Electronic Supplementary Material (ESI) for RSC Advances.

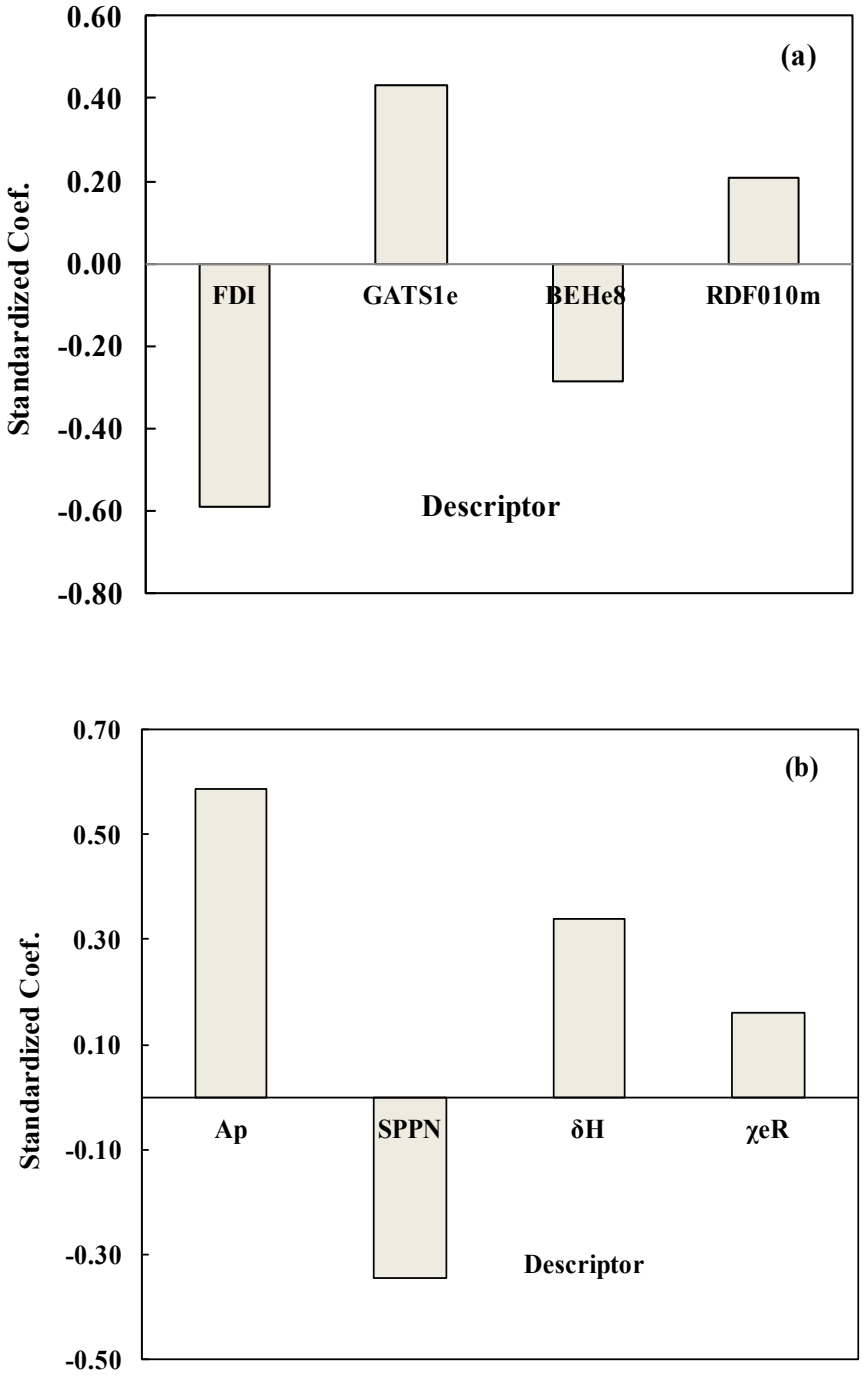

Fig S1. Standardized coefficient of (a) QSPR model based on the structural parameters of solvents and (b) LSER model based on the experimental solvent scale.

Table S1. Unstandardized and standardized coefficients of model 1 and their statistical t and p-values.

Model	Unstandardized Coefficients		Standardized Coefficients	t	p-value
	B	Std. Error	Beta		
(Constant)	0.895	0.024	-----	36.582	0.000
FDI	-0.283	0.025	-0.589	-11.417	0.000
GATS1e	0.236	0.030	0.432	7.872	0.000
BEHe8	-0.148	0.033	-0.287	-4.508	0.000
RDF010m	0.106	0.034	0.206	3.095	0.004

Table S2. Unstandardized and standardized coefficients of model 2 and their statistical t and p-values.

Model	Unstandardized Coefficients		Standardized Coefficients	t	p-value
	B	Std. Error	Beta		
(Constant)	-0.360	0.182	-----	46.088	0.000
Ap	0.062	0.007	0.586	8.456	0.000
SPP^N	-1.697	0.199	-.345	-8.526	0.000
δ	0.031	0.006	0.341	5.637	0.000
χ_e^R	0.751	0.239	0.161	3.135	0.003

Table S3. "Good" and "Bad" solvents from the view of ΔR_{rel}. "Good" solvents, which led to significant resistance changes of the CPC during immersion, whereas "bad" solvents which led to very small resistance changes (ΔRrel < 1% after 1 h).

No.	Solvent	ΔR_{rel}	No.	Solvent	ΔR_{rel}
1	Acetophenon	Good	**31**	n-Butyl acetate	Good
2	Cyclohexanone	Good	**32**	Morpholin	Good
3	n-Metyl-2-pyrrolidone	Good	**33**	Aniline	Good
4	Ethylene dichloride	Good	**34**	Furan	Good
5	Isophorone	Good	**35**	Nitromethane	Good
6	2-Nitropropane	Good	**36**	Toluene	Good
7	o-Dichlorobenzene	Good	**37**	Diethylene glycol monomethyl ether	Good
8	Methyl ethyl ketone	Good	**38**	Ethylene glycol monoethyl ether acetate	Good
9	Methylene dichloride	Good	**39**	Isoamyl acetate	Good
10	Mesityl oxide	Good	**40**	1,4-dioxane	Good
11	Diethyl ketone	Good	**41**	m-Cresol	Good
12	Butyronitrile	Good	**42**	Ethyl benzene	Good
13	Acetone	Good	**43**	Mesitylene	Good
14	Nitroethane	Good	**44**	Benzene	Good
15	Chlorobenzene	Good	**45**	Diethyl ether	Good
16	Anisole	Good	**46**	Dipropyl amine	Bad
17	Tetrahydrofuran	Good	**47**	Cyclohexanol	Bad
18	Methyl acetate	Good	**48**	Cyclohexane	Bad
19	Propylene carbonate	Good	**49**	Ethylene glycol monomethyl ether	Bad
20	Acetic anhydride	Good	**50**	n-Hexane	Bad
21	Methyl butyl ketone	Good	**51**	1-Butanol	Bad
22	Methyl isobutyl ketone	Good	**52**	Diethylene glycol	Bad

23	Trichloroethylene	Good	**53**	Ethanol	Bad
24[d]	Dimethyl formamide	Good	**54**	Propylene glycol	Bad
25[d]	Chloroform	Good	**55**	Ethanolamine	Bad
26[c]	Diethyl carbonate	Good	**56**	Methanol	Bad
27	Dimethyl sulfoxide	Good	**57**	Formamide	Bad
28[c]	Ethyl acetate	Good	**58**	Ethylene glycol	Bad
29	Di-(2-methoxyethyl) ether	Good	**59**	Water	Bad
30	Diethylene glycol monobutyl ether	Bad			

Data of this table was adapted from: Villmow T, John A, Pötschke P, Heinrich G. Polymer/carbon nanotube composites for liquid sensing: Selectivity against different solvents. Polymer (Guildf) 2012;53:2908–18.

Table S4 Experimental and predicted RED number of R polycarbonate polymer [ref. 17] in various solvents

No.	Solvent	RED (Exp)	No.	Solvent	RED (Exp)
1	Acetophenon	0.188	**31**	n-Butyl acetate	0.813
2[c]	Cyclohexanone	0.298	**32**	Morpholin	0.719
3[d]	n-Metyl-2-pyrrolidone	0.277	**33**	Aniline	0.678
4[c]	Ethylene dichloride	0.352	**34**	Furan	0.828
5	Isophorone	0.422	**35**[c]	Nitromethane	0.855
6[c]	2-Nitropropane	0.496	**36**	Toluene	0.846
7	o-Dichlorobenzene	0.409	**37**[c]	Diethylene glycol monomethyl ether	0.824
8	Methyl ethyl ketone	0.536	**38**	Ethylene glycol monoethyl ether acetate	0.865
9	Methylene dichloride	0.486	**39**	Isoamyl acetate	0.914
10	Mesityl oxide	0.541	**40**	1,4-dioxane	0.860
11[d]	Diethyl ketone	0.611	**41**[c]	m-Cresol	0.805
12[d]	Butyronitrile	0.640	**42**	Ethyl benzene	0.930
13[d]	Acetone	0.617	**43**	Mesitylene	0.947
14	Nitroethane	0.640	**44**[d]	Benzene	0.944
15	Chlorobenzene	0.603	**45**	Diethyl ether	1.008
16[c]	Anisole	0.597	**46**[c]	Dipropyl amine	1.009
17[d]	Tetrahydrofuran	0.622	**47**	Cyclohexanol	0.936
18	Methyl acetate	0.700	**48**[c]	Cyclohexane	1.058
19	Propylene carbonate	0.611	**49**[d]	Ethylene glycol monomethyl ether	0.991
20	Acetic anhydride	0.667	**50**	n-Hexane	1.213
21	Methyl butyl ketone	0.747	**51**	1-Butanol	1.109

22	Methyl isobutyl ketone	0.747	**52**	Diethylene glycol	1.224
23	Trichloroethylene	0.670	**53**[d]	Ethanol	1.313
24[d]	Dimethyl formamide	0.629	**54**[c,d]	Propylene glycol	1.392
25[d]	Chloroform	0.681	**55**	Ethanolamine	1.411
26[c]	Diethyl carbonate	0.774	**56**[d]	Methanol	1.601
27	Dimethyl sulfoxide	0.631	**57**[c]	Formamide	1.737
28[c]	Ethyl acetate	0.736	**58**	Ethylene glycol	1.762
29	Di-(2-methoxyethyl) ether	0.755	**59**	Water	3.160
30	Diethylene glycol monobutyl ether	0.757			

[c] Compounds in the test set using model 1
[d] Compounds in the test set using model 2

Table S5. Unstandardized and standardized coefficients of model constructed for new polymer (R polycarbonate) using the parameters of model 1 and their statistical t and p-values.

Model	Unstandardized Coefficients		Standardized Coefficients	t	p-value
	B	Std. Error	Beta		
(Constant)	0.857	0.022	------	39.157	0.000
FDI	-0.267	0.022	-0.624	-12.023	0.000
GATS1e	0.196	0.027	0.404	7.317	0.000
BEHe8	-0.121	0.029	-0.263	-4.112	0.000
RDF010m	0.089	0.031	0.195	2.917	0.006

Table S6. Unstandardized and standardized coefficients of model 2 and their statistical t and p-values.

Model	Unstandardized Coefficients		Standardized Coefficients	t	p-value
	B	Std. Error	Beta		
(Constant)	-0.069	0.187	------	-0.369	0.0714
Ap	0.052	0.008	0.546	6.846	0.000
SPP^N	-1.681	0.204	-0.384	-8.242	0.000
δ	0.030	0.006	0.366	5.262	0.000
χ_e^R	0.687	0.245	0.165	2.799	0.008

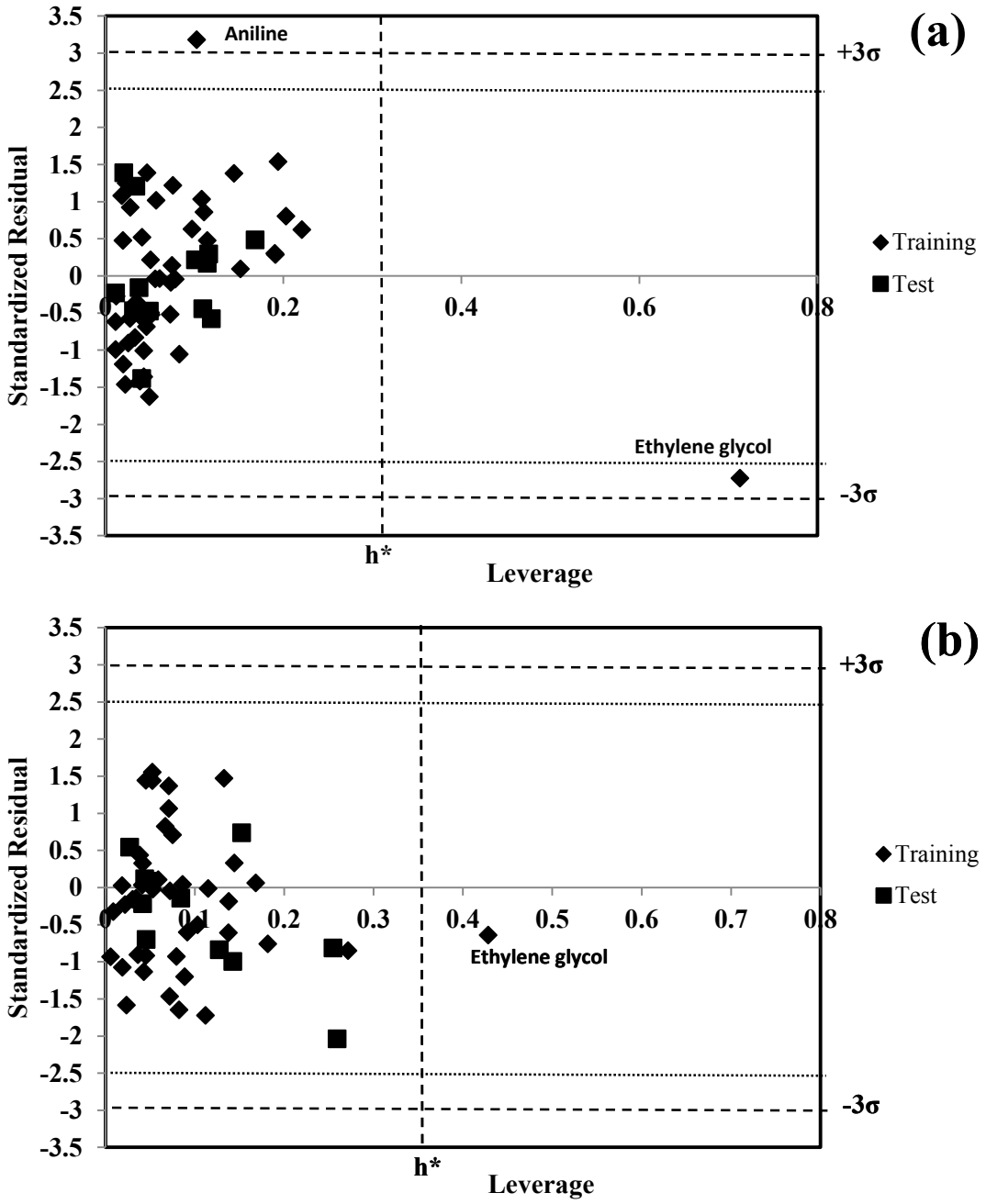

Fig. S2. Williams plot of the entire set of solvents for the models for new polymer (R polycarbonate) constructed using the parameters of model 1 (a) and model 2 (b). Cut off values of leverage (h^*) and standardized residual (±3 times the standards deviation) are depicted by vertical and horizontal dashed lines, respectively. Ethylene glycol is out of the applicable domain in model 1; Ethylene glycol and water are out of the applicable domain in model 2.