

# Itzia Irene Padilla-Martinez

## List of Publications by Citations

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papers

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20  
g-index

97  
ext. papers

781  
ext. citations

3.2  
avg, IF

3.58  
L-index

#	Paper	IF	Citations
90	π-Stacking Interactions and CH...X (X = O, Aryl) Hydrogen Bonding as Directing Features of the Supramolecular Self-Association in 3-Carboxy and 3-Amido Coumarin Derivatives. <i>Crystal Growth and Design</i> , <b>2003</b> , 3, 35-45	3.5	60
89	Azolyborane adducts. Structural and conformational analysis by x-ray diffraction and NMR. Protic-hydric (C?H...-B) and Protic-Fluoride (C?H...-F) interactions. <i>Chemische Berichte</i> , <b>1996</b> , 129, 441-449		45
88	Synthesis and Reactivity of [Ir(C <sub>2</sub> H <sub>4</sub> ) <sub>2</sub> TpmMe <sub>2</sub> ]PF <sub>6</sub> (TpmMe <sub>2</sub> = Tris(3,5-dimethylpyrazolyl)methane): Comparison with the Analogous TpMe <sub>2</sub> Derivatives (TpMe <sub>2</sub> = Hydrotris(3,5-dimethylpyrazolyl)borate). <i>Organometallics</i> , <b>2002</b> , 21, 93-104	3.8	31
87	New Imidazole Derivatives: Dimers of Carbene-Borane Adducts. <i>European Journal of Inorganic Chemistry</i> , <b>1998</b> , 1998, 1547-1553	2.3	26
86	NMR Study of isolobal N-CH <sub>3</sub> <sup>+</sup> , N-BH <sub>3</sub> and N-BF <sub>3</sub> imidazole derivatives. <i>Magnetic Resonance in Chemistry</i> , <b>1993</b> , 31, 189-193	2.1	25
85	N-(2-hydroxyphenyl)-2-propylpentanamide, a valproic acid aryl derivative designed in silico with improved anti-proliferative activity in HeLa, rhabdomyosarcoma and breast cancer cells. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , <b>2016</b> , 31, 140-149	5.6	25
84	From Azole-Borane Adducts to Azaboles [Molecular Structure of an Imidazole. <i>Chemische Berichte</i> , <b>1994</b> , 127, 343-346		22
83	Carbonyl-carbonyl, carbonyl-π and carbonyl-halogen dipolar interactions as the directing motifs of the supramolecular structure of ethyl 6-chloro-2-oxo-2H-chromene-3-carboxylate and ethyl 6-bromo-2-oxo-2H-chromene-3-carboxylate. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , <b>2007</b> , 63, 0239-42		20
82	Design of multi-target compounds as AChE, BACE1, and amyloid-β(1-42) oligomerization inhibitors: in silico and in vitro studies. <i>Journal of Alzheimers Disease</i> , <b>2014</b> , 41, 1073-85	4.3	18
81	Synthesis and Crystal Structure of Iridium-1,4-benzoquinone Complexes of Tris(3,5-dimethylpyrazolyl)methane Ligand: Decarbonylation, Protonation, and Substitution Reactions. <i>Organometallics</i> , <b>2012</b> , 31, 5438-5451	3.8	16
80	Competition between OH...O and multiple halogen...dipole interactions on the formation of intramolecular three-centred hydrogen bond in 3-acyl coumarins. <i>CrystEngComm</i> , <b>2009</b> , 11, 1451	3.3	16
79	9-(2-Methylphenyl)-3,4,5,6,9,10-hexa-hydroxanthene-1,8(2H,7H)-dione. <i>Journal of Chemical Crystallography</i> , <b>1999</b> , 29, 759-763	0.5	16
78	Benzazole-N(SINGLE BOND)BH <sub>3</sub> adducts. Reductive transposition of 2-benzimidazole, 2-benzothiazole, and 2-benzoxazole N(SINGLE BOND)BH <sub>3</sub> adducts to 1,3,2-benzimidazaborole, 1,3,2-benzoxaborole, and 1,3,2-benzothiazaborole. <i>Heteroatom Chemistry</i> , <b>1996</b> , 7, 323-335	1.2	16
77	Through space charge transfer and quadratic nonlinear optical (NLO) properties in alternated stacks of 2-amino-1,3-benzothiazole-ethylcoumarin-3-carboxylate charge transfer complexes: from the molecular to the bulk NLO response. <i>New Journal of Chemistry</i> , <b>2004</b> , 28, 542-547	3.6	15
76	Molecular Complexes of Diethyl N,N'-1,3-Phenyldioxalamate and Resorcinols: Conformational Switching through Intramolecular Three-Centered Hydrogen-Bonding. <i>Crystal Growth and Design</i> , <b>2014</b> , 14, 628-642	3.5	14
75	Further insight into three center hydrogen bonding. Participation in tautomeric equilibria of heterocyclic amides. <i>Perkin Transactions II RSC</i> , <b>2001</b> , 1817-1823		14
74	Solid state structure and solution thermodynamics of three-centered hydrogen bonds (O...H...O) using N-(2-benzoyl-phenyl) oxalyl derivatives as model compounds. <i>Molecules</i> , <b>2014</b> , 19, 14446-60	4.8	12

73	Supramolecular architectures of conformationally controlled 1,3-phenyl-dioxalamic molecular clefts through hydrogen bonding and steric restraints. <i>CrystEngComm</i> , <b>2011</b> , 13, 4748	3.3	12
72	Ethers and esters derived from apocynin avoid the interaction between p47phox and p22phox subunits of NADPH oxidase: evaluation in vitro and in silico. <i>Bioscience Reports</i> , <b>2013</b> , 33,	4.1	11
71	Design, synthesis and in vitro evaluation of (R)-4-(2-(tert-butylamino)-1-hydroxyethyl)-2-(hydroxymethyl)phenyl hydrogen phenylboronate: a novel salbutamol derivative with high intrinsic efficacy on the $\beta_2$ adrenoceptor. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2010</b> , 20, 5623-9	2.9	11
70	Reactivity of chlorodeoxypseudoephedrines with oxo-, thio-, and selenocyanates. <i>Tetrahedron: Asymmetry</i> , <b>2007</b> , 18, 123-130		11
69	Design, in silico studies, synthesis and in vitro evaluation of oseltamivir derivatives as inhibitors of neuraminidase from influenza A virus H1N1. <i>European Journal of Medicinal Chemistry</i> , <b>2017</b> , 128, 154-167	6.8	10
68	Anti-inflammatory effect and inhibition of nitric oxide production by targeting COXs and iNOS enzymes with the 1,2-diphenylbenzimidazole pharmacophore. <i>Bioorganic and Medicinal Chemistry</i> , <b>2020</b> , 28, 115427	3.4	10
67	NMR structural study of the prototropic equilibrium in solution of Schiff bases as model compounds. <i>Molecules</i> , <b>2013</b> , 19, 459-81	4.8	10
66	X-ray supramolecular structure, NMR spectroscopy and synthesis of 3-methyl-1-phenyl-1H-chromeno[4,3-c]pyrazol-4-ones formed by the unexpected cyclization of 3-[1-(phenyl-hydrazono)ethyl]-chromen-2-ones. <i>Molecules</i> , <b>2011</b> , 16, 915-32	4.8	10
65	In silico design, chemical synthesis and toxicological evaluation of 1,3-thiazolidine-2,4-dione derivatives as PPAR $\alpha$ agonists. <i>Regulatory Toxicology and Pharmacology</i> , <b>2017</b> , 86, 25-32	3.4	9
64	Iridaoxacyclohexadiene-Bridged Mixed-Valence Iridium Cyclooctadiene Complex: Oxidative Addition and Hydrogen-Transfer to Coordinated Cyclooctadiene. <i>Organometallics</i> , <b>2014</b> , 33, 6305-6318	3.8	9
63	DiethylN,N'-m-phenylenedioxamate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , <b>2003</b> , 59, o825-o827		9
62	Fluorine-containing benzothiazole as a novel trypanocidal agent: design, in silico study, synthesis and activity evaluation. <i>Medicinal Chemistry Research</i> , <b>2016</b> , 25, 211-224	2.2	8
61	Insights on the role of boron containing moieties in the design of new potent and efficient agonists targeting the $\beta_2$ adrenoceptor. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2015</b> , 25, 820-5	2.9	8
60	Novel synthesis of isoindoline/isoindoline-1,3-dione derivatives under solventless conditions and evaluation with the human D2 receptor. <i>Medicinal Chemistry Research</i> , <b>2017</b> , 26, 2420-2431	2.2	8
59	Thermal [4 + 2] cycloadditions of 3-acetyl-, 3-carbamoyl-, and 3-ethoxycarbonyl-coumarins with 2,3-dimethyl-1,3-butadiene under solventless conditions: a structural study. <i>Molecules</i> , <b>2010</b> , 15, 1513-30	4.8	8
58	Ethyl N-phenyloxamate. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , <b>2003</b> , 59, O541-3		8
57	Evaluation of a new benzothiazole derivative with antioxidant activity in the initial phase of acetaminophen toxicity. <i>Arabian Journal of Chemistry</i> , <b>2019</b> , 12, 3871-3882	5.9	8
56	Positional Isomerism and Steric Effects in the Self-Assemblies of Phenylene Bis-Monothiooxalamides. <i>Crystal Growth and Design</i> , <b>2017</b> , 17, 2513-2528	3.5	7

55	Crystal structure, DFT calculations and evaluation of 2-(2-(3,4-dimethoxyphenyl)ethyl)isoindoline-1,3-dione as AChE inhibitor. <i>Chemistry Central Journal</i> , <b>2018</b> , 12, 74		6
54	Aromatic Regions Govern the Recognition of NADPH Oxidase Inhibitors as Diapocynin and its Analogues. <i>Archiv Der Pharmazie</i> , <b>2017</b> , 350, 1700041	4.3	6
53	The zwitterion of 4-nitro-2-((E)-[2-(piperidin-1-yl)ethyl]iminomethyl)phenol. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , <b>2009</b> , 65, o8-o10		6
52	An efficient synthesis of aziridines from ephedrines. <i>Tetrahedron: Asymmetry</i> , <b>2010</b> , 21, 909-913		6
51	Switching from twisted to planar oxamide molecular cavities through intramolecular three centered hydrogen bonding. <i>Arkivoc</i> , <b>2005</b> , 2005, 401-415	0.9	6
50	2-Acetyl-4-aminoresorcinol derivatives: synthesis, antioxidant activity and molecular docking studies. <i>Medicinal Chemistry Research</i> , <b>2018</b> , 27, 1186-1197	2.2	5
49	A synthetic method to access symmetric and non-symmetric 2-(N,NRdisubstituted)guanidinebenzothiazoles. <i>Molecules</i> , <b>2012</b> , 17, 10178-91	4.8	5
48	1,3-Heterazolidines-2-heterounsaturated compounds derived from ephedrines. <i>Tetrahedron: Asymmetry</i> , <b>2006</b> , 17, 1499-1505		5
47	Three amino acid derivatives of valproic acid: design, synthesis, theoretical and experimental evaluation as anticancer agents. <i>Anti-Cancer Agents in Medicinal Chemistry</i> , <b>2014</b> , 14, 984-93	2.2	5
46	Supramolecular assembly of 2-aminobenzothiazole and N-[(2-oxo-2H-1-benzopyran-3-yl)carboxyl]phenethylamide donor-acceptor complex. A comparative study. <i>Arkivoc</i> , <b>2006</b> , 2003, 100-111	0.9	5
45	Surface Modification of the Ti-6Al-4V Alloy by Anodic Oxidation and Its Effect on Osteoarticular Cell Proliferation. <i>Coatings</i> , <b>2020</b> , 10, 491	2.9	4
44	Inhibitory activity on cholinesterases produced by aryl-phthalimide derivatives: green synthesis, in silico and in vitro evaluation. <i>Medicinal Chemistry Research</i> , <b>2020</b> , 29, 1030-1040	2.2	4
43	Theoretical studies, synthesis, and biological activity of 1-[(4-methylphenyl)sulfonyl]-5-oxo-2,3,4,5-tetrahydro-1H-1-benzazepine-4-carbonitrile (C9) as a non-peptide antagonist of the arginine vasopressin V1a and V2 receptors. <i>Medicinal Chemistry Research</i> , <b>2014</b> , 23, 1581-1590	2.2	4
42	Efficient synthesis of cis-thiazolidinethiones derived from ephedrines. <i>Tetrahedron: Asymmetry</i> , <b>2011</b> , 22, 394-398		4
41	Mechanochemical Synthesis and Structure of the Tetrahydrate and Mesoporous Anhydrous Metforminium(2+)-,R1,4-Phenylenedioxalamic Acid (1:2) Salt: The Role of Hydrogen Bonding and n- $\pi$ Charge Assisted Interactions. <i>Pharmaceutics</i> , <b>2020</b> , 12,	6.4	4
40	Repurposing FDA Drug Compounds against Breast Cancer by Targeting EGFR/HER2. <i>Pharmaceutics</i> , <b>2021</b> , 14,	5.2	4
39	Carbonyl-carbonyl interactions and amide $\pi$ -stacking as the directing motifs of the supramolecular assembly of ethyl N-(2-acetylphenyl)oxalamate in a synperiplanar conformation. <i>Acta Crystallographica Section C, Structural Chemistry</i> , <b>2015</b> , 71, 381-5	0.8	3
38	Ephedrines as Chiral Auxiliaries in Enantioselective Alkylation Reactions of Acyl Ephedrine Amides and Esters: A Review. <i>Current Organic Synthesis</i> , <b>2018</b> , 15, 38-83	1.9	3

37	π-Stacking and C-X...D (X = H, NO <sub>2</sub> ; D = O, N) interactions in the crystal network of both C-H...N and π-Stacked dimers of 1,2-bis(4-bromophenyl)-1H-benzimidazole and 2-(4-bromophenyl)-1-(4-nitrophenyl)-1H-benzimidazole. <i>Acta Crystallographica Section C, Structural Chemistry</i> , <b>2014</b> , 70, 55-9	0.8	3
36	Mechanochemical Complexation of Diethyl N,N'-[1,3-(2-methyl)phenyl]dioxalamate and Resorcinol: Conformational Twist and X-Ray Helical Supramolecular Architecture. <i>Journal of Chemical Crystallography</i> , <b>2015</b> , 45, 244-250	0.5	3
35	Synthesis and structure of sulfur derivatives from 2-aminobenzimidazole. <i>Molecules</i> , <b>2014</b> , 19, 13878-93	4.8	3
34	2-Amino-1,3-benzothiazole-ethyl coumarin-3-carboxylate (1/1). <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , <b>2003</b> , 59, O544-6		3
33	DiethylN,N'-cyclohexane-1,4-diyl dioxalamate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , <b>2005</b> , 61, o2994-o2996		3
32	Modifications on the Tetrahydroquinoline Scaffold Targeting a Phenylalanine Cluster on GPER as Antiproliferative Compounds against Renal, Liver and Pancreatic Cancer Cells. <i>Pharmaceuticals</i> , <b>2021</b> , 14,	5.2	3
31	Isothioureas, Ureas, and Their N-Methyl Amides from 2-Aminobenzothiazole and Chiral Amino Acids. <i>Molecules</i> , <b>2019</b> , 24,	4.8	2
30	Helical supramolecular assembly of N2,N2'-bis[3-(morpholin-4-yl)propyl]-N1,N1'R(1,2-phenylene)dioxalamide dimethyl sulfoxide monosolvate. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , <b>2013</b> , 69, 66-9		2
29	Helical Arrangement of 2-(4-hydroxy-3-methoxyphenyl)-Benzothiazole in Crystal Formation and Biological Evaluation on HeLa Cells. <i>Crystals</i> , <b>2017</b> , 7, 171	2.3	2
28	Facial π...Cl...π interactions as the directing motif of the supramolecular structures of Mg <sup>2+</sup> and Ca <sup>2+</sup> bis[hydrotris(pyrazolyl)borate] chloroform disolvates. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , <b>2006</b> , 62, m132-5		2
27	The E and Z isomers of 3-(benzoxazol-2-yl)prop-2-enoic acid. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , <b>2004</b> , 60, o723-6		2
26	The 2-aminobenzothiazole-N-benzyl-2-oxo-2H-1-benzopyran-3-carboxamide (1/1) donor-acceptor complex. <i>Acta Crystallographica Section E: Structure Reports Online</i> , <b>2003</b> , 59, o1628-o1630		2
25	Design, synthesis, molecular docking and in vitro evaluation of benzothiazole derivatives as 11β-hydroxysteroid dehydrogenase type 1 inhibitors. <i>Molecular Diversity</i> , <b>2020</b> , 24, 1-14	3.1	2
24	A New Symmetrical Thiazolidinedione Derivative: In Silico Design, Synthesis, and In Vivo Evaluation on a Streptozotocin-Induced Rat Model of Diabetes. <i>Processes</i> , <b>2021</b> , 9, 1294	2.9	2
23	Design, synthesis and in vitro evaluation of a Dopa-organoboron compound that acts as a bladder relaxant through non-catecholamine receptors. <i>Molecular Diversity</i> , <b>2019</b> , 23, 361-370	3.1	2
22	Synthesis, In Silico, and Biological Evaluation of a Borinic Tryptophan-Derivative That Induces Melatonin-like Amelioration of Cognitive Deficit in Male Rat.. <i>International Journal of Molecular Sciences</i> , <b>2022</b> , 23,	6.3	2
21	Solventless Synthesis of Poly(pyrazolyl)phenyl-methane Ligands and Thermal Transformation of Tris(3,5-dimethylpyrazol-1-yl)phenylmethane. <i>Molecules</i> , <b>2017</b> , 22,	4.8	1
20	Profiling the interaction of 1-phenylbenzimidazoles to cyclooxygenases. <i>Journal of Molecular Recognition</i> , <b>2019</b> , 32, e2801	2.6	1

19	Carbonyl-carbonyl and carbonyl-π interactions as directing motifs in the supramolecular structure of carbonyl(3-oxopenta-1,4-diene-1,5-diyl)[tris(3,5-dimethyl-1H-pyrazol-1-yl-N2)methane]iridium(III) trifluoromethanesulfonate. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , <b>2018</b> , 74, o125-8		1
18	2-(4-Hydroxyphenyl)-1H-benzimidazol-3-ium chloride monohydrate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , <b>2013</b> , 69, o1485-6		1
17	N,NRBis(4-amino-benz-yl)oxalamide. <i>Acta Crystallographica Section E: Structure Reports Online</i> , <b>2011</b> , 67, o398		1
16	Intramolecular Carbonyl-Carbonyl Interaction as the Directing Motif of the Opposed Conformational Preferences Among [4 + 2] Cycloadducts of 3-Ethoxycarbonyl- and 3-Acetyl-Coumarins with 2,3-Dimethyl-1,3-Butadiene. <i>Journal of Chemical Crystallography</i> , <b>2010</b> , 40, 1024-1028	0.5	1
15	Two isomeric butadiene-N-(acetoxyphenyl)maleimide Diels-Alder adducts: supramolecular structure directed by C-H...X (X = O and pi) hydrogen bonds and perpendicular dipole carbonyl-carbonyl interactions. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , <b>2006</b> , 62, o125-8		1
14	N-Cyclohexyl-2-oxo-2H-1-benzopyran-3-carboxamide. <i>Acta Crystallographica Section E: Structure Reports Online</i> , <b>2004</b> , 60, o2306-o2308		1
13	1,1,2,2-Tetrachloro-1,2-diphenylethane. <i>Acta Crystallographica Section E: Structure Reports Online</i> , <b>2005</b> , 61, o678-o680		1
12	Di-Ediphenylphosphido-bis[tricarbonyliron(II)] dichloromethane solvate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , <b>2005</b> , 61, m1475-m1477		1
11	Involvement of conformational isomerism in the complexity of the crystal network of 1-(4-nitrophenyl)-1H-1,3-benzimidazole derivatives driven by C-H...A (A = NO, N and π) and orthogonal N...NO and ONO...Csp interactions. <i>Acta Crystallographica Section C, Structural Chemistry</i> , <b>2018</b> , 74, 428-436	0.8	1
10	Benzothiazoles from Condensation of α-Aminothiophenols with Carboxylic Acids and Their Derivatives: A Review. <i>Molecules</i> , <b>2021</b> , 26,	4.8	1
9	Crystal Structure and Supramolecular Architecture of Antiallergic Diphenylene Diethyl Dioxalamates. <i>Crystals</i> , <b>2020</b> , 10, 1048	2.3	1
8	Myeloperoxidase Inhibitory and Antioxidant Activities of (E)-2-Hydroxy-β-aminocinnamic Acids Obtained through Microwave-Assisted Synthesis. <i>Pharmaceuticals</i> , <b>2021</b> , 14,	5.2	1
7	Dihydropyrazole-Carbohydrazone Derivatives with Dual Activity as Antioxidant and Anti-Proliferative Drugs on Breast Cancer Targeting the HDAC6. <i>Pharmaceuticals</i> , <b>2022</b> , 15, 690	5.2	1
6	2,2?-Bi-1,3-thiazolidine. <i>Acta Crystallographica Section E: Structure Reports Online</i> , <b>2006</b> , 62, o525-o527		
5	Exo Diels-Alder adducts between ortho- and para-N-acetoxyphenylmaleimides and furan. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , <b>2004</b> , 60, o427-30		
4	Ethyl (E)-3-(2-hydroxyphenyl)-2-(morpholinocarbonyl)propenoate. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , <b>2004</b> , 60, o517-9		
3	Diethyl piperazine-1,4-diyl dioxalate. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , <b>2004</b> , 60, o699-701		
2	1,1?,3,3?-Tetrabenzyl-2,2?-biimidazolidine. <i>Acta Crystallographica Section E: Structure Reports Online</i> , <b>2005</b> , 61, o2464-o2466		

- 1 Microcrystalline solid-solid transformations of conformationally-responsive solvates, desolvates and a salt of N,N'-(1,4-phenylene)dioxalamic acid: the energetics of hydrogen bonding and n- $\pi$  interactions. *CrystEngComm*, **2022**, 24, 1017-1034 33