**Figure S 2**

**Visualizations of energy-related trends for the calculated conformers of tetraflavaspidic acid BBBB**

**Note**

The graphs in this figure report the conformers of tetraflavaspidic acid BBBB, denoting them with numbers (in order of increasing energy in the DFT/B3LYP/6-31+G(d,p)-D3 results), according to the following table

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| conformer | number | conformer | number | conformer | number | conformer | number |
| 1-a-α | 1 | 8-a-τ | 17 | 5-e-η | 33 | 1-b-ξ1 | 49 |
| 2-a-γ | 2 | 7-b-β | 18 | 4-b-λ | 34 | 2-c-ξ2 | 50 |
| 3-a-ε | 3 | 7-e-β | 19 | 4-c-λ | 35 | 7-c-ξ7 | 51 |
| 2-c-γ | 4 | 3-c-ε | 20 | 4-e-λ | 36 | 8-c-ξ8 | 52 |
| 1-c-α | 5 | 3-e-ε | 21 | 1-a-ξ1 | 37 | 1-e-ξ1 | 53 |
| 2-b-γ | 6 | 8-b-τ | 22 | 4-c-ξ4 | 38 | 4-e-ξ4 | 54 |
| 4-a-λ | 7 | 5-c-η | 23 | 3-c-ξ3 | 39 | 5-b-ξ5 | 55 |
| 5-a-η | 8 | 4-a-ξ4 | 24 | 4-b-ξ4 | 40 | 6-e-ξ6 | 56 |
| 3-b-ε | 9 | 5-a-ξ5 | 25 | 3-b-ξ3 | 41 | 3-e-ξ3 | 57 |
| 1-b-α | 10 | 7-a-ξ7 | 26 | 6-b-ξ6 | 42 | 2-e-ξ2 | 58 |
| 1-e-α | 11 | 8-a-ξ8 | 27 | 1-c-ξ1 | 43 | 7-b-ξ7 | 59 |
| 6-b-ρ | 12 | 5-b-η | 28 | 6-c-ξ6 | 44 | 5-e-ξ5 | 60 |
| 7-a-β | 13 | 2-a-ξ2 | 29 | 3-a-ξ3 | 45 | 7-e-ξ7 | 61 |
| 6-c-ρ | 14 | 6-e-ρ | 30 | 2-b-ξ2 | 46 | 8-e-ξ8 | 62 |
| 2-e-γ | 15 | 8-c-τ | 31 | 5-c-ξ5 | 47 |  |  |
| 7-c-β | 16 | 8-e-τ | 32 | 8-b-ξ8 | 48 |  |  |

**a) Relative energies (kcal/mol, vertical axis)) of the calculated conformers of tetraflavaspidic acid BBBB**

HF/6-31G(d,p) {  }, DFT/B3LYP/6-31+G(d,p) { } and DFT/B3LYP/6-31+G(d,p)-D3 { } results

conformers (denoted by numbers)

**b) Lowering effect (kcal/mol, vertical axis) of the Grimme’s correction on the estimation of the energy of the calculated conformers of tetraflavaspidic acid BBBB**

The lowerings (difference in the estimations of the conformers’ energies, taken as «energy in the DFT/6-31+G(d,p) result without the Grimme’s correction minus energy in the DFT/6-31+G(d,p) result comprising the Grimme’s correction») are reported in table S3.

conformers (denoted by numbers)

**c) Comparison of the relative energies (kcal/mol, vertical axis) not corrected for ZPE {****} and corrected for ZPE {** **}, and relative Gibbs free energies {** **}, of the calculated conformers of tetraflavaspidic acid**

The values are reported in table S5.

**c) i) HF/6-31G(d,p) results**

conformers (denoted by numbers)

**c) ii) DFT/B3LYP/6-31+G(d,p) results**

conformers (denoted by numbers)

**c) iii) DFT/B3LYP/6-31+G(d,p)-D3 results**

conformers (denoted by numbers)

**d) ZPE correction (kcal/mol, vertical axis) for the calculated conformers of tetraflavaspidic acid BBBB**

HF/6-31G(d,p) {  }, DFT/B3LYP/6-31+G(d,p) { } and DFT/B3LYP/6-31+G(d,p)-D3 { } results. The values are reported in table S6.

conformers (denoted by numbers)