BIOGRAPHICAL SKETCH

NAME	POSITION TITLE
Paola Posocco	Associate Professor
Date of birth 31/07/1978	

EDUCATION/TRAINING

INSTITUTION AND LOCATION	DEGREE	YEARs	FIELD OF STUDY
University of Trieste, Italy	PhD	2007-2010	Nanotechnology and Molecular modeling
University of Trieste, Italy	Major Degree with Honor	1997-2005	Chemical Engineering

EMPLOYMENT

2017-present	Associate Professor (ING-IND 24), University of Trieste (UNITS), Italy
2014-2017	Assistant Professor (ING-IND 24), UNITS, Italy
2010-2014	Post-doc (ING-IND 24), Molecular Simulation Engineering Laboratory (MOSE), UNITS, Italy
2007-2009	PhD student, MOSE, UNITS, Italy
2008-2009	Associated scientist, SUPSI, Switzerland
2006-2007	Research collaborator, MOSE, UNITS, Italy
2005-2006	Research collaborator, Centro Ricerche Plast-Optica, Amaro (UD), Italy

TEACHING ACTIVITIES

2015-	Assistant Professor **- Chemical and Biochemical Reactors**, University of Trieste, Italy
2011-2016	Lecturer - **Molecular Simulation**, University of Trieste, Italy

INSTITUTIONAL RESPONSIBILITIES

2017-	Member of the Teaching Board of the School of Nanotechnology, UNITS, Italy
2017-	Referent for the Quality Assurance, Department of Engineering and Architecture, UNITS, Italy
2015-	Member of the Committee for Quality Assurance, Process and Materials Engineering Course, UNITS, Italy

MEMBERSHIPS OF SCIENTIFIC AND PROFESSIONAL SOCIETIES

2016-	Royal Society of Chemistry
2014-	European Materials Modelling Council
2013-	Consorzio Interuniversitario per la Scienza e Tecnologia dei Materiali
2006-	Ordine degli ingegneri della Provincia di Trieste (sezione A)

CAREER BREAKS

2015 **Maternity Leave**, Oct 2014- Feb 2015

AWARDS

2016 Cover for “Mastering dendrimer self-assembly for efficient siRNA, delivery: from conceptual design to *in vivo* efficient gene silencing”, Chen et al. Small 2016, 12, 3667

2015 Finalist at Start Cup FVG with “SmartNanoLab” start-up project

2014 TOYP (The Outstanding Young Person) Prize, "Research", Junior Chamber International Lom Trieste

2012 Finalist at Nanochallenge international competition with “EpiDyne” start-up project

2012 National Science Foundation-sponsored fellowship award to attend FOMMS

2012 Cover for “Rationalizing the F···S interaction discovered within a tetrafluorophenylazido-containing bolaphospholipid”, Xia et al. Chem. Commun. 2012, 36, 4261

2011 Finalist at Premio Nazionale Innovazione-Working Capital 2011 with a research project entitled “Design of multifunctional materials for thin films by multiscale molecular modeling”

BIBLIOMETRICS

- Pubblications: 77 original papers and 9 chapter books
- Times cited (Google Scholar): 1970
- H-index (Google Scholar): 26

INTERNATIONAL PUBLISHED COLLABORATIONS

Ling Peng (CNRS Marseille, 15 publications), David K. Smith (University of York, 15 publications), Kostas Karatasos (University of Thessaloniki, 5 publications), Alfonso Quintás-Cardama (University of Texas MD Anderson Cancer Center, 3 publications), Johannes Fraije (Leiden Institute of Chemistry, 3 publications), Marcelo Calderon (Freie Universität Berlin, 4 publications), Martin Lísal (J. E. Purkinje University, 4 publications), Carlo V. Catapano (Institute of Oncology Research Bellinzona, 2 publications), Laurence Charles (Aix-Marseille Université, 2 publication), Julian Rodriguez-Lopez (Universidad de Castilla la Mancha, 1 publication), Francesco Stellacci (1 publication)

PARTICIPATION TO RESEARCH PROJECTS

2017-2019 **POR-FESR**, Plastic Cover for Marine Engine

2015-2018 **SIR**, Structure and Function at the nanoparticle bioInterfAce

2015-2016 **FRA**, Combined Computational/Experimental Evidences for Multivalent Amphiphilic Nanoscale Carriers

2014-2016 **FP7**, Modelling of morphology Development of micro- and NAno Structures

2013-2013 **ISCRA**, A multiscale modeling approach for the rational design of self-assembling multivalent nanovectors for gene therapy

2013-2014 **ISCRA**, Dendrimer Illuminated using what’s offered by molecular simulation

2012-2016 **FP7**, Soft Materials Advanced Research Training Network

2012-2015 **P.O.N. RICERCA E COMPETITIVITA**’, PRocessi Ausiliari: le giunzioni aDesive e il rEpairing

2012-2015 **Industria 2015**, Rivestimenti multifunzionali nanostrutturati su materiali soft per migliorare la qualità dei prodotti del made in Italy

2010-2013 **Euronanomed ERA-NET**, Dendrimers as nanovectors for targeted RNA delivery in gene therapy

2010 - 2012 **PRIN**, Modellazione molecolare multiscala di sistemi nanostrutturati biodegradabili: previsione di strutture e proprietà

2010-2012 **FP7**, Multi-Scale Modelling of Nano-Structured Polymeric Materials: From Chemistry to Materials Performance

2010-2012 **POR-FESR**, Green boat design: nautica da diporto a basso impatto

2009-2011 **Swiss National Science Foundation**, Nanovectors for drug delivery in oncology: a combined modeling/experimental study

2009-2010 **PRIN**, Modellazione numerica della nascita e dello sviluppo di interfacce mediante il metodo delle discontinuita' forti intraelemento

2008-2012 **COST Action**, Dendrimers in Biomedical Applications

2008-2010 **RINAVE**, Metodologie innovative di ricollocazione di materie plastiche nanocomposite per la sostituzione dei compositi in fibre di vetro e matrice termoindurente

2007-2010 **FP6,** Innovative sensor-based processing technology of nanostructured multifunctional hybrids and composites

2007-2009 **FP6**, Design of "tailor to made" multifunctional organic materials by molecular modelling of structure property relationship, experimentation and processing

2004-2007 **FP6**, Innovative molecular modelling approach to up-grade polymeric materials from post-industrial rejects

SUPERVISION of PhD STUDENTS and POST-DOCS

4 Post-Docs: Filomena Guida (2016-), Elena Pellizzoni (2017-), Maria Sologan (2016-), Domenico Marson (2015-); 1 PhD student in Nanotechnology: Silvia Boccardo (2015-)

SUPERVISION of STUDENTS

26 undergraduate and graduate students in Process and Materials Engineering

REVIEWER

Biomacromolecules, Langmuir, Macromolecules, Journal Of Nanoparticle Research, New Journal of Chemistry, Journal of Chemical Physics, Nanoscale

PUBLICATIONS, ORIGINAL AND PEER-REVIEWED

1. Vieira, V. M. P.; Liljeström, V.; **Posocco, P**.; Laurini , E.; Pricl, S.; Kostiainen, M. A.; Smith, D. K., Emergence of highly-ordered hierarchical nanoscale aggregates on electrostatic binding of self-assembled multivalent (samul) cationic micelles with polyanionic heparin. *J. Mater. Chem. B* **2017**, *5*, 341-347.

2. Pengo, P.; Şologan, M.; Pasquato, L.; Guida, F.; Pacor, S.; Tossi, A.; Stellacci, F.; Marson, D.; Boccardo, S.; Pricl, S.; **Posocco, P.**, Gold nanoparticles with patterned surface monolayers for nanomedicine: Current perspectives" *Eur. Biophys. J.* **2017**, DOI:10.1007/s00249-017-1250-6.

3. Chiarappa, G.; Piccolo, A.; Colombo, I.; Hasa, D.; Voinovich, D.; Moneghini, M.; Grassi, G.; Farra, R.; Abrami, M.; **Posocco, P.**; Pricl, S.; Grassi, M., Exploring the shape influence on melting temperature, enthalpy, and solubility of organic drug nanocrystals by a thermodynamic model. *Cryst. Growth Des.* **2017**, *17* (8), 4072-4083.

4. Albanyan, B.; Laurini, E.; **Posocco, P.**; Pricl, S.; Smith, D. K., Self-assembled multivalent (samul) polyanion binding—impact of hydrophobic modifications in the micellar core on DNA and heparin binding at the peripheral cationic ligands. *Chem.–Eur. J.* **2017**, *23* (26), 6391-6397.

5. Rodrigo, A. C.; Bromfield, S. M.; Laurini, E.; **Posocco, P.**; Pricl, S.; Smith, D. K., Morphological control of self-assembled multivalent (samul) heparin binding in highly competitive media. *Chem. Commun.* **2017**, *53* (47), 6335-6338.

6. Hinman, S. S.; Ruiz, C. J.; Cao, Y.; Ma, M. C.; Tang, J.; Laurini, E.; Posocco, P.; Giorgio, S.; Pricl, S.; Peng, L.; Cheng, Q., Mix and match: Coassembly of amphiphilic dendrimers and phospholipids creates robust, modular, and controllable interfaces. *ACS Appl Mater Interfaces* **2017**, 9, 1029–1035.

7. Sologan, M.; Marson, D.; Polizzi, S.; Pengo, P.; Boccardo, S.; Pricl, S.; **Posocco, P.**; Pasquato, L., Patchy and janus nanoparticles by self-organization of mixtures of fluorinated and hydrogenated alkanethiolates on the surface of a gold core. *ACS Nano* **2016**, *10*, 9316−9325.

8. **Posocco, P.**; Perazzo, A.; Preziosi, V.; Laurini, E.; Pricl, S.; Guido, S. Interfacial Tension of Oil/Water Emulsions with Mixed Non-Ionic Surfactants: Comparison between Experiments and Molecular Simulations. *RSC Advances* **2016**, *6*, 4723-4729.

9. **Posocco, P.**; Hassan, Y. M.; Barandiaran, I.; Kortaberria, G.; Pricl, S.; Fermeglia, M. Combined Mesoscale/Experimental Study of Selective Placement of Magnetic Nanoparticles in Diblock Copolymer Films Via Solvent Vapor Annealing. *J. Phys. Chem. C* **2016**, *120*, 7403-7411.

10. Posel, Z.; **Posocco, P.**; Lisal, M.; Fermeglia, M.; Pricl, S. Highly Grafted Polystyrene/Polyvinylpyridine Polymer Gold Nanoparticles in a Good Solvent: Effects of Chain Length and Composition. *Soft Matter* **2016**, *12*, 3600-3611.

11. Marizza, P., et al. Synthesis and Characterization of Uv Photocrosslinkable Hydrogels with Poly(N-Vinyl-2-Pyrrolidone): Determination of the Network Mesh Size Distribution. *International Journal of Polymeric Materials and Polymeric Biomaterials* **2016**, *65*, 516-525.

12. Laurini, E.; Marson, D.; **Posocco, P.**; Fermeglia, M.; Pricl, S. Structure and Binding Thermodynamics of Viologen-Phosphorous Dendrimers to Human Serum Albumin: A Combined Computational/Experimental Investigation. *Fluid Phase Equilibria* **2016**, *422*, 18-31.

13. Fechner, L. E.; Albanyan, B.; Vieira, V. M. P.; Laurini, E.; **Posocco, P.**; Pricl, S.; Smith, D. K. Electrostatic Binding of Polyanions Using Self-Assembled Multivalent (SAMUL) Ligand Displays - Structure-Activity Effects on DNA/Heparin Binding. *Chem. Sci.* **2016**, 7, 4653-4659.

14. Chen, C., et al. Mastering Dendrimer Self-Assembly for Efficient Sirna Delivery: From Conceptual Design to in Vivo Efficient Gene Silencing. *Small* **2016**, 12, 3667-3676.

15. Chan, C. W.; Laurini, E.; **Posocco, P.**; Pricl, S.; Smith, D. K. Chiral Recognition at Self-Assembled Multivalent (Samul) Nanoscale Interfaces - Enantioselectivity in Polyanion Binding. *Chem. Commun.* **2016**, 52, 10540-10543.

16. Laurini, E.; **Posocco, P.**; Fermeglia, M.; Pricl, S., Modena Nanotools: An Integrated Multiscale Simulation Workflow to Predict Thermophysical Properties of Thermoplastic Polyurethanes. *J. Comput. Sci.* **2016**, 15, 24-33.

17. Mehrabadi, F. S.; Hirsch, O.; Zeisig, R.; **Posocco, P.**; Laurini, E.; Pricl, S.; Haag, R.; Kemmner, W.; Calderon, M. Structure-Activity Relationship Study of Dendritic Polyglycerolamines for Efficient SiRNA Transfection. *RSC Advances* **2015**, 5, 78760-78770.

18. Chendo, C.; Moreira, G.; Tintaru, A.; **Posocco,P.**; Laurini, E.; Lefay,C.; Gigmes, D.; Viel, S.; Pricl, S.; Charles, L., Anomerization of Acrylated Glucose During Traveling Wave Ion Mobility Spectrometry. *J. Am. Soc. Mass. Spectrom.* **2015**, 26, 1483-1493.

19. Wei, T.; Chen, C.; Liu, J.; Liu, C.; **Posocco, P.**; Liu, X.; Cheng, Q.; Huo, S.; Liang, Z.; Fermeglia, M.; Pricl, S.; Liang, X.-J.; Rocchi, P.; Peng, L., Anticancer drug nanomicelles formed by self-assembling amphiphilic dendrimer to combat cancer drug resistance. *PNAS* **2015**, 112, 2978-2983.

20. Marson, D.; Laurini, E.; **Posocco, P.**; Fermeglia, M.; Pricl, S., Cationic carbosilane dendrimers and oligonucleotide binding: An energetic affair. *Nanoscale* **2015**, *7*, 3876-3887.

21. Liu, X.; Zhou, J.; Yu, T.; Chen, C.; Cheng, Q.; Sengupta, K.; Huang, Y.; Li, H.; Liu, C.; Wang, Y.; **Posocco, P.**; Wang, M.; Cui, Q.; Giorgio, S.; Fermeglia, M.; Qu, F.; Pricl, S.; Shi, Y.; Liang, Z.; Rocchi, P.; Rossi, J. J.; Peng, L., Adaptive Amphiphilic Dendrimer-Based Nanoassemblies as Robustand Versatile siRNA Delivery Systems. *Angew. Chem. Int. Ed.* **2014**, *53*, 11822-11827.

22. Kala, S.; Mak, A. S.; Liu, X.; **Posocco, P.**; Pricl, S.; Peng, L.; Wong, A. S., Combination of Dendrimer Nanovector Mediated Small Interfering RNA Delivery to Target Akt with Clinical Anticancer Drug Paclitaxel for Effective and Potent Anticancer Activity in Treating Ovarian Cancer. *J. Med. Chem.* **2014,** *57*, 2634-2642.

23. Wang, Y.; Liu, X.; Laurini, E.; **Posocco, P.**; Ziarelli, F.; Fermeglia, M.; Qu, F.; Pricl, S.; Zhang, C.-C.; Peng, L., Mimicking the 2-oxoglutaric acid signalling function using molecular probes: insights from structural and functional investigations. *Org. Biomol. Chem.* **2014,** *12* (26), 4723-4729.

24. Bromfield, S. M.; **Posocco, P.**; Fermeglia, M.; Tolosa, J.; Herreros-López, A.; Pricl, S.; Rodríguez-López, J.; Smith, D. K., Shape-Persistent and Adaptive Multivalency: Rigid Transgeden (TGD) and Flexible PAMAM Dendrimers for Heparin Binding. *Chem. Eur. J.* **2014,** *20* (31), 9666-9674.

25. Gibbons, D. L.; Pricl, S.; **Posocco, P.**; Laurini, E.; Fermeglia, M.; Sun, H.; Talpaz, M.; Donato, N.; Quintás-Cardama, A., Molecular dynamics reveal BCR-ABL1 polymutants as a novel mechanism of resistance to pan-BCR-ABL1 kinase inhibitor therapy. *PNAS* **2014**, 111(9), 3550-3555.

26. Bromfield, S. M.; **Posocco, P.**; Chan, C. W.; Calderon,M.; Guimond, S. R.; Turnbull, J. E.; Pricl, Smith, D. K., Nanoscale Self-Assembled Multivalent (SAMul) Heparin Binders in Highly Competitive, Biologically Relevant, Aqueous Media. *Chem. Sci.* **2014**, 5(4), 1484-1492.

27. Barnard, A.; **Posocco, P.**; Fermeglia, M.; Tschiche, A.; Calderon, M.; Pricl, S.; Smith, D. K., Double-degradable responsive self-assembled multivalent arrays - temporary nanoscale recognition between dendrons and DNA. *Org. Biomol. Chem.* **2014**, *12* (3), 446-455.

28. Tintaru, A.; Chendo, C.; Wang, Q.; Viel, S.; Quelever, G.; Peng, L.; **Posocco, P.**; Pricl, S.; Charles, L., Conformational sensitivity of conjugated poly(ethylene oxide)-poly(amidoamine) molecules to cations adducted upon electrospray ionization - A mass spectrometry, ion mobility and molecular modeling study. *Anal. Chim. Acta* **2014**, *808*, 163-174.

29. Ottaviani, M. F.; Cangiotti, M.; Fattori, A.; Coppola, C.; **Posocco, P.**; Laurini, E.; Liu, X.; Liu, C.; Fermeglia, M.; Peng, L.; Pricl, S., Copper(II) binding to flexible triethanolamine-core PAMAM dendrimers: a combined experimental/in silico approach. *Phys. Chem.Chem.Phys.* **2014**, *16* (2), 685-694.

30. Liu, X.; Wang, Y.; Laurini, E.; **Posocco, P.**; Chen, H.; Ziarelli, F.; Janicki, A.; Qu, F.; Fermeglia, M.; Pricl, S.; Zhang, C.-C.; Peng, L., Structural requirements of 2-oxoglutaric acid analogues to mimic its signaling function. *Org. Lett.* **2013**, *15* (18), 4662–4665.

31. Bozzi, F.; Conca, E.; Laurini, E.; **Posocco, P.**; Lo Sardo, A.; Jocolle, G.; Sanfilippo, R.; Gronchi, A.; Perrone, F.; Tamborini, E.; Pelosi, G.; Pierotti, M. A.; Maestro, R.; Pricl, S.; Pilotti, S., In vitro and in silico studies of MDM2/MDMX isoforms predict Nutlin-3A sensitivity in well/de-differentiated liposarcomas. *Lab. Invest.* **2013**, *93* (11), 1232-1240.

32. Tanis, I.; Karatasos, K.; **Posocco, P.**; Laurini, E.; Pricl, S., Complexes between poly(amido amine) dendrimers and poly(methacrlyic acid): insight from molecular dynamics simulations. *Macromol. Symp.* **2013**, *331-332* (1), 34-42.

33. **Posocco, P.**; Liu, X.; Laurini, E.; Marson, D.; Chen, C.; Liu, C.; Fermeglia, M.; Rocchi, P.; Pricl, S.; Peng, L., Impact of siRNA overhangs for dendrimer-mediated siRNA delivery and gene silencing. *Mol. Pharm.* **2013**, *10* (8), 3262-73.

34. Bromfield, S. M.; **Posocco, P.**; Fermeglia, M.; Pricl, S.; Rodriguez-Lopez, J.; Smith, D. K., A simple new competition assay for heparin binding in serum applied to multivalent PAMAM dendrimers. *Chem. Commun.* **2013**, *49* (42), 4830-4832.

35. Bromfield, S. M.; Barnard, A.; **Posocco, P.**; Fermeglia, M.; Pricl, S.; Smith, D. K., Mallard Blue: A high-affinity selective heparin sensor that operates in highly competitive media. *J. Am. Chem. Soc.* **2013**, *135* (8), 2911-2914.

36. Welsh, D. J.; **Posocco, P.**; Pricl, S.; Smith, D. K., Self-assembled multivalent RGD-peptide arrays--morphological control and integrin binding. *Org. Biomol. Chem.* **2013**, *11* (19), 3177-86.

37. Laurini, E.; **Posocco, P.**; Fermeglia, M.; Gibbons, D. L.; Quintas-Cardama, A.; Pricl, S., Through the open door: Preferential binding of dasatinib to the active form of BCR-ABL unveiled by in silico experiments. *Mol. Oncol.* **2013**, *7* (5), 968-975.

38. Fermeglia, M.; **Posocco, P.**; Pricl, S., Nano tools for macro problems: multiscale molecular modeling of nanostructured polymer systems. *Compos. Interfaces* **2013**, *20* (6), 379-394.

39. Posel, Z.; **Posocco, P.**; Fermeglia, M.; Lisal, M.; Pricl, S., Modeling hierarchically structured nanoparticle/diblock copolymer systems. *Soft Matter* **2013**, *9* (10), 2936-2946.

40. Pricl, S.; **Posocco, P.**; Laurini, E.; Fermeglia, M.; Talpaz, M.; Cortes, J. E.; Donato, N. J.; Quintas-Cardama, A., Acquisition of compound BCR-ABL1 alleles as a mechanism of resistance to ponatinib in chronic myeloid leukemia. *Blood* **2013**, *122* (21), 853.

41. **Posocco, P.**; Gentilini, C.; Bidoggia, S.; Pace, A.; Franchi, P.; Lucarini, M.; Fermeglia, M.; Pricl, S.; Pasquato, L., Self-organization of mixtures of fluorocarbon and hydrocarbon amphiphilic thiolates on the surface of gold nanoparticles. *ACS Nano* **2012**, *6* (8), 7243-7253.

42. Nieto, D. R.; Santese, F.; Toth, R.; **Posocco, P.**; Pricl, S.; Fermeglia, M., Simple, fast, and accurate in silico estimations of contact angle, surface tension, and work of adhesion of water and oil nanodroplets on amorphous polypropylene surfaces. *ACS Appl. Mater. Interfaces* **2012**, *4* (6), 2855–2859.

43. Toth, R.; Santese, F.; Pereira, S. P.; Nieto, D. R.; Pricl, S.; Fermeglia, M.; **Posocco, P.**, Size and shape matter! A multiscale molecular simulation approach to polymer nanocomposites. *J. Mater. Chem.* **2012**, *22* (12), 5398-5409.

44. Marson, D.; Dal Col, V.; **Posocco, P.**; Laurini, E.; Fermeglia, M.; Pricl, S., Genes within bottles. synergism between simulation and experiment in designing nanovectors for DNA/RNA delivery. *Chem. Biochem. Eng. Q.* **2012**, *26* (4), 447–465.

45. **Posocco, P.**; Laurini, E.; Dal Col, V.; Marson, D.; Karatasos, K.; Fermeglia, M.; Pricl, S., Tell me something I do not know. Multiscale molecular modeling of dendrimer/dendron organization and self-assembly in gene therapy. *Curr. Med. Chem.* **2012**, *19* (29), 5062-5087.

46. Karatasos, K.; **Posocco, P.**; Laurini, E.; Pricl, S., Poly(amidoamine)-based dendrimer/siRNA complexation studied by computer simulations: effects of pH and generation on dendrimer structure and siRNA binding. *Macromol. Biosci.* **2012**, *12* (2), 225-240.

47. Liu, X.; Liu, C.; Laurini, E.; **Posocco, P**.; Pricl, S.; Qu, F.; Rocchi, P.; Peng, L., Efficient delivery of sticky siRNA and potent gene silencing in a prostate cancer model using a generation 5 triethanolamine-core PAMAM dendrimer. *Mol. Pharm.* **2012**, *9* (3), 470-81.

48. Xia, Y.; Viel, S.; Wang, Y.; Ziarelli, F.; Laurini, E.; **Posocco, P.**; Fermeglia, M.; Qu, F.; Pricl, S.; Peng, L., Rationalizing the F-S interaction discovered within a tetrafluorophenylazido-containing bola-phospholipid. *Chem. Commun.* **2012**, *48* (36), 4284-4286.

49. Pereira, S. P.; Scocchi, G.; Toth, R.; **Posocco, P.**; Nieto, D. R.; Pricl, S.; Fermeglia, M., Multiscale modeling of polymer/clay nanocomposites *Journal of Multiscale Modelling* **2011**, *3* (3), 151-176.

50. Barnard, A.; **Posocco, P.**; Pricl, S.; Calderon, M.; Haag, R.; Hwang, M. E.; Shum, V. W.; Pack, D. W.; Smith, D. K., Degradable self-assembling dendrons for gene delivery: experimental and theoretical insights into the barriers to cellular uptake. *J. Am. Chem. Soc.* **2011**, *133* (50), 20288-20300.

51. Liu, X.; Wu, J.; Yammine, M.; Zhou, J.; **Posocco, P.**; Viel, S.; Liu, C.; Ziarelli, F.; Fermeglia, M.; Pricl, S.; Victorero, G.; Nguyen, C.; Erbacher, P.; Behr, J.-P.; Peng, L., Structurally flexible triethanolamine core PAMAM dendrimers

are effective nanovectors for DNA transfection in vitro and in vivo to the mouse thymus. *Bioconjug. Chem.* **2011**, *22* (12), 2461-2473.

52. Laurini, E.; Col, V. D.; Mamolo, M. G.; Zampieri, D.; **Posocco, P.**; Fermeglia, M.; Vio, L.; Pricl, S., Homology model and docking-based virtual screening for ligands of the σ1 receptor. *ACS Med. Chem. Lett.* **2011**, *2* (11), 834-839.

53. Jones, S. P.; Gabrielson, N. P.; Wong, C.-H.; Chow, H.-F.; Pack, D. W.; **Posocco, P.**; Fermeglia, M.; Pricl, S.; Smith, D. K., Hydrophobically modified dendrons: developing structure-activity relationships for DNA binding and gene transfection. *Mol. Pharm.* **2011**, *8* (2), 416-429.

54. Liu, X.; Chen, H.; Laurini, E.; Wang, Y.; Dal Col, V.; **Posocco, P.**; Ziarelli, F.; Fermeglia, M.; Zhang, C.-C.; Pricl, S.; Peng, L., 2-difluoromethylene-4-methylenepentanoic acid, a paradoxical probe able to mimic the signaling role of 2-oxoglutaric acid in cyanobacteria. *Org. Lett.* **2011**, *13* (11), 2924-2927.

55. Dileo, P.; Pricl, S.; Tamborini, E.; Negri, T.; Stacchiotti, S.; Gronchi, A.; **Posocco, P.**; Laurini, E.; Coco, P.; Fumagalli, E.; Casali, P. G.; Pilotti, S., Imatinib response in two GIST patients carrying two hitherto functionally uncharacterized PDGFRA mutations: an imaging, biochemical and molecular modeling study. *Int. J. Cancer* **2011**, *128* (4), 983-990.

56. Carta, A.; Briguglio, I.; Piras, S.; Boatto, G.; La Colla, P.; Loddo, R.; Tolomeo, M.; Grimaudo, S.; Di Cristina, A.; Pipitone, R. M.; Laurini, E.; Paneni, M. S.; **Posocco, P.**; Fermeglia, M.; Pricl, S., 3-Aryl-2-[1H-benzotriazol-1-yl]acrylonitriles: a novel class of potent tubulin inhibitors. *Eur. J. Med. Chem.* **2011**, *46* (9), 4151-4167.

57. Tonelli, M.; Boido, V.; Colla, P. L.; Loddo, R.; **Posocco, P.**; Paneni, M. S.; Fermeglia, M.; Pricl, S., Pharmacophore modeling, resistant mutant isolation, docking, and MM-PBSA analysis: Combined experimental/computer-assisted approaches to identify new inhibitors of the bovine viral diarrhea virus (BVDV). *Bioorg. Med. Chem.* **2010**, *18* (6), 2304-2316.

58. Giliberti, G.; Ibba, C.; Marongiu, E.; Loddo, R.; Tonelli, M.; Boido, V.; Laurini, E.; **Posocco, P.**; Fermeglia, M.; Pricl, S., Synergistic experimental/computational studies on arylazoenamine derivatives that target the bovine viral diarrhea virus RNA-dependent RNA polymerase. *Bioorg. Med. Chem.* **2010**, *18* (16), 6055-6068.

59. Laurini, E.; Zampieri, D.; Mamolo, M. G.; Vio, L.; Zanette, C.; Florio, C.; **Posocco, P.**; Fermeglia, M.; Pricl, S., A 3D-pharmacophore model for σ2 receptors based on a series of substituted benzo[d]oxazol-2(3H)-one derivatives. *Bioorg. Med. Chem. Lett.* **2010**, *20* (9), 2954-2957.

60. **Posocco, P.**; Fermeglia, M.; Pricl, S., Morphology prediction of block copolymers for drug delivery by mesoscale simulations. *J. Mater. Chem.* **2010**, *20* (36), 7742-7753.

61. Pavan, G. M.; **Posocco, P.**; Tagliabue, A.; Maly, M.; Malek, A.; Danani, A.; Ragg, E.; Catapano, C. V.; Pricl, S., PAMAM Dendrimers for siRNA Delivery: Computational and Experimental Insights. *Chem. Eur. J.* **2010**, *16* (26), 7781-7795.

62. **Posocco, P.**; Pricl, S.; Jones, S.; Barnard, A.; Smith, D. K., Less is more – multiscale modelling of self-assembling multivalency and its impact on DNA binding and gene delivery. *Chem. Sci.* **2010**, *1* (3), 393-404.

63. Piscitelli, F.; **Posocco, P.**; Toth, R.; Fermeglia, M.; Pricl, S.; Mensitieri, G.; Lavorgna, M., Sodium montmorillonite silylation: unexpected effect of the aminosilane chain length. *J. Colloid Interface Sci.* **2010**, *351* (1), 108-15.

64. **Posocco, P.**; Posel, Z.; Fermeglia, M.; Lísal, M.; Pricl, S., A molecular simulation approach to the prediction of the morphology of self-assembled nanoparticles in diblock copolymers. *J. Mater. Chem.* **2010**, *20* (46), 10511–10520.

65. Zampieri, D.; Mamolo, M. G.; Laurini, E.; Florio, C.; Zanette, C.; Fermeglia, M.; **Posocco, P.**; Paneni, M. S.; Pricl, S.; Vio, L., Synthesis, biological evaluation, and three-dimensional in silico pharmacophore model for σ1 receptor ligands based on a series of substituted benzo[d]oxazol-2(3h)-one derivatives. *J. Med. Chem.* **2009**, *52* (17), 5380-5393.

66. Zampieri, D.; Mamolo, M. G.; Laurini, E.; Fermeglia, M.; **Posocco, P.**; Pricl, S.; Banfi, E.; Scialino, G.; Vio, L., Antimycobacterial activity of new 3,5-disubstituted 1,3,4-oxadiazol-2(3H)-one derivatives. Molecular modeling investigations. *Bioorg. Med. Chem.* **2009**, *17* (13), 4693-4707.

67. Tonelli, M.; Vazzana, I.; Tasso, B.; Boido, V.; Sparatore, F.; Fermeglia, M.; Paneni, M. S.; **Posocco, P.**; Pricl, S.; Colla, P. L.; Ibba, C.; Secci, B.; Collu, G.; Loddo, R., Antiviral and cytotoxic activities of aminoarylazo compounds and aryltriazene derivatives. *Bioorg. Med. Chem.* **2009**, *17* (13), 4425-4440.

68. Scocchi, G.; **Posocco, P.**; Handgraaf, J.-W.; Fraaije, J. G. E. M.; Fermeglia, M.; Pricl, S., A complete multiscale modelling approach for polymer–clay nanocomposites. *Chem. Eur. J.* **2009**, *15* (31), 7586-7592.

69. Toth, R.; Voorn, D.-J.; Handgraaf, J.-W.; Fraaije, J. G. E. M.; Fermeglia, M.; Pricl, S.; **Posocco, P.**, Multiscale computer simulation studies of water-based montmorillonite/poly(ethylene oxide) nanocomposites. *Macromolecules* **2009**, *42* (21), 8260-8270.

70. Maly, M.; **Posocco**, **P.**; Pricl, S.; Fermeglia, M., Self-Assembly of nanoparticle mixtures in diblock copolymers: multiscale molecular modeling. *Ind. Eng. Chem. Res.* **2008**, *47* (15), 5023–5038.

71. Maly, M.; **Posocco, P.**; Fermeglia, M.; Pricl, S., Scripting approach in hybrid organic–inorganic condensation simulation: the GPTMS proof-of-concept. *Mol. Simulat.* **2008**, *34* (10-15), 1215–1236.

72. Fermeglia, M.; Maly, M.; **Posocco, P.**; Pricl, S., Multiscale molecular modeling of hybrid organic-inorganic nanocomposites of type I and II. *Advances in Science and Technology* **2008**, *54*, 265-269.

73. **Posocco, P.**; Pavan, G. M.; Scocchi, G.; Handgraaf, J.-W.; Malek, A.; Maly, M.; Fermeglia, M.; Fraaije, J. G. E. M.; Catapano, C. V.; Danani, A.; Pricl, S., Base invaders. Coupling experiments and multiscale modeling of dendrimer-based siRNA delivery agents. *Advances in Science and Technology* **2008**, *57*, 154-159.

74. **Posocco, P.**; Ferrone, M.; Fermeglia, M.; Pricl, S., Binding at the core. Computational study of structural and ligand binding properties of naphthyridine-based dendrimers. *Macromolecules* **2007**, *40*, 2257-2266.

75. Scocchi, G.; **Posocco, P.**; Fermeglia, M.; Pricl, S., Polymer−clay nanocomposites: a multiscale molecular modeling approach. *J. Phys. Chem. B* **2007**, *111* (9), 2143-2151.

76. Scocchi, G.; **Posocco, P.**; Danani, A.; Pricl, S.; Fermeglia, M., To the nanoscale, and beyond! Multiscale molecular modeling of polymer-clay nanocomposites. *Fluid Phase Equilibria* **2007**, *261* (1-2), 366-374.

77. Fermeglia, M.; Ferrone, M.; Cosoli, P.; Paneni, M. S.; Venica, R.; Pricl, S.; Sinesi, S.; **Posocco, P.**; Martinelli, L., Many-scale simulation of ABS/PC blends for the automotive industry. *Advances in Science and Technology* **2006**, *51*, 134-139.

CHAPTER BOOKS

1. Marson, M.; Yang, Y.; Guldin, S.; **Posocco, P.**; "Noble metal nanoparticles with anisotropy in shape and surface functionality for biomedical applications" in "Anisotropic Particle Assemblies: Synthesis, Assembly, Modeling, and Applications", Elsevier Ltd, **2018**, in press.

2. Laurini E.; **Posocco P.**; Fermeglia M; Pricl S; "Multiscale molecular modeling of clay-polymer nanocomposites" in "Clay-polymer nanocomposites. Morphology, structure, properties and applications", Jlassi K, Chehimi MM, Thomas S (eds.) Elsevier Ltd, **2017**.

3. **Posocco, P.**; Pricl, S.; Fermeglia, M., "Modelling and Simulation of Sol-Gel Nanocomposites" in "Sol-Gel Nanocomposites. Advances in Sol-Gel Derived Materials and Technologies"", Eds: M. Guglielmi, G. Kickelbick, A. Martucci, Springer, **2014,** pp: 21-49.

4. **Posocco, P**.; Pricl, S.; Fermeglia, M., "Multiscale Modeling Approach for Polymeric Nanocomposites" in "Modeling and Prediction of Polymer Nanocomposite Properties", Wiley-VCH Verlag GmbH & Co. KGaA: **2013**, pp: 95-128.

5. Liu, X.; **Posocco, P**.; Liu, C.; Yu, T.; Wang, Q.; Dal Col, V.; Chen, C.; Wang, Y.; Rocchi, P.; Pricl, S; Peng, L., "Poly(amidoamine) dendrimes as non-viral vectors for the delivery of RNA therapeutics" in "Dendrimers in Biomedical Applications", Eds: V. Cena, B. Klajnert, L. Peng, RSC publishing, **2013**, pp: 73-83.
6. **Posocco, P.**; Laurini, E.; Dal Col, V.; Marson, D.; Peng, L.; Smith, D. K.; Klajnert , B.; Bryszewska, M.; Caminade, A.-M.; Majoral, J. P.; Fermeglia, M.; Karatasos, K.; Pricl, S.; "Multiscale modeling of dendrimers and dendrons for drug and nucleic acid delivery" in "Dendrimers in Biomedical Applications", Eds: V. Cena, B. Klajnert, L. Peng, RSC publishing, **2013**, pp: 148-166.
7. **Posocco, P**.; Fermeglia, M.; Pricl S., "Multiscale modeling approach for polymer nanocomposites", in "Modeling and Prediction of Polymer Nanocomposite Properties", Eds: V. Mittal, Wiley-VCH Verlag GmbH & Co., **2013,** pp: 95-128.
8. Pricl, S.; **Posocco, P.**; Scocchi, G; Fermeglia, M., "Polymer-clay nanocomposites", in "Handbook of Nanophysics", Klaus Sattler Editor, CRC Taylor&Francis Publisher, **2009**.
9. Paneni MS; Posocco P; Fermeglia M; Pricl S., "Molecular Modeling of HCV NS5B Inhibitors", in "RNA viruses. Enzymatic and receptorial inhibitors", Ed: A. Carta, Research Signpost: Trivandrum, Kerala, India, **2009**, pp: 375-394.

CONFERENCE PROCEEDINGS

1. Boccardo S, Guida F, Sologan M, Marson D, Pricl S, Tossi A, Pasquato L, Pacor S, **Posocco P** *Membranes & Proteins VS Engineered Nanoparticles: A Computational and Experimental Investigation at the Bio-Nanointerface*, ICONAN, Barcelona (Spain), 2017.
2. Marson D, Boccardo S, Guida F, Sologan M, Pricl S, Pasquato L, Tossi A, Pacor S, **Posocco P** *A trip for two: computational/experimental insights into the interactions of gold nanoparticles protected by self-assembling mixtures of ligands in biological systems*, CLINAM, Basel (Switzerland), 2017.
3. Guida F, Iacuzzi V, Sologan M, Marson D, Boccardo S, Pengo P, Pasquato L, Tossi A, **Posocco P**, Pacor S *Effects of gold nanoparticles, protected by self-assembling mixtures of ligands, on eukaryotic cells and model membranes*. Regional Biophysical Conference, Trieste (Italy), 2016.
4. Marson D, Şologan M, Boccardo S, Pengo P, Pricl S, Pasquato L, **Posocco P** *CLEAR! ComputationaL and Experimental design Rules in tailoring the monolayer organization of fluorocarbon/hydrocarbon thiolates mixtures on gold nanoparticles*. Nanoparticles with Morphological and Functional Anisotropy: Faraday Discussion, Glasgow (UK), 2016.
5. Guida F, Şologan M, Marson D, Boccardo S, Pricl S, Pasquato L, Tossi A, Pacor S, **Posocco *P*** *Insights on the morphology and biological activity of gold nanoparticles protected by self-assembling mixtures of ligands*. Regional Biophysical Conference, Trieste (Italy), 2016.
6. Mio A, **Posocco P**, Laurini E, Pricl S, Fermeglia M, *Development of a methodology for the sustainability evaluation of industrial pharmaceutical processes*. PEPPD, Porto (Portugal), 2016.
7. Laurini E, **Posocco P**, Marson D, Fermeglia M, Pricl S, *Modeling: A Tool for Experimentalists. Design, Synthesis and Evaluation of Self-Assembling Dendrons for Gene/Drug Delivery*. AIChE, San Francisco (USA), 2016.
8. Chen C, **Posocco P**, Liu X et al.; *Self-assembling of amphiphilic dendrons for functional siRNA delivery: from the design to in vivo gene silencing*. SACS, San Sebastian (Spain), 2016.
9. Marson M, Boccardo S, Guida M, Sologan M, Pengo P, Lucarini M, Pasquato L, Tossi A, Pacor S, **Posocco P**, *Computational and experimental investigation on the morphology and biological activity of gold nanoparticles protected by self-assembling mixtures of ligands*. SACS, San Sebastian (Spain), 2016.

10. Laurini E, **Posocco P**, Fermeglia M, Pricl S, *Multiscale molecular modeling of thermoplastic polyurethane-based nanocomposites*. ICSM, Shangai, 2016.

11. **Posocco P**, Mohamed Y, Barandiaran I, Zweyer M, Baldini G, Laurini E, Fermeglia M, Kortaberria G, Pricl S, *Still looking for the magic spot: dispersing modified Fe_2O_3 in lamellar PS-PMMA diblock copolymer by vapor annealing deposition*. AIChe, Salt Lake City, USA (2015).

12. Laurini E, **Posocco P**, Fermeglia M, Pricl S, Of (computers and cells) mice and men: Integration of Simulations and Experiments in biomedical sciences FOMMS, Mt. Hood (Oregon), USA, (2015).

13. Pricl S, Fermeglia M, **Posocco P**, Marson D, Laurini E, Of (computers, cells) mice and men: Integration of simulations and experiments in molecular medicine, International Computational Science and Engineering Conference, Doha, Qatar (2015).

14. Laurini E, **Posocco P**, Fermeglia M, Pricl S, MoDeNa: Modeling of morphology Development of micro and Nano Structures International Computational Science and Engineering Conference, Doha, Qatar (2015).

15. Posel Z, **Posocco P**, Pricl S, Lísal M, Fermeglia M, *Scaling Laws for Hairy Nanoparticle in Good Solvent*. 9th Conference on the Statistical Mechanics of Liquids, Liblice, Czech Republic, (2014).

16. P. Marizza; M. Abrami; S.S. Keller; A. Boisen; K. Goswami; A.L. Skov; **P. Posocco**; R. Lapasin; G. Grassi; M. Grassi Hdrogel Basati Sul PVP Per Il Drug Delivery Da Microcontainer. Convegno Nazionale dell'Associazione Italiana di Reologia – SIR (2014), 67-72.

17. Pricl S, Gibbons DL, **Posocco P**, Laurini E, Giabbai B, Storici P, Fermeglia M , Sun H, Cortes J, Talpaz M , Donato N, Quintas-Cardama A, *Polymutant BCR-ABL1 proteins during chronic myeloid leukemia therapy: novel mechanisms of resistance from clinical, in vitro, and in silico evidences*. AACR-NCI-EORTC International Conference on Molecular Targets and Cancer Therapeutics. Boston, USA, (2013).

18. Fermeglia M, **Posocco P**, Pricl S *Nano Tools For Macro Problems: Multiscale Molecular Modeling For Nano-Bio-Tecnology. 3rd Summer Symposium on Nanomaterials and their application to Biology and Medicine*. Poznan, Poland, (2013).

19. Marson D, Laurini E, **Posocco P**, Peng L, Klajnert B, Majoral J-P, Caminade A-M, Pricl S *Odd Man Out: Molecular Dynamic Studies On Dendrimers And Their Interactions With Albumin And Oligodeoxynucleotides*. 22° National Meeting on Medicinal Chemistry, Rome, Italy, (2013).

20. **Posocco P**, Laurini E, Dal Col V, Peng L, Smith DK, Karatasos K, Fermeglia M, Pricl S *Dal computer alla cellula: evidenze sperimentali/computazionali per il design di nanovettori efficienti per terapia genica*. GRICU, Montesilvano, Italy, (2012).

21. Laurini E, Dal Col V, Marson D, **Posocco P**, Fermeglia M, Tamborini E, Quintas-Cardama A, Pricl S *Approccio di ingegneria molecolare per lo studio della farmaco-resistenza nella terapia oncologica*. GRICU, Montesilvano, Italy, (2012).

22. Marson D, Dal Col V, Barnard A, Jones SP, Laurini E, **Posocco P**, Smith DK, Fermeglia M, Pricl S *Nanozapped! DNA and its dendritic nanovectors: a combined in silico/in vitro approach*. FOMMS, Mt. Hood (Oregon), USA, (2012).

23. Dal Col V, Laurini E, **Posocco P**, Marson D, Wang Q, Fermeglia M, Peng L, Pricl S *Catch me if you can: ligand/antibody conjugated PAMAM dendrimer*. RCOM-7, Marseille, France, (2012).

24. **Posocco P**, Bidoggia S, Pasquato L, Lucarini M, Fermeglia M, Pricl S *Flying under the radar. Morphology prediction of the self-assembly of PEG-modified thiolate mixtures on the surface of stealth gold nanoparticles by experiment and multiscale modeling*. FOMMS, Mt. Hood (Oregon), USA, (2012).

25. **Posocco P**, Santese F, Handgraaf JW, Meyer M, Pravaz O, Fermeglia M, Pricl S *Multiscale Molecular Modeling of Nanocomposite Materials. An integrated experimental/computational approach to the characterization of polymer-grafted silica-based polymer nanocomposites*. FOMMS, Mt. Hood (Oregon), USA, (2012).

26. Fermeglia M, Pricl S, **Posocco P** *Nano tools for macro problems: multiscale molecular modeling of nanostructured polymer systems*. 11th European Symposium on Polymer Blends, Donostia-San Sebastian, Spain, (2012).

27. **Posocco P** *L'unione fa la forza! Approccio combinato computazionale/sperimentale allo studio di materiali nanostrutturati*. Macrogiovani, Milano, Italy, (2012).

28. Fermeglia M, **Posocco P**, Santese F, Handgraaf JW, Meyer M, Pravaz O, Pricl S *An integrated experimental/computational approach to the characterization of polymer-grafted silica-based polymer nanocomposites*. ESAT, Berlin, (2012).

29. Fermeglia M, **Posocco P**, Pricl S Nano tools for macro problems: multiscale molecular modeling of nanostructured polymer systems. 15th European Conference on Composite Materials, Venice, Italy, (2012).

30. **Posocco P**, Peng L, Behr J-P, Smith DK, Pack DW, Pricl S *From computer to in vivo: computational/experimental evidences for designing efficient nanovectors for gene therapy*. Nuove Prospettive in Chimica Farmaceutica, Trieste, Italy, (2011).

31. Pricl S, **Posocco P**, Fermeglia M, Malek a, Catapano CV *Short RNAs go a long way. Combined experimental/multiscale modeling studies of PAMAM-based dendrimers binding to different siRNAs*. AACR Nano in Cancer, Miami, USA, (2011).

32. Pricl S, **Posocco P**, Fermeglia M, Jones SP, Barnard A, Smith DK *Genes with bottles. Combined experimental/modeling investigations of dendron-based nanovectors for DNA delivery*. AACR Nano in Cancer, Miami, USA, (2011).

33. Dal Col V, Laurini E, **Posocco P**, Pricl P, Liu XX, Peng L, Jones SP, Barnard A, Smith DK *Nanozapped! DNA, siRNA, and their dendritic nanovectors: a combined in silico/in vitro/in vivo approach*. Computational Driven Drug Discovery, L'Aquila, Italy, (2011).

34. Laurini E, Dal Col V, Zampieri D, Mamolo MG, **Posocco P**, Vio L, Pricl S *The sigma-enigma. A multistep homology modeling of σ_1 receptors*. Computational Driven Drug Discovery, L'Aquila, Italy, (2011).

35. Fermeglia M, **Posocco P**, Toth R, Romero D, Santese F, Pricl S *The Factory of the Future: Integrating Multiscale Modeling and Experiments to Produce New, Better Nanocomposite Materials*. AIChE Annual Meeting, Minneapolis, USA, (2011).

36. Fermeglia M, **Posocco P**, Toth R, Romero D, Santese F, Pricl S *Chemistry and shape effects in polymer based nanocomposites: a multiscale modeling study*. Eurofillers, Dresden, Germany, (2011).

37. Fermeglia M, **Posocco P**, Toth R, Pereira SP, Pricl S *Multiscale molecular modeling of polymer nanocomposites*. VI International Materials Symposium MATERIAIS, Guimarães, Portugal, (2011).

38. Karatasos K, **Posocco P**, Laurini E, Pricl S *Computational study of complexes of dendrimers with siRNA for gene delivery applications*. 8th Panhellenic Scientific Chemical Engineering Congress, Thessaloniki, Greece, (2010).

39. Karatasos K, Pricl S, **Posocco P**, Laurini E *A Molecular Dynamics Simulation Study On siRNA/TEA-PAMAM Dendrimer Complexation*. 8th Hellenic Polymer Society Symposium, Hersonissos, Greece, (2010).

40. Pricl S, **Posocco P**, Laurini E, Fermeglia M, Karatasos K, Peng L, Smith DK *When virtual and real meet: computational/experimental evidences for designing efficient nanovectors for siRNA/DNA delivery*. NanotechItaly, Venezia, Italia, (2010).

41. Pricl S, **Posocco P**, Fermeglia M, Karatasos K, Peng L, Smith DK *The Sound of Silence. Multiscale Molecular Simulations and Experiments in Developing Nanocarrier/Nucleic Acid Systems.* AIChE Annual Meeting, Salt Lake City, USA, (2010).

42. **Posocco P**, Fermeglia M, Liu X, Peng L, Malek A, Catapano CV, Smith DK, Pricl S *Is variety the spice of life? Multiscale molecular simulations support experiments in nanocarrier/nucleic acid systems design*. ACS National meeting, Boston, USA, (2010).

43. Laurini E, Zampieri D, Mamolo MG, Vio L, **Posocco P**, Fermeglia M, Pricl S, Zanette C, Florio C *Synthesis, Molecular Modeling And Experimental Activity Of Some New Acetamide, Benzamide And Phenylmethanone Derivatives As Sigma Ligands*. XX National Meeting on Medicinal Chemistry, Abano Terme, Italy, (2010).

44. Pricl S, Gibbons DL, **Posocco P**, Laurini E, Fermeglia M, Kantarjian H, Talpaz M, Cortes J, Donato N, Quintás Cardama A *In Silico Modeling of Sensitivity to Novel Tyrosine Kinase Inhibitors of Highly Resistant Single-Point Mutant and Polymutant BCR-ABL1 Proteins*. Annual Meeting of the American Society of Hematology, Orlando, USA, (2010).

45. Pricl S, Gibbons DL, **Posocco P**, Laurini E, Fermeglia M, Kantarjian HM, Talpaz M, Cortes J, , Young M, Sun H, Peterson LF, Donato N, Quintás Cardama A *The Novel BCR-ABL1 V304D Mutation Induces Pan-Tyrosine Kinase Inhibitor Resistance by a Unique Kinase Lateral Escape Mechanism and Is Associated with Very Poor Prognosis In Patients (PTS) with Chronic Myeloid Leukemia (CML)*. Annual Meeting of the American Society of Hematology, Orlando, USA, (2010).

46. Fermeglia M, **Posocco P**, Toth R, Pereira SPSB, Pricl S *Multiscale Molecular Modeling of Polymer/Silica Nanocomposites*. NanotechItaly, Venezia, Italia, (2010).

47. Fermeglia M, **Posocco P**, Pricl S, Handgraaf JW *Multiscale Molecular Modeling of Polymer/Silica Nanocomposites*. AIChE Annual Meeting, Salt Lake City, USA, (2010).

48. Pricl S, **Posocco P**, Pavan GM, Fermeglia M, Scocchi G, Malek A, Maly M, Danani A, Catapano C, Peng L, Smith D. *The sound of silence. Experimental/computational investigations of dendrimer-based sirna/dna delivery systems*. FOMMS, Blaine, USA, (2009).

49. Pricl S, Pavan GM, **Posocco P**, Scocchi G, Malek A, Maly M, Fermeglia M, Ragg EM, Danani A, Catapano C. *Nanopackages ready for dispatch. A combined experimental/in silico approach to denrimer/siRNA systems*. 6th International Dendrimer Symposium, Stockholm, Sweden, (2009).

50. **Posocco P**, Fermeglia M, Pricl S. *The Long and Winding Road. Multiscale Molecular Modeling Approach to the Self-Assembly of Di/Triblock Copolymers for Drug Delivery in Aqueous Solution*. AIChE Annual meeting, Nashville, USA, (2009).

51. **Posocco P**, Fermeglia M, Pricl S *Multiscale molecular modeling of di/triblock copolymers for drug delivery*. FOMMS, Blaine, USA, (2009).

52. Fermeglia M, **Posocco P**, Pricl S, Fraaije JGEM, Handgraaf JW, Deglmann P, Kurkal-Siebert V, Weiss H. *On the DPD Parameter Estimation From Atomistic/Quantum Mechanics Information*. AIChE Annual meeting, Nashville, USA, (2009).

53. Fermeglia M, Scocchi G, Pricl S, Handgraaf JW, Fraaije JGEM, **Posocco P**. *A Complete Multiscale Modeling Approach for Polymer-Clay Nanocomposites*. AIChE Annual Meeting, Nashville, USA, (2009).

54. Fermeglia M, **Posocco P**, Pricl S, Fraaije JGEM, Handgraaf JW, Scocchi G, Danani A. *A complete multiscale modeling approach for nanocomposites*. Eurofillers, Alessandria, Italy, (2009).

55. Danani A, Scocchi G, **Posocco P**, Pricl S, Fermeglia M. *Multiscale modeling applied to polymer-clay nanocomposites*. 5th International Conference NANOFUN-POLY, Paris, France, (2009).

56. **Posocco P** *Modellistica molecolare multiscala per la progettazione di materiali nanostrutturati*. I giovani e la chimica in FVG, Trieste, (2009).

57. Malek A, **Posocco P**, Pavan GM, Fermeglia M, Scocchi G, Maly M, Danani A, Catapano C, Pricl S. *Experimental and computational simulation studies of co-polymeric nanocarriers for delivery of small interfering RNA therapeutics*. 2nd Saint-Petersburg International Conference on NanoBiotechnologies NANOBIO, Saint-Petersburg, Russia, (2008).

58. Pricl S, **Posocco P**, Pavan GM, Fermeglia M, Scocchi G, Danani A, Malek A, Catapano C *Designing nanovectors for siRNA delivery: coupled experimental/modeling investigations*. 20th EORTC–NCI–AACR Symposium on Molecular Targets and Cancer Therapeutics, Geneva, Switzerland, (2008).

59. Pricl S, **Posocco P**, Fermeglia M, Scocchi G, Danani A, Catapano C, Maly M, Handgraaf J-W Fraaije JGEM *Base Invaders. Coupling Experiments and Multiscale Modeling of Dendrimer-Based siRNA Delivery Agents*. 12th International Conferences on "Modern Materials and Technologies" CIMTEC, Acireale, Italia, (2008).

60. **Posocco P**, Pavan GM, Fermeglia M, Scocchi G, Malek A, Maly M, Danani A, Catapano C, Pricl S *Packed to go. Experimental/simulation studies of nanocarriers /siRNA delivery systems in cancer therapeutics*. 1th European Conference for Clinical Nanomedicine, Basilea, Switzerland, (2008).

61. **Posocco P**, Handgraaf JW, Fraaije JGEM, Scocchi G, Fermeglia M, Pricl S *A multiscale approach to the self-assembly of dendrimers in solution*. CECAM, Lausanne, Switzerland, (2008).

62. Pavan GM, **Posocco P**, Scocchi G, Danani A, Malek A, Catapano C, Maly M, Fermeglia M, Pricl S. *How far can you go? Dendrimer-siRNA interactions analyzed by computer simulations*. 1st Symposium on Biomedical Properties and Applications of Dendrimers BIO-Dendrimers, Lodz, Poland, (2008).

63. Pricl S, **Posocco P**, Pavan GM, Scocchi G, Mály M, Malek A, Fermeglia M, Danani A, Catapano *C Finding your way. The DRUDE initiative for nanocarriers in delivery of small interfering RNA therapeutics*. AIChE, Philadelphia, USA, (2008).

64. **Posocco P**, Toth R, Voorn DJ, Handgraaf JW, Fermeglia M, Pricl S. *Paving the way to new nanocomposite materials: multiscale computer simulations of PEO and exfoliated layer silicates in aqueous dispersions*. 1st Transalp' Nano Conference, Lyon, France, (2008).

65. Paneni M, **Posocco P**, del Santo I, Causa F, Netti PA, Pricl S. *"Math"-odological insights into smart nanochannels: a multiscale molecular modeling of molecular motion in confined nanospaces*. 1st Transalp' Nano Conference, Lyon, France, (2008).

66. Paneni MS, **Posocco P**, De Santo I, Causa F, Netti PA, Pricl S *Nanochannels versus macromolecules:a multiscale computational approch of macromolecular transport in confined nanospaces*. NNC: National nanomedicine Conference, Genova, Italia, (2008).

67. Fermeglia M, Pricl S, **Posocco P**, Mály M, Lisal M. *Computer Simulation of Hybrid Organic-Inorganic Nanocomposites*. AICHE Annual meeting, Philadelphia, USA, (2008).

68. Pricl S, **Posocco P**, Mály M, Lisal M, Fermeglia M. *Beyond Patterns to Mechanisms. Multiscale Molecular Simulations of Nanoparticles/block Copolymers Self-Assembled Bulk Nanocomposites*. AICHE Annual meeting, Philadelphia, USA, (2008).

69. **Posocco P**, Scocchi G, Fermeglia M, Handgraaf JW, Fraaije JGEM, Pricl S. *A Complete Multiscale Modeling Approach for Nanocomposites*. AICHE Annual meeting, Philadelphia, USA, (2008).

70. Fermeglia M, **Posocco P**, Pricl S, Maly M. *Multiscale Molecular Modeling of Hybrid Organic-Inorganic Nanocomposites of Type I and II*. 12th International Conferences on "Modern Materials and Technologies" CIMTEC, Acireale, Italia, (2008).

71. **Posocco P**, Scocchi G, Fermeglia M, Pricl S, Ferrari M *The nanoroad less travelled. A multiscale approach to self-assembly of dendrimers for cancer therapy*. 11th International Conference on "Properties and Phase Equilibria for Product and Process Design" PPEPPD, Crete, Greece, (2007).

72. Scocchi G, **Posocco P**, Pricl S, Fermeglia M *To the nanoscale and beyond! Multiscale molecular modelling of polymer-clay nanocomposites*. 11th International Conference on "Properties and Phase Equilibria for Product and Process Design" PPEPPD, Crete, Greece, (2007).

73. Fermeglia M, **Posocco P**, Maly M, Pricl S *Enthalpy/entropy effect in the self-assembly of a nanoparticle complex system: a multiscale molecular modelling approach*. AIChE Annual Meeting, Salt Lake City, UT, USA, (2007).

74. Cosoli P, Fermeglia M, Ferrone M, **Posocco P**, Pricl S, Scocchi G. *New materials from multiscale modeling procedures: properties prediction and customization of polymeric nanocomposites*. ICheaP-8, Ischia, Italia, (2007).

75. Pricl S, **Posocco P**, Fermeglia M, Scocchi G, Danani A, Handgraaf JW, Fraaije JGEM. *What goes around comes around. Multiscale molecular modeling of dendrimers self-assembly*. IDS:5 fifth international dendrimer symposium, Tolouse, France, (2007).

76. Fermeglia M, Ferrone M, Cosoli P, Paneni MS, Venica R, Sinesi S, **Posocco P**, Martinelli L *Many scale simulation of ABS/PC blends for the automotive industry*. 11th International Conferences on "Modern Materials and Technologies" CIMTEC, Acireale, Italia (2006).

77. Martinelli L, Sinesi S, Baron Toaldo A, Fermeglia M, **Posocco P**, Szczurek T, Kozlowski M *Innovative molecular modelling approach to up-grade polymeric materials from post-industrial rejects*. 5th Central European Conference on "Plastics recycling and recovery Science - Industry – Government", Wroclaw, Poland, (2006).