Itzia Irene Padilla-Martnez

List of Publications by Year in Descending Order

90 papers	697 citations	14 h-index	20 g-index
97 ext. papers	781 ext. citations	3.2 avg, IF	3.58 L-index

#	Paper	IF	Citations
90	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/□-p□ interactions. *CrystEngComm*, **2022**, 24, 1017-1034	3.3	
89	Synthesis, In Silico, and Biological Evaluation of a Borinic Tryptophan-Derivative That Induces Melatonin-like Amelioration of Cognitive Deficit in Male Rat.. *International Journal of Molecular Sciences*, **2022**, 23,	6.3	2
88	Dihydropyrazole-Carbohydrazide Derivatives with Dual Activity as Antioxidant and Anti-Proliferative Drugs on Breast Cancer Targeting the HDAC6. *Pharmaceuticals*, **2022**, 15, 690	5.2	1
87	Benzothiazoles from Condensation of -Aminothiophenoles with Carboxylic Acids and Their Derivatives: A Review. *Molecules*, **2021**, 26,	4.8	1
86	Myeloperoxidase Inhibitory and Antioxidant Activities of ()-2-Hydroxy-□aminocinnamic Acids Obtained through Microwave-Assisted Synthesis. *Pharmaceuticals*, **2021**, 14,	5.2	1
85	A New Symmetrical Thiazolidinedione Derivative: In Silico Design, Synthesis, and In Vivo Evaluation on a Streptozotocin-Induced Rat Model of Diabetes. *Processes*, **2021**, 9, 1294	2.9	2
84	Modifications on the Tetrahydroquinoline Scaffold Targeting a Phenylalanine Cluster on GPER as Antiproliferative Compounds against Renal, Liver and Pancreatic Cancer Cells. *Pharmaceuticals*, **2021**, 14,	5.2	3
83	Repurposing FDA Drug Compounds against Breast Cancer by Targeting EGFR/HER2. *Pharmaceuticals*, **2021**, 14,	5.2	4
82	Surface Modification of the Ti-6Al-4V Alloy by Anodic Oxidation and Its Effect on Osteoarticular Cell Proliferation. *Coatings*, **2020**, 10, 491	2.9	4
81	Anti-inflammatory effect and inhibition of nitric oxide production by targeting COXs and iNOS enzymes with the 1,2-diphenylbenzimidazole pharmacophore. *Bioorganic and Medicinal Chemistry*, **2020**, 28, 115427	3.4	10
80	Inhibitory activity on cholinesterases produced by aryl-phthalimide derivatives: green synthesis, in silico and in vitro evaluation. *Medicinal Chemistry Research*, **2020**, 29, 1030-1040	2.2	4
79	Design, synthesis, molecular docking and in vitro evaluation of benzothiazole derivatives as 11□hydroxysteroid dehydrogenase type 1 inhibitors. *Molecular Diversity*, **2020**, 24, 1-14	3.1	2
78	Crystal Structure and Supramolecular Architecture of Antiallergic Diphenylene Diethyl Dioxalamates. *Crystals*, **2020**, 10, 1048	2.3	1
77	Mechanochemical Synthesis and Structure of the Tetrahydrate and Mesoporous Anhydrous Metformin(2+)-,R1,4-Phenylenedioxalamic Acid (1:2) Salt: The Role of Hydrogen Bonding and n-p□ Charge Assisted Interactions. *Pharmaceutics*, **2020**, 12,	6.4	4
76	Isothioureas, Ureas, and Their -Methyl Amides from 2-Aminobenzothiazole and Chiral Amino Acids. *Molecules*, **2019**, 24,	4.8	2
75	Profiling the interaction of 1-phenylbenzimidazoles to cyclooxygenases. *Journal of Molecular Recognition*, **2019**, 32, e2801	2.6	1
74	Design, synthesis and in vitro evaluation of a Dopa-organoboron compound that acts as a bladder relaxant through non-catecholamine receptors. *Molecular Diversity*, **2019**, 23, 361-370	3.1	2

73	Evaluation of a new benzothiazole derivative with antioxidant activity in the initial phase of acetaminophen toxicity. *Arabian Journal of Chemistry*, **2019**, 12, 3871-3882	5.9	8
72	2-Acetyl-4-aminoresorcinol derivatives: synthesis, antioxidant activity and molecular docking studies. *Medicinal Chemistry Research*, **2018**, 27, 1186-1197	2.2	5
71	Ephedrines as Chiral Auxiliaries in Enantioselective Alkylation Reactions of Acyl Ephedrine Amides and Esters: A Review. *Current Organic Synthesis*, **2018**, 15, 38-83	1.9	3
70	Crystal structure, DFT calculations and evaluation of 2-(2-(3,4-dimethoxyphenyl)ethyl)isoindoline-1,3-dione as AChE inhibitor. *Chemistry Central Journal*, **2018**, 12, 74		6
69	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) and orthogonal N...NO and ONO...Csp interactions. *Acta Crystallographica Section C, Structural Chemistry*, **2018**, 74, 428-436	0.8	1
68	Design, in silico studies, synthesis and in vitro evaluation of oseltamivir derivatives as inhibitors of neuraminidase from influenza A virus H1N1. *European Journal of Medicinal Chemistry*, **2017**, 128, 154-167	4.8	10
67	In silico design, chemical synthesis and toxicological evaluation of 1,3-thiazolidine-2,4-dione derivatives as PPAR agonists. *Regulatory Toxicology and Pharmacology*, **2017**, 86, 25-32	3.4	9
66	Positional Isomerism and Steric Effects in the Self-Assemblies of Phenylene Bis-Monothiooxalamides. *Crystal Growth and Design*, **2017**, 17, 2513-2528	3.5	7
65	Solventless Synthesis of Poly(pyrazolyl)phenyl-methane Ligands and Thermal Transformation of Tris(3,5-dimethylpyrazol-1-yl)phenylmethane. *Molecules*, **2017**, 22,	4.8	1
64	Aromatic Regions Govern the Recognition of NADPH Oxidase Inhibitors as Diapocynin and its Analogues. *Archiv Der Pharmazie*, **2017**, 350, 1700041	4.3	6
63	Novel synthesis of isoindoline/isoindoline-1,3-dione derivatives under solventless conditions and evaluation with the human D2 receptor. *Medicinal Chemistry Research*, **2017**, 26, 2420-2431	2.2	8
62	Helical Arrangement of 2-(4-hydroxy-3-methoxyphenyl)-Benzothiazole in Crystal Formation and Biological Evaluation on HeLa Cells. *Crystals*, **2017**, 7, 171	2.3	2
61	Fluorine-containing benzothiazole as a novel trypanocidal agent: design, in silico study, synthesis and activity evaluation. *Medicinal Chemistry Research*, **2016**, 25, 211-224	2.2	8
60	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. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2016**, 31, 140-149	5.6	25
59	Insights on the role of boron containing moieties in the design of new potent and efficient agonists targeting the adrenoceptor. *Bioorganic and Medicinal Chemistry Letters*, **2015**, 25, 820-5	2.9	8
58	Carbonyl-carbonyl interactions and amide stacking as the directing motifs of the supramolecular assembly of ethyl N-(2-acetylphenyl)oxalamate in a synperiplanar conformation. *Acta Crystallographica Section C, Structural Chemistry*, **2015**, 71, 381-5	0.8	3
57	Mechanochemical Complexation of Diethyl N,N′-[1,3-(2-methyl)phenyl]dioxalamate and Resorcinol: Conformational Twist and X-Ray Helical Supramolecular Architecture. *Journal of Chemical Crystallography*, **2015**, 45, 244-250	0.5	3
56	Molecular Complexes of Diethyl N,N?-1,3-Phenyldioxalamate and Resorcinols: Conformational Switching through Intramolecular Three-Centered Hydrogen-Bonding. *Crystal Growth and Design*, **2014**, 14, 628-642	3.5	14

55	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. *Medicinal Chemistry Research*, **2014**, 23, 1581-1590	2.2	4
54	Design of multi-target compounds as AChE, BACE1, and amyloid-β (1-42) oligomerization inhibitors: in silico and in vitro studies. *Journal of Alzheimer's Disease*, **2014**, 41, 1073-85	4.3	18
53	π-stacking and C-X...D (X = H, NO2; D = O, π) 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. *Acta Crystallographica Section C, Structural Chemistry*, **2014**, 70, 55-9	0.8	3
52	Synthesis and structure of sulfur derivatives from 2-aminobenzimidazole. *Molecules*, **2014**, 19, 13878-93	4.8	3
51	Solid state structure and solution thermodynamics of three-centered hydrogen bonds (OHO) using N-(2-benzoyl-phenyl) oxalyl derivatives as model compounds. *Molecules*, **2014**, 19, 14446-60	4.8	12
50	Iridaoxacyclohexadiene-Bridged Mixed-Valence Iridium Cyclooctadiene Complex: Oxidative Addition and Hydrogen-Transfer to Coordinated Cyclooctadiene. *Organometallics*, **2014**, 33, 6305-6318	3.8	9
49	Three amino acid derivatives of valproic acid: design, synthesis, theoretical and experimental evaluation as anticancer agents. *Anti-Cancer Agents in Medicinal Chemistry*, **2014**, 14, 984-93	2.2	5
48	Helical supramolecular assembly of N2,N2′-bis[3-(morpholin-4-yl)propyl]-N1,N1′-(1,2-phenylene)dioxalamide dimethyl sulfoxide monosolvate. *Acta Crystallographica Section C: Crystal Structure Communications*, **2013**, 69, 66-9		2
47	NMR structural study of the prototropic equilibrium in solution of Schiff bases as model compounds. *Molecules*, **2013**, 19, 459-81	4.8	10
46	2-(4-Hy-droxy-phen-yl)-1H-benzimidazol-3-ium chloride monohydrate. *Acta Crystallographica Section E: Structure Reports Online*, **2013**, 69, o1485-6		1
45	Ethers and esters derived from apocynin avoid the interaction between p47phox and p22phox subunits of NADPH oxidase: evaluation in vitro and in silico. *Bioscience Reports*, **2013**, 33,	4.1	11
44	Synthesis and Crystal Structure of Iridium-1,4-benzoquinone Complexes of Tris(3,5-dimethylpyrazolyl)methane Ligand: Decarbonylation, Protonation, and Substitution Reactions. *Organometallics*, **2012**, 31, 5438-5451	3.8	16
43	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-κN2)methane]iridium(III) trifluoromethanesulfonate. *Acta Crystallographica Section C: Crystal Structure Communications*, [illegible]		1
42	A synthetic method to access symmetric and non-symmetric 2-(N,N′-disubstituted)guanidinebenzothiazoles. *Molecules*, **2012**, 17, 10178-91	4.8	5
41	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. *Molecules*, **2011**, 16, 915-32	4.8	10
40	Supramolecular architectures of conformationally controlled 1,3-phenyl-dioxalamic molecular clefts through hydrogen bonding and steric restraints. *CrystEngComm*, **2011**, 13, 4748	3.3	12
39	Efficient synthesis of cis-thiazolidinethiones derived from ephedrines. *Tetrahedron: Asymmetry*, **2011**, 22, 394-398		4
38	N,N′-Bis(4-amino-benz-yl)oxalamide. *Acta Crystallographica Section E: Structure Reports Online*, **2011**, 67, o398		1

37	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. *Molecules*, **2010**, 15, 1513-30	4.8	8
36	An efficient synthesis of aziridines from ephedrines. *Tetrahedron: Asymmetry*, **2010**, 21, 909-913		6
35	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. *Journal of Chemical Crystallography*, **2010**, 40, 1024-1028	0.5	1
34	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 □2 adrenoceptor. *Bioorganic and Medicinal Chemistry Letters*, **2010**, 20, 5623-9	2.9	11
33	The zwitterion of 4-nitro-2-{(E)-[2-(piperidin-1-yl)ethyl]iminomethyl}phenol. *Acta Crystallographica Section C: Crystal Structure Communications*, **2009**, 65, o8-o10		6
32	Competition between OH?O and multiple halogen□dipole interactions on the formation of intramolecular three-centred hydrogen bond in 3-acyl coumarins. *CrystEngComm*, **2009**, 11, 1451	3.3	16
31	Carbonyl-carbonyl, carbonyl-pi 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. *Acta Crystallographica Section C: Crystal Structure Communications*, **2007**, 63, o239-42		20
30	Reactivity of chlorodeoxypseudoephedrines with oxo-, thio-, and selenocyanates. *Tetrahedron: Asymmetry*, **2007**, 18, 123-130		11
29	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. *Acta Crystallographica Section C: Crystal Structure Communications*, **2006**, 62, o125-8		1
28	Facial pi...Cl...pi interactions as the directing motif of the supramolecular structures of Mg2+ and Ca2+ bis[hydrotris(pyrazolyl)borate] chloroform disolvates. *Acta Crystallographica Section C: Crystal Structure Communications*, **2006**, 62, m132-5		2
27	2,2?-Bi-1,3-thiazolidine. *Acta Crystallographica Section E: Structure Reports Online*, **2006**, 62, o525-o527		
26	1,3-Heterazolidines-2-heterounsaturated compounds derived from ephedrines. *Tetrahedron: Asymmetry*, **2006**, 17, 1499-1505		5
25	Supramolecular assembly of 2-aminobenzothiazole and N-[(2-oxo-2H-1-benzopyran-3-yl)carboxyl]phenethylamide donor-acceptor complex. A comparative study. *Arkivoc*, **2006**, 2003, 100-111	0.9	5
24	1,1,2,2-Tetrachloro-1,2-diphenylethane. *Acta Crystallographica Section E: Structure Reports Online*, **2005**, 61, o678-o680		1
23	Di-□diphenylphosphido-bis[tricarbonyliron(II)] dichloromethane solvate. *Acta Crystallographica Section E: Structure Reports Online*, **2005**, 61, m1475-m1477		1
22	1,1?,3,3?-Tetrabenzyl-2,2?-biimidazolidine. *Acta Crystallographica Section E: Structure Reports Online* , **2005**, 61, o2464-o2466		
21	DiethylN,N?-cyclohexane-1,4-diyldioxalamate. *Acta Crystallographica Section E: Structure Reports Online*, **2005**, 61, o2994-o2996		3
20	Switching from twisted to planar oxamide molecular cavities through intramolecular three centered hydrogen bonding. *Arkivoc*, **2005**, 2005, 401-415	0.9	6

19	Exo Diels-Alder adducts between ortho- and para-N-acetoxyphenylmaleimides and furan. *Acta Crystallographica Section C: Crystal Structure Communications*, **2004**, 60, o427-30		
18	Ethyl (E)-3-(2-hydroxyphenyl)-2-(morpholinocarbonyl)propenoate. *Acta Crystallographica Section C: Crystal Structure Communications*, **2004**, 60, o517-9		
17	The E and Z isomers of 3-(benzoxazol-2-yl)prop-2-enoic acid. *Acta Crystallographica Section C: Crystal Structure Communications*, **2004**, 60, o723-6		2
16	Diethyl piperazine-1,4-diyldioxalate. *Acta Crystallographica Section C: Crystal Structure Communications*, **2004**, 60, o699-701		
15	N-Cyclohexyl-2-oxo-2H-1-benzopyran-3-carboxamide. *Acta Crystallographica Section E: Structure Reports Online*, **2004**, 60, o2306-o2308		1
14	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. *New Journal of Chemistry*, **2004**, 28, 542-547	3.6	15
13	2-Amino-1,3-benzothiazole-ethyl coumarin-3-carboxylate (1/1). *Acta Crystallographica Section C: Crystal Structure Communications*, **2003**, 59, O544-6		3
12	Ethyl N-phenyloxamate. *Acta Crystallographica Section C: Crystal Structure Communications*, **2003**, 59, O541-3		8
11	DiethylN,N?-m-phenylenedioxamate. *Acta Crystallographica Section E: Structure Reports Online*, **2003**, 59, o825-o827		9
10	The 2-aminobenzothiazole–N-benzyl-2-oxo-2H-1-benzopyran-3-carboxamide (1/1) donor–acceptor complex. *Acta Crystallographica Section E: Structure Reports Online*, **2003**, 59, o1628-o1630		2
9	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. *Crystal Growth and Design*, **2003**, 3, 35-45	3.5	60
8	Synthesis and Reactivity of [Ir(C2H4)2TpmMe2]PF6 (TpmMe2 = Tris(3,5-dimethylpyrazolyl)methane): Comparison with the Analogous TpMe2 Derivatives (TpMe2 = Hydrotris(3,5-dimethylpyrazolyl)borate). *Organometallics*, **2002**, 21, 93-104	3.8	31
7	Further insight into three center hydrogen bonding. Participation in tautomeric equilibria of heterocyclic amides. *Perkin Transactions II RSC*, **2001**, 1817-1823		14
6	9-(2-Methylphenyl)-3,4,5,6,9,10-hexa- hydroxanthene-1,8(2H,7H)-dione. *Journal of Chemical Crystallography*, **1999**, 29, 759-763	0.5	16
5	New Imidazabole Derivatives: Dimers of Carbene–Borane Adducts. *European Journal of Inorganic Chemistry*, **1998**, 1998, 1547-1553	2.3	26
4	Benzazole-N(SINGLE BOND)BH3 adducts. Reductive transposition of 2-benzimidazole, 2-benzothiazole, and 2-benzoxazole N(SINGLE BOND)BH3 adducts to 1,3,2-benzimidazaborole, 1,3,2-benzoxaborole, and 1,3,2-benzothiazaborole. *Heteroatom Chemistry*, **1996**, 7, 323-335	1.2	16
3	Azolylborane adducts. Structural and conformational analysis by x-ray diffraction and NMR. Protic-hydric (C?H□+-□H?B) and Protic-Fluoride (C?H□+-□F?B) interactions. *Chemische Berichte*, **1996**, 129, 441-449		45
2	From Azole–Borane Adducts to Azaboles □Molecular Structure of an Imidazabole. *Chemische Berichte*, **1994**, 127, 343-346		22

1	NMR Study of isolobal N-CH3+, N-BH3 and N-BF3 imidazole derivatives. *Magnetic Resonance in Chemistry*, **1993**, 31, 189-193	2.1	25