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MDPI

Supplementary Material

Potent and Selective Inhibitors of Human Monoamine Oxidase A from an Endogenous Lichen Fungus *Diaporthe mahothocarpus*

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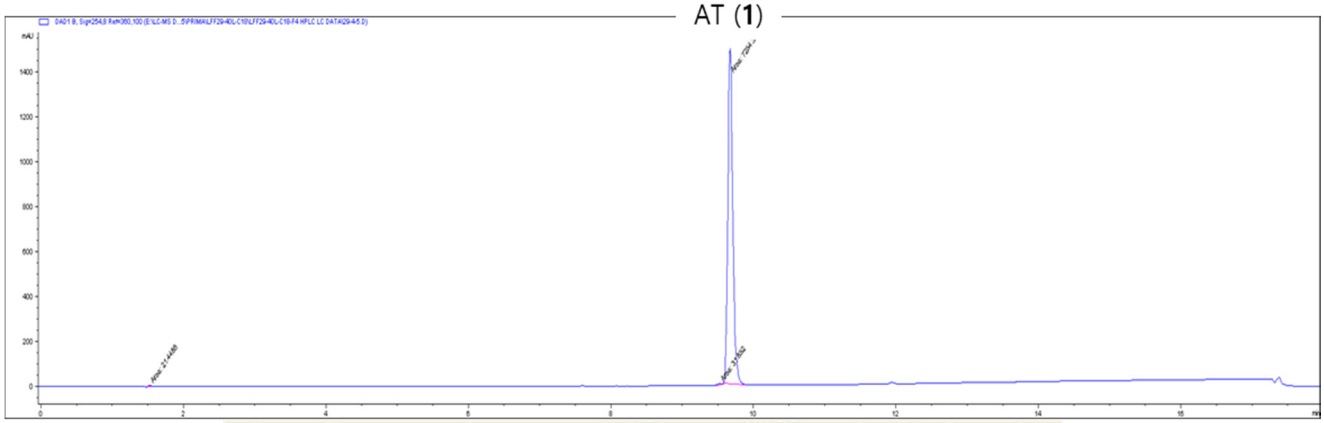
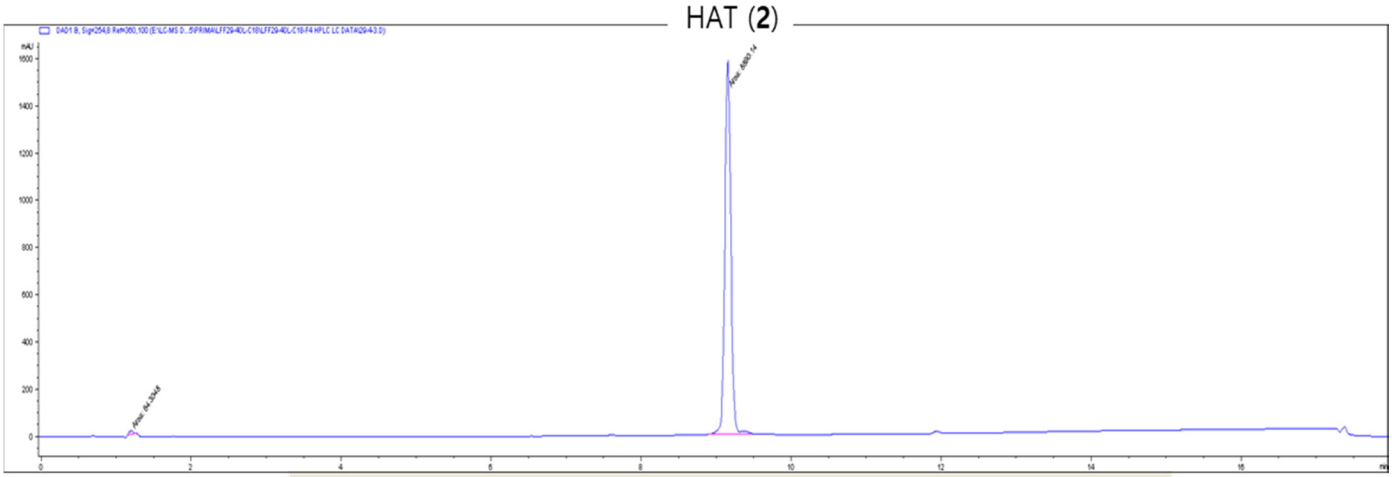


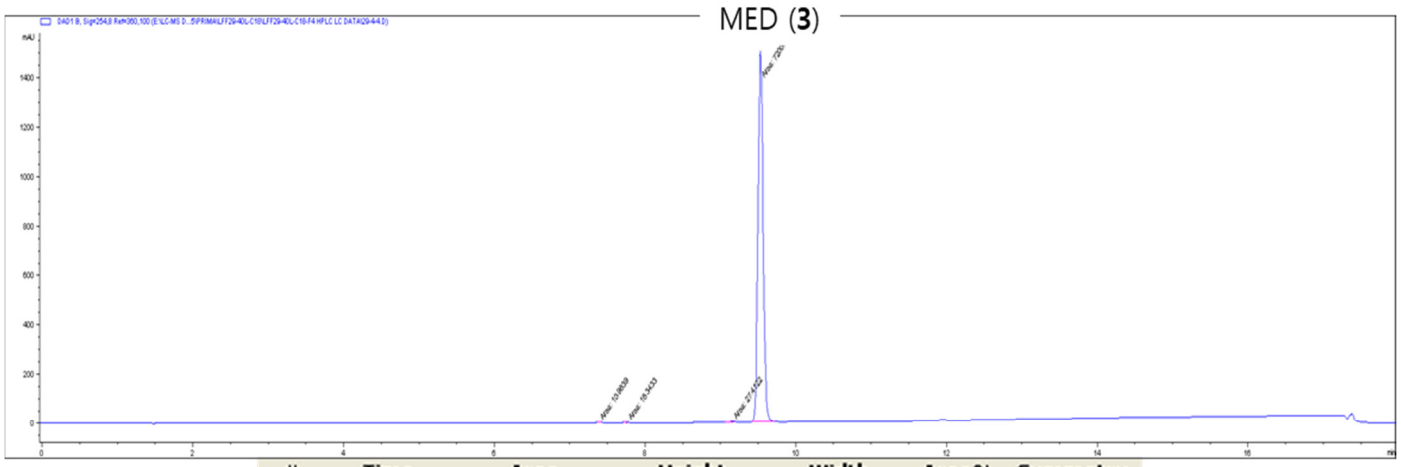
#	Time	Area	Height	Width	Area%	Symmetry
1	1.52	21.4	8	0.0448	0.294	0.827
2	9.526	31.9	9.7	0.0545	0.436	1.5
3	9.669	7254.4	1495.7	0.0808	99.271	0.806

Figure S1. Percentage purity of AT (**1**).



#	Time	Area	Height	Width	Area%	Symmetry
1	1.196	64.3	16.9	0.0633	0.718	1.018
2	9.153	8890.1	1585.9	0.0934	99.282	0.959

Figure S2. Percentage purity of HAT (**2**).



#	Time	Area	Height	Width	Area%	Symmetry
1	7.393	11	4.4	0.0414	0.151	1.291
2	7.762	16.3	6.7	0.0404	0.225	0.581
3	9.166	27.4	6.6	0.069	0.378	4.287
4	9.528	7200	1504.2	0.0798	99.246	0.906

Figure S3. Percentage purity of MED (**3**).

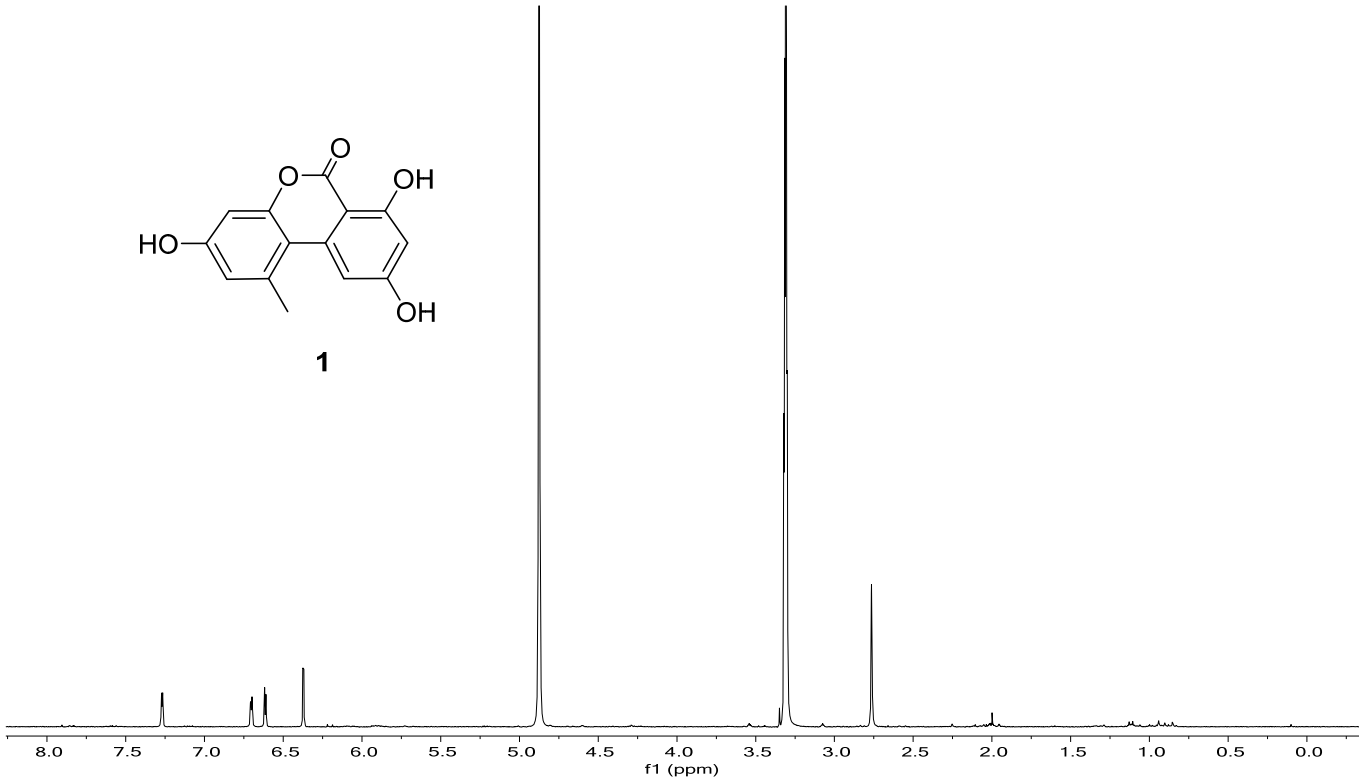


Figure S4. ^{1}H NMR spectrum of Alternariol (AT) (**1**) in CD_3OD.

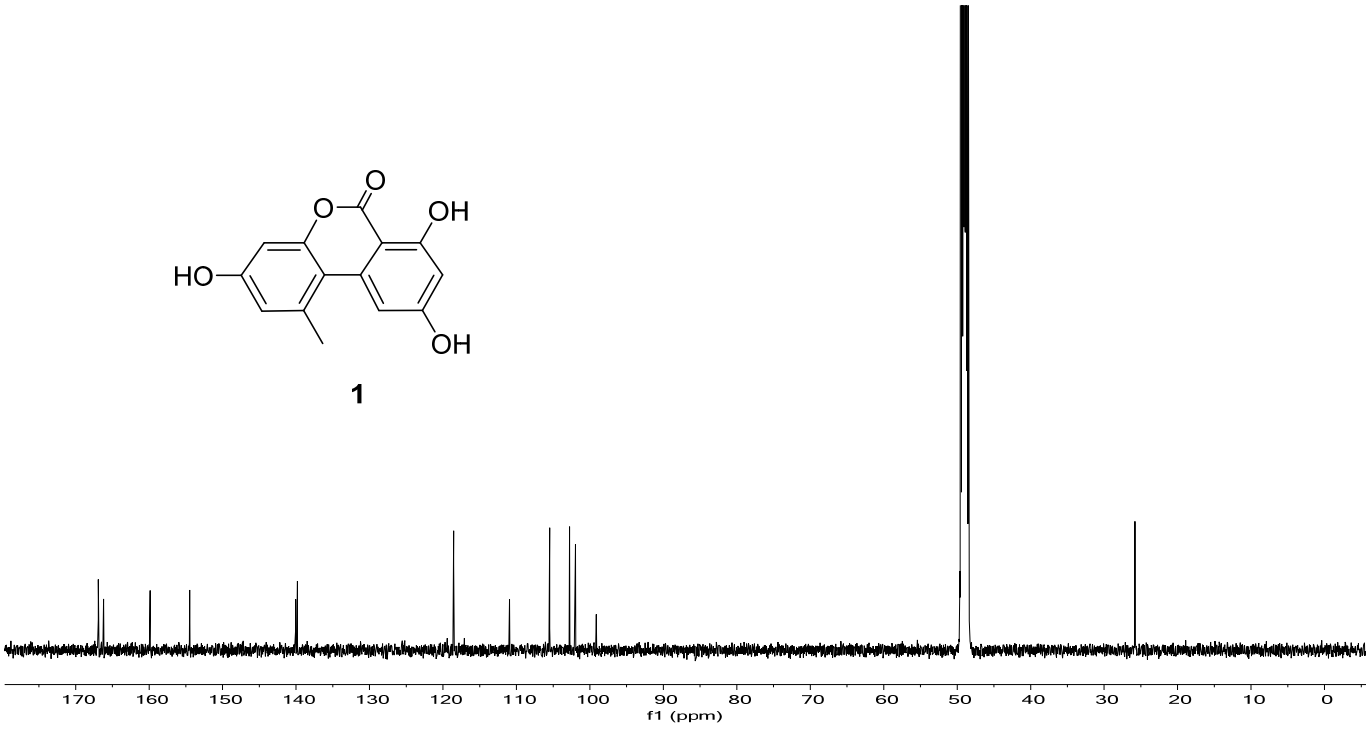


Figure S5. ^{13}C NMR spectrum of Alternariol (AT) (**1**) in CD_3OD.

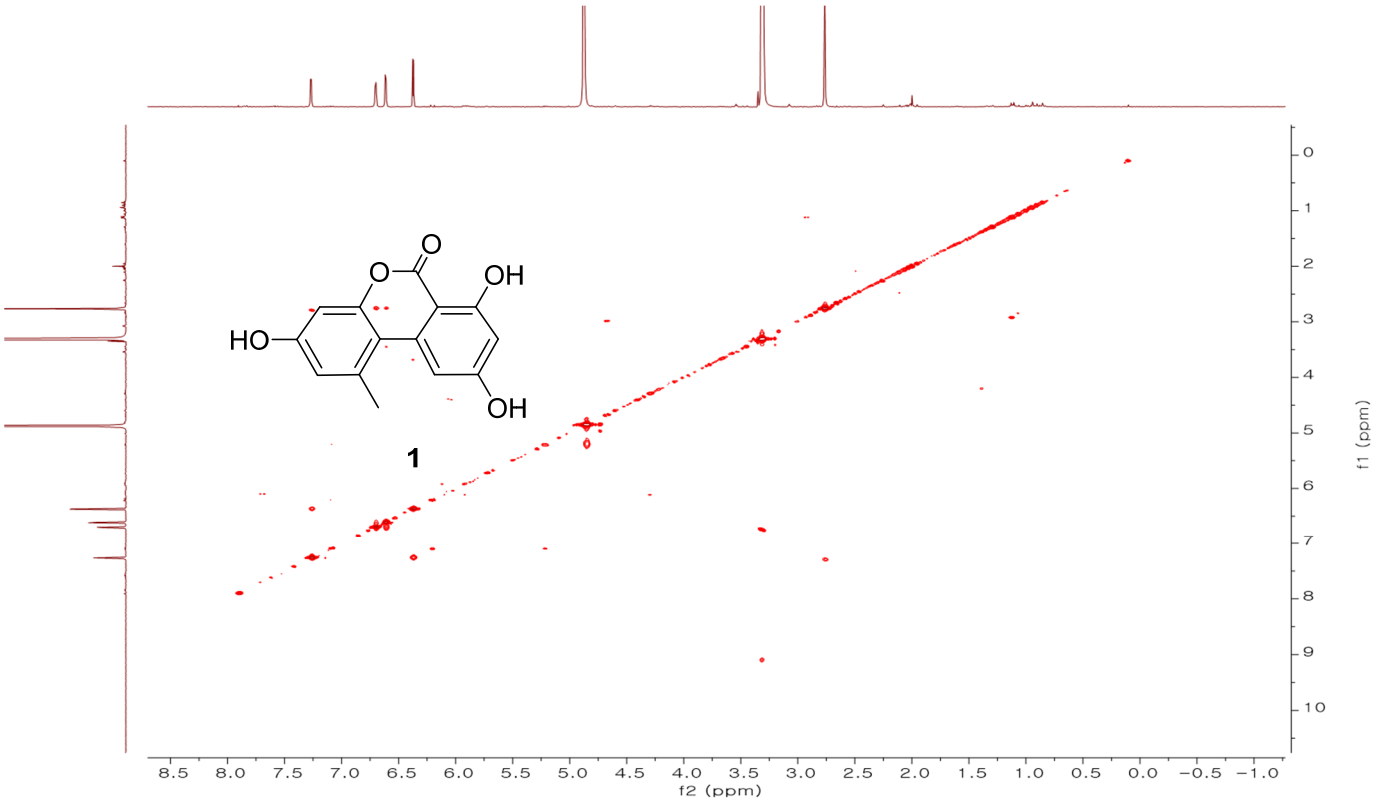


Figure S6. COSY spectrum of Alternariol (AT) (**1**) in CD_3OD.

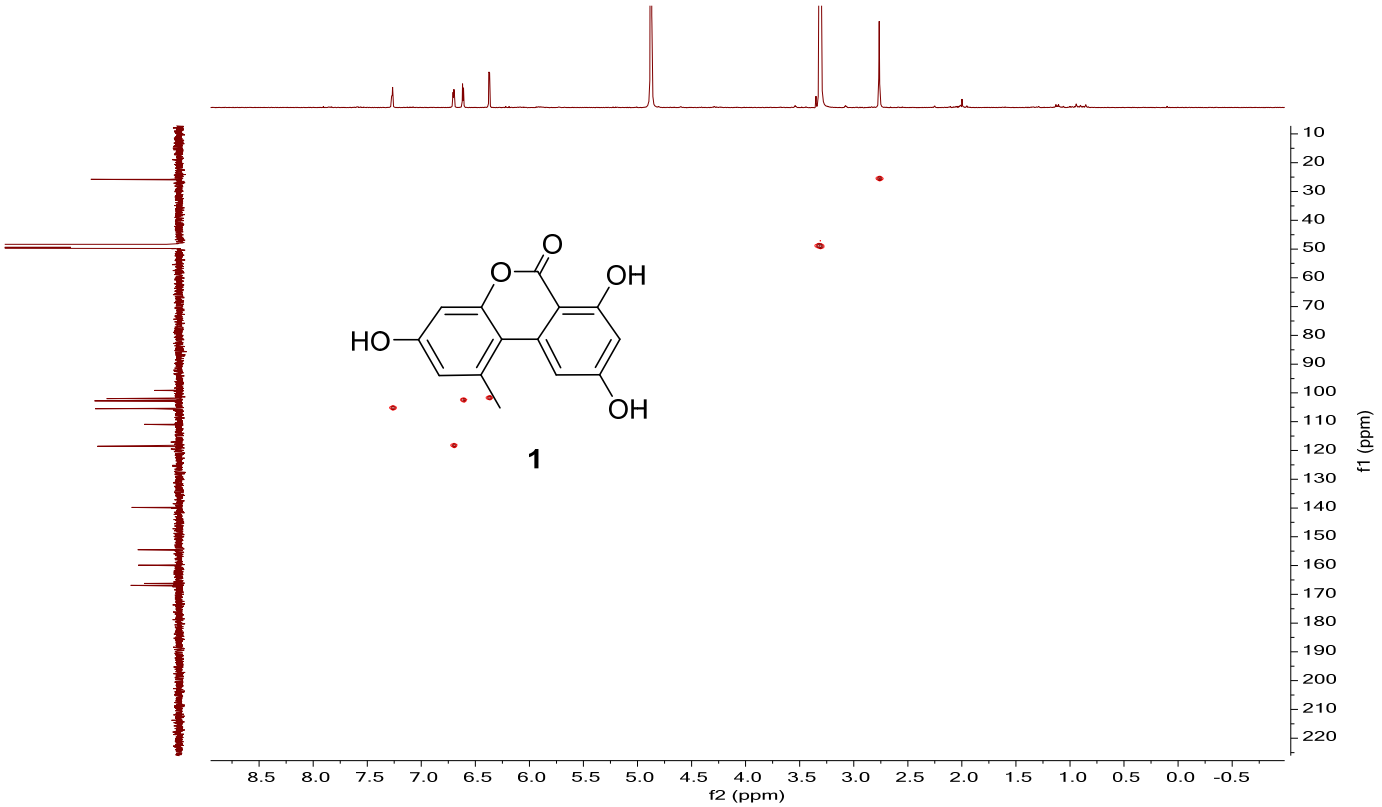


Figure S7. HSQC spectrum of Alternariol (AT) (**1**) in CD_3OD.

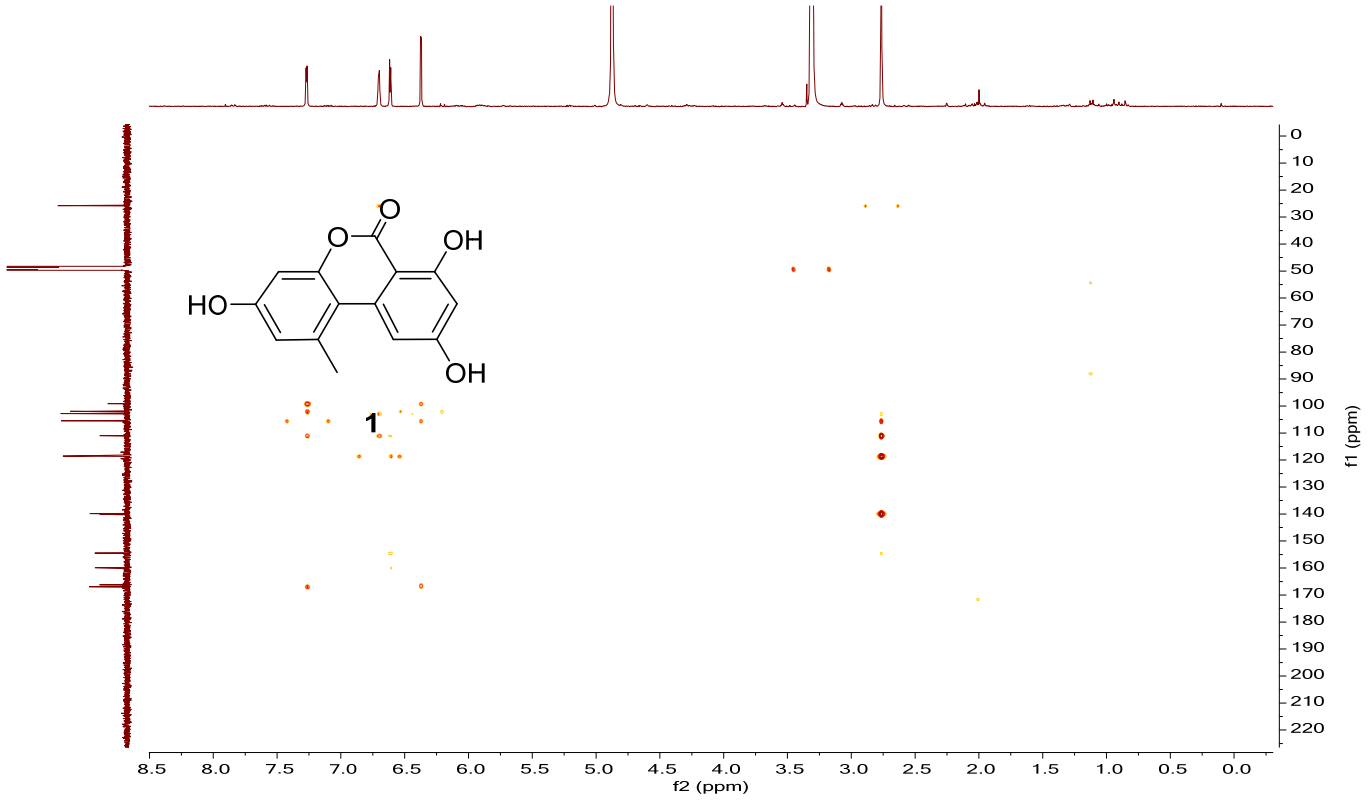


Figure S8. HMBC spectrum of Alternariol (AT) (**1**) in CD_3OD.

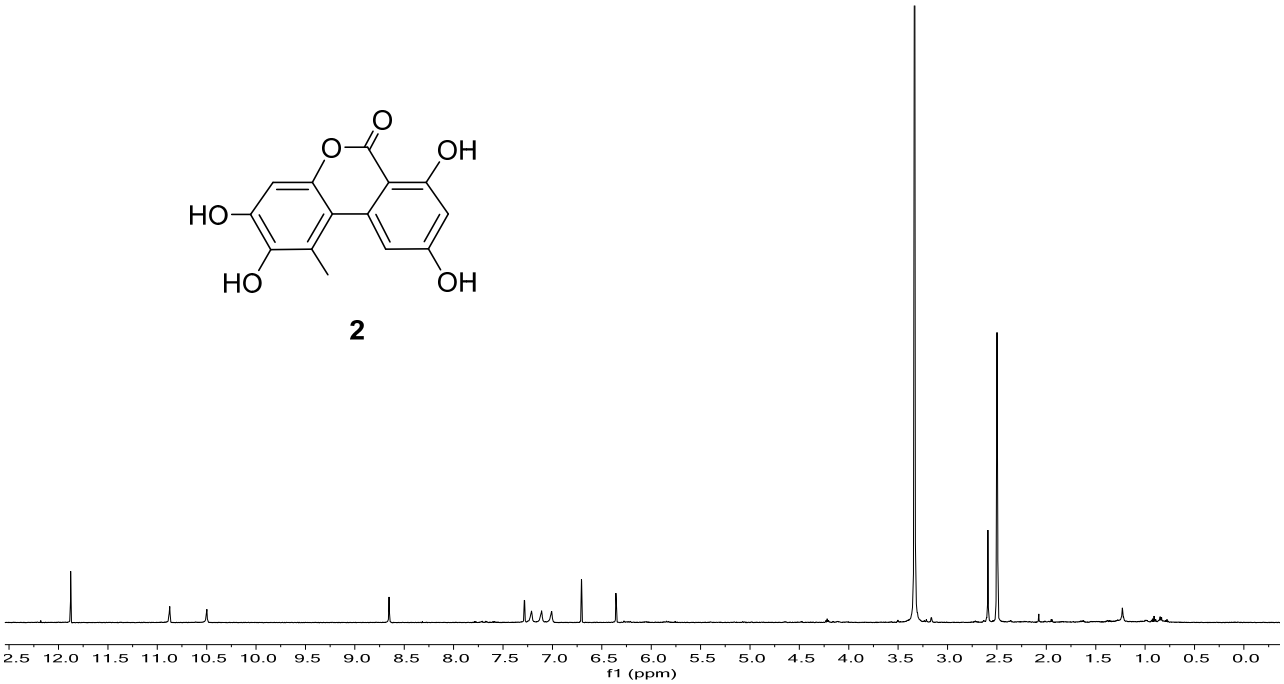


Figure S9. ^1H NMR Spectrum of 5'-hydroxy-alternariol (HAT) (**2**) in DMSO-d_6.

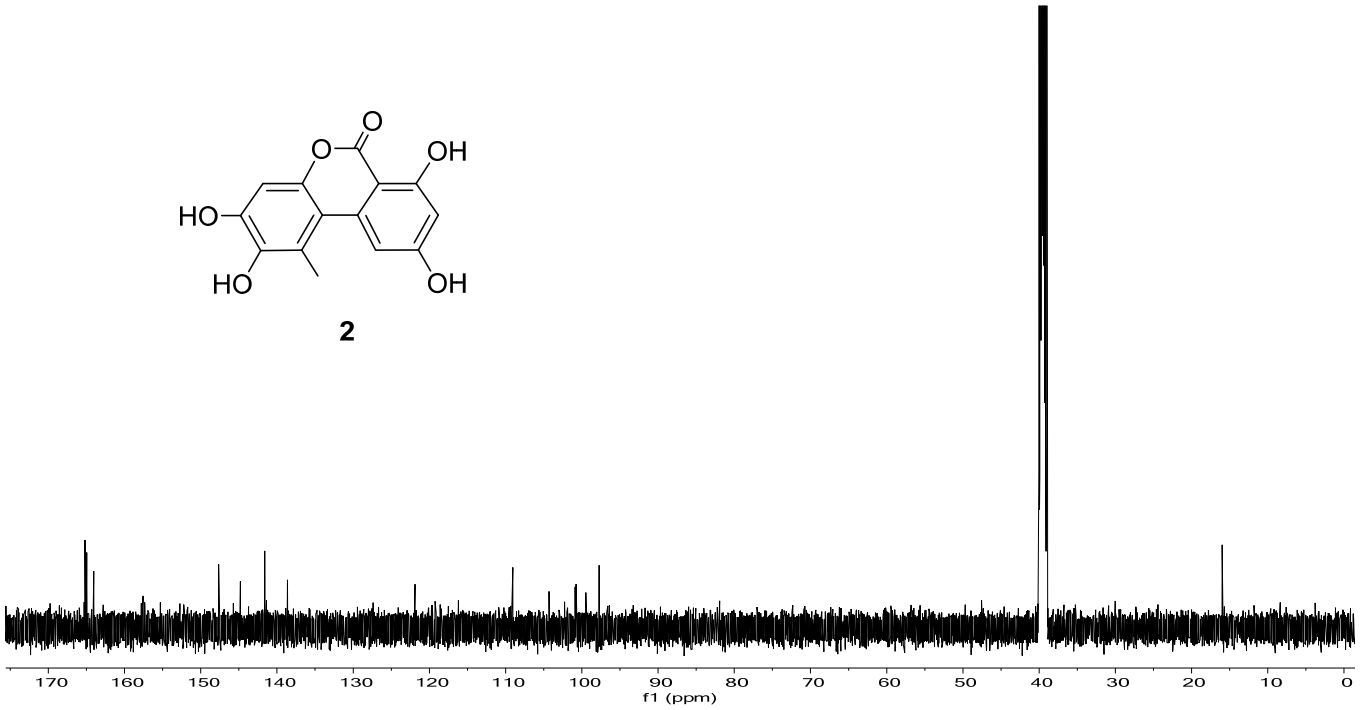


Figure S10. ^{13}C NMR Spectrum of 5'-hydroxy-alternariol (HAT) (**2**) in DMSO-*d*$_6$.

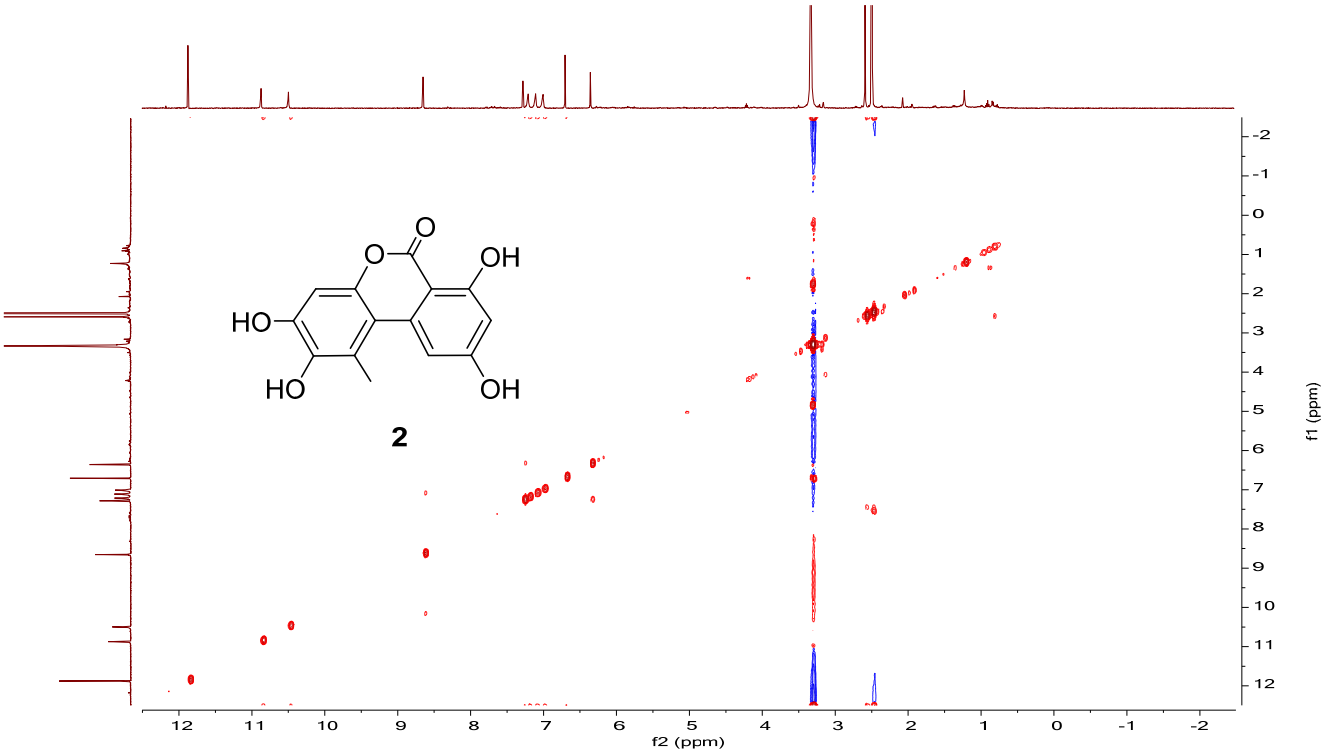


Figure S11. COSY Spectrum of 5'-hydroxy-alternariol (HAT) (**2**) in DMSO-*d*$_6$.

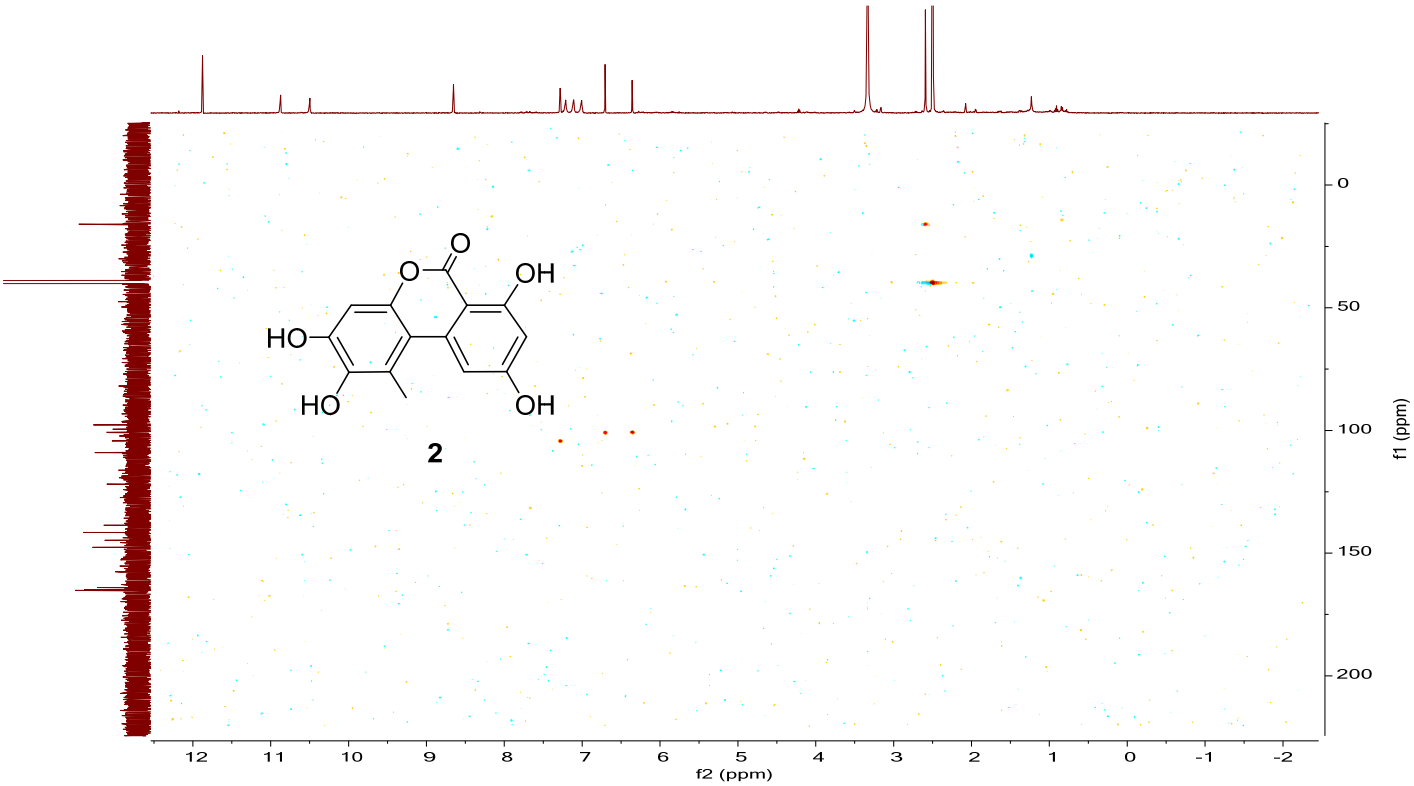


Figure S12. HSQC Spectrum of 5'-hydroxy-alternariol (HAT) (**2**) in DMSO-*d*6.

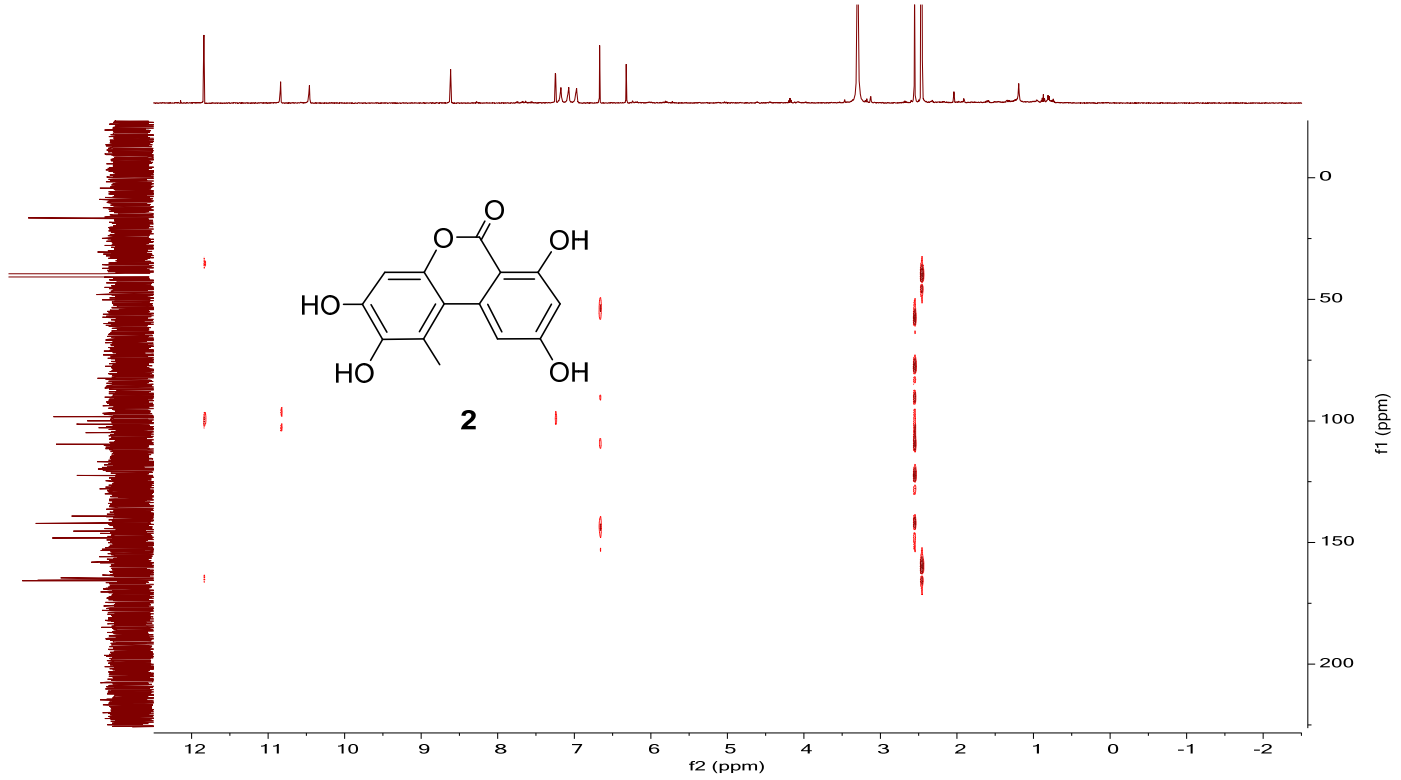


Figure S13. HMBC Spectrum of 5'-hydroxy-alternariol (HAT) (**2**) in DMSO-*d*6.

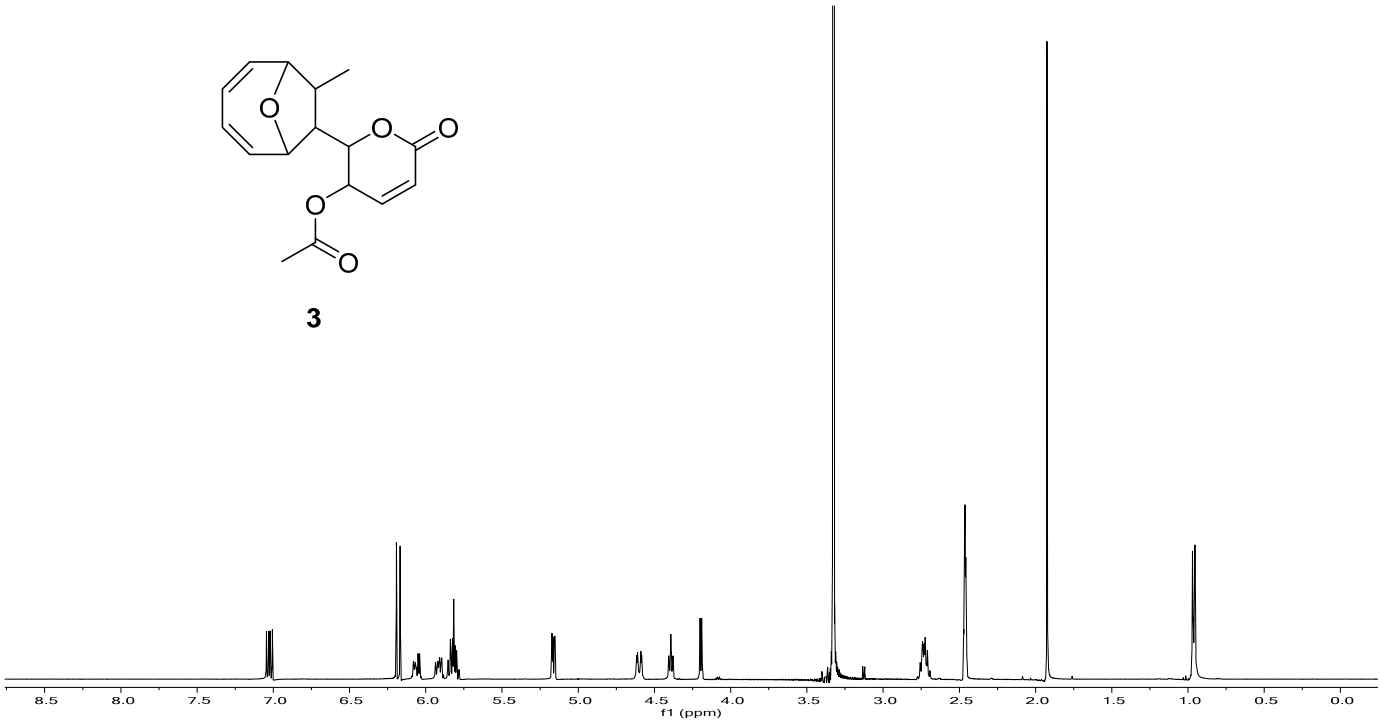


Figure S14. [1]H NMR spectrum of Mycoepoxydiene (MED) (**3**) in DMSO-*d*6.

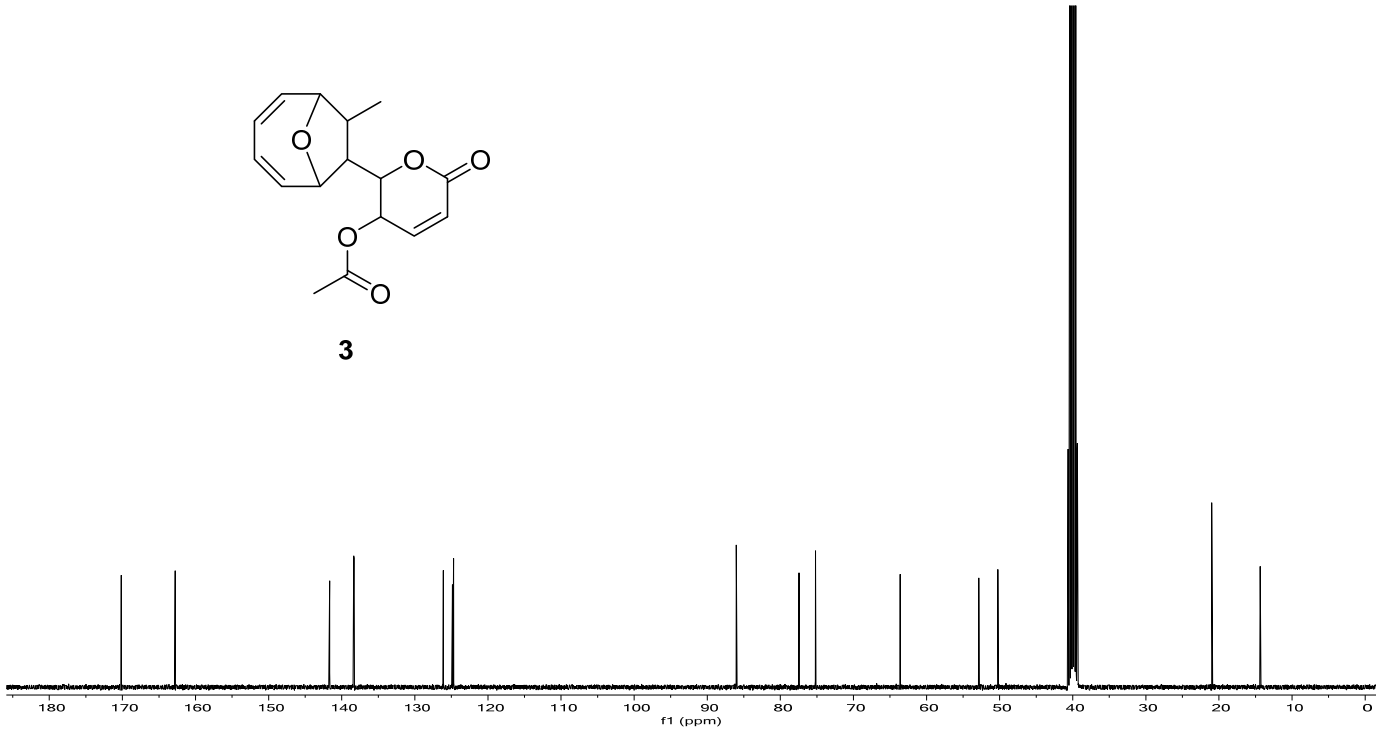


Figure S15. [13]C NMR Spectrum of Mycoepoxydiene (MED) (**3**) in DMSO-*d*6.

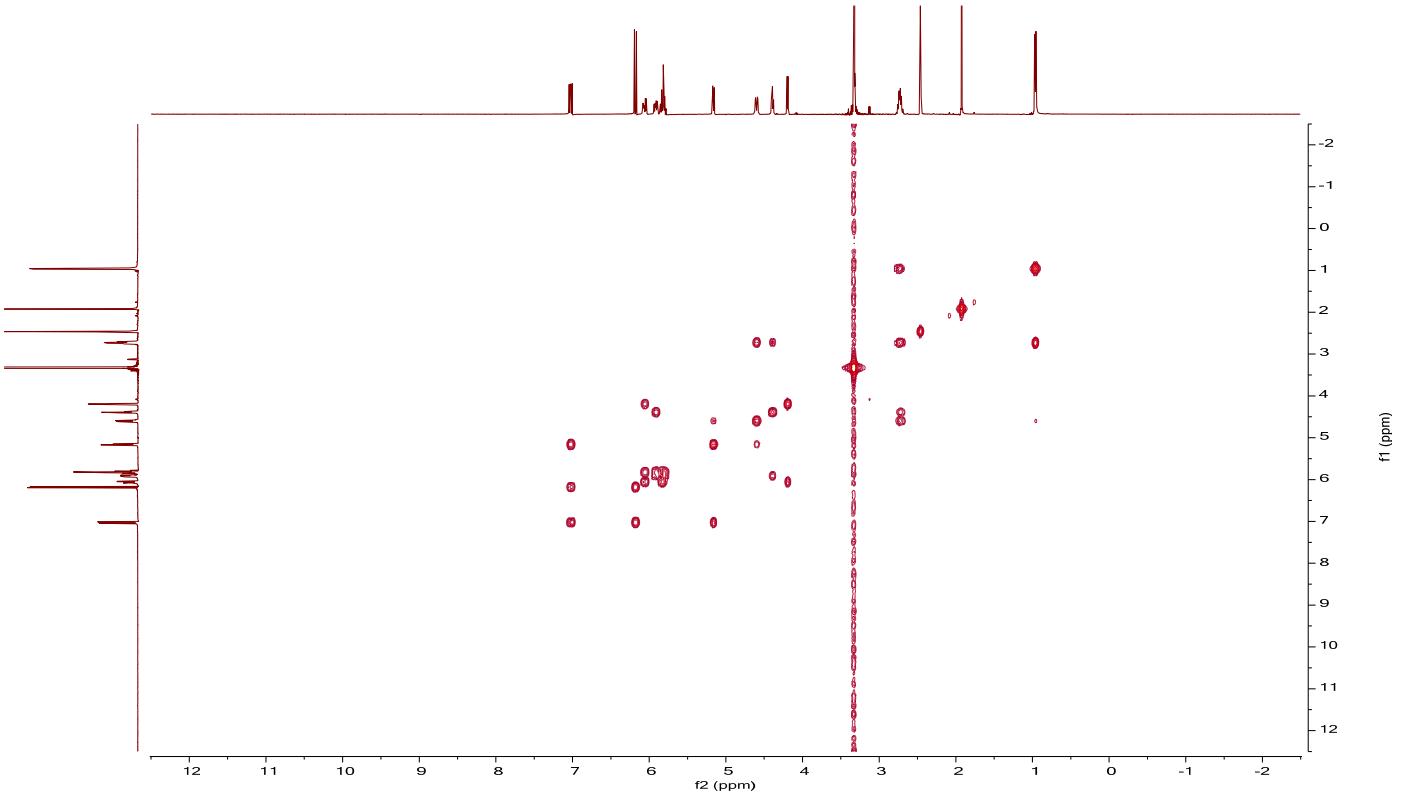


Figure S16. COSY Spectrum of Mycoepoxydiene (MED) (**3**) in DMSO-*d*6.

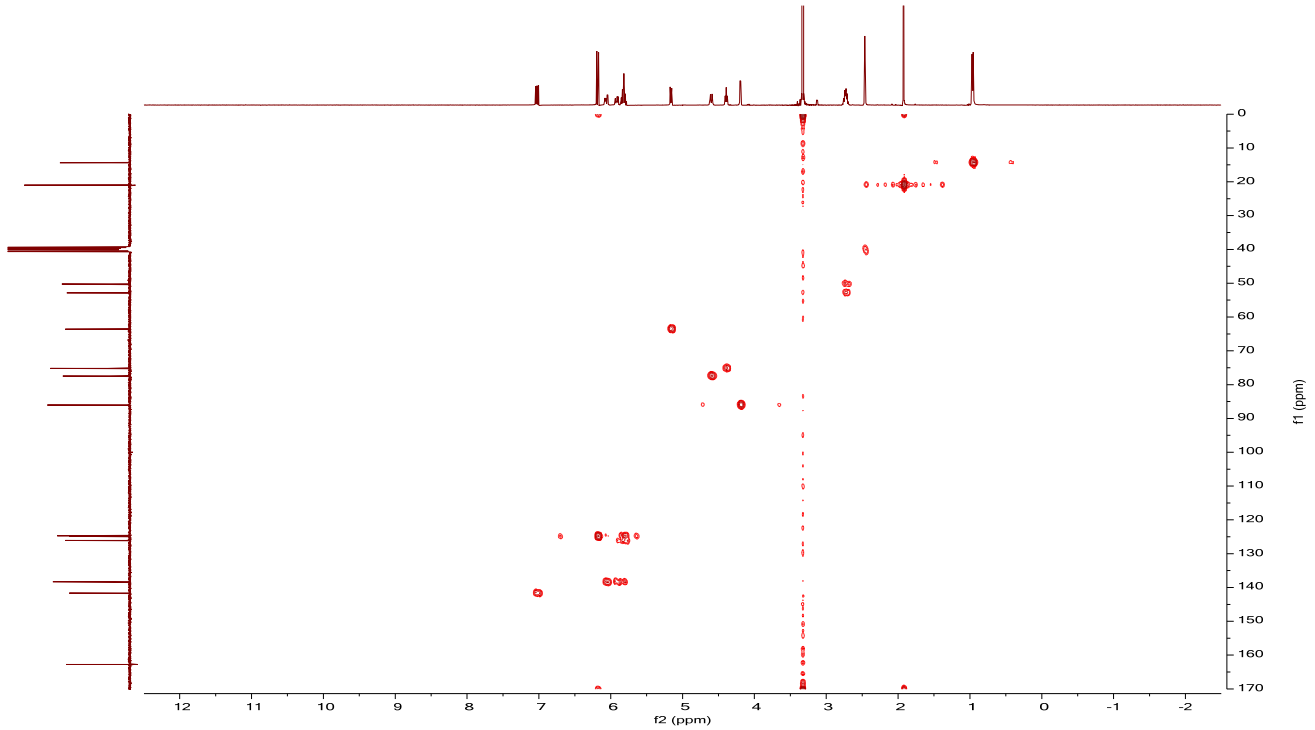


Figure S17. HSQC Spectrum of Mycoepoxydiene (MED) (**3**) in DMSO-*d*6.

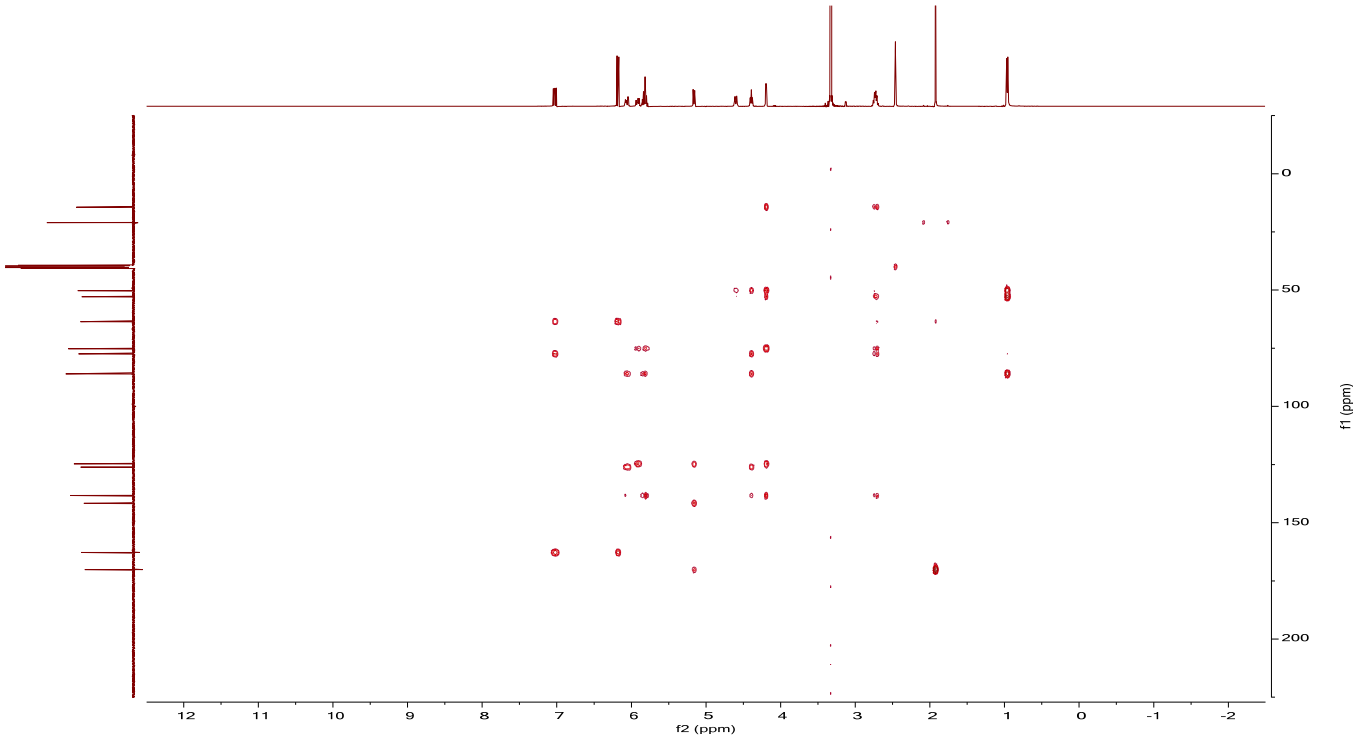


Figure S18. HMBC Spectrum of Mycoepoxydiene (MED) (**3**) in DMSO-d_6.

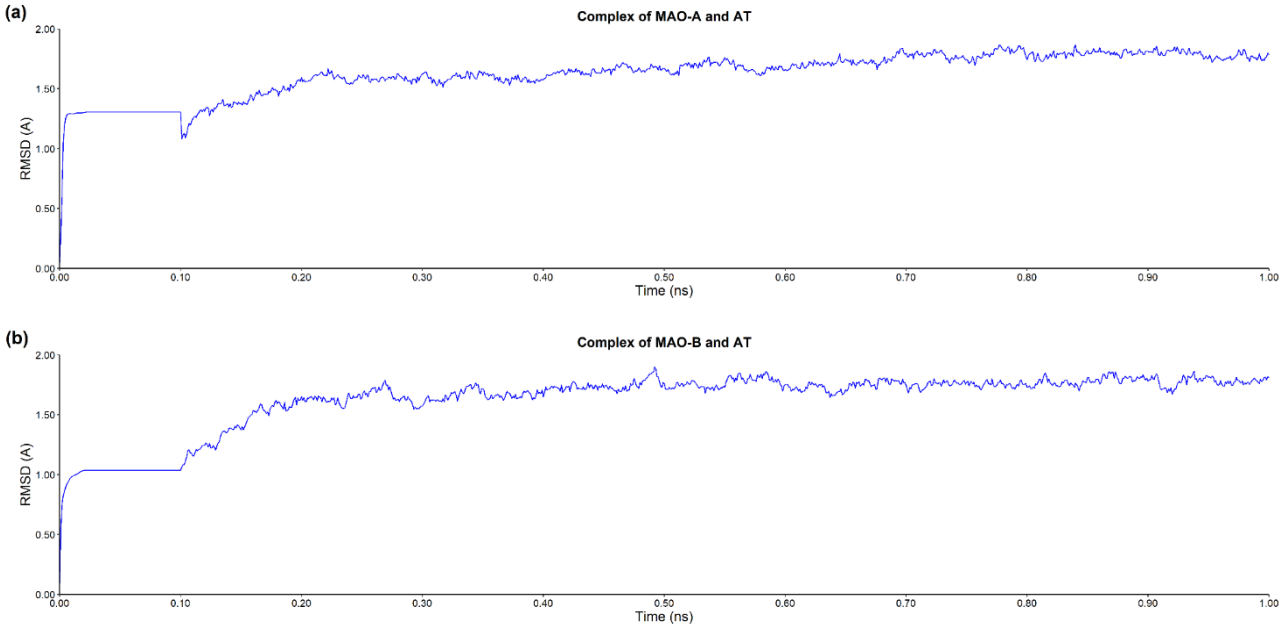


Figure S19. Plots of root mean square deviation (RMSD) during 1 ns MD simulation of (a) hMAO-A and (b) hMAO-B complexes with AT.