Supporting information (tables) to

Large-scale Modeling of Multi-Species Acute Toxicity Endpoints using Conse

Sankalp Jain, Vishal B. Siramshetty, Vinicius M. Alves, Eugene N. Muratov, N
*Corresponding author: Alexey V. Zakharov (Email: alexey.zakharov@nih.gov

Species	Route of administration	Toxicity type
mouse	intraperitoneal	lethal dose fifty
mouse	oral	lethal dose fifty
mouse	intravenous	lethal dose fifty
rat	oral	lethal dose fifty
mouse	subcutaneous	lethal dose fifty
rat	intraperitoneal	lethal dose fifty
rat	intravenous	lethal dose fifty
rat	subcutaneous	lethal dose fifty
mouse	unreported	lethal dose fifty
rabbit	skin	lethal dose fifty
mammal (species unspecified)	unreported	lethal dose fifty
rabbit	oral	lethal dose fifty
rat	skin	lethal dose fifty
rat	unreported	lethal dose fifty
guinea pig	oral	lethal dose fifty
rabbit	intravenous	lethal dose fifty
rat	oral	lethal dose low
rat	intraperitoneal	lethal dose low
mouse	intraperitoneal	lethal dose low
mouse	oral	lethal dose low
mouse	subcutaneous	lethal dose low
man	oral	toxic dose low
women	oral	toxic dose low
mammal (species unspecified)	oral	lethal dose fifty
dog	oral	lethal dose fifty
mouse	intramuscular	lethal dose fifty
mammal (species unspecified)	intraperitoneal	lethal dose fifty
dog	intravenous	lethal dose fifty
dog	intravenous	lethal dose low
chicken	oral	lethal dose fifty
quail	oral	lethal dose fifty
rabbit	intravenous	lethal dose low
bird - wild	oral	lethal dose fifty
mouse	parenteral	lethal dose fifty
rat	intramuscular	lethal dose fifty
cat	intravenous	lethal dose fifty
rabbit	oral	lethal dose low
guinea pig	intraperitoneal	lethal dose fifty
rabbit	subcutaneous	lethal dose low

mouse	skin	lethal dose fifty
duck	oral	lethal dose fifty
dog	oral	lethal dose low
rabbit	skin	lethal dose low
guinea pig	subcutaneous	lethal dose low
guinea pig	skin	lethal dose fifty
rat	subcutaneous	lethal dose low
cat	oral	lethal dose fifty
guinea pig	subcutaneous	lethal dose fifty
cat	intravenous	lethal dose low
rabbit	subcutaneous	lethal dose fifty
guinea pig	intravenous	lethal dose fifty
cat	oral	lethal dose low
human	oral	toxic dose low
rat	intravenous	lethal dose low
rabbit	intraperitoneal	lethal dose fifty
mammal (species unspecified)	subcutaneous	lethal dose fifty
guinea pig	intravenous	lethal dose low
frog	subcutaneous	lethal dose low
mouse	intravenous	lethal dose low
mouse	intraperitoneal	toxic dose low
mouse	oral	toxic dose low
rat	intraperitoneal	toxic dose low
rat	intravenous	toxic dose low
rat	oral	toxic dose low
rat	subcutaneous	toxic dose low

nsus of Multi-Task Deep Learning Methods

icole Kleinstreuer, Alexander Tropsha, Marc C. Nicklaus, Anton Simeonov, Alexey V. Zakharov*
)

Number of measurements (threshold 100)	Number of measurements in Sosn	Group
36295	37202	a
23373	24355	a
16978	17742	a
10190	10743	a
6769	7221	a
5021	5041	a
2472	2538	a
1896	2014	a
1739	1804	a
1495	1734	a
1129	1121	a
894	910	a
835	930	a
806	838	a
793	799	a
792	764	a
322	966	a
318	1029	a
266	2965	b
264	1565	b
252	921	b
163	512	b
156	490	b
674	0	c
649	0	c
571	0	c
545	0	c
468	0	c
360	0	c
353	0	c
352	0	c
346	0	c
338	0	c
302	0	c
300	0	c
261	0	c
249	0	c
248	0	c
241	0	c

214	0	c
192	0	c
187	0	c
181	0	c
179	0	c
176	0	c
174	0	c
171	0	c
169	0	c
159	0	c
156	0	c
153	0	c
142	0	c
140	0	c
135	0	c
131	0	c
125	0	c
121	0	c
112	0	c
102	0	c
0	1057	d
0	646	d
0	1117	d
0	608	d
0	955	d
0	555	d

a
b
c
d

a+b+c

endpoints compared with Sosnin et al. [49] (number of measuremnets > 300)
endpoint included in our study but not included in the comparison with Sosnin et al. [49] (as number of measurem
endpoint included in our study but not included in the study by Sosnin et al. [49]
endpoint not included in our study but included in the study by Sosnin et al. [49]

endpoints used for multi-task modeling in this study

Supporting information (tables) to

Large-scale Modeling of Multi-Species Acute Toxicity Endpoints using Consensus of Multi-Task

Sankalp Jain, Vishal B. Siramshetty, Vinicius M. Alves, Eugene N. Muratov, Nicole Kleinstreuer, .
*Corresponding author: Alexey V. Zakharov (Email: alexey.zakharov@nih.gov)

Model architectures for MT-DNN	**Parameter**
	number of hidden layers
	number of neurons for each layer
	optimizer
	learning rate
	activation function
	batch size
	number of epochs

Model architectures for ST-DNN	**Parameter**
	number of hidden layers
	number of neurons for each layer
	optimizer
	learning rate
	activation function
	batch size
	number of epochs

Parameters for Hyperparameter optimization for MT-DNN	
Fixed parameters	
	Parameter
	activation function
	optimizer
Tuned Parameters	
	Parameter
	dense_size_candidates
	learning rate (Adam)
	number of epochs
	batch size
Parameters for Hyperparameter optimization for ST-DNN	
Fixed parameters	
	Parameter
	activation function
	optimizer
Tuned Parameters	number of epochs
	batch size
	Parameter
	learning rate (Adam)

Model architectures for DLCA	Parameter
Descriptor 1-3 (Fingerprints)	number of hidden layers
	number of neurons for each layer
Descriptor 4 (RDKit physicochemical properties)	number of hidden layers
	number of neurons for each layer
	Dropout
Descriptor 5 (SMILES)	architecture
	Pooling
	number of hidden layers
	number of neurons for each layer
	optimizer
	learning rate
	activation function
	batch size
	number of epochs

Optimized hyperparameter parameter for GCNN v2	
Random Split	
	Parameter
	depth
	dropout
	ffn_num_layers
	hidden_size
Scaffold Split	
	Parameter
	depth
	dropout
	ffn_num_layers
	hidden_size

Deep Learning Methods

Alexander Tropsha, Marc C. Nicklaus, Anton Simeonov, Alexey V. Zakharov*

Value
3
2000, 700, 500
Adam
0.0001
relu
32
20

Value
3
500, 300, 100 (train_size<=700)
2000, 700, 500 (train_size>700)
Adam
0.0001
relu
32
20

Value
ReLu
Adam

Values	**Best Value**
[2000, 700, 500, 1], [1500, 500, 100, 1]	[1500, 500, 100, 1]
0.01, 0.001, 0.0001, 0.00001	0.0001
20, 50	50
128, 256, 512, 1024	128

Value
ReLu
Adam
20
32
Values
0.01, 0.001, 0.0001, 0.00001

Value
4
8000, 2000, 1000, 700
4
8000, 2000, 1000, 700
0.3
1D convolutional
GlobalMaxPooling1D
1
200
Adagrad
0.01
relu
128
20

Value
5
0.3
3
1700
Value
5
0.15
3
2200

Supporting information (tables) to

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Sankalp Jain, Vishal B. Siramshetty, Vinicius M. Alves, Eugene N. Muratov, Nicole Kleinstre

*Corresponding author: Alexey V. Zakharov (Email: alexey.zakharov@nih.gov)

Species	Route of administration	Toxicity type
mouse	intraperitoneal	lethal dose fifty
mouse	oral	lethal dose fifty
mouse	intravenous	lethal dose fifty
rat	oral	lethal dose fifty
mouse	subcutaneous	lethal dose fifty
rat	intraperitoneal	lethal dose fifty
rat	intravenous	lethal dose fifty
rat	subcutaneous	lethal dose fifty
mouse	unreported	lethal dose fifty
rabbit	skin	lethal dose fifty
mammal (sp	unreported	lethal dose fifty
rabbit	oral	lethal dose fifty
rat	skin	lethal dose fifty
rat	unreported	lethal dose fifty
guinea pig	oral	lethal dose fifty
rabbit	intravenous	lethal dose fifty
rat	oral	lethal dose low
rat	intraperitoneal	lethal dose low
mouse	intraperitoneal	lethal dose low
mouse	oral	lethal dose low
mouse	subcutaneous	lethal dose low
man	oral	toxic dose low
women	oral	toxic dose low
mammal (sp	oral	lethal dose fifty
dog	oral	lethal dose fifty
mouse	intramuscular	lethal dose fifty
mammal (sp	intraperitoneal	lethal dose fifty
dog	intravenous	lethal dose fifty
dog	intravenous	lethal dose low
chicken	oral	lethal dose fifty
quail	oral	lethal dose fifty
rabbit	intravenous	lethal dose low
bird - wild	oral	lethal dose fifty
mouse	parenteral	lethal dose fifty
rat	intramuscular	lethal dose fifty
cat	intravenous	lethal dose fifty
rabbit	oral	lethal dose low
guinea pig	intraperitoneal	lethal dose fifty
rabbit	subcutaneous	lethal dose low

mouse	skin	lethal dose fifty
duck	oral	lethal dose fifty
dog	oral	lethal dose low
rabbit	skin	lethal dose low
guinea pig	subcutaneous	lethal dose low
guinea pig	skin	lethal dose fifty
rat	subcutaneous	lethal dose low
cat	oral	lethal dose fifty
guinea pig	subcutaneous	lethal dose fifty
cat	intravenous	lethal dose low
rabbit	subcutaneous	lethal dose fifty
guinea pig	intravenous	lethal dose fifty
cat	oral	lethal dose low
human	oral	toxic dose low
rat	intravenous	lethal dose low
rabbit	intraperitoneal	lethal dose fifty
mammal (sp	subcutaneous	lethal dose fifty
guinea pig	intravenous	lethal dose low
frog	subcutaneous	lethal dose low
mouse	intravenous	lethal dose low

·**Task Deep Learning Methods**

euer, Alexander Tropsha, Marc C. Nicklaus, Anton Simeonov, Alexey V. Zakharov*

Number of measurements	% of available measurements	% of missing measurements
36295	45.32	54.68
23373	29.19	70.81
16978	21.20	78.80
10190	12.72	87.28
6769	8.45	91.55
5021	6.27	93.73
2472	3.09	96.91
1896	2.37	97.63
1739	2.17	97.83
1495	1.87	98.13
1129	1.41	98.59
894	1.12	98.88
835	1.04	98.96
806	1.01	98.99
793	0.99	99.01
792	0.99	99.01
322	0.40	99.60
318	0.40	99.60
266	0.33	99.67
264	0.33	99.67
252	0.31	99.69
163	0.20	99.80
156	0.19	99.81
674	0.84	99.16
649	0.81	99.19
571	0.71	99.29
545	0.68	99.32
468	0.58	99.42
360	0.45	99.55
353	0.44	99.56
352	0.44	99.56
346	0.43	99.57
338	0.42	99.58
302	0.38	99.62
300	0.37	99.63
261	0.33	99.67
249	0.31	99.69
248	0.31	99.69
241	0.30	99.70

214	0.27	99.73
192	0.24	99.76
187	0.23	99.77
181	0.23	99.77
179	0.22	99.78
176	0.22	99.78
174	0.22	99.78
171	0.21	99.79
169	0.21	99.79
159	0.20	99.80
156	0.19	99.81
153	0.19	99.81
142	0.18	99.82
140	0.17	99.83
135	0.17	99.83
131	0.16	99.84
125	0.16	99.84
121	0.15	99.85
112	0.14	99.86
102	0.13	99.87

Supporting information (tables) to

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*Corresponding author: Alexey V. Zakharov (Email: alexey.zakharov@nih.gov)

MT-DNN					
Average Performance- Random Split					
Metric	**Fold_0**	**Fold_1**	**Fold_2**	**Fold_3**	**Fold_4**
r2_score	0.51 +/- 0.18	0.50 +/- 0.18	0.52 +/- 0.16	0.52 +/- 0.13	0.51 +/- 0.16
mae	0.52 +/- 0.16	0.51 +/- 0.14	0.48 +/- 0.13	0.49 +/- 0.13	0.50 +/- 0.14
mse	0.56 +/- 0.34	0.55 +/- 0.28	0.47 +/- 0.26	0.48 +/- 0.24	0.49 +/- 0.25
rmse	0.72 +/- 0.20	0.72+/- 0.18	0.66 +/- 0.17	0.67 +/- 0.16	0.68 +/- 0.17
Average Performance- Scaffold Split					
Metric	**Fold_0**	**Fold_1**	**Fold_2**	**Fold_3**	**Fold_4**
r2_score	0.34 +/- 0.21	0.31 +/- 0.22	0.32 +/- 0.45	0.27 +/- 0.20	0.38 +/- 0.17
mae	0.55 +/- 0.15	0.58 +/- 0.18	0.54 +/- 0.14	0.56 +/- 0.16	0.55 +/- 0.16
mse	0.60 +/- 0.34	0.73 +/- 0.49	0.60 +/- 0.32	0.65 +/- 0.39	0.60 +/- 0.38
rmse	0.75 +/- 0.20	0.82 +/- 0.26	0.75 +/- 0.19	0.77 +/- 0.21	0.75 +/- 0.21

ep Learning Methods

xander Tropsha, Marc C. Nicklaus, Anton Simeonov, Alexey V. Zakharov*

5-CV (mean)
0.51 +/- 0.16
0.50 +/- 0.14
0.51 +/- 0.23
0.69 +/- 0.18
5-CV (mean)
0.32 +/- 0.25
0.56 +/- 0.16
0.64 +/- 0.38
0.77 +/- 0.21

ST-RF

Average Performance- Random Split

Metric	Fold_0	Fold_1	Fold_2
r2_score	0.34 +/- 0.20	0.31 +/- 0.19	0.38 +/- 0.17
mae	0.61 +/- 0.19	0.62 +/- 0.20	0.57 +/- 0.18
mse	0.76 +/- 0.41	0.79 +/- 0.46	0.61 +/- 0.36
rmse	0.84 +/- 0.23	0.86 +/- 0.24	0.76 +/- 0.20

Average Performance- Scaffold Split

Metric	Fold_0	Fold_1	Fold_2
r2_score	0.21 +/- 0.26	0.18 +/- 0.27	0.27 +/- 0.24
mae	0.61 +/- 0.18	0.66 +/- 0.20	0.59 +/- 0.17
mse	0.73 +/- 0.39	0.85 +/- 0.50	0.68 +/- 0.33
rmse	0.82 +/- 0.22	0.89 +/- 0.26	0.80 +/- 0.20

ST-DNN

Average Performance- Random Split

Metric	Fold_0	Fold_1	Fold_2
r2_score	0.25 +/- 0.23	0.13 +/- 0.31	0.23 +/- 0.29
mae	0.64 +/- 0.19	0.69 +/- 0.23	0.62 +/- 0.18
mse	0.87 +/- 0.45	1.01 +/- 0.61	0.75 +/- 0.38
rmse	0.9 +/- 0.24	0.96 +/- 0.29	0.84 +/- 0.22

Average Performance- Scaffold Split

Metric	Fold_0	Fold_1	Fold_2
r2_score	0 +/- 0.5	-0.01 +/- 0.4	0.14 +/- 0.34
mae	0.68 +/- 0.2	0.73 +/- 0.25	0.65 +/- 0.2
mse	0.89 +/- 0.47	1.05 +/- 0.64	0.81 +/- 0.42
rmse	0.91 +/- 0.25	0.98 +/- 0.31	0.87 +/- 0.24

Fold_3	Fold_4	5-CV (mean)
0.36 +/- 0.16	0.34 +/- 0.20	**0.35 +/- 0.18**
0.58 +/- 0.17	0.58 +/- 0.17	**0.59 +/- 0.18**
0.66 +/- 0.34	0.66 +/- 0.33	**0.70 +/- 0.38**
0.79 +/- 0.20	0.79 +/- 0.20	**0.81 +/- 0.21**
Fold_3	**Fold_4**	**5-CV (mean)**
0.19 +/- 0.26	0.23 +/- 0.22	**0.22 +/- 0.25**
0.61 +/- 0.19	0.63 +/- 0.17	**0.62 +/- 0.18**
0.83 +/- 0.22	0.74 +/- 0.37	**0.74 +/- 0.40**
0.81 +/- 0.22	0.83 +/- 0.21	**0.83 +/- 0.22**

Fold_3	Fold_4	5-CV (mean)
0.21 +/- 0.27	0.19 +/- 0.28	**0.20 +/- 0.28**
0.63 +/- 0.19	0.64 +/- 0.19	**0.64 +/- 0.19**
0.81 +/- 0.43	0.81 +/- 0.39	**0.85 +/- 0.45**
0.87 +/- 0.24	0.87 +/- 0.22	**0.89 +/- 0.24**
Fold_3	**Fold_4**	**5-CV (mean)**
-0.01 +/- 0.3	0.11 +/- 0.31	**0.05 +/- 0.39**
0.67 +/- 0.2	0.66 +/- 0.19	**0.68 +/- 0.21**
0.87 +/- 0.46	0.84 +/- 0.48	**0.89 +/- 0.49**
0.9 +/- 0.24	0.89 +/- 0.24	**0.91 +/- 0.26**

Average Performance- Random Split

Metric	Fold_0
r2_score	0.50 +/- 0.18
mae	0.53 +/- 0.17
mse	0.58 +/- 0.37
rmse	0.73 +/- 0.21
Average Performance- Scaffold Split	
Metric	**Fold_0**
r2_score	0.32 +/- 0.26
mae	0.56 +/- 0.18
mse	0.64 +/- 0.44
rmse	**0.76 +/- 0.23**

GCNN				
Fold_1	**Fold_2**	**Fold_3**	**Fold_4**	**5-CV (mean)**
0.48 +/- 0.18	0.50 +/- 0.18	0.53 +/- 0.13	0.49 +/- 0.16	**0.50 +/- 0.17**
0.53 +/- 0.16	0.49 +/- 0.17	0.49 +/- 0.13	0.51 +/- 0.16	**0.51 +/- 0.16**
0.58 +/- 0.33	0.49 +/- 0.33	0.48 +/- 0.24	0.52 +/- 0.31	**0.53 +/- 0.32**
0.74 +/- 0.19	0.67 +/- 0.19	0.67 +/- 0.16	0.70 +/- 0.18	**0.70 +/- 0.19**
Fold_1	**Fold_2**	**Fold_3**	**Fold_4**	**5-CV (mean)**
0.36 +/- 0.18	0.35 +/- 0.27	0.3 +/- 0.2	0.41 +/- 0.2	0.35 +/- 0.22
0.57 +/- 0.16	0.54 +/- 0.16	0.54 +/- 0.16	0.54 +/- 0.19	0.55 +/- 0.17
0.67 +/- 0.41	0.61 +/- 0.37	0.62 +/- 0.36	0.58 +/- 0.41	0.62 +/- 0.40
0.79 +/- 0.23	**0.75 +/- 0.22**	**0.76 +/- 0.21**	**0.73 +/- 0.22**	**0.77 +/- 0.22**

DLCA					
Average Performance- Random Split					
Metric	**Fold_0**	**Fold_1**	**Fold_2**	**Fold_3**	**Fold_4**
r2_score	0.54 +/- 0.16	0.51 +/- 0.17	0.55 +/- 0.16	0.55 +/- 0.12	0.54 +/- 0.14
mae	0.5 +/- 0.16	0.51 +/- 0.15	0.46 +/- 0.15	0.48 +/- 0.13	0.47 +/- 0.14
mse	0.52 +/- 0.31	0.55 +/- 0.3	0.44 +/- 0.29	0.47 +/- 0.25	0.46 +/- 0.26
rmse	**0.7 +/- 0.19**	**0.71 +/- 0.19**	**0.64 +/- 0.17**	**0.66 +/- 0.17**	**0.66 +/- 0.17**
Average Performance- Scaffold Split					
Metric	**Fold_0**	**Fold_1**	**Fold_2**	**Fold_3**	**Fold_4**
r2_score	0.34 +/- 0.21	0.37 +/- 0.21	0.39 +/- 0.22	0.32 +/- 0.15	0.40 +/- 0.15
mae	0.55 +/- 0.17	0.55 +/- 0.18	0.52 +/- 0.14	0.54 +/- 0.16	0.54 +/- 0.16
mse	0.62 +/- 0.37	0.66 +/- 0.43	0.57 +/- 0.31	0.61 +/- 0.38	0.59 +/- 0.34
rmse	**0.75 +/- 0.22**	**0.78 +/- 0.24**	**0.73 +/- 0.2**	**0.75 +/- 0.22**	**0.74 +/- 0.20**

5-CV (mean)
0.54 +/- 0.15
0.48 +/- 0.15
0.49 +/- 0.28
0.67 +/- 0.18

5-CV (mean)
0.36 +/- 0.18
0.54 +/- 0.16
0.61 +/- 0.36
0.75 +/- 0.21

Consensus A

age Performance- Random

Metric	Fold_0	Fold_1	Fold_2	Fold_3
r2_score	0.56 +/- 0.16	0.53 +/- 0.17	0.57 +/- 0.15	0.58 +/- 0.12
mae	0.49 +/- 0.16	0.49 +/- 0.15	0.46 +/- 0.15	0.46 +/- 0.12
mse	0.5 +/- 0.31	0.52 +/- 0.29	0.42 +/- 0.27	0.63 +/- 0.22
rmse	0.68 +/- 0.19	0.69 +/- 0.18	0.63 +/- 0.17	0.64 +/- 0.15

Consensus B

age Performance- Random

Metric	Fold_0	Fold_1	Fold_2	Fold_3
r2_score	0.57 +/- 0.16	0.54 +/- 0.17	0.58 +/- 0.14	0.58 +/- 0.11
mae	0.48 +/- 0.16	0.49 +/- 0.15	0.45 +/- 0.15	0.45 +/- 0.12
mse	0.49 +/- 0.3	0.51 +/- 0.28	0.41 +/- 0.27	0.42 +/- 0.22
rmse	0.68 +/- 0.19	0.69 +/- 0.18	0.62 +/- 0.17	0.63 +/- 0.16

Fold_4	5-CV (mean)
0.56 +/- 0.14	**0.56 +/- 0.15**
0.47 +/- 0.14	**0.47 +/- 0.14**
0.44 +/- 0.25	**0.50 +/- 0.27**
0.64 +/- 0.17	**0.66 +/- 0.17**

Fold_4	5-CV (mean)
0.57 +/- 0.13	0.57 +/- 0.14
0.46 +/- 0.14	0.46 +/- 0.14
0.43 +/- 0.24	0.45 +/- 0.26
0.63 +/- 0.16	**0.65 +/- 0.17**

MT-DNN
ST-RF
ST-DNN
GCNN
DLCA
Consensus A
Consensus B

Multi-task DNN
Single Task - Random Forests
Single Task - DNN
Multi-task GCNN
Multi-task DLCA
Consensus-MT-DNN + GCNN
Consensus-MT-DNN + GCNN + DLCA

Large-scale Modeling of Multi-Species Acute Toxicity Endpoints using Consensus of Multi-Task D

Sankalp Jain, Vishal B. Siramshetty, Vinicius M. Alves, Eugene N. Muratov, Nicole Kleinstreuer, A
*Corresponding author: Alexey V. Zakharov (Email: alexey.zakharov@nih.gov)

ML-Method	RMSE	R2
MT-DNN	0.69	0.51
ST-RF	0.81	0.35
ST-DNN	0.89	0.2
GCNN	0.7	0.5
DLCA	0.67	0.54
Cosensus A	0.66	0.56
Cosensus B	0.65	0.57

Wilcoxon-test	MT-DNN vs. ST-RF	ST-RF vs. ST-DNN	MT-DNN vs. GCNN	DLCA vs. MT-DNN
P value (RMSE)	<0.0001	<0.0001	0.1331	<0.0001
P value (R2)	<0.0001	<0.0001	0.081	<0.0001
Significantly different (P < 0.05)?	Yes	Yes	No	Yes

Deep Learning Methods

Alexander Tropsha, Marc C. Nicklaus, Anton Simeonov, Alexey V. Zakharov*

DLCA vs. GCNN	Consensus A vs. DLCA	Consensus B vs. DLCA	Consensus B vs. Consensus A
<0.0001	0.0027	<0.0001	<0.0001
<0.0001	0.0064	<0.0001	<0.0001
Yes	Yes	Yes	Yes

MT-DNN	Multi-task DNN

Supporting information (tables) to

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*Corresponding author: Alexey V. Zakharov (Email: alexey.zakharov@nih.gov)

Task	**MT-DNN**		**ST-DNN**	
	RMSE	**R^2**	**RMSE**	**R^2**
mouse_intravenous_LDLo	0.83	0.53	1.14	0.10
frog_subcutaneous_LDLo	0.84	0.54	0.98	0.37
guinea pig_intravenous_LDLo	0.65	0.61	0.98	0.06
mammal (species unspecified)_subcutaneous_LD50	0.47	0.20	0.58	-0.24
rabbit_intraperitoneal_LD50	0.66	0.43	1.00	-0.28
rat_intravenous_LDLo	0.80	0.48	1.20	-0.15
cat_oral_LDLo	0.69	0.41	0.94	-0.04
human_oral_TDLo	1.27	0.32	1.55	-0.02
guinea pig_intravenous_LD50	0.75	0.62	1.23	0.00
rabbit_subcutaneous_LD50	0.81	0.62	1.11	0.28
women_oral_TDLo	1.04	0.20	1.14	0.04
cat_intravenous_LDLo	0.68	0.71	1.04	0.32
man_oral_TDLo	1.11	0.17	1.31	-0.14
guinea pig_subcutaneous_LD50	0.81	0.58	1.07	0.27
cat_oral_LD50	0.83	0.47	1.10	0.08
rat_subcutaneous_LDLo	0.66	0.68	0.98	0.30
guinea pig_skin_LD50	0.77	0.33	0.92	0.06
guinea pig_subcutaneous_LDLo	0.75	0.65	0.98	0.40
rabbit_skin_LDLo	0.67	0.47	0.91	0.02
dog_oral_LDLo	0.83	0.52	1.23	-0.08
duck_oral_LD50	0.92	0.48	1.09	0.26
mouse_skin_LD50	0.79	0.36	0.99	0.02
rabbit_subcutaneous_LDLo	0.66	0.73	0.84	0.56
guinea pig_intraperitoneal_LD50	0.61	0.57	0.94	-0.02
rabbit_oral_LDLo	0.58	0.57	0.76	0.28
mouse_subcutaneous_LDLo	0.76	0.31	0.97	-0.12
cat_intravenous_LD50	0.80	0.63	1.10	0.31
mouse_oral_LDLo	0.68	0.34	0.91	-0.16
mouse_intraperitoneal_LDLo	0.67	0.46	0.94	-0.06
rat_intramuscular_LD50	0.70	0.57	1.00	0.15
mouse_parenteral_LD50	0.71	0.46	0.84	0.21
rat_intraperitoneal_LDLo	0.58	0.53	0.84	0.00
rat_oral_LDLo	0.68	0.37	0.87	-0.06
bird - wild_oral_LD50	0.72	0.38	0.90	0.04
rabbit_intravenous_LDLo	0.74	0.61	1.00	0.27
quail_oral_LD50	0.74	0.46	0.89	0.22
chicken_oral_LD50	0.84	0.36	1.04	0.01

dog_intravenous_LDLo	0.71	0.62	1.00	0.26
dog_intravenous_LD50	0.66	0.64	0.91	0.32
mammal (species unspecified)_intraperitoneal_LD50	0.40	0.64	0.55	0.29
mouse_intramuscular_LD50	0.58	0.58	0.78	0.25
dog_oral_LD50	0.77	0.38	0.93	0.10
mammal (species unspecified)_oral_LD50	0.49	0.63	0.68	0.30
guinea pig_oral_LD50	0.72	0.61	0.80	0.52
rabbit_intravenous_LD50	0.63	0.72	0.85	0.49
rat_unreported_LD50	0.64	0.56	0.79	0.31
rat_skin_LD50	0.66	0.36	0.77	0.13
rabbit_oral_LD50	0.62	0.56	0.74	0.37
mammal (species unspecified)_unreported_LD50	0.44	0.50	0.50	0.35
rabbit_skin_LD50	0.56	0.43	0.63	0.27
mouse_unreported_LD50	0.50	0.68	0.60	0.54
rat_subcutaneous_LD50	0.68	0.53	0.77	0.40
rat_intravenous_LD50	0.56	0.67	0.65	0.56
rat_intraperitoneal_LD50	0.56	0.56	0.62	0.46
mouse_subcutaneous_LD50	0.55	0.59	0.59	0.54
rat_oral_LD50	0.57	0.60	0.58	0.58
mouse_intravenous_LD50	0.48	0.57	0.48	0.57
mouse_oral_LD50	0.42	0.51	0.43	0.49
mouse_intraperitoneal_LD50	0.45	0.59	0.45	0.58

earning Methods

ler Tropsha, Marc C. Nicklaus, Anton Simeonov, Alexey V. Zakharov*

random_split							
ST-RF		GCNN		DLCA		Consensus A	
RMSE	R^2	RMSE	R^2	RMSE	R^2	RMSE	R^2
1.05	0.25	0.86	0.49	0.79	0.58	0.80	0.56
0.97	0.38	0.82	0.56	0.84	0.54	0.80	0.58
0.74	0.49	0.67	0.57	0.61	0.66	0.64	0.62
0.43	0.33	0.45	0.28	0.48	0.18	0.42	0.36
0.85	0.08	0.62	0.51	0.63	0.48	0.61	0.51
1.00	0.21	0.88	0.37	0.76	0.55	0.79	0.50
0.88	0.08	0.70	0.39	0.64	0.51	0.67	0.45
1.46	0.11	1.44	0.11	1.32	0.27	1.29	0.31
0.89	0.47	0.77	0.60	0.71	0.66	0.71	0.66
1.07	0.36	0.83	0.59	0.86	0.56	0.76	0.66
1.06	0.17	1.05	0.19	1.09	0.13	1.01	0.26
0.86	0.54	0.74	0.66	0.66	0.72	0.67	0.72
1.21	0.02	1.13	0.15	1.04	0.28	1.06	0.26
1.10	0.21	0.88	0.48	0.83	0.56	0.80	0.58
0.90	0.38	0.84	0.46	0.76	0.56	0.79	0.52
0.93	0.36	0.69	0.65	0.66	0.68	0.67	0.67
0.76	0.38	0.78	0.32	0.74	0.40	0.75	0.37
0.88	0.52	0.72	0.68	0.75	0.65	0.70	0.70
0.89	0.09	0.77	0.31	0.70	0.45	0.68	0.46
1.11	0.14	0.88	0.46	0.84	0.51	0.84	0.51
0.99	0.39	0.94	0.44	0.85	0.55	0.88	0.52
0.89	0.21	0.71	0.49	0.79	0.38	0.73	0.46
0.85	0.55	0.61	0.76	0.61	0.77	0.59	0.78
0.79	0.28	0.66	0.49	0.62	0.56	0.63	0.55
0.72	0.36	0.63	0.49	0.61	0.53	0.59	0.55
0.90	0.03	0.73	0.36	0.77	0.30	0.73	0.38
0.88	0.55	0.78	0.65	0.78	0.65	0.76	0.67
0.77	0.16	0.68	0.36	0.68	0.35	0.66	0.39
0.83	0.17	0.65	0.49	0.62	0.53	0.62	0.53
0.93	0.25	0.67	0.61	0.70	0.58	0.65	0.63
0.76	0.39	0.72	0.44	0.72	0.44	0.66	0.53
0.77	0.18	0.55	0.58	0.56	0.57	0.54	0.58
0.78	0.15	0.69	0.33	0.64	0.44	0.64	0.42
0.75	0.33	0.71	0.41	0.67	0.46	0.68	0.45
0.92	0.39	0.75	0.59	0.71	0.63	0.71	0.64
0.81	0.35	0.75	0.44	0.71	0.51	0.72	0.49
0.90	0.27	0.87	0.31	0.77	0.45	0.81	0.41

0.93	0.36	0.72	0.61	0.70	0.64	0.68	0.66
0.81	0.45	0.64	0.67	0.64	0.66	0.62	0.69
0.48	0.48	0.45	0.54	0.43	0.59	0.40	0.63
0.71	0.39	0.57	0.61	0.55	0.63	0.54	0.64
0.87	0.22	0.76	0.39	0.73	0.44	0.73	0.44
0.60	0.44	0.54	0.54	0.53	0.57	0.48	0.63
0.77	0.55	0.70	0.63	0.69	0.64	0.66	0.67
0.79	0.55	0.64	0.71	0.62	0.72	0.61	0.74
0.73	0.41	0.62	0.57	0.60	0.60	0.59	0.61
0.71	0.25	0.63	0.41	0.62	0.43	0.62	0.44
0.70	0.43	0.61	0.56	0.60	0.57	0.60	0.59
0.47	0.41	0.46	0.45	0.44	0.49	0.42	0.53
0.63	0.28	0.55	0.44	0.54	0.47	0.53	0.48
0.56	0.59	0.54	0.63	0.48	0.70	0.48	0.71
0.75	0.43	0.68	0.53	0.65	0.58	0.64	0.58
0.64	0.57	0.57	0.65	0.54	0.69	0.54	0.70
0.62	0.47	0.56	0.56	0.55	0.59	0.54	0.60
0.58	0.54	0.56	0.58	0.53	0.62	0.52	0.63
0.58	0.58	0.56	0.61	0.53	0.64	0.53	0.65
0.48	0.56	0.47	0.58	0.44	0.64	0.44	0.63
0.43	0.50	0.43	0.50	0.40	0.55	0.40	0.56
0.45	0.58	0.45	0.57	0.42	0.63	0.42	0.63

		scaffold_s				
Consensus B		MT-DNN		ST-DNN		ST-
RMSE	R^2	RMSE	R^2			RMSE
0.78	0.58	0.82	0.46	1.22	-0.32	1.13
0.80	0.58	1.06	0.20	1.15	-0.13	0.93
0.61	0.66	0.58	0.61	0.82	0.14	0.58
0.44	0.32	0.55	-0.63	0.59	-0.57	0.52
0.60	0.53	0.70	0.32	0.98	-0.32	0.88
0.78	0.52	1.04	0.13	1.35	-0.47	1.15
0.64	0.50	0.71	0.40	1.02	-0.21	0.87
1.29	0.30	1.37	0.16	1.49	-0.01	1.38
0.70	0.67	0.89	0.46	1.19	0.05	0.83
0.78	0.65	0.81	0.42	0.92	0.26	0.96
1.01	0.26	1.17	-0.03	1.18	-0.10	1.14
0.65	0.73	0.73	0.54	1.08	-0.02	0.77
1.04	0.28	1.10	0.00	1.35	-0.48	1.21
0.79	0.59	0.74	0.38	1.00	-0.14	1.01
0.76	0.56	0.85	0.56	0.96	0.46	0.87
0.63	0.71	0.84	0.44	1.14	-0.03	1.08
0.72	0.42	1.01	-0.11	1.00	-0.08	0.86
0.70	0.69	1.02	0.24	0.98	0.27	0.93
0.68	0.46	0.60	0.12	0.87	-0.91	0.73
0.82	0.54	1.05	0.14	1.30	-0.36	1.19
0.86	0.54	0.96	0.39	1.02	0.31	1.00
0.73	0.47	0.67	0.27	0.78	-0.01	0.82
0.57	0.79	0.91	0.36	0.90	0.33	0.80
0.60	0.58	0.65	0.40	0.85	-0.06	0.73
0.58	0.58	0.65	0.49	0.73	0.36	0.77
0.72	0.38	0.71	0.40	0.95	-0.08	0.88
0.75	0.67	0.80	0.61	1.04	0.33	0.92
0.65	0.40	0.70	0.25	0.98	-0.50	0.80
0.61	0.55	0.71	0.33	0.92	-0.14	0.86
0.65	0.64	0.71	0.34	0.87	0.00	0.81
0.67	0.52	0.80	0.44	1.00	0.09	0.89
0.52	0.62	0.68	0.39	0.88	-0.04	0.82
0.63	0.44	0.71	0.32	0.97	-0.28	0.86
0.67	0.47	0.89	0.20	1.11	-0.26	0.95
0.69	0.66	0.88	0.34	1.04	0.09	0.96
0.70	0.52	0.72	0.38	0.86	0.11	0.75
0.79	0.43	0.81	0.37	0.98	0.08	0.92

0.67	0.67	0.88	0.45	1.14	0.06	1.01
0.60	0.70	0.75	0.48	0.88	0.28	0.80
0.40	0.64	0.48	0.41	0.58	0.13	0.50
0.53	0.66	0.66	0.39	0.80	0.11	0.77
0.71	0.47	0.85	0.25	0.98	0.00	0.92
0.48	0.64	0.72	0.19	0.77	0.06	0.70
0.66	0.67	1.01	0.37	1.05	0.32	1.04
0.59	0.75	0.77	0.50	0.82	0.44	0.78
0.58	0.62	0.67	0.36	0.76	0.18	0.70
0.61	0.46	0.64	0.13	0.65	0.09	0.65
0.58	0.61	0.72	0.31	0.80	0.13	0.75
0.42	0.54	0.47	0.30	0.49	0.22	0.49
0.53	0.50	0.59	0.26	0.66	0.08	0.63
0.47	0.72	0.59	0.57	0.67	0.43	0.63
0.63	0.60	0.76	0.38	0.86	0.21	0.83
0.52	0.71	0.65	0.49	0.70	0.41	0.70
0.52	0.62	0.64	0.36	0.68	0.28	0.66
0.51	0.65	0.65	0.38	0.66	0.35	0.67
0.52	0.66	0.68	0.40	0.70	0.36	0.70
0.43	0.65	0.54	0.42	0.53	0.43	0.53
0.39	0.58	0.48	0.30	0.48	0.29	0.47
0.41	0.65	0.52	0.43	0.52	0.42	0.52

split				
RF	GCNN		DLCA	
R^2	RMSE	R^2	RMSE	R^2
-0.04	0.91	0.34	0.81	0.47
0.36	0.97	0.34	0.98	0.33
0.61	0.58	0.54	0.57	0.63
-0.19	0.43	0.02	0.47	0.00
-0.05	0.66	0.40	0.72	0.29
-0.05	1.01	0.17	0.99	0.21
0.12	0.81	0.22	0.69	0.43
0.14	1.54	-0.08	1.39	0.13
0.52	0.77	0.59	0.81	0.56
0.23	0.86	0.34	0.88	0.33
0.01	1.04	0.19	1.11	0.08
0.48	0.77	0.50	0.73	0.53
-0.18	1.11	-0.03	1.03	0.14
-0.14	0.79	0.28	0.77	0.34
0.55	0.85	0.58	0.88	0.53
0.09	0.75	0.56	0.87	0.41
0.20	0.94	0.09	0.99	-0.05
0.35	0.92	0.37	0.94	0.32
-0.19	0.68	-0.07	0.62	0.05
-0.11	1.10	0.08	1.03	0.19
0.34	1.00	0.35	0.98	0.37
-0.13	0.63	0.34	0.64	0.34
0.47	0.87	0.40	0.93	0.31
0.23	0.57	0.56	0.63	0.43
0.30	0.71	0.41	0.70	0.42
0.07	0.73	0.37	0.77	0.29
0.48	0.82	0.60	0.84	0.57
0.03	0.70	0.27	0.71	0.25
0.02	0.73	0.29	0.67	0.41
0.13	0.76	0.22	0.73	0.31
0.29	0.82	0.39	0.85	0.37
0.11	0.64	0.44	0.67	0.40
0.02	0.82	0.09	0.74	0.27
0.11	0.84	0.29	0.77	0.40
0.23	0.82	0.41	0.86	0.37
0.32	0.73	0.35	0.68	0.44
0.19	0.85	0.32	0.77	0.43

MT-DNN
ST-DNN
ST-RF
GCNN
DLCA
Consensus A
Consensus B

0.26	0.84	0.49	0.88	0.45
0.41	0.70	0.55	0.71	0.54
0.35	0.45	0.46	0.46	0.45
0.17	0.68	0.35	0.66	0.40
0.13	0.82	0.29	0.84	0.26
0.23	0.65	0.32	0.72	0.19
0.33	0.90	0.49	0.99	0.40
0.50	0.70	0.59	0.74	0.55
0.31	0.65	0.41	0.63	0.44
0.10	0.62	0.18	0.56	0.32
0.24	0.72	0.30	0.69	0.36
0.22	0.46	0.32	0.45	0.37
0.15	0.59	0.26	0.56	0.32
0.50	0.56	0.60	0.55	0.62
0.25	0.77	0.36	0.74	0.41
0.40	0.63	0.52	0.61	0.54
0.31	0.62	0.40	0.61	0.43
0.35	0.64	0.40	0.62	0.44
0.38	0.67	0.41	0.66	0.43
0.43	0.51	0.48	0.49	0.52
0.32	0.48	0.31	0.46	0.36
0.42	0.49	0.49	0.49	0.50

Multi-task DNN
Single Task - DNN
Single Task - Random Forests
Multi-task GCNN
Multi-task DLCA
Consensus-MT-DNN v2 + GCNN v2
Consensus-MT-DNN v2 + GCNN v2 + DLCA

Supporting information (tables) to

Large-scale Modeling of Multi-Species Acute Toxicity Endpoints using Consensus of Multi-Task Deep

Sankalp Jain, Vishal B. Siramshetty, Vinicius M. Alves, Eugene N. Muratov, Nicole Kleinstreuer, Alexa
*Corresponding author: Alexey V. Zakharov (Email: alexey.zakharov@nih.gov)

Task	Sosnin et al. [49]		MT-D
	RMSE	R^2	RMSE
mouse_intraperitoneal_LD50	0.41	0.65	0.45
mouse_oral_LD50	0.42	0.54	0.42
mouse_intravenous_LD50	0.43	0.66	0.48
rat_oral_LD50	0.53	0.65	0.57
mouse_subcutaneous_LD50	0.51	0.65	0.55
rat_intraperitoneal_LD50	0.55	0.62	0.56
rat_intravenous_LD50	0.54	0.71	0.56
rat_subcutaneous_LD50	0.64	0.61	0.68
mouse_unreported_LD50	0.51	0.69	0.50
rabbit_skin_LD50	0.56	0.44	0.56
mammal (species unspecified)_unreported_LD50	0.40	0.59	0.44
rabbit_oral_LD50	0.58	0.58	0.62
rat_skin_LD50	0.63	0.36	0.66
rat_unreported_LD50	0.60	0.46	0.64
rabbit_intravenous_LD50	0.68	0.69	0.63
guinea pig_oral_LD50	0.70	0.64	0.72
rat_oral_LDLo	0.61	0.56	0.68
rat_intraperitoneal_LDLo	0.43	0.61	0.58
Average for 18 tasks	**0.54**	**0.60**	**0.57**