## Giuseppe Musumarra

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Aromaticity as a quantitative concept. 1. A statistical demonstration of the orthogonality of classical and magnetic aromaticity in five- and six-membered heterocycles. Journal of the American Chemical Society, 1989, 111, 7-15.	13.7	446
2	Aromaticity as a Quantitative Concept. 2. Sixteen familiar five- and six-membered monocyclic heterocycles. Journal FÃ1⁄4r Praktische Chemie, 1990, 332, 853-869.	0.2	99
3	Aromaticity as a Quantitative Concept. 3. Benzo-fused five- and six-membered heterocycles. Journal Für Praktische Chemie, 1990, 332, 870-884.	0.2	95
4	Design and synthesis of trans 2-(furan-2-yl)vinyl heteroaromatic iodides with antitumour activity. Bioorganic and Medicinal Chemistry, 2008, 16, 4150-4159.	3.0	76
5	A Bioinformatic Approach to the Identification of Candidate Genes for the Development of New Cancer Diagnostics. Biological Chemistry, 2003, 384, 321-327.	2.5	70
6	Qualitative organic analysis. Journal of Chromatography A, 1985, 350, 151-168.	3.7	59
7	Design, Synthesis, and Biological Evaluation of 4-Alkyliden-beta Lactams:  New Products with Promising Antibiotic Activity Against Resistant Bacteria. Journal of Medicinal Chemistry, 2006, 49, 2804-2811.	6.4	57
8	A C-13 study of the reaction of 2,4,6-triarylpyrylium cations with amines. Tetrahedron, 1980, 36, 1643-1647.	1.9	51
9	New insights into aliphatic nucleophilic substitution reactions from the use of pyridines as leaving groups. Chemical Society Reviews, 1984, 13, 47.	38.1	51
10	Design, synthesis and inÂvitro antitumour activity of new heteroaryl ethylenes. European Journal of Medicinal Chemistry, 2012, 47, 221-227.	5.5	51
11	Chemometrics and cultural heritage. Chemometrics and Intelligent Laboratory Systems, 1998, 44, 363-372.	3.5	47
12	New linezolid-like 1,2,4-oxadiazoles active against Gram-positive multiresistant pathogens. European Journal of Medicinal Chemistry, 2013, 65, 533-545.	5.5	42
13	Acid Catalyzed Transesterification as a Route to Poly(3-hydroxybutyrate-co-ε-caprolactone) Copolymers from Their Homopolymers. Biomacromolecules, 2002, 3, 835-840.	5.4	38
14	A 3D-QSAR Study on the Structural Requirements for Binding to CB1 and CB2 Cannabinoid Receptors. Journal of Medicinal Chemistry, 2000, 43, 2300-2309.	6.4	36
15	A New Set of Principal Properties for Heteroaromatics Obtained by GRID. QSAR and Combinatorial Science, 1996, 15, 108-120.	1.2	34
16	Photophysics and photochemistry of 2,6-distyrylpyridine and some heteroanalogues. Physical Chemistry Chemical Physics, 2000, 2, 4005-4012.	2.8	34
17	Design, synthesis and in vitro antitumor activity of new trans 2-[2-(heteroaryl)vinyl]-1,3-dimethylimidazolium iodides. Bioorganic and Medicinal Chemistry, 2004, 12, 1689-1695.	3.0	33
18	Photochemistry and DNA-affinity of some stilbene and distyrylbenzene analogues containing pyridinium and imidazolium iodides. Journal of Photochemistry and Photobiology A: Chemistry, 2010, 216, 66-72.	3.9	33

GIUSEPPE MUSUMARRA

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19	¢€œClassical―and "Magnetic―Aromaticities as new Descriptors for Heteroaromatics in Ç Principal Properties for Heteroaromatics. QSAR and Combinatorial Science, 1993, 12, 146-151.	SAR, Part	3 [1].
20	Prediction of gas chromatographic response factors by the PLS method. Tetrahedron Computer Methodology, 1989, 2, 17-36.	0.2	29
21	Synthesis and NLO properties of new trans 2-(thiophen-2-yl)vinyl heteroaromatic iodides. Organic and Biomolecular Chemistry, 2011, 9, 1608.	2.8	29
22	Ultraviolet and infrared absorption spectra of 2-thiophenesulfonamides. Spectrochimica Acta Part A: Molecular Spectroscopy, 1974, 30, 611-618.	0.1	26
23	Cancer Institute gene expression databasea ^fa ft Supplementary information is available on Elseviera€™s World Wide Web site (http://www.elsevier.nl) or from the corresponding authors.11Abbreviations: NCI, National Cancer Institute; PLS, partial least squares modelling in latent variables or projections to latent structures: SIMCA, soft independent modelling of class analogy: PCA, principal component	4.4	26
24	analysis; PC, princ. Biochemical Pharmacology, 2001, 62, 547-553. Modeling, design and synthesis of new heteroaryl ethylenes active against the MCF-7 breast cancer cell-line. Molecular BioSystems, 2013, 9, 2426.	2.9	26
25	Application of principal components analysis to the evaluation and selection of eluent systems for the thin-layer chromatography of basic and neutral drugs. Journal of Chromatography A, 1984, 295, 31-47.	3.7	25
26	Design, synthesis and biological evaluation of trans 2-(thiophen-2-yl)vinyl heteroaromatic iodides. Bioorganic and Medicinal Chemistry, 2010, 18, 4516-4523.	3.0	24
27	In vitro antitumor activities of 2,6-di-[2-(Heteroaryl)vinyl]pyridines and pyridiniums. Bioorganic and Medicinal Chemistry, 2002, 10, 2899-2904.	3.0	22
28	A multivariate insight into ionic liquids toxicities. RSC Advances, 2014, 4, 23985-24000.	3.6	22
29	A multivariate insight into the in vitro antitumour screen database of the National Cancer Institute: classification of compounds, similarities among cell lines and the influence of molecular targets. Journal of Computer-Aided Molecular Design, 2001, 15, 219-234.	2.9	21
30	New potent antibacterials against Gram-positive multiresistant pathogens: Effects of side chain modification and chirality in linezolid-like 1,2,4-oxadiazoles. Bioorganic and Medicinal Chemistry, 2014, 22, 6814-6825.	3.0	21
31	Reactions of aromatic sulphonyl chlorides with anilines. Tetrahedron, 1977, 33, 105-111.	1.9	19
32	Studies of substituent effects by carbon-13 NMR spectroscopy. Thiophene and furan chalcone analogues. Magnetic Resonance in Chemistry, 1980, 14, 384-391.	0.7	19
33	Genome-based identification of diagnostic molecular markers for human lung carcinomas by PLS-DA. Computational Biology and Chemistry, 2005, 29, 183-195.	2.3	19
34	Cyto- and enzyme toxicities of ionic liquids modelled on the basis of VolSurf+ descriptors and their principal properties. SAR and QSAR in Environmental Research, 2016, 27, 221-244.	2.2	19
35	Application of principal component analysis to13C NMR shifts of chalcones and their thiophene and furan analogues: A useful tool for the shift assignment and for the study of substituent effects. Magnetic Resonance in Chemistry, 1981, 17, 118-123.	0.7	18
36	Structure-based rationalization of antitumor drugs mechanism of action by a MIF approach. European Journal of Medicinal Chemistry, 2004, 39, 281-289.	5.5	18

GIUSEPPE MUSUMARRA

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37	Modelling the aquatic toxicity of ionic liquids by means of VolSurf <i>in silico</i> descriptors. SAR and QSAR in Environmental Research, 2016, 27, 1-15.	2.2	18
38	Solvent effects in the benzylation of aniline. Journal of Organic Chemistry, 1977, 42, 1415-1418.	3.2	17
39	Geographical classification of sicilian olive oils in terms of sterols and fatty acids content. Journal of the Science of Food and Agriculture, 1991, 56, 445-455.	3.5	16
40	The Reaction of 2,4,6-Triarylpyrylium Cations with Methoxide-Ion. Heterocycles, 1979, 12, 775.	0.7	16
41	Kinetics and mechanisms of nucleophilic displacements with heterocycles as leaving groups. 3. N-(substituted benzyl)-2,4,6-triphenylpyridiniums: effects of benzyl substitution on first- and second-order rates. Journal of Organic Chemistry, 1981, 46, 3831-3835.	3.2	15
42	Kinetics and mechanisms of nucleophilic displacements with heterocycles as leaving groups. 2. N-benzylpyridinium cations: rate variation with steric effects in the leaving group. Journal of Organic Chemistry, 1981, 46, 3823-3830.	3.2	15
43	Kinetics and mechanisms of nucleophilic displacements with heterocycles as leaving groups. Part 4. 2,4,6-Triaryl-N-benzylpyridinium cations: rate variation with electronic effects in the leaving group. Journal of the Chemical Society Perkin Transactions II, 1982, , 1041.	0.9	15
44	Nucleophilic substitution in the side chain of 5-membered heterocycles—I. Tetrahedron, 1975, 31, 2523-2527.	1.9	14
45	Nucleophilic substitution in the side chain of five-membered heterocycles. 3. Reactions of heterocyclic aldehydes with aniline and with benzoylmethylenetriphenyl phosphorane. Journal of Organic Chemistry, 1977, 42, 3024-3028.	3.2	14
46	Formation of (N-Heteroaryl)heteroarymethanamines from Heteroaromatic Aldehydes and Heteroaromatic Amines. Heterocycles, 1994, 37, 1033.	0.7	14
47	Photobehaviour of some 1-heteroaryl-2-(1-methylpyridinium-2-yl)ethene iodides (free and complexed) Tj ETQq1 1	0,784314	rgBT /Over
48	On the nitration of 2â€benzylthiophene and the spectroscopic behaviour of nitroâ€2â€benzylthiophenes. Journal of Heterocyclic Chemistry, 1972, 9, 849-852.	2.6	13
49	A QSPR approach to the ecotoxicity of ionic liquids (Vibrio fischeri) using VolSurf principal properties. Toxicology Research, 2016, 5, 1090-1096.	2.1	13
50	Principal properties (PPs) for lanthanide triflates as Lewis-acid catalysts. Journal of Chemometrics, 2006, 20, 418-424.	1.3	12
51	Nucleophilic substitution at sulphonyl sulphur. Part 1. Reactivity of thiophen-2-sulphonyl halides in water and methanol–acetonitrile. Journal of the Chemical Society Perkin Transactions II, 1981, , 221-227.	0.9	11
52	Studies of substituent effects by carbon-13 NMR spectroscopy.V—Ethyl (E)-(α-cyano)cinnamates, (E)-(α-cyano)cinnamamides and ethyl (α-ethoxycarbonyl)cinnamates. Magnetic Resonance in Chemistry, 1986, 24, 31-34.	1.9	11
53	"Classical―and "Magnetic―Aromaticities as new Descriptors for Heteroaromatics in QS Prediction of Tetrahymena Pyriformis Growth Inhibition by Heteroaromatics. QSAR and Combinatorial Science, 1991, 10, 101-106.	SARs. PLS 1.2	11
54	Studies on the Interactions of the New 2,6-Bis[2-(heteroaryl)vinyl]1-methylpyridinium Cations with the Decamer d(CGTACGTACG)2. European Journal of Organic Chemistry, 2002, 2002, 145-150.	2.4	11

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55	N-benzoxazol-2-yl-N′-1-(isoquinolin-3-yl-ethylidene)-hydrazine, a novel compound with antitumor activity, induces radicals and dissipation of mitochondrial membrane potential. Investigational New Drugs, 2009, 27, 189-202.	2.6	11
56	Synthesis, spectroscopic characterization and in vitro antitumor activity of new trans 1-heteroaryl-2-(1-methylpyridinium-2-yl) ethylenes. Arkivoc, 2003, 2003, 105-117.	0.5	11
57	Infrared and ultraviolet spectra of 2-thienyl-phenyl-ketone nitro-derivatives. Spectrochimica Acta Part A: Molecular Spectroscopy, 1973, 29, 161-167.	0.1	10
58	Unimolecular and bimolecular transfer of N-substituents from pyridinium cations: Evidence for a clear mechanistic changeover. Tetrahedron Letters, 1980, 21, 2697-2699.	1.4	10
59	Synthesis and basicity of 2,6-di-[2-(heteroaryl)vinyl]pyridines. Tetrahedron, 1998, 54, 9721-9730.	1.9	10
60	OPLS-DA as a Suitable Method for Selecting a Set of Gene Transcripts Discriminating RAS- and PTPN11-Mutated Cells in Acute Lymphoblastic Leukaemia. Combinatorial Chemistry and High Throughput Screening, 2011, 14, 36-46.	1.1	10
61	Kinetics and mechanisms of nucleophilic displacements with heterocycles as leaving groups. 1. 1-Benzyl-2,4,6-triphenylpyridinium. Journal of Organic Chemistry, 1981, 46, 3820-3823.	3.2	9
62	The mass spectra of some thiophene chalcone analogues. Organic Mass Spectrometry, 1981, 16, 54-54.	1.3	9
63	Multiariate characterization, using the SIMCA method, of mortars from two frescoes in Chiaravalle Abbey. Thermochimica Acta, 1995, 269-270, 797-807.	2.7	9
64	Successful Application of OPLSâ€DA for the Discrimination of Wildâ€Type and Mutated Cells in Acute Lymphoblastic Leukemia. QSAR and Combinatorial Science, 2009, 28, 822-828.	1.4	9
65	Metal-free synthesis of bisthiophene-core donor acceptor organic photosensitizers for dye-sensitized solar cells. Tetrahedron, 2015, 71, 7260-7266.	1.9	9
66	Use of the Hammett equation in substituted thiophenes. Journal of the Chemical Society Perkin Transactions II, 1985, , 485-490.	0.9	8
67	Effects of the heteroaromatic moiety on spectroscopic properties, pKa and reactivity of azoles: A chemometric study. Journal of Physical Organic Chemistry, 1990, 3, 651-658.	1.9	8
68	Prediction of ionic liquid's heat capacity by means of their in silico principal properties. RSC Advances, 2016, 6, 36085-36089.	3.6	8
69	ldentification of genes involved in the sensitivity to antitumour drug 17-allylamino,17-demethoxygeldanamycin (17AAG). Molecular BioSystems, 2006, 2, 231.	2.9	7
70	Polarity study of ionic liquids with the solvatochromic dye Nile Red: a QSPR approach using in silico VolSurf+ descriptors. Tetrahedron, 2016, 72, 3282-3287.	1.9	7
71	Substituent effects in five-membered rings: σHetconstants for thia- and oxa-substituents from the reaction of arenesulphonyl chlorides with aniline. Journal of the Chemical Society Perkin Transactions II, 1976, , 906-908.	0.9	6
72	The protonation of furan- and thiophen-carboxamides. Journal of the Chemical Society Perkin Transactions II, 1979, , 1700.	0.9	6

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73	Nucleophilic displacement of N-benzyl groups: effect of pyridinium on rates and mechanism. Tetrahedron Letters, 1980, 21, 2701-2703.	1.4	6
74	Kinetics and mechanisms of nucleophilic displacements with heterocycles as leaving groups. Part 25. X-Ray structure determinations, crystallographic evidence for steric crowding, and correlation with acceleration of rates. Journal of the Chemical Society Perkin Transactions II, 1987, , 1391.	0.9	6
75	( <i>E</i> )â€2â€Cyanoâ€3â€(5â€2â€piperidinâ€1â€ylâ€2,2â€2â€bithienâ€5â€yl)acrylic Acid: A Fluorescent Prob Prefibrillar Oligomers. European Journal of Organic Chemistry, 2013, 2013, 3635-3639.	e for Dete 2.4	cting
76	Synthesis and applications of new trans 1-indolyl-2-(1-methyl pyridinium and quinolinium-2-yl) ethylenes. Arkivoc, 2009, 2009, 222-229.	0.5	6
77	QSAR Study of Heteroaromatic Modifications in the Side Chain of Bradycardic Benzazepinones by Response Surface Modelling [1]. QSAR and Combinatorial Science, 1993, 12, 256-260.	1.2	5
78	Spectroscopic evidence of a free-radical mechanism in the reduction of Schiff bases by formic acid. Tetrahedron, 1997, 53, 6907-6916.	1.9	5
79	2,6-Di(heteroarylvinyl)pyridines as new potential �antitumor agents. Journal of Physical Organic Chemistry, 2000, 13, 344-346.	1.9	5
80	Kinetics and mechanisms of nucleophilic displacements with heterocycles as leaving groups. Part 8. Conductimetric and spectrophotometric rate constants for the reactions of pyridinium and related cations with piperidine in chlorobenzene. Journal of the Chemical Society Perkin Transactions II, 1983, , 1421.	0.9	4
81	X-ray structure determination of cyclobutane photodimers from (Z)-?, ?-diarylacrylonitriles. Journal of Crystallographic and Spectroscopic Research, 1989, 19, 791-808.	0.2	4
82	Modeling from Theory and Modeling from Data: Complementary or Alternative Approaches? The Case of Ionic Liquids. ChemistryOpen, 2017, 6, 90-101.	1.9	4
83	The acid dissociation of arenesulphonamides: ÏfHetconstants for thia- and oxa-substituents in five-membered S-linked heterocycles and effects of substituents in the N-linked aromatic ring. Journal of the Chemical Society Perkin Transactions II, 1977, , 984-987.	0.9	3
84	Nuclear magnetic resonance studies of (Z)- and (E)-3-amino-3-(p-substituted phenyl)propenenitriles. Journal of the Chemical Society Perkin Transactions II, 1986, , 1847.	0.9	3
85	E/Z photoisomerization of 3-amino-3-phenylprop-2-enenitriles. Journal of the Chemical Society Perkin Transactions II, 1988, , 1591.	0.9	3
86	Effects of the Heteroaromatic Moiety on the Antisecretory Activities of Heteroarylmethyl Heteroaryl Sulfides [1]. QSAR and Combinatorial Science, 1991, 10, 107-109.	1.2	3
87	Identification of genes involved in radiationâ€induced G <sub>1</sub> arrest. Journal of Chemometrics, 2007, 21, 398-405.	1.3	3
88	Election Impact Mass Spectra of para-Substituted N-Heteroaryl Benzylamines. Heterocycles, 1994, 37, 367.	0.7	3
89	Kinetics and mechanisms of nucleophilic displacements with heterocycles as leaving groups. Part 5. Solvent effects. Journal of the Chemical Society Perkin Transactions II, 1982, , 1049.	0.9	2
90	Kinetics and mechanisms of nucleophilic displacements with heterocycles as leaving groups. Part 6. Reactions of N-(substituted benzyl)azaheterocyclonium compounds with piperidine. Journal of the Chemical Society Perkin Transactions II, 1982, , 1055.	0.9	2

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91	Kinetics and mechanisms of nucleophilic displacements with heterocycles as leaving groups. Part 9. N-substituted 2,4,6-triphenylpyridiniums, 5,6-dihydro-2,4-diphenylbenzo[h]quinoliniums, and 5,6,8,9-tetrahydro-7-phenyldibenzo[c,h]acridiniums: kinetic rate variation with structure of the N-substituent. Journal of the Chemical Society Perkin Transactions II, 1983, , 1427.	0.9	2
92	Kinetics and mechanisms of nucleophilic displacements with heterocycles as leaving groups. Part 14. The preparation and reactions of some further α-heteroaryl-pyridinium salts. Journal of the Chemical Society Perkin Transactions II, 1983, , 1463-1469.	0.9	2
93	Kinetics and mechanisms of nucleophilic displacements with heterocycles as leaving groups. Part 12. Regio- and stereo-chemistry of nucleophilic displacement and solvolysis reactions of N-(l±-methylallyl)-and N-(l±-phenylethyl)-pyridiniums. Journal of the Chemical Society Perkin Transactions II. 1983 1449-1453.	0.9	2
94	A Discussion of Principal Component Analysis: Reply. Journal of Analytical Toxicology, 1985, 9, 187-188.	2.8	2
95	Kinetics and mechanisms of nucleophilic displacements with heterocycles as leaving groups. Part 19. Chemometric investigation of the simultaneous dependence of S N 2 rates on alkyl group structure and leaving group nucleofugacity. Journal of the Chemical Society Perkin Transactions II, 1985, , 1887.	0.9	2
96	Studies of substituent effects by carbon-13 NMR spectroscopy. Vl—Application of multivariate data analysis to13C NMR chemical shifts of protonated chalcones and thiophene chalcone analogues. Magnetic Resonance in Chemistry, 1986, 24, 209-212.	1.9	2
97	Kinetics and mechanisms of nucleophilic displacements with heterocycles as leaving groups. Part 22. Reactions with various nucleophiles and a study of the effects of substrate concentration, traces of water, and nature of the gegenion on the rates. Journal of the Chemical Society Perkin Transactions II, 1987 73.	0.9	2
98	Carbon-13 NMR spectra of substituted 2-thiophenecarboxanilides. Magnetic Resonance in Chemistry, 1987, 25, 277-279.	1.9	2
99	Design, synthesis and antimycotic activity of (N-heteroaryl)arylmethanamines. Journal of Physical Organic Chemistry, 1996, 9, 61-65.	1.9	2
100	Gas principal properties as new compact descriptors for data-driven gas solubility modelling. Arkivoc, 2017, 2017, 356-369.	0.5	1
101	Dataâ€Ðriven Modelling of Gas Solubility in Ionic Liquids Using Principal Properties as Orthogonal Descriptors. ChemistrySelect, 2018, 3, 2181-2184.	1.5	1
102	Nucleophilic Displacements with Pyridine, Quinoline and Acridine Leaving Groups: Rate Variation with Structure of the N-Substituent. Bulletin Des Sociétés Chimiques Belges, 2010, 91, 417-417.	0.0	0
103	Celebrating the 150th anniversary of the Periodic Table: an outlook in the circular economy era. Bulletin of the Gioenia Academy of Catania, 2020, 53, FP1-FP10.	0.2	Ο