## Paola Gratteri

List of Publications by Year in descending order

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138 papers 3,970 citations

94433 37 h-index 54 g-index

141 all docs

141 docs citations

times ranked

141

4147 citing authors

| #  | Article  | IF          | CITATIONS |
|----|--|-------------|-----------|
| 1  | Novel benzenesulfonamideâ€bearing pyrazoles and 1,2,4â€thiadiazoles as selective carbonic anhydrase inhibitors. Archiv Der Pharmazie, 2022, 355, e2100241.   | 4.1         | 11        |
| 2  | Natural inspired ligustrazine-based SLC-0111 analogues as novel carbonic anhydrase inhibitors. European Journal of Medicinal Chemistry, 2022, 228, 114008.   | 5.5         | 12        |
| 3  | 2-(2-Hydroxyethyl)piperazine derivatives as potent human carbonic anhydrase inhibitors: Synthesis, enzyme inhibition, computational studies and antiglaucoma activity. European Journal of Medicinal Chemistry, 2022, 228, 114026.   | 5.5         | 1         |
| 4  | The three-tails approach as a new strategy to improve selectivity of action of sulphonamide inhibitors against tumour-associated carbonic anhydrase IX and XII. Journal of Enzyme Inhibition and Medicinal Chemistry, 2022, 37, 930-939.   | 5.2         | 19        |
| 5  | Calixarenes Incorporating Sulfonamide Moieties: Versatile Ligands for Carbonic Anhydrases<br>Inhibition. Chemistry - A European Journal, 2022, 28, .   | 3.3         | 3         |
| 6  | Computationally enhanced X-ray diffraction analysis of a gold(III) complex interacting with the human telomeric DNA G-quadruplex. Unravelling non-unique ligand positioning. International Journal of Biological Macromolecules, 2022, 211, 506-513.                               | 7.5         | 1         |
| 7  | Novel 3-substituted coumarins as selective human carbonic anhydrase IX and XII inhibitors: Synthesis, biological and molecular dynamics analysis. European Journal of Medicinal Chemistry, 2021, 209, 112897.  | <b>5.</b> 5 | 38        |
| 8  | Ninhydrins inhibit carbonic anhydrases directly binding to the metal ion. European Journal of Medicinal Chemistry, $2021, 209, 112875$ .   | 5.5         | 18        |
| 9  | Identification of N-phenyl-2-(phenylsulfonyl)acetamides/propanamides as new SLC-0111 analogues:<br>Synthesis and evaluation of the carbonic anhydrase inhibitory activities. European Journal of<br>Medicinal Chemistry, 2021, 218, 113360.  | 5.5         | 24        |
| 10 | Novel benzenesulfonamides aryl and arylsulfone conjugates adopting tail/dual tail approaches: Synthesis, carbonic anhydrase inhibitory activity and molecular modeling studies. European Journal of Medicinal Chemistry, 2021, 221, 113486.  | 5.5         | 19        |
| 11 | Inhibition of α-, β- and γ-carbonic anhydrases from the pathogenic bacterium <i>Vibrio cholerae</i> with aromatic sulphonamides and clinically licenced drugs – a joint docking/molecular dynamics study. Journal of Enzyme Inhibition and Medicinal Chemistry, 2021, 36, 469-479. | 5.2         | 14        |
| 12 | Selective Inhibition of Helicobacter pylori Carbonic Anhydrases by Carvacrol and Thymol Could Impair Biofilm Production and the Release of Outer Membrane Vesicles. International Journal of Molecular Sciences, 2021, 22, 11583.  | 4.1         | 35        |
| 13 | Discovery of New $1,1\hat{a}\in^2$ -Biphenyl-4-sulfonamides as Selective Subnanomolar Human Carbonic Anhydrase II Inhibitors. ACS Medicinal Chemistry Letters, 2020, $11,633-637$ .  | 2.8         | 2         |
| 14 | Synthesis, biological and molecular dynamics investigations with a series of triazolopyrimidine/triazole-based benzenesulfonamides as novel carbonic anhydrase inhibitors. European Journal of Medicinal Chemistry, 2020, 185, 111843.   | 5.5         | 38        |
| 15 | Bioisosteric Development of Multitarget Nonsteroidal Anti-Inflammatory Drug–Carbonic Anhydrases Inhibitor Hybrids for the Management of Rheumatoid Arthritis. Journal of Medicinal Chemistry, 2020, 63, 2325-2342.   | 6.4         | 26        |
| 16 | Sulfonamide-based ring-fused analogues for CAN508 as novel carbonic anhydrase inhibitors endowed with antitumor activity: Design, synthesis, and inÂvitro biological evaluation. European Journal of Medicinal Chemistry, 2020, 189, 112019.                                       | 5.5         | 42        |
| 17 | 3-Methylthiazolo[3,2-a]benzimidazole-benzenesulfonamide conjugates as novel carbonic anhydrase inhibitors endowed with anticancer activity: Design, synthesis, biological and molecular modeling studies. European Journal of Medicinal Chemistry, 2020, 207, 112745.              | 5.5         | 45        |
| 18 | Novel insights on saccharin- and acesulfame-based carbonic anhydrase inhibitors: design, synthesis, modelling investigations and biological activity evaluation. Journal of Enzyme Inhibition and Medicinal Chemistry, 2020, 35, 1891-1905.  | 5.2         | 14        |

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|----|--|--------------|-----------|
| 19 | Synthesis, Computational Studies and Assessment of <i>in Vitro</i> Activity of Squalene Derivatives as Carbonic Anhydrase Inhibitors. ChemMedChem, 2020, 15, 2052-2057.  | 3.2          | 4         |
| 20 | Benzoxaboroles: New Potent Inhibitors of the Carbonic Anhydrases of the Pathogenic Bacterium <i>Vibrio cholerae</i> . ACS Medicinal Chemistry Letters, 2020, 11, 2277-2284.  | 2.8          | 25        |
| 21 | Phenyl(thio)phosphon(amid)ate Benzenesulfonamides as Potent and Selective Inhibitors of Human<br>Carbonic Anhydrases II and VII Counteract Allodynia in a Mouse Model of Oxaliplatin-Induced<br>Neuropathy. Journal of Medicinal Chemistry, 2020, 63, 5185-5200.                             | 6.4          | 16        |
| 22 | Halogenated isophthalamides and dipicolineamides: the role of the halogen substituents in the anion binding properties. Dalton Transactions, 2020, 49, 9231-9238.  | 3.3          | 5         |
| 23 | Sulfonamide Inhibitors of Human Carbonic Anhydrases Designed through a Three-Tails Approach: Improving Ligand/Isoform Matching and Selectivity of Action. Journal of Medicinal Chemistry, 2020, 63, 7422-7444.   | 6.4          | 75        |
| 24 | Discovery of first-in-class multi-target adenosine A2A receptor antagonists-carbonic anhydrase IX and XII inhibitors. 8-Amino-6-aryl-2-phenyl-1,2,4-triazolo [4,3-a]pyrazin-3-one derivatives as new potential antitumor agents. European Journal of Medicinal Chemistry, 2020, 201, 112478. | 5 <b>.</b> 5 | 9         |
| 25 | Sensing Zn2+ in Aqueous Solution with a Fluorescent Scorpiand Macrocyclic Ligand Decorated with an Anthracene Bearing Tail. Molecules, 2020, 25, 1355.   | 3.8          | 21        |
| 26 | Perfluoroalkyl Substances of Significant Environmental Concern Can Strongly Inhibit Human Carbonic Anhydrase Isozymes. Analytical Chemistry, 2020, 92, 4614-4622.  | 6.5          | 28        |
| 27 | Pyridine Derivative of the Natural Alkaloid Berberine as Human Telomeric G <sub>4</sub> -DNA Binder: A Solution and Solid-State Study. ACS Medicinal Chemistry Letters, 2020, 11, 645-650.   | 2.8          | 20        |
| 28 | Aryl-4,5-dihydro-1H-pyrazole-1-carboxamide Derivatives Bearing a Sulfonamide Moiety Show Single-digit Nanomolar-to-Subnanomolar Inhibition Constants against the Tumor-associated Human Carbonic Anhydrases IX and XII. International Journal of Molecular Sciences, 2020, 21, 2621.         | 4.1          | 5         |
| 29 | The antibiotic furagin and its derivatives are isoform-selective human carbonic anhydrase inhibitors.<br>Journal of Enzyme Inhibition and Medicinal Chemistry, 2020, 35, 1011-1020.  | 5.2          | 27        |
| 30 | Phosphorus versus Sulfur: Discovery of Benzenephosphonamidates as Versatile Sulfonamideâ€Mimic Chemotypes Acting as Carbonic Anhydrase Inhibitors. Chemistry - A European Journal, 2019, 25, 1188-1192.  | 3.3          | 59        |
| 31 | Carbonic anhydrases from pathogens. , 2019, , 419-448.   |              | 1         |
| 32 | Synthesis, biological evaluation and in silico studies with 4-benzylidene-2-phenyl-5(4H)-imidazolone-based benzenesulfonamides as novel selective carbonic anhydrase IX inhibitors endowed with anticancer activity. Bioorganic Chemistry, 2019, 90, 103102.                                 | 4.1          | 21        |
| 33 | 3-Hydrazinoisatin-based benzenesulfonamides as novel carbonic anhydrase inhibitors endowed with anticancer activity: Synthesis, inÂvitro biological evaluation and in silico insights. European Journal of Medicinal Chemistry, 2019, 184, 111768.   | 5.5          | 49        |
| 34 | From random to rational: A discovery approach to selective subnanomolar inhibitors of human carbonic anhydrase IV based on the Castagnoli-Cushman multicomponent reaction. European Journal of Medicinal Chemistry, 2019, 182, 111642.   | 5.5          | 10        |
| 35 | Continued exploration and tail approach synthesis of benzenesulfonamides containing triazole and dual triazole moieties as carbonic anhydrase I, II, IV and IX inhibitors. European Journal of Medicinal Chemistry, 2019, 183, 111698.   | 5.5          | 38        |
| 36 | New Rigid Nicotine Analogues, Carrying a Norbornane Moiety, Are Potent Agonists of $\hat{l}\pm7$ and $\hat{l}\pm3^*$ Nicotinic Receptors. Journal of Medicinal Chemistry, 2019, 62, 1887-1901.   | 6.4          | 6         |

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| 37 | Selenols: a new class of carbonic anhydrase inhibitors. Chemical Communications, 2019, 55, 648-651.  | 4.1              | 56        |
| 38 | Effect of structure levels on surface-enhanced Raman scattering of human telomeric G-quadruplexes in diluted and crowded media. Analytical and Bioanalytical Chemistry, 2019, 411, 5197-5207.  | 3.7              | 3         |
| 39 | Novel Diamide-Based Benzenesulfonamides as Selective Carbonic Anhydrase IX Inhibitors Endowed with Antitumor Activity: Synthesis, Biological Evaluation and In Silico Insights. International Journal of Molecular Sciences, 2019, 20, 2484.   | 4.1              | 21        |
| 40 | Solid State and Solution Study on the Formation of Inorganic Anion Complexes with a Series of Tetrazine-Based Ligands. Molecules, 2019, 24, 2247.  | 3.8              | 11        |
| 41 | Appraisal of anti-protozoan activity of nitroaromatic benzenesulfonamides inhibiting carbonic anhydrases from <i>Trypanosoma cruzi</i> and <i>Leishmania donovani</i> Inhibition and Medicinal Chemistry, 2019, 34, 1164-1171.   | 5.2              | 18        |
| 42 | Tales of the Unexpected: The Case of Zirconium(IV) Complexes with Desferrioxamine. Molecules, 2019, 24, 2098.  | 3.8              | 24        |
| 43 | Î <sup>2</sup> 3-Adrenoreceptor Activity Limits Apigenin Efficacy in Ewing Sarcoma Cells: A Dual Approach to Prevent<br>Cell Survival. International Journal of Molecular Sciences, 2019, 20, 2149.  | 4.1              | 9         |
| 44 | Polypharmacology of epacadostat: a potent and selective inhibitor of the tumor associated carbonic anhydrases IX and XII. Chemical Communications, 2019, 55, 5720-5723.  | 4.1              | 18        |
| 45 | Induction of a Fourâ€Way Junction Structure in the DNA Palindromic Hexanucleotide 5′â€d(CGTACG)â€3′ b<br>Mononuclear Platinum Complex. Angewandte Chemie, 2019, 131, 9478-9482.  | y <sub>2.0</sub> | 4         |
| 46 | Induction of a Fourâ€Way Junction Structure in the DNA Palindromic Hexanucleotide 5′â€d(CGTACG)â€3′ b Mononuclear Platinum Complex. Angewandte Chemie - International Edition, 2019, 58, 9378-9382.  | y a<br>13.8      | 24        |
| 47 | $\hat{l}_{\pm}, \hat{l}^{3}$ -Diketocarboxylic Acids and Their Esters Act as Carbonic Anhydrase IX and XII Selective Inhibitors. ACS Medicinal Chemistry Letters, 2019, 10, 661-665.   | 2.8              | 18        |
| 48 | 4-Substituted benzenesulfonamides featuring cyclic imides moieties exhibit potent and isoform-selective carbonic anhydrase II/IX inhibition. Bioorganic Chemistry, 2019, 83, 198-204.  | 4.1              | 23        |
| 49 | Enhancement of the tail hydrophobic interactions within the carbonic anhydrase IX active site via structural extension: Design and synthesis of novel N-substituted isatins-SLC-0111 hybrids as carbonic anhydrase inhibitors and antitumor agents. European Journal of Medicinal Chemistry, 2019, 162, 147-160.           | 5.5              | 81        |
| 50 | N-Nitrosulfonamides as Carbonic Anhydrase Inhibitors: A Promising Chemotype for Targeting Chagas Disease and Leishmaniasis. ACS Medicinal Chemistry Letters, 2019, 10, 413-418.  | 2.8              | 21        |
| 51 | Deciphering the Mechanism of Human Carbonic Anhydrases Inhibition with Sulfocoumarins:<br>Computational and Experimental Studies. Chemistry - A European Journal, 2018, 24, 7840-7844.   | 3.3              | 62        |
| 52 | Natural Polyphenols Selectively Inhibit β arbonic Anhydrase from the Dandruffâ€Producing Fungus <i>Malassezia globosa</i> : Activity and Modeling Studies. ChemMedChem, 2018, 13, 816-823.   | 3.2              | 32        |
| 53 | 2-Benzylpiperazine: A new scaffold for potent human carbonic anhydrase inhibitors. Synthesis, enzyme inhibition, enantioselectivity, computational and crystallographic studies and inÂvivo activity for a new class of intraocular pressure lowering agents. European Journal of Medicinal Chemistry, 2018, 151, 363-375. | 5.5              | 29        |
| 54 | Dual-tail arylsulfone-based benzenesulfonamides differently match the hydrophobic and hydrophilic halves of human carbonic anhydrases active sites: Selective inhibitors for the tumor-associated hCA IX isoform. European Journal of Medicinal Chemistry, 2018, 152, 1-9.   | 5.5              | 60        |

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| 55 | Synthesis, biological evaluation and computational studies of novel iminothiazolidinone benzenesulfonamides as potent carbonic anhydrase II and IX inhibitors. Bioorganic Chemistry, 2018, 77, 381-386.   | 4.1  | 27        |
| 56 | Use of Innovative (Micro)Extraction Techniques to Characterise <scp><i>Harpagophytum procumbens</i></scp> Root and its Commercial Food Supplements. Phytochemical Analysis, 2018, 29, 233-241.  | 2.4  | 38        |
| 57 | Interaction of a gold( <scp>i</scp> ) dicarbene anticancer drug with human telomeric DNA G-quadruplex: solution and computationally aided X-ray diffraction analysis. Dalton Transactions, 2018, 47, 16132-16138.   | 3.3  | 35        |
| 58 | 4-Hydroxy-3-nitro-5-ureido-benzenesulfonamides Selectively Target the Tumor-Associated Carbonic Anhydrase Isoforms IX and XII Showing Hypoxia-Enhanced Antiproliferative Profiles. Journal of Medicinal Chemistry, 2018, 61, 10860-10874.                             | 6.4  | 48        |
| 59 | Steroids interfere with human carbonic anhydrase activity by using alternative binding mechanisms. Journal of Enzyme Inhibition and Medicinal Chemistry, 2018, 33, 1453-1459.   | 5.2  | 69        |
| 60 | Discovery of β-Adrenergic Receptors Blocker–Carbonic Anhydrase Inhibitor Hybrids for Multitargeted Antiglaucoma Therapy. Journal of Medicinal Chemistry, 2018, 61, 5380-5394.   | 6.4  | 53        |
| 61 | Assessment of human telomeric G-quadruplex structures using surface-enhanced Raman spectroscopy. Analytical and Bioanalytical Chemistry, 2017, 409, 2285-2295.  | 3.7  | 23        |
| 62 | Novel indolin-2-one-based sulfonamides as carbonic anhydrase inhibitors: Synthesis, inÂvitro biological evaluation against carbonic anhydrases isoforms I, II, IV and VII and molecular docking studies. European Journal of Medicinal Chemistry, 2017, 127, 521-530. | 5.5  | 56        |
| 63 | Solution NMR Structure of a Ligand/Hybridâ€2â€Gâ€Quadruplex Complex Reveals Rearrangements that Affect Ligand Binding. Angewandte Chemie - International Edition, 2017, 56, 7102-7106.  | 13.8 | 52        |
| 64 | Solution NMR Structure of a Ligand/Hybridâ€2â€Gâ€Quadruplex Complex Reveals Rearrangements that Affect Ligand Binding. Angewandte Chemie, 2017, 129, 7208-7212.   | 2.0  | 20        |
| 65 | Inhibition of Malassezia globosa carbonic anhydrase with phenols. Bioorganic and Medicinal Chemistry, 2017, 25, 2577-2582.  | 3.0  | 41        |
| 66 | Dithiocarbamates effectively inhibit the $\hat{l}^2$ -carbonic anhydrase from the dandruff-producing fungus Malassezia globosa. Bioorganic and Medicinal Chemistry, 2017, 25, 1260-1265.  | 3.0  | 45        |
| 67 | Benzoxaboroles as Efficient Inhibitors of the $\hat{l}^2$ -Carbonic Anhydrases from Pathogenic Fungi: Activity and Modeling Study. ACS Medicinal Chemistry Letters, 2017, 8, 1194-1198.   | 2.8  | 47        |
| 68 | Lipoyl-Homotaurine Derivative (ADM_12) Reverts Oxaliplatin-Induced Neuropathy and Reduces Cancer Cells Malignancy by Inhibiting Carbonic Anhydrase IX (CAIX). Journal of Medicinal Chemistry, 2017, 60, 9003-9011.  | 6.4  | 12        |
| 69 | [Au(9â€methylcaffeinâ€8â€ylidene) <sub>2</sub> ] <sup>+</sup> /DNA Tel23 System: Solution, Computational, and Biological Studies. Chemistry - A European Journal, 2017, 23, 13784-13791.  | 3.3  | 7         |
| 70 | Synthesis and carbonic anhydrase inhibition of polycyclic imides incorporating N-benzenesulfonamide moieties. Bioorganic and Medicinal Chemistry, 2017, 25, 5373-5379.  | 3.0  | 23        |
| 71 | Novel 4/3-((4-oxo-5-(2-oxoindolin-3-ylidene)thiazolidin-2-ylidene)amino) benzenesulfonamides: Synthesis, carbonic anhydrase inhibitory activity, anticancer activity and molecular modelling studies. European Journal of Medicinal Chemistry, 2017, 139, 250-262.    | 5.5  | 110       |
| 72 | Inhibition of the $\hat{I}^2$ -carbonic anhydrase from the dandruff-producing fungus < i> Malassezia globosa < /i> with monothic carbamates. Journal of Enzyme Inhibition and Medicinal Chemistry, 2017, 32, 1064-1070.   | 5.2  | 33        |

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| 73 | Discovery of New Sulfonamide Carbonic Anhydrase IX Inhibitors Incorporating Nitrogenous Bases. ACS Medicinal Chemistry Letters, 2017, 8, 1314-1319.   | 2.8          | 61        |
| 74 | Role of the Benzodioxole Group in the Interactions between the Natural Alkaloids Chelerythrine and Coptisine and the Human Telomeric G-Quadruplex DNA. A Multiapproach Investigation. Journal of Natural Products, 2017, 80, 3128-3135.   | 3.0          | 11        |
| 75 | Cation, Anion and Ion-Pair Complexes with a G-3 Poly(ethylene imine) Dendrimer in Aqueous Solution. Molecules, 2017, 22, 816.   | 3.8          | 4         |
| 76 | Solution and Solidâ€State Analysis of Binding of 13â€Substituted Berberine Analogues to Human Telomeric<br>Gâ€quadruplexes. Chemistry - an Asian Journal, 2016, 11, 1107-1115.  | 3.3          | 24        |
| 77 | Determinants for Tight and Selective Binding of a Medicinal Dicarbene Gold(I) Complex to a Telomeric DNA Gâ€Quadruplex: a Joint ESI MS and XRD Investigation. Angewandte Chemie, 2016, 128, 4328-4331.  | 2.0          | 45        |
| 78 | Benzenesulfonamides Incorporating Flexible Triazole Moieties Are Highly Effective Carbonic Anhydrase Inhibitors: Synthesis and Kinetic, Crystallographic, Computational, and Intraocular Pressure Lowering Investigations. Journal of Medicinal Chemistry, 2016, 59, 10692-10704. | 6.4          | 93        |
| 79 | Determinants for Tight and Selective Binding of a Medicinal Dicarbene Gold(I) Complex to a Telomeric DNA Gâ€Quadruplex: a Joint ESI MS and XRD Investigation. Angewandte Chemie - International Edition, 2016, 55, 4256-4259.   | 13.8         | 93        |
| 80 | Enhanced curcumin permeability by SLN formulation: The PAMPA approach. LWT - Food Science and Technology, 2016, 66, 475-483.  | 5.2          | 66        |
| 81 | Antagonism/Agonism Modulation to Build Novel Antihypertensives Selectively Triggering I <sub>1</sub> -Imidazoline Receptor Activation. ACS Medicinal Chemistry Letters, 2015, 6, 496-501.   | 2.8          | 9         |
| 82 | Interactions of selected gold( <scp>iii</scp> ) complexes with DNA G quadruplexes. Dalton Transactions, 2015, 44, 3633-3639.  | 3.3          | 22        |
| 83 | Anion and ion-pair binding by a G-2 poly(ethylene imine) dendrimer. Dalton Transactions, 2013, 42, 12130.   | 3.3          | 6         |
| 84 | Metal Ion Binding by a G-2 Poly(ethylene imine) Dendrimer. Ion-Directed Self-Assembling of Hierarchical Mono- and Two-Dimensional Nanostructured Materials. Inorganic Chemistry, 2013, 52, 2125-2137.   | 4.0          | 27        |
| 85 | The crystal structure of human telomeric DNA complexed with berberine: an interesting case of stacked ligand to G-tetrad ratio higher than 1:1. Nucleic Acids Research, 2013, 41, 632-638.  | 14.5         | 129       |
| 86 | Selective binding and fluorescence sensing of diphosphate in H <sub>2</sub> OviaZn <sup>2+</sup> -induced allosteric regulation of the receptor structure. Chemical Communications, 2012, 48, 139-141.  | 4.1          | 33        |
| 87 | Insights into the Conformational Switching Mechanism of the Human Vascular Endothelial Growth Factor Receptor Type 2 Kinase Domain. Journal of Chemical Information and Modeling, 2012, 52, 483-491.  | 5 <b>.</b> 4 | 5         |
| 88 | Spectroscopic, Molecular Modeling, and NMR-Spectroscopic Investigation of the Binding Mode of the Natural Alkaloids Berberine and Sanguinarine to Human Telomeric G-Quadruplex DNA. ACS Chemical Biology, 2012, 7, 1109-1119.   | 3.4          | 102       |
| 89 | Bis(2-pyridylmethyl)alkyl(thioalkyl)diamines as promising scaffolds for the construction of fluorescent and redox chemosensors for transition and post-transition metal ions. Inorganica Chimica Acta, 2012, 381, 170-180.  | 2.4          | 7         |
| 90 | Thermodynamic and fluorescence emission properties of the Zn(II), Cd(II) and Pb(II) complexes with a fluorescent chelator bearing phenanthroline and naphthalene subunits. Inorganica Chimica Acta, 2012, 381, 229-235.   | 2.4          | 7         |

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|-----|---|-----|-----------|
| 91  | X-Ray diffraction analyses of the natural isoquinoline alkaloids Berberine and Sanguinarine complexed with double helix DNA d(CGTACG). Chemical Communications, 2011, 47, 4917.   | 4.1 | 48        |
| 92  | Diversity-oriented syntheses of 7-substituted lentiginosines. Tetrahedron, 2011, 67, 9555-9564.   | 1.9 | 18        |
| 93  | Hypericins and thioredoxin reductase: Biochemical and docking studies disclose the molecular basis for effective inhibition by naphthodianthrones. Bioorganic and Medicinal Chemistry, 2011, 19, 631-641.   | 3.0 | 11        |
| 94  | Modeling and Biological Investigations of an Unusual Behavior of Novel Synthesized Acridineâ€Based Polyamine Ligands in the Binding of Double Helix and Gâ€Quadruplex DNA. ChemMedChem, 2010, 5, 1995-2005.   | 3.2 | 12        |
| 95  | Synthesis, Biological Evaluation and Docking Studies of Casuarine Analogues: Effects of Structural Modifications at Ring B on Inhibitory Activity Towards Glucoamylase. European Journal of Organic Chemistry, 2010, 2010, 5574-5585.   | 2.4 | 47        |
| 96  | A highly pH-sensitive Zn(ii) chemosensor. Dalton Transactions, 2010, 39, 7080.  | 3.3 | 14        |
| 97  | Binding of H+ and Zn(ii) ions with a new fluorescent macrocyclic phenanthrolinophane. Dalton Transactions, 2010, 39, 10128.   | 3.3 | 14        |
| 98  | DNA interaction with Ru(ii) and Ru(ii)/Cu(ii) complexes containing azamacrocycle and dppz residues. A thermodynamic, kinetic and theoretical study Dalton Transactions, 2010, 39, 9838.   | 3.3 | 14        |
| 99  | Total Syntheses of Casuarine and Its 6â€ <i>O</i> àâ€ì±â€Glucoside: Complementary Inhibition towards Glycoside Hydrolases of the GH31 and GH37 Families. Chemistry - A European Journal, 2009, 15, 1627-1636.   | 3.3 | 92        |
| 100 | Insights into docking and scoring neuronal $\hat{l}\pm4\hat{l}^22$ nicotinic receptor agonists using molecular dynamics simulations and QM/MM calculations. Journal of Computational Chemistry, 2009, 30, 2443-2454.  | 3.3 | 23        |
| 101 | DNA Binding by a New Metallointercalator that Contains a Proflavine Group Bearing a Hanging<br>Chelating Unit. Chemistry - A European Journal, 2008, 14, 184-196.   | 3.3 | 27        |
| 102 | Synthesis, SAR and in vitro evaluation of new cyclic Arg-Gly-Asp pseudopentapeptides containing a s-cis peptide bond as integrin $\hat{l}\pm v\hat{l}^2$ 3 and $\hat{l}\pm v\hat{l}^2$ 5 ligands. Bioorganic and Medicinal Chemistry, 2008, 16, 4262-4271.  | 3.0 | 14        |
| 103 | Tuning the Activity of Zn(II) Complexes in DNA Cleavage: Clues for Design of New Efficient<br>Metallo-Hydrolases. Inorganic Chemistry, 2008, 47, 5473-5484.   | 4.0 | 52        |
| 104 | Synthesis and Biological Evaluation of Novel 9-Heteroaryl Substituted 7-Chloro-4,5-dihydro-4-oxo-1,2,4-triazolo[1,5-a]quinoxaline-2-carboxylates (TQX) as (R,S)-2-amino-3-(3-hydroxy-5-methylisoxazol-4-yl)propionic Acid (AMPA) Receptor Antagonists. Chemical and Pharmaceutical Bulletin, 2008, 56, 1085-1091. | 1.3 | 5         |
| 105 | Central Nicotinic Receptors: Structure, Function, Ligands, and Therapeutic Potential. ChemMedChem, 2007, 2, 746-767.  | 3.2 | 168       |
| 106 | Structural Investigation of the 7-Chloro-3-hydroxy-1H-quinazoline-2,4-dione Scaffold to Obtain AMPA and Kainate Receptor Selective Antagonists. Synthesis, Pharmacological, and Molecular Modeling Studies. Journal of Medicinal Chemistry, 2006, 49, 6015-6026.  | 6.4 | 48        |
| 107 | Design, synthesis and binding affinity of new nicotinic ligands. Arkivoc, 2006, 2006, 50-65.  | 0.5 | 4         |
| 108 | Insight into 2-phenylpyrazolo[1,5-a]pyrimidin-3-yl acetamides as peripheral benzodiazepine receptor ligands: Synthesis, biological evaluation and 3D-QSAR investigation. Bioorganic and Medicinal Chemistry, 2005, 13, 4821-4834.   | 3.0 | 63        |

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| 109 | A Novel Selective GABAAÎ $\pm 1$ Receptor Agonist Displaying Sedative and Anxiolytic-like Properties in Rodents. Journal of Medicinal Chemistry, 2005, 48, 6756-6760.   | 6.4          | 68        |
| 110 | Searching for a Reliable Orientation of Ligands in Their Binding Site: Comparison between a Structure-Based (Glide) and a Ligand-Based (FIGO) Approach in the Case Study of PDE4 Inhibitorsâ€. Journal of Medicinal Chemistry, 2005, 48, 1657-1665.   | 6.4          | 9         |
| 111 | Field Interaction and Geometrical Overlap:Â A New Simplex and Experimental Design Based<br>Computational Procedure for Superposing Small Ligand Molecules. Journal of Medicinal Chemistry,<br>2003, 46, 1359-1371.  | 6.4          | 34        |
| 112 | New docking CFF91 parameters specific for cyclodextrin inclusion complexes. Chemical Physics Letters, 2003, 370, 280-292.   | 2.6          | 14        |
| 113 | Synthesis and Benzodiazepine Receptor Affinity of Pyrazolo $[1,5-a]$ pyrimidine Derivatives. 3. New 6-(3-Thienyl) Series as $\hat{l}\pm 1$ Selective Ligands. Journal of Medicinal Chemistry, 2003, 46, 310-313.  | 6.4          | 36        |
| 114 | Compatibility Studies of Multicomponent Tablet Formulations. DSC and experimental mixture design. Magyar AprA³vad KözlemÃ@nyek, 2002, 68, 541-551.  | 1.4          | 38        |
| 115 | FILO (field interaction ligand optimization): a simplex strategy for searching the optimal ligand interaction field in drug design. Journal of Computer-Aided Molecular Design, 2001, 15, 57-66.  | 2.9          | 2         |
| 116 | 3D-QSAR, GRID Descriptors and Chemometric Tools in the Development of Selective Antagonists of Muscarinic Receptor., 2000, , 334-335.   |              | 0         |
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