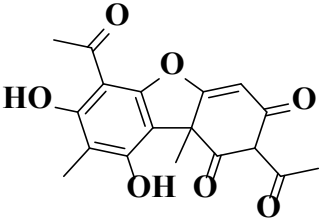
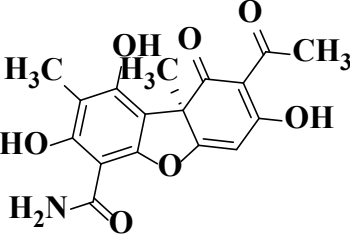
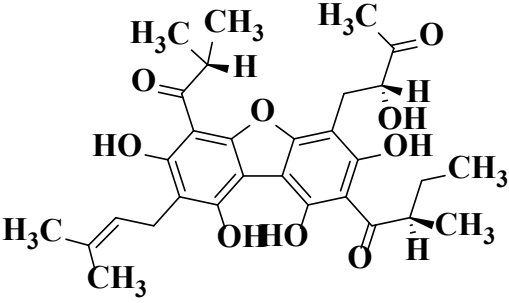
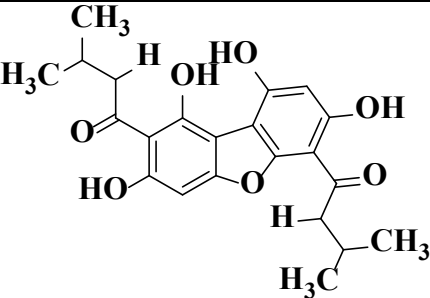
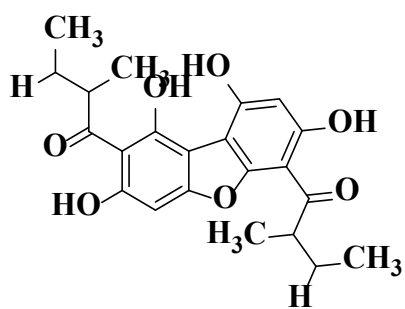


Supplementary data

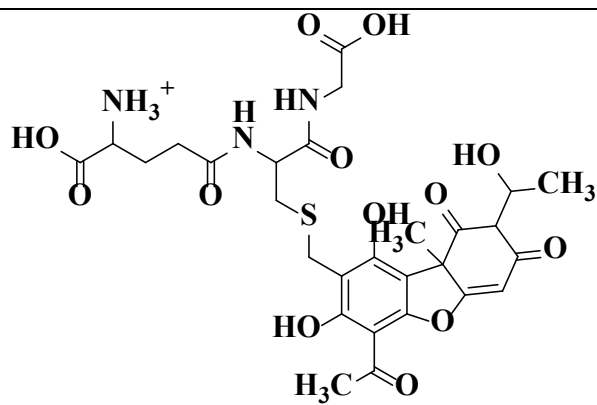
Table S1. Usnic acid derivatives (340)

Compound Number	Structure
1	
2	
3	
4	

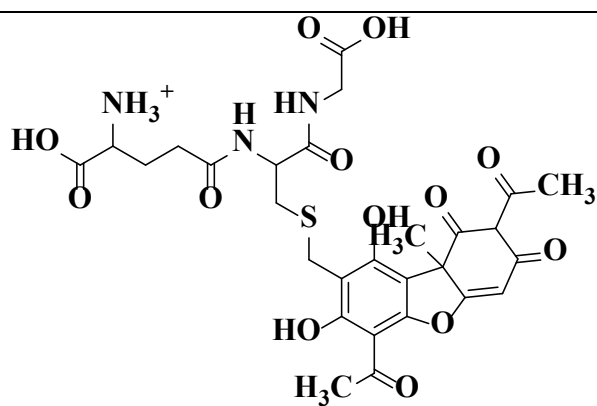
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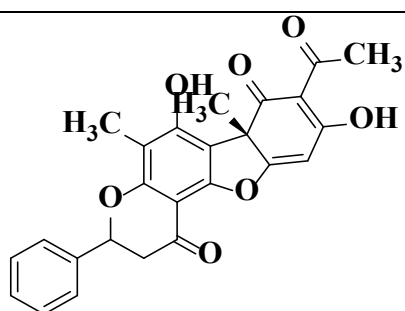
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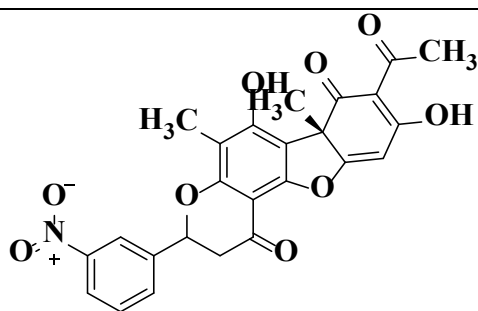
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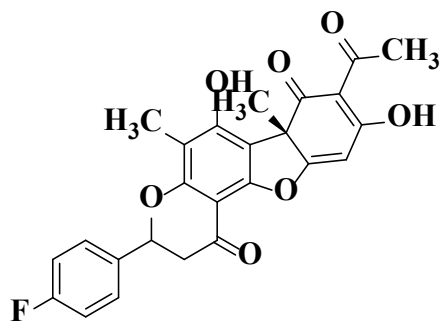
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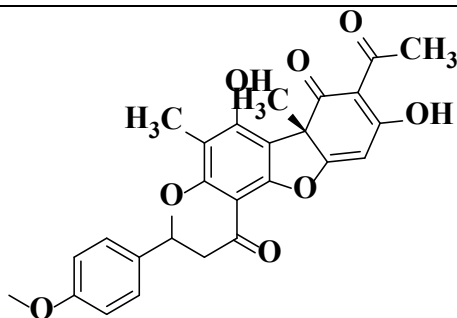
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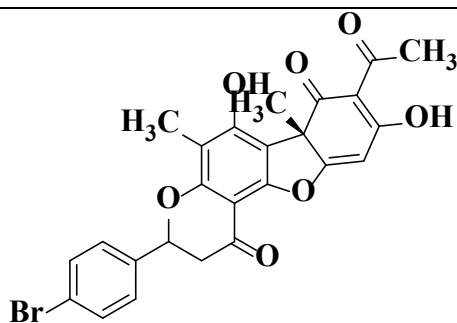
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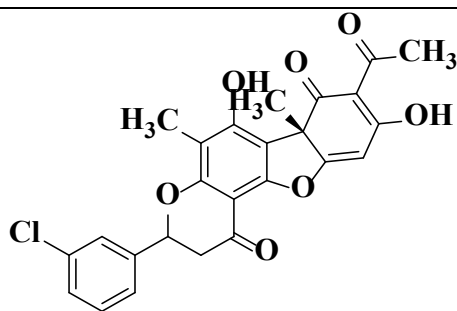
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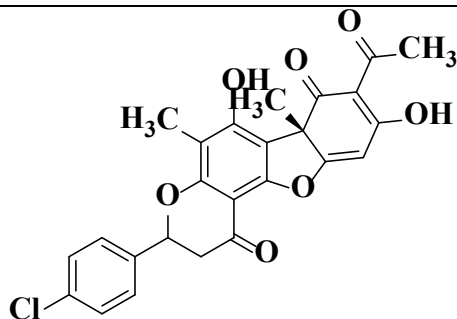
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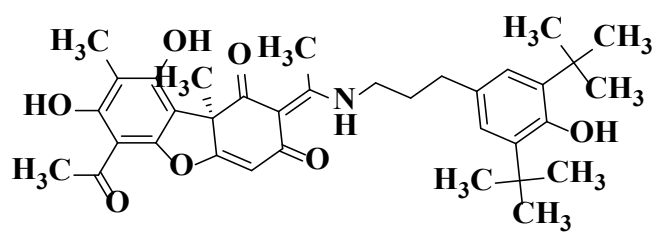
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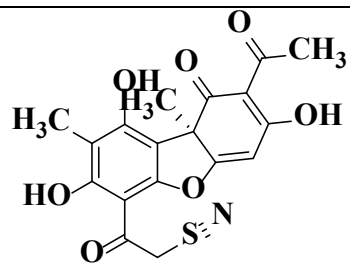
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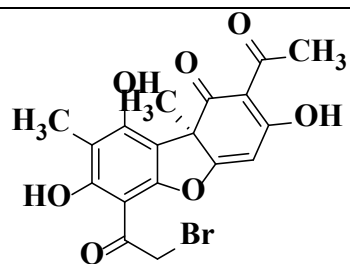
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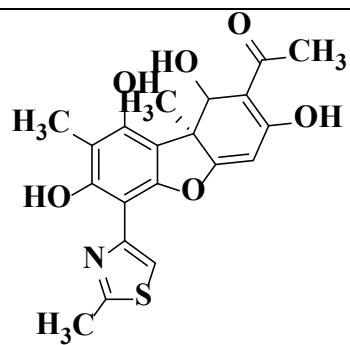
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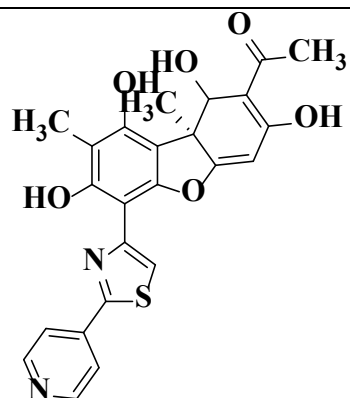
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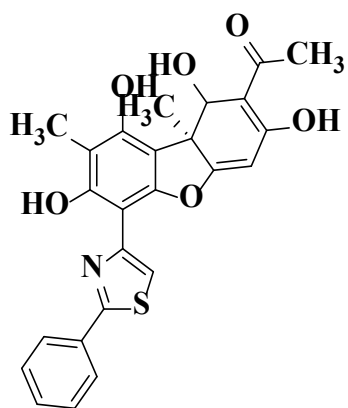
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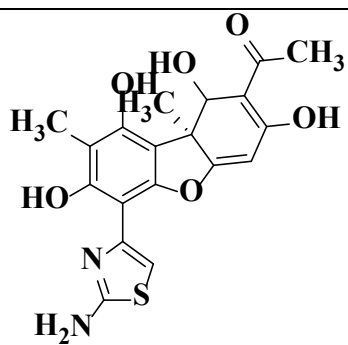
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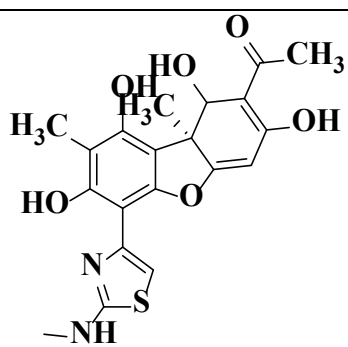
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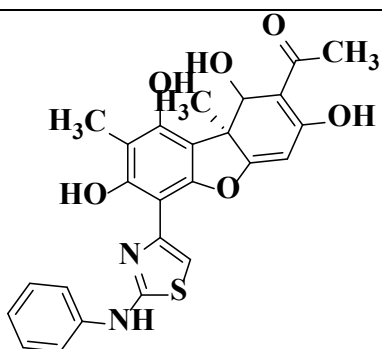
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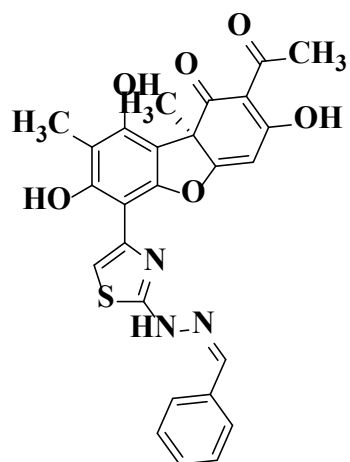
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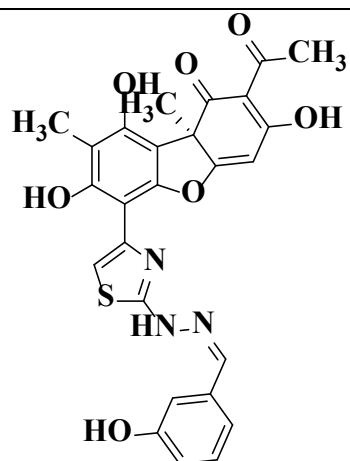
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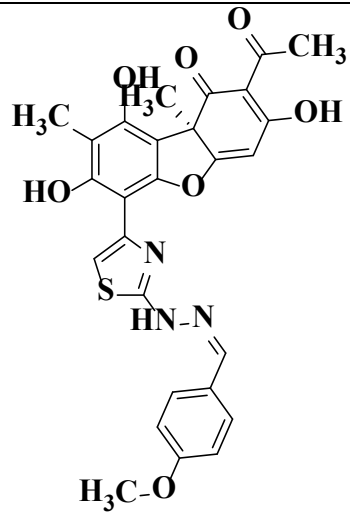
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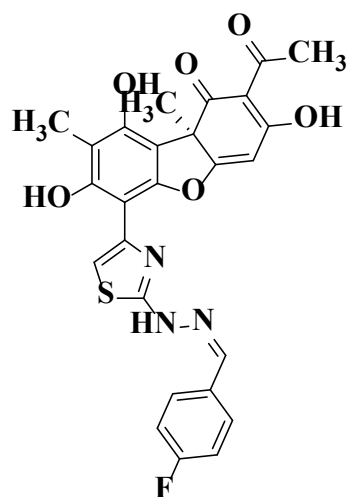
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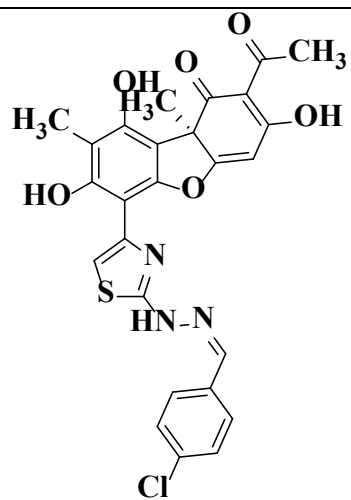
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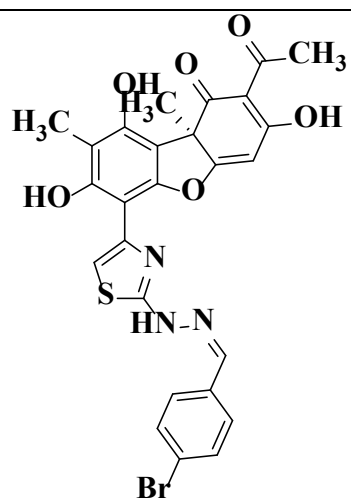
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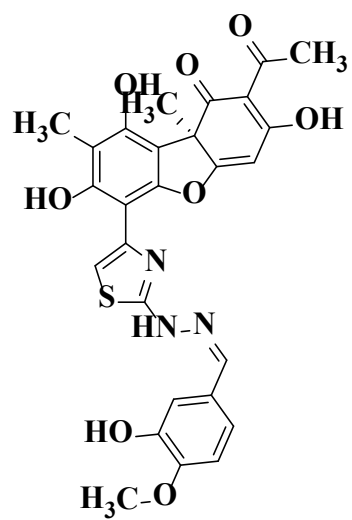
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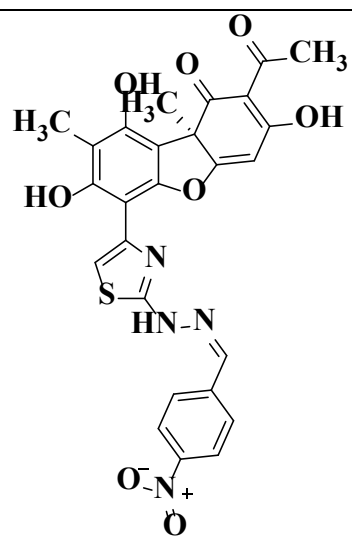
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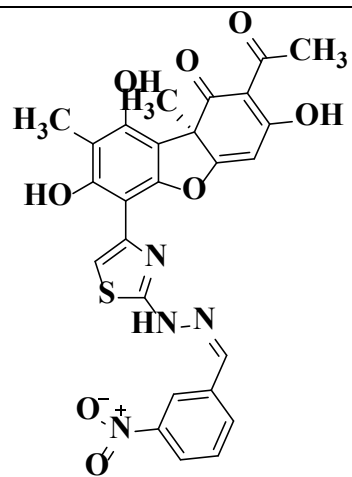
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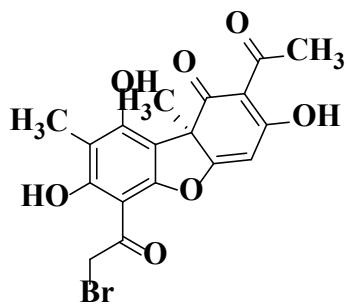
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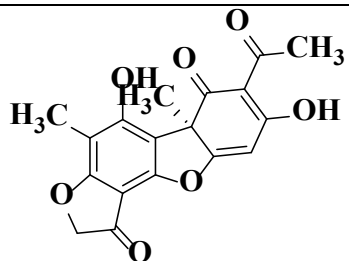
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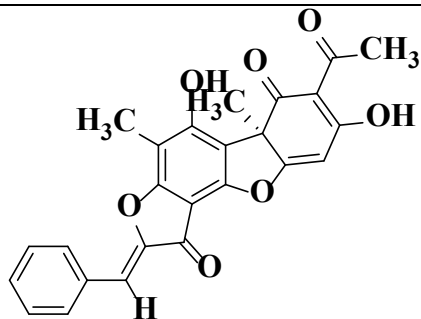
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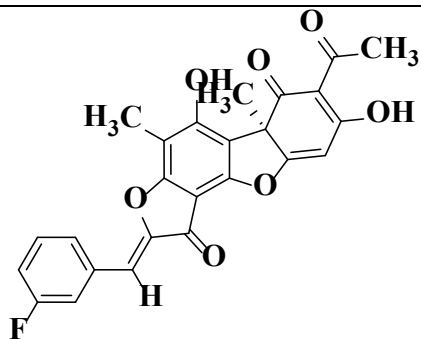
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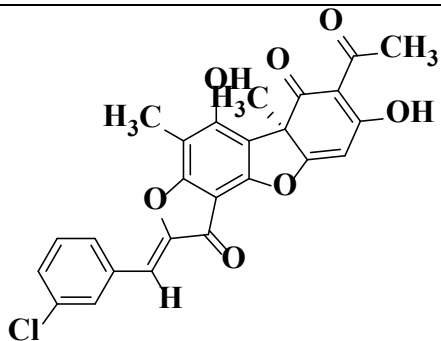
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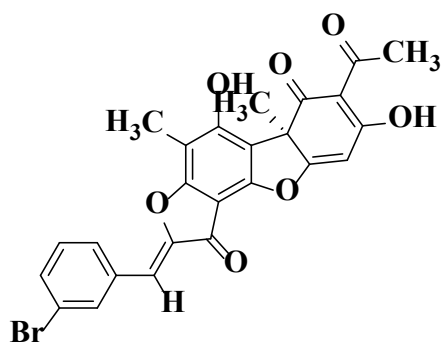
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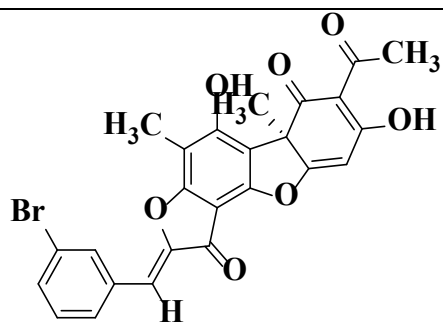
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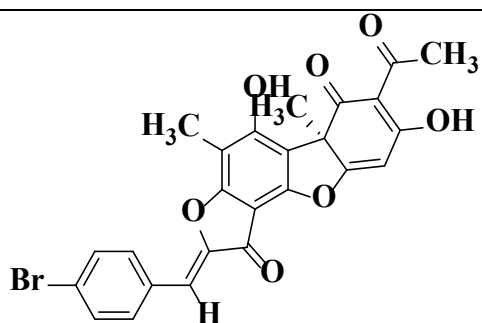
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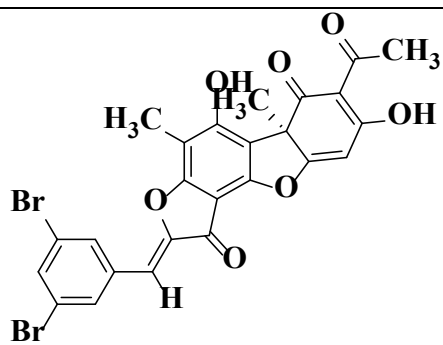
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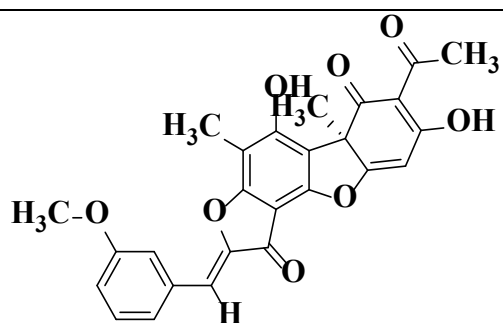
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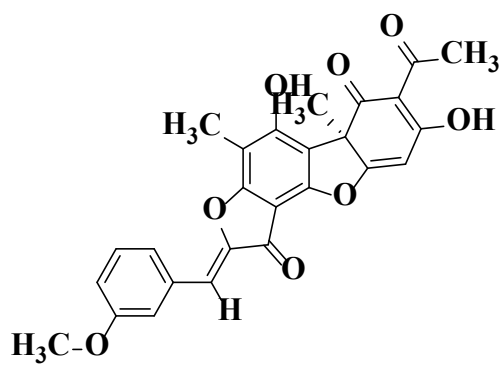
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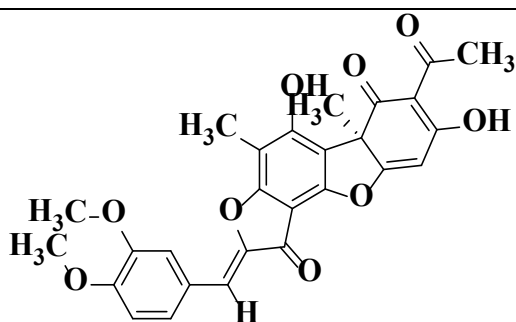
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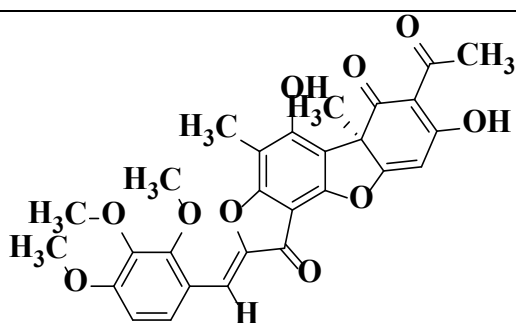
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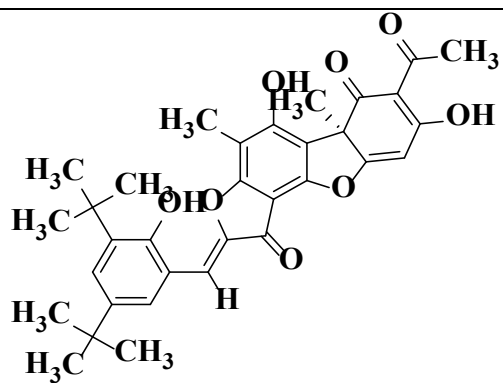
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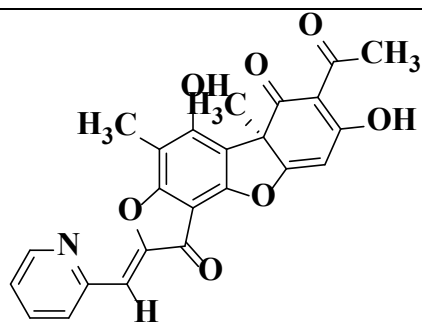
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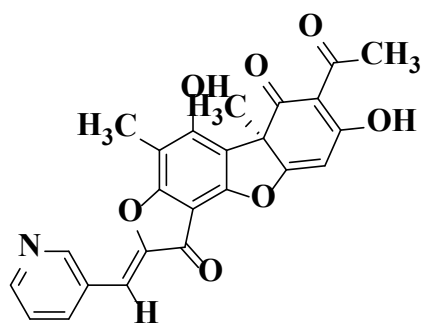
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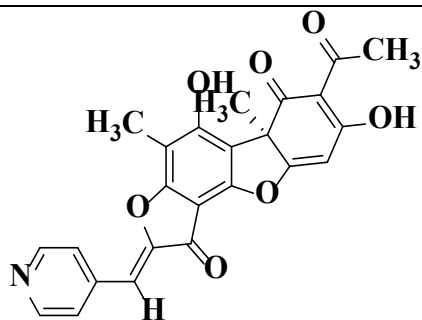
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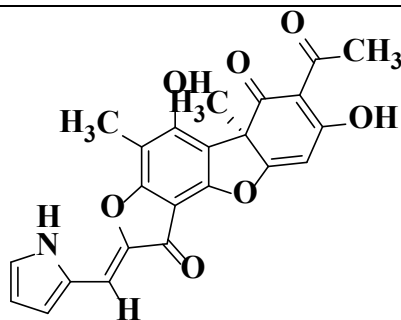
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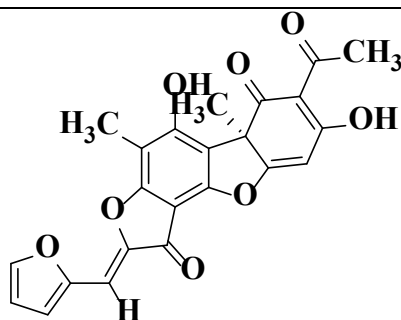
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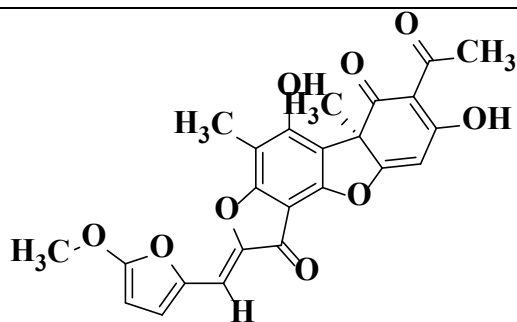
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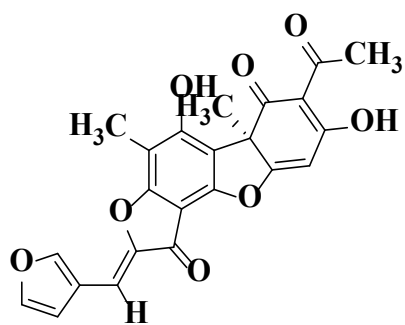
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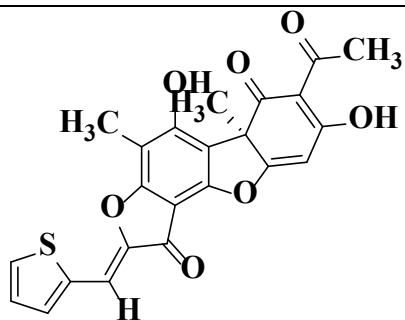
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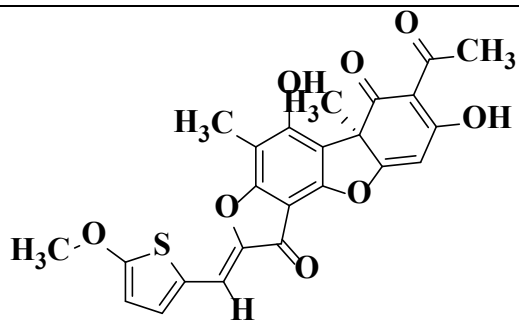
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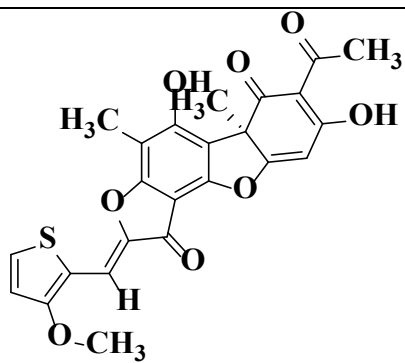
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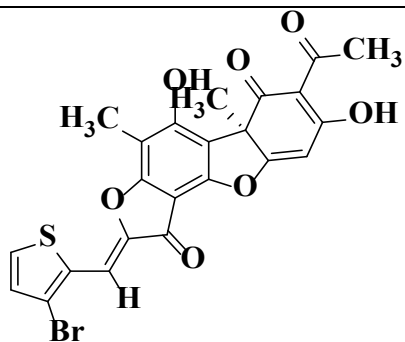
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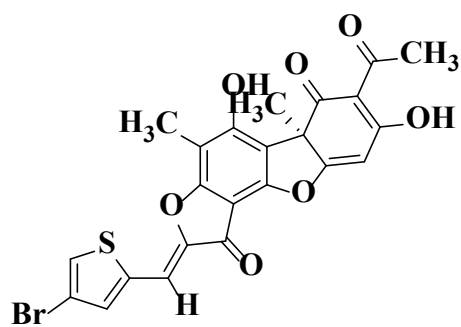
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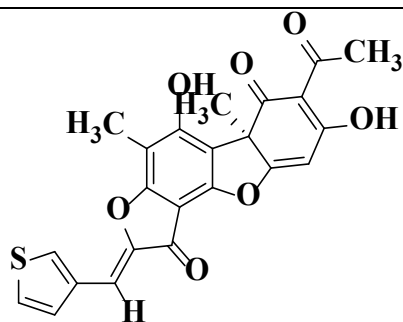
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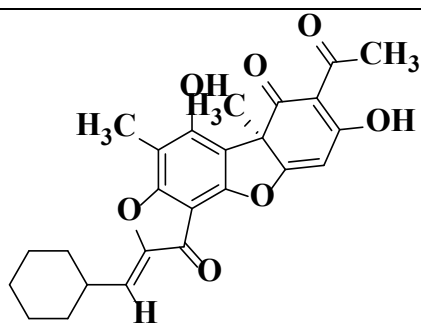
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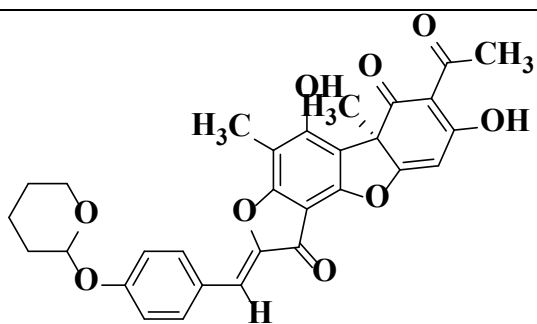
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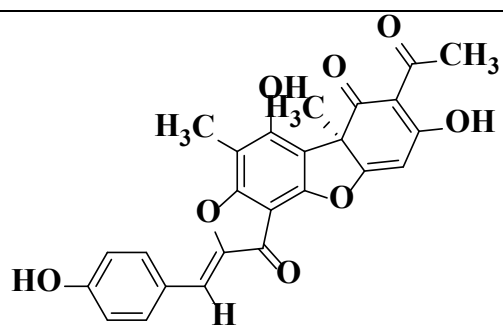
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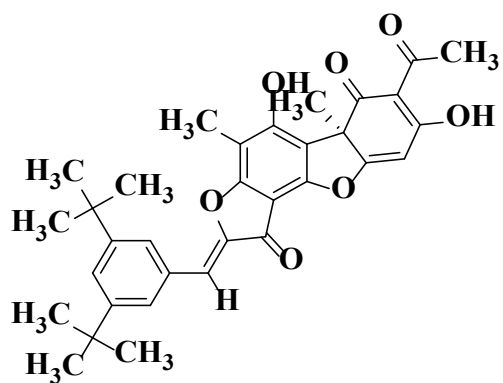
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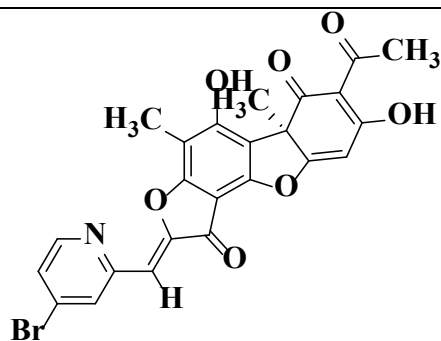
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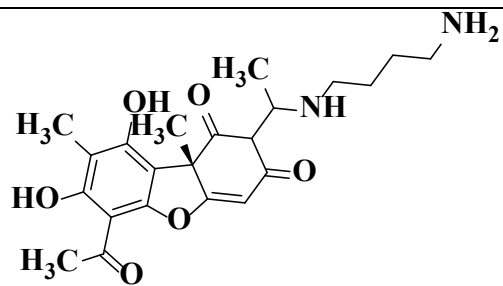
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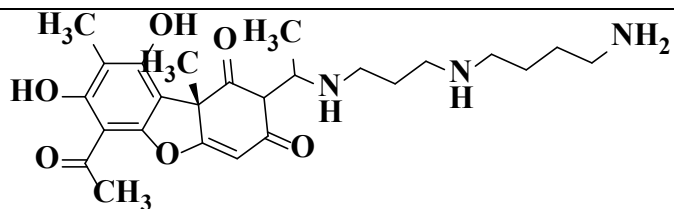
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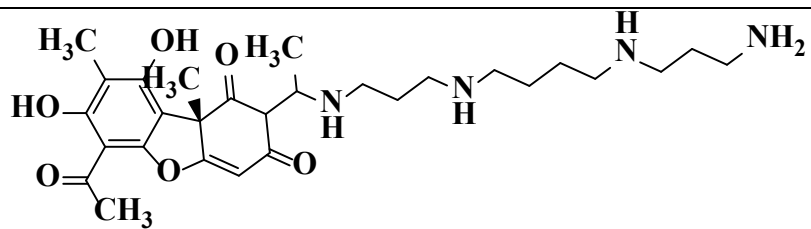
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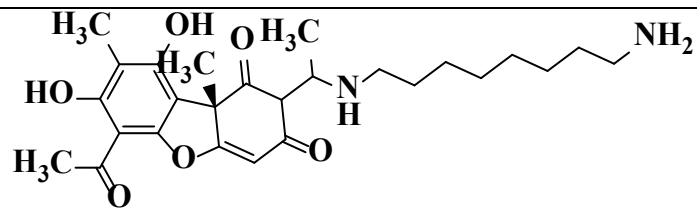
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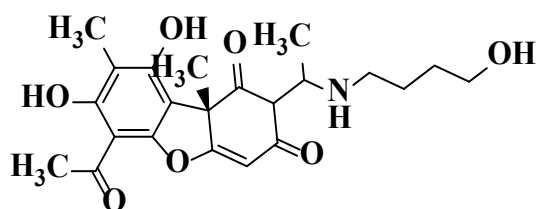
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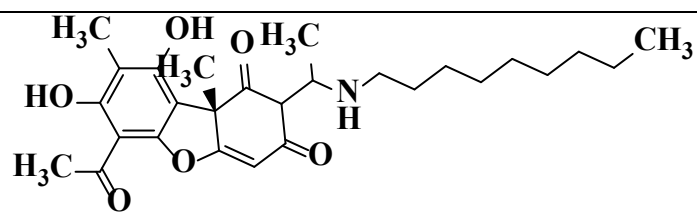
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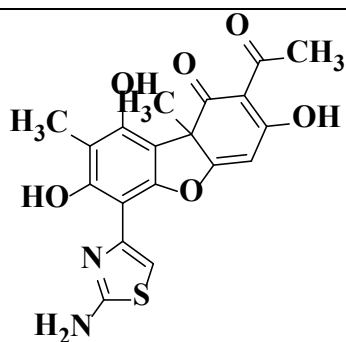
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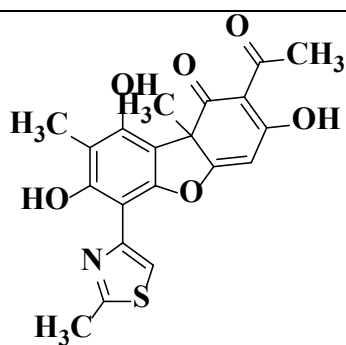
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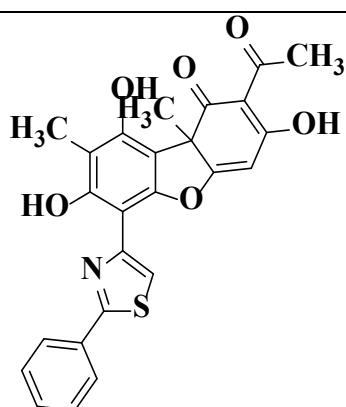
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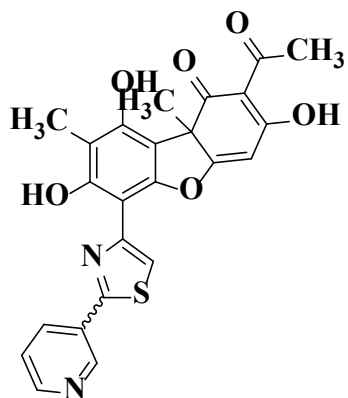
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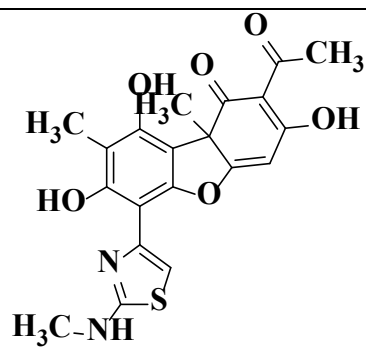
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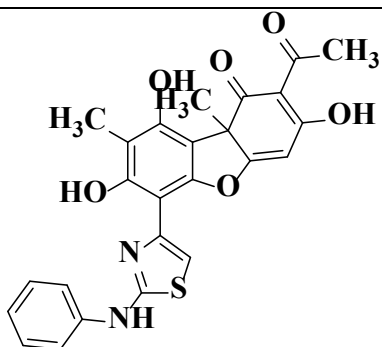
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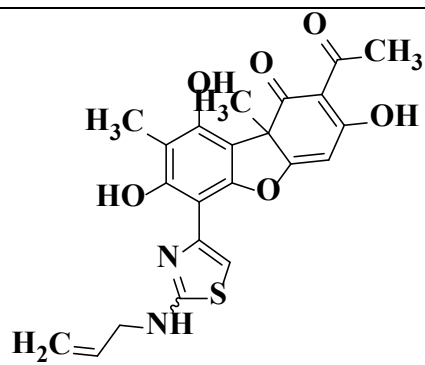
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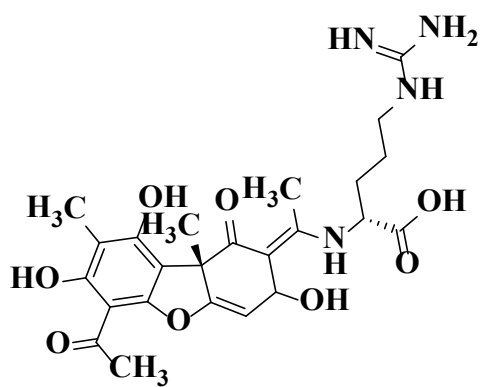
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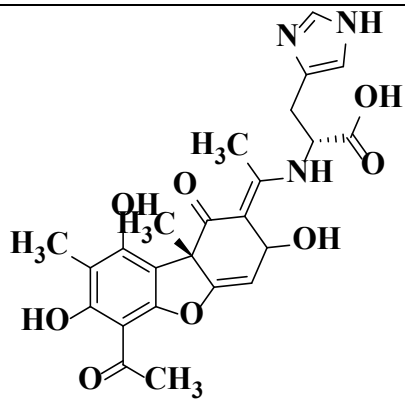
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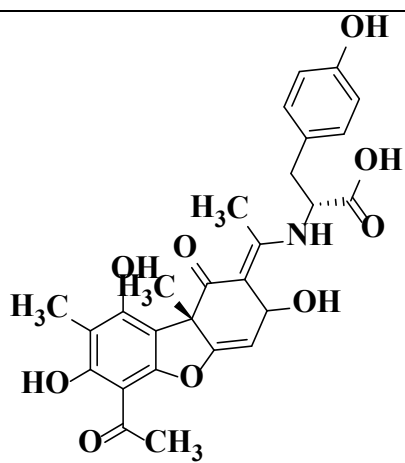
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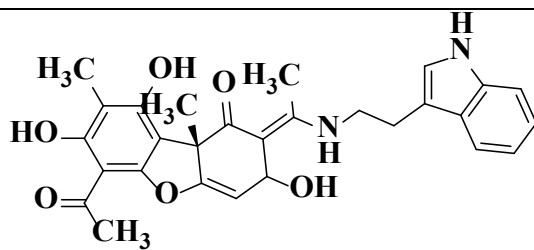
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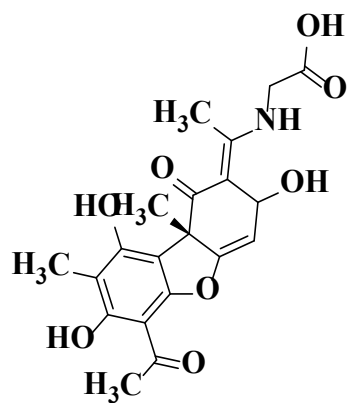
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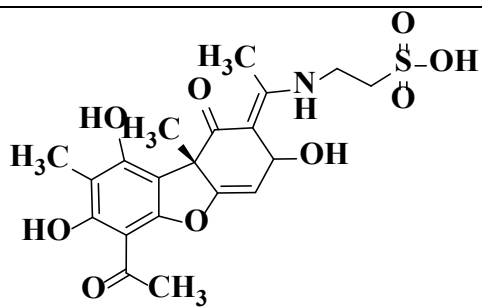
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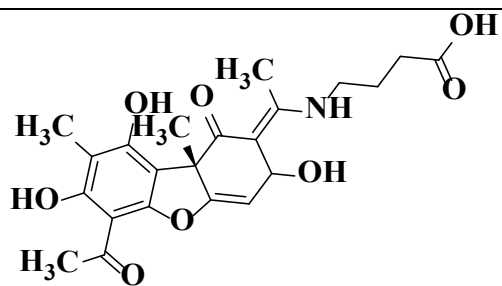
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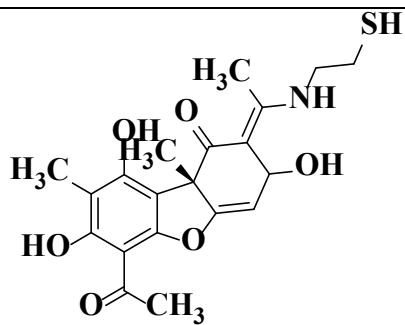
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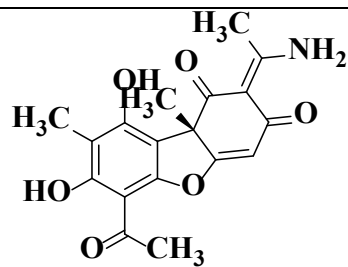
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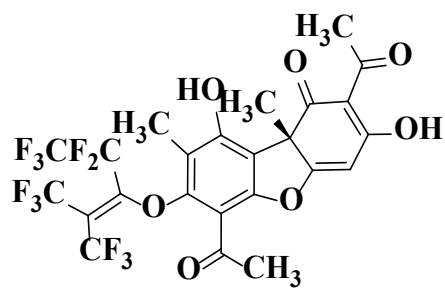
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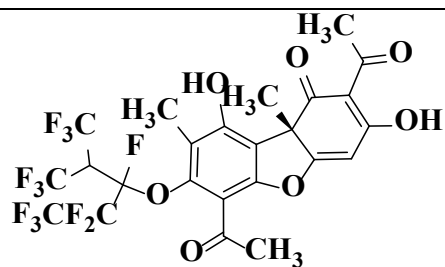
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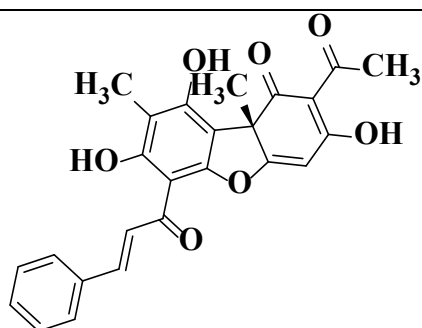
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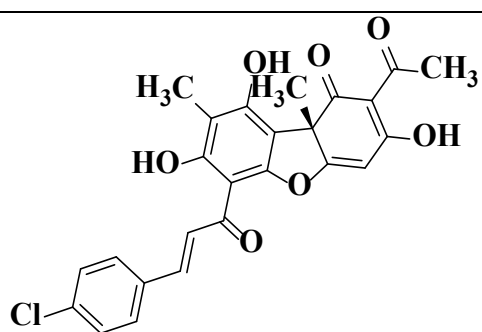
88



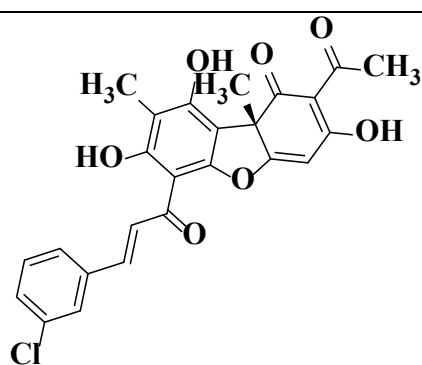
89



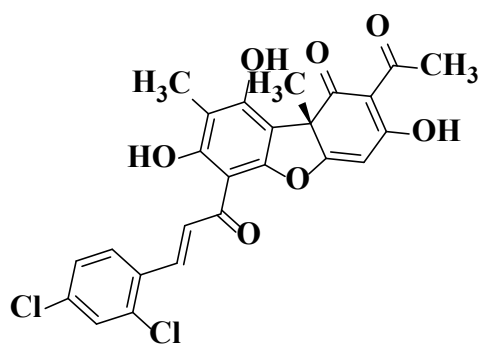
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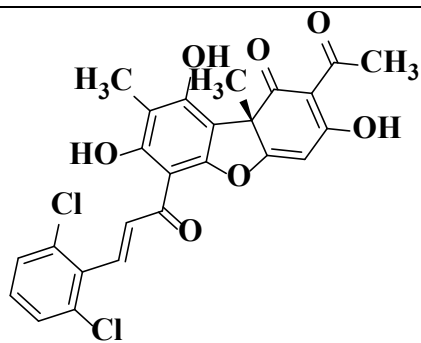
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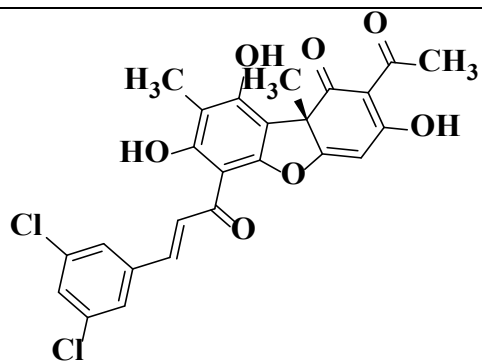
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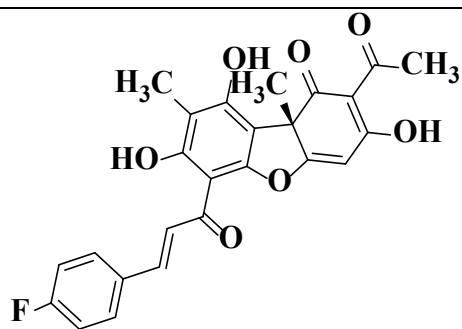
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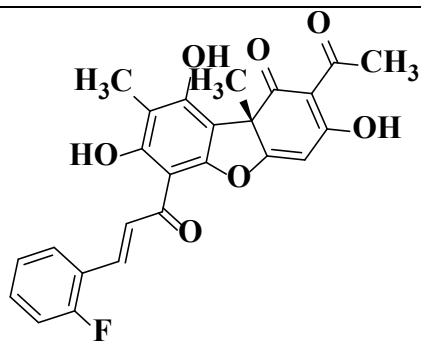
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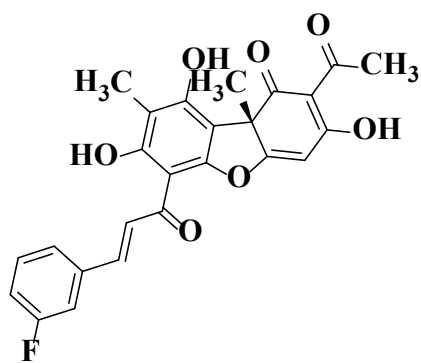
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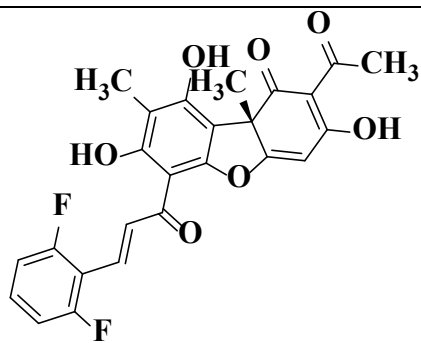
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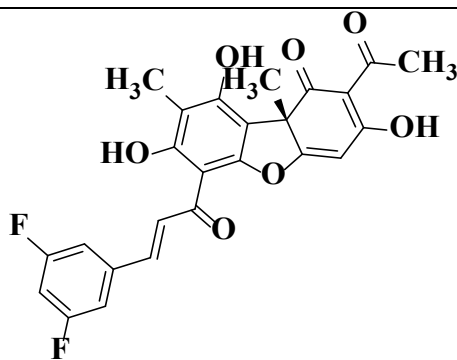
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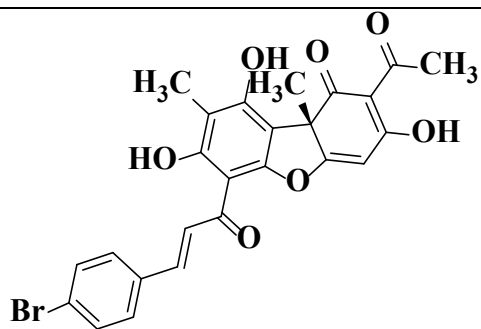
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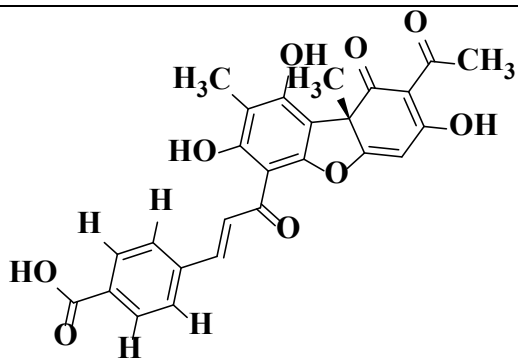
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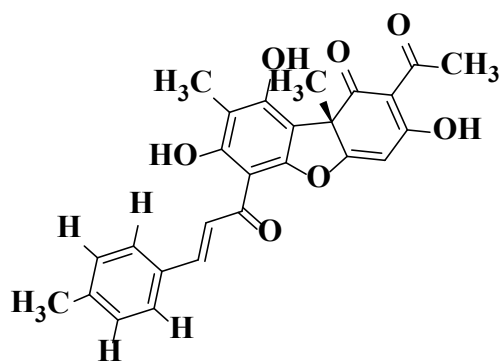
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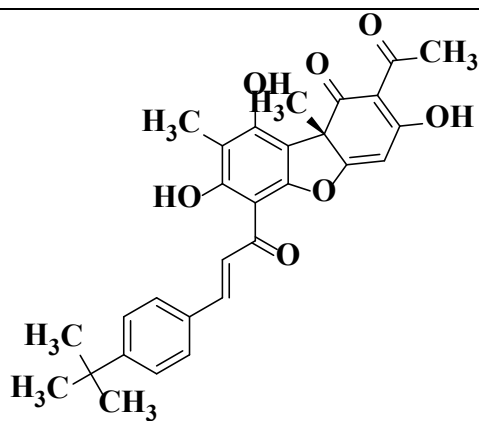
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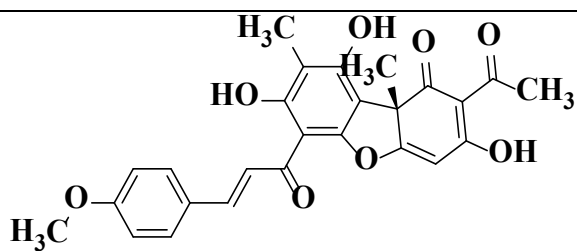
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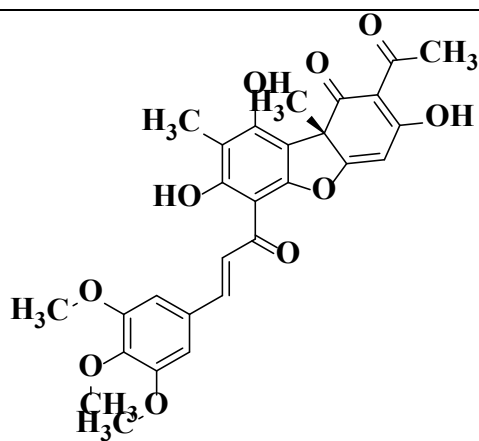
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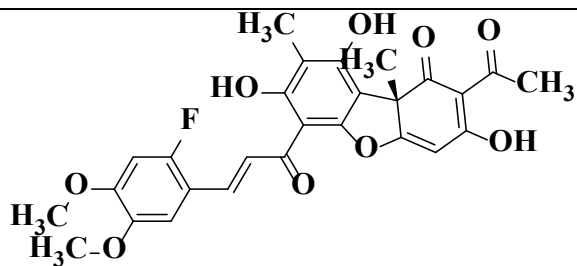
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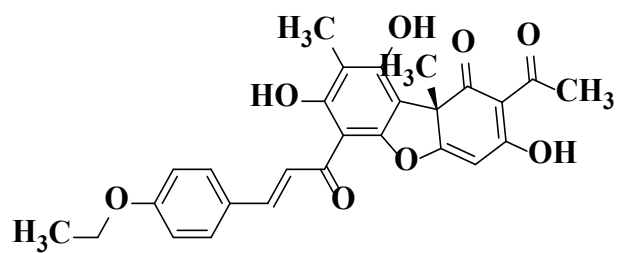
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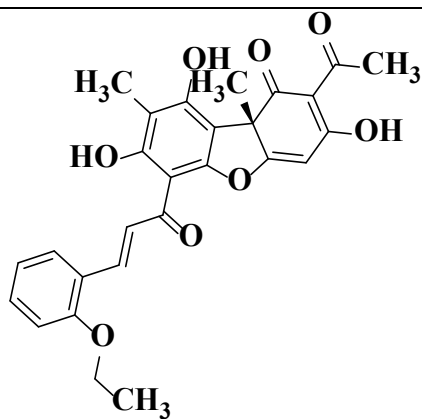
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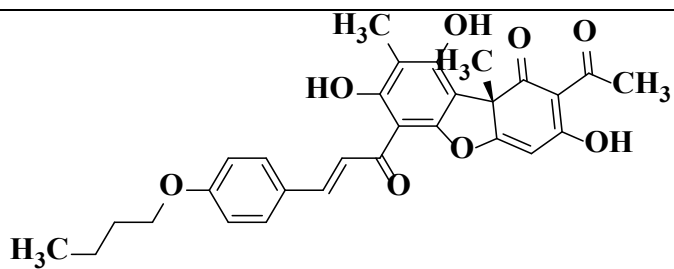
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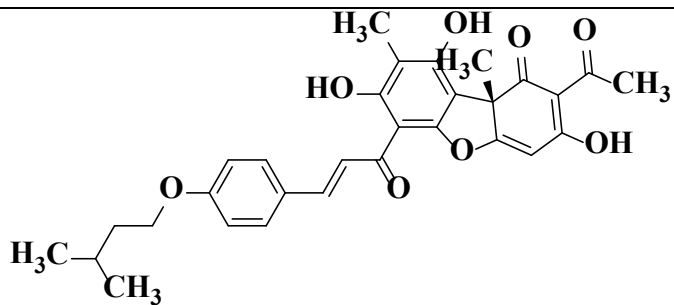
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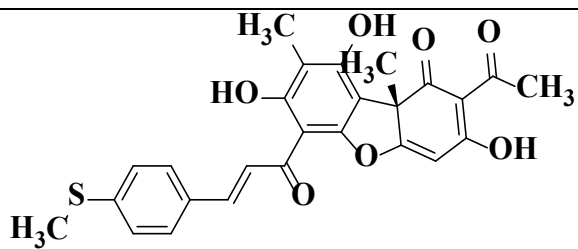
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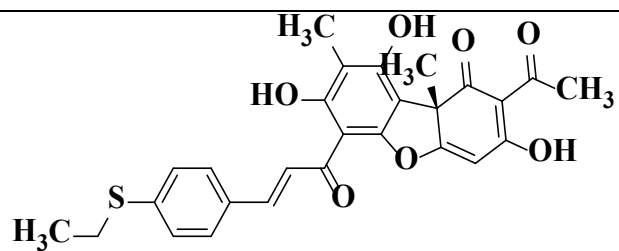
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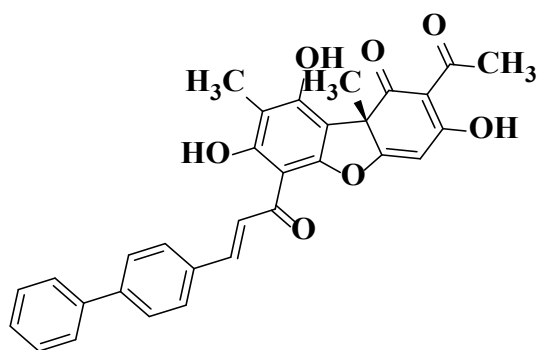
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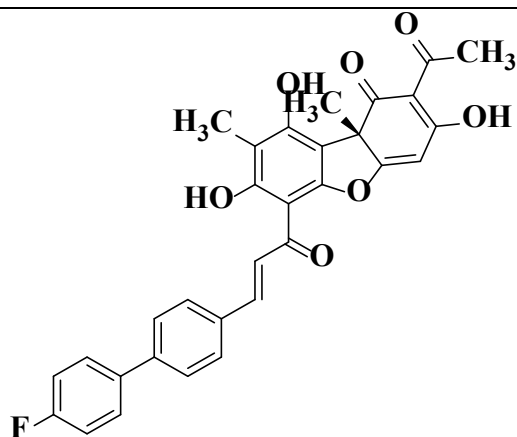
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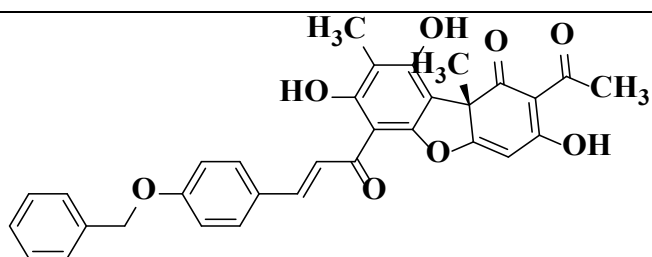
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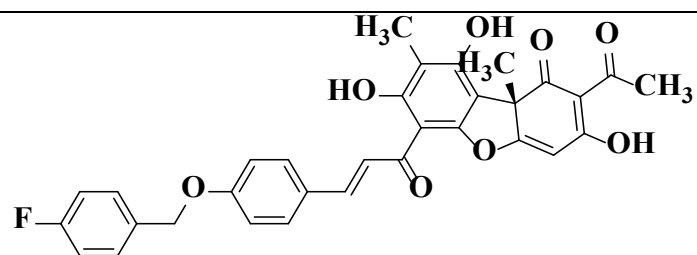
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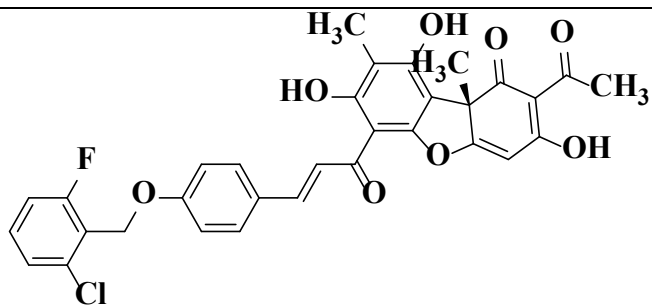
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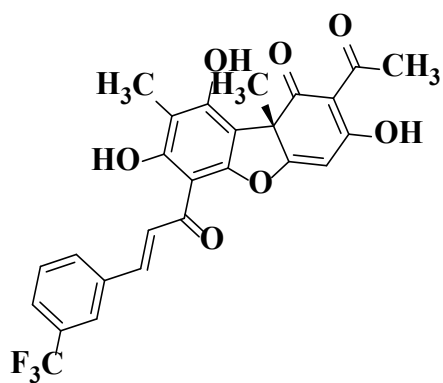
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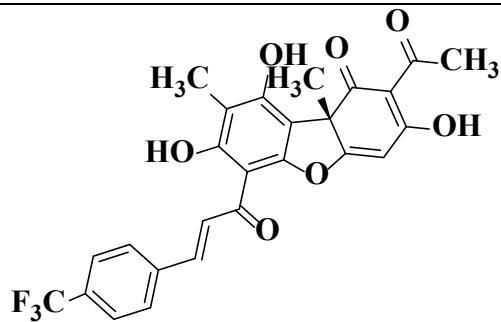
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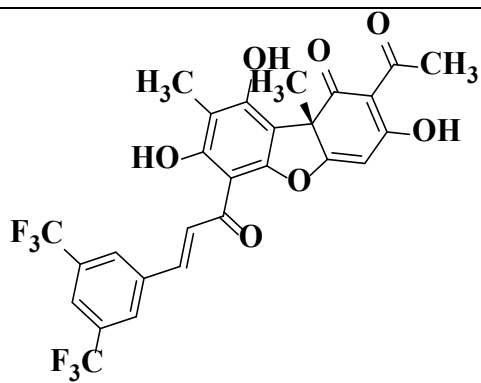
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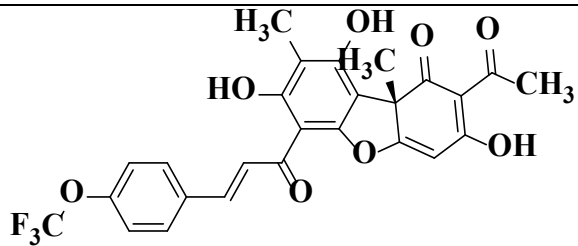
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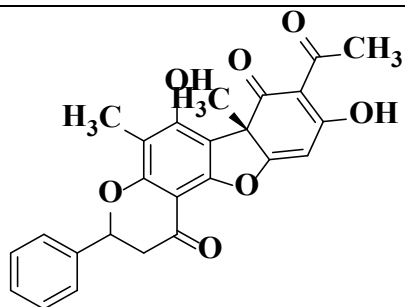
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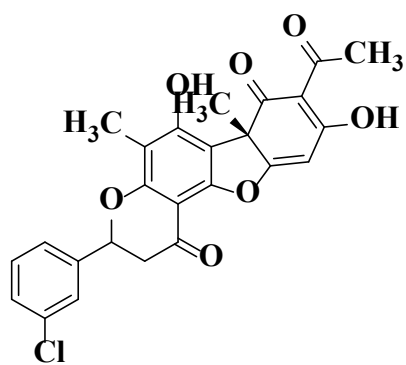
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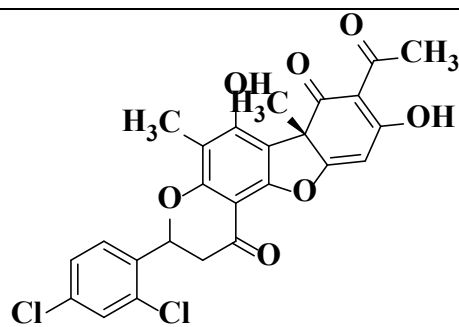
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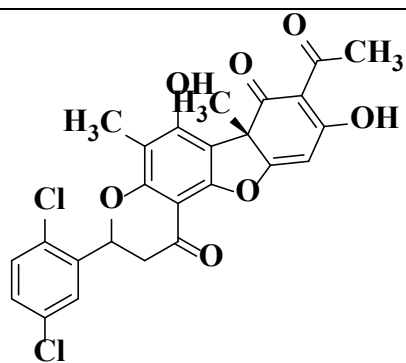
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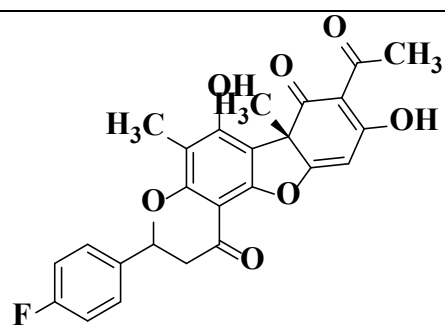
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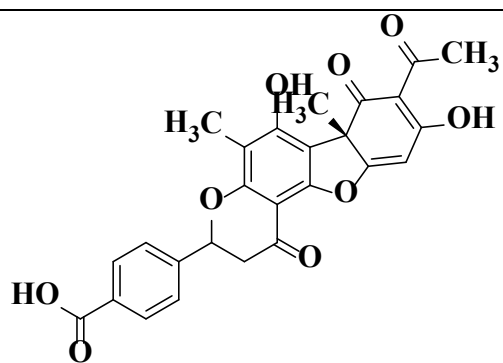
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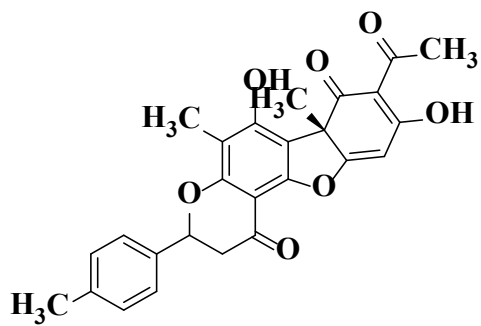
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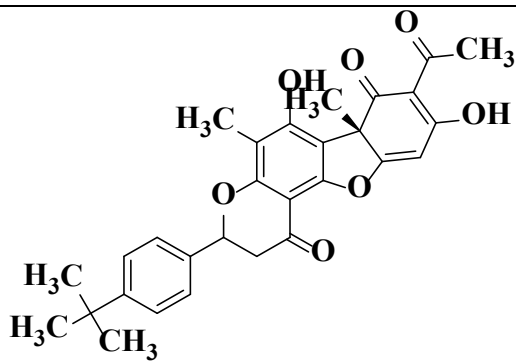
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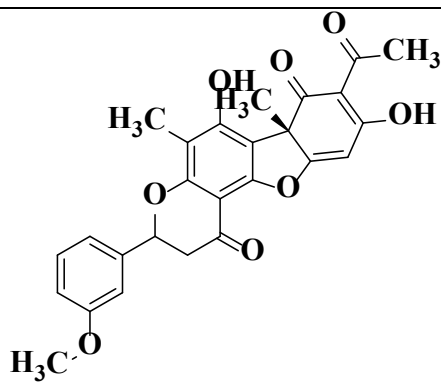
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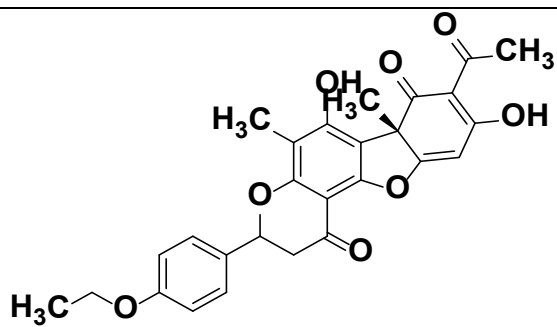
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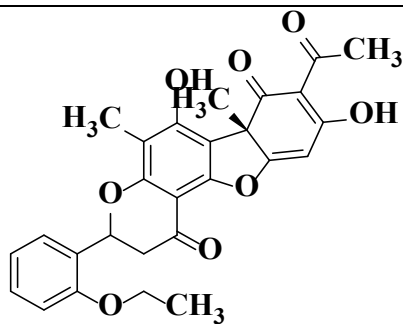
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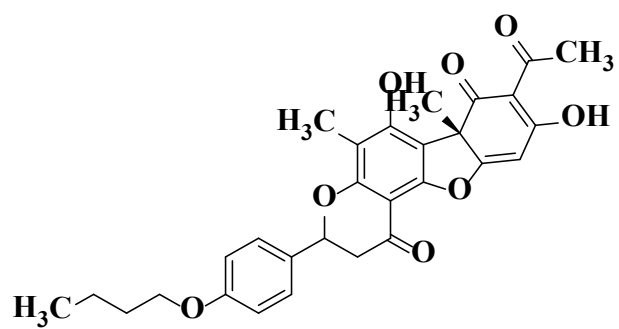
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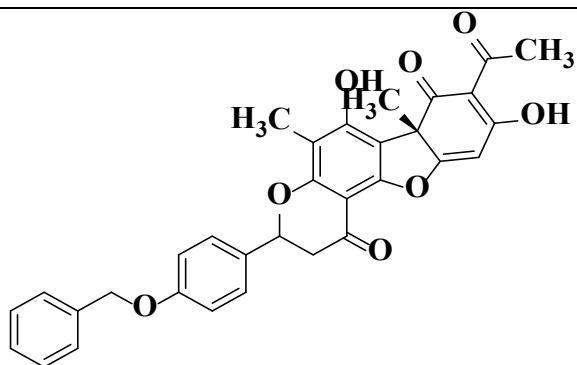
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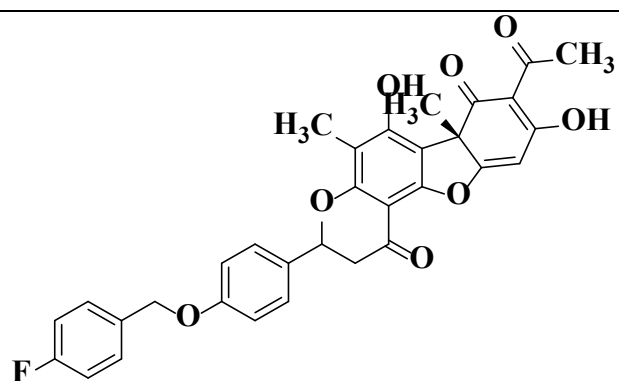
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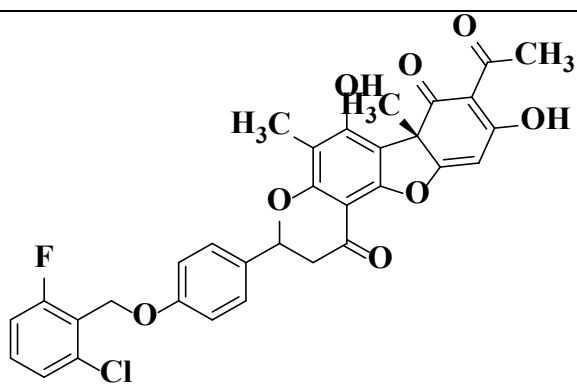
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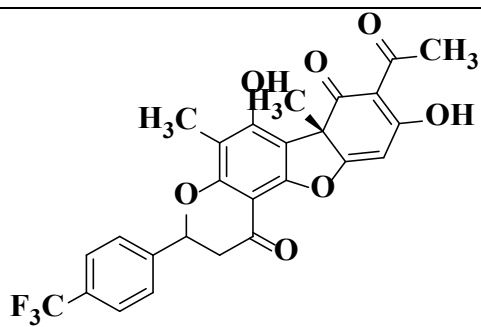
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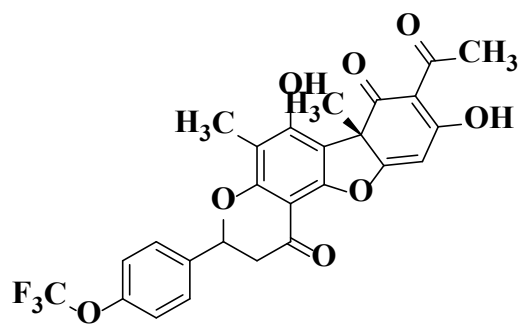
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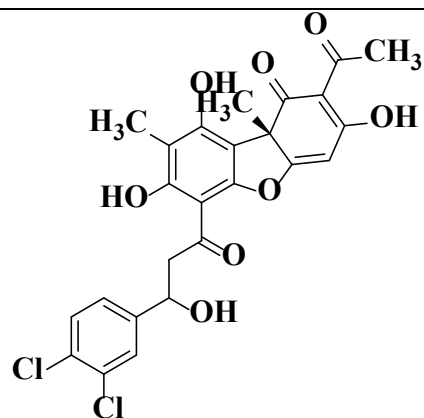
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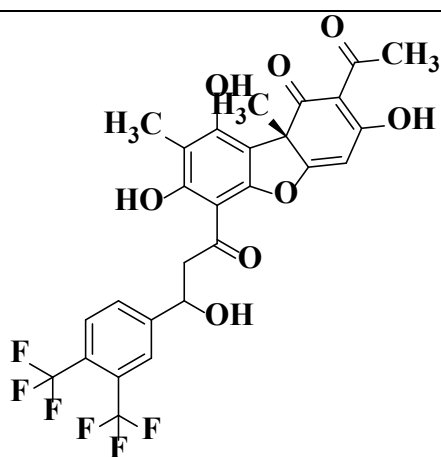
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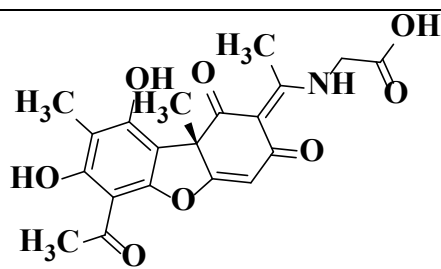
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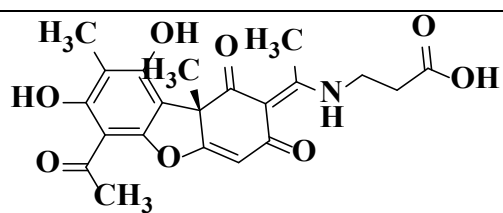
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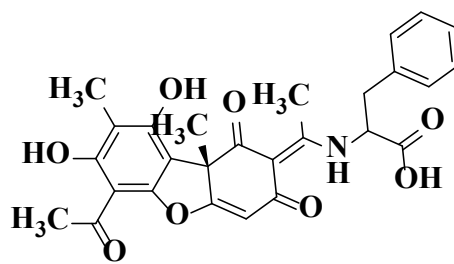
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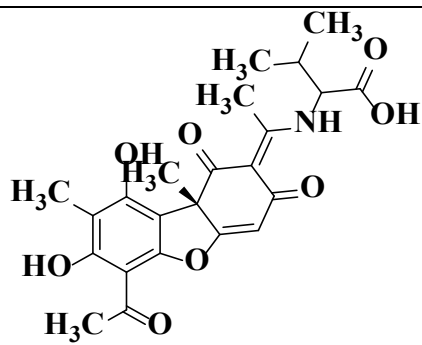
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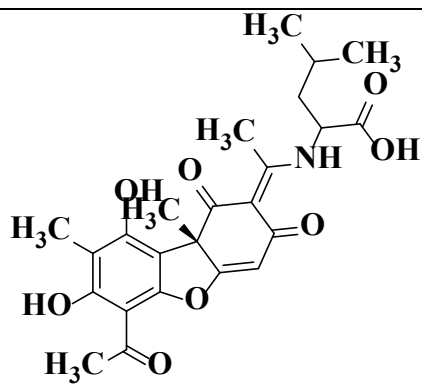
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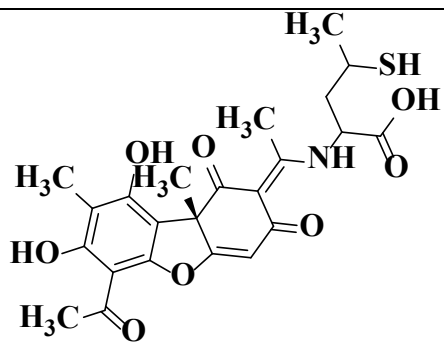
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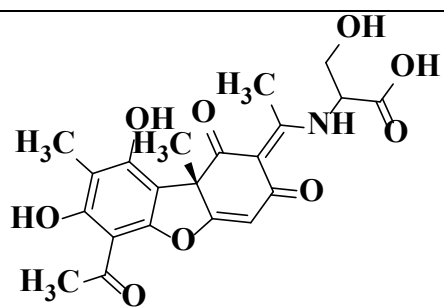
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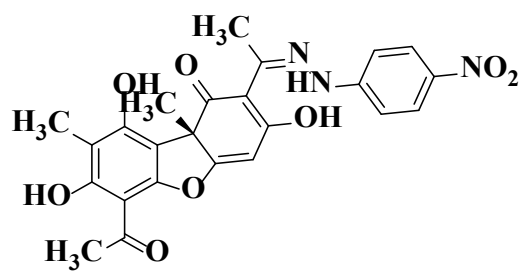
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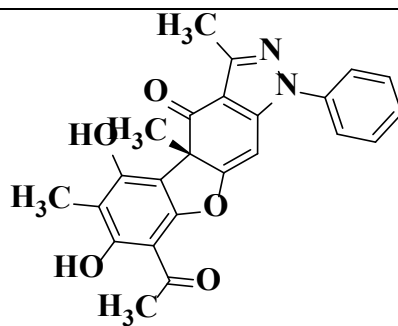
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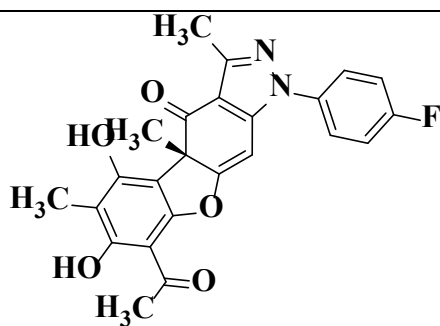
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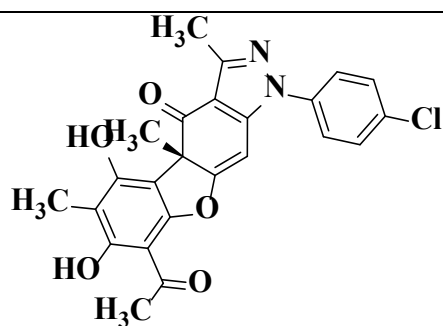
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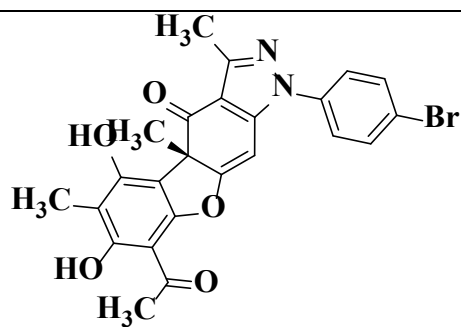
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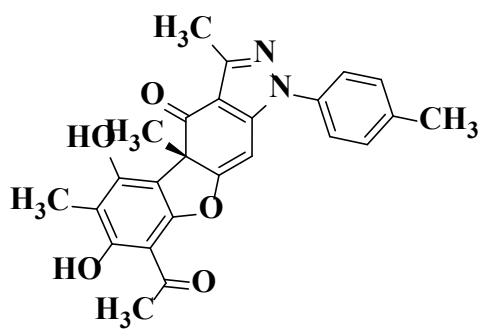
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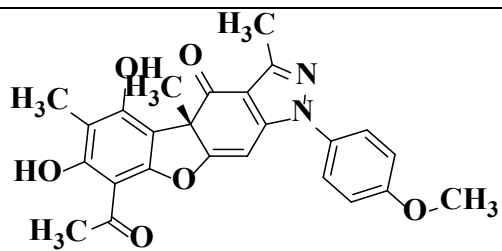
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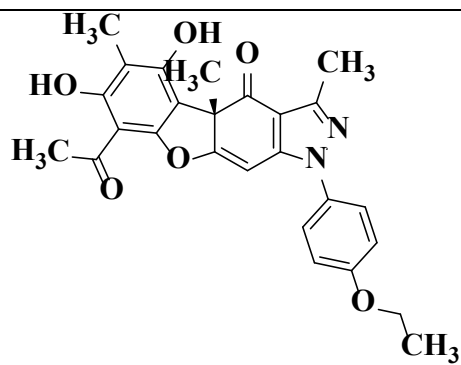
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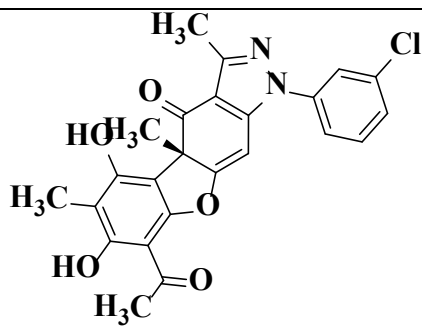
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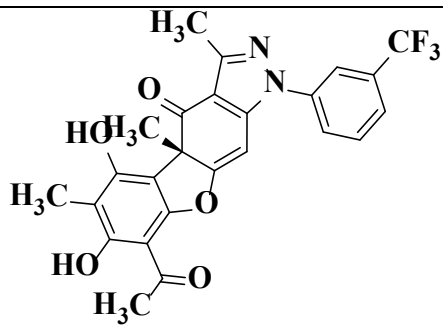
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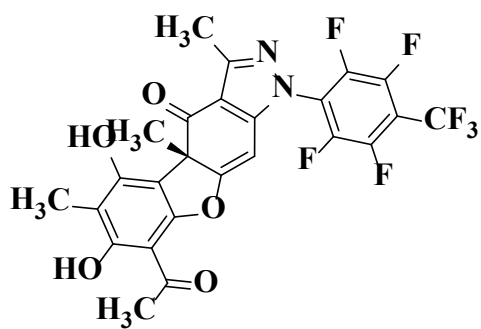
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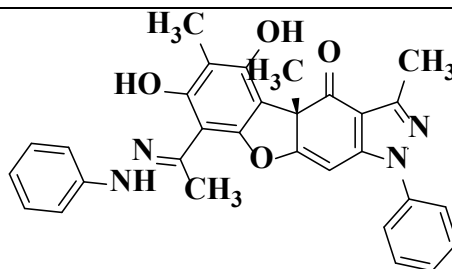
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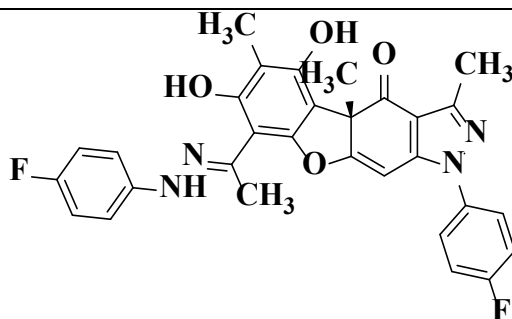
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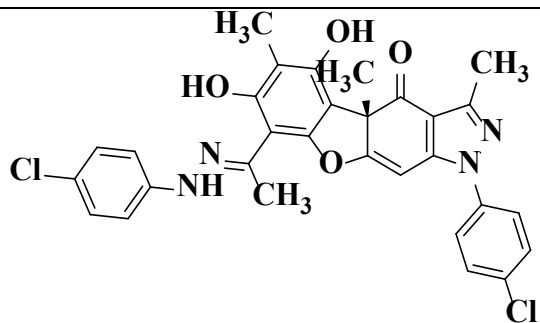
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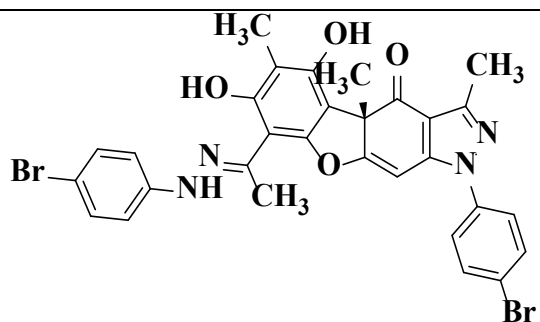
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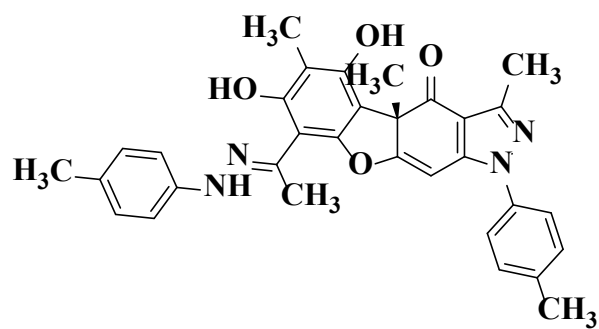
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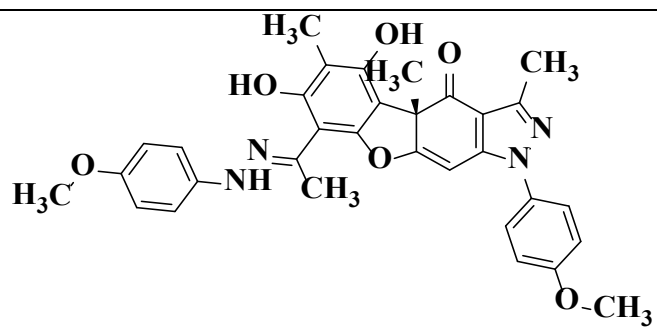
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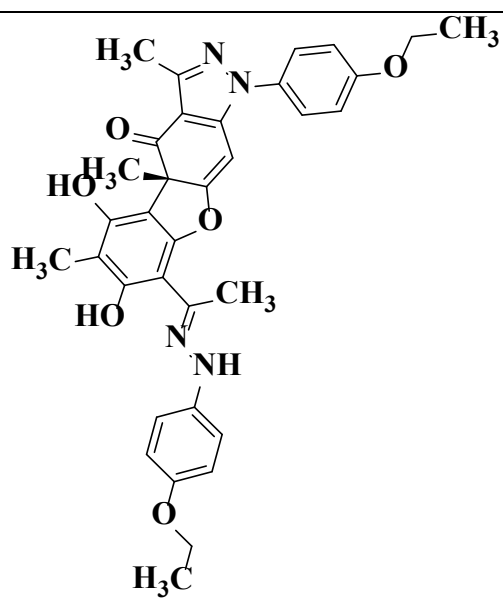
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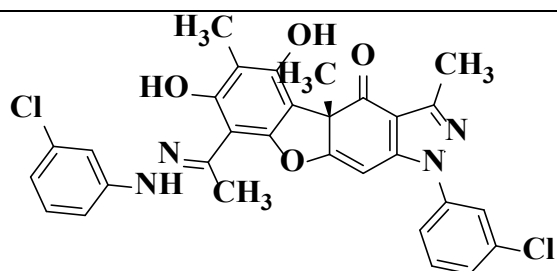
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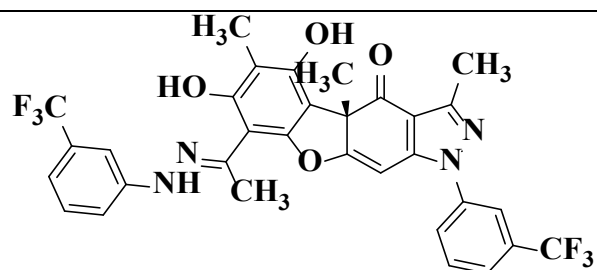
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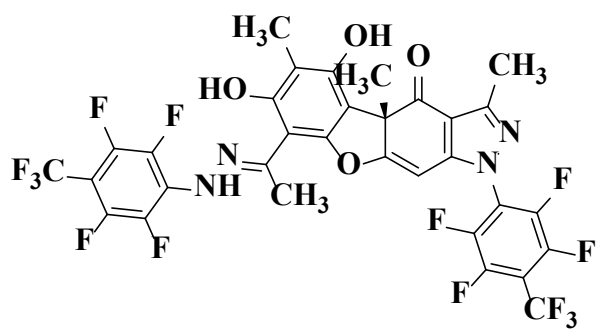
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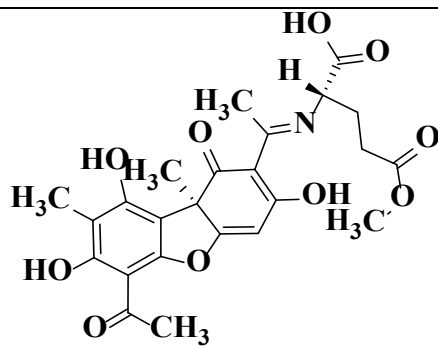
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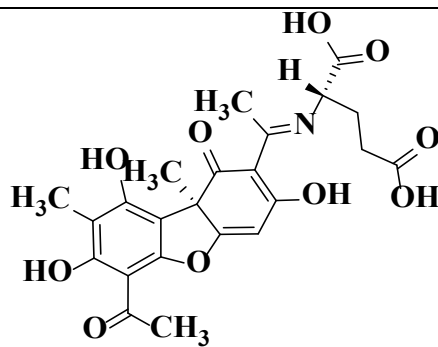
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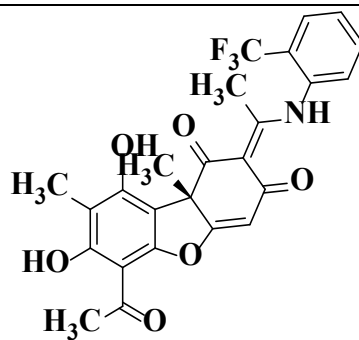
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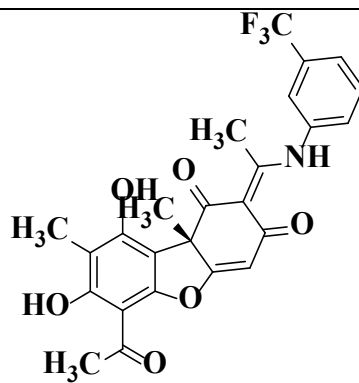
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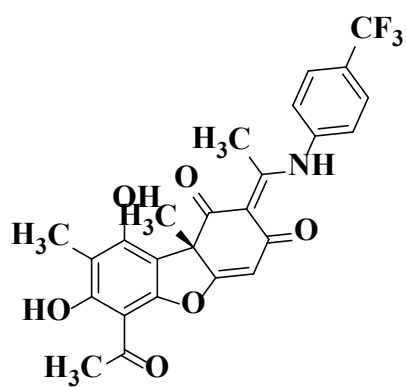
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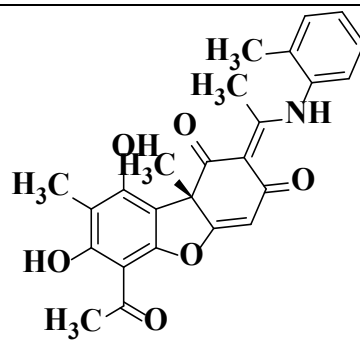
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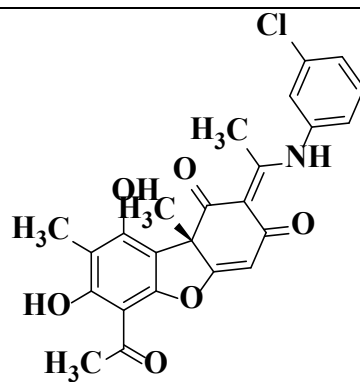
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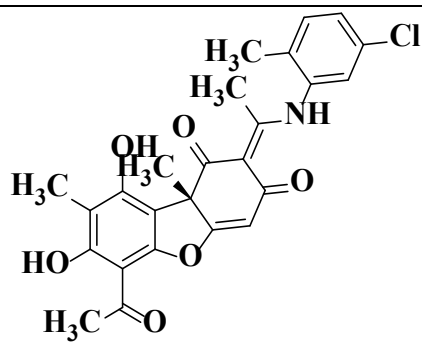
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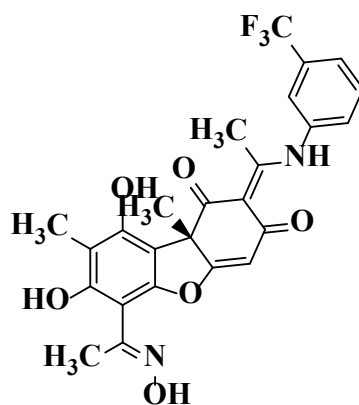
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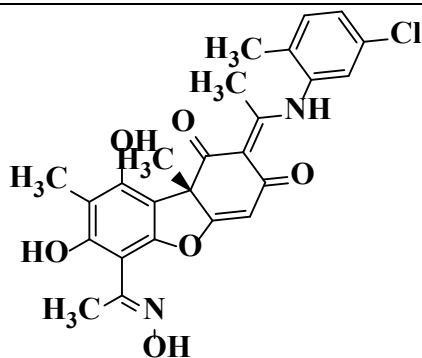
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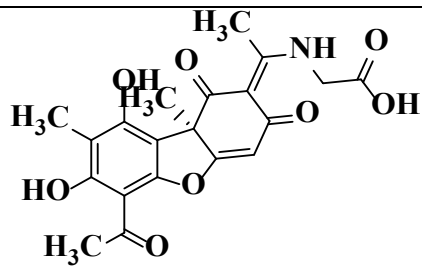
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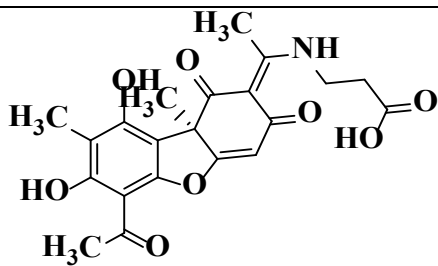
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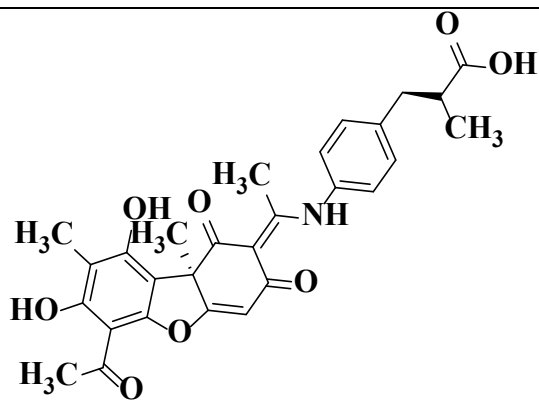
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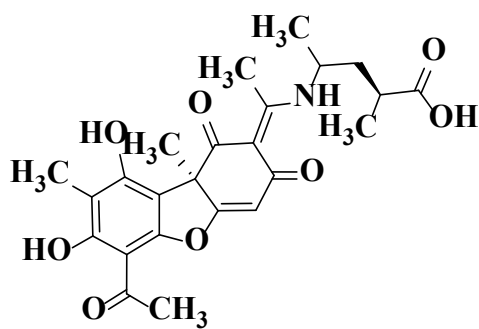
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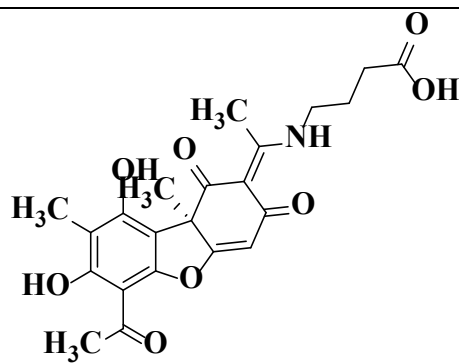
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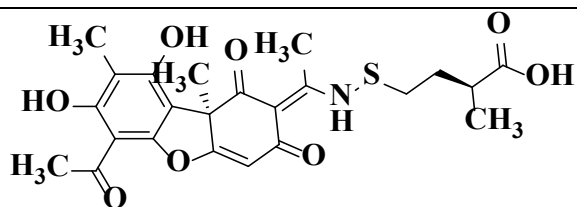
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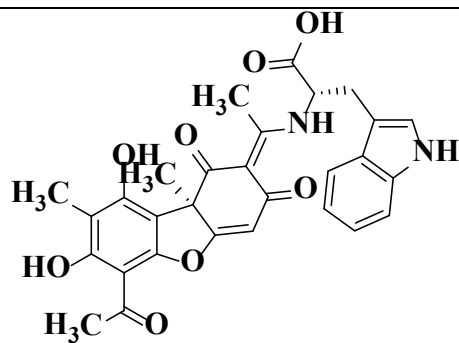
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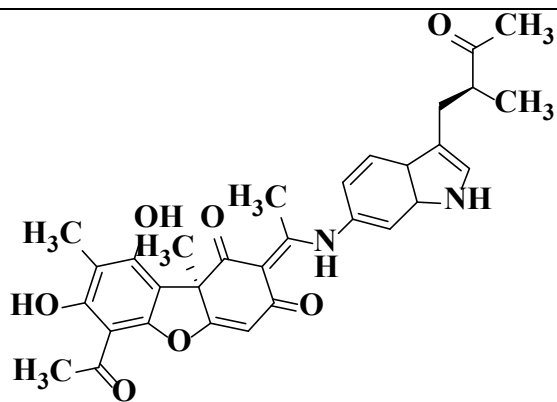
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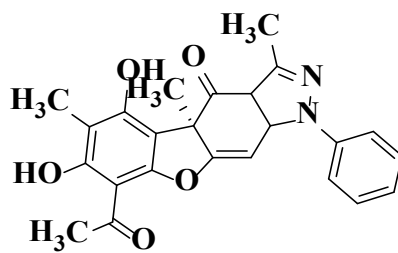
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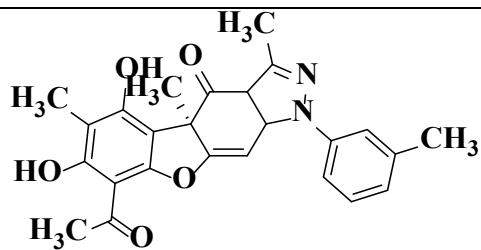
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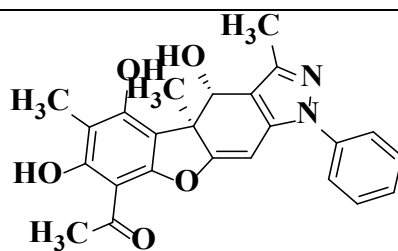
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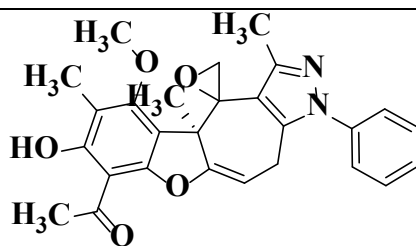
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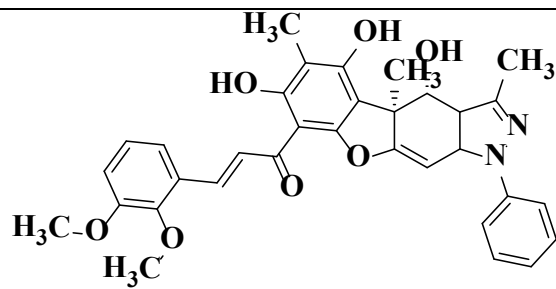
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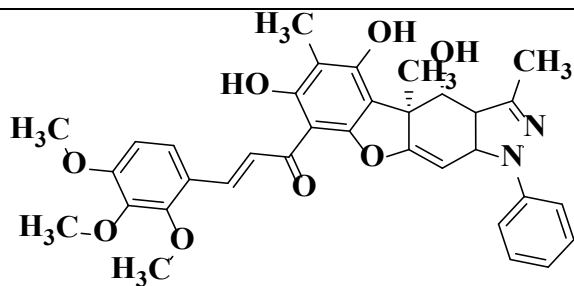
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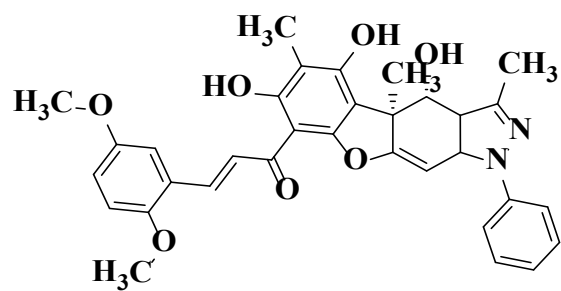
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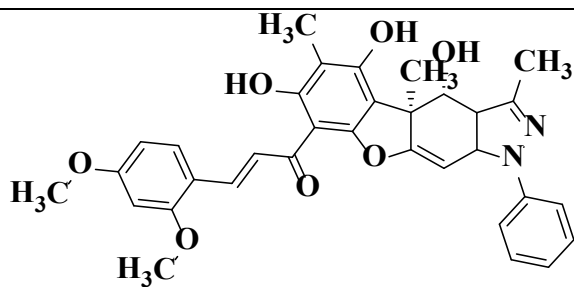
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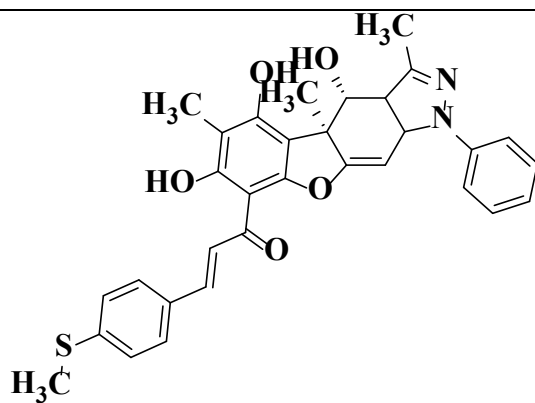
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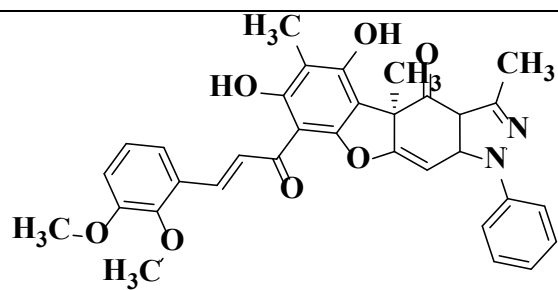
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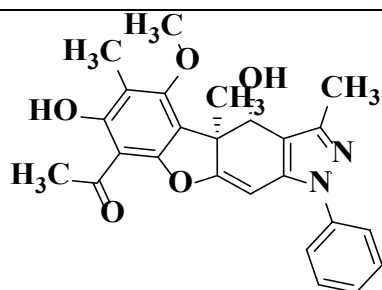
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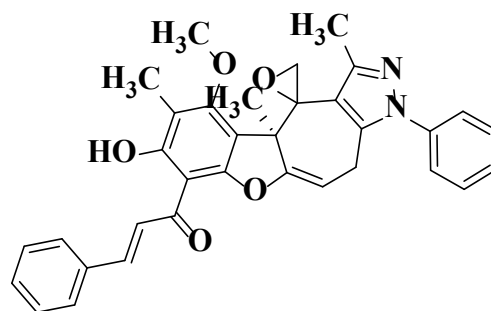
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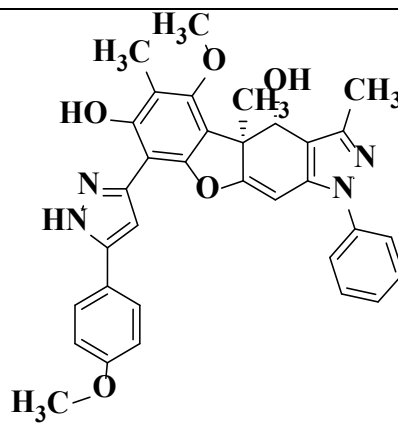
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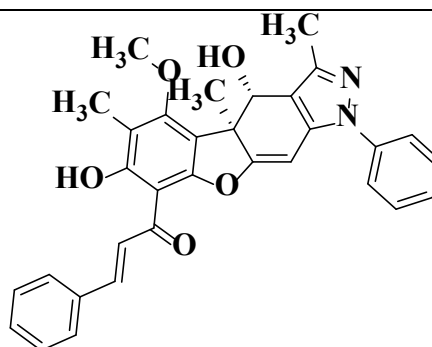
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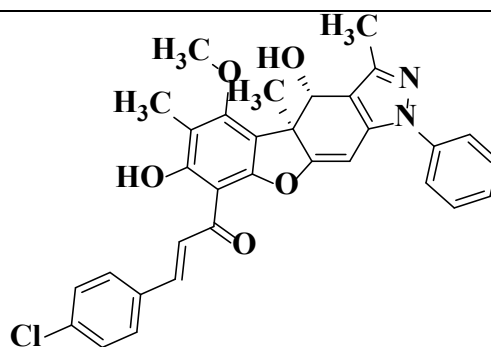
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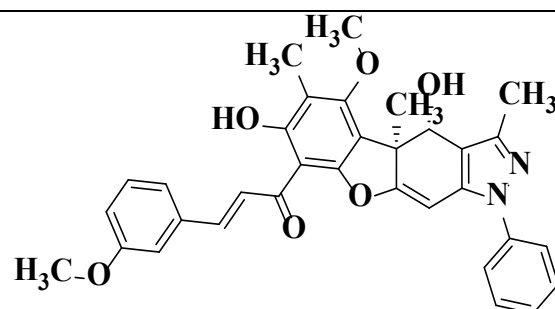
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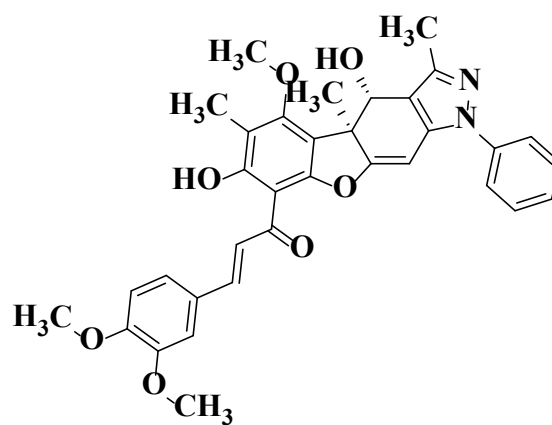
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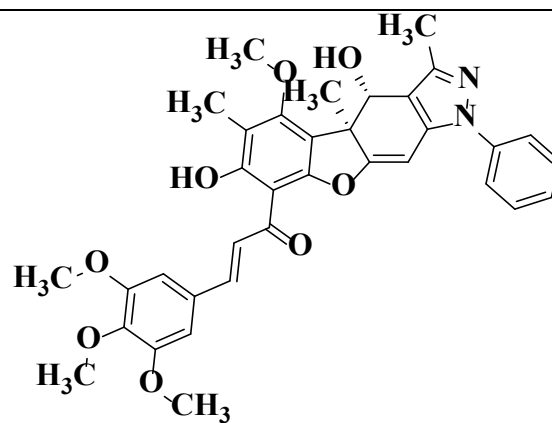
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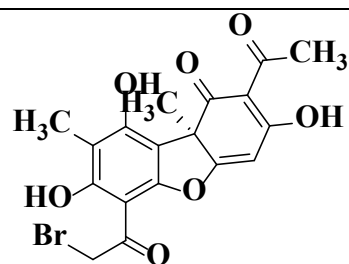
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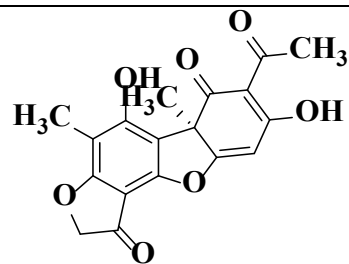
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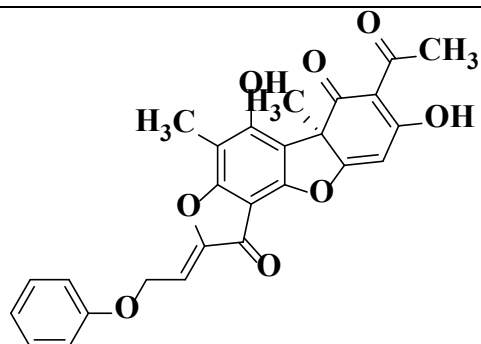
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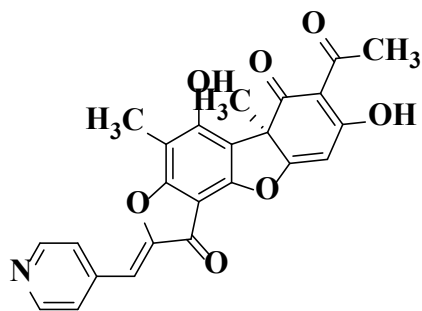
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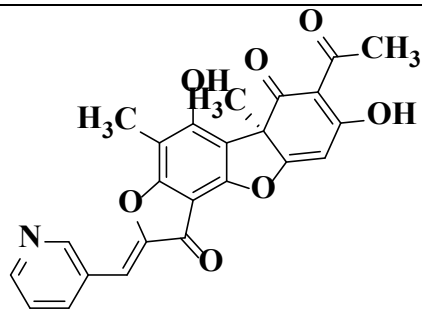
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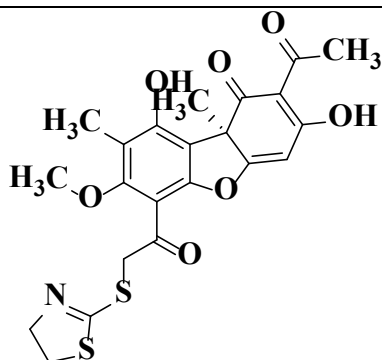
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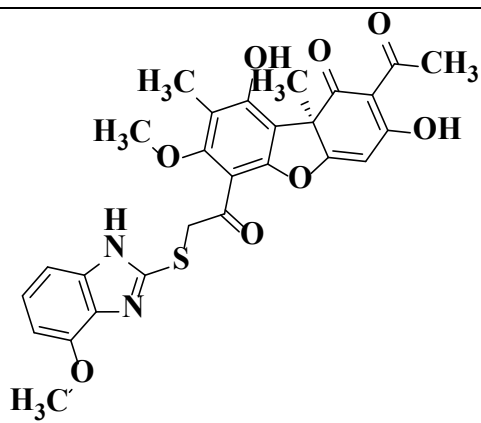
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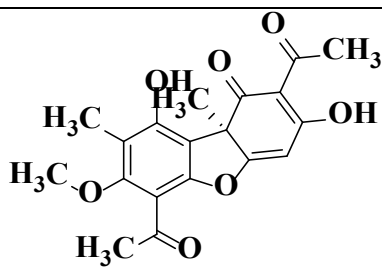
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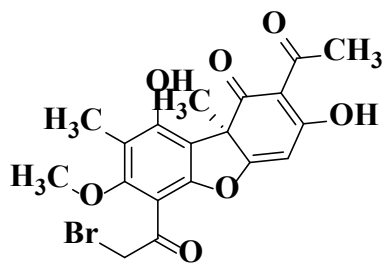
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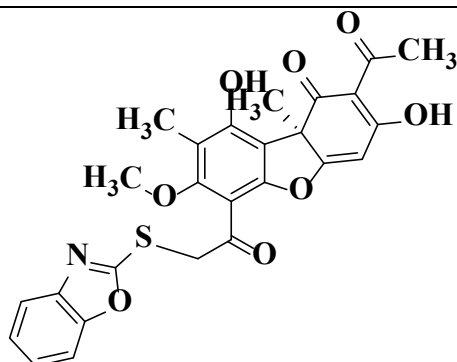
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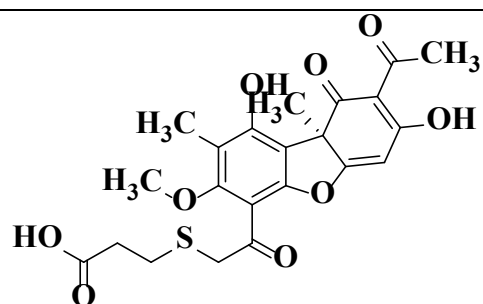
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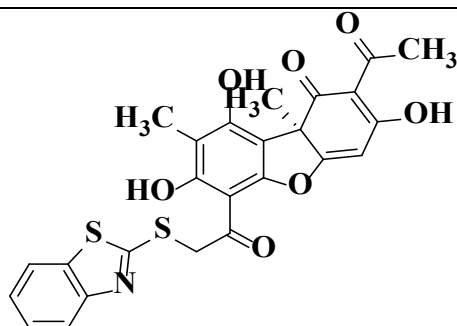
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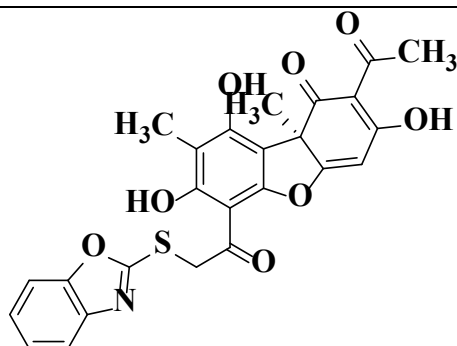
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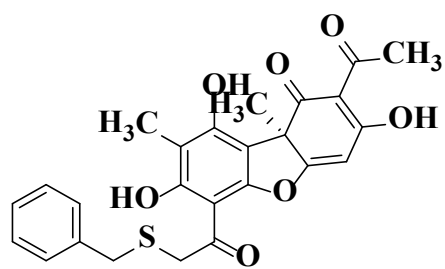
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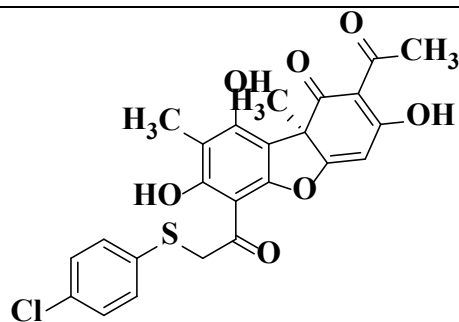
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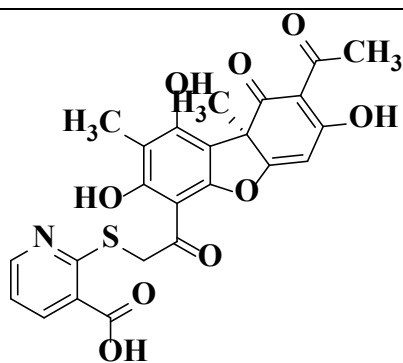
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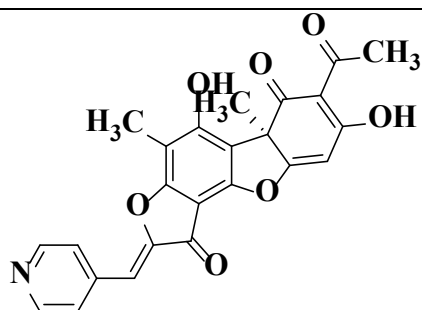
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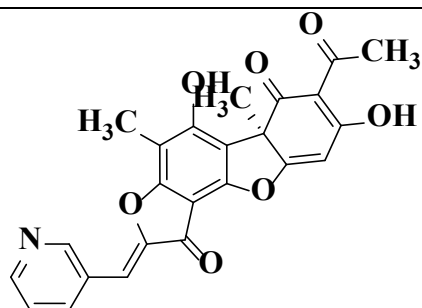
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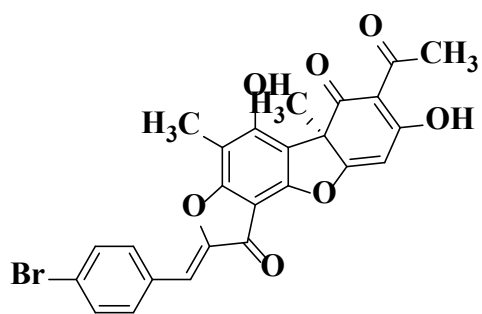
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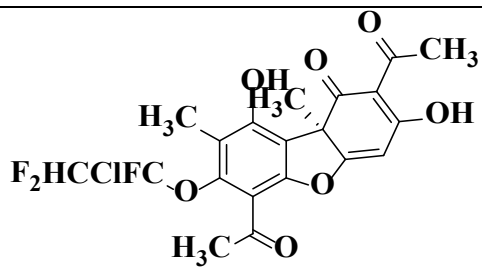
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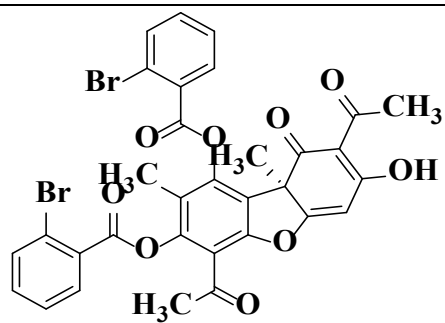
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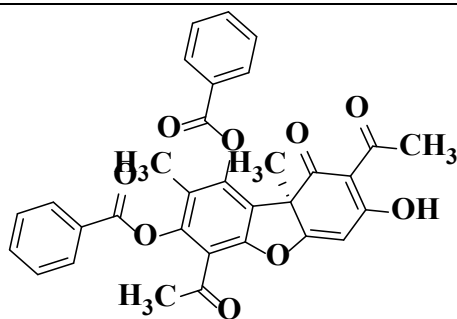
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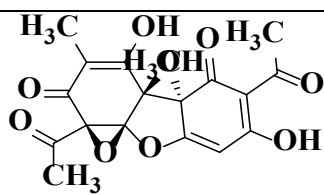
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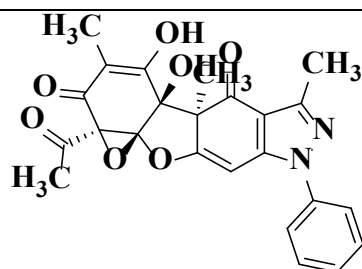
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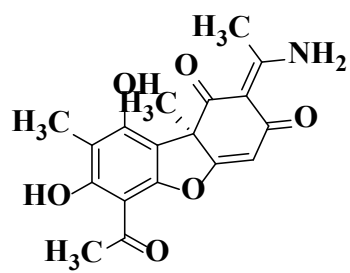
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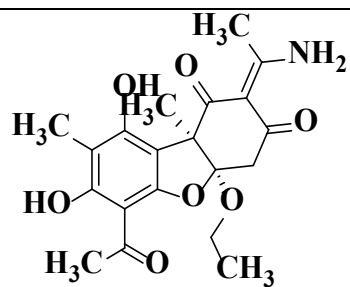
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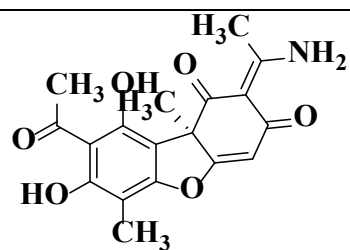
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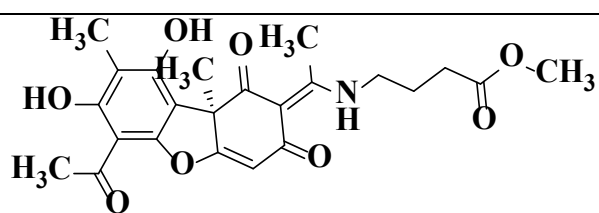
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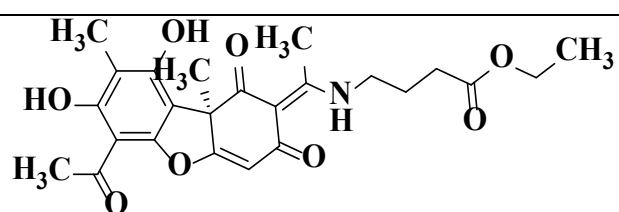
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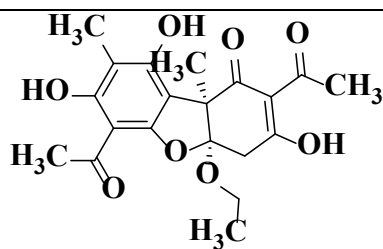
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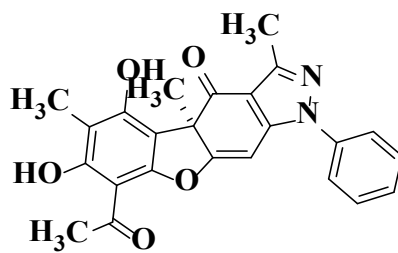
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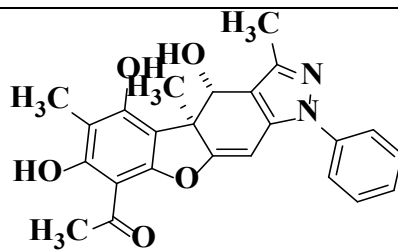
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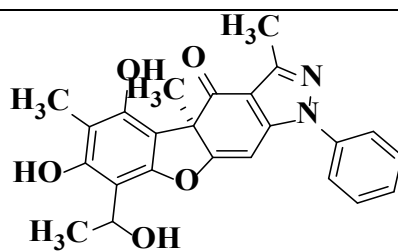
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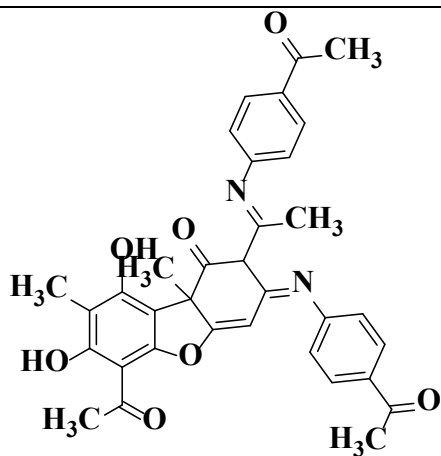
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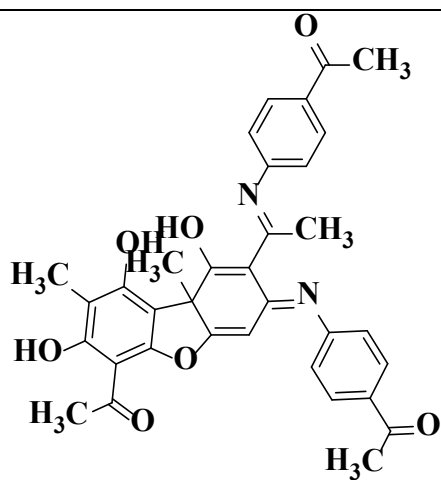
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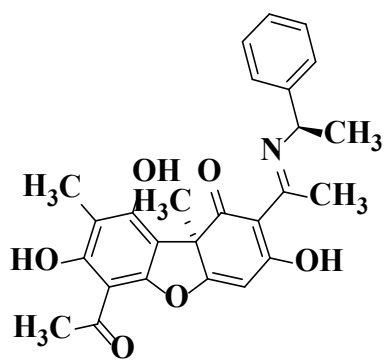
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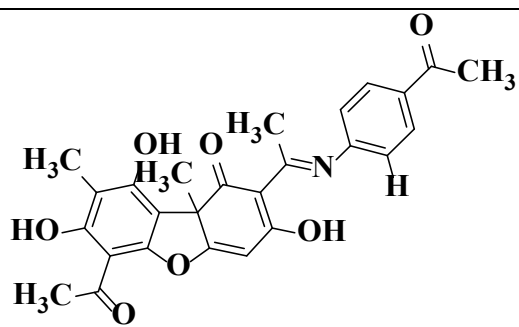
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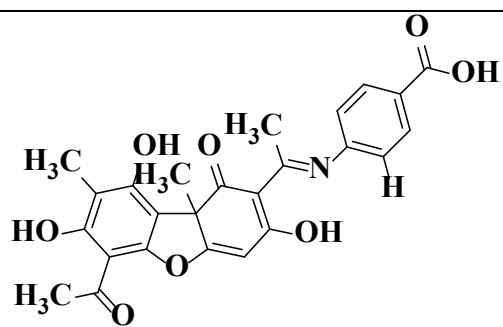
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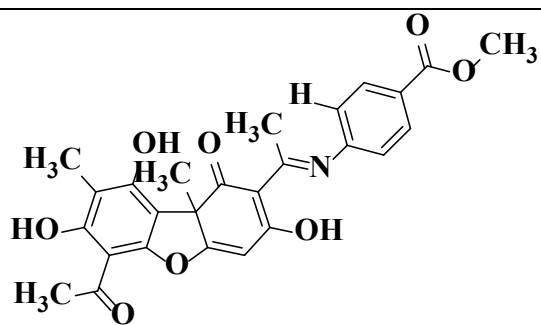
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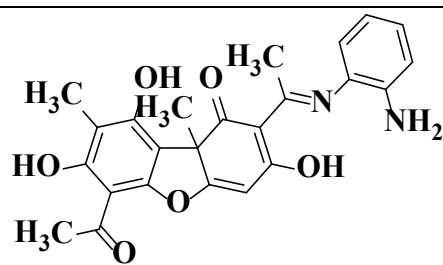
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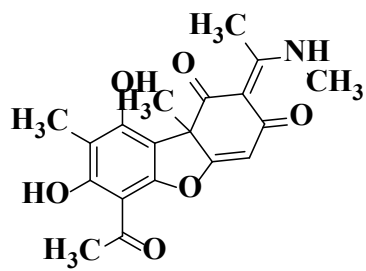
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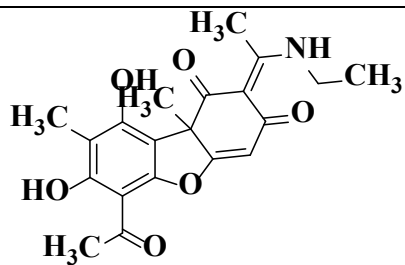
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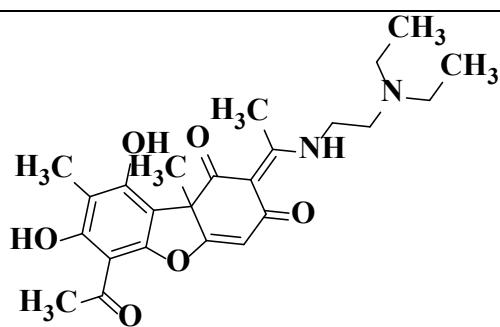
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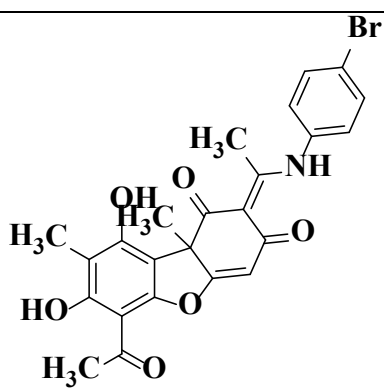
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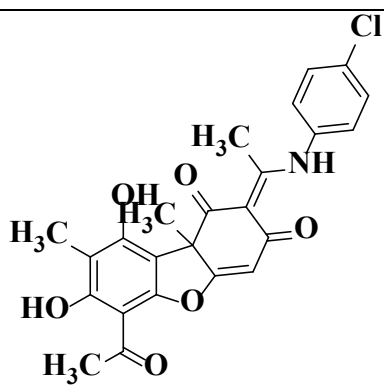
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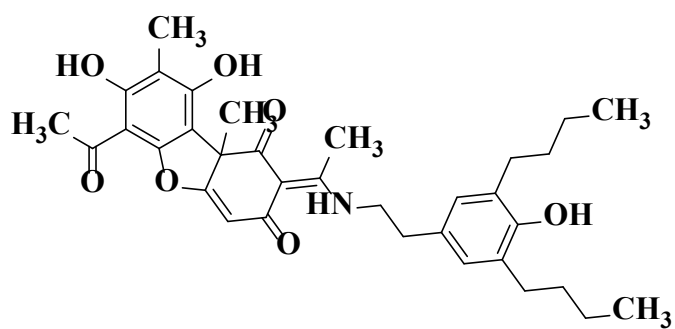
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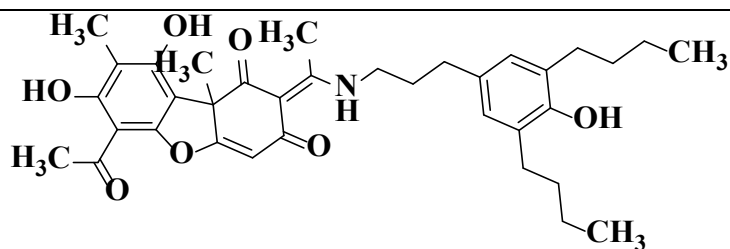
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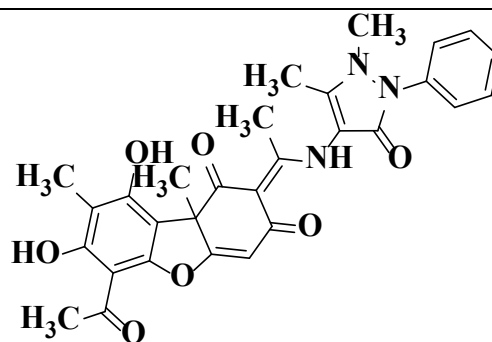
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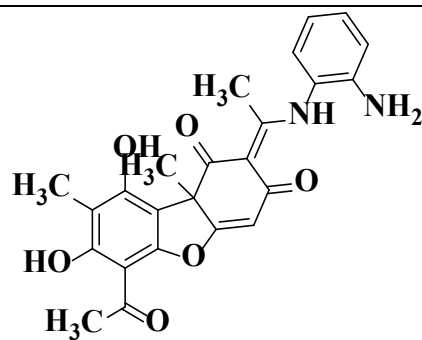
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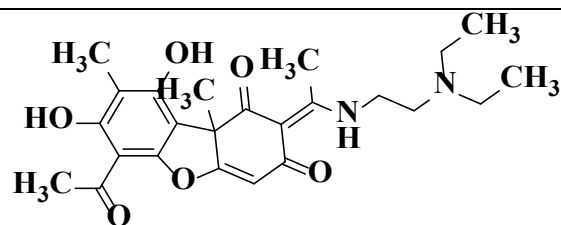
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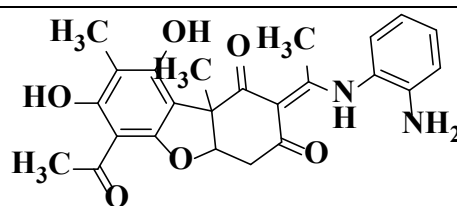
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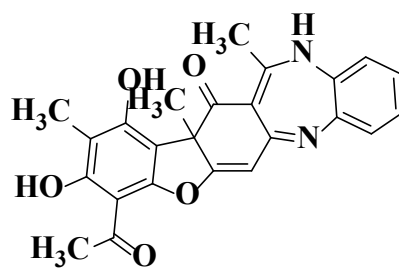
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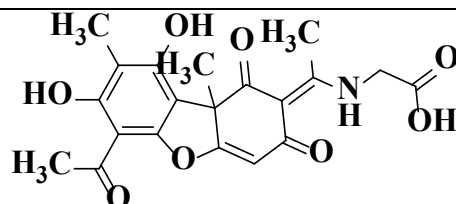
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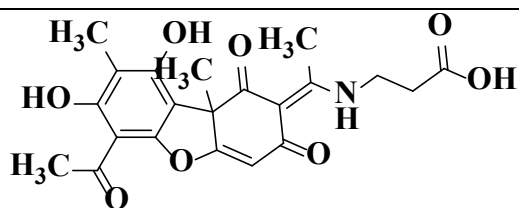
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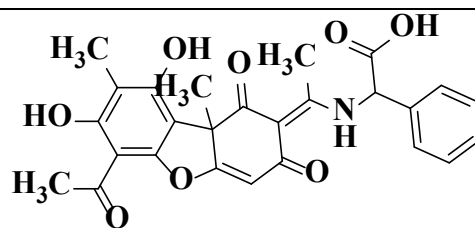
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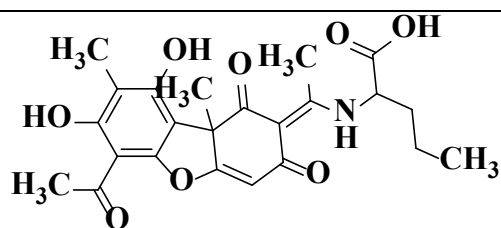
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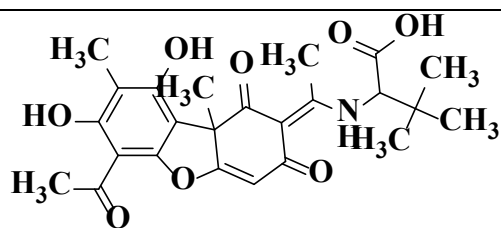
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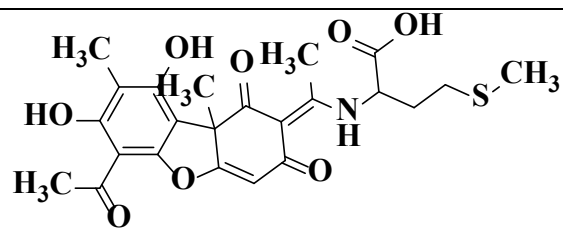
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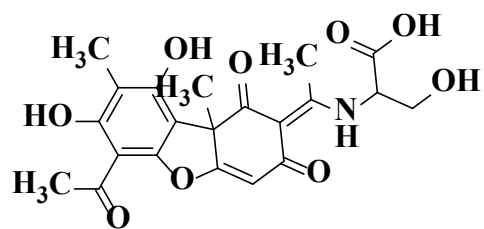
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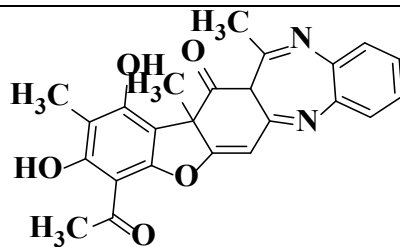
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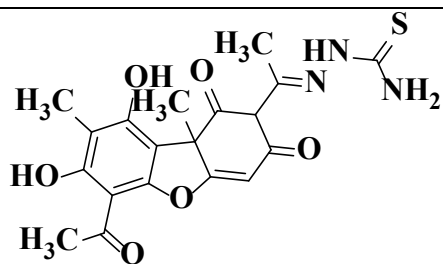
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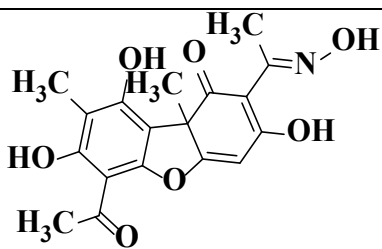
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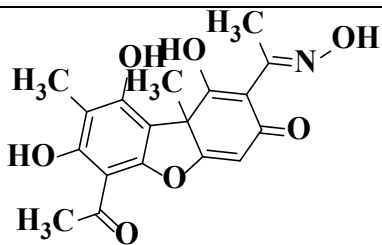
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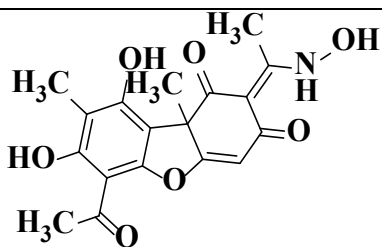
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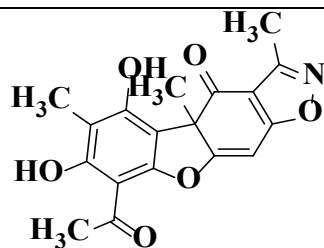
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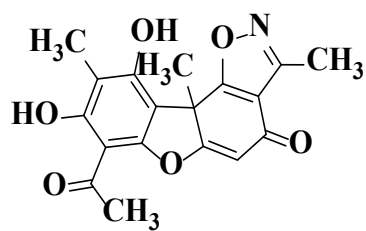
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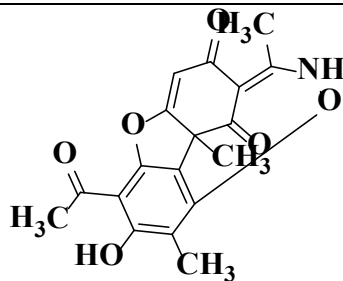
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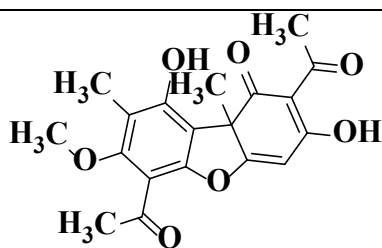
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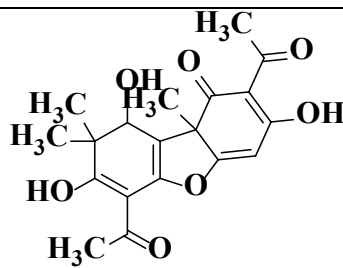
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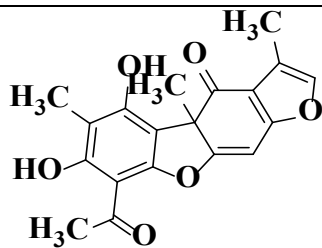
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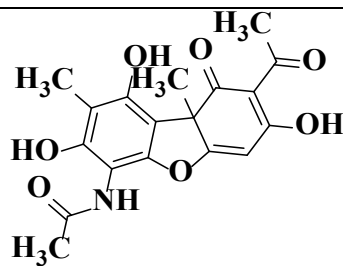
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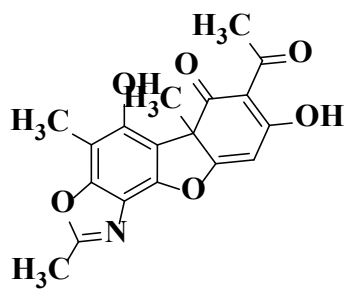
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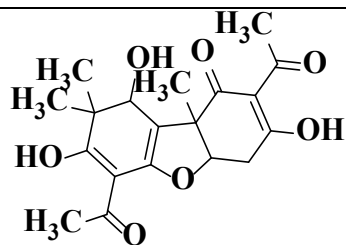
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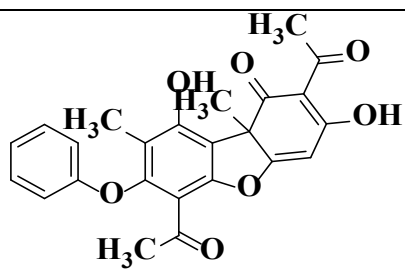
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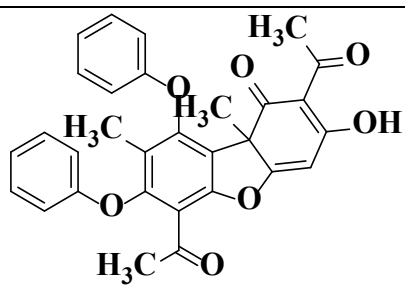
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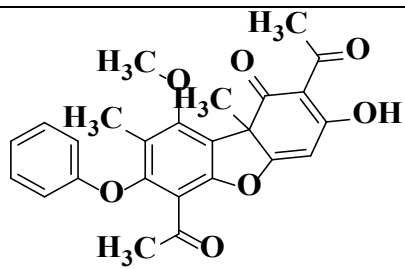
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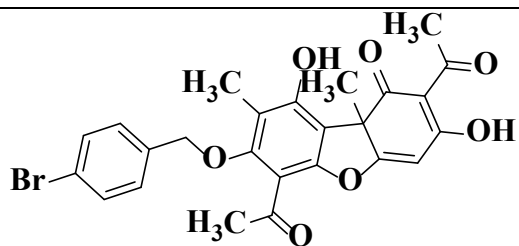
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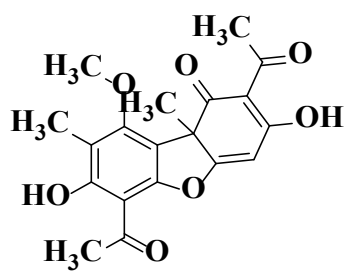
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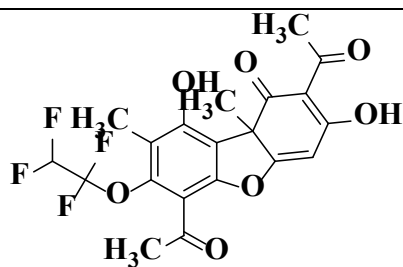
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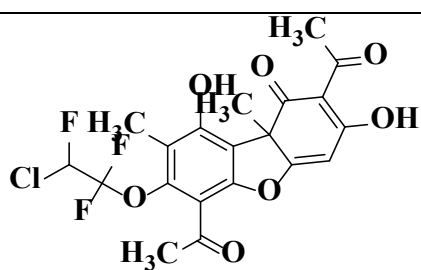
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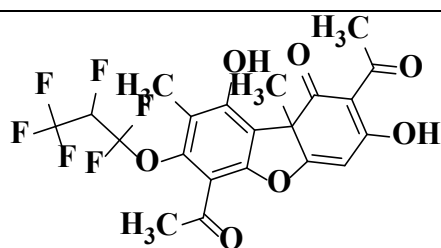
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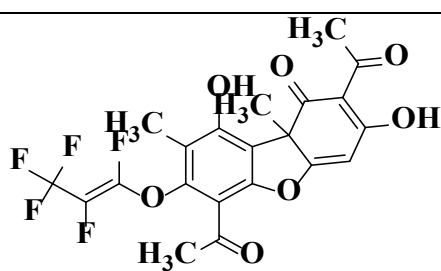
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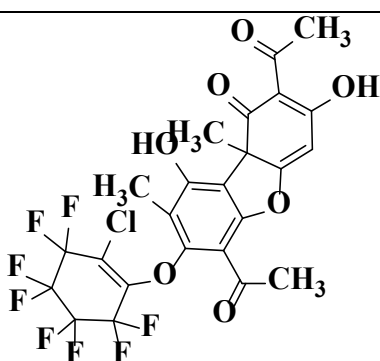
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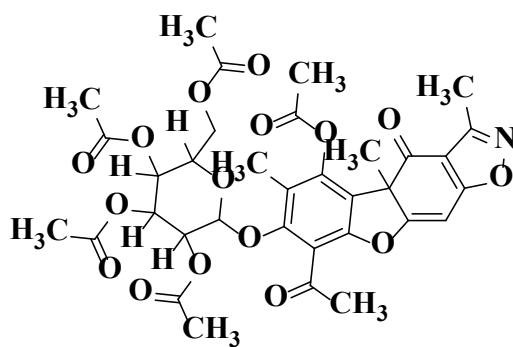


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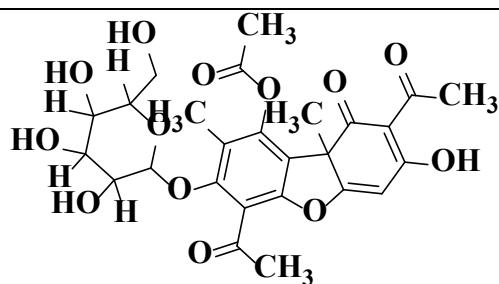


CC(=O)c1cc(O)c2c(c1)oc3c(O)c(C(F)(F)F)c(Cl)c(Cl)c3C(=O)c2CCOC1=C(C)C(=C2C(=C1)OC(=O)C2=CC=C3C(=C(C)C)N(C)C3=O)C(=O)CCc1cc(O)c2c(c1)oc3c2C(=O)C(C)(C)C(=O)C3(C)CCC(=O)OC1=C(C)C(=C(C(=O)O)C(=C1C2=C(C)C(=C(C(=O)O)C=C2)OC3=C(C)C(=O)N=C3)OCC(=O)c1cc2c(c1)c3c(c2)oc(=O)c4c3c(N)cc(=O)c4OC[C@H]5C[C@@H](O)[C@H](O)[C@@H](O)[C@H]5O

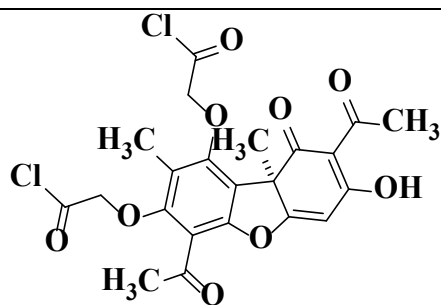
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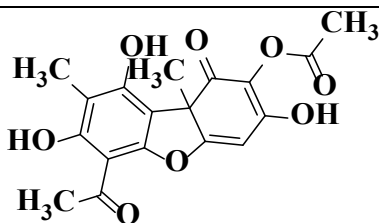
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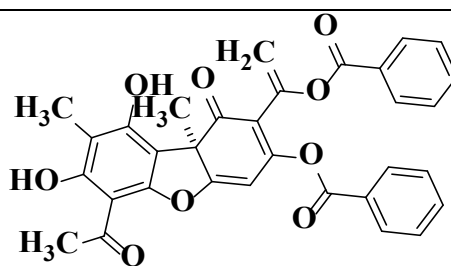
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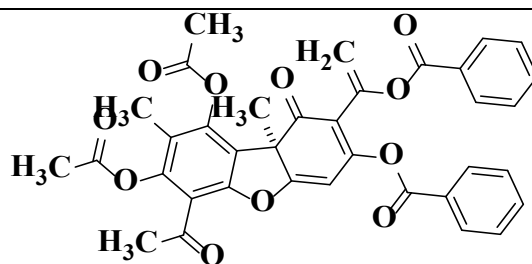
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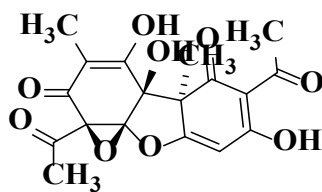
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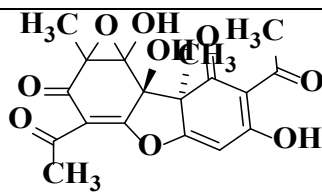
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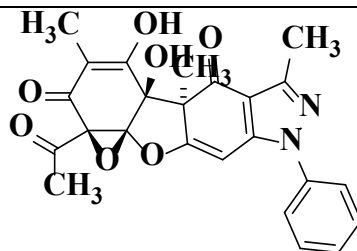
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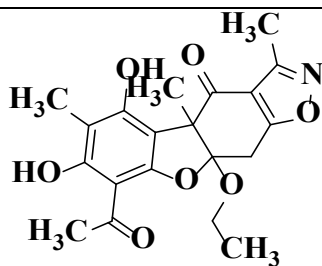
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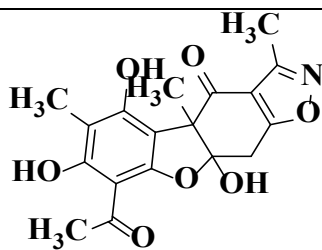
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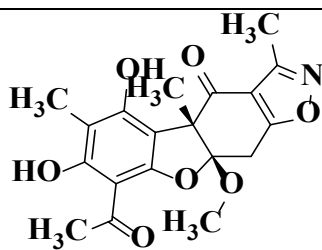
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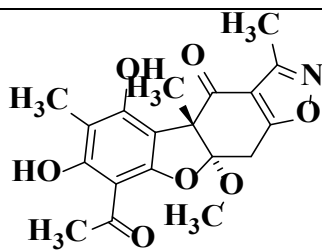
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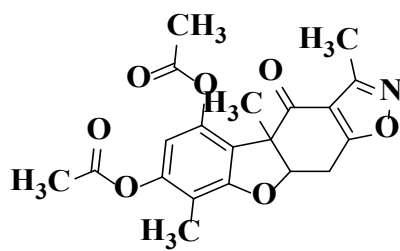
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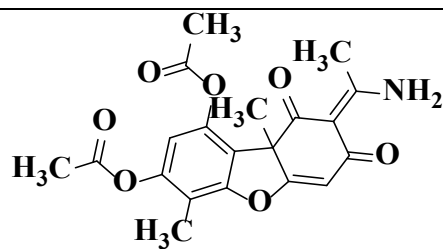
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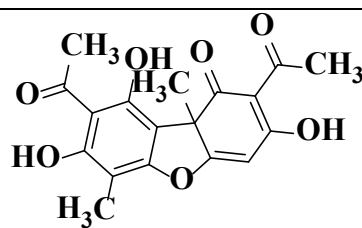
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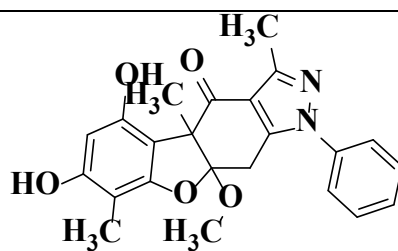
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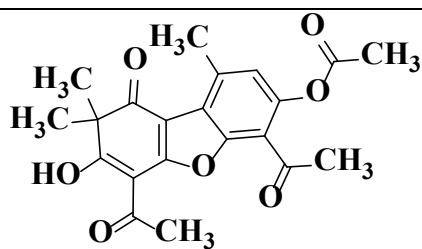
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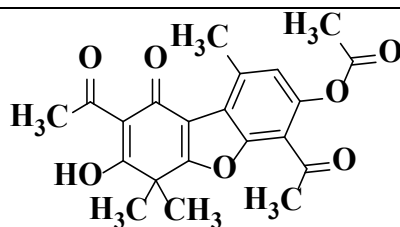
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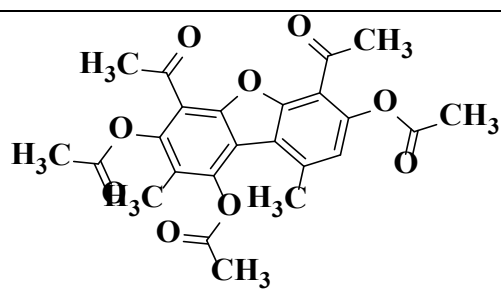
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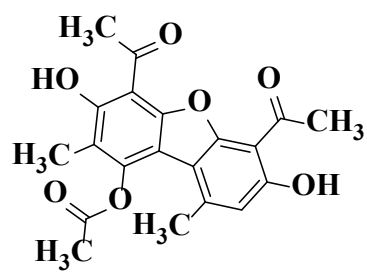
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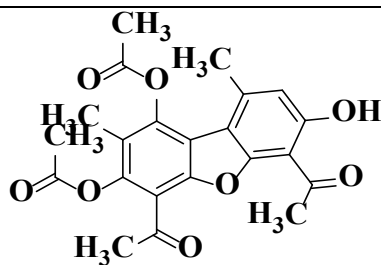
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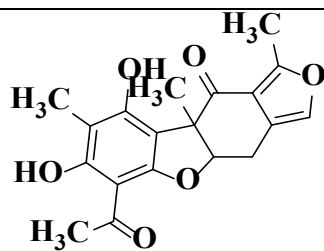
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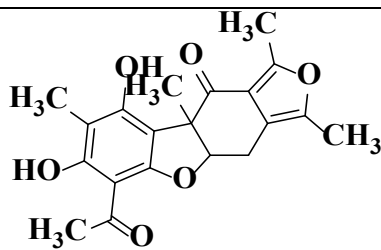
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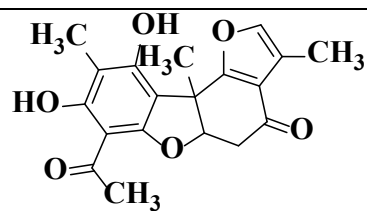
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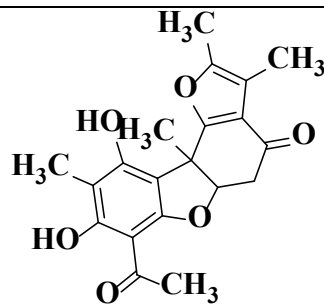
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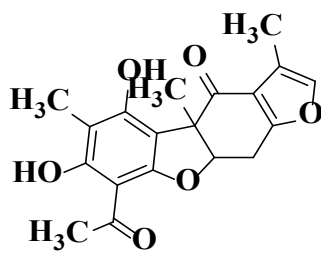
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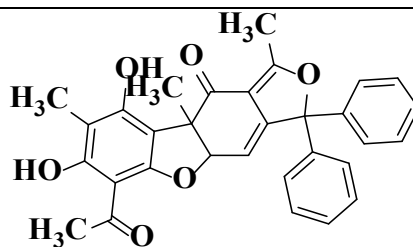
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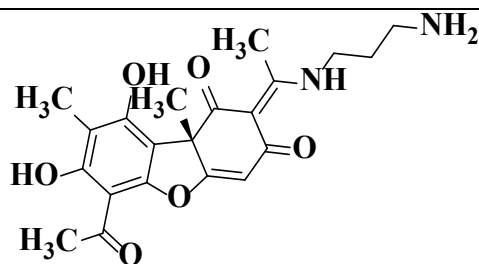
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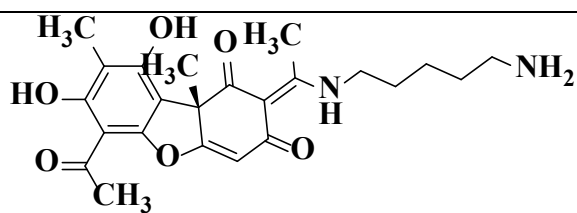
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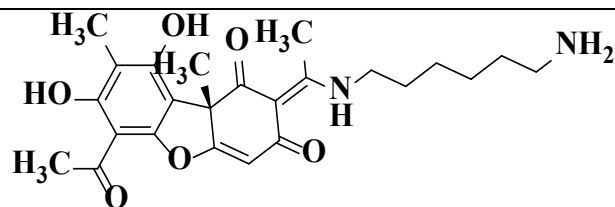
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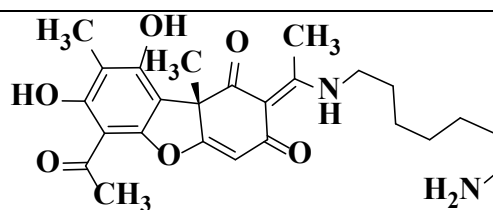
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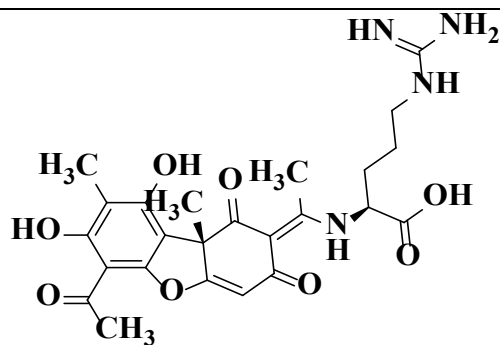
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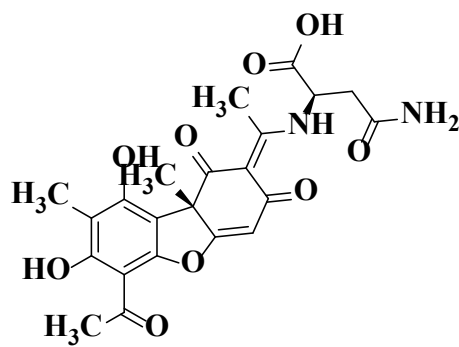
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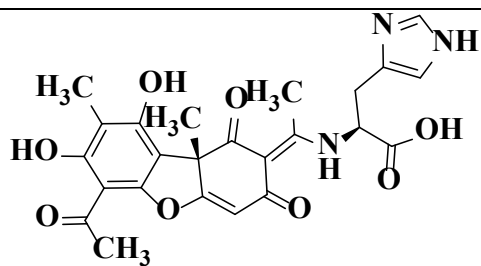
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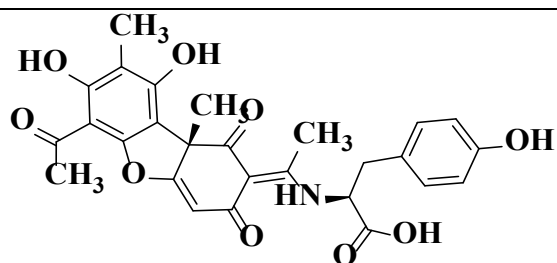
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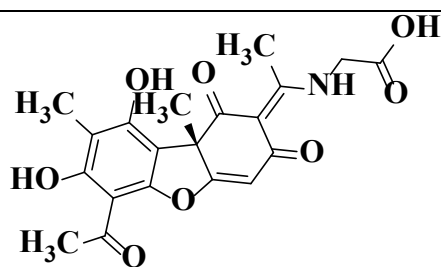
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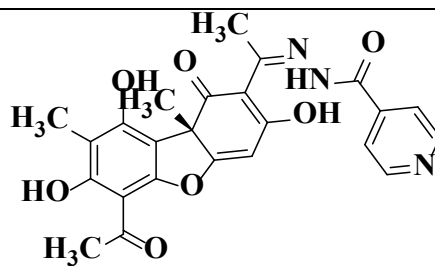
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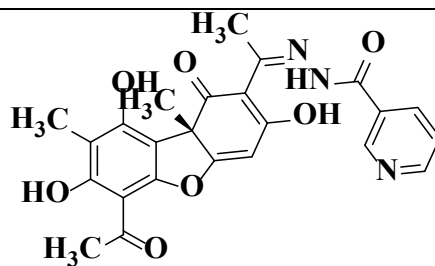
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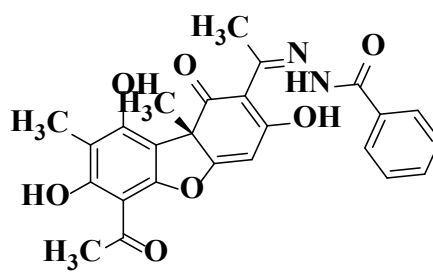
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338



339



340

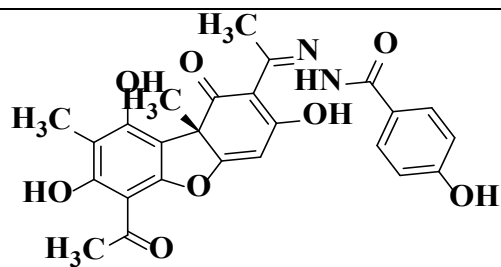


Table S2. Pharmacophore Filtering

Compound Number	Fit Value (>3.30)
3	3.51587
5	3.34017
219	3.55323
305	3.69827
215	3.45441
301	3.56383
29	3.72617
140	3.57668
70	3.46804
139	3.54672
214	3.33978
78	3.90888
300	3.56301
87	3.45912
193	3.62649
299	3.47006
110	3.34021
198	3.33202
204	3.35229
225	3.59074
256	3.44933

Table S3. Molecular Docking Result

Compound Number	CDOCKER Interaction Energy (kcal/mol)	Amino Acid Residues
Co-crystallized ligand	-48.2195	Arg119, Glu120, Glu278, Arg372, Glu279, Ile224, Arg226
3	-57.1741	Arg119, Asp152, Arg226, Ile150, Ile429, Pro433
5	-49.9863	Glu229, Glu278, Arg372, Arg226, Asp152, Glu279, Arg153, Trp180, Ile224
29	-48.6009	Glu120, Arg153, Asn348, Ile150, Asn347, Arg119, Arg372, Ile224, Ala248
70	-52.187	Arg153, Arg372, Tyr406, Leu135
78	-52.1765	Ile150, Asp152, Ser181, Glu229, Arg226, Pro433, Arg153, Ile224
87	-52.0339	Arg119, Asp152, Arg153, Ser181, Glu229, Lys294, Arg372, Arg226, Trp180, Asp152, Glu279, Trp180, Ile224
110	-49.8924	Arg119, Arg153, Arg372, Arg226
139	-56.9771	Arg119, Ser181, Glu229, Arg372, Glu279, Pro433
140	-54.5009	Arg119, Ser181, Glu278, Lys294, Asn348, Arg372, Lys434, Arg372, Glu279, Pro433
193	-55.4167	Ile150, Asp152, Arg119, Arg372, Ile224, Ala248, Ile429, Pro433
198	-46.8648	Asn348, Arg372, Asn347, Arg119, Arg153, Arg226, Ala248, Pro433
204	-54.4001	Asn348, Arg372, Lys434, Ala370, Asp152, Arg153, Ile224, Ala248, Pro433
214	-50.8905	Arg119, Glu120, Asp152, Arg153, Lys294, Glu278, Glu279, Ala248, Tyr406

215	-41.7198	Glu120, Arg153, Glu229, Lys294, Asn296, Arg372, Tyr406, Ile224, Ala248
219	-44.7888	Asp152, Arg153, Ser181, Glu229, Asn296, Arg372, Ile224
225	-51.4035	Arg119, Arg153, Trp180, Glu229, Arg372, Ser181, Asp152, Ile224, Ala248, Pro433
256	-42.0317	Arg153, Arg372, Asp152, Arg226, Ala248
299	-51.2603	Arg119, Arg153, Trp180, Glu229, Arg372, Asn348, Gly349, Asp152
300	-62.0523	Arg153, Arg226, Lys294, Asp152, Arg226, Arg119, Pro433
301	-52.9625	Arg119, Arg153, Trp180, Glu229, Asn347, Arg372, Ser181, Asn296, Asn348, Asp152
305	-54.2907	Asn348, Arg372, Lys434, Arg153, Ala248

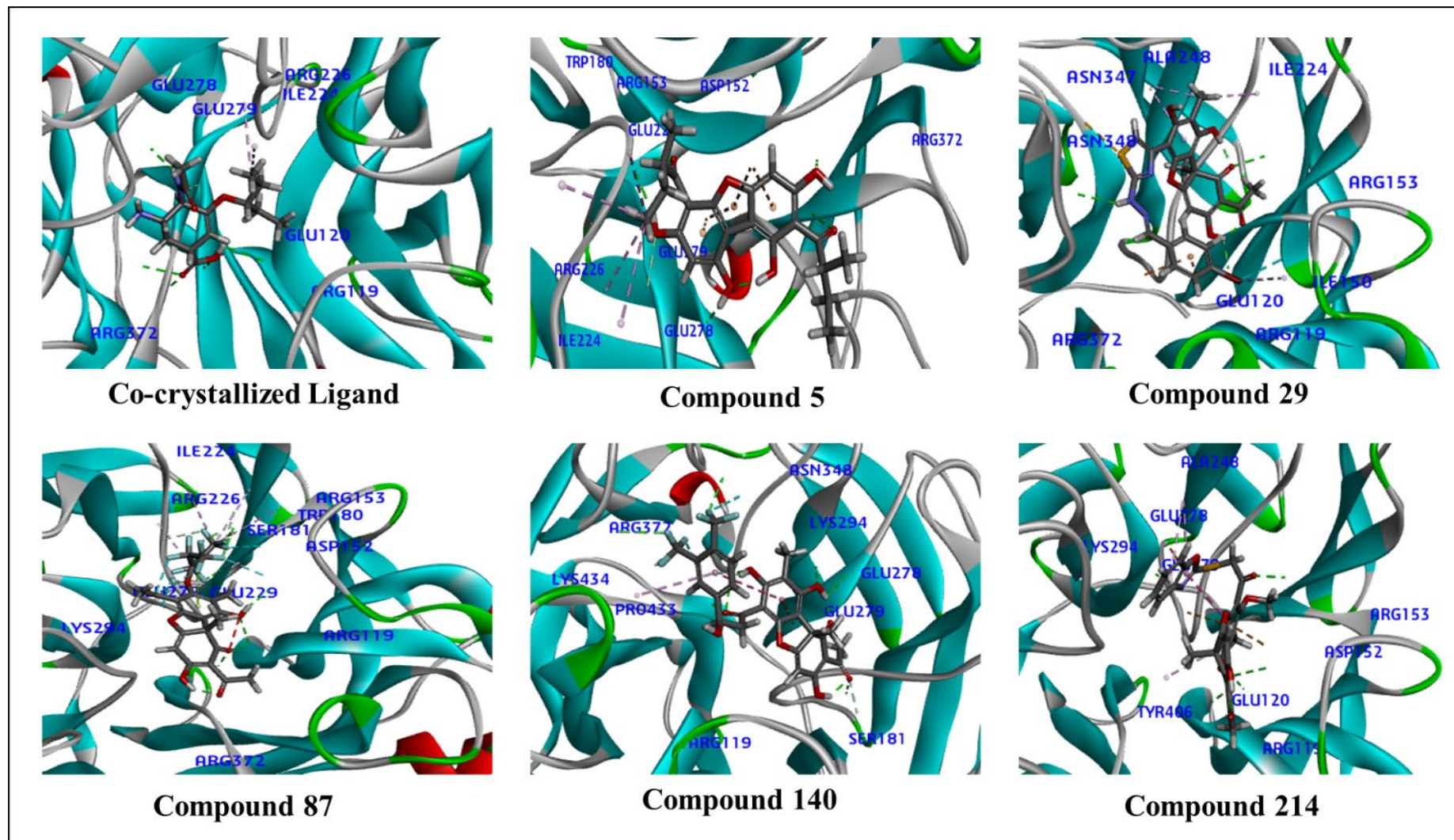


Figure S1. Molecular docking interaction analysis of Co-crystallized ligand and compound 5, 29, 87, 140, 214 with Avian Influenza A (4MWW).