Free radical scavenging activity of five benzoic acid derivatives: a theoretical M06-2X study

Bienfait Kabuyaya Isamura \*, [a], [b], Issofa Patouossa [c], Isaac Kaba Elaka [d], Aristote Matondo [b], and Pius Tshimankinda Mpiana \*, [b]

[a] Department of Chemistry, Rhodes University, 6140, Makhanda, South Africa

[b] Department of Chemistry, Faculty of Sciences, University of Kinshasa, Kinshasa XI, Democratic Republic of the Congo

[c] Physical and Theoretical chemistry unit of the Laboratory of applied Physical and Analytical Chemistry, Faculty of Sciences, University of Yaoundé I, Yaoundé , Cameroon

[d] College of Pharmacy and Pharmaceutical Sciences, University of Toledo,Toledo, Ohio, USA

SUPPORTING INFORMATION

Table S1. O-H and C=O bonds lengths predicted at the M06-2X/6-311++G(d,p) level. Values expressed in Å. Also given are the dipolar momenta in vacuum (DM in Debye).

|  |  |  |  |
| --- | --- | --- | --- |
| Antioxidant | DM | Bond | Bond length (Å) |
|  |  |  | **Vacuum** | **Water** | **Methanol** |
| **GA** | 4.59  | O11-H12 | 0.966 | 0.968 | 0.968 |
| O16-H17 | 0.961 | 0.963 | 0.963 |
| O13-H14 | 0.965 | 0.966 | 0.966 |
| O15-H18 | 0.964 | 0.966 | 0.966 |
| C9=O10 | 1.201 | 1.208 | 1.208 |
| **PHBA** | 3.23 | O12-H13 | 0.966 | 0.968 | 0.966 |
| O14-H15 | 0.961 | 0.964 | **0.968** |
|  | C10=O11 | 1.203 | 1.209 | **1.209** |
| **PCA** | 3.49 | O11-H12 | 0.968 | 0.968 | 0.978 |
| O15-H16 | 0.962 | 0.963 | 0.963 |
| O13-H14 | 0.967 | 0.967 | 0.967 |
|  | C9=O10 | 1.202 | 1.208 | 1.208 |
| **SA** | 4.46 | O23-H24 | 0.966 | 0.968 | 0.968 |
| O10-H11 | 0.966 | 0.968 | 0.968 |
|  | C21=O22 | 1.202 | 1.208 | 1.208 |
| **VA** | 4.17 | O11-H12 | 0.966 | 0.968 | 0.968 |
| O13-H14 | 0.961 | 0.964 | 0.964 |
| C9=O10 | 1.202 | 1.208 | 1.208 |