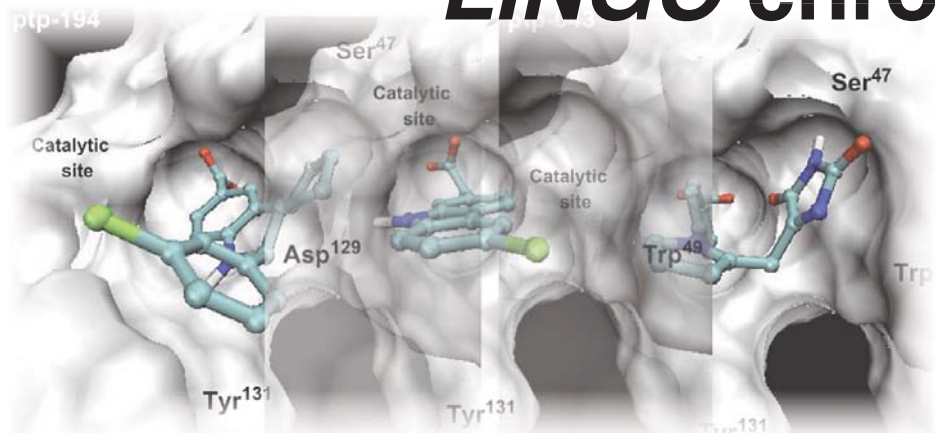


Structuring chemical space for virtual screening applications and virtual *LINGO* chromatography



Tuesday 11 May 2010
S0.21
10.00

Professor Miquel Pons

*Institute for Research in Biomedicine and
Department of Organic Chemistry, University of Barcelona*



The PubChem collection exceeds 26 million compounds - an opportunity and challenge when screening for drug candidates. To increase search efficiency, we are exploring the concept of chemical space using *LINGO* methods, developed in our group, to identify functional relationships between molecules to generate a PubChem “yellow pages” by grouping molecules with expected similar biological properties.



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