



DIPARTIMENTO DI CHIMICA E TECNOLOGIE DEL FARMACO
CURRICULUM DIDATTICO-SCIENTIFICO DEL PROF. RINO RAGNO

DATI PERSONALI

Nome e Cognome	RINO RAGNO
<i>Luogo e data di nascita:</i>	Roma, 07/06/21965
<i>Stato Civile:</i>	Coniugato
Dipartimento	Dipartimento di Chimica e Tecnologie del Farmaco
Indirizzo	Piazzale Aldo Moro, 5 00185
Telefono uff./lab./mobile	06/49913937/0649913152/338 9094019
Fax	0649913627
E-mail	rino.ragno@uniroma1.it


Settore Scientifico-Disciplinare: CHIM08
Orario di Ricevimento: 08:00-09:00
ATTUALE POSIZIONE

➤ Professore Associato

CARRIERA E TITOLI

1989	Laurea in Chimica e Tecnologia Farmaceutiche
1990	Tecnico Laureato presso il Dipartimento di Chimica e Tecnologia delle Sostanze Biologicamente Attive
1991	Abilitazione all'Esercizio della Professione di Farmacista
1992	Laurea in Farmacia
1996-1998	Post-Doc presso il Center for Molecular Design della Washington University di Saint Louis diretto dal prof. Garland R. Marshall.
1999	Responsabile del Laboratorio di Chimica Farmaceutica Computazionale Rome Center for Molecular Design (www.rcmd.it)
2000	Nominato ricercatore in seguito a concorso pubblico riservato a n° 4 posti per titoli ed esami (G.U. n° 23 del 21.3.2000) presso la Facoltà di Farmacia dell'Università degli Studi di Roma "La Sapienza".
2010	Nominato Professore Associato in seguito a concorso pubblico presso la Facoltà di Farmacia e Medicina - Università degli Studi di ROMA "La Sapienza", nel Settore CHIM/08 - CHIMICA FARMACEUTICA

ATTIVITA' DIDATTICA

- 1) Esercitazioni pratiche di laboratorio didattico negli insegnamenti di Chimica Farmaceutica e Tossicologica II, Analisi dei Medicinali II, Analisi dei Farmaci II, Analisi dei Medicinali (1991-2000)
- 2) Chimica Organica presso la Facoltà di Agraria dell'Università degli Studi di della Tuscia. (2000-2001)
- 3) Chimica Farmaceutica e Tossicologica I (Corso di Laurea di I° Livello in Scienze e Tecnologie dei Prodotto Erboristici – SSD CHIM08) (2001-2009)
- 4) Chimica Farmaceutica e Tossicologica I (Corso di Laurea di I° Livello in Scienze e Tecnologie dei Prodotto Erboristici – SSD CHIM08) (2002-2012)



- 5) Chimica Farmaceutica e Tossicologica I (Corso di Laurea di I° Livello in Scienze e Tecnologie dei Prodotti Erboristici – SSD CHIM08) Chimica Farmaceutica e Tossicologica I (Corso di Laurea di I° Livello in Scienze e Tecnologie dei Prodotti Erboristici – SSD CHIM08) (2010-)
- 6) Chimica Farmaceutica e Tossicologica (Corso di Laurea in Biotecnologie – SSD CHIM08) (2011-)
- 7) Professore visitatore (A.A. 2009-2010 e 2011-2012) presso il Laboratoire d'Ingénierie Moléculaire et Biochimie Pharmacologique diretto dal Professeur Gilbert KIRSCH - Université Paul Verlaine Metz (Francia)
- 8) Professore visitatore (A.A. 2013-2014) presso il Laboratoire d'Ingénierie Moléculaire et Biochimie Pharmacologique diretto dal Professeur Gilbert KIRSCH - UMR CNRS 7565 SRSMC Université de Lorraine Metz (Francia)

ATTIVITA' SCIENTIFICA

- A. Sintesi chimica di nuovi composti a struttura azolica a potenziale attività antifungina analoghi del bifonazolo e del miconazolo.
- B. Sintesi chimica di nuovi composti ad attività anti-rhinovirale analoghi del disoxaril.
- C. Studi computazionali su composti ad attività anti-HRV volto alla determinazione di una relazione QSAR che hanno permesso la descrizione delle interazioni atomiche che intercorrono tra il potenziale farmaco e la proteina ricoprente (capside).
- D. Studi computazionali su composti a struttura azolica ad attività antifungina volto alla determinazione di una relazione QSAR che hanno permesso la formulazione di un modello farmacoforico utile allo sviluppo di nuove strutture.
- E. Studi di modellazione e progettazione molecolare (Molecular Modeling), relazioni quantitative struttura-attività bi e tridimensionali (QSAR e 3D QSAR), progettazione molecolare a partire da informazioni strutturali del recettore conosciute (Structure Based Drug Design) o da serie molecolari in caso di non conoscenza della struttura tridimensionale del recettore (Ligand Based Design) e studi di accostamento molecolare ligando-recettore (Docking) sui seguenti sistemi biologici di interesse chimico-farmaceutico:
- F. Sviluppo di nuove tecniche miste di relazione quantitativa struttura-attività, volte al *De Novo Ligand Design* ed alla valutazione di complessi ligando-recettore (docking).
- G. Sviluppo di modelli ibridi QSAR/*Scoring Function* generalizzati per diverse classi di inibitori a target variabile (VALIDATE) e costante (VALIDATE II)
- H. Ricerche sull'Attività antibatterica ed antimicotica di olii essenziali
- I. Collaborazioni internazionali con
 - Prof. Garland Marshall, Washington University in Saint Louis – Missouri – USA
 - Prof.ssa Neerja Kaushik-Basu, Department of Biochemistry and Molecular Biology, UMDNJ-New Jersey Medical School, Newark, NJ – USA
 - Professeur Gilbert KIRSCH Laboratoire d'Ingénierie Moléculaire et Biochimie Pharmacologique Université Paul Verlaine Metz, Metz – France.

PUBBLICAZIONI SCIENTIFICHE

- [1] S. Massa, M. Artico, A. Mai, R. Ragno, F. Corelli, Synthesis of new disoxaril analogs with potent and selective anti-human rhinovirus 14 activity, *Bioorg. Med. Chem. Lett.*, 1 (1991) 575-578.
- [2] S. Massa, R. Ragno, G.C. Porretta, A. Mai, A. Retico, M. Artico, N. Simonetti, Antifungal agents. II. Synthesis and antifungal activities of aryl-1H-pyrrol-2-yl-1H-imidazol-1-ylmethane derivatives with unsaturated chains, *Arch. Pharm. (Weinheim, Ger.)*, 326 (1993) 539-546.
- [3] S. Massa, A. Mai, R. Ragno, G.C. Porretta, A. Retico, G. Simonetti, M. Artico, Antifungal agents. 7. Dichlorophenylpyrrolimidazolylmethane derivatives: synthesis and antifungal activities, *Farmaco*, 49 (1994) 51-55.



- [4] S. Massa, F. Corelli, M. Artico, A. Mai, R. Ragno, M.A. De, A.G. Loi, S. Corrias, M.E. Marongiu, C.P. La, [(((Thienylcarbonyl)alkyl[oxy]phenyl)- and [(((Pyrrylcarbonyl)alkyl[oxy]phenyl)]oxazoline Derivatives with Potent and Selective Antihuman Rhinovirus Activity, *J. Med. Chem.*, 38 (1995) 803-809.
- [5] M. Artico, M. Botta, F. Corelli, A. Mai, S. Massa, R. Ragno, Investigation on QSAR and binding mode of a new class of human rhinovirus-14 inhibitors by CoMFA and docking experiments, *Bioorg. Med. Chem.*, 4 (1996) 1715-1724.
- [6] M. Artico, R. Ragno, G.C. Porretta, S. Massa, C. Musiu, M.G. Spiga, S. Corrias, C.P. La, Iso-miconazole and related derivatives: synthesis and antifungal activities, *Med. Chem. Res.*, 6 (1996) 137-147.
- [7] A. Mai, M. Artico, S. Massa, R. Ragno, M.A. De, S. Corrias, M.G. Spiga, C.P. La, Methyl-2-thienylketopolymethyleneoxyphenyl derivatives of alkyl-substituted 4,5-dihydro-oxazoles with anti-human picornavirus activity, *Antiviral Chem. Chemother.*, 7 (1996) 213-220.
- [8] A. Tafi, J. Anastassopoulou, T. Theophanides, M. Botta, F. Corelli, S. Massa, M. Artico, R. Costi, S.R. Di, R. Ragno, Molecular Modeling of Azole Antifungal Agents Active against *Candida albicans*. 1. A Comparative Molecular Field Analysis Study, *J. Med. Chem.*, 39 (1996) 1227-1235.
- [9] A. Ettore, M. Artico, A. Mai, R. Ragno, G.C. Porretta, S. Massa, Crystal structure of 2-[5-(4-carbethoxyphenoxy)pentanoyl]-5-chlorothiophene, C₁₈H₁₉O₄ClS, *Z. Kristallogr. - New Cryst. Struct.*, 213 (1998) 129-130.
- [10] R. Ragno, R. Head, G.R. Marshall, A predictive model for HIV protease inhibitors, in, American Chemical Society, 1998, pp. COMP-032.
- [11] G.R. Marshall, R. Ragno, G.M. Makara, R. Arimoto, O. Kisselev, Bound conformations for ligands for G-protein coupled receptors, *Lett. Pept. Sci.*, 6 (1999) 283-288.
- [12] G.R. Marshall, R. Arimoto, R. Ragno, R.D. Head, Predicting affinity: The sine qua non of activity, in, American Chemical Society, 2000, pp. COMP-056.
- [13] G.R. Marshall, R.D. Head, R. Ragno, Affinity prediction: The sine qua non, in, Oxford University Press, Inc., 2000, pp. 87-111.
- [14] G.R. Marshall, R. Ragno, G.M. Makara, R. Arimoto, O. Kisselev, Bound conformations for ligands of G-protein coupled receptors, in, Kluwer Academic Publishers, 2000, pp. 583-584.
- [15] R. Ragno, G.R. Marshall, S.R. Di, R. Costi, S. Massa, R. Rompei, M. Artico, Antimycobacterial pyrroles: synthesis, anti-*Mycobacterium tuberculosis* activity and QSAR studies, *Bioorg. Med. Chem.*, 8 (2000) 1423-1432.
- [16] A. Mai, G. Sbardella, M. Artico, R. Ragno, S. Massa, E. Novellino, G. Greco, A. Lavecchia, C. Musiu, C.M. La, C. Murgioni, C.P. La, R. Loddo, Structure-based design, synthesis, and biological evaluation of conformationally restricted novel 2-alkylthio-6-[1-(2,6-difluorophenyl)alkyl]-3,4-dihydro-5-alkylpyrimidin-4(3H)-ones as non-nucleoside inhibitors of HIV-1 reverse transcriptase, *J. Med. Chem.*, 44 (2001) 2544-2554.
- [17] S. Massa, A. Mai, G. Sbardella, M. Esposito, R. Ragno, P. Loidl, G. Brosch, 3-(4-Aroyl-1H-pyrrol-2-yl)-N-hydroxy-2-propenamides, a new class of synthetic histone deacetylase inhibitors, *J. Med. Chem.*, 44 (2001) 2069-2072.
- [18] M.G. Quaglia, A. Mai, G. Sbardella, M. Artico, R. Ragno, S. Massa, P.D. Del, G. Setzu, S. Doratiotto, V. Cotichini, Chiral resolution and molecular modeling investigation of rac-2-cyclopentylthio-6-[1-(2,6-difluorophenyl)ethyl]-3,4-dihydro-5-methylpyrimidin-4(3H)-one (MC-1047), a potent anti-HIV-1 reverse transcriptase agent of the DABO class, *Chirality*, 13 (2001) 75-80.
- [19] S.R. Di, R. Costi, M. Artico, S. Massa, R. Ragno, G.R. Marshall, C.P. La, Design, synthesis and QSAR studies on N-aryl heteroarylisopropanolamines, a new class of non-peptidic HIV-1 protease inhibitors, *Bioorg. Med. Chem.*, 10 (2002) 2511-2526.
- [20] S.R. Di, R. Costi, M. Artico, R. Ragno, S. Massa, C.M. La, R. Loddo, C.P. La, A. Pani, Arylthiopyridylmethylisopropylpyrrole carbinols, novel NNRTIs endowed with potent anti-HIV-1 activity, *Med. Chem. Res.*, 11 (2002) 153-167.



- [21] A. Mai, S. Massa, R. Ragno, M. Esposito, G. Sbardella, G. Nocca, R. Scatena, F. Jesacher, P. Loidl, G. Brosch, Binding mode analysis of 3-(4-benzoyl-1-methyl-1H-2-pyrrolyl)-N-hydroxy-2-propenamide: A new synthetic histone deacetylase inhibitor inducing histone hyperacetylation, growth inhibition, and terminal cell differentiation, *J. Med. Chem.*, 45 (2002) 1778-1784.
- [22] R. Silvestri, M. Artico, M.G. De, R. Ragno, S. Massa, R. Loddo, C. Murgioni, A.G. Loi, C.P. La, A. Pani, Synthesis, Biological Evaluation, and Binding Mode of Novel 1-[2-(Diarylmethoxy)ethyl]-2-methyl-5-nitroimidazoles Targeted at the HIV-1 Reverse Transcriptase, *J. Med. Chem.*, 45 (2002) 1567-1576.
- [23] R. Silvestri, M.G. De, M. Artico, R.G. La, R. Ragno, R. Loddo, C.P. La, M.E. Marongiu, C.M. La, A. Pani, Anti-HIV-1 NNRT agents: acylamino pyrrol aryl sulfones (APASs) as truncated analogues of tricyclic PBTDS, *Med. Chem. Res.*, 11 (2002) 195-218.
- [24] A. Mai, M. Artico, M. Esposito, R. Ragno, G. Sbardella, S. Massa, Synthesis and biological evaluation of enantiomerically pure pyrrolyl-oxazolidinones as a new class of potent and selective monoamine oxidase type A inhibitors, *Farmaco*, 58 (2003) 231-241.
- [25] A. Mai, S. Massa, R. Ragno, I. Cerbara, F. Jesacher, P. Loidl, G. Brosch, 3-(4-Aroyl-1-methyl-1H-2-pyrrolyl)-N-hydroxy-2-alkylamides as a New Class of Synthetic Histone Deacetylase Inhibitors. 1. Design, Synthesis, Biological Evaluation, and Binding Mode Studies Performed through Three Different Docking Procedures, *J. Med. Chem.*, 46 (2003) 512-524.
- [26] R. Costi, S.R. Di, M. Artico, S. Massa, R. Ragno, R. Loddo, C.M. La, E. Tramontano, C.P. La, A. Pani, 2,6-Bis(3,4,5-trihydroxybenzylidene) derivatives of cyclohexanone: novel potent HIV-1 integrase inhibitors that prevent HIV-1 multiplication in cell-based assays, *Bioorg. Med. Chem.*, 12 (2004) 199-215.
- [27] R. Costi, S.R. Di, M. Artico, A. Roux, R. Ragno, S. Massa, E. Tramontano, C.M. La, R. Loddo, M.E. Marongiu, A. Pani, C.P. La, 6-Aryl-2,4-dioxo-5-hexenoic acids, novel integrase inhibitors active against HIV-1 multiplication in cell-based assays, *Bioorg. Med. Chem. Lett.*, 14 (2004) 1745-1749.
- [28] A. Mai, S. Massa, I. Cerbara, S. Valente, R. Ragno, P. Bottoni, R. Scatena, P. Loidl, G. Brosch, 3-(4-Aroyl-1-methyl-1H-2-pyrrolyl)-N-hydroxy-2-propenamides as a New Class of Synthetic Histone Deacetylase Inhibitors. 2. Effect of Pyrrole-C2 and/or -C4 Substitutions on Biological Activity, *J. Med. Chem.*, 47 (2004) 1098-1109.
- [29] R. Ragno, A. Mai, S. Massa, I. Cerbara, S. Valente, P. Bottoni, R. Scatena, F. Jesacher, P. Loidl, G. Brosch, 3-(4-Aroyl-1-methyl-1H-pyrrol-2-yl)-N-hydroxy-2-propenamides as a New Class of Synthetic Histone Deacetylase Inhibitors. 3. Discovery of Novel Lead Compounds through Structure-Based Drug Design and Docking Studies, *J. Med. Chem.*, 47 (2004) 1351-1359.
- [30] R. Ragno, A. Mai, G. Sbardella, M. Artico, S. Massa, C. Musiu, M. Mura, F. Marturana, A. Cadeddu, C.P. La, Computer-aided design, synthesis, and anti-HIV-1 activity in vitro of 2-alkylamino-6-[1-(2,6-difluorophenyl)alkyl]-3,4-dihydro-5-alkylpyrimidin-4(3H)-ones as novel potent non-nucleoside reverse transcriptase inhibitors, also active against the Y181C variant, *J. Med. Chem.*, 47 (2004) 928-934.
- [31] M. Agamennone, C. Campestre, S. Prezioso, V. Consalvi, M. Crucianelli, F. Mazza, V. Politi, R. Ragno, P. Tortorella, C. Gallina, Synthesis and evaluation of new tripeptide phosphonate inhibitors of MMP-8 and MMP-2, *Eur. J. Med. Chem.*, 40 (2005) 271-279.
- [32] R. Cancio, R. Silvestri, R. Ragno, M. Artico, M.G. De, R.G. La, E. Crespan, S. Zanolli, U. Hubscher, S. Spadari, G. Maga, High potency of indolyl aryl sulfone nonnucleoside inhibitors towards drug-resistant human immunodeficiency virus type 1 reverse transcriptase mutants is due to selective targeting of different mechanistic forms of the enzyme, *Antimicrob. Agents Chemother.*, 49 (2005) 4546-4554.
- [33] M.G. De, R.G. La, P.A. Di, R. Ragno, A. Bergamini, C. Ciaprini, A. Sinistro, G. Maga, E. Crespan, M. Artico, R. Silvestri, Novel 1-[2-(Diarylmethoxy)ethyl]-2-methyl-5-nitroimidazoles as HIV-1 Non-Nucleoside Reverse Transcriptase Inhibitors. A Structure-Activity Relationship Investigation, *J. Med. Chem.*, 48 (2005) 4378-4388.



- [34] S.R. Di, R. Costi, M. Artico, R. Ragno, G. Greco, E. Novellino, C. Marchand, Y. Pommier, Design, synthesis and biological evaluation of heteroaryl diketohexenoic and diketobutanoic acids as HIV-1 integrase inhibitors endowed with antiretroviral activity, *Farmaco*, 60 (2005) 409-417.
- [35] A. Mai, M. Artico, R. Ragno, G. Sbardella, S. Massa, C. Musiu, M. Mura, F. Marturana, A. Cadeddu, G. Maga, C.P. La, 5-Alkyl-2-alkylamino-6-(2,6-difluorophenylalkyl)-3,4-dihydropyrimidin-4(3H)-ones, a new series of potent, broad-spectrum non-nucleoside reverse transcriptase inhibitors belonging to the DABO family, *Bioorg. Med. Chem.*, 13 (2005) 2065-2077.
- [36] A. Mai, S. Massa, S. Lavu, R. Pezzi, S. Simeoni, R. Ragno, F.R. Mariotti, F. Chiani, G. Camilloni, D.A. Sinclair, Design, Synthesis, and Biological Evaluation of Sirtinol Analogues as Class III Histone/Protein Deacetylase (Sirtuin) Inhibitors, *J. Med. Chem.*, 48 (2005) 7789-7795.
- [37] A. Mai, S. Massa, D. Rotili, I. Cerbara, S. Valente, R. Pezzi, S. Simeoni, R. Ragno, Histone deacetylation in epigenetics: An attractive target for anticancer therapy, *Med. Res. Rev.*, 25 (2005) 261-309.
- [38] R. Ragno, M. Artico, M.G. De, R.G. La, A. Coluccia, P.A. Di, R. Silvestri, Docking and 3-D QSAR Studies on Indolyl Aryl Sulfones. Binding Mode Exploration at the HIV-1 Reverse Transcriptase Non-Nucleoside Binding Site and Design of Highly Active N-(2-Hydroxyethyl)carboxamide and N-(2-Hydroxyethyl)carbohydrazide Derivatives, *J. Med. Chem.*, 48 (2005) 213-223.
- [39] R. Ragno, S. Frasca, F. Manetti, A. Brizzi, S. Massa, HIV-Reverse Transcriptase Inhibition: Inclusion of Ligand-Induced Fit by Cross-Docking Studies, *J. Med. Chem.*, 48 (2005) 200-212.
- [40] M.G. De, R.G. La, R. Ragno, A. Coluccia, A. Bergamini, C. Ciapriani, A. Sinistro, G. Maga, E. Crespan, M. Artico, R. Silvestri, Indolyl aryl sulphones as HIV-1 non-nucleoside reverse transcriptase inhibitors: synthesis, biological evaluation and binding mode studies of new derivatives at indole-2-carboxamide, *Antiviral Chem. Chemother.*, 17 (2006) 59-77.
- [41] S.R. Di, R. Costi, M. Artico, R. Ragno, A. Lavecchia, E. Novellino, E. Gavuzzo, T.F. La, R. Cirilli, R. Cancio, G. Maga, Design, synthesis, biological evaluation, and molecular modeling studies of TIBO-like cyclic sulfones as non-nucleoside HIV-1 reverse transcriptase inhibitors, *ChemMedChem*, 1 (2006) 82-95.
- [42] A. Mai, S. Massa, D. Rotili, S. Simeoni, R. Ragno, G. Botta, A. Nebbioso, M. Miceli, L. Altucci, G. Brosch, Synthesis and biological properties of novel, uracil-containing histone deacetylase inhibitors, *J. Med. Chem.*, 49 (2006) 6046-6056.
- [43] A. Mai, S. Massa, S. Valente, S. Simeoni, R. Ragno, P. Bottoni, R. Scatena, G. Brosch, Aroyl-pyrrolyl hydroxyamides: influence of pyrrole C4-phenylacetyl substitution on histone deacetylase inhibition, *ChemMedChem*, 1 (2006) 225-237.
- [44] F. Manetti, C. Tintori, M. Armand-Ugon, I. Clotet-Codina, S. Massa, R. Ragno, J.A. Este, M. Botta, A Combination of Molecular Dynamics and Docking Calculations to Explore the Binding Mode of ADS-J1, a Polyanionic Compound Endowed with Anti-HIV-1 Activity, *J. Chem. Inf. Model.*, 46 (2006) 1344-1351.
- [45] R. Ragno, A. Coluccia, R.G. La, M.G. De, F. Piscitelli, A. Lavecchia, E. Novellino, A. Bergamini, C. Ciapriani, A. Sinistro, G. Maga, E. Crespan, M. Artico, R. Silvestri, Design, Molecular Modeling, Synthesis, and Anti-HIV-1 Activity of New Indolyl Aryl Sulfones. Novel Derivatives of the Indole-2-carboxamide, *J. Med. Chem.*, 49 (2006) 3172-3184.
- [46] R. Ragno, S. Simeoni, S. Valente, S. Massa, A. Mai, 3-D QSAR Studies on Histone Deacetylase Inhibitors. A GOLPE/GRID Approach on Different Series of Compounds, *J. Chem. Inf. Model.*, 46 (2006) 1420-1430.
- [47] A. Mai, M. Artico, D. Rotili, D. Tarantino, I. Clotet-Codina, M. Armand-Ugon, R. Ragno, S. Simeoni, G. Sbardella, M.B. Nawrozkij, A. Samuele, G. Maga, J.A. Este, Synthesis and Biological Properties of Novel 2-Aminopyrimidin-4(3H)-ones Highly Potent against HIV-1 Mutant Strains, *J. Med. Chem.*, 50 (2007) 5412-5424.



- [48] A. Mai, S. Valente, D. Cheng, A. Perrone, R. Ragno, S. Simeoni, G. Sbardella, G. Brosch, A. Nebbioso, M. Conte, L. Altucci, M.T. Bedford, Synthesis and biological validation of novel synthetic histone/protein methyltransferase inhibitors, *ChemMedChem*, 2 (2007) 987-991.
- [49] R. Ragno, A. Coluccia, R.G. La, R. Silvestri, Indolyl aryl sulphones as HIV-1 reverse transcriptase inhibitors: docking and 3D QSAR studies, *Expert Opin. Drug Discovery*, 2 (2007) 87-114.
- [50] R. Ragno, A. Mai, S. Simeoni, A. Caroli, Beta-Secretase Inhibitors: Structure-Based 3-D QSAR Studies, in, American Chemical Society, Division of Medicinal Chemistry, 2007, pp. COMC-064.
- [51] R. Ragno, A. Mai, S. Simeoni, A. Caroli, E. Caffarelli, N.P. La, U. Gioia, I. Bozzoni, Structure-Based Drug Discovery of XendoU Inhibitors through Multi-Docking Virtual Screening, in, American Chemical Society, Division of Medicinal Chemistry, 2007, pp. COMC-063.
- [52] R. Ragno, A. Mai, S. Simeoni, A. Caroli, I. Musmuca, Interferon Inducers: Definition of a Pharmacophore Model through GRID/GOLPE 3-D QSAR Studies, in, American Chemical Society, Division of Medicinal Chemistry, 2007, pp. COMC-062.
- [53] R. Ragno, A. Mai, S. Simeoni, A. Caroli, D. Rotili, G. Botta, Docking and 3-D QSAR Studies on SIRT2 Inhibitors: A GRID/GOLPE Approach on Different Series of Compounds, in, American Chemical Society, Division of Medicinal Chemistry, 2007, pp. COMC-009.
- [54] R. Ragno, A. Mai, S. Simeoni, A. Caroli, S. Valente, A. Perrone, New Aroyl-Pyrrolyl-Hydroxy-Amides APHAs: Class I and II Histone Deacetylase Inhibiting Activity and Binding Mode Analysis through Molecular Docking Experiments, in, American Chemical Society, Division of Medicinal Chemistry, 2007, pp. COMC-008.
- [55] R. Ragno, A. Mai, S. Simeoni, A. Caroli, S. Valente, A. Perrone, S. Castellano, G. Sbardella, Small Molecule Inhibitors of Histone Arginine Methyltransferases: Updated Structure-Based 3-D QSAR Models with Improved Robustness and Predictive Ability, in, American Chemical Society, Division of Medicinal Chemistry, 2007, pp. COMC-010.
- [56] R. Ragno, S. Simeoni, S. Castellano, C. Vicidomini, A. Mai, A. Caroli, A. Tramontano, C. Bonaccini, P. Trojer, I. Bauer, G. Brosch, G. Sbardella, Small Molecule Inhibitors of Histone Arginine Methyltransferases: Homology Modeling, Molecular Docking, Binding Mode Analysis, and Biological Evaluations, *J. Med. Chem.*, 50 (2007) 1241-1253.
- [57] S. Castellano, G. Stefancich, R. Ragno, K. Schewe, M. Santoriello, A. Caroli, R.W. Hartmann, G. Sbardella, CYP19 (aromatase): Exploring the scaffold flexibility for novel selective inhibitors, *Bioorg. Med. Chem.*, 16 (2008) 8349-8358.
- [58] P. Laneve, U. Gioia, R. Ragno, F. Altieri, F.C. Di, T. Santini, M. Arceci, I. Bozzoni, E. Caffarelli, The Tumor Marker Human Placental Protein 11 Is an Endoribonuclease, *J. Biol. Chem.*, 283 (2008) 34712-34719.
- [59] M.B. Nawrozkij, D. Rotili, D. Tarantino, G. Botta, A.S. Eremiychuk, I. Musmuca, R. Ragno, A. Samuele, S. Zanolì, M. Armand-Ugon, I. Clotet-Codina, I.A. Novakov, B.S. Orlinson, G. Maga, J.A. Este, M. Artico, A. Mai, 5-Alkyl-6-benzyl-2-(2-oxo-2-phenylethylsulfanyl)pyrimidin-4(3H)-ones, a Series of Anti-HIV-1 Agents of the Dihydro-alkoxy-benzyl-oxopyrimidine Family with Peculiar Structure-Activity Relationship Profile, *J. Med. Chem.*, 51 (2008) 4641-4652.
- [60] R. Ragno, S. Simeoni, D. Rotili, A. Caroli, G. Botta, G. Brosch, S. Massa, A. Mai, Class II-selective histone deacetylase inhibitors. Alignment-independent GRIND 3-D QSAR, homology and docking studies, *Eur. J. Med. Chem.*, 43 (2008) 621-632.
- [61] R. Ragno, S. Sivric, G. Sartorelli, A. Serilli, E. Vavala, L. Angiolella, In vitro activity of essential oil of *Myrtus communis* L. against *Candida albicans*. Comments, *Int. J. Essent. Oil Ther.*, 2 (2008) 156-157.
- [62] A. Mai, S. Valente, A. Nebbioso, S. Simeoni, R. Ragno, S. Massa, G. Brosch, B.F. De, F. Manzo, L. Altucci, New pyrrole-based histone deacetylase inhibitors: Binding mode, enzyme- and cell-based investigations, *Int. J. Biochem. Cell Biol.*, 41 (2009) 235-247.
- [63] I. Musmuca, S. Simeoni, A. Caroli, R. Ragno, Small-Molecule Interferon Inducers. Toward the Comprehension of the Molecular Determinants through Ligand-Based Approaches, *J. Chem. Inf. Model.*, 49 (2009) 1777-1786.



- [64] E. Vavala, R. Ragno, S. Sivric, G. Sartorelli, A. Filippi, A.T. Palamara, L. Angiolella, Antimycotic activity of *Achillea ageratum* L. essential oil, *Int. J. Essent. Oil Ther.*, 3 (2009) 101-105.
- [65] L. Angiolella, E. Vavala, S. Sivric, D.A.F. Diodata, R. Ragno, In vitro activity of *Mentha suaveolens* essential oil against *Cryptococcus neoformans* and dermatophytes, *Int. J. Essent. Oil Ther.*, 4 (2010) 35-36.
- [66] S. Castellano, C. Milite, R. Ragno, S. Simeoni, A. Mai, V. Limongelli, E. Novellino, I. Bauer, G. Brosch, A. Spannhoff, D. Cheng, M.T. Bedford, G. Sbardella, Design, synthesis and biological evaluation of carboxy analogues of arginine methyltransferase inhibitor 1 (AMI-1), *ChemMedChem*, 5 (2010) 398-414.
- [67] I. Musmuca, A. Caroli, A. Mai, N. Kaushik-Basu, P. Arora, R. Ragno, Combining 3-D Quantitative Structure-Activity Relationship with Ligand Based and Structure Based Alignment Procedures for in Silico Screening of New Hepatitis C Virus NS5B Polymerase Inhibitors, *J. Chem. Inf. Model.*, 50 (2010) 662-676.
- [68] L. Angiolella, R. Ragno, *Mentha suaveolens* essential oil and therapeutic activities thereof, in, *Universita Degli Studi di Roma "La Sapienza"*, Italy . 2011, pp. 24pp.
- [69] G. Nocca, R. Ragno, V. Carbone, G.E. Martorana, D.V. Rossetti, G. Gambarini, B. Giardina, A. Lupi, Identification of glutathione-methacrylates adducts in gingival fibroblasts and erythrocytes by HPLC-MS and capillary electrophoresis, *Dent. Mater.*, 27 (2011) e87-e98.
- [70] F. Pepi, A. Tata, S. Garzoli, P. Giacomello, R. Ragno, A. Patsilinakos, F.M. Di, A. D'Annibale, S. Cannistraro, C. Baldacchini, G. Favero, M. Frascioni, F. Mazzei, Chemically Modified Multiwalled Carbon Nanotubes Electrodes with Ferrocene Derivatives through Reactive Landing, *J. Phys. Chem. C*, 115 (2011) 4863-4871.
- [71] D. Pietrella, L. Angiolella, E. Vavala, A. Rachini, F. Mondello, R. Ragno, F. Bistoni, A. Vecchiarelli, Beneficial effect of *Mentha suaveolens* essential oil in the treatment of vaginal candidiasis assessed by real-time monitoring of infection, *BMC Complement Altern Med*, 11 (2011) 18.
- [72] R. Ragno, U. Gioia, P. Laneve, I. Bozzoni, A. Mai, E. Caffarelli, Identification of Small-Molecule Inhibitors of the XendoU Endoribonucleases Family, *ChemMedChem*, 6 (2011) 1797-1805.
- [73] S. Valente, M. Tardugno, M. Conte, R. Cirilli, A. Perrone, R. Ragno, S. Simeoni, A. Tramontano, S. Massa, A. Nebbioso, M. Miceli, G. Franci, G. Brosch, L. Altucci, A. Mai, Novel Cinnamyl Hydroxyamides and 2-Aminoanilides as Histone Deacetylase Inhibitors: Apoptotic Induction and Cytodifferentiation Activity, *ChemMedChem*, 6 (2011) 698-712.
- [74] F. Ballante, I. Musmuca, G.R. Marshall, R. Ragno, Comprehensive model of wild-type and mutant HIV-1 reverse transcriptases, *J. Comput.-Aided Mol. Des.*, 26 (2012) 907-919.
- [75] F. Ballante, R. Ragno, 3-D QSAutogrid/R: An Alternative Procedure To Build 3-D QSAR Models. Methodologies and Applications, *J. Chem. Inf. Model.*, 52 (2012) 1674-1685.
- [76] D.B. Nichols, G. Fournet, K.R. Gurukumar, A. Basu, J.-C. Lee, N. Sakamoto, F. Kozielski, I. Musmuca, B. Joseph, R. Ragno, N. Kaushik-Basu, Inhibition of hepatitis C virus NS5B polymerase by S-trityl-L-cysteine derivatives, *Eur. J. Med. Chem.*, 49 (2012) 191-199.
- [77] A. Ricci, S. Piccolella, F. Pepi, A. Patsilinakos, R. Ragno, S. Garzoli, P. Giacomello, Gas-phase basicity of 2-furaldehyde, *J. Mass Spectrom.*, 47 (2012) 1488-1494.
- [78] D. Rotili, A. Samuele, D. Tarantino, R. Ragno, I. Musmuca, F. Ballante, G. Botta, L. Morera, M. Pierini, R. Cirilli, M.B. Nawrozkij, E. Gonzalez, B. Clotet, M. Artico, J.A. Este, G. Maga, A. Mai, 2-(Alkyl/Aryl)Amino-6-Benzylpyrimidin-4(3H)-ones as Inhibitors of Wild-Type and Mutant HIV-1: Enantioselectivity Studies, *J. Med. Chem.*, 55 (2012) 3558-3562.
- [79] L. Silvestri, F. Ballante, A. Mai, G.R. Marshall, R. Ragno, Histone Deacetylase Inhibitors: Structure-Based Modeling and Isoform-Selectivity Prediction, *J. Chem. Inf. Model.*, 52 (2012) 2215-2235.
- [80] G. Ortar, E. Morera, L. De Petrocellis, A. Ligresti, A.S. Moriello, L. Morera, M. Nalli, R. Ragno, A. Pirolli, V. Di Marzo, Biaryl tetrazolyl ureas as inhibitors of endocannabinoid metabolism: modulation at the N-portion and distal phenyl ring, *European Journal of Medicinal Chemistry*. 63 (2013) 118-132



- [81] E. Perspicace, V. Jouan-Hureau, R. Ragno*, F. Ballante, S. Sartini, C. La Motta, F. Da Settimo, B. Chen, G. Kirsch, S. Schneider, B. Faivre, S. Hesse, Design, synthesis and biological evaluation of new classes of thieno[3,2-d]pyrimidinone and thieno[1,2,3]triazine as inhibitor of vascular endothelial growth factor receptor-2 (VEGFR-2), *European Journal of Medicinal Chemistry*. (2013), doi: 10.1016/j.ejmech.2013.03.022, 63, 765–781
- [82] Laura Friggeri, Flavio Ballante, Rino Ragno*, Ira Musmuca, Daniela De Vita, Fabrizio Manetti, Mariangela Biava, Luigi Scipione, Roberto Di Santo, Roberta Costi, Marta Feroci and Silvano Tortorella. Pharmacophore Assessment Through 3-D QSAR:evaluation of the predictive ability on new derivatives by the application on a serie of antitubercularagents. DOI: 10.1021/ci400132q.
- [83] L. Civitelli; S. Panella; M.E.Marcocci; A. De Petris; A. Garzoli; F. Pepi; E. Vavala; R. Ragno; L. Nencioni; A.T. Palamara; L. Angiolella. n vitro inhibition of herpes simplex virus type 1 replication by Mentha suaveolens essential oil and its main component piperitenone oxide. *Phytomedicine* (2014), Accepted for publication.
- [84] Maria Chatzopoulou, Alexandros Patsilidakos, Theodosia Vallianatou, Marta Soltesova Prnova, Simon Žakelj, Rino Ragno, Milan Stefek, Albin Kristl, Anna Tsantili-Kakoulidou, and Vassilis J. Demopoulos . Decreasing acidity in a series of aldose reductase inhibitors: 2-fluoro-4-(1H-pyrrol- 1-yl)phenol as a scaffold for improved membrane permeation *Biorganic Medicinal Chemistry* (2014), in press
- [85] Flavio Ballante, Antonia Caroli, Richard B. Wickersham III‡ and Rino Ragno. Hsp90 Inhibitors (I). Definition of 3-D QSAutogrid/R Models as a Tool for Virtual Screening, *J. Chem. Inf. Model.*, (2014). In press. doi: 10.1021/ci400759t
- [86] Antonia Caroli, Flavio Ballante, Richard B. Wickersham III, Federico Corelli and Rino Ragno. Hsp90 Inhibitors (II). Combining ligand-based and structure-based approaches for Virtual Screening application. *J. Chem. Inf. Model.*, (2014). In press. doi: 10.1021/ci400760a
- [87] Annarita Stringaro, Elisabetta Vavala, Marisa Colone, Federico Pepi, Giuseppina Mignogna, Stefania Garzoli, Serena Cecchetti, Rino Ragno, and Letizia Angiolella. Effects of Mentha suaveolens Essential Oil Alone or in Combination with Other Drugs in Candida albicans, *Evidence-Based Complementary and Alternative Medicine*, vol. 2014, Article ID 125904, 9 pages, 2014. doi:10.1155/2014/125904. In press

LIBRI

1. GARLAND R. MARSHALL, RICHARD D. HEAD AND **RINO RAGNO**. Affinity Prediction: The Sine Qua Non. *Thermodynamics in Biology*, Enrico di Cera, Editor, Oxford University Press. 87-111. **2000**.
2. Rino Ragno. Tecniche di Screening per i nuovi farmaci. Alla ricerca del farmaco perduto, Carlo Tomino, Medi Servis 2010, ISBN: 8890545925, ISBN-13: 9788890545924.