Electronic Supplementary Material (ESI) for Toxicology Research.

Supporting information

Development of predictive QSAR models for *Vibrio fischeri* toxicity of ionic liquids and their true external and experimental validation tests

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Table S1. Categorical list of the used descriptor pool.

Descriptor group	Variables
ETA indices	First generation: $\sum\alpha$, $\sum\alpha/N_v$, $(\sum\alpha)_P/\sum\alpha$, $(\sum\alpha)_Y/\sum\alpha$, $(\sum\alpha)_X/\sum\alpha$, $\sum\beta'$, $\sum\beta'_s$, $\sum\beta'_{ns}$, η' (η/N_v), η'_F, η'^{local}, $\eta'_F{}^{local}$, η'_B
	Second generation: $\Delta\alpha_B$, $\Delta\varepsilon_A$, $\Delta\varepsilon_B$, $\Delta\varepsilon_C$, $\Delta\varepsilon_D$, $\Delta\psi_A$, $\Delta\psi_B$, $\Delta\beta'$
QTMS parameters	ρ, λ_1, λ_2, λ_3, $\nabla^2\rho$, ε, K, G, R_e
Lipophilicity parameters	$\log k_0$ (using ETA and QTMS variables), ALOGP
Constitutional indices	MW, AMW, Sv, Se, Sp, Si, Mv, Me, Mp, Mi, nAT, nSK, nBT, nBO, nBM, SCBO, RBN, RBF, nDB, nTB, nAB, nH, nC, nN, nO, nP, nS, nF, nCL, nBR, nI, nB, nHM, nHet, nX, H%, C%, N%, O%, X%, nCsp3, nCsp2, nCsp
Ring descriptors	nCIC, Rbrid, MCD, RCI, NNRS, nR05, nR06, nR07, nR09, nBnz, ARR, D/Dtr05, D/Dtr06
Topological indices	ZM1, ZM1V, ZM1Kup, ZM1Mad, ZM1Per, ZM1MulPer, ZM2, ZM2V, ZM2Kup, ZM2Mad, ZM2Per, ZM2MulPer, ON0, ON0V, ON1, ON1V, Qindex, BBI, DBI, SNar, HNar, GNar, Xt, Dz, Ram, BLI, Pol, LPRS, MSD, SPI, PJI2, ECC, AECC, DECC, MDDD, UNIP, CENT, VAR, ICR, SMTI, SMTIV, GMTI, GMTIV, Xu, CSI, Wap, S1K, S2K, S3K, PHI, PW2, PW3, PW4, PW5, MAXDN, MAXDP, DELS, TIE, Psi_i_s, Psi_i_A, Psi_i_0, Psi_i_1, Psi_i_t, Psi_i_0d, Psi_i_1d, Psi_i_1s, Psi_e_A, Psi_e_0, Psi_e_1, Psi_e_t, Psi_e_0d, Psi_e_1d, Psi_e_1s, BAC, LOC
Connectivity indices	X0, X1, X2, X3, X4, X5, X0A, X1A, X2A, X3A, X4A, X5A, X0v, X1v, X2v, X3v, X4v, X5v, X0Av, X1Av, X2Av, X3Av, X4Av, X5Av, X0sol, X1sol, X2sol, X3sol, X4sol, X5sol, XMOD, RDCHI, RDSQ, X1Kup, X1Mad, X1Per, X1MulPer
Information indices	ISIZ, IAC, AAC, IDE, IDM, IDDE, IDDM, IDET, IDMT, IVDE, IVDM, S0K, HVcpx, HDcpx, Uindex, Vindex, Xindex, Yindex, IC0, IC1, IC2, IC3, IC4, IC5, TIC0, TIC1, TIC2, TIC3, TIC4, TIC5, SIC0, SIC1, SIC2, SIC3, SIC4,SIC5, CIC0, CIC1, CIC2, CIC3, CIC4, CIC5, BIC0, BIC1, BIC2, BIC3, BIC4, BIC5
Functional group counts	nCp, nCs, nCt, nCq, nCrs, nCrt, nCrq, nCar, nCbH, nCb-, nCconj, nR=Cp, nR=Cs, nR=Ct, n=C=, nR#CH/X, nR#C-, nROCN, nArOCN, nRNCO, nArNCO, nRSCN, nArSCN, nRNCS, nArNCS, nRCOOH, nArCOOH, nRCOOR, nArCOOR, nRCONH2, nArCONH2, nRCONHR, nArCONHR, nRCONR2, nArCONR2, nROCON, nArOCON, nRCOX, nArCOX, nRCSOH, nArCSOH, nRCSSH, nArCSSH, nRCOSR, nArCOSR, nRCSSR, nArCSSR, nRCHO, nArCHO, nRCO, nArCO, nCONN, nC=O(O)2, nN=C-N<, nC(=N)N2, nRC=N, nArC=N, nRCNO, nArCNO, nRNH2, nArNH2, nRNHR, nArNHR, nRNR2, nArNR2, nN-N, nN=N, nRCN, nArCN, nN+, nNq, nRNHO, nArNHO, nRNNOx nArNNOx, nRNO, nArNO, nRNO2, nArNO2, nN(CO)2, nC=N-N<, nROH, nArOH, nOHp, nOHs, nOHt, nROR, nArOR, nROX, nArOX, nO(C=O)2, nH2O, nSH, nC=S, nRSR, nRSSR, nSO, nS(=O)2, nSOH, nSOOH, nSO2OH, nSO3OH, nSO2, nSO3, nSO4, nSO2N, nPO3, nPO4, nPR3, nP(=O)O2R, nP(=O)R3/nPR5, nCH2RX, nCHR2X, nCR3X, nR=CHX, nR=CRX, nR#CX, nCHRX2, nCR2X2, nR=CX2, nCRX3, nArX, nCXr, nCXr=, nCconjX, nAziridines, nOxiranes, nThiranes, nAzetidines, nOxetanes, nThioethanes, nBeta-Lactams, nPyrrolidines, nOxolanes,

	ntH-Thiophenes, nPyrroles, nPyrazoles, nImidazoles, nFuranes, nThiophenes, nOxazoles, nIsoxazoles, nThiazoles, nIsothiazoles, nTriazoles, nPyridines, nPyridazines, nPyrimidines, nPyrazines, n135-Triazines, n124-Triazines, nHDon, nHAcc, nHBonds, N-aromatics, naAromAtom
Atom-centred fragments	C-001, C-002, C-003, C-004, C-005, C-006, C-007, C-008, C-009, C-010, C-011, C-012, C-013, C-014, C-015, C-016, C-017, C-018, C-019, C-020, C-021, C-022, C-023, C-024, C-025, C-026, C-027, C-028, C-029, C-030, C-031, C-032, C-033, C-034, C-035, C-036, C-037, C-038, C-039, C-040, C-041, C-042, C-043, C-044, H-046, H-047, H-048, H-049, H-050, H-051, H-052, H-053, H-054, H-055, O-056, O-057, O-058, O-059, O-060, O-061, O-062, O-063, N-066, N-067, N-068, N-069, N-070, N-071, N-072, N-073, N-074, N-075, N-076, N-077, N-078, N-079, F-081, F-082, F-083,F-084, F-085, Cl-086, Cl-087, Cl-088, Cl-089, Cl-090, Br-091, Br-092, Br-093, Br-094, Br-095, I-096, I-097, I-098, I-099, I-100, F-101, Cl-102, Br-103, I-104, S-106, S-107, S-108, S-109, S-110, P-115, P-116, P-117, P-118, P-119, P-120
Atom-type E-state indices	SsCH3, SdCH2, SssCH2, StCH, SdsCH, SaaCH, SsssCH, SddC, StsC, SdssC, SaasC, SaaaC, SssssC, SsNH2, SssNH, SdNH, SsssN, SdsN, SaaN, StN, SsNH3+, SssNH2+, SdNH2+, SsssNH+, SssssN+, SddsN, SaasN, SaaNH, SsOH, SdO, SssO, SaaO, SsPH2, SssPH, SsssP, SdsssP, SddsP, SssssssP, SsSH, SdS, SssS, SaaS, SdssS, SddssS, SssssssS, SsF, SsCl, SsBr, SsI
2D atom pairs	T(N..N), T(N..O), T(N..S), T(N..P), T(N..F), T(N..Cl), T(N..Br), T(N..I), T(O..O), T(O..S), T(O..P), T(O..F), T(O..Cl), T(O..Br), T(O..I), T(S..S), T(S..P), T(S..F), T(S..Cl), T(S..Br), T(S..I), T(P..P), T(P..F), T(P..Cl), T(P..Br), T(P..I), T(F..F), T(F..Cl), T(F..Br), T(F..I), T(Cl..Cl), T(Cl..Br), T(Cl..I), T(Br..Br), T(Br..I), T(I..I), B01[C-C], B01[C-N], B01[C-O], B01[C-S], B01[C-P], B01[C-F], B01[C-Cl], B01[C-Br], B01[C-I], B01[C-B], B01[C-Si], B01[C-X], B01[N-N], B01[N-O], B01[N-S], B01[N-P], B01[N-F], B01[N-Cl], B01[N-Br], B01[N-I], B01[N-B], B01[N-Si], B01[N-X], B01[O-O], B01[O-S], B01[O-P], B01[O-F], B01[O-Cl], B01[O-Br], B01[O-I], B01[O-B], B01[O-Si], B01[O-X], B01[S-S], B01[S-P], B01[S-F], B01[S-Cl], B01[S-Br], B01[S-I], B01[S-B], B01[S-Si], B01[S-X], B01[P-P], B01[P-F], B01[P-Cl], B01[P-Br], B01[P-I], B01[P-B], B01[P-Si], B01[P-X], B01[F-F], B01[F-Cl], B01[F-Br], B01[F-I], B01[F-B], B01[F-Si], B01[F-X], B01[Cl-Cl], B01[Cl-Br], B01[Cl-I], B01[Cl-B], B01[Cl-Si], B01[Cl-X], B01[Br-Br], B01[Br-I], B01[Br-B], B01[Br-Si], B01[Br-X], B01[I-I], B01[I-B], B01[I-Si], B01[I-X], B01[B-B], B01[B-Si], B01[B-X], B01[Si-Si], B01[Si-X], B01[X-X], B02[C-C], B02[C-N], B02[C-O], B02[C-S], B02[C-P], B02[C-F], B02[C-Cl], B02[C-Br], B02[C-I], B02[C-B], B02[C-Si], B02[C-X], B02[N-N], B02[N-O], B02[N-S], B02[N-P], B02[N-F], B02[N-Cl], B02[N-Br], B02[N-I], B02[N-B], B02[N-Si], B02[N-X], B02[O-O], B02[O-S], B02[O-P], B02[O-F], B02[O-Cl], B02[O-Br], B02[O-I], B02[O-B], B02[O-Si], B02[O-X], B02[S-S], B02[S-P], B02[S-F], B02[S-Cl], B02[S-Br], B02[S-I], B02[S-B], B02[S-Si], B02[S-X], B02[P-P], B02[P-F], B02[P-Cl], B02[P-Br], B02[P-I], B02[P-B], B02[P-Si], B02[P-X], B02[F-F], B02[F-Cl], B02[F-Br], B02[F-I], B02[F-B], B02[F-Si], B02[F-X], B02[Cl-Cl], B02[Cl-Br], B02[Cl-I], B02[Cl-B], B02[Cl-Si], B02[Cl-X], B02[Br-Br], B02[Br-I], B02[Br-B], B02[Br-Si], B02[Br-X], B02[I-I], B02[I-B], B02[I-Si], B02[I-X], B02[B-B], B02[B-Si], B02[B-X], B02[Si-Si], B02[Si-X], B02[X-X], B03[C-C], B03[C-N], B03[C-O], B03[C-S], B03[C-P], B03[C-F], B03[C-Cl], B03[C-Br], B03[C-I], B03[C-B], B03[C-Si],

	B03[C-X], B03[N-N], B03[N-O], B03[N-S], B03[N-P], B03[N-F], B03[N-Cl], B03[N-Br], B03[N-I], B03[N-B], B03[N-Si], B03[N-X], B03[O-O], B03[O-S], B03[O-P], B03[O-F], B03[O-Cl], B03[O-Br], B03[O-I], B03[O-B], B03[O-Si], B03[O-X], B03[S-S], B03[S-P], B03[S-F], B03[S-Cl], B03[S-Br], B03[S-I], B03[S-B], B03[S-Si], B03[S-X], B03[P-P], B03[P-F], B03[P-Cl], B03[P-Br], B03[P-I], B03[P-B], B03[P-Si], B03[P-X], B03[F-F], B03[F-Cl], B03[F-Br], B03[F-I], B03[F-B], B03[F-Si], B03[F-X], B03[Cl-Cl], B03[Cl-Br], B03[Cl-I], B03[Cl-B], B03[Cl-Si], B03[Cl-X], B03[Br-Br], B03[Br-I], B03[Br-B], B03[Br-Si], B03[Br-X], B03[I-I], B03[I-B], B03[I-Si], B03[I-X], B03[B-B], B03[B-Si], B03[B-X], B03[Si-Si], B03[Si-X], B03[X-X], B04[C-C], B04[C-N], B04[C-O], B04[C-S], B04[C-P], B04[C-F], B04[C-Cl], B04[C-Br], B04[C-I], B04[C-B], B04[C-Si], B04[C-X], B04[N-N], B04[N-O], B04[N-S], B04[N-P], B04[N-F], B04[N-Cl], B04[N-Br], B04[N-I], B04[N-B], B04[N-Si], B04[N-X], B04[O-O], B04[O-S], B04[O-P], B04[O-F], B04[O-Cl], B04[O-Br], B04[O-I], B04[O-B], B04[O-Si], B04[O-X], B04[S-S], B04[S-P], B04[S-F], B04[S-Cl], B04[S-Br], B04[S-I], B04[S-B], B04[S-Si], B04[S-X], B04[P-P], B04[P-F], B04[P-Cl], B04[P-Br], B04[P-I], B04[P-B], B04[P-Si], B04[P-X], B04[F-F], B04[F-Cl], B04[F-Br], B04[F-I], B04[F-B], B04[F-Si], B04[F-X], B04[Cl-Cl], B04[Cl-Br], B04[Cl-I], B04[Cl-B], B04[Cl-Si], B04[Cl-X], B04[Br-Br], B04[Br-I], B04[Br-B], B04[Br-Si], B04[Br-X], B04[I-I], B04[I-B], B04[I-Si], B04[I-X], B04[B-B], B04[B-Si], B04[B-X], B04[Si-Si], B04[Si-X], B04[X-X], B05[C-C], B05[C-N], B05[C-O], B05[C-S], B05[C-P], B05[C-F], B05[C-Cl], B05[C-Br], B05[C-I], B05[C-B], B05[C-Si], B05[C-X], B05[N-N], B05[N-O], B05[N-S], B05[N-P], B05[N-F], B05[N-Cl], B05[N-Br], B05[N-I],B05[N-B], B05[N-Si], B05[N-X], B05[O-O], B05[O-S], B05[O-P], B05[O-F], B05[O-Cl], B05[O-Br], B05[O-I], B05[O-B], B05[O-Si], B05[O-X], B05[S-S], B05[S-P], B05[S-F], B05[S-Cl], B05[S-Br], B05[S-I], B05[S-B], B05[S-Si], B05[S-X], B05[P-P], B05[P-F], B05[P-Cl], B05[P-Br], B05[P-I], B05[P-B], B05[P-Si], B05[P-X], B05[F-F], B05[F-Cl], B05[F-Br], B05[F-I], B05[F-B], B05[F-Si], B05[F-X], B05[Cl-Cl], B05[Cl-Br], B05[Cl-I], B05[Cl-B], B05[Cl-Si], B05[Cl-X], B05[Br-Br], B05[Br-I], B05[Br-B], B05[Br-Si], B05[Br-X], B05[I-I], B05[I-B], B05[I-Si], B05[I-X], B05[B-B], B05[B-Si], B05[B-X], B05[Si-Si], B05[Si-X], B05[X-X], B06[C-C], B06[C-N], B06[C-O], B06[C-S], B06[C-P], B06[C-F], B06[C-Cl], B06[C-Br], B06[C-I], B06[C-B], B06[C-Si], B06[C-X], B06[N-N], B06[N-O], B06[N-S], B06[N-P], B06[N-F], B06[N-Cl], B06[N-Br], B06[N-I], B06[N-B], B06[N-Si], B06[N-X], B06[O-O], B06[O-S], B06[O-P], B06[O-F], B06[O-Cl], B06[O-Br], B06[O-I], B06[O-B], B06[O-Si], B06[O-X], B06[S-S], B06[S-P], B06[S-F], B06[S-Cl], B06[S-Br], B06[S-I], B06[S-B], B06[S-Si], B06[S-X], B06[P-P], B06[P-F], B06[P-Cl], B06[P-Br], B06[P-I], B06[P-B], B06[P-Si], B06[P-X], B06[F-F], B06[F-Cl], B06[F-Br], B06[F-I], B06[F-B], B06[F-Si], B06[F-X], B06[Cl-Cl], B06[Cl-Br], B06[Cl-I], B06[Cl-B], B06[Cl-Si], B06[Cl-X], B06[Br-Br], B06[Br-I], B06[Br-B], B06[Br-Si], B06[Br-X], B06[I-I], B06[I-B], B06[I-Si], B06[I-X], B06[B-B], B06[B-Si], B06[B-X], B06[Si-Si], B06[Si-X], B06[X-X], B07[C-C], B07[C-N], B07[C-O], B07[C-S], B07[C-P], B07[C-F], B07[C-Cl], B07[C-Br], B07[C-I], B07[C-B], B07[C-Si], B07[C-X], B07[N-N], B07[N-O], B07[N-S], B07[N-P], B07[N-F], B07[N-Cl], B07[N-Br], B07[N-I], B07[N-B], B07[N-Si], B07[N-X], B07[O-O], B07[O-S], B07[O-P], B07[O-F], B07[O-Cl], B07[O-Br], B07[O-I], B07[O-B], B07[O-Si], B07[O-X], B07[S-S], B07[S-P], B07[S-F], B07[S-

	Cl], B07[S-Br], B07[S-I], B07[S-B], B07[S-Si], B07[S-X], B07[P-P], B07[P-F], B07[P-Cl], B07[P-Br], B07[P-I], B07[P-B], B07[P-Si], B07[P-X], B07[F-F], B07[F-Cl], B07[F-Br], B07[F-I], B07[F-B], B07[F-Si], B07[F-X], B07[Cl-Cl], B07[Cl-Br], B07[Cl-I], B07[Cl-B], B07[Cl-Si], B07[Cl-X], B07[Br-Br], B07[Br-I], B07[Br-B], B07[Br-Si], B07[Br-X], B07[I-I], B07[I-B], B07[I-Si], B07[I-X], B07[B-B], B07[B-Si], B07[B-X], B07[Si-Si], B07[Si-X], B07[X-X], B08[C-C], B08[C-N], B08[C-O], B08[C-S], B08[C-P], B08[C-F], B08[C-Cl], B08[C-Br], B08[C-I], B08[C-B], B08[C-Si], B08[C-X], B08[N-N], B08[N-O], B08[N-S], B08[N-P], B08[N-F], B08[N-Cl], B08[N-Br], B08[N-I], B08[N-B], B08[N-Si], B08[N-X], B08[O-O], B08[O-S], B08[O-P], B08[O-F], B08[O-Cl], B08[O-Br], B08[O-I], B08[O-B], B08[O-Si], B08[O-X], B08[S-S], B08[S-P], B08[S-F], B08[S-Cl], B08[S-Br], B08[S-I], B08[S-B], B08[S-Si], B08[S-X], B08[P-P], B08[P-F], B08[P-Cl], B08[P-Br], B08[P-I], B08[P-B], B08[P-Si], B08[P-X], B08[F-F], B08[F-Cl], B08[F-Br], B08[F-I], B08[F-B], B08[F-Si], B08[F-X], B08[Cl-Cl], B08[Cl-Br], B08[Cl-I], B08[Cl-B], B08[Cl-Si], B08[Cl-X], B08[Br-Br], B08[Br-I], B08[Br-B], B08[Br-Si], B08[Br-X], B08[I-I], B08[I-B], B08[I-Si], B08[I-X], B08[B-B], B08[B-Si], B08[B-X], B08[Si-Si], B08[Si-X], B08[X-X], B09[C-C], B09[C-N], B09[C-O], B09[C-S], B09[C-P], B09[C-F], B09[C-Cl], B09[C-Br], B09[C-I], B09[C-B], B09[C-Si], B09[C-X], B09[N-N], B09[N-O], B09[N-S], B09[N-P], B09[N-F], B09[N-Cl], B09[N-Br], B09[N-I], B09[N-B], B09[N-Si], B09[N-X], B09[O-O], B09[O-S], B09[O-P], B09[O-F], B09[O-Cl], B09[O-Br], B09[O-I], B09[O-B], B09[O-Si], B09[O-X], B09[S-S], B09[S-P], B09[S-F], B09[S-Cl], B09[S-Br], B09[S-I], B09[S-B], B09[S-Si], B09[S-X], B09[P-P], B09[P-F], B09[P-Cl], B09[P-Br], B09[P-I], B09[P-B], B09[P-Si], B09[P-X], B09[F-F], B09[F-Cl], B09[F-Br], B09[F-I], B09[F-B], B09[F-Si], B09[F-X], B09[Cl-Cl], B09[Cl-Br], B09[Cl-I], B09[Cl-B], B09[Cl-Si], B09[Cl-X], B09[Br-Br], B09[Br-I], B09[Br-B], B09[Br-Si], B09[Br-X], B09[I-I], B09[I-B], B09[I-Si], B09[I-X], B09[B-B], B09[B-Si], B09[B-X], B09[Si-Si], B09[Si-X], B09[X-X], B10[C-C], B10[C-N], B10[C-O], B10[C-S], B10[C-P], B10[C-F], B10[C-Cl], B10[C-Br], B10[C-I], B10[C-B], B10[C-Si], B10[C-X], B10[N-N], B10[N-O], B10[N-S], B10[N-P], B10[N-F], B10[N-Cl], B10[N-Br], B10[N-I], B10[N-B], B10[N-Si], B10[N-X], B10[O-O], B10[O-S], B10[O-P], B10[O-F], B10[O-Cl], B10[O-Br], B10[O-I], B10[O-B], B10[O-Si], B10[O-X], B10[S-S], B10[S-P], B10[S-F], B10[S-Cl], B10[S-Br], B10[S-I], B10[S-B], B10[S-Si], B10[S-X], B10[P-P], B10[P-F], B10[P-Cl], B10[P-Br], B10[P-I], B10[P-B], B10[P-Si], B10[P-X], B10[F-F], B10[F-Cl], B10[F-Br], B10[F-I], B10[F-B], B10[F-Si], B10[F-X], B10[Cl-Cl], B10[Cl-Br], B10[Cl-I], B10[Cl-B], B10[Cl-Si], B10[Cl-X], B10[Br-Br], B10[Br-I], B10[Br-B], B10[Br-Si], B10[Br-X], B10[I-I], B10[I-B], B10[I-Si], B10[I-X], B10[B-B], B10[B-Si], B10[B-X], B10[Si-Si], B10[Si-X], B10[X-X]
CATS 2D parameters	CATS2D_00_DD, CATS2D_01_DD, CATS2D_02_DD, CATS2D_03_DD, CATS2D_04_DD, CATS2D_05_DD, CATS2D_06_DD,CATS2D_07_DD, CATS2D_08_DD, CATS2D_09_DD, CATS2D_00_DA, CATS2D_01_DA, CATS2D_02_DA, CATS2D_03_DA, CATS2D_04_DA, CATS2D_05_DA, CATS2D_06_DA, CATS2D_07_DA, CATS2D_08_DA, CATS2D_09_DA, CATS2D_00_DP, CATS2D_01_DP, CATS2D_02_DP, CATS2D_03_DP, CATS2D_04_DP, CATS2D_05_DP, CATS2D_06_DP, CATS2D_07_DP, CATS2D_08_DP, CATS2D_09_DP, CATS2D_00_DN, CATS2D_01_DN, CATS2D_02_DN, CATS2D_03_DN, CATS2D_04_DN, CATS2D_05_DN,

	CATS2D_06_DN, CATS2D_07_DN, CATS2D_08_DN, CATS2D_09_DN, CATS2D_00_DL, CATS2D_01_DL, CATS2D_02_DL, CATS2D_03_DL, CATS2D_04_DL, CATS2D_05_DL, CATS2D_06_DL, CATS2D_07_DL, CATS2D_08_DL, CATS2D_09_DL, CATS2D_00_AA, CATS2D_01_AA, CATS2D_02_AA, CATS2D_03_AA, CATS2D_04_AA, CATS2D_05_AA, CATS2D_06_AA, CATS2D_07_AA, CATS2D_08_AA, CATS2D_09_AA, CATS2D_00_AP, CATS2D_01_AP, CATS2D_02_AP, CATS2D_03_AP, CATS2D_04_AP, CATS2D_05_AP, CATS2D_06_AP, CATS2D_07_AP, CATS2D_08_AP, CATS2D_09_AP, CATS2D_00_AN, CATS2D_01_AN, CATS2D_02_AN, CATS2D_03_AN, CATS2D_04_AN, CATS2D_05_AN, CATS2D_06_AN, CATS2D_07_AN, CATS2D_08_AN, CATS2D_09_AN, CATS2D_00_AL, CATS2D_01_AL, CATS2D_02_AL, CATS2D_03_AL, CATS2D_04_AL, CATS2D_05_AL, CATS2D_06_AL, CATS2D_07_AL, CATS2D_08_AL, CATS2D_09_AL, CATS2D_00_PP, CATS2D_01_PP, CATS2D_02_PP, CATS2D_03_PP, CATS2D_04_PP, CATS2D_05_PP, CATS2D_06_PP, CATS2D_07_PP, CATS2D_08_PP, CATS2D_09_PP, CATS2D_00_PN, CATS2D_01_PN, CATS2D_02_PN, CATS2D_03_PN, CATS2D_04_PN, CATS2D_05_PN, CATS2D_06_PN, CATS2D_07_PN, CATS2D_08_PN, CATS2D_09_PN, CATS2D_00_PL, CATS2D_01_PL, CATS2D_02_PL, CATS2D_03_PL, CATS2D_04_PL, CATS2D_05_PL, CATS2D_06_PL, CATS2D_07_PL, CATS2D_08_PL, CATS2D_09_PL, CATS2D_00_NN, CATS2D_01_NN, CATS2D_02_NN, CATS2D_03_NN, CATS2D_04_NN, CATS2D_05_NN, CATS2D_06_NN, CATS2D_07_NN, CATS2D_08_NN, CATS2D_09_NN, CATS2D_00_NL, CATS2D_01_NL, CATS2D_02_NL, CATS2D_03_NL, CATS2D_04_NL, CATS2D_05_NL, CATS2D_06_NL, CATS2D_07_NL, CATS2D_08_NL, CATS2D_09_NL, CATS2D_00_LL, CATS2D_01_LL, CATS2D_02_LL, CATS2D_03_LL, CATS2D_04_LL, CATS2D_05_LL, CATS2D_06_LL, CATS2D_07_LL, CATS2D_08_LL, CATS2D_09_LL

Table S2. Compound Nos. of the test set molecules with respect to the employed clusters.

Cluster number	Sl. No. of test set chemicals
1	29, 33, 34, 51, 56, 57, 63, 65, 109, 112, 115, 118, 132, 145, 197, 199, 217
2	188
3	95, 97, 99, 100, 155, 170
4	7, 9, 17, 36, 38, 39, 74, 88, 90, 163, 213, 228, 236, 264, 267, 290, 291
5	2, 4, 20, 32, 46, 48, 77, 82, 102, 103, 138, 141, 149, 150, 151, 154, 165, 167, 174, 187, 190, 196, 198, 201, 205, 207, 208, 210, 212, 223, 239, 243, 244, 248, 250, 254, 256, 259, 261, 268, 281, 283, 284, 285, 286, 288, 298, 300, 303, 304, 305
6	–

Table S3. Definition of some of the employed statistical validation metrics.

Type	Mathematical definition*	Refs.
Model fitness measures	$R^2 = 1 - \frac{\sum (Y_{obs(train)} - Y_{calc(train)})^2}{\sum (Y_{obs(train)} - \overline{Y}_{train})^2}$ $R_a^2 = \frac{(n_{train} - 1) \times R^2 - p}{n_{train} - p - 1}$ $F = \frac{\left[\sum (Y_{calc(train)} - \overline{Y}_{\text{train}})^2\right] / p}{\left[\sum (Y_{obs(train)} - Y_{calc(train)})^2\right] / (n_{train} - p - 1)}$	7, 43
Internal validation metric	$Q^2_{LOO} = 1 - \frac{\sum (Y_{obs(train)} - Y_{pred(train)})^2}{\sum (Y_{obs(train)} - \overline{Y}_{train})^2}$	7
External validation metrics	$Q^2_{ext(F1)} = R^2_{pred} = 1 - \frac{\sum (Y_{obs(test)} - Y_{pred(test)})^2}{\sum (Y_{obs(test)} - \overline{Y}_{train})^2}$ $Q^2_{ext(F2)} = 1 - \frac{\sum (Y_{obs(test)} - Y_{pred(test)})^2}{\sum (Y_{obs(test)} - \overline{Y}_{test})^2}$	7

* The terms used in the equations are explained below.

n_{train}= Number of compounds in the training set
n_{test} = Number of compounds in the test set
p = Number of descriptors present in the model
$Y_{\text{obs(train)}}$ = Experimental response values of the training set compounds
$Y_{\text{calc(train)}}$ = Calculated response values of the training set compounds
$\overline{Y}_{train}$ = Mean experimental response value of the training set compounds
$Y_{\text{pred(train)}}$ = Predicted response values of the training set compounds
$Y_{\text{obs(test)}}$ = Experimental response values of the test set compounds
$Y_{\text{pred(test)}}$ = Predicted response values of the test set compounds
$\overline{Y}_{test}$ = Mean experimental response value of the test set compounds

Table S4. Experimental and computed *Vibrio fischeri* toxicity of ILs.

Sl. No.	Formulae of the ILs	Ecotoxicity to *Vibrio fischeri* (pEC_{50} considering EC_{50} in mol L^{-1})		
		Expt. values	Predicted values (consensus)	Refs
Training set chemicals				
1	[IM1,3][N(CF3SO2)2]	3.2277	3.2128	30
3	[IM1,4][N(CF3SO2)2]	3.4704	3.3560	29
5	[IM1,6][PF6]	3.8901	3.7548	29
6	[IM1,8][PF6]	5.2989	4.5707	29
8	[TMGC7]I	5.0725	5.5746	31
10	[DMG(di-h)2]Cl	5.0821	5.3928	31
11	[DMG(C3O)4]Cl	3.5591	3.9135	31
12	[IM1,2O2O1]Cl	3.7359	2.6391	31
13	[P6,6,6,14]Br	4.9464	4.6255	31
14	[P6,6,6,14]Cl	5.0144	5.0127	31
15	[P6,6,6,14][CH3SO3]	5.0594	4.7463	31
16	[P4,4,4,4]Br	3.2932	3.0180	31
18	[P1,(4,4,4)i][ToS]	3.3601	2.7312	31
19	[IM1,4]Br	2.4739	2.6554	31
21	[IM1,4][ToS]	2.6769	2.4797	31
22	[IM1,3][PF6]	2.4452	2.8468	32
23	[PYR1,3][PF6]	1.9894	2.4514	32
24	[PYD1,3][PF6]	3.2137	3.2223	32
25	[PIP1,3][PF6]	2.4102	2.5499	32
26	[N1,1,1,2OH][Bic]	3.7474	2.5862	34
27	[N1,1,1,2OH]Cl	2.9469	2.7694	34
28	[N1,1,1,2OH][Ac]	2.7913	2.5800	34
30	[N1,1,1,2OH][DHCit]	4.1268	3.1859	34
31	[N1,1,1,2OH][Sal]	3.5078	2.7451	34
35	[N4,4,4,6][N(CF3SO2)2]	4.5189	4.0170	24
37	[N4,4,4,6][PF6]	3.8241	4.0125	24
40	[P4,4,4,4][PF6]	3.5557	3.3520	24
41	[N1,8,8,8][N(CF3SO2)2]	4.4449	5.0451	24
42	[P1,8,8,8][N(CF3SO2)2]	5.1829	4.9840	24
43	[IM1,4i][N(CF3SO2)2]	3.1696	3.1802	25
44	[PYD1,4][N(CF3SO2)2]	4.0218	3.7216	25
45	[PYD1,4i][N(CF3SO2)2]	3.5409	3.7345	25
47	[PYR1,4i][N(CF3SO2)2]	3.0604	3.1350	25
49	[PIP1,4i][N(CF3SO2)2]	3.3493	3.4818	25
50	[IM1,2][CHES]	2.9427	2.9486	28
52	[IM1,2][MES]	1.3157	2.1728	28

53	[IM1,2][TES]	2.0022	2.3038	28
54	[IM1,2][TRICINE]	2.7115	2.6558	28
55	[N1,1,1,1][CHES]	3.1011	3.2497	28
58	[N2,2,2,2][CHES]	3.1504	2.6585	28
59	[N2,2,2,2][HEPES]	1.8180	2.0140	28
60	[N2,2,2,2][MES]	0.8648	1.8828	28
61	[N2,2,2,2][TES]	1.2309	2.0137	28
62	[N2,2,2,2][TRICINE]	2.3984	2.3658	28
64	[N4,4,4,4][HEPES]	3.3455	2.9070	28
66	[N4,4,4,4][TES]	3.2390	2.9352	28
67	[N4,4,4,4][TRICINE]	3.3681	3.3981	28
68	[N1,1,2,2OH]Br	0.8884	1.7669	27
69	[N1,1,3,2OH]Br	0.7955	1.8348	27
70	[N1,1,4,2OH]Br	1.2260	1.8621	27
71	[N1,1,5,2OH]Br	1.9010	2.1396	27
72	[N1,1,6,2OH]Br	2.5323	2.5175	27
73	[N1,1,8,2OH]Br	3.2386	3.2687	27
75	[N1,1,2OH,CH2CHCH2]Br	1.0045	1.7581	27
76	[N1,1,2OH,CH2CCH]Br	2.9455	1.7191	27
78	[N1,3,2OH,2OH]Br	2.1797	2.1173	27
79	[N1,6,2OH,2OH]Br	3.0113	2.7910	27
80	[N1,12,2OH,2OH]Br	4.6395	4.2878	27
81	[N1,2OH,2OH,CH2CHCH2]Br	1.9418	2.0796	27
83	[N1,2OH,2OH,(CH2)4CHCH2]Br	2.3328	2.7527	27
84	[N6,2OH,2OH,2OH]Br	4.2020	3.0338	27
85	[N1,2OH,2OH,6,N1,2OH,2OH][2Br]	1.8968	2.8376	27
86	[N1,2OH,2OH,8,N1,2OH,2OH][2Br]	1.9613	3.4734	27
87	[N1,2OH,2OH,10,N1,2OH,2OH][2Br]	3.1413	4.0239	27
89	[N2OH,2OH,2OH,6,N2OH,2OH,2OH][2Br]	3.1137	2.7644	27
91	[N2OH,2OH,2OH,10,N2OH,2OH,2OH][2Br]	4.7283	3.7703	27
92	[N2OH,2OH,2OH,12,N2OH,2OH,2OH][2Br]	5.0081	3.9015	27
93	[PYD1(PhOOCH2)(COOCH3)]Br	3.1523	2.7641	33
94	[IM1,1(COOCH3)(PhOOCH2)]Cl	3.6412	3.0673	33
96	[IM1(PhOOCH2)(COOC4H9)]Br	3.6596	2.9427	33
98	[PYDCH2COOCH(COOCH3)(PhOOCH2)][Br]	2.6588	3.1743	33
101	[DABCO2]Br	0.4000	1.4952	20
104	[DABCO8]Br	3.7000	3.5290	20
105	[DABCO10]Br	4.7000	4.3714	20
106	[N1,1,2OH][Ace]	1.7100	2.3882	23
107	[2-HEA][But]	1.8202	2.6784	16
108	[2-HDEA][Ace]	1.9743	2.0194	16
110	[2-HDEA][For]	2.2757	2.0104	16
111	[2-HDEA][iB]	2.3565	2.0681	16

113	[2-HDEA][Pr]	2.4401	2.1490	16
114	[N1,1,2,2O1][N(CF3SO2)2]	2.6500	2.6841	23
116	[N1,1,2,1COO2][N(CF3SO2)2]	2.6800	2.7562	23
117	[N4,4,4,4]Br	2.7300	3.0264	23
119	[N1,1,2,4][N(CF3SO2)2]	2.7852	3.2582	16
120	[2-HDEA][Pe]	2.7721	2.4569	16
121	[N4,4,4,4]Cl	3.3100	3.2743	23
122	[N2,2,2,6]Br	3.5400	3.1169	23
123	[N1,1,Bn,2O2OPh((4-C(CH3)2CH2C(CH3)3)][N(CF3SO2)2]	3.8620	4.5351	16
124	[N1,1,Bn,2O2OPh((4-C(CH3)2CH2C(CH3)3)][Sal]	4.1851	4.5063	16
125	[N1,1,Bn,2O2OPh((4-C(CH3)2CH2C(CH3)3)][Cl]	4.3883	4.8491	16
126	[N1,1,8,Bn]Cl	4.7235	5.0626	16
127	[N1,1,8,Bn][Sal]	4.8210	5.0383	16
128	[N1,1,1,16]Cl	5.6000	5.3560	23
129	[N1,1,1,16]Br	5.9600	5.1081	23
130	[N1,1,12,Bn]Cl	6.2300	5.2362	23
131	[N1,1,16,Bn]Cl	6.3100	5.3163	23
133	[IM1,2][FAP]	3.2549	3.1382	35
134	[IM1,8]Br	3.5607	4.2320	35
135	[IM1,6]Br	3.6073	3.4156	35
136	[IM1,1][CH3SO4]	1.2400	1.9641	22
137	[IM1,2]Cl	1.4500	2.5320	22
139	[IM1,2O2]Br	1.7167	2.0376	16
140	[IM1,2][TFA]	1.7200	2.4781	23
142	[IM1,2O1]Cl	1.8239	2.1808	16
143	[IM1,2][SCN]	1.8500	2.3747	23
144	[IM1,2O1][BF4]	1.8533	2.0754	16
146	[IM][TFA]	1.9300	2.3015	23
147	[IM1,2O1][N(CN)2]	1.9352	1.9559	16
148	[IM1,2OH][N(CF3SO2)2]	1.9547	2.4825	16
152	[IM1,3][BF4]	2.0600	2.5478	22
153	[IM1,2OH]Cl	2.1100	2.0298	16
156	[IM1,1CN][N(CF3SO2)2]	2.1871	2.2178	16
157	[IM1,3OH][N(CF3SO2)2]	2.1871	2.6066	16
158	[IM][TFO]	2.1900	2.4178	23
159	[IM1,2O2O1][BF4]	2.2147	2.5379	16
160	[IM1,2O2O2O1][N(CN)2]	2.3098	2.7530	16
161	[IM1,4][N(CN)2]	2.3300	2.5718	23
162	[IM][Ace]	2.3900	2.1661	23
164	[IM1,4]I	2.4100	2.6961	23

166	[IM1,2][B(CN)4]	2.4400	2.4714	23
168	[IM1,4][pToS]	2.4800	2.3731	16
169	[IM1,4][N(CF3)2]	2.5300	2.8496	23
171	[IM4][Ace]	2.6800	2.7231	16
172	[IM4][TFA]	2.7200	2.8585	23
173	[IM1,3O1][N(CF3SO2)2]	2.7959	2.7335	16
175	[IM1,6][BF4]	2.8200	3.5582	22
176	[IM1,5][BF4]	2.8600	3.1431	22
177	[IM1,2][Sal]	2.8684	2.5077	16
178	[IM1,2][(C2F5)2PO2]	2.9500	3.0601	23
179	[IM1,2O1][N(CF3SO2)2]	3.0000	2.6336	23
180	[IM1,1O2][N(CF3SO2)2]	3.0000	2.6363	16
181	[IM1,2][B(2-OPhO)2]	3.0200	2.7659	23
182	[IM1,2O2][N(CF3SO2)2]	3.0400	2.7383	23
183	[IM1,4]Cl	3.0500	2.7968	22
184	[IM1][For]	3.1700	2.5406	23
185	[IM1,2O1][N(CF3SO2)2]	3.1739	2.6336	16
186	[IM2,4][BF4]	3.2000	2.6143	22
189	[IM1,2O2O2O2O1][N(CN)2]	3.3468	2.9882	16
191	[IM1,7][BF4]	3.5600	3.9700	22
192	[IM][CAP]	3.7100	3.0928	23
193	[IM1,2O2O1]Cl	3.7358	2.6433	16
194	[IM2,6][BF4]	3.8500	3.5276	22
195	[IM1][Cap]	3.8700	3.3071	23
200	[IM1,1,6]Cl	4.2600	3.5660	22
202	[IM1,4][FeCl4]	4.4900	3.0387	23
203	[IM1,8][BF4]	4.5900	4.3745	22
204	[IM1,18]Cl	4.6500	5.5458	23
206	[IM1,10COO2]Br	4.9222	4.5520	16
209	[IM1,9][BF4]	5.2800	4.7722	22
211	[IM1,16]Cl	5.7700	5.5094	23
214	[IM1,10][BF4]	6.1800	5.1632	22
215	[IM1,10][FeCl4]	6.4300	5.5105	23
216	[Melanime][TfO]	3.5500	3.4184	16
218	[Melanime][TFA]	3.7600	3.3022	16
219	[MOR1,4][CF3SO3]	1.6000	1.9222	16
220	[MOR1,8]Br	3.6000	3.1829	20
221	[MOR1,4]Br	0.5500	1.6120	16
222	[MOR1,4][N(CN)2]	1.1100	1.6350	16
224	[MOR1,6]Br	2.0500	2.3629	20
225	[MOR1,1O2][N(CF3SO2)2]	2.6200	3.1924	23
226	[MOR1,1(CH)OH1OH][Br]	2.7700	2.0582	20
227	[MOR1,4][N(CF3SO2)2]	3.5086	2.3031	16

229	[P2,4,4,4][(CH3CH2)2PO4]	2.9300	3.1319	23
230	[TROP8][N(CN)2]	3.4800	3.4328	16
231	[P6,6,6,14][P(C2F5)3F3]	4.3000	4.7259	23
232	[PIP2,8][BPh4]	3.2277	4.2060	35
233	[PIP2,8]Br	3.4522	3.7811	35
234	[PIP1,8]Br	3.5346	3.9461	35
235	[PIP2,8]I	3.5376	3.9284	35
237	[PIP1,6]Br]	3.0600	3.1110	16
238	[PIP1,4]Br	3.6271	2.3430	35
240	[PIP1,3][N(CF3SO2)2]	2.9900	2.9159	17
241	[PYD3OH][N(CF3SO2)2]	1.9900	2.4969	23
242	[PYD4]Br]	2.2800	2.5468	16
245	[PYD1,4][BF4]	2.9800	3.1636	23
246	[PYD4][Al2Cl7]	2.9900	3.3086	23
247	[PYD1,1,4]Br]	3.0700	3.5621	16
249	[PYD1,1,4][CF3SO3]	3.1600	3.8724	16
251	[PYD1,1,4]Br	3.3111	3.4838	16
252	[PYD1,4][N(CN)2]	3.3437	3.0440	16
253	[PYD4,N(CH3)2]Cl	3.4800	3.1217	23
255	[PYD1,1,4][N(CN2)2]	3.6181	3.5068	16
257	[PYD8]Br	4.1100	4.1648	16
258	[PYD1,1,4][N(CF3SO2)2]	4.1439	4.1562	16
260	[PYD1,1,1,4][N(CF3SO2)2]	4.4377	4.6753	16
262	[PYD1,6]Cl	4.5600	3.2685	22
263	[PYD6,N(CH3)2][N(CF3SO2)2]	4.6200	4.1850	23
265	[PYD1,1,8]Br	4.8761	5.0359	16
266	[PYD1,1,8][BF4]	5.0300	5.1784	16
269	[PYD1,1,1,8][N(CF3SO2)2]	5.3768	5.4746	16
270	[PYD1,2,8]Br	5.4100	4.9790	16
271	[PYD1,1,8][N(CF3SO2)2]	5.6400	5.5323	23
272	[PYD1,8]Br	5.7500	4.6028	22
273	[PYR1,8][N(CF3SO2)2]	3.3206	4.4541	35
274	[TROP8][N(CF3SO2)2]	3.8300	3.7995	16
275	[PYR1,4][CF3SO3]	3.5361	2.4152	35
276	[PYR1,8]Br	3.5560	3.8887	35
277	[Pyr1,6]Br]	2.8100	3.0343	16
278	[PYR1,8]Cl	3.6308	4.1366	35
279	[PYR1,4][N(CN)2]	3.6819	2.2697	35
280	[PYR4,3CN]Br	0.6700	1.4445	16
282	[PYR4]Cl	1.7000	2.5652	26
287	[PYR4][N(CF3SO2)2]	3.4600	3.0179	26
289	[PYR1,4][P(C2F5)3F3]	4.3000	3.0153	23
292	[QUINU4]Br	1.5500	1.0683	16

293	[S2,2,2][N(CF3SO2)2]	2.7400	3.3762	23
294	[TMG][TfO]	2.4800	3.3835	23
295	[TMG][Ace]	2.8300	3.1318	23
296	[TMG][Cap]	3.7100	4.0585	23
297	[TMG][TFA]	5.5300	3.2672	23
299	[TROP4]I	1.2600	1.9499	16
301	[TROP4][N(CF3SO2)2]	3.3900	2.3682	16
302	[IM1,1,4]Br	2.7477	2.3882	36
Test set chemicals				
2	[IM1,2][N(CF3SO2)2]	3.4310	2.9944	29
4	[IM1,4][PF6]	2.9301	2.9901	29
7	[TMGC4]I	4.0649	3.5502	31
9	[TMGC12]I	4.5702	5.2516	31
17	[P1,(4,4,4)i][CH3SO4]	3.1457	2.5415	31
20	[IM1,4][CH3SO3]	2.4147	2.8239	31
29	[N1,1,1,2OH][DHPhosp]	3.3315	2.6959	34
32	[N1,1,Bn,2OH]Cl	2.5296	3.0187	34
33	[N1,1,1,2OH][Prop]	3.1383	2.7097	34
34	[N1,1,1,2OH][But]	2.7873	2.8597	34
36	[P4,4,4,6][N(CF3SO2)2]	5.0390	3.9573	24
38	[N4,4,4,4][PF6]	3.5371	3.3571	24
39	[P4,4,4,6][PF6]	4.0071	4.0059	24
46	[PYR1,4][N(CF3SO2)2]	2.9961	2.9467	25
48	[PIP1,4][N(CF3SO2)2]	3.1515	3.0403	25
51	[IM1,2][HEPES]	1.7839	2.3040	28
56	[N1,1,1,1][HEPES]	1.3131	2.6052	28
57	[N1,1,1,1][MES]	2.4135	2.4740	28
63	[N4,4,4,4][CHES]	3.3974	3.6488	28
65	[N4,4,4,4][MES]	2.8995	2.9108	28
74	[N1,1,11,2OH][Br]	5.6210	4.0805	27
77	[N3,2OH,2OH][Br]	2.7900	2.0533	27
82	[N2OH,2OH,2OH,CH2CHCH2]Br	2.0299	2.2546	27
88	[N1,2OH,2OH,12,N1,2OH,2OH][2Br]	3.7625	4.2057	27
90	[N2OH,2OH,2OH,8,N2OH,2OH,2OH][2Br]	4.9130	3.2803	27
95	[PYD1(PhOOCH2)(COOC4H9)]Br	3.6664	2.9036	33
97	[PYD1(Ph-3,4-(OCH3)2)(COOCH3)]Cl	3.5860	3.3149	33
99	[PYDCH2COOCH(COOC4H9)(PhOOCH2)]Br	4.3130	3.2621	33
100	[IM1,CH2COOCH(COOC4H9)(PhOOCH2)]Br	4.2434	3.2739	33
102	[DABCO4]Br	1.1500	1.8527	20
103	[DABCO6]Br	2.3000	2.6671	20
109	[2-HEA][For]	2.1844	2.3941	16
112	[2-HDEA][But]	2.3820	2.2991	16

115	[2-HTEA][But]	2.6757	2.6137	16
118	[2-HTEA][Pe]	2.7352	2.7715	16
132	[N1,1,1,2OH][N(CF3SO2)2]	1.8500	3.2222	23
138	[IM1][TFO]	1.6500	2.6321	23
141	[IM1,2O2]Cl	1.7200	2.2856	16
145	[IM1][Ace]	1.9300	2.3805	23
149	[IM1,2][C2H5SO4]	1.9800	1.9982	22
150	[IM1,1O2]Cl	1.9900	2.1835	16
151	[IM1,1O2][N(CN)2]	2.0088	1.9586	16
154	[IM1,2OH]I	2.1135	1.9291	16
155	[IM1,2O2O1][N(CN)2]	2.1249	2.4184	16
163	[TROP8][BF4]	3.2300	3.5523	16
165	[IM1][TFA]	2.4300	2.5159	23
167	[IM1,4][BF4]	2.4500	2.6914	22
170	[IM1,2O2O2O1][BF4]	2.5528	2.8725	16
174	[IM4][For]	2.8100	2.7141	16
187	[IM4][TFO]	3.2300	2.9747	16
188	[IM1,6][N(2-SO2PhCO)]	3.3300	3.2701	23
190	[IM1,6][P(C2F5)3F3]	3.3500	4.1058	23
196	[IM1,6][N(CF3SO2)2]	3.9500	4.0785	23
197	[IM4][Cap]	4.0000	3.6497	16
198	[IM1,6]Cl	4.0600	3.6636	22
199	[IM1,4][8OSO3]	4.1700	3.2350	23
201	[IM1,2][FeCl4]	4.4900	2.7739	23
205	[IM1,8]Cl	4.8100	4.4799	22
207	[IM1,8][N(CF3SO2)2]	5.1700	4.8070	23
208	[IM16]Br	5.1900	3.4156	22
210	[IM1,10]Cl	5.5000	5.2686	22
212	[IM1,8]Br	5.9300	4.2320	22
213	[IM1,14]Cl	6.1500	5.4510	23
217	[Melanime][Ace]	3.6100	3.1668	16
223	[MOR1,2]Br	0.8000	1.3079	20
228	[MOR1,10]Br	4.6500	3.9548	20
236	[PIP2,8][SCN]	3.5467	3.8717	35
239	[PIP2,4]Br]	2.0400	2.1289	16
243	[PYD4][N(CN)2]	2.7000	2.5698	23
244	[PYD4]Cl	2.7645	2.7947	16
248	[PYD6]Br	3.1500	3.3270	16
250	[PYD1,4]Br	3.2464	3.0211	16
254	[PYD1,1,1,4]Br	3.5214	4.0469	16
256	[PYD1,1,4][SCN]	3.7500	3.5744	16
259	[PYD4,N(CH3)2][N(CF3SO2)2]	4.1549	3.4990	16
261	[PYD1,6]Br	4.5200	3.7796	22

264	[PYD-16]Cl	4.7212	5.4878	16
267	[PYD-16][Sal]	5.0857	5.4438	16
268	[PYD1,1,1,8]Br	5.3585	5.0221	16
281	[PYR1,4]Br	1.6000	2.2467	16
283	[PYR1,3OH][N(CF3SO2)2]	2.0900	2.2013	23
284	[PYR1,1COO2][N(CF3SO2)2]	2.7700	2.4873	23
285	[PYR1,6]Cl	3.0100	3.2822	22
286	[PYR1,2O2][N(CF3SO2)2]	3.0300	2.2309	23
288	[PYR1,6][N(CF3SO2)2]	3.6000	3.6876	23
290	[QUINU8]Br	3.4949	2.7025	35
291	[QUINU8][N(CN)2]	3.5143	2.7255	35
298	[TROP4]Br	0.6400	1.8026	16
300	[TROP4][SCN]	1.9300	1.8932	16
303	[IM1,1,6]Br	2.9350	3.3180	36
304	[IM1,1,8]Br	4.2423	4.1862	36
305	[IM1,2]Br	1.7312	2.2841	36