APPENDIX

for
Research Article

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Comparative Adsorption of Ibuprofen and Ciprofloxacin from Aqueous Solution Using Natural Bentonite Clay: Experimental and DFT Study

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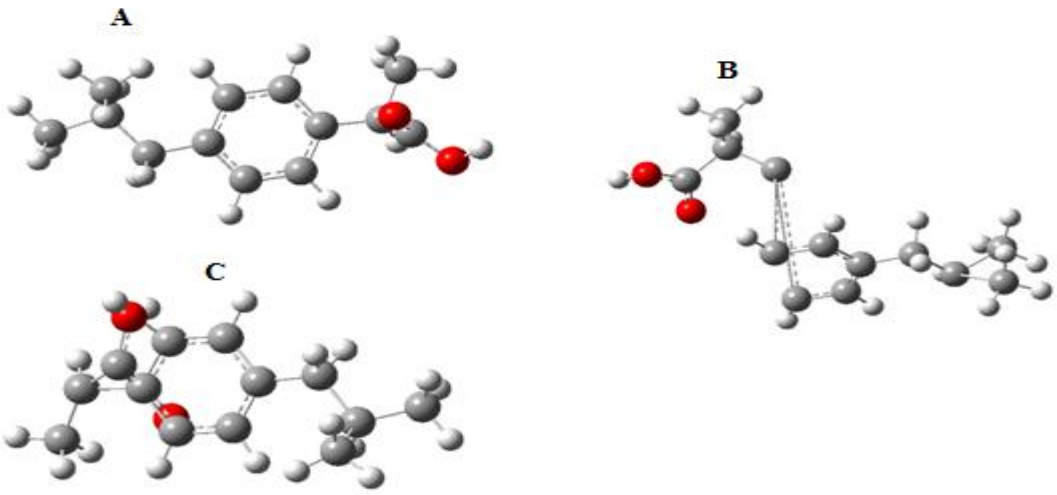

Fig. A1. *Possible optimized conformers of ibuprofen generated using DFT and B3LYP/6-31G(d)*

(A) - Anti-conformer (most stable):
- Energy: -434.64 Hartrees (optimized)
- Dihedral angle (C2-C1-C7-C8): 180.0°

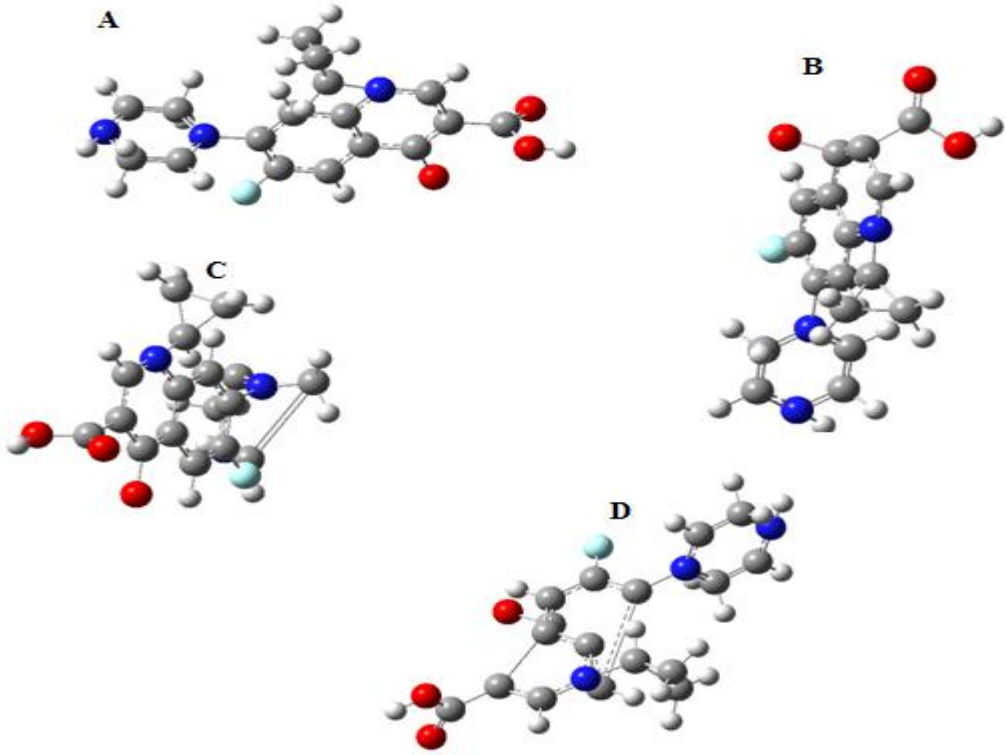

Fig. A2. *Possible optimized conformers of ciprofloxacin generated using DFT and B3LYP/6-31G(d)*

(A) - Global Minimum Energy Conformation
- Energy: -1046.44 Hartrees
- Dihedral angles:
- C5-C6-C7-N8: -179.6°
- C6-C7-N8-C9: 179.5°
- N8-C9-C10-N11: -179.9°
This is the most stable conformer

Table A1. *Bond lengths and bond angles for the Ibuprofen molecule calculated using DFT and B3LYP/6-31G(d)*

Bond Lengths(Å)	
-C1-C2:	1.539
-C1-C6:	1.543
-C2-C3:	1.525
-C3-C4:	1.538
-C4-C5:	1.523
-C5-C6:	1.541
-C6-C7:	1.494
-C7-C8:	1.509
-C8-C9:	1.523
-C9-C10:	1.538
-C10-C11:	1.525
-C11-O12:	1.227
-C11-O13:	1.343
-O13-H14:	0.970
-C2-H15:	1.090
-C3-H16:	1.090
-C5-H17:	1.090
-C8-H18:	1.090
-C9-H19:	1.090
-C10-H20:	1.090
Bond Angles(°)	
-C2-C1-C6:	111.4
-C3-C2-C1:	113.4
-C4-C3-C2:	111.1
-C5-C4-C3:	113.4
-C6-C5-C4:	111.1
-C7-C6-C5:	112.9
-C8-C7-C6:	112.2
-C9-C8-C7:	112.9
-C10-C9-C8:	112.2
-O12-C11-C10:	123.4
-O13-C11-C10:	113.4
-O13-C11-O12:	123.2
-H14-O13-C11:	109.5
-H15-C2-C1:	107.8
-H16-C3-C2:	107.8
-H17-C5-C4:	107.8
-H18-C8-C7:	107.8
-H19-C9-C8:	107.8
-H20-C10-C9:	107.8

Table A2. *Bond lengths and bond angles for the Ciprofloxacin molecule calculated using DFT and B3LYP/6-31G(d)*

Bond Lengths (Å)	
-C1-C2:	1.397
-C1-C6:	1.404
-C2-C3:	1.391
-C3-C4:	1.397
-C4-C5:	1.384
-C5-C6:	1.398
-C6-N7:	1.305
-N7-C8:	1.448
-C8-C9:	1.354
-C9-F10:	1.362
-C9-C11:	1.444
-C11-C12:	1.397
-C12-C13:	1.384
-C13-C14:	1.397
-C14-C15:	1.398
-C15-N16:	1.305
-N16-C17:	1.448
-C17-C18:	1.354
-C18-O19:	1.227
-C18-O20:	1.343
-O20-H21:	0.970
Bond Angles(°)	
-C2-C1-C6:	119.4
-C3-C2-C1:	120.5
-C4-C3-C2:	118.6
-C5-C4-C3:	121.1
-C6-C5-C4:	118.3
-N7-C6-C5:	124.9
-C8-N7-C6:	127.4
-C9-C8-N7:	125.6
-F10-C9-C8:	109.4
-F10-C9-C11:	109.4
-C11-C9-C8:	114.5
-C12-C11-C9:	121.4
-C14-C13-C12:	121.1
-C15-C14-C13:	118.6
-N16-C15-C14:	124.9
-C17-N16-C15:	127.4
-C18-C17-N16:	125.6
-O19-C18-C17:	123.4
-O20-C18-C17:	113.4
-O20-C18-O19:	123.2
-H21-O20-C18:	109.5