Table 2. Optimized paramters of our hybrid model to reproduce the results for various types of toxicity data sets.

Task	Mini-batch	Epochs	Drop-Out	Activation	Initilization	Threshold	Features Selected	AUROC for Held-out CV	AUROC of Individual Models	Ensemble Neural Network AUROC	Random Forrest	SVM
NR-ahr												
1									0.911			
2	32	20	0.6	relu	he_normal	1.5*mean	270	0.802233	0.912	0.919		
3									0.903	0.919		
4									0.916	0.921	0.907	0.889
NR-ar	Mini-batch	Epochs	Drop-Out	Activation	Initilization	Threshold	Features Selected	AUROC for Held-out CV	AUROC of Individual Models	Ensemble Neural Network AUROC		
1									0.744			
2	2048	20	0.1	sigmoid	he_normal	1.5*mean	284	0.619164	0.743	0.744		
3									0.744	0.743		
4									0.744	0.743	0.638	0.730
NR-ar-lbd	Mini-batch	Epochs	Drop-Out	Activation	Initilization	Threshold	Features Selected	AUROC for Held-out CV	AUROC of Individual Models	Ensemble Neural Network AUROC		
1									0.882			
2	4096	20	0.9	relu	he_uniform	1.2*mean	365	0.769197	0.876	0.879		
3									0.879	0.881		
4									0.877	0.881	0.800	0.702
NR-aromatase	Mini-batch	Epochs	Drop-Out	Activation	Initilization	Threshold	Features Selected	AUROC for Held-out CV	AUROC of Individual Models	Ensemble Neural Network AUROC		
1									0.794			
2	4096	20	0	sigmoid	normal	0.7*mean	815	0.76325	0.792	0.794		
3									0.794	0.794		
4									0.790	0.794	0.792	0.782
NR-er	Mini-batch	Epochs	Drop-Out	Activation	Initilization	Threshold	Features Selected	AUROC for Held-out CV	AUROC of Individual Models	Ensemble Neural Network AUROC		
1									0.823			
2	8192	40	0.2	relu	he_uniform	1.7*mean	292	0.689923	0.822	0.823		
3									0.823	0.823		
4									0.818	0.822	0.778	0.791
NR-er-lbd	Mini-batch	Epochs	Drop-Out	Activation	Initilization	Threshold	Features Selected	AUROC for Held-out CV	AUROC of Individual Models	Ensemble Neural Network AUROC		
1									0.840			
2	1024	60	0.3	relu	he_uniform	0.8*mean	755	0.606101	0.831	0.835		
3									0.832	0.836		
4									0.834	0.836	0.768	0.786
NR-pparg	Mini-batch	Epochs	Drop-Out	Activation	Initilization	Threshold	Features Selected	AUROC for Held-out CV	AUROC of Individual Models	Ensemble Neural Network AUROC		
1									0.864			
2	512	10	0.3	relu	he_normal	1*mean	517	0.678438	0.852	0.860		
3									0.857	0.858		
4									0.849	0.858	0.789	0.744
									Average	0.836	0.782	0.775
SR-are	Mini-batch	Epochs	Drop-Out	Activation	Initilization	Threshold	Features Selected	AUROC for Held-out CV	AUROC of Individual Models	Ensemble Neural Network AUROC		
1									0.825			
2	1024	20	0.8	sigmoid	he_normal	1*mean	615	0.769482	0.822	0.827		
3									0.825	0.827		
4									0.825	0.828	0.774	0.779
SR-hse	Mini-batch	Epochs	Drop-Out	Activation	Initilization	Threshold	Features Selected	AUROC for Held-out CV	AUROC of Individual Models	Ensemble Neural Network AUROC		
1									0.833			
2	2048	20	0.4	relu	he_normal	0.3*mean	1028	0.774243	0.829	0.832		
3									0.834	0.832		
4									0.829	0.832	0.859	0.798
SR-mmp	Mini-batch	Epochs	Drop-Out	Activation	Initilization	Threshold	Features Selected	AUROC for Held-out CV	AUROC of Individual Models	Ensemble Neural Network AUROC		
1									0.955			
2	1024	20	0.5	relu	he_normal	0.9*mean	685	0.898425	0.953	0.959		
3									0.954	0.959		
4									0.953	0.958	0.978	0.916
SR-p53	Mini-batch	Epochs	Drop-Out	Activation	Initilization	Threshold	Features Selected	AUROC for Held-out CV	AUROC of Individual Models	Ensemble Neural Network AUROC		
1									0.874			
2	512	20	0.7	relu	he_normal	1.7*mean	223	0.665071	0.875	0.876		
3									0.873	0.875		
4									0.877	0.875	0.847	0.810
SR-atad5	Mini-batch	Epochs	Drop-Out	Activation	Initilization	Threshold	Features Selected	AUROC for Held-out CV	AUROC of Individual Models	Ensemble Neural Network AUROC		
1									0.819			
2	4096	20	0.1	relu	he_normal	1.1*mean	390	0.644897	0.820	0.820		
3									0.820	0.820		
4									0.819	0.820	0.812	0.765
									Average	0.862	0.854	0.814
AM	Mini-batch	Epochs	Drop-Out	Activation	Initilization	Threshold	Features Selected	AUROC for Held-out CV	AUROC of Individual Models	Ensemble Neural Network AUROC		
1									0.874			
2	1024	250	0.1	Sigmoid	he_normal	1.5*mean	145	0.870	0.872	0.880		
3									0.872	0.880		
4									0.869	0.878	0.842	0.810
									5 Fold Cross Validation	0.879	0.831	0.815
IGC50	Mini-batch	Epochs	Drop-Out	Activation	Initilization	Threshold	Features Selected	R^2 for Held-out CV	R^2 of Individual Models	Ensemble Neural Network AUROC		
1									0.804			
2	1024	400	0.1	Sigmoid>Relu	glorot_normal	1.5*mean	117	0.805	0.805	0.808		
3									0.805	0.808		
4									0.806	0.810		
									5 Fold Cross Validation	0.807		
LC50	Mini-batch	Epochs	Drop-Out	Activation	Initilization	Threshold	Features Selected	R^2 for Held-out CV	R^2 of Individual Models	Ensemble Neural Network AUROC		
1									0.672			
2	128	40	0.3	Sigmoid>Relu	glorot_normal	0.1*mean	857	0.678	0.661	0.669		
3									0.653	0.665		
4									0.677	0.678		
									5 Fold Cross Validation	0.675		
LD50	Mini-batch	Epochs	Drop-Out	Activation	Initilization	Threshold	Features Selected	R^2 for Held-out CV	R^2 of Individual Models	Ensemble Neural Network AUROC		
1									0.621			
2	32	200	0.6	Sigmoid>Relu	glorot_normal	0.1*mean	817	0.613	0.626	0.621		
3									0.625	0.626		
4									0.627	0.629		
									5 Fold Cross Validation	0.618		
LC50-DM	Mini-batch	Epochs	Drop-Out	Activation	Initilization	Threshold	Features Selected	R^2 for Held-out CV	R^2 of Individual Models	Ensemble Neural Network AUROC		
1									0.612			
2	128	50	0.3	Sigmoid>Relu	glorot_normal	0.1*mean	854	0.611	0.612	0.615		
3									0.613	0.616		
4									0.614	0.616		
									5 Fold Cross Validation	0.612		