

[PD1-20] [ 04/20/2001 (Fri) 13:30 – 14:30 / Hall 4 ]

### HQSAR of 3-quaternary ammonium cephalosporins for antibiotic activity

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Hologram quantitative structure activity relationship (HQSAR) of 3-quaternary ammonium cephalosporins for their antibiotic activity was conducted. HQSAR attempted to correlated molecular structure with their biological activity for a series of compounds using molecular holograms constructed from counts of sub-structure molecular fragments. Since HQSAR did not require conformational analysis and structural alignment, it gave rapid QSAR screening of large number of compounds.

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### CoMFA analysis of 2-phenyl-1,8-naphthyridin-4-ones for cytotoxicity

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The structure of 2-phenyl-1,8-naphthyridin-4-one derivatives have been studied and optimized for their cytotoxic activity. The three dimensional quantitative structure activity relationship (QSAR) was investigated using comparative molecular field analysis (CoMFA). The result suggested that electrostatic and steric factors of 2-phenyl-1,8-naphthyridin-4-one derivatives were correlated well with cytotoxic activity.

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### A First Total Synthesis of Naturally Occurring Isocoumarin: Sescandelin and AGI-7

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Among the naturally occurring isocoumarin derivatives, 4-substituted-3-nonsubstituted isocoumarin are very rare, and only a few synthetic methods for construction of the skeleton have been developed. Sescandelin and AGI-7 are representatives of 4-substituted-3-nonsubstituted natural isocoumarins. In order to further investigate the biochemical and pharmaceutical effects of sescandelin and AGI-7, especially in growth and proliferation of new blood vessels, we need to synthesize these isocoumarins in large quantities. The first total synthesis of these isocoumarins are accomplished from readily available homophthalate in seven steps in high overall yield. The key step of our synthesis involved the intramolecular cyclization of the vinylogous amide ester.

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