DOTTORANDO: Simone Brogi

CICLO: XXIII

TUTOR: Prof. Andrea Tafi

TITOLO DELLA TESI: "Computational Approaches in Drug Discovery"

La tesi è stata discussa il 20/12/2010

PUBBLICAZIONI
Peer-reviewed scientific articles:

Three-dimensional quantitative structure–selectivity relationships analysis guided rational design of a highly selective ligand for the cannabinoid receptor 2
Simone Brogi, Federico Corelli, Vincenzo Di Marzo, Alessia Ligresti, Claudia Mugnaini, Serena Pasquini and Andrea Tafi Eur. J. Med. Chem. 2010, Accepted doi:10.1016/j.ejmech.2010.11.034 (I.F. 3,269)

Pharmacophore Modeling for Qualitative Prediction of Antiestrogenic Activity
Simone Brogi, Maria Kladi, Constantinos Vagias, Panagiota Papazafiri, Vassilios Roussis and Andrea Tafi J. Chem. Inf. Model. 2009, 49, 2489-2497 http://pubs.acs.org/doi/abs/10.1021/ci900254b (I.F. 3,643)
Tetrahydrofuran Acetogenins from Laurencia glandulifera
Maria Kladi, Constantinos Vagias, Panagiota Papazafiri, Simone Brogi, Andrea Tafi and Vassilios Roussis J. Nat. Prod. 2009, 72(2), 190-193 DOI:10.1021/np800481w (I.F. 2.843)

Chapter in book:

New Perspectives in Medicinal Chemistry, 2009, Vol.1: 13-23
Pharmacophore modeling: A continuously evolving tool for computational drug design
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