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**for**

**Structural characterization of kaempferol: spectroscopic and computational study**

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**Table S1.**   Bond angles and torsion angles in structure kaempferol, optimized with B3LYP-D3/6-311+G(d,p) model (the atom numbering is in line with Figure 1). Experimental values are also included.

|  |  |
| --- | --- |
| Bond angles (˚) | Kaempferol |
| Experimental | B3LYP-D3 |
| Ol-C2-C3 | 117.3 | 119.1 |
| Ol-C2-C1` | 113.7 | 112.3 |
| C2-Ol-C9 | 122.2 | 122.8 |
| C3-C2-Cl` | 128.7 | 128.6 |
| C2-C3-C4 | 122.5 | 121.6 |
| C2-C3-O3 | 120.4 | 123.3 |
| C4-C3-O3 | 117.1 | 115.1 |
| C3-C4-C10 | 117.8 | 116.8 |
| C3-C4-O4 | 120.6 | 119.0 |
| C10-C4-O4 | 121.6 | 124.2 |
| C4-C10-C5 | 121.7 | 122.2 |
| C4-C10-C9 | 120.1 | 119.3 |
| C5-C10-C9 | 118.2 | 118.6 |
| C10-C5-C6 | 121.7 | 119.8 |
| C10-C5-O5 | 117.1 | 120.7 |
| C6-C5-O5 | 121.1 | 119.5 |
| C5-C6-C7 | 119.3 | 119.6 |
| C6-C7-C8 | 119.7 | 122.0 |
| C6-C7-O7 | 120.5 | 121.5 |
| C8-C7-O7 | 119.8 | 116.5 |
| C7-C8-C9 | 120.5 | 117.7 |
| Ol-C9-C10 | 120.0 | 120.5 |
| Ol-C9-C8 | 119.4 | 117.2 |
| C10-C9-C8 | 120.6 | 122.3 |
| C2-Cl`-C2` | 117.2 | 122.2 |
| C2-Cl`-C6` | 123.5 | 119.9 |
| Cl`-C2`-C3` | 121.2 | 120.8 |
| C2`-C3`-C4` | 118.9 | 120.4 |
| C3`-C4`-C5` | 120.4 | 119.7 |
| C3`-C4`-O4` | 120.8 | 123.0 |
| C5`-C4`-O4` | 118.8 | 117.4 |
| C4`-C5`-C6` | 120.2 | 119.9 |
| Cl`-C6`-C5` | 120.1 | 121.4 |
| τ(C3-C2-C1`-C2`) | 168.9 | 0.0 |

**Table S2.**  The total electric dipole moment μ (debye), the mean polarizability αtot (×10-24 esu) and the total first order static hyperpolarizability βtotal (×10-30 esu).

|  |  |  |  |
| --- | --- | --- | --- |
|  Parameters |

|  | **Values** |
| --- | --- |

 |
| µx | 1.374602 |
| µy | -1.136802 |
| µz | 0.0002 |
| µtot | **1.783774** |
| αxx | 353.470000 |
| αxy | -7.556910 |
| αyy | 228.796000 |
| αxz | 0.000932 |
| αyz | 0.006826 |
| αzz | 96.664100 |
| **αtot** | **33.53688 ×10-24 esu** |
| Δα | 222.816468 |
| βxxx | 3729.690000 |
| βxxy | -899.012000 |
| βxyy | -532.409000 |
| βyyy | 61.513200 |
| βxxz | -0.030886 |
| βxyz | -0.010685 |
| βyyz | 0.008098 |
| βxzz | -6.133230 |
| βyzz | 34.853400 |
| βzzz | -0.002287 |
| **βtot** | **28.42771×10-30 esu** |

**Table S3.**  Estimated free energy of binding (Δ*G*bind) in kcal/mol, and inhibition constant (Ki) (μM) of different poses of ligand against human Procalcitonin.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Conformations of ligand | $Δ$Δ*G*bind(kcal/mol) |  Ki (μM) | Hydrogen Bond | Hydrophobic Contact |
| 1 | -2.68 | 1.04x104 | A:ASP53  | A:LEU52A:PRO55A:ARG56 |
| 2 | -2.66 | 1.12x104 | A:ASP53  | A:LEU52A:PRO55A:ARG56 |
| 3 | -2.64 | 1.15x104 | A:ASP53  | A:LEU52A:PRO55A:ARG56 |
| 4 | -2.61 | 1.22x104 | /  | A:LEU52A:PRO55A:ARG56 |
| 5 | -2.29 | 2.11x104 | A:ARG56 | A:PRO55A:ARG56A:LEU52 |
| 6 | -2.27 | 2.16x104 | A:ASP53A:ARG60 | A:ARG56  |
| 7 | -2.26 | 2.19x104 | A:ARG56 | A:PRO55A:ARG56A:LEU52 |
| 8 | -1.97 | 3.62x104 | A:ASN64 | A:MET69A:LEU65 |
| 9 | -1.94 | 3.79x104 | / | A:LEU52A:PRO55A:ARG56 |
| 10 | -1.79 | 4.84x104 | / | A:TYR73A:MET69A:LEU70 |

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**Fig. S1**. IR spectrum of kaempferol.



**Fig. S2**. Raman spectrum of kaempferol.



**Fig. S3**: 13C NMR spectrum of kaempferol in DMSO.



**Fig. S4.** 1H NMR spectrum of kaempferol in DMSO.