Tudor Ionel Oprea, M.D., Ph.D.

Translational Informatics Division
University of New Mexico School of Medicine
Building 289, Room 2115, MSC10 5550
Albuquerque, NM 87131-0001, USA
Tel.: (+1 505) 272 3694
Fax: (+1 505) 272 8738
E-mail: toprea@salud.unm.edu

Home:
335 Washington St. NE

Albuquerque, NM 87108, USA
Phone: (+1 505) 550 7744
E-mail: tudorzinho@gmail.com

SUMMARY

Over two decades of knowledge management, with proven track record in in drug repurposing, focused on small molecule drug informatics, cheminformatics, translational informatics and data acquisition and mining in medical informatics. Fifteen years of conceptual development for chemical space exploration, including leadlike and druglike properties for high-throughput screening and synthesis. Three years of electronic medical record evaluation and data mining. Strong biomedical background with previous clinical and pharmaco-physiological training. Excellent communication and interpersonal skills. One book as editor (Wiley-VCH), one as author (on molecular modeling; in Romanian), over 20 book chapters, 3 awarded patents, 7 patent applications pending, and over 130 peer-reviewed papers co-authored and published since 1993. Google Scholar profile link.

PROFESSIONAL APPOINTMENTS

• *Professor of Medicine* and *Chief*, Division of Translational Informatics, Department of Internal Medicine, University of New Mexico, Albuquerque, USA (07/12 – present).
• Visiting Professor, Sahlgrenska Institute of Medicine, Department of Rheumatology and Inflammation Research, University of Gothenburg, Gothenburg, Sweden (07/11 – present).
• Guest Professor, Center for Biological Sequence Analysis, Department of Systems Biology, Technical University of Denmark, Lyngby, Denmark (01/09 – present).
• Visiting Professor, Chemometrics Lab, Univ. of Perugia, Perugia, Italy (04/09 – 12/09).
• Professor of Biochemistry and Molecular Biology and Chief, Division of Biocomputing, University of New Mexico, Albuquerque, USA (08/02 – 06/12).
• Founder and CEO, Sunset Molecular Discovery LLC, Santa Fe, USA – from 07/02.
• *Associate Director*, EST Lead Informatics, Enabling Science and Technology, AstraZeneca, Mölndal, Sweden - between 11/00 and 07/02; *Research Scientist*, Computational Chemistry Group, Medicinal Chemistry, AstraZeneca R&D Mölndal, Sweden (04/96 - 03/00).
• *Professor*, Faculty of Chemistry, University of West, Timisoara, Romania (02/02 – 11/03); *Associate Professor* (10/99 – 01/02); and *Visiting Professor* (10/96 – 06/99) at the same Faculty.
• *Postdoctoral Fellow* (with Dr. A.E. García), Theoretical Biology and Biophysics Group, Los Alamos National Laboratory, Los Alamos, New Mexico, USA (07/94 - 03/96)
• *Postdoctoral Research Associate* (with Prof. G.R. Marshall), Center for Molecular Design, Washington University, St. Louis, Missouri, USA (09/92 - 06/94);
• *Visiting Researcher* (with Dr. J.G. Vinter), Molecular Graphics Unit, University Chemical Laboratory, Cambrigde, UK (10-12/93)
• *Assistant Professor* (with Prof. Fr. Schneider), Department of Physiology, University of Medicine and Pharmacy, Timisoara, Romania (02/91 - 07/92)
• *Visiting Scientist* with Prof. F.P. Nijkamp, Dept. Pharmacology, and Prof. L.H.M. Janssen, Dept. Pharmacochemistry, Utrecht University, The Netherlands (10/90 - 12/91)
• *Assistant Researcher* (with Prof. Fr. Schneider), Department of Physiology, University of Medicine and Pharmacy, Timisoara, Romania and Clinical Physiology Laboratory, Timis County Hospital, Timisoara, Romania (07/85 - 09/90)

PROFESSIONAL ACTIVITIES

• Chair, 2005-2012, The Cheminformatics and QSAR Society (former QSAR Society)
• Member of the Scientific Advisory Board, *ChemDiv, Inc.*, San Diego, CA
• Member of the External Advisory Board, *IMIM*, Barcelona, Spain
• Member of the Chemistry Advisory Board, EBI, Hinxton, UK
• Member of the Editorial Board, *Journal of Chemical Information and Modeling* (2006-2012), *QSAR and Combinatorial Sciences* (2004-2009), *ChemMedChem* (since 2005), *Molecular Informatics*
• Ad-hoc referee for *Angew. Chem.*, *Science Translational Medicine, Science Signaling*, *Nature Biotechnology, Nature Chem. Biol., Nature Reviews Drug Discov., Molecular Systems Biology, Proc. Natl. Acad. Sci. USA, Bioorg. Med. Chem. Lett.*, *ChemMedChem*, *Eur. J. Pharm. Sci., J. Med. Chem., J. Comput.-Aided Mol. Design, J. Chem. Inf. Model., J. Mol. Graphics Model., J. Mol. Mod., Org. Lett.*, *Pharm. Res….* and others

Invited Lectures: (selected from over 300):

- Gordon Research Conferences in: *Combinatorial Chemistry*, Oxford UK, 08/06 and Tilton NH, 07/03; *Computer-Aided Drug Design*, Tilton NH, 07/03, and 08/95; *Drug Metabolism*, Plymouth NH, 07/07. Keystone Symposium, 04/06;
- *European QSAR Symposia*: 18th (Rhodes, Greece) 09/10; 17th (Uppsala, Sweden) 09/08; 15th (Istanbul, Turkey) 09/04; 14th (Portsmouth, UK) 09/02; 13th (Düsseldorf, Germany) 08/00; and 10th, Barcelona, Spain, 09/94.
- *ACS National Meetings:* 29 oral presentations between 1995 and 2012;
- BrazMedChem, 4th (11/08), 3rd (11/06), and 1st (11/01);
- FIGON Dutch Medicine Days (Keynote Speaker, 10/10).

• **Invited Faculty:** School for Advanced Sciences, São Paulo, Brazil (April 2012), Institute for Pure and Applied Mathematics at UCLA (Spring 2011); Summer school in Medicinal Chemistry at University of Regensburg (09/08) and at University of Rio de Janeiro (02/08); UCSF, 04/08 and 01/95; Obernai (Alsace), 06/08 and 06/06; University of São Paulo, 11/08, 11/06 and 11/01; Max Planck Institute Dortmund, 12/06.

Awards and prizes:

- Recipient of the STC.UNM 11th (2014) and 8th (2011) Annual Creative Award, in recognition for issued patents
- Recipient of the AAPS Journal Award with LZ Benet and F Broccatelli, 11/13;
- Recipient of the Hansch Award from the QSAR and Modelling Society, 09/02;
- AstraZeneca Global Discovery Conference Poster Awards (three awards), Stockholm, 03/02;
- 1st prize, National Contest in Human Physiology (Romania, 1986);
- ranked 5th (1979) and 3rd (1981) at the National Chemistry Olympiad in Romania.

EDUCATION

- Ph.D. – Molecular Physiology with Francisc Schneider, University of Medicine and Pharmacy, Timisoara, Romania, 1992
- M.D. – General Medicine, University of Medicine and Pharmacy, Timisoara, Romania, 1990
- Baccalauréat (B.Sc.) – Organic Chemistry, Banat College, Timisoara, Romania, 1983

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SCIENTIFIC IMPACT (using Harzing's Publish Or Perish)

- over 8500 citations (1993 to 2013); h-index: 48; g-index: 86
- 4 authors/paper (median); 13.5 citations/paper (median)
- 10 papers with over 200 citations; 19 papers with over 100 citations

LIST OF PUBLICATIONS

Symbols: ≥50 (▼), ≥100 (▲), ≥150 (●) and ≥200 (○) citations (using Harzing's Publish or Perish)

- BOOKS

TI Oprea (Editor). **Chemoinformatics in Drug Discovery**. Wiley, New York, **2005**. ISBN: 3-527-30753-2.

TI Oprea, with L Kurunczi and OM Martin. **Computer-Aided Drug Design** *(in Romanian)*. Mirton Publishing House, Timisoara, Romania, **1999**, ISBN 973-578-990-6

- INVITED BOOK CHAPTERS:

1. TI Oprea, L Kurunczi, Molecular Recognition Processes During Receptor Ligand Interactions. Applications to Receptor Mapping in **Specific Interactions and Biological Recognition Processes,** N Voiculetz, I Motoc, Z Simon (Eds), CRC Press, Boca Raton, **1993**, pp. 295-326

2. TI Oprea, CL Waller, GR Marshall,Viral Proteases: Structure and Function in **Cellular Proteolytic Systems** , A Ciechanover, A Schwartz (Eds), Wiley-Liss, New York, **1994**, pp. 183-221

3. TI Oprea, CMW Ho, GR Marshall *, De Novo* Design: Ligand construction and prediction of affinity in **Computer-Aided Molecular Design**, CH Reynolds, MK Holloway, H Cox (Eds), ACS, Washington DC, **1995**, pp 64-81

4. ▼ TI Oprea, CL Waller, Theoretical and Practical Aspects of Three Dimensional Quantitative Structure-Activity Relationships , in **Reviews in Computational Chemistry**, **vol 11** KB Lipkowitz, DB Boyd (Eds), Wiley, New York, **1997**, pp 127-182

5. TI Oprea, I Zamora, P Svensson, Qvo Vadis, Scoring Functions? Toward an Integrated Pharmacokinetic and Binding Affinity Prediction Framework, in **Combinatorial Library Design and Evaluation for Drug Design.** AK Ghose, VN Viswanadhan (Eds), Marcel Dekker Inc, New York, **2001**, pp 233-266

6. TI Oprea, Chemoinformatics and the Quest for Leads in Drug Discovery. In **Handbook of Chemoinformatics vol 4** J Gasteiger, T Engel (Eds), VCH-Wiley, New York, **2003**, pp 1508-1531

7. TI Oprea, Global Positioning in Chemical Space – the ChemGPS Concept, in **Combinatorial Approaches for New Materials Discovery,** Knowledge Press, Boston MA, **2003**, pp 7-37

8. TI Oprea, 3D-QSAR Modeling in Drug Design, in **Computational Medicinal Chemistry and Drug Discovery** J Tollenaere, H De Winter, W Langenaeker, P Bultinck (Eds), Marcel Dekker Inc, New York, **2004**, pp 571-616

9. TI Oprea, Chemoinformatics in Lead Discovery, in **Chemoinformatics in Drug Discovery.** TI Oprea (Ed), Wiley-VCH, New York, **2005**, pp. 24-41

10. ▼ M Olah, M Mracec, L Ostopovici, R Rad, A Bora, N Hadaruga, I Olah, M Banda, Z Simon, M Mracec, **TI Oprea**. WOMBAT: World of Molecular Bioactivity, in **Chemoinformatics in Drug Discovery**. TI Oprea (Ed), Wiley-VCH, New York, **2005**, pp. 223-239

11. TI Oprea, C Bologa, M Olah, Compound Selection for Virtual Screening, in **Virtual Screening in Drug Discovery.** J Alvarez, B Shoichet(Eds), CRC Press Inc, Boca Raton, **2005**, pp. 89-106

12. LA Sklar, PC Simmons, A Waller, SM Biggs, SM Young, M Olah, C Bologa, **TI Oprea**, ER Prossnitz, BS Edwards. High Throughput Flow Cytommetry. In **Drug Discovery Handbook**, SC Gad (Ed), John Wiley and Sons, **2005**, pp. 185-226

13. CG Bologa, M Olah and **TI Oprea**. Chemical Database Preparation for Compound Acquisition or Virtual Screening. In: Bioinformatics in Drug Discovery. Larson RS (Ed), Humana Press, New York, **2005**, pp 375-388

14. TI Oprea, P Benedetti, G Berellini, M Olah, K Fejgin, S Boyer. Rapid ADME Filters for Lead Discovery, in **Molecular Interaction Fields.** G Cruciani (Ed), Wiley-VCH, New York, **2006**, pp. 249-272

15. TI Oprea, J Blaney. Cheminformatics Approaches to Fragment-based Lead Discovery. In **Fragment-based Approaches in Drug Discovery**, W Jahnke, DA Erlanson (Eds), Wiley-VCH, New York, **2006**, 99-121

16. M Olah, TI Oprea. Bioactivity Databases. In **Comprehensive Medicinal Chemistry II vol 3**, JB Taylor, DJ Triggle (Eds), Elsevier, Oxford, **2006**, 293-313

17. M Olah, R Rad, L Ostopovici, A Bora, N Hadaruga, D Hadaruga, R Moldovan, A Fulias, M Mracec, **TI Oprea**. WOMBAT and WOMBAT-PK: Bioactivity Databases for Lead and Drug Discovery. In *Chemical Biology: From Small Molecules to Systems Biology and Drug Design*, SL Schreiber, TM Kapoor, G Wess (Eds), Wiley-VCH, pp 760-786, **2007**

18. IV Tetko, **TI Oprea**. Early ADME/T Predictions: Toy or Tool? In **Chemoinformatics: An approach to virtual screening**, A Varnek, A Tropsha (Eds), Royal Society of Chemistry, London, **2008**, 240-267

19. TI Oprea. Sense and Nonsense in Drug Discovery: A Chemical Perspective. In **Towards Drugs of the Future**, CG Kruse, H Timmerman (Eds), IOS Press, Amsterdam, **2008**, 29-36

20. TI Oprea, L Ostopovici-Halip, R Rad-Curpan. Databases for chemical and biological information. In **Pharmaceutical Data Mining**, KV Balakin (Ed), Wiley & Sons, Hoboken NJ, **2010**, 491-520

21. TI Oprea, EE May, A Leitão, A Tropsha. Computational Systems Chemical Biology. In *Methods in Molecular Biology,* vol. 672, J Bajorat (Ed), **2011**, 459-488

22. PD Leeson, **TI Oprea**. Drug-like physicochemical properties. In *RSC Drug Discovery Series,* vol. 13, DJ Livingstone, AM Davis (Ed), **2012**, 35-59 **doi**:10.1039/9781849733410-00035

23. TI Oprea, CG Bologa. Compound collection preparation for virtual screening. In *Methods in Molecular Biology,* vol. 910, RS Larson (Ed), **2012**, 125-143

- SCIENTIFIC PUBLICATIONS IN PEER-REVIEWED JOURNALS:

1. Oprea TI, Ciubotariu D, Sulea T, Simon Z. Comparative analysis by the minimal steric difference (MTD), comparative molecular field analysis (CoMFA) methods for binding of steroids to carrier proteins. *Quant. Struct.-Act. Relat.*, 12:21-26, **1993**.
2. Ciubotariu D, Deretey E, **Oprea TI**, Sulea TI, Simon Z, Kurunczi L, Chiriac A. Multiconformational minimal steric difference. Structure-acetylcholinesterase hydrolysis rates relations for acetic acid esters. *Quant. Struct.-Act. Relat.*, 12:367-372, **1993**.
3. ● Waller CL, **Oprea TI**, Giolitti A, Marshall GR. 3D-QSAR of Human Immunodeficiency Virus (I) Protease Inhibitors. I. A CoMFA Study Employing Experimentally-Determined Alignment Rules. *J. Med. Chem.,* 36:4152-4160, **1993**.
4. ▲ Oprea TI, Waller CL, Marshall GR. 3D-QSAR of Human Immunodeficiency Virus (I) Protease Inhibitors. II. Predictive power using limited exploration of alternate binding modes. *J. Med. Chem.*, 37:2206-2215, **1994**.

5. ▼ Oprea TI, Waller CL, Marshall GR. 3D-QSAR of Human Immunodeficiency Virus (I) Protease Inhibitors. III. Interpretation of CoMFA Results. *Drug Design Discov.,* 12:29-51, **1994**.

6. Kurunczi L, Sulea T, **Oprea TI**. Conformational analysis, experimental dipole moments. Comments on a furan derivatives study. *J. Mol. Struct. (Theochem),* 306**:**93-100, **1994.**

7. ▼ Oprea TI, García AE. Three-dimensional quantitative structure activity relationships of steroid Aromatase inhibitors. *J. Comput.-Aided Mol. Design*, 10:186-200, **1996**.

8. ● Waller CL, **Oprea TI**, Chae K, Park H-K, Korach KS, Laws SC, Wiese TE, Kelce WR & Gray LE. Ligand-Based Identification of Environmental Estrogens. *Chem. Res. Toxicol.*, 9:1240-1248, **1996**.

9. ○ Head RD, Smythe ML, **Oprea TI**, Waller CL, Green SM, Marshall GR. VALIDATE: A new method for the receptor-based prediction of binding affinities of novel ligands. *J. Am. Chem. Soc.,* 118:3959-3969, **1996.**

10. Tung C-S, **Oprea TI**, Hummer G, García AE. Three-Dimensional Model of a Selective Theophylline-Binding RNA Molecule. *J. Mol. Recognition*, 9:273-286, **1996**.

11. ▼ Oprea TI, Hummer G, García AE. Identification of a Functional Water Channel in Cytochrome P450 enzymes. *Proc. Natl. Acad. Sci. USA*, 94:2133-2138, **1997**.

12. Sulea T, **Oprea TI**, Muresan S, Chan SL. A Different Method for Steric Field Evaluation in CoMFA Improves Model Robustness. *J. Chem. Inf. Comput. Sci.*, 37:1162-1170, **1997**.

13. Oprea TI, Kurunczi L, Timofei S. Quantitative Structure-Activity Relationship Studies of Disperse Azo Dyes. Towards the negation of the pharmacophore theory of dye-fiber interaction? *Dyes Pigm.*, 33:41-64, **1997.**

14. ▼ Oprea TI, Marshall GR. Receptor-Based Prediction of Affinity. *Perspect. Drug Discov. Des.*, 9-11:35-61, **1998**.

15. Sulea T, Kurunczi L, **Oprea TI**, Simon Z. MTD-ADJ: A multiconformational minimal topologic difference for determining bioactive conformers using adjusted biological activities. *J. Comput.-Aided Mol. Design*, 12, 133-146, **1998**.

16. ○ Teague SJ, Davis AM, Leeson PD, **Oprea TI**. The Design of Leadlike Combinatorial Libraries. *Angew. Chem. Intl. Ed.*, 38:3743-3748, **1999**. German version: *Angew. Chemie*, 111:3962-3967, **1999**.

17. ▼ Oprea TI, Gottfries J. Toward a minimalist model of oral drug absorbtion. *J. Mol. Graph. Model.*, 17, 261-274, **1999**.

18. ○ Oprea TI. Property distribution of drug-related chemical databases. *J. Comput.-Aided Mol. Design*, 14:251-264, **2000**.

19. Oprea TI, Gottfries J, Sherbuhin V, Svensson P, Kühler TC. Chemical information management in drug discovery: Optimizing the computational, combinatorial chemistry interfaces. *J. Mol. Graph. Model.*, 18:512-524, **2000**.

20. Mracec Maria, **Oprea TI**, Mracec M. Correlation between experimental electron affinities for aromatic derivatives, the values calculated with semiempirical MO methods. *Rev. Roum. Chimie*, 45:949-954, **2000**.

21. Oprea TI. Rapid Estimation of Hydrophobicity for Virtual Combinatorial Library Analysis. *SAR QSAR Environ. Res.*, 12:129-141, **2001**.

22. Oprea TI, Kurunczi L, Olah M, Simon Z. MTD-PLS: A PLS-based Variant of the MTD Method. A 3D-QSAR Analysis of Receptor Affinities for a Series of Halogenated Dibenzoxin, Biphenyl Derivatives. *SAR QSAR Environ. Res.*, 12:75-92, **2001**.

23. ● Oprea TI, Gottfries J. Chemography: the art of chemical space navigation. *J. Comb. Chem.*, 3:157-166, **2001**.

24. ○ Oprea TI, Davis AM, Teague SJ, Leeson PD. Is there a difference between leads, drugs? A historical perspective. *J. Chem. Inf. Comput. Sci.*, 41:1308-1315, **2001**.

25. Olsson T, Oprea TI. Cheminformatics: A Tool for Decision Makers in Drug Discovery. *Curr. Op. Drug Discov. Dev.*, 4:308-313, **2001**.

26. Nilsson JW, Thorstensson F, Kvarnström I, **Oprea TI**, Samuelsson B, Nilsson I. Solid phase synthesis of libraries around the 4-phenyl-2-carboxy-piperazine scaffold. *J. Comb. Chem.*, 3, 546-553, **2001**.

27. ▼ Oprea TI. Virtual Screening in Lead Discovery: A Viewpoint. *Molecules*, 7:51-62, **2002**.

28. ▼ Oprea TI. Chemical space navigation in lead discovery. *Curr. Op. Chem. Biol.* 6:384-389, **2002**.

29. ▼ Oprea TI, Zamora I, Ungell AL. Pharmacokinetically based mapping device for chemical space navigation. *J. Comb. Chem.*, 4:258-266, **2002**.

30. Kurunczi L, Olah M, **Oprea TI**, Bologa C, Simon Z. MTD-PLS: A PLS-Based Variant of the MTD Method. 2. Mapping Ligand-Receptor Interactions. Enzymatic Acetic Acid Esters Hydrolysis. *J. Chem. Inf. Comput. Sci.*, 42: 841-846, **2002**.

31. ● Oprea TI. Current trends in lead discovery: Are we looking at the appropriate properties? *J. Comput. Aided Mol. Design* 16:325-334, **2002**

32. Pastor M, Benedetti P, Carotti A, Carrieri A, Diaz C, Herraiz C, H-D Hoeltje, M Loza, **Oprea TI**, F Padin, F Pubill, F Sanz, F Stoll. Distant collaboration in drug discovery: The LINK3D project. *J. Comput.-Aided Mol. Design* 16:809-818, **2002**

33. Oprea TI. On the information content of 2D, 3D descriptors for QSAR. *J. Braz. Chem. Soc.*, 13:811-815, **2002**

34. ▼ Zamora I, **Oprea TI**, Cruciani G, Pastor M, Ungell A-L. Surface descriptors for protein-ligand affinity prediction. *J. Med. Chem.*, 46:25-33, **2003**

35. Oprea TI. Next generation therapeutics. *Curr. Op. Chem. Biol.* 8:347-348, **2004**.

36. ○ Hann MM, Oprea TI. Pursuing the leadlikeness concept in pharmaceutical research. *Curr. Opin. Chem. Biol.,* 8:255-263, **2004**.

37. ● Oprea TI, Matter H. Integrating virtual screening in lead discovery. *Curr. Opin. Chem. Biol.,* 8:349-358, **2004**.

38. ▲ Edwards BS, **Oprea TI**, Prossnitz ER, Sklar LA. Flow Cytometry for High Throughput, High Content Screening. *Curr. Opin. Chem. Biol.,* 8:392-398, **2004**.

39. ▼ Olah MM, Bologa CG, **Oprea TI**. Strategies for Compound Selection, *Curr. Drug Discov. Tech.,* 1:211-220, **2004**.

40. Mracec Maria, Mracec M, Olah M, **Oprea TI**. QSAR study for 2-carboxy-4-carboxamido-tetrahydroquinolines as antagonists of the NMDA receptor. *Rev. Roum. Chim.* 49:567-572, **2004**

41. Olah M, Bologa C, **Oprea TI**. An automated PLS search for biologically-relevant QSAR descriptors. *J. Comput.-Aided Mol. Design*, 18:437-449, **2004**

42. Larson RS, Davis T, Bologa C, Semenuk G, Vivayan S, Li Y, **Oprea TI**, Chigaev A, Wagner CR, Sklar LA. Dissociation of I domain, global conformational changes in LFA-1: Refinement of small molecule-I domain structure-activity relationships. *Biochemistry*, 44:4322-4331, **2005**

43. Young SM, Bologa CG, **Oprea TI**, Prossnitz ER, Sklar LA, Edwards BS. Screening with HyperCyt high throughput flow cytometry to detect small-molecule formyl peptide receptor ligands., *J. Biomol. Screening,* 10:374-382, **2005**

44. Oprea TI, Bologa CG, Edwards BS, Prossnitz ER, Sklar LA. Post-HTS compound prioritization analysis: An empirical evaluation scheme. *J. Biomol. Screening,* 10:419-425, **2005**.

45. Allu TK, Oprea TI. Rapid Evaluation of Synthetic, Molecular Complexity for In Silico Chemistry. *J. Chem. Inf. Model.* 45:1237 – 1243, **2005**

46. Kurunczi L, Secleman E, **Oprea TI**, Crisan L, Simon Z. MTD-PLS: A PLS Variant of the Minimal Topologic Difference Method. III. Mapping Interactions between Estradiol Derivatives, the Alpha Estrogenic Receptor. *J. Chem. Inf. Model.* 45:1275 – 1281, **2005**

47. ▼ Edwards BS, Bologa CG, Young SM, Prossnitz ER, Sklar LA, **Oprea TI**. Integration of virtual screening with high throughput flow cytometry to identify novel small molecule formylpeptide receptor antagonists. *Mol. Pharmacol.* 368:1301-1310, **2005**

48. Bologa CG, Allu TK, Olah M, Kappler MA, **Oprea TI**. Descriptor collision, confusion: Toward the design of descriptors to mask chemical structures. *J. Comput.-Aided Mol. Design*, 19:625-635, **2005**

49. Tetko IV, Abagyan R, **Oprea TI**. Surrogate data -- a secure way to share corporate data. *J. Comput.-Aided Mol. Design*, 19:749-764, **2005**

50. Lloyd DG, Golfis G, Knox AJS, Fayne D, Meegan MJ, **Oprea TI**. Oncology exploration: charting cancer medicinal chemistry space. *Drug Discov. Today*, 11:149-159, **2006**

51. ○ Bologa CG, Revankar CM, Young SM, Edwards BS, Arterburn JB, Parker MA, Tkachenko SE, Savchuck NP, Sklar LA, **Oprea TI**, Prossnitz ER. Virtual, Biomolecular Screening Converge on a Selective Agonist for GPR30. *Nature Chem. Biol.*, 2:207-212, **2006**

52. Edwards BS, Young SM, **Oprea TI**, Bologa CG, Prossnitz ER, Sklar LA. Biomolecular screening of formylpeptide receptor ligands with a sensitive, quantitative, high-throughput flow cytometry platform. *Nature Protocols*, 1:59-66, **2006**

53. Prossnitz ER, Arterburn JB, Edwards BS, Sklar LA, **Oprea TI**. Steroid-binding GPCRs: new drug discovery targets for old ligands. *Expert Opin. Drug Discov*., 1:137-150, **2006**

54. Oprea TI, Tropsha A. Target, chemical, bioactivity databases – integration is key. *Drug Discov. Today Technol.*, 3:357-365, **2006**

55. Fara DC, **Oprea TI**, Prossnitz ER, Bologa CG, Edwards BS, Sklar LA. Integration of virtual, physical screening. *Drug Discov. Today Technol.*, 3:377-385, **2006**

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57. ▼ Oprea TI, Allu TK, Fara DC, Rad RF, Ostopovici L, Bologa CG. Lead-like, drug-like or ''Pub-like'': how different are they? *J. Comput. Aided Mol. Des.*, 21:113–119, **2007**

58. • Brailoiu E, Dun SL, Brailoiu GC, Mizuo K, Sklar LA, **Oprea TI**, Prossnitz ER, Dun NJ. Distribution, characterization of estrogen receptor GPR30 in the rat central nervous system. *J. Endocrinol.* 193:311-321, **2007**

59. Burchiel SW, Thompson TA, Lauer FT, **Oprea TI**. Activation of dioxin response element (DRE)-associated genes by benzo(a)pyrene 3,6-quinone, benzo(a)pyrene 1,6-quinone in MCF-10A human mammary epithelial cells. *Toxicol. Applied Pharmacol.*, 221:203-214, **2007**

60. Edwards BS, Young SM, Saunders MJ, Bologa CG, **Oprea TI**, Ye RD, Prossnitz ER, Graves SW, Sklar LA. High-throughput flow cytometry for drug discovery. *Expert Opin. Drug Discov*., 2:685-696, **2007**

61. ▼ Oprea TI, Tropsha A, Faulon J-L, Rintoul MD. Systems chemical biology. *Nature Chem. Biol.* , 3, 447-450, **2007**

62. ▼ Paunescu V, Deak E, Herman D, Siska IR, Tanasie G, Bunu C, Anghel S, Tatu CA, **Oprea TI**, Henschler R, Ruester B, Bistrian R, Seifried E. In vitro differentiation of human mesenchymal stem cells to epithelial lineage. *J. Cell. Mol. Medicine*, 11:502-508, **2007**

63. Hristozov D, **Oprea TI**, Gasteiger J. Ligand-Based Virtual Screening by Novelty Detection with Self-Organizing Maps. *J. Chem. Inf. Model.* , 47:2044-2062, **2007**

64. Ariazi EA, Leitão A, **Oprea TI**, Chen B, Louis T, Bertucci AM, Sharma CG, Gill SD, Kim HR, Shupp HA, Pyle JR, Madrack A, Donato AL, Cheng D, Paige JR, Jordan VC. Exemestane's 17-hydroxylated metabolite exerts biological effects as an androgen. *Mol. Cancer Therapeutics*, 6:2817-2827, **2007**

65. Freitas RF, **Oprea TI**, Montanari CA. 2D QSAR, similarity studies on cruzain inhibitors aimed at improving selectivity over cathepsin L. *Bioorganic Med. Chem.*, 16:838-853, **2008**

66. Li Q, Jorgensen FS, **Oprea TI**, Brunak S, Taboureau O. hERG Classification Model Based on a Combination of Support Vector Machine Method, GRIND Descriptors. *Mol. Pharmaceutics*, 5:117-127, **2008**

67. ○ Prossnitz ER, Arterburn JB, Smith HO, **Oprea TI**, Sklar LA, Hathaway HJ. Estrogen signaling through the transmembrane G protein–coupled receptor GPR30. *Annu. Rev. Physiol.,* 70:165–190, **2008**

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Gottfries J and Oprea TI. Global method for mapping property spaces. US Patent 6,675,136.

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methods of treating disease states and conditions mediated through these receptors and identification thereof. US Patents 7,875,721 and 8,487,100

- PATENT REQUESTS (PENDING):

Paunescu V, Suciu EI, Tatu CA, **Oprea TI**. Isolation and purification of human insulin producing cells for the treatment of insulin dependent diabetes. PCT Int. Appl. (2006), Application nr 20060148079

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Hromas R, Leitao A, **Oprea TI**, Sklar LA, Williamson EA, Wray J. Metnase and Intnase inhibitors and their use in treating cancer. PCT Int. Appl. (2010), A1 20120093917

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Oprea TI, Bologa CG, Ursu O. Methods for chemical mixture informatics. Provisional Patent Application STC 2013-021-01 (2013)

ON-GOING RESEARCH SUPPORT:

Title: Molecular Libraries Bioactivity Database (MLBD) – U54 supplement
PI: Stuart Schreiber, Chris Austin, Larry Sklar
Agency: NIH **1U54MH084690**
Period: 3/1/2012 - 2/28/2013, *extended through 3/1/2014*
This supplement aims to maximize return on the chemical biology investment of the Roadmap by reshaping knowledge management at NIH ("MLBD"). Total budget: ~8.5 MUSD; UNM Budget ~0.65 MUSD. Oprea wrote the UNM part of the proposal

Title: OpenPHACTS
PI: Gerhard F Ecker (Uni Vienna); PI for DTU: T. Oprea
Agency: Innovative Medicines Initiative (EU)
Period: 3/01/2011 - 2/28/2014
This consortium involves 14 academic partners and 8 major pharmaceutical companies, and aims to establish transparent, effective, semantic-web compliant technologies for data and knowledge mining. Budget ~14 MEuro. Oprea was part of the 4-people core team that wrote the grant.

Title: Givaudan Flavors Corporation
PI: Tudor Oprea
Agency: Private sector funding for consulting
Period: 1/1/2005 - 12/31/2013 *renewed for the 9th consecutive year*
This contract is designed to assist Givaudan with compound selection and analysis for taste and flavor research. Annual budget ~0.33 MUSD

Title: Visiting Professorship Agreement, Gothenburg University
PI: Claes Dahlgren, T. Oprea
Agency: Gothenburg University (GU), Sweden
Period: 7/1/2011 - 6/30/2013 *funding for visiting professorship*
This contract is designed to support research in the group of Prof Claes Dahlgren at the Department of Rheumatology and Inflammation Research. Annual budget ~100k USD

Title: Guest Professorship Agreement, Technical University of Denmark
PI: Søren Brunak, T. Oprea
Agency: Technical University of Denmark (DTU), Denmark
Period: 1/1/2009 - 12/31/2014 *funding for visiting professorship*
This contract is designed to support research in the computational chemical biology group at the Department of Systems Biology. Annual budget ~120k USD

Title: Research Support Agreement, AstraZeneca R&D
PI: Anders Hogner, T. Oprea
Agency: AstraZeneca, Gothenburg Sweden
Period: 1/1/2013 - 12/31/2013
This contract is designed to support the drugs database project. Budget ~10k USD

Title: Subsetting the Small Molecules Repository
PI: T. Oprea
Agency: Evotec and NIH
Period: 5/1/2013 - 12/31/2013
This contract is designed to support the subsetting of the NIH Molecular Libraries program Small Molecules Repository (MLSMR). Budget ~38k USD

Title: Caspase Inhibitors in Neurodegeneration
PI: T. Oprea
Agency: New Mexico Clinical and Translational Science Center (CTSC)
Period: 5/1/2013 - 4/30/2014
This contract is designed to support the identification of Caspase 3, 7 and 8 modulators, as potential targets in neurodegenerative diseases. Annual budget ~18k USD

RECENT PAST RESEARCH SUPPORT:

Title: Development of GPR30-Selective Ligands
MPI: Jeffrey Arterburn, Tudor Oprea, Eric Prossnitz (Multiple PIs)
Agency: NIH **R01CA127731-01A2**
Period: 12/01/2007 - 11/30/2012
This proposal seeks to identify novel GPR30 agonists and antagonists. Budget ~1.4 MUSD

Title: Chemical Pattern Detection and Visualization in Biological Networks
PI: Tudor Oprea
Agency: NIH **5R21GM095952-02**
Period: 1/01/2011 - 11/30/2012
This proposal seeks to develop bioactivity visualization tools in Cytoscape. Budget 475k USD

Title: University of New Mexico Center for Molecular Discovery
PI: Larry Sklar Co-PI and Informatics core director Tudor Oprea
Agency: NIH **1U54MH084690**
Period: 7/1/2008 - 5/28/2012
This facility core provides informatics infrastructure support to the UNMCMD. Budget ~15 MUSD

Title: New Mexico Molecular Library Screening Center
PI: Larry Sklar Co-PI and Cheminformatics core director Tudor Oprea
Agency: NIH **1U54 MH074425-01**
Period: 7/1/2005 - 6/30/2008
This facility core provided informatics infrastructure support to the NM MLS Center. Budget ~9 MUSD. Oprea was part of the 4-people core team that wrote the grant.