Supplementary Material

Prediction of the endocrine disruption profile of pesticides

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CAS RN of the 220 pesticides. The unstated stereochemistry CAS RN was indicated below in priority to facilitate the retrieval of structural information but as indicated in the text, when necessary, isomeric CAS RNs were used to run the EDS.

Acetamiprid (135410-20-7), Acetochlor (34256-82-1), Acifluorfen-methyl (50594-67-7), Aclonifen (74070-46-5), Amitraz (33089-61-1), Amitrole (61-82-5), Anthraquinone (84-65-1), Asulam (3337-71-1), Bflubutamid (113614-08-7), Benalaxyl (71626-11-4), Benfluralin (1861-40-1), Benfuracarb (82560-54-1), Benoxacor (98730-04-2), Bentazone (25057-89-0), Benthiavalicarb (177406-68-7), Bifenox (42576-02-3), Bifenthrin (82657-04-3), Boscalid (188425-85-6), Brodifacoum (56073-10-0), Bromadiolone (28772-56-7), Bromopropylate (18181-80-1), Bromoxynil octanoate (1689-99-2), Bromuconazole (116255-48-2), Bupirimate (41483-43-6), Carboxin (5234-68-4), Carfentrazone-ethyl (128639-02-1), Chlormethoxyfen (32861-85-1), Chlorantraniliprole (500008-45-7), Chloridazon (1698-60-8), Chlorobenzilate (510-15-6), Chloropropylate (5836-10-2), Chlorotoluron (15545-48-9), Chlorpropham (101-21-3), Chlorpyrifos-ethyl (2921-88-2), Chlorpyrifos-methyl (5598-13-0), Chlorsulfuron (64902-72-3), Clethodim (99129-21-2), Clodinafop-propargyl (105512-06-9), Clomazone (81777-89-1), Clopyralid (1702-17-6), Cloquintocet-mexyl (99607-70-2), Coumatetralyl (5836-29-3), Cyanamide (420-04-2), Cyazofamid (120116-88-3), Cycloxydim (101205-02-1), Cyfluthrin (68359-37-5), Cymoxanil (57966-95-7), α -Cypermethrin (67375-30-8), Cyproconazole (94361-06-5), Cyprodinil (121552-61-2), 2,4-D (94-75-7), 2,4-DB (94-82-6), Deltamethrin (52918-63-5), Desmedipham (13684-56-5), Diazinon (333-41-5), Dicamba (1918-00-9), Dichlorprop-P (15165-67-0), Diclofop-methyl (51338-27-3), Difenacoum (56073-07-5), Difenoconazole (119446-68-3), Difethialone (104653-34-1), Diflufenican (83164-33-4), Dimethachlor (50563-36-5), Dimethenamid-P (163515-14-8), Dimethoate (60-51-5), Dimethomorph (110488-70-5), Dinocap (131-72-6), Diphacinone (82-66-6), Diquat (2764-72-9), Dodemorph (1593-77-7), α -Endosulfan (959-98-8), EPN (2104-64-5), Epoxiconazole (133855-98-8), Ergocalciferol (50-14-6), Esfenvalerate (66230-04-4), Ethephon (16672-87-0), Ethofumesate (26225-79-6), Ethoprophos (13194-48-4), Ethylene dibromide (106-93-4), Ethylene dichloride (107-06-3), Fenamidone (161326-34-7), Fenarimol (60168-88-9), Fenazaquin (120928-09-8), Fenoxaprop-P-ethyl (71283-80-2), Fenpropidin (67306-00-7), Fenpropimorph (67564-91-4), Fenvalerate (51630-58-1), Flocoumafen (90035-08-8), Flonicamid (158062-67-0), Florasulam (145701-23-1), Fluazifop-butyl (79241-46-6), Fluazinam (79622-59-6), Flucycloxuron (113036-88-7), Flucythrinate (70124-77-5), Fludioxonil (131341-86-1), Fluopicolide (239110-15-7), Fluoxastrobin (361377-29-9), Flupyrsulfuron-methyl (144740-53-4), Flurochloridone (61213-25-0), Flurtamone (96525-23-4), Fluthiamide (142459-58-3), Flutolanil (66332-96-5), Flutriafol (76674-21-0), Foramsulfuron (173159-57-4), Glyphosate (1071-83-6), Hexaconazole (79983-71-4), Hexythiazox (78587-05-0), Hydramethylnon (67485-29-4), Imazamox (114311-32-9), Imazaquin (81335-37-7), Imidacloprid (138261-41-3), Indanofan (133220-30-1), Iodosulfuron (1144097-22-2), Ioxynil octanoate (3861-47-0), Ipconazole (125225-28-7), Iprodione (36734-19-7), Iprovalicarb (140923-17-7), Isoproturon (34123-59-6), Isoxaben (82558-50-7), Isoxadifen-ethyl (163520-33-0), Isoxaflutole (141112-29-0), Kresoxim-methyl (143390-89-0), lambda-Cyhalothrin (91465-08-6), Lenacil (2164-08-1), Linuron (330-55-2), Maleic hydrazide (123-33-1), Mandipropamid (374726-62-2), Mecoprop (7085-19-0), Mecoprop-P (16484-77-8), Mefenpyr-diethyl (135590-

91-9), Mepiquat chloride (24307-26-4), Mesosulfuron-methyl (208465-21-8), Mesotrione (104206-82-8), Metalaxyl-M (70630-17-0), Metaldehyde (108-62-3), Metam (144-54-7), Metamitron (41394-05-2), Metazachlor (67129-08-2), Metconazole (125116-23-6), Methiocarb (2032-65-7), Methyl isothiocyanate (556-61-6), Metobenzuron (111578-32-6), S-Metolachlor (87392-12-9), Metosulam (139528-85-1), Metrafenone (220899-03-6), Metribuzin (21087-64-9), Metsulfuron-methyl (74223-64-6), Myclobutanil (88671-89-0), Napropamide (15299-99-7), Nicosulfuron (111991-09-4), Nonylphenol ethoxylate (9016-45-9), Oxadiargyl (39807-15-3), Oxadiazon (19666-30-9), Oxyfluorfen (42874-03-3), Paclobutrazol (76738-62-0), Penconazole (66246-88-6), Pencycuron (66063-05-6), Pendimethalin (40487-42-1), Permethrin (52645-53-1), Phenmedipham (13684-63-4), 2-Phenylphenol (90-43-7), Picolinafen (137641-05-5), Pinoxaden (243973-20-8), Pirimicarb (23103-98-2), Prochloraz (67747-09-5), Procymidone (32809-16-8), Propamocarb (24579-73-5), Propaquizafop (111479-05-1), Propiconazole (60207-90-1), Propyzamide (23950-58-5), Proquinazid (189278-12-4), Prosulfocarb (52888-80-9), Prosulfuron (94125-34-5), Prothioconazole (178928-70-6), Pymetrozine (123312-89-0), Pyraclostrobin (175013-18-0), Pyrazoxyfen (71561-11-0), Pyridate (55512-33-9), Pyrimethanil (53112-28-0), Pyriproxyfen (95737-68-1), Pyroxulam (422556-08-9), Quinmerac (90717-03-6), Quinoxifen (124495-18-7), Quizalofop-ethyl (76578-14-8), Quizalofop-P-ethyl (100646-51-3), Rimsulfuron (122931-48-0), Rotenone (83-79-4), RU 15525 (58769-20-3), Spiroxamine (118134-30-8), Sulcotrione (99105-77-8), Sulfosulfuron (141776-32-1), Sulfuramid (4151-50-2), Tau-Fluvalinate (102851-06-9), Tebuconazole (107534-96-3), Tebufenozide (112410-23-8), Tebufenpyrad (119168-77-3), Tefluthrin (79538-32-2), Tembotrione (335104-84-2), Tetraconazole (112281-77-3), Thiacloprid (111988-49-9), Thiamethoxam (153719-23-4), Thifensulfuron-methyl (79277-27-3), Thiocyclam (31895-21-3), Thiophanate-methyl (23564-05-8), Thiram (137-26-8), Transfluthrin (118712-89-3), Triadimefon (43121-43-3), Triadimenol (55219-65-3), Triallate (2303-17-5), Triazoxide (72459-58-6), Tribenuron-methyl (101200-48-0), Trifloxystrobin (141517-21-7), Triflumizole (99387-89-0), Trifluralin (1582-09-8), Triflusulfuron-methyl (126535-15-7), Trinexapac-ethyl (95266-40-3), Triticonazole (131983-72-7), Vinclozolin (50471-44-8), Warfarin (5543-58-8), Zoxamide (156052-68-5).