Itzia Irene Padilla-MartÃ-nez

List of Publications by Year
in descending order

96 papers	865 citations	516215 16 h-index	610482 24 g-index
97 all docs	97 docs citations	97 times ranked	1141 citing authors

#	Article	IF	Citations
1	Ï€-Stacking Interactions and CHÂ·Â·Â·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.	1.4	64
2	Azolylborane adducts. Structural and conformational analysis by xâ€ray diffraction and NMR. Proticâ€hydric (Cï£¾H^{Î´+}â€¦^{Î´â€“}Hï£¾B) and Proticâ€Fluoride (Cï£¾H^{Î´+}â€¦^{Î´â€“}Fï£ interactions. Chemische Berichte, 1996, 129, 441-449.		
3	Synthesis and Reactivity of [Ir(C2H4)2TpmMe2]PF6 (TpmMe2 = Tris(3,5-dimethylpyrazolyl)methane):â€‰ Comparison with the Analogous TpMe2 Derivatives (TpMe2 = Hydrotris(3,5-dimethylpyrazolyl)borate). Organometallics, 2002, 21, 93-104.	1.1	33
4	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.	2.5	32
5	NMR Study of isolobalN-CH3+,N-BH3 andN-BF3 imidazole derivatives. Magnetic Resonance in Chemistry, 1993, 31, 189-193.	1.1	29
6	New Imidazabole Derivatives: Dimers of Carbeneâ€“Borane Adducts. European Journal of Inorganic Chemistry, 1998, 1998, 1547-1553.	1.0	29
7	From Azoleâ€”Borane Adducts to Azaboles â€” Molecular Structure of an Imidazabole. Chemische Berichte, 1994, 127, 343-346.	0.2	25
8	Design of Multi-Target Compounds as AChE, BACE1, and Amyloid-Î²1-42 Oligomerization Inhibitors: In Silico and In Vitro Studies. Journal of Alzheimer's Disease, 2014, 41, 1073-1085.	1.2	23
9	Carbonylâ€“carbonyl, carbonylâ€“Ï€ and carbonylâ€“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-o242.	0.4	21
10	Through space charge transfer and quadratic nonlinear optical (NLO) properties in alternated stacks of 2-amino-1,3-benzothiazoleâ€“ethylcoumarin-3-carboxylate charge transfer complexes: from the molecular to the bulk NLO response. New Journal of Chemistry, 2004, 28, 542-547.	1.4	20
11	Competition between OHâ‹¯O and multiple halogenâ€“dipole interactions on the formation of intramolecular three-centred hydrogen bond in 3-acyl coumarins. CrystEngComm, 2009, 11, 1451.	1.3	19
12	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.	0.4	18
13	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.	1.1	18
14	Fluorine-containing benzothiazole as a novel trypanocidal agent: design, in silico study, synthesis and activity evaluation. Medicinal Chemistry Research, 2016, 25, 211-224.	1.1	18
15	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	17
16	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.	1.4	17
17	Evaluation of a new benzothiazole derivative with antioxidant activity in the initial phase of acetaminophen toxicity. Arabian Journal of Chemistry, 2019, 12, 3871-3882.	2.3	16
18	Ethers and esters derived from apocynin avoid the interaction between p47phox and p22phox subunits of NADPH oxidase: evaluation inÂvitro and in silico. Bioscience Reports, 2013, 33, .	1.1	15

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19	NMR Structural Study of the Prototropic Equilibrium in Solution of Schiff Bases as Model Compounds. Molecules, 2014, 19, 459-481.	1.7	15
20	Further insight into three center hydrogen bonding. Participation in tautomeric equilibria of heterocyclic amides. Perkin Transactions II RSC, 2001, , 1817-1823.	1.1	14
21	Solid State Structure and Solution Thermodynamics of Three-Centered Hydrogen Bonds (Oâ^™â^™â^™Hâ^™â^™â^™O) Using N-(2-Benzoyl-phenyl) Oxalyl Derivatives as Model Compounds. Molecules, 2014, 19, 14446-14460.	1.7	14
22	Molecular Complexes of Diethyl N,Nâ€²-1,3-Phenyldioxalamate and Resorcinols: Conformational Switching through Intramolecular Three-Centered Hydrogen-Bonding. Crystal Growth and Design, 2014, 14, 628-642.	1.4	14
23	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 Î²2 adrenoceptor. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 5623-5629.	1.0	13
24	Supramolecular architectures of conformationally controlled 1,3-phenyl-dioxalamic molecular clefts through hydrogen bonding and steric restraints. CrystEngComm, 2011, 13, 4748.	1.3	13
25	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, 915-932.	1.7	13
26	Design, in silico studies, synthesis and inÂvitro evaluation of oseltamivir derivatives as inhibitors of neuraminidase from influenza A virus H1N1. European Journal of Medicinal Chemistry, 2017, 128, 154-167.	2.6	13
27	Reactivity of chlorodeoxypseudoephedrines with oxo-, thio-, and selenocyanates. Tetrahedron: Asymmetry, 2007, 18, 123-130.	1.8	12
28	Iridaoxacyclohexadiene-Bridged Mixed-Valence Iridium Cyclooctadiene Complex: Oxidative Addition and Hydrogen-Transfer to Coordinated Cyclooctadiene. Organometallics, 2014, 33, 6305-6318.	1.1	11
29	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.	1.1	11
30	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, 1513-1530.	1.7	10
31	In silico design, chemical synthesis and toxicological evaluation of 1,3-thiazolidine-2,4-dione derivatives as PPARÎ³ agonists. Regulatory Toxicology and Pharmacology, 2017, 86, 25-32.	1.3	10
32	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.	2.6	10
33	DiethylN,Nâ€²-m-phenylenedioxamate. Acta Crystallographica Section E: Structure Reports Online, 2003, 59, o825-o827.	0.2	9
34	Surface Modification of the Ti-6Al-4V Alloy by Anodic Oxidation and Its Effect on Osteoarticular Cell Proliferation. Coatings, 2020, 10, 491.	1.2	9
35	Benzothiazoles from Condensation of o-Aminothiophenoles with Carboxylic Acids and Their Derivatives: A Review. Molecules, 2021, 26, 6518.	1.7	9
36	EthylN-phenyloxamate. Acta Crystallographica Section C: Crystal Structure Communications, 2003, 59, o541-o543.	0.4	8

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37	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.	0.4	8
38	An efficient synthesis of aziridines from ephedrines. Tetrahedron: Asymmetry, 2010, 21, 909-913.	1.8	8
39	Insights on the role of boron containing moieties in the design of new potent and efficient agonists targeting the Î²2 adrenoceptor. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 820-825.	1.0	8
40	Positional Isomerism and Steric Effects in the Self-Assemblies of Phenylene Bis-Monothiooxalamides. Crystal Growth and Design, 2017, 17, 2513-2528.	1.4	8
41	Modifications on the Tetrahydroquinoline Scaffold Targeting a Phenylalanine Cluster on GPER as Antiproliferative Compounds against Renal, Liver and Pancreatic Cancer Cells. Pharmaceuticals, 2021, 14, 49.	1.7	8
42	Aromatic Regions Govern the Recognition of NADPH Oxidase Inhibitors as Diapocynin and its Analogues. Archiv Der Pharmazie, 2017, 350, 1700041.	2.1	7
43	Repurposing FDA Drug Compounds against Breast Cancer by Targeting EGFR/HER2. Pharmaceuticals, 2021, 14, 791.	1.7	7
44	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, 3229.	1.8	7
45	Efficient synthesis of cis-thiazolidinethiones derived from ephedrines. Tetrahedron: Asymmetry, 2011, 22, 394-398.	1.8	6
46	A Synthetic Method to Access Symmetric and Non-Symmetric 2-(N,N'-disubstituted)guanidinebenzothiazoles. Molecules, 2012, 17, 10178-10191.	1.7	6
47	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.	1.3	6
48	Switching from twisted to planar oxamide molecular cavities through intramolecular three centered hydrogen bonding. Arkivoc, 2005, 2005, 401-415.	0.3	6
49	1,3-Heterazolidines-2-heterounsaturated compounds derived from ephedrines. Tetrahedron: Asymmetry, 2006, 17, 1499-1505.	1.8	5
50	2-Acetyl-4-aminoresorcinol derivatives: synthesis, antioxidant activity and molecular docking studies. Medicinal Chemistry Research, 2018, 27, 1186-1197.	1.1	5
51	Ephedrines as Chiral Auxiliaries in Enantioselective Alkylation Reactions of Acyl Ephedrine Amides and Esters: A Review. Current Organic Synthesis, 2018, 15, 38-83.	0.7	5
52	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.	2.1	5
53	Mechanochemical Synthesis and Structure of the Tetrahydrate and Mesoporous Anhydrous Metforminium(2+)-N,Nâ€²-1,4-Phenylenedioxalamic Acid (1:2) Salt: The Role of Hydrogen Bonding and nâ†'Ï€ * Charge Assisted Interactions. Pharmaceutics, 2020, 12, 998.	2.0	5
54	Inhibitory activity on cholinesterases produced by aryl-phthalimide derivatives: green synthesis, in silico and in vitro evaluation. Medicinal Chemistry Research, 2020, 29, 1030-1040.	1.1	5

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55	Myeloperoxidase Inhibitory and Antioxidant Activities of (E)-2-Hydroxy-Î±-aminocinnamic Acids Obtained through Microwave-Assisted Synthesis. Pharmaceuticals, 2021, 14, 513.	1.7	5
56	Three Amino Acid Derivatives of Valproic Acid: Design, Synthesis, Theoretical and Experimental Evaluation as Anticancer Agents. Anti-Cancer Agents in Medicinal Chemistry, 2014, 14, 984-993.	0.9	5
57	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.	0.3	5
58	2-Amino-1,3-benzothiazoleâ€“ethyl coumarin-3-carboxylate (1/1). Acta Crystallographica Section C: Crystal Structure Communications, 2003, 59, o544-o546.	0.4	4
59	Synthesis and Structure of Sulfur Derivatives from 2-Aminobenzimidazole. Molecules, 2014, 19, 13878-13893.	1.7	4
60	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.	1.1	4
61	Carbonylâ€“carbonyl interactions and amide Ï€-stacking as the directing motifs of the supramolecular assembly of ethylN-(2-acetylphenyl)oxalamate in a synperiplanar conformation. Acta Crystallographica Section C, Structural Chemistry, 2015, 71, 381-385.	0.2	4
62	Helical Arrangement of 2-(4-hydroxy-3-methoxyphenyl)-Benzothiazole in Crystal Formation and Biological Evaluation on HeLa Cells. Crystals, 2017, 7, 171.	1.0	4
63	Isothioureas, Ureas, and Their N-Methyl Amides from 2-Aminobenzothiazole and Chiral Amino Acids. Molecules, 2019, 24, 3391.	1.7	4
64	TheEandZisomers of 3-(benzoxazol-2-yl)prop-2-enoic acid. Acta Crystallographica Section C: Crystal Structure Communications, 2004, 60, o723-o726.	0.4	3
65	DiethylN,Nâ€²-cyclohexane-1,4-diyldioxalamate. Acta Crystallographica Section E: Structure Reports Online, 2005, 61, o2994-o2996.	0.2	3
66	Ï€-stacking and Câ€”X...D(X= H, NO₂;D= O, Ï€) interactions in the crystal network of both Câ€”H...N and Ï€-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, 55-59.	0.2	3
67	Mechanochemical Complexation of Diethyl N,NÂ´-[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
68	Design, synthesis, molecular docking and in vitro evaluation of benzothiazole derivatives as 11Î²-hydroxysteroid dehydrogenase type 1 inhibitors. Molecular Diversity, 2020, 24, 1-14.	2.1	3
69	The 2-aminobenzothiazoleâ€“N-benzyl-2-oxo-2H-1-benzopyran-3-carboxamide (1/1) donorâ€“acceptor complex. Acta Crystallographica Section E: Structure Reports Online, 2003, 59, o1628-o1630.	0.2	2
70	1,1,2,2-Tetrachloro-1,2-diphenylethane. Acta Crystallographica Section E: Structure Reports Online, 2005, 61, o678-o680.	0.2	2
71	Facial Ï€...Cl...Ï€ 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-m135.	0.4	2
72	Helical supramolecular assembly ofN²,N^{2â€²}-bis[3-(morpholin-4-yl)propyl]-N¹,N^{1â€²}-(1, dimethyl sulfoxide monosolvate. Acta Crystallographica Section C: Crystal Structure Communications, 2013, 69, 66-69.	0.4	2

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73	S-Methyl-(-N-aryl and -N-alkyl)isothioureas derived from 2-aminobenzothiazole. Arkivoc, 2007, 2008, 200-209.	0.3	2
74	Synthesis, Optical Characterization in Solution and Solid-State, and DFT Calculations of 3-Acetyl and 3-(1â€²-(2â€²-Phenylhydrazono)ethyl)-coumarin-(7)-substituted Derivatives. Molecules, 2022, 27, 3677.	1.7	2
75	N-Cyclohexyl-2-oxo-2H-1-benzopyran-3-carboxamide. Acta Crystallographica Section E: Structure Reports Online, 2004, 60, o2306-o2308.	0.2	1
76	Di-Î¼-diphenylphosphido-bis[tricarbonyliron(II)] dichloromethane solvate. Acta Crystallographica Section E: Structure Reports Online, 2005, 61, m1475-m1477.	0.2	1
77	Two isomeric butadieneâ€“N-(acetoxyphenyl)maleimide Dielsâ€“Alder adducts: supramolecular structure directed by Câ€”H...X(X= O and Ï€) hydrogen bonds and perpendicular dipole carbonylâ€“carbonyl interactions. Acta Crystallographica Section C: Crystal Structure Communications, 2006, 62, o125-o128.	0.4	1
78	Intramolecular Carbonylâ€“Carbonyl Interaction as the Directing Motif of the Opposed Conformational Preferences Among [4Â+Â2] 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
79	N,Nâ€²-Bis(4-aminobenzyl)oxalamide. Acta Crystallographica Section E: Structure Reports Online, 2011, 67, o398-o398.	0.2	1
80	Carbonylâ€“carbonyl and carbonylâ€“Ï€ 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-ÎºN2)methane]iridium(III) trifluoromethanesulfonate. Acta Crystallographica Section C: Crystal Structure Communications, 2012, 68, m367-m369.	0.4	1
81	2-(4-Hydroxyphenyl)-1H-benzimidazol-3-ium chloride monohydrate. Acta Crystallographica Section E: Structure Reports Online, 2013, 69, o1485-o1486.	0.2	1
82	Solventless Synthesis of Poly(pyrazolyl)phenyl-methane Ligands and Thermal Transformation of Tris(3,5-dimethylpyrazol-1-yl)phenylmethane. Molecules, 2017, 22, 441.	1.7	1
83	Profiling the interaction of 1â€phenylbenzimidazoles to cyclooxygenases. Journal of Molecular Recognition, 2019, 32, e2801.	1.1	1
84	Crystal Structure and Supramolecular Architecture of Antiallergic Diphenylene Diethyl Dioxalamates. Crystals, 2020, 10, 1048.	1.0	1
85	Involvement of conformational isomerism in the complexity of the crystal network of 1-(4-nitrophenyl)-1H-1,3-benzimidazole derivatives driven by Câ€”H...A (A =) Tj ETQq1 1 0.784314 rgBT /Overloc ONO...Csp ² interactions. Acta Crystallographica Section C, Structural Chemistry, 2018, 74, 428-436.	0.2	1
86	Preclinical Pharmacokinetics and Acute Toxicity in Rats of 5-{[(2E)-3-Bromo-3-carboxyprop-2-enoyl]amino}-2-hydroxybenzoic Acid: A Novel 5-Aminosalicylic Acid Derivative with Potent Anti-Inflammatory Activity. Molecules, 2021, 26, 6801.	1.7	1
87	Dihydropyrazole-Carbohydrazide Derivatives with Dual Activity as Antioxidant and Anti-Proliferative Drugs on Breast Cancer Targeting the HDAC6. Pharmaceuticals, 2022, 15, 690.	1.7	1
88	ExoDielsâ€“Alder adducts betweenortho- andpara-N-acetoxyphenylmaleimides and furan. Acta Crystallographica Section C: Crystal Structure Communications, 2004, 60, o427-o430.	0.4	0
89	Ethyl (E)-3-(2-hydroxyphenyl)-2-(morpholinocarbonyl)propenoate. Acta Crystallographica Section C: Crystal Structure Communications, 2004, 60, o517-o519.	0.4	0
90	Diethyl piperazine-1,4-diyldioxalate. Acta Crystallographica Section C: Crystal Structure Communications, 2004, 60, o699-o701.	0.4	0

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91	DimethylN,Nâ€²-(1,2-phenylene)dicarbamate. Acta Crystallographica Section E: Structure Reports Online, 2004, 60, o1488-o1490.	0.2	0
92	The E and Z Isomers of 3-(Benzoxazol-2-yl)prop-2-enoic Acid. ChemInform, 2005, 36, no.	0.1	0
93	1,1â€²,3,3â€²-Tetrabenzyl-2,2â€²-biimidazolidine. Acta Crystallographica Section E: Structure Reports Online, 2005, 61, o2464-o2466.	0.2	0
94	2,2â€²-Bi-1,3-thiazolidine. Acta Crystallographica Section E: Structure Reports Online, 2006, 62, o525-o527.	0.2	0
95	Microcrystalline solidâ€“solid transformations of conformationally-responsive solvates, desolvates and a salt of N,Nâ€²-(1,4-phenylene)dioxalamic acid: the energetics of hydrogen bonding and nÍ€ â†' Ï€* interactions. CrystEngComm, 2022, 24, 1017-1034.	1.3	0
96	N-substitution Reactions of 2-Aminobenzimidazoles to Access Pharmacophores. Current Organic Synthesis, 2022, 19, .	0.7	0