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Representation of the Structure—A Key Point of Building QSAR/QSPR Models for Ionic Liquids

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Table S1. The experimental data of ILs' toxicity towards Escherichia coli collected from the literature.

ID	Cation	Cation's Abbreviation	Cation's SMILES	Anion	Anion's Abbreviation	Anion's SMILES	Set	EC50 [mM]	log_EC50 [mM]
1	1−butyl−3−methylpyridinium	C4mpy	CCCC[N+]1=CC=CC(=C1)C	bromide	Br	[Br−]	T	45.12	1.65
2	1−butyl−3−methylpyridinium	C4mpy	CCCC[N+]1=CC=CC(=C1)C	thiocyanate	SCN	C(#N)[S−]	V	55.47	1.74
3	1−hexyl−3−methylpyridinium	C6mpy	CCCCCC[N+]1=CC=CC(=C1)C	bromide	Br	[Br−]	T	9.75	0.99
4	1−hexyl−3−methylpyridinium	C6mpy	CCCCCC[N+]1=CC=CC(=C1)C	thiocyanate	SCN	C(#N)[S−]	T	14.29	1.16
5	1−octyl−3−methylpyridinium	C8mpy	CCCCCCCC[N+]1=CC=CC(=C1)C	bromide	Br	[Br−]	V	1.09	0.04
6	1−octyl−3−methylpyridinium	C8mpy	CCCCCCCC[N+]1=CC=CC(=C1)C	thiocyanate	SCN	C(#N)[S−]	V	0.57	−0.24
7	1−decyl−3−methylpyridinium	C10mpy	CCCCCCCCCC[N+]1=CC=CC(=C1)C	bromide	Br	[Br−]	T	0.27	−0.57
8	1−decyl−3−methylpyridinium	C10mpy	CCCCCCCCCC[N+]1=CC=CC(=C1)C	thiocyanate	SCN	C(#N)[S−]	T	0.02	−1.70
9	1−ethyl−1−methylpyrrolidinium	C2mpyrr	CC[N+]1(CCCC1) C	bromide	Br	[Br−]	T	222.19	2.35
10	1−butyl−1−methylpyrrolidinium	C4mpyrr	CCCC[N+]1(CCCC1)C	bromide	Br	[Br−]	T	108.88	2.04
11	1−octyl−1−methylpyrrolidinium	C8mpyrr	CCCCCCCC[N+]1(CCCC1)C	bromide	Br	[Br−]	V	3.22	0.51
12	1−decyl−1−methylpyrrolidinium	C10mpyrr	CCCCCCCCCC[N+]1(CCCC1)C	bromide	Br	[Br−]	T	0.52	−0.28
13	1−butyl−1−methylpiperidinium	C4mpip	CCCC[N+]1(CCCCC1)C	bromide	Br	[Br−]	T	80.4	1.91
14	1−hexyl−1−methylpiperidinium	C6mpip	CCCCCC[N+]1(CCCCC1)C	bromide	Br	[Br−]	V	10.83	1.03
15	1−octyl−1−methylpiperidinium	C8mpip	CCCCCCCC[N+]1(CCCCC1)C	bromide	Br	[Br−]	T	1.91	0.28

16	1−octyl−3−methylimidazolium	C8mim	CCCCCCCCN1C=C[N+](=C1)C	thiocyanate	SCN	C(#N)[S−]	T	2.53	0.40
17	1−butyl−3−methylimidazolium	C4mim	CCCCN1C=C[N+](=C1)C	bis(trifluoromethylsulfonyl)amide	NTf2	C(F)(F)(F)S(=O)(=O)[N−]S(=O)(=O)C(F)(F)F	T	1.64	0.21
18	1−butylpyridinium	C4py	CCCC[N+]1=CC=CC=C1	bis(trifluoromethylsulfonyl)amide	NTf2	C(F)(F)(F)S(=O)(=O)[N−]S(=O)(=O)C(F)(F)F	T	2.3	0.36
19	1−butyl−1−methylpyrrolidinium	C4mpyrr	CCCC[N+]1(CCCC1)C	bis(trifluoromethylsulfonyl)amide	NTf2	C(F)(F)(F)S(=O)(=O)[N−]S(=O)(=O)C(F)(F)F	T	3.29	0.52
20	1−butyl−1−methylpiperidinium	C4mpip	CCCC[N+]1(CCCCC1)C	bis(trifluoromethylsulfonyl)amide	NTf2	C(F)(F)(F)S(=O)(=O)[N−]S(=O)(=O)C(F)(F)F	V	2.05	0.31
21	1−octyl−3−methylimidazolium	C8mim	CCCCCCCCN1C=C[N+](=C1)C	bis(trifluoromethylsulfonyl)amide	NTf2	C(F)(F)(F)S(=O)(=O)[N−]S(=O)(=O)C(F)(F)F	V	0.35	−0.46
22	1−octylpyridinium	C8py	CCCCCCCC[N+]1=CC=CC=C1	bis(trifluoromethylsulfonyl)amide	NTf2	C(F)(F)(F)S(=O)(=O)[N−]S(=O)(=O)C(F)(F)F	T	0.47	−0.33
23	1−octyl−1−methylpyrrolidinium	C8mpyrr	CCCCCCCC[N+]1(CCCC1)C	bis(trifluoromethylsulfonyl)amide	NTf2	C(F)(F)(F)S(=O)(=O)[N−]S(=O)(=O)C(F)(F)F	T	0.64	−0.19
24	1−octyl−1−methylpiperidinium	C8mpip	CCCCCCCC[N+]1(CCCCC1)C	bis(trifluoromethylsulfonyl)amide	NTf2	C(F)(F)(F)S(=O)(=O)[N−]S(=O)(=O)C(F)(F)F	T	0.9	−0.05

T—training set, V—validation set

Table S2. Details of the model based on 2D descriptors calculated for each of the cations and anions separately (M1).

Variable	**Coeff.**	**Std. Error**
Intercept	2.49	0.18
Psi_i_0^{A}	−0.14	0.02
SMTIV^{C}	−0.001	0.0001
Quality Parameters:		
Fitting criteria	*Internal validation criteria*	*External validation criteria*

R^2	0.91	Q^2loo	0.86	$R^2ext/Q^2–F1$	0.83
$RMSE_C$	0.30	$RMSE_{CV}$	0.38	$RMSE_{EXT}$	0.30
R^2adj	0.90	$R^2–Q^2loo$	0.05	$Q^2–F2$	0.83
$R^2–R^2adj$	0.01	MAE_{CV}	0.31	MAE_{EXT}	0.28
MAE_C	0.25			r^2m aver.	0.76
RSS_C	1.53			r^2m delta	0.11
				r^2	0.85
				$r0^2$	0.84
				reverse $r0^2$	0.82

Golbraikh and Tropsha Acceptable Model Criteria's:			
1. Q^2	0.86	$Q^2 > 0.5$	Passed
2. r^2	0.85	$r^2 > 0.6$	Passed
3. $\|r0^2–r'^2\|$	0.03	$\|r0^2–r'0^2\| < 0.3$	Passed
4. k	0.89	[0.85 < k < 1.15 and ((r²–r0^2)/r^2 < 0.1]	Passed
$[(r^2–r0^2)/r^2]$	0.01		
OR*			
k'	1.00	[0.85 < k' < 1.15 and $((r^2–r'0^2)/ r^2) < 0.1$])	Passed
$[(r^2–r'0^2)/r^2]$	0.04		

ID	**Set**	**Psi_i_0[A]**	**SMTIV[C]**	**Exp. Endpoint**	**Pred. by Model eq.**	**Pred.Mod.Eq.Res.**	**Outlier or out of AD? (StdAD)**
1	T	0	900	1.65	1.58	0.08	No
3	T	0	1480	0.99	0.99	0.00	No
4	T	1.56	1480	1.16	0.76	0.39	No
7	T	0	3370	−0.57	−0.93	0.36	No
8	T	1.56	3370	−1.70	−1.15	−0.55	No
9	T	0	262	2.35	2.22	0.12	No
10	T	0	518	2.04	1.96	0.07	No

12	T	0	2370	−0.28	0.08	−0.37	No
13	T	0	669	1.91	1.81	0.10	No
15	T	0	1840	0.28	0.62	−0.34	No
16	T	1.56	1960	0.40	0.28	0.13	No
17	T	8.09	721	0.22	0.60	−0.38	No
18	T	8.09	740	0.36	0.58	−0.22	No
19	T	8.09	518	0.52	0.80	−0.29	No
22	T	8.09	1990	−0.33	−0.69	0.36	No
23	T	8.09	1540	−0.19	−0.23	0.04	No
24	T	8.09	1840	−0.05	−0.54	0.49	No
2	V	1.56	900	1.74	1.35	0.39	No
5	V	0	2300	0.04	0.16	−0.12	No
6	V	1.56	2300	−0.24	−0.07	−0.18	No
11	V	0	1540	0.51	0.93	−0.42	No
14	V	0	1150	1.04	1.32	−0.29	No
20	V	8.09	669	0.31	0.65	−0.34	No
21	V	8.09	1960	−0.46	−0.66	0.20	No

Table S3. Details of the model based on 3D descriptors calculated for each of the cations and anions separately (M2).

Variable	**Coef.**	**Std. Error**
Intercept	2.52	0.20
$L1m^C$	−0.12	0.01
$L1i^A$	−0.19	0.03

Quality Parameters:					
Fitting criteria		*Internal validation criteria*		*External validation criteria*	
R^2	0.90	Q^2loo	0.85	$R^2ext/Q^2–F1$	0.85

$RMSE_C$	0.33	$RMSE_{CV}$	0.40	$RMSE_{EXT}$	0.27
R^2adj	0.89	$R^2–Q^2loo$	0.05	$Q^2–F2$	0.85
$R^2–R^2adj$	0.01	MAE_{CV}	0.33	MAE_{EXT}	0.25
MAE_C	0.27			r^2m aver.	0.80
RSS_C	1.80			r^2m delta	0.10
				r^2	0.86
				$r0^2$	0.86
				reverse $r0^2$	0.85

Golbraikh and Tropsha Acceptable Model Criteria's:

1. Q^2	0.85	$Q^2 > 0.5$	Passed
2. r^2	0.86	$r^2 > 0.6$	Passed
3. $\|r0^2–r'0^2\|$	0.01	$\|r0^2–r'0^2\| < 0.3$	Passed
4. k	0.93		
[(r^2−r0^2)/r^2]	0.002	[0.85 < k < 1.15 and $((r^2–r0^2)/r^2 < 0.1$]	Passed
OR*			
k'	0.96		
$[(r^2–r'0^2)/r^2]$	0.02	[0.85 < k' < 1.15 and $((r^2–r'0^2)/r^2) < 0.1$])	Passed

ID	Set	$L1m^C$	$L1i^A$	Exp. Endpoint	Pred. by Model eq.	Pred.Mod.Eq.Res.	Outlier or out of AD? (StdAD)
1	T	6.779	0	1.65	1.68	−0.03	No
3	T	11.763	0	0.99	1.07	−0.08	No

4	T	11.763	1.378	1.16	0.81	0.35	No
7	T	26.051	0	−0.57	−0.69	0.12	No
8	T	26.051	1.378	−1.70	−0.95	−0.75	No
9	T	2.543	0	2.35	2.20	0.15	No
10	T	4.483	0	2.04	1.96	0.08	No
12	T	22.202	0	−0.28	−0.22	−0.06	No
13	T	6.231	0	1.91	1.75	0.16	No
15	T	15.419	0	0.28	0.62	−0.34	No
16	T	18.4	1.378	0.40	−0.01	0.41	No
17	T	6.996	5.665	0.22	0.59	−0.38	No
18	T	6.482	5.665	0.36	0.65	−0.29	No
19	T	4.483	5.665	0.52	0.90	−0.38	No
22	T	17.744	5.665	−0.33	−0.73	0.40	No
23	T	15.31	5.665	−0.19	−0.43	0.24	No
24	T	15.419	5.665	−0.05	−0.45	0.40	No
2	V	6.779	1.378	1.74	1.42	0.32	No
5	V	18.237	0	0.04	0.27	−0.23	No
6	V	18.237	1.378	−0.24	0.01	−0.26	No
11	V	15.31	0	0.51	0.63	−0.12	No
14	V	11.166	0	1.04	1.14	−0.11	No
20	V	6.231	5.665	0.31	0.68	−0.37	No
21	V	18.4	5.665	−0.46	−0.81	0.36	No

Table 4. Details of the model based on 2D and 3D descriptors calculated for each of the cations and anions separately (M3).

Variable	**Coeff.**	**Std. Error**			
Intercept	2.304	0.1653			
Psi_i_0[A]	−0.142	0.0217			
QZZm[C]	−0.006	0.0005			
Quality Parameters:					
Fitting criteria		*Internal validation criteria*		*External validation criteria*	
R^2	0.92	Q^2loo	0.87	R^2ext/Q^2−F1	0.86
$RMSE_C$	0.30	$RMSE_{CV}$	0.38	$RMSE_{EXT}$	0.27
R^2adj	0.905	R^2−Q^2loo	0.05	Q^2−F2	0.86
R^2−R^2adj	0.012	MAE_{CV}	0.32	MAE_{EXT}	0.26
MAE_C	0.25			r^2m aver.	0.75
RSS_C	1.50			r^2m delta	0.10
				r^2	0.89
				$r0^2$	0.87
				reverse r0^2	0.84
Golbraikh and Tropsha acceptable model criteria's:					
1. Q^2	0.86	$Q^2 > 0.5$		Passed	
2. r^2	0.89	$r^2 > 0.6$		Passed	
3. $\|r0^2-r'0^2\|$	0.03	$\|r0^2-r'0^2\| < 0.3$		Passed	
4. k	0.91	$[0.85 < k < 1.15$ and $((r^2-r0^2)/r^2 < 0.1]$		Passed	
$[(r^2-r0^2)/r^2]$	0.02				
OR*					
k'	0.99	$[0.85 < k' < 1.15$ and $((r^2-r'0^2)/r^2) < 0.1])$		Passed	

$[(r^2-r'0^2)/r^2]$	0.06

ID	Set	Psi_i_0[A]	QZZm[C]	Exp. Endpoint	Pred. by Model eq.	Pred.Mod.Eq.Res.	Outlier or out of AD? (StdAD)
1	T	0	99	1.65	1.71	−0.06	No
3	T	0	190.258	0.99	1.17	−0.18	No
4	T	1.56	190.258	1.16	0.95	0.21	No
7	T	0	525.383	−0.57	−0.83	0.26	No
8	T	1.56	525.383	−1.70	−1.05	−0.65	No
9	T	0	30.861	2.35	2.12	0.23	No
10	T	0	67.211	2.04	1.90	0.13	No
12	T	0	436.357	−0.28	−0.29	0.01	No
13	T	0	91.447	1.91	1.76	0.15	No
15	T	0	290.62	0.28	0.57	−0.29	No
16	T	1.56	307.266	0.40	0.25	0.15	No
17	T	8.09	87.871	0.22	0.63	−0.42	No
18	T	8.09	81.203	0.36	0.67	−0.31	No
19	T	8.09	67.211	0.52	0.76	−0.24	No
22	T	8.09	292.369	−0.33	−0.59	0.26	No
23	T	8.09	266.49	−0.19	−0.43	0.24	No
24	T	8.09	290.62	−0.05	−0.57	0.53	No
2	V	1.56	99	1.74	1.49	0.25	No
5	V	0	329.776	0.04	0.34	−0.30	No
6	V	1.56	329.776	−0.24	0.12	−0.36	No
11	V	0	266.49	0.51	0.72	−0.21	No
14	V	0	182.483	1.04	1.22	−0.18	No
20	V	8.09	91.447	0.31	0.61	−0.30	No

21	V	8.09	307.266	−0.46	−0.67	0.22	No

Table S5. Details of the model based on 2D descriptors calculated for whole ionic pairs (M4).

Variable	**Coeff.**	**Std. Error**
Intercept	4.15	0.40
GMTI	−0.001	0.0001
MDDD	−0.09	0.02
AMW	−0.16	0.04

Quality Parameters:

Fitting criteria		*Internal validation criteria*		*External validation criteria*	
R^2	0.97	Q^2loo	0.94	$R^2ext/Q^2–F1$	0.91
$RMSE_C$	0.18	$RMSE_{CV}$	0.25	$RMSE_{EXT}$	0.21
R^2adj	0.96	$R^2–Q^2loo$	0.03	$Q^2–F2$	0.91
$R^2–R^2adj$	0.01	MAE_{CV}	0.19	MAE_{EXT}	0.21
MAE_C	0.14			r^2m aver.	0.74
RSS_C	0.52			r^2m delta	0.07
				r^2	0.97
				$r0^2$	0.92
				reverse $r0^2$	0.89

Golbraikh and Tropsha acceptable model criteria's:

1. Q^2	0.94	$Q^2 > 0.5$	Passed
2. r^2	0.97	$r^2 > 0.6$	Passed
3. $\|r0^2 - r'0^2\|$	0.03	$\|r0^2 - r'0^2\| < 0.3$	Passed
4. k	0.93	[0.85 < k < 1.15 and $((r^2 - r0^2)/r^2 < 0.1]$	Passed
$[(r^2 - r0^2)/r^2]$	0.06		
OR*			
k'	1.01	[0.85 < k' < 1.15 and $((r^2 - r'0^2)/r^2) < 0.1]$	Passed
$[(r^2 - r'0^2)/r^2]$	0.09		

ID	Set	GMTI	MDDD	AMW	Exp. Endpoint	Pred. by Model eq.	Pred.Mod.Eq.Res.	Outlier or out of AD? (StdAD)
1	T	609	7.17	8.22	1.65	1.66	−0.01	No
3	T	1080	10.3	7.59	0.99	1.07	−0.08	No
4	T	1090	14.1	6.57	1.16	0.87	0.29	No
7	T	2690	17.9	6.83	−0.57	−0.90	0.33	No
8	T	2690	24	6.09	−1.70	−1.34	−0.36	No
9	T	201	3.65	7.77	2.35	2.41	−0.06	No
10	T	435	5.95	7.17	2.04	2.09	−0.05	No
12	T	2230	16	6.25	−0.28	−0.23	−0.05	No
13	T	577	7	6.95	1.91	1.91	0.00	No
15	T	1700	13.5	6.36	0.28	0.43	−0.15	No
16	T	1490	17.3	6.34	0.40	0.27	0.13	No
17	T	1420	10.4	10.5	0.22	0.31	−0.10	No
18	T	1440	10.3	10.7	0.36	0.27	0.09	No
19	T	1390	10.9	9.39	0.52	0.46	0.06	No
22	T	2460	8.73	9.27	−0.33	−0.23	−0.10	No

23	T	2370	8.28	8.4	−0.19	0.02	−0.21	No
24	T	2660	9.65	8.21	−0.05	−0.32	0.27	No
2	V	615	9.92	6.95	1.74	1.60	0.14	No
5	V	1770	14	7.16	0.04	0.20	−0.17	No
6	V	1770	18.9	6.3	−0.24	−0.12	−0.13	No
11	V	1420	12.1	6.47	0.51	0.79	−0.28	No
14	V	1040	10	6.61	1.04	1.29	−0.25	No
20	V	1530	9.54	9.09	0.31	0.52	−0.21	No
21	V	2430	8.66	9.15	−0.46	−0.18	−0.27	No

Table S6. Details of the model based on 3D descriptors calculated from the optimized geometries of whole ionic pairs (M5).

Variable	**Coeff.**	**Std. Error**			
Intercept	6.91	0.34			
L/Bw	−0.24	0.02			
RTv	−1.05	0.07			
L3u	0.53	0.18			
Quality Parameters:					
Fitting criteria		*Internal validation criteria*		*External validation criteria*	
R^2	0.97	Q^2loo	0.94	$R^2ext/Q^2–F1$	0.84
$RMSE_C$	0.18	$RMSE_{CV}$	0.26	$RMSE_{EXT}$	0.28
R^2adj	0.96	$R^2–Q^2loo$	0.04	$Q^2–F2$	0.85
$R^2–R^2adj$	0.01	MAE_{CV}	0.20	MAE_{EXT}	0.25
MAE_C	0.14			r^2m aver.	0.77
RSS_C	0.52			r^2m delta	0.09
				r^2	0.89
				$r0^2$	0.88
				reverse $r0^2$	0.89
Golbraikh and Tropsha Acceptable Model Criteria's:					
1. Q^2	0.94	$Q^2 > 0.5$		Passed	
2. r^2	0.89	$r^2 > 0.6$		Passed	
3. $\|r0^2–r'0^2\|$	0.01	$\|r0^2–r'0^2\| < 0.3$		Passed	
4. k	0.86	$[0.85 < k < 1.15$ and $((r^2–r0^2)/r^2 < 0.1]$		Passed	
$[(r^2–r0^2)/r^2]$	0.02				
OR*				Passed	
k'	1.06	$[0.85 < k' < 1.15$ and $((r^2–r'0^2)/r^2) < 0.1]$		Passed	
$[(r^2–r'0^2)/r^2]$	0.01				

ID	Set	L/Bw	RTv	L3u	Exp. Endpoint	Pred. by model eq.	Pred.Mod.Eq .Res.	Outlier or out of AD? (StdAD)
1	T	1.6	4.874	0.746	1.65	1.81	−0.16	No
3	T	4.37	5.002	0.903	0.99	1.08	−0.09	No
4	T	4.18	5.474	1.454	1.16	0.92	0.24	No
7	T	9.44	5.509	0.905	−0.57	−0.69	0.12	No
8	T	10.52	6.068	0.941	−1.70	−1.52	−0.18	No
9	T	3.76	4.232	1.147	2.35	2.17	0.18	No
10	T	1.59	4.725	1.094	2.04	2.15	−0.11	No
12	T	7.66	5.532	0.992	−0.28	−0.23	−0.05	No
13	T	1.29	5.175	1.284	1.91	1.85	0.06	No
15	T	4.61	5.671	1.151	0.28	0.45	−0.17	No
16	T	6.58	5.298	0.941	0.40	0.25	0.15	No
17	T	1.96	6.685	2.292	0.22	0.64	−0.43	No
18	T	1.68	6.651	1.392	0.36	0.27	0.09	No
19	T	2.3	6.749	2.127	0.52	0.40	0.12	No
22	T	2.2	7.163	1.557	−0.33	−0.31	−0.02	No
23	T	2.05	6.929	1.277	−0.19	−0.18	−0.01	No
24	T	2.23	7.341	1.896	−0.05	−0.32	0.27	No
2	V	2.8	4.732	1.003	1.74	1.80	−0.06	No
5	V	8.96	5.498	1.127	0.04	−0.44	0.48	No
6	V	7.86	5.778	1.185	−0.24	−0.43	0.19	No
11	V	4.56	5.3	1.018	0.51	0.78	−0.27	No
14	V	2.41	5.458	1.22	1.04	1.25	−0.21	No
20	V	2.03	6.818	1.391	0.31	0.01	0.31	No

21	V	2.85	7.201	2.126	−0.46	−0.21	−0.25	No

Table S7. Details of the model based on 2D and 3D descriptors from the optimized geometries of whole ionic pairs (M6).

Variable	**Coeff.**	**Std. Error**						
Intercept	3.49	0.53						
GMTI	−0.001	0.00						
E1e	−3.21	0.81						
DISPm	0.04	0.02						
Quality Parameters:								
Fitting criteria			*Internal validation criteria*		*External validation criteria*			
R^2	0.96		Q^2loo	0.91	R^2ext/Q^2-F1	0.90		
$RMSE_C$	0.20		$RMSE_{CV}$	0.30	$RMSE_{EXT}$	0.23		
R^2adj	0.95		R^2-Q^2loo	0.05	Q^2-F2	0.90		
R^2-R^2adj	0.01		MAE_{CV}	0.22	MAE_{EXT}	0.21		
MAE_C	0.16				r^2m aver.	0.65		
RSS_C	0.68				r^2m delta	0.11		
					r^2	0.98		
					$r0^2$	0.90		
					reverse $r0^2$	0.85		
Golbraikh and Tropsha Acceptable Model Criteria's:								
1. Q^2	0.91		$Q^2 > 0.5$		Passed			
2. r^2	0.98		$r^2 > 0.6$		Passed			
3. $\|r0^2-r'0^2\|$	0.05		$\|r0^2-r'0^2\| < 0.3$		Passed			
4. k	1.03		$[0.85 < k < 1.15$ and $((r^2-r0^2)/r^2 <$		Passed			
$[(r^2-r0^2)/r^2]$	0.08		$0.1]$					
OR*					Passed			

k'	0.90	[0.85 < k' < 1.15 and ((r²−r'0²)/r²) < 0.1]	Passed
[(r²−r'0²)/r²]	0.13		

ID	Set	GMTI	E1e	DISPm	Exp. Endpoint	Pred. by Model eq.	Pred.Mod.Eq.Res.	Outlier or out of AD? (StdAD)
1	T	609	0.528	11.096	1.65	1.49	0.16	No
3	T	1080	0.562	17.687	0.99	1.06	−0.07	No
4	T	1090	0.546	11.082	1.16	0.80	0.36	No
7	T	2690	0.568	23.257	−0.57	−0.83	0.26	No
8	T	2690	0.547	13.135	−1.70	−1.21	−0.49	No
9	T	201	0.446	16.767	2.35	2.55	−0.20	No
10	T	435	0.464	14.929	2.04	2.10	−0.06	No
12	T	2230	0.557	17.057	−0.28	−0.47	0.19	No
13	T	577	0.452	13.776	1.91	1.90	0.01	No
15	T	1700	0.52	14.36	0.28	0.23	0.05	No
16	T	1490	0.537	12.694	0.40	0.38	0.02	No
17	T	1420	0.622	15.915	0.21	0.34	−0.13	No
18	T	1440	0.616	17.52	0.36	0.40	−0.04	No
19	T	1390	0.616	19.885	0.52	0.57	−0.05	No
22	T	2460	0.454	21.417	−0.33	−0.24	−0.09	No
23	T	2370	0.41	21.32	−0.19	0.01	−0.20	No
24	T	2660	0.385	20.641	−0.05	−0.32	0.27	No
2	V	615	0.545	11.476	1.74	1.45	0.30	No
5	V	1770	0.579	23.399	0.04	0.35	−0.31	No
6	V	1770	0.553	14.124	−0.24	0.02	−0.26	No
11	V	1420	0.536	15.651	0.51	0.60	−0.10	No

14	V	1040	0.488	13.477	1.04	1.16	−0.13	No
20	V	1530	0.613	20.523	0.31	0.43	−0.12	No
21	V	2430	0.446	20.942	−0.46	−0.20	−0.26	No