

表 S1 不同流动相条件下中性化合物 $\log k$ - ϕ 关系及外推 $\log k_w$ 值

Table S1 Correlations of $\log k$ - ϕ and extrapolated $\log k_w$ values for neutral compounds by different mobile phases

No.	Methanol-Water					Acetonitrile-Water						
	ϕ	$\log k$	N	Equation 2		ϕ	$\log k$	N	Equation 2		Equation 4	
				Adj. R^2	$\log k_w$				Adj. R^2	$\log k_w$	Adj. R^2	$\log k_w$
N1	0.05-0.80	-0.956-0.293	16	0.9952	0.30	0.05-0.80	-0.915-0.211	16	0.9943	0.24	0.9987	0.61
N2	0.05-0.95	-1.143-0.919	19	0.9992	1.04	0.05-0.95	-1.143-0.761	19	0.9779	0.66	0.9989	1.43
N3	0.30-0.95	-0.670-1.147	14	0.9986	2.00	0.05-0.95	-0.978-1.125	19	0.9921	1.12	0.9991	1.59
N4	0.30-0.95	-0.606-1.164	14	0.9993	2.01	0.05-0.95	-0.810-1.636	19	0.9911	1.66	0.9988	1.96
N5	0.40-0.95	-0.631-0.916	12	0.9990	2.06	0.05-0.95	-0.753-1.446	19	0.9960	1.56	0.9982	1.49
N6	0.40-0.95	-0.588-1.299	12	0.9990	2.67	0.25-0.95	-0.788-1.357	15	0.9926	1.97	0.9995	5.44
N7	0.45-0.95	-0.865-1.212	12	0.9981	2.66	0.20-0.95	-0.932-1.468	16	0.9802	1.83	0.9998	5.54
N8	0.40-0.95	-0.477-1.527	12	0.9990	2.76	0.25-0.95	-0.603-1.402	15	0.9904	1.96	0.9996	5.12
N9	0.40-0.95	-0.409-1.521	12	0.9993	2.92	0.25-0.95	-0.543-1.521	15	0.9879	2.08	0.9997	5.63
N10	0.45-0.95	-0.350-1.460	11	0.9990	3.08	0.30-0.95	-0.529-1.410	14	0.9913	2.15	0.9997	7.07
N11	0.45-0.95	-0.347-1.521	11	0.9990	3.19	0.30-0.95	-0.505-1.468	14	0.9910	2.22	0.9997	7.14
N12	0.45-0.95	-0.404-1.471	11	0.9990	3.16	0.25-0.95	-0.545-1.674	15	0.9883	2.28	0.9996	5.95
N13	0.45-0.95	-0.345-1.520	11	0.9990	3.18	0.30-0.95	-0.506-1.468	14	0.9907	2.21	0.9997	7.24
N14	0.45-0.95	-0.379-1.572	11	0.9996	3.29	0.30-0.95	-0.510-1.493	14	0.9878	2.23	0.9998	7.66
N15	0.45-0.95	-0.327-1.606	11	0.9991	3.32	0.30-0.95	-0.460-1.526	14	0.9886	2.26	0.9998	7.58
N16	0.50-0.95	-0.266-1.505	10	0.9994	3.44	0.30-0.95	-0.389-1.622	14	0.9879	2.36	0.9998	7.76
N17	0.55-0.95	-0.151-1.494	9	0.9992	3.72	0.35-0.95	-0.371-1.562	13	0.9894	2.51	0.9998	10.31
N18	0.55-0.95	-0.198-1.513	9	0.9989	3.83	0.35-0.95	-0.443-1.582	13	0.9891	2.57	0.9999	10.89
N19	0.60-0.95	0.013-1.438	8	0.9990	3.89	0.40-0.95	-0.308-1.455	12	0.9924	2.59	0.9998	12.20
N20	0.60-0.95	-0.005-1.516	8	0.9990	4.11	0.40-0.95	-0.154-1.554	12	0.9944	2.66	0.9999	11.25
N21	0.55-0.95	-0.314-1.434	9	0.9989	3.79	0.35-0.95	-0.519-1.546	13	0.9899	2.56	0.9998	11.17
N22	0.65-0.95	0.141-1.445	7	0.9991	4.25	0.40-0.95	-0.161-1.662	12	0.9903	2.82	0.9999	13.65

N23	0.65-0.95	0.206-1.584	7	0.9990	4.56	0.45-0.95	0.035-1.599	11	0.9960	2.89	0.9998	15.56
N24	0.70-0.95	0.293-1.471	6	0.9990	4.75	0.45-0.95	-0.003-1.652	11	0.9961	3.02	0.9998	15.54
N25	0.80-0.95	0.964-1.804	4	0.9990	6.29	0.65-0.95	0.589-1.600	7	0.9990	3.77	0.9999	21.04
N26	0.40-0.95	-0.490-1.307	12	0.9990	2.60	0.25-0.95	-0.632-1.331	15	0.9926	1.90	0.9996	4.74
N27	0.70-0.95	0.337-1.576	6	0.9990	5.02	0.45-0.95	0.091-1.758	11	0.9959	3.14	0.9998	16.34
N28	0.35-0.95	-0.729-1.418	13	0.9944	2.61	0.20-0.95	-0.872-1.670	16	0.9809	2.07	0.9996	5.84
N29	0.80-0.95	0.875-1.707	4	0.9990	6.14	0.65-0.95	0.590-1.583	7	0.9990	3.72	0.9999	20.89

N : the number of $\log k$ values used; $\text{adj.}R^2$: the adjusted squared correlation coefficient.

表 S2 不同流动相条件下弱酸性化合物 $\log k$ - φ 关系及外推 $\log k_w$ 值

Table S2 Correlations of $\log k$ - φ and extrapolated $\log k_w$ values for weak acidic compounds by different mobile phases

No.	Methanol-20 mmol/L KH ₂ PO ₄ (pH 2.5)					Methanol-20 mmol/L KH ₂ PO ₄ (pH 4.0)				
	φ	$\log k$	N	Equation 2		φ	$\log k$	N	Equation 2	
				Adj. R^2	$\log k_w$				Adj. R^2	$\log k_w$
A1	0.05-0.70	-1.286-0.019	14	0.9990	0.13	0.05-0.60	-1.100-0.045	12	0.9992	0.16
A2	0.05-0.70	-1.055-0.366	14	0.9998	0.49	0.05-0.60	-0.839-0.392	12	0.9993	0.52
A3	0.05-0.70	-0.796-0.461	14	0.9991	0.59	0.05-0.60	-0.596-0.485	12	0.9983	0.61
A4	0.05-0.70	-0.640-0.944	14	0.9995	1.07	0.05-0.60	-0.437-0.970	12	0.9996	1.10
A5	0.10-0.70	-0.479-1.158	13	0.9999	1.43	0.10-0.60	-0.310-1.024	11	0.9999	1.30
A6	0.10-0.70	-0.383-1.247	13	0.9993	1.55	0.10-0.60	-0.248-1.062	11	0.9991	1.36
A7	0.15-0.70	-0.197-1.279	12	0.9998	1.68	0.15-0.60	0.055-1.296	10	0.9996	1.71
A8	0.10-0.70	-0.275-1.274	13	0.9994	1.56	0.10-0.60	-0.020-1.298	11	0.9992	1.57
A9	0.10-0.70	-0.341-1.302	13	0.9992	1.61	0.05-0.60	-0.530-0.649	12	0.9998	0.75
A10	0.25-0.70	-0.182-1.096	10	0.9997	1.82	0.25-0.60	0.088-1.133	8	0.9999	1.88
A11	0.25-0.70	-0.281-1.011	10	0.9996	1.74	0.05-0.60	-0.444-0.721	12	0.9997	0.83
A12	0.30-0.70	-0.061-1.355	9	0.9999	2.42	0.30-0.60	0.168-1.203	7	0.9998	2.24
A13	0.30-0.70	-0.172-1.167	9	0.9998	2.17	0.30-0.60	0.023-1.005	7	0.9996	1.99
A14	0.30-0.70	0.059-1.360	9	0.9999	2.35	0.30-0.60	0.357-1.354	7	0.9998	2.36
A15	0.30-0.70	0.060-1.433	9	0.9999	2.46	0.30-0.60	0.165-1.152	7	0.9997	2.14
A16	0.30-0.70	0.315-1.757	9	0.9994	2.85	0.30-0.60	0.648-1.769	7	0.9998	2.90
A17	0.30-0.70	0.171-1.797	9	0.9990	3.01	0.30-0.60	0.368-1.597	7	0.9994	2.82
A18	0.30-0.70	0.254-1.681	9	0.9996	2.78	0.30-0.60	0.580-1.698	7	0.9999	2.82
A19	0.35-0.70	0.180-1.663	8	0.9993	3.16	0.35-0.60	0.462-1.529	6	0.9994	3.03

A20	0.40-0.70	0.653-1.857	7	0.9998	3.46			0.40-0.70	0.637-1.829	8	0.9996	3.41		
A21	0.60-0.90	0.451-1.871	7	0.9999	4.71			0.60-0.80	0.650-1.677	5	0.9999	4.75		
A22	0.05-0.70	-0.463-1.051	14	0.9998	1.16			0.05-0.60	-0.249-1.032	12	0.9999	1.15		
A23	0.30-0.70	0.123-1.548	9	0.9995	2.63			0.30-0.60	0.180-1.191	7	0.9997	2.20		
A24	0.20-0.70	-0.301-1.233	11	0.9998	1.85			0.20-0.60	-0.089-1.103	9	0.9999	1.70		
A25	0.25-0.70	-0.293-1.156	10	0.9997	1.97			0.20-0.60	-0.093-1.137	9	0.9998	1.76		
A26	0.30-0.70	-0.062-1.455	9	0.9994	2.59			0.30-0.60	0.196-1.337	7	0.9994	2.47		
A27	0.30-0.70	0.049-1.585	9	0.9994	2.74			0.30-0.60	0.264-1.449	7	0.9999	2.64		
A28	0.50-0.90	0.090-1.750	9	0.9998	3.80			0.50-0.80	0.444-1.722	7	0.9998	3.84		
Acetonitrile-20 mmol/L KH ₂ PO ₄ (pH 2.5)								Acetonitrile-20 mmol/L KH ₂ PO ₄ (pH 4.0)						
No.	φ	logk	N	Equation (2)		Equation (4)		φ	logk	N	Equation (2)		Equation (4)	
				Adj. <i>R</i> ²	log <i>k</i> _w	Adj. <i>R</i> ²	log <i>k</i> _w				Adj. <i>R</i> ²	log <i>k</i> _w	Adj. <i>R</i> ²	log <i>k</i> _w
A1	0.05-0.70	-1.124-0.043	14	0.9708	-0.03	0.9997	0.81	0.05-0.70	-1.109-0.025	14	0.9744	-0.04	0.9992	0.65
A2	0.05-0.70	-1.045-0.451	14	0.9588	0.32	0.9998	1.41	0.05-0.70	-1.023-0.427	14	0.9601	0.31	0.9998	1.27
A3	0.05-0.70	-0.886-0.571	14	0.9695	0.48	0.9999	1.33	0.05-0.70	-0.872-0.558	14	0.9688	0.47	0.9999	1.27
A4	0.05-0.70	-0.816-0.945	14	0.9487	0.78	0.9999	1.96	0.05-0.70	-0.795-0.928	14	0.9479	0.77	0.9999	1.85
A5	0.10-0.70	-0.716-0.994	13	0.9716	1.08	0.9999	2.27	0.10-0.70	-0.723-0.853	13	0.9707	0.93	0.9999	2.06
A6	0.10-0.70	-0.671-1.020	13	0.9664	1.09	0.9999	2.34	0.10-0.70	-0.688-0.840	13	0.9667	0.91	0.9999	2.02
A7	0.10-0.70	-0.461-1.204	13	0.9853	1.35	0.9999	1.98	0.10-0.70	-0.454-1.200	13	0.9837	1.34	0.9999	1.97
A8	0.10-0.70	-0.515-1.159	13	0.9833	1.30	0.9999	2.04	0.10-0.70	-0.503-1.154	13	0.9814	1.29	0.9999	2.00
A9	0.10-0.70	-0.601-1.142	13	0.9706	1.24	0.9999	2.31	0.05-0.70	-0.757-0.559	14	0.9617	0.51	0.9982	0.85
A10	0.10-0.70	-0.449-1.322	13	0.9833	1.48	0.9999	2.12	0.10-0.70	-0.446-1.316	13	0.9827	1.47	0.9999	2.08
A11	0.10-0.70	-0.560-1.235	13	0.9699	1.33	0.9999	2.37	0.05-0.70	-0.721-0.641	14	0.9435	0.53	0.9994	1.12
A12	0.15-0.70	-0.478-1.511	12	0.9619	1.79	0.9999	4.34	0.15-0.70	-0.489-1.328	12	0.9621	1.59	0.9999	3.74
A13	0.10-0.70	-0.534-1.493	13	0.9591	1.56	0.9999	3.00	0.10-0.70	-0.551-1.339	13	0.9596	1.40	0.9999	2.80
A14	0.15-0.70	-0.352-1.460	12	0.9755	1.77	0.9999	3.40	0.15-0.70	-0.348-1.439	12	0.9762	1.75	0.9999	3.07

A15	0.15-0.70	-0.412-1.457	12	0.9595	1.71	0.9999	4.20	0.15-0.70	-0.466-1.182	12	0.9605	1.41	0.9999	3.52
A16	0.20-0.70	-0.195-1.542	11	0.9781	2.08	0.9999	4.17	0.20-0.70	-0.192-1.533	11	0.9771	2.07	0.9999	3.87
A17	0.20-0.70	-0.338-1.450	11	0.9629	1.94	0.9999	5.27	0.20-0.70	-0.359-1.307	11	0.9621	1.76	0.9999	4.76
A18	0.20-0.70	-0.120-1.557	11	0.9828	2.10	0.9999	3.63	0.20-0.70	-0.117-1.550	11	0.9820	2.09	0.9999	3.31
A19	0.20-0.70	-0.300-1.591	11	0.9649	2.11	0.9999	5.82	0.20-0.70	-0.316-1.492	11	0.9671	2.01	0.9999	4.75
A20	0.25-0.70	0.054-1.649	10	0.9826	2.41	0.9999	4.96	0.25-0.70	0.054-1.639	10	0.9812	2.39	0.9999	4.34
A21	0.40-0.80	0.237-1.552	9	0.9852	2.76	0.9999	8.86	0.40-0.80	0.161-1.471	9	0.9851	2.66	0.9999	12.64
A22	0.05-0.70	-0.631-0.943	14	0.9852	0.92	0.9999	1.42	0.05-0.70	-0.631-0.943	14	0.9838	0.91	0.9999	1.39
A23	0.20-0.70	-0.360-1.230	11	0.9685	1.68	0.9999	4.43	0.15-0.70	-0.434-1.220	12	0.9574	1.44	0.9999	3.73
A24	0.10-0.70	-0.611-1.033	13	0.9675	1.42	0.9999	2.77	0.10-0.70	-0.618-1.200	13	0.9666	1.28	0.9999	2.51
A25	0.10-0.70	-0.594-1.106	13	0.9658	1.50	0.9999	2.81	0.10-0.70	-0.608-1.218	13	0.9651	1.29	0.9999	2.58
A26	0.20-0.70	-0.464-1.285	11	0.9682	1.77	0.9999	5.17	0.20-0.70	-0.466-1.168	11	0.9684	1.63	0.9999	4.47
A27	0.20-0.70	-0.391-1.289	11	0.9668	1.76	0.9999	4.94	0.20-0.70	-0.407-1.183	11	0.9692	1.64	0.9999	4.22
A28	0.30-0.80	0.027-1.702	11	0.9786	2.54	0.9999	7.44	0.30-0.80	0.025-1.692	11	0.9769	2.52	0.9999	7.28

N : the number of $\log k$ values used; $\text{adj.}R^2$: the adjusted squared correlation coefficient.