Grace Patlewicz

List of Publications by Year
in descending order

134 papers	9,217 citations	44069 48 h-index	42399 92 g-index
142 all docs	142 docs citations	142 times ranked	4822 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	The CompTox Chemistry Dashboard: a community data resource for environmental chemistry. Journal of Cheminformatics, 2017, 9, 61.	6.1	674
3	ToxCast Chemical Landscape: Paving the Road to 21st Century Toxicology. Chemical Research in Toxicology, 2016, 29, 1225-1251.	3.3	456
4	An evaluation of the implementation of the Cramer classification scheme in the Toxtree software. SAR and QSAR in Environmental Research, 2008, 19, 495-524.	2.2	359
5	Applying Adverse Outcome Pathways (AOPs) to support Integrated Approaches to Testing and Assessment (IATA). Regulatory Toxicology and Pharmacology, 2014, 70, 629-640.	2.7	291
6	A Stepwise Approach for Defining the Applicability Domain of SAR and QSAR Models. Journal of Chemical Information and Modeling, 2005, 45, 839-849.	5.4	243
7	The Next Generation Blueprint of Computational Toxicology at the U.S. Environmental Protection Agency. Toxicological Sciences, 2019, 169, 317-332.	3.1	225
8	A roadmap for the development of alternative (non-animal) methods for systemic toxicity testing. ALTEX: Alternatives To Animal Experimentation, 2012, 29, 3-91.	1.5	190
9	Skin Sensitization:â€‰ Reaction Mechanistic Applicability Domains for Structureâˆ'Activity Relationships. Chemical Research in Toxicology, 2005, 18, 1420-1426.	3.3	165
10	In silico toxicology protocols. Regulatory Toxicology and Pharmacology, 2018, 96, 1-17.	2.7	159
11	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
12	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
13	Toward Good Read-Across Practice (GRAP) guidance. ALTEX: Alternatives To Animal Experimentation, 2016, 33, 149-166.	1.5	134
14	A New OECD Definition for Per- and Polyfluoroalkyl Substances. Environmental Science & Technology, 2021, 55, 15575-15578.	10.0	134
15	The role of the European Chemicals Bureau in promoting the regulatory use of (Q)SAR methods. SAR and QSAR in Environmental Research, 2007, 18, 111-125.	2.2	130
16	A chemical dataset for evaluation of alternative approaches to skinâ€sensitization testing. Contact Dermatitis, 2004, 50, 274-288.	1.4	129
17	Use of category approaches, read-across and (Q)SAR: General considerations. Regulatory Toxicology and Pharmacology, 2013, 67, 1-12.	2.7	105
18	Skinâ€sensitization structureâ€activity relationships for aldehydes. Contact Dermatitis, 2001, 44, 331-336.	1.4	98

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19	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
20	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
21	Read-across approaches - misconceptions, promises and challenges ahead. ALTEX: Alternatives To Animal Experimentation, 2014, 31, 387-396.	1.5	90
22	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
23	Proposing a scientific confidence framework to help support the application of adverse outcome pathways for regulatory purposes. Regulatory Toxicology and Pharmacology, 2015, 71, 463-477.	2.7	87
24	Computer-Aided Knowledge Generation for Understanding Skin Sensitization Mechanisms: The TOPS-MODE Approach. Chemical Research in Toxicology, 2003, 16, 1226-1235.	3.3	81
25	GRADE Guidelines 30: the GRADE approach to assessing the certaintyÂof modeled evidenceâ€"An overview in the context of healthÂdecision-making. Journal of Clinical Epidemiology, 2021, 129, 138-150.	5.0	81
26	Navigating through the minefield of read-across tools: A review of in silico tools for grouping. Computational Toxicology, 2017, 3, 1-18.	3.3	80
27	Skin Sensitization: Modeling Based on Skin Metabolism Simulation and Formation of Protein Conjugates. International Journal of Toxicology, 2005, 24, 189-204.	1.2	79
28	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
29	A Chemical Category-Based Prioritization Approach for Selecting 75 Per- and Polyfluoroalkyl Substances (PFAS) for Tiered Toxicity and Toxicokinetic Testing. Environmental Health Perspectives, 2019, 127, 14501.	6.0	75
30	Current and Future Perspectives on the Development, Evaluation, and Application of <i>in Silico</i> Approaches for Predicting Toxicity. Chemical Research in Toxicology, 2016, 29, 438-451.	3.3	72
31	Systematically evaluating read-across prediction and performance using a local validity approach characterized by chemical structure and bioactivity information. Regulatory Toxicology and Pharmacology, 2016, 79, 12-24.	2.7	70
32	Skin Sensitisation and Epidermal Disposition: The Relevance of Epidermal Disposition for Sensitisation Hazard Identification and Risk Assessment. ATLA Alternatives To Laboratory Animals, 2007, 35, 137-154.	1.0	69
33	Structure-activity relationships for selected fragrance allergens. Contact Dermatitis, 2002, 47, 219-226.	1.4	68
34	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
35	Pathway-based predictive approaches for non-animal assessment of acute inhalation toxicity. Toxicology in Vitro, 2018, 52, 131-145.	2.4	66
36	Toxmatchâ€"a new software tool to aid in the development and evaluation of chemically similar groups. SAR and QSAR in Environmental Research, 2008, 19, 397-412.	2.2	64

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37	CATMoS: Collaborative Acute Toxicity Modeling Suite. Environmental Health Perspectives, 2021, 129, 47013.	6.0	63
38	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
39	Alternative approaches for acute inhalation toxicity testing to address global regulatory and non-regulatory data requirements: An international workshop report. Toxicology in Vitro, 2018, 48, 53-70.	2.4	62
40	Predictive models for acute oral systemic toxicity: A workshop to bridge the gap from research to regulation. Computational Toxicology, 2018, 8, 21-24.	3.3	62
41	Current Topics on Software Use in Medicinal Chemistry: Intellectual Property, Taxes, and Regulatory Issues. Current Topics in Medicinal Chemistry, 2008, 8, 1666-1675.	2.1	60
42	Guidance on assessing the methodological and reporting quality of toxicologically relevant studies: A scoping review. Environment International, 2016, 92-93, 630-646.	10.0	58
43	Bioactivity profiling of per- and polyfluoroalkyl substances (PFAS) identifies potential toxicity pathways related to molecular structure. Toxicology, 2021, 457, 152789.	4.2	57
44	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
45	Building scientific confidence in the development and evaluation of read-across. Regulatory Toxicology and Pharmacology, 2015, 72, 117-133.	2.7	56
46	Predicting Drugs and Proteins in Parasite Infections with Topological Indices of Complex Networks: Theoretical Backgrounds, Applications and Legal Issues. Current Pharmaceutical Design, 2010, 16, 2737-2764.	1.9	54
47	QSARs for the skin sensitization potential of aldehydes and related compounds. QSAR and Combinatorial Science, 2003, 22, 196-203.	1.4	53
48	Utilizing Threshold of Toxicological Concern (TTC) with high throughput exposure predictions (HTE) as a risk-based prioritization approach for thousands of chemicals. Computational Toxicology, 2018, 7, 58-67.	3.3	53
49	QUANTITATIVE STRUCTUREâ€"ACTIVITY RELATIONSHIPS FOR PREDICTING MUTAGENICITY AND CARCINOGENICITY. Environmental Toxicology and Chemistry, 2003, 22, 1885.	4.3	50
50	Validation of counter propagation neural network models for predictive toxicology according to the OECD principles: a case study. SAR and QSAR in Environmental Research, 2006, 17, 265-284.	2.2	50
51	Predicting Organ Toxicity Using <i>in Vitro</i> Bioactivity Data and Chemical Structure. Chemical Research in Toxicology, 2017, 30, 2046-2059.	3.3	49
52	Structure?activity relationships for skin sensitization: recent improvements to Derek for Windows. Contact Dermatitis, 2006, 55, 342-347.	1.4	48
53	Internationalization of read-across as a validated new approach method (NAM) for regulatory toxicology. ALTEX: Alternatives To Animal Experimentation, 2020, 37, 579-606.	1.5	48
54	From Knowledge Generation to Knowledge Archive. A General Strategy Using TOPS-MODE with DEREK To Formulate New Alerts for Skin Sensitization. Journal of Chemical Information and Computer Sciences, 2004, 44, 688-698.	2.8	47

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55	The challenge of using read-across within the EU REACH regulatory framework; how much uncertainty is too much? Dipropylene glycol methyl ether acetate, an exemplary case study. Regulatory Toxicology and Pharmacology, 2014, 68, 212-221.	2.7	47
56	An exposure:activity profiling method for interpreting high-throughput screening data for estrogenic activityâ€"Proof of concept. Regulatory Toxicology and Pharmacology, 2015, 71, 398-408.	2.7	45
57	A Minireview of Available Skin Sensitization (Q)SARs/Expert Systems. QSAR and Combinatorial Science, 2008, 27, 60-76.	1.4	44
58	Navigating through the minefield of read-across frameworks: A commentary perspective. Computational Toxicology, 2018, 6, 39-54.	3.3	44
59	The adverse outcome pathway for rodent liver tumor promotion by sustained activation of the aryl hydrocarbon receptor. Regulatory Toxicology and Pharmacology, 2015, 73, 172-190.	2.7	42
60	Evidence-based toxicology for the 21st century: Opportunities and challenges. ALTEX: Alternatives To Animal Experimentation, 2013, 30, 74-104.	1.5	42
61	The local lymph node assay and skin sensitization: a cut-down screen to reduce animal requirements?. Contact Dermatitis, 2006, 54, 181-185.	1.4	41
62	Creating molecular diversity from antioxidants in Brazilian propolis. Combination of TOPS-MODE QSAR and virtual structure generation. Molecular Diversity, 2004, 8, 21-33.	3.9	40
63	Global (Q)SARs for skin sensitisationâ€"assessment against OECD principlesâ€–. SAR and QSAR in Environmental Research, 2007, 18, 343-365.	2.2	39
64	A feasibility study developing an integrated testing strategy assessing skin irritation potential of chemicals. Toxicology Letters, 2008, 180, 9-20.	0.8	38
65	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
66	A QSAR model for the eye irritation of cationic surfactants. Toxicology in Vitro, 2000, 14, 79-84.	2.4	36
67	A Comparison of Reactivity Schemes for the Prediction Skin Sensitization Potential. Chemical Research in Toxicology, 2008, 21, 521-541.	3.3	36
68	Systematic Evidence Map for Over One Hundred and Fifty Per- and Polyfluoroalkyl Substances (PFAS). Environmental Health Perspectives, 2022, 130, 56001.	6.0	36
69	Use and validation of HT/HC assays to support 21st century toxicity evaluations. Regulatory Toxicology and Pharmacology, 2013, 65, 259-268.	2.7	35
70	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
71	Evaluating potential refinements to existing Threshold of Toxicological Concern (TTC) values for environmentally-relevant compounds. Regulatory Toxicology and Pharmacology, 2019, 109, 104505.	2.7	34
72	QUANTITATIVE STRUCTUREâ€"ACTIVITY RELATIONSHIPS FOR PREDICTING PERCUTANEOUS ABSORPTION RATES. Environmental Toxicology and Chemistry, 2003, 22, 1870.	4.3	33

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73	A Mechanistic Approach to Modeling Respiratory Sensitization. Chemical Research in Toxicology, 2014, 27, 219-239.	3.3	33
74	Generalized Read-Across (GenRA): A workflow implemented into the EPA CompTox Chemicals Dashboard. ALTEX: Alternatives To Animal Experimentation, 2019, 36, 462-465.	1.5	33
75	Investigation of the skin sensitizing activity of linalool. Contact Dermatitis, 2002, 47, 161-164.	1.4	32
76	A Review of (Q)SAR Models for Skin and Eye Irritation and Corrosion. QSAR and Combinatorial Science, 2008, 27, 49-59.	1.4	32
77	Toxmatchâ€"A chemical classification and activity prediction tool based on similarity measures. Regulatory Toxicology and Pharmacology, 2008, 52, 77-84.	2.7	32
78	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
79	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
80	QUANTITATIVE STRUCTUREâ€"ACTIVITY RELATIONSHIPS FOR PREDICTING SKIN AND RESPIRATORY SENSITIZATION. Environmental Toxicology and Chemistry, 2003, 22, 1855.	4.3	29
81	Identification of Branched and Linear Forms of PFOA and Potential Precursors: A User-Friendly SMILES Structure-based Approach. Frontiers in Environmental Science, 2022, 10, 1-865488.	3.3	29
82	Developing scientific confidence in HTS-derived prediction models: Lessons learned from an endocrine case study. Regulatory Toxicology and Pharmacology, 2014, 69, 443-450.	2.7	27
83	Assembly and Curation of Lists of Per- and Polyfluoroalkyl Substances (PFAS) to Support Environmental Science Research. Frontiers in Environmental Science, 2022, 10, .	3.3	25
84	Mechanism based structure-activity relationships for skin sensitisation--the carbonyl group domain. SAR and QSAR in Environmental Research, 2002, 13, 145-152.	2.2	24
85	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
86	Evaluation of SARs for the prediction of skin irritation/corrosion potentialâ€"structural inclusion rules in the BfR decision support systemâ€. SAR and QSAR in Environmental Research, 2007, 18, 331-342.	2.2	23
87	Investigating the Relationship between in Vitroâ€"in Vivo Genotoxicity: Derivation of Mechanistic QSAR Models for in Vivo Liver Genotoxicity and in Vivo Bone Marrow Micronucleus Formation Which Encompass Metabolism. Chemical Research in Toxicology, 2012, 25, 277-296.	3.3	23
88	Exploring current read-across applications and needs among selected U.S. Federal Agencies. Regulatory Toxicology and Pharmacology, 2019, 106, 197-209.	2.7	23
89	Use of Genotoxicity Information in the Development of Integrated Testing Strategies (ITS) for Skin Sensitization. Chemical Research in Toxicology, 2010, 23, 1519-1540.	3.3	22
90	Using chemical structure information to develop predictive models for in vitro toxicokinetic parameters to inform high-throughput risk-assessment. Computational Toxicology, 2020, 16, 100136.	3.3	22

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91	Evaluation of Variability Across Rat Acute Oral Systemic Toxicity Studies. Toxicological Sciences, 2022, 188, 34-47.	3.1	22
92	QUANTITATIVE STRUCTUREâ€“ACTIVITY RELATIONSHIPS FOR PREDICTING SKIN AND EYE IRRITATION. Environmental Toxicology and Chemistry, 2003, 22, 1862.	4.3	20
93	NAM-supported read-across: From case studies to regulatory guidance in safety assessment. ALTEX: Alternatives To Animal Experimentation, 2021, 38, 140-150.	1.5	19
94	A feasibility study: Can information collected to classify for mutagenicity be informative in predicting carcinogenicity?. Regulatory Toxicology and Pharmacology, 2015, 72, 17-25.	2.7	18
95	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
96	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
97	Predicting estrogen receptor activation by a group of substituted phenols: An integrated approach to testing and assessment case study. Regulatory Toxicology and Pharmacology, 2019, 106, 278-291.	2.7	17
98	Non-testing approaches under REACH â€“ help or hindrance? Perspectives from a practitioner within industry. SAR and QSAR in Environmental Research, 2011, 22, 67-88.	2.2	16
99	Retrospective mining of toxicology data to discover multispecies and chemical class effects: Anemia as a case study. Regulatory Toxicology and Pharmacology, 2017, 86, 74-92.	2.7	15
100	A systematic evaluation of analogs and automated read-across prediction of estrogenicity: A case study using hindered phenols. Computational Toxicology, 2017, 4, 22-30.	3.3	15
101	Integrated Approaches to Testing and Assessment. Advances in Experimental Medicine and Biology, 2016, 856, 317-342.	1.6	15
102	Network Topological Indices from Chem-Bioinformatics to Legal Sciences and back. Current Bioinformatics, 2011, 6, 53-70.	1.5	14
103	Transitioning the generalised read-across approach (GenRA) to quantitative predictions: A case study using acute oral toxicity data. Computational Toxicology, 2019, 12, 100097.	3.3	14
104	Validation of Computational Methods. Advances in Experimental Medicine and Biology, 2016, 856, 165-187.	1.6	13
105	Extending the Generalised Read-Across approach (GenRA): A systematic analysis of the impact of physicochemical property information on read-across performance. Computational Toxicology, 2018, 8, 34-50.	3.3	13
106	Identification of novel activators of the metal responsive transcription factor (MTF-1) using a gene expression biomarker in a microarray compendium. Metallomics, 2020, 12, 1400-1415.	2.4	13
107	A mechanistic framework for integrating chemical structure and high-throughput screening results to improve toxicity predictions. Computational Toxicology, 2018, 8, 1-12.	3.3	12
108	Derivation of New Threshold of Toxicological Concern Values for Exposure via Inhalation for Environmentally-Relevant Chemicals. Frontiers in Toxicology, 2020, 2, 580347.	3.1	12

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109	Generalized Read-Across prediction using genra-py. Bioinformatics, 2021, 37, 3380-3381.	4.1	12
110	An evaluation of existing QSAR models and structural alerts and development of new ensemble models for genotoxicity using a newly compiled experimental dataset. Computational Toxicology, 2021, 18, 100167.	3.3	12
111	Integrating data gap filling techniques: A case study predicting TEFs for neurotoxicity TEQs to facilitate the hazard assessment of polychlorinated biphenyls. Regulatory Toxicology and Pharmacology, 2019, 101, 12-23.	2.7	11
112	Integrated testing and assessment approaches for skin sensitization: a commentary. Journal of Applied Toxicology, 2014, 34, 436-440.	2.8	10
113	Predicting Toxicological and Ecotoxicological Endpoints. , 2007, , 427-465.		9
114	An evaluation of the performance of selected (Q)SARs/expert systems for predicting acute oral toxicity. Computational Toxicology, 2020, 16, 100135.	3.3	9
115	Can mutagenicity information be useful in an Integrated Testing Strategy (ITS) for skin sensitization?. SAR and QSAR in Environmental Research, 2010, 21, 619-656.	2.2	8
116	Quantitative prediction of repeat dose toxicity values using GenRA. Regulatory Toxicology and Pharmacology, 2019, 109, 104480.	2.7	8
117	Repeat-dose toxicity prediction with Generalized Read-Across (GenRA) using targeted transcriptomic data: A proof-of-concept case study. Computational Toxicology, 2021, 19, 100171.	3.3	8
118	Skin, drug and chemical reactions. Drug Discovery Today Disease Mechanisms, 2008, 5, e211-e220.	0.8	7
119	Chemistry Based Nonanimal Predictive Modeling for Skin Sensitization. Emerging Topics in Ecotoxicology, 2009, , 61-83.	1.5	7
120	Comparing the performance and coverage of selected in silico (liver) metabolism tools relative to reported studies in the literature to inform analogue selection in read-across: A case study. Computational Toxicology, 2022, 21, 100208.	3.3	7
121	Application of IATA â€“ A case study in evaluating the global and local performance of a Bayesian network model for skin sensitization. SAR and QSAR in Environmental Research, 2017, 28, 297-310.	2.2	6
122	Implementing in vitro bioactivity data to modernize priority setting of chemical inventories. ALTEX: Alternatives To Animal Experimentation, 2021, , .	1.5	6
123	Navigating the Minefield of Computational Toxicology and Informatics: Looking Back and Charting a New Horizon. Frontiers in Toxicology, 2020, 2, 2.	3.1	5
124	Markov Entropy Centrality: Chemical, Biological, Crime, and Legislative Networks. , 2011, , 199-258.		5
125	Principles and procedures for assessment of acute toxicity incorporating in silico methods. Computational Toxicology, 2022, 24, 100237.	3.3	5
126	Integrating publicly available information to screen potential candidates for chemical prioritization under the Toxic Substances Control Act: A proof of concept case study using genotoxicity and carcinogenicity. Computational Toxicology, 2021, 20, 100185.	3.3	4

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127	Development of the InTelligence And Machine LEarning (TAME) Toolkit for Introductory Data Science, Chemical-Biological Analyses, Predictive Modeling, and Database Mining for Environmental Health Research. Frontiers in Toxicology, 0, 4, .	3.1	4
128	Comparing and contrasting the coverage of publicly available structural alerts for protein binding. Computational Toxicology, 2019, 12, 100100.	3.3	3
129	Computational Methods to Predict Drug Safety. Current Computer-Aided Drug Design, 2006, 2, 151-168.	1.2	1
130	Editorial: Advances and Refinements in the Development and Application of Threshold of Toxicological Concern. Frontiers in Toxicology, 2022, 4, 882321.	3.1	1
131	From Knowledge Generation to Knowledge Archive. A General Strategy Using TOPS-MODE with DEREK to Formulate New Alerts for Skin Sensitization.. ChemInform, 2004, 35, no.	0.0	0
132	A Stepwise Approach for Defining the Applicability Domain of SAR and QSAR Models.. ChemInform, 2005, 36, no.	0.0	0
133	FS04.3â€¨Hair dyes, prediction of sensitization potential with QSAR. Contact Dermatitis, 2008, 50, 137-137.	1.4	0
134	P38â€¨Quantitative structure activity relationships for fragrance aldehydes. Contact Dermatitis, 2008, 50, 192-192.	1.4	0