International Journal of
Molecular Sciences

MDPI

Supplementary Material

New arylethanolimidazole derivatives as HO-1 inhibitors with cytotoxicity against MCF-7 breast cancer cells

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Table of contents

Table S1. Elemental analysis data for compounds **2a–c**, **5a–f**, and **6a**,**b**.

			Calcd			Found		
Compd	Formula	Mw	C	H	N	C	H	N
2a	$C_{11}H_{11}BrN_2$	251.12	52.61	4.42	11.16	52.69	4.48	11.19
2b	$C_{18}H_{17}BrN_2O_2$	357.24	60.52	4.80	7.84	60.48	4.86	7.80
2c	$C_{17}H_{16}N_2$	248.32	82.22	6.49	11.28	82.25	6.54	11.33
5a	$C_{18}H_{17}BrN_2O_2$	373.24	57.92	4.59	7.51	57.95	4.62	7.55
5b	$C_{18}H_{17}BrN_2O_2$	373.24	57.92	4.59	7.51	57.89	4.64	7.53
5c	$C_{18}H_{17}BrN_2O_2$	373.24	57.92	4.59	7.51	57.96	4.64	7.56
5d	$C_{18}H_{17}BrN_2O_2$	373.24	57.92	4.59	7.51	57.94	4.63	7.49
5e	$C_{18}H_{17}BrN_2O_2$	373.24	57.92	4.59	7.51	57.96	4.57	7.53
5f	$C_{18}H_{17}BrN_2O_2$	373.24	57.92	4.59	7.51	57.94	4.61	7.48
6a	$C_{18}H_{16}BrClN_2O$	391.69	55.19	4.12	7.15	55.17	4.10	7.19
6b	$C_{18}H_{15}BrCl_2N_2O$	426.13	50.73	3.55	6.57	50.77	3.59	6.53

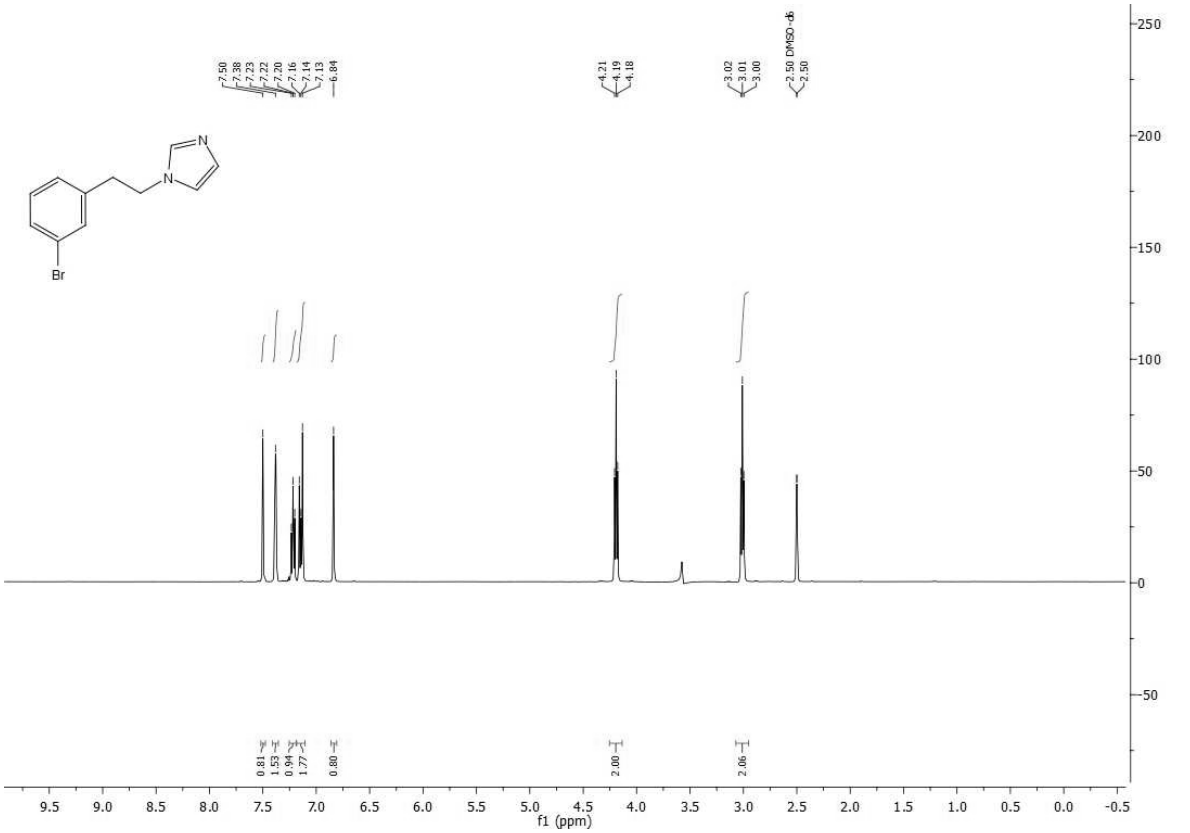

Figure S1. [1]H NMR of compound **2a.**

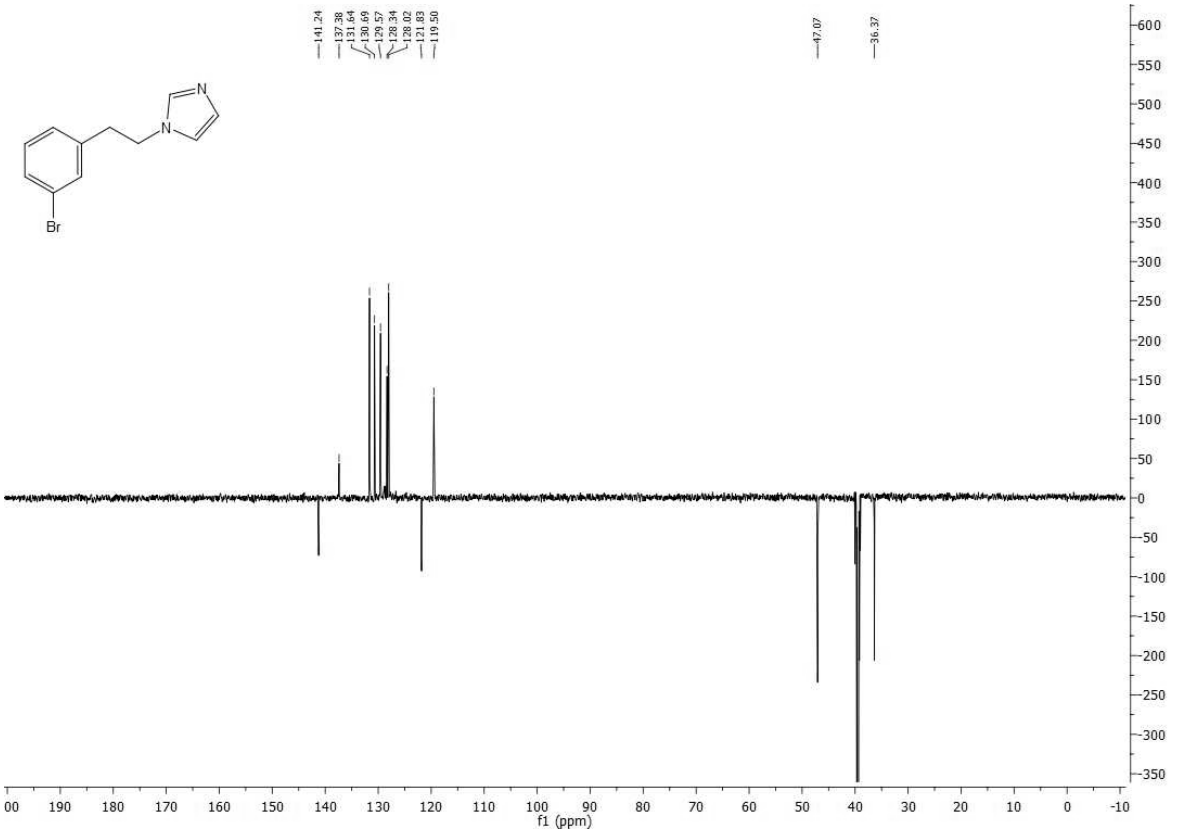

Figure S2. [13]C NMR of compound **2a.**

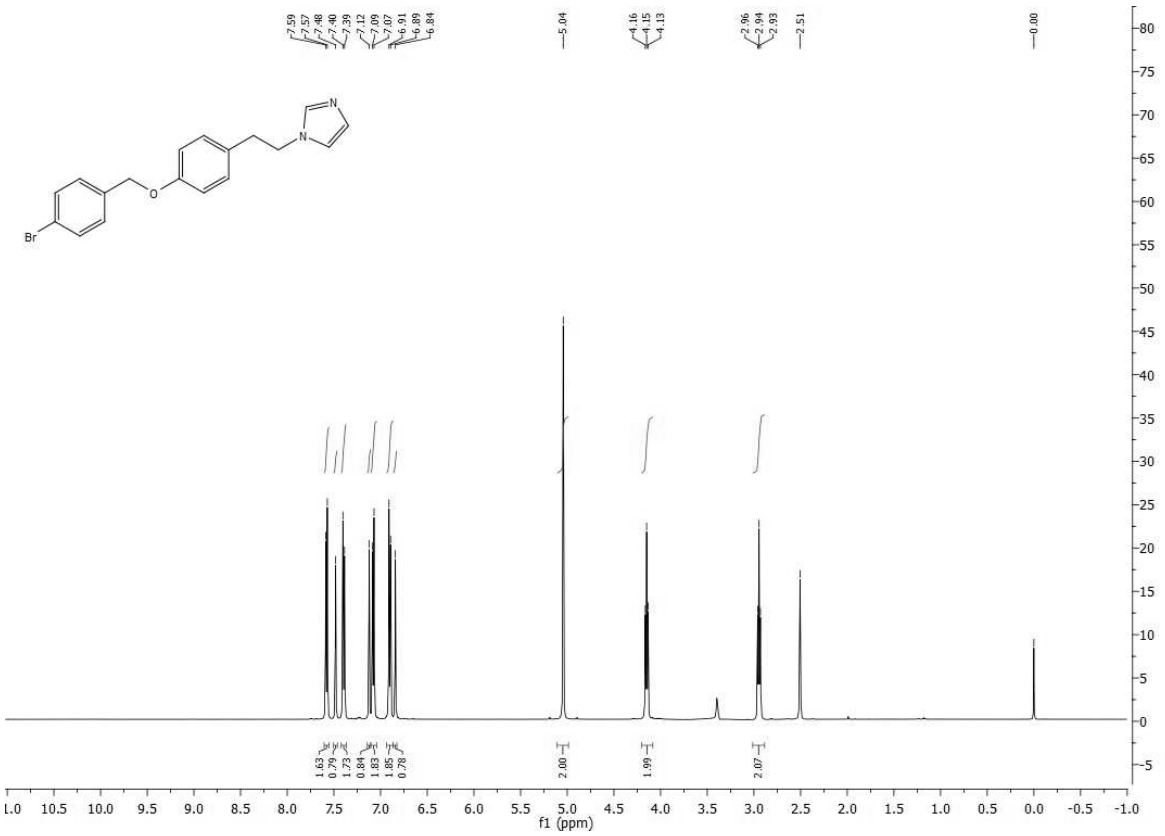

Figure S3. [1]H NMR of compound **2b.**

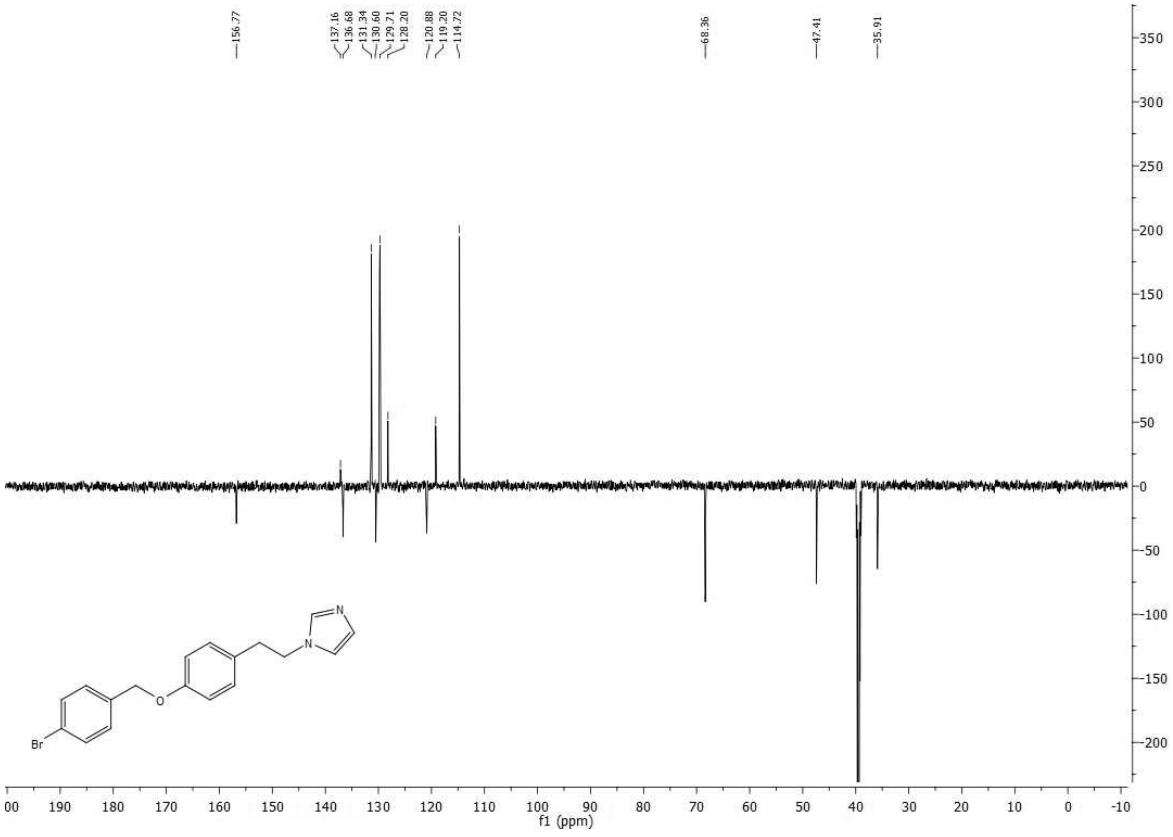

Figure S4. [13]C NMR of compound **2b.**

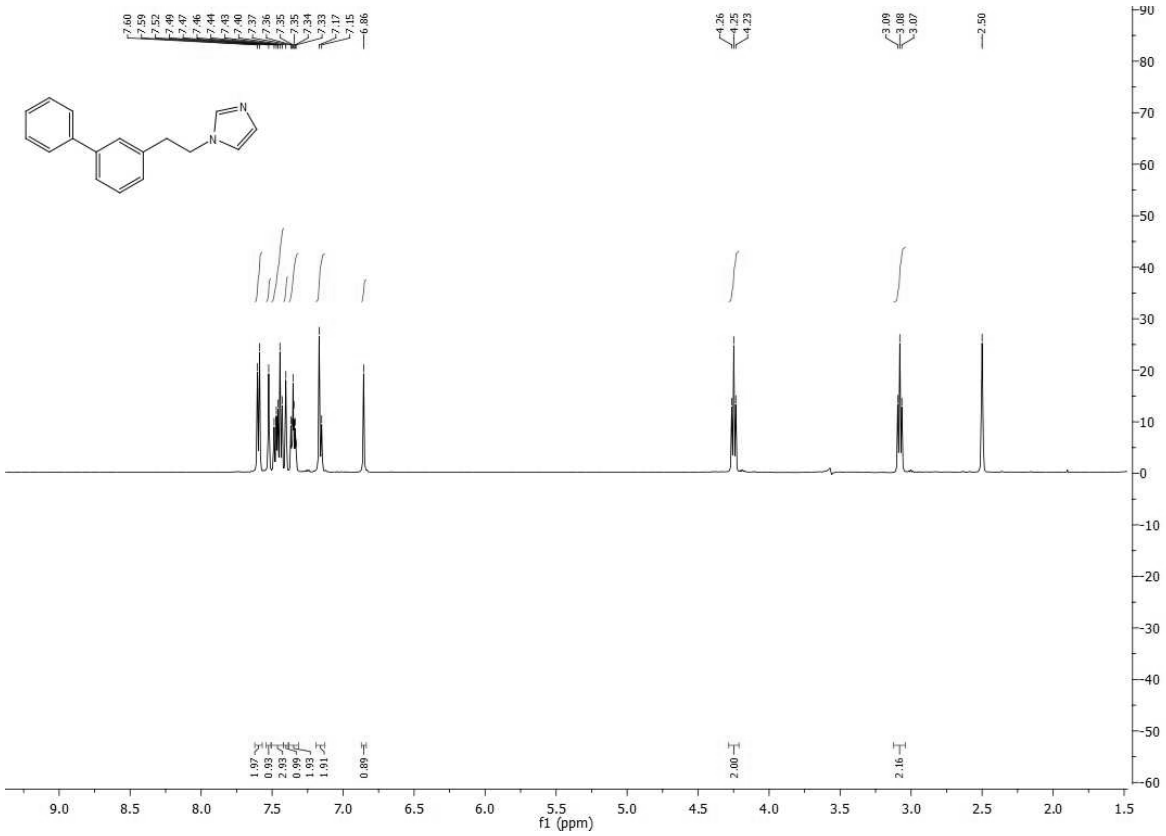

Figure S5. [1]H NMR of compound **2c.**

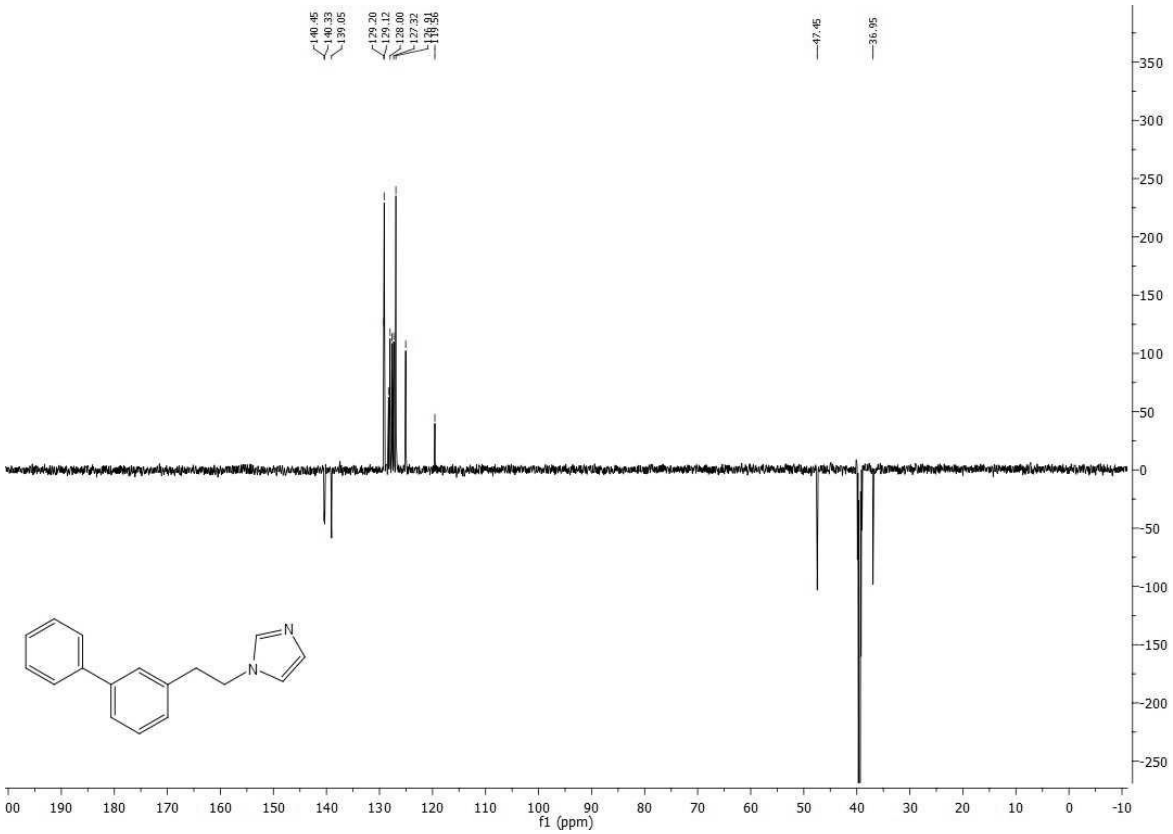

Figure S6. [13]C NMR of compound **2c.**

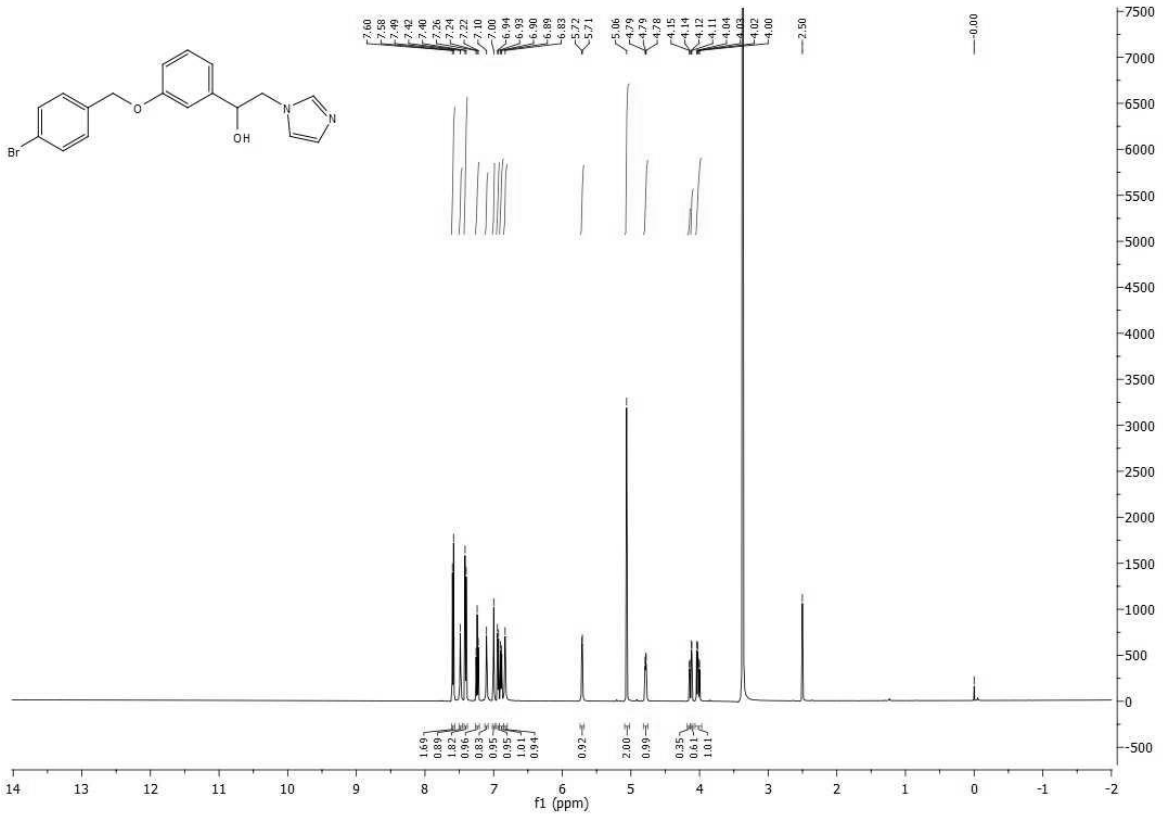

Figure S7. [1]H NMR of compound **5a.**

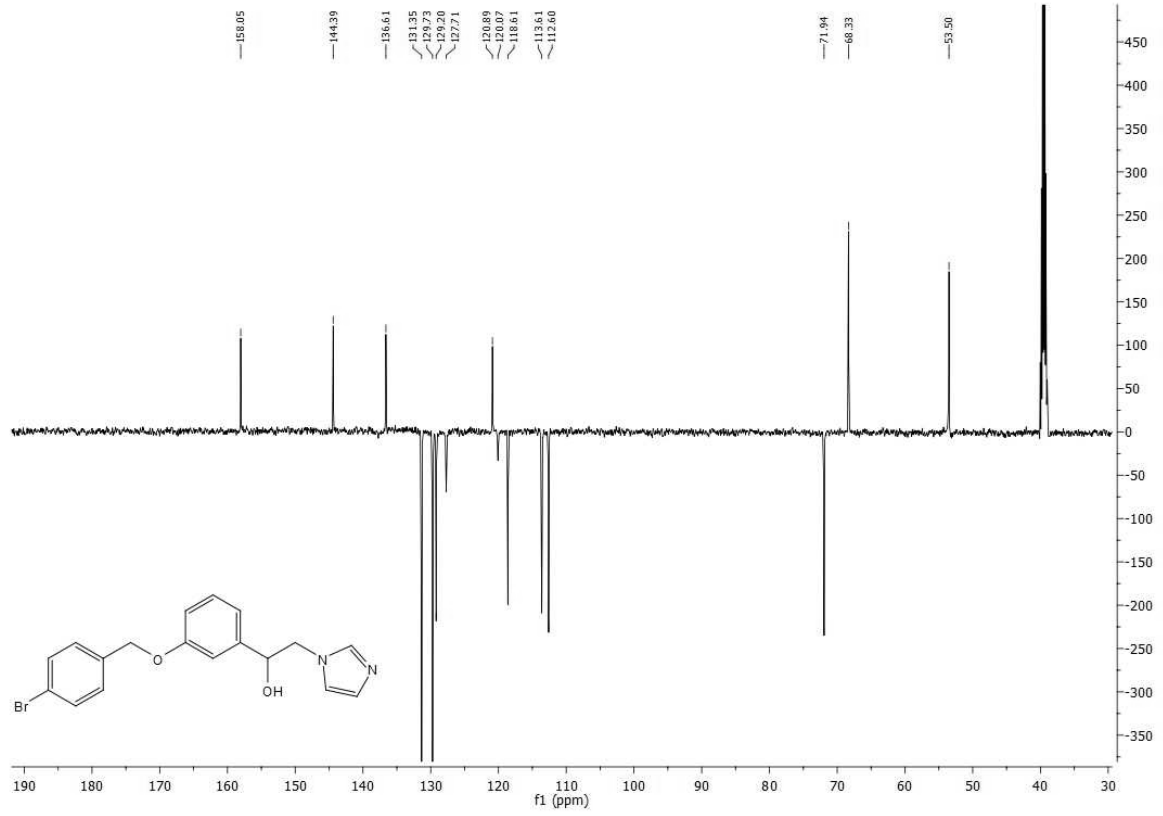

Figure S8. [13]C NMR of compound **5a.**

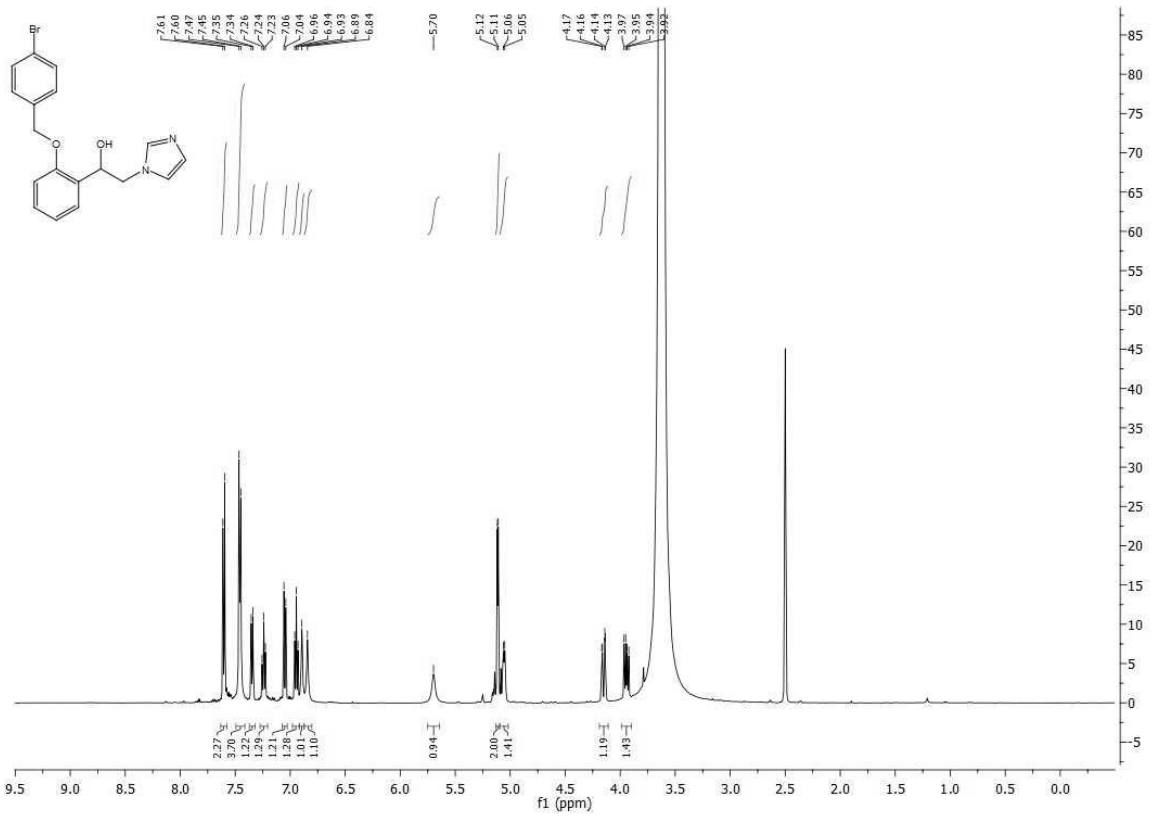

Figure S9. [1]H NMR of compound **5b.**

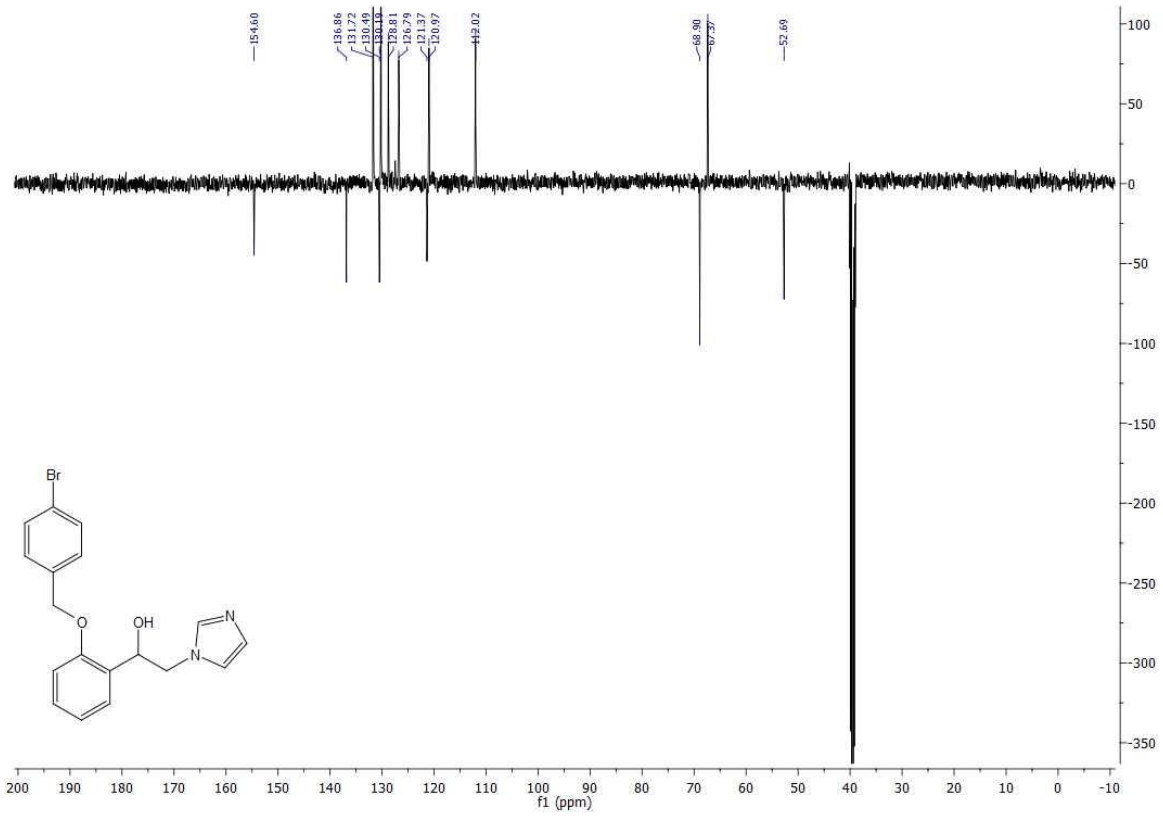

Figure S10. [13]C NMR of compound **5b.**

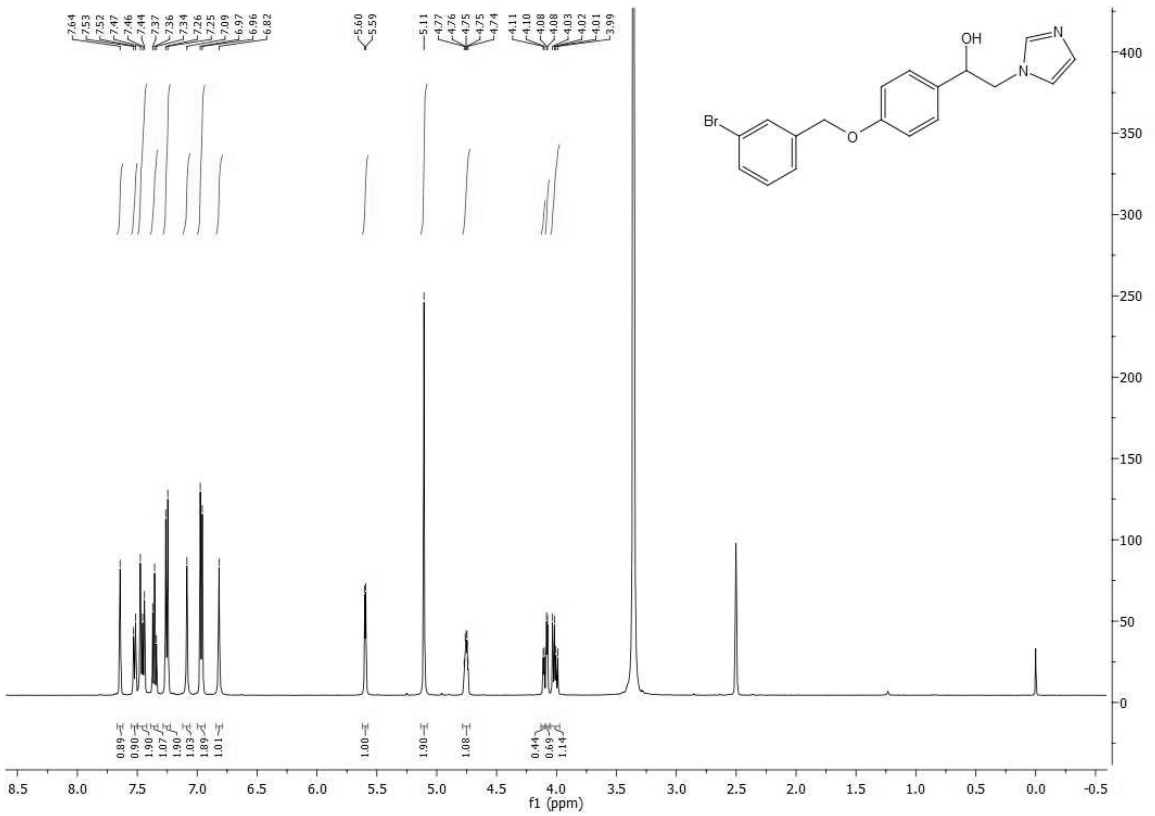

Figure S11. [1]H NMR of compound **5c.**

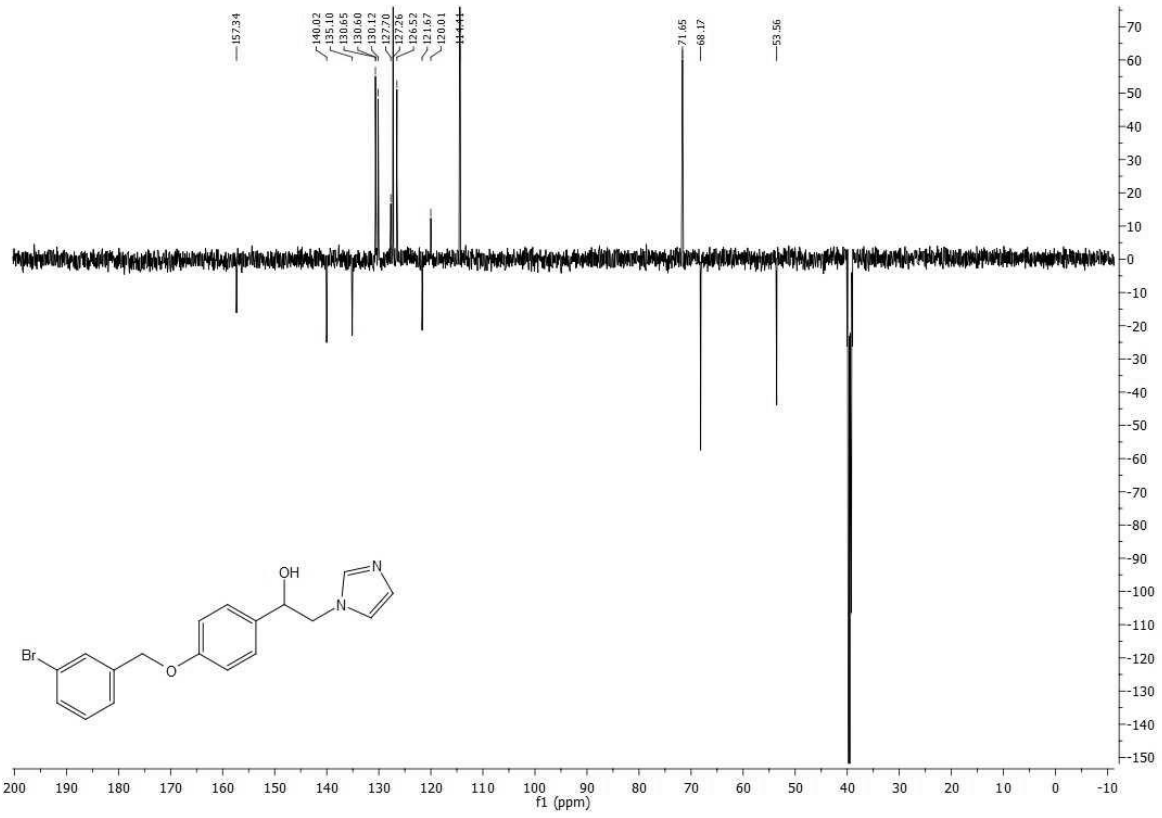

Figure S12. [13]C NMR of compound **5c.**

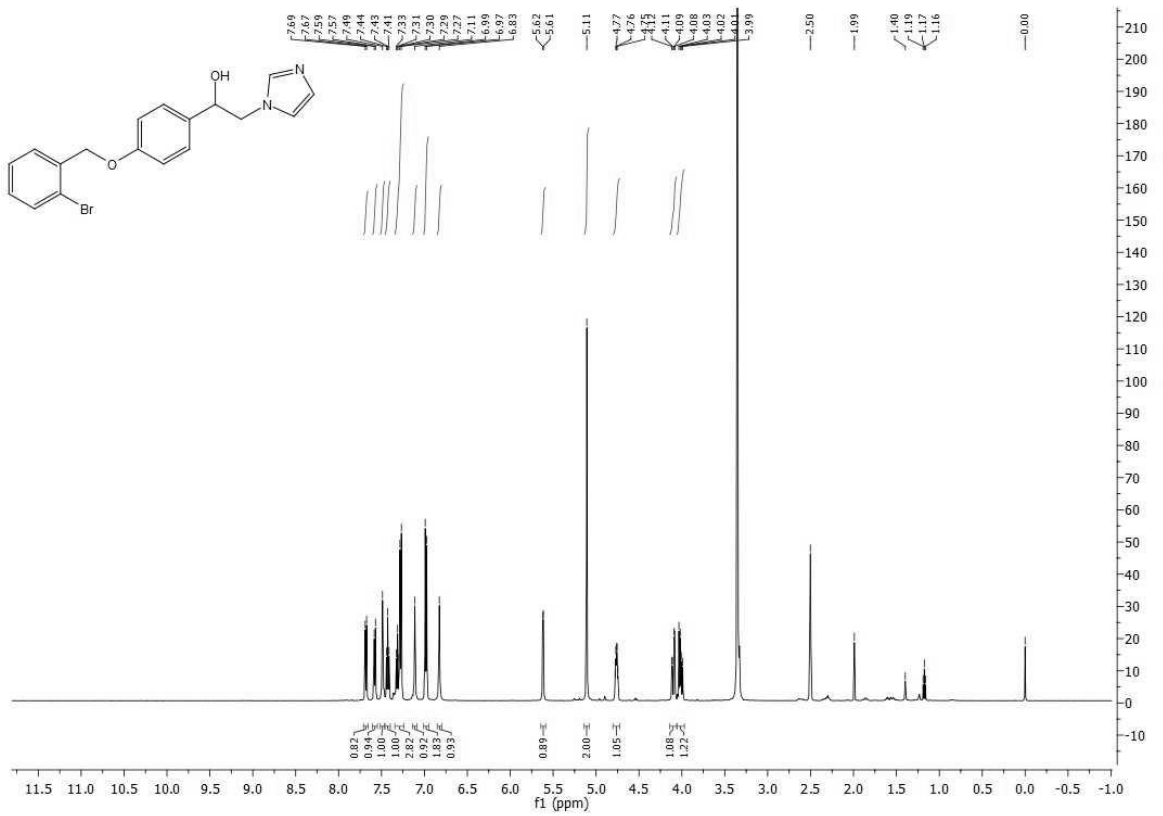

Figure S13. ^{1}H NMR of compound **5d.**

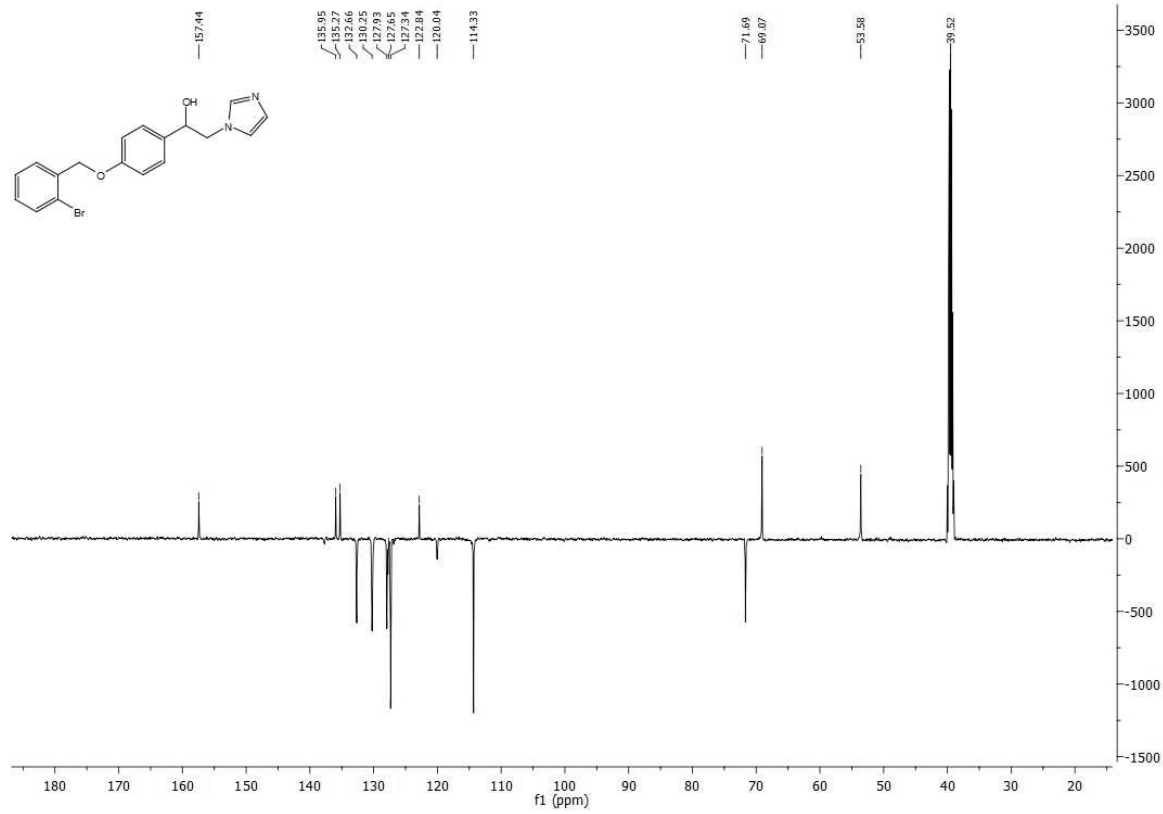

Figure S14. ^{13}C NMR of compound **5d.**

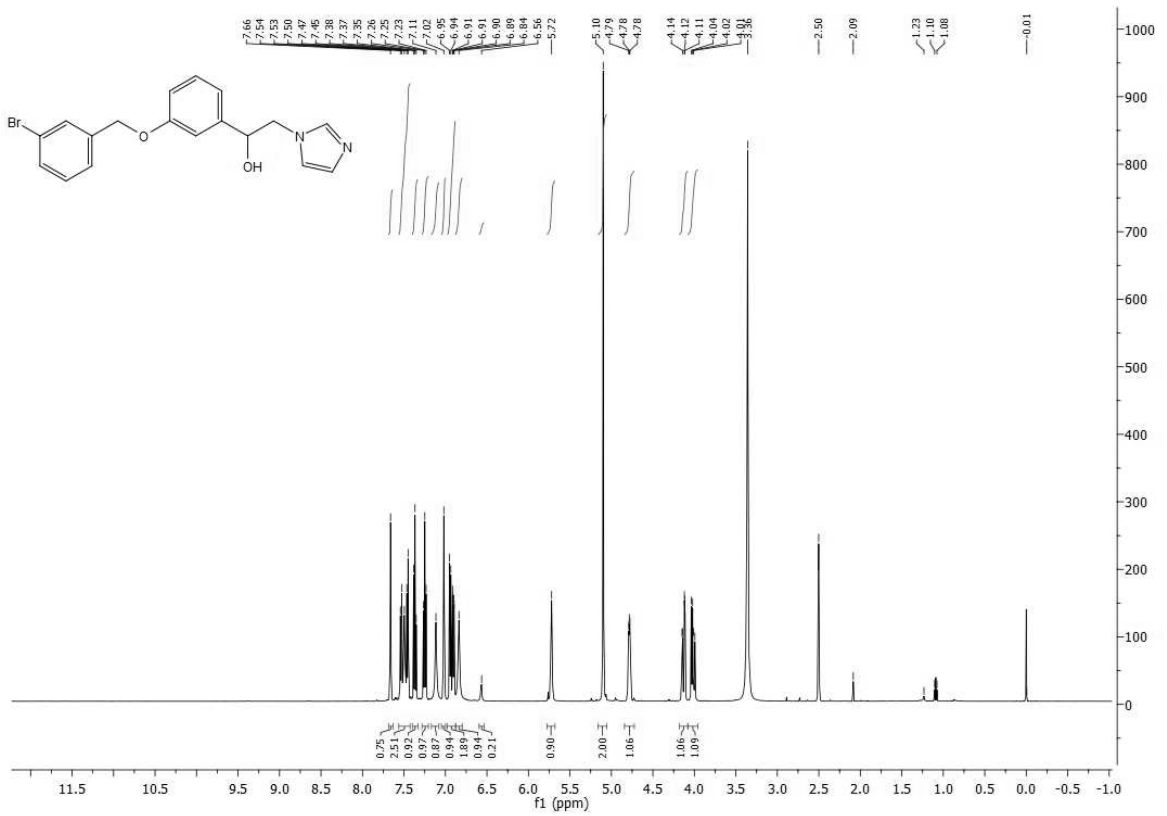

Figure S15. ^{1}H NMR of compound **5e.**

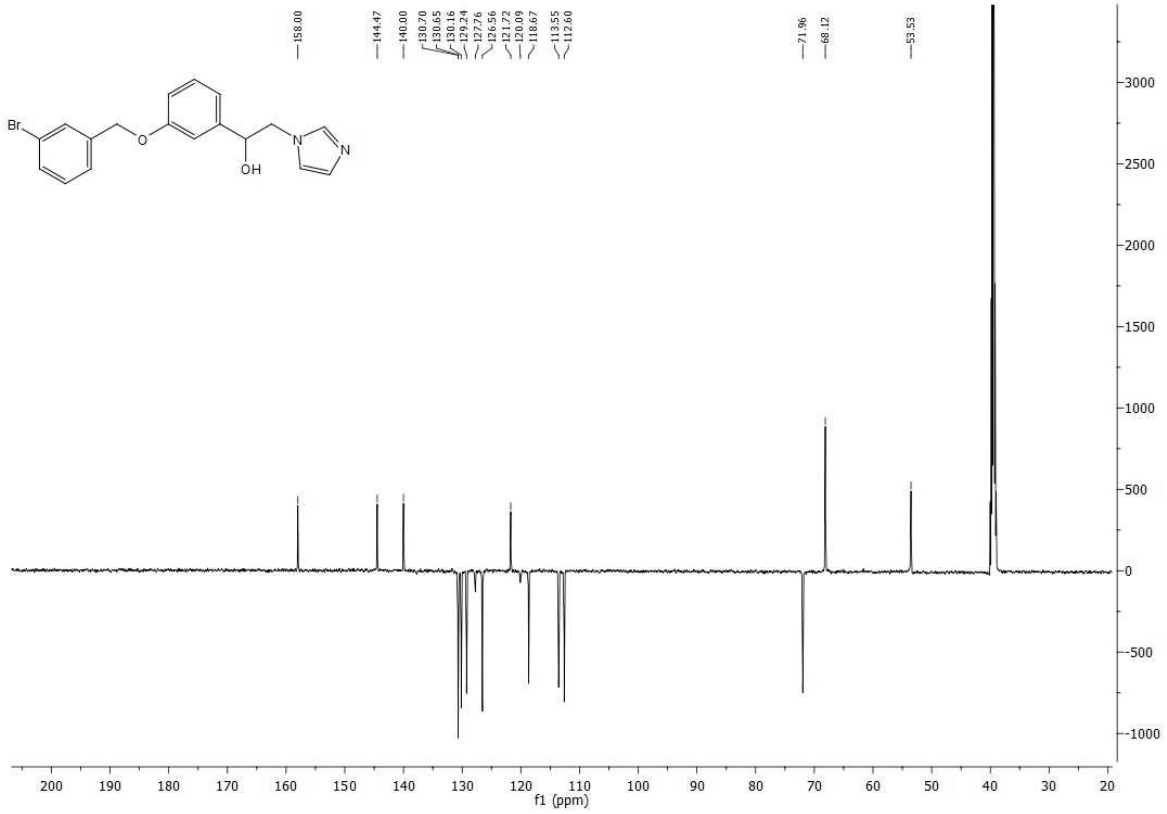

Figure S16. ^{13}C NMR of compound **5e.**

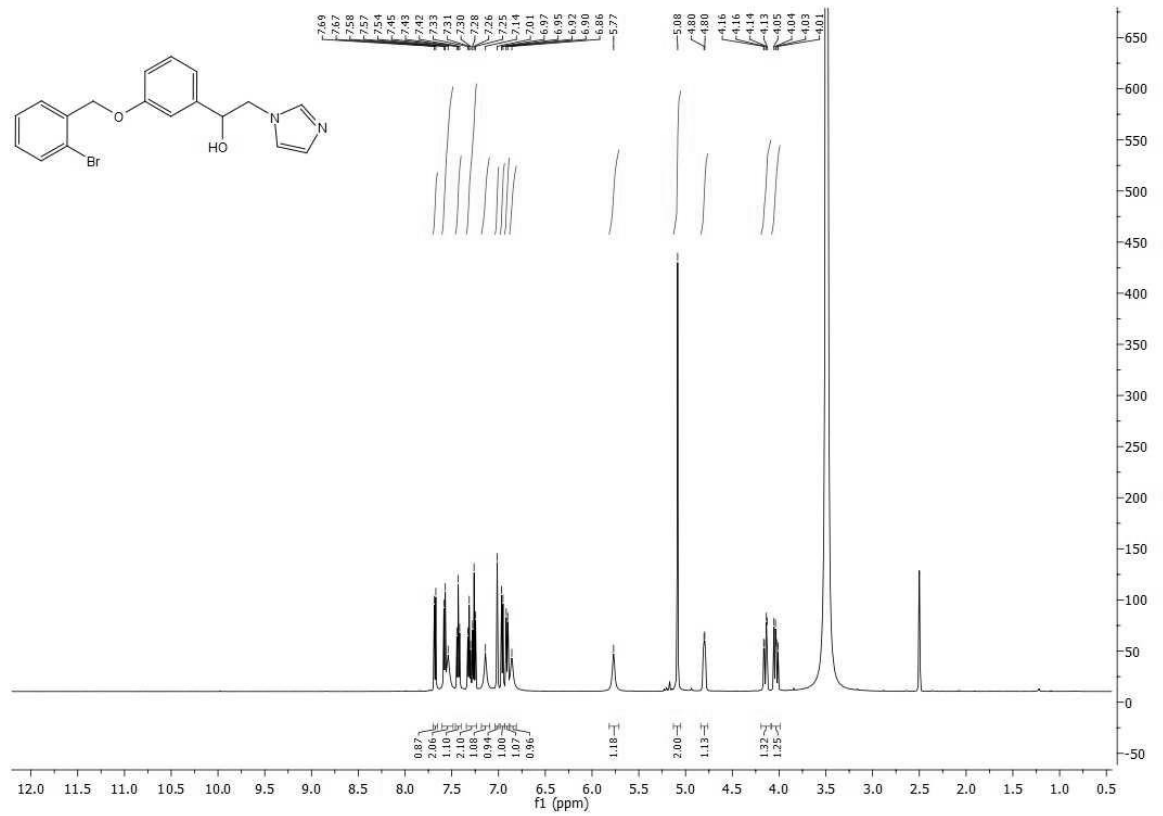

Figure S17. ^{1}H NMR of compound **5f.**

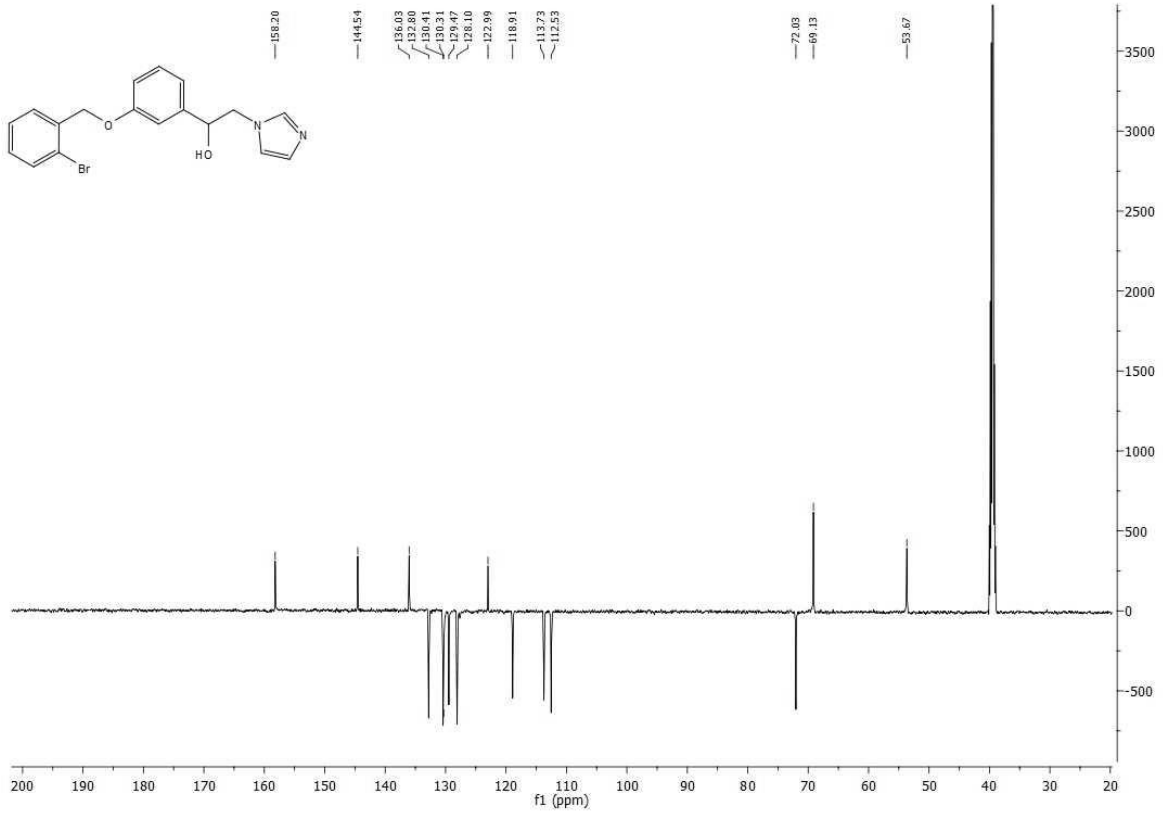

Figure S18. ^{13}C NMR of compound **5f.**

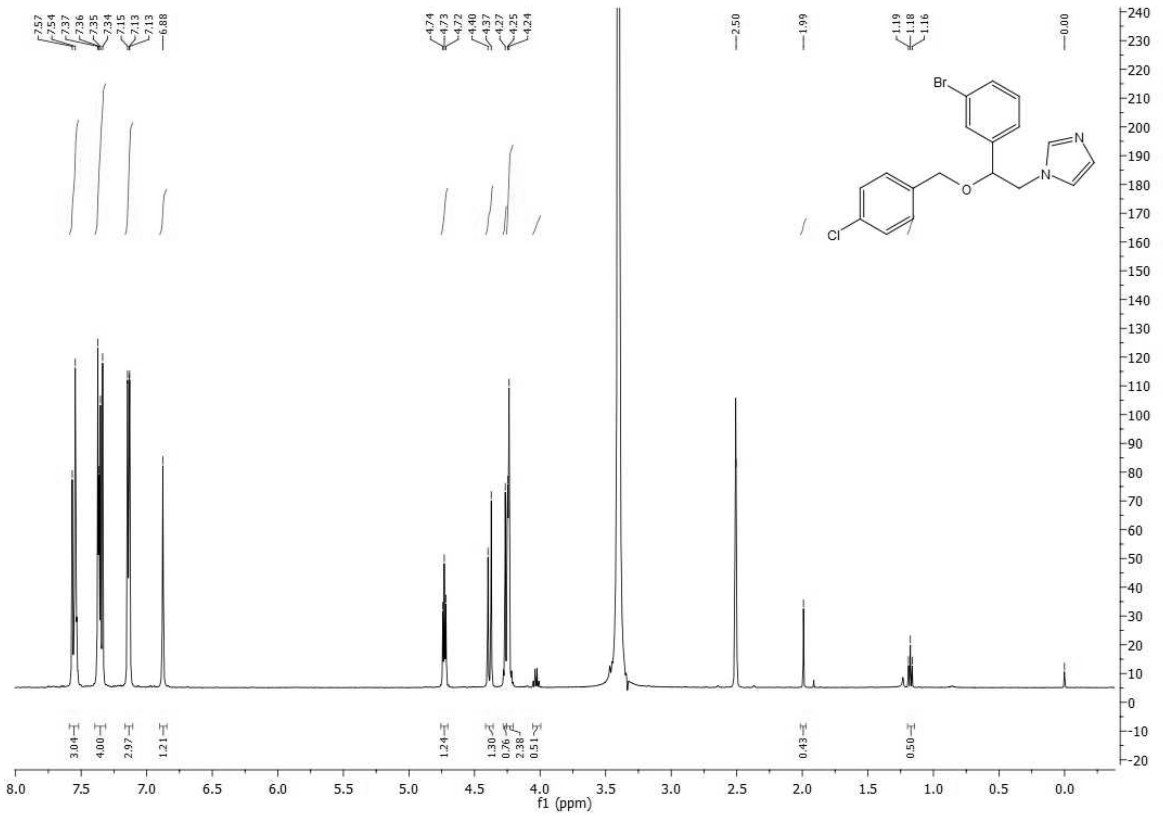

Figure S19. [1]H NMR of compound **6a.**

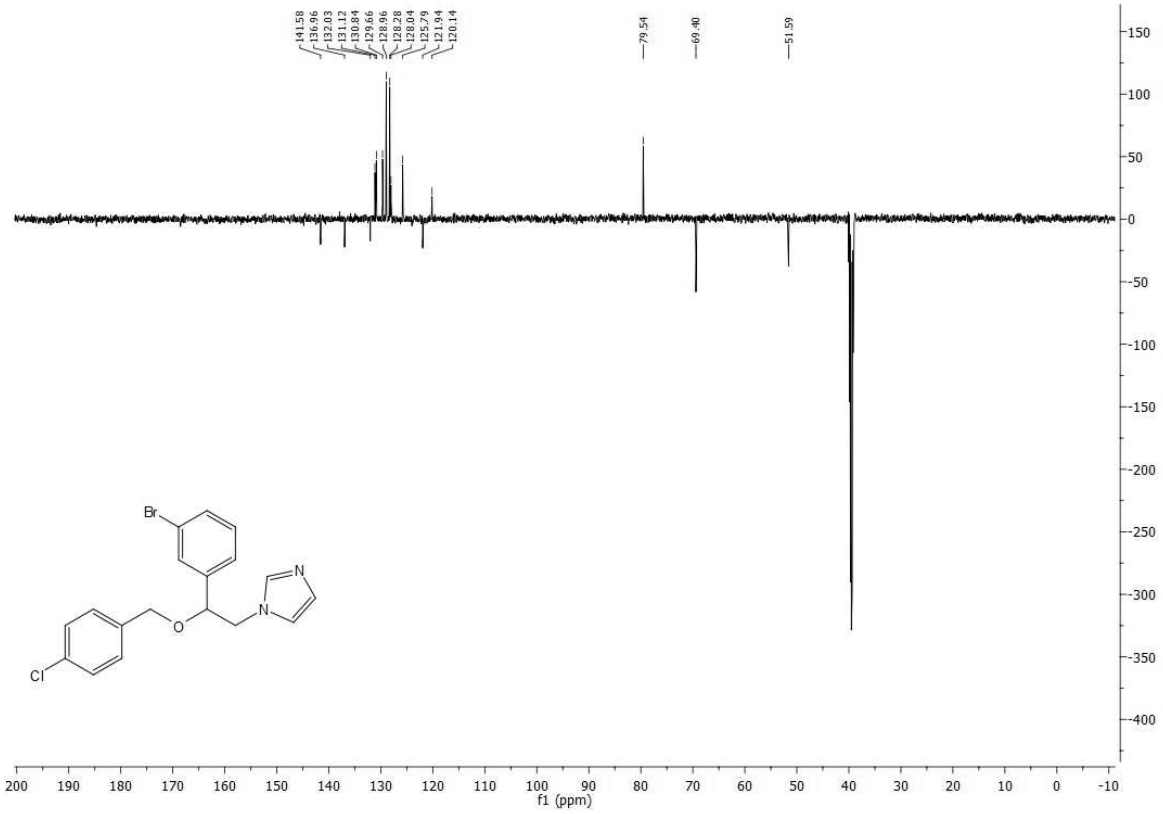

Figure S20. [13]C NMR of compound **6a.**

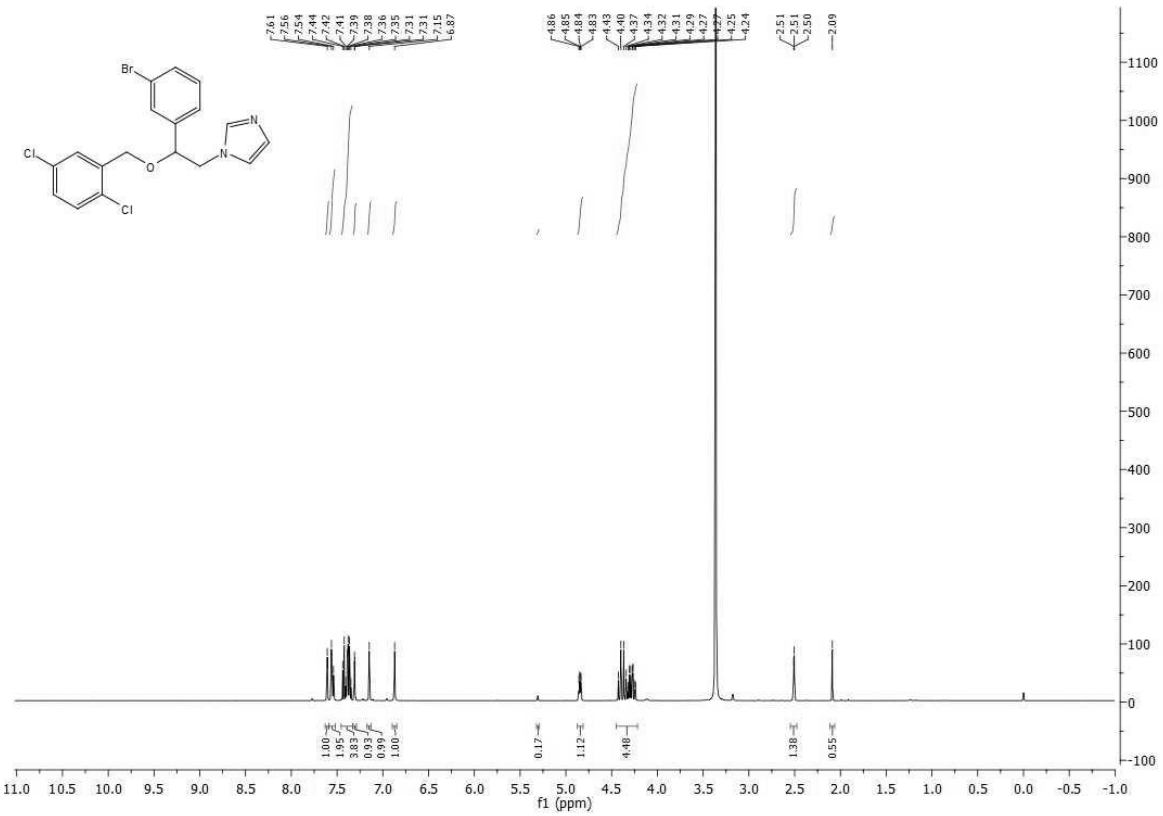

Figure S21. [1]H NMR of compound **6b.**

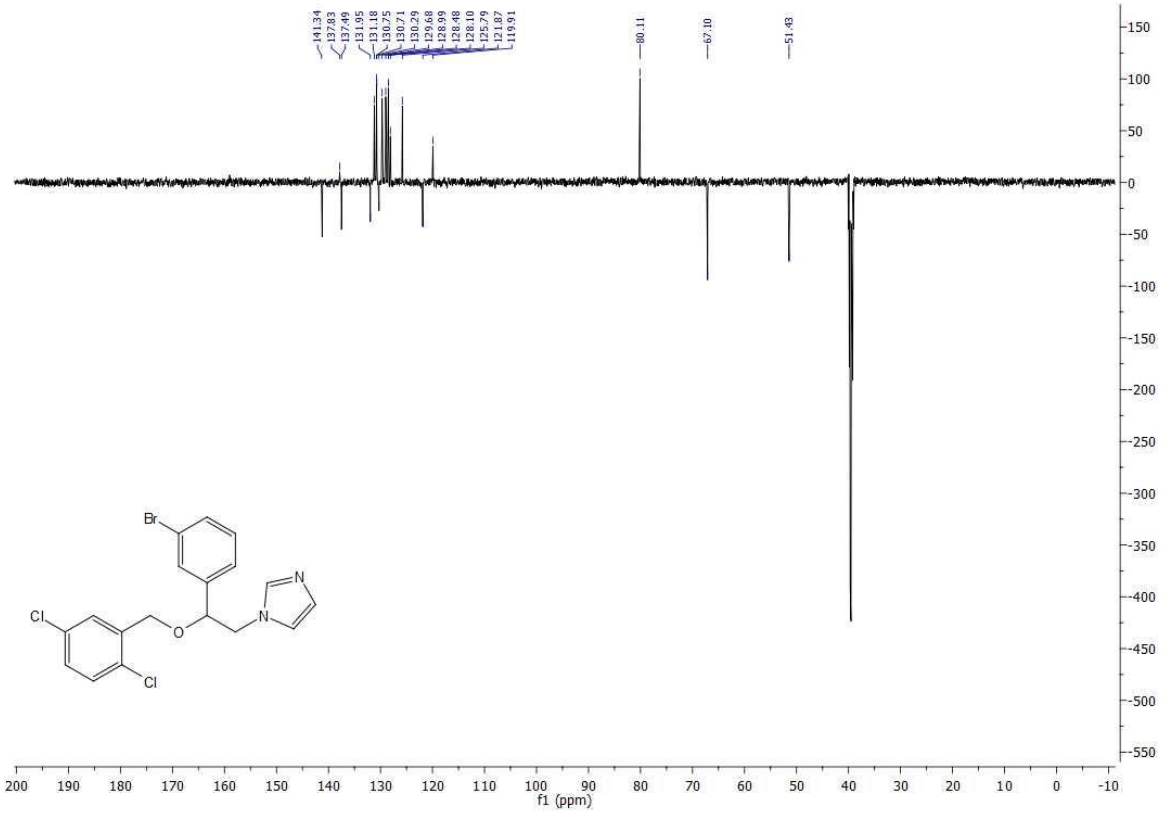

Figure S22. [13]C NMR of compound **6b.**

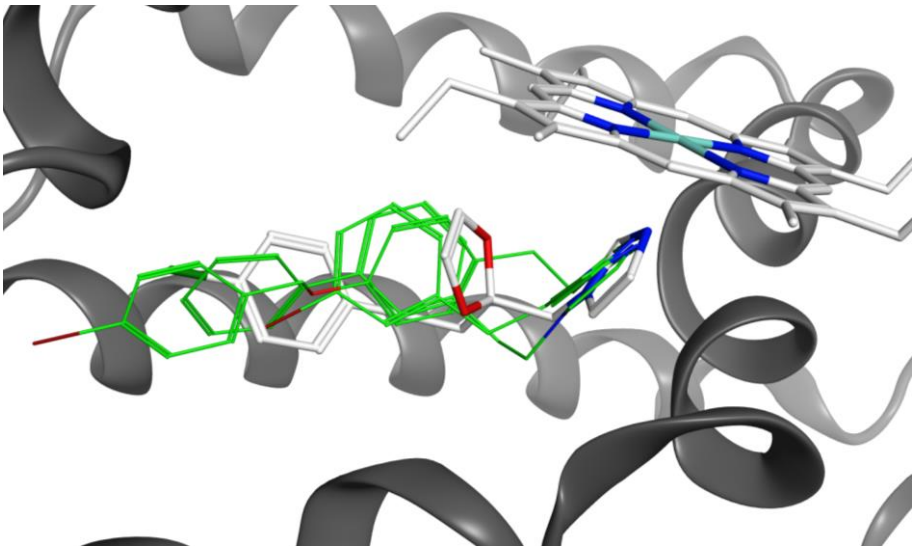

Figure S23. Binding poses of molecules **2a–c** (green) compared to the crystallized pose of QC-15 (white).

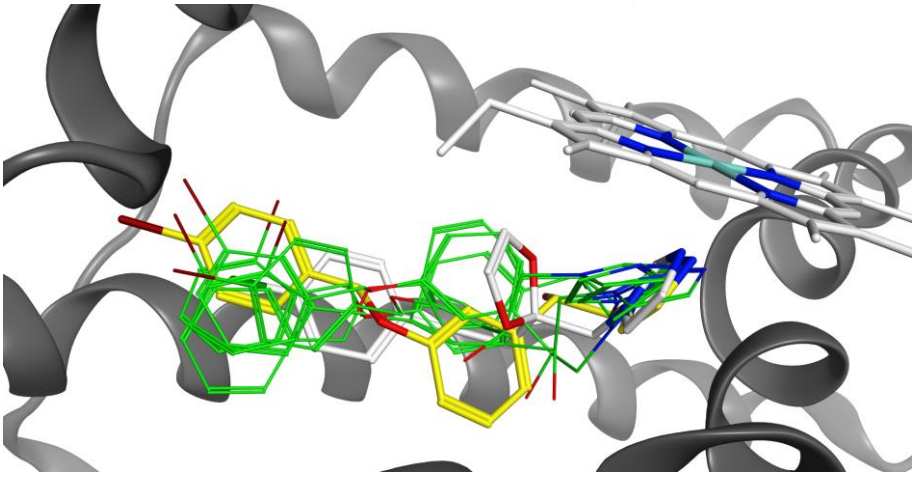

Figure S24. Binding poses of molecules **5b–f** (green) compared to the crystallized pose of QC-15 (white). In yellow the binding pose of the most potent compound **5a**.

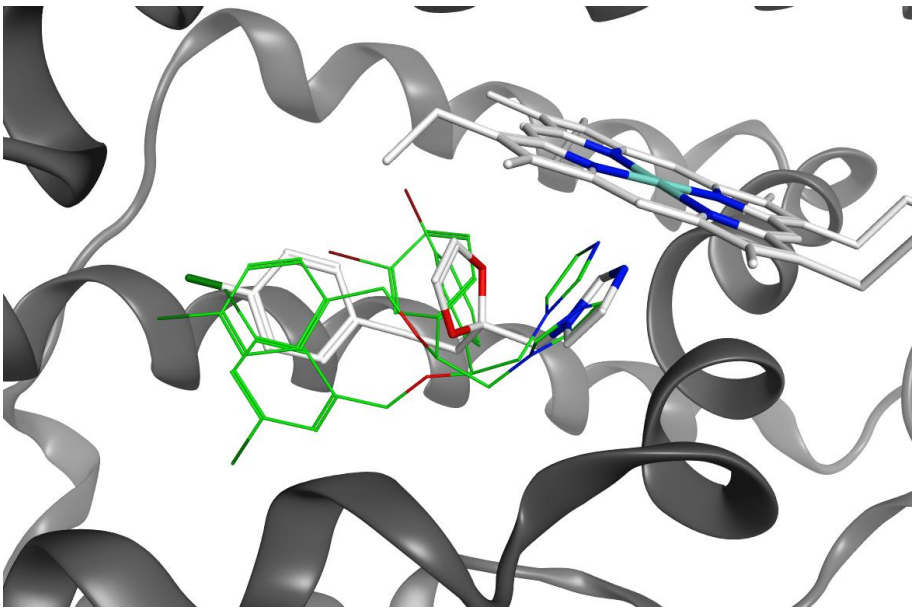

Figure S25. Binding poses of molecules **6a, b** (green) compared to the crystallized pose of QC-15 (white).

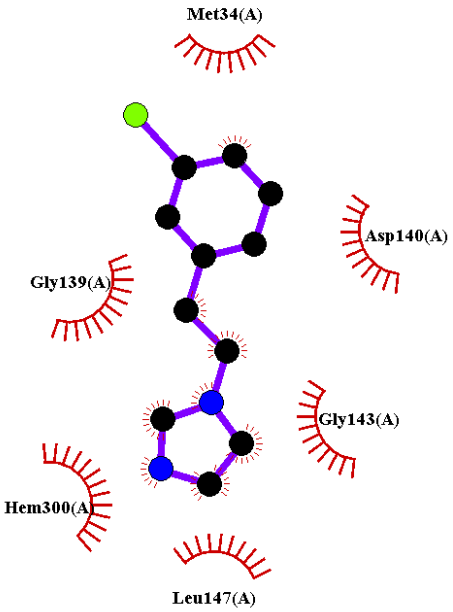

Figure S26. 2D representations of HO-1-molecule **2a** complex.

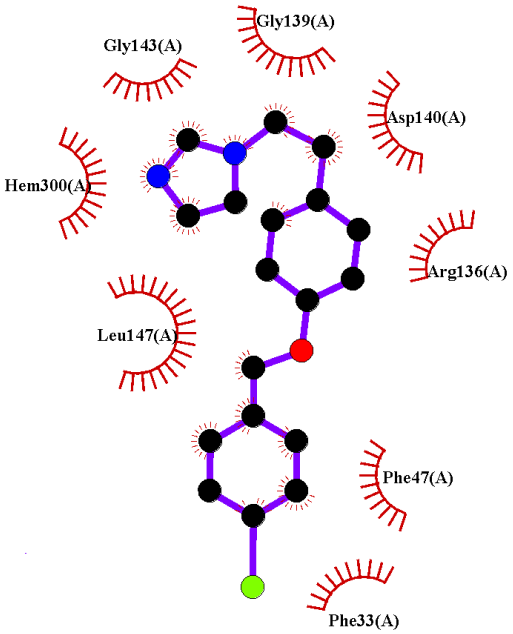

Figure S7. 2D representations of HO-1-molecule **2b** complex.

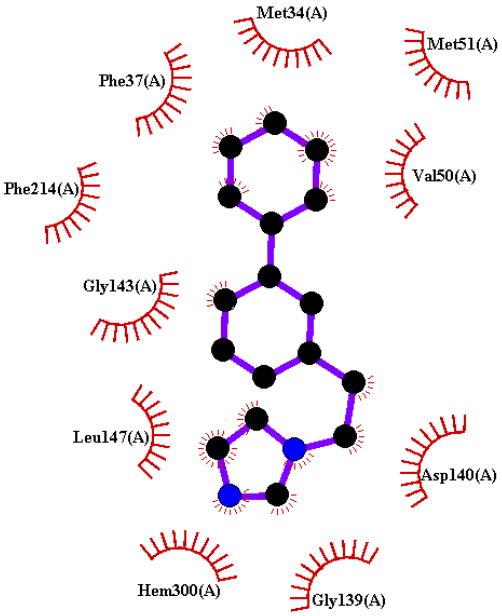

Figure S28. 2D representations of HO-1-molecule **2c** complex.

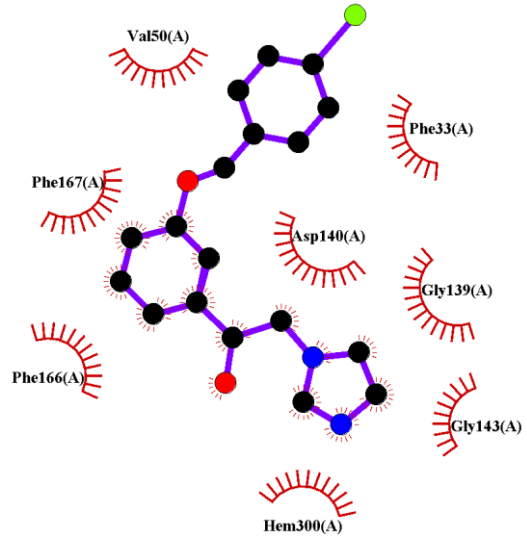

Figure S29. 2D representations of HO-1-molecule **5a** complex.

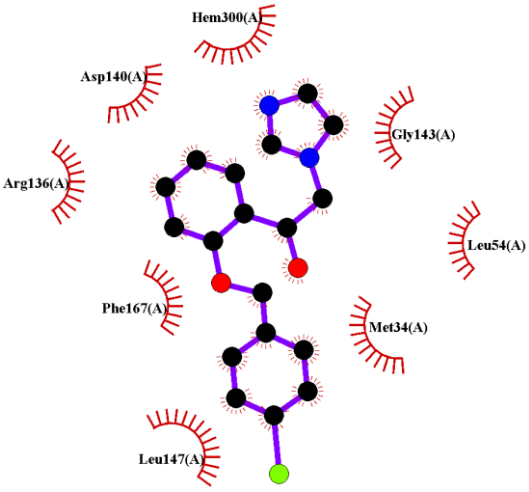

Figure S30. 2D representations of HO-1-molecule **5b** complex.

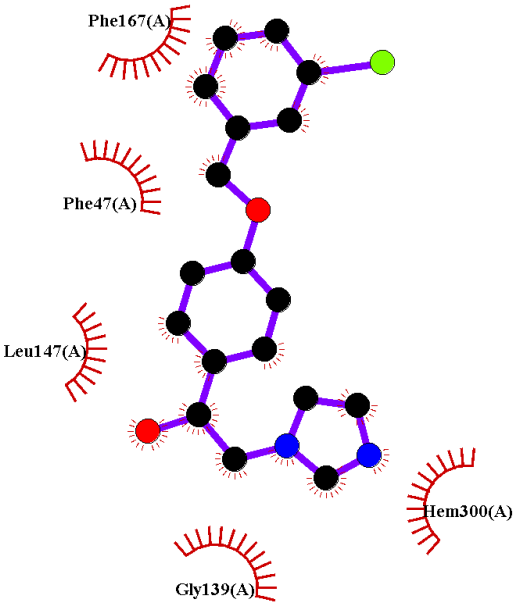

Figure S31. 2D representations of HO-1-molecule **5c** complex.

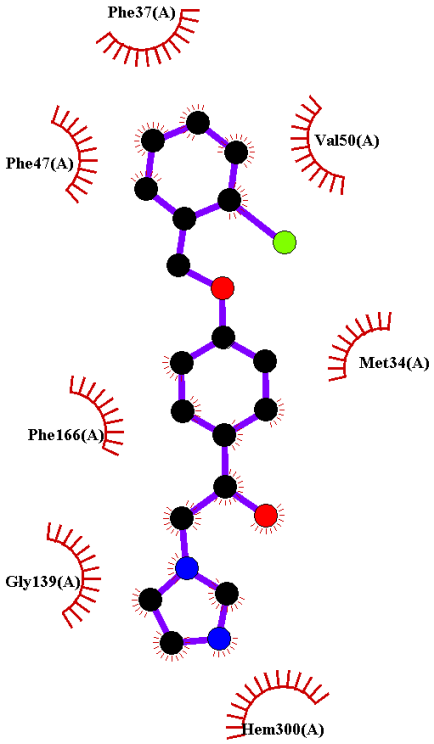

Figure S32. 2D representations of HO-1-molecule **5d** complex.

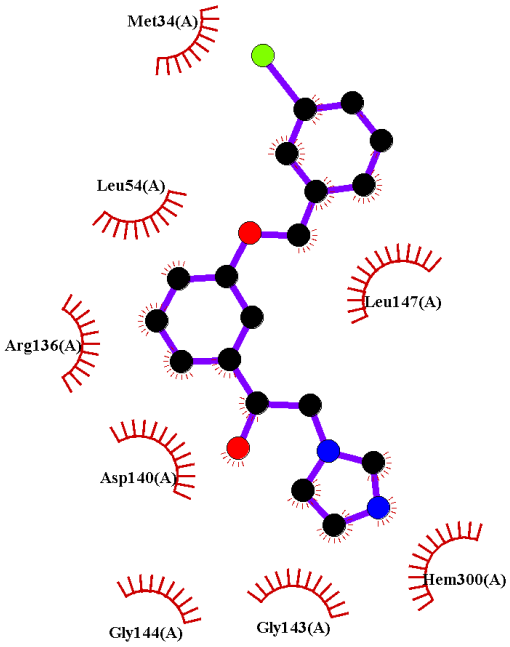

Figure S33. 2D representations of HO-1-molecule **5e** complex.

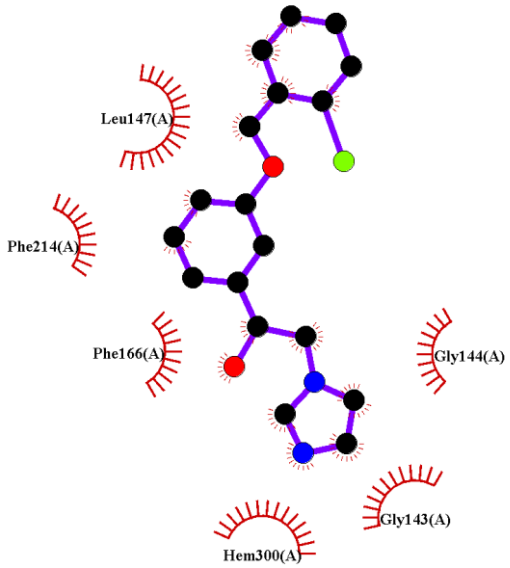

Figure S34. 2D representations of HO-1-molecule **5f** complex.

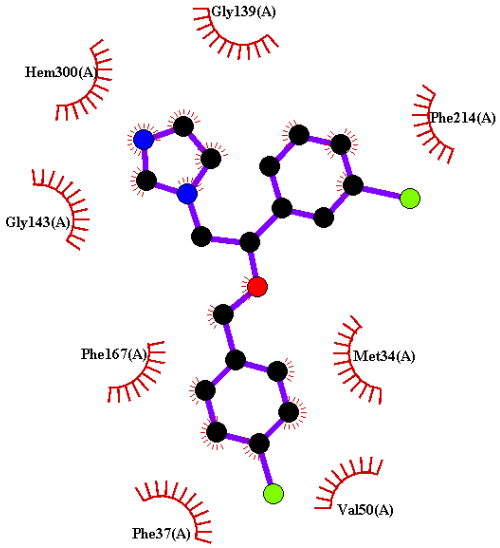

Figure S35. 2D representations of HO-1-molecule **6a** complex.

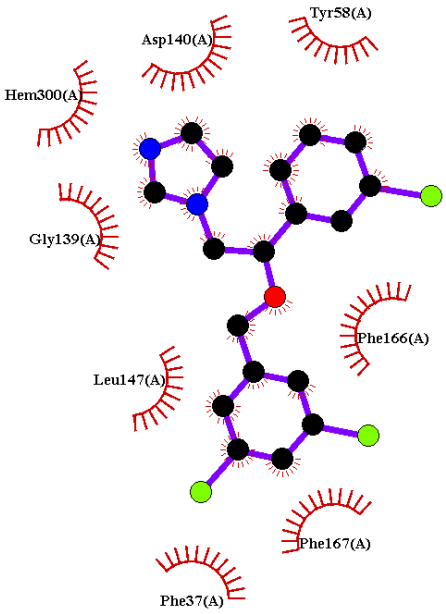

Figure S36. 2D representations of HO-1-molecule **6b** complex.