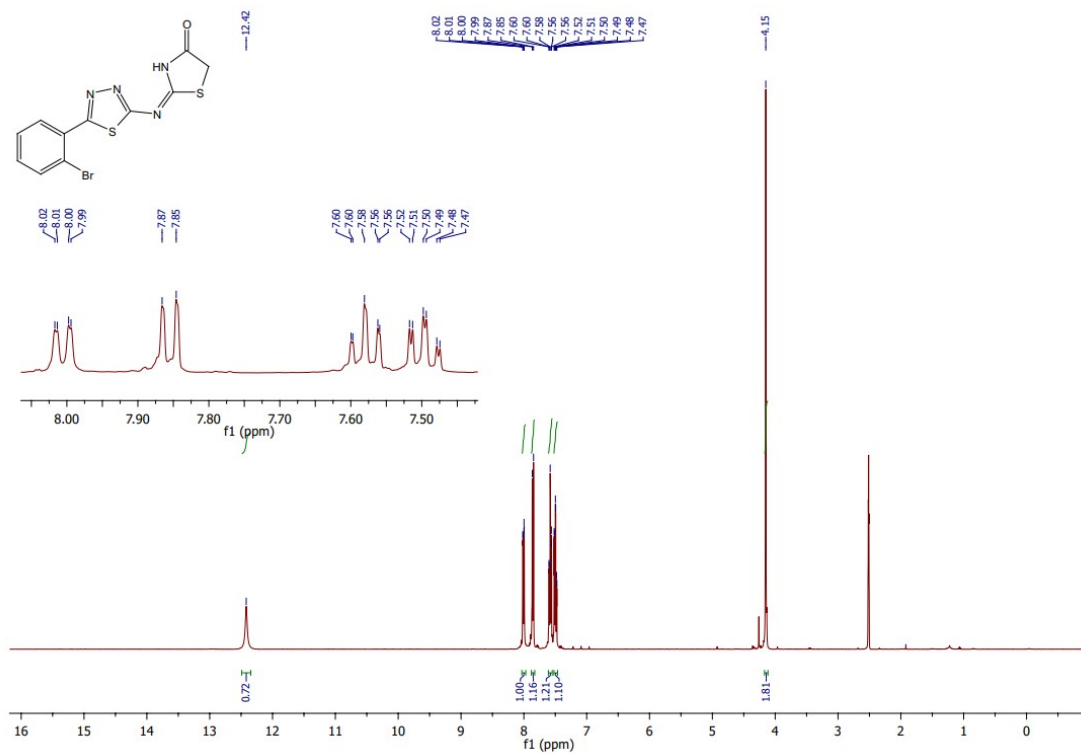


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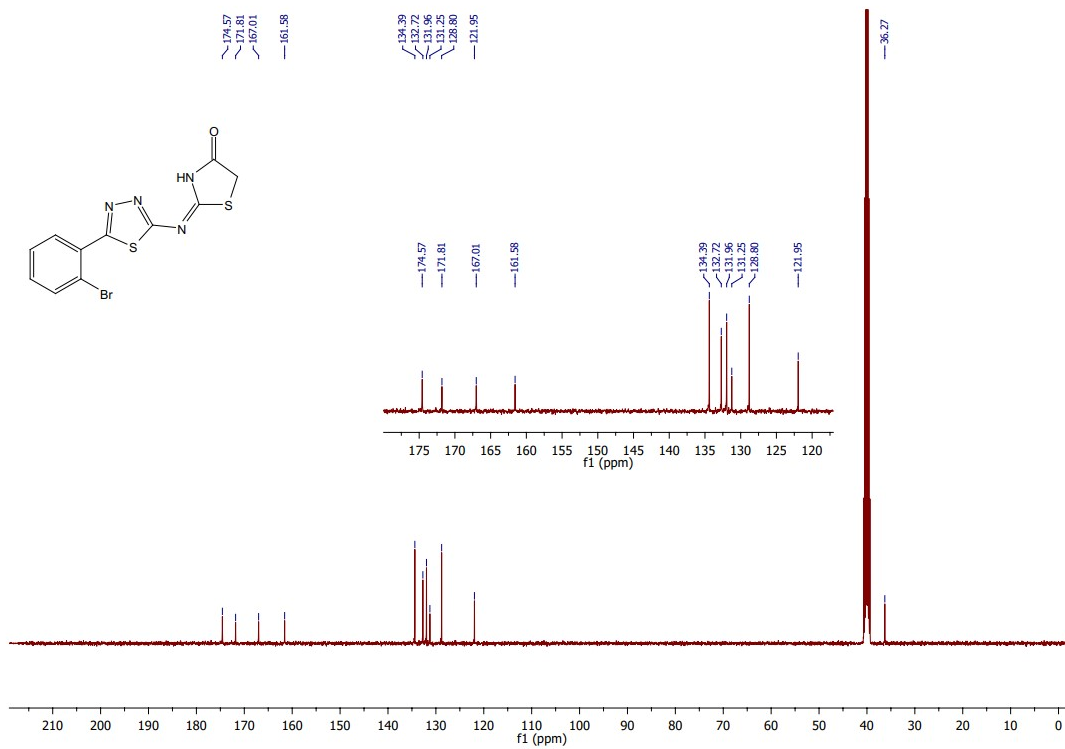


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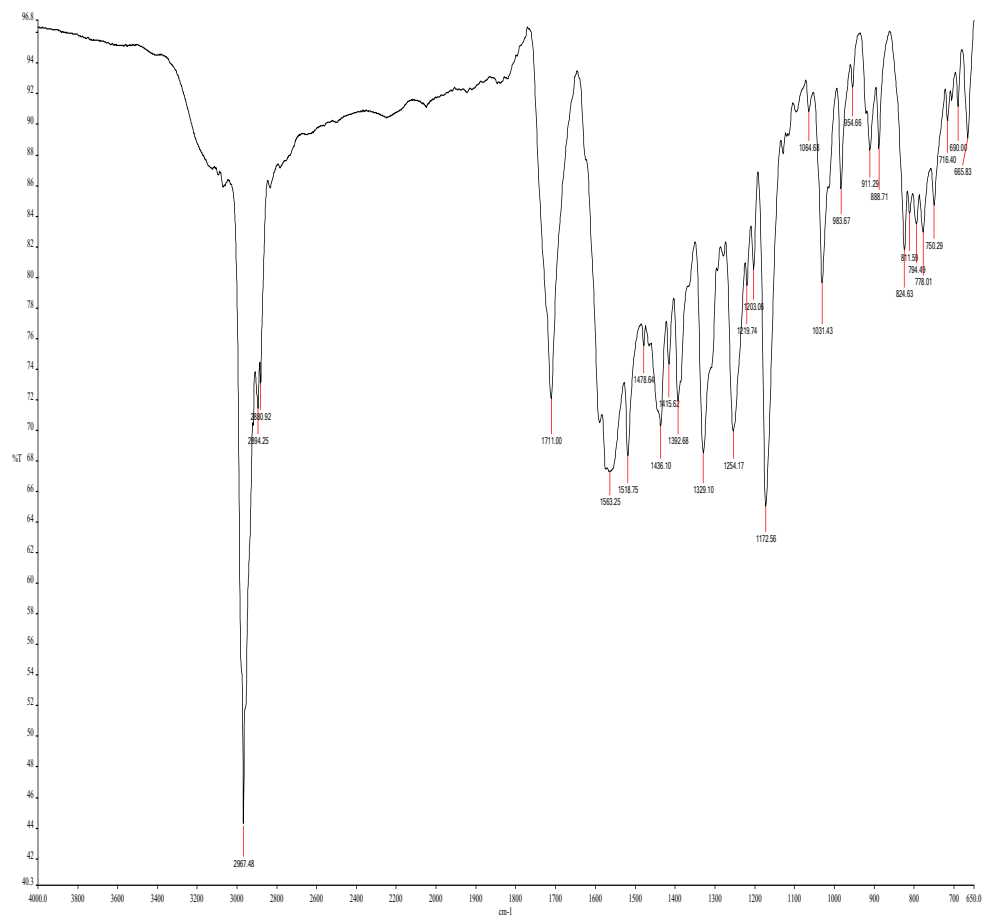


Fig. S16, ES⁺

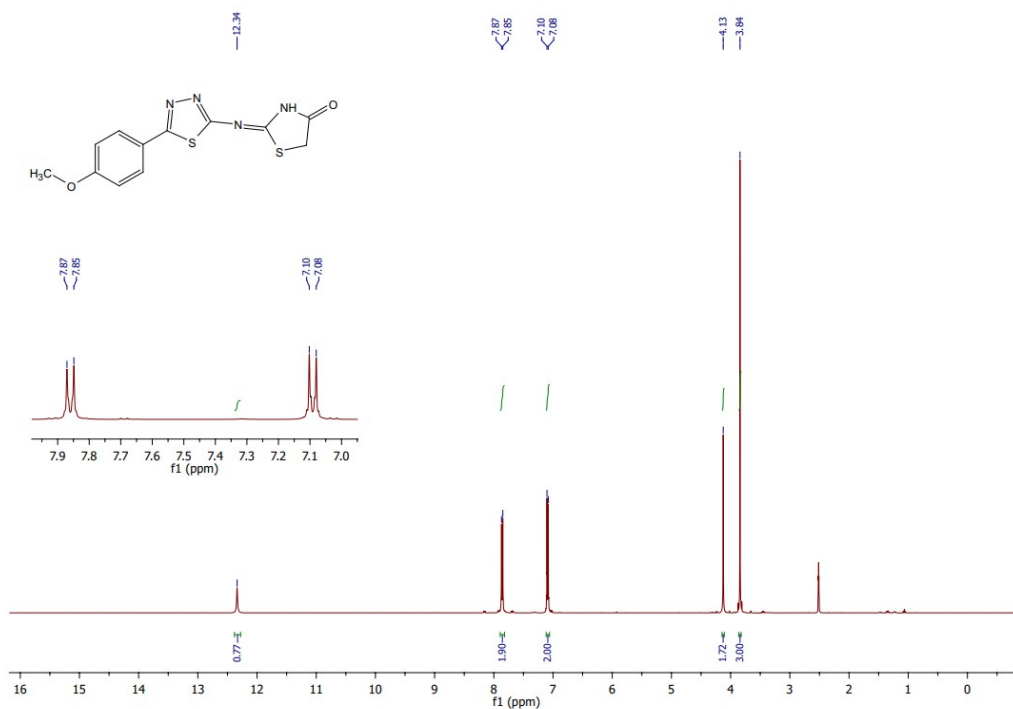


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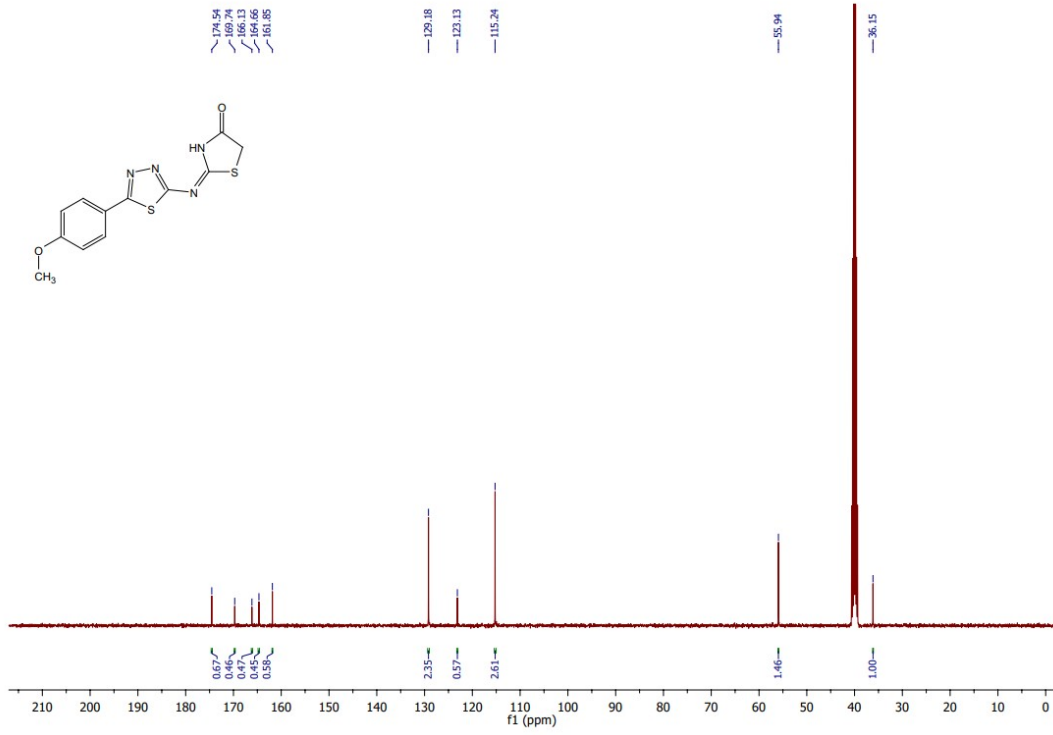


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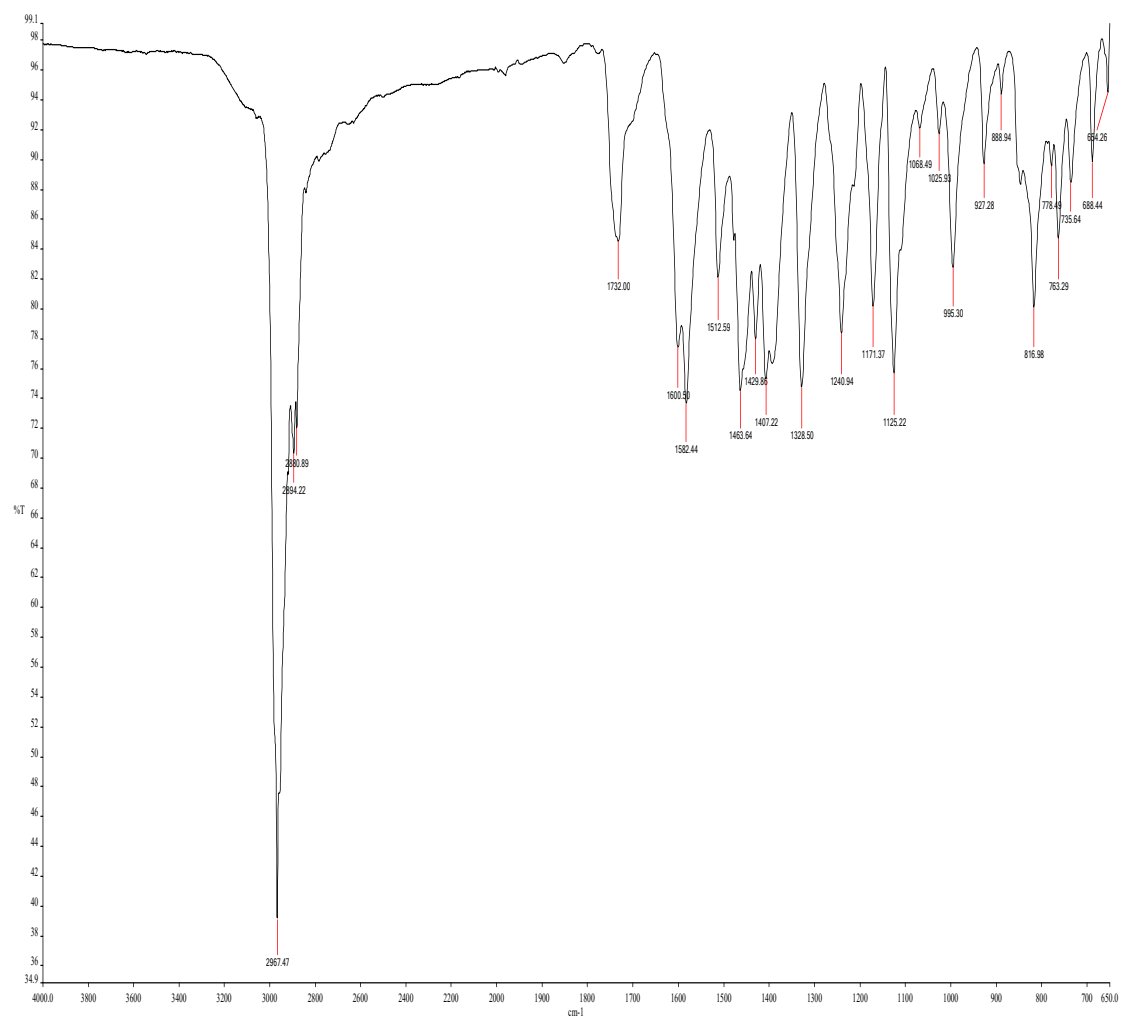


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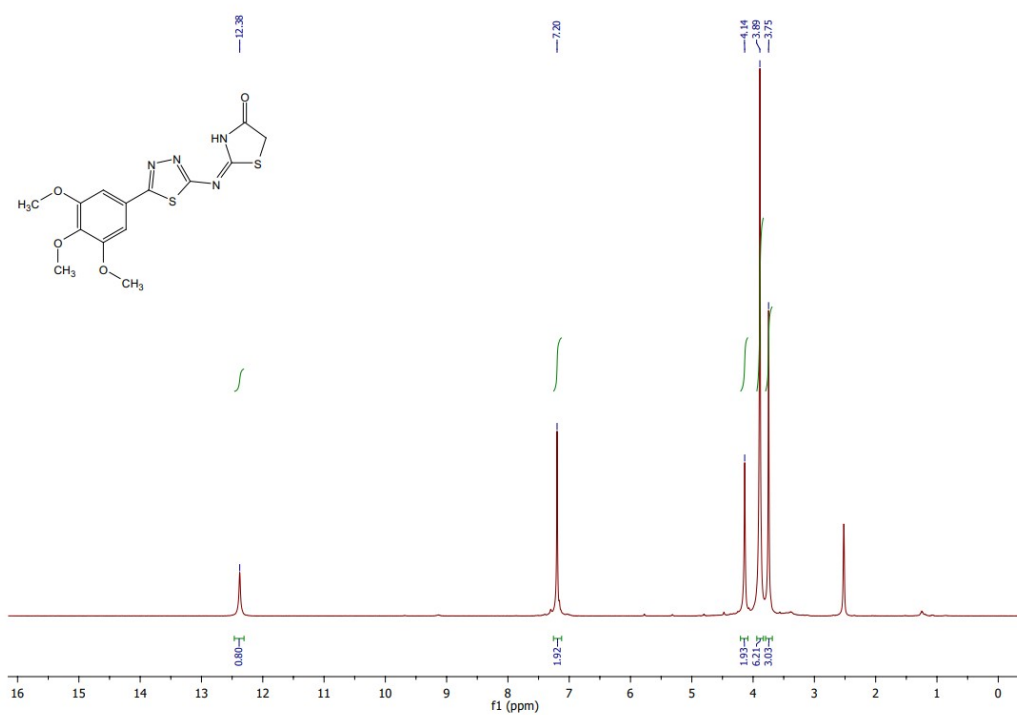


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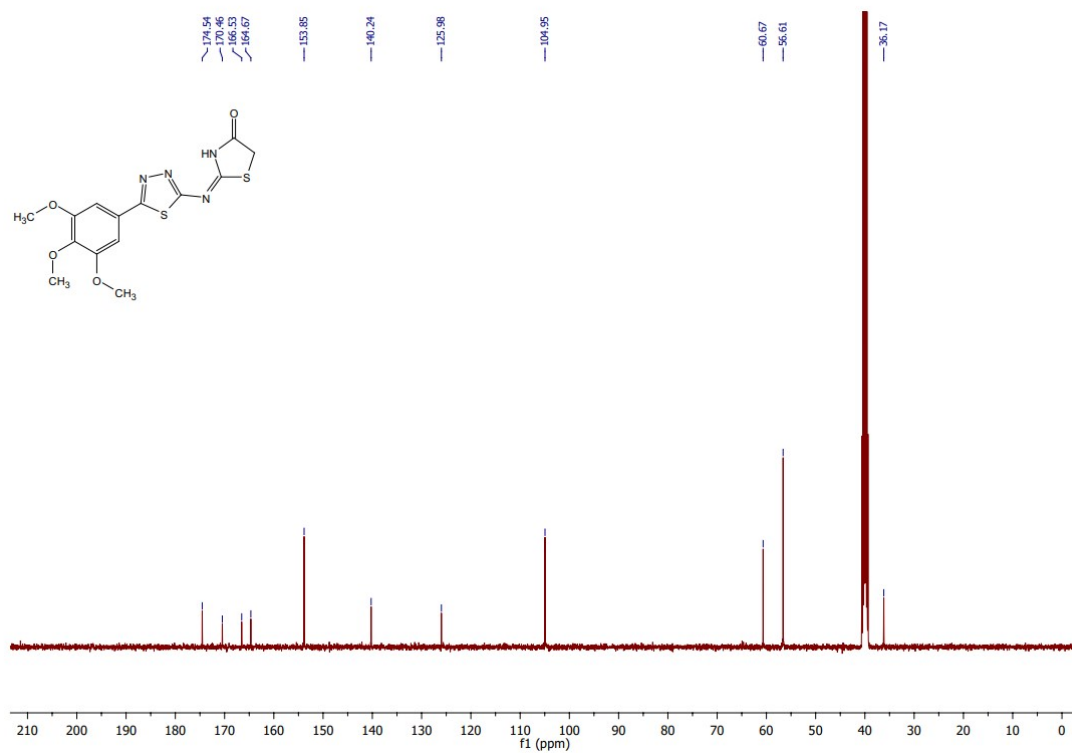


Fig. S21, ES†

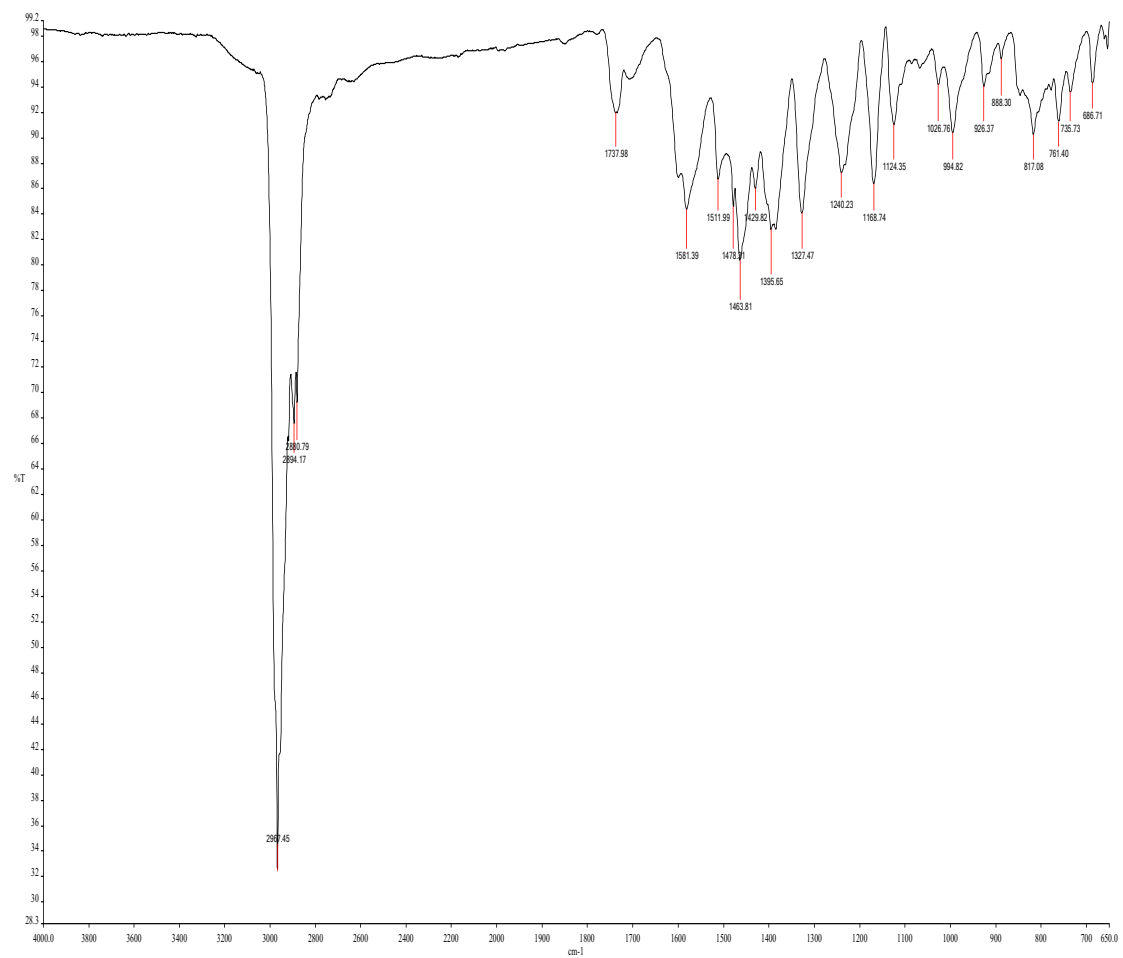


Fig. S22, ES†

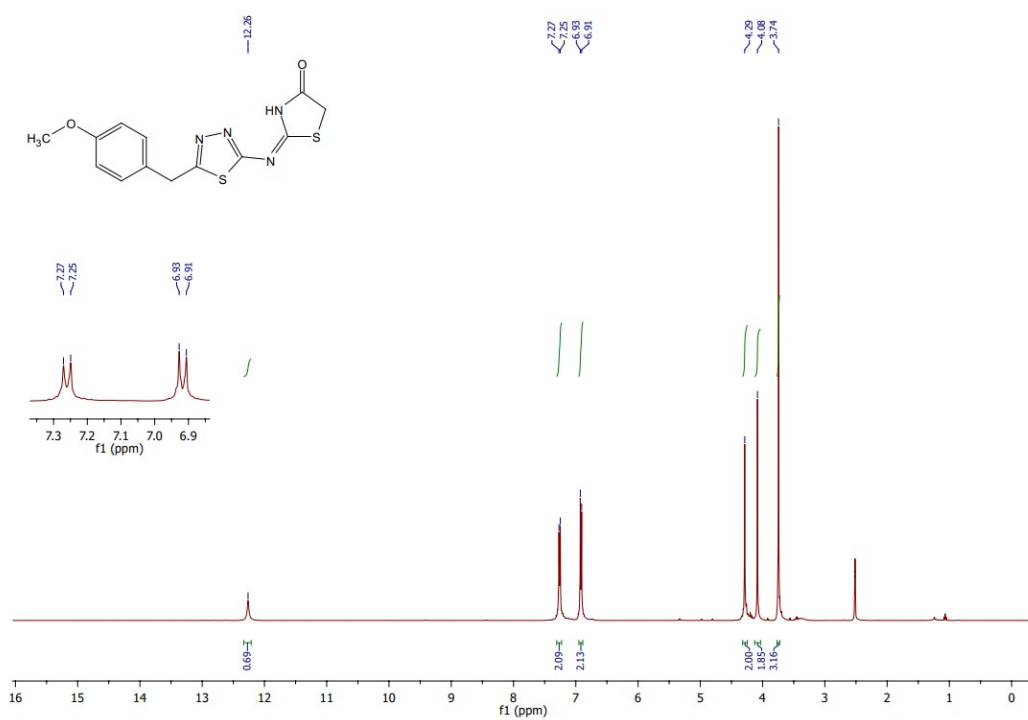


Fig. S23, ES†

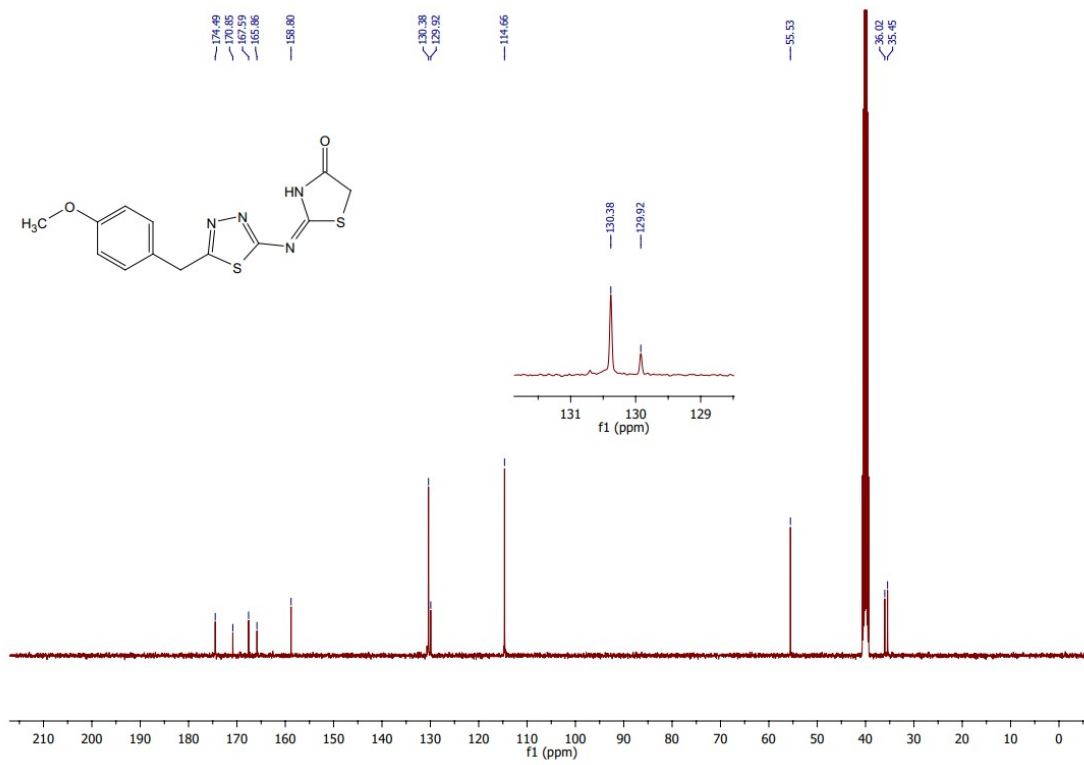


Fig. S24, ES†

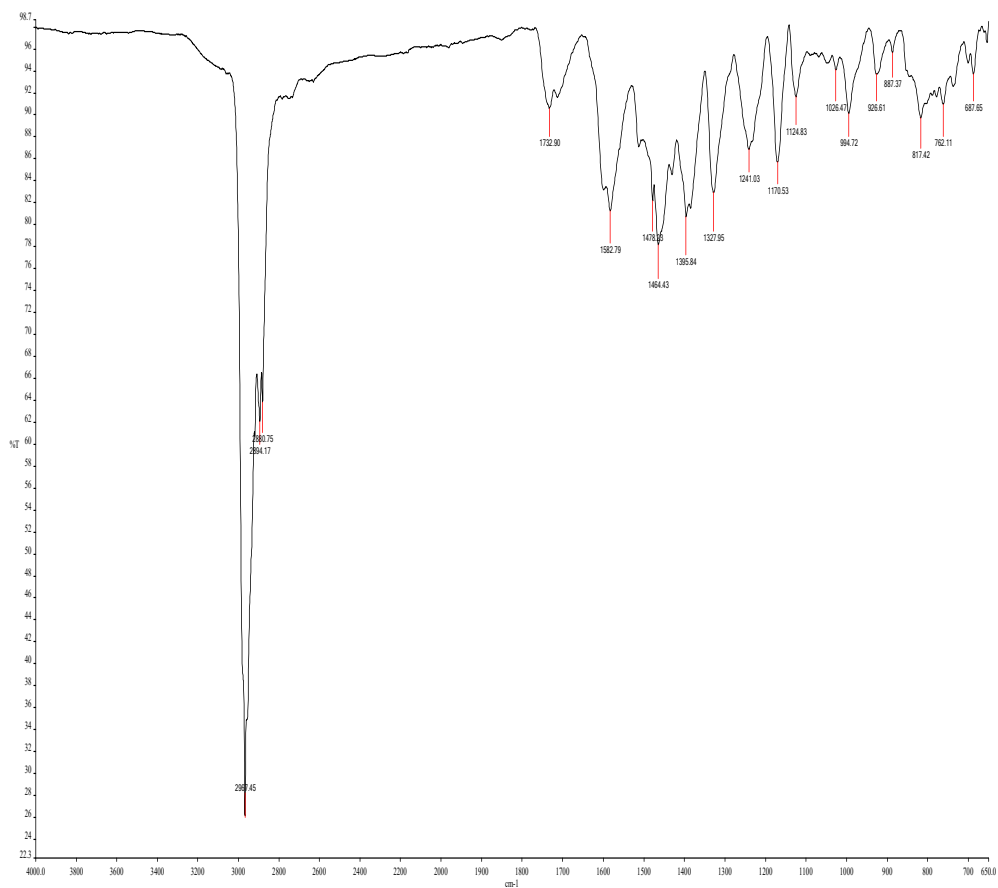


Fig. S25, ES†

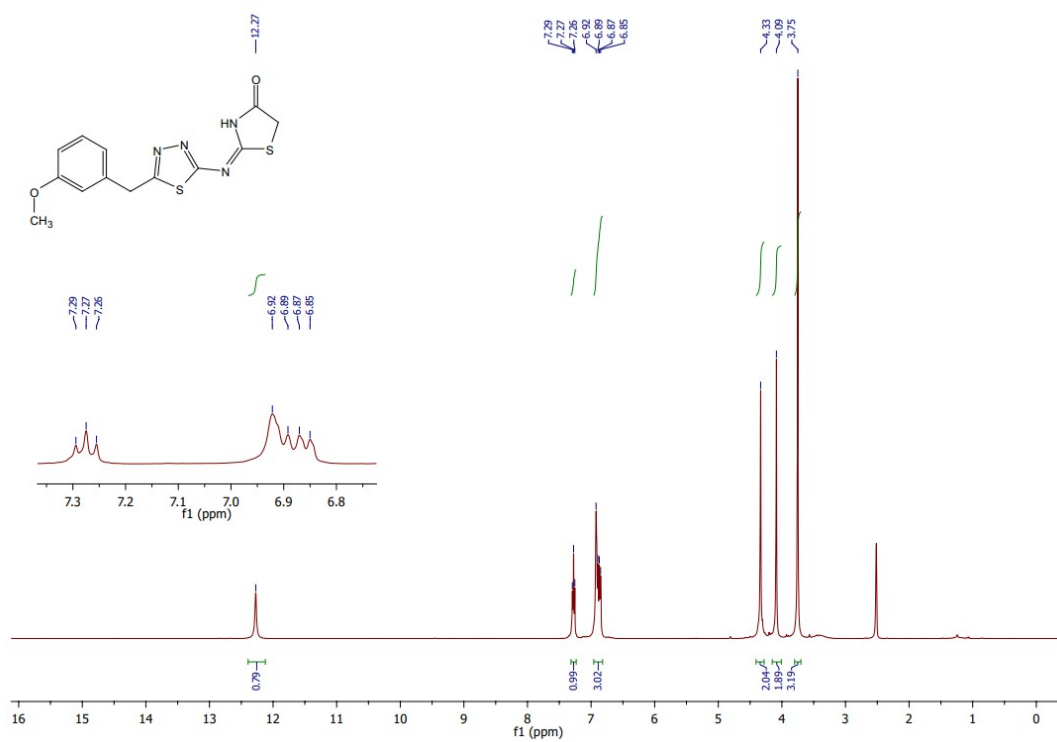


Fig. S26, ES†

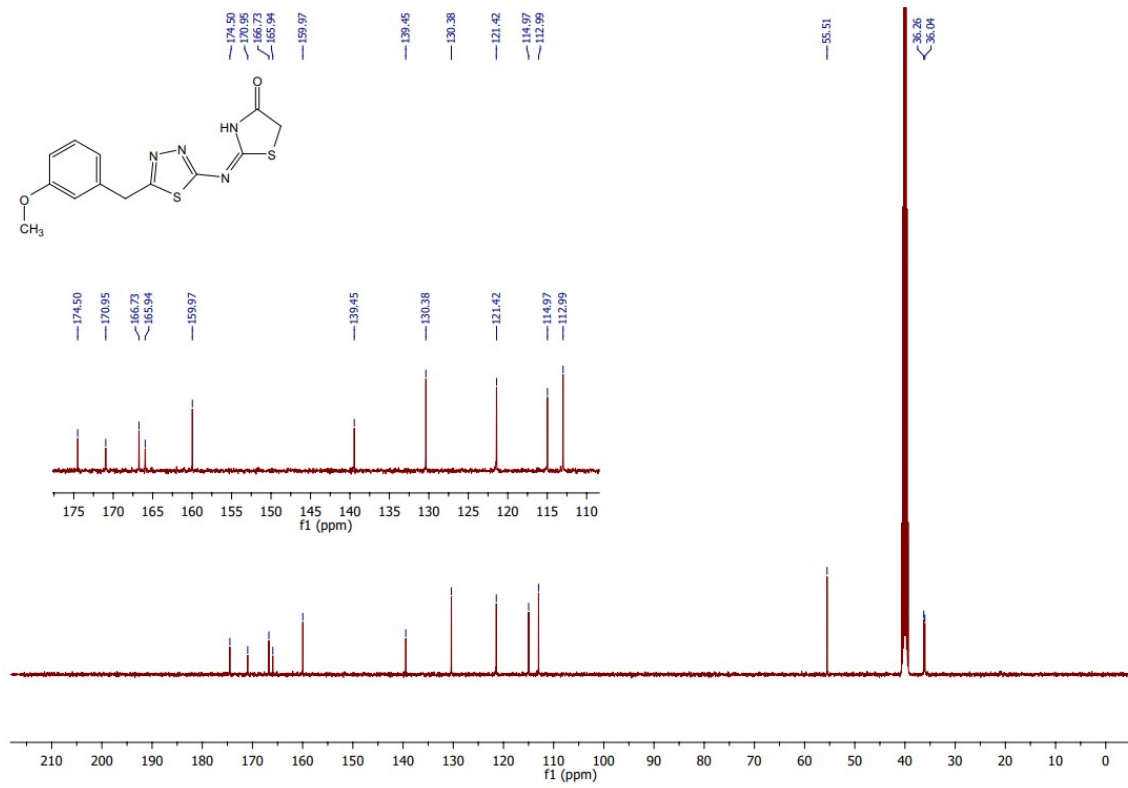


Fig. S27, ES†

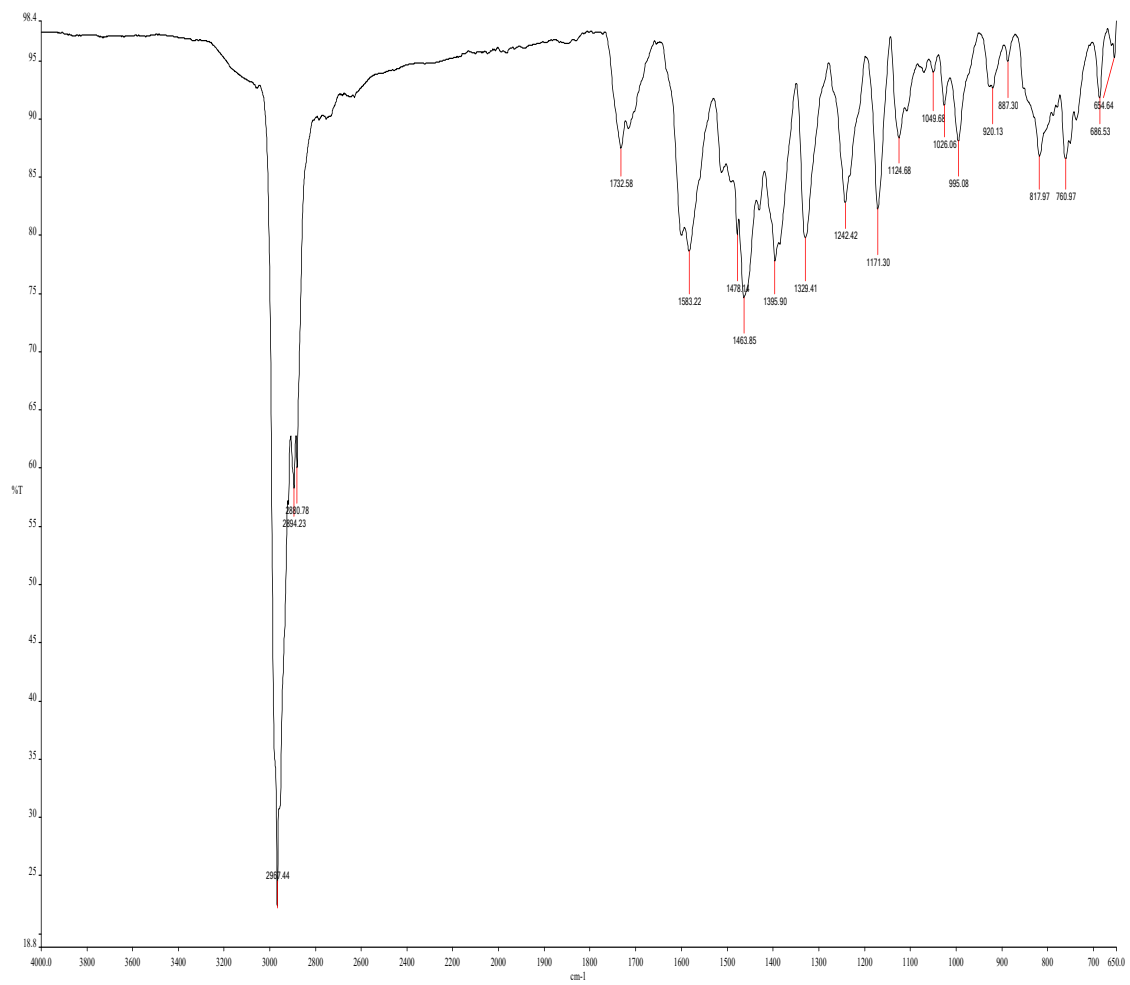


Fig. S28, ES[‡]

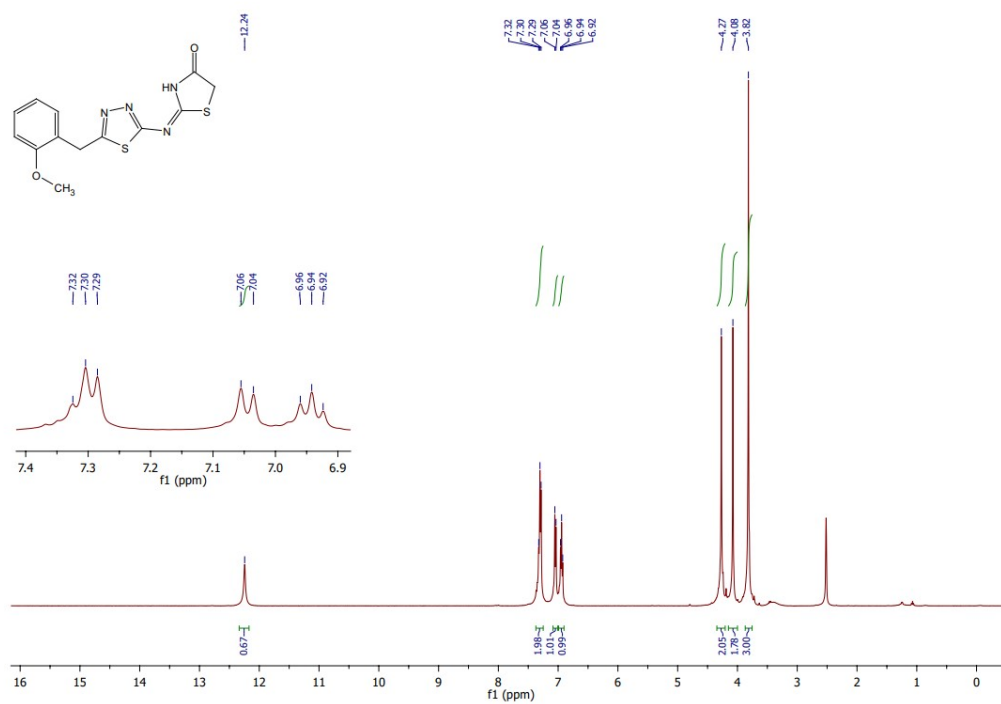


Fig. S29, ES⁺

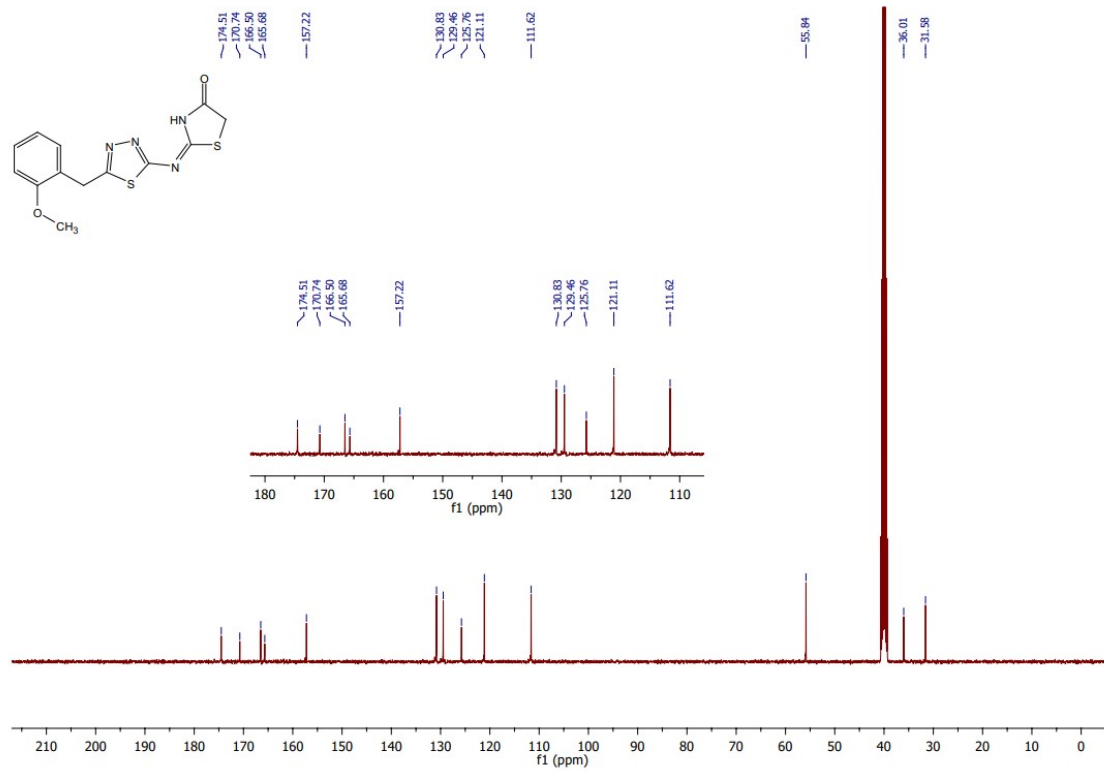


Fig. S30, ES⁺

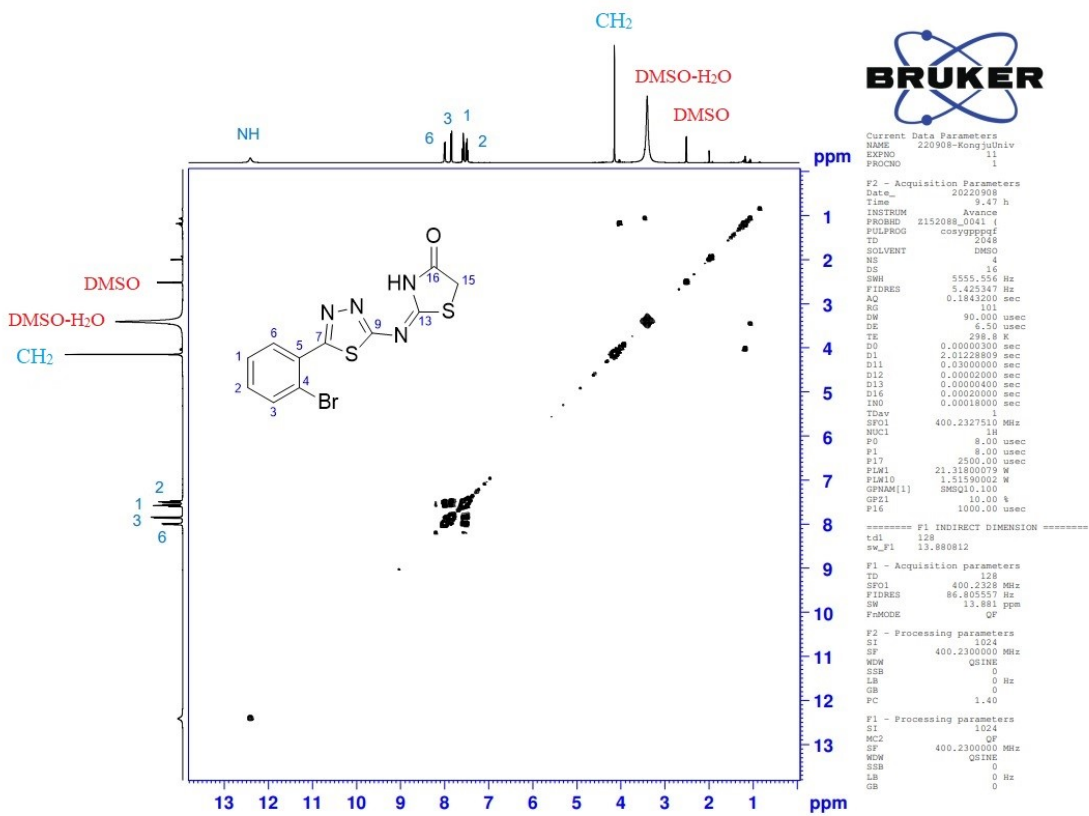


Fig. S31, ES†

HSQC

CH₂-15

DMSO-H₂O
DMSO



Current Data Parameters
NAME 220908-KongjuUniv
EXPNO 1
PROCNO 1

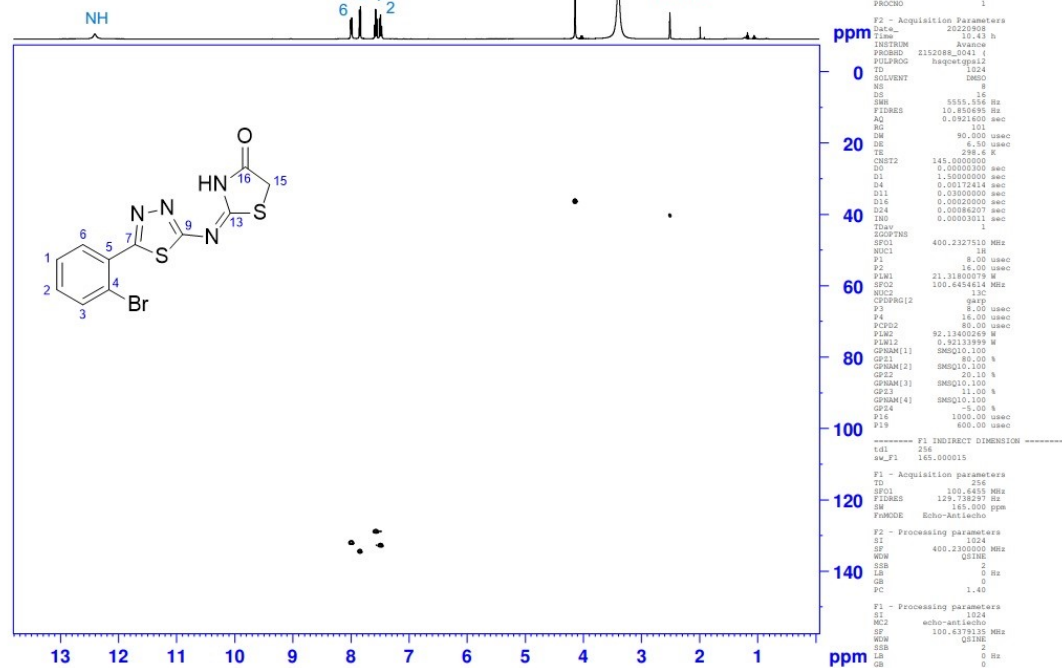


Fig. S32, ES†

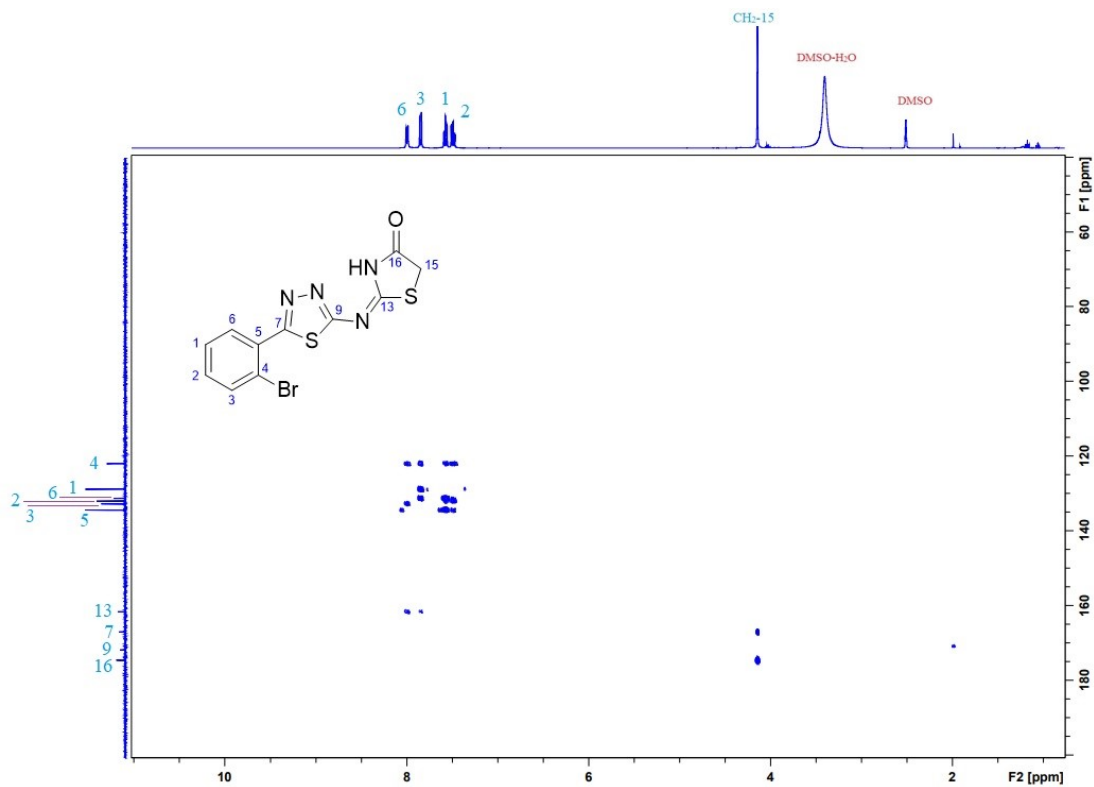


Fig. S33, ES‡

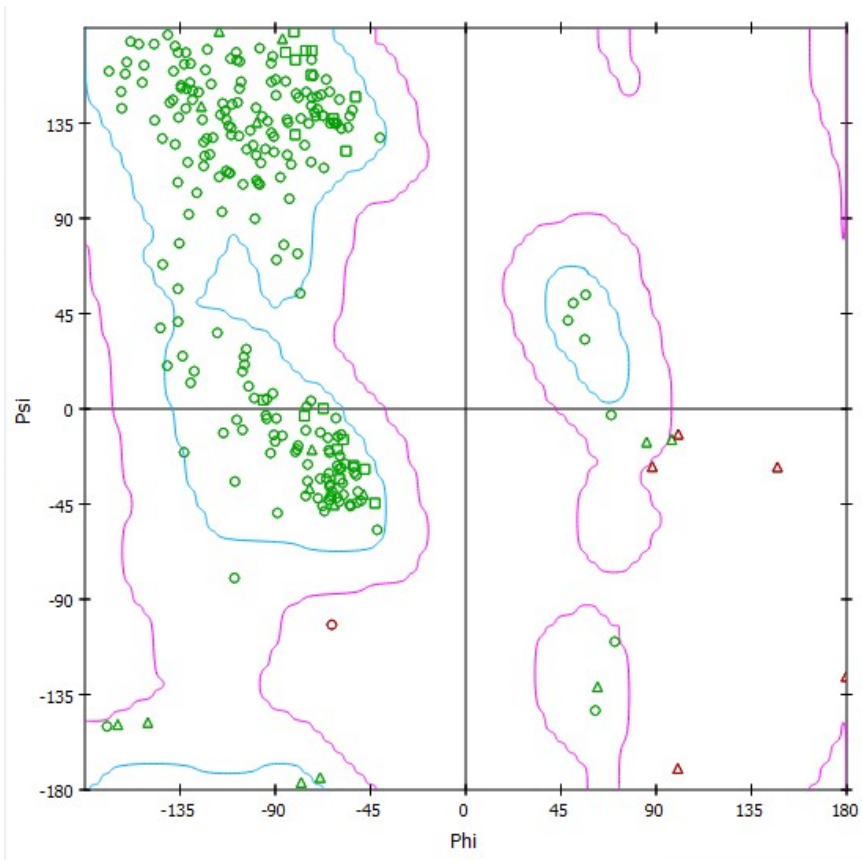


Fig. S34, ES‡

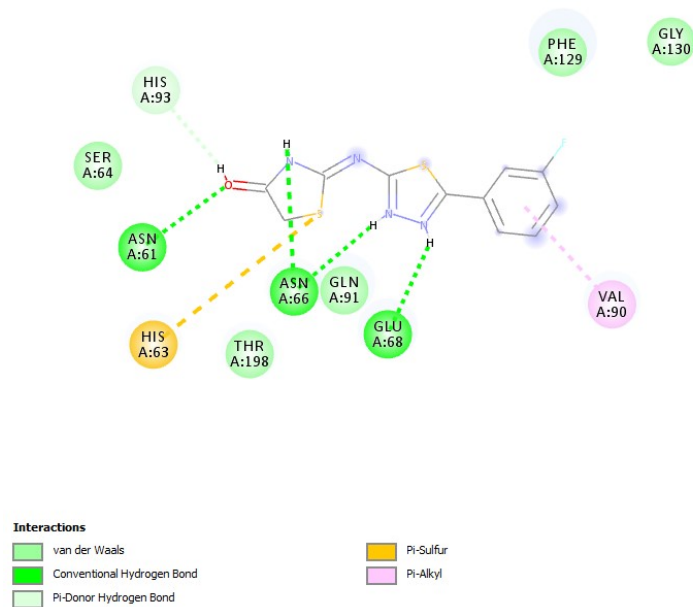


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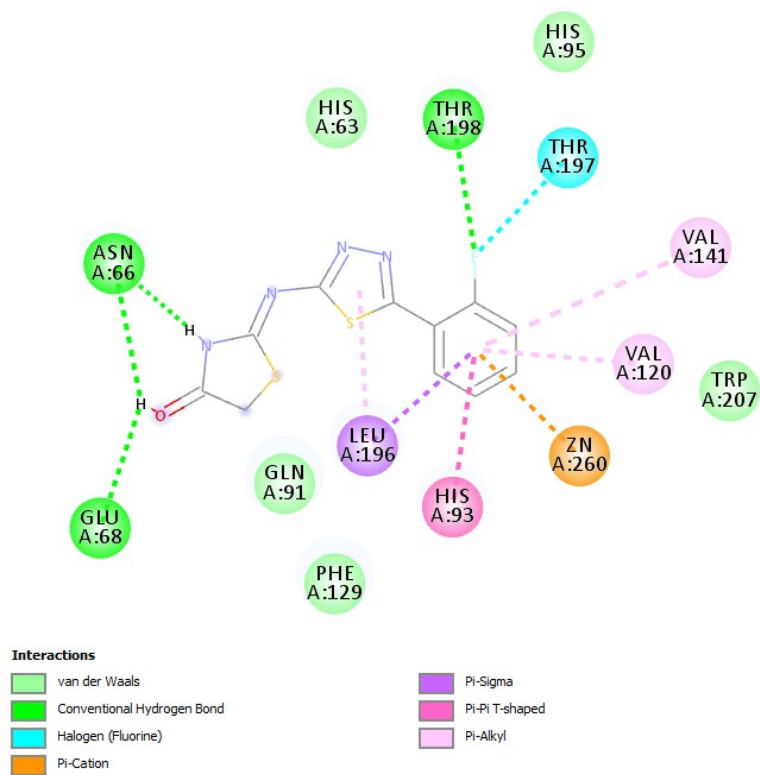


Fig. S36, ES‡

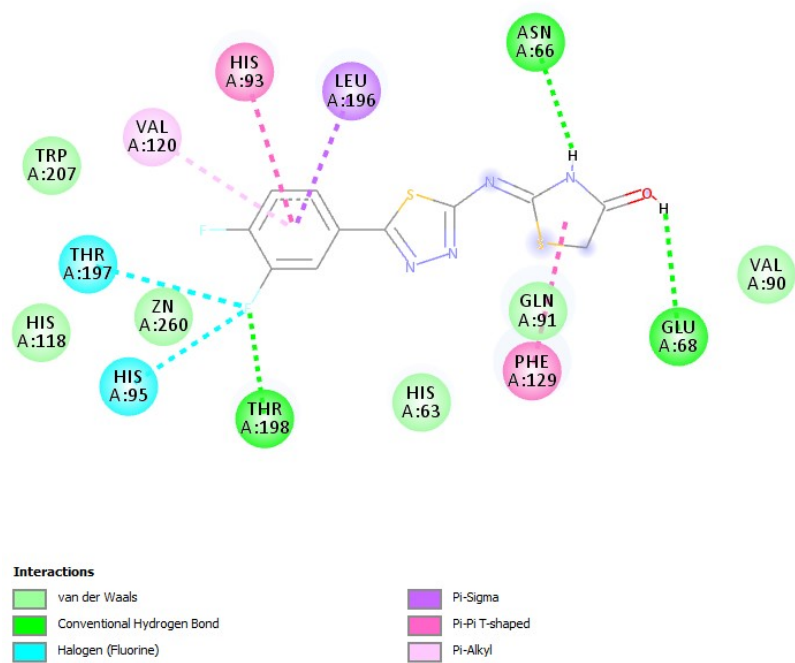


Fig. S37, ES‡

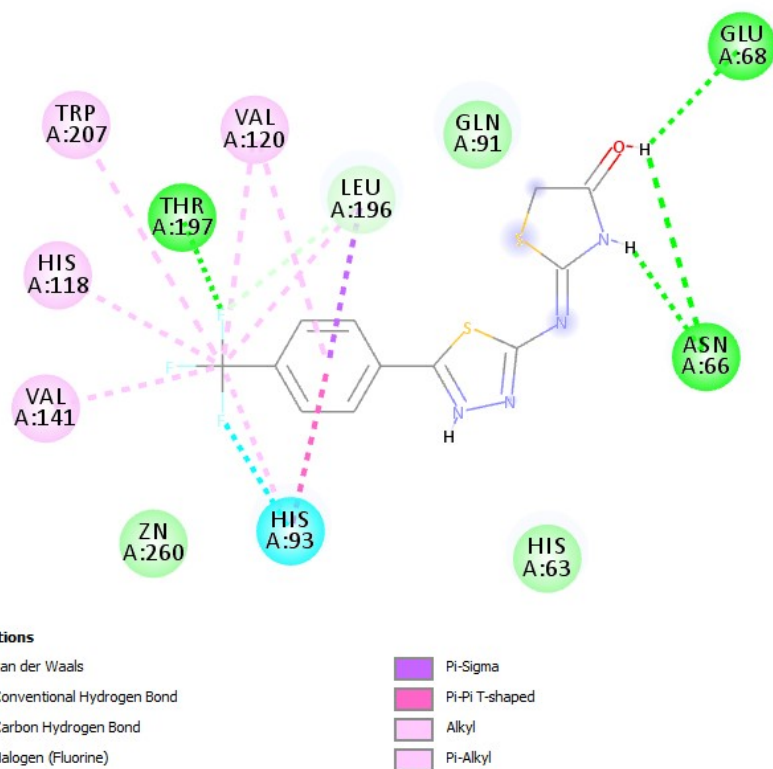


Fig. S38, ES‡

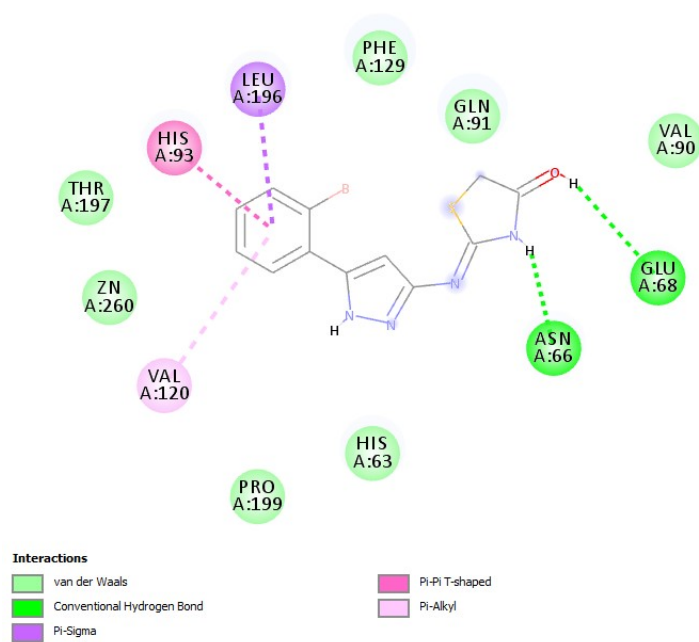


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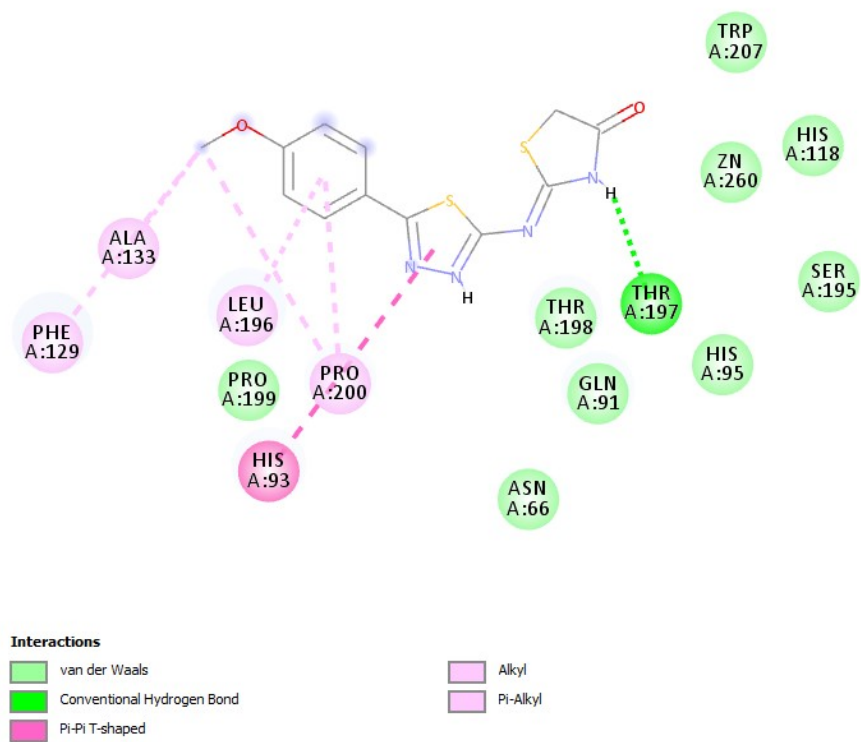


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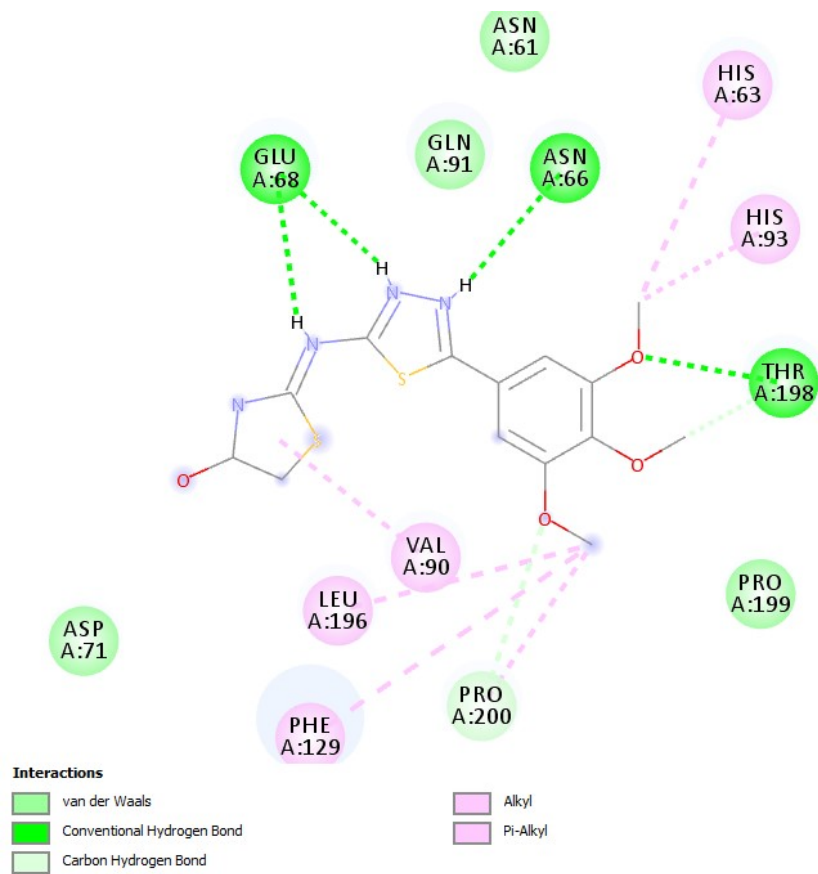


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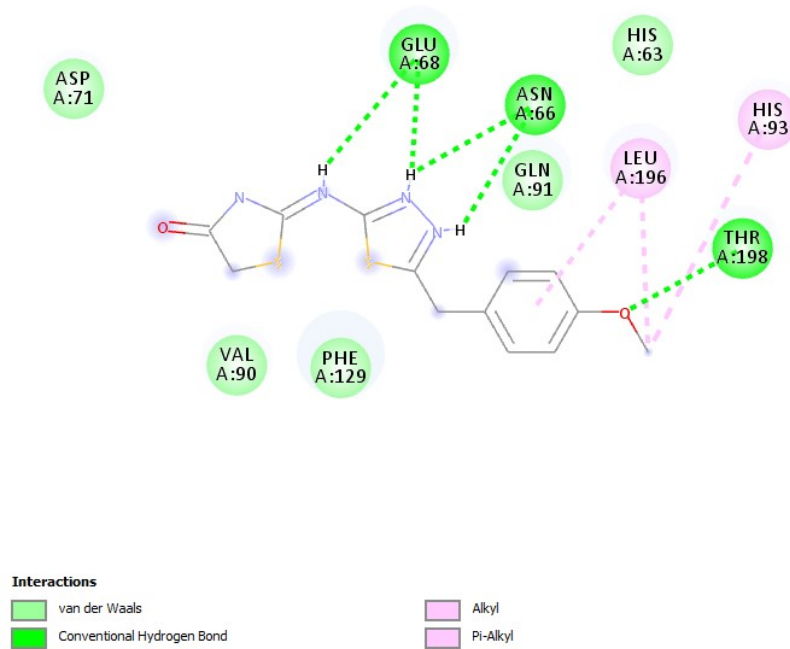


Fig. S42, ES‡

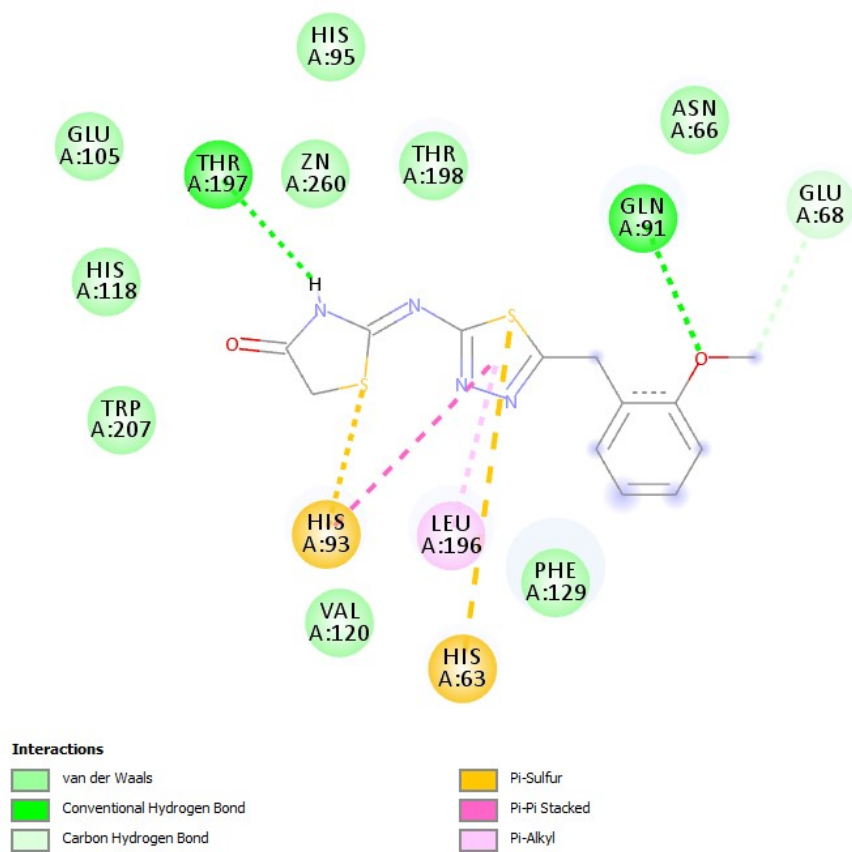


Fig. S43, ES‡