

**Table S1.** The 16 reference databases

Reference database	Website address	Provided test data		
		Physicochemical properties	Health hazard	Environmental hazard
NCIS (Korea)	ncis.nier.go.kr/ncis.jsp	○	○	○
Safety test (Korea)	ncis.nier.go.kr/ncis.jsp	○	○	○
OECD SIDS (EU)	www.chem.unep.ch/irptc/sids/OECD/SIDS/indexcasnumb.htm	○	○	○
GHS classification result (EU)	esis.jrc.ec.europa.eu/index.html	○	○	○
GHS classification result (Korea)	ncis.nier.go.kr/ghs/search/toxic_contain_chem_label.jsp	○	○	○
ECB IUCLID (EU)	esis.jrc.ec.europa.eu/	○	○	○
HSDB (US)	toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen-HSDB	○	○	○
IPCS EHC (EU)	http://www.inchem.org/pages/ehc.html	-	○	○
ATSDR (US)	www.atsdr.cdc.gov/toxprofiles/index.asp	-	○	-
Japanese safety assessment report (Japan)	www.safe.nite.go.jp/english/sougou/view/TotalSrchInput_en.faces	-	○	○
CCRIS (US)	toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?CCRIS	-	○	-
GENETOX (US)	toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?GENETOX	-	○	-
EPA IRIS (US)	cfpub.epa.gov/ncea/iris/index.cfm?fuseaction=iris.showsubstanceList	-	○	-
ECOTOX (US)	cfpub.epa.gov/ecotox/quick_query.htm	-	-	○
Chemical DB (US)	ull.chemistry.uakron.edu/erd/	○	-	-
ChemID Plus (US)	chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp	○	-	-
Total	16	9	13	10

NCIS, National Chemicals Information System; OECD, Organization for Economic Cooperation and Development; SIDS, Screening Information Data Set; GHS, Globally Harmonized System; EU, European Union; European Chemical Bureau; IUCLID, International Uniform Chemical Information Database; HSDB, Hazardous Substances Data Bank; IPCS EHC, International Programme on Chemical Safety Environmental Health Criteria; ATSDR, Agency for Toxic Substances and Disease Registry; CCRIS, Chemical Carcinogenesis Research Information System; GENETOX, Genetic Toxicology Data Bank; EPA IRIS, US Environmental Protection Agency Integrated Risk Information System.