

## **On the Pro-oxidant Activity of Curcumin in Lipid Media: A Theoretical Study**

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## **Supplementary Information**

<sup>1</sup>CUR

E0=-1262.740551

H=-1262.714526

G=-1262.798243

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<sup>1</sup>CUR\*

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<sup>3</sup>CUR

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C,0.5060525207,3.1215647352,-0.1915398699  
C,-0.8842614113,3.1109302444,-0.206400638  
C,-1.5730623121,1.9097448065,-0.0977434684  
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H,1.023911437,4.0707962082,-0.2801204989  
H,-1.4543925982,4.0289838834,-0.3027831893  
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H,3.2032273671,3.952253297,-0.1084106821  
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O,5.4869256226,1.5400298489,-0.0062742164  
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CUR<sup>++</sup>

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C,7.1927662534,3.8408063907,-0.0335148449  
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C,9.3966243469,4.9225963592,-0.0154964717  
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CUR<sup>-</sup>

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