| Endpoint | N in training set | **(Cross) validation result (%)a** | QMRF |
|---|---|---|---|
| Water solubility v1.0.1 (mg/L) | 4014 | Test set in AD: n=341; Q2=0.91; RMSE=0.69 | VEGA |
| Air Half-Life (CORAL) v1.0.1 (hr) | 76+77+74 | Test set in AD: n=34; Q2=0.89; RMSE=0.29 | VEGA |
| Not ready biodegradability (POS=Not Ready) | 735 | Sens=68.9, Spec=87.8, Conc=77.2 | CASE Ultra |
| | | Sens=87.3, Spec=85.2, Conc=86.4 | Leadscope |
| | | Sens=63.0, Spec=92.7, Conc=77.8 | SciQSAR |
| Ready Biodegradability model v1.0.10 (POS=Not Ready) | 582 | Test set in AD: n=71, Sens=100, Spec=87, BA=94 | VEGA |
| Log BCF (CAESAR) v2.1.15 (L/kg) | 378 | Test set in AD: n=31; Q2=0.85; RMSE=0.52 | VEGA |
| Fathead minnow 96h LC50 (mg/L) | 565 | R2=0.75, Q2=0.73 | Leadscope |
| | | R2=0.74, Q2=0.72 | SciQSAR |
| Daphnia magna 48h EC50 (mg/L) | 626 | R2=0.67, Q2=0.64 | Leadscope |
| | | R2=0.65, Q2=0.63 | SciQSAR |
| Pseudokirchneriella s. 72h EC50 (mg/L) | 531 | R2=0.74, Q2=0.71 | Leadscope |

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| | | R2=0.64, Q2=0.60 | SciQSAR |
| Daphnia magna 48h EC50 v1.0.1 (mg/L) | 312 | Test set in AD: n=44; Q2=0.66; RMSE = 0.60 | VEGA |
| Daphnia magna 21d NOEC v1.0.1 (mg/L)) | 215 | Test set in AD: n=23; Q2=0.76; RMSE=0.46 | VEGA |
| Algae 72h ErC50 v1.0.1 (mg/L) | 252 | Test set in AD: n=17, Q2=0.83, RMSE=0.53 | VEGA |
| Sludge Classification, 3h EC50 < 100 mg/L v1.0.1 | 60 | Test set in AD: n=6, Sens=100, Spec=0.67 | VEGA |
| Sludge 3h EC50 v1.0.1 (mg/L) | 35 | R2 = 0.70, Q2 LOO = 0.69 | VEGA |
| MOA Toxicity classification (EPA T.E.S.T) v1.0.2 | 757 | Test set in AD: n=125, Acc=0.97 | VEGA |
| Cytochrome P450 2D6 (CYP2D6) substrates (human clinical data) | 746 | Sens=43.9, Spec=87.0, Conc=74.1 | CASE Ultra |
| | | Sens=60.0, Spec=89.4, Conc=80.1 | Leadscope |
| | | Sens=59.5, Spec=79.8, Conc=73.1 | SciQSAR |
| | | Sens=30.6, Spec=83.6, Conc=68.8 | CASE Ultra |
| Cytochrome P450 2C9 (CYP2C9) substrates (human clinical data) | 736 | | |

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| | | Sens=30.0, Spec=89.6, Conc=75.4 | Leadscope |
| | | Sens=26.3, Spec=91.5, Conc=74.7 | SciQSAR |
| Rat oral | 6464 | Ext. validation, RI>0.5, Q2=0.64 | ACDLabs |
| Rat intraperitoneal | 3751 | Ext. validation, RI>0.5, Q2=0.56 | ACDLabs |
| Mouse oral | 14,678 | Ext. validation, RI>0.5, Q2=0.55 | ACDLabs |
| Mouse intraperitoneal | 27,004 | Ext. validation, RI>0.5, Q2=0.61 | ACDLabs |
| Mouse intravenous | 14,972 | Ext. validation, RI>0.5, Q2=0.66 | ACDLabs |
| Mouse subcutaneous | 6432 | Ext. validation, RI>0.5, Q2=0.57 | ACDLabs |
| Maximum recommended daily dose (MRDD) in humans ≤ 2.69 mg/kg-2bw/d | 1222 | Sens=69.4, Spec=92.5, Conc=82.5 | CASE Ultra |
| | | Sens=78.6, Spec=82.5, Conc=80.7 | Leadscope |
| | | Sens=73.1, Spec=77.3, Conc=75.3 | SciQSAR |

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| Hepatotoxicity Model v1.0.1 | 760 | Sens=85, Spec=37, Conc=66 | VEGA |
| Severe skin irritation in rabbit | 836 | Sens=63.4, Spec=86.7, Conc=75.8 | CASE Ultra |
| | | Sens=79.5, Spec=81.7, Conc=80.6 | Leadscope |
| | | Sens=77.3, Spec=71.3, Conc=74.3 | SciQSAR |
| Allergic contact dermatitis in guinea pig and human | 1032 | Sens=76.7, Spec=93.9, Conc=89.3 | CASE Ultra |
| | | Sens=75.0, Spec=96.3, Conc=90.8 | Leadscope |
| | | Sens=61.6, Spec=96.8, Conc=85.8 | SciQSAR |
| Respiratory sensitisation in humans | 80 | Sens=68.2, Spec=96.3, Conc=86.4 | CASE Ultra |
| | | Sens=91.7, Spec=95.5, Conc=93.9 | Leadscope |
| | | Sens=80.0, Spec=87.5, Conc=83.8 | SciQSAR |
| Estrogen Receptor α binding (human in vitro) ALL | 802 | Sens=60.9, Spec=95.2, Conc=85.7 | CASE Ultra |
| | | Sens=75.2, Spec=90.1, Conc=84.7 | Leadscope |
| | | Sens=67.3, Spec=89.0, Conc=81.3 | SciQSAR |

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| Estrogen Receptor α binding (human in vitro) Balanced | 595 | Sens=81.7, Spec=89.2, Conc=85.4 | CASE Ultra |
| | | Sens=83.7, Spec=89.0, Conc=86.3 | Leadscope |
| | | Sens=76.1, Spec=83.3 Conc=79.8 | SciQSAR |
| Estrogen Receptor α activation (human in vitro) | 481 | Sens=73.7, Spec=86.6, Conc=80.9 | CASE Ultra |
| | | Sens=73.1, Spec=86.6, Conc=80.7 | Leadscope |
| | | Sens=77.9, Spec=80.8, Conc=79.6 | SciQSAR |
| Estrogen Receptor activation (in vitro, CERAPP data) | 1420 | Sens=78.5, Spec=96.7, BA=87.6 (2*5-fold cross-validation) | Leadscope |
| Androgen Receptor inhibition (human in vitro) | 874 | Sens=57.4, Spec=87.2, Conc=78.3 | CASE Ultra |
| | | Sens=51.7, Spec=91.2, Conc=80.4 | Leadscope |
| | | Sens=56.3 Spec=91.1, Conc=81.9 | SciQSAR |
| Androgen Receptor binding (in vitro, CoMPARA data) | 1662 | Sens=80.4, Spec=93.3, BA=86.9 (2*5-fold cross-validation) | Leadscope |

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| Androgen Receptor activation (in vitro, CoMPARA data) | 1659 | Sens=76.3, Spec=99.3, BA=87.8 (2*5-fold cross-validation) | Leadscope |
| Androgen Receptor inhibition (in vitro, CoMPARA data) | 1525 | Sens=81.5, Spec=92.2, BA=86.9 (2*5-fold cross-validation) | Leadscope |
| Thyroperoxidase (TPO) inhibition QSAR1 (rat in vitro) | 877 | Sens=72.4, Spec=89.0, BA=80.6 Ext. validation: Sens=79.7, Spec=90.8, BA=85.3 | Leadscope |
| Thyroperoxidase (TPO) inhibition QSAR2 (rat in vitro) | 1519 | Sens=75.6, Spec=89.8, BA=82.7 | Leadscope |
| Thyroid receptor α binding – log(IC50 in μM) (human in vitro) | 118 | Q2=0.59 | CASE Ultra |
| | | R2=0.83, Q2=0.68 | Leadscope |
| | | R2=0.64, Q2=0.57 | SciQSAR |
| Thyroid receptor β binding – log(IC50 in μM) (human in vitro) | 130 | Q2=0.61 | CASE Ultra |
| | | R2=0.83, Q2=0.64 | Leadscope |
| | | R2=0.65, Q2=0.58 | SciQSAR |
| Pregnane X receptor binding (human in vitro) | 631 | Sens=72.4, Spec=83.9, Conc=78.5 | CASE Ultra |

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| | | Sens=80.4, Spec=80.4, Conc=80.4 | Leadscope |
| | | Sens=79.9, Spec=82.7, Conc=81.4 | SciQSAR |
| Pregnane X Receptor (PXR) Binding (Human in vitro) NEW | 1504 | Sens=86.6, Spec=98.5, Conc=92.6 (2*5-fold cross-validation) | Leadscope |
| Pregnane X Receptor (PXR) Activation (Human in vitro) | 2176 | Sens=89.1, Spec=98.6, BA=93.9 (2*5-fold cross-validation) | Leadscope |
| Pregnane X Receptor (PXR) Activation (Rat in vitro) | 2330 | Sens=86.5, Spec=97.4, BA=92.0 (2*5-fold cross-validation) | Leadscope |
| CYP3A4 Induction (Human in vitro) | 2271 | Sens=86.7, Spec=98.2, BA=92.5 (2*5-fold cross-validation) | Leadscope |
| Arylhydrocarbon (AhR) Activation – Rational final model | 4625 | Sens=75.4, Spec=87.0, BA=80.8 (2*5-fold cross-validation) | Leadscope |

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| Arylhydrocarbon (AhR) Activation – Random final model | 4625 | Sens=86.4, Spec=91.5, BA=88.9 (2*5-fold cross-validation) | Leadscope |
| Constitutive Androstane Receptor (CAR) activation at max. 20 µM | 924 | Sens=72.2, Spec=93.5, BA=82.8 (2*5-fold cross-validation) | Leadscope |
| Constitutive Androstane Receptor (CAR) activation at max. 50 µM | 1903 | Sens=78.4, Spec=91.4, BA=84.9 (2*5-fold cross-validation) | Leadscope |
| Constitutive Androstane Receptor (CAR) inhibition at max. 20 µM | 1408 | Sens=58.4, Spec=97.1, BA=77.8 (2*5-fold cross-validation) | Leadscope |
| Constitutive Androstane Receptor (CAR) inhibition at max. 50 µM | 1870 | Sens=72.4, Spec=91.6, BA=82.0 (2*5-fold cross-validation) | Leadscope |
| Teratogenic potential in Humans | 323 | Sens=65.0, Spec=85.1, Conc=76.4 | CASE Ultra |
| | | Sens=72.0, Spec=85.5, Conc=80.1 | Leadscope |
| | | Sens=64.6, Spec=92.7, Conc=81.4 | SciQSAR |

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| Developmental/Reproductive Toxicity library (PG) v1.1.2 | 685 | NA | VEGA |
| | | Sens=89.7, Spec=95.1, Conc=91.9 | CASE Ultra |
| | | Sens=87.5, Spec=90.7, Conc=88.5 | Leadscope |
| Ashby structural alerts | 782 | Sens=81.7, Spec=80.6, Conc=81.1 | SciQSAR |
| | | Sens=83.9, Spec=89.1, Conc=86.4 | CASE Ultra |
| | | Sens=84.3, Spec=85.7, Conc=84.9 | Leadscope |
| Bacterial reverse mutation test (Ames test in S. typhimurium in vitro) | 4102 | Sens=79.3, Spec=79.1, Conc=79.2 | SciQSAR |
| | 3367 | Test set in AD: n=3129, Sens=81, Spec=86 | VEGA-SARPy |
| | 670 | Test set in AD: n=2404, Sens=92, Spec=0.80 | VEGA-ISS |
| | 5770 | Test set in AD: n=2437, Sens=62, Spec=0.84 | VEGA-KNN |
| Mutagenicity (Ames test) | 3367 | Test set in AD: n=3106, Sens=83, Spec=0.82 | VEGA-CAESAR |

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| Direct acting Ames mutagens (without S9) – ONLY use for Ames POS_IN | 388 | Sens=63.5, Spec=90.4, Conc=79.5 | CASE Ultra |
| | | Sens=66.9, Spec=78.9, Conc=74.0 | Leadscope |
| | | Sens=56.5, Spec=72.9, Conc=68.6 | SciQSAR |
| Base pair Ames mutagens - ONLY use for Ames POS_IN | 204 | Sens=52.8, Spec=88.4, Conc=71.9 | CASE Ultra |
| | | Sens=70.2, Spec=66.4, Conc=68.4 | Leadscope |
| | | Sens=68.6, Spec=67.7, Conc=68.1 | SciQSAR |
| Frame shift Ames mutagens - ONLY use for Ames POS_IN | 309 | Sens=73.5, Spec=84.1, Conc=78.9 | CASE Ultra |
| | | Sens=74.4, Spec=78.6, Conc=76.6 | Leadscope |
| | | Sens=68.3, Spec=78.2, Conc=73.8 | SciQSAR |
| Potent Ames mutagens, reversions ≥ 10 times controls - ONLY use for Ames POS_IN | 187 | Sens=73.7, Spec=87.7, Conc=81.2 | CASE Ultra |
| | | Sens=68.9, Spec=70.0, Conc=69.8 | Leadscope |
| | | Sens=75.0, Spec=74.7, Conc=74.9 | SciQSAR |
| Chromosome aberrations in CHO cells (in vitro) | 233 | Sens=40.4, Spec=94.5, Conc=74.4 | CASE Ultra |

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| | | Sens=54.1, Spec=79.3, Conc=68.8 | Leadscope |
| | | Sens=50.5, Spec=84.3, Conc=70.3 | SciQSAR |
| Chromosome aberrations in CHL cells (in vitro) | 600 | Sens=63.3, Spec=86.7, Conc=76.4 | CASE Ultra |
| | | Sens=74.6, Spec=75.2, Conc=74.9 | Leadscope |
| | | Sens=73.0, Spec=72.8, Conc=72.9 | SciQSAR |
| Mutations in thymidine kinase locus in mouse lymphoma cells (in vitro) | 555 | Sens=76.5, Spec=86.3, Conc=81.2 | CASE Ultra |
| | | Sens=85.1, Spec=83.8, Conc=84.4 | Leadscope |
| | | Sens=79.1, Spec=80.5, Conc=79.8 | SciQSAR |
| Mutations in HGPRT locus in CHO cells (in vitro) | 239 | Sens=75.4, Spec=84.5, Conc=78.9 | CASE Ultra |
| | | Sens=81.7, Spec=78.4, Conc=80.5 | Leadscope |
| | | Sens=80.0, Spec=73.0, Conc=76.5 | SciQSAR |
| Unscheduled DNA synthesis (UDS) in rat hepatocytes (in vitro) | 415 | Sens=60.6, Spec=87.0, Conc=74.1 | CASE Ultra |
| | | Sens=74.1, Spec=70.1, Conc=72.4 | Leadscope |

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| | | Sens=69.6, Spec=72.5, Conc=71.1 | SciQSAR |
| Micronucleus VERMEER (in vitro) v1.0.1 | 293 | Test set in AD: n=27, Sens=93, Spec=0.83 | VEGA |
| Syrian hamster embryo (SHE) cell transformation (in vitro) | 363 | Sens=50.8, Spec=86.9, Conc=74.0 | CASE Ultra |
| | | Sens=71.6, Spec=76.5, Conc=74.5 | Leadscope |
| | | Sens=76.1, Spec=66.5, Conc=71.3 | SciQSAR |
| Sex-linked recessive lethal (SLRL) test in Drosophila m. (in vivo) | 367 | Sens=75.4, Spec=92.0, Conc=83.6 | CASE Ultra |
| | | Sens=79.1, Spec=80.3, Conc=79.6 | Leadscope |
| | | Sens=74.2, Spec=78.3, Conc=76.2 | SciQSAR |
| Micronucleus test in mouse erythrocytes (in vivo) | 357 | Sens=31.2, Spec=95.2, Conc=75.7 | CASE Ultra |
| | | Sens=64.1, Spec=77.6, Conc=72.3 | Leadscope |
| | | Sens=52.1, Spec=83.3, Conc=69.7 | SciQSAR |
| Dominant lethal mutations in rodents (in vivo) | 191 | Sens=42.4, Spec=92.7, Conc=73.7 | CASE Ultra |
| | | Sens=61.5, Spec=80.4, Conc=71.8 | Leadscope |

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| | | Sens=57.7, Spec=81.4, Conc=71.7 | SciQSAR |
| Sister chromatid exchange in mouse bone marrow cells (in vivo) | 265 | Sens=91.8, Spec=94.8, Conc=93.9 | CASE Ultra |
| | | Sens=88.6, Spec=95.9, Conc=94.0 | Leadscope |
| | | Sens=76.7, Spec=93.2, Conc=86.8 | SciQSAR |
| Comet assay in mouse (in vivo) | 286 | Sens=60.1, Spec=93.1, Conc=82.9 | CASE Ultra |
| | | Sens=86.6, Spec=80.8, Conc=83.1 | Leadscope |
| | | Sens=82.4, Spec=82.0, Conc=82.2 | SciQSAR |
| FDA RCA cancer male rat (in vivo) | 1324 | Sens=34.2, Spec=95.0, Conc=63.9 | CASE Ultra |
| | | Sens=62.6, Spec=74.7, Conc=69.2 | Leadscope |
| FDA RCA cancer female rat (in vivo) | 1321 | Sens=44.4, Spec=93.3, Conc=71.6 | CASE Ultra |
| | | Sens=57.7, Spec=83.6, Conc=72.7 | Leadscope |
| FDA RCA cancer rat (in vivo) | 1379 | Sens=41.7, Spec=94.0, Conc=66.9 | CASE Ultra |
| | | Sens=57.1, Spec=82.3, Conc=71.2 | Leadscope |

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| FDA RCA cancer male mouse (in vivo) | 1197 | Sens=38.4, Spec=86.1, Conc=66.1 | CASE Ultra |
| | | Sens=58.6, Spec=81.4, Conc=71.9 | Leadscope |
| FDA RCA cancer female mouse (in vivo) | 1208 | Sens=41.5, Spec=85.9, Conc=65.6 | CASE Ultra |
| | | Sens=59.2, Spec=80.6, Conc=71.3 | Leadscope |
| FDA RCA cancer mouse (in vivo) | 1221 | Sens=43.1, Spec=86.9, Conc=66.9 | CASE Ultra |
| | | Sens=56.5, Spec=83.9, Conc=72.7 | Leadscope |
| FDA RCA cancer rodent (in vivo) | 1530 | Sens=51.4, Spec=88.3, Conc=68.2 | CASE Ultra |
| | | Sens=65.9, Spec=76.2, Conc=71.3 | Leadscope |
| Liver specific cancer in rat or mouse (in vivo) | 320 | Sens=31.1, Spec=92.0, Conc=70.9 | CASE Ultra |
| | | Sens=35.6, Spec=88.6, Conc=69.3 | Leadscope |
| | | Sens=38.5, Spec=84.8, Conc=69.1 | SciQSAR |