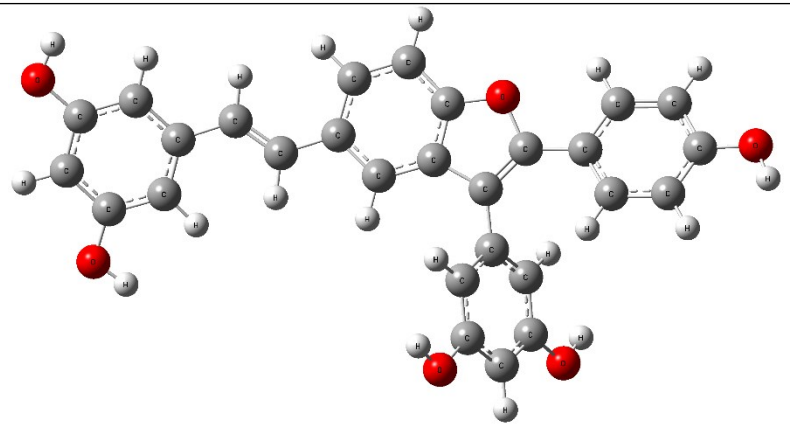
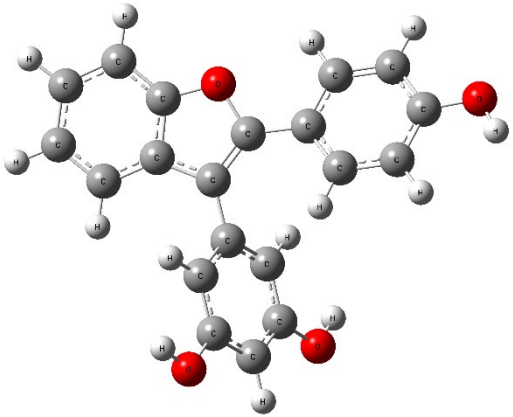
Electronic Supplementary Material (ESI) for RSC Advances.

Compound **1**



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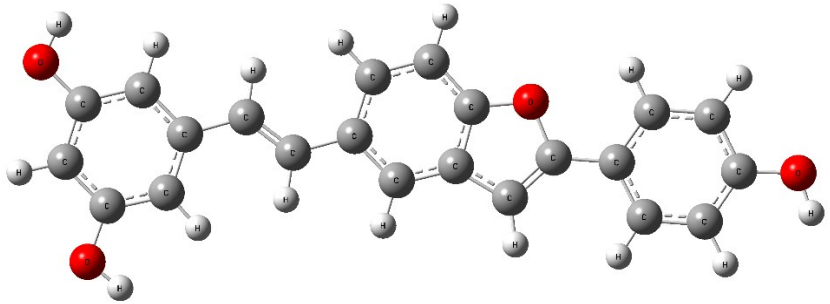

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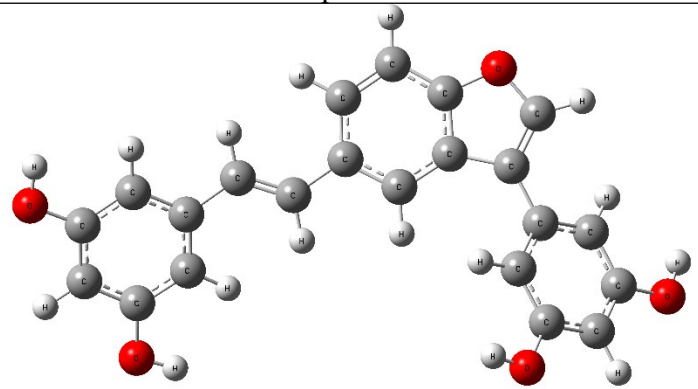
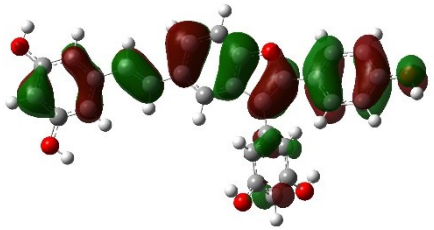
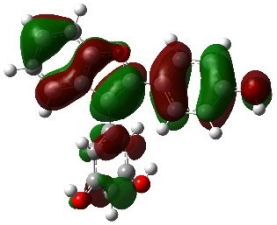
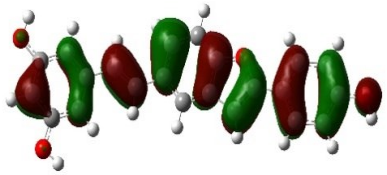
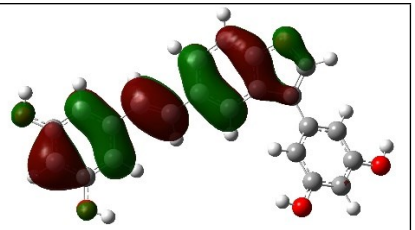
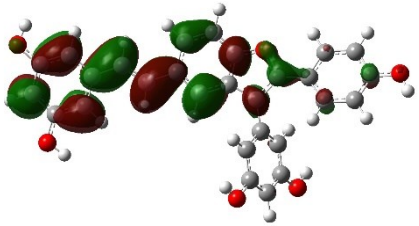
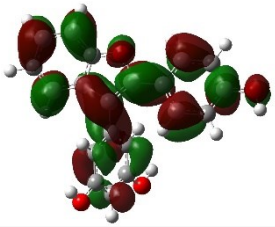
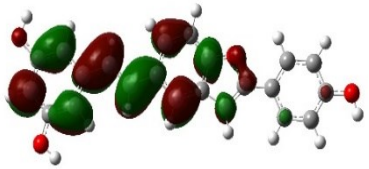
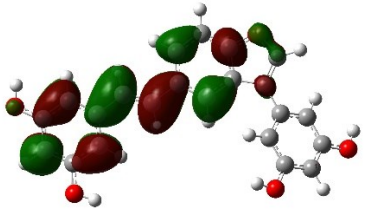
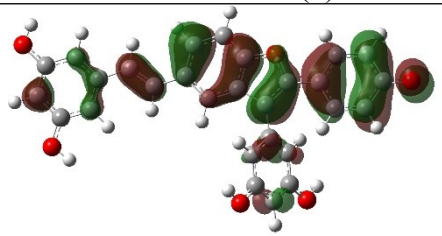
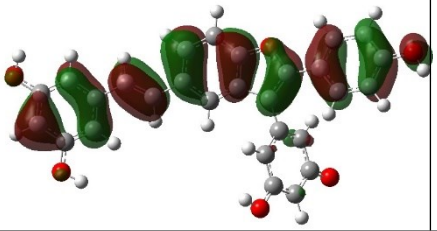
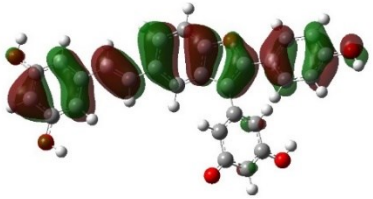
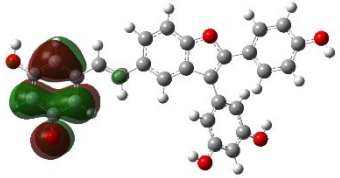
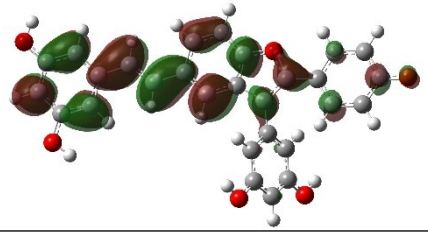
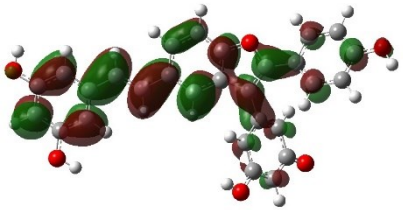
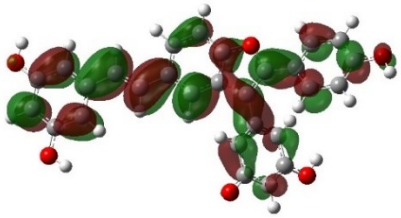
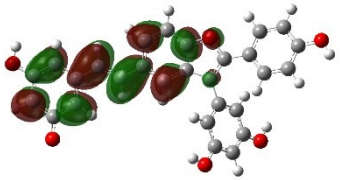
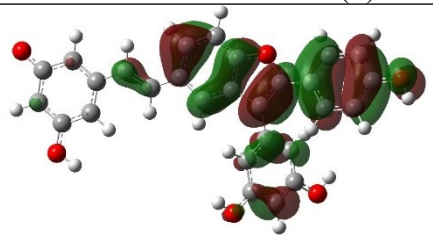
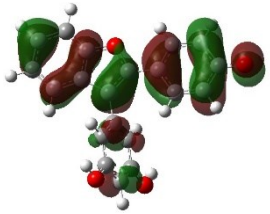
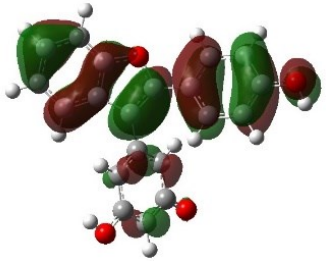
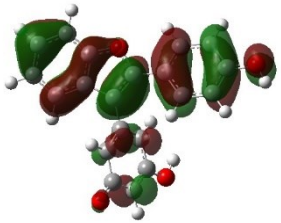
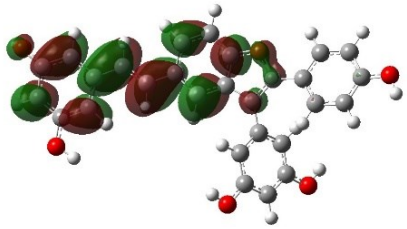
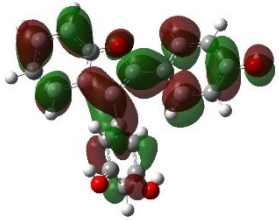
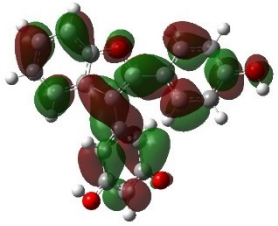
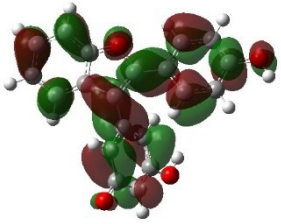
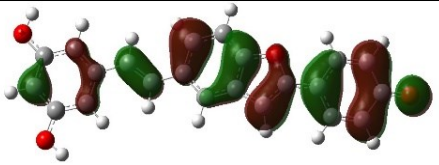
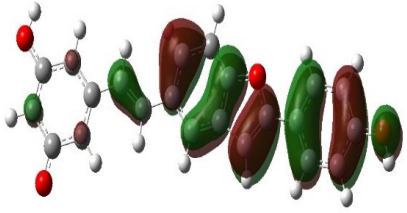
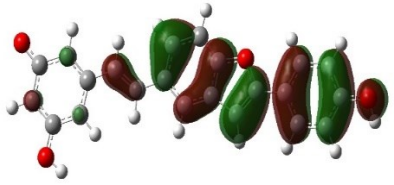
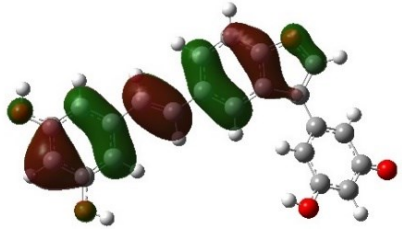


Compound **4**

**Fig. S1.** The state forms of studied compounds **1-4** in studied media at B3LYP/6-311G(d,p) level of theory

| | | | |
|---|---|---|---|
|  |  |  |  |
| HOMO-neutral (**1**) | HOMO-neutral (**2**) | HOMO-neutral (**3**) | HOMO-neutral (**4**) |
|  |  |  |  |
| LUMO-neutral (**1**) | LUMO-neutral (**2**) | LUMO-neutral (**3**) | LUMO-neutral (**4**) |
|  |  |  |  |
| HOMO-4'-OH radical (**1**) | HOMO-3''-OH radical (**1**) | HOMO-5''-OH radical (**1**) | HOMO-3'''-OH radical (**1**) |

| | | | |
|---|---|---|---|
|  |  |  |  |
| LUMO-4'-OH radical (**1**) | LUMO-3"-OH radical (**1**) | LUMO-5"-OH radical (**1**) | LUMO-3'"-OH radical (**1**) |
|  |  |  |  |
| HOMO-5'"-OH radical (**1**) | HOMO-4'-OH radical (**2**) | HOMO-3"-OH radical (**2**) | HOMO-5"-OH radical (**2**) |
|  |  |  |  |
| LUMO-5'"-OH radical (**1**) | LUMO-4'-OH radical (**2**) | LUMO-3"-OH radical (**2**) | LUMO-5"-OH radical (**2**) |
|  |  |  |  |
| HOMO-4'-OH radical (**3**) | HOMO-3'"-OH radical (**3**) | HOMO-5'"-OH radical (**3**) | HOMO-3"-OH radical (**4**) |

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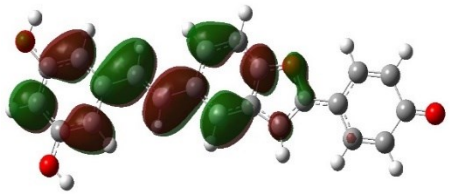
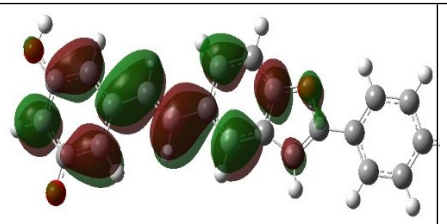
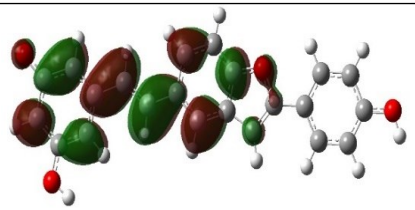
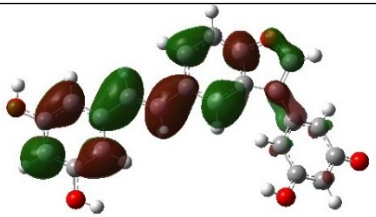
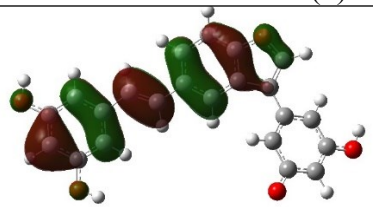
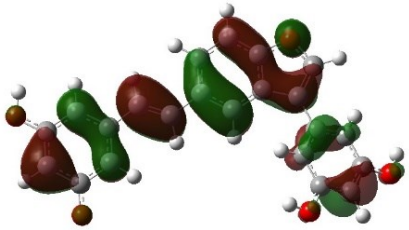
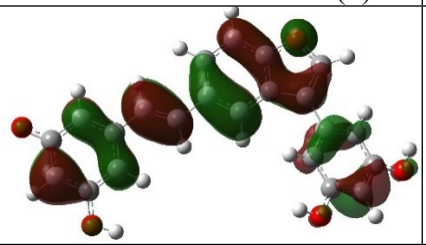
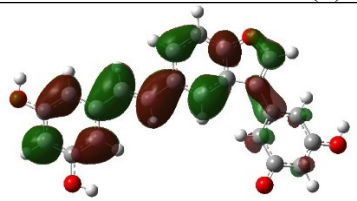
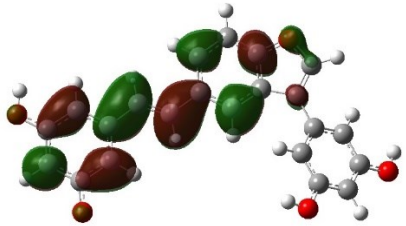
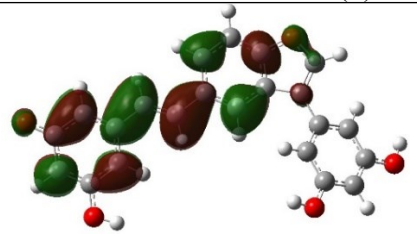
|---|---|---|---|
|  |  |  |  |
| LUMO-4'-OH radical (**3**) | LUMO-3'''-OH radical (**3**) | LUMO-5'''-OH radical (**3**) | LUMO-3''-OH radical (**4**) |
|  |  |  | |
| HOMO-5''-OH radical (**4**) | HOMO-3'''-OH radical (**4**) | HOMO-5'''-OH radical (**4**) | |
|  |  |  | |
| LUMO-5''-OH radical (**4**) | LUMO-3'''-OH radical (**4**) | LUMO-5'''-OH radical (**4**) | |

**Fig. S2.** HOMO and LUMO images of neutral and radical forms of compounds **1-4** in all studied mediums at B3LYP/6-311G(d,p) level of theory

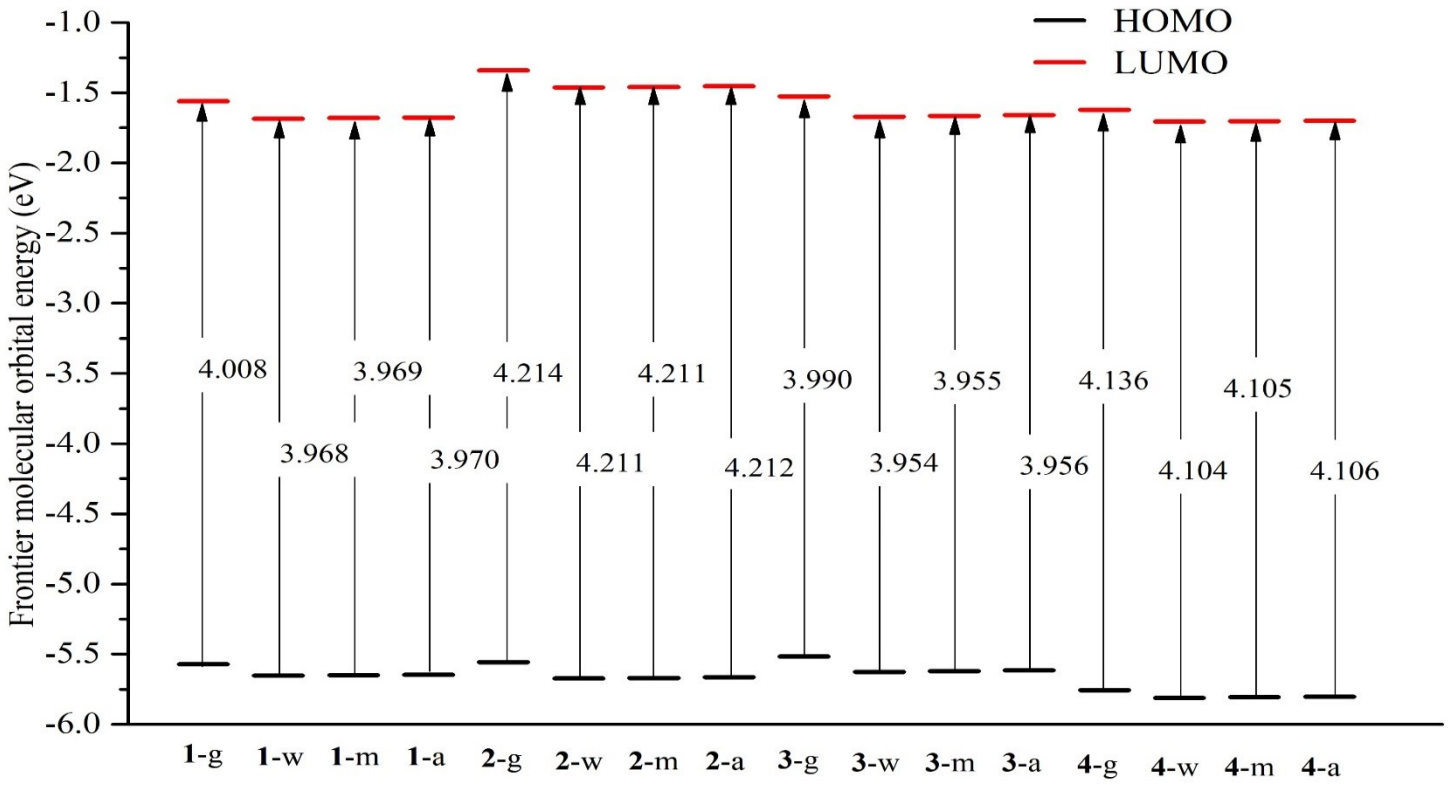
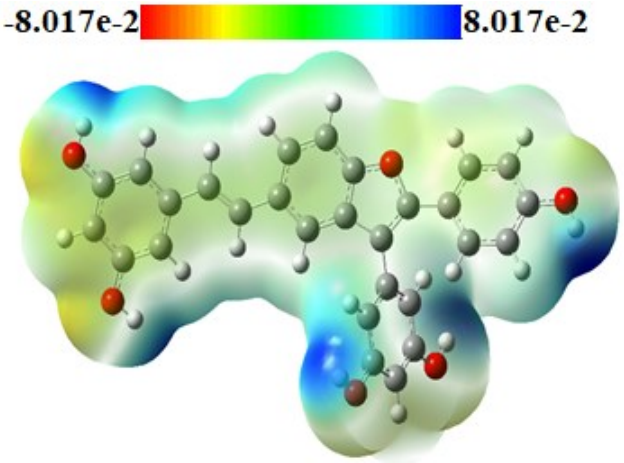
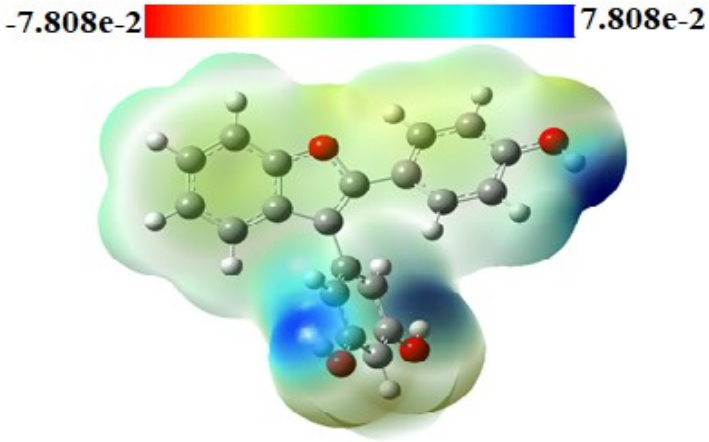


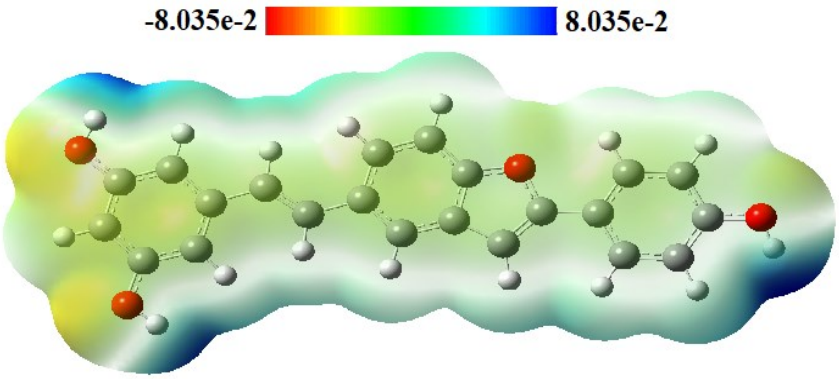

**Fig. S3.** Egap = $E_L - E_H$ of the neutral structures **1-4** in four studied mediums at B3LYP/6-311G(d,p) level of theory



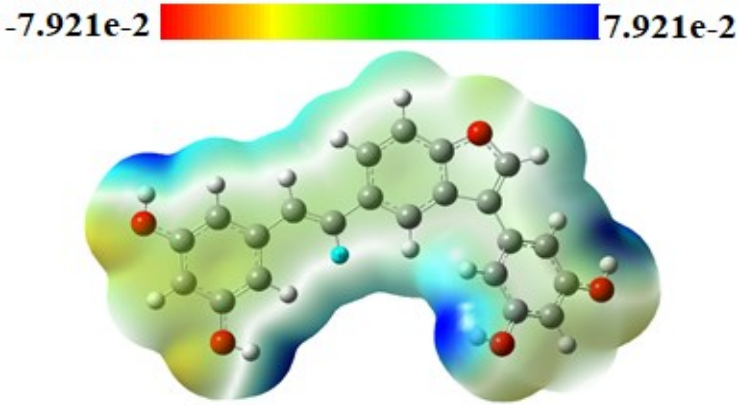

Compound **1**




Compound **2**

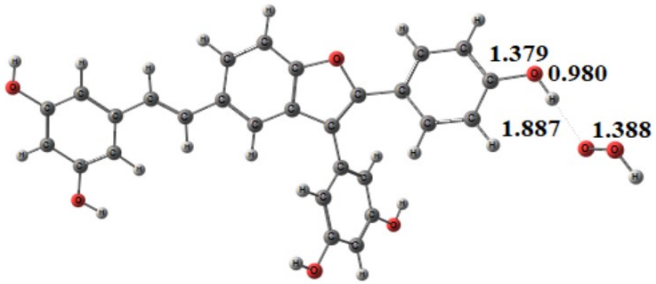
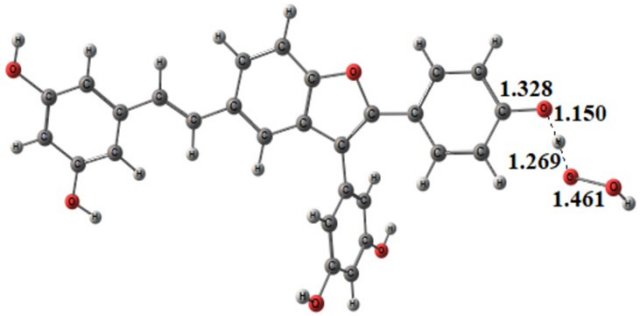
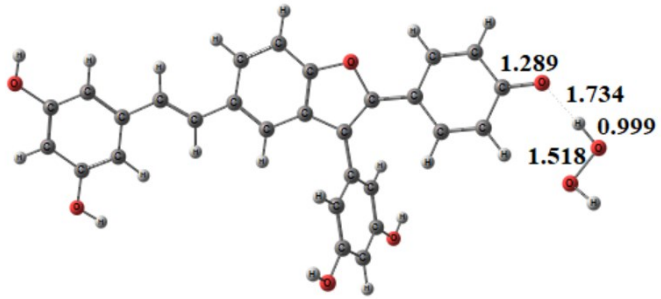
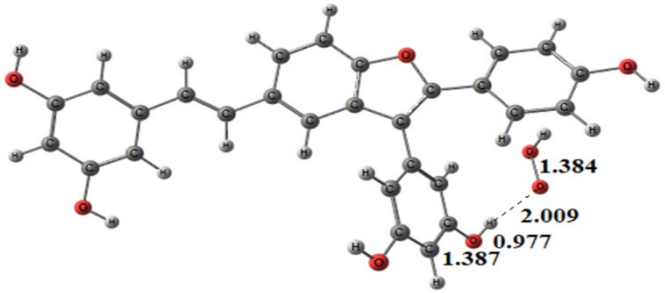
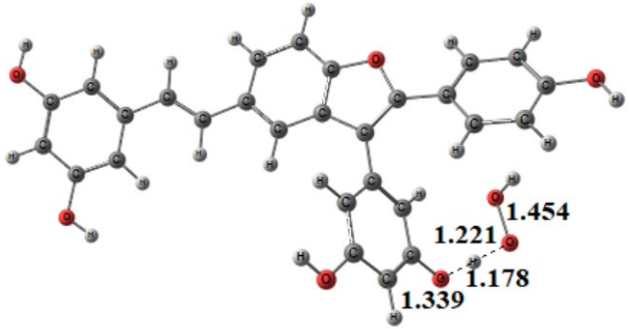
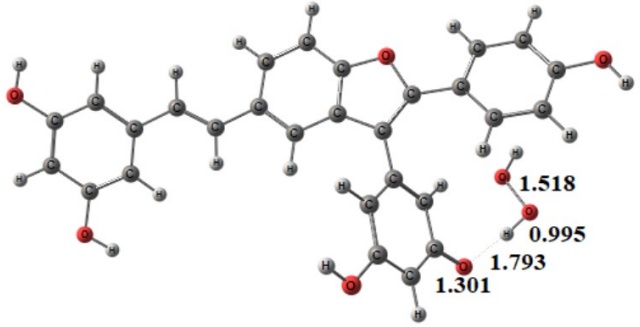


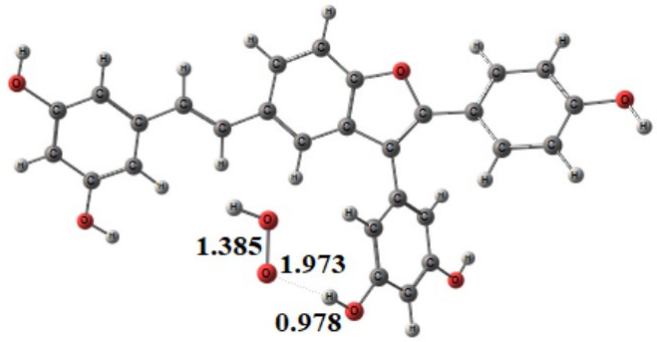
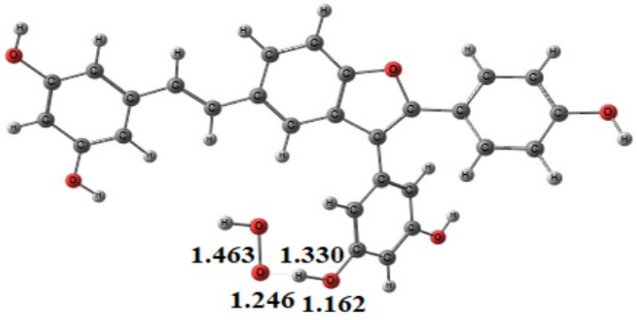
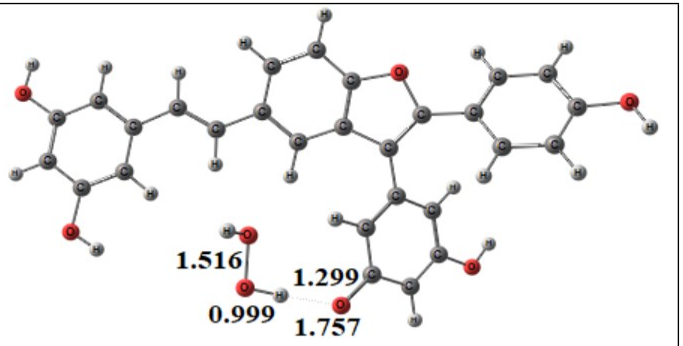
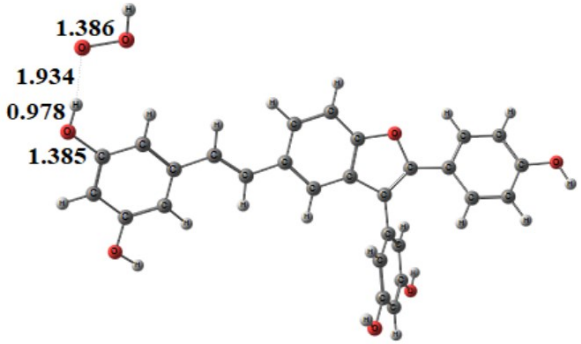
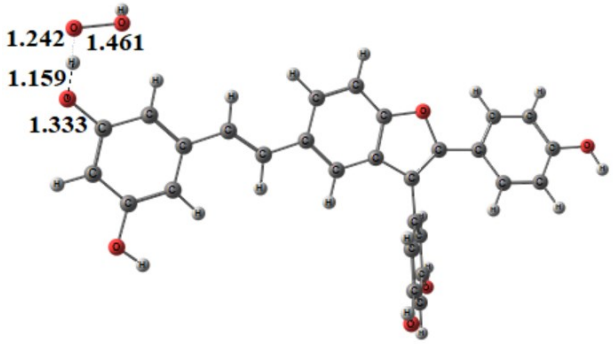
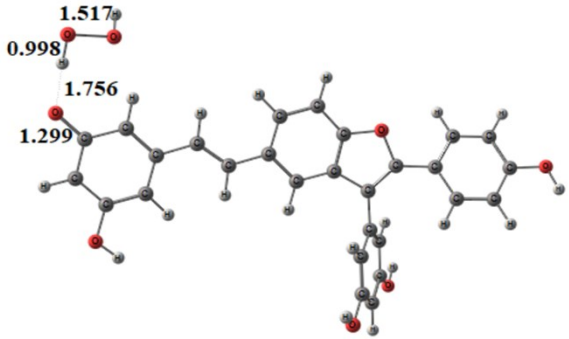
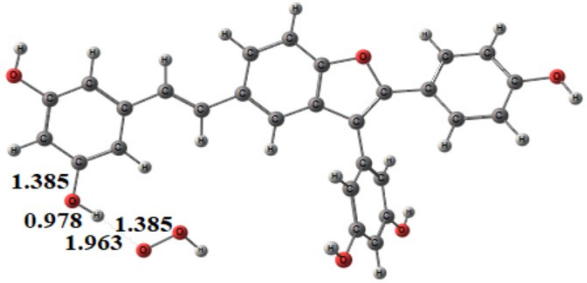
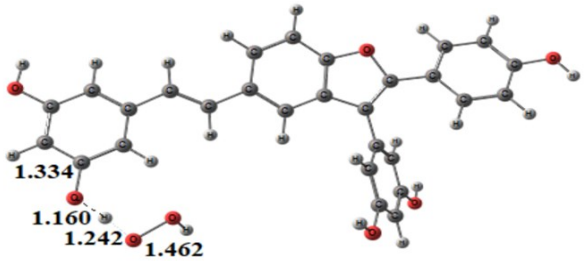
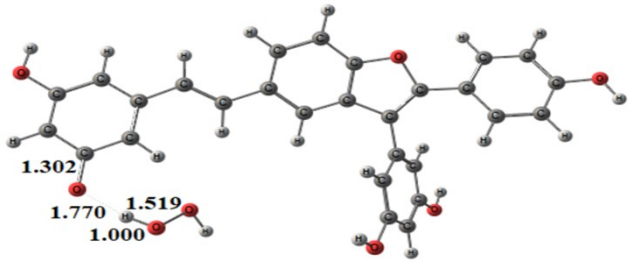

Compound **3**

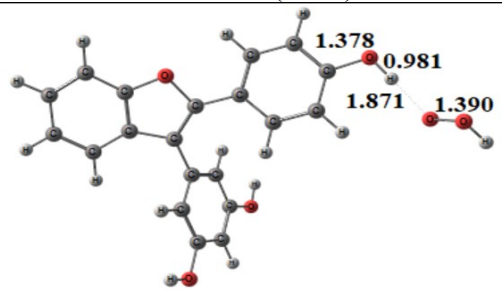
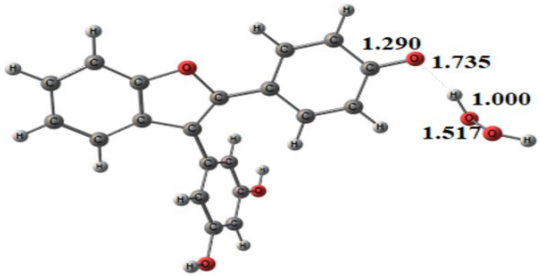
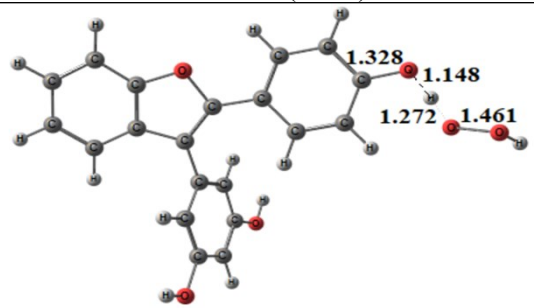
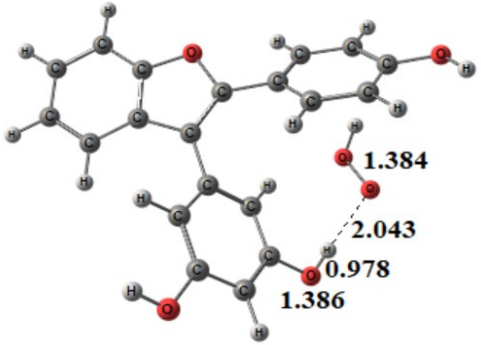
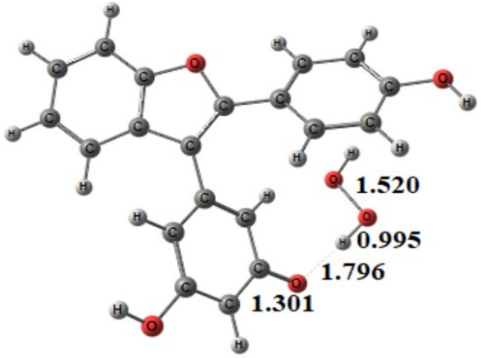
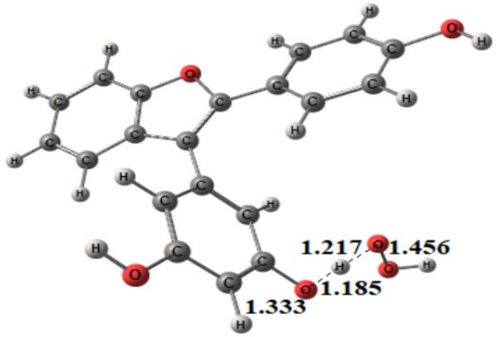


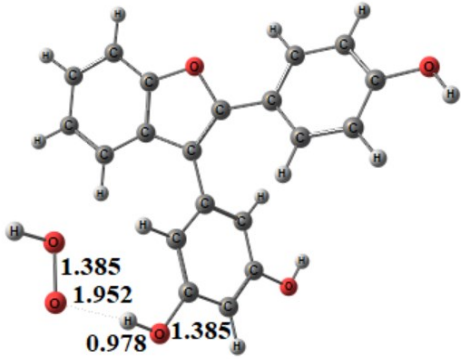
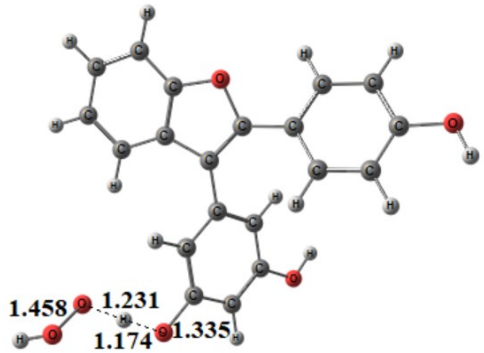
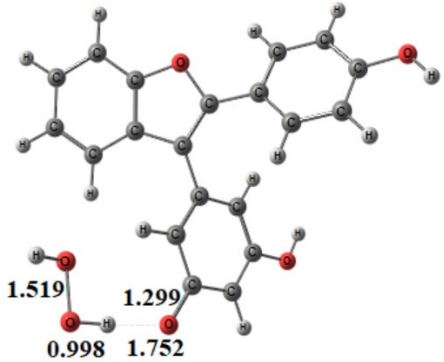
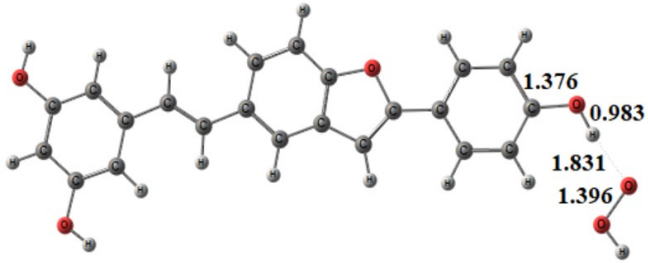
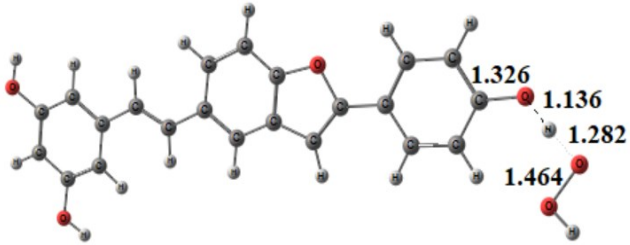
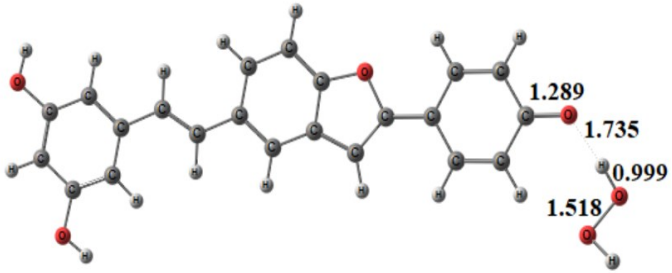
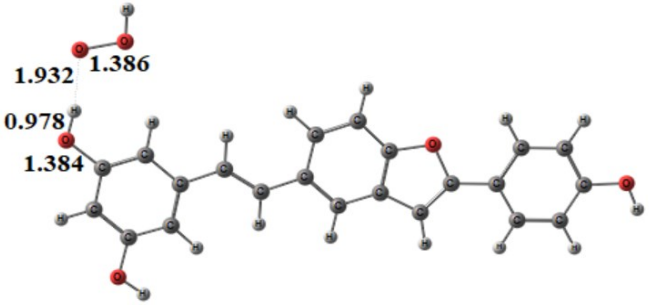
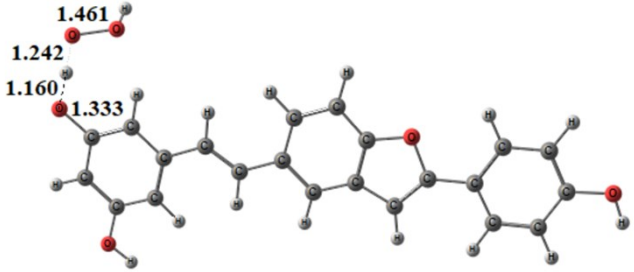
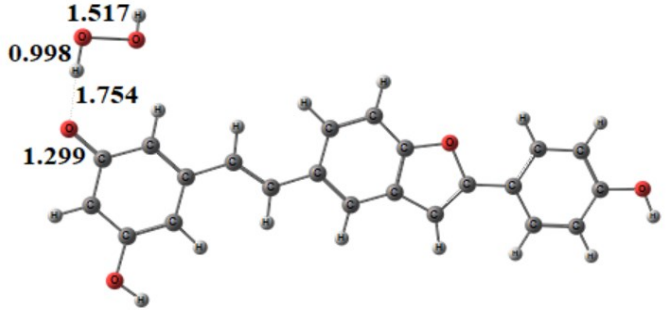

Compound **4**

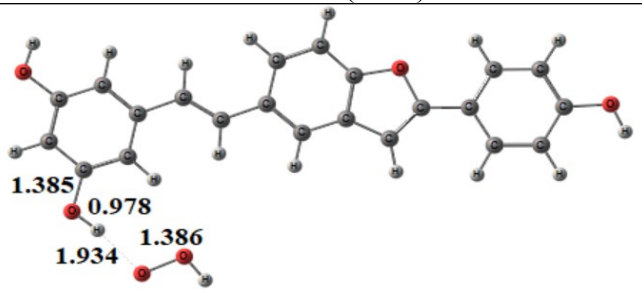
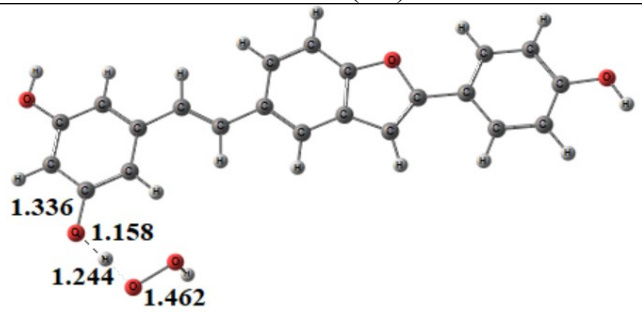
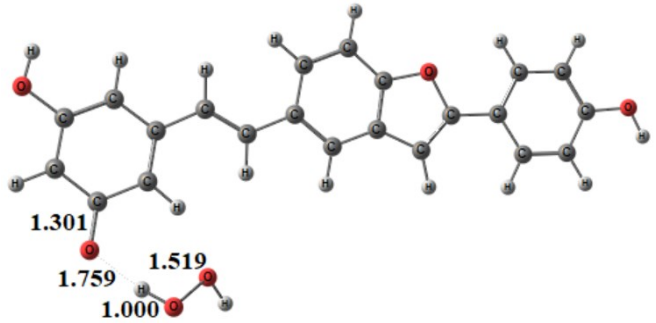
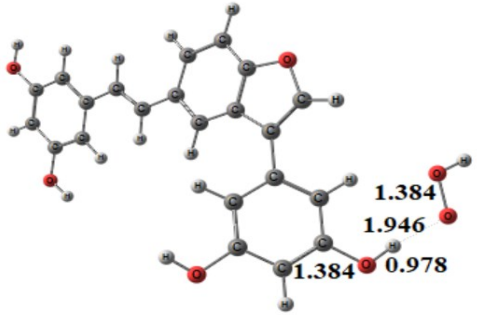
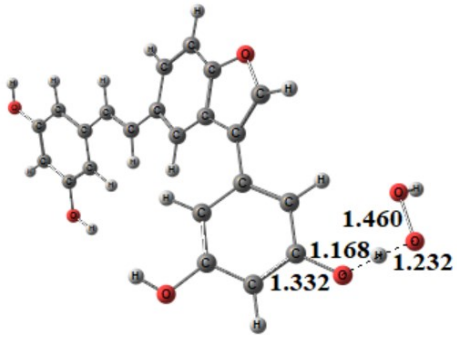
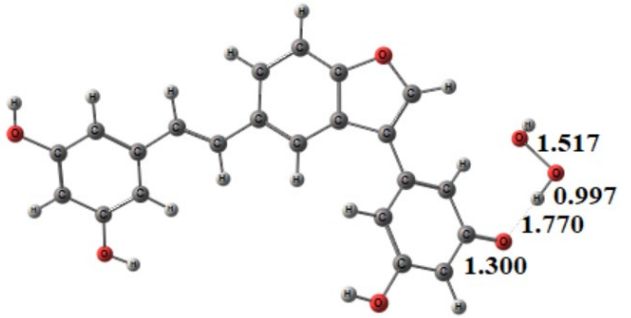
**Fig. S4**. Molecular electrostatic potential map on the isodensity surfaces in gaseous phase at B3LYP/6-311G(d,p) level of theory

| | | |
|---|---|---|
|  |  |  |
| **1**-4'-OH (Int-1) | **1**-4'-OH (TS) | **1**-4'-OH (Int-2) |
|  |  |  |
| **1**-3"-OH (Int-1) | **1**-3"-OH (TS) | **1**-3"-OH (Int-2) |

| | | |
|---|---|---|
|  |  |  |
| **1**-5"-OH (Int-1) | **1**-5"-OH (TS) | **1**-5"-OH (Int-2) |
|  |  |  |
| **1**-3'''-OH (Int-1) | **1**-3'''-OH (TS) | **1**-3'''-OH (Int-2) |
|  |  |  |

| **1**-5'''-OH (Int-1) | **1**-5'''-OH (TS) | **1**-5'''-OH (Int-2) |
|---|---|---|
|  |  |  |
| **2**-4'-OH (Int-1) | **2**-4'-OH (TS) | **2**-4'-OH (Int-2) |
|  |  |  |
| **2**-3"-OH (Int-1) | **2**-3"-OH (TS) | **2**-3"-OH (Int-2) |

| | | |
|---|---|---|
|  |  |  |
| **2**-5"-OH (Int-1) | **2**-5"-OH (TS) | **2**-5"-OH (Int-2) |
|  |  |  |
| **3**-4'-OH (Int-1) | **3**-4'-OH (TS) | **3**-4'-OH (Int-2) |
|  |  |  |

| **3**-3'''-OH (Int-1) | **3**-3'''-OH (TS) | **3**-3'''-OH (Int-2) |
|---|---|---|
|  |  |  |
| **3**-5'''-OH (Int-1) | **3**-5'''-OH (TS) | **3**-5'''-OH (Int-2) |
|  |  |  |
| **4**-3"-OH (Int-1) | **4**-3"-OH (TS) | **4**-3"-OH (Int-2) |

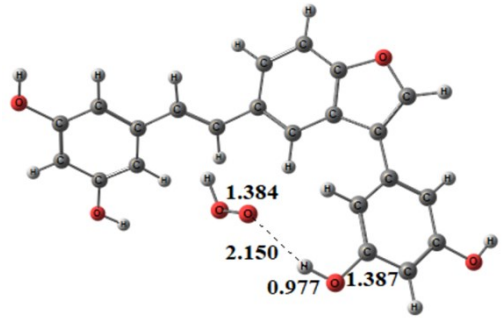
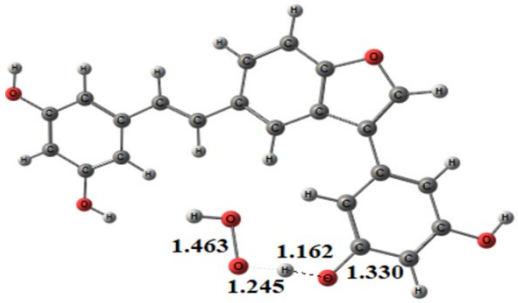
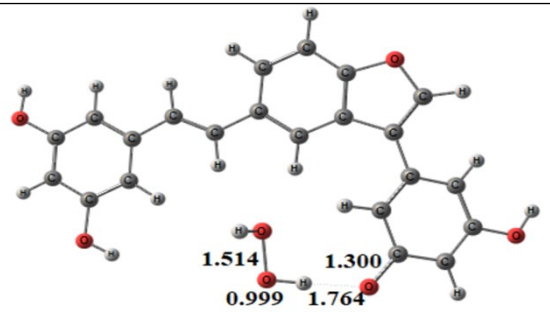
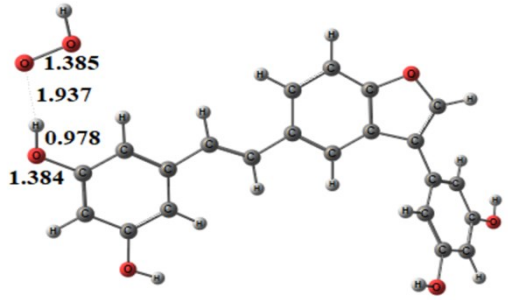
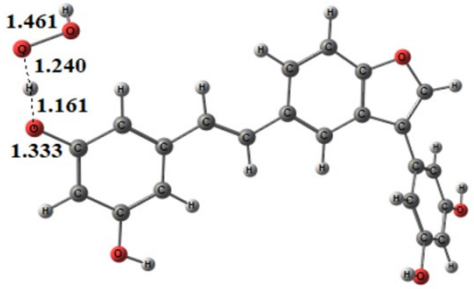
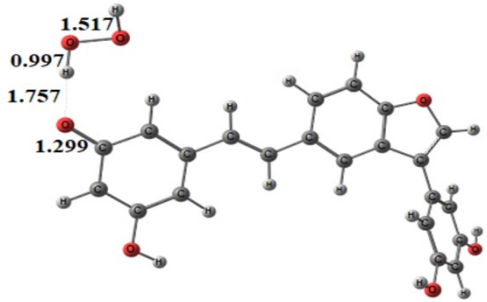
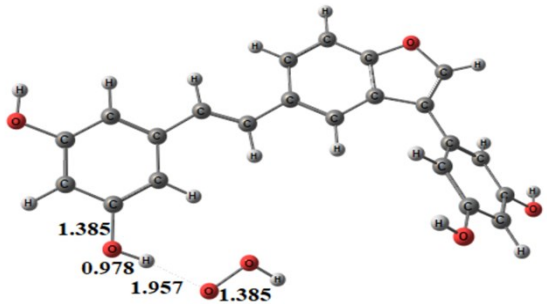
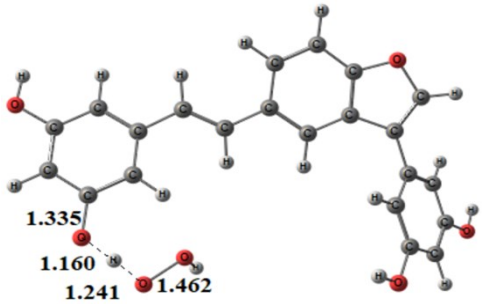
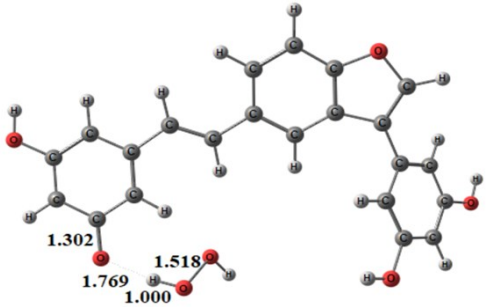
| | | |
|---|---|---|
|  |  |  |
| **4**-5''-OH (Int-1) | **4**-5''-OH (TS) | **4**-5''-OH (Int-2) |
|  |  |  |
| **4**-3'''-OH (Int-1) | **4**-3'''-OH (TS) | **4**-3'''-OH (Int-2) |
|  |  |  |
| **4**-5'''-OH (Int-1) | **4**-5'''-OH (TS) | **4**-5'''-OH (Int-2) |

**Fig. S5**. The optimized structures of intermediates and transition states of HOO• attack to the compounds **1-4** at B3LYP/6-311G(d,p) level

**Table S1** Optimized bond distances and dihedral angles (θ) of studied compounds **1-4** in mediums gas, methanol, water and acetone at B3LYP/6-311G(d,p) level of theory

| No | | Bond lengths | | | | | Dihedral angles | |
|---|---|---|---|---|---|---|---|---|
| | | 4' (O-H) | 3" (O-H) | 5"(O-H) | 3"'(O-H) | 5"'(O-H) | $\theta_{11}$(C3-C2-C1'-C2') | $\theta_{12}$(C2-C3-C1"-C2") |
| **1** | Gas | 0.963 | 0.963 | 0.963 | 0.963 | 0.963 | −22.0 | −57.3 |
| | Water | 0.965 | 0.964 | 0.964 | 0.964 | 0.964 | −24.7 | −55.0 |
| | Methanol | 0.965 | 0.964 | 0.964 | 0.964 | 0.964 | −24.6 | −55.2 |
| | Acetone | 0.965 | 0.964 | 0.964 | 0.964 | 0.964 | −24.4 | −55.4 |
| **2** | Gas | 0.963 | 0.963 | 0.963 | | | −21.4 | −57.9 |
| | Water | 0.965 | 0.965 | 0.964 | | | −23.8 | −55.3 |
| | Methanol | 0.965 | 0.964 | 0.964 | | | −23.8 | −55.4 |
| | Acetone | 0.965 | 0.964 | 0.964 | | | −23.7 | −55.5 |
| **3** | Gas | 0.963 | | | 0.963 | 0.963 | 0.0 | |
| | Water | 0.965 | | | 0.965 | 0.965 | 0.0 | |
| | Methanol | 0.965 | | | 0.965 | 0.965 | 0.0 | |
| | Acetone | 0.965 | | | 0.965 | 0.965 | 0.0 | |
| **4** | Gas | | 0.963 | 0.963 | 0.963 | 0.963 | | −42.8 |
| | Water | | 0.965 | 0.964 | 0.964 | 0.964 | | −38.1 |
| | Methanol | | 0.965 | 0.964 | 0.964 | 0.964 | | −38.7 |
| | Acetone | | 0.965 | 0.964 | 0.964 | 0.964 | | −39.1 |

**Table S2** The optimized energies versus torsional angles (θ) at B3LYP/6-311G(d) level of theory

| Degree | $\theta_{11}$(C3-C2-C1'-C2') | | $\theta_{12}$(C2-C3-C1"-C2") | | $\theta_{11}$(C3-C2-C1'-C2') | | $\theta_{12}$(C2-C3-C1"-C2") | |
|---|---|---|---|---|---|---|---|---|
| | Compound **1** (au) | ΔE (kcal/mol) | Compound **1** (au) | ΔE (kcal/mol) | Compound **2** (au) | ΔE (kcal/mol) | Compound **2** (au) | ΔE (kcal/mol) |
| −180 | −1530.742395 | 0.40 | −1530.732391 | **6.68** | −1071.723044 | 0.39 | −1071.713396 | **6.44** |
| −170 | −1530.742799 | 0.15 | −1530.735894 | 4.48 | −1071.723433 | 0.14 | −1071.716714 | 4.36 |
| −160 | −1530.743036 | **0.00** | −1530.738923 | 2.58 | −1071.723661 | **0.00** | −1071.719716 | 2.47 |
| −150 | −1530.742762 | 0.17 | −1530.741127 | 1.19 | −1071.723385 | 0.17 | −1071.721833 | 1.14 |
| −140 | −1530.742092 | 0.59 | −1530.742367 | 0.42 | −1071.722752 | 0.57 | −1071.723073 | 0.37 |
| −130 | −1530.741009 | 1.27 | −1530.742965 | 0.04 | −1071.721622 | 1.28 | −1071.723604 | 0.03 |
| −120 | −1530.739643 | 2.13 | −1530.743029 | **0.00** | −1071.720278 | 2.12 | −1071.723656 | **0.00** |
| −110 | −1530.738174 | 3.05 | −1530.742781 | 0.16 | −1071.718813 | 3.04 | −1071.723423 | 0.15 |
| −100 | −1530.736816 | 3.90 | −1530.742505 | 0.33 | −1071.717482 | 3.88 | −1071.723126 | 0.33 |
| −90 | −1530.735946 | 4.45 | −1530.742381 | **0.41** | −1071.716584 | 4.44 | −1071.723039 | **0.39** |
| −80 | −1530.735661 | **4.63** | −1530.742552 | 0.30 | −1071.716318 | **4.61** | −1071.723177 | 0.30 |
| −70 | −1530.735995 | 4.42 | −1530.742826 | 0.13 | −1071.716607 | 4.43 | −1071.723465 | 0.12 |
| −60 | −1530.739955 | 1.93 | −1530.743029 | **0.00** | −1071.720596 | 1.92 | −1071.723656 | **0.00** |
| −50 | −1530.741287 | 1.10 | −1530.742904 | 0.08 | −1071.721911 | 1.10 | −1071.723558 | 0.06 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| –40 | −1530.742316 | 0.45 | −1530.742229 | 0.50 | −1071.722989 | 0.42 | −1071.722925 | 0.46 |
| –30 | −1530.742907 | 0.08 | −1530.740876 | 1.35 | −1071.723517 | 0.09 | −1071.721573 | 1.31 |
| –20 | −1530.743036 | **0.00** | −1530.738631 | 2.76 | −1071.723661 | **0.00** | −1071.719408 | 2.67 |
| –10 | −1530.742799 | 0.15 | −1530.735629 | 4.64 | −1071.723420 | 0.15 | −1071.716430 | 4.53 |
| 0 | −1530.742401 | **0.40** | −1530.732040 | **6.90** | −1071.723061 | **0.38** | −1071.713016 | **6.68** |
| 10 | −1530.742799 | 0.15 | −1530.735651 | 4.63 | −1071.723420 | 0.15 | −1071.716460 | 4.52 |
| 20 | −1530.743036 | **0.00** | −1530.738620 | 2.77 | −1071.723661 | **0.00** | −1071.719412 | 2.66 |
| 30 | −1530.742907 | 0.08 | −1530.740843 | 1.37 | −1071.723517 | 0.09 | −1071.721548 | 1.32 |
| 40 | −1530.742316 | 0.45 | −1530.742177 | 0.53 | −1071.722989 | 0.42 | −1071.722873 | 0.49 |
| 50 | −1530.741287 | 1.10 | −1530.742841 | 0.12 | −1071.721911 | 1.10 | −1071.723504 | 0.10 |
| 60 | −1530.739955 | 1.93 | −1530.743029 | **0.00** | −1071.720597 | 1.92 | −1071.723602 | **0.00** |
| 70 | −1530.738537 | 2.82 | −1530.742760 | 0.17 | −1071.719164 | 2.82 | −1071.723396 | 0.16 |
| 80 | −1530.737259 | 3.63 | −1530.742493 | 0.34 | −1071.717906 | 3.61 | −1071.723124 | 0.33 |
| 90 | −1530.736384 | 4.17 | −1530.742336 | **0.43** | −1071.717017 | 4.17 | −1071.722998 | **0.41** |
| 100 | −1530.735944 | **4.45** | −1530.742445 | 0.37 | −1071.716603 | **4.43** | −1071.723075 | 0.36 |
| 110 | −1530.735986 | 4.42 | −1530.742711 | 0.20 | −1071.716600 | 4.43 | −1071.723352 | 0.19 |
| 120 | −1530.739643 | 2.13 | −1530.743029 | **0.00** | −1071.720278 | 2.12 | −1071.723656 | **0.00** |
| 130 | −1530.741009 | 1.27 | −1530.742904 | 0.08 | −1071.721622 | 1.28 | −1071.723553 | 0.06 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 140 | −1530.742092 | 0.59 | −1530.742320 | 0.44 | −1071.722752 | 0.57 | −1071.723021 | 0.40 |
| 150 | −1530.742762 | 0.17 | −1530.741098 | 1.21 | −1071.723385 | 0.17 | −1071.721810 | 1.16 |
| 160 | −1530.743036 | **0.00** | −1530.738914 | 2.58 | −1071.723661 | **0.00** | −1071.719720 | 2.47 |
| 170 | −1530.742799 | 0.15 | −1530.735914 | 4.46 | −1071.723433 | 0.14 | −1071.716738 | 4.34 |
| 180 | −1530.742395 | 0.40 | −1530.732391 | **6.68** | −1071.723044 | 0.39 | −1071.713396 | **6.44** |
| Degree | $\theta_{11}$(C3-C2-C1'-C2') | | | | | | $\theta_{12}$(C2-C3-C1"-C2") | |
| | Compound **3** (au) | ΔE (kcal/mol) | | | | | Compound **4** (au) | ΔE (kcal/mol) |
| −180 | −1149.148565 | **0.00** | | | | | −1224.380416 | **2.75** |
| −170 | −1149.092597 | 0.06 | | | | | −1224.381332 | 2.18 |
| −160 | −1148.909979 | 0.24 | | | | | −1224.382857 | 1.22 |
| −150 | −1148.523069 | 0.63 | | | | | −1224.384265 | 0.34 |
| −140 | −1147.914680 | 1.23 | | | | | −1224.384799 | **0.00** |
| −130 | −1147.091162 | 2.06 | | | | | −1224.384700 | 0.06 |
| −120 | −1146.121446 | 3.03 | | | | | −1224.384085 | 0.45 |
| −110 | −1145.151630 | 4.00 | | | | | −1224.383295 | 0.94 |
| −100 | −1144.378281 | 4.77 | | | | | −1224.382613 | 1.37 |
| −90 | −1144.132837 | **5.02** | | | | | −1224.382399 | **1.51** |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| −80 | −1144.406005 | 4.74 | | | | | −1224.382651 | 1.35 |
| −70 | −1145.127383 | 4.02 | | | | | −1224.383314 | 0.93 |
| −60 | −1146.044859 | 3.10 | | | | | −1224.384057 | 0.47 |
| −50 | −1146.993716 | 2.15 | | | | | −1224.384682 | 0.07 |
| −40 | −1147.804420 | 1.34 | | | | | −1224.384799 | **0.00** |
| −30 | −1148.406076 | 0.74 | | | | | −1224.384354 | 0.28 |
| −20 | −1148.785958 | 0.36 | | | | | −1224.383257 | 0.97 |
| −10 | −1148.964070 | 0.18 | | | | | −1224.381693 | 1.95 |
| 0 | −1149.148565 | **0.00** | | | | | −1224.380417 | **2.75** |
| 10 | −1148.964102 | 0.18 | | | | | −1224.381507 | 2.07 |
| 20 | −1148.785877 | 0.36 | | | | | −1224.383257 | 0.97 |
| 30 | −1148.406089 | 0.74 | | | | | −1224.384354 | 0.28 |
| 40 | −1147.804420 | 1.34 | | | | | −1224.384799 | **0.00** |
| 50 | −1146.993703 | 2.15 | | | | | −1224.384682 | 0.07 |
| 60 | −1146.044871 | 3.10 | | | | | −1224.384086 | 0.45 |
| 70 | −1145.118341 | 4.03 | | | | | −1224.383332 | 0.92 |
| 80 | −1144.392482 | 4.76 | | | | | −1224.382651 | 1.35 |
| 90 | −1144.132843 | **5.02** | | | | | −1224.382398 | **1.51** |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 100 | −1144.394603 | 4.75 | | | | | −1224.382613 | 1.37 |
| 110 | −1145.146460 | 4.00 | | | | | −1224.383279 | 0.95 |
| 120 | −1146.121440 | 3.03 | | | | | −1224.384057 | 0.47 |
| 130 | −1147.091155 | 2.06 | | | | | −1224.384700 | 0.06 |
| 140 | −1147.914680 | 1.23 | | | | | −1224.384799 | **0.00** |
| 150 | −1148.523032 | 0.63 | | | | | −1224.384265 | 0.34 |
| 160 | −1148.909948 | 0.24 | | | | | −1224.383068 | 1.09 |
| 170 | −1149.092616 | 0.06 | | | | | −1224.381505 | 2.07 |
| 180 | −1149.148565 | **0.00** | | | | | −1224.380416 | **2.75** |

**Table S3** Chemical reactivity indices obtained using DFT method in the studied mediums at B3LYP/6-311G(d,p) level of theory

| No | Medium | η (eV) | χ (eV) | μ (eV) | ω (eV) | | | Polarizability (au) | $E_{HOMO}$ (eV) | $E_{LUMO}$ (eV) |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | ω | $\omega^-$ | $\omega^+$ | | | |
| **1** | Gas | 2.004 | 3.566 | −3.566 | 3.172 | 5.206 | 1.640 | 394.760 | −5.570 | −1.562 |
| | Water | 1.984 | 3.669 | −3.669 | 3.393 | 5.476 | 1.806 | 525.107 | −5.653 | −1.685 |
| | Methanol | 1.985 | 3.665 | −3.665 | 3.384 | 5.465 | 1.800 | 520.533 | −5.649 | −1.680 |
| | Acetone | 1.985 | 3.661 | −3.661 | 3.376 | 5.454 | 1.793 | 516.088 | −5.646 | −1.676 |
| **2** | Gas | 2.107 | 3.449 | −3.449 | 2.823 | 4.811 | 1.362 | 247.853 | −5.556 | −1.342 |
| | Water | 2.105 | 3.568 | −3.568 | 3.023 | 5.071 | 1.503 | 339.324 | −5.673 | −1.463 |
| | Methanol | 2.106 | 3.563 | −3.563 | 3.015 | 5.060 | 1.497 | 336.008 | −5.669 | −1.458 |
| | Acetone | 2.106 | 3.559 | −3.559 | 3.007 | 5.049 | 1.491 | 332.801 | −5.664 | −1.453 |
| **3** | Gas | 1.995 | 3.522 | −3.522 | 3.109 | 5.119 | 1.597 | 323.816 | −5.517 | −1.527 |
| | Water | 1.977 | 3.648 | −3.648 | 3.365 | 5.436 | 1.788 | 425.582 | −5.625 | −1.671 |
| | Methanol | 1.977 | 3.642 | −3.642 | 3.354 | 5.423 | 1.780 | 422.234 | −5.620 | −1.665 |
| | Acetone | 1.978 | 3.637 | −3.637 | 3.344 | 5.410 | 1.773 | 418.961 | −5.615 | −1.659 |
| **4** | Gas | 2.068 | 3.688 | −3.688 | 3.288 | 5.390 | 1.703 | 294.364 | −5.756 | −1.620 |
| | Water | 2.052 | 3.758 | −3.758 | 3.441 | 5.576 | 1.819 | 395.357 | −5.810 | −1.706 |
| | Methanol | 2.052 | 3.754 | −3.754 | 3.435 | 5.568 | 1.814 | 391.815 | −5.806 | −1.702 |
| | Acetone | 2.052 | 3.751 | −3.751 | 3.429 | 5.560 | 1.810 | 388.396 | −5.803 | −1.699 |

**Table S4** Condensed Fukui indices of studied compounds in the gaseous medium at B3LYP/6-311G(d,p) level of theory

| No | **1** | | | | **2** | | | | **3** | | | | **4** | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | $f_t^+$ | $f_t^-$ | $f_t^o$ | $\Delta f_t$ | $f_t^+$ | $f_t^-$ | $f_t^o$ | $\Delta f_t$ | $f_t^+$ | $f_t^-$ | $f_t^o$ | $\Delta f_t$ | $f_t^+$ | $f_t^-$ | $f_t^o$ | $\Delta f_t$ |
| C-2 | 0.029 | 0.027 | 0.028 | 0.002 | 0.047 | 0.043 | 0.045 | 0.004 | 0.017 | 0.016 | 0.017 | 0.001 | 0.041 | 0.024 | 0.033 | 0.017 |
| C-3 | 0.033 | 0.022 | 0.028 | 0.011 | 0.040 | 0.046 | 0.043 | −0.006 | 0.051 | 0.042 | 0.047 | 0.009 | 0.011 | 0.013 | 0.012 | −0.002 |
| C-3a | −0.012 | −0.003 | −0.008 | −0.009 | −0.001 | −0.003 | −0.002 | 0.002 | −0.021 | −0.009 | −0.015 | −0.012 | −0.013 | −0.009 | −0.011 | −0.004 |
| C-4 | 0.055 | 0.028 | 0.042 | 0.026 | 0.051 | 0.040 | 0.046 | 0.011 | 0.060 | 0.030 | 0.045 | 0.030 | 0.049 | 0.051 | 0.050 | −0.002 |
| C-5 | −0.003 | −0.006 | −0.005 | 0.003 | 0.009 | 0.014 | 0.012 | −0.005 | −0.005 | 0.159 | 0.077 | −0.164 | −0.002 | −0.002 | −0.002 | 0.000 |
| C-6 | 0.008 | 0.040 | 0.024 | −0.032 | 0.036 | 0.043 | 0.040 | −0.007 | 0.008 | 0.041 | 0.025 | −0.033 | 0.015 | 0.013 | 0.014 | 0.002 |
| C-7 | 0.038 | 0.022 | 0.030 | 0.015 | 0.046 | 0.029 | 0.038 | 0.017 | 0.041 | 0.025 | 0.033 | 0.016 | 0.033 | 0.034 | 0.034 | −0.001 |
| C-7a | 0.010 | 0.034 | 0.022 | −0.024 | 0.002 | 0.016 | 0.009 | −0.014 | 0.013 | 0.038 | 0.026 | −0.025 | 0.032 | 0.019 | 0.026 | 0.013 |
| C-8 | 0.030 | 0.106 | 0.068 | −0.076 | | | | | 0.036 | 0.028 | 0.032 | 0.008 | 0.048 | 0.035 | 0.042 | 0.013 |
| C-9 | 0.035 | 0.031 | 0.033 | 0.004 | | | | | 0.038 | 0.034 | 0.036 | 0.004 | 0.053 | 0.043 | 0.048 | 0.010 |
| C-1' | −0.001 | 0.006 | 0.003 | −0.007 | 0.003 | 0.011 | 0.007 | −0.008 | −0.001 | 0.005 | 0.002 | −0.006 | | | | |
| C-2' | 0.021 | 0.019 | 0.020 | 0.002 | 0.036 | 0.029 | 0.033 | 0.007 | 0.020 | 0.022 | 0.021 | −0.002 | | | | |
| C-3' | 0.012 | 0.021 | 0.017 | −0.009 | 0.016 | 0.030 | 0.023 | −0.014 | 0.015 | 0.020 | 0.018 | −0.005 | | | | |
| C-4' | 0.029 | 0.019 | 0.024 | 0.010 | 0.044 | 0.027 | 0.036 | 0.017 | 0.030 | 0.021 | 0.026 | 0.009 | | | | |
| 4'-OH | 0.027 | 0.040 | −0.034 | −0.013 | 0.037 | 0.056 | −0.047 | −0.019 | 0.027 | 0.041 | −0.034 | −0.014 | | | | |
| C-5' | 0.002 | 0.022 | 0.012 | −0.020 | 0.017 | 0.030 | 0.024 | −0.013 | 0.012 | 0.023 | 0.018 | −0.011 | | | | |
| C-6' | 0.024 | 0.020 | 0.022 | 0.004 | 0.038 | 0.026 | 0.032 | 0.012 | 0.030 | 0.019 | 0.025 | 0.011 | | | | |
| C-1" | −0.007 | −0.005 | −0.006 | −0.002 | −0.006 | −0.008 | −0.007 | 0.002 | | | | | 0.005 | 0.001 | 0.003 | 0.004 |

| | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| C-2" | 0.005 | 0.003 | 0.004 | 0.002 | 0.006 | 0.010 | 0.008 | −0.004 | | | | | 0.015 | 0.018 | 0.017 | −0.003 |
| C-3" | 0.001 | 0.001 | 0.001 | 0.000 | 0.002 | 0.001 | 0.001 | 0.001 | | | | | 0.003 | 0.004 | 0.004 | −0.001 |
| 3"-OH | 0.029 | 0.008 | 0.019 | −0.021 | 0.025 | 0.026 | 0.026 | −0.001 | | | | | 0.018 | 0.028 | 0.023 | −0.010 |
| C-4" | 0.025 | 0.022 | 0.024 | 0.003 | 0.038 | 0.040 | 0.039 | −0.002 | | | | | −0.195 | 0.037 | −0.079 | −0.232 |
| C-5" | 0.018 | 0.019 | 0.019 | −0.001 | 0.025 | 0.328 | 0.177 | −0.303 | | | | | 0.018 | 0.020 | 0.019 | −0.002 |
| 5"-OH | 0.003 | 0.002 | 0.002 | 0.001 | 0.005 | 0.004 | 0.004 | 0.001 | | | | | 0.003 | 0.001 | 0.002 | 0.002 |
| C-6" | 0.000 | 0.002 | 0.001 | −0.002 | 0.013 | 0.012 | 0.013 | 0.001 | | | | | 0.000 | 0.012 | 0.006 | −0.012 |
| C-1‴ | −0.003 | −0.009 | −0.006 | 0.006 | | | | | −0.001 | −0.010 | −0.006 | 0.009 | −0.004 | −0.010 | −0.007 | 0.006 |
| C-2‴ | 0.030 | 0.026 | 0.028 | 0.004 | | | | | 0.034 | 0.031 | 0.033 | 0.003 | 0.042 | 0.037 | 0.040 | 0.005 |
| C-3‴ | 0.003 | 0.002 | 0.003 | 0.001 | | | | | 0.003 | 0.002 | 0.003 | 0.001 | 0.003 | 0.003 | 0.003 | 0.000 |
| 3‴-OH | 0.022 | 0.023 | 0.023 | −0.001 | | | | | 0.024 | 0.025 | 0.025 | −0.001 | 0.028 | 0.031 | 0.030 | −0.003 |
| C-4‴ | 0.045 | 0.048 | 0.047 | −0.003 | | | | | 0.050 | 0.055 | 0.053 | −0.005 | 0.058 | 0.070 | 0.064 | −0.012 |
| C-5‴ | 0.005 | 0.004 | 0.005 | 0.001 | | | | | 0.006 | 0.004 | 0.005 | 0.002 | 0.007 | 0.005 | 0.006 | 0.002 |
| 5‴-OH | 0.023 | 0.025 | 0.024 | −0.002 | | | | | 0.025 | 0.027 | 0.026 | −0.002 | 0.029 | 0.032 | 0.031 | −0.003 |
| C-6‴ | 0.024 | 0.027 | 0.026 | −0.003 | | | | | 0.026 | 0.030 | 0.028 | −0.004 | 0.031 | 0.039 | 0.035 | −0.008 |