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 Å) 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

^aexperiment: ref. 9 (powder x-ray)

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

6-31G(d)	6-31+G(d,p)	6-311+G(d,p)	6-311++G(d,p)	cc-PVTZ	TZVP
2.7777	2.7819	2.7850	2.7853	2.7819	2.7822

^aexperiment: 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/6-31G(d) Levels in Gas Phase and Water Solution

Conformers (Gas Phase)	Diheral Angles		Total Energies ^a	Conformers	Dihedral Angles		Total Energy ^a
	Ψ_1	Ψ_2	(E, hartree)	(Water)	Ψ_1	Ψ_2	(E, hartree)
<u>(2RS,3RS)-(I)</u>				<u>(2RS,3RS)-(I)</u>			
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

^aTotal energies in atomic units

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

M06-2X	B3LYP	LSDA	B3PW91	PBEPBE	B3P86
193.1 ^a	133.8 ^a	80.4 ^a	133.1 ^a	75.6 ^a	138.6 ^a
7.38 ^b	5.11 ^b	3.08 ^b	5.09 ^b	2.89 ^b	5.30 ^b

^aIt 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 cm⁻¹) between calculated vibrational frequencies (cm⁻¹) and experimental values (cm⁻¹) using various basis sets for (2RS,3RS)-(I) at PBEPBE level

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

"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





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 Å. The BIg and CIIg are 1.92 Å.

Figure S2. Preferred conformational structures AIs, BIs, and CIs of (2RS,3RS)-(I) at LSDA/6-31G(d) level in water solution. Hydrogen bonds are represented by dashed line. The distances of hydrogen bond for AIs and CIs are 1.88 Å. The BIs is 1.85 Å. (2RS,3RS)-(II) shows the structures of AIIs, BIIs, and CIIs in water. The hydrogen bond distances are from 1.90 Å to 1.85 Å.





LSDA

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







PBEPBE



B3P86

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



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TZVP

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 cc-PVTZ for (2RS,3RS)-(I) by PBEPBE method.



(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.