

## 別添 4

## 研究成果の刊行に関する一覧表

## 書籍

著者氏名	論文タイトル名	書籍全体の 編集者名	書 籍 名	出版社名	出版地	出版年	ページ
本間正充	化学物質毒性ビッグデータベースと、インシリコによる毒性予測		IT・ビッグデータと薬学	日本学術協力財団		2019	89-100
山田隆志	OECDにおけるQSAR、AOPの開発状況		皮膚の安全性・有用性評価法	技術情報協会		2018	151-157

## 雑誌

発表者氏名	論文タイトル名	発表誌名	巻号	ページ	出版年
Mishima M, Hashizume T, Haranosono Y, Nagato Y, Takeshita K, Fukuchi J, and Homma M.	Meeting report, ICH M7 relevant workshop: use of (Q)SAR systems and expert judgment.	Genes and Environment	40	19-25	2018
Benfenati E, Golbamaki A, Raitano G, Roncaglioni A, Manganelli S, Lemke F, Norinder U, Lo Piparo E, Honma M, Manganaro A, Gini G.	A large comparison of integrated SAR/QSAR models of the Ames test for mutagenicity.	SAR QSAR Environ Res.	29	591-611	2018

<p>Myatt GJ, Ahlberg E, Akahori Y, Allen D, Amberg A, Anger LT, Aptula A, Auerbach S, Beilke L, Bellion P, Benigni R, Bercu J, Booth ED, Bower D, Brigo A, Burden N, Cammerer Z, Cronin MTD, Cross KP, Custer L, Dettwiler M, Dobo K, Ford KA, Fortin MC, Gad-McDonald SE, Gellatly N, Gervais V, Glover KP, Glowienke S, Van Gompel J, Gutsell S, Hardy B, Harvey JS, Hillegass J, Honma M, Hsieh JH, Hsu CW, Hughes K, Johnson C, Jolly R, Jones D, Kemper R, Kenyon MO, Kim MT, Kruhlak NL, Kulkarni SA, Kümmerer K, Leavitt P, Majer B, Masten S, Miller S, Moser J, Mumtaz M, Muster W, Neilson L, Oprea TI, Patlewicz G, Paulino A, Lo Piparo E, Powley M, Quigley DP, Reddy MV, Richarz AN, Ruiz P, Schilter B, Serafimova R, Simpson W, Stavitskaya L, Stidl R, Suarez-Rodriguez D, Szabo DT, Teasdale A, Trejo-Martin A, Valentin JP, Vuorinen A, Wall BA, Watts P, White AT, Wichard J, Witt KL, Woolley A, Woolley D, Zwickl C, Hasselgren C.</p>	<p><i>In silico</i> toxicology protocols.</p>	<p>Regul Toxicol Pharmacol.</p>	<p>96</p>	<p>1-17</p>	<p>2018</p>
--	---	---------------------------------	-----------	-------------	-------------

Amberg A, Andaya RV, Anger LT, Barber C, Beilke L, Bercu J, Bower D, Brigo A, Cammerer Z, Cross KP, Custer L, Dobo K, Gerets H, Gervais V, Glowienke S, Gomez, S, Van Gompel J, Harvey J, Hasselgren C, Honma M, Johnson C, Jolly R, Kemper R, Kenyon M, Kruhlak N, Leavitt P, Miller S, Muster W, Naven R, Nicolette J, Parenty A, Powley M, Quigley DP, Reddy MV, Sasaki JC, Stavitskaya L, Teasdale A, Trejo-Martin A, Weiner S, Welch DS, White A, Wichard J, Woolley D, Myatt GJ.	Principles and procedures for handling out-of-domain and indeterminate results as part of ICH M7 recommended (Q)SAR analyses.	Regul Toxicol Pharmacol.	102	59-64	2019
Honma M, Kitazawa A, Cayley A, Williams RV, Barber C, Hanser T, Saiakhov R, Chakravarti S, Myatt GJ, Cross KP, Benfenati E, Raitano G, Mekenyan O, Petkov P, Bossa C, Benigni R, Battistelli CL, Giuliani A, Tcheremenskaia O, DeMeo C, Norinder U, Koga H, Jose C, Jeliazkova N, Kochev N, Paskaleva V, Yang C, Daga PR, Clark RD, Rathman J.	Improvement of quantitative structure-activity relationship (QSAR) tools for predicting Ames mutagenicity: outcomes of the Ames/QSAR International Challenge Project.	Mutagenesis	34	3-16	2019
Fukuchi J, Kitazawa A, Hirabayashi K, Honma M.	A practice of expert review by read-across using QSAR Toolbox.	Mutagenesis	34	49-54	2019
Amberg A, Anger LT, Bercu J, Bower D, Cross KP, Custer L, Harvey JS, Hasselgren C, Honma M, Johnson C, Jolly R, Kenyon MO, Kruhlak NL, Leavitt P, Quigley DP, Miller S, Snodin D, Stavitskaya L, Teasdale A, Trejo-Martin A, White AT, Wichard J, Myatt GJ.	Extending (Q)SARs to incorporate proprietary knowledge for regulatory purposes: is aromatic N-oxide a structural alert for predicting DNA-reactive mutagenicity?	Mutagenesis	34	67-82	2019

Petkov PI, Schultz TW, Honma M, Yamada T, Kaloyanova E, Mekenyan OG.	Validation of the performance of TIMES genotoxicity models with EFSA pesticide data.	Mutagenesis	34	83-90	2019
Morita T, Shigeta Y, Kawamura T, Fujita Y, Honda H, Honma M.	<i>In silico</i> prediction of chromosome damage: comparison of three (Q)SAR models.	Mutagenesis	34	91-100	2019
Fujita Y, Honda H, Matsumura S, Yamane M, Morita T, Matsuda T, Morita O	A decision tree-based integrated testing strategy for the tailor-made carcinogenicity evaluation of test substances using genotoxicity test results and chemical spaces.	Mutagenesis	34	101-109	2019
Tennant RE, Guesné SJ, Canipa S, Cayley A, Drewe WC, Honma M, Masumura K, Morita T, Stalford SA, Williams RV.	Extrapolation of <i>in vitro</i> structural alerts for mutagenicity to the <i>in vivo</i> endpoint.	Mutagenesis	34	111-121	2019

Hasselgren C, Ahlberg E, Akahori Y, Amberg A, Anger LT, Atienzar F, Auerbach S, Beilke L, Bellion P, Benigni R, Bercu J, Booth ED, Bower D, Brigo A, Cammerer Z, Cronin MTD, Crooks I, Cross KP, Custer L, Dobo K, Doktorova T, Faulkner D, Ford KA, Fortin MC, Frericks M, Gad-McDonald SE, Gellatly N, Gerets H, Gervais V, Glowienke S, Van Gompel J, Harvey JS, Hillegass J, Honma M, Hsieh JH, Hsu CW, Barton-Maclaren TS, Johnson C, Jolly R, Jones D, Kemper R, Kenyon MO, Kruhlak NL, Kulkarni SA, Kümmerer K, Leavitt P, Masten S, Miller S, Moudgal C, Muster W, Paulino A, Lo Piparo E, Powley M, Quigley DP, Reddy MV, Richarz AN, Schilter B, Snyder RD, Stavitskaya L, Stidl R, Szabo DT, Teasdale A, Tice RR, Trejo-Martin A, Vuorinen A, Wall BA, Watts P, White AT, Wichard J, Witt KL, Woolley A, Woolley D, Zwickl C, Myatt GJ.	Genetic toxicology in silico protocol.	Regul Toxicol Pharmacol	107	doi: 10.1016/j.yrtph.2019.104403.	2019
Petkov PI, Kuseva C, Kotov S, Honma M, Kitazawa A, Kulkarni S, Schultz TW, Mekenyan OG.	Procedure for toxicological predictions based on mechanistic weight of evidences: Application to Ames mutagenicity.	Computational Toxicology	12	doi.org/10.1016/J.COMTOX.2017.02.004	2019
本間正充	医薬品中の変異原性不純物の安全性評価と管理—ICH-M7を踏まえた遺伝毒性物質の許容値の設定に関する科学—	PHARM TECH JAPAN	35	1461-1469	2019

本間正充	化学物質の遺伝毒性評価と定量的構造相関 (Q) SAR)	ポリ衛協会報	65	5-25	2019
本間正充	毒性試験の未来を考える — (定量的) 構造活性相関による化学物質の変異原性評価 —	国立医薬品食品衛生研究所報告	137	20-31	2019
本間正充	食品中に混在する微量な化学物質の安全性評価 — 定量的構造活性相関 (QSAR) による変異原性化学物質の同定 —	日本包装学会誌	29	27-42	2020
Honma M	An assessment of mutagenicity of chemical substances by (quantitative) structure-activity relationship.	Genes Environ.	42:23	doi: 10.1186/s41021-020-00163-1. PMID: 32626544.	2020
Van Bossuyt M, Raitano G, Honma M, Van Hoeck E, Vanhaecke T, Rogiers V, Mertens B, Benfenati E.	New QSAR models to predict chromosome damaging potential based on the in vivo micronucleus test.	Toxicol Lett.	329	80-84	2020
Honma M, Kitazawa A, Kasamatsu T, Sugiyama KI.	Screening for Ames mutagenicity of food flavor chemicals by (quantitative) structure-activity relationship.	Genes Environ.	42:32	doi: 10.1186/s41021-020-00171-1.	2020
Igarashi T, Takashima H, Takabe M, Suzuki H, Ushida K, Kawamura T, Matsumoto M, Iso T, Tanabe S, Inoue K, Ono A, Yamada T, Hirose A.	Initial hazard assessment of benzyl salicylate: <i>In vitro</i> genotoxicity test and combined repeated-dose and reproductive/developmental toxicity screening test in rats.	Regul. Toxicol. Pharmacol.	100	105-117	2018
Chesnut M, Yamada T, Adams T, Knight D, Kleinstreuer N, Kass G, Luechtefeld T, Hartung T.	Regulatory acceptance of read-across.	ALTEX	35	413-419	2018

Igarashi T, Serizawa H, Kobayashi K, Suzuki H, Matsumoto M, Iso T, Kawamura T, Inoue K, Ono A, Yamada T, Hirose A.	Initial hazard assessment of 4-benzylphenol, a structural analog of bisphenol F: Genotoxicity tests <i>in vitro</i> and a 28-day repeated-dose toxicity study in rats.	Regul. Toxicol. Pharmacol.	96	64-75	2018
Yamada T, Tanaka Y, Hasegawa R, Igarashi T, Hirose A.	Male-specific prolongation of prothombin time by industrial chemicals.	Fundam. Toxicol. Sci.	5	75-82	2018
Matsumoto M, Furukawa M, Kobayashi K, Iso T, Igarashi T, Yamada T, Hirose A.	A 28-day repeated oral-dose toxicity study of insecticide synergist N-(2-ethylhexyl)-1-isopropyl-4-methylbicyclo[2.2.2]oct-5-ene-2,3-dicarbo-ximide in rats.	Fundam. Toxicol. Sci.	5	1-11	2018
Inoue K, Suzuki H, Yamada T.	Comprehensive toxicity evaluation of cyclopentyl methyl ether (CPME) for establishing a permitted daily exposure level.	Fundam. Toxicol. Sci.	6	145-165	2019
Jojima K, Yamada T, Hirose A.	Development of a hepatotoxicity prediction model using <i>in vitro</i> assay data of key molecular events.	Fundam. Toxicol. Sci.	6	327-32	2019
Yamada T, Matsumoto M, Miura M, Hirose A.	Case study on the use of integrated approaches to testing and assessment for testicular toxicity of ethylene glycol methyl ether (EGME)-related chemicals.	Organisation for Economic Co-operation and Development (OECD), Series on Testing & Assessment.	308	1-75	2019

Patlewicz G, Lizarraga LE, Rua D, Allen DG, Daniel AB, Fitzpatrick SC, Garcia-Reyero N, Gordon J, Hakkinen P, Howard AS, Karmaus A, Matheson J, Mumtaz M, Richarz A, Ruiz P, Scarano L, Yamada T, Kleinstreuer N.	Exploring current read-across applications and needs among selected U.S. Federal Agencies.	Regul. Toxicol. Pharmacol.	106	197-209	2019
Tachibana K, Kass GEN, Ono A, Yamada T, Tong W, Doerge DR, Yamazoe Y.	A Summary Report of FSCJ Workshop "Future Challenges and Opportunities in Developing Methodologies for Improved Human Risk Assessments".	Food Safety	7	83-89	2019
山田隆志, 足利太可雄, 小島肇, 広瀬明彦.	AOP (Adverse Outcome Pathway; 有害性発現経路) に基づいた化学物質の安全性評価へ向けたチャレンジ.	YAKUGAKU ZASSHI	140	481-484	2020
Shigeta Y, Iso T, Inoue K, Yamada T, Hirose A, Matsumoto M.	Summary information of human health hazard assessment of existing chemical substances (VI).	Bull. Natl Inst. Health Sci.	138	33-39	2020
Kawashima A, Inoue K, Yoshizaki Y, Ushida K, Kai K, Suzuki H, Takano M, Fujii S, Yabe K, Matsumoto M, Yamada T, Hirose A.	Combined repeated-dose and reproductive/developmental oral toxicity of 3-methylpentane, isooctane, and isononane in rats.	Fundam. Toxicol. Sci.	7	259-279	2020
Yamazoe Y, Yamada T, Nagata K.	Prediction and Characterization of CYP3A4-mediated metabolisms of azole fungicides: an application of the fused-grid template system.	Food Saf (Tokyo).	8	34-51	2020



Rovida C, Barton-Maclaren T, Benfenati E, Caloni F, Chandrasekera PC, Chesné C, Cronin MTD, De Knecht J, Dietrich DR, Escher SE, Fitzpatrick S, Flannery B, Herzler M, Hougaard Bennekou S, Hubesch B, Kamp H, Kisitu J, Kleinstreuer N, Kovarich S, Leist M, Maertens A, Nugent K, Pallocca G, Pastor M, Patlewicz G, Pavan M, Presgrave O, Smirnova L, Schwarz M, Yamada T, Hartung T.	Internationalization of read-across as a validated new approach method (NAM) for regulatory toxicology.	ALTEX	37	579-606	2020
山田隆志	IATAの実践および毒性データベースと <i>in silico</i> ツールの利用から学んだ知見.	フロンティア	2(3)	133-139	2020
Rovida C, Escher SE, Herzler M, Hougaard Bennekou S, Kamp H, Kroese, DE, Maslankiewicz L, Moné MJ, Patlewicz G, Sipes, N, van Aerts L, White A, Yamada T, van de Water B.	NAM-supported read-across: From case studies to regulatory guidance in safety assessment.	ALTEX	38	140-150	2021
Yamazoe Y, Yamada T, Hirose A, Murayama N.	Deciphering key interactions of ligands with CYP3A4-Template system.	Food Saf (Tokyo).	9	10-21	2021
Yamada T, Kurimoto M, Hirose A, Yang C, Rathman J.	Development of a new threshold of toxicological concern database of non-cancer toxicity endpoints for industrial chemicals.	Front. Toxicol.	3	1-9	2021
Matsumoto M, Iso T, Igarashi T, Tanabe S, Inoue K, Hirose A.	Summary information of human health hazard assessment of existing chemical substances(IV).	Bull. Natl Inst. Health Sci.	136	108-113	2018

Kohara A, Matsumoto M, Hirose A, Hayashi M, Honma M, Suzuki T.	Mutagenic properties of dimethylaniline isomers in mice as evaluated by comet, micronucleus and transgenic mutation assays.	Genes Environ.	40	18-27	2018
Matsumoto M, Hirata-Koizumi M, Kawamura T, Sakuratani S, Ono A, Hirose A.	Validation of the statistical parameters and model selection criteria of the benchmark dose methods for the evaluation of various endpoints in repeated-dose toxicity studies.	Fundam. Toxicol. Sci.	6	125-136	2019
Matsumoto M, Iso T, Igarashi T, Tanabe S, Inoue K, Hirose A.	Summary information of human health hazard assessment of existing chemical substances(V).	Bull. Natl Inst. Health Sci.	137	66-72	2019
田邊思帆里, 広瀬明彦, Maurice Whelan, 山田隆志.	遺伝子ネットワーク解析による分子パスウェイ解明及びAOP開発状況について.	YAKUGAKU ZASSHI	140	485-489	2020
Igarashi T, Suzuki H, Ushida K, Matsumoto M, Inoue K, Kanno T, Miwa Y, Ishii T, Nagase T, Katsumata Y, Hirose A.	Initial hazard assessment of 1,4-dichlorobutane: Genotoxicity tests, 28-day repeated-dose toxicity test, and reproductive/developmental toxicity screening test in rats.	Regul Toxicol Pharmacol.	112:1046-1050	doi: 10.1016/j.rpth.2020.104610.	2020