Fluid Phase Equilibria 606 (2026) 114696

Contents lists available at ScienceDirect

Fluid Phase Equilibria

journal homepage: www.journals.elsevier.com/fluid-phase-equilibria

The Fermeglia *Continuum*: From classical thermodynamics to multiscale molecular engineering

Sabrina Pricl *

Molecular Biology and Nanotechnology Laboratory (MolBNL@UniTs), Department of Engineering and Architecture (DIA), University of Trieste, 34127 Trieste, Italy

ARTICLE INFO

Keywords:
Phase equilibria
Multiscale modeling
Property predictions
Molecular dynamics
Mesoscopic simulations
Process simulation

ABSTRACT

This review offers my personal perspective on the evolution of fluid phase equilibria, traced through the scientific arc of Professor Maurizio Fermeglia. Beginning with classical thermodynamics, his work advanced equations of state and activity-coefficient models, strengthening the thermophysical-property foundations that enable reliable phase-equilibria prediction for complex mixtures and supercritical fluids of industrial relevance. As the limits of purely analytical descriptions became clear, he helped consolidate a molecular viewpoint, using quantum chemistry and molecular simulation to derive physically meaningful parameters and to connect microscopic interactions with macroscopic phase behavior. That vision matured into multiscale molecular engineering, linking quantum and atomistic descriptions to coarse-grained models and process-simulation tools, and enabling predictive design of nanostructured polymers, membranes, and later biomedical systems such as dendrimer-based carriers and protein–ligand complexes. In his final phase, the same "deployable modeling" philosophy expanded to energy and sustainability: process-level simulations and multiscale workflows were coupled to decision-oriented metrics, life-cycle assessment, and circularity considerations, turning impact and boundary conditions into computable design variables. Rather than an exhaustive catalog, this article follows an intellectual arc from classical foundations to simulation-informed thermodynamics, multiscale frameworks, biological translation, and sustainability-by-design, while reflecting on the person who made that trajectory coherent. In honoring Maurizio, I also highlight a standard of practice: rigorous, integrative, and purpose-driven that continues to guide our research*.

1. Introduction

I did not intend to write a memorial. I set out to tell a story: that of a field in motion and of the person who taught many of us how to move with it. Maurizio believed that thermodynamics is not a static collection of formulas but a living language that connects molecules to matter and matter to technology. He began where our discipline began: with equations of state (EOS) and activity-coefficient models, with carefully measured densities, viscosities, and refractive indices, and with ternary liquid-liquid equilibria (LLE) tie lines checked and rechecked, guided by the conviction that good theory grows from good data. He also believed that no single scale could capture reality. When analytical models fell short, he turned to molecular simulations, not as an embellishment but as a bridge. When systems became too large or too complex for atomistic treatment alone, he built coarse-grained (CG) pathways across scales. When applications demanded relevance, he moved toward polymers, membranes, and ultimately the life sciences. In his later work, that same discipline widened its horizon: models had to remain auditable and transferable, but their outputs had to speak the language of decisions - energy performance, cost, life-cycle impact, and circularity - so that sustainability became something engineers could compute rather than merely claim. This review follows that trajectory, from classical foundations to simulation-informed thermodynamics and multiscale modeling, to biomedical design, and finally to sustainability-by-design, guided throughout by Maurizio's clarity of purpose and generosity of thought. We begin by revisiting the classical foundations that shaped his early work and then follow the molecular and multiscale transitions that defined his broader legacy.

In loving memory of Professor Maurizio Fermeglia (1955–2024), a beloved husband and colleague, whose scientific vision, rigor, curiosity, and human warmth still shape the way I work and think.

* Corresponding author at: University of Trieste Italy

* During the preparation of this manuscript, I received the sad news of the passing of Karel Haim, a distinguished scientist in our community and a long-time friend of Maurizio. He was also a cherished personal friend of our family. I remember him with gratitude and affection, and I honor his scientific legacy.

https://doi.org/10.1016/j.fluid.2026.114696
Received 30 January 2026; Received in revised form 17 February 2026; Accepted 17 February 2026
Available online 18 February 2026

2. Classical foundations

The practice of modern fluid phase equilibria grew out of classical thermodynamics, where EOS and excess Gibbs-energy (G^E) models became the central instruments for correlating and predicting phase behavior. From the start, Maurizio consistently framed thermodynamic modeling as testable and data-anchored, prioritizing predictivity over curve fitting and making limitations explicit rather than implicit. This position is clear in early work on what infinite-dilution information can (and cannot) support when extrapolated to finite concentrations in azeotropic and partially miscible systems, and in later contributions emphasizing how EOS choice, mixing rules, and parameter-estimation strategy shape what can legitimately be predicted from available data [1,2]. In parallel, he reinforced the connection between EOS structure and measurable caloric properties through excess-enthalpy calculations, underscoring that "good phase behavior" is not, by itself, a sufficient test of thermodynamic realism [3].

A second, tightly connected pillar is the disciplined use of benchmark equilibrium datasets to separate correlation from prediction. Across LLE and vapor-liquid equilibria (VLE), Maurizio helped expand and consolidate experimental reference points for mixtures relevant to separations and process windows, while maintaining thermodynamic consistency checks and clear parameter reporting as part of the scientific content rather than a technical appendix [4–10]. He also extended the predictivity of group-contribution to more demanding electrolyte-containing mixtures by embedding UNIFAC within frameworks suited to mixed solvent-salt systems, broadening classical predictive thermodynamics beyond neutral fluids [11] (Fig. 1, top left). This validation-first logic was complemented by explicit attention to dilute-region behavior, both as an information-rich regime (for constraints and extrapolation) and as a regime where experimental and inferential pitfalls must be confronted directly [12,13].

Concomitantly, Maurizio built a broad experimental backbone of thermophysical-property data (e.g., densities, viscosities, excess volumes, and refractive indices) often in temperature ranges relevant to engineering use. These datasets serve as calibration and validation targets that keep EOS/G^E development grounded in measurable reality and expand confidence beyond narrow benchmark points [14–22].

These classical foundations naturally extend to high-pressure and supercritical regimes, where asymmetry, chain character, and size disparity dominate behavior and where predictivity is most valuable (and most fragile). Here, Maurizio contributed to a coherent "predictive toolkit" that links EOS development, parameterization from accessible data, and applicability in pressure and composition ranges relevant to supercritical-fluid extraction and related technologies [23–30] (Fig. 1, top right). This stream also includes petroleum-relevant mixtures (heavy ends and fractions) where characterization constraints (e.g., Henry's constants and pseudocomponents) become part of the predictive strategy rather than a *post hoc* fit [31,32]. He further strengthened perturbed hard-sphere-chain (PHSC) EOS families for refrigerants and

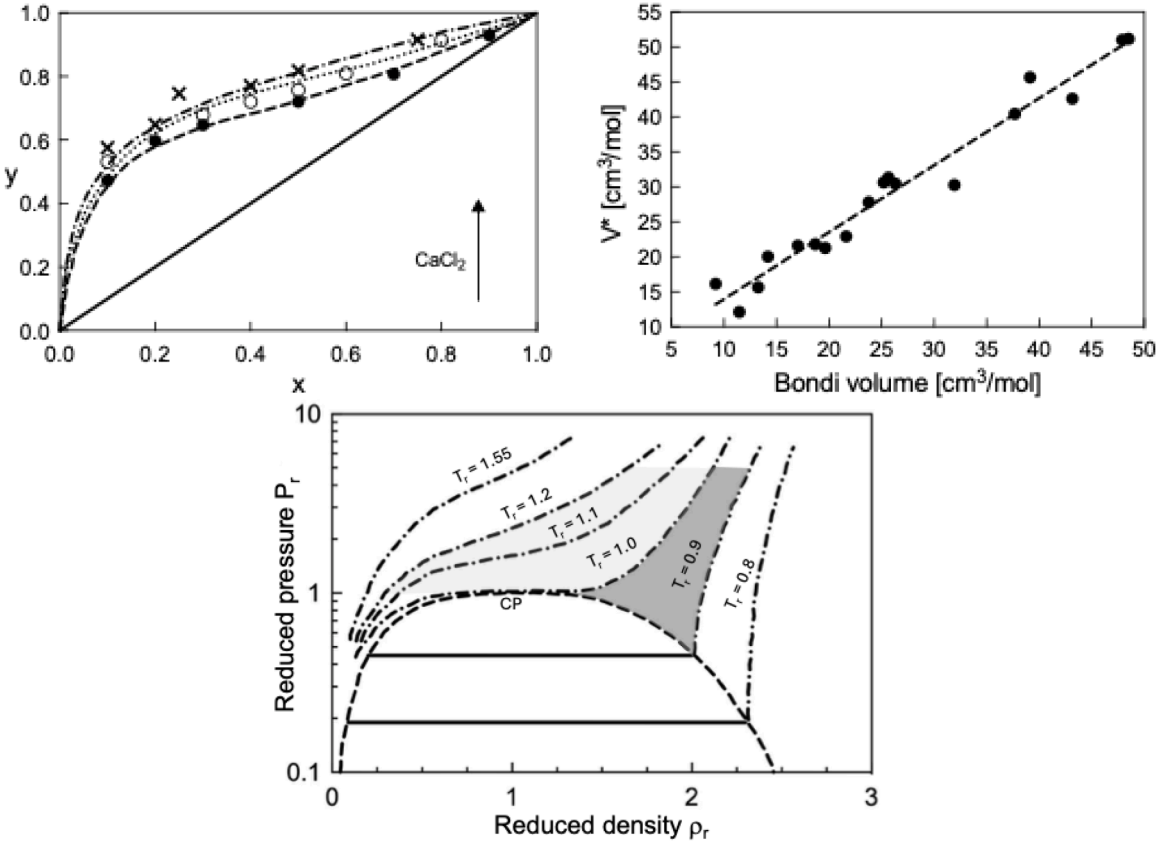

Fig. 1. From predictive thermodynamics to deployable process modeling in classical fluid phase equilibria. (Top, left) Example of UNIFAC-based modeling for a mixed solvent-salt system, showing the comparison between calculated (lines) and experimental VLE behavior (symbols) for ethanol-water in the presence of increasing $CaCl_2$ concentrations (from 5 to 15 %), highlighting how electrolyte effects reshape phase equilibria in ways that must be captured by predictive models (redrawn and adapted with permission from [11], Copyright© 1991 Pergamon Press plc). (Top, right) Illustration of parameter transferability in PHCT, linking an effective molecular-size descriptor (V*) to Bondi volumes for different compounds, supporting physically grounded parameter estimation for predictive EOS (redrawn and adapted with permission from [25], Copyright© 1991 Pergamon Press plc). (Bottom) Example of deployable process modeling for supercritical separations, showing the reduced density as a function of reduced pressure with reduced temperature as a parameter (and the critical point indicated), illustrating how EOS-based reduced-property representations support generalized, operating-window-spanning simulations for multistage, multicomponent supercritical separation processes (adapted and redrawn with permission from [37], Copyright© 1992 Pergamon Press plc).

hydrocarbons and extended them to highly asymmetric, industrially relevant refrigerant-lubricant mixtures [33–35].

A recurring theme throughout Maurizio's scientific thinking is that thermodynamics becomes industrially actionable when it is computationally deployable, i.e., embedded in algorithms, flash calculations, and process simulations that operationalize validated models within separation-unit workflows, optimization loops, and recovery strategies [8,31,36–38] (Fig. 1, bottom).

Finally, within the same "classical foundations" arc, Maurizio's equilibrium thinking and data discipline also reach complex fluids and soft matter, including LLE-based separations in polymer-rich aqueous systems and coupled equilibrium-kinetics descriptions in responsive materials, natural bridges from molecular-fluid thermodynamics toward the broader multiscale and application-focused themes he would later develop [39,40].

3. The molecular turn: From simulation to predictive thermodynamics

The limits of purely analytical models opened the door to molecular information as a physically grounded route to predictive thermodynamics. In the late 1990s and early 2000s, Maurizio made this shift systematic by extracting physically meaningful EOS parameters directly from simulation. Using chloro-fluoro-hydrocarbons (CFCs) as a test case, he combined quantum mechanics (QM)-based and molecular dynamics (MD)-based simulations to compute molecular size, surface, and interaction energy, and then transferred those quantities into a PHSC framework for property prediction. This provided a clear proof of concept for a molecules-to-EOS pipeline that preserved interpretability while improving parameter transferability [41]. Closely related work extended the same strategy to "real systems," combining CFCs and polymers within a unified simulation-driven perspective for thermophysical prediction [42]. In parallel, computational chemistry was used to support the prediction of thermophysical properties of alternative refrigerants, reinforcing the broader idea that refrigerant screening can be anchored to molecular-level descriptors rather than empirical correlations alone [43]. Contextually, he extended the same logic to polymeric targets by deriving EOS parameters for pure polymers directly from molecular simulation, demonstrating that physically meaningful parameterization can be obtained without relying exclusively on empirical fitting [44] (Fig. 2).

He then formalized the bridge from molecular calculations to process simulation. In a series of contributions, he showed how atomistic and quantum-derived information can generate EOS parameters that feed phase-equilibria and PVT calculations in process while retaining a transparent link to underlying physics, turning molecular modeling from a *post hoc* explanation into a predictive front end [45,46]. Concurrently, perturbation-theory EOSs were extended to polymer-containing mixtures, strengthening the ability of these approaches to address multiphase, multicomponent equilibria under strong asymmetry [47]. To broaden coverage while retaining parsimony, he advanced a group-contribution variant of the PHSC framework that estimates EOS parameters from molecular structure and relies on a minimal set of binary interaction terms to describe complex mixtures, including systems exhibiting both upper and lower critical solution temperatures [48].

At the same time, he pushed direct atomistic simulations into

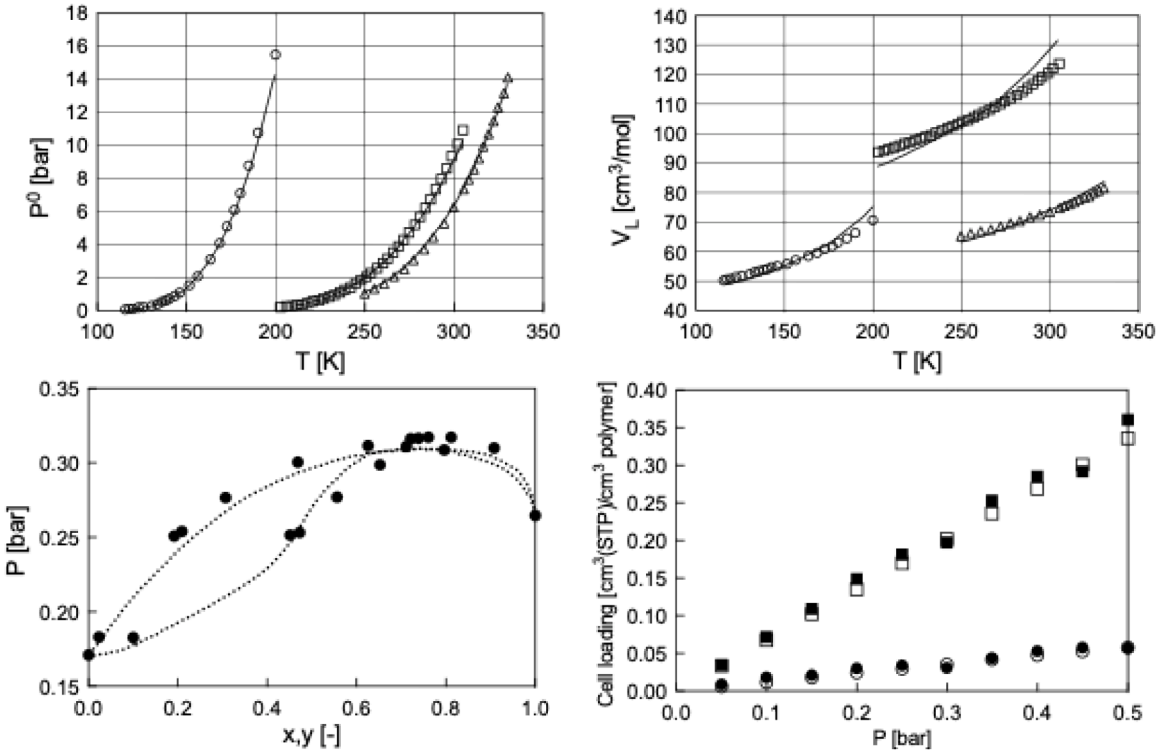

Fig. 2. The "molecular turn" from simulation to predictive thermodynamics. (Top) Vapor pressure (left) and saturated-liquid molar volume (right) as a function of temperature for selected CFCs, showing agreement between experimental data (symbols) and PHSC EOS predictions based on simulation-derived parameters (lines), and illustrating how molecular-level descriptors can be translated into transferable EOS inputs without sacrificing interpretability (adapted and redrawn with permission from [41], Copyright© 1999 Elsevier Science B.V.). (Bottom, left) Experimental VLE behavior of a trichloromethane/ethanol system (symbols) compared with the corresponding PHSC EOS prediction (dotted line) obtained using parameter values derived from MD simulations, highlighting the export of molecular information into phase-equilibria calculations in a process-relevant form (adapted and redrawn with permission from [46], Copyright© 2001 American Institute of Chemical Engineers (AIChE)). (Bottom, right) Comparison of experimental (open symbols) and simulated (filled symbols) sorption isotherms for O_2 (circles) and CO_2 (squares) in poly(isobutylene) as obtained from MD/GCMC simulations, exemplifying the extension of the same paradigm to polymer/soft-matter systems where transport and sorption become design-relevant targets (adapted and redrawn with permission from [52], Copyright© 2003 Taylor & Francis).

transport-relevant and materials settings. Virtual rheology of confined linear alkanes between titanium walls linked molecular alignment to non-equilibrium response and provided a template for probing shear-driven behavior by MD [49]. Early host-guest studies showed how dendritic architectures control the inclusion of small molecules, foreshadowing later biomedical directions [50]. These were not detours. They were steppingstones that established a second principle of the molecular turn: simulation earns its place when it both explains mechanisms and yield compact, transferable quantities that predictive tools engineers can actually use [45,46].

The gains from this period were twofold. First, predictive thermodynamics became more physical because EOS parameters were anchored to molecular geometry and energetics rather than fitted in isolation [41,44,46–48]. Second, simulations became more consequential for polymer and soft-matter design, including transport and sorption in polymer matrices and nanostructured systems, where atomistic MD simulations (and related Monte Carlo sampling strategies) can deliver diffusion and solubility trends consistent with available measurements [51,52]. This logic prepared the ground for seamless handovers to mesoscopic and process scales, and it naturally led to systematic multiscale frameworks in which bottom-up and top-down routes coexist and properties travel from atoms to continuum models with quantified fidelity [53,54].

4. Multiscale molecular simulations

4.1. From atomistic truth to mesoscopic reach

Maurizio approached multiscale modeling as an engineering discipline: not merely a change of resolution, but a controlled transfer of information across levels, as summarized in (Fig. 3).

The starting point was always an explicit decision about what must remain invariant, e.g., local structure, interfacial energetics, chain statistics, or emergent morphology. The mesoscale (MS) model was then constructed to match those invariants and to reach length and time scales inaccessible to atomistic simulation. This philosophy is already explicit in his early polymer-clay program, where atomistic simulations were used to resolve clay gallery organization and polymer-surface interactions, and the resulting descriptors guided coarse-grained (CG) models toward realistic morphologies and materials response [55–59]. Within the same arc, atomistic energetics were used to quantify polymer/clay affinity and rationalize how surfactant chemistry and matrix composition tune interfacial strength [60]. As the work matured, the methodology was codified into hierarchical, transferable procedures that connect atomistic descriptors to mesoscopic organization and, when needed, to the prediction of continuum properties [61,62].

4.2. Polymer-clay nanocomposites as a benchmark multiscale problem

Polymer-layered silicate (or polymer-clay) nanocomposites (PCNs) became a defining testbed because they force multiscale consistency: local adsorption motifs and surface chemistry control intercalation/exfoliation, which in turn determines mesoscale morphology and ultimately macroscopic performance. In PCNs based on montmorillonite (MMT) and nylon-6 (PA6), atomistic simulations clarified the structural and energetic determinants of intercalation [55]. The strategy was then generalized to polypropylene (PP)/organoclay nanocomposites, preserving molecular fidelity while enabling morphology and property prediction [56]. Already in 2007, Maurizio and his collaborators argued that polymer-clay systems require explicit bridges "to the nanoscale, and beyond," because topology, polymer architecture, and processing constraints couple through scales [57–59]. Later, this program expanded to water-based clay/poly(ethylene oxide) (PEO) nanocomposites, showing that the same cross-scale logic can be applied when hydration and solvent-mediated forces dominate the interphase physics [61]. Importantly, the principle of "what must be preserved" was also used to interpret and constrain modifier effects at the nanoscale: even ostensibly simple design variables (e.g., the chain length of aminosilanes used as polymer-clay compatibilizers) can produce non-intuitive trends in gallery spacing that are only rationalized when atomistic organization is explicitly modeled [63]. Finally, the polymer-mineral framework was extended to functional, biocompatible PNCs systems, again emphasizing that the design of reliable materials requires an energetically-aware description of the confined structure in both dry and solvated environments [64] (Fig. 4).

4.3. Self-assembled hybrids and nanoparticle-polymer architectures

A second multiscale line targeted hybrid soft matter, where emergent structure is controlled by molecular features (ligands, brushes, block incompatibility), but only becomes observable (and designable) at the mesoscale. In nanoparticle (NP)-diblock copolymer (DBCP) systems,

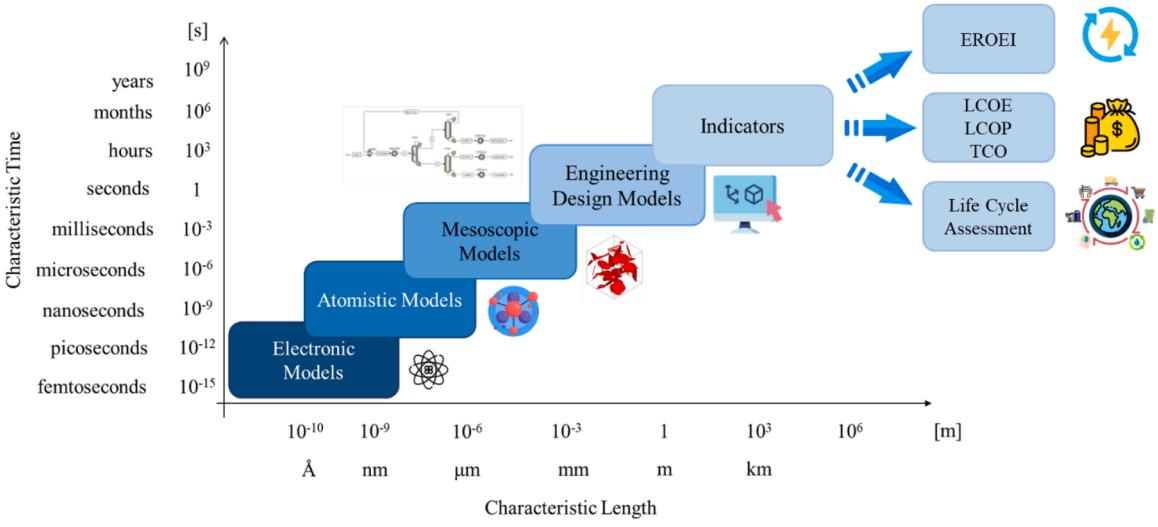

Fig. 3. Multiscale information handoff from molecular physics to engineering decision metrics. Conceptual schematic showing how models at increasing levels of resolution (electronic, atomistic, and mesoscopic) feed into engineering design models and, ultimately, decision-relevant outputs such as selected performance indicators (e.g., energy return on energy invested (EROEI), levelized cost metrics including energy (LCOE), product (LCOP), and total cost of ownership (TCO)) and life-cycle assessment.

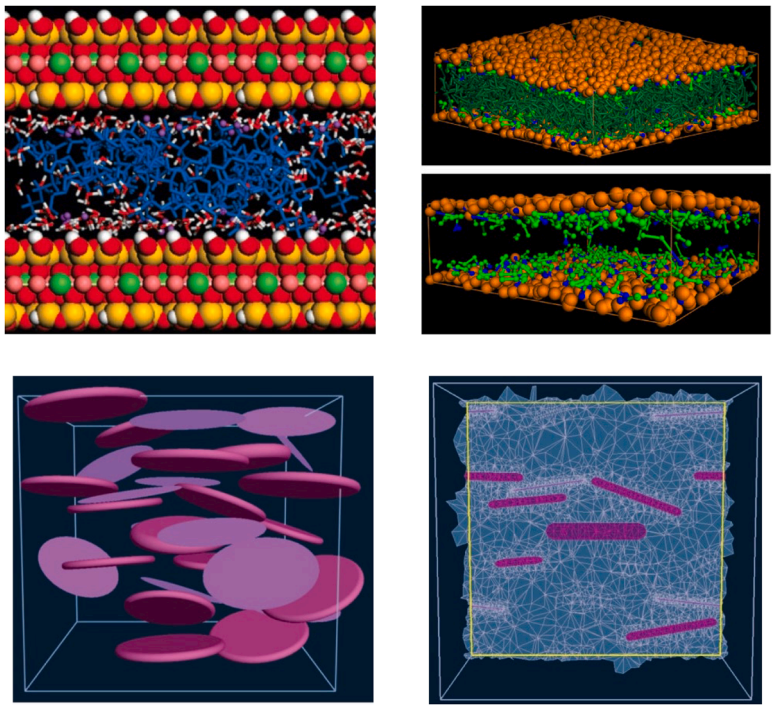

Fig. 4. Polymer–clay nanocomposites as a benchmark multiscale problem. (Top, left) Equilibrated atomistic MD snapshot of a solvated MMT system with intercalated PEO chains (adapted with permission from [61], Copyright© 2009 American Chemical Society). (Top, right) Example of a dissipative particle dynamics (DPD)-derived mesoscale morphology for a PCN system, shown as the full ternary morphology (MMT, PA6, and M_3C_{18} as compatibilizer; top) and a zoomed interfacial detail (bottom) (adapted with permission from [57], Copyright© 2007 Elsevier B.V.). (Bottom, left) Finite-element (FE) representative volume element configuration generated from mesoscale structural descriptors (platelets/stacks) and (bottom, right) the corresponding FE mesh used to compute macroscopic properties (adapted with permission from [61], Copyright© 2009 American Chemical Society).

Maurizio and collaborators used multiscale simulation to predict self-assembled morphologies of NP mixtures embedded in microphase-separating media [65], later developing molecular simulation routes to morphology prediction for self-assembled NPs in DBCPs [66]. The same MS logic was applied to drug-delivery block copolymers, linking composition/segregation strength to morphology selection relevant to function [67] (Fig. 5).

Concomitantly, ligand chemistry was treated as a *bona fide* design variable: mixtures of fluorocarbon/hydrocarbon ligands were shown to self-organize on NP surfaces into distinct patterns that propagate to mesoscale phase behavior [68]. Geometry was likewise promoted from "detail" to "control knob," with NP size and shape demonstrated to govern structure in polymer nanocomposites within a consistent modeling framework [69]. Hierarchical organization followed naturally, including NP/DBCP systems with higher-order structure [70] and strongly grafted hybrid objects where corona physics controls effective interactions and stability windows [71]. The same processing-aware perspective extended to selective NP placement in DBCP films via solvent-vapor annealing, where MS modeling and experiment were combined to show that ordered morphologies and domain-selective NP localization can be achieved through fabrication steps compatible with industrial workflows [72].

In parallel, Maurizio's group used dendritic architectures as model "functional nanoparticles," using molecular simulation to connect dendrimer topology to structure and emergent properties [73–75]. This emphasis on structure-property transferability was also carried into hybrid organic-inorganic networks, where recipe-style simulation protocols were developed to generate atomistic models of crosslinked materials and benchmark their thermophysical/mechanical signatures against available experimental ranges [76].

4.4. *From multiscale materials models to industrially actionable workflows*

A recurring message in Maurizio's work is that multiscale models matter only if they can be operationalized, that is translated into auditable workflows that deliver parameters, properties, and (where possible) uncertainty bounds usable in materials selection and process decisions. This "engineering closure" is a central theme of his contribution linking multiscale molecular modeling with nanostructured materials design and process systems engineering [77], and is further developed in later work explicitly framed around industrial applications and decision-oriented multiscale pipelines [54].

Within this same logic, multiscale strategies were applied to polymer systems of direct industrial relevance, including many-scale modeling of poly(ethylene terephthalate) (PET)/poly(ethylene naphtalate) (PEN) blends as barrier materials, where molecular-to-continuum handoffs are used to predict phase behavior and transport-relevant properties in blends and compatibilized systems [78]. The MoDeNa project then formalized integrated multiscale toolchains for nanostructured materials and connected microscale physics to higher-level models used in design [79]. A particularly illustrative example of "deployable multiscale" is polyurethane foams, where molecular inputs derived from MD/grand canonical Monte Carlo (GCMC) simulations are coupled to continuum computational fluid dynamics (CFD) to predict morphology and density evolution under processing conditions [80], and where heat-transfer performance is predicted by linking quantum chemistry, non-equilibrium MD, surrogate modeling, and experimentally validated macroscopic insulation models [81].

Industrial actionability was also explicitly pursued at the interface between materials modeling and business decision processes. In the COMPOSELECTOR framework, multimodel/multiscale pipelines were organized around industry-driven key performance indicators (KPIs) to support material selection under competitive time constraints, with

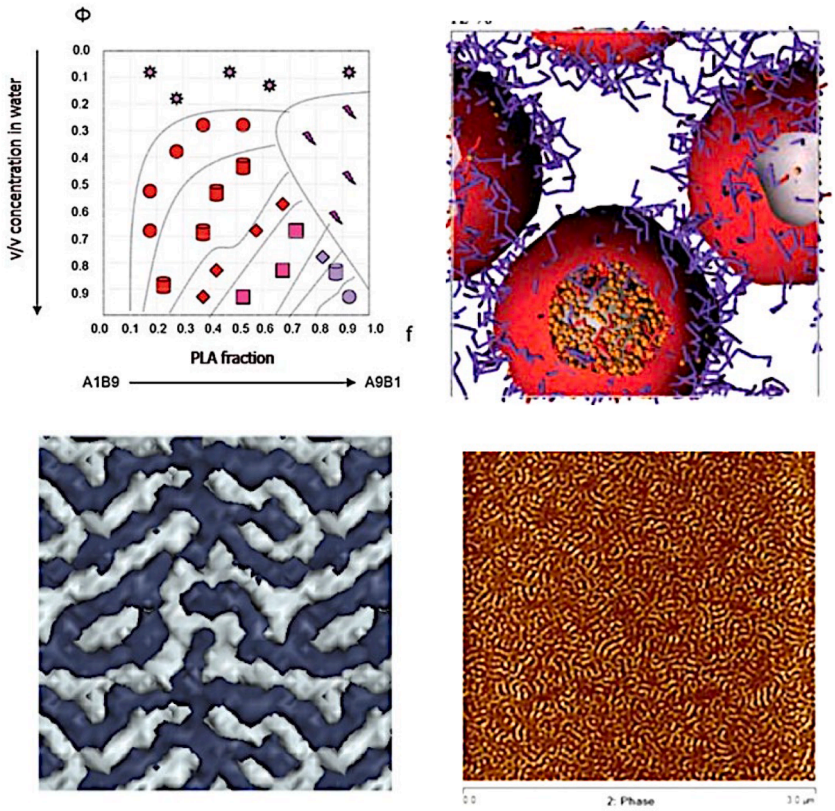

Fig. 5. Self-assembled hybrids and nanoparticle–polymer architectures. (Top, left) Predicted phase diagram for an AB-type poly(lactic acid) (PLA)/PEO DBCP in water, highlighting regimes associated with distinct self-assembled structures (adapted with permission from [67], Copyright© 2010 Royal Society of Chemistry). (Top, right) Representative mesoscale configuration illustrating a micellar aggregate morphology for PLA/PEO at volume fraction (F) = 0.15 v/v and PLA fraction (f_{PLA}) = 0.3, at 12 % (v/v) nifedipine loading (adapted with permission from [67], Copyright© 2010 Royal Society of Chemistry). (Bottom, left) 2D rendering of a representative bi-continuous microphase-separated morphology of a polystyrene (PS)/poly(methyl methacrylate) (PMMA) film from mesoscale simulations, emphasizing domain connectivity and characteristic length scales (adapted with permission from [72], Copyright© 2016 American Chemical Society). (Bottom, right) Experimental atomic force microscope (AFM) image (two-phase contrast) providing an observable benchmark for mesoscale structural signatures (adapted with permission from [72], Copyright© 2016 American Chemical Society).

clear emphasis on reliability, efficiency, and traceability of the model chain [82,83]. Finally, the same systems-level mindset extends to sustainability-aware modeling: multiscale techniques were assessed as enablers for more credible life-cycle assessments when microstructure-property relations and processing are coupled [84], and hierarchical workflows were proposed to connect molecular modeling outputs to process simulation and environmental-impact estimation when key toxicological/thermophysical inputs are missing from standard databases [85].

Beyond structural materials, Maurizio also demonstrated how molecular simulation can feed directly into environmentally relevant separation and mitigation strategies in porous media and adsorbents: volatile organic compound (VOC) adsorption in zeolites [86], multicomponent adsorption for exhaust-stream cleanup in zeolites and activated carbon [87], and selective H_2S removal from biogas *via* coupled GCMC/MD protocols [88,89]. The same concept of "validated, transferable quantities" appears in sorption/transport problems spanning nanoporous polymers [90] and upcycling/recycling-relevant nanocomposite platforms [91,92], and extends to contaminant adhesion/diffusion in saturated porous media [93]. At the material-interface level, fast MD-based recipes for contact angles, surface tension, and work of adhesion further exemplify Maurizio's drive toward experimentally verifiable, design-ready interfacial metrics [94].

Taken together, these contributions show that, for Maurizio, multiscale simulation was never an end in itself: it was a method to make molecular truth usable, carrying physically grounded descriptors from atoms to mesoscopic structure and, ultimately, to engineering decisions. Once this "information handover" became reliable, the same playbook could be applied well beyond structural polymers and nanocomposites. In the next section, the focus shifts to life-science problems, where multiscale thinking becomes even more consequential: the relevant "invariants" are no longer only morphology or transport, but also recognition, binding, responsiveness, and function in complex biological environments.

5. Life sciences: Drug design, nanomedicine, and mechanism in disease

By the time these multiscale workflows had matured, the next step was almost inevitable: moving from engineered soft matter to biological complexity. Proteins, drug nanocarriers, and nanoparticles in aqueous media are, in practice, complex fluids governed by the same ingredients that defined Maurizio's materials program: interfacial chemistry, self-assembly, transport, and the disciplined handoff of physically meaningful descriptors through scales. Accordingly, Maurizio and collaborators transferred the rigor of chemical-engineering modeling (quantitative, predictive, and oriented toward design) into life-science problems (Fig. 6).

5.1. *Molecular recognition and drug design*

A recurring theme across the life-science work is that binding was treated as a controllable, testable design variable, quantified whenever possible, and interpreted mechanistically rather than descriptively.

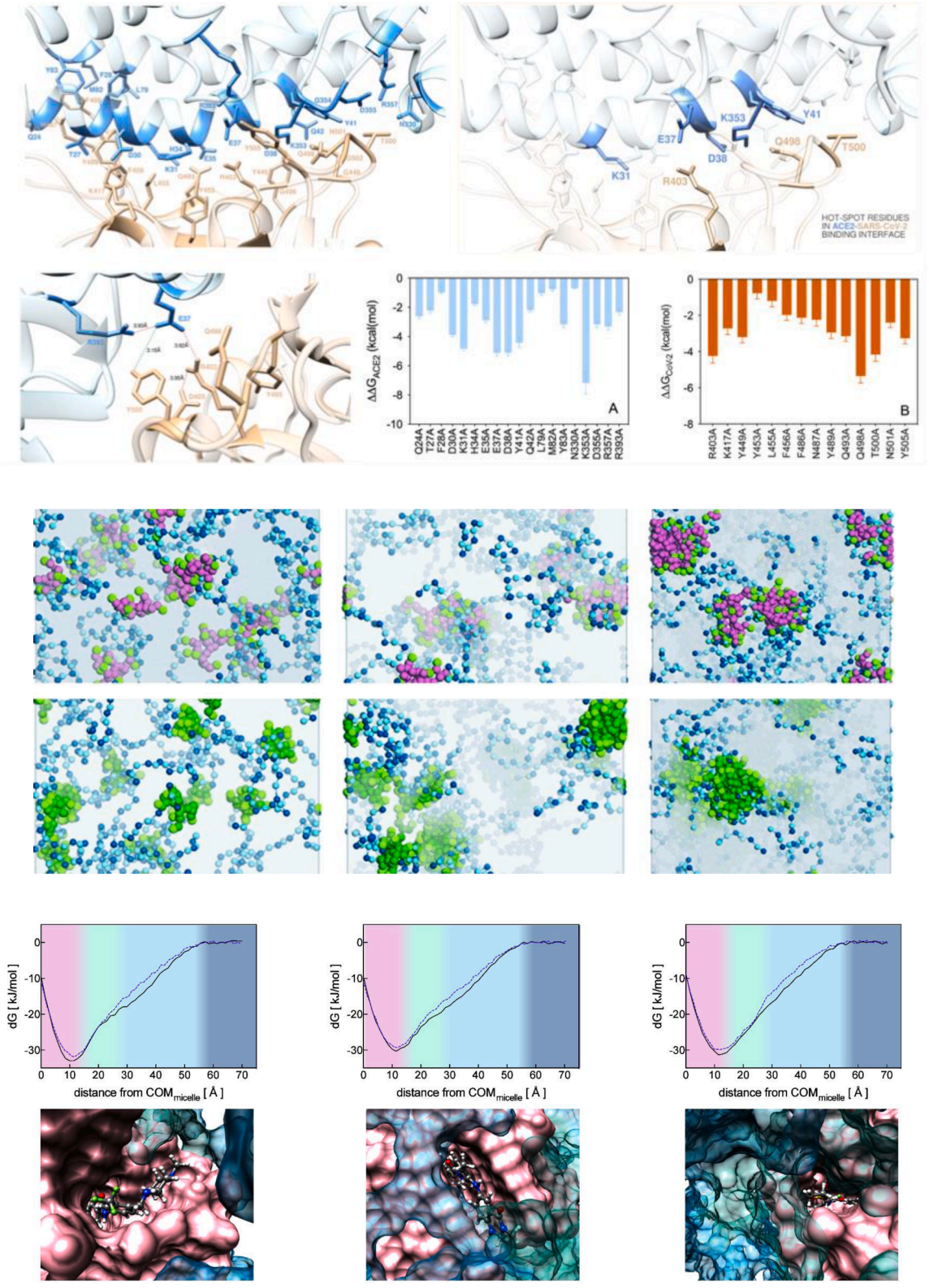

Fig. 6. Life sciences: multivalent recognition, emergent threats, and predictive nanocarrier design. (Top) Structural views of the SARS-CoV-2 Spike receptor-binding domain bound to human ACE2 highlight the binding interface, while alanine-scanning free-energy profiles (ΔΔG upon mutation to alanine; bottom right) identify a small set of hot-spot residues that dominate binding energetics, explaining how single substitutions can disproportionately bias recognition (adapted with permission from [128], Copyright© 2020 American Chemical Society). (Middle) Mesoscale snapshots of heparin complexation by rigid transgeden dendrimers (TGD, pink spheres; top row) and poly(amidoamine) (PAMAM, green spheres; bottom row) across generations (G1-G3, left to right), illustrating architecture-dependent multivalent recognition of heparin (light/dark blue spheres) in complex media (adapted with permission from [139], Copyright© 2014 Royal Society of Chemistry) [139]. (Bottom) Quantitatively predictive encapsulation workflows: Conductor-like Screening Model (COSMO)-derived free-energy/partitioning descriptors combined with atomistic MD rationalize micellar localization/affinity and guide optimization of self-assembled nanomicelles for three oncology payloads: ponatinib (left), AZ6 (center), and vemurafenib (right) (adapted with permission from [146], Copyright© 2024 American Chemical Society).

Early enzyme-substrate studies on α-chymotrypsin exemplify this approach: docking and conformational/energetic analyses were used to rationalize experimentally observed substrate specificity and enantioselectivity and later refined through combined MD and free-energy calculations to dissect the balance of contributions underlying the binding free energy (ΔG_{bind}) and stereochemical outcomes [95–97].

In host-guest systems, the same logic translated atomistic structure into binding trends that matter for formulation. Modeling supported the design and interpretation of cyclodextrin-based constructs for drug inclusion and delivery, including β-cyclodextrin (CDX) inclusion complexes with anticancer drugs and folate-CDX bioconjugates whose physicochemical behavior was experimentally characterized and structurally rationalized [98–99].

As the program expanded into medicinal chemistry, modeling became a practical engine for hypothesis generation and prioritization. Ligand- and structure-based pipelines, including pharmacophore hypotheses, docking, MD, and end-point free energy calculation-based scoring, were used to connect chemical features to activity and selectivity in antiviral and broader anti-infective targets. This included pharmacophore-driven modeling for Hepatitis C virus (HCV) polymerase inhibitors and multi-step experimental/computational workflows for *Flaviviridae* inhibitor discovery where pharmacophore constraints, docking, MD-based ranking, and mechanism-oriented validation were integrated into a design loop [100–106]. Parallel efforts addressed additional antiviral targets such as viral helicases (via homology modeling and interaction analysis), expanded the scaffold space with new chemotypes supported by *in silico binding* rationales, and extended antiviral strategy beyond enzymatic targets to entry/fusion inhibition guided by selective cell assays, discriminating functional tests, and modeling [107–111]. Beyond antivirals, target-based anti-infective design also coupled synthesis and microbiological profiling with structure-guided modeling to rationalize binding modes on bacterial enzymes and prioritize leads active against clinically relevant, including resistant, strains [112–115].

A particularly coherent arc is the σ-receptor program, where model building, validation, and prospective design were iterated in a genuinely deployable workflow. Starting from 3D pharmacophore models (for both σ_1 and σ_2 receptors), the group advanced to homology modeling and docking-based virtual screening strategies, then to MD-based affinity ranking and residue-level analysis, and finally to *in silico/in vitro* site-directed mutagenesis that mapped how specific residues shape ligand binding. This platform supported optimization of σ_1 agonists and systematic structure-activity relationship (SAR) campaigns that explicitly balanced affinity, σ_1 over σ_2 selectivity, and developability-oriented properties, while simulations rationalized trade-offs through interaction- and solvation-aware energetic decompositions [116–127].

Finally, the same interface-level recognition logic was rapidly extended to emerging viral threats. Atomistic frameworks were applied to SARS-CoV-2 Spike-human ACE2 protein-protein recognition to identify key binding hot spots and provide structurally grounded determinants relevant to entry and neutralization strategies [128] (Fig. 6, top).

5.2. Nanomedicine and dendrimer/nanoparticle carriers

A second meta-theme is that nanoscale carriers were treated as physical objects whose performance can be traced back to architecture, solvation, and self-assembly, again with explicit handoffs through scales. In dendrimer-based delivery, atomistic and multiscale modeling were repeatedly coupled to experiments to connect molecular structure to complexation mechanisms, stability in aqueous media, and functional outcomes. Early work established dendrimer architectures and design rules relevant to drug delivery and nucleic-acid complexation [129]. In triethanolamine (TEA)-core poly(amido amine) (PAMAM) families, structural flexibility and internal accessibility were leveraged to design effective nanovectors for nucleic acid delivery, and subsequent combined experimental/computational work quantified how small-interfering RNA (siRNA) overhang length, chemistry, and complementarity modulate binding cooperativity and ultimately gene silencing performance [130,131]. Broader design logic questioning how focal-point hydrophobic moieties drive dendron self-assembly into micellar aggregates, how that controls surface charge density, and how these parameters correlate with DNA binding and transfection, was also established through mesoscale modeling tightly coupled with experimental readouts [132]. This self-assembly paradigm was then translated into functional supramolecular carriers enabling efficient siRNA delivery and gene silencing from challenging cell models to in vivo settings, and into drug-loaded amphiphilic dendrimer nanomicelles that improved anticancer payload performance and mitigated resistance-linked phenotypes through carrier-enabled transport effects [133,134]. Responsiveness was pushed further via double-degradable self-assembled multivalent systems engineered for temporary high-affinity binding and triggered breakdown/release [135]. Complementary mechanistic descriptors relevant to biomedical use were obtained by probing metal binding and solvation effects in flexible TEA-core PAMAM families [136].

A related branch focused on multivalent recognition in highly competitive media, conditions that matter in vivo. Here, modeling helped rationalize experimental results and generalize how dendrimer architecture governs binding to polyanionic biopolymers such as heparin, spanning dye-based sensing in serum, competition assays that quantify dendrimer binding under realistic conditions, and multiscale explanations of "shape-persistent" versus "adaptive" multivalency in rigid and flexible dendrimer families [137–139] (Fig. 6, center). This theme was extended to quantify thermodynamics and competitive displacement driven by self-assembly, while also benchmarking compatibility with abundant serum proteins in complex physiological environments [140].

Protein-nanocarrier recognition was also framed in thermodynamic terms to support "protein-as-carrier" concepts. Combined computational/experimental pipelines mapped binding sites and rationalized differential binding free energies for dendrimer-human serum albumin (HSA) complexes with orthogonal biophysical validation, and more broadly showed how supramolecular recognition motifs can modulate HSA exposure states and enhance drug-loading performance in hybrid protein-based vectors [141,142]. In parallel, fully atomistic simulations were used to dissect oligonucleotide binding by non-PAMAM dendrimer families and to extract physically interpretable performance descriptors (e.g., effective binding strength normalized by the number of active branches) that explain sequence-dependent affinity beyond gross size/shape similarities [143].

Finally, the same multiscale discipline was applied to protein-surface interactions and transport phenomena relevant to biomedical microdevices: atomistic simulations were used to derive molecular parameters for adsorption and to build predictive diffusion models in nanochannels, explicitly bridging nanoscale interactions to macroscale release/diffusion behavior [144,145]. More recently, quantitatively predictive encapsulation metrics were extended by coupling experimental encapsulation readouts with atomistic MD and conductor-like screening model (COSMO)-derived free-energy/partitioning profiles to rationalize micellar localization and affinity, supporting principled optimization of self-assembled nanomicelles for oncology payloads [146] (Fig. 6, bottom).

5.3. Mechanism in disease

A third meta-theme is fully mechanistic modeling, where the goal is not only ranking ligands, but explaining why specific molecular events drive functional outcomes in disease contexts. In oncology and resistance biology, kinase systems became prime case studies. Accordingly, Maurizio and his group used molecular simulations to move beyond single-interaction narratives and to show how resistance mutations reshape binding networks and conformational landscapes, including

mechanistic studies of drug resistance and mutation landscapes for different disease-relevant oncogenes, and clinically anchored mutant analyses where computed trends were aligned with functional/clinical correlates [147–153]. This thread deepened into conformation-selective binding and the emergent problem of polymutants, clarifying how complex mutation constellations can drive resistance and suggesting thermodynamically grounded strategies for inhibitor choice [154,155]. Resistance mechanisms beyond kinases were likewise resolved structurally, exemplified by the interpretation of function-preserving mutations in tumor suppressor systems such as p53 and Smoothened (SMO) mutations that remodel drug-entry pathways and/or binding-site geometry and thereby abrogate inhibitor efficacy [156,157].

Mechanism-of-action elucidation also combined in vitro and *in silico* approaches to connect antiproliferative phenotypes to defined molecular targets, integrating functional assays with thermodynamic binding characterization and modeling to rationalize activity in terms of target engagement [158–160]. Mechanism-driven workflows were also extended to therapeutically relevant protein-protein interactions, mapping disease-linked interfaces and identifying small molecules able to disrupt pro-survival signaling nodes with functional validation in resistant cancer models [161]. Beyond cancer pharmacology, mutation-stratified disease biology integrated protein-structure and protein-protein interaction modeling with transcriptomic and immune-marker profiling, linking specific variants to altered interaction propensities and to distinct gene-expression and immune-context signatures relevant to clinical behavior [162].

Beyond disease, Maurizio and his group applied the same mechanistic mindset to biological signaling: atomistic modeling rationalized how structurally altered 2-oxoglutarate analogues can retain signaling function through receptor-binding accommodation and SAR constraints, enabling functional probe design [163–165].

6. Legacy and outlook: Energy, impact, and circularity

Taken together, these life-science contributions complete the arc that naturally opens onto Maurizio's later outlook themes. Once molecular mechanisms are traced all the way to function in proteins, carriers, and complex biological media the next questions become unavoidable: how do we compare alternatives under realistic constraints, and how do we quantify trade-offs that matter outside the laboratory? This is where his work converged with today's most urgent priorities: energy transition, sustainability-aware development, circularity, and credible impact assessment, closing the loop from molecular-scale understanding to societal-scale value.

6.1. Energy transition as a modeling-and-decision problem

A recurring lesson in Maurizio's later work is that the energy transition is not a single-technology story. It is a systems problem that demands models able to connect device-level physics to plant-scale performance and, ultimately, to decision variables. Early process-level studies on molten carbonate fuel cells framed this approach clearly: detailed steady-state simulations embedded custom unit models within flowsheets to identify efficiency drivers via sensitivity analysis, and then extended the same strategy to biomass-derived feeds, emphasizing feasibility under realistic operating constraints rather than idealized conditions [166,167]. In these studies, simulation is used in its most "Fermeglia" sense: as an actionable bridge between mechanism and decisions.

A similar multiscale logic was later applied to assess potential breakthroughs, such as integrating carbon capture and storage (CCS) into natural-gas combined-cycle power plants, and comparing performance and trade-offs against alternative generation options [168]. This system framing culminated in broader energy outlook work that treats photovoltaics not as an isolated solution, but as a lever within tightly coupled energy–carbon–resource dynamics. The key message is methodological as much as technological: credible transition planning requires quantitative baselines, transparent assumptions, and explicit links between scenarios and measurable outcomes [169].

6.2. Sustainability metrics that are deployable in design workflows

A second enduring contribution is the insistence that sustainability must be computed where design happens: inside the tools and pipelines that generate process options. This view appears early in the implementation of process sustainability evaluation as a reusable CAPE-OPEN module that operationalizes WAR/PEI-type indicators within standard simulation environments, turning "environmental impact" into something engineers can evaluate alongside mass and energy balances [170].

More recent work pushes this idea toward multi-criteria decision support under uncertainty and incomplete early-stage information. By combining process simulation with indicator sets spanning the sustainability pillars and using data envelopment analysis (DEA) for screening and ranking, the workflow addresses what practitioners face in real projects: many alternatives, competing objectives, and the need to identify why designs underperform - and where retrofits matter - committing to detailed development [171].

6.3. Quantified impact assessment under realistic conditions

If sustainability indicators make design choices comparable, life-cycle thinking makes them meaningful. A hallmark of this body of work is the disciplined coupling of detailed process simulation (to avoid "black-box inventories") with Life Cycle Assessment (LCA) (to capture upstream and downstream burdens). In separations, the combined contributions of thermodynamic analysis, process simulation, and full LCA enable solvent/process comparisons that remain consistent at the level of mass and energy requirements, and explicit about how utilities and supply chains shape impact categories [172]. A forward-looking extension is the use of multiscale modeling to generate life-cycle inventory data for complex or novel materials, precisely where conventional LCA struggles most. Here, atomistic/mesoscale/continuum simulations become a controlled source of inventory parameters during early product design, allowing environmental evaluation before full industrial datasets are available and making eco-design more than an *ex post* accounting exercise [84]. Hydrogen studies then extend the framework from production to use contexts (including transportation and logistics), using consistent KPI triads (energy return, levelized costs, and LCA) and, when relevant, ownership/cost metrics that stakeholders and policy actually use (Fig. 3) [173,174]. Across these analyses, the methodological point is the same: sustainability is conditional on boundary choices, operating profiles, and infrastructure constraints, and must be assessed as such.

Finally, the inclusion of broader impact categories such as biodiversity and land-use, and the explicit identification of operational thresholds (e.g., demand/occupancy levels required to outperform incumbent systems) challenge simplistic "green-by-default" narratives. This is responsible modeling in its most consequential form: it prevents well-intended projects from being justified by incomplete metrics [175].

6.4. Circularity and end-of-life as first-class design variables

A unifying theme behind these contributions is that circularity is not an afterthought. Recycling rates, reuse scenarios, and end-of-life pathways can invert rankings between competing solutions, so the "best material" or "best technology" is often a system-level property rather than an intrinsic attribute. Making these dependencies explicit enables more honest optimization: identifying which levers (collection logistics, recycling infrastructure, energy mix, and operational profiles) must change for a solution to remain favorable over its full life cycle [84,174,175].

6.5. Outlook: From multiscale modeling to auditable sustainability-by-design

What emerges from Maurizio's later work is not a new technical niche, but a coherent philosophy of practice: build models that can be audited, couple them to measurable indicators, and use them to guide decisions under realistic constraints. In that sense, the "Fermeglia Continuum" naturally extends from molecular truth to societal value: it treats sustainability, circularity, and impact not as externalities, but as quantities that can, and should, be computed within the same disciplined multiscale workflows that previously carried structure into properties, and properties into design.

Through energy systems, sustainable process design, and circular materials, Maurizio insisted that models must earn the right to guide decisions, and that numbers should always travel with their assumptions. His work makes that lesson explicit: multiscale workflows can compare competing options on equal footing, quantify trade-offs (efficiency, cost, footprint), and keep impact assessment auditable rather than rhetorical.

Writing these last pages, I found myself returning less to milestones and more to a habit of mind Maurizio gave many of us: the insistence that rigor is a form of care: care for the truth in the numbers, for the people who will rely on them, and for the consequences that follow when models leave our notebooks and enter decisions. I first learned this from his classical thermodynamics and equation-of-state contributions, where reliable properties are not an academic luxury but a prerequisite for designing processes that are safe, controllable, and trustworthy in the hands of industry. I saw it again in the life-science work, where rigor becomes accountability because modeling can influence experimental priorities, mechanistic interpretation, and translational choices. And I recognized it most explicitly in his later work on energy transition, sustainability-by-design, life-cycle thinking, and circularity: the same ethic carried into domains where the cost of weak assumptions is paid in real constraints and real outcomes.

If we carry this discipline forward: open data, reusable pipelines, and training that reads clearly across scales, his work will keep doing what it always did: turning molecular truth into societal value. That is the Fermeglia continuum, and it remains open.

CRediT authorship contribution statement

Sabrina Pricl: Writing – review & editing, Writing – original draft, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

I am personally grateful to the colleagues, collaborators, students, and friends who accompanied this journey over the years, and to the broader communities of thermodynamics, fluid phase equilibria, molecular simulation, and multiscale modeling for the conversations, critiques, and shared standards, and for the constructive debate that keep our field rigorous, open, and in motion.

Data availability

No data was used for the research described in the article.

References

[1] I. Kikic, P. Alessi, M. Fermeglia, Prediction of finite concentration behavior from infinite dilution equilibrium data, Fluid Ph. Equilib 14 (C) (1983) 363–372, https://doi.org/10.1016/0378-3812(83)80142-3.
[2] P. Alessi, A. Bertucco, M. Fermeglia, Correlation of thermodynamic properties of fluids by means of equations of state, Thermochim. Acta 137 (1) (1988) 21–38, https://doi.org/10.1016/0040-6031(88)87462-8.
[3] M. Fermeglia, I. Kikic, Excess enthalpy calculations by means of equations of state, J. Therm. Anal. 29 (4) (1984) 687–695, https://doi.org/10.1007/BF01913526.
[4] M. Orlandini, M. Fermeglia, I. Kikic, P. Alessi, Liquid-liquid equilibria for water-propanol- and water-butanol-chlorocompound systems, Chem. Eng. J. 26 (3) (1983) 245–250, https://doi.org/10.1016/0300-9467(83)80020-3.
[5] P. Alessi, I. Kikic, M. Fermeglia, C. Nonino, Liquid–liquid equilibrium data for ternary systems containing organic acid, hydrocarbon and water, Fluid Ph. Equilib 18 (1) (1984) 93–102, https://doi.org/10.1016/0378-3812(84)80024-2.
[6] L. Fele, M. Fermeglia, P. Alessi, J.R. Rarey, J. Golob, Vapor-liquid and liquid-liquid equilibria for the toluene + 1,2-propanediol + water system, J. Chem. Eng. Data 39 (4) (1994) 735–741, https://doi.org/10.1021/je00016a023.
[7] P. Alessi, M. Fermeglia, I. Kikic, Liquid-liquid equilibrium of cyclohexane-n-hexane-methanol mixtures: effect of water content, J. Chem. Eng. Data 34 (2) (1989) 236–240, https://doi.org/10.1021/je00056a026.
[8] G. Soave, M. Fermeglia, On the application of cubic equations of state to synthetic high-pressure VLE measurements, Fluid Ph. Equilib 60 (3) (1990) 261–271, https://doi.org/10.1016/0378-3812(90)85056-G.
[9] C. Pettenati, P. Alessi, M. Fermeglia, I. Kikic, Vapor liquid equilibrium data for systems containing morpholine, Fluid Ph. Equilib 54 (1990) 81–91, https://doi.org/10.1016/0378-3812(90)85072-I.
[10] E. Neau, M. Rogalski, P. Alessi, M. Fermeglia, VLE of alkanol-alkane systems with the modified CRG model, Fluid Ph. Equilib 56 (1990) 189–202, https://doi.org/10.1016/0378-3812(90)85102-G.
[11] I. Kikic, M. Fermeglia, P. Rasmussen, Unifac prediction of vapor-liquid equilibria in mixed solvent-salt systems, Chem. Eng. Sci. 46 (11) (1991) 2775–2780, https://doi.org/10.1016/0009-2509(91)85146-O.
[12] P. Alessi, M. Fermeglia, I. Kikic, Limitations of differential static apparatus in dilute regions, Fluid Ph. Equilib 43 (2-3) (1988) 355–358, https://doi.org/10.1016/0378-3812(88)87015-8.
[13] P. Alessi, M. Fermeglia, I. Kikic, Significance of dilute regions, Fluid Ph. Equilib 70 (1-2) (1991) 239–250, https://doi.org/10.1016/0378-3812(91)85037-U.
[14] M. Fermeglia, G. Torriano, Density, viscosity, and refractive index for binary systems of n-C16 and four nonlinear alkanes at 298.15 K, J. Chem. Eng. Data 44 (5) (1999) 965–969, https://doi.org/10.1021/je9900171.
[15] M. Fermeglia, R. Lapasin, Excess volumes and viscosities of binary mixtures of organics, J. Chem. Eng. Data 33 (4) (1988) 415–417, https://doi.org/10.1021/je00054a008.
[16] M. Fermeglia, R. Lapasin, G. Torriano, Excess volumes and viscosities of binary systems containing 4-methyl-2-pentanone, J. Chem. Eng. Data 35 (3) (1990) 260–265, https://doi.org/10.1021/je00061a011.
[17] C. Pettenati, P. Alessi, M. Fermeglia, I. Kikic, Excess volumes of binary mixtures containing morpholine, Thermochim. Acta 162 (1) (1990) 203–212, https://doi.org/10.1016/0040-6031(90)80342-V.
[18] L. de Lorenzi, M. Fermeglia, G. Torriano, Densities and viscosities of 1,1,1-trichloroethane + paraffins and + cycloparaffins at 298.15 K, J. Chem. Eng. Data 39 (3) (1994) 483–487, https://doi.org/10.1021/je00015a018.
[19] L. de Lorenzi, M. Fermeglia, G. Torriano, Densities and viscosities of 1,1,1-trichloroethane with 13 different solvents at 298.15 K, J. Chem. Eng. Data 40 (6) (1995) 1172–1177, https://doi.org/10.1021/je00022a003.
[20] L. de Lorenzi, M. Fermeglia, G. Torriano, Density and viscosity of 1-methoxy-2-propanol, 2-methyltetrahydrofuran, α,α,α-trifluorotoluene, and their binary mixtures with 1,1,1-trichloroethane at different temperatures, J. Chem. Eng. Data 41 (5) (1996) 1121–1125, https://doi.org/10.1021/je9601220.
[21] L. de Lorenzi, M. Fermeglia, G. Torriano, Density, refractive index, and kinematic viscosity of diesters and triesters, J. Chem. Eng. Data 42 (5) (1997) 919–923, https://doi.org/10.1021/je970036f.
[22] L. de Lorenzi, M. Fermeglia, G. Torriano, Density, kinematic viscosity, and refractive index for bis(2-ethylhexyl) adipate, tris(2-ethylhexyl) trimellitate, and diisononyl phthalate, J. Chem. Eng. Data 43 (2) (1998) 183–186, https://doi.org/10.1021/je970200z.
[23] A. Bertucco, M. Fermeglia, I. Kikic, Modified Carnahan-Starling-Van der Waals equation for supercritical fluid extraction, Chem. Eng. J. 32 (1) (1986) 21–30, https://doi.org/10.1016/0300-9467(86)85003-1.
[24] P. Alessi, M. Fermeglia, I. Kikic, Correlation of 1-alkanol-n-alkane activity coefficients at infinite dilution by means of GCEOS equation, Fluid Ph. Equilib 27 (C) (1986) 93–102, https://doi.org/10.1016/0378-3812(86)87043-1.
[25] J. Gregorowicz, M. Fermeglia, G. Soave, I. Kikic, The perturbed hard chain theory for the prediction of supercritical fluid extraction: pure component properties, Chem. Eng. Sci. 46 (5-6) (1991) 1427–1436, https://doi.org/10.1016/0009-2509(91)85069-A.
[26] M. Fermeglia, I. Kikic, The perturbed hard chain theory for the prediction of supercritical fluid extraction: binary mixtures, Chem. Eng. Sci. 48 (23) (1993) 3889–3896, https://doi.org/10.1016/0009-2509(93)80367-Y.
[27] F. Donaggio, M. Fermeglia, V. de Leeuw, Prediction of high-pressure multicomponent phase equilibria using a perturbed hard chain equation of state, J. Supercrit. Fluids. 9 (4) (1996) 207–215, https://doi.org/10.1016/S0896-8446(96)90050-9.

[28] E. Neau, P. Alessi, M. Fermeglia, I. Kikic, Low-pressure equilibrium data for the prediction of solubility in carbon dioxide, Chem. Eng. Sci. 45 (4) (1990) 795–808, https://doi.org/10.1016/0009-2509(90)85003-V.
[29] B. Spicka, A. Cortesi, M. Fermeglia, I. Kikic, Determination of partial molar volumes at infinite dilution using SFC technique, J. Supercrit. Fluids 7 (3) (1994) 171–176, https://doi.org/10.1016/0896-8446(94)90022-1.
[30] P. Alessi, M. Fermeglia, I. Kikic, E. Neau, Phase behavior prediction for binary volatile-nonvolatile mixtures of N-paraffins, J. Supercrit. Fluids 5 (3) (1992) 151–156, https://doi.org/10.1016/0896-8446(92)90001-Z.
[31] P. Alessi, A. Cortesi, M. Fermeglia, M. Fontana, I. Kikic, Prediction of solubility in heavy ends by means of PHCT, Fluid Ph. Equilib 53 (1989) 397–406, https://doi.org/10.1016/0378-3812(89)80105-0.
[32] M. Zuliani, A. Barreau, J. Vidal, P. Alessi, Fermeglia M. Measurements, correlation and prediction of Henry's constants of light alkanes in model heavy hydrocarbons and petroleum fractions, Fluid Ph. Equilib 82 (1993) 141–148, https://doi.org/10.1016/0378-3812(93)87137-P.
[33] M. Fermeglia, A. Bertucco, D. Patrizio, Thermodynamic properties of pure hydrofluorocarbons by a perturbed hard-sphere-chain equation of state, Chem. Eng. Sci. 52 (9) (1997) 1517–1527, https://doi.org/10.1016/S0009-2509(96)00503-9.
[34] M. Fermeglia, A. Bertucco, S. Bruni, A perturbed hard sphere chain equation of state for applications to hydrofluorocarbons, hydrocarbons and their mixtures, Chem. Eng. Sci. 53 (7) (1998) 3117–3128, https://doi.org/10.1016/S0009-2509(98)00087-6.
[35] A. Bertucco, N. Elvassore, M. Fermeglia, J.M. Prausnitz, A perturbed-hard-sphere-chain equation of state for phase equilibria of mixtures containing a refrigerant and a lubricant oil, Fluid Ph. Equilib 158-160 (1999) 183–191, https://doi.org/10.1016/S0378-3812(99)00152-1.
[36] G. Cesari, M. Fermeglia, I. Kikic, M. Policastro, A computer program for the dynamic simulation of a semi-batch supercritical fluid extraction process, Comput. Chem. Eng. 13 (10) (1989) 1175–1181, https://doi.org/10.1016/0098-1354(89)87020-6.
[37] I. Colussi, M. Fermeglia, V. Gallo, I. Kikic, Supercritical multistaged multicomponent separation: process simulation, Comput. Chem. Eng. 16 (3) (1992) 211–224, https://doi.org/10.1016/0098-1354(92)85007-U.
[38] L. Fele, P. Vidali, P. Alessi, M. Fermeglia, Recovery of N-methylmorpholine from waste aqueous streams by distillation, Chem. Eng. Sci. 49 (21) (1994) 3677–3680, https://doi.org/10.1016/0009-2509(94)00169-3.
[39] L. Fele, M. Fermeglia, Partition coefficients of proteins in poly(ethylene glycol) + dextran + water at 298 K, J. Chem. Eng. Data 41 (2) (1996) 331–334, https://doi.org/10.1021/je9502298.
[40] I. Colombo, M. Grassi, M. Fermeglia, R. Lapasin, S. Pricl, Modeling phase transitions and sorption desorption kinetics in thermo-sensitive gels for controlled drug delivery systems, Fluid Ph. Equilib 116 (1-2) (1996) 148–161, https://doi.org/10.1016/0378-3812(95)02883-8.
[41] M. Fermeglia, S. Pricl, A novel approach to thermophysical properties prediction for chloro-fluoro-hydrocarbons, Fluid Ph. Equilib 166 (1) (1999) 21–37, https://doi.org/10.1016/S0378-3812(99)00295-2.
[42] M. Fermeglia, S. Pricl, Molecular dynamics simulations of real systems: application to chloro-fluoro-hydrocarbons and polymers, Fluid Ph. Equilib 158-160 (1999) 49–58, https://doi.org/10.1016/S0378-3812(99)00093-X.
[43] O. Milocco, M. Fermeglia, S. Pricl, Prediction of thermophysical properties of alternative refrigerants by computational chemistry, Fluid Ph. Equilib 199 (1-2) (2002) 15–21, https://doi.org/10.1016/S0378-3812(01)00811-1.
[44] M. Fermeglia, S. Pricl, Equation-of-state parameters for pure polymers by molecular dynamics simulations, AIChE J. 45 (12) (1999) 2619–2627, https://doi.org/10.1002/aic.690451218.
[45] F. Belloni, M. Fermeglia, S. Pricl, From molecular to process simulation: novel approaches to the prediction of phase equilibria and PVT behavior based on molecular/quantum mechanics and molecular dynamics simulations, Mol. Simul. 25 (1-2) (2000) 53–71, https://doi.org/10.1080/08927020008044112.
[46] M. Fermeglia, S. Pricl, Prediction of phase equilibria for binary mixtures by molecular modeling, AIChE J. 47 (10) (2001) 2371–2382, https://doi.org/10.1002/aic.690471021.
[47] F. Favari, A. Bertucco, N. Elvassore, M. Fermeglia, Multiphase multicomponent equilibria for mixtures containing polymers by the perturbation theory, Chem. Eng. Sci. 55 (13) (2000) 2379–2392, https://doi.org/10.1016/S0009-2509(99)00517-5.
[48] N. Elvassore, A. Bertucco, M. Fermeglia, Phase-equilibria calculation by group-contribution perturbed hard sphere chain equation of state, AIChE J. 48 (2) (2002) 359–368, https://doi.org/10.1002/aic.690480219.
[49] S. Pricl, M. Fermeglia, Virtual rheological experiments on linear alkane chains confined between titanium walls, Rheol. Acta 40 (2) (2001) 104–110, https://doi.org/10.1007/s003970000148.
[50] S. Pricl, M. Fermeglia, Molecular simulation of host-guest inclusion compounds: an approach to the lactodendrimers case, Carbohydr. Polym. 45 (1) (2001) 23–33, https://doi.org/10.1016/S0144-8617(00)00241-1.
[51] M. Fermeglia, M. Ferrone, S. Pricl, Computer simulation of nylon 6/organoclay nanocomposites, Fluid Ph. Equilib 212 (1-2) (2003) 315–329, https://doi.org/10.1016/S0378-3812(03)00273-5.
[52] S. Pricl, M. Fermeglia, Atomistic molecular dynamics simulations of gas diffusion and solubility in rubbery amorphous hydrocarbon polymers, Chem. Eng. Commun. 190 (10) (2003) 1267–1292, https://doi.org/10.1080/00986440302153.
[53] M. Fermeglia, S. Pricl, Multiscale molecular modeling in nanostructured material design and process system engineering, Comput. Chem. Eng. 33 (10) (2009) 1701–1710, https://doi.org/10.1016/j.compchemeng.2009.04.006.
[54] M. Fermeglia, A. Mio, S. Aulic, D. Marson, E. Laurini, S. Pricl, Multiscale molecular modelling for the design of nanostructured polymer systems: industrial applications, Mol. Syst. Des. Eng. 5 (9) (2020) 1447–1476, https://doi.org/10.1039/d0me00109k.
[55] M. Fermeglia, M. Ferrone, S. Pricl, Computer simulation of nylon 6/organoclay nanocomposites, Fluid Ph. Equilib 212 (1-2) (2003) 315–329, https://doi.org/10.1016/S0378-3812(03)00273-5.
[56] R. Toth, A. Coslanich, M. Ferrone, M. Fermeglia, S. Pricl, S. Miertus, Computer simulation of polypropylene/organoclay nanocomposites, Polym. (Guildf) 45 (23) (2004) 8075–8083, https://doi.org/10.1016/j.polymer.2004.09.025.
[57] G. Scocchi, P. Posocco, A. Danani, S. Pricl, M. Fermeglia, To the nanoscale, and beyond! multiscale molecular modelling of polymer–clay nanocomposites, Fluid Ph. Equilib 261 (1-2) (2007) 366–374, https://doi.org/10.1016/j.fluid.2007.07.046.
[58] G. Scocchi, P. Posocco, M. Fermeglia, S. Pricl, Polymer-clay nanocomposites: A multiscale molecular modeling approach, J. Phys. Chem. B 111 (9) (2007) 2143–2151, https://doi.org/10.1021/jp067649w.
[59] G. Scocchi, P. Posocco, M. Fermeglia, S. Pricl, A complete multiscale molecular modeling approach to polymer-clay nanocomposites, Chem. - Eur. J. 15 (31) (2009) 7586–7592, https://doi.org/10.1002/chem.200900995.
[60] M. Fermeglia, M. Ferrone, S. Pricl, Estimation of the binding energy in random poly butylene terephtalate-co-thiodiethylene terephtalate copolyesters/clay nanocomposites via molecular simulation, Mol. Simul. 30 (5) (2004) 289–300, https://doi.org/10.1080/08927020410001659385.
[61] R. Toth, D.J. Voorn, J.W. Handgraaf, J.G.E.M. Fraije, M. Fermeglia, S. Pricl, P. Posocco, Multiscale computer simulation studies of water-based montmorillonite/poly(ethylene oxide) nanocomposites, Macromolecules. 42 (21) (2009) 8260–8270, https://doi.org/10.1021/ma901584w.
[62] M. Fermeglia, S. Pricl, Multiscale modeling for polymer systems of industrial interest, Prog. Org. Coat. 58 (2-3) (2007) 187–199, https://doi.org/10.1016/j.porgcoat.2006.08.028.
[63] F. Piscitelli, P. Posocco, R. Toth, M. Fermeglia, S. Pricl, G. Mensitieri, M. Lavorgna, Sodium montmorillonite silylation: unexpected effect of the aminosilane chain length, J. Colloid. Interface Sci. 351 (1) (2010) 108–115, https://doi.org/10.1016/j.jcis.2010.07.059.
[64] R. Toth, M. Ferrone, S. Miertus, E. Chiellini, M. Fermeglia, S. Pricl, Structure and energetics of biocompatible polymer nanocomposite systems: A molecular dynamics study, Biomacromolecules. 7 (6) (2006) 1714–1719, https://doi.org/10.1021/bm050937y.
[65] M. Maly, P. Posocco, S. Pricl, M. Fermeglia, Self-assembly of nanoparticle mixtures in diblock copolymers: multiscale molecular modeling, Ind. Eng. Chem. Res. 47 (15) (2008) 5023–5038, https://doi.org/10.1021/ie071311m.
[66] P. Posocco, Z. Posel, M. Fermeglia, M. Lísal, S. Pricl, A molecular simulation approach to the prediction of the morphology of self-assembled nanoparticles in diblock copolymers, J. Mater. Chem. 20 (2010) 10511–10520, https://doi.org/10.1039/C0JM01561J.
[67] P. Posocco, M. Fermeglia, S. Pricl, Morphology prediction of drug-delivery block copolymers via mesoscopic simulation, J. Mater. Chem. 20 (2010) 7742–7753, https://doi.org/10.1039/c0jm01301c.
[68] P. Posocco, C. Gentilini, S. Bidoggia, A. Pace, P. Franchi, M. Lucarini, M. Fermeglia, S. Pricl, L. Pasquato, Self-organization of mixtures of fluorocarbon and hydrocarbon amphiphilic thiolates on the surface of gold nanoparticles, ACS. Nano 6 (8) (2012) 7243–7253, https://doi.org/10.1021/nn302366q.
[69] R. Toth, F. Santese, S.P. Pereira, D.R. Nieto, S. Pricl, M. Fermeglia, Size and shape matter: nanoparticle geometry governs structure in polymer-nanocomposites, J. Mater. Chem. 22 (2012) 5398–5409, https://doi.org/10.1039/c2jm15763b.
[70] Z. Posel, P. Posocco, M. Fermeglia, M. Lísal, S. Pricl, Modeling hierarchically structured nanoparticle/diblock copolymer system, Soft. Matter. 9 (10) (2013) 2936–2946, https://doi.org/10.1039/c2sm27360h.
[71] Z. Posel, P. Posocco, M. Lísal, M. Fermeglia, S. Pricl, Highly grafted polymer-gold nanostars in good solvent: simulation of core–corona structure and interparticle interactions, Soft. Matter. 12 (15) (2016) 3600–3611, https://doi.org/10.1039/c5sm02867a.
[72] P. Posocco, Y.M. Hassan, I. Barandiaran, G. Kortaberria, S. Pricl, M. Fermeglia, Combined mesoscale/experimental study of selective placement of magnetic nanoparticles in diblock copolymer films via Solvent Vapor annealing, J. Phys. Chem. C 120 (13) (2016) 7403–7411, https://doi.org/10.1021/Acs.Jpcc.6b01050.
[73] E. Blasizza, M. Fermeglia, S. Pricl, Dendrimers as functional materials. A molecular simulation study of poly(propylene) imine starburst molecules, Mol. Simul. 24 (1-3) (2000) 167–189, https://doi.org/10.1080/08927020008024194.
[74] S. Pricl, M. Fermeglia, M. Ferrone, A. Asquini, Scaling properties in the molecular structure of three-dimensional, nanosized phenylene-based dendrimers as studied by atomistic molecular dynamics simulations, Carbon. N. Y. 41 (12) (2003) 2269–2283, https://doi.org/10.1016/S0008-6223(03)00254-9.
[75] P. Posocco, M. Ferrone, M. Fermeglia, S. Pricl, Binding at the core. Computational study of structural and ligand binding properties of naphthyridine-based dendrimers, Macromolecules. 40 (6) (2007) 2257–2266, https://doi.org/10.1021/ma062610a.
[76] M. Maly, P. Posocco, M. Fermeglia, S. Pricl, Scripting approach in hybrid organic–inorganic condensation simulation: the GPTMS proof-of-concept, Mol. Simul. 34 (10-15) (2008) 1215–1236, https://doi.org/10.1080/08927020802235706.

[77] M. Fermeglia, S. Pricl, Multiscale molecular modeling in nanostructured material design and process system engineering, Comput. Chem. Eng. 33 (10) (2009) 1701–1710, https://doi.org/10.1016/j.compchemeng.2009.04.006.
[78] M. Fermeglia, P. Cosoli, M. Ferrone, S. Piccarolo, G. Mensitieri, S. Pricl, PET/PEN blends of industrial interest as barrier materials. Part I. Many-scale molecular modeling of PET/PEN blends, Polym. (Guildf) 47 (16) (2006) 5979–5989, https://doi.org/10.1016/j.polymer.2006.05.070.
[79] E. Laurini, P. Posocco, M. Fermeglia, Pricl S.MoDeNa Nanotools, An integrated multiscale simulation workflow to predict thermophysical properties of thermoplastic polyurethanes, J. Comput. Sci. 15 (2017) 24–33, https://doi.org/10.1016/j.jocs.2015.11.006.
[80] M. Karimi, D. Marchisio, E. Laurini, M. Fermeglia, S. Pricl, Bridging the gap across scales: coupling CFD and MD/GCMC in polyurethane foam simulation, Chem. Eng. Sci. 178 (2018) 39–47, https://doi.org/10.1016/j.ces.2017.12.030.
[81] P. Ferkl, M. Toulec, E. Laurini, S. Pricl, M. Fermeglia, S. Auffarth, B. Eling, V. Settels, J. Kosek, Multi-scale modelling of heat transfer in polyurethane foams, Chem. Eng. Sci. 172 (2017) 323–334, https://doi.org/10.1016/j.ces.2017.06.035.
[82] E. Laurini, D. Marson, M. Fermeglia, S. Pricl, Multimodel approach for accurate determination of industry-driven properties for polymer nanocomposite materials, J. Comput. Sci. 26 (2018) 28–38, https://doi.org/10.1016/j.jocs.2018.03.002.
[83] E. Laurini, D. Marson, S. Aulic, A. Mio, M. Fermeglia, S. Pricl, Integrating multiscale simulations for composite materials with industrial business decision: the EU H2020 COMPOSELECTOR project experience, Chem. Eng. Trans. 74 (2019) 619–624, https://doi.org/10.3303/CET1974104.
[84] A. Mio, S. Bertagna, L. Cozzarini, E. Laurini, V. Bucci, A. Marinò, M. Fermeglia, Multiscale modelling techniques in life cycle assessment: application to nanostructured polymer systems in the maritime industry, Sustain. Mater. Technol. 29 (2021) e00327, https://doi.org/10.1016/j.susmat.2021.e00327.
[85] M. Fermeglia, G. Longo, L. Petrescu, A hierarchical approach for the estimation of environmental impact of a chemical process: from molecular modeling to process simulation, Comput. Aided Chem. Eng. 24 (2007) 1199–1204, https://doi.org/10.1016/S1570-7946(07)80224-0.
[86] P. Cosoli, M. Ferrone, S. Pricl, M. Fermeglia, Grand Canonical Monte-Carlo simulations for VOCs adsorption in non-polar zeolites, Int. J. Environ. Technol. Manag. 7 (1-2) (2007) 228–243, https://doi.org/10.1504/IJETM.2007.013247.
[87] P. Cosoli, M. Fermeglia, M. Ferrone, GCMC simulations in zeolite MFI and activated carbon for benzene removal from exhaust gaseous streams, Mol. Simul. 34 (10-15) (2008) 1321–1327, https://doi.org/10.1080/08927020802350919.
[88] P. Cosoli, M. Ferrone, S. Pricl, M. Fermeglia, Hydrogen sulphide removal from biogas by zeolite adsorption. Part I. GCMC molecular simulations, Chem. Eng. J. 145 (1) (2008) 86–92, https://doi.org/10.1016/j.cej.2008.07.034.
[89] P. Cosoli, M. Ferrone, S. Pricl, M. Fermeglia, Hydrogen sulfide removal from biogas by zeolite adsorption. Part II. MD simulations, Chem. Eng. J. 145 (1) (2008) 93–99, https://doi.org/10.1016/j.cej.2008.08.013.
[90] G. Mensitieri, D. Larobina, G. Guerra, V. Venditto, M. Fermeglia, S. Pricl, Chloroform sorption in nanoporous crystalline and amorphous phases of syndiotactic polystyrene, J. Polym. Sci. B: Polym. Phys. 46 (1) (2008) 8–15, https://doi.org/10.1002/polb.21303.
[91] P. Cosoli, G. Scocchi, S. Pricl, M. Fermeglia, Many-scale molecular simulation for ABS-MMT nanocomposites: upgrading of industrial scraps, Microporous Mesoporous Mater. 107 (1-2) (2008) 169–179, https://doi.org/10.1016/j.micromeso.2007.03.017.
[92] L. Martin, G. Kortaberria, A. Vazquez, M. Fermeglia, et al., A comparative study of nanocomposites based on a recycled poly(methyl methacrylate) matrix containing several nanoclays, Polym. Compos. 29 (7) (2008) 782–790, https://doi.org/10.1002/pc.20438.
[93] P. Cosoli, M. Fermeglia, M. Ferrone, Molecular simulation of atrazine adhesion and diffusion in a saturated sand model, Soil Sediment Contam. 19 (1) (2010) 72–87, https://doi.org/10.1080/15320380903390505.
[94] D.R. Nieto, F. Santese, R. Toth, P. Posocco, S. Pricl, M. Fermeglia, 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. 4 (6) (2012) 2855–2859, https://doi.org/10.1021/am3004818.
[95] F. Felluga, M. Fermeglia, M. Ferrone, G. Pitacco, S. Pricl, E. Valentin, Computational studies on the enantioselectivity of α-chymotrypsin towards β-carbomethoxy-γ-lactams, Tetrahedron: Asymmetry 13 (5) (2002) 475–489, https://doi.org/10.1016/S0957-4166(02)00144-1.
[96] F. Felluga, M. Fermeglia, M. Ferrone, G. Pitacco, S. Pricl, E. Valentin, Chemo-enzymatic synthesis and determination of the absolute configuration of both enantiomers of methyl trans-5-oxo-2-pentylpyrrolidine-3-carboxylate precursors of the aza analogues of (+)- and (−)-methylenolactocin, Helv. Chim. Acta 85 (11) (2002) 4046–4054, https://doi.org/10.1002/1522-2675(200211)85:11%3C4046::AID-HLCA4046%3E3.0.CO;2-F.
[97] F. Felluga, G. Pitacco, E. Valentin, A. Coslanich, M. Fermeglia, M. Ferrone, S. Pricl, Studying enzyme enantioselectivity using combined ab initio and free energy calculations: α-chymotrypsin and methyl cis- and trans-5-oxo-2-pentylpirrolidine-3-carboxylates, Tetrahedron: Asymmetry 14 (21) (2003) 3385–3399, https://doi.org/10.1016/j.tetasy.2003.09.003.
[98] M. Fermeglia, M. Ferrone, A. Lodi, S. Pricl, Host-guest inclusion complexes between anticancer drugs and β-cyclodextrin: computational studies, Carbohydr. Polym. 53 (1) (2003) 15–44, https://doi.org/10.1016/S0144-8617(03)00011-0.
[99] P. Caliceti, S. Salmaso, A. Semenzato, T. Carofiglio, R. Fornasier, M. Fermeglia, M. Ferrone, S. Pricl, Synthesis and physicochemical characterization of folate-cyclodextrin bioconjugate for active drug delivery, Bioconjug, Chem 14 (5) (2003) 899–908, https://doi.org/10.1021/bc034080i.
[100] R. Di Santo, M. Fermeglia, M. Ferrone, M.S. Paneni, R. Costi, M. Artico, A. Roux, M. Gabriele, KD. Tardif, A. Siddiqui, S. Pricl, Simple but highly effective three-dimensional chemical-feature-based pharmacophore model for diketo acid derivatives as hepatitis C virus RNA-dependent RNA polymerase inhibitors, J. Med, Chem 48 (20) (2005) 6304–6314, https://doi.org/10.1021/jm0504454.
[101] A. Carta, M. Loriga, G. Paglietti, M. Ferrone, M. Fermeglia, S. Pricl, T. Sanna, C. Ibba, P. La Colla, R. Loddo, Design, synthesis, and preliminary in vitro and in silico antiviral activity of [4,7]phenantrolines and 1-oxo-1,4-dihydro-[4,7]phenantrolines against single-stranded positive-sense RNA genome viruses, Bioorg, Med, Chem 15 (5) (2007) 1914–1927, https://doi.org/10.1016/j.bmc.2007.01.005.
[102] M. Mazzei, E. Nieddu, M. Miele, A. Balbi, M. Ferrone, M. Fermeglia, MT. Mazzei, S. Pricl, P. La Colla, F. Marongiu, C. Ibba, R. Loddo, Activity of Mannich bases of 7-hydroxycoumarin against Flaviviridae, Bioorg, Med, Chem 16 (5) (2008) 2591–2605, https://doi.org/10.1016/j.bmc.2007.11.045.
[103] M. Tonelli, V. Boido, C. Canu, A. Sparatore, F. Sparatore, M.S. Paneni, M. Fermeglia, S. Pricl, P. La Colla, L. Casula, C. Ibba, D. Collu, R. Loddo, Antimicrobial and cytotoxic arylazoenamines. Part III: antiviral activity of selected classes of arylazoenamines, Bioorg, Med, Chem 16 (18) (2008) 8447–8465, https://doi.org/10.1016/j.bmc.2008.08.028.
[104] M. Tonelli, I. Vazzana, B. Tasso, V. Boido, F. Sparatore, M. Fermeglia, M. S. Paneni, P. Posocco, S. Pricl, P. La Colla, C. Ibba, B. Secci, G. Collu, R. Loddo, Antiviral and cytotoxic activities of aminoarylazo compounds and aryltriazene derivatives, Bioorg, Med, Chem 17 (13) (2009) 4425–4440, https://doi.org/10.1016/j.bmc.2009.05.020.
[105] M. Tonelli, V. Boido, P. Colla, R. Loddo, P. Posocco, M.S. Paneni, M. Fermeglia, S. Pricl, 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 18 (6) (2010) 2304–2316, https://doi.org/10.1016/j.bmc.2010.01.058.
[106] G. Giliberti, C. Ibba, E. Marongiu, R. Loddo, M. Tonelli, V. Boido, E. Laurini, P. Posocco, M. Fermeglia, S. Pricl, Synergistic experimental/computational studies on arylazoenamine derivatives that target the bovine viral diarrhea virus RNA-dependent RNA polymerase, Bioorg, Med, Chem 18 (16) (2010) 6055–6068, https://doi.org/10.1016/j.bmc.2010.06.065.
[107] A. Carta, M. Loriga, S. Piras, G. Paglietti, M. Ferrone, M. Fermeglia, S. Pricl, P. La Colla, G. Collu, T. Sanna, R. Loddo, Synthesis and in vitro evaluation of the anti-viral activity of N-[4-(1H/2H-benzotriazol-1/2-yl)phenyl]alkylcarboxamides: homology model of the Sabin 1 polio virus helicase, Med Chem (Angeles) 3 (6) (2007) 520–553, https://doi.org/10.2174/1573406410602060577.
[108] I. Briguglio, R. Loddo, E. Laurini, M. Fermeglia, S. Piras, P. Corona, P. Giunchedi, E. Gavini, G. Sanna, G. Giliberti, C. Ibba, P. Farci, P. La Colla, S. Pricl, A. Carta, Synthesis, cytotoxicity and antiviral evaluation of new series of imidazo[4,5-g] quinoline and pyrido[2,3-g]quinoxalinone derivatives, Eur. J. Med. Chem. 105 (2015) 63–79, https://doi.org/10.1016/j.ejmech.2015.10.002.
[109] A. Carta, G. Sanna, I. Briguglio, S. Madeddu, G. Vitale, S. Piras, P. Corona, AT. Peana, E. Laurini, M. Fermeglia, S. Pricl, A. Serra, E. Carta, R. Loddo, G. Giliberti, Quinoxaline derivatives as new inhibitors of coxsackievirus B5, Eur. J. Med. Chem. 145 (2018) 559–569, https://doi.org/10.1016/j.ejmech.2017.12.083.
[110] S. Piras, G. Sanna, A. Carta, P. Corona, R. Ibba, R. Loddo, S. Madeddu, P. Caria, S. Aulic, E. Laurini, M. Fermeglia, S. Pricl, Dichloro-phenyl-benzotriazoles: a new selective class of human respiratory syncytial virus entry inhibitors, Front. Chem. 7 (2019) 247, https://doi.org/10.3389/fchem.2019.00247.
[111] R. Loddo, V. Francesconi, E. Laurini, S. Boccardo, S. Aulic, M. Fermeglia, S. Pricl, M. Tonelli, 9-Aminoacridine-based agents impair the bovine viral diarrhea virus (BVDV) replication targeting the RNA-dependent RNA polymerase (RdRp), Bioorg, Med, Chem 26 (4) (2018) 855–868, https://doi.org/10.1016/j.bmc.2018.01.001.
[112] E. Banfi, G. Scialino, D. Zampieri, M.G. Mamolo, L. Vio, M. Ferrone, M. Fermeglia, M.S. Paneni, S. Pricl, Antifungal and antimycobacterial activity of new imidazole and triazole derivatives. A combined experimental and computational approach, J. Antimicrob. Chemother. 58 (1) (2006) 76–84, https://doi.org/10.1093/jac/dkl182.
[113] M.G. Mamolo, D. Zampieri, L. Vio, M. Fermeglia, M. Ferrone, S. Pricl, G. Scialino, E. Banfi, Antimycobacterial activity of new 3-substituted 5-(pyridin-4-yl)-3H-1,3,4-oxadiazol-2-one and 2-thione derivatives. Preliminary molecular modeling investigations, Bioorg, Med, Chem 13 (11) (2005) 3797–3809, https://doi.org/10.1016/j.bmc.2005.03.013.
[114] D. Zampieri, M.G. Mamolo, E. Laurini, M. Fermeglia, P. Posocco, S. Pricl, E. Banfi, G. Scialino, L. Vio, Antimycobacterial activity of new 3,5-disubstituted 1,3,4-oxadiazol-2(3H)-one derivatives. Molecular modeling investigations, Bioorg, Med, Chem 17 (13) (2009) 4693–4707, https://doi.org/10.1016/j.bmc.2009.04.055.
[115] A. Carta, A. Bua, P. Corona, S. Piras, I. Briguglio, P. Molicotti, S. Zanetti, E. Laurini, S. Aulic, M. Fermeglia, Pricl S. Design, synthesis and antitubercular activity of 4-alkoxy-triazoloquinolones able to inhibit the M. tuberculosis DNA gyrase, Eur. J. Med. Chem. 161 (2019) 399–415, https://doi.org/10.1016/j.ejmech.2018.10.031.
[116] D. Zampieri, E. Laurini, L. Vio, M. Fermeglia, S. Pricl, B. Wünsch, D. Schepmann, M.G. Mamolo, Improving selectivity preserving affinity: new piperidine-4-carboxamide derivatives as effective sigma-1-ligands, Eur. J. Med. Chem. 90 (2015) 797–808, https://doi.org/10.1016/j.ejmech.2014.12.018.

[117] D. Zampieri, M.G. Mamolo, E. Laurini, C. Florio, C. Zanette, M. Fermeglia, P. Posocco, M.S. Paneni, S. Pricl, L. Vio, Synthesis, biological evaluation, and three-dimensional in silico pharmacophore model for sigma(1) receptor ligands based on a series of substituted benzo[d]oxazol-2(3H)-one derivatives, J. Med, Chem 52 (17) (2009) 5380–5393, https://doi.org/10.1021/jm900366z.
[118] E. Laurini, D. Zampieri, MG. Mamolo, L. Vio, C. Zanette, C. Florio, P. Posocco, M. Fermeglia, S.A Pricl, 3D-pharmacophore model for sigma2 receptors based on a series of substituted benzo[d]oxazol-2(3H)-one derivatives, Bioorg, Med, Chem, Lett 20 (9) (2010) 2954–2957, https://doi.org/10.1016/j.bmcl.2010.03.009.
[119] E. Laurini, V. Dal Col, M.G. Mamolo, D. Zampieri, P. Posocco, M. Fermeglia, L. Vio, S. Pricl, Homology model and docking-based virtual screening for ligands of the σ1 receptor, ACS. Med. Chem. Lett. (11) (2011) 834–839, https://doi.org/10.1021/ml2001505.
[120] E. Laurini, D. Marson, V. Dal Col, M. Fermeglia, M.G. Mamolo, D. Zampieri, L. Vio, S. Pricl, Another brick in the wall. Validation of the σ1 receptor 3D model by computer-assisted design, synthesis, and activity of new σ1 ligands, Mol, Pharm 9 (11) (2012) 3107–3126, https://doi.org/10.1021/mp300233y.
[121] D. Rossi, A. Marra, P. Picconi, M. Serra, L. Catenacci, M. Sorrenti, E. Laurini, M. Fermeglia, S. Pricl, S. Brambilla, N. Almirante, M. Peviani, D. Curti, S. Collina, Identification of RC-33 as a potent and selective σ1 receptor agonist potentiating NGF-induced neurite outgrowth in PC12 cells. Part 2: g-scale synthesis, physicochemical characterization and in vitro metabolic stability, Bioorg, Med, Chem 21 (9) (2013) 2577–2586, https://doi.org/10.1016/j.bmc.2013.02.029.
[122] D. Rossi, A. Pedrali, R. Gaggeri, A. Marra, L. Pignataro, E. Laurini, V. Dal Col, M. Fermeglia, S. Pricl, D. Schepmann, B. Wünsch, M. Peviani, D. Curti, Collina S. Chemical, pharmacological, and in vitro metabolic stability studies on enantiomerically pure RC-33 compounds: promising neuroprotective agents acting as σ_1 receptor agonists, ChemMedChem. 8 (9) (2013) 1514–1527, https://doi.org/10.1002/cmdc.201300218.
[123] D. Zampieri, E. Laurini, L. Vio, S. Golob, M. Fermeglia, S. Pricl, M.G. Mamolo, Synthesis and receptor binding studies of some new arylcarboxamide derivatives as sigma-1 ligands, Bioorg, Med, Chem, Lett 24 (4) (2014) 1021–1025, https://doi.org/10.1016/j.bmcl.2014.01.032.
[124] S. Brune, D. Schepmann, KH. Klempnauer, D. Marson, V. Dal Col, E. Laurini, M. Fermeglia, B. Wünsch, S. Pricl, The sigma enigma: in vitro/in silico site-directed mutagenesis studies unveil σ1 receptor ligand binding, Biochemistry 53 (18) (2014) 2993–3003, https://doi.org/10.1021/bi401575g.
[125] D. Rossi, A. Marra, M. Rui, E. Laurini, M. Fermeglia, S. Pricl, D. Schepmann, B. Wünsch, M. Peviani, D. Curti, S. Collina, A step forward in the sigma enigma: a role for chirality in the sigma1 receptor–ligand interaction? Medchemcomm. 6 (2015) 138–146, https://doi.org/10.1039/C4MD00349G.
[126] F. Weber, S. Brune, F. Börgel, C. Lange, K. Korpis, P.J. Bednarski, E. Laurini, M. Fermeglia, S. Pricl, D. Schepmann, B. Wünsch, Rigidity versus flexibility: is this an issue in σ1 receptor ligand affinity and activity? J. Med, Chem 59 (11) (2016) 5505–5519, https://doi.org/10.1021/acs.jmedchem.6b00585.
[127] A.K. Kokornaczyk, D. Schepmann, J. Yamaguchi, K. Itami, E. Laurini, M. Fermeglia, S. Pricl, B. Wünsch, Thiazole-based σ1 receptor ligands: diversity by late-stage C-H arylation of thiazoles, structure-affinity and selectivity relationships, and molecular interactions, ChemMedChem. 12 (13) (2017) 1070–1080, https://doi.org/10.1002/cmdc.201700166.
[128] E. Laurini, D. Marson, S. Aulic, M. Fermeglia, S. Pricl, Computational alanine scanning and structural analysis of the SARS-CoV-2 spike/ACE2 complex, ACS. Nano 14 (9) (2020) 11821–11830, https://doi.org/10.1021/acsnano.0c04674.
[129] L. Metullio, M. Ferrone, A. Coslanich, S. Fuchs, M. Fermeglia, M.S. Paneni, Pricl S. Polyamidoamine, yet not PAMAM) dendrimers as bioinspired materials for drug delivery: structure-activity relationships by molecular simulations, Biomacromolecules. 5 (4) (2004) 1371–1378, https://doi.org/10.1021/bm049858x.
[130] X. Liu, J. Wu, M. Yammine, J. Zhou, P. Posocco, S. Viel, C. Liu, F. Ziarelli, M. Fermeglia, S. Pricl, G. Victorero, C. Nguyen, P. Erbacher, J.P. Behr, L. Peng, Structurally flexible triethanolamine core PAMAM dendrimers are effective nanovectors for DNA transfection in vitro and in vivo to the mouse thymus, Bioconjug, Chem 22 (12) (2011) 2461–2473, https://doi.org/10.1021/bc200275g.
[131] P. Posocco, X. Liu, E. Laurini, D. Marson, C. Chen, C. Liu, M. Fermeglia, P. Rocchi, S. Pricl, L. Peng, Impact of siRNA overhangs for dendrimer-mediated siRNA delivery and gene silencing, Mol, Pharm 10 (8) (2013) 3262–3273, https://doi.org/10.1021/mp400329g.
[132] S.P. Jones, N.P. Gabrielson, C.H. Wong, H.F. Chow, D.W. Pack, P. Posocco, M. Fermeglia, S. Pricl, D.K. Smith, Hydrophobically modified dendrons: developing structure-activity relationships for DNA binding and gene transfection, Mol, Pharm 8 (2) (2011) 416–429, https://doi.org/10.1021/mp100260c.
[133] C. Chen, P. Posocco, X. Liu, Q. Cheng, E. Laurini, J. Zhou, C. Liu, Y. Wang, J. Tang, V. Dal Col, T. Yu, S. Giorgio, M. Fermeglia, F. Qu, Z. Liang, J.J. Rossi, M. Liu, P. Rocchi, S. Pricl, L. Peng, Mastering dendrimer self-assembly for efficient siRNA delivery: from conceptual design to in vivo efficient gene silencing, Small. 12 (27) (2016) 3667–3676, https://doi.org/10.1002/smll.201503866.
[134] T. Wei, C. Chen, J. Liu, C. Liu, P. Posocco, X. Liu, Q. Cheng, S. Huo, Z. Liang, M. Fermeglia, S. Pricl, X.J. Liang, P. Rocchi, L. Peng, Anticancer drug nanomicelles formed by self-assembling amphiphilic dendrimer to combat cancer drug resistance, Proc. Natl. Acad. Sci. U. S. A. 112 (10) (2015) 2978–2983, https://doi.org/10.1073/pnas.1418494112.
[135] A. Barnard, P. Posocco, M. Fermeglia, A. Tschiche, M. Calderon, S. Pricl, DK. Smith, Double-degradable responsive self-assembled multivalent arrays–temporary nanoscale recognition between dendrons and DNA, Org, Biomol, Chem 12 (3) (2013) 446–455, https://doi.org/10.1039/c3ob42202j.
[136] M.F. Ottaviani, M. Cangiotti, A. Fattori, C. Coppola, P. Posocco, E. Laurini, X. Liu, M. Fermeglia, L. Peng, Pricl S. Copper(ii) binding to flexible triethanolamine-core PAMAM dendrimers: a combined experimental/in silico approach, Phys. Chem. Chem. Phys. 16 (2013) 685–694, https://doi.org/10.1039/C3CP54005G.
[137] S.M. Bromfield, A. Barnard, P. Posocco, M. Fermeglia, S. Pricl, D.K. Smith, Mallard blue: a high-affinity selective heparin sensor that operates in highly competitive media, J. Am, Chem, Soc 135 (8) (2013) 2911–2914, https://doi.org/10.1021/ja311734d.
[138] S.M. Bromfield, P. Posocco, M. Fermeglia, S. Pricl, J. Rodriguez-Lopez, D. K. Smith, A simple new competition assay for heparin binding in serum applied to multivalent PAMAM dendrimers, Chem. Commun. 49 (2013) 4830–4832, https://doi.org/10.1039/C3CC41251B.
[139] S.M. Bromfield, P. Posocco, M. Fermeglia, J. Tolosa, A. Herreros-Lopez, S. Pricl, J. Rodríguez-Lopez, D.K. Smith, Shape-persistent and adaptive multivalency: rigid transgeden (TGD) and flexible PAMAM dendrimers for heparin binding, Chem. (Easton) 20 (31) (2014) 9666–9674, https://doi.org/10.1002/chem.201402237.
[140] D. Marson, E. Laurini, M. Fermeglia, D.K. Smith, Pricl S. Mallard, Blue binding to heparin, its SDS micelle-driven de-complexation, and interaction with human serum albumin: A combined experimental/modeling investigation, Fluid Ph. Equilib 470 (2018) 259–267.
[141] E. Laurini, D. Marson, P. Posocco, M. Fermeglia, S. Pricl, Structure and binding thermodynamics of viologen-phosphorous dendrimers to human serum albumin: A combined computational/experimental investigation, Fluid Ph. Equilib 422 (2016) 18–31, https://doi.org/10.1016/j.fluid.2016.02.014.
[142] Z. Beiranvand, F. Bani, A. Kakanejadifard, E. Laurini, M. Fermeglia, S. Pricl, M. Adeli, Drug delivery systems based on specific interactions between albumin and polyglycerol, RSC. Adv. 6 (2016) 11266–11277, https://doi.org/10.1039/C5RA25463A.
[143] D. Marson, E. Laurini, P. Posocco, M. Fermeglia, S. Pricl, Cationic carbosilane dendrimers and oligonucleotide binding: an energetic affair, Nanoscale 7 (2015) 3876–3887, https://doi.org/10.1039/C4NR04510F.
[144] S. Pricl, M. Ferrone, M. Fermeglia, F. Amato, C. Cosentino, MM. Cheng, R. Walczak, M. Ferrari, Multiscale modeling of protein transport in silicon membrane nanochannels. Part 1. Derivation of molecular parameters from computer simulations, Biomed. MicroDevices 8 (4) (2006) 277–290, https://doi.org/10.1007/s10544-006-0031-2.
[145] F. Amato, C. Cosentino, S. Pricl, M. Ferrone, M. Fermeglia, MM. Cheng, R. Walczak, M. Ferrari, Multiscale modeling of protein transport in silicon membrane nanochannels. Part 2. From molecular parameters to a predictive continuum diffusion model, Biomed. MicroDevices 8 (4) (2006) 291–298, https://doi.org/10.1007/s10544-006-0032-1.
[146] A. Mio, D. Marson, G. Cavalieri, M. Fermeglia, E. Laurini, S. Pricl, Beyond the veil: free energy profiles and partition coefficients for antimelanoma drugs in self-assembled nanomicelles via COSMOmic and atomistic molecular dynamics simulations, J. Chem. Eng. Data 69 (10) (2024) 3450–3461, https://doi.org/10.1021/acs.jced.4c00076.
[147] S. Pricl, M. Fermeglia, M. Ferrone, E. Tamborini, T315I-mutated bcr-abl in chronic myeloid leukemia and imatinib: insights from a computational study, Mol, Cancer Ther 4 (8) (2005) 1167–1174, https://doi.org/10.1158/1535-7163.MCT-05-0101.
[148] E. Tamborini, S. Pricl, T. Negri, M.S. Lagonigro, F. Miselli, A. Greco, A. Gronchi, P.G. Casali, M. Ferrone, M. Fermeglia, A. Carbone, M.A. Pierotti, S. Pilotti, Functional analyses and molecular modeling of two c-kit mutations responsible for imatinib secondary resistance in GIST patients, Oncogene 25 (45) (2006) 6140–6146, https://doi.org/10.1038/sj.onc.1209639.
[149] T. Negri, G.M. Pavan, E. Virdis, A. Greco, M. Fermeglia, M. Sandri, S. Pricl, M. A. Pierotti, S. Pilotti, E. Tamborini, T670X KIT mutations in gastrointestinal stromal tumors: making sense of missense, J. Natl, Cancer Inst 101 (3) (2009) 194–204, https://doi.org/10.1093/jnci/djn477.
[150] S.E. Woodman, J.C. Trent, K. Stemke-Hale, A.J. Lazar, S. Pricl, G.M. Pavan, M. Fermeglia, Y.N. Gopal, D. Yang, D.A. Podoloff, D. Ivan, K.B. Kim, N. Papadopoulos, P. Hwu, G.B. Mills, M.A. Davies, Activity of dasatinib against L576P KIT mutant melanoma: molecular, cellular, and clinical correlates, Mol, Cancer Ther 8 (8) (2009) 2079–2085, https://doi.org/10.1158/1535-7163.MCT-09-0459.
[151] E. Conca, T. Negri, A. Gronchi, E. Fumagalli, E. Tamborini, G.M. Pavan, M. Fermeglia, M.A. Pierotti, S. Pricl, S. Pilotti, Activate and resist: L576P-KIT in GIST, Mol, Cancer Ther 8 (9) (2009) 2491–2495, https://doi.org/10.1158/1535-7163.MCT-09-0662.
[152] E. Conca, C. Miranda, V. Dal Col, E. Fumagalli, G. Pelosi, M. Mazzoni, M. Fermeglia, E. Laurini, MA. Pierotti, S. Pilotti, A. Greco, S. Pricl, E. Tamborini, Are two better than one? A novel double-mutant KIT in GIST that responds to Imatinib, Mol. Oncol. 7 (4) (2013) 756–762, https://doi.org/10.1016/j.molonc.2013.02.019.
[153] V. Perfetti, E. Laurini, S. Aulic, M. Fermeglia, R. Riboni, M. Lucioni, E. Dallera, S. Delfanti, L. Pugliese, F.S. Latteri, A. Pietrabissa, S. Pricl, Molecular and functional characterization of a new 3′ end KIT juxtamembrane deletion in a duodenal GIST treated with neoadjuvant Imatinib, Oncotarget. 8 (34) (2017) 56158–56167, https://doi.org/10.18632/oncotarget.19341.
[154] E. Laurini, P. Posocco, M. Fermeglia, D.L. Gibbons, 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. 7 (5) (2013) 968–975, https://doi.org/10.1016/j.molonc.2013.06.001.

[155] D.L. Gibbons, S. Pricl, P. Posocco, E. Laurini, M. Fermeglia, H. Sun, M. Talpaz, N. Donato, A. Quintas-Cardama, Molecular dynamics reveal BCR-ABL1 polymutants as a unique mechanism of resistance to PAN-BCR-ABL1 kinase inhibitor therapy, Proc. Natl. Acad. Sci. U. S. A. 111 (9) (2014) 3550–3555, https://doi.org/10.1073/pnas.1321173111.

[156] M. Ferrone, F. Perrone, E. Tamborini, M.S. Paneni, M. Fermeglia, S. Suardi, E. Pastore, D. Delia, M.A. Pierotti, S. Pricl, S. Pilotti, Functional analysis and molecular modeling show a preserved wild-type activity of p53(C238Y), Mol, Cancer Ther 5 (6) (2006) 1467–1473, https://doi.org/10.1158/1535-7163.MCT-06-0012.

[157] S. Pricl, B. Cortelazzi, V. Dal Col, D. Marson, E. Laurini, M. Fermeglia, L. Licitra, S. Pilotti, P. Bossi, Perrone F. Smoothened, SMO) receptor mutations dictate resistance to vismodegib in basal cell carcinoma, Mol. Oncol. 9 (2) (2015) 389–397, https://doi.org/10.1016/j.molonc.2014.09.003.

[158] A. Carta, I. Briguglio, S. Piras, G. Boatto, P. La Colla, R. Loddo, M. Tolomeo, S. Grimaudo, A. Di Cristina, R.M. Pipitone, E. Laurini, M.S. Paneni, P. Posocco, M. Fermeglia, S. Pricl, 3-Aryl-2-[1H-benzotriazol-1-yl]acrylonitriles: a novel class of potent tubulin inhibitors, Eur. J. Med. Chem. 46 (9) (2011) 4151–4167, https://doi.org/10.1016/j.ejmech.2011.06.018.

[159] I. Briguglio, E. Laurini, M.A. Pirisi, S. Piras, P. Corona, M. Fermeglia, S. Pricl, A. Carta, Triazolopyridinyl-acrylonitrile derivatives as antimicrotubule agents: synthesis, in vitro and in silico characterization of antiproliferative activity, inhibition of tubulin polymerization and binding thermodynamics, Eur. J. Med. Chem. 141 (2017) 460–472, https://doi.org/10.1016/j.ejmech.2017.09.065.

[160] L. Brambilla, D. Genini, E. Laurini, J. Merulla, L. Perez, M. Fermeglia, G. M. Carbone, S. Pricl, C.V. Catapano, Hitting the right spot: mechanism of action of OPB-31121, a novel and potent inhibitor of the signal transducer and activator of transcription 3 (STAT3), Mol. Oncol. 9 (6) (2015) 1194–1206, https://doi.org/10.1016/j.molonc.2015.02.012.

[161] H. Ziouziou, C. Andrieu, E. Laurini, S. Karaki, M. Fermeglia, R. Oueslati, D. Taieb, M. Camplo, O. Siri, S. Pricl, M. Katsogiannou, P. Rocchi, Targeting Hsp27/eIF4E interaction with phenazine compound: a promising alternative for castration-resistant prostate cancer treatment, Oncotarget. 8 (44) (2017) 77317–77329, https://doi.org/10.18632/oncotarget.20469.

[162] C. Colombo, A. Belfiore, N. Paielli, L. De Cecco, S. Canevari, E. Laurini, M. Fermeglia, S. Pricl, P. Verderio, S. Bottelli, M. Fiore, S. Stacchiotti, E. Palassini, A. Gronchi, S. Pilotti, Perrone F. β-catenin in desmoid-type fibromatosis: deep insights into the role of T41A and S45F mutations on protein structure and gene expression, Mol. Oncol. 11 (11) (2017) 1495–1507, https://doi.org/10.1002/1878-0261.12101.

[163] X. Liu, H. Chen, E. Laurini, Y. Wang, V. Dal Col, P. Posocco, F. Ziarelli, M. Fermeglia, C.C. Zhang, S. Pricl, L. Peng, 2-difluoromethylene-4-methylenepentanoic acid, a paradoxical probe able to mimic the signaling role of 2-oxoglutaric acid in cyanobacteria, Org, Lett 13 (11) (2011) 2924–2927, https://doi.org/10.1021/ol2009544.

[164] X. Liu, Y. Wang, E. Laurini, P. Posocco, H. Chen, F. Ziarelli, A. Janicki, F. Qu, M. Fermeglia, S. Pricl, C.C. Zhang, L. Peng, Structural requirements of 2-oxoglutaric acid analogues to mimic its signaling function, Org, Lett 15 (18) (2013) 4662–4665, https://doi.org/10.1021/ol401914z.

[165] Y. Wang, X. Liu, E. Laurini, P. Posocco, F. Ziarelli, M. Fermeglia, F. Qu, S. Pricl, C. C. Zhang, L. Peng, Mimicking the 2-oxoglutaric acid signalling function using molecular probes: insights from structural and functional investigations, Org, Biomol, Chem 12 (26) (2014) 4723–4729, https://doi.org/10.1039/c4ob00630e.

[166] G. de Simon, F. Parodi, M. Fermeglia, R. Taccani, Simulation of process for electrical energy production based on molten carbonate fuel cells, J. Power. Sources. 115 (2) (2003) 210–218, https://doi.org/10.1016/S0378-7753(02)00728-0.

[167] G. Donolo, G.D. De Simon, M. Fermeglia, Steady state simulation of energy production from biomass by molten carbonate fuel cells, J. Power. Sources. 158 (2) (2006) 1282–1289, https://doi.org/10.1016/j.jpowsour.2005.10.045.

[168] E. Barbera, A. Mio, A. Massi Pavan, A. Bertucco, M. Fermeglia, Fuelling power plants by natural gas: an analysis of energy efficiency, economical aspects and environmental footprint based on detailed process simulation of the whole carbon capture and storage system, Energy Convers. Manag. 252 (2022) 115072, https://doi.org/10.1016/j.enconman.2021.115072.

[169] M. Fermeglia, V. Lughi, A. Massi Pavan, How to avoid the perfect storm: the role of energy and photovoltaics, MRS Energy Sustain. 7 (1) (2020) E34, https://doi.org/10.1557/mre.2020.36.

[170] M. Fermeglia, G. Longo, L. Petrescu, COWAR: A CAPE OPEN software module for the evaluation of process sustainability, Environ. Prog. 27 (3) (2008) 373–382, https://doi.org/10.1002/ep.10262.

[171] A. Mio, P. Limleamthong, G. Guillén-Gosálbez, M. Fermeglia, Sustainability evaluation of alternative routes for fine chemicals production in an early stage of process design adopting process simulation along with data envelopment analysis, Ind. Eng. Chem. Res. 57 (23) (2018) 7946–7960, https://doi.org/10.1021/acs.iecr.7b05126.

[172] L. Petrescu, S. Burca, M. Fermeglia, A. Mio, C.C. Cormo, Process simulation coupled with LCA for the evaluation of liquid–liquid extraction processes of phenol from aqueous streams, J. Water Process Eng. 4 (2021) 102077, https://doi.org/10.1016/j.jwpe.2021.102077.

[173] A. Mio, E. Barbera, A. Massi Pavan, R. Danielis, A. Bertucco, M. Fermeglia, Analysis of the energetic, economic, and environmental performance of hydrogen utilization for port logistic activities, Appl. Energy 347 (2023) 121431, https://doi.org/10.1016/j.apenergy.2023.121431.

[174] A. Mio, E. Barbera, A. Massi Pavan, A. Bertucco, M. Fermeglia, Sustainability analysis of hydrogen production processes, Int J Hydrog. Energy 54 (2024) 540–553, https://doi.org/10.1016/j.ijhydene.2023.06.122.

[175] A. Vujanovic, A. Mio, R. Pucnik, N. Blasuttigh, D. Krajnc, M. Fermeglia, The environmental and biodiversity impacts of a new cableway system: A comprehensive life cycle assessment, J. Clean. Prod. 482 (2024) 144201, https://doi.org/10.1016/j.jclepro.2024.144201.