The geometries were succesfuly optimized and the results of optimizations correspond to energy minima. Total energies were calculated at B3LYP/ 6-31G(d) level of theory. For parallel complexes of ferutinin **1a** and antiparallel complexes of ferutinin **1b** the results of optimization do not correspond to energy minima since some imaginery frequencies were detected and thus these complexes are not presented.

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| --- | --- |
| **Ferutinin 1a (enol)**  **E=-1157.27327127 Hartree** | **Ferutinin 1b (keto)**  **E=-1157.25132705 Hartree** |
|  |  |
| **Two ferutinin 1a molecules without H-bond**  **E=-2314.58242457 Hartree**  **dO…H=2.91 Å** | **Two H-bonded ferutinin 1a molecules**  **E=-2314.59035393 Hartree**  **dO…H=1.95 Å** |
|  |  |
| **Ferutinin 1a-Ca2+ complex (antiparallel)**  **E=-2991.82674481 Hartree**  **Coordination bonds : 2.36 – 2.65 Å** | **Ferutinin 1b-Ca2+ complex (parallel)**  **E=-2991.68193580 Hartree**  **Coordination bonds : 2.40 – 2.52 Å** |
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