**Molecular structure, vibrational spectra and density functional theory of spiro-conjugated anticancer active molecule rubrocurcumin**

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**Supplementary Tables**

**Supplementary Table 1.Optimized bond angle of compound I and II by B3LYP/6-311G(d,p) basis set in comparison with X-ray diffraction data.**

|  |  |  |  |
| --- | --- | --- | --- |
| **Bond angle** | **Experimental value (o)** | **Calculated value (o)** | |
| **(I)** | **(II)** |
| C2-C1-C3 | 118.0 | 118.4 | 118.5 |
| C2-C1-C7 | 118.4 | 123.6 | 123.6 |
| C3-C1-C7 | 122.7 | 117.9 | 117.9 |
| C1-C2-C4 | 120.9 | 121.0 | 121.0 |
| C1-C2-H44 | 119.1 | 120.0 | 120.1 |
| C4-C2-H44 | 119.2 | 118.9 | 118.9 |
| C1-C3-C5 | 120.2 | 120.6 | 120.7 |
| C1-C3-H48 | 120.0 | 118.9 | 118.9 |
| C5-C3-H48 | 120.0 | 120.4 | 120.5 |
| C2-C4-C6 | 119.3 | 120.1 | 120.1 |
| C2-C4-H45 | 120.4 | 121.5 | 121.5 |
| C6-C4-H45 | 120.3 | 118.4 | 118.4 |
| C3-C5-C6 | 120.0 | 121.0 | 120.0 |
| C3-C5-O47 | 123.9 | 126.5 | 123.6 |
| C6-C5-O47 | 114.0 | 113.4 | 113.4 |
| C4-C6-C5 | 120.2 | 119.7 | 119.7 |
| C4-C6-H46 | 117.7 | 120.1 | 120.2 |
| C5-C6-H46 | 122.1 | 120.1 | 120.1 |
| C1-C7-C8 | 126.4 | 128.0 | 128.1 |
| C1-C7-H43 | 116.9 | 115.8 | 115.8 |
| C8-C7-H43 | 116.7 | 116.1 | 116.0 |
| C7-C8-C9 | 123.8 | 122.0 | 121.9 |
| C7-C8-H42 | 116.3 | 121.9 | 121.8 |
| C9-C8-H42 | 119.9 | 116.0 | 116.3 |
| C8-C9-C10 | 125.9 | 121.7 | 119.9 |
| C8-C9-O14 | 111.9 | 117.4 | 117.5 |
| C10-C9-O14 | 122.1 | 120.8 | 122.6 |
| C9-C10-C11 | 117.1 | 119.6 | 124.7 |
| C9-C10-H35 | 121.6 | 120.1 | 117.7 |
| C11-C10-H35 | 121.4 | 120.1 | 117.7 |
| C10-C11-O12 | 122.1 | 120.8 | 122.6 |
| C10-C11-C15 | 121.1 | 121.8 | 119.9 |
| O12-C11-C15 | 116.7 | 117.4 | 117.5 |
| C11-O12-B13I / C11-O12-Al13II | 118.2 | 123.8 | 125.6 |
| O12-B13-O14I / O12-Al13-O14II | 108.5 | 111.2 | 99.0 |
| O12-B13-O36I / O12-Al13-O36II | 109.3 | 109.7 | 116.2 |
| O12-B13-O39I / O12-Al13-O39II | 111.1 | 109.7 | 116.2 |
| O14-B13-O36I / O14-Al13-O36II | 107.7 | 109.7 | 116.2 |
| O14-B13-O39I / O14-Al13-O39II | 110.0 | 109.7 | 116.2 |
| O36-B13-O39I / O36-Al13-O39II | 111.2 | 106.7 | 94.0 |
| C9-O14-B13I / C9-O14-Al13II | 119.4 | 123.8 | 125.6 |
| C11-C15-C16 | 122.7 | 122.0 | 121.9 |
| C11-C15-H34 | 118.6 | 116.0 | 116.3 |
| C16-C15-H34 | 118.7 | 121.9 | 121.8 |
| C15-C16-C17 | 129.6 | 128.0 | 128.1 |
| C15-C16-H33 | 115.3 | 116.1 | 116.0 |
| C17-C16-H33 | 115.2 | 115.8 | 115.8 |
| C16-C17-C18 | 119.2 | 117.9 | 117.9 |
| C16-C17-C22 | 122.7 | 123.6 | 123.6 |
| C18-C17-C22 | 118.1 | 118.4 | 118.5 |
| C17-C18-C19 | 122.1 | 120.6 | 120.7 |
| C17-C18-H26 | 118.8 | 118.9 | 118.9 |
| C19-C18-H26 | 119.0 | 120.5 | 120.5 |
| C18-C19-C20 | 119.4 | 120.0 | 120.0 |
| C18-C19-O24 | 125.9 | 126.5 | 126.6 |
| C20-C19-O24 | 113.9 | 113.4 | 113.4 |
| C19-C20-C21 | 120.0 | 119.7 | 119.7 |
| C19-C20-O23 | 120.6 | 120.1 | 120.1 |
| C21-C20-O23 | 119.5 | 120.1 | 120.2 |
| C20-C21-C22 | 119.4 | 120.1 | 120.1 |
| C20-C21-H27 | 120.3 | 118.4 | 118.4 |
| C22-C21-H27 | 120.4 | 121.5 | 121.4 |
| C17-C22-C21 | 120.1 | 121.0 | 121.0 |
| C17-C22-H28 | 120.0 | 120.0 | 120.1 |
| C21-C22-H28 | 119.0 | 118.9 | 118.9 |
| C20-O23-H29 | 109.4 | 107.3 | 107.3 |
| C19-O24-C25 | 118.4 | 118.3 | 118.3 |
| O24-C25-H30 | 109.5 | 111.1 | 111.1 |
| O24-C25-H31 | 109.5 | 106.1 | 106.1 |
| O24-C25-H32 | 109.4 | 111.1 | 111.2 |
| H30-C25-H31 | 109.5 | 109.5 | 109.5 |
| H30-C25-H32 | 109.5 | 109.5 | 109.5 |
| H31-C25-H32 | 109.5 | 109.5 | 109.5 |
| B13-O36-C37I / Al13-O36-C37II | 108.9 | 109.5 | 165.2 |
| O36-C37-C38 | 108.4 | 107.1 | 112.2 |
| O36-C37-O41 | 124.9 | 126.2 | 125.1 |
| C38-C37-O41 | 126.8 | 126.6 | 122.6 |
| C37-C38-O39 | 107.8 | 107.2 | 112.2 |
| C37-C38-O40 | 127.0 | 126.6 | 122.6 |
| O39-C38-O40 | 125.2 | 126.2 | 125.1 |
| B13-O39-C38I / Al13-O39-C38II | 108.7 | 109.4 | 111.3 |
| C6-O46-H49 | 109.5 | 107.3 | 107.3 |
| C5-O47-C50 | 118.9 | 118.3 | 118.3 |
| O47-C50-H51 | 109.5 | 111.1 | 111.2 |
| O47-C50-H52 | 109.4 | 111.2 | 111.2 |
| O47-C50-H53 | 109.5 | 106.1 | 106.1 |
| H51-C50-H52 | 109.4 | 109.5 | 109.5 |
| H51-C50-H53 | 109.5 | 109.5 | 109.5 |
| H52-C50-H53 | 109.5 | 109.5 | 109.5 |

**Supplementary Table 2. Optimized dihedral angle of compound I and II by B3LYP/6-311G(d,p) basis set in comparison with X-ray diffraction data.**

|  |  |  |  |
| --- | --- | --- | --- |
| **Dihedral angle** | **Experimental value (o)** | **Calculated value (o)** | |
| **(I)** | **(II)** |
| C3-C1-C2-C4 | -1.6 | 0 | 0 |
| C3-C1-C2-H44 | 178.4 | -179.9 | 179.9 |
| C7-C1-C2-C4 | 177.0 | -179.9 | -179.9 |
| C7-C1-C2-H44 | -3 | 0 | 0 |
| C2-C1-C3-C5 | 1.7 | 0 | 0 |
| C2-C1-C3-H48 | 178.3 | 179.9 | -179.9 |
| C7-C1-C3-C5 | -176.9 | 179.9 | 179.9 |
| C7-C1-C3-H48 | 3.2 | 0 | 0 |
| C2-C1-C7-C8 | 2.3 | 0 | 0 |
| C2-C1-C7-H43 | 2.3 | 179.9 | 179.9 |
| C3-C1-C7-C8 | 0.8 | -179.9 | 179.9 |
| C3-C1-C7-H43 | -179.2 | 0 | 0 |
| C1-C2-C4-C6 | 0.9 | 0 | 0 |
| C1-C2-C4-H45 | -179.7 | 179.9 | 179.9 |
| H44-C2-C4-C6 | -179.7 | 179.9 | -179.9 |
| H44-C2-C4-H45 | 0.2 | 0 | 0 |
| C1-C3-C5-C6 | -0.5 | 0 | 0 |
| C1-C3-C5-O47 | 166.6 | 179.9 | 179.9 |
| H48-C3-C5-C6 | 179.5 | 179.9 | 179.9 |
| H48-C3-C5-O47 | 0.9 | 0 | 0 |
| C2-C4-C6-C5 | 0.9 | 0 | 0 |
| C2-C4-C6-O46 | -177.3 | -179.9 | -179.9 |
| H45-C4-C6-C5 | -179.1 | 179.9 | 179.9 |
| H45-C4-C6-O46 | 2.7 | 0 | 0 |
| C3-C5-C6-C4 | -1 | 0 | 0 |
| C3-C5-C6-O46 | 177.3 | -180.0 | -179.9 |
| O47-C5-C6-C4 | 177.9 | -179.9 | -179.9 |
| O47-C5-C6-O46 | -4 | 0 | 0 |
| C3-C5-O47-C50 | -7 | 0 | 0 |
| C6-C5-O47-C50 | 174.7 | 179.9 | 179.9 |
| C4-C6-O46-H49 | -171.3 | -179.9 | -179.9 |
| C5-C6-O46-H49 | 10.5 | 0 | 0 |
| C1-C7-C8-C9 | 176.6 | 179.9 | 180.0 |
| C1-C7-C8-H42 | -3.5 | 0 | 0 |
| H43-C7-C8-C9 | -3.4 | 0 | 0 |
| H43-C7-C8-H42 | 176.5 | -179.9 | -179.9 |
| C7-C8-C9-C10 | 1.73 | -179.9 | 180.0 |
| C7-C8-C9-O14 | 179.3 | 0 | 0 |
| H42-C8-C9-C10 | -178.2 | 0 | 0 |
| H42-C8-C9-O14 | -1 | -179.9 | -179.9 |
| C8-C9-C10-C11 | 1.73 | -179.9 | -179.9 |
| C8-C9-C10-H35 | -6.2 | 0 | 0 |
| O14-C9-C10-C11 | -3.7 | 0 | 0 |
| O14-C9-C10-H35 | 176.5 | 179.9 | 180.0 |
| C8-C9-O14-B13/  C8-C9-O14-Al13 | 164.7 | -179.9 | -179.9 |
| C10-C9-O14-B13I/  C10-C9-O14-Al13II | -17.6 | 0 | 0 |
| C9-C10-C11-O12 | 1.3 | 0 | 0 |
| C9-C10-C11-C15 | -176.1 | 179.9 | 179.9 |
| H35-C10-C11-O12 | -178.8 | -179.9 | -180.0 |
| H35-C10-C11-C15 | 3.8 | 0 | 0 |
| C10-C11-O12-B13/  C10-C11-O12-Al13 | 21.9 | 0 | 0 |
| C15-C11-O12-B13I/  C15-C11-O12-Al13II | -160.5 | 179.9 | 179.9 |
| C10-C11-C15-C16 | -173.2 | 179.9 | -180.0 |
| C10-C11-C15-H34 | 6.7 | 0 | 0 |
| O12-C11-C15-C16 | 9.2 | 0 | 0 |
| O12-C11-C15-H34 | -170.9 | 0 | 179.9 |
| C11-O12-B13-O14I/  C11-O12-Al13-O14II | -38.9 | 0 | 0 |
| C11-O12-B13-O36I/  C11-O12-Al13-O36II | -156.2 | -121.2 | -124.9 |
| C11-O12-B13-O39I/  C11-O12-Al13-O39II | -92.9 | 121.8 | 125.4 |
| O12-B13-O14-C9I/  O12-Al13-O14-C9II | -23.51 | 0 | 0 |
| O36-B13-O14-C9I/  O36-Al13-O14-C9II | 155.2 | 121.2 | 124.9 |
| O39-B13-O14-C9I/  O39-Al13-O14-C9II | 96.5 | -121.8 | -125.4 |
| O12-B13-O36-C37I/  O12-Al13-O36-C37II | 123.5 | -118.8 | -122.3 |
| O14-B13-O36-C37I/  O14-Al13-O36-C37II | -115.0 | 118.8 | 122.3 |
| O39-B13-O36-C37I/  O39-Al13-O36-C37II | 3.8 | 0 | 0 |
| O12-B13-O39-C38I/  O12-Al13-O39-C38II | -124.1 | 118.8 | 122.3 |
| O14-B13-O39-C38I/  O14-Al13-O39-C38II | 115.7 | -118.8 | -122.3 |
| O36-B13-O39-C38I/  O36-Al13-O39-C38II | -3 | 0 | 0 |
| C11-C15-C16-C17 | 177.9 | -179.9 | -180.0 |
| C11-C15-C16-H33 | -2.2 | 0 | 0 |
| H34-C15-C16-C17 | -2 | 0 | 0 |
| H34-C15-C16-H33 | 177.9 | 179.9 | 179.9 |
| C15-C16-C17-C18 | 178.6 | 179.9 | -179.9 |
| C15-C16-C17-C22 | -1.3 | 0 | 0 |
| H33-C16-C17-C18 | -1.3 | 0 | 0 |
| H33-C16-C17-C22 | 178.8 | -179.9 | -179.9 |
| C16-C17-C18-C19 | -179.3 | -179.9 | -179.9 |
| C16-C17-C18-H26 | 1 | 0 | 0 |
| C22-C17-C18-C19 | 1 | 0 | 0 |
| C22-C17-C18-H26 | -179.4 | 179.9 | 179.9 |
| C16-C17-C22-C21 | 179.7 | 179.9 | 179.9 |
| C16-C17-C22-H28 | 0 | 0 | 0 |
| C18-C17-C22-C21 | 0 | 0 | 0 |
| C18-C17-C22-H28 | 180.0 | 179.9 | -179.9 |
| C17-C18-C19-C20 | 1 | 0 | 0 |
| C17-C18-C19-O24 | 177.8 | -179.9 | -179.9 |
| H26-C18-C19-C20 | 178.6 | -179.9 | -179.9 |
| H26-C18-C19-O24 | -2.3 | 0 | 0 |
| C18-C19-C20-C21 | 2.9 | 0 | 0 |
| C18-C19-C20-O23 | -178.8 | 180.0 | 179.9 |
| O24-C19-C20-C21 | -176.8 | 179.9 | 179.9 |
| O24-C19-C20-O23 | 2 | 0 | 0 |
| C18-C19-O24-C25 | 0 | 0 | 0 |
| C20-C19-O24-C25 | 178.5 | -179.9 | -179.9 |
| C19-C20-C21-C22 | -2 | 0 | 0 |
| C19-C20-C21-H27 | 178.0 | -179.9 | -179.9 |
| O23-C20-C21-C22 | 179.2 | 179.9 | 179.9 |
| O23-C20-C21-H27 | -1 | 0 | 0 |
| C19-C20-O23-H29 | 11.65 | 0 | 0 |
| C21-C20-O23-H29 | 169.5 | 179.9 | 179.9 |
| C20-C21-C22-C17 | 0 | 0 | 0 |
| C20-C21-C22-H28 | 179.5 | -179.9 | 179.9 |
| H27-C21-C22-C17 | -179.4 | -179.9 | -179.9 |
| H27-C21-C22-H28 | 0 | 0 | 0 |
| C19-O24-C25-H30 | -57.1 | 61.1 | 61.1 |
| C19-O24-C25-H31 | -177.1 | 179.9 | 179.9 |
| C19-O24-C25-H32 | -57.1 | -61.1 | -61.1 |
| B13-O36-C37-C38I/  Al13-O36-C37-C38II | -3.2 | 0 | 0 |
| B13-O36-C37-O41I/  Al13-O36-C37-O41II | 178.4 | 180.0 | -180.0 |
| O36-C37-C38-C39 | 1.3 | 0 | 0 |
| O36-C37-C38-O40 | 179.8 | 179.9 | -179.9 |
| O41-C37-C38-O39 | 179.8 | -180.0 | -179.9 |
| O41-C37-C38-O40 | 0 | 0 | 0 |
| C37-C38-O39-B13I/  C37-C38-O39-Al13II | 1.1 | 0 | 0 |
| O40-C38-O39-B13I/  O40-C38-O39-Al13II | -178.4 | -179.9 | 180.0 |
| C5-O47-C50-H51 | -54.0 | -61.1 | -61.1 |
| C5-O47-C50-H52 | 65.9 | 61.1 | 61.1 |
| C5-O47-C50-H53 | -174.2 | -179.9 | -179.9 |

**Supplementary Table 3. Natural charges of compound I and II**

|  |  |  |
| --- | --- | --- |
| **Atom** | **Natural charge (e)** | |
| **I** | **II** |
| C1 | -0.099 | -0.100 |
| C2 | -0.163 | -0.163 |
| C3 | -0.240 | -0.240 |
| C4 | -0.243 | -0.243 |
| C5 | 0.262 | 0.262 |
| C6 | 0.334 | 0.335 |
| C7 | -0.078 | -0.079 |
| C8 | -0.276 | -0.278 |
| C9 | 0.479 | 0.478 |
| C10 | -0.392 | -0.388 |
| C11 | 0.479 | 0.478 |
| O12 | -0.646 | -0.842 |
| B13I/Al13II | 1.218 | 2.049 |
| O14 | -0.646 | -0.842 |
| C15 | -0.276 | -0.278 |
| C16 | -0.078 | -0.079 |
| C17 | -0.099 | -0.100 |
| C18 | -0.240 | -0.240 |
| C19 | 0.262 | 0.262 |
| C20 | 0.334 | 0.335 |
| C21 | -0.243 | -0.243 |
| C22 | -0.163 | -0.163 |
| O23 | -0.651 | -0.651 |
| O24 | -0.555 | -0.555 |
| C25 | -0.193 | -0.193 |
| H26 | 0.216 | 0.216 |
| H27 | 0.221 | 0.221 |
| H28 | 0.203 | 0.203 |
| H29 | 0.483 | 0.483 |
| H30 | 0.172 | 0.172 |
| H31 | 0.189 | 0.190 |
| H32 | 0.172 | 0.172 |
| H33 | 0.216 | 0.215 |
| H34 | 0.202 | 0.201 |
| H35 | 0.220 | 0.215 |
| O36 | -0.693 | -0.904 |
| C37 | 0.706 | 0.701 |
| C38 | 0.706 | 0.701 |
| O39 | -0.693 | -0.904 |
| O40 | -0.539 | -0.539 |
| O41 | -0.539 | -0.539 |
| H42 | 0.202 | 0.201 |
| H43 | 0.216 | 0.215 |
| H44 | 0.203 | 0.203 |
| H45 | 0.221 | 0.221 |
| O46 | -0.651 | -0.651 |
| O47 | -0.555 | -0.555 |
| H48 | 0.216 | 0.216 |
| H49 | 0.483 | 0.483 |
| C50 | -0.193 | -0.193 |
| H51 | 0.172 | 0.172 |
| H52 | 0.172 | 0.172 |
| H53 | 0.189 | 0.190 |

**Supplementary Table 4a. Second order perturbation theory analysis of Fock matrix in natural bond orbital basis for compound I.**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Donor**  **NBO(i)** | **E.D.(e)** | **Acceptor NBO(j)** | **E.D.(e)** | **E(2)**  **kJmol-1** |
| σ (C1-C3) | 1.96652  -0.69760 | σ \* (C5-O47) | 0.03058  0.33067 | 21.50 |
| σ (C1-C7) | 1.97267  -0.68731 | σ \* (C8-O9) | 0.02929  0.47809 | 10.75 |
| σ (C2-C4) | 1.97535  -0.71788 | σ \* (C1-C7) | 0.02335  0.49649 | 15.15 |
| σ (C3-C5) | 1.97740  -0.74040 | σ \* (C5-C6) | 0.04005  0.50453 | 20.58 |
| σ(C3-O5) | 1.97740  -0.74040 | σ \* (C6-O46) | 0.01934  0.34804 | 11.21 |
| σ (C7-C43) | 1.97412  -0.52515 | σ \* (C8-H42) | 0.01614  0.41660 | 22.76 |
| σ (C10-H35) | 1.97313  -0.54196 | σ \* (C11-O12) | 0.02735  0.41607 | 22.76 |
| σ (C15-C34) | 1.97633  -0.53857 | σ \* (C11-O12) | 0.02735  0.41607 | 20.25 |
| σ (C16-H33) | 1.97412  -0.52515 | σ \* (C17-C22) | 0.02711  0.54763 | 20.83 |
| σ (C17-C18) | 1.96652  -0.69760 | σ \* (C19-O24) | 0.03058  0.03058 | 21.50 |
| σ (C18-C19) | 1.97740  -0.74040 | σ \* (C19-C20) | 0.04005  0.50453 | 20.58 |
| σ (O23-H29) | 1.98718  -0.75363 | σ \* (C20-C21) | 0.02327  0.54296 | 20.92 |
| σ (O46-H49) | 1.98718  -0.75363 | σ \* (C4-C6) | 0.02327  0.54296 | 20.92 |
| σ (B13-O36) | 1.98190  -0.78498 | σ \* (C37-O41) | 0.01765  0.67193 | 23.13 |
| σ (B13-O39) | 1.98189  -0.78511 | σ \* (C38-O40) | 0.01765  0.67194 | 23.13 |
| σ (O36-C37) | 1.99007  -0.89176 | σ \* (B13-O39) | 0.05447  0.38885 | 4.184 |
| σ (O36-C37) | 1.99007  -0.89176 | σ \* (C38-O40) | 0.01765  0.67194 | 4.39 |
| σ(C37-C38) | 1.99046  -0.62819 | σ \* (B13-O36) | 0.05463  0.38875 | 13.47 |
| σ(C37-O38) | 1.99046  -0.62819 | σ \* (B13-O39) | 0.05447  0.38885 | 13.43 |

i, donor orbital; j, acceptor orbital; E(2), energy of hyperconjugative interactions.

**Supplementary Table 4b. Second Second order perturbation theory analysis of Fock matrix in natural bond orbital basis for compound II.**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Donor**  **NBO(i)** | **E.D.(e)** | **Acceptor NBO(j)** | **E.D.(e)** | **E(2)**  **kJmol-1** |
| σ (C1-C3) | 1.96653  -0.69973 | σ \* (C5-O47) | 0.03056  0.32898 | 21.50 |
| σ (C1-C7) | 1.9727  -0.68998 | σ \* (C8-C9) | 0.03374  0.47229 | 10.63 |
| σ (C2-C4) | 1.97539  -0.72015 | σ \* (C1-C7) | 0.02338  0.49488 | 15.15 |
| σ (C3-C5) | 1.97741  -0.74275 | σ \* (C5-C6) | 0.04009  0.50196 | 20.58 |
| σ (C3-C5) | 1.71414  -0.29.94 | σ \* (C6-O46) | 0.01930  0.34641 | 11.21 |
| σ (C7-C43) | 1.97412  -0.52515 | σ \* (C8-H42) | 0.01626  0.41539 | 22.76 |
| σ (C10-H35) | 1.97156  -0.53856 | σ \* (C11-O12) | 0.02446  0.40808 | 25.27 |
| σ (C15-C34) | 1.97651  -0.54070 | σ \* (C11-O12) | 0.02446  0.40808 | 19.58 |
| σ (C16-H33) | 1.97408  -0.52729 | σ \* (C17-C22) | 0.02715  0.54512 | 20.88 |
| σ (C17-C18) | 1.96653  -0.69973 | σ \* (C19-O24) | 0.03056  0.32898 | 21.51 |
| σ (C18-C19) | 1.97741  -0.74275 | σ \* (C19-C20) | 0.04009  0.50196 | 20.59 |
| σ (O36-C37) | 1.99131  -0.90709 | σ \* (C38-C40) | 0.02233  0.67580 | 3.59 |
| σ (O23-H29) | 1.98715  -0.75569 | σ \* (C20-C21) | 0.02328  0.54050 | 20.96 |
| σ (O46-H49) | 1.98715  -0.75569 | σ \* (C4-C6) | 0.02328  0.54050 | 20.96 |

i, donor orbital; j, acceptor orbital; E(2), energy of hyperconjugative interactions.

**Supplementary Table 5a. Possible Hydrogen Bonding of compound I**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Donor NBO**  **(i)** | **E.D (e)** | **Acceptor NBO**  **(j)** | **E.D (e)** | **E(2) kJmol-1** | **H.O** | **D-H (Å)** | **H-A (Å)** | **D-A (Å)** | **D-H..A (o)** |
| n1O24 | 1.95839  -0.58122 | σ \*(O23-H29) | 0.01366  0.38889 | 6.40 | sp1.64 | 2.08 | 0.968 | 2.636 | 114.7 |
| n1O47 | 1.95839  -0.58122 | σ \*(O46-H49) | 0.01366  0.38889 | 6.40 | sp1.64 | 2.08 | 0.968 | 2.636 | 114.7 |

i, donor orbital; j, acceptor orbital; E(2), energy of hyperconjugative interactions; H.O, hybrid orbital; Å, angstrong unit.

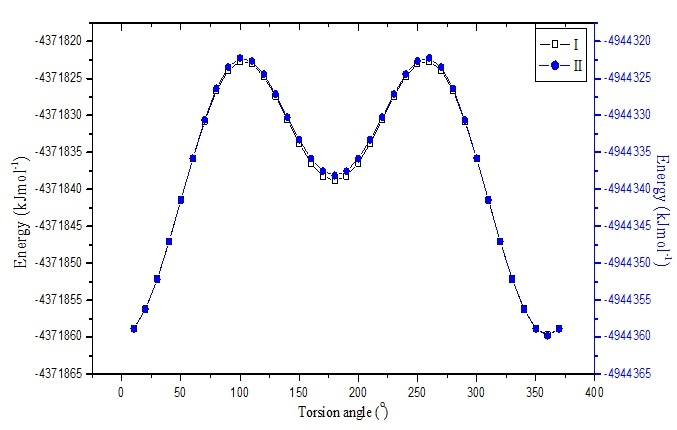
**Supplementary Table 5b. Possible Hydrogen Bonding of compound II**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Donor NBO**  **(i)** | **E.D (e)** | **Acceptor NBO**  **(j)** | **E.D (e)** | **E(2) kJmol-1** | **H.O** | **D-H (Å)** | **H-A (Å)** | **D-A (Å)** | **D-H..A (o)** |
| n1O24 | 1.95835  -0.58306 | σ \*(O23-H29) | 0.01369  0.38688 | 6.44 | sp1.64 | 2.08 | 0.968 | 2.636 | 114.7 |
| n1O47 | 1.95835  -0.58306 | σ \*(O46-H49) | 0.01369  0.38688 | 6.44 | sp1.64 | 2.08 | 0.968 | 2.636 | 114.7 |

i, donor orbital; j, acceptor orbital; E(2), energy of hyperconjugative interactions; H.O, hybrid orbital; Å, angstrong unit.

**Supplementary Figures**

**Supplementary Figure 1. Potential energy surface plot for torsion around O46-H49**



**Supplementary Figure 2. HOMO-LUMO plot of compound I and II**

**(A) - LUMO of compound I; (B) - LUMO of compound II**

**(C) - HOMO of compound I; (D) - HOMO of compound II**

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