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Supporting information for article:

Biotransformation, spectroscopic investigation, crystal structure and the electrostatic properties of 3,7 α -dihydroxyestra-1,3,5(10)-trien-17-one monohydrate studied using transferred electron-density parameters

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Table S1:

Topological properties at the critical points of **O**···**H** and **C**···**H** intermolecular interactions in the crystal packing of compound 2 for the ELMAM2 model. Where d_{12} , $d_{1\text{CP}}$ and $d_{2\text{CP}}$ are the distances (\AA) between the two atoms, between the first atom and the CP, and between the CP and the second atom. ρ_{CP} is the total electron density (e\AA^{-3}) at the CP and $\nabla^2\rho_{\text{cp}}$, its Laplacian (e\AA^{-5}). λ_1 , λ_2 , λ_3 are the eigenvalues (e\AA^{-5}) of the Hessian matrix $\partial^2\rho/\partial x_i \partial x_j$; $\epsilon = \lambda_1/\lambda_2 - 1$ is the ellipticity. Gcp = Bond Kinetic energy Vcp= Bond Potential Energy (KJ /mol/Bohr³)

Interacting atoms	d_{12} (\AA)	$d_{1\text{CP}}$ (\AA)	$d_{2\text{CP}}$ (\AA)	$\rho(\text{rb})$ (e\AA^{-3})	$\nabla^2\rho(\text{cp})$ (e\AA^{-5})	λ_1 (e\AA^{-5})	λ_2 (e\AA^{-5})	λ_3 (e\AA^{-5})	ϵ	Gcp	Vcp
H1A···O1W	1.7302	0.5906	1.1412	0.3158	1.40	-2.19	-2.15	5.73	0.02	71.15	-104.28
H2···O1W	2.6170	1.5289	1.0895	0.0413	0.71	-0.14	-0.06	0.91	1.45	14.45	-9.54
O1W···H14	2.644	1.5491	1.0951	0.0456	0.58	-0.16	-0.13	0.87	0.28	12.38	-8.92
H1W···O3 ⁱ	1.8605	0.6845	1.177	0.2608	1.32	-1.66	-1.64	4.62	0.01	57.25	-78.56
H2W···O2 ⁱⁱ	1.8065	0.6549	1.1522	0.2902	1.3	-1.92	-1.89	5.1	0.02	63.4	-91.38
H2A···O1 ⁱⁱ	1.8791	0.6767	1.2043	0.2332	1.16	-1.44	-1.42	4.02	0.01	48.8	-65.86
H6A···C3 ⁱⁱⁱ	2.4644	0.9726	1.5253	0.084	0.8	-0.29	-0.19	1.27	0.54	19.48	-17.3
H2···O2 ^{iv}	2.5084	1.0326	1.4773	0.0544	0.64	-0.21	-0.18	1.04	0.15	14.11	-10.72
H16B···O3 ^v	2.4533	1.0125	1.4413	0.0591	0.88	-0.23	-0.21	1.31	0.1	18.82	-13.61
H12A···H15B ^{vi}	2.1682	1.0843	1.084	0.046	0.57	-0.19	-0.14	0.89	0.322	12.08	-8.76
H6B···H11B ^{vii}	2.2434	1.1065	1.1537	0.043	0.55	-0.15	-0.1	0.8	0.385	11.61	-8.27
H1···H6B ^{vi}	2.2803	1.2065	1.1057	0.041	0.57	-0.13	-0.1	0.8	0.243	11.94	-8.29
H18A···H16B ^{viii}	2.351	1.1219	1.2559	0.036	0.59	-0.11	-0.08	0.79	0.48	12	-7.85
H6B···H9 ^{vii}	2.3546	1.1434	1.2758	0.035	0.54	-0.1	-0.03	0.68	2.151	11.04	-7.25
H15A···H16A ^{ix}	2.3897	1.2019	1.1886	0.031	0.31	-0.12	-0.1	0.53	0.213	6.62	-4.76

Symmetry codes: (i) $x, y, z+1$ (ii) $1-x, 1/2+y, 1-z$; (iii) $-x+1, y+1/2, -z+1$ (vi) $-x+2, y-1/2, -z+1$ (v) $-x+2, y+1/2, -z$; (vi) $x+1, y, z$; (vii) $x-1, y, z$; (viii) $-x+1 ; y-1/2 ; -z$; (ix) $-x+1 ; y+1/2 ; -z$;