

## **AI4NAMS - Deliverable 5**

Draft case study report – Supplementary data

Case study 3

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# 1. Initial data collection, Unstructured data sources

## 1.1 Full search string for PubMed

((in vitro) OR (in chemico) OR (in silico) OR (QSAR) OR (zebrafish) OR (danio rerio) OR (c. elegans) OR (cell culture) OR (organ chip) OR (ex vivo) OR (cell line) OR (organoid) OR (Drosophila melanogaster)) AND ((hypothyroidism) OR (thyrotoxicosis) OR (endocrine) OR (thyroid) OR (Thyroperoxidase) OR (Thyroid peroxidase) OR (iodide peroxidase) OR (TPO) OR (Sodium Iodide Symporter) OR (Na<sup>+</sup>/I<sup>-</sup> symporter) OR (Sodium Iodide antiporter) OR (Na<sup>+</sup>/I<sup>-</sup> antiporter) OR (NIS) OR (Sodium Iodide Transporter) OR (Na<sup>+</sup>/I<sup>-</sup> Transporter) OR (Glucuronosyltransferase) OR (Glucuronosyl transferase) OR (Uridine 5'-diphospho-glucuronosyltransferase) OR (UDP-GT) OR (Sulfotransferase) OR (SULT) OR ({iodothyronine deiodinase}) OR ({iodothyronine 5'-deiodinase}) OR ({iodothyronine 5'-monodeiodinase}) OR (deiodinase) OR (Monodeiodinase) OR (DIO) OR (Transthyretin) OR (TTR) OR (TBPA) OR (Thyroxine Binding Prealbumin)) AND ("2,4-dichlorophenoxyacetic acid"[Title/Abstract] OR "94-75-7"[Title/Abstract] OR "2-(2,4-dichlorophenoxy)acetic acid"[Title/Abstract] OR "2,4-D"[Title/Abstract] OR "(2,4-Dichlorophenoxy)acetic acid"[Title/Abstract] OR "2,4-D acid"[Title/Abstract] OR "Amitrole"[Title/Abstract] OR "3-amino-1,2,4-triazole"[Title/Abstract] OR "61-82-5"[Title/Abstract] OR "4H-1,2,4-triazol-3-amine"[Title/Abstract] OR "1H-1,2,4-Triazol-3-amine"[Title/Abstract] OR "1H-1,2,4-Triazol-5-amine"[Title/Abstract] OR "Aminotriazole"[Title/Abstract] OR "3-Aminotriazole"[Title/Abstract] OR "Amitrol"[Title/Abstract] OR "Clofentazine"[Title/Abstract] OR "74115-24-5"[Title/Abstract] OR "3,6-Bis(2-chlorophenyl)-1,2,4,5-tetrazine"[Title/Abstract] OR "Bisclorfentazin"[Title/Abstract] OR "Bisclorfentazine"[Title/Abstract] OR "1,2,4,5-Tetrazine, 3,6-bis(2-chlorophenyl)-"[Title/Abstract] OR "3,6-Bis(o-chlorophenyl)-1,2,4,5-tetrazine"[Title/Abstract] OR "imidazolidine-2-thione"[Title/Abstract] OR "2-Imidazolidinethione"[Title/Abstract] OR "Ethylenethiourea"[Title/Abstract] OR "96-45-7"[Title/Abstract] OR "ETHYLENE THIOUREA"[Title/Abstract] OR "2-Mercaptoimidazoline"[Title/Abstract] OR "Imidazolidinethione"[Title/Abstract] OR "N,N'-Ethylenethiourea"[Title/Abstract] OR "Ethlenethiourea"[Title/Abstract] OR "Fluopyram"[Title/Abstract] OR "658066-35-4"[Title/Abstract] OR "N-[2-[3-Chloro-5-(trifluoromethyl)-2-pyridinyl]ethyl]-2-(trifluoromethyl)benzamide"[Title/Abstract] OR "N-[2-[3-chloro-5-(trifluoromethyl)pyridin-2-yl]ethyl]-2-(trifluoromethyl)benzamide"[Title/Abstract] OR "N-{2-[3-chloro-5-(trifluoromethyl)-2-pyridyl]ethyl}-alpha,alpha,alpha-trifluoro-o-toluamide"[Title/Abstract] OR "N-[2-[3-chloro-5-(trifluoromethyl)pyridin-2-yl]ethyl]-2-(trifluoromethyl)benzamide"[Title/Abstract] OR "Benzamide, N-[2-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]ethyl]-2-(trifluoromethyl)-"[Title/Abstract] OR "n-[2-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]ethyl]-2-trifluoromethylbenzamide"[Title/Abstract] OR "N-{2-[3-chloro-5-(trifluoromethyl)-2-pyridyl]ethyl}-alpha,alpha,alpha-trifluoro-o-toluamide"[Title/Abstract] OR "Ioxynil"[Title/Abstract] OR "4-Hydroxy-3,5-diiodobenzonitrile"[Title/Abstract] OR "1689-83-4"[Title/Abstract] OR "Benzonitrile, 4-hydroxy-3,5-diiodo-"[Title/Abstract] OR "3,5-Diiodo-4-hydroxybenzonitrile"[Title/Abstract] OR "2,6-Diiodo-4-cyanophenol"[Title/Abstract] OR "4-Cyano-2,6-diiodophenol"[Title/Abstract] OR "4-Cyano-2,6-dijodphenol"[Title/Abstract] OR "Isoxaflutole"[Title/Abstract] OR "141112-29-0"[Title/Abstract] OR "(5-Cyclopropylisoxazol-4-yl)(2-(methylsulfonyl)-4-(trifluoromethyl)phenyl)methanone"[Title/Abstract] OR "(5-cyclopropyl-1,2-oxazol-4-yl)-[2-methylsulfonyl-4-(trifluoromethyl)phenyl)methanone"[Title/Abstract] OR "(5-Cyclopropyl-4-isoxazolyl)(2-(methylsulfonyl)-4-(trifluoromethyl)phenyl)methanone"[Title/Abstract] OR "(5-cyclopropyl-4-isoxazolyl)[2-(methylsulfonyl)-4-(trifluoromethyl)phenyl)methanone"[Title/Abstract] OR "MANCOZEB"[Title/Abstract] OR "8018-01-7"[Title/Abstract] OR "Manganese Zinc ethylenebis(dithiocarbamate)"[Title/Abstract] OR "18-METHYLNONADECANOICACID"[Title/Abstract] OR "manganese(2+) ethane-1,2-diylbis(dithiocarbamate) zinc ethane-1,2-diylbis(dithiocarbamate)"[Title/Abstract] OR "MANEB"[Title/Abstract] OR "12427-38-2"[Title/Abstract] OR "Manganese ethylenebisthiocarbamate"[Title/Abstract] OR "manganese(II) ethane-1,2-diylidcarbomodithioate"[Title/Abstract] OR "manganese(2+) ethane-1,2-diylbis(dithiocarbamate)"[Title/Abstract] OR "manganese(2+);N-[2-(sulfidocarbothioylamino)ethyl]carbomodithioate"[Title/Abstract] OR "ZINEB"[Title/Abstract] OR "METIRAM"[Title/Abstract] OR "Polyram"[Title/Abstract] OR "9006-42-2"[Title/Abstract] OR "12122-67-7"[Title/Abstract] OR "Zinc ethylenebisthiocarbamate"[Title/Abstract] OR "Zinc ammoniate ethylenebis(dithiocarbamate)-poly(ethylenethiuram disulfide)"[Title/Abstract] OR "zinc ethane-1,2-diylbis(dithiocarbamate)"[Title/Abstract] OR "Proquinazid"[Title/Abstract] OR "189278-12-4"[Title/Abstract] OR "6-iodo-2-propoxy-3-propylquinazolin-4(3H)-one"[Title/Abstract] OR "6-iodo-2-

propoxy-3-propylquinazolin-4-one"[Title/Abstract] OR "6-iodo-2-propoxy-3-propyl-4(3H)-quinazolinone"[Title/Abstract] OR "6-Iodo-2-propoxy-3-propyl-4(3H)quinazolinone"[Title/Abstract] OR "4(3H)-Quinazolinone, 6-iodo-2-propoxy-3-propyl-"[Title/Abstract] OR "6 -Iodo-2 -propoxy-3-propyl-4(3H)-quinazolinone"[Title/Abstract] OR "thiabendazole"[Title/Abstract] OR "148-79-8"[Title/Abstract] OR "Thiabendazole"[Title/Abstract] OR "2-(4-Thiazolyl)benzimidazole"[Title/Abstract] OR "2-(1,3-Thiazol-4-yl)-1H-benzimidazole"[Title/Abstract] OR "4-(1H-Benzo[d]imidazol-2-yl)thiazole"[Title/Abstract] OR "1H-Benzimidazole, 2-(4-thiazolyl)-"[Title/Abstract] OR "2-(4-Thiazolyl)-1H-benzimidazole"[Title/Abstract] OR "Thiacloprid"[Title/Abstract] OR "111988-49-9"[Title/Abstract] OR "(Z)-thiacloprid"[Title/Abstract] OR "(3-((6-Chloro-3-pyridinyl)methyl)-2-thiazolidinylidene)cyanamide"[Title/Abstract] OR "[3-[(6-chloropyridin-3-yl)methyl]-1,3-thiazolidin-2-ylidene]cyanamide"[Title/Abstract] OR "{(2Z)-3-[(6-chloropyridin-3-yl)methyl]-1,3-thiazolidin-2-ylidene}cyanamide"[Title/Abstract] OR "{3-[(6-chloropyridin-3-yl)methyl]-1,3-thiazolidin-2-ylidene}cyanamide"[Title/Abstract] OR "N-(3-((6-Chloropyridin-3-yl)methyl)thiazolidin-2-ylidene)cyanamide"[Title/Abstract] OR "Topramezone"[Title/Abstract] OR "210631-68-8"[Title/Abstract] OR "4-[3-(4,5-dihydro-1,2-oxazol-3-yl)-2-methyl-4-methylsulfonylbenzoyl]-2-methyl-1H-pyrazol-3-one"[Title/Abstract] OR "[3-(4,5-Dihydro-3-isoxazolyl)-2-methyl-4-(methylsulfonyl)phenyl](5-hydroxy-1-methyl-1H-pyrazol-4-yl)methanone"[Title/Abstract] OR "Methanone, [3-(4,5-dihydro-3-isoxazolyl)-2-methyl-4-(methylsulfonyl)phenyl](5-hydroxy-1-methyl-1H-pyrazol-4-yl)-"[Title/Abstract] OR "(3-(4,5-dihydro-3-isoxazolyl)-2-methyl-4-(methylsulfonyl)phenyl)(5-hydroxy-1-methyl-1H-pyrazol-4-yl)methanone"[Title/Abstract] OR "[3-(4,5-dihydro-1,2-oxazol-3-yl)-2-methyl-4-methylsulfonylphenyl]-(5-hydroxy-1-methylpyrazol-4-yl)methanone"[Title/Abstract] OR "ZIRAM"[Title/Abstract] OR "Zinc dimethyldithiocarbamate"[Title/Abstract] OR "137-30-4"[Title/Abstract] OR "Zinc Bis(dimethyldithiocarbamate)"[Title/Abstract] OR "Dimethyldithiocarbamic acid zinc salt"[Title/Abstract] OR "Zinc, bis(dimethyldithiocarbamate)-"[Title/Abstract] OR "Zinc, bis(dimethylcarbamodithioato-S,S')-, (T-4)-"[Title/Abstract] OR ("bromide"[Title/Abstract] NOT "[3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide]"[Title/Abstract])OR"Bromide ion"[Title/Abstract] OR "24959-67-9"[Title/Abstract] OR "3-Acetyl-1-benzyl-pyridinium bromide"[Title/Abstract] OR "3-Carbamoyl-1-dodecyl-pyridinium bromide"[Title/Abstract] OR "3-Carbamoyl-1-(3-phenyl-propyl)-pyridinium bromide"[Title/Abstract] OR ("Perchlorate"[Title/Abstract]NOT"Perchlorate discharge"[Title/Abstract]) OR "14797-73-0"[Title/Abstract] OR "Perchlorate ion"[Title/Abstract] OR "Chlorat(VII)"[Title/Abstract]OR"ClO4-"[Title/Abstract]OR"ClO(4)(-)"[Title/Abstract]OR"ClO4"[Title/Abstract])

## 1.2 Full search string for Scopus

TITLE-ABS-KEY( "in vitro"OR "in chemico"OR "in silico"OR "QSAR"OR "zebrafish"OR "danio rerio"OR "c. elegans"OR "cell culture"OR "organ chip"OR "ex vivo"OR "cell line"OR "organoid"OR "Drosophila melanogaster" ) AND TITLE-ABS-KEY ("hypothyroidism"OR "thyrotoxicosis"OR "endocrine"OR "thyroid"OR"Thyroperoxidase"OR"Thyroid peroxidase"OR"iodide peroxidase"OR"TPO"OR"Sodium Iodide Symporter"OR"Na+/I- symporter"OR"Sodium Iodide antiporter"OR"Na+/I- antiporter"OR"NIS"OR"Sodium Iodide Transporter"OR"Na+/I- Transporter"OR"Glucuronosyltransferase"OR"Glucuronosyl transferase"OR"Uridine 5'-diphospho-glucuronosyltransferase"OR"UDP-GT"OR"Sulfotransferase"OR"SULT"OR"{iodothyronine deiodinase}"OR"{iodothyronine 5'-deiodinase}"OR"{iodothyronine 5'-monodeiodinase}"OR"deiodinase"OR"Monodeiodinase"OR"DIO"OR"Transthyretin"OR"TTR"OR"TBPA"OR"Thyroxine Binding Prealbumin") AND TITLE-ABS-KEY ({2,4-dichlorophenoxyacetic acid}OR {94-75-7}OR {2-(2,4-dichlorophenoxy)acetic acid}OR{2,4-D}OR{(2,4-Dichlorophenoxy)acetic acid}OR{2,4-D acid}OR{Amitrole}OR{3-amino-1,2,4-triazole}OR{61-82-5}OR{4H-1,2,4-triazol-3-amine}OR{1H-1,2,4-Triazol-3-amine}OR{1H-1,2,4-Triazol-5-amine}OR{Aminotriazole}OR{3-

Aminotriazole}OR{Amitrol}OR{Clofentezine}OR{74115-24-5}OR{3,6-Bis(2-chlorophenyl)-  
 1,2,4,5-tetrazine}OR{Bisclofentazin}OR{Bisclofentazine}OR{1,2,4,5-Tetrazine, 3,6-bis(2-  
 chlorophenyl)-}OR{3,6-Bis(o-chlorophenyl)-1,2,4,5-tetrazine}OR{imidazolidine-2-  
 thione}OR{2-Imidazolidinethione}OR{Ethylenethiourea}OR{96-45-7}OR{ETHYLENE  
 THIOUREA}OR{2-Mercaptoimidazoline}OR{Imidazolidinethione}OR{N,N'-  
 Ethylenethiourea}OR{Ethlenethiourea}OR{Fluopyram}OR{658066-35-4}OR{N-[2-[3-Chloro-5-  
 (trifluoromethyl)-2-pyridinyl]ethyl]-2-(trifluoromethyl)benzamide}OR{N-[2-[3-chloro-5-  
 (trifluoromethyl)pyridin-2-yl]ethyl]-2-(trifluoromethyl)benzamide}OR{N-2-(3-chloro-5-  
 (trifluoromethyl)-2-pyridyl)ethyl-alpha,alpha,alpha-trifluoro-o-toluamide}OR{N-2-[3-chloro-5-  
 (trifluoromethyl)pyridin-2-yl]ethyl-2-(trifluoromethyl)benzamide}OR{Benzamide, N-[2-[3-  
 chloro-5-(trifluoromethyl)-2-pyridinyl]ethyl]-2-(trifluoromethyl)-}OR{n-[2-[3-chloro-5-  
 (trifluoromethyl)-2-pyridinyl]ethyl]-2-trifluoromethylbenzamide}OR{N-2-[3-chloro-5-  
 (trifluoromethyl)-2-pyridyl]ethyl-alpha,alpha,alpha-trifluoro-o-toluamide}OR{Ioxynil}OR{4-  
 Hydroxy-3,5-diiodobenzonitrile}OR{1689-83-4}OR{Benzonitrile, 4-hydroxy-3,5-diiodo-  
 }OR{3,5-Diiodo-4-hydroxybenzonitrile}OR{2,6-Diiodo-4-cyanophenol}OR{4-Cyano-2,6-  
 diiodophenol}OR{4-Cyano-2,6-dijodphenol}OR{Isoxaflutole}OR{141112-29-0}OR{(5-  
 Cyclopropylisoxazol-4-yl)(2-(methylsulfonyl)-4-(trifluoromethyl)phenyl)methanone}OR{(5-  
 cyclopropyl-1,2-oxazol-4-yl)-[2-methylsulfonyl-4-(trifluoromethyl)phenyl]methanone}OR{(5-  
 Cyclopropyl-4-isoxazolyl)(2-(methylsulfonyl)-4-(trifluoromethyl)phenyl)methanone}OR{(5-  
 cyclopropyl-4-isoxazolyl)[2-(methylsulfonyl)-4-  
 (trifluoromethyl)phenyl]methanone}OR{MANCOZEB}OR{8018-01-7}OR{Manganese Zinc  
 ethylenebis(dithiocarbamate)}OR{18-METHYLNONADECANOICACID}OR{manganese(2+)  
 ethane-1,2-diylbis(dithiocarbamate) zinc ethane-1,2-  
 diylbis(dithiocarbamate)}OR{MANEB}OR{12427-38-2}OR{Manganese  
 ethylenebisthiocarbamate}OR{manganese(II) ethane-1,2-  
 diyldicarbamodithioate}OR{manganese(2+) ethane-1,2-  
 diylbis(dithiocarbamate)}OR{manganese(2+);N-[2-  
 (sulfidocarbothioylamino)ethyl]carbamodithioate}OR{ZINEB}OR{METIRAM}OR{Polyram}OR{  
 9006-42-2}OR{12122-67-7}OR{Zinc ethylenebisthiocarbamate}OR{Zinc ammoniate  
 ethylenebis(dithiocarbamate)-poly(ethylenethiuram disulfide)}OR{zinc ethane-1,2-  
 diylbis(dithiocarbamate)}OR{Proquinazid}OR{189278-12-4}OR{6-iodo-2-propoxy-3-  
 propylquinazolin-4(3H)-one}OR{6-iodo-2-propoxy-3-propylquinazolin-4-one}OR{6-iodo-2-  
 propoxy-3-propyl-4(3H)-quinazolinone}OR{6-Iodo-2-propoxy-3-propyl-  
 4(3H)quinazolinone}OR{4(3H)-Quinazolinone, 6-iodo-2-propoxy-3-propyl-}OR{6 -Iodo-2 -  
 propoxy-3-propyl-4(3H)-quinazolinone}OR{thiabendazole}OR{148-79-  
 8}OR{Tiabendazole}OR{2-(4-Thiazolyl)benzimidazole}OR{2-(1,3-Thiazol-4-yl)-1H-  
 benzimidazole}OR{4-(1H-Benzo[d]imidazol-2-yl)thiazole}OR{1H-Benzimidazole, 2-(4-  
 thiazolyl)-}OR{2-(4-Thiazolyl)-1H-benzimidazole}OR{Thiacloprid}OR{111988-49-9}OR{(Z)-  
 thiacloprid}OR{(3-((6-Chloro-3-pyridinyl)methyl)-2-thiazolidinylidene)cyanamide}OR{(3-[(6-  
 chloropyridin-3-yl)methyl]-1,3-thiazolidin-2-ylidene)cyanamide}OR{(2Z)-3-[(6-chloropyridin-3-  
 yl)methyl]-1,3-thiazolidin-2-ylidenecyanamide}OR{3-[(6-chloropyridin-3-yl)methyl]-1,3-  
 thiazolidin-2-ylidenecyanamide}OR{N-(3-((6-Chloropyridin-3-yl)methyl)thiazolidin-2-  
 ylidene)cyanamide}OR{Topramezone}OR{210631-68-8}OR{4-[3-(4,5-dihydro-1,2-oxazol-3-  
 yl)-2-methyl-4-methylsulfonylbenzoyl]-2-methyl-1H-pyrazol-3-one}OR{(3-(4,5-Dihydro-3-  
 isoxazolyl)-2-methyl-4-(methylsulfonyl)phenyl)(5-hydroxy-1-methyl-1H-pyrazol-4-  
 yl)methanone}OR{Methanone, [3-(4,5-dihydro-3-isoxazolyl)-2-methyl-4-  
 (methylsulfonyl)phenyl](5-hydroxy-1-methyl-1H-pyrazol-4-yl)-}OR{(3-(4,5-dihydro-3-

isoxazolyl)-2-methyl-4-(methylsulfonyl)phenyl)(5-hydroxy-1-methyl-1H-pyrazol-4-yl)methanone}OR{[3-(4,5-dihydro-1,2-oxazol-3-yl)-2-methyl-4-methylsulfonylphenyl]-(5-hydroxy-1-methylpyrazol-4-yl)methanone}OR{ZIRAM}OR{Zinc dimethyldithiocarbamate}OR{137-30-4}OR{Zinc Bis(dimethyldithiocarbamate)}OR{Dimethyldithiocarbamic acid zinc salt}OR{Zinc, bis(dimethyldithiocarbamate)-}OR{Zinc, bis(dimethylcarbamodithioato-S,S')-, (T-4)-}OR({bromide}AND NOT{[3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide]})OR{Bromide ion}OR{24959-67-9}OR{3-Acetyl-1-benzyl-pyridinium bromide}OR{3-Carbamoyl-1-dodecyl-pyridinium bromide}OR{3-Carbamoyl-1-(3-phenyl-propyl)-pyridinium bromide}OR({Perchlorate}AND NOT{Perchlorate discharge})OR{14797-73-0}OR{Perchlorate ion}OR{Chlorat(VII)}OR{ClO4-}OR{ClO(4)(-)}OR{ClO4})