MS7-P5 **Structural studies of cisplatin and carboplatin binding to histidine in a protein upto 1 year**
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The anti-cancer complexes cisplatin and carboplatin target the DNA major groove, but do have toxic side effects. We show that, over a timescale of several days, both cisplatin and carboplatin bind to lysozyme as a test protein with DMSO but not in aqueous media [1]. Furthermore two molecules of either cisplatin or carboplatin bind to its His15 residue. This structural unit (one histidine and two platinum centres) means that in the imidazole of this histidine, the usual *N*-hydrogen of such a residue is absent and that both nitrogens are sp^2 hybridised with nitrogen lone pairs in the plane of the imidazole ring – effectively it is an imidazolyl anion. This effect seen with DMSO, a widely used super-solvent for drug delivery, should be considered in toxicity assessments of these drugs. In further experiments [2] after a ~1 year shelf life, binding of cisplatin or carboplatin to His-15 in hen egg white lysozyme are seen at higher occupancies in the 'with DMSO' conditions. Surprisingly, this much extended shelf life also leads to cisplatin binding to His-15 in aqueous conditions; this could also be significant in prolonged medical and/or veterinary treatments of cancers in people and animals using cisplatin or carboplatin.

[1] Tanley SWM, Schreurs AMM, Kroon-Batenburg LMJ, Meredith J, Prendergast R, Walsh D, Bryant P, Levy C, Helliwell JR (2012) Structural studies of the effect dimethyl sulfoxide (DMSO) has on cisplatin and carboplatin binding to histidine in a protein" *Acta Crystallographica D in press*
[2] Tanley SWM, Schreurs AMM, Kroon-Batenburg LMJ and Helliwell JR (2012) to be published

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MS7-P6 **Supramolecular Structure of Flavanone**.
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Flavonoids are a group of polyphenolic compounds of low molecular weight [1] that present a common benzo-γ-pyrone structure [2]. They occur naturally in fruit, vegetables, nuts, seeds, flowers, leaves, roots, and bark. They are categorized into various subclasses including flavones, flavonols, flavanones, isoflavanones, anthocyanidins, and catechins. Their various properties make them attractive for pharmaceutical, cosmetic, and nutraceutical products. They are pharmacologically active, and have a wide range of useful biological effects, including antioxidative, anti-inflammatory, antibacterial, antiviral, and vasodilatory properties [3,4].

The crystal structure of flavanone, 2-phenyl-2,3-dihydro-*4H-chromen 4-One,* was determined by single crystal X-ray analysis. Data were collected on a Nonius KappaCCD diffractometer equipped with a graphite-monochromated fine-focus molybdenum X-ray source and a 0.3 mm *ifg* capilliary collimator. Structure solution and refinement utilized SIR97, MaXus, and the SHELXTL system.

***Crystal data*:** $C_{15}H_{12}O_2$; M_r = 224.26 Daltons; transparent colorless; monoclinic; $P2_1/n$ (No.14); a = 10.611(5), b = 5.531(5), c = 19.362(5) A, V = 1136.32 A^3; Z = 4; D_{calc} = 1.230 Mg/m^3; $\lambda_{MoK\alpha}$ = 0.71073 A; ĕ = 0.9 cm^{-1}; T = 298(2) K; 16,476 data collected, R_{int} = 0.0752, 1068 unique data.

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