## Supporting Information

## Conformations and Vibrational Frequencies of a Precursor of Benzovesamicol Analogues Studied by Density Functional Theories

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Table S1. Comparison of root-mean-square deviation (RMSD in $\AA$ ) between calculated coordinates in gas phase and experiment ${ }^{a}$ using different DFT methods at 6-31G(d) basis set for (2RS,3RS)-(I)

| M06-2X | B3LYP | LSDA | B3PW91 | PBEPBE | B3P86 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 2.7793 | 2.7923 | 2.7777 | 2.7854 | 2.7958 | 2.7849 |

${ }^{a}$ experiment: ref. 9 (powder x-ray)

Table S2. Comparison of root-mean-square deviation (RMSD in $\AA$ ) between calculated coordinates and experiment ${ }^{a}$ using various basis sets for (2RS,3RS)-(I) at LSDA level theory

| $6-31 \mathrm{G}(\mathrm{d})$ | $6-31+\mathrm{G}(\mathrm{d}, \mathrm{p})$ | $6-311+\mathrm{G}(\mathrm{d}, \mathrm{p})$ | $6-311++\mathrm{G}(\mathrm{d}, \mathrm{p})$ | cc-PVTZ | TZVP |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 2.7777 | 2.7819 | 2.7850 | 2.7853 | 2.7819 | 2.7822 |

${ }^{a}$ experiment: ref. 9

Table S3. Molecular Dihedral Angles, and Total Energies of (2RS,3RS)-(I) and (2RS,3RS)-(II) Optimized at the LSDA/6-31G(d)//HF/631G(d) Levels in Gas Phase and Water Solution

| Conformers (Gas Phase) | Diheral Angles |  | Total Energies ${ }^{a}$ (E, hartree) | Conformers <br> (Water) | Dihedral Angles |  | Total Energy ${ }^{a}$ (E, hartree) |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $\Psi_{1}$ | $\Psi_{2}$ |  |  | $\Psi_{1}$ | $\Psi_{2}$ |  |
| (2RS,3RS)-(I) |  |  |  | (2RS,3RS)-(I) |  |  |  |
| AIg | 4 | -162 | -1011.07502683 | AIs | -18 | -163 | -1011.10061081 |
| BIg | -174 | -161 | -1011.07502380 | BIs | 40 | -160 | -1011.10041814 |
| CIg | -168 | -168 | -1011.07451734 | CIs | 136 | -166 | -1011.10019340 |
| DIg | 156 | -156 | -1011.07440201 |  |  |  |  |
| (2RS,3RS)-(II) |  |  |  | (2RS,3RS)-(II) |  |  |  |
| AIIg | 6 | -156 | -1011.07509615 | AIIs | 11 | -166 | -1011.10017823 |
| BIIg | -40 | -160 | -1011.07506485 | BIIs | 167 | -167 | -1011.10016484 |
| CIIg | 155 | -155 | -1011.07454298 | CIIs | 4 | -154 | -1011.09941041 |

[^0]Table S4. Comparison of mean absolute deviation (MAD in $\mathrm{cm}^{-1}$ ) between calculated vibrational frequencies $\left(\mathrm{cm}^{-1}\right)$ and experimental values $\left(\mathrm{cm}^{-1}\right)$ using different DFT methods at $6-31 \mathrm{G}(\mathrm{d})$ basis set for (2RS,3RS)-(I)

| M06-2X | B3LYP | LSDA | B3PW91 | PBEPBE | B3P86 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $193.1^{\mathrm{a}}$ | $133.8^{\mathrm{a}}$ | $80.4^{\mathrm{a}}$ | $133.1^{\mathrm{a}}$ | $75.6^{\mathrm{a}}$ | $138.6^{\mathrm{a}}$ |
| $7.38^{\mathrm{b}}$ | $5.11^{\mathrm{b}}$ | $3.08^{\mathrm{b}}$ | $5.09^{\mathrm{b}}$ | $2.89^{\mathrm{b}}$ | $5.30^{\mathrm{b}}$ |

${ }^{\text {a }}$ It is mean absolute deviation(MAD) between calculated vibrational frequency and experimental value in normal frequencies.
Mean absolute deviations of normal frequencies $\times 100=\%$
bMean normal frequencies of experimental value

Table S5. Comparison of mean absolute deviation (MAD in $\mathrm{cm}^{-1}$ ) between calculated vibrational frequencies $\left(\mathrm{cm}^{-1}\right)$ and experimental values $\left(\mathrm{cm}^{-1}\right)$ using various basis sets for (2RS,3RS)-(I) at PBEPBE level

| $6-31 \mathrm{G}(\mathrm{d})$ | $6-31+\mathrm{G}(\mathrm{d}, \mathrm{p})$ | $6-311+\mathrm{G}(\mathrm{d}, \mathrm{p})$ | $6-311++\mathrm{G}(\mathrm{d}, \mathrm{p})$ | cc-PVTZ | TZVP |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $75.6^{\mathrm{a}}$ | $51.7^{\mathrm{a}}$ | $50.7^{\mathrm{a}}$ | $50.6^{\mathrm{a}}$ | $45.9^{\mathrm{a}}$ | $122.6^{\mathrm{a}}$ |
| $2.89^{\mathrm{b}}$ | $1.98^{\mathrm{b}}$ | $1.93^{\mathrm{b}}$ | $1.93^{\mathrm{b}}$ | $1.59^{\mathrm{b}}$ | $4.69^{\mathrm{b}}$ |

${ }^{a}$ It is mean absolute deviation(MAD) between calculated vibrational frequency and experimental value in normal frequencies.
$\frac{\text { Mean absolute deviations of normal frequencies }}{\text { bMean normal frequencies of experimental value }} \times 100=\%$


Figure S1. Preferred conformational structures AIIg, BIIg, and CIIg of (2RS,3RS)-(II) at LSDA/6-31G(d) level in gas phase. Hydrogen bonds are represented by dashed line. The distance of hydrogen bond for AIIg is $1.91 \AA$. The BIg and CIIg are $1.92 \AA$.



Figure S3. Calculated IR spectrum using different methods, including M06-2X, B3LYP, and LSDA at $6-31 \mathrm{G}(\mathrm{d})$ basis set for (2RS, 3RS)-(I).


Figure S4. Calculated IR spectrum using different methods, including B3PW91, PBEPBE, and B3P86 at $6-31 \mathrm{G}(\mathrm{d})$ basis set for (2RS,3RS)-(I).


Figure S5. Calculated IR spectrum using various basis sets, including $6-31+G(d, p), 6-311+G(d, p), 6-311++G(d, p)$, and ccPVTZ for (2RS,3RS)-(I) by PBEPBE method.

(2RS, 3RS)-(I) in Water Solution
(2RS, 3RS)-(II) in Gaseous Phase

(2RS, 3RS)-(II) in Water Solution
Figure S6. Calculated IR spectrum of gaseous and water solution for (2RS, 3RS)-(I) and (2RS, 3RS)-(II) by PBEPBE method.


[^0]:    ${ }^{a}$ Total energies in atomic units

