

# Poster Presentations

[MS32-P01] Absolute structure of 3-hydroxy-2-[(2*E*)-1-(2-hydroxy-6-oxocyclohex-1-en-1-yl)-3-(2-substitutedphenyl)prop-2-en-1-yl]cyclohex-2-en-1-one.

Joo Hwan Cha,<sup>a</sup> Jae Kyun Lee,<sup>b</sup> Yong Seo Cho,<sup>b a</sup>

<sup>a</sup>Advanced Analysis Center, Korea Institute of Science & Technology, Hwarangro 14-gil, Seongbuk-gu, Seoul, South Korea,

<sup>b</sup>Center for Neuro-Medicine, Korea Institute of Science & Technology, Hwarangro 14-gil, Seongbuk-gu, Seoul, South Korea

E-mail: jhcha@kist.re.kr

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Herewith we present the crystal structure of 3-hydroxy-2[(2*E*)-1-(2-hydroxy-6-oxocyclohex-1-en-1-yl)-3-(2-methoxyphenyl)prop-2-en-1-yl]cyclohex-2-en-1-one (**A**)[1], (E)-2,2-[3-(2-nitrophenyl)prop-2-ene-1,1-diyl]bis(3-hydroxycyclohex-2-en-1-one) (**B**)[2] and (E)-2,2-[3-(2-nitrophenyl)prop-2-ene-1,1-diyl]bis(3hydroxy-5,5-dimethylcyclohex-2-en-1-one) (**C**)[3]. In the compound (**A**), C<sub>22</sub>H<sub>24</sub>O<sub>5</sub>, each of the cyclohexenone rings adopts a half-chair conformation. The hydroxy and carbonyl O atoms face each other and are orientated to allow for the formation of the two intramolecular O—H---O hydrogen bonds which are typical of xanthene derivatives. In the crystal, weak intermolecular C—H---O hydrogen bonds link molecules into layers parallel to the *ab* plane. The compound (**B**) has similar structural data as like the compound (**A**). In the compound(**C**), C<sub>25</sub>H<sub>29</sub>NO<sub>6</sub>, the nitro group is rotationally disordered over two orientations in a 0.544 (6):0.456 (6) ratio. In the crystal, weak intermolecular C—H---O hydrogen bonds link molecules into layers parallel to the *ab* plane.

[1] Cha, J. H., Son, M. H., Min, S. J., Cho, Y. S. & Lee, J. K. (2011). *Acta Cryst.* E67, o2739.

[2] Cha, J. H., Kim, Y. H., Lee, J. K. & Cho, Y. S. (2012). *Acta Cryst.* E68, o245. [3] Cha, J. H.,

Kim, Y. H., Min, S. J., Cho, Y. S. & Lee, J. K. (2011). *Acta Cryst.* E67, o3153.