Supporting Information

A solvent selection strategy on hydrogenation reaction inside tubular-flow reactor through statistic approach

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Table S1. Detail of nitrobenzene hydrogenation reaction

Solvents	Substrate		Products										Material balance (%)	Retention time (s)	k_0 (s^{-1})	Remarks
	NB, t_R ~ 3.80 min		PHA, t_R ~ 2.80 min		AN, t_R ~ 3.10 min		HAB, t_R ~ 4.05 min.		NSB, t_R ~ 4.16 min.		AXB, t_R ~ 6.30 min.					
	Initial (mM)	Conv. (%)	Yield (%)	Selectivity (%)	Yield (%)	Selectivity (%)	Yield (%)	Selectivity (%)	Yield (%)	Selectivity (%)	Yield (%)	Selectivity (%)				
MeOH	50	55.97	3.08	5.50	46.09	82.35	0.00	0.00	0.90	1.61	0.00	0.01	94.11	172	0.00477	Statistical analysis
	50	56.59	3.87	6.83	42.29	74.73	0.00	0.00	1.97	3.47	0.04	0.08	91.62	227	0.00368	
	50	46.38	3.10	6.69	36.39	78.46	0.00	0.00	1.52	3.28	0.00	0.00	94.64	170	0.00367	
EtOH	50	38.01	3.01	7.91	25.74	67.72	0.00	0.00	8.05	21.17	0.24	0.64	99.26	137	0.00349	Statistical analysis
	50	42.54	3.84	9.04	32.99	77.55	0.00	0.00	16.00	37.61	0.02	0.05	110.34	131	0.00423	
	50	41.42	3.94	9.52	32.11	77.53	0.00	0.00	14.16	34.18	0.07	0.17	108.93	122	0.00438	
n-PrOH	50	62.08	4.06	6.53	54.94	88.49	0.00	0.00	1.01	1.63	0.01	0.02	97.94	170	0.00570	Statistical analysis
	50	64.64	3.79	5.86	56.38	87.23	0.00	0.00	0.74	1.15	0.01	0.01	96.30	171	0.00608	
	50	64.69	4.11	6.36	56.74	87.71	0.00	0.00	0.78	1.21	0.01	0.01	96.96	170	0.00612	
i-PrOH	50	47.59	2.42	5.10	34.23	71.93	0.00	0.00	2.58	5.42	1.10	2.32	93.85	189	0.00342	Statistical analysis
	50	28.83	4.96	17.20	18.66	64.72	0.00	0.00	1.94	6.72	0.09	0.32	96.91	263	0.00129	
	50	31.72	5.22	16.47	22.18	69.92	0.00	0.00	1.09	3.44	0.06	0.19	96.90	263	0.00145	
	50	99.50	0.33	0.33	91.99	92.46	0.00	0.00	0.37	0.37	0.01	0.01	93.22	*N/A*	*N/A*	5 min data collection
	50	58.50	0.00	0.00	55.55	94.96	0.00	0.00	0.28	0.48	0.42	0.72	98.17	*N/A*	*N/A*	5 min data collection
n-BuOH	50	33.32	4.22	12.68	25.21	75.69	0.00	0.00	0.34	1.03	0.01	0.03	96.48	105	0.00386	Statistical analysis
	50	30.87	5.35	17.33	21.84	70.74	0.00	0.00	0.65	2.10	0.11	0.35	97.18	105	0.00352	
	50	25.36	4.82	18.99	18.54	73.11	0.00	0.00	0.63	2.49	0.03	0.14	98.70	105	0.00279	
tert-BuOH	50	24.99	4.86	19.43	14.75	59.01	0.00	0.00	0.67	2.67	0.01	0.02	95.29	147	0.00196	Statistical analysis
	50	33.04	7.12	21.54	23.64	71.55	0.00	0.00	0.78	2.37	0.01	0.03	98.52	146	0.00275	
	50	44.36	7.25	16.35	35.00	78.90	0.00	0.00	1.84	4.16	0.01	0.02	99.75	144	0.00407	
Acetone	50	17.07	0.00	0.00	3.17	18.57	0.00	0.00	0.30	1.77	0.03	0.20	86.47	199	0.00094	Statistical analysis
AN	50	23.99	2.45	10.21	12.64	52.69	0.00	0.00	1.05	4.38	0.03	0.13	92.21	251	0.00109	Statistical analysis
AcOEt	50	2.87	0.38	13.38	3.80	132.12	0.00	0.00	0.14	4.92	0.00	0.00	101.45	176	0.00017	Statistical analysis
DMSO	50	8.03	0.08	1.01	0.04	0.46	0.00	0.00	0.06	0.77	0.00	0.00	92.15	291	0.00029	Statistical analysis
Dioxane	50	16.27	0.03	0.20	0.28	1.69	0.00	0.00	0.00	0.00	0.00	0.00	84.04	312	0.00057	Statistical analysis
n-hexane	50	12.04	0.00	0.00	0.49	4.10	0.00	0.00	0.00	0.00	0.00	0.00	88.46	284	0.00045	Statistical analysis
THF	50	15.37	0.02	0.13	0.13	0.87	0.00	0.00	0.00	0.00	0.00	0.00	84.78	329	0.00051	Statistical analysis
Toluene	50	9.47	0.04	0.46	0.89	9.38	0.00	0.00	0.00	0.00	0.19	1.97	91.83	246	0.00040	Statistical analysis
CH_2Cl_2	50	12.37	0.02	0.16	0.28	2.22	0.00	0.00	0.00	0.00	0.01	0.05	87.94	299	0.00044	Statistical analysis
$CHCl_3$	50	20.98	0.01	0.07	0.29	1.37	0.00	0.00	0.24	1.12	0.00	0.00	79.56	291	0.00081	Statistical analysis
CCl_4	50	16.80	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.21	7.20	85.62	326	0.00056	Statistical analysis
2,2,2-trifluoroethanol	50	71.89	0.30	0.42	61.41	85.42	0.00	0.00	20.81	28.94	0.07	0.10	110.78	300	0.00423	Validation

NB: nitrobenzene
PHA: *N*-phenylhydroxylamine
AN: aniline
HAB: hydrazobenzene
NSB: nitrosobenzene
AXB: azoxybenzene

Conversion of nitrobenzene (%) = {Concentration of reacted nitrobenzene (mM) / Concentration of initial nitrobenzene (mM)} × 100 %
Yield of product (%) = {Concentration of product (mM) / Concentration of initial nitrobenzene (mM)} × 100 %
Selectivity of product (%) = {Concentration of product (mM) / Concentration of reacted nitrobenzene (mM)} × 100 %
Material balance (%) = Remaining nitrobenzene (%) + Yield of *N*-phenylhydroxylamine (%) + Yield of aniline (%) + (2 × Yield of Hydrazobenzene) + Yield of nitrosobenzene + (2 × Yield of Azoxybenzene)
$\boldsymbol{k_0}$ (s^{-1}) = [– ln {1 – (Concentration of reacted nitrobenzene (mM) / Concentration of initial nitrobenzene (mM))}] / retention time (s)

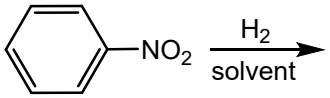

Table S2. List of abbreviations

Abbreviation	Parameter
ACNTRC	Acentric factor
AQUEOS	Aqueous solibility (log S_w)
BOILPT	Normal boiling point (K)
BPP40C	Boiling point pressure at 313 K (kPa)
CATASA	Catalán's acidity parameter
CATASB	Catalán's basicity parameter
CATASP	Catalán's polarizability parameter
COHESI	Hildebrand cohesion energy density
COMBUS	Heat of combustion ($J \cdot mol^{-1}$)
CRITCP	Critical pressure (kPa)
CRITCT	Critical temperature (K)
CRITCV	Critical volume ($m^3 \cdot kmol^{-1}$)
CRITIC	Critical compressibility factor
DIELEC	Dielectric constant
DIMREN	Dimroth and Reichardt's hydrogen donor donation (normalization)
DIMRET	Dimroth and Reichardt's hydrogen donor donation
DIPOLE	Dipole moment (Deybe)
DNSITY	Density ($g \cdot mL^{-1}$)
ENTFOR	Enthalphy of formation ($J \cdot mol^{-1}$)
GIBENR	Gibbs energy of formation ($J \cdot mol^{-1}$)
GUTACN	Gutmann's acceptor number
GUTDNN	Gutmann's donor number
HEATEV	Heat evaporation
HEATVA	Lower heating value ($J \cdot mol^{-1}$)
HETFUS	Heat of fusion ($J \cdot mol^{-1}$)
HILDEX	Hildebrand's solubility parameter (shodex)
HILTHO	Hildebrand's solubility parameter
HISOLU	Hydrogen solubility ($\cdot 10^{-4}$)
HSNDIS	Hansen's dispersion parameter
HSNHYB	Hansen's hydrogen bonding parameter

Table S2. List of abbreviations (continue)

Abbreviation	Parameter
HSNMOL	Hansen's molar volume
HSNPOL	Hansen's polarizability parameter
HYDDEF	Hydrogen deficiency number
KAMALP	Taft's hydrogen bond donation parameter
KAMBET	Taft's hydrogen bond acceptor parameter
KAMPHI	Taft's polarizability parameter
KIRDIE	Kirkwood function on dielectric constant
KIRREF	Kirkwood function on reflactive index
LOQMOL	Liquid molar volume ($m^3 \cdot kmol^{-1}$)
MELTPT	Normal melting point (K)
PRACHR	Parachor
PRPENE	PR Peneloux ($m^3 \cdot kmol^{-1}$)
RADGYR	Radius of gyration (mm)
REFRAC	Refractive index
SOLPAR	Solubility parameter $[(cal \cdot cc)^{0.5}]$
SOLTAN	Solvent's solubility in *n*-octane (log *P*)
SOLWAT	Solvent's solubility in H_2O (%w/w)
SRPENE	SRK Peneloux ($m^3 \cdot kmol^{-1}$)
SWAIAC	Swain's acidity parameter
SWAIBS	Swain's- basicity parameter
TNSION	Surface tension ($N \cdot m^{-1}$)
TRIPRS	Triple point pressure (kPa)
TRITEM	Triple point temperature (K)
UNIFAQ	UNIFAC Q
UNIFAR	UNIFAC R
VISCOS	Viscosity (*cP*)
WEIGHT	Molecular weight ($g \cdot mol^{-1}$)

Table S3. Solvent's properties database from simulation with Aveva Pro II software

Solvents	Parameters	
	BOILPT	**HEATEV**
MeOH	337.9	35.27
EtOH	351.4	38.65
n-PrOH	370.4	41.65
i-PrOH	355.4	39.38
n-BuOH	390.8	43.18
tert-BuOH	355.6	39.04
Acetone	329.4	29.57
Acetonitrile	354.8	30.21
AcOEt	350.2	32.23
DMSO	464.0	43.87
Dioxane	374.5	34.37
n-hexane	341.9	28.79
THF	339.1	29.86
Toluene	383.8	33.51
CH_2Cl_2	312.9	28.38
$CHCl_3$	334.3	29.51
CCl_4	349.8	29.77

Table S4. Solvent's properties database from literatures

Solvents	Parameters				
	AQUEOS[1]	**DIELEC[2]**	**DIPOLE[3-4]**	**HISOLU[5]**	**REFRAC[10]**
MeOH	1.49	32.60	2.87	7.90[6]	1.3284
EtOH	1.34	24.60	1.69	2.06	1.3614
n-PrOH	1.22	20.10	3.09	2.31	1.3856
i-PrOH	1.22	18.30	1.66	2.66	1.3772
n-BuOH	0.00	17.80	1.66	2.69[7]	1.3993
tert-BuOH	1.13	12.50	1.70	3.00	1.3877
Acetone	1.24	21.01	2.69	2.87[8]	1.3586
Acetonitrile	0.26	36.64	3.44	1.78[8]	1.3441
AcOEt	-0.04	6.00	1.88	3.46	1.3724
DMSO	1.11	47.00	4.10	0.76	1.4793
Dioxane	1.05	2.21	0.45	1.76	1.4224
n-hexane	-3.84	1.89	0.00	0.01[8]	1.3749
THF	1.15	7.52	1.75	0.01[8]	1.4072
Toluene	-2.21	2.38	0.31	3.15	1.4969
CH_2Cl_2	-0.63	9.08	1.14	1.78[9]	1.4241
$CHCl_3$	-1.17	4.81	1.15	0.25[9]	1.4458
CCl_4	-2.31	2.24	0.00	0.04[9]	1.4601

Table S4. Solvent's properties database from literatures (continue)

Solvents	Parameters			
	SOLTAN[11]	**SOLWAT[12-13]**	**TNSION[14]**	**VISCOS[15]**
MeOH	-0.82	100	0.023	0.59
EtOH	-0.32	100	0.022	1.10
n-PrOH	0.34	100	0.023	2.30
i-PrOH	0.26	100	0.022	2.40
n-BuOH	2.34	0.43	0.025	2.98
tert-BuOH	0.40	100	0.021	3.38
Acetone	-0.24	100	0.024	0.36
Acetonitrile	-0.34	100	0.029	0.38
AcOEt	0.73	8.70	0.024	0.45
DMSO	-1.35	100	0.043	2.24
Dioxane	-0.42	100	0.033	1.37
n-hexane	3.80	0.00	0.018	0.31
THF	0.46	100	0.027	0.55
Toluene	2.69	0.05	0.028	0.59
CH_2Cl_2	1.25	1.60	0.028	0.44
$CHCl_3$	1.97	0.82	0.027	0.57
CCl_4	2.64	0.08	0.027	0.97

Table S5. Hildebrand's cohesion energy density parameter of solvents

Solvents	Parameters			
	HEATEV[16]	***T* (K)**[16]	**HSNMOL**[17]	**COHESI**
MeOH	36.7	313	40.7	0.84
EtOH	42.2	313	58.5	0.68
n-PrOH	46.4	313	75.2	0.58
i-PrOH	44.8	315	76.8	0.55
n-BuOH	53	310	91.5	0.55
tert-BuOH	44.9	313	95.8	0.44
Acetone	30.7	313	74.0	0.38
Acetonitrile	34.8	315	52.6	0.61
AcOEt	34.6	313	98.5	0.32
DMSO	52.1	318	71.3	0.69
Dioxane	37	318	85.7	0.40
n-hexane	30.7	313	131.6	0.21
THF	31.9	311	81.7	0.36
Toluene	37.3	318	106.8	0.32
CH_2Cl_2	29.2	308	63.9	0.42
$CHCl_3$	30.8	321	80.7	0.35
CCl_4	32.3	308	97.1	0.31

Hildebrand's cohesion energy density (**COHESI**), kJ · mol^{-1} = (BPP40C – R*T*) / **BOILPT**

R : molar gas constant, 8.314 J · mol^{-1} · K^{-1}

Table S6. Kirkwood function on dielectric constant and refractive index

Solvents	Parameters	
	KIRDIE	**KIRREF**
MeOH	0.477	0.203
EtOH	0.470	0.221
n-PrOH	0.464	0.235
i-PrOH	0.460	0.230
n-BuOH	0.459	0.242
tert-BuOH	0.442	0.236
Acetone	0.465	0.220
Acetonitrile	0.480	0.212
AcOEt	0.385	0.227
DMSO	0.484	0.284
Dioxane	0.223	0.254
n-hexane	0.186	0.229
THF	0.406	0.246
Toluene	0.240	0.293
CH_2Cl_2	0.422	0.255
$CHCl_3$	0.359	0.267
CCl_4	0.226	0.274

KIRDIE[5] = (**DIELEC** – 1) / (2 × **DIELEC** + 1)

KIRREF[5] = (**REFRAC**^2 – 1) / (**REFRAC**^2 + 2)

Table S7. Solvent parameters on Linear Solvation Energy Relationship (LSER) based on Abraham-About-Kamlet-Talf model[18]

Solvents	Abraham-Abbout-Kamlet-Talf				
	KAMALP	**KAMBET**	**KAMPHI**	**CORPOL[19-20]**	**COHESI**
MeOH	0.93	0.62	0.60	0.00	0.84
EtOH	0.83	0.77	0.54	0.00	0.68
n-PrOH	0.84	0.90	0.52	0.00	0.58
i-PrOH	0.76	0.84	0.48	0.00	0.55
n-BuOH	0.84	0.84	0.47	0.00	0.55
tert-BuOH	0.42	0.93	0.41	0.00	0.44
Acetone	0.08	0.48	0.40	0.00	0.38
Acetonitrile	0.19	0.40	0.75	0.00	0.61
AcOEt	0.00	0.45	0.55	0.00	0.32
DMSO	0.00	0.76	0.40	0.00	0.69
Dioxane	0.00	0.37	0.55	0.00	0.40
n-hexane	0.00	0.00	-0.04	0.00	0.21
THF	0.00	0.55	0.58	0.00	0.36
Toluene	0.00	0.11	0.54	1.00	0.32
CH_2Cl_2	0.13	0.10	0.82	0.50	0.42
$CHCl_3$	0.20	0.10	0.58	0.50	0.35
CCl_4	0.00	0.10	0.28	0.50	0.31

Correction on polarizability (**CORPOR**)

Table S8. Solvent parameters on LSER based on Catalán model[21]

Solvents	Catalán		
	CATASA	**CATASB**	**CATASP**
MeOH	0.86	0.55	0.61
EtOH	0.85	0.66	0.40
n-PrOH	0.85	0.78	0.37
i-PrOH	0.85	0.83	0.28
n-BuOH	0.84	0.81	0.34
tert-BuOH	0.83	0.93	0.15
Acetone	0.88	0.48	0.00
Acetonitrile	0.90	0.29	0.04
AcOEt	0.80	0.54	0.00
DMSO	1.00	0.65	0.07
Dioxane	0.70	0.44	0.00
n-hexane	0.52	0.06	0.00
THF	0.84	0.59	0.00
Toluene	0.66	0.13	0.00
CH_2Cl_2	0.88	0.18	0.04
$CHCl_3$	0.79	0.07	0.05
CCl_4	0.63	0.04	0.00

Table S9. Solvent parameters on LSER based on Gutmann model[22]

Solvents	Gutmann	
	GUTACN	**GUTDNN**
MeOH	41.50	19.00
EtOH	37.90	19.20
n-PrOH	37.30	19.80
i-PrOH	33.50	21.10
n-BuOH	36.80	19.50
tert-BuOH	27.10	38.00
Acetone	12.50	17.00
Acetonitrile	18.90	14.10
AcOEt	9.30	17.10
DMSO	19.30	29.80
Dioxane	10.30	14.30
n-hexane	0.00	0.00
THF	8.00	20.00
Toluene	0.00	0.10
CH_2Cl_2	20.40	1.00
$CHCl_3$	23.10	4.00
CCl_4	8.60	0.00

Table S10. Solvent parameters on LSER based on Hansen model[17]

Solvents	Hansen			
	HSNDIS	**HSNHYB**	**HSNMOL**	**HSNPOL**
MeOH	15.10	22.30	40.70	12.30
EtOH	15.80	19.40	58.50	8.80
n-PrOH	16.00	17.40	75.20	6.80
i-PrOH	15.80	16.40	76.80	6.10
n-BuOH	16.00	15.80	91.50	5.70
tert-BuOH	15.20	14.70	95.80	5.10
Acetone	15.50	7.00	74.00	10.40
Acetonitrile	15.30	6.10	52.60	18.00
AcOEt	15.80	7.20	98.50	5.30
DMSO	18.40	10.20	71.30	16.40
Dioxane	19.00	7.40	85.70	1.80
n-hexane	14.90	0.00	131.60	0.00
THF	16.80	8.00	81.70	5.70
Toluene	18.00	2.00	106.80	1.40
CH_2Cl_2	18.20	6.10	63.90	6.30
$CHCl_3$	17.80	5.70	80.70	3.10
CCl_4	17.80	0.60	97.10	0.00

Table S11. Solvent parameters on LSER based on Koppel–Palm (KP) model

Solvents	Koppel-Palm				
	KIRDIE[5]	**KIRREF[5]**	**COHESI**	**SWAIBS[23]**	**DIMRET[24]**
MeOH	0.48	0.20	0.84	0.50	0.76
EtOH	0.47	0.22	0.68	0.45	0.65
n-PrOH	0.46	0.23	0.58	0.44	0.62
i-PrOH	0.46	0.23	0.55	0.44	0.57
n-BuOH	0.46	0.24	0.55	0.43	0.60
tert-BuOH	0.44	0.24	0.44	0.50	0.40
Acetone	0.47	0.22	0.38	0.81	0.57
Acetonitrile	0.48	0.21	0.61	0.86	0.46
AcOEt	0.38	0.23	0.32	0.59	0.23
DMSO	0.48	0.28	0.69	1.08	0.44
Dioxane	0.22	0.25	0.40	0.67	0.16
n-hexane	0.19	0.23	0.21	-0.01	0.01
THF	0.41	0.25	0.36	0.67	0.21
Toluene	0.24	0.29	0.32	0.54	0.10
CH_2Cl_2	0.42	0.26	0.42	0.80	0.31
$CHCl_3$	0.36	0.27	0.35	0.73	0.26
CCl_4	0.23	0.27	0.31	0.34	0.05

Table S12. Solvent parameters on LSER based on Swain model[23]

Solvents	Swain	
	SWAIAC	SWAIBS
MeOH	0.75	0.50
EtOH	0.66	0.45
n-PrOH	0.63	0.44
i-PrOH	0.59	0.44
n-BuOH	0.61	0.43
tert-BuOH	0.45	0.50
Acetone	0.25	0.81
Acetonitrile	0.37	0.86
AcOEt	0.21	0.59
DMSO	0.34	1.08
Dioxane	0.19	0.67
n-hexane	0.01	-0.01
THF	0.17	0.67
Toluene	0.13	0.54
CH_2Cl_2	0.33	0.80
$CHCl_3$	0.42	0.73
CCl_4	0.09	0.34

Table S13. R^2-values from single regression analysis

R^2-value	ACNTRC	AQUEOS	BOILPT	BPP40C	CATASA	CATASB	CATASP	COHESI	COMBUS	CRITCP
NBCONV	0.626	0.218	0.008	0.059	0.070	0.259	0.784	0.433	0.054	0.223
ANYIEL	0.727	0.233	0.000	0.102	0.094	0.353	0.819	0.474	0.016	0.166
k_0	0.743	0.217	0.000	0.100	0.081	0.363	0.865	0.448	0.017	0.169

R^2-value	CRITCT	CRITCV	CRITIC	DIELEC	DIMREN	DIMRET	DIPOLE	DNSITY	ENTFOR	GIBENR
NBCONV	0.106	0.259	0.025	0.126	0.566	0.586	0.110	0.106	0.030	0.060
ANYIEL	0.080	0.203	0.052	0.165	0.607	0.685	0.172	0.196	0.070	0.104
k_0	0.078	0.180	0.018	0.132	0.626	0.674	0.120	0.161	0.078	0.108

R^2-value	GUTACN	GUTDNN	HEATEV	HEATVA	HETFUS	HILDEX	HILTHO	HISOLU	HSNDIS	HSNHYB
NBCONV	0.706	0.100	0.243	0.052	0.260	0.063	0.276	0.237	0.192	0.654
ANYIEL	0.693	0.151	0.337	0.015	0.206	0.093	0.267	0.345	0.260	0.711
k_0	0.757	0.142	0.379	0.015	0.204	0.144	0.315	0.286	0.223	0.741

Table S13. R^2-value from single-regression analysis (continue)

R^2-value	HSNMOL	HSNPOL	HYDDEF	KAMALP	KAMBET	KAMPHI	KIRDIE	KIRREF	LOQMOL	MELTPT
NBCONV	0.237	0.044	0.232	**0.841**	0.354	0.020	0.229	0.250	0.240	0.131
ANYIEL	0.197	0.071	0.255	**0.852**	0.444	0.021	0.282	0.286	0.199	0.152
k_0	0.171	0.040	0.278	**0.925**	0.457	0.011	0.265	0.237	0.173	0.157

R^2-value	PRACHR	PRPENE	RADGYR	REFRAC	SOLPAR	SOLTAN	SOLWAT	SRPENE	SWAIAC	SWAIBS
NBCONV	0.193	0.403	0.253	0.249	0.436	0.082	0.202	0.047	0.709	0.082
ANYIEL	0.205	0.426	0.224	0.284	0.478	0.094	0.175	0.053	0.717	0.081
k_0	0.170	0.468	0.181	0.236	0.457	0.059	0.135	0.067	0.760	0.102

R^2-value	TNSION	TRIPRS	TRITEM	UNIFAQ	UNIFAR	VISCOS	WEIGHT
NBCONV	0.164	0.004	0.131	0.187	0.233	0.150	0.275
ANYIEL	0.165	0.008	0.151	0.137	0.186	0.179	0.350
k_0	0.172	0.005	0.157	0.112	0.156	0.226	0.294

Note:

Value with a bold-style indicates the best R2-value on each category (**NBCONV**, **ANYIEL**, or k_0)

Table S14. R^2-values of multi regression analysis of k_0 on existing LSER models

No.	LSER model	R^2-value		
		k_0		
		Entire solvents	**Protic solvents**	**Aprotic solvents**
1	AKT	0.929	0.866	0.582
2	AKT w/ polarity cor.	0.929	0.880	0.583
3	AKT w/ polarity and cohesion cor.	0.929	*N/A*	0.590
4	Catalán	0.885	0.749	0.307
5	Gutmann	0.762	0.627	0.168
6	Hansen	0.798	0.647	0.615
7	KP	0.889	0.726	0.441
8	KP w/ cohesion cor.	0.894	*N/A*	0.441
9	Swain	0.883	0.598	0.197

Table S15. *P*-value of each parameter on existing LSER models for entire solvents

No.	LSER model	Entire solvents					
		NBCONV	***P*-value (%)**	**ANYIEL**	***P*-value (%)**	**k_0**	***P*-value (%)**
1	AKT	**KAMALP**	<1	**KAMALP**	<1	**KAMALP**	<1
2	AKT w/ polarity cor.	**KAMALP**	<1	**KAMALP**	<1	**KAMALP**	<1
3	AKT w/ polarity and cohesion cor.	**KAMALP**	<1	**KAMALP**	<1	**KAMALP**	<1
4	Catalán	**CATASP**	<1	**CATASP**	<1	**CATASP**	<1
5	Gutmann	**GUTACN**	<1	**GUTACN**	<1	**GUTACN**	<1
6	Hansen	**HSNHYB**	1.33	**HSNHYB**	<1	**HSNHYB**	<1
7	KP	**DIMRET**	<1	**DIMRET**	<1	**DIMRET**	<1
				SWAIBS	2.28	**SWAIBS**	<1
8	KP w/ cohesion cor.	N/A	N/A	**SWAIBS**	1.65	**DIMRET**	1.16
						SWAIBS	<1
9	Swain	**SWAIAC**	<1	**SWAIAC**	<1	**SWAIAC**	<1
		SWAIBS	1.64	**SWAIBS**	1.47	**SWAIBS**	<1

Table S16. Mathematic equations generating from experimental outputs and some parameters from the existing LSER models

Model	*y*-axis	Mathematic equations
AKT		$y = A_0 + A_1 \cdot$ **(KAMALP)** $+ A_2 \cdot$ **(KAMBET)** $+ A_3 \cdot$ **(KAMPHI)**
	NBCONV	$y = 12.77 + 44.19 \cdot$ **(KAMALP)** $- 2.90 \cdot$ **(KAMBET)** $- 0.77 \cdot$ **(KAMPHI)**
	ANYIEL	$y = -1.47 + 41.95 \cdot$ **(KAMALP)** $+ 3.99 \cdot$ **(KAMBET)** $- 0.50 \cdot$ **(KAMPHI)**
	k_0	$y = 0.47 + 4.53 \cdot$ **(KAMALP)** $+ 0.21 \cdot$ **(KAMBET)** $- 0.49 \cdot$ **(KAMPHI)**
AKT w/ polarizability correction		$y = A_0 + A_1 \cdot$ **(KAMALP)** $+ A_2 \cdot$ **(KAMBET)** $+ A_3 \cdot$ **(KAMPHI)** $+ A_4 \cdot$ **(CORPOL)**
	NBCONV	$y = 13.88 + 44.60 \cdot$ **(KAMALP)** $- 5.59 \cdot$ **(KAMBET)** $+ 0.54 \cdot$ **(KAMPHI)** $- 3.89 \cdot$ **(CORPOL)**
	ANYIEL	$y = -0.53 + 42.30 \cdot$ **(KAMALP)** $+ 1.72 \cdot$ **(KAMBET)** $+ 0.61 \cdot$ **(KAMPHI)** $- 3.29 \cdot$ **(CORPOL)**
	k_0	$y = 0.47 + 4.54 \cdot$ **(KAMALP)** $+ 0.21 \cdot$ **(KAMBET)** $- 0.49 \cdot$ **(KAMPHI)** $- 0.00 \cdot$ **(CORPOL)**
AKT w/ polarizability and cohesion corrections		$y = A_0 + A_1 \cdot$ **(KAMALP)** $+ A_2 \cdot$ **(KAMBET)** $+ A_3 \cdot$ **(KAMPHI)** $+ A_4 \cdot$ **(POLCOR)** $+ A_5 \cdot$ **(COHESI)**
	NBCONV	$y = 14.00 + 54.24 \cdot$ **(KAMALP)** $- 2.55 \cdot$ **(KAMBET)** $- 4.30 \cdot$ **(KAMPHI)** $- 2.34 \cdot$ **(CORPOL)** $+ 1.48 \cdot$ **(COHESI)**
	ANYIEL	$y = -1.27 + 14.37 \cdot$ **(KAMALP)** $- 3.91 \cdot$ **(KAMBET)** $+ 3.04 \cdot$ **(KAMPHI)** $- 4.74 \cdot$ **(CORPOL)** $+ 8.27 \cdot$ **(COHESI)**
	k_0	$y = 0.58 + 3.31 \cdot$ **(KAMALP)** $+ 0.31 \cdot$ **(KAMBET)** $- 0.36 \cdot$ **(KAMPHI)** $- 0.01 \cdot$ **(POLCOR)** $- 0.28 \cdot$ **(COHESI)**

Table S16. Mathematic equations generating from experimental outputs and some parameters from the existing LSER models (continue)

Model	*y*-axis	Mathematic equations
Catalán		$y = C_0 + C_1 \cdot$ **(CATASA)** $+ C_2 \cdot$ **(CATASB)** $+ C_3 \cdot$ **(CATASP)**
	NBCONV	$y = 19.41 - 9.48 \cdot$ **(CATASA)** $+ 3.79 \cdot$ **(CATASB)** $+ 79.38 \cdot$ **(CATASP)**
	ANYIEL	$y = 6.24 - 11.25 \cdot$ **(CATASA)** $+ 10.75 \cdot$ **(CATASB)** $+ 78.48 \cdot$ **(CATASP)**
	k_0	$y = 1.47 - 1.77 \cdot$ **(CATASA)** $+ 1.16 \cdot$ **(CATASB)** $+ 8.16 \cdot$ **(CATASP)**
Gutmann		$y = G_0 + G_1 \cdot$ **(GUTACN)** $+ G_2 \cdot$ **(GUTDNN)**
	NBCONV	$y = 4.50 + 1.16 \cdot$ **(GUTACN)** $- 0.23 \cdot$ **(GUTDNN)**
	ANYIEL	$y = -8.58 + 1.12 \cdot$ **(GUTACN)** $- 0.07 \cdot$ **(GUTDNN)**
	k_0	$y = -0.49 + 0.12 \cdot$ **(GUTACN)** $- 0.01 \cdot$ **(GUTDNN)**
Hansen		$y = H_0 + H_1 \cdot$ **(HSNDIS)** $+ H_2 \cdot$ **(HSNHYB)** $+ H_3 \cdot$ **(HSNMOL)** $+ H_4 \cdot$ **(HSNPOL)**
	NBCONV	$y = 106.95 - 3.56 \cdot$ **(HSNDIS)** $+ 1.57 \cdot$ **(HSNHYB)** $- 0.35 \cdot$ **(HSNMOL)** $- 1.48 \cdot$ **(HSNPOL)**
	ANYIEL	$y = 68.96 - 3.50 \cdot$ **(HSNDIS)** $+ 1.93 \cdot$ **(HSNHYB)** $- 0.14 \cdot$ **(HSNMOL)** $- 0.77 \cdot$ **(HSNPOL)**
	k_0	$y = 6.01 - 0.28 \cdot$ **(HSNDIS)** $+ 0.21 \cdot$ **(HSNHYB)** $- 0.01 \cdot$ **(HSNMOL)** $- 0.10 \cdot$ **(HSNPOL)**

Table S16. Mathematic equations generating from experimental outputs and some parameters from the existing LSER models (continue)

Model	*y*-axis	Mathematic equations
KP		$y = K_0 + K_1 \cdot$ **(KIRDIE)** $+ K_2 \cdot$ **(KIRREF)** $+ K_3 \cdot$ **(SWAIBS)** $+ K_4 \cdot$ **(DIMRET)**
	NBCONV	$y = 6.17 - 41.91 \cdot$ **(KIRDIE)** $+ 81.58 \cdot$ **(KIRREF) -** $28.76 \cdot$ **(SWAIBS)** $+ 83.93 \cdot$ **(DIMRET)**
	ANYIEL	$y = -11.19 - 8.76 \cdot$ **(KIRDIE)** $+ 78.85 \cdot$ **(KIRREF**$) - 34.53 \cdot$ **(SWAIBS)** $+ 75.92 \cdot$ **(DIMRET)**
	k_0	$y = -2.45 - 1.79 \cdot$ **(KIRDIE)** $+ 15.98 \cdot$ **(KIRREF)** $- 3.90 \cdot$ **(SWAIBS)** $+ 8.66 \cdot$ **(DIMRET)**
KP w/ cohesion correction		$y = K_0 + K_1 \cdot$ **(KIRDIE)** $+ K_2 \cdot$ **(KIRREF)** $+ K_3 \cdot$ **(COHESI)** $+ K_4 \cdot$ **(SWAIBS)** $+ K_5 \cdot$ **(DIMRET)**
	NBCONV	$y = 4.27 - 33.33 \cdot$ **(KIRDIE)** $+ 66.09 \cdot$ **(KIRREF)** $+ 21.64 \cdot$ **(COHESI)** $- 31.16 \cdot$ **(SWAIBS)** $+ 66.62 \cdot$ **(DIMRET)**
	ANYIEL	$y = -13.83 + 3.13 \cdot$ **(KIRDIE)** $+ 57.35 \cdot$ **(KIRREF)** $+ 30.05 \cdot$ **(COHESI)** $- 37.86 \cdot$ **(SWAIBS)** $+ 51.89 \cdot$ **(DIMRET)**
	k_0	$y = -2.58 - 1.21 \cdot$ **(KIRDIE)** $+ 14.92 \cdot$ **(KIRREF)** $+ 1.47 \cdot$ **(COHESI)** $- 4.06 \cdot$ **(SWAIBS)** $+ 7.49 \cdot$ **(DIMRET)**
Swain		$y = S_1 + S_2 \cdot$ **(SWAIAC)** $+ S_3 \cdot$ **(SWAIBS)**
	NBCONV	$y = 13.28 + 66.11 \cdot$ **(SWAIAC)** $- 22.21 \cdot$ **(SWAIBS)**
	ANYIEL	$y = 1.31 + 68.87 \cdot$ **(SWAIAC)** $- 23.01 \cdot$ **(SWAIBS)**
	k_0	$y = 0.61 + 7.12 \cdot$ **(SWAIAC)** $- 2.55 \cdot$ **(SWAIBS)**

Table S17. R^2-values from a combination of acidity and basicity of solvent

Parameter		R^2-score		Parameter		R^2-score	
1	**2**	**NBCONV**	**ANYIEL**	**1**	**2**	**NBCONV**	**ANYIEL**
CATASA	CATASB	0.261	0.356	DIMREN	CATASB	0.566	0.615
CATASA	GUTACN	0.781	0.739	DIMREN	GUTACN	0.707	0.702
CATASA	KAMBET	0.375	0.466	DIMREN	KAMBET	0.568	0.621
CATASA	SWAIBS	0.574	0.666	DIMREN	SWAIBS	0.759	0.805
GUTDNN	CATASB	0.386	0.488	**KAMALP**	**CATASB**	**0.846**	**0.853**
GUTDNN	GUTACN	0.722	0.694	**KAMALP**	**GUTACN**	**0.842**	**0.857**
GUTDNN	KAMBET	0.634	0.704	**KAMALP**	**KAMBET**	**0.842**	**0.855**
GUTDNN	SWAIBS	0.248	0.315	**KAMALP**	**SWAIBS**	**0.841**	**0.852**
HSNHYB	CATASB	0.714	0.732	SWAIAC	CATASB	0.710	0.722
HSNHYB	GUTACN	0.715	0.732	SWAIAC	GUTACN	0.713	0.717
HSNHYB	KAMBET	0.683	0.719	SWAIAC	KAMBET	0.709	0.725
HSNHYB	SWAIBS	0.727	0.783	**SWAIAC**	**SWAIBS**	**0.810**	**0.817**

NB: bold letter indicates top five R^2-score

Table S18. Statistical analysis of KAMALP–CATASB–SOLWAT multiple regression for nitrobenzene conversion

Summary Output

Regression Statistics	
Multiple R	0.95
R Square	0.91
Adjusted R Square	0.89
Standard Error	5.76
Observations	17

ANOVA

	df	**SS**	**MS**	**F**	**Significance F**
Regression	3	4310.9	1437.0	43.3	5.0E-07
Residual	13	431.0	33.2		
Total	16	4741.9			

	Coefficients	**Standard Error**	***t* Stat**	***P*-value**	**Lower 95%**	**Upper 95%**
Intercept	12.22	2.73	4.48	0.00	6.32	18.11
KAMALP	46.54	4.94	9.43	0.00	35.87	57.20
CATASB	-18.22	7.56	-2.41	0.03	-34.56	-1.88
SOLWAT	0.11	0.04	3.00	0.01	0.03	0.19

Table S19. Statistical analysis of KAMALP–SWAIBS–DIPOLE multiple regression model for aniline production

Summary Output

Regression Statistics	
Multiple R	0.95
R Square	0.90
Adjusted R Square	0.88
Standard Error	6.15
Observations	17

ANOVA

	df	**SS**	**MS**	**F**	**Significance F**
Regression	3	4599.8	1533.3	40.5	7.3E-07
Residual	13	491.8	37.8		
Total	16	5091.6			

	Coefficients	**Standard Error**	***t* Stat**	***P*-value**	**Lower 95%**	**Upper 95%**
Intercept	5.07	4.96	1.02	0.33	-5.65	15.79
KAMALP	34.92	5.55	6.29	0.00	22.93	46.91
SWAIBS	-20.72	9.92	-2.09	0.06	-42.15	0.71
DIPOLE	5.35	2.05	2.62	0.02	0.93	9.77

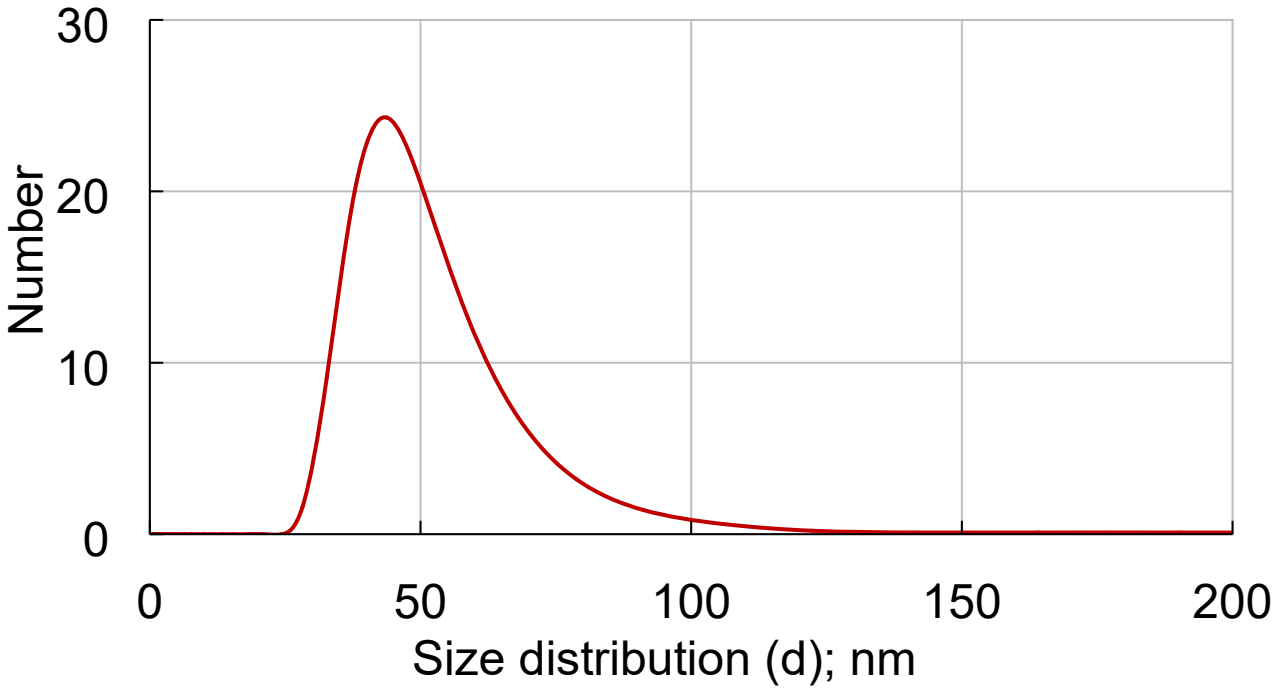

Fig. S1. The size distribution of PdNPs-stabilized-PVP particles in reaction solution

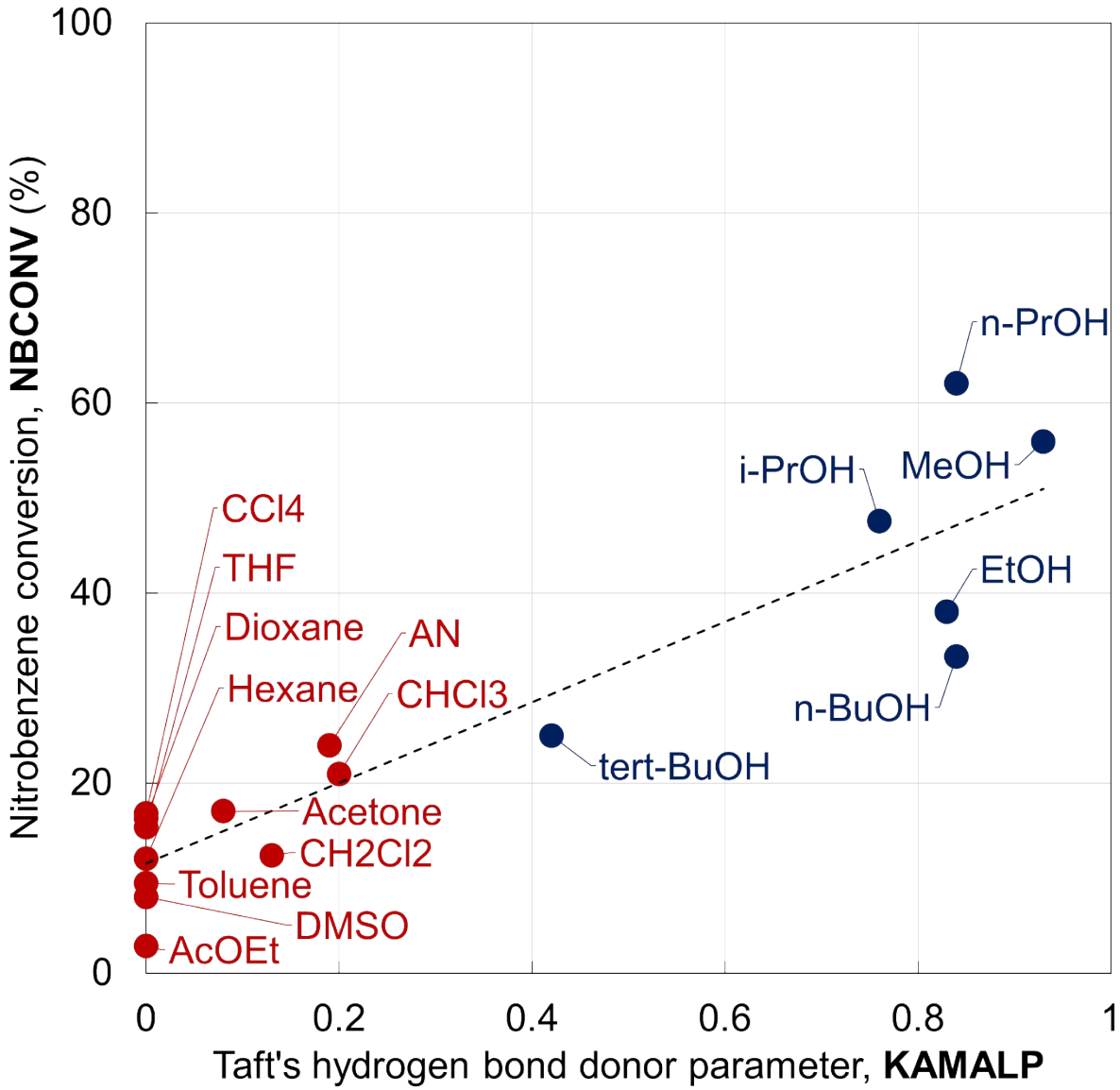

Fig. S2. Single regression analysis of aniline yield *vs.* **KAMALP**. Blue: protic solvents/alcohols, red: aprotic solvents

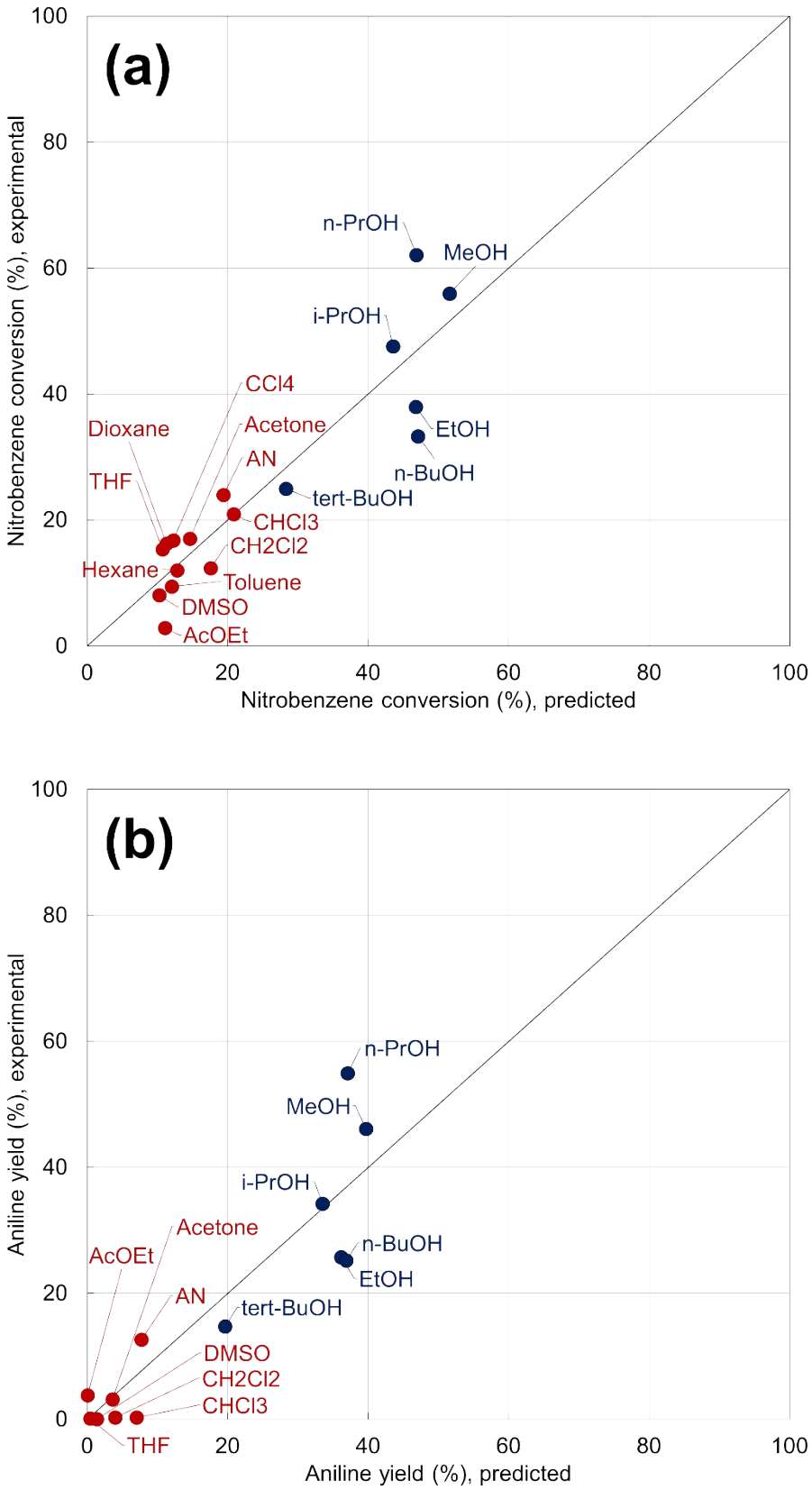

Fig. S3. Multiple regression analysis of (a) **NBCONV** and (b) **ANYIEL** on AKT model. Blue: protic solvents/alcohols, red: aprotic solvents

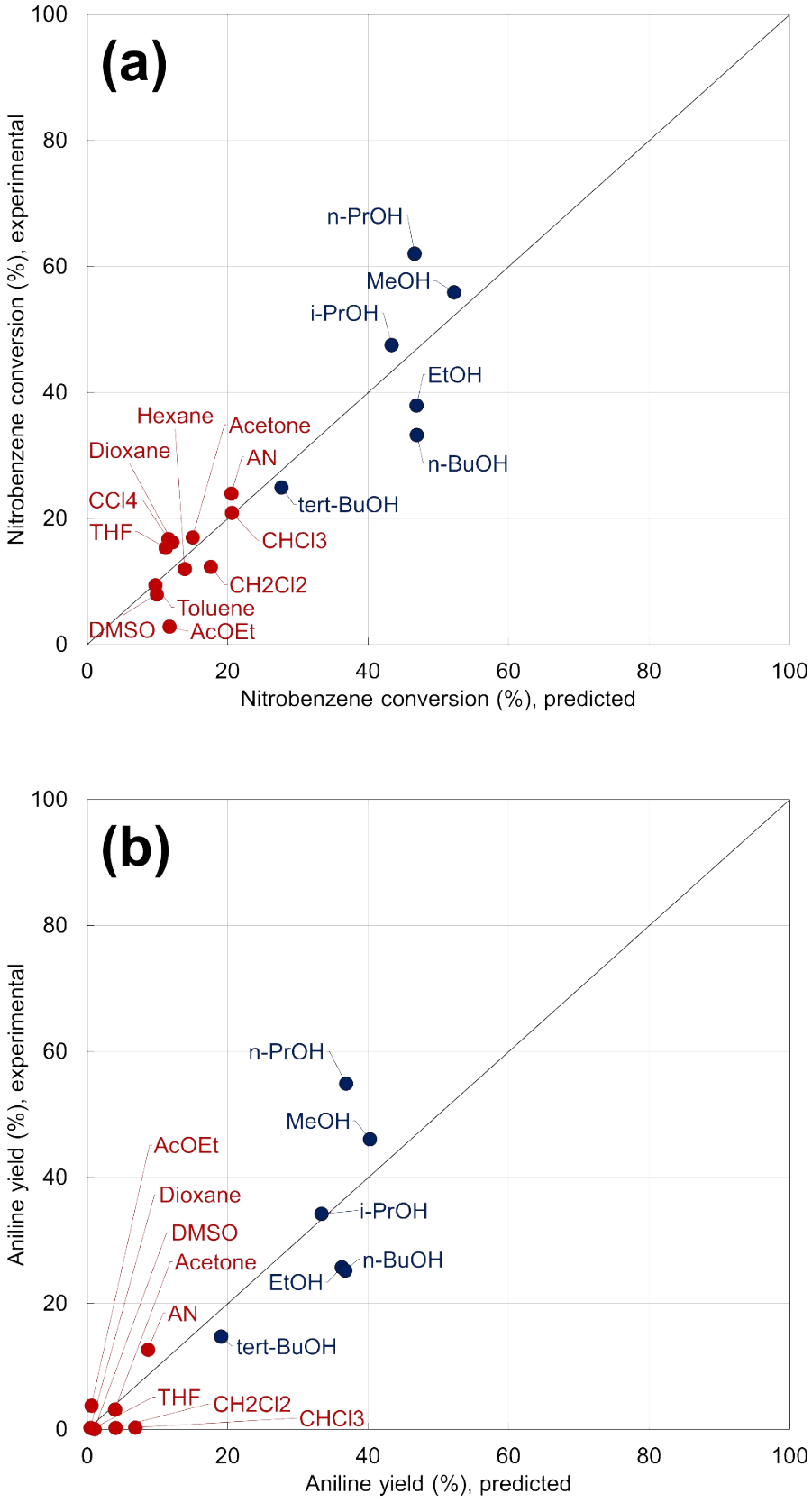

Fig. S4. Multiple regression analysis of (a) **NBCONV** and (b) **ANYIEL** on AKT model with correction on polarizability. Blue: protic solvents/alcohols, red: aprotic solvents

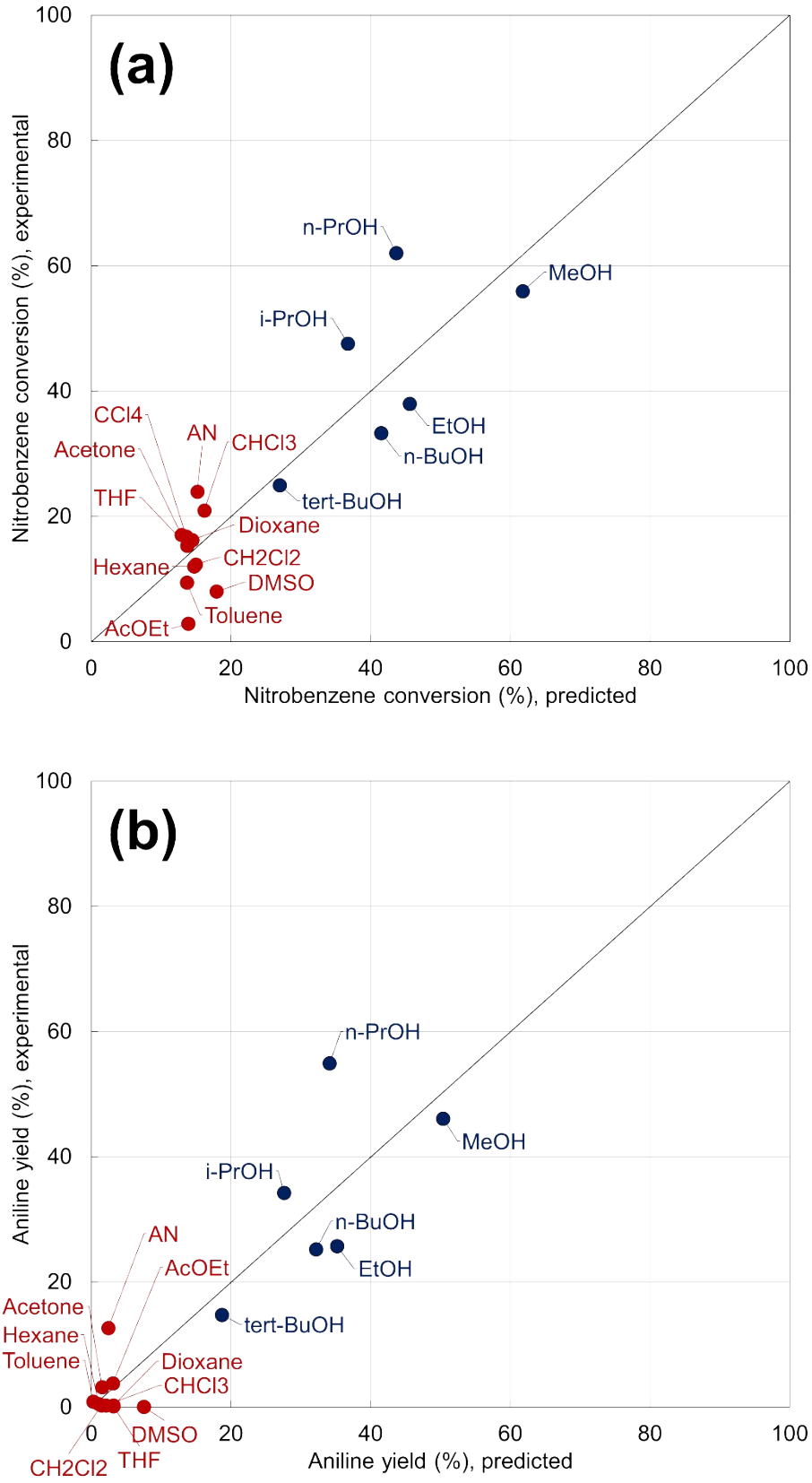

Fig. S5. Multiple regression analysis of (a) **NBCONV** and (b) **ANYIEL** on Catalán model. Blue: protic solvents/alcohols, red: aprotic solvents

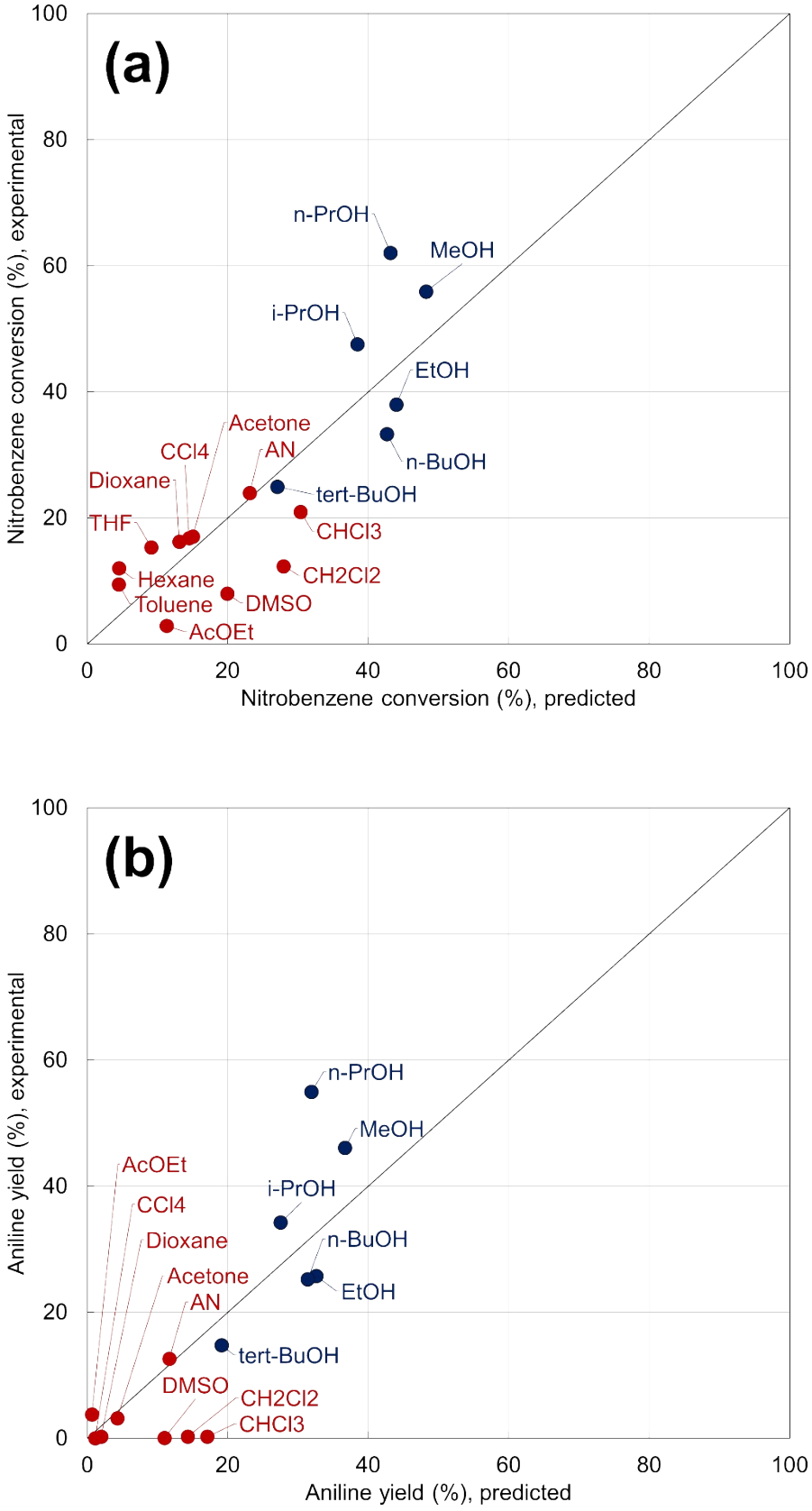

Fig. S6. Multiple regression analysis of (a) **NBCONV** and (b) **ANYIEL** on Gutmann model. Blue: protic solvents/alcohols, red: aprotic solvents

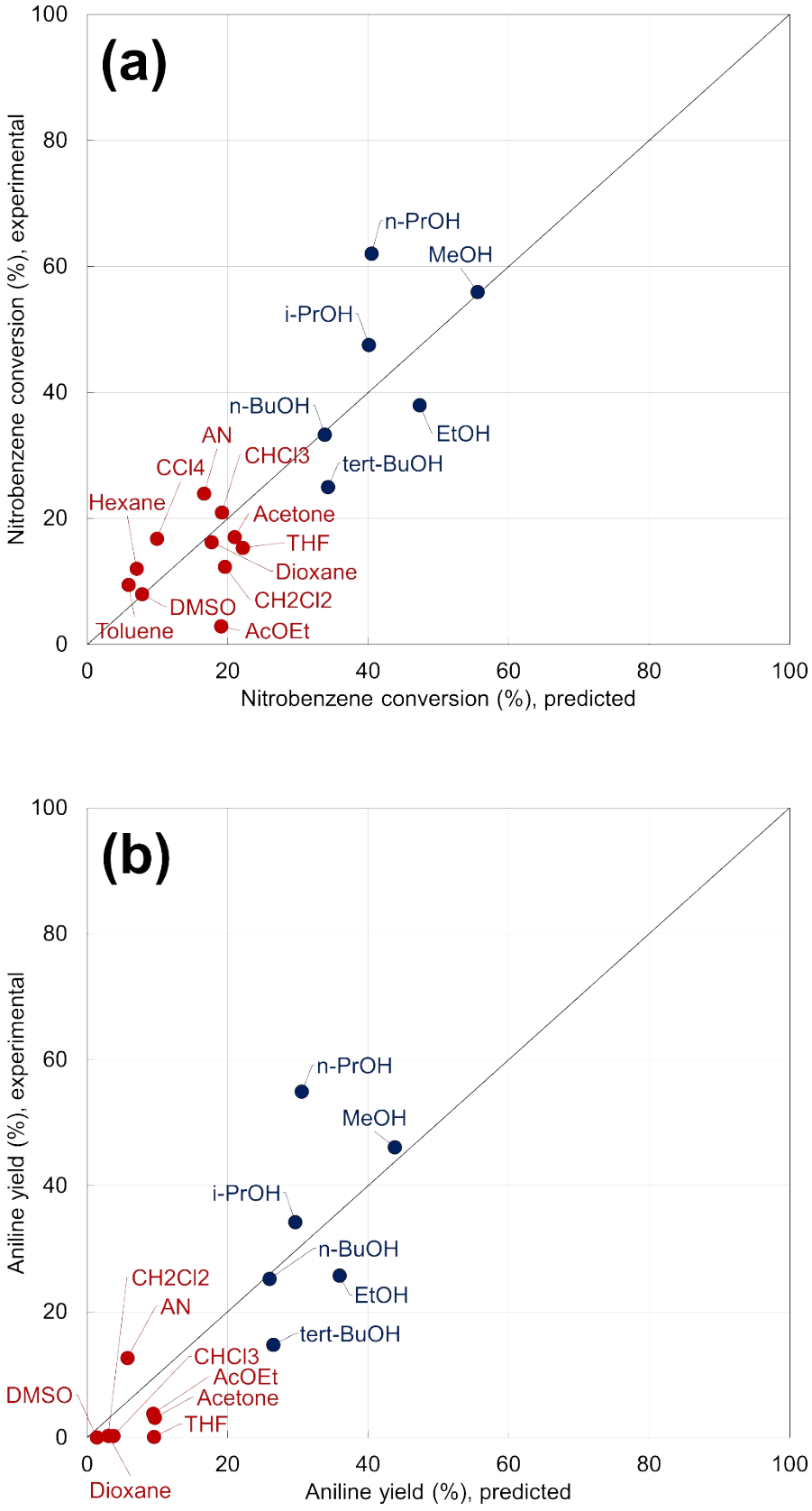

Fig. S7. Multiple regression analysis of (a) **NBCONV** and (b) **ANYIEL** on Hansen model. Blue: protic solvents/alcohols, red: aprotic solvents

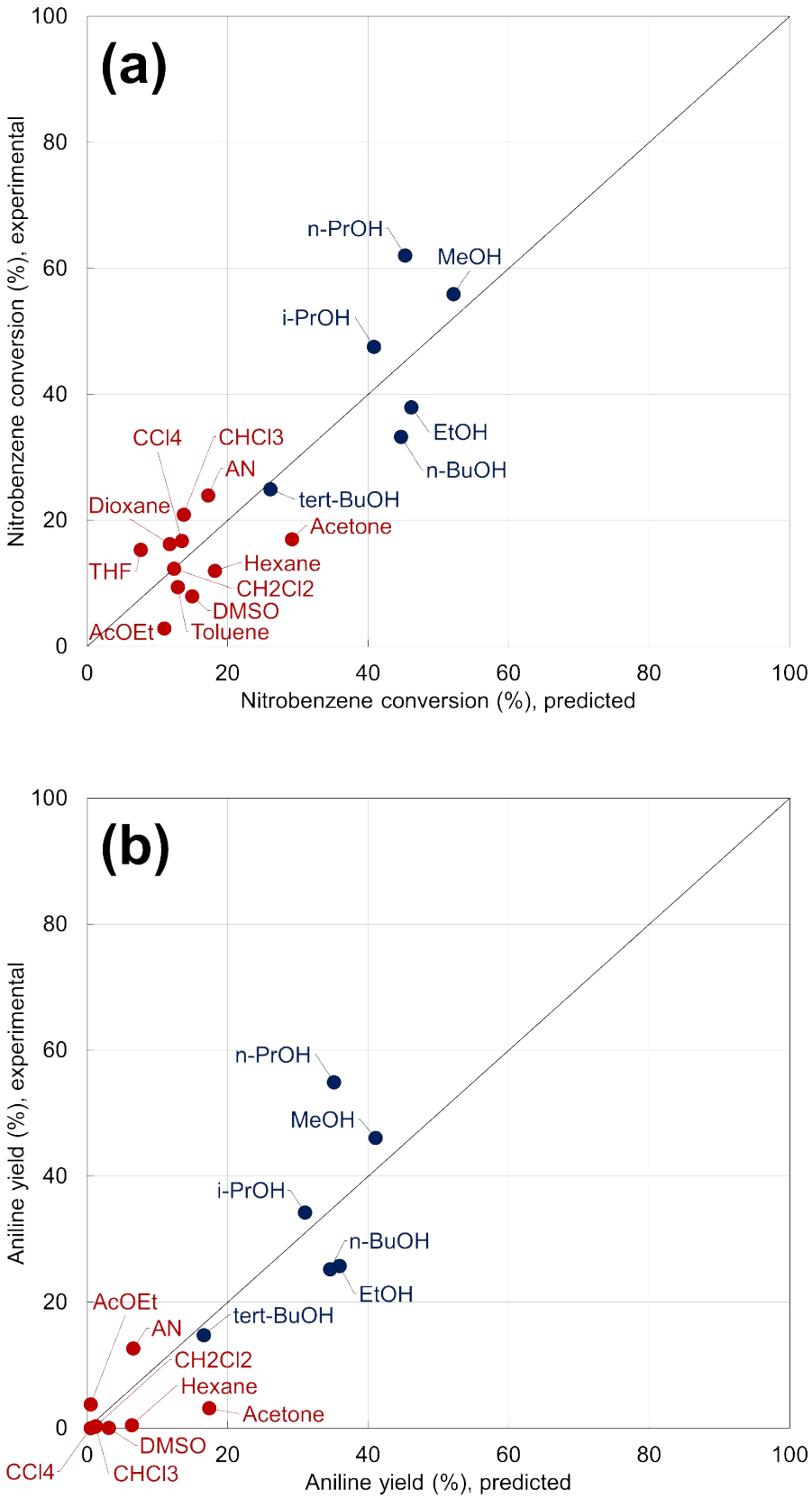

Fig. S8. Multiple regression analysis of (a) **NBCONV** and (b) **ANYIEL** on KP model. Blue: protic solvents/alcohols, red: aprotic solvents

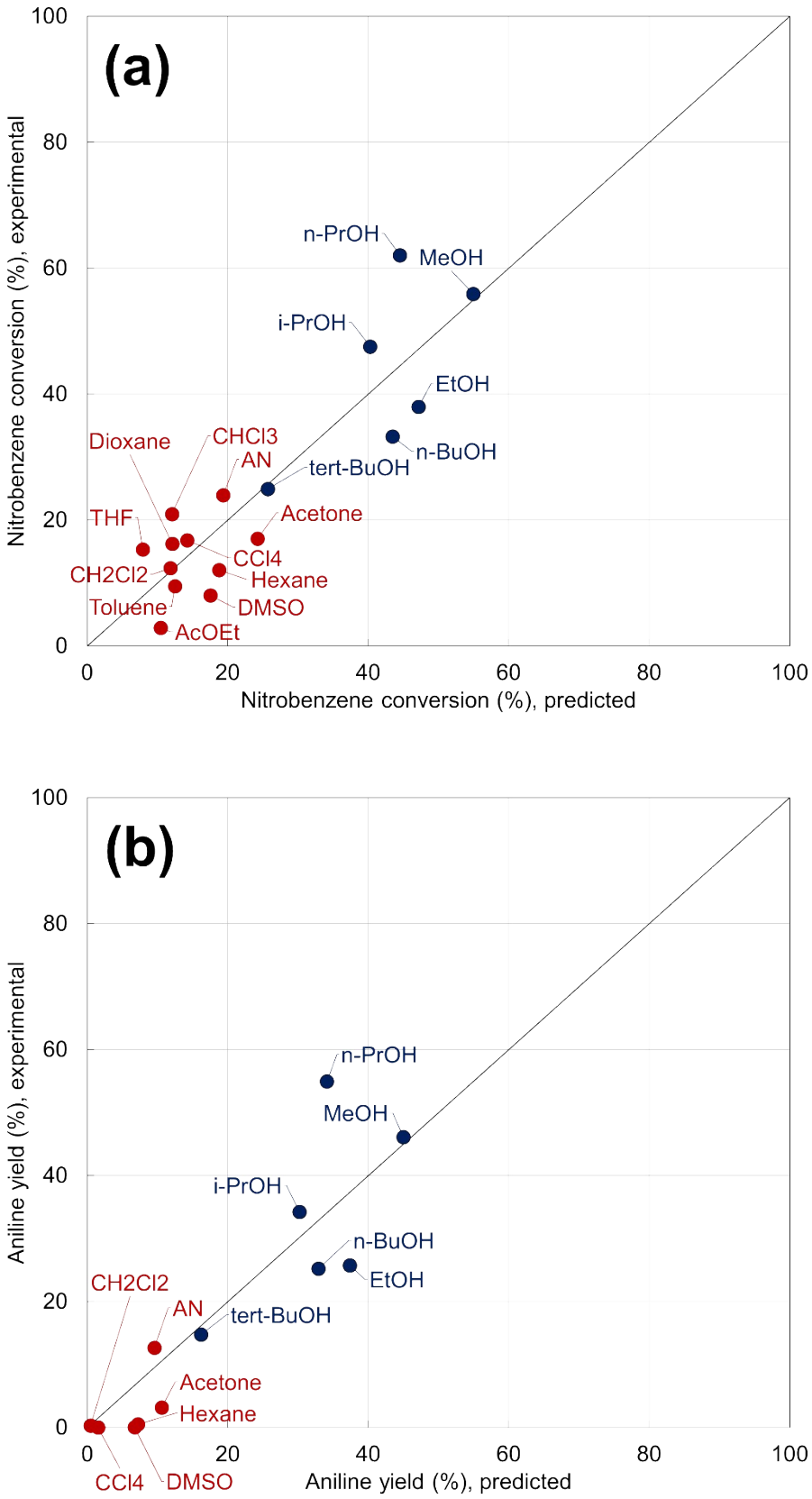

Fig. S9. Multiple regression analysis of (a) **NBCONV** and (b) **ANYIEL** on KP model with correction on Hildebrand's cohesion energy density. Blue: protic solvents/alcohols, red: aprotic solvents

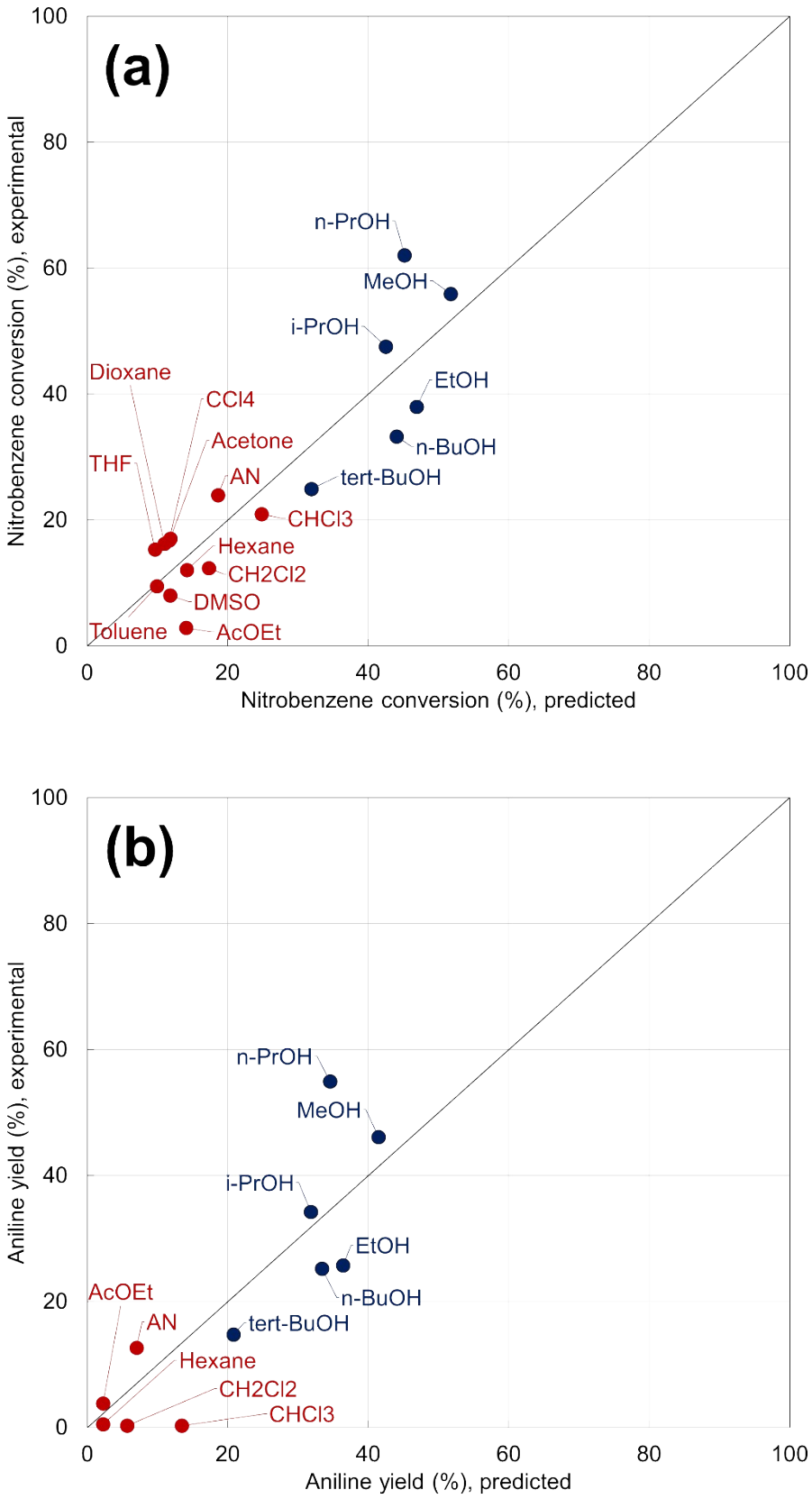

Fig. S10. Multiple regression analysis of (a) **NBCONV** and (b) **ANYIEL** on Swain model. Blue: protic solvents/alcohols, red: aprotic solvents

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