

Supporting Information

Exploitation of multitarget role of new ferulic and gallic acid derivatives in oxidative stress-related Alzheimer's disease Therapies: Design, synthesis and bioevaluation

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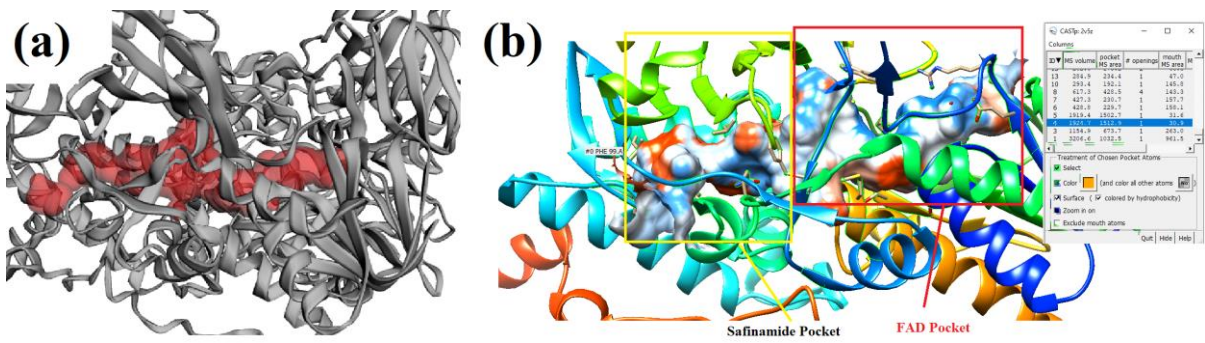


Figure S-1: (a) Shape and binding pocket volume of MAO-B (2V5Z) generated *via* Computed Atlas of Surface Topography of proteins (CASTp) online server (b) 3D modelled ribbon diagram with co-crystallized ligand (surface diagram) obtained *via* MOE software

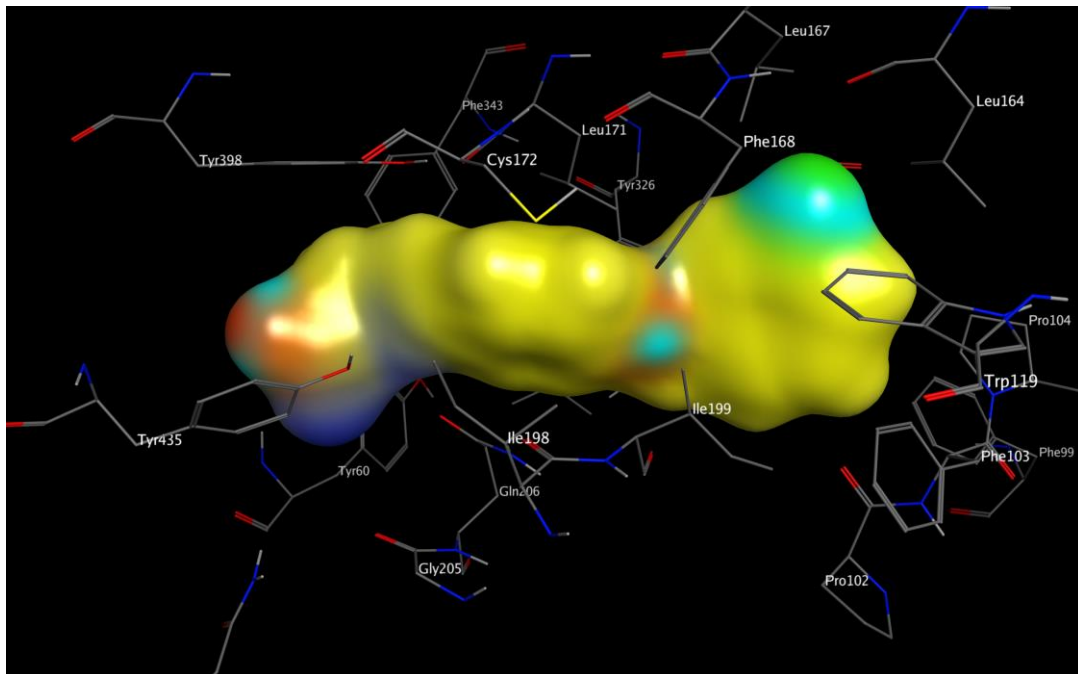


Figure S-2: Shape and binding pocket of MAO-B (2V5Z) with co-crystallized ligand safinamide (Surface diagram) generated *via* MOE

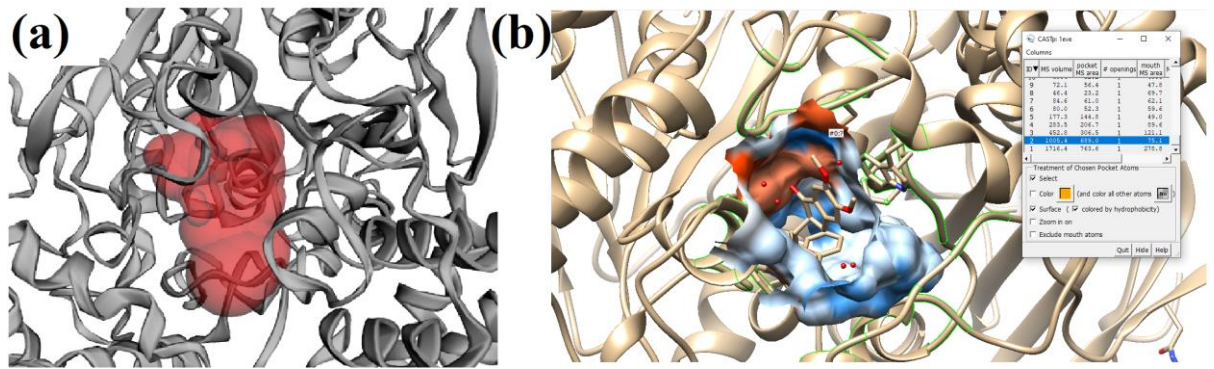


Figure S-3: (a) Shape and binding pocket volume of *TcAChE* (1EVE) generated *via* CASTp online server (b) 3D modelled ribbon diagram with co-crystallized ligand (surface diagram) obtained *via* MOE software

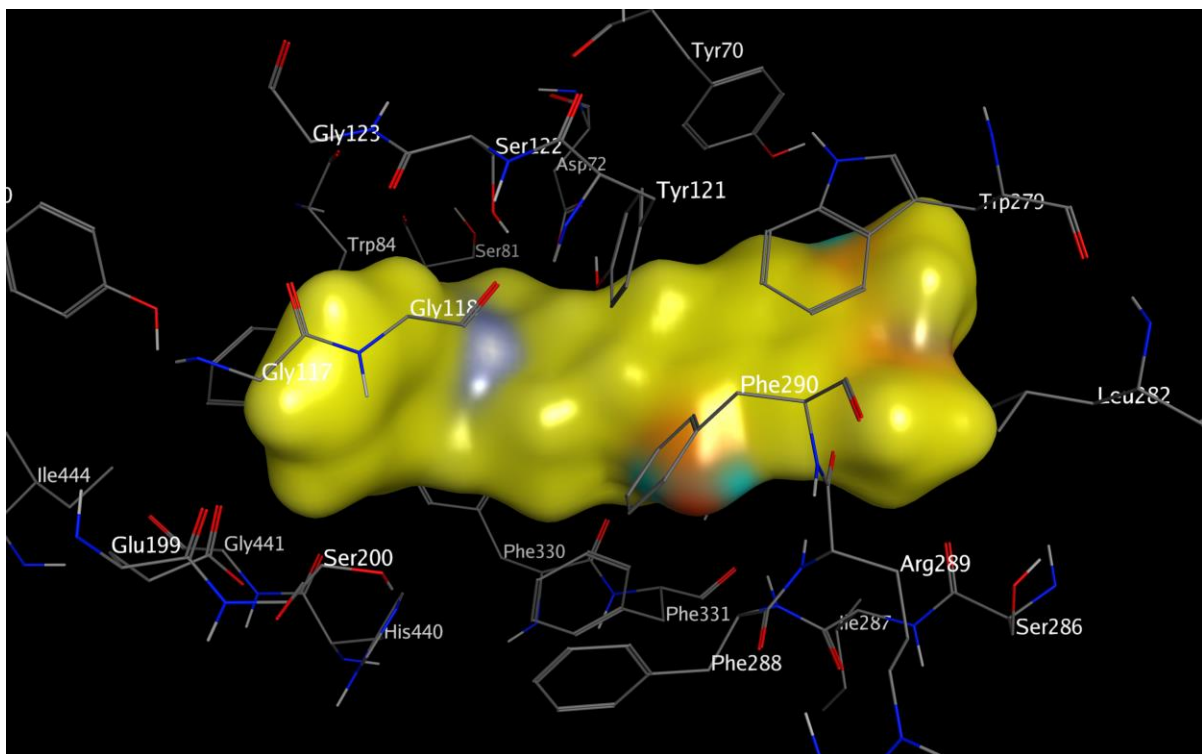


Figure S-4: Shape and binding pocket of *TcAChE* (1EVE) with co-crystallized ligand donepezil (Surface diagram) generated *via* MOE

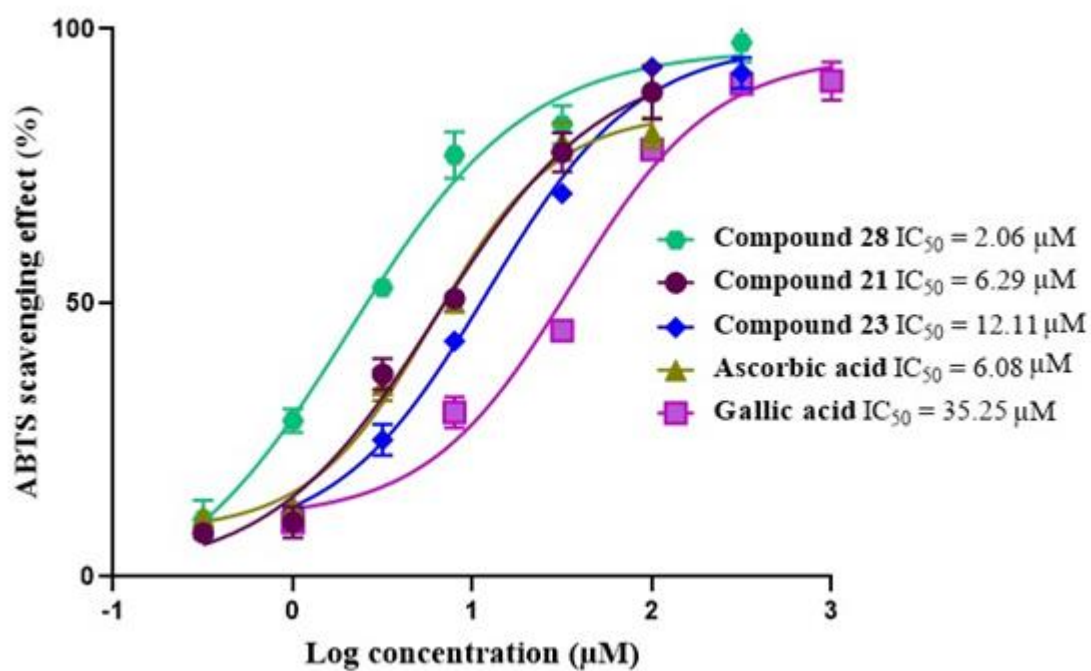


Figure S-5: Dose-response curve of synthesized compounds obtained from the percent ABTS scavenging effect and concentration values.

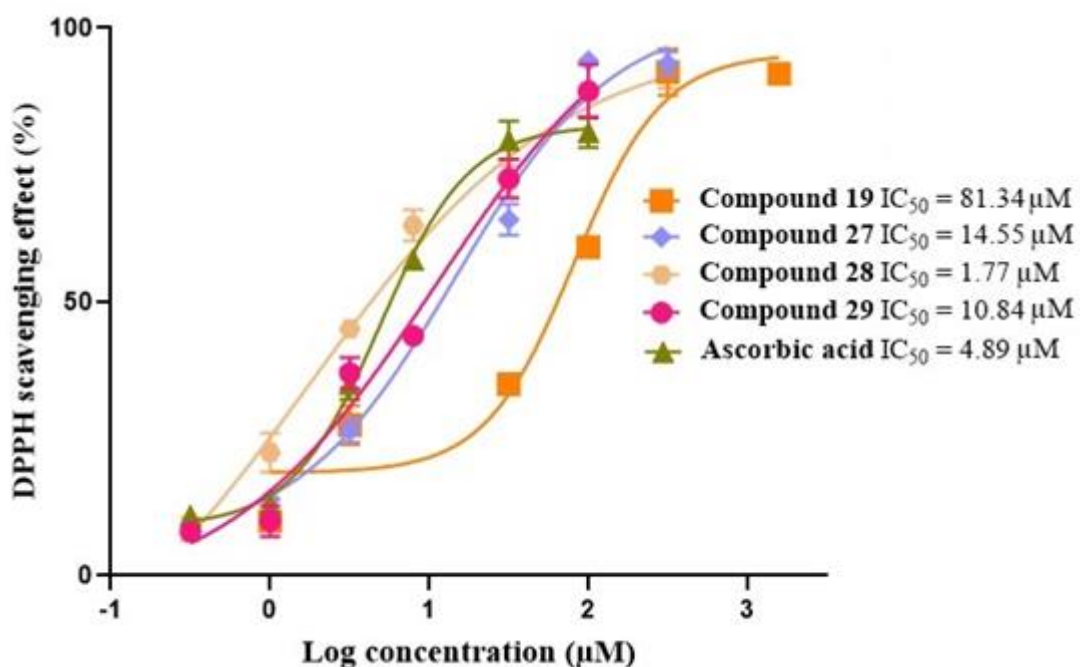


Figure S-6: Dose-response curve of synthesized compounds obtained from the percent DPPH scavenging effect and concentration values.

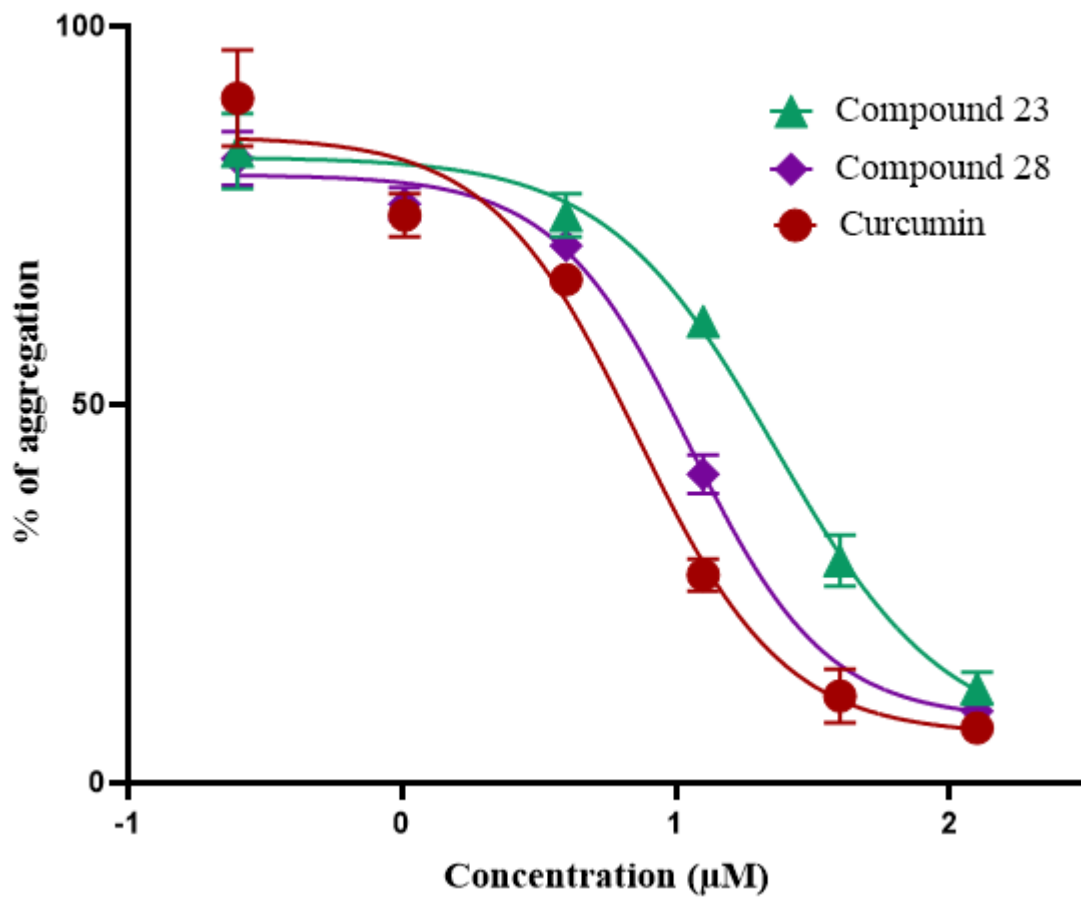


Figure S-7: Dose–response effect of inhibitors (**23**, **28**) and standard drug curcumin) from ThT assay on A β aggregation.

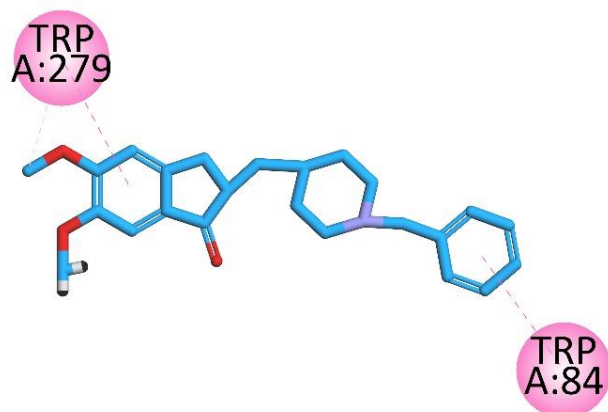


Figure S-8: 2D interaction plot of standard drug donepezil in the binding site of AChE (1EVE) modelled by using Discovery Studio visualizer

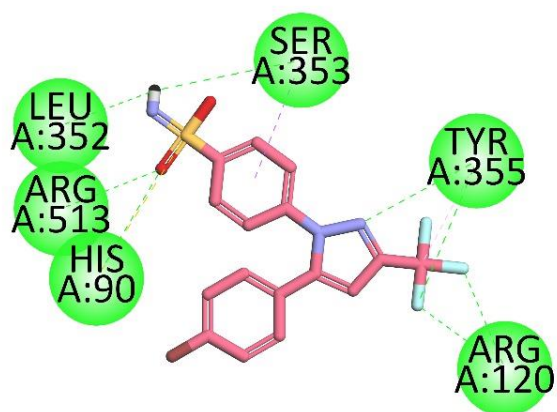


Figure S-9: 2D interaction plot of standard drug Celecoxib in the binding site of COX-2 (1CX2) modelled by using Discovery Studio visualizer

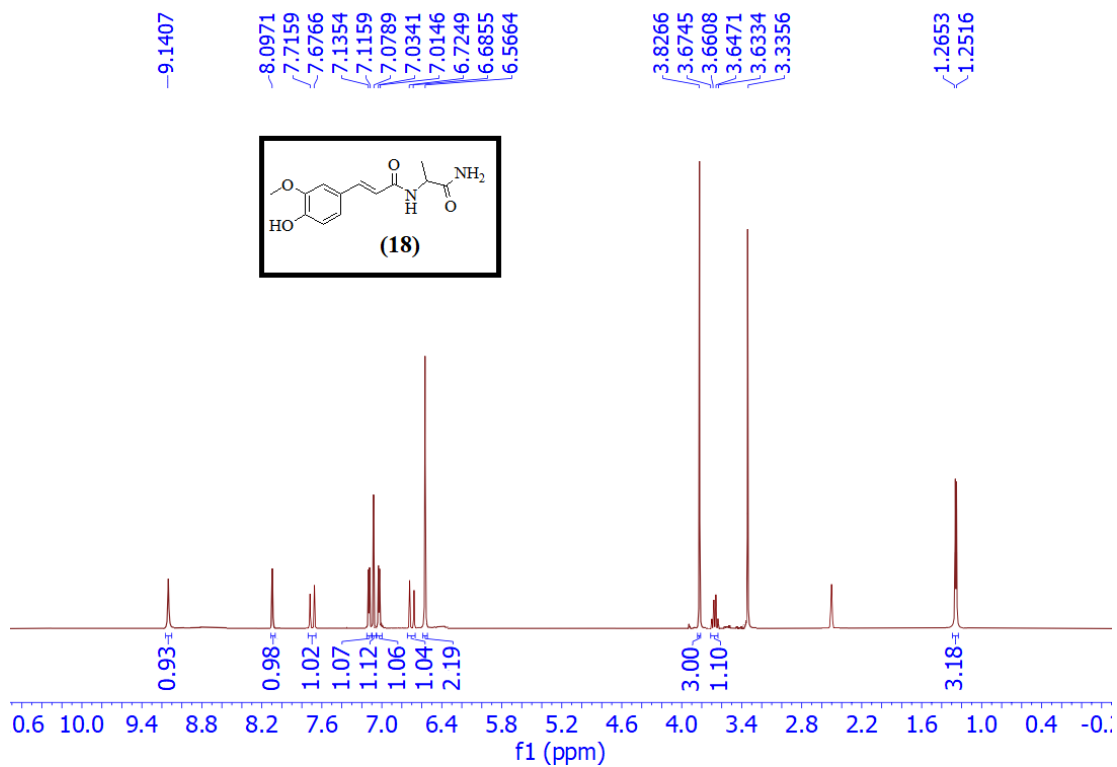


Figure S-10: ¹H NMR (400 MHz) spectrum of compound **18** in DMSO-*d*₆

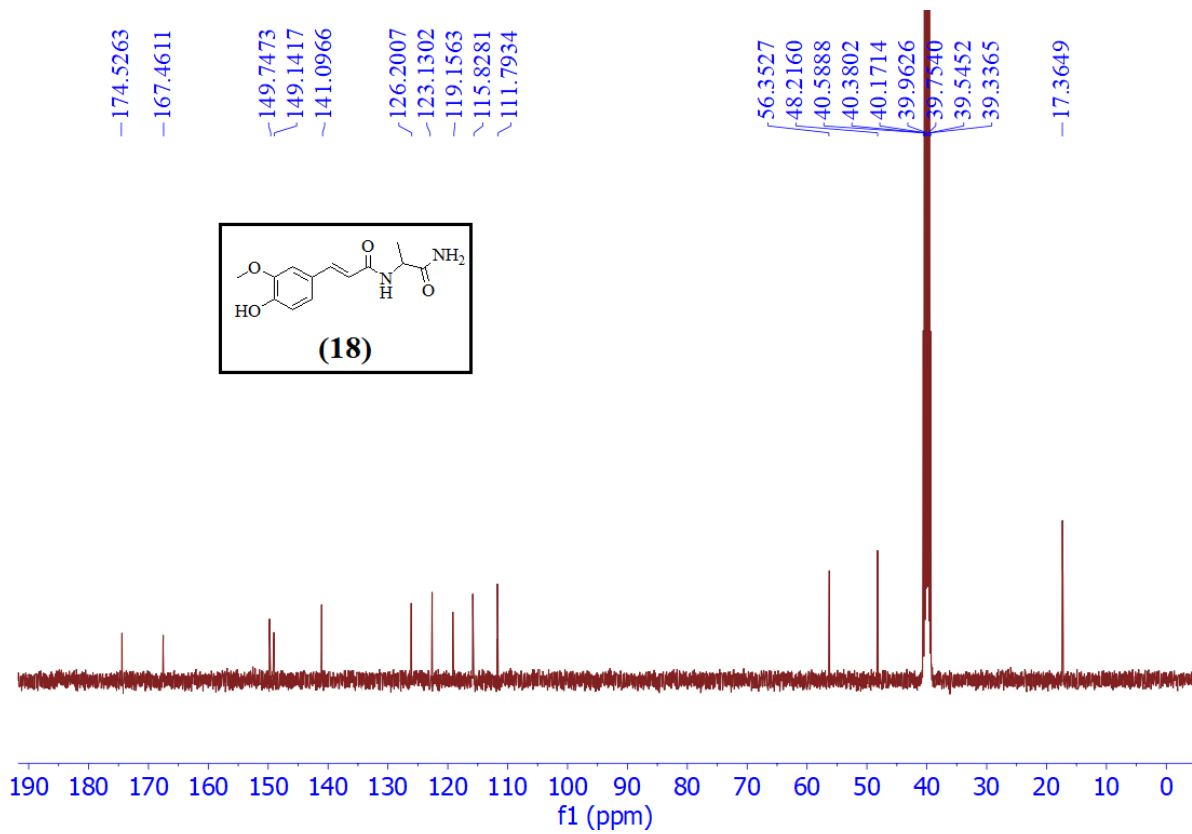


Figure S-11: ¹³C NMR (100 MHz) spectrum of compound **18** in DMSO-*d*₆

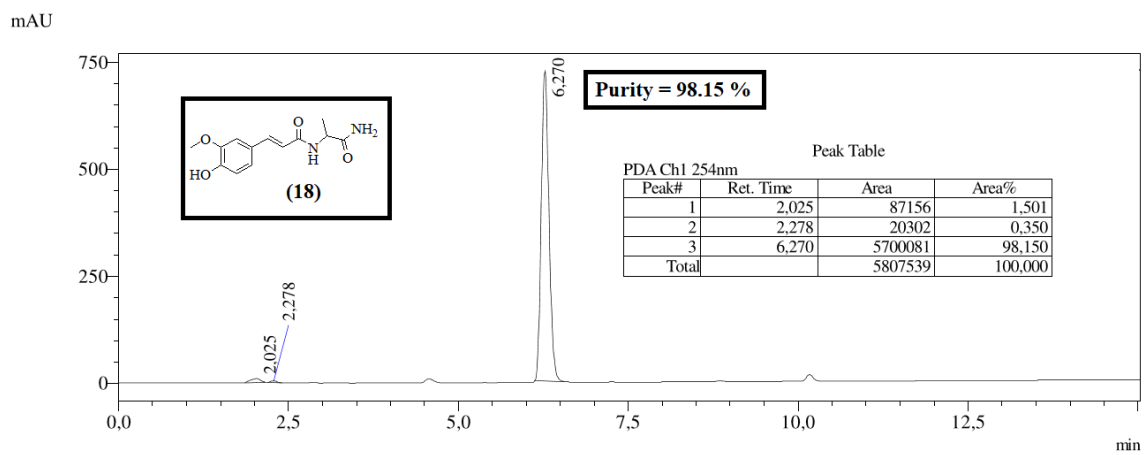


Figure S-12: HPLC Chromatogram of compound **18**

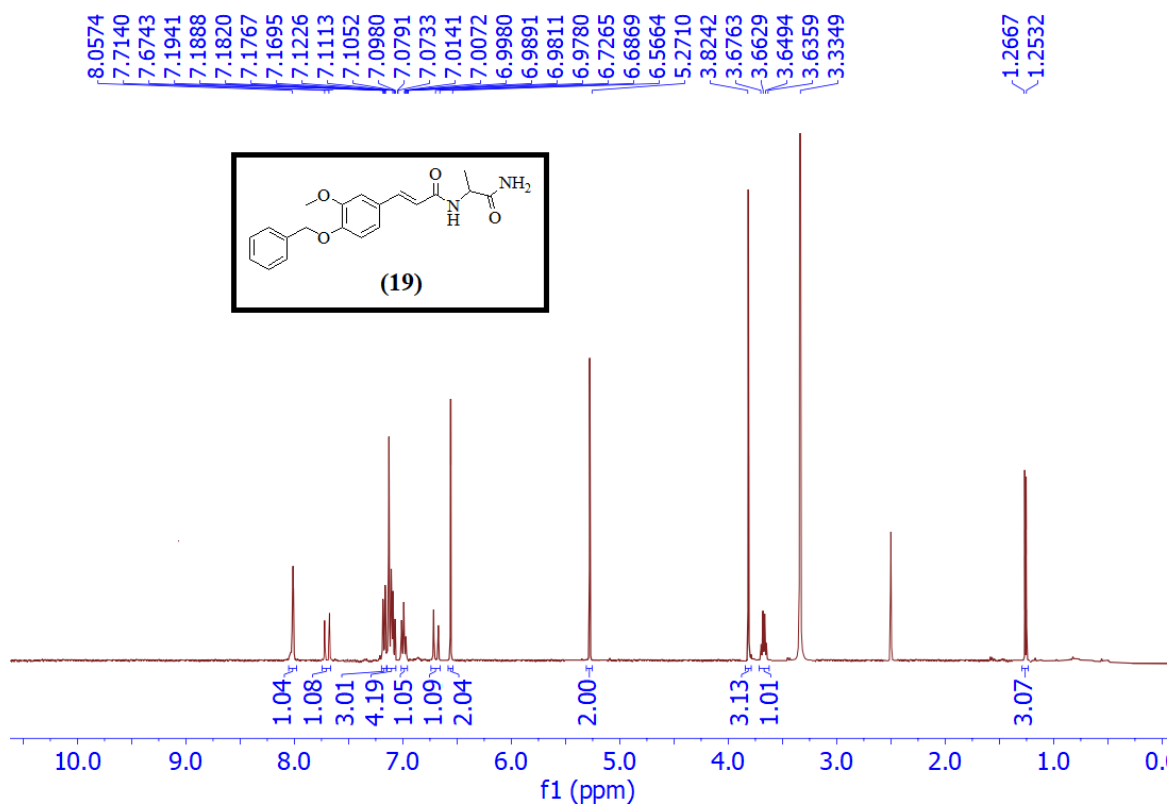


Figure S-13: ¹H NMR (400 MHz) spectrum of compound **19** in DMSO-*d*₆

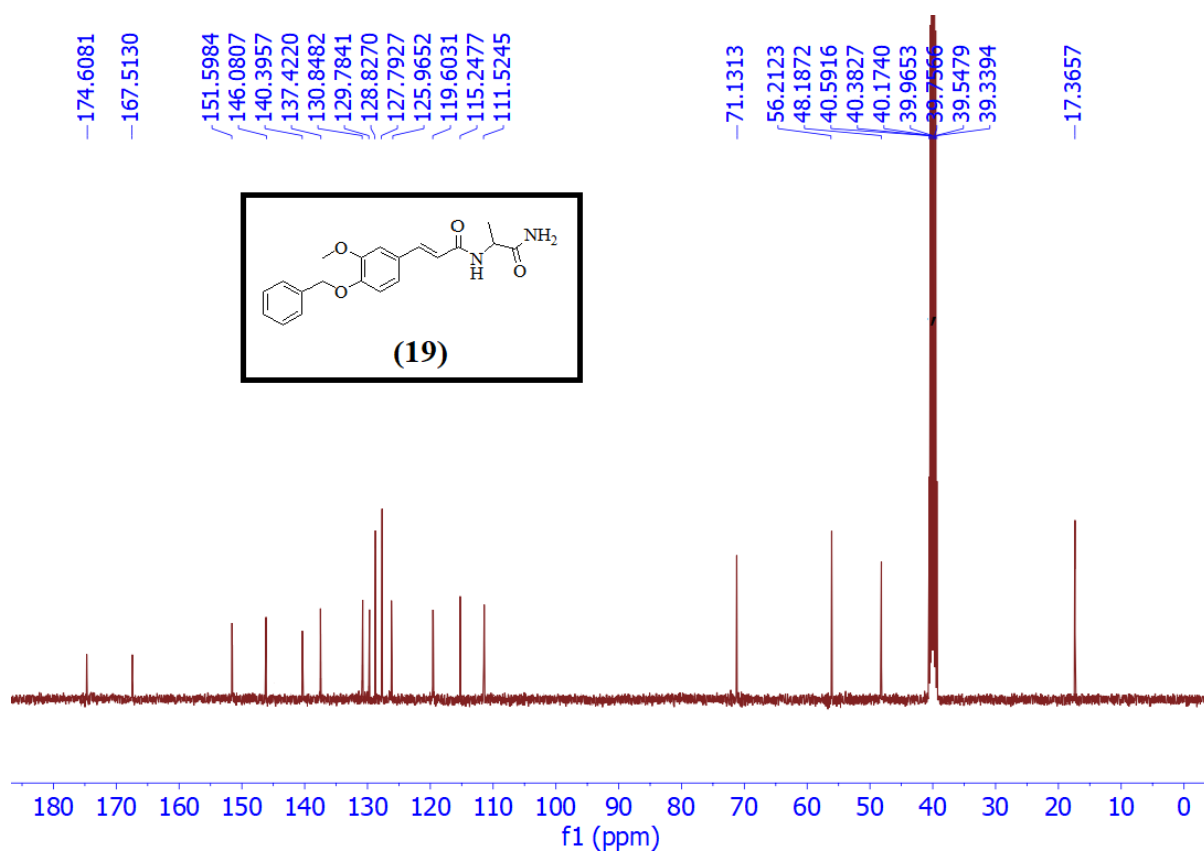


Figure S-14: ^{13}C NMR (100 MHz) spectrum of compound **19** in $\text{DMSO-}d_6$

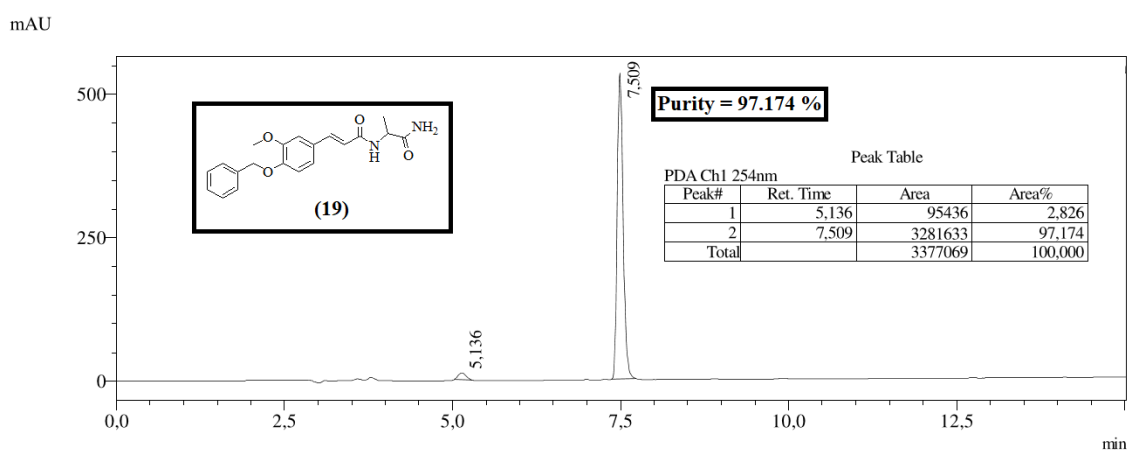


Figure S-15: HPLC Chromatogram of compound **19**

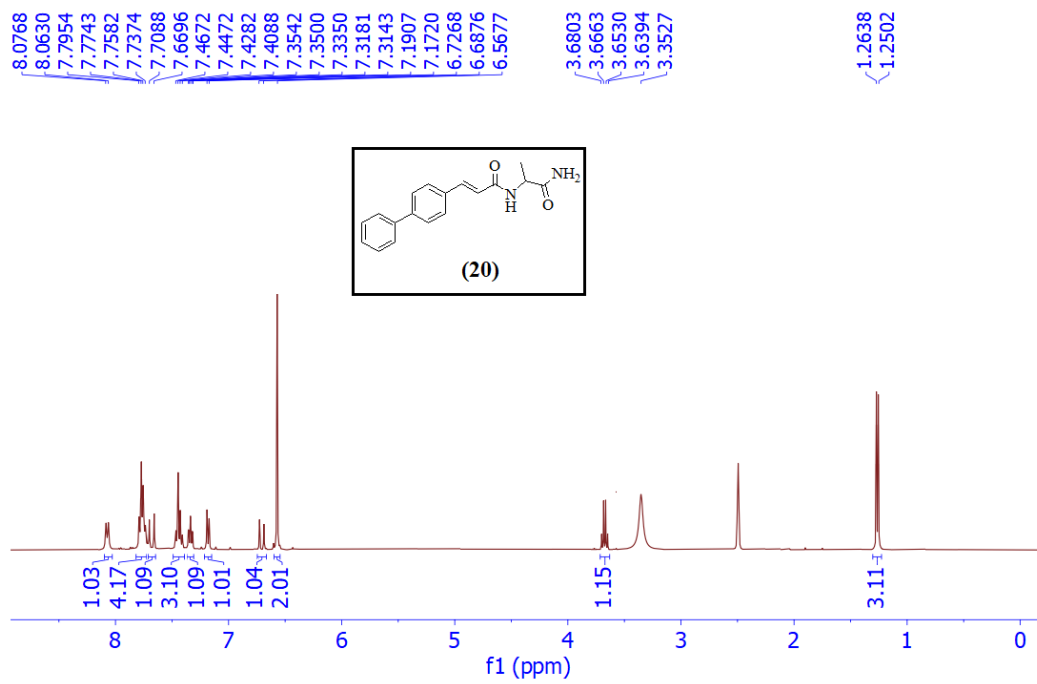


Figure S-16: ¹H NMR (400 MHz) spectrum of compound **20** in DMSO-*d*₆

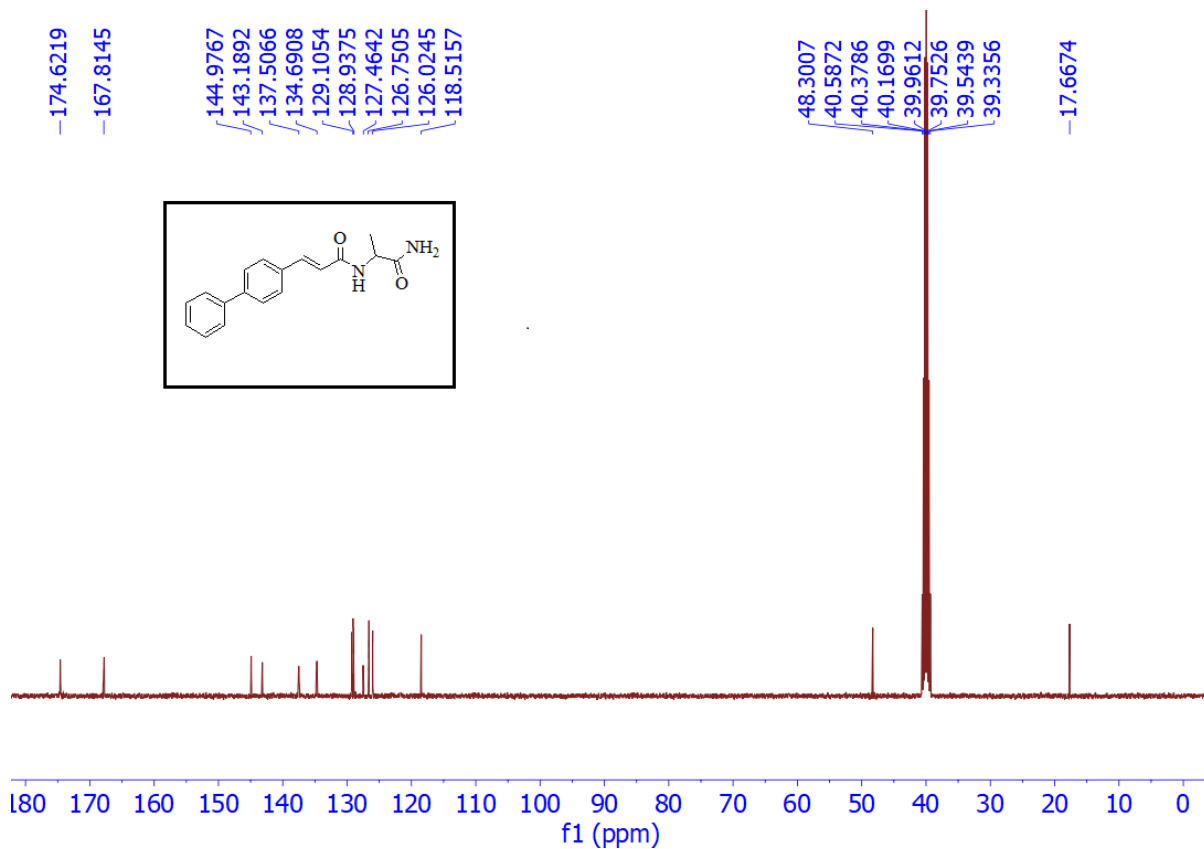


Figure S-17: ¹³C NMR (100 MHz) spectrum of compound 20 in DMSO-*d*₆

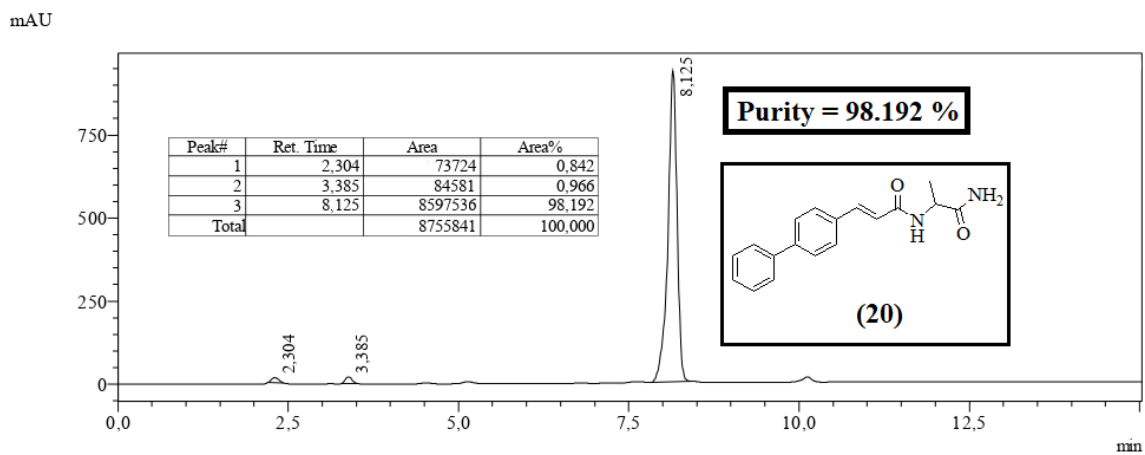


Figure S-18: HPLC Chromatogram of compound 20

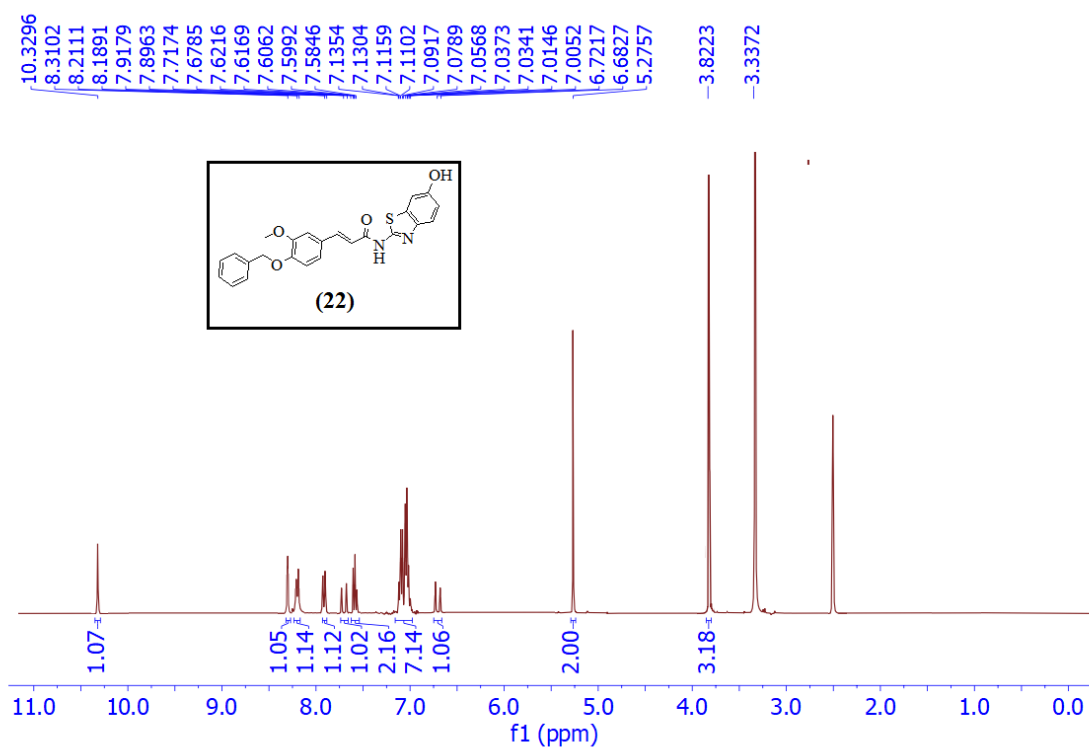


Figure S-19: $^1\text{H NMR}$ (400 MHz) spectrum of compound **22** in $\text{DMSO-}d_6$

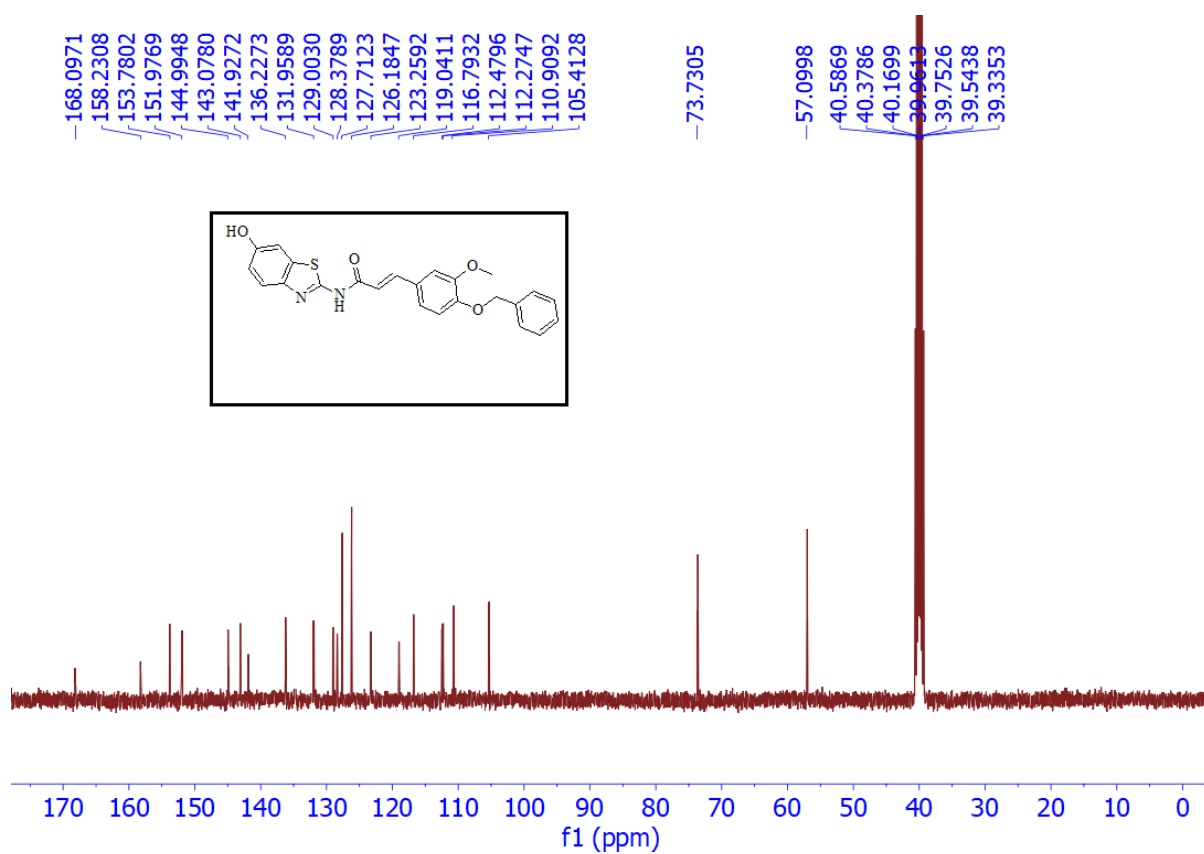


Figure S-20: ^{13}C NMR (100 MHz) spectrum of compound **22** in $\text{DMSO-}d_6$

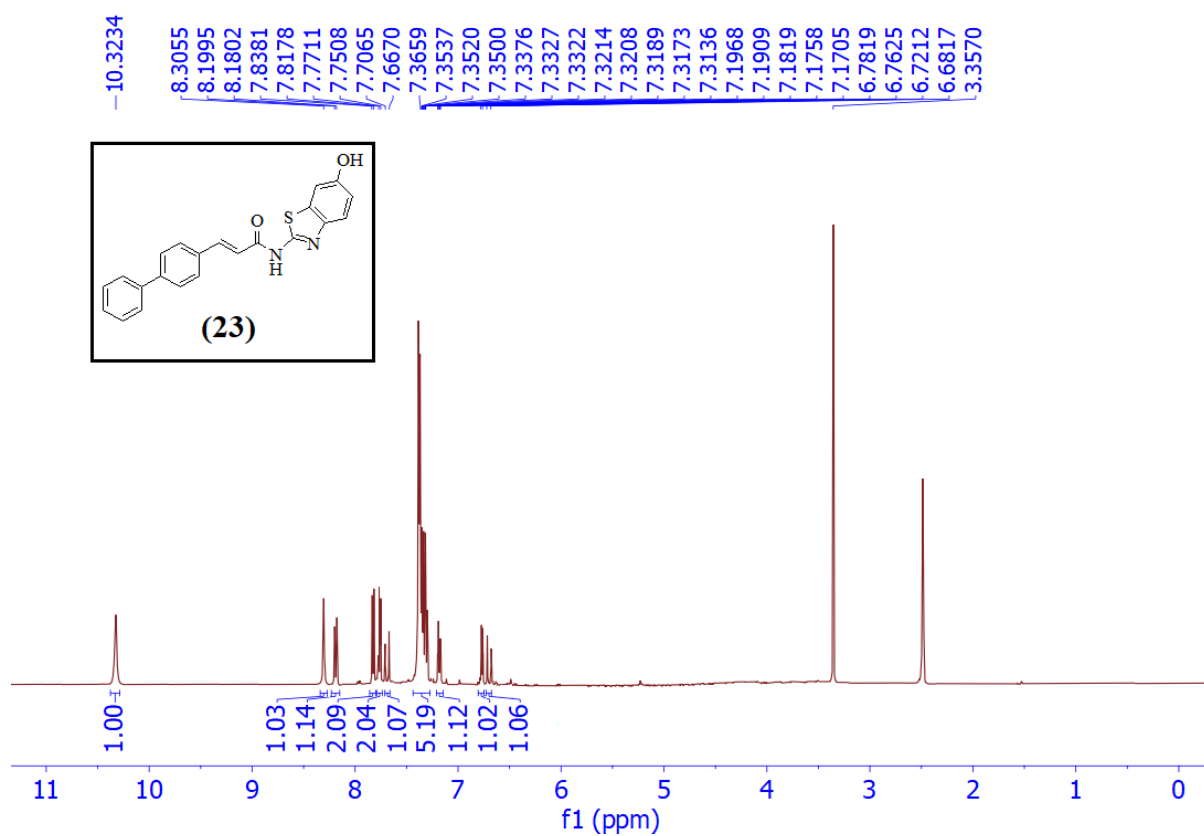


Figure S-21: ^1H NMR (400 MHz) spectrum of compound **23** in $\text{DMSO-}d_6$

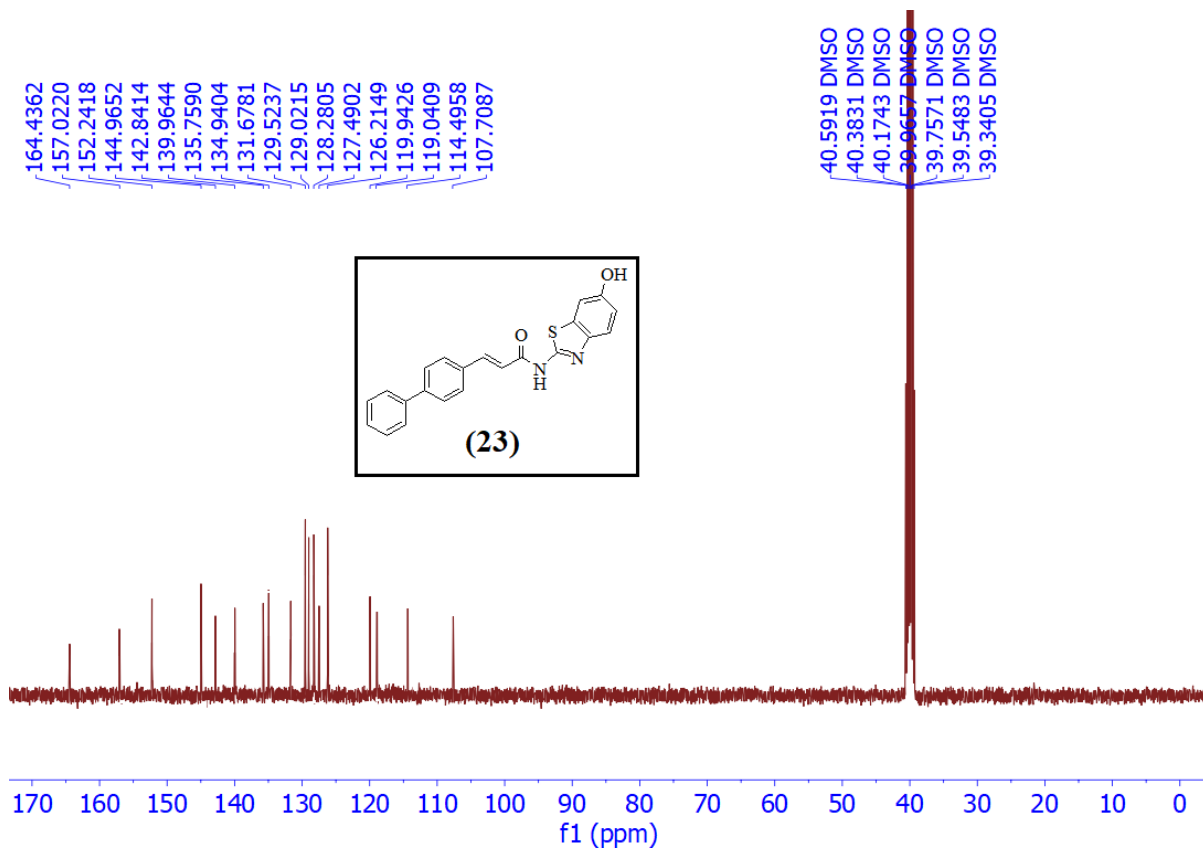


Figure S-22: ^{13}C NMR (100 MHz) spectrum of compound **23** in $\text{DMSO-}d_6$

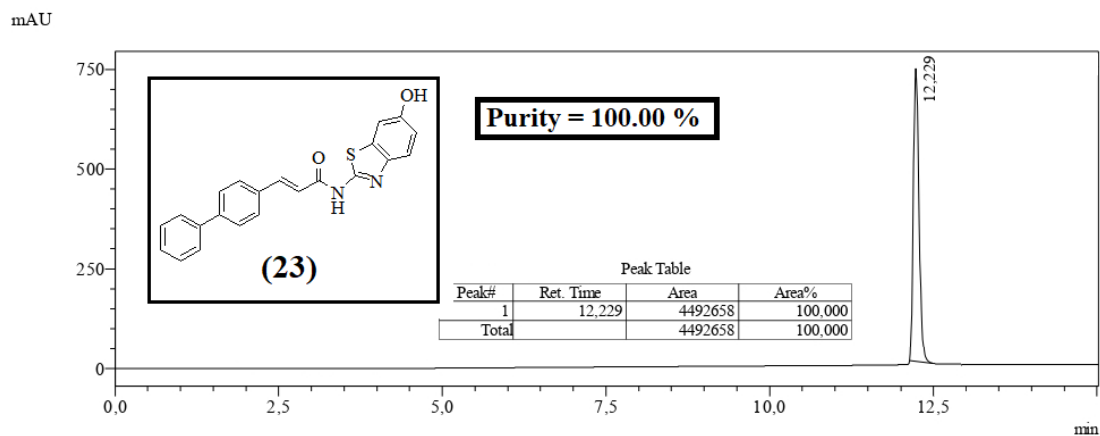


Figure S-23: HPLC Chromatogram of compound **23**

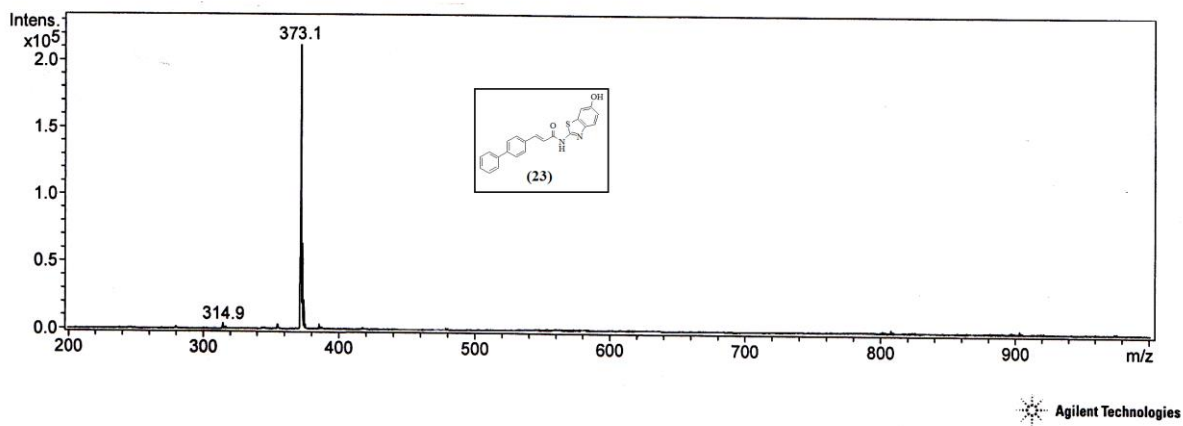


Figure S-24: LC-MS Chromatogram of compound **23**

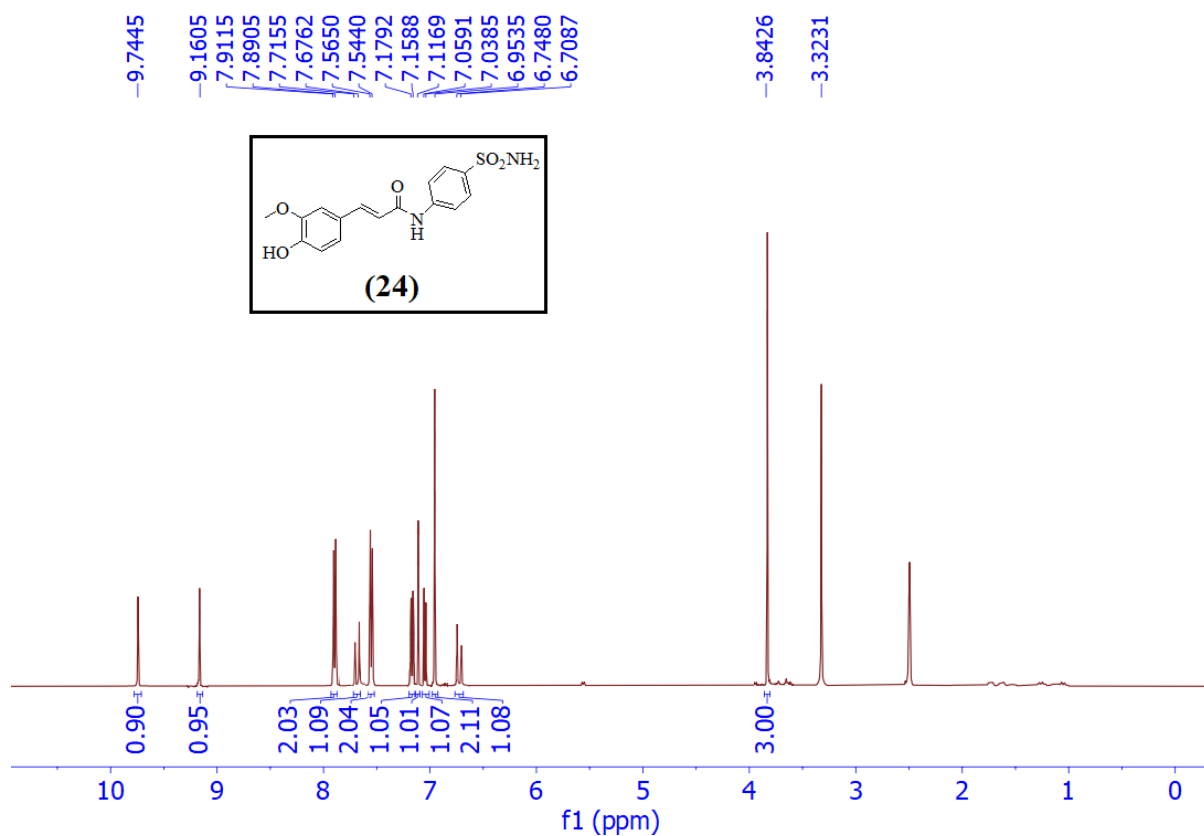


Figure S-25: ¹H NMR (400 MHz) spectrum of compound **24** in DMSO-*d*₆

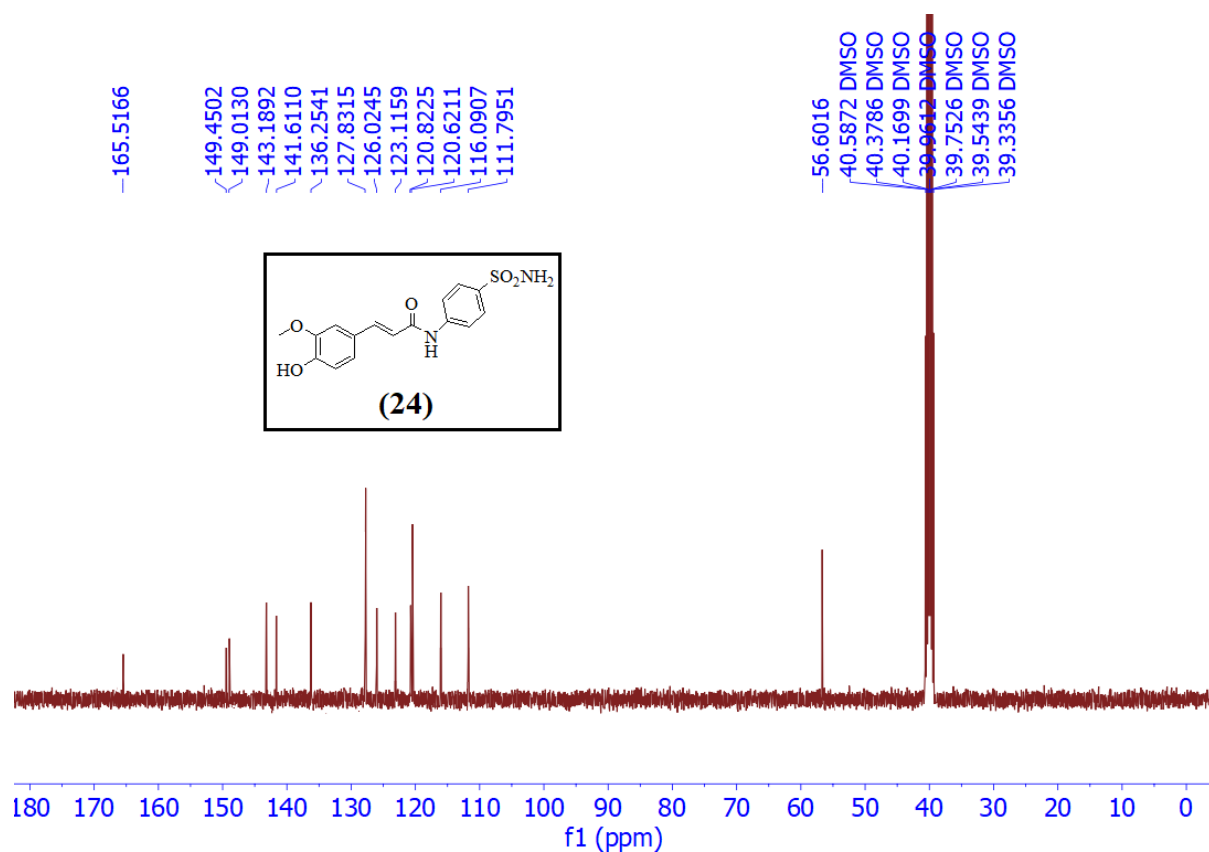


Figure S-26: ¹³C NMR (100 MHz) spectrum of compound **24** in DMSO-*d*₆

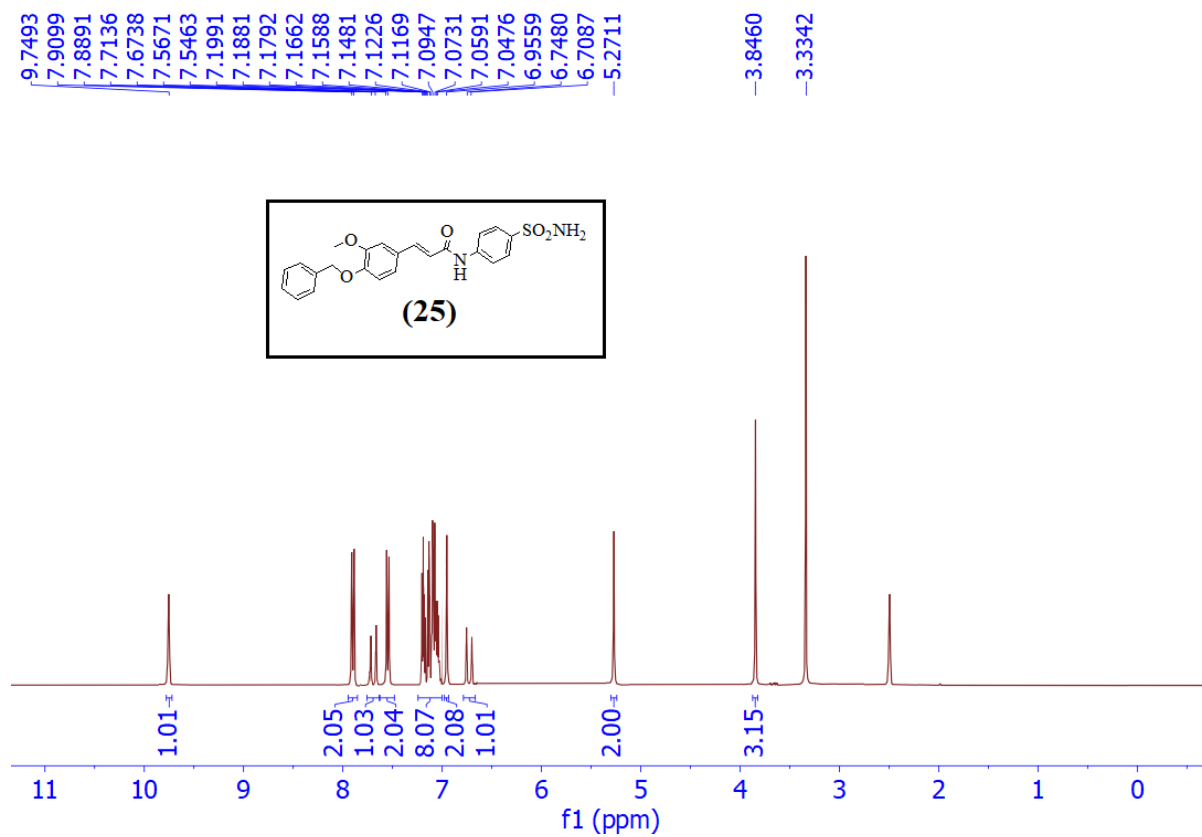


Figure S-27: $^1\text{H NMR}$ (400 MHz) spectrum of compound **25** in $\text{DMSO-}d_6$

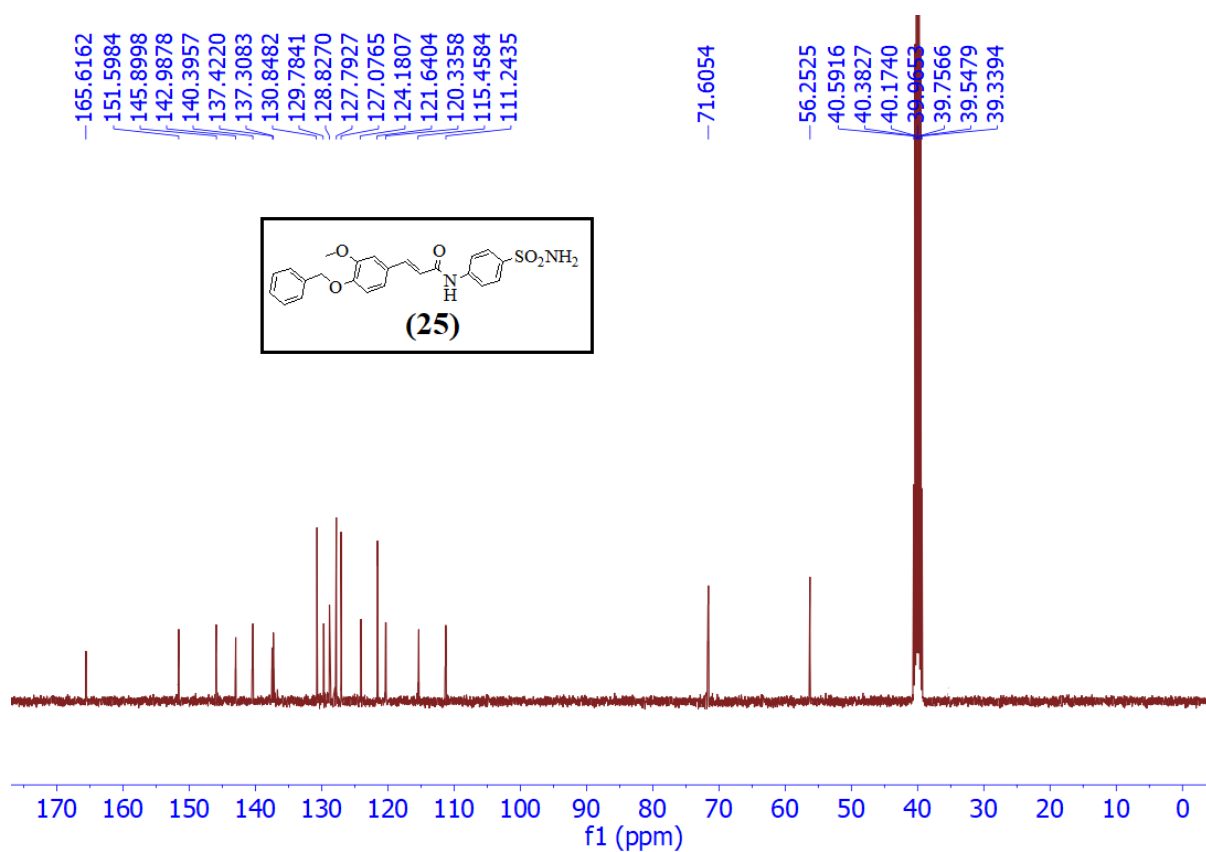


Figure S-28: ¹³C NMR (100 MHz) spectrum of compound **(25)** in DMSO-*d*₆

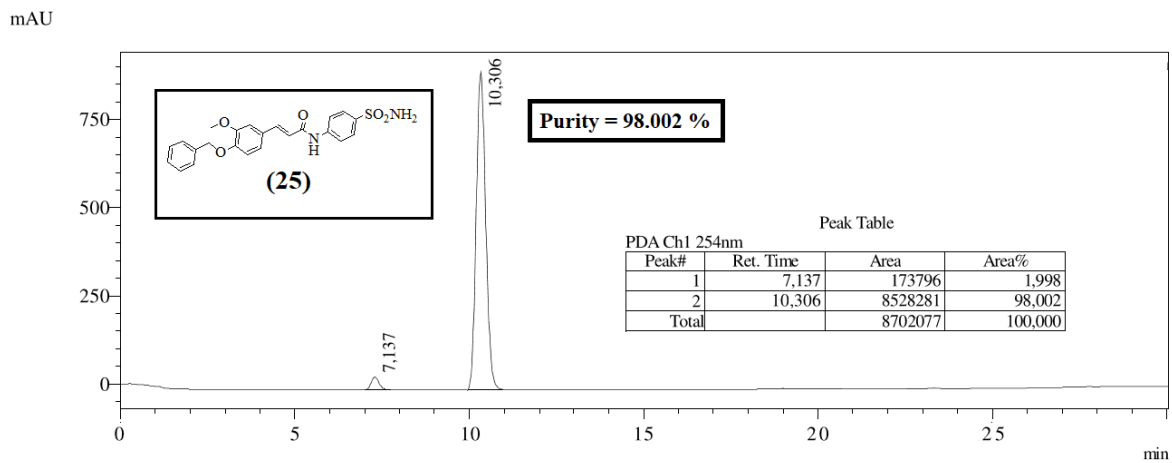
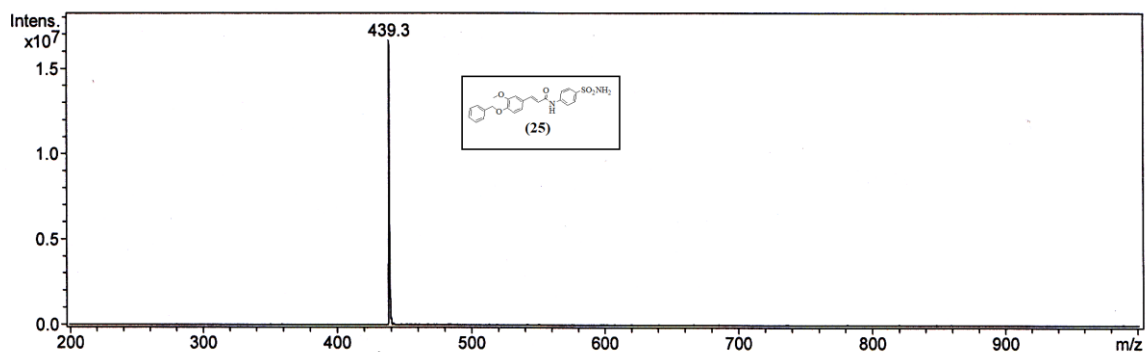


Figure S-29: HPLC Chromatogram of compound **(25)**



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Figure S-30: LC-MS Chromatogram of compound 25

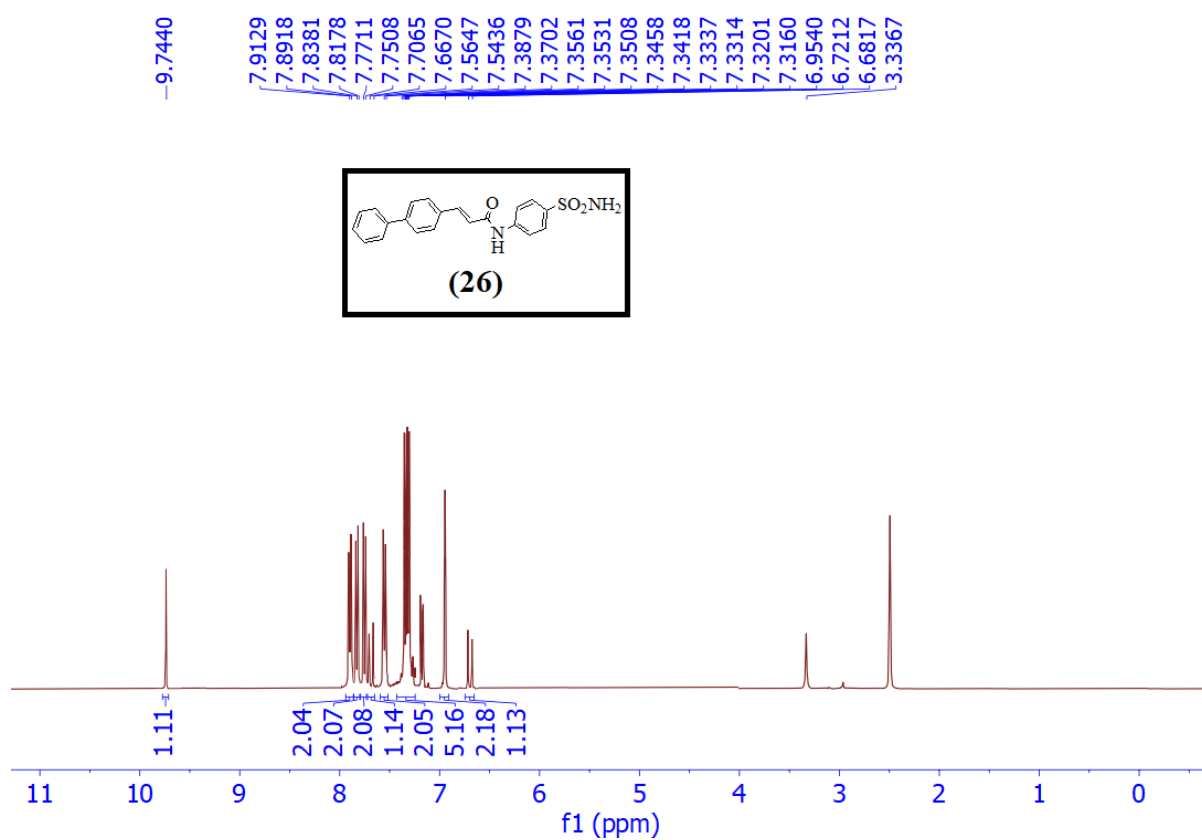


Figure S-31: ¹H NMR (400 MHz) spectrum of compound 26 in DMSO-*d*₆

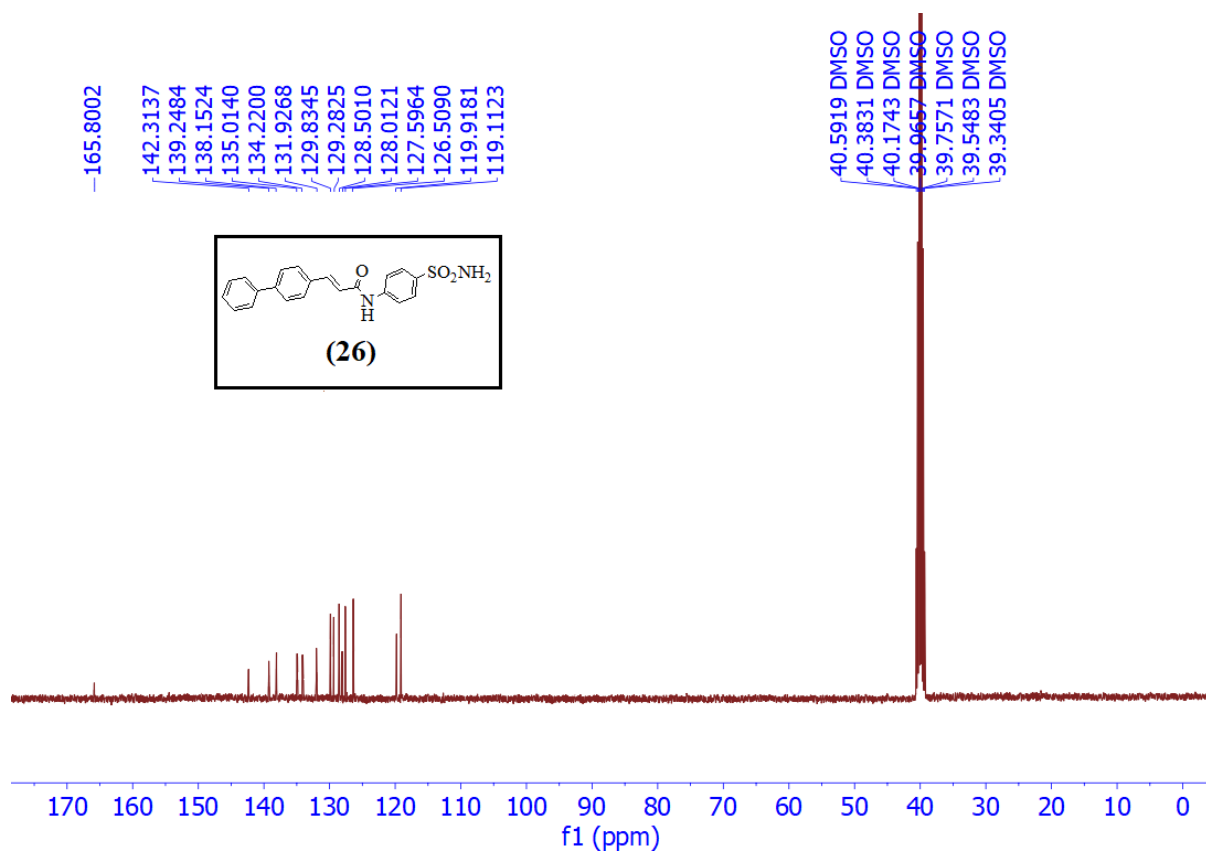


Figure S-32: ¹³C NMR (100 MHz) spectrum of compound **26** in DMSO-*d*₆

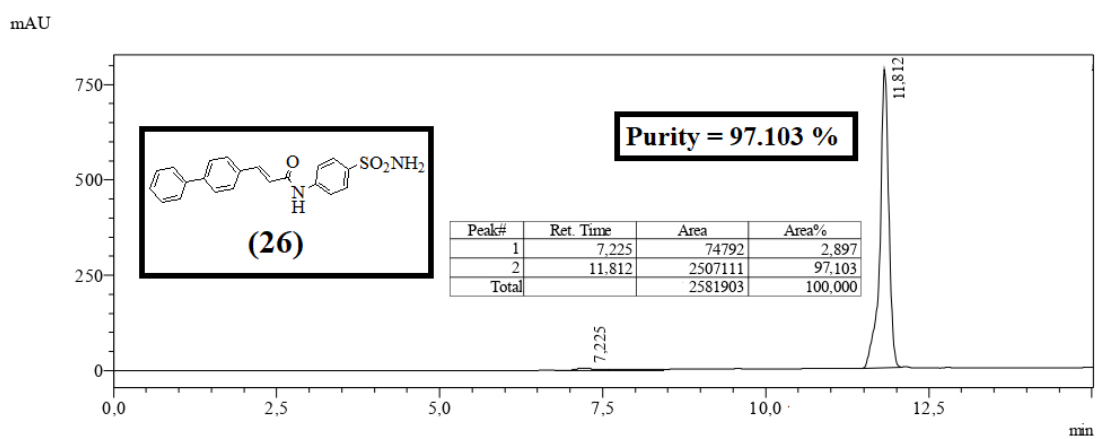


Figure S-33: HPLC Chromatogram of compound **26**

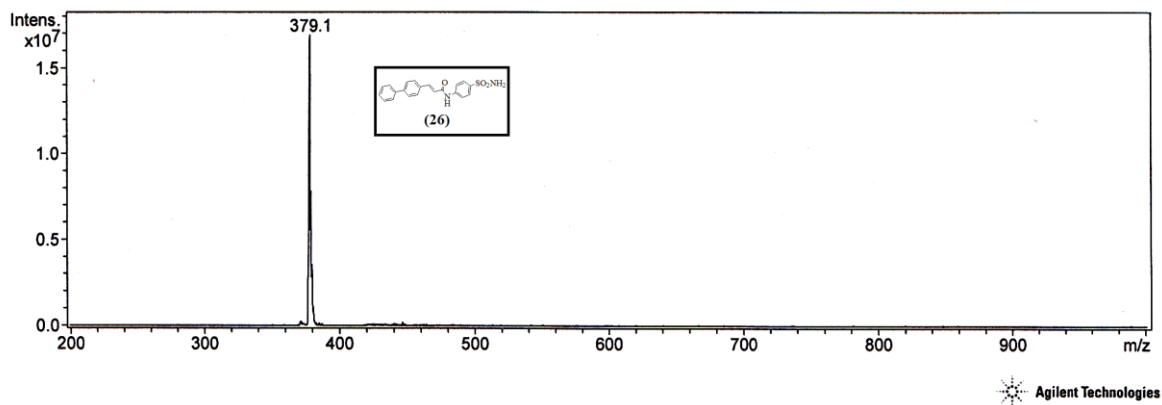


Figure S-34: LC-MS Chromatogram of compound **26**

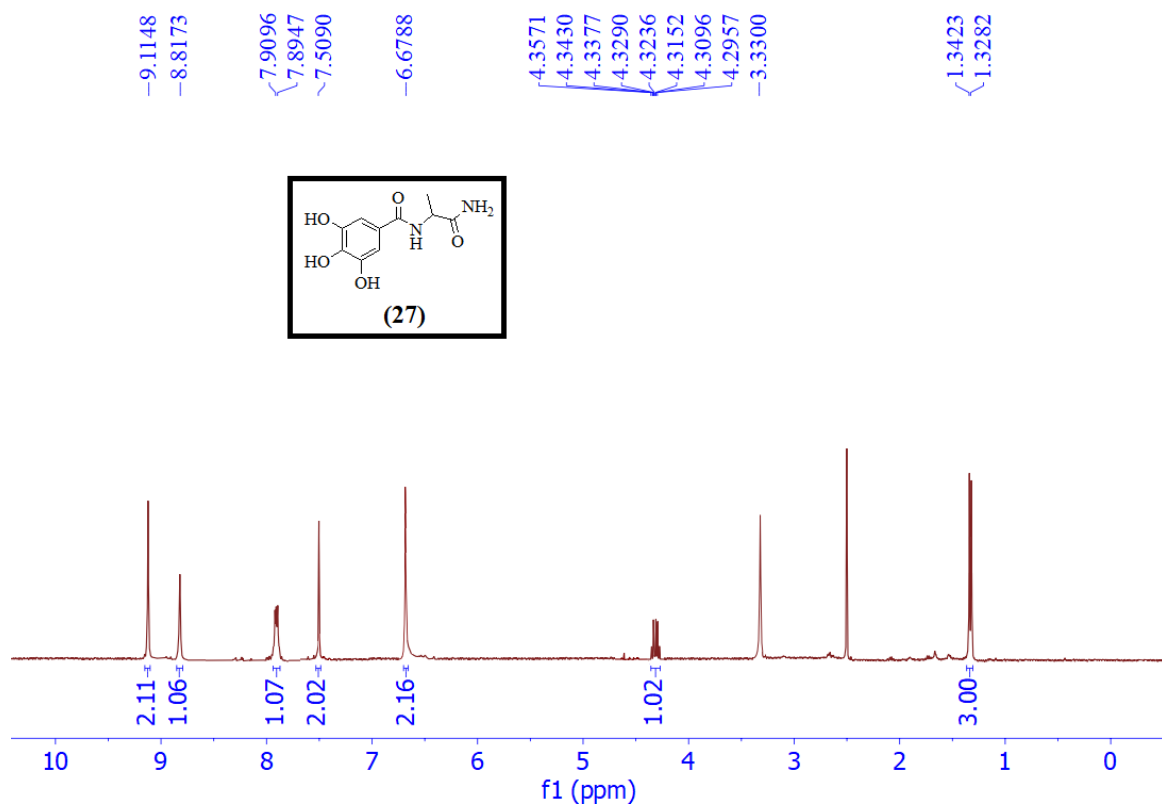


Figure S-35: ^1H NMR (400 MHz) spectrum of compound **27** in $\text{DMSO-}d_6$

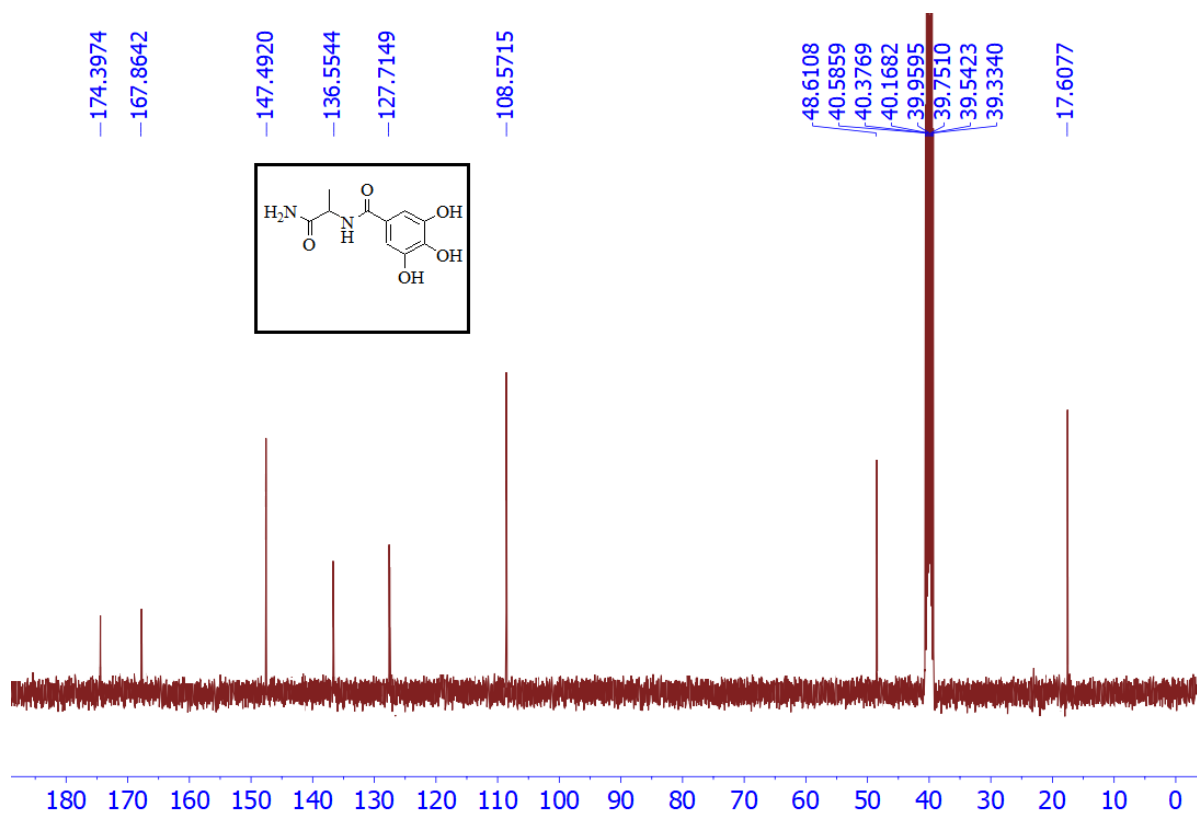


Figure S-36: ^{13}C NMR (100 MHz) spectrum of compound **27** in $\text{DMSO-}d_6$

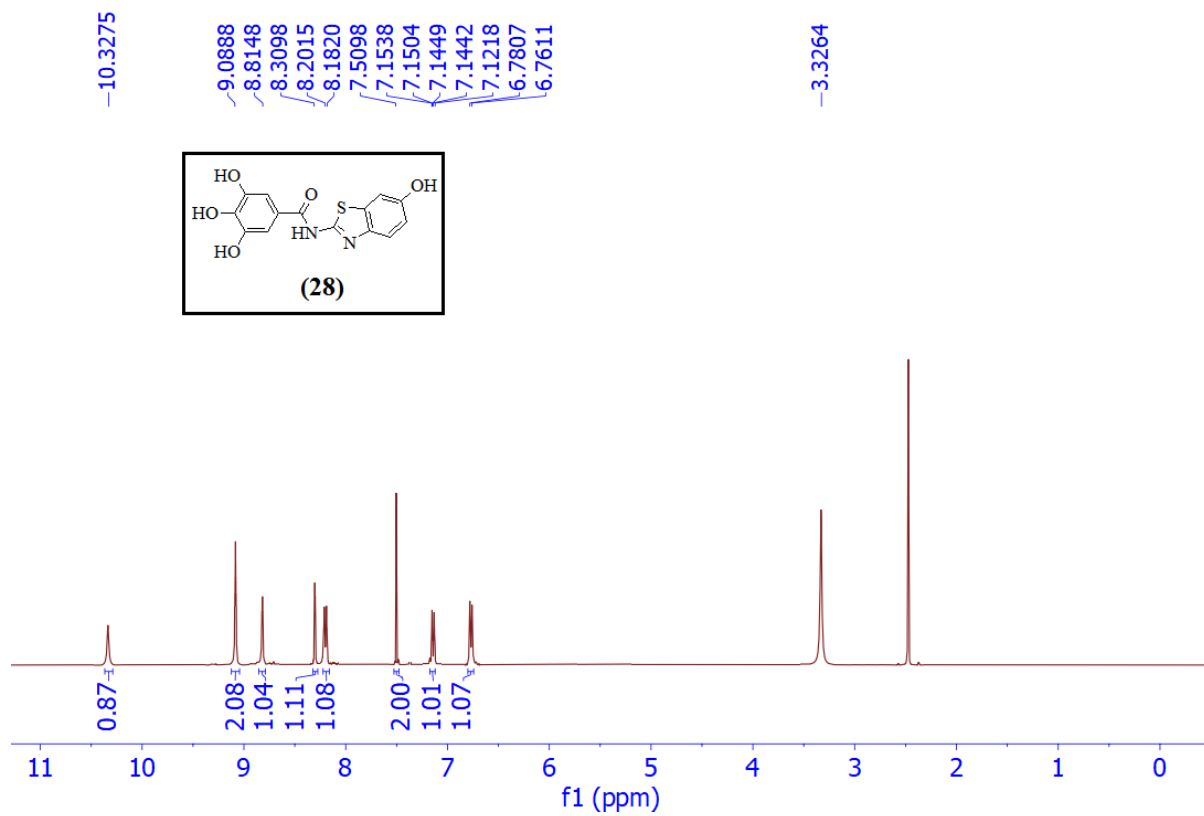


Figure S-37: ^1H NMR (400 MHz) spectrum of compound **28** in $\text{DMSO-}d_6$

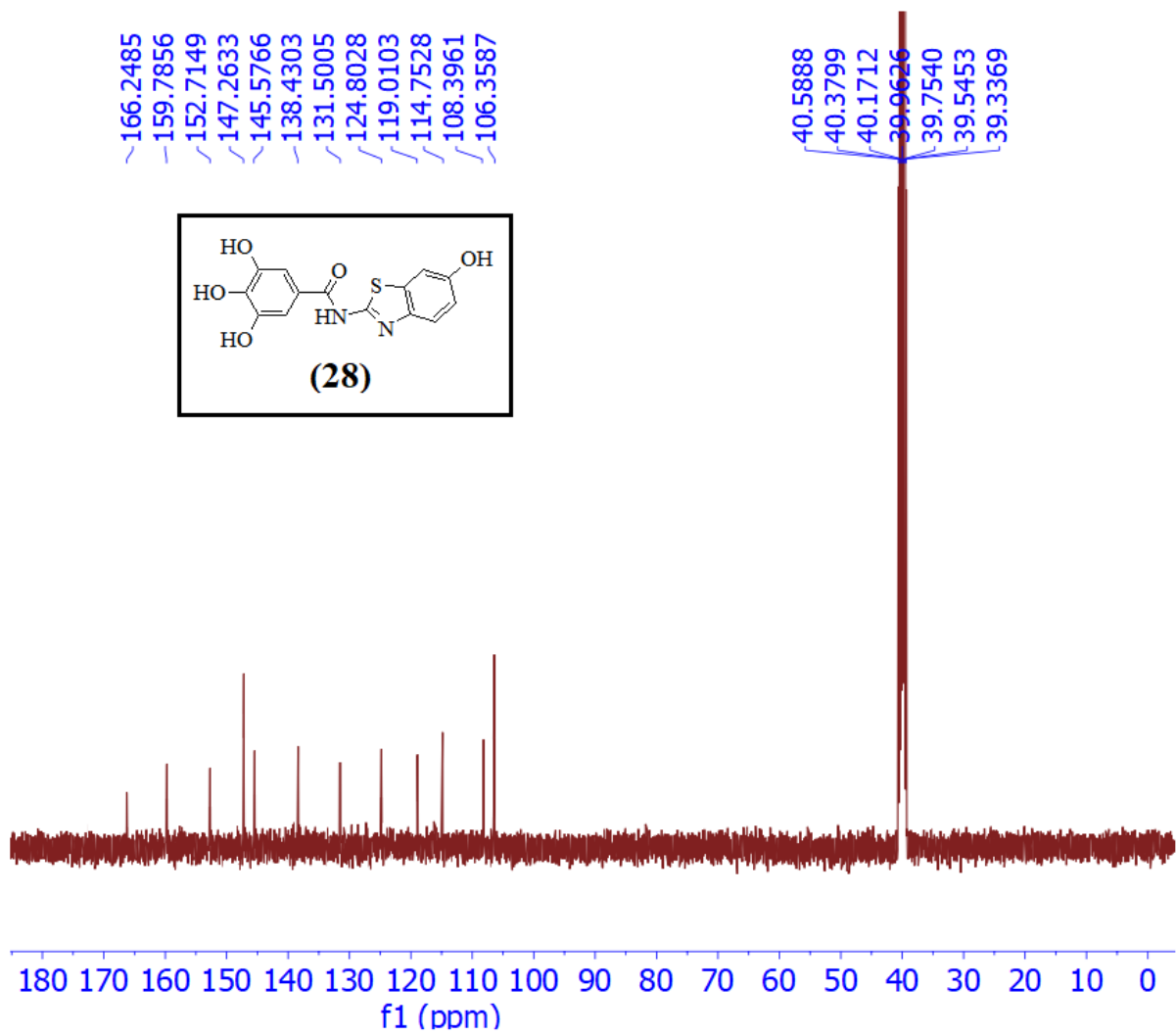


Figure S-38: ^{13}C NMR (100 MHz) spectrum of compound **28** in DMSO

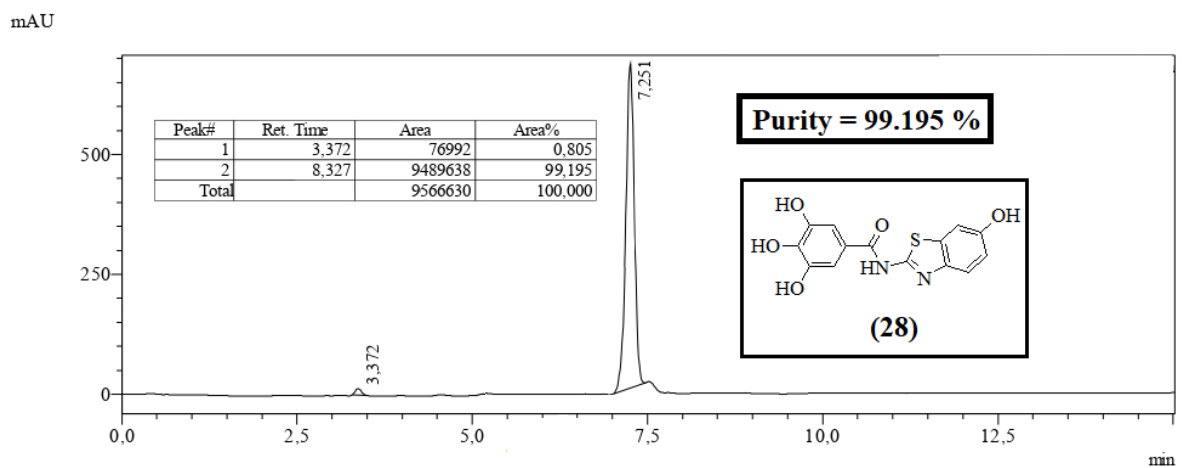


Figure S-39: HPLC Chromatogram of compound **28**

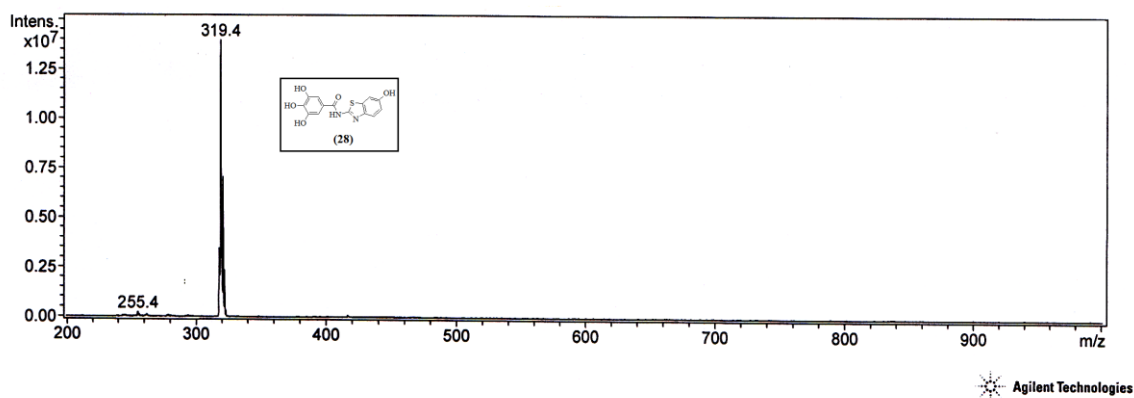


Figure S-40: LC-MS Chromatogram of compound 28

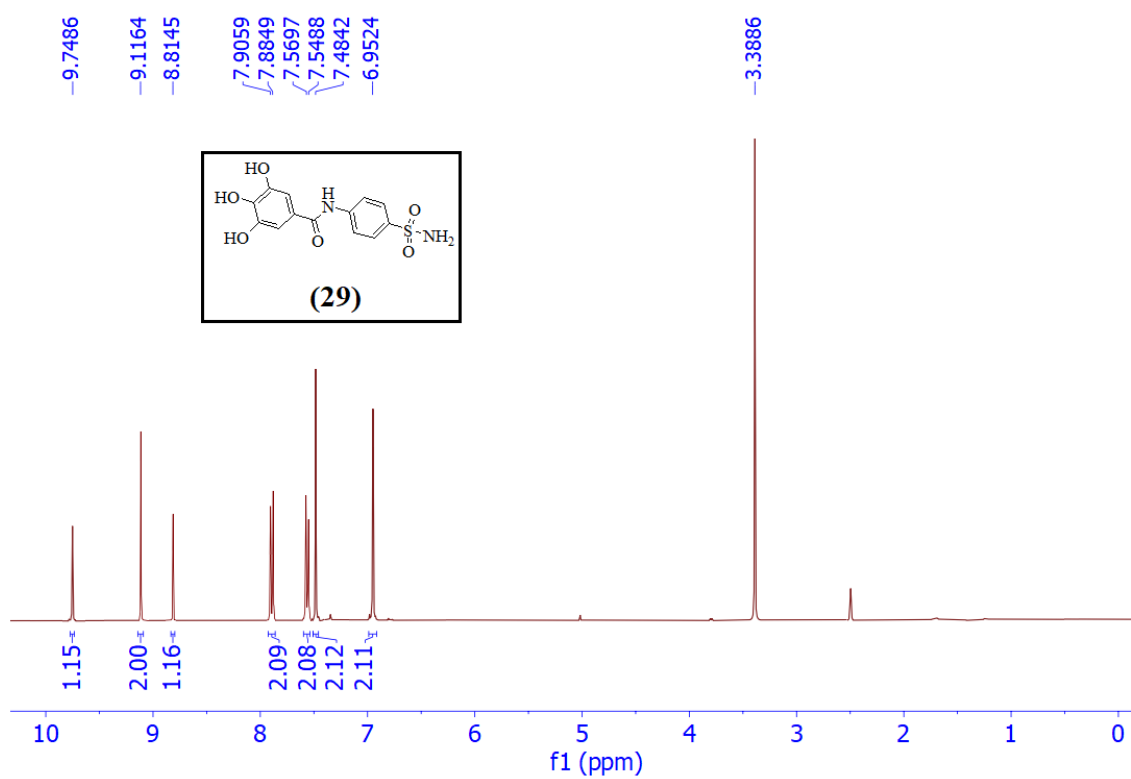


Figure S-41: ¹H NMR (400 MHz) spectrum of compound 29 in DMSO-*d*₆

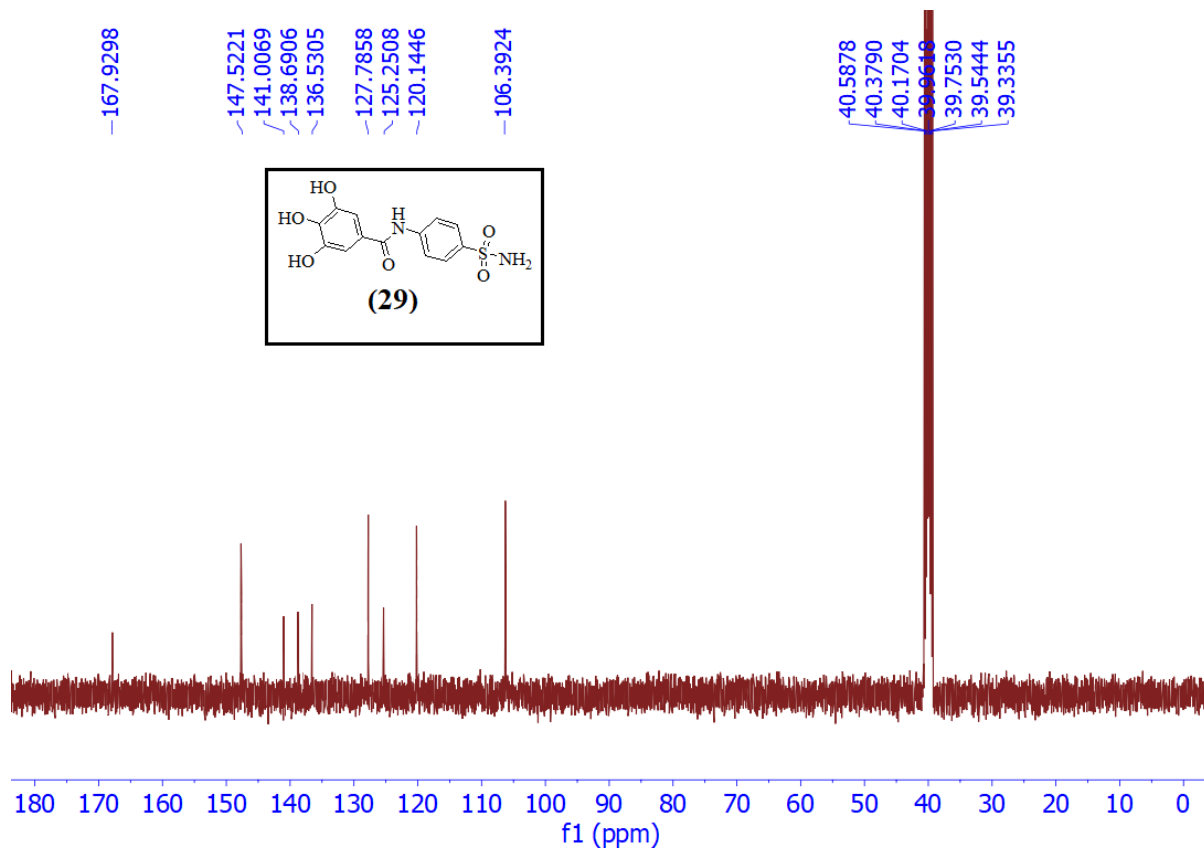


Figure S-42: ^{13}C NMR (100 MHz) spectrum of compound **29** in $\text{DMSO-}d_6$

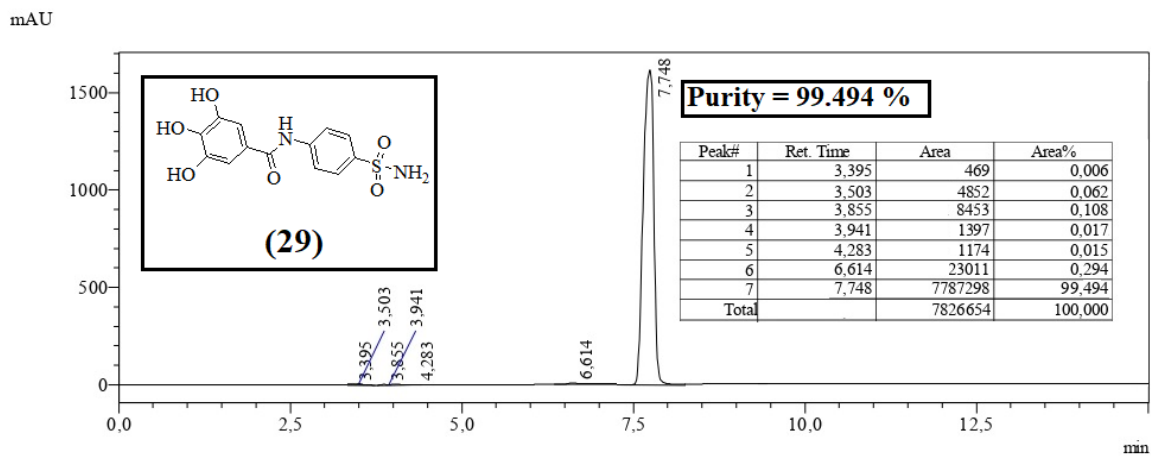


Figure S-43: HPLC Chromatogram of compound **29**