GI-MS48-P16 | Absolute structure of (E)-2,2'-[3-(4-Fluorophenyl)prop-2-ene-1,1-diyl]bis(3-hydroxy-5,5-dimethylcyclohex-2-en-1-one)

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Herewith we present the crystal structure of (E)-2,20-[3-(4-Fluorophenyl)prop-2-ene-1,1-diyl]bis(3-hydroxy-5,5-dimethylcyclohex-2-en-1-one) (**A**)[1], (E)-9-(4-Fluorostyryl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-2Hxanthene-1,8-dione (**B**)[2]. In the compound (**A**), $C_{25}H_{29}FO_4$, each cyclohexenone ring has an envelope conformation with the dimethyl-substituted atom as the flap. The hydroxy and carbonyl groups form two intramolecular O—H---O hydrogen bonds, as is typical for xanthene derivatives. In the crystal, very weak C—H---O hydrogen bonds link molecules into dimers. The compound (**B**), $C_{25}H_{27}FO_3$, each of the cyclohexanone rings adopts a half-chair conformation, whereas the sixmembered pyran ring adopts a flattened boat conformation, with the O and methine C atoms deviating by 0.0769 (15) and 0.196 (2) Å , respectively, from the plane of the other four atoms (r.m.s. deviation = 0.004 Å). The C=C double bond adopts an *E* conformation. The dihedral angle between the benzene and pyran (all atoms) rings is 89.94 (10)º. In the crystal, weak C—H---O hydrogen bonds link the molecules into chains running parallel to the *b* axis.

[1] Cha, J, H., Min, S. J., Cho, Y. S., Lee, J. K. & Park, J. H. (2013). *Acta Cryst.* E**69**, o397. [2] Lee, J. K., Min, S. J., Cho, Y. S., Cha, J, H. & Won, S. O. (2013). *Acta Cryst.* E**69**, o985.