## **Rafel Prohens**

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Oxyma: An Efficient Additive for Peptide Synthesis to Replace the Benzotriazoleâ€Based HOBt and HOAt with a Lower Risk of Explosion <sup>[1]</sup> . Chemistry - A European Journal, 2009, 15, 9394-9403.	1.7	326
2	COMU: A Safer and More Effective Replacement for Benzotriazoleâ€Based Uronium Coupling Reagents. Chemistry - A European Journal, 2009, 15, 9404-9416.	1.7	260
3	Virtual cocrystal screening. Chemical Science, 2011, 2, 883.	3.7	245
4	Squaramido-based receptors: Molecular recognition of carboxylate anions in highly competitive media. Tetrahedron Letters, 1998, 39, 1063-1066.	0.7	88
5	A squaramide fluorescent ensemble for monitoring sulfate in water. Chemical Communications, 2001, , 1456-1457.	2.2	77
6	Squaramido-Based Receptors:Â Design, Synthesis, and Application to the Recognition of Tetraalkylammonium Compounds. Journal of Organic Chemistry, 1996, 61, 9394-9401.	1.7	73
7	A theoretical study of aromaticity in squaramide complexes with anions. Chemical Physics Letters, 2002, 351, 115-120.	1.2	57
8	Application of heparin as a dual agent with antimalarial and liposome targeting activities toward Plasmodium-infected red blood cells. Nanomedicine: Nanotechnology, Biology, and Medicine, 2014, 10, 1719-1728.	1.7	55
9	Polymorphism of Norfloxacin:  Evidence of the Enantiotropic Relationship between Polymorphs A and B. Crystal Growth and Design, 2006, 6, 1463-1467.	1.4	52
10	An Effective Fluorescent Sensor for Choline-Containing Phospholipids. Angewandte Chemie - International Edition, 1999, 38, 2208-2211.	7.2	49
11	Virtual Screening Identifies New Cocrystals of Nalidixic Acid. Crystal Growth and Design, 2014, 14, 1749-1755.	1.4	49
12	Adaptation of targeted nanocarriers to changing requirements in antimalarial drug delivery. Nanomedicine: Nanotechnology, Biology, and Medicine, 2017, 13, 515-525.	1.7	49
13	A new polymorph of Norfloxacin. Journal of Thermal Analysis and Calorimetry, 2007, 89, 687-692.	2.0	46
14	Thermodynamic characterization of the squaramide–carboxylate interaction in squaramide receptors. Tetrahedron Letters, 2001, 42, 4933-4936.	0.7	44
15	Thermodynamics of Cd2+ and Zn2+ binding by the phytochelatin (γ-Glu-Cys)4-Gly and its precursor glutathione. Analytical Biochemistry, 2008, 375, 82-89.	1.1	41
16	Modulation of Reactivity in the Cavity of Liposomes Promotes the Formation of Peptide Bonds. Journal of the American Chemical Society, 2015, 137, 12269-12275.	6.6	39
17	Cocrystals of spironolactone and griseofulvin based on an in silico screening method. CrystEngComm, 2017, 19, 3592-3599.	1.3	39
18	Competitive Binding of Cd and Zn with the Phytochelatin (γ-Clu-Cys) <sub>4</sub> -Gly: Comparative Study by Mass Spectrometry, Voltammetry-Multivariate Curve Resolution, and Isothermal Titration Calorimetry. Environmental Science & Technology, 2008, 42, 2860-2866.	4.6	38

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19	Polymorphism of Cocrystals: The Promiscuous Behavior of Agomelatine. Crystal Growth and Design, 2016, 16, 1063-1070.	1.4	38
20	Combined Virtual/Experimental Multicomponent Solid Forms Screening of Sildenafil: New Salts, Cocrystals, and Hybrid Salt–Cocrystals. Crystal Growth and Design, 2018, 18, 7618-7627.	1.4	35
21	H-Bonded anion–anion complex trapped in a squaramido-based receptor. Chemical Communications, 2018, 54, 1841-1844.	2.2	32
22	Molecular Architecture of the Mn2+-dependent Lactonase UlaG Reveals an RNase-like Metallo-β-lactamase Fold and a Novel Quaternary Structure. Journal of Molecular Biology, 2010, 398, 715-729.	2.0	31
23	Quaternary Structural Transitions in the DeoR-Type Repressor UlaR Control Transcriptional Readout from the <scp>l</scp> -Ascorbate Utilization Regulon in <i>Escherichia coli</i> . Biochemistry, 2008, 47, 11424-11433.	1.2	30
24	Kâ€Oxyma: a Strong Acylationâ€Promoting, 2â€CTC Resinâ€Friendly Coupling Additive. European Journal of Organic Chemistry, 2013, 2013, 6372-6378.	1.2	29
25	New polymorphic hydrogen bonding donor–acceptor system with two temperature coincident solid–solid transitions. CrystEngComm, 2009, 11, 52-54.	1.3	27
26	H-Bonded anion–anion complexes in fentanyl citrate polymorphs and solvates. Chemical Communications, 2019, 55, 115-118.	2.2	26
27	Experimental and Theoretical Study of Aromaticity Effects in the Solid State Architecture on Squaric Acid Derivatives. Crystal Growth and Design, 2014, 14, 2578-2587.	1.4	24
28	DNA structure directs positioning of the mitochondrial genome packaging protein Abf2p. Nucleic Acids Research, 2017, 45, 951-967.	6.5	23
29	Effect of Preorganization on the Polymorphism and Cocrystallization of a Squaramide Compound. Crystal Growth and Design, 2012, 12, 4548-4553.	1.4	22
30	Cooperative induction in double H-bonding donor/acceptor compounds: Chains vs. ribbons. CrystEngComm, 2012, 14, 5745.	1.3	22
31	The Ca2+–EDTA chelation as standard reaction to validate Isothermal Titration Calorimeter measurements (ITC). Talanta, 2016, 154, 354-359.	2.9	22
32	Calorimetric Studies of Binary and Ternary Molecular Interactions between Transthyretin, Aβ Peptides, and Small-Molecule Chaperones toward an Alternative Strategy for Alzheimer's Disease Drug Discovery. Journal of Medicinal Chemistry, 2020, 63, 3205-3214.	2.9	22
33	A Novel, Extremely Bioavailable Cocrystal of Pterostilbene. Crystal Growth and Design, 2021, 21, 2315-2323.	1.4	22
34	Ziprasidone malate, a new trimorphic salt with improved aqueous solubility. CrystEngComm, 2009, 11, 791.	1.3	21
35	Solid form and solubility. CrystEngComm, 2017, 19, 23-26.	1.3	19
36	DFT Analysis of Uncommon π···H-Bond Array Interaction in a New Pterostilbene/Theophylline Cocrystal. Crystal Growth and Design, 2020, 20, 6691-6698.	1.4	19

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37	Revisiting the Solid State of Norfloxacin. Crystal Growth and Design, 2010, 10, 2948-2953.	1.4	18
38	Safety Evaluation of an Unexpected Incident with a Nitro Compound. Organic Process Research and Development, 2007, 11, 1131-1134.	1.3	17
39	Cooperativity in Solid-State Squaramides. Crystal Growth and Design, 2011, 11, 3725-3730.	1.4	17
40	Self-Assembling of Zwitterionic Squaramides through Electrostatically Compressed Face-to-Face Ï€-Stacking: A New Supramolecular Synthon. Crystal Growth and Design, 2013, 13, 4200-4203.	1.4	17
41	Polymorphism of Sildenafil: A New Metastable Desolvate. Crystal Growth and Design, 2018, 18, 3740-3746.	1.4	17
42	DNA specificities modulate the binding of human transcription factor A to mitochondrial DNA control region. Nucleic Acids Research, 2019, 47, 6519-6537.	6.5	17
43	New Cocrystal of Ubiquinol with High Stability to Oxidation. Crystal Growth and Design, 2020, 20, 5583-5588.	1.4	16
44	Synthesis and Characterization of a New Norfloxacin/Resorcinol Cocrystal with Enhanced Solubility and Dissolution Profile. Pharmaceutics, 2022, 14, 49.	2.0	16
45	Single-Stranded Molecular Helical Assembly from a Self-Complementary Squaramide Compound. Crystal Growth and Design, 2014, 14, 397-400.	1.4	15
46	Sildenafil–Resorcinol Cocrystal: XRPD Structure and DFT Calculations. Crystals, 2020, 10, 1126.	1.0	15
47	Targeting transthyretin in Alzheimer's disease: Drug discovery of small-molecule chaperones as disease-modifying drug candidates for Alzheimer's disease. European Journal of Medicinal Chemistry, 2021, 226, 113847.	2.6	15
48	Polymorphism in secondary squaramides: on the importance of π-interactions involving the four membered ring. CrystEngComm, 2018, 20, 237-244.	1.3	14
49	Experimental and theoretical study of weak intermolecular interactions in crystalline tertiary squaramides. CrystEngComm, 2016, 18, 6437-6443.	1.3	13
50	Water wires in the nanoporous form II of carbamazepine: a single-crystal X-ray diffraction analysis. CrystEngComm, 2013, 15, 845-847.	1.3	12
51	Morphotropism and "Quasi-Isostructurality―in the Three High Z′ Concomitant Polymorphs of Efinaconazole. Crystal Growth and Design, 2020, 20, 4238-4242.	1.4	11
52	A New and Highly Stable Cocrystal of Vitamin D3 for Use in Enhanced Food Supplements. Crystal Growth and Design, 2021, 21, 1418-1423.	1.4	11
53	A cocrystal is the key intermediates for the production of a new polymorph of Vorinostat. CrystEngComm, 2012, 14, 362-365.	1.3	10
54	Gallic Acid Dimer As a Double π–Hole Donor: Evidence from X-ray, Theoretical Calculations, and Generalization from the Cambridge Structural Database. Crystal Growth and Design, 2019, 19, 3989-3997.	1.4	10

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55	Hydrogen Bond Polarization Overcomes Unfavorable Packing in the Most Stable High Z′ Polymorph of Pterostilbene. Crystal Growth and Design, 2019, 19, 2552-2556.	1.4	10
56	A late appearing polymorph of nutraceutical pterostilbene. CrystEngComm, 2020, 22, 4680-4684.	1.3	10
57	Polymorphism in the 1/1 Pterostilbene/Picolinic Acid Cocrystal. Crystal Growth and Design, 2022, 22, 590-597.	1.4	10
58	X-Ray structure of the 1:1 complex of a tripodal receptor and cis-cyclohexane-1,3,5-tricarboxylic acid. Chemical Communications, 1997, , 357-358.	2.2	9
59	Two New Polymorphic Cocrystals of Zafirlukast: Preparation, Crystal Structure, and Stability Relations. Crystal Growth and Design, 2015, 15, 4162-4169.	1.4	9
60	Expanding the Crystal Form Landscape of the Antiviral Drug Adefovir Dipivoxil. Crystal Growth and Design, 2015, 15, 475-484.	1.4	9
61	A combined crystallographic and theoretical study of weak intermolecular interactions in crystalline squaric acid esters and amides. CrystEngComm, 2017, 19, 3071-3077.	1.3	9
62	Hydrogen bonding <i>versus</i> π-interactions: their key competition in sildenafil solvates. CrystEngComm, 2018, 20, 4526-4530.	1.3	9
63	Novel Polymorphic Cocrystals of the Non-Steroidal Anti-Inflammatory Drug Niflumic Acid: Expanding the Pharmaceutical Landscape. Pharmaceutics, 2021, 13, 2140.	2.0	9
64	Mechanistic Understanding of Competitive Destabilization of Carbamazepine Cocrystals under Solvent Free Conditions. Crystal Growth and Design, 2020, 20, 6024-6029.	1.4	7
65	Combination of chemometrically assisted voltammetry, calorimetry, and circular dichroism as a new method for the study of bioinorganic substances: application to selenocystine metal complexes. Journal of Biological Inorganic Chemistry, 2012, 17, 321-329.	1.1	6
66	Crystal structure solution of an elusive polymorph of Dibenzylsquaramide. Powder Diffraction, 2013, 28, S470-S480.	0.4	6
67	Property prediction and pharmacokinetic evaluation of mixed stoichiometry cocrystals of zafirlukast, a drug delivery case study. CrystEngComm, 2018, 20, 1346-1351.	1.3	6
68	The Solid State Landscape of the Sildenafil Drug. Journal of Pharmaceutical Sciences, 2022, 111, 1104-1109.	1.6	6
69	Solid-State Competitive Destabilization of Caffeine Malonic Acid Cocrystal: Mechanistic and Kinetic Investigations. Crystal Growth and Design, 2020, 20, 7598-7605.	1.4	5
70	Polymorphism of (S)-triphenylglycol: kinetic dependent transformation of a new multipolymorphic system. Chemical Communications, 2007, , 3538.	2.2	4
71	An improved methodology to compute surface site interaction points using high density molecular electrostatic potential surfaces. Journal of Computational Chemistry, 2018, 39, 2371-2377	1.5	4
72	An Assay for Screening Potential Drug Candidates for Alzheimer's Disease That Act as Chaperones of the Transthyretin and Amyloidâ€i² Peptides Interaction. Chemistry - A European Journal, 2020, 26, 17462-17469.	1.7	4

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73	Crystal engineering of nutraceutical phytosterols: new cocrystal solid solutions. CrystEngComm, 2020, 22, 4210-4214.	1.3	4
74	Assembling the Puzzle of Apixaban Solid Forms. Molecular Pharmaceutics, 2018, 15, 1909-1916.	2.3	3
75	Computational screens can speed up the discovery of pharmaceutical cocrystals. ADMET and DMPK, 2018, 6, 284-287.	1.1	3
76	Static discrete disorder in the crystal structure of iododiflunisal: on the importance of hydrogen bond, halogen bond and π-stacking interactions. CrystEngComm, 0, , .	1.3	3
77	A surface site interaction point methodology for macromolecules and huge molecular databases. Journal of Computational Chemistry, 2017, 38, 419-426.	1.5	2
78	Derisking Development by a Cocrystallization Screen of a Novel Selective Inhaled JAK-STAT inhibitor. Crystal Growth and Design, 2019, 19, 403-414.	1.4	2
79	Potentiometric CheqSol and standardized shake-flask solubility methods are complimentary tools in physicochemical profiling. European Journal of Pharmaceutical Sciences, 2020, 148, 105305.	1.9	2
80	Combined crystallographic and computational investigation of the solvent disorder present in a new tipiracil hydrochloride methanol solvate–hydrate. CrystEngComm, 0, , .	1.3	1
81	Revision of the Crystal Structure of the Orthorhombic Polymorph of Oxyma: On the Importance of π–Hole Interactions and Their Interplay with H–Bonds. Crystals, 2022, 12, 823.	1.0	1