Supplementary Materials for

Molecular insights into Herniarin: structural, spectroscopic, electronic and thermodynamic characterization via Density Functional Theory

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Table S1: Bond length, bond angle and dihedral angle in the optimized geometry of the molecule

Bond Length	Values(Å)	Bond Angle	Values (°)	Dihedral angle	Values (°)
O15-C12	1.20	C11-C12-O15	126.47	O16-C3-C2-C1	-179.99
C12-O16	1.40	C11-C12-O16	115.99	O17-C1-C2-C3	179.99
O16-C3	1.36	C12-O16-C3	122.91	O17-C1-C6-C5	-179.99
C2-C3	1.38	C4-C3-O16	121.01	C18-O17-C1-C2	179.93
C2-H7	1.08	C1-C2-C3	119.23	O15-C12-C11-C18	179.98
C1-C2	1.39	C2-C3-O16	117.33	O16-C3-C4-C5	-179.99
C1-O17	1.35	C2-C3-C4	121.64	O15-C12-O16-C3	-179.97
O17-C18	1.42	C1-C2-C6	120.42	H14-C11-C12-16	179.98
C18-H20	1.09	C2-C1-O17	115.45	C1-O17-C18-H21	-179.98
C18-H21	1.08	C1-C5-C6	119.32	C4-O16-C5-O16	179.98
C11-C12	1.45	C6-C1-O17	124.12	H14-C11-C8-C4	-180.00
C11-H14	1.08	C1-O17-C18	119.10	H13-C8-C11-C12	-179.99
C8-C11	1.35	O17-C18-H19	111.29	H13-C8-C4-C3	-179.99
C8-H13	1.08	O17-C18-H20	111.29	H9-C5-C4-C3	179.99

C4-C8	1.43	C4-C5-C6	121.49	H9-C5-C6-C1	179.99
C4-C3	1.41	O17-C18-H21	105.64	H10-C6-C5-C4	179.99
C4-C5	1.40	C8-C11-C12	121.57	H10-C6-C1-C2	-179.99
C5-H9	1.08	C3-C4-C5	117.87	H7-C2-C3-C4	179.99
C5-C6	1.38	O15-C12-O16	117.53	H7-C2-C1-C6	179.98