Supplementary materials

Anti-inflammatory properties of novel 1,2-benzothiazine derivatives and their interaction with phospholipid model membranes

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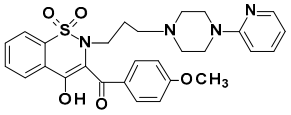
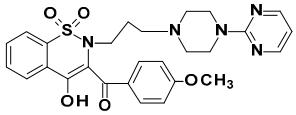
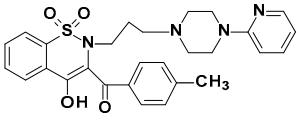
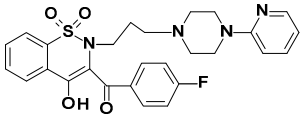
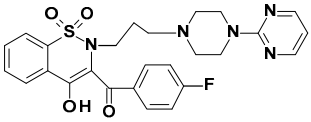
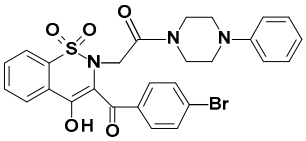
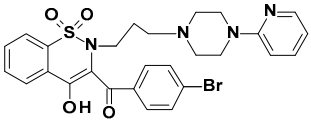
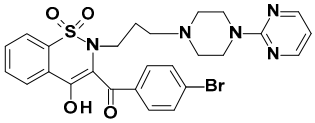
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^{1}H NMR and ^{13}C NMR spectra of new compounds

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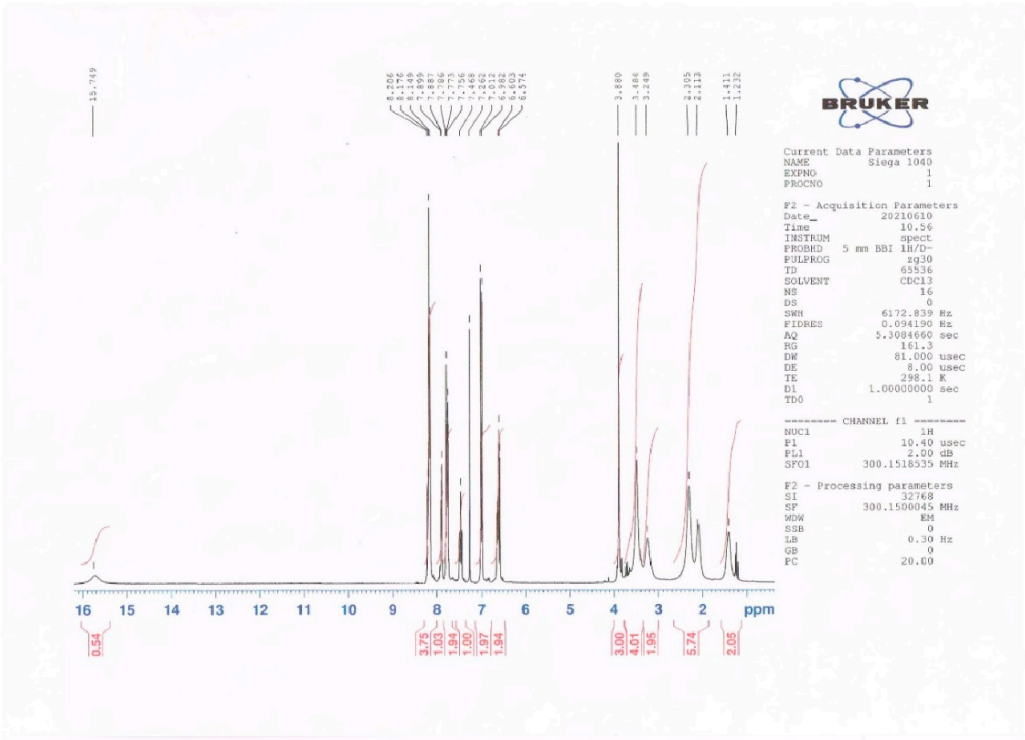


Figure S1. ^{1}H NMR spectrum of **BS23** in $CDCl_3$.

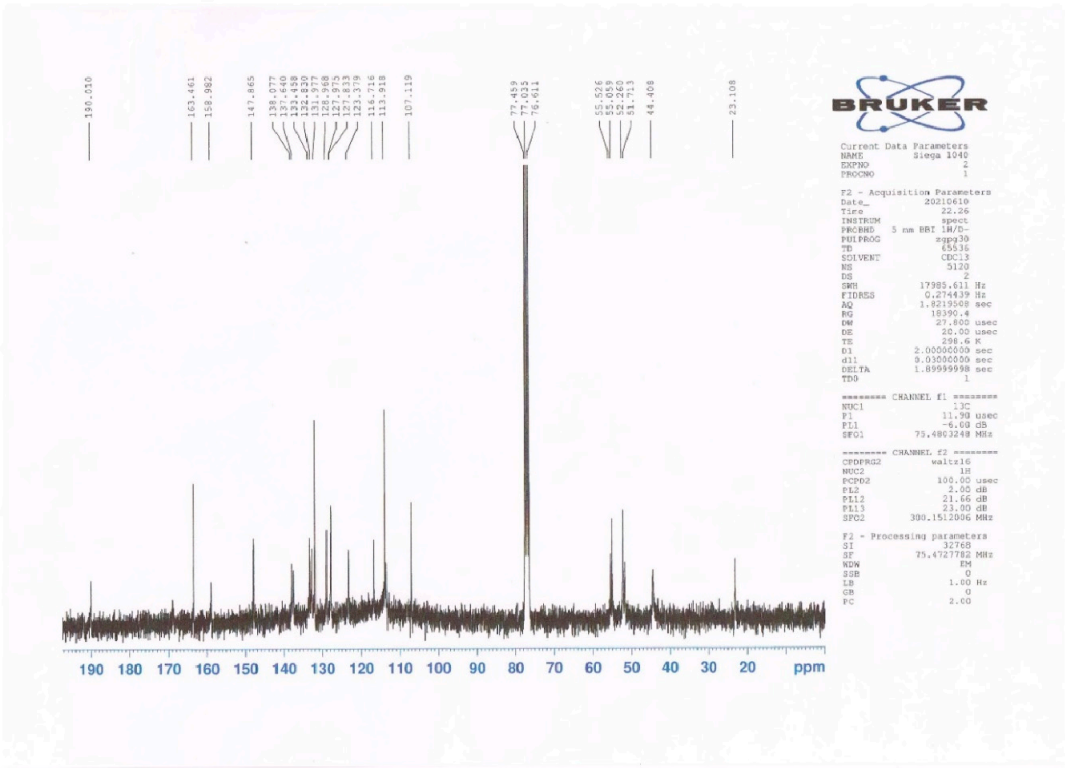


Figure S2. ^{13}C NMR spectrum of **BS23** in $CDCl_3$.

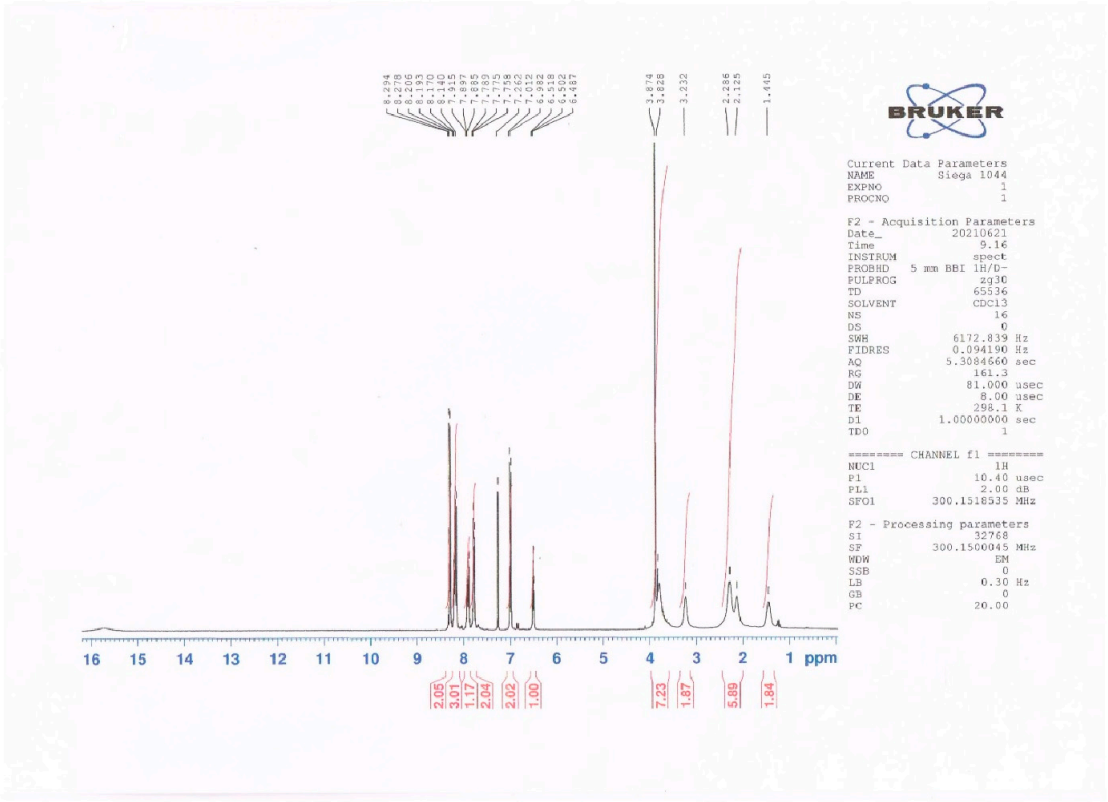


Figure S3. ^{1}H NMR spectrum of **BS24** in $CDCl_3$.

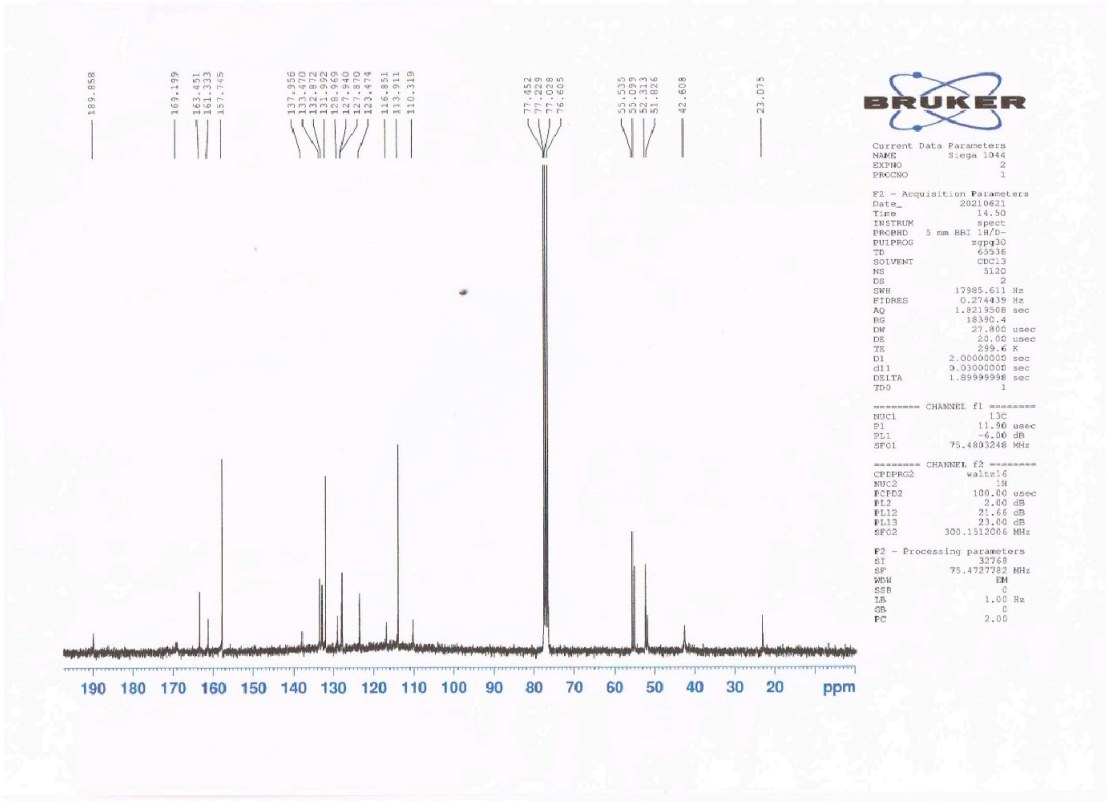


Figure S4. ^{13}C NMR spectrum of **BS24** in $CDCl_3$.

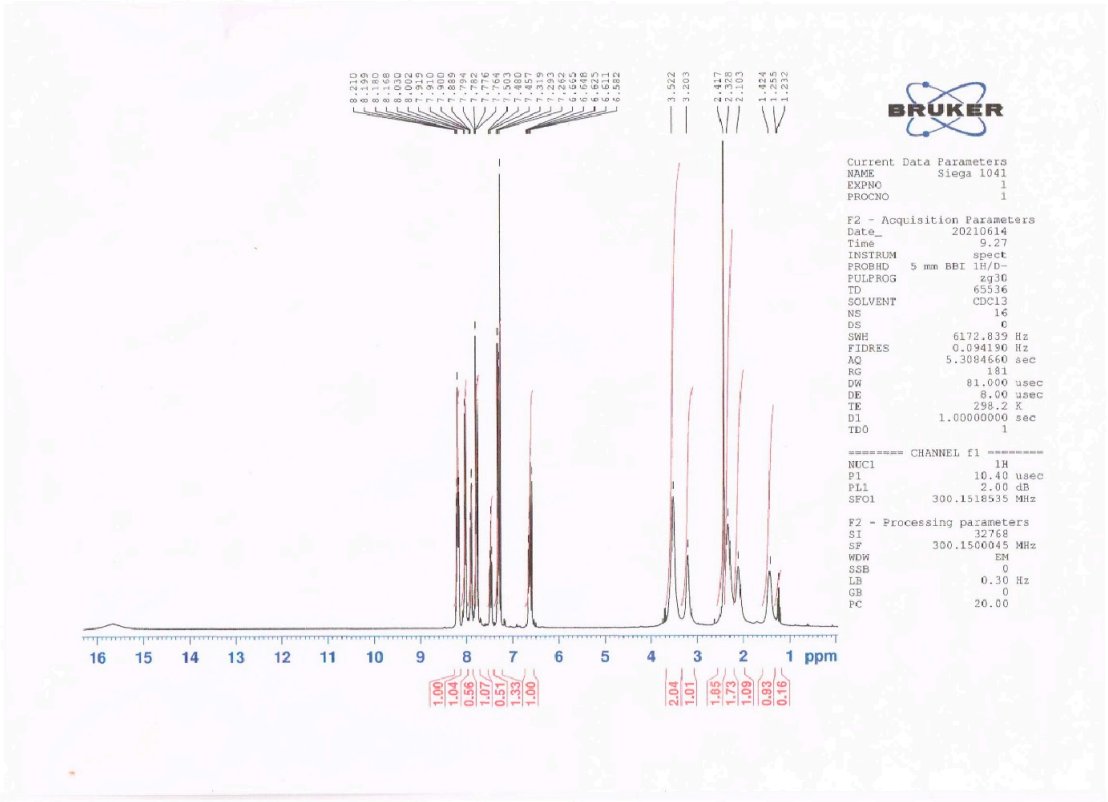


Figure S5. ^{1}H NMR spectrum of **BS25** in $CDCl_3$.

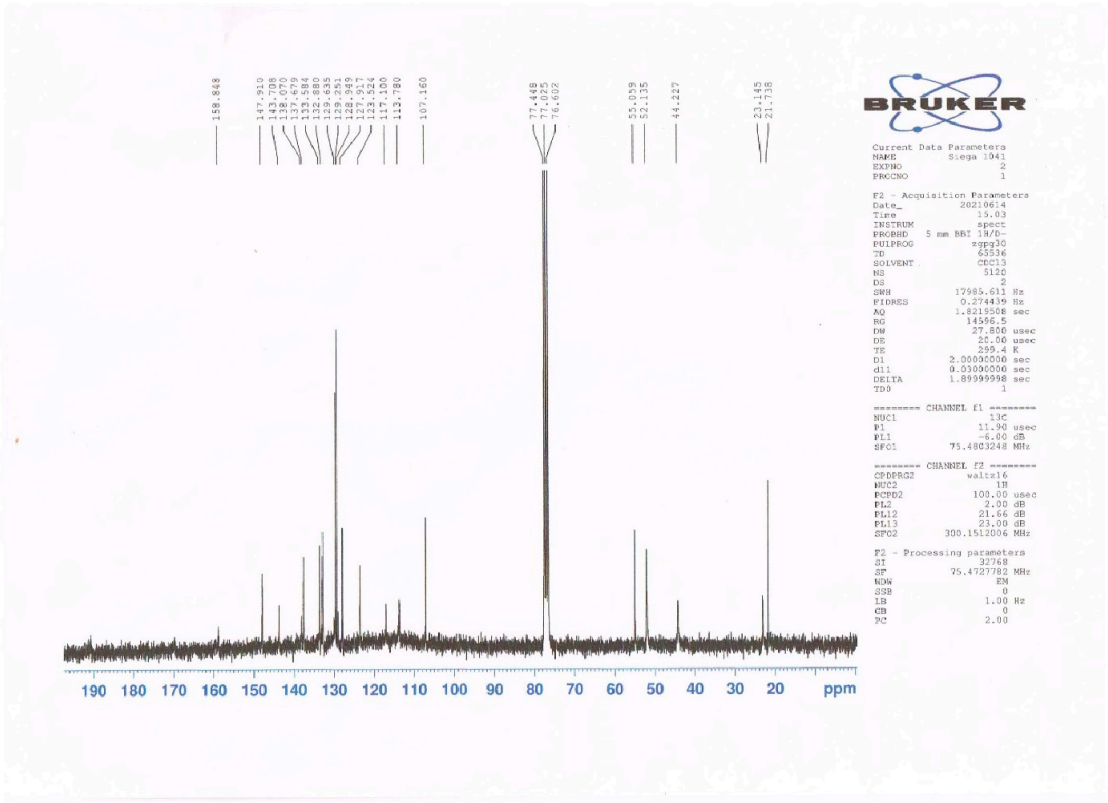


Figure S6. ^{13}C NMR spectrum of **BS25** in $CDCl_3$.

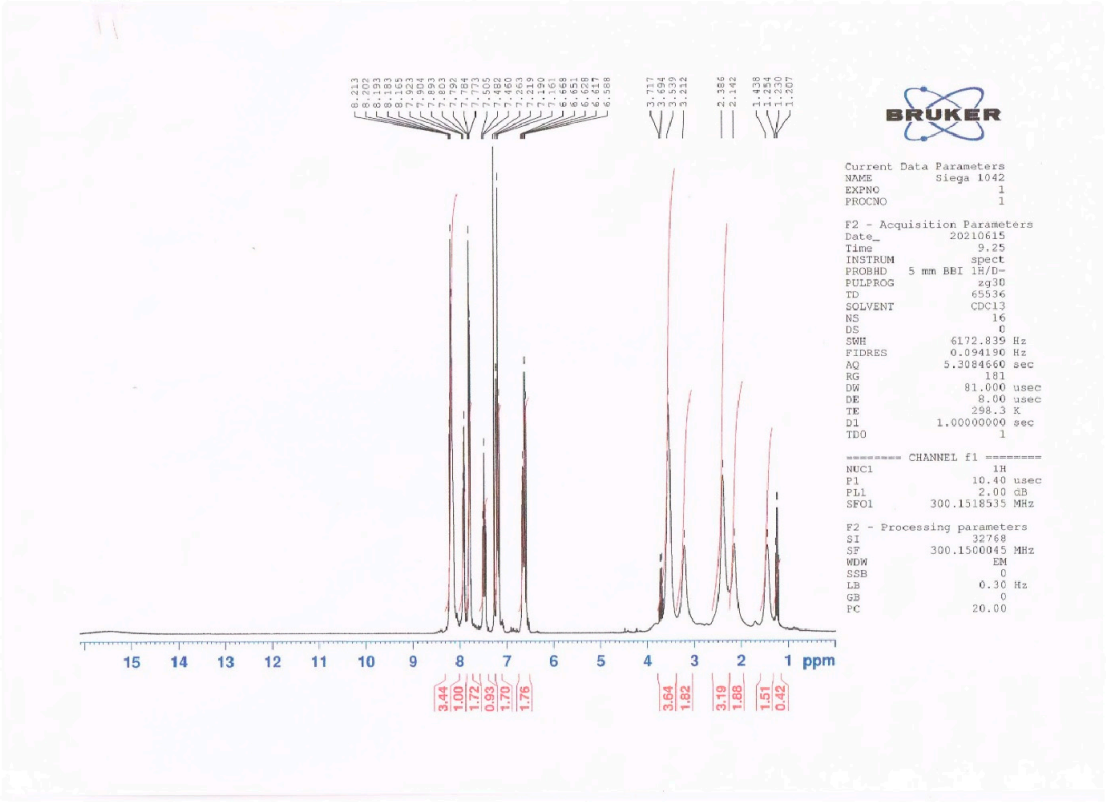


Figure S7. ^{1}H NMR spectrum of **BS26** in $CDCl_3$.

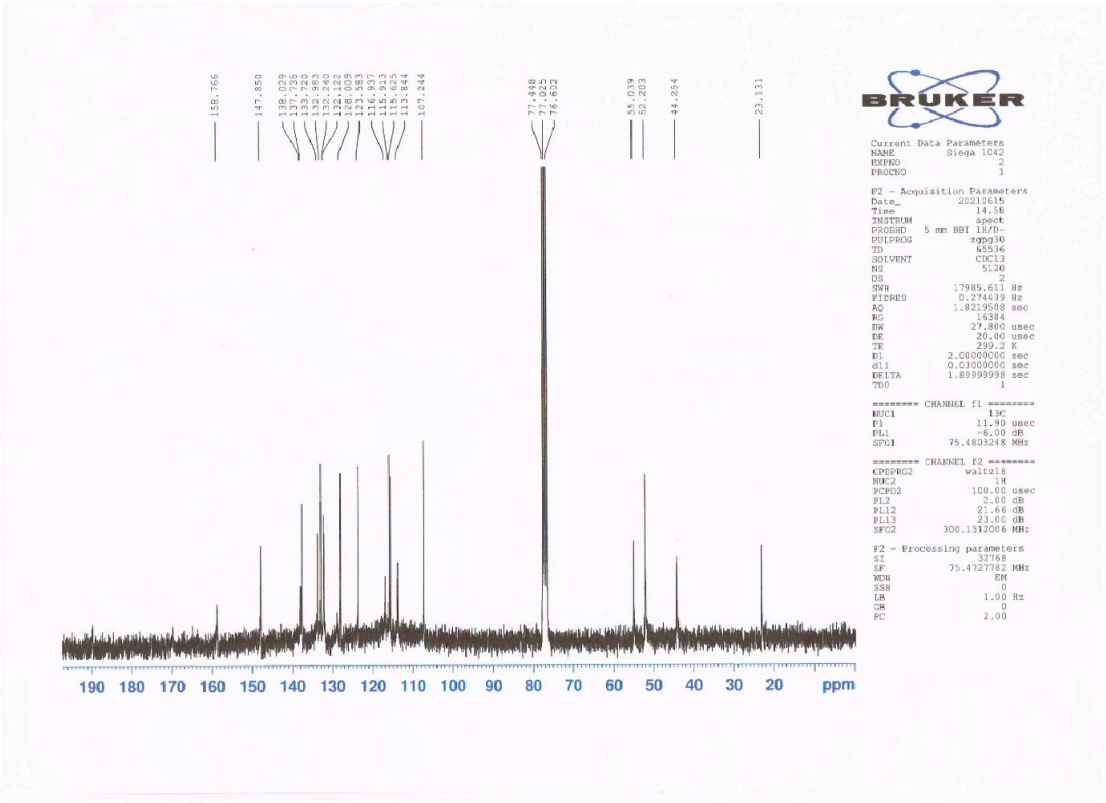


Figure S8. ^{13}C NMR spectrum of **BS26** in $CDCl_3$.

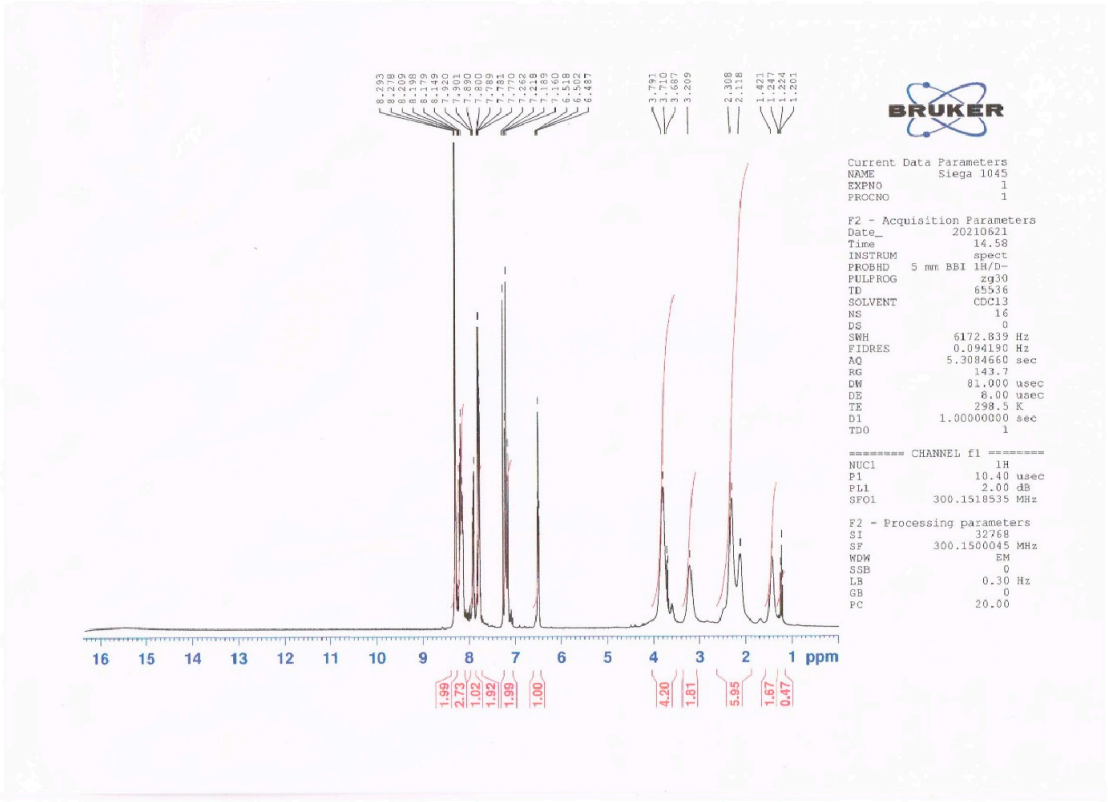


Figure S9. ^{1}H NMR spectrum of **BS27** in $CDCl_3$.

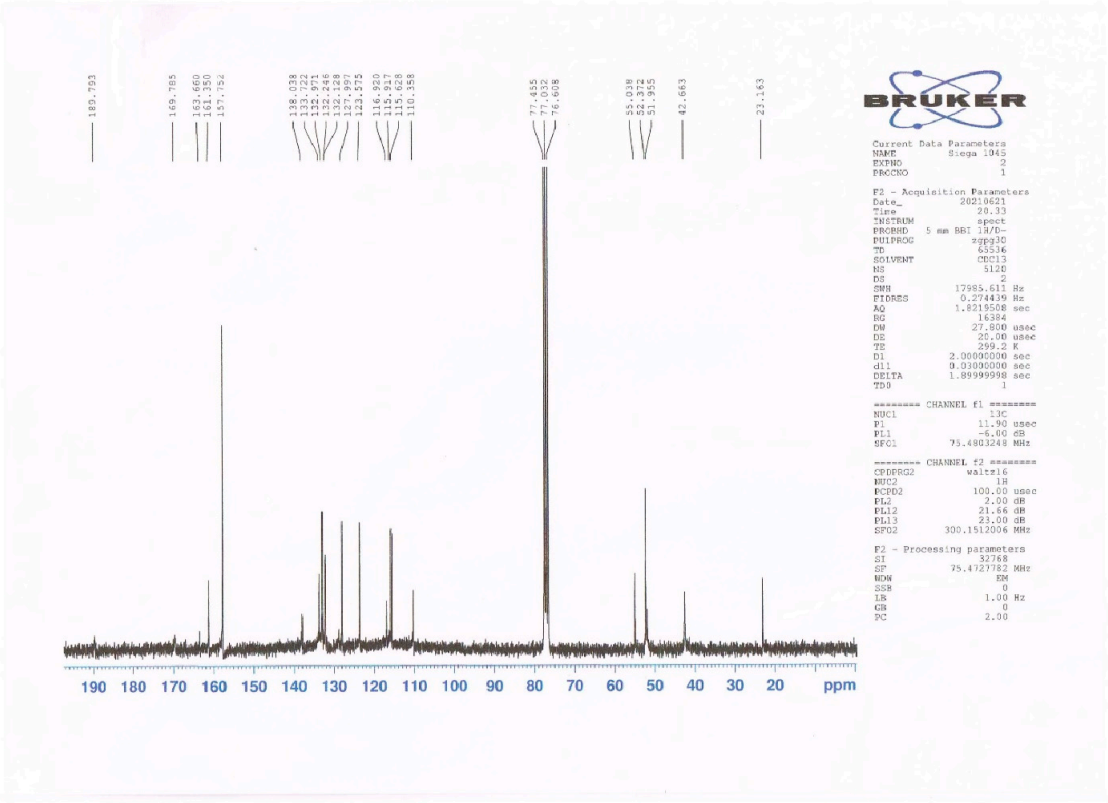


Figure S10. ^{13}C NMR spectrum of **BS27** in $CDCl_3$.

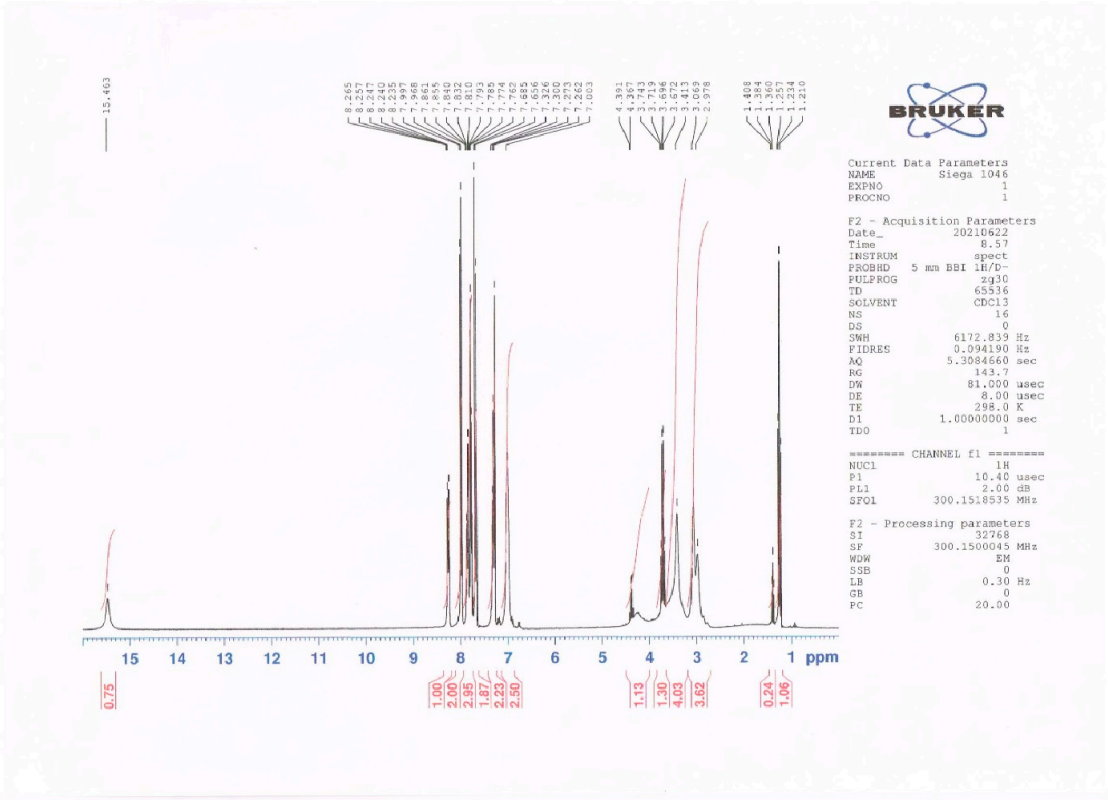


Figure S11. ^{1}H NMR spectrum of **BS28** in $CDCl_3$.

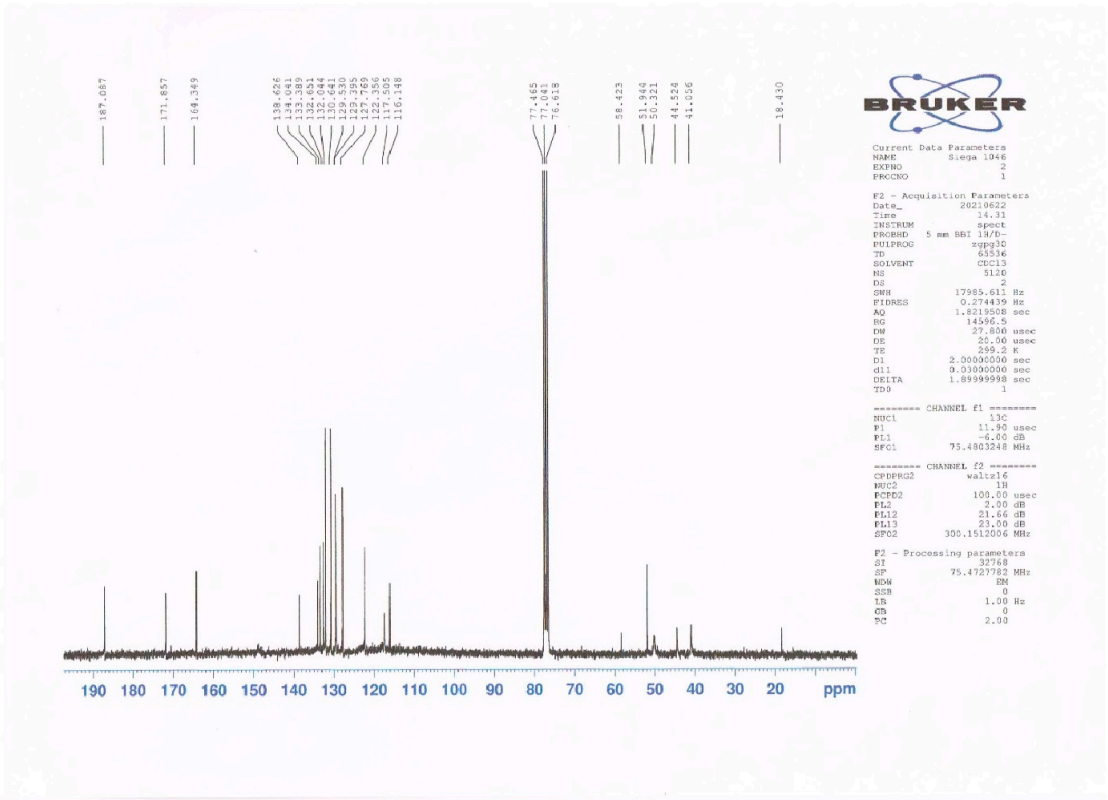


Figure S12. ^{13}C NMR spectrum of **BS28** in $CDCl_3$.

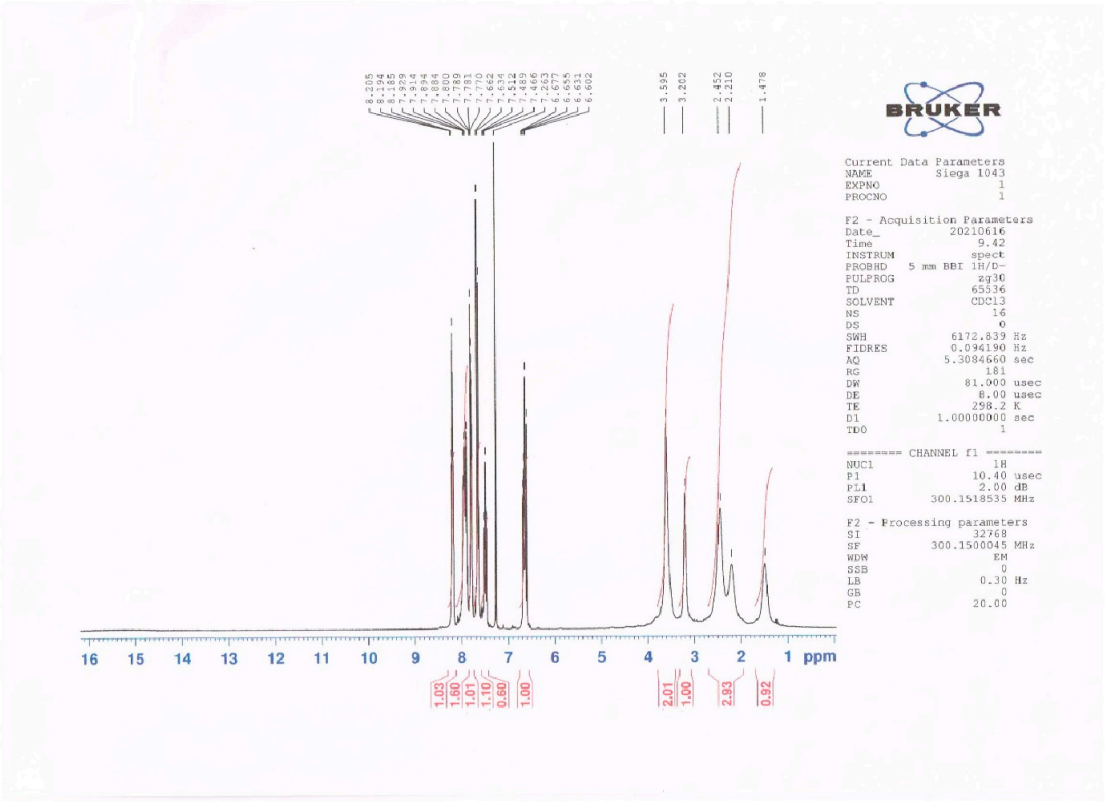


Figure S13. ^{1}H NMR spectrum of **BS29** in $CDCl_3$.

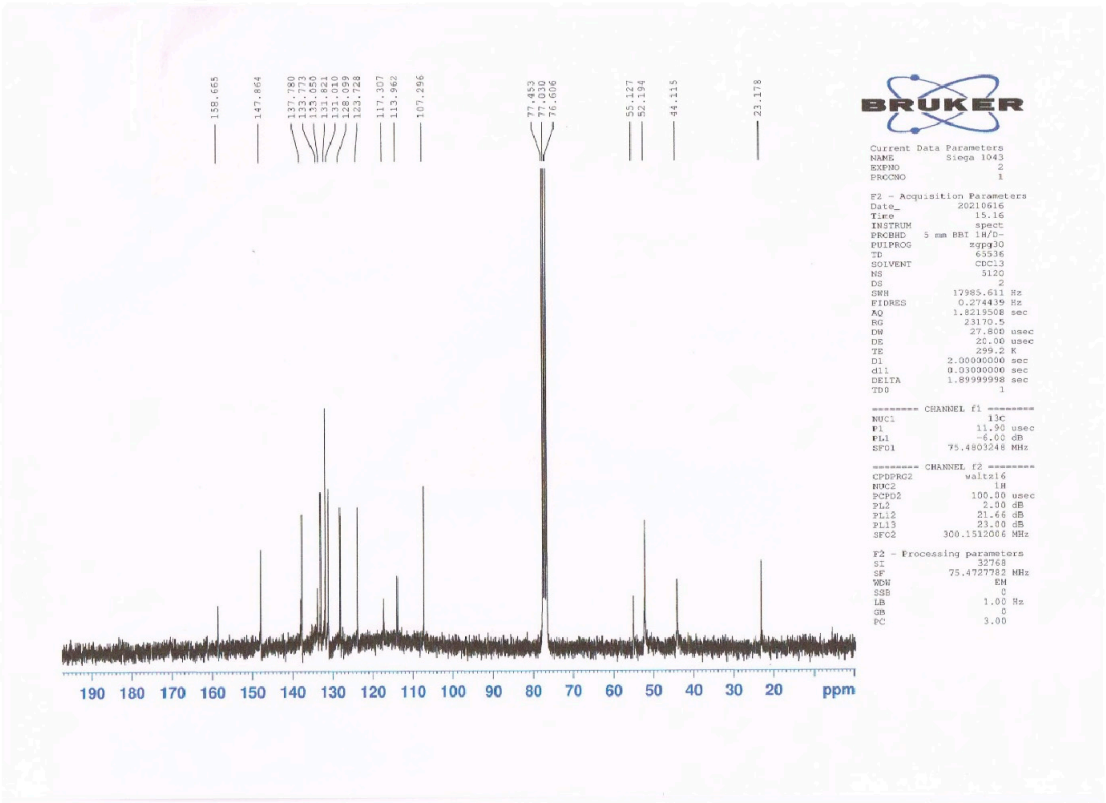


Figure S14. ^{13}C NMR spectrum of **BS29** in $CDCl_3$.

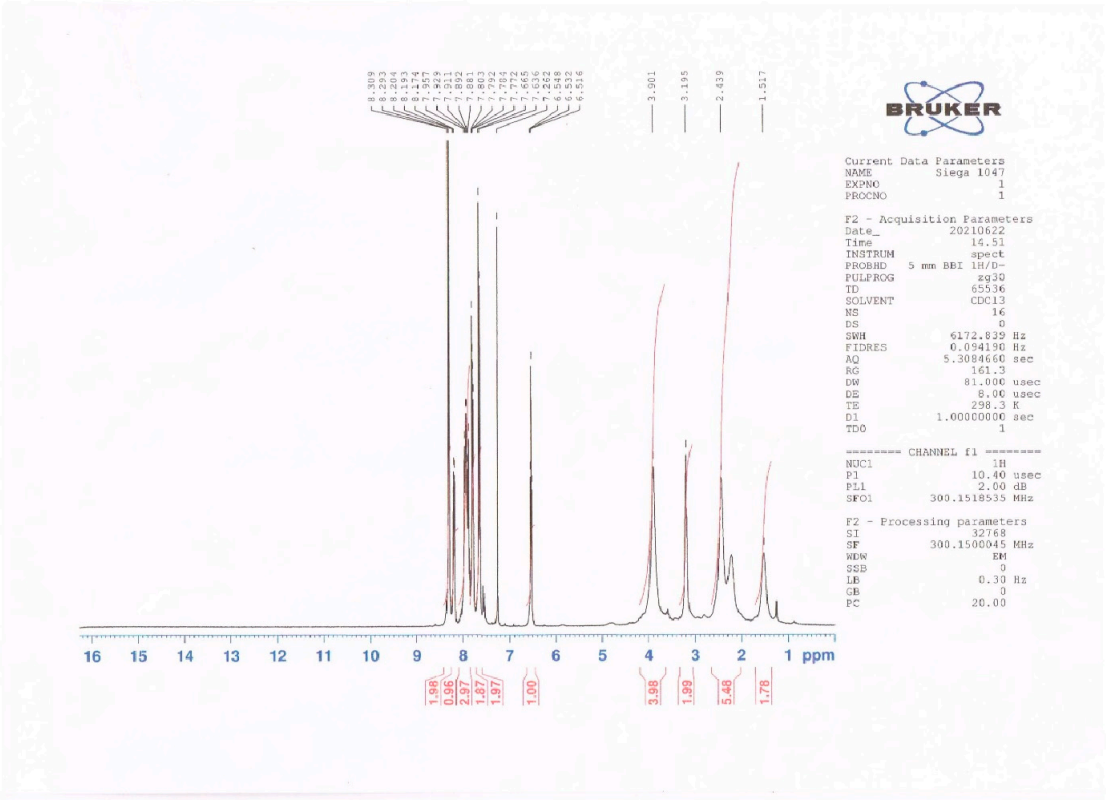


Figure S15. ^{1}H NMR spectrum of **BS30** in $CDCl_3$.

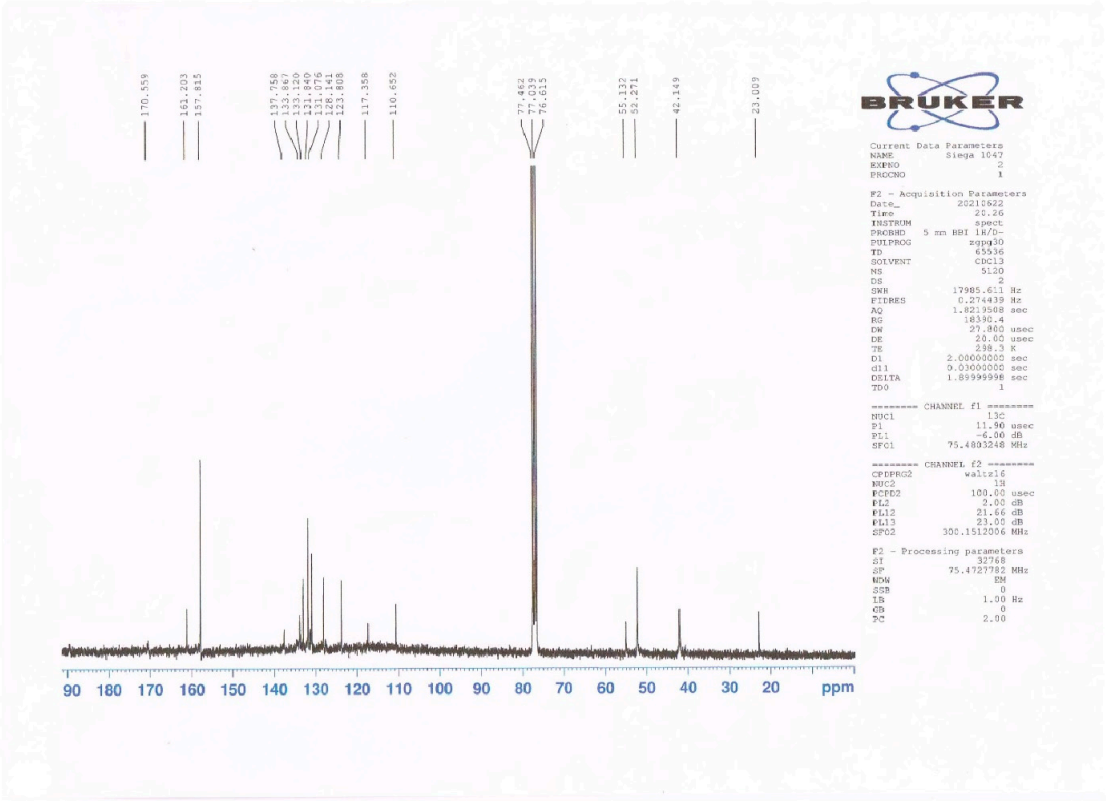


Figure S16. ^{13}C NMR spectrum of **BS30** in $CDCl_3$.

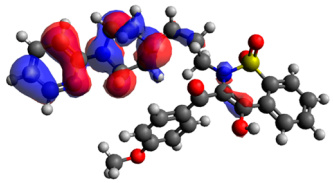
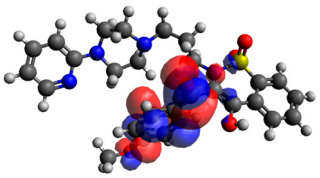
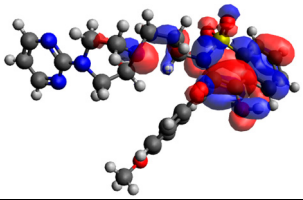
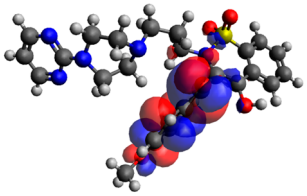
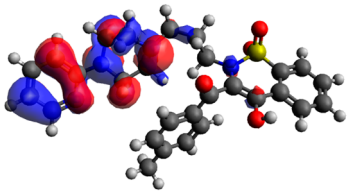
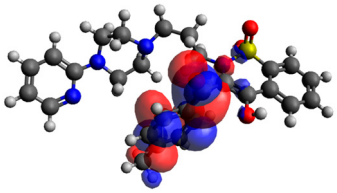
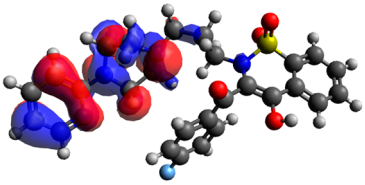
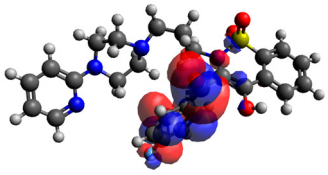
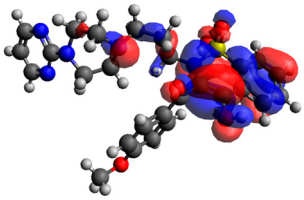
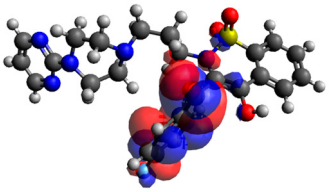
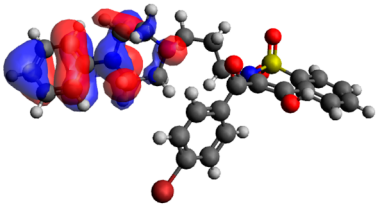
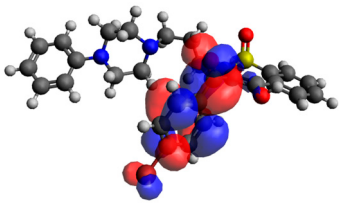
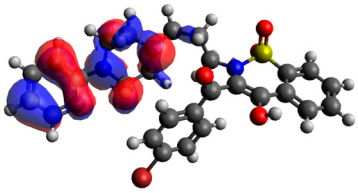
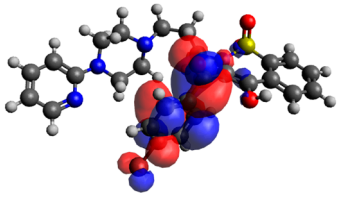
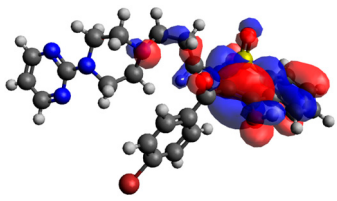
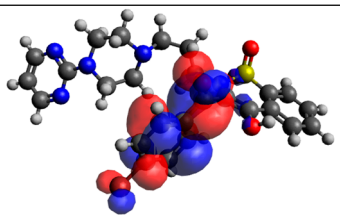
	HOMO	LUMO
BS23		
BS24		
BS25		
BS26		
BS27		
BS28		
BS29		
BS30		

Figure S17. The distribution map of HOMO/LUMO densities. The negative electron density is presented in blue color while the red color indicates the positive electron density.

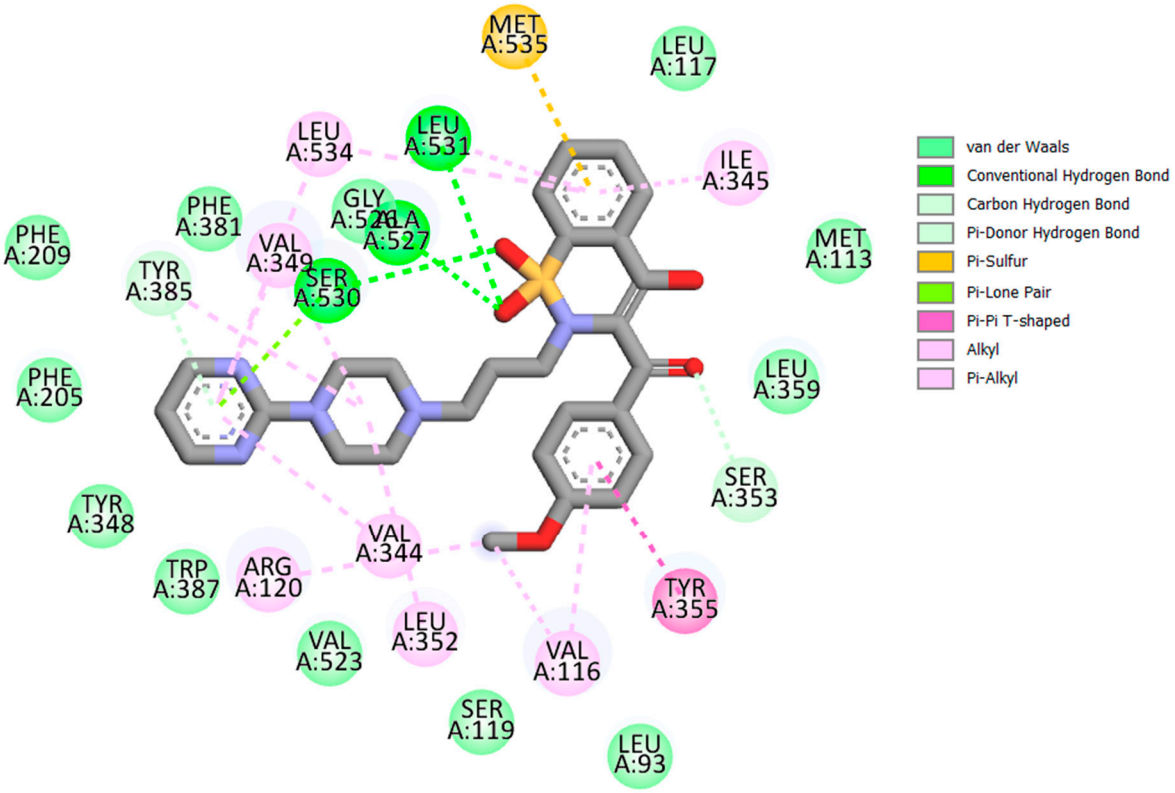


Figure S18. The binding mode of designed compound **BS24 – COX-2** in the active center of COX-2

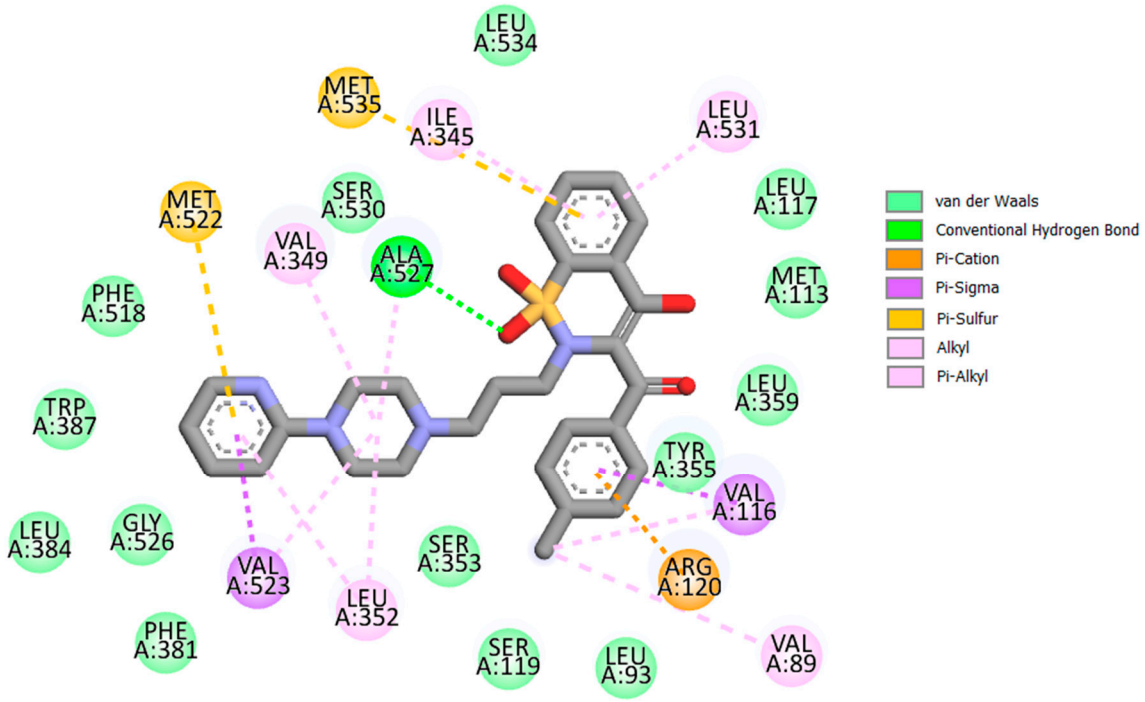


Figure S19. The binding mode of designed compound **BS25 – COX-2** in the active center of COX-2

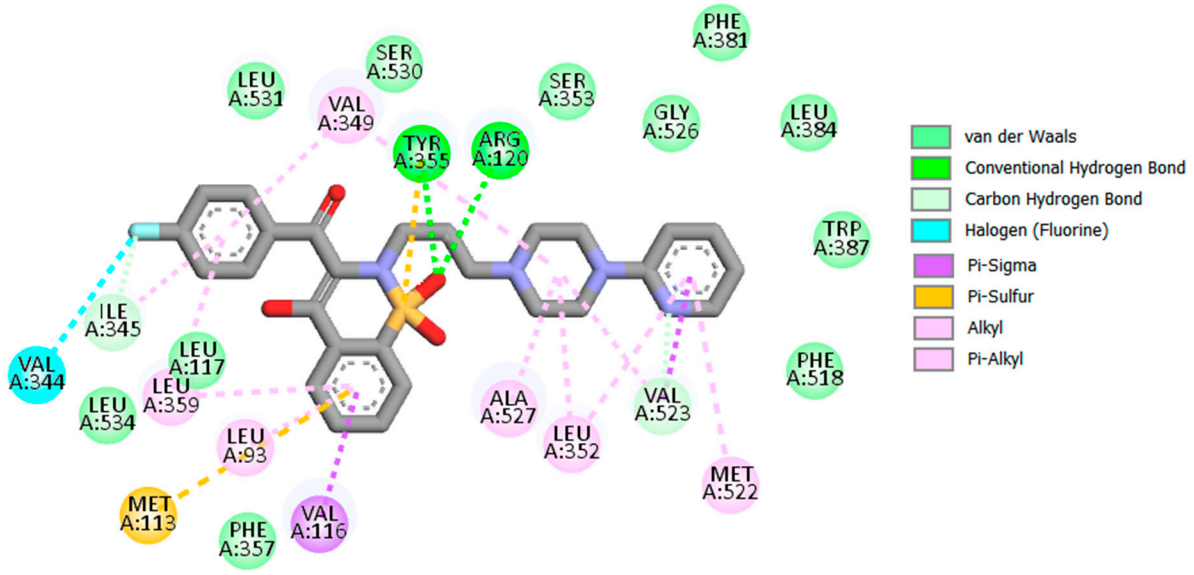


Figure S20. The binding mode of designed compound **BS26 – COX-2** in the active center of COX-2

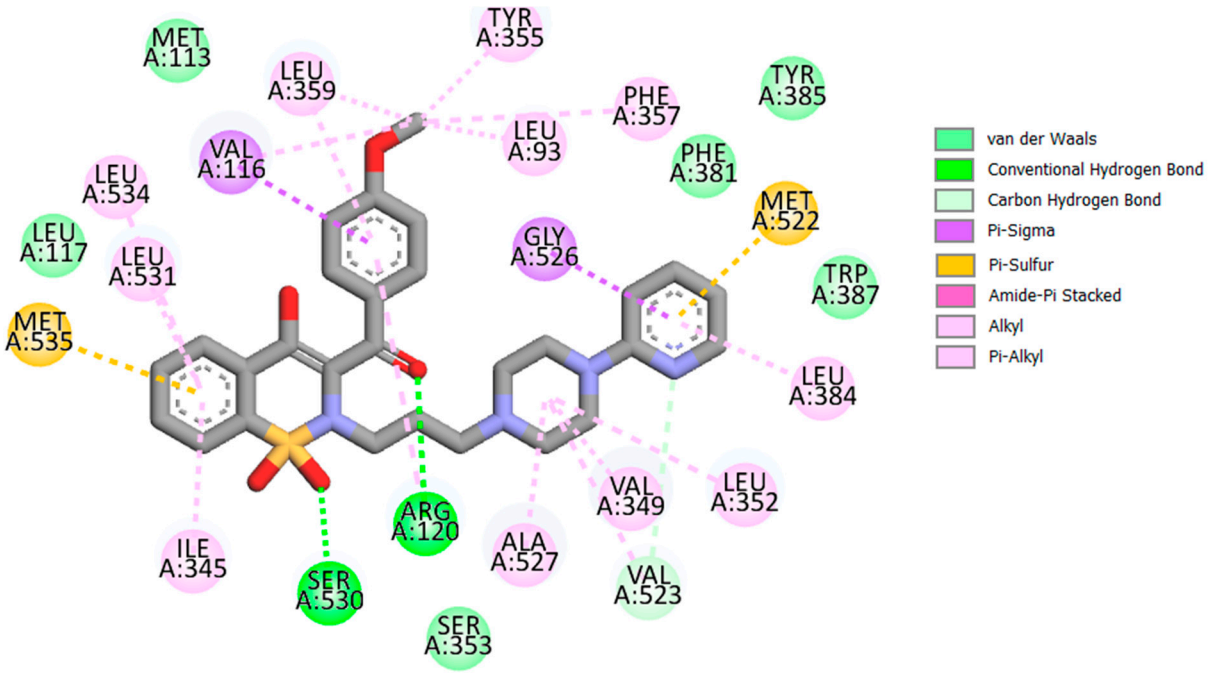


Figure S21. The binding mode of designed compound **BS27 – COX-2** in the active center of COX-2

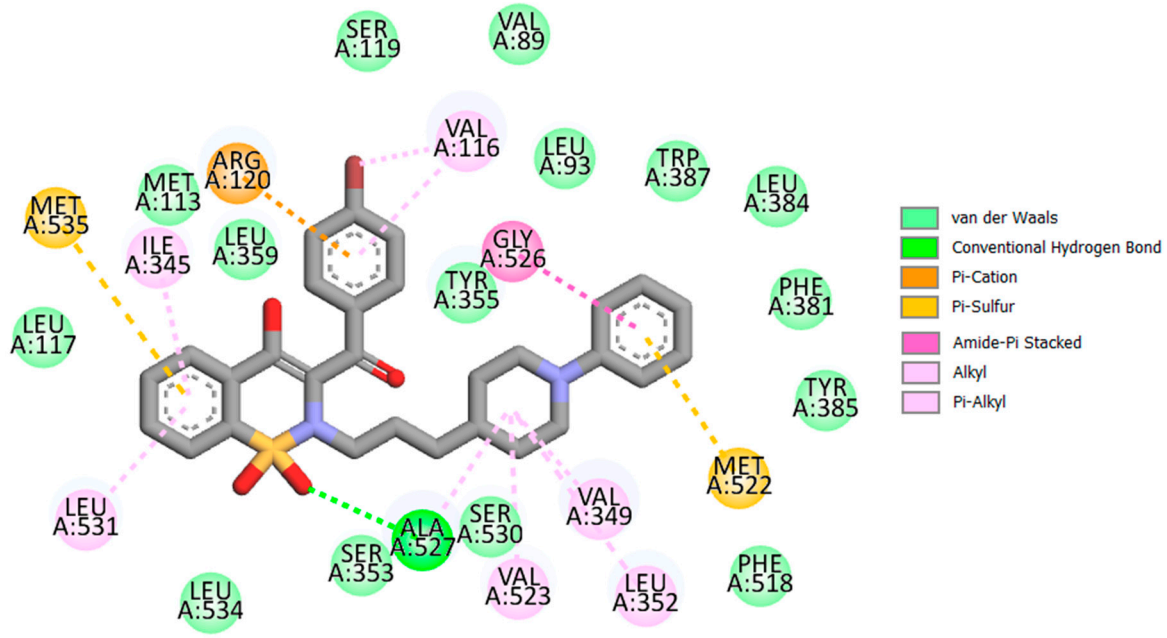


Figure S22. The binding mode of designed compound **BS28 – COX-2** in the active center of COX-2

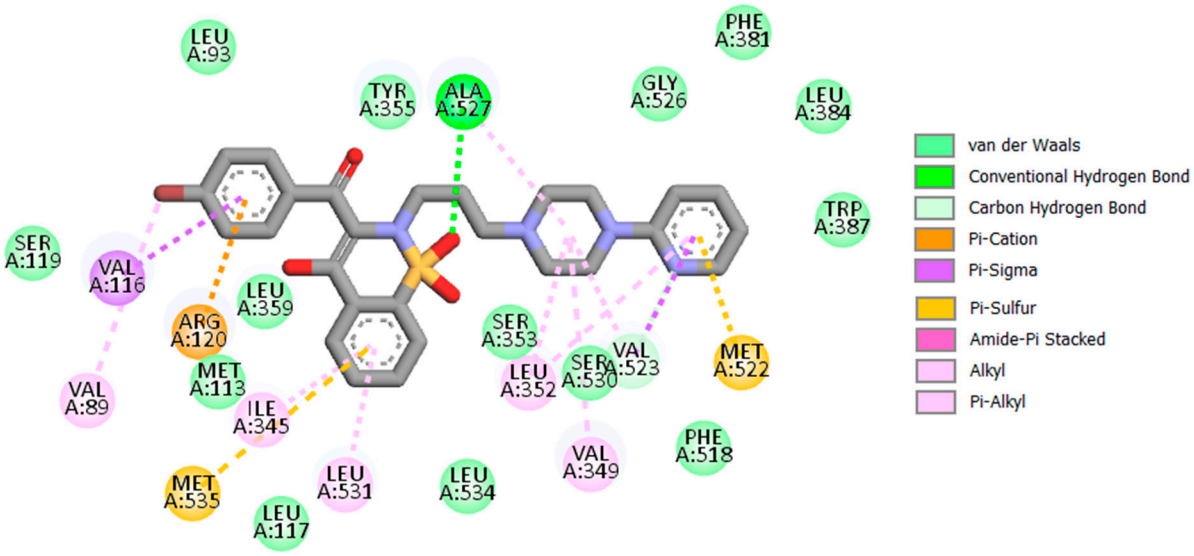


Figure S23. The binding mode of designed compound **BS29 – COX-2** in the active center of COX-2

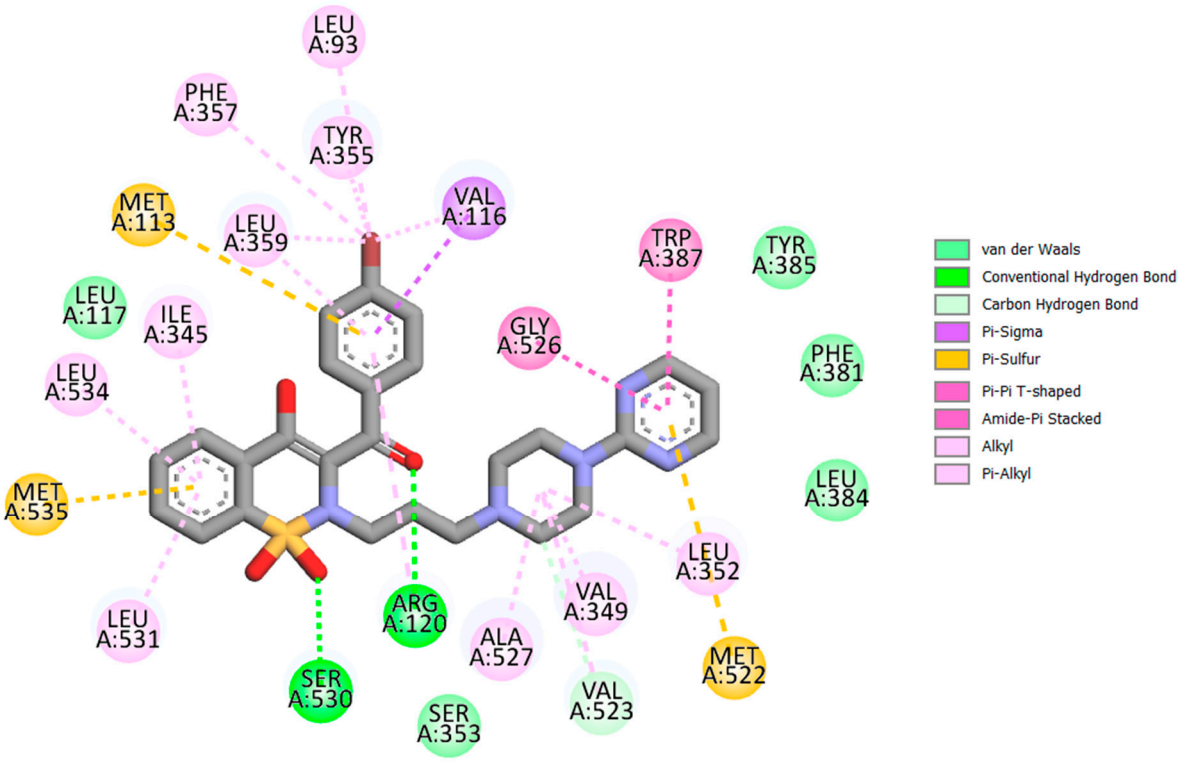


Figure S24. The binding mode of designed compound **BS30 – COX-2** in the active center of COX-2

Table S1. Intermolecular interactions in the active center of COX-1.

	$\Delta G_{binding}$ [kcal/mol]	van der Waals	hydrogen bonds	π-type interactions
BS23	-13.9	Ser353, Phe361, Phe518, Gly526, Leu534	Arg120, Ala527, Ser530, Tyr355	Leu93, Ile89, Met113, Val16, Leu117, Ile345, Leu357, Ile523, Leu535
BS24	-13.4	Ser353, Phe361, Phe518, Leu534, Gly526	Arg120, Tyr355, Ala527, Leu531	Ile89, Leu93, Val116, Ile345, Tyr355, Leu357, Leu359, Ile523, Leu531
BS25	-14.9	Met113, Leu117, Arg120, Phe321, Leu359, Trp387, Leu534, Leu535,	Ser353, Ala527	Val116, Ile345, Tyr355, Leu384, Tyr385, Met522, Gly526, Leu531
BS26	-13.9	Ser353, Phe361, Phe518, Leu534, Gly526	Ser530	Ile345, Leu357, Ile523, Leu531, Leu535
BS27	-14.1	Leu93, Arg120, Leu357, Tyr385, Phe381, Trp387, Ser530	Ser353, Ala527	Vla116, Leu117, Ile345, Tyr355, Leu384
BS28	-12.9	Met113, Arg120, Ser353, Leu357, Trp387, Leu535, Leu543	Ala527	Val116, Leu117, Ile345, Tyr355, Tyr385, Met522, Leu531,
BS29	-14.5	Arg120, Ser353, Leu357, Leu359, Phe381, Tyr385, Trp387, Phe518, Leu534, Leu535	Ala527	Leu93, Met113, Val116, Leu117, Ile345, Leu348, Tyr355, Leu384, Met522, Gly526, Leu531,
BS30	-13.8	Ile89, Met113, Arg120 Tyr348, Leu359, Phe381, Tyr385, Gly526, leu534, Leu535	Ser353, Ala527, Ser530, Leu531	Leu117, Val116, Ile345, Tyr355, Trp387, Leu531,