David W Roberts

List of Publications by Year
in descending order

112 papers	6,335 citations	87888 38 h-index	69250 77 g-index
115 all docs	115 docs citations	115 times ranked	1941 citing authors

#	Article	IF	Citations
1	Mechanistic Applicability Domain Classification of a Local Lymph Node Assay Dataset for Skin Sensitization. Chemical Research in Toxicology, 2007, 20, 1019-1030.	3.3	1,334
2	Extension of the Dermal Sensitisation Threshold (DST) approach to incorporate chemicals classified as reactive. Regulatory Toxicology and Pharmacology, 2015, 72, 694-701.	2.7	380
3	Principles for identification of High Potency Category Chemicals for which the Dermal Sensitisation Threshold (DST) approach should not be applied. Regulatory Toxicology and Pharmacology, 2015, 72, 683-693.	2.7	350
4	Mechanistic Applicability Domains for Nonanimal-Based Prediction of Toxicological End Points:â€‰ General Principles and Application to Reactive Toxicity. Chemical Research in Toxicology, 2006, 19, 1097-1105.	3.3	243
5	Measurement and Estimation of Electrophilic Reactivity for Predictive Toxicology. Chemical Reviews, 2011, 111, 2562-2596.	47.7	178
6	Skin Sensitization:â€‰ Reaction Mechanistic Applicability Domains for Structureâ^'Activity Relationships. Chemical Research in Toxicology, 2005, 18, 1420-1426.	3.3	165
7	The derivation of quantitative correlations between skin sensitisation and physio-chemical parameters for alkylating agents, and their application to experimental data for sultones. Journal of Theoretical Biology, 1982, 99, 807-825.	1.7	147
8	Electrophilic Chemistry Related to Skin Sensitization. Reaction Mechanistic Applicability Domain Classification for a Published Data Set of 106 Chemicals Tested in the Mouse Local Lymph Node Assay. Chemical Research in Toxicology, 2007, 20, 44-60.	3.3	142
9	Mechanistic Applicability Domains for Non-Animal Based Prediction of Toxicological Endpoints. QSAR Analysis of the Schiff Base Applicability Domain for Skin Sensitization. Chemical Research in Toxicology, 2006, 19, 1228-1233.	3.3	141
10	High Throughput Kinetic Profiling Approach for Covalent Binding to Peptides: Application to Skin Sensitization Potency of Michael Acceptor Electrophiles. Chemical Research in Toxicology, 2009, 22, 592-603.	3.3	120
11	Skin Sensitization to Eugenol and Isoeugenol in Mice:â€‰ Possible Metabolic Pathways Involving ortho-Quinone and Quinone Methide Intermediates. Chemical Research in Toxicology, 1997, 10, 335-343.	3.3	107
12	Determinants of skin sensitisation potential. Journal of Applied Toxicology, 2008, 28, 377-387.	2.8	106
13	Skinâ€sensitization structureâ€activity relationships for aldehydes. Contact Dermatitis, 2001, 44, 331-336.	1.4	98
14	The value of the local lymph node assay in quantitative structureâ€activity investigations. Contact Dermatitis, 1992, 27, 137-142.	1.4	95
15	Non-enzymatic glutathione reactivity and in vitro toxicity: A non-animal approach to skin sensitization. Toxicology in Vitro, 2006, 20, 239-247.	2.4	91
16	TIMES-SSâ€”A promising tool for the assessment of skin sensitization hazard. A characterization with respect to the OECD validation principles for (Q)SARs and an external evaluation for predictivity. Regulatory Toxicology and Pharmacology, 2007, 48, 225-239.	2.7	91
17	Towards AOP application â€“ Implementation of an integrated approach to testing and assessment (IATA) into a pipeline tool for skin sensitization. Regulatory Toxicology and Pharmacology, 2014, 69, 529-545.	2.7	89
18	QSAR issues in aquatic toxicity of surfactants. Science of the Total Environment, 1991, 109-110, 557-568.	8.0	86

#	Article	IF	Citations
19	Electrophilic Reaction Chemistry of Low Molecular Weight Respiratory Sensitizers. Chemical Research in Toxicology, 2009, 22, 1447-1453.	3.3	78
20	An evaluation of selected global (Q)SARs/expert systems for the prediction of skin sensitisation potential. SAR and QSAR in Environmental Research, 2007, 18, 515-541.	2.2	77
21	Chemistryâ^'Toxicity Relationships for the Effects of Di- and Trihydroxybenzenes to Tetrahymena pyriformis. Chemical Research in Toxicology, 2005, 18, 844-854.	3.3	68
22	Chemical reactivity indices and mechanismâ€based readâ€across for nonâ€animal based assessment of skin sensitisation potential. Journal of Applied Toxicology, 2008, 28, 443-454.	2.8	67
23	Further evaluation of quantitative structure-activity relationship models for the prediction of the skin sensitization potency of selected fragrance allergens. Contact Dermatitis, 2004, 50, 91-97.	1.4	62
24	Development of Mechanism-Based Structural Alerts for Respiratory Sensitization Hazard Identification. Chemical Research in Toxicology, 2012, 25, 2490-2498.	3.3	60
25	Quantitative structure-activity relationships: sulfonate esters in the local lymph node assay. Contact Dermatitis, 2000, 42, 154-161.	1.4	56
26	TIMES-SSâ€”A Mechanistic Evaluation of an External Validation Study Using Reaction Chemistry Principles. Chemical Research in Toxicology, 2007, 20, 1321-1330.	3.3	56
27	The aquatic toxicity of anionic surfactants to Daphnia magnaâ€”A comparative QSAR study of linear alkylbenzene sulphonates and ester sulphonates. Chemosphere, 2006, 63, 1443-1450.	8.2	53
28	Correlations between skin sensitization potential and chemical reactivity for p-nitrobenzyl Compounds. Food and Chemical Toxicology, 1983, 21, 811-813.	3.6	52
29	Structure-activity relationships for skin sensitisation potential of diacrylates and dimethacrylates. Contact Dermatitis, 1987, 17, 281-289.	1.4	51
30	Skin sensitization structure-activity relationships for phenyl benzoates. Toxicology in Vitro, 1994, 8, 823-826.	2.4	51
31	Structure-activity relationships in the murine local lymph node assay for skin sensitization: ?,?-diketones. Contact Dermatitis, 1999, 41, 14-17.	1.4	51
32	A quantitative structure activity/dose response relationship for contact allergic potential of alkyl group transfer agents. Contact Dermatitis, 1990, 23, 331-335.	1.4	47
33	Sulfonation Technology for Anionic Surfactant Manufacture. Organic Process Research and Development, 1998, 2, 194-202.	2.7	44
34	Haptens, prohaptens and prehaptens, or electrophiles and proelectrophiles. Contact Dermatitis, 2007, 56, 54-56.	1.4	44
35	Structure-Activity Relationships for Contact Allergenic Potential of .gamma.,.gamma.-Dimethyl-.gamma.-butyrolactone Derivatives. 2. Quantitative Structure-Skin Sensitization Relationships for .alpha.-Substituted-.alpha.-methyl-.gamma.,.gamma.-dimethyl-.gamma.-butyrolactones. Chemical Research in Toxicology, 1994, 7, 307-312.	3.3	43
36	Linear Free Energy Relationships for Reactions of Electrophilic Halo- and Pseudohalobenzenes, and Their Application in Prediction of Skin Sensitization Potential for SNAr Electrophiles. Chemical Research in Toxicology, 1995, 8, 545-551.	3.3	43

#	Article	IF	Citations
37	Molecular Orbital Parameters as Predictors of Skin Sensitization Potential of Halo- and Pseudohalobenzenes Acting as SNAr Electrophiles. Chemical Research in Toxicology, 1997, 10, 994-1000.	3.3	42
38	Experimental Reactivity Parameters for Toxicity Modeling: Application to the Acute Aquatic Toxicity of S_N2 Electrophiles to Tetrahymena pyriformis. Chemical Research in Toxicology, 2010, 23, 228-234.	3.3	41
39	Global (Q)SARs for skin sensitisationâ€“assessment against OECD principlesâ€“. SAR and QSAR in Environmental Research, 2007, 18, 343-365.	2.2	39
40	The In Chemicoâ€“In Silico Interface: Challenges for Integrating Experimental and Computational Chemistry to Identify Toxicity. ATLA Alternatives To Laboratory Animals, 2009, 37, 513-521.	1.0	37
41	Nonâ€animal assessment of skin sensitization hazard: Is an integrated testing strategy needed, and if so what should be integrated?. Journal of Applied Toxicology, 2018, 38, 41-50.	2.8	37
42	A Comparison of Reactivity Schemes for the Prediction Skin Sensitization Potential. Chemical Research in Toxicology, 2008, 21, 521-541.	3.3	36
43	Mechanism-Based QSAR Modeling of Skin Sensitization. Chemical Research in Toxicology, 2015, 28, 1975-1986.	3.3	36
44	Chemistry-Based Risk Assessment for Skin Sensitization: Quantitative Mechanistic Modeling for the SNAr Domain. Chemical Research in Toxicology, 2011, 24, 1003-1011.	3.3	34
45	Electrophilic Reactivity and Skin Sensitization Potency of S_NAr Electrophiles. Chemical Research in Toxicology, 2014, 27, 240-246.	3.3	34
46	Structureâ€“activity relationships for abiotic thiol reactivity and aquatic toxicity of halo-substituted carbonyl compounds. SAR and QSAR in Environmental Research, 2007, 18, 21-29.	2.2	33
47	Chemical Mechanisms for Skin Sensitization by Aromatic Compounds with Hydroxy and Amino Groups. Chemical Research in Toxicology, 2009, 22, 1541-1547.	3.3	33
48	A Mechanistic Approach to Modeling Respiratory Sensitization. Chemical Research in Toxicology, 2014, 27, 219-239.	3.3	33
49	Structure-Activity Relationships for Contact Allergenic Potential of .gamma.,.gamma.-Dimethyl-.gamma.-butyrolactone Derivatives. 1. Synthesis and Electrophilic Reactivity Studies of .alpha.-(.omega.-Substituted-alkyl)-.gamma.,.gamma.-dimethyl-.gamma.-butyrolactones and Correlation of Skin Sensitization Potential and Cross-Sensitization Patterns with Structure. Chemical Research in Toxicology, 1994, 7, 297-306.	3.3	31
50	Predicting Skin Sensitization Potency for Michael Acceptors in the LLNA Using Quantum Mechanics Calculations. Chemical Research in Toxicology, 2013, 26, 767-774.	3.3	30
51	TIMES-SS â€“ Recent refinements resulting from an industrial skin sensitisation consortium. SAR and QSAR in Environmental Research, 2014, 25, 367-391.	2.2	30
52	What determines skin sensitization potency: Myths, maybes and realities. The 500 molecular weight cutâ€off: An updated analysis. Journal of Applied Toxicology, 2017, 37, 105-116.	2.8	30
53	Skin sensitization in silico protocol. Regulatory Toxicology and Pharmacology, 2020, 116, 104688.	2.7	27
54	Aquatic toxicityâ€”Are surfactant properties relevant?. Journal of Surfactants and Detergents, 2000, 3, 309-315.	2.1	25

#	Article	IF	Citations
55	Methylisothiazolinone is categorised as a strong sensitiser in the <scp>M</scp>urine <scp>L</scp>ocal <scp>L</scp>ymph <scp>N</scp>ode <scp>A</scp>ssay. Contact Dermatitis, 2013, 69, 261-262.	1.4	25
56	Structure/activity relationships in contact allergy. International Journal of Cosmetic Science, 1990, 12, 81-90.	2.6	24
57	Is skin penetration a determining factor in skin sensitization potential and potency? Refuting the notion of a LogKow threshold for skin sensitization. Journal of Applied Toxicology, 2017, 37, 117-127.	2.8	24
58	Methyl groups as antigenic determinants in skin sensitisation. Contact Dermatitis, 1988, 18, 219-225.	1.4	23
59	What determines skin sensitization potencyâ€“myths, maybes and realities. Part 1. The 500 molecular weight cutâ€off. Contact Dermatitis, 2013, 68, 32-41.	1.4	22
60	A practical guidance for Cramer class determination. Regulatory Toxicology and Pharmacology, 2015, 73, 971-984.	2.7	21
61	From Experiment to Theory:Â Molecular Orbital Parameters to Interpret the Skin Sensitization Potential of 5-Chloro-2-methylisothiazol-3-one and 2-Methylisothiazol-3-one. Chemical Research in Toxicology, 2005, 18, 324-329.	3.3	20
62	An Integrated Decision-tree Testing Strategy for Skin Sensitisation with Respect to the Requirements of the EU REACH Legislation. ATLA Alternatives To Laboratory Animals, 2007, 35, 683-697.	1.0	20
63	Adsorption and self-assembly in methyl ester sulfonate surfactants, their eutectic mixtures and the role of electrolyte. Journal of Colloid and Interface Science, 2018, 516, 456-465.	9.4	20
64	Further evaluation of the quantitative structure-activity relationship for skin-sensitizing alkyl transfer agents. Contact Dermatitis, 1997, 37, 107-112.	1.4	19
65	Electrophilic Reactions of Skin-Sensitizing Sultones. Chemical Research in Toxicology, 2007, 20, 61-71.	3.3	19
66	Practical methods for the measurement of logP for surfactants. Ecotoxicology and Environmental Safety, 2010, 73, 1484-1489.	6.0	19
67	Chemical applicability domain of the Local Lymph Node Assay (LLNA) for skin sensitisation potency. Part 2. The biological variability of the murine Local Lymph Node Assay (LLNA) for skin sensitisation. Regulatory Toxicology and Pharmacology, 2016, 80, 255-259.	2.7	19
68	Skin Sensitization QMM for HRIPT NOEL Data: Aldehyde Schiff-Base Domain. Chemical Research in Toxicology, 2017, 30, 1309-1316.	3.3	19
69	Adsorption of Methyl Ester Sulfonate at the Airâ€“Water Interface: Can Limitations in the Application of the Gibbs Equation be Overcome by Computer Purification?. Langmuir, 2017, 33, 9944-9953.	3.5	18
70	An evaluation of selected (Q)SARs/expert systems for predicting skin sensitisation potential. SAR and QSAR in Environmental Research, 2018, 29, 439-468.	2.2	18
71	The impact of electrolyte on the adsorption of the anionic surfactant methyl ester sulfonate at the air-solution interface: Surface multilayer formation. Journal of Colloid and Interface Science, 2018, 512, 231-238.	9.4	18
72	Chemical applicability domain of the local lymph node assay (LLNA) for skin sensitisation potency. Part 4. Quantitative correlation of LLNA potency with human potency. Regulatory Toxicology and Pharmacology, 2018, 96, 76-84.	2.7	18

#	Article	IF	Citations
73	Chemical Basis for the Extreme Skin Sensitization Potency of (E)-4-(Ethoxymethylene)-2-phenyloxazol-5(4H)-one. Chemical Research in Toxicology, 2010, 23, 1913-1920.	3.3	17
74	Chemical applicability domain of the Local Lymph Node Assay (LLNA) for skin sensitization potency. Part 1. Underlying physical organic chemistry principles and the extent to which they are represented in the LLNA validation dataset. Regulatory Toxicology and Pharmacology, 2016, 80, 247-254.	2.7	17
75	Estimating skin sensitization potency from a single dose LLNA. Regulatory Toxicology and Pharmacology, 2015, 71, 437-443.	2.7	16
76	Structureâ€“Potency Relationships for Epoxides in Allergic Contact Dermatitis. Chemical Research in Toxicology, 2017, 30, 524-531.	3.3	16
77	QUANTITATIVE STRUCTUREâ€“ACTIVITY RELATIONSHIP MODELING OF ACUTE TOXICITY OF QUATERNARY ALKYLAMMONIUM SULFOBETAINES TO DAPHNIA MAGNA. Environmental Toxicology and Chemistry, 2004, 23, 2111.	4.3	15
78	The structure of alkyl ester sulfonate surfactant micelles: The impact of different valence electrolytes and surfactant structure on micelle growth. Journal of Colloid and Interface Science, 2019, 557, 124-134.	9.4	15
79	Chemical applicability domain of the Local Lymph Node Assay (LLNA) for skin sensitisation potency. Part 3. Apparent discrepancies between LLNA and GPMT sensitisation potential: False positives or differences in sensitivity?. Regulatory Toxicology and Pharmacology, 2016, 80, 260-267.	2.7	14
80	Is a combination of assays really needed for non-animal prediction of skin sensitization potential? Performance of the GARDâ„¢ (Genomic Allergen Rapid Detection) assay in comparison with OECD guideline assays alone and in combination. Regulatory Toxicology and Pharmacology, 2018, 98, 155-160.	2.7	14
81	Impact of molecular structure, headgroup and alkyl chain geometry, on the adsorption of the anionic ester sulfonate surfactants at the air-solution interface, in the presence and absence of electrolyte. Journal of Colloid and Interface Science, 2019, 544, 293-302.	9.4	14
82	Does the extreme skin sensitization potency of benzoquinone result from special chemistry?. Contact Dermatitis, 2009, 61, 332-336.	1.4	13
83	The respiratory allergen glutaraldehyde in the local lymph node assay: Sensitization by skin exposure, but not by inhalation. Toxicology, 2011, 279, 115-122.	4.2	13
84	Aquatic toxicity of cationic surfactants toDaphnia magna. SAR and QSAR in Environmental Research, 2013, 24, 417-427.	2.2	13
85	Development of an In Silico Profiler for Respiratory Sensitisation. ATLA Alternatives To Laboratory Animals, 2014, 42, 367-375.	1.0	13
86	Application of the dermal sensitization threshold concept to chemicals classified as high potency category for skin sensitization assessment of ingredients for consumer products. Regulatory Toxicology and Pharmacology, 2020, 117, 104732.	2.7	13
87	Updating the Skin Sensitization in Vitro Data Assessment Paradigm in 2009 â€“ a chemistry and QSAR perspective. Journal of Applied Toxicology, 2010, 30, 286-288.	2.8	12
88	Is Diacetyl a Respiratory Sensitizer? A Reconsideration Using QSAR, QMM, and Competition Experiments. Chemical Research in Toxicology, 2013, 26, 631-633.	3.3	12
89	AQUATIC TOXICITY OF ETHOXYLATED AND PROPOXYLATED ALCOHOLS TO DAPHNIA MAGNA. Environmental Toxicology and Chemistry, 2007, 26, 68.	4.3	11
90	Sodium metabisulfite as a contact allergen â€“ an example of a rare chemical mechanism for protein modification. Contact Dermatitis, 2012, 66, 123-127.	1.4	11

#	Article	IF	Citations
91	Integrated testing and assessment approaches for skin sensitization: a commentary. Journal of Applied Toxicology, 2014, 34, 436-440.	2.8	10
92	The role of competitive counterion adsorption on the electrolyte induced surface ordering in methyl ester sulfonate surfactants at the air-water interface. Journal of Colloid and Interface Science, 2019, 533, 154-160.	9.4	10
93	Evaluating confidence in toxicity assessments based on experimental data and in silico predictions. Computational Toxicology, 2022, 21, 100204.	3.3	10
94	An Integrated Decision-tree Testing Strategy for Skin Sensitisation with Respect to the Requirements of the EU REACH Legislation. ATLA Alternatives To Laboratory Animals, 2008, 36, 75-89.	1.0	9
95	Updating the Dermal Sensitisation Thresholds using an expanded dataset and an in silico expert system. Regulatory Toxicology and Pharmacology, 2022, 133, 105200.	2.7	8
96	Skin, drug and chemical reactions. Drug Discovery Today Disease Mechanisms, 2008, 5, e211-e220.	0.8	7
97	Chemistry Based Nonanimal Predictive Modeling for Skin Sensitization. Emerging Topics in Ecotoxicology, 2009, , 61-83.	1.5	7
98	A critical review of the kinetic direct peptide reactivity assay (kDPRA) for skin sensitizer potency assessment â€“ taking it forward. Critical Reviews in Toxicology, 2021, 51, 805-819.	3.9	6
99	Nonanimal Alternatives for Skin Sensitization: Letter to the Editor. Toxicological Sciences, 2008, 106, 572-574.	3.1	4
100	Contact allergy to capryloyl salicylic acid: a mechanistic chemistry and structureâ€“activity perspective. Contact Dermatitis, 2015, 72, 347-351.	1.4	4
101	Î±-Sulfo alkyl ester surfactants: Impact of changing the alkyl chain length on the adsorption, mixing properties and response to electrolytes of the tetradecanoate. Journal of Colloid and Interface Science, 2021, 586, 876-890.	9.4	4
102	Interpretation of murine local lymph node assay (LLNA) data for skin sensitization: Overload effects, danger signals and chemistry-based read-across. Current Research in Toxicology, 2021, 2, 53-63.	2.7	4
103	Reactivity assays, substances, samples and in vitro alternatives: why should we care?. Contact Dermatitis, 2009, 61, 310-311.	1.4	3
104	Allergic contact dermatitis: is the reactive chemistry of skin sensitizers the whole story? A response. Contact Dermatitis, 2013, 68, 245-249.	1.4	3
105	Comparing and contrasting the coverage of publicly available structural alerts for protein binding. Computational Toxicology, 2019, 12, 100100.	3.3	3
106	Reactivity assays: dealing with substances and samples in an in vitro world â€“ the solution and the real problem. Contact Dermatitis, 2010, 63, 55-56.	1.4	2
107	Interconversion between local lymph node assay EC3 units. Contact Dermatitis, 2011, 65, 59-59.	1.4	2
108	Allergic contact dermatitis caused by a skinâ€lightening agent, 5,5â€²â€dipropylbiphenylâ€2,2â€²â€diol. A comment. Contact Dermatitis, 2012, 66, 357-359.	1.4	2

#	Article	IF	Citations
109	Quantifying skin sensitization potency. Contact Dermatitis, 2012, 66, 356-357.	1.4	1
110	Letter to the editor. Food and Chemical Toxicology, 2014, 70, 260-261.	3.6	0
111	Letter to the Editor Regarding the Article by Natsch et al., 2015. Chemical Research in Toxicology, 2015, 28, 2085-2085.	3.3	0
112	Response to the comments of Natsch and Landsiedel on my paper â€œIs a combination of assays really needed for non-animal prediction of skin sensitization potential? Performance of the GARD (genomic) Tj ETQq0 0 0 rgBT /Overlock 10 Tf Regulatory Toxicology and Pharmacology, 2019, 102, 95-97.	2.7	0