

Itzia Irene Padilla-Martínez

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Microcrystalline solid-solid transformations of conformationally-responsive solvates, desolvates and a salt of N,N ² -(1,4-phenylene)dioxalamic acid: the energetics of hydrogen bonding and n/í€ â†' í€* interactions. <i>CrystEngComm</i> , 2022, 24, 1017-1034.	1.3	0
2	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> , 2022, 23, 3229.	1.8	7
3	N-substitution Reactions of 2-Aminobenzimidazoles to Access Pharmacophores. <i>Current Organic Synthesis</i> , 2022, 19, .	0.7	0
4	Dihydropyrazole-Carbohydrazide Derivatives with Dual Activity as Antioxidant and Anti-Proliferative Drugs on Breast Cancer Targeting the HDAC6. <i>Pharmaceuticals</i> , 2022, 15, 690.	1.7	1
5	Synthesis, Optical Characterization in Solution and Solid-State, and DFT Calculations of 3-Acetyl and 3-(1 ² -(2 ² -Phenylhydrazono)ethyl)-coumarin-(7)-substituted Derivatives. <i>Molecules</i> , 2022, 27, 3677.	1.7	2
6	Modifications on the Tetrahydroquinoline Scaffold Targeting a Phenylalanine Cluster on GPER as Antiproliferative Compounds against Renal, Liver and Pancreatic Cancer Cells. <i>Pharmaceuticals</i> , 2021, 14, 49.	1.7	8
7	Myeloperoxidase Inhibitory and Antioxidant Activities of (E)-2-Hydroxy-1 ² -aminocinnamic Acids Obtained through Microwave-Assisted Synthesis. <i>Pharmaceuticals</i> , 2021, 14, 513.	1.7	5
8	A New Symmetrical Thiazolidinedione Derivative: In Silico Design, Synthesis, and In Vivo Evaluation on a Streptozotocin-Induced Rat Model of Diabetes. <i>Processes</i> , 2021, 9, 1294.	1.3	6
9	Repurposing FDA Drug Compounds against Breast Cancer by Targeting EGFR/HER2. <i>Pharmaceuticals</i> , 2021, 14, 791.	1.7	7
10	Benzothiazoles from Condensation of o-Aminothiophenoles with Carboxylic Acids and Their Derivatives: A Review. <i>Molecules</i> , 2021, 26, 6518.	1.7	9
11	Preclinical Pharmacokinetics and Acute Toxicity in Rats of 5-[[[(2E)-3-Bromo-3-carboxyprop-2-enoyl]amino]-2-hydroxybenzoic Acid: A Novel 5-Aminosalicyclic Acid Derivative with Potent Anti-Inflammatory Activity. <i>Molecules</i> , 2021, 26, 6801.	1.7	1
12	Design, synthesis, molecular docking and in vitro evaluation of benzothiazole derivatives as 11 ² -hydroxysteroid dehydrogenase type 1 inhibitors. <i>Molecular Diversity</i> , 2020, 24, 1-14.	2.1	3
13	Crystal Structure and Supramolecular Architecture of Antiallergic Diphenylene Diethyl Dioxalamates. <i>Crystals</i> , 2020, 10, 1048.	1.0	1
14	Mechanochemical Synthesis and Structure of the Tetrahydrate and Mesoporous Anhydrous Metforminium(2+)-N,N ² -1,4-Phenylenedioxalamic Acid (1:2) Salt: The Role of Hydrogen Bonding and nâ†'í€* Charge Assisted Interactions. <i>Pharmaceutics</i> , 2020, 12, 998.	2.0	5
15	Surface Modification of the Ti-6Al-4V Alloy by Anodic Oxidation and Its Effect on Osteoarticular Cell Proliferation. <i>Coatings</i> , 2020, 10, 491.	1.2	9
16	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> , 2020, 28, 115427.	1.4	17
17	Inhibitory activity on cholinesterases produced by aryl-phthalimide derivatives: green synthesis, in silico and in vitro evaluation. <i>Medicinal Chemistry Research</i> , 2020, 29, 1030-1040.	1.1	5
18	Profiling the interaction of 1 ² -phenylbenzimidazoles to cyclooxygenases. <i>Journal of Molecular Recognition</i> , 2019, 32, e2801.	1.1	1

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19	Isothioureas, Ureas, and Their N-Methyl Amides from 2-Aminobenzothiazole and Chiral Amino Acids. <i>Molecules</i> , 2019, 24, 3391.	1.7	4
20	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> , 2019, 23, 361-370.	2.1	5
21	Evaluation of a new benzothiazole derivative with antioxidant activity in the initial phase of acetaminophen toxicity. <i>Arabian Journal of Chemistry</i> , 2019, 12, 3871-3882.	2.3	16
22	2-Acetyl-4-aminoresorcinol derivatives: synthesis, antioxidant activity and molecular docking studies. <i>Medicinal Chemistry Research</i> , 2018, 27, 1186-1197.	1.1	5
23	Ephedrines as Chiral Auxiliaries in Enantioselective Alkylation Reactions of Acyl Ephedrine Amides and Esters: A Review. <i>Current Organic Synthesis</i> , 2018, 15, 38-83.	0.7	5
24	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> , 2018, 12, 74.	2.6	10
25	Involvement of conformational isomerism in the complexity of the crystal network of 1-(4-nitrophenyl)-1 <i>H</i> -1,3-benzimidazole derivatives driven by Câ€”H...<i>A</i> (<i>A</i> =) Tj ETQq1 1 0.784314 rgBT /Overloc ONO...C<i>sp</i> ² interactions. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2018, 74, 128-136.	0.2	1
26	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> , 2017, 128, 154-167.	2.6	13
27	In silico design, chemical synthesis and toxicological evaluation of 1,3-thiazolidine-2,4-dione derivatives as PPAR β agonists. <i>Regulatory Toxicology and Pharmacology</i> , 2017, 86, 25-32.	1.3	10
28	Positional Isomerism and Steric Effects in the Self-Assemblies of Phenylene Bis-Monothiooxalamides. <i>Crystal Growth and Design</i> , 2017, 17, 2513-2528.	1.4	8
29	Aromatic Regions Govern the Recognition of NADPH Oxidase Inhibitors as Diapocynin and its Analogues. <i>Archiv Der Pharmazie</i> , 2017, 350, 1700041.	2.1	7
30	Novel synthesis of isoindoline/isoindoline-1,3-dione derivatives under solventless conditions and evaluation with the human D2 receptor. <i>Medicinal Chemistry Research</i> , 2017, 26, 2420-2431.	1.1	11
31	Helical Arrangement of 2-(4-hydroxy-3-methoxyphenyl)-Benzothiazole in Crystal Formation and Biological Evaluation on HeLa Cells. <i>Crystals</i> , 2017, 7, 171.	1.0	4
32	Solventless Synthesis of Poly(pyrazolyl)phenyl-methane Ligands and Thermal Transformation of Tris(3,5-dimethylpyrazol-1-yl)phenylmethane. <i>Molecules</i> , 2017, 22, 441.	1.7	1
33	N-(2-hydroxyphenyl)-2-propylpentanamide, a valproic acid aryl derivative designed <i>in silico</i> with improved anti-proliferative activity in HeLa, rhabdomyosarcoma and breast cancer cells. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2016, 31, 140-149.	2.5	32
34	Fluorine-containing benzothiazole as a novel trypanocidal agent: design, in silico study, synthesis and activity evaluation. <i>Medicinal Chemistry Research</i> , 2016, 25, 211-224.	1.1	18
35	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> , 2015, 45, 244-250.	0.5	3
36	Insights on the role of boron containing moieties in the design of new potent and efficient agonists targeting the β_2 adrenoceptor. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2015, 25, 820-825.	1.0	8

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37	Carbonylâ€“carbonyl interactions and amide Î€-stacking as the directing motifs of the supramolecular assembly of ethylN-(2-acetylphenyl)oxalamate in a synperiplanar conformation. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2015, 71, 381-385.	0.2	4
38	NMR Structural Study of the Prototropic Equilibrium in Solution of Schiff Bases as Model Compounds. <i>Molecules</i> , 2014, 19, 459-481.	1.7	15
39	Synthesis and Structure of Sulfur Derivatives from 2-Aminobenzimidazole. <i>Molecules</i> , 2014, 19, 13878-13893.	1.7	4
40	Solid State Structure and Solution Thermodynamics of Three-Centered Hydrogen Bonds (Oâ€“Hâ€“O) Using N-(2-Benzoyl-phenyl) Oxalyl Derivatives as Model Compounds. <i>Molecules</i> , 2014, 19, 14446-14460.	1.7	14
41	Iridaoxacyclohexadiene-Bridged Mixed-Valence Iridium Cyclooctadiene Complex: Oxidative Addition and Hydrogen-Transfer to Coordinated Cyclooctadiene. <i>Organometallics</i> , 2014, 33, 6305-6318.	1.1	11
42	Molecular Complexes of Diethyl 1,3-Phenyldioxalamate and Resorcinols: Conformational Switching through Intramolecular Three-Centered Hydrogen-Bonding. <i>Crystal Growth and Design</i> , 2014, 14, 628-642.	1.4	14
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> , 2014, 23, 1581-1590.	1.1	4
44	Design of Multi-Target Compounds as AChE, BACE1, and Amyloid-Î²1-42 Oligomerization Inhibitors: In Silico and In Vitro Studies. <i>Journal of Alzheimer's Disease</i> , 2014, 41, 1073-1085.	1.2	23
45	Î€-stacking and Caâ€“H...N (â€“Xâ€“Y)â€“D (â€“Xâ€“Y) = H, NO ₂ ; â€“D = O, Î€) interactions in the crystal network of both Caâ€“H...N and Î€-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> , 2014, 70, 55-59.	0.2	3
46	Three Amino Acid Derivatives of Valproic Acid: Design, Synthesis, Theoretical and Experimental Evaluation as Anticancer Agents. <i>Anti-Cancer Agents in Medicinal Chemistry</i> , 2014, 14, 984-993.	0.9	5
47	Helical supramolecular assembly of 2,2-bis[3-(morpholin-4-yl)propyl]-N,N-dimethyl sulfoxide monosolvate. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2013, 69, 66-69.	0.4	1
48	2-(4-Hydroxyphenyl)-1H-benzimidazol-3-ium chloride monohydrate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2013, 69, o1485-o1486.	0.2	1
49	Ethers and esters derived from apocynin avoid the interaction between p47 ^{phox} and p22 ^{phox} subunits of NADPH oxidase: evaluation <i>in vitro</i> and <i>in silico</i> . <i>Bioscience Reports</i> , 2013, 33, .	1.1	15
50	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> , 2012, 31, 5438-5451.	1.1	18
51	Carbonylâ€“carbonyl and carbonylâ€“Î€ 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-Î²-N2)methane]iridium(III) trifluoromethanesulfonate. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2012, 68, m367-m369.	0.4	1
52	A Synthetic Method to Access Symmetric and Non-Symmetric 2-(N,N'-disubstituted)guanidinebenzothiazoles. <i>Molecules</i> , 2012, 17, 10178-10191.	1.7	6
53	Supramolecular architectures of conformationally controlled 1,3-phenyl-dioxalamic molecular clefts through hydrogen bonding and steric restraints. <i>CrystEngComm</i> , 2011, 13, 4748.	1.3	13
54	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> , 2011, 16, 915-932.	1.7	13

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55	Efficient synthesis of cis-thiazolidinethiones derived from ephedrines. <i>Tetrahedron: Asymmetry</i> , 2011, 22, 394-398.	1.8	6
56	N,Nâ€²-Bis(4-aminobenzyl)oxalamide. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2011, 67, o398-o398.	0.2	1
57	An efficient synthesis of aziridines from ephedrines. <i>Tetrahedron: Asymmetry</i> , 2010, 21, 909-913.	1.8	8
58	Intramolecular Carbonylâ€“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> , 2010, 40, 1024-1028.	0.5	1
59	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 I ₂ adrenoceptor. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2010, 20, 5623-5629.	1.0	13
60	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> , 2010, 15, 1513-1530.	1.7	10
61	The zwitterion of 4-nitro-2-[(2-(piperidin-1-yl)ethyl)iminomethyl]phenol. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2009, 65, o8-o10.	0.4	8
62	Competition between OHâ€“O and multiple halogenâ€“dipole interactions on the formation of intramolecular three-centred hydrogen bond in 3-acyl coumarins. <i>CrystEngComm</i> , 2009, 11, 1451.	1.3	19
63	Carbonylâ€“carbonyl, carbonylâ€“F 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. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2007, 63, o239-o242.	0.4	21
64	Reactivity of chlorodeoxypseudoephedrines with oxo-, thio-, and selenocyanates. <i>Tetrahedron: Asymmetry</i> , 2007, 18, 123-130.	1.8	12
65	S-Methyl-(N-aryl and -N-alkyl)isothioureas derived from 2-aminobenzothiazole. <i>Arkivoc</i> , 2007, 2008, 200-209.	0.3	2
66	Two isomeric butadieneâ€“N-(acetoxyphenyl)maleimide Dielsâ€“Alder adducts: supramolecular structure directed by Câ€“H...X (X= O and F) hydrogen bonds and perpendicular dipole carbonylâ€“carbonyl interactions. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2006, 62, o125-o128.	0.4	1
67	Facial F...Cl...F interactions as the directing motif of the supramolecular structures of Mg ²⁺ and Ca ²⁺ bis[hydrotris(pyrazolyl)borate] chloroform disolvates. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2006, 62, m132-m135.	0.4	2
68	2,2â€“Bi-1,3-thiazolidine. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2006, 62, o525-o527.	0.2	0
69	1,3-Heterazolidines-2-heterounsaturated compounds derived from ephedrines. <i>Tetrahedron: Asymmetry</i> , 2006, 17, 1499-1505.	1.8	5
70	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> , 2006, 2003, 100-111.	0.3	5
71	The E and Z Isomers of 3-(Benzoxazol-2-yl)prop-2-enoic Acid. <i>ChemInform</i> , 2005, 36, no.	0.1	0
72	1,1,2,2-Tetrachloro-1,2-diphenylethane. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2005, 61, o678-o680.	0.2	2

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73	Di-1/4-diphenylphosphido-bis[tricarbonyliron(II)] dichloromethane solvate. Acta Crystallographica Section E: Structure Reports Online, 2005, 61, m1475-m1477.	0.2	1
74	1,1,3,3-Tetrabenzyl-2,2-biimidazolidine. Acta Crystallographica Section E: Structure Reports Online, 2005, 61, o2464-o2466.	0.2	0
75	DiethylN-cyclohexane-1,4-diylidioxalamate. Acta Crystallographica Section E: Structure Reports Online, 2005, 61, o2994-o2996.	0.2	3
76	Switching from twisted to planar oxamide molecular cavities through intramolecular three centered hydrogen bonding. Arkivoc, 2005, 2005, 401-415.	0.3	6
77	ExoDiels-Alder adducts betweenortho- andpara-N-acetoxyphenylmaleimides and furan. Acta Crystallographica Section C: Crystal Structure Communications, 2004, 60, o427-o430.	0.4	0
78	Ethyl (E)-3-(2-hydroxyphenyl)-2-(morpholinocarbonyl)propenoate. Acta Crystallographica Section C: Crystal Structure Communications, 2004, 60, o517-o519.	0.4	0
79	TheEandZisomers of 3-(benzoxazol-2-yl)prop-2-enoic acid. Acta Crystallographica Section C: Crystal Structure Communications, 2004, 60, o723-o726.	0.4	3
80	Diethyl piperazine-1,4-diylidioxalate. Acta Crystallographica Section C: Crystal Structure Communications, 2004, 60, o699-o701.	0.4	0
81	DimethylN-(1,2-phenylene)dicarbamate. Acta Crystallographica Section E: Structure Reports Online, 2004, 60, o1488-o1490.	0.2	0
82	N-Cyclohexyl-2-oxo-2H-1-benzopyran-3-carboxamide. Acta Crystallographica Section E: Structure Reports Online, 2004, 60, o2306-o2308.	0.2	1
83	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.	1.4	20
84	2-Amino-1,3-benzothiazole-ethyl coumarin-3-carboxylate (1/1). Acta Crystallographica Section C: Crystal Structure Communications, 2003, 59, o544-o546.	0.4	4
85	EthylN-phenyloxamate. Acta Crystallographica Section C: Crystal Structure Communications, 2003, 59, o541-o543.	0.4	8
86	DiethylN-m-phenylenedioxamate. Acta Crystallographica Section E: Structure Reports Online, 2003, 59, o825-o827.	0.2	9
87	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.	0.2	2
88	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.	1.4	64
89	Synthesis and Reactivity of [Ir(C ₂ H ₄) ₂ Tp ^{Me} Me ₂][PF ₆] (Tp ^{Me} Me ₂ = Tris(3,5-dimethylpyrazolyl)methane): Comparison with the Analogous Tp ^{Me} Me ₂ Derivatives (Tp ^{Me} Me ₂ = Hydrotris(3,5-dimethylpyrazolyl)borate). Organometallics, 2002, 21, 93-104.	1.1	33
90	Further insight into three center hydrogen bonding. Participation in tautomeric equilibria of heterocyclic amides. Perkin Transactions II RSC, 2001, , 1817-1823.	1.1	14

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91	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
92	New Imidazabole Derivatives: Dimers of Carbene-Borane Adducts. European Journal of Inorganic Chemistry, 1998, 1998, 1547-1553.	1.0	29
93	Benzazole-N(SINGLE BOND)BH ₃ adducts. Reductive transposition of 2-benzimidazole, 2-benzothiazole, and 2-benzoxazole N(SINGLE BOND)BH ₃ adducts to 1,3,2-benzimidazaborole, 1,3,2-benzoxaborole, and 1,3,2-benzothiazaborole. Heteroatom Chemistry, 1996, 7, 323-335.	0.4	18
94	Azolyborane adducts. Structural and conformational analysis by x-ray diffraction and NMR. Protic hydroxydic (C ₁₂ H ₁₀ O ₂) and Protic fluoride (C ₁₂ H ₁₀ F ₂) interactions. Chemische Berichte, 1996, 129, 441-449.	0.5	19
95	From Azole-Borane Adducts to Azaboles Molecular Structure of an Imidazabole. Chemische Berichte, 1994, 127, 343-346.	0.2	25
96	NMR Study of isolobal N-CH ₃ ⁺ , N-BH ₃ and N-BF ₃ imidazole derivatives. Magnetic Resonance in Chemistry, 1993, 31, 189-193.	1.1	29