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Supplementary Material for:

Influence of water molecular bridges on sequestration of phenol in soil organic matter of sapric histosol

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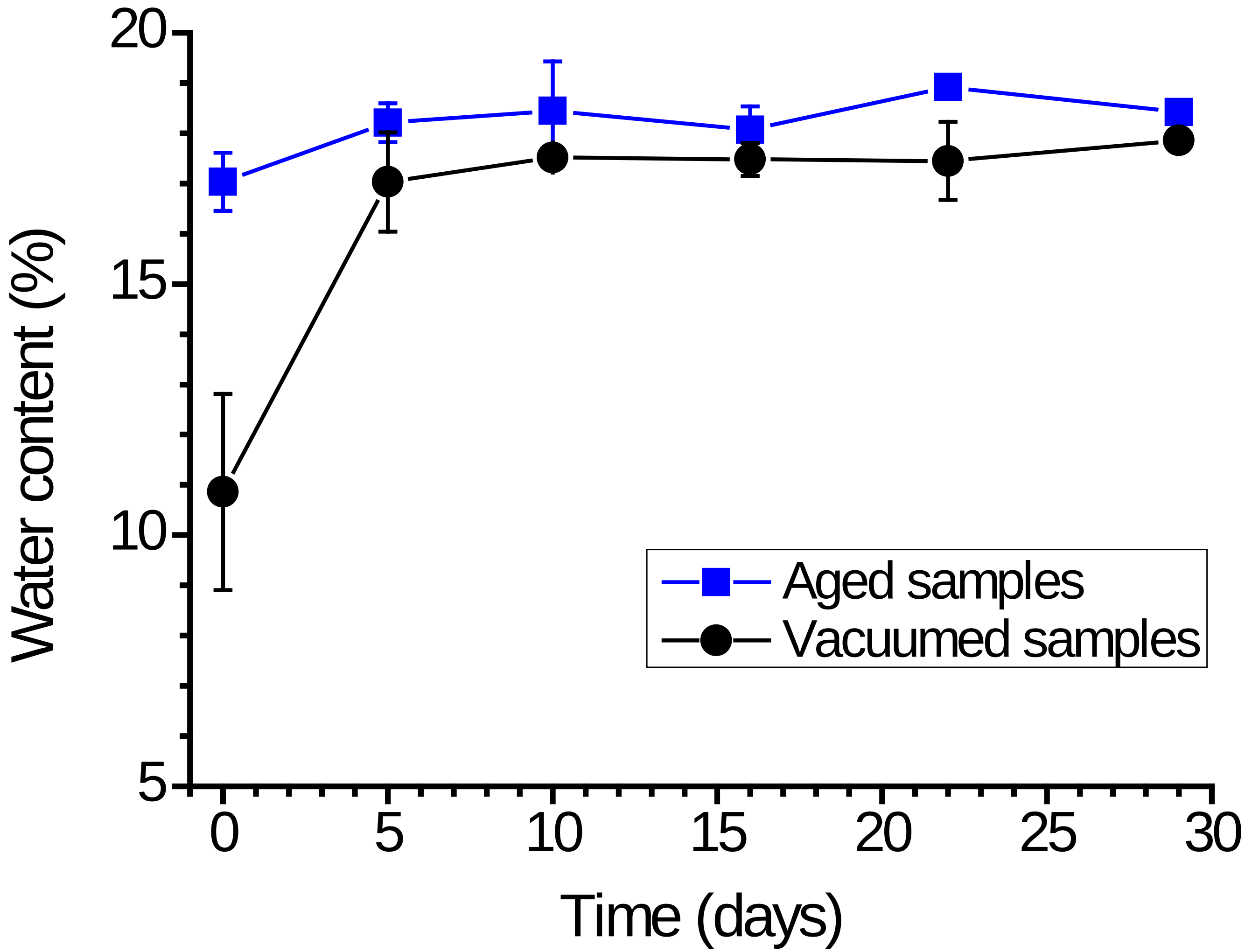

Figure S1. *Development of water content in vacuumed and aged samples.*

Table S1. *Fitting parameters obtained from desorption kinetics of phenol from vacuumed and pre-aged samples.*[1]

Sample	Cont.-e	A_{FAST}	Corr. R^2	Chisquare	y_0	SE_y_0	A_1	SE_A_1	t_1	SE_t_1	A2	SE_A_2	t_2	SE_t_2	Integral
	days		V^2	V^2	V	V	V	V	days	days	V	V	days	days	Vh
Vac 1	0	0.70	0.9988	2.1E-07	-0.085	2.1E-06	0.120	1.6E-04	0.909	0.001	0.052	4.9E-05	5.623	0.004	0.40
	5	0.75	0.9995	1.7E-07	-0.085	3.0E-06	0.118	4.0E-05	1.713	0.001	0.038	5.6E-05	7.747	0.008	0.50
	10	0.75	0.9891	3.7E-06	-0.015	2.9E-05	0.142	3.0E-04	1.212	0.004	0.048	1.6E-04	7.447	0.031	0.53
	16	0.73	0.9999	2.8E-08	-0.085	8.2E-07	0.134	3.4E-05	1.739	0.001	0.050	4.5E-05	5.295	0.002	0.50
	22	0.70	0.9985	5.0E-07	-0.009	4.1E-06	0.117	7.6E-05	1.640	0.002	0.051	9.6E-05	6.560	0.008	0.52
	29	0.68	0.9994	2.0E-07	-0.010	2.7E-06	0.106	5.2E-05	1.770	0.002	0.051	6.9E-05	6.631	0.006	0.52
Vac 2	0	0.75	0.9999	3.2E-08	-0.009	7.9E-07	0.140	2.5E-05	1.395	0.001	0.047	3.4E-05	4.942	0.002	0.43
	6	0.78	0.9981	9.2E-07	-0.010	6.9E-06	0.142	1.5E-04	2.191	0.003	0.039	1.9E-04	7.302	0.022	0.60
	10	0.71	0.9999	3.2E-08	-0.008	1.4E-06	0.099	1.5E-05	1.792	0.001	0.041	1.7E-05	8.320	0.003	0.52
	16	0.73	0.9999	3.0E-08	-0.008	1.4E-06	0.094	1.5E-05	1.731	0.001	0.035	1.5E-05	8.669	0.003	0.46
	22	0.75	0.9997	2.9E-08	-0.007	1.0E-06	0.075	1.9E-05	1.445	0.001	0.025	1.6E-05	6.948	0.004	0.28
Vac 3	0	0.78	0.9997	3.2E-08	-0.008	1.0E-06	0.099	2.6E-05	1.248	0.000	0.027	1.4E-05	6.752	0.003	0.31
	7	0.68	0.9998	3.7E-08	-0.007	1.2E-06	0.089	1.8E-05	1.608	0.001	0.042	2.0E-05	7.355	0.003	0.45
	10	0.71	0.9998	2.8E-08	-0.008	1.1E-06	0.084	1.6E-05	1.628	0.001	0.035	1.7E-05	7.417	0.003	0.40
	16	0.73	0.9992	1.4E-07	-0.006	2.8E-06	0.084	3.4E-05	1.694	0.001	0.031	3.6E-05	8.157	0.008	0.40
	*22	0.64	0.9961	8.4E-07	0.008	8.4E-03	0.124	4.8E-03	2.100	0.203	0.070	3.4E-02	8.011	3.260	0.82
	29	0.80	0.9997	1.9E-07	-0.010	1.3E-05	0.151	8.1E-05	2.231	0.002	0.038	9.4E-05	10.683	0.028	0.73
Pre-aged 1	0	0.79	0.9992	2.4E-07	-0.085	4.3E-06	0.140	5.7E-05	1.423	0.001	0.037	2.8E-05	9.475	0.008	0.54
	10	0.58	0.9996	2.2E-07	-0.014	3.5E-06	0.101	2.1E-04	1.871	0.003	0.075	2.5E-04	4.739	0.007	0.54
	16	0.68	0.9998	7.2E-08	-0.009	1.7E-06	0.112	6.4E-05	2.186	0.001	0.053	7.7E-05	6.316	0.005	0.58
	22	0.78	0.9999	2.4E-08	-0.009	9.5E-07	0.155	1.7E-05	1.735	0.000	0.045	2.2E-05	6.743	0.002	0.57
	29	0.75	0.9970	1.2E-06	-0.009	7.5E-06	0.132	1.3E-04	1.917	0.003	0.044	1.6E-04	7.250	0.018	0.57
Pre-aged 2	0	0.77	0.9985	5.1E-07	-0.010	7.1E-06	0.131	1.0E-04	2.472	0.003	0.040	1.3E-04	8.770	0.020	0.67
	4	0.77	0.9998	7.6E-08	-0.009	2.0E-06	0.157	3.2E-05	1.540	0.001	0.046	4.1E-05	6.167	0.004	0.52
	10	0.67	0.9998	7.0E-08	-0.008	1.7E-06	0.105	2.6E-05	1.659	0.001	0.053	3.0E-05	7.210	0.003	0.55
	16	0.86	0.9998	7.0E-08	-0.009	2.9E-06	0.162	2.9E-05	2.030	0.001	0.027	3.5E-05	8.835	0.010	0.57
	23	0.73	0.9998	3.3E-08	-0.008	1.4E-06	0.080	1.6E-05	1.687	0.001	0.029	1.5E-05	8.574	0.004	0.38

[*] *The fitting function for Vac_3 at 22 days did not converge. Here a two-step fitting procedure was chosen: (1) Determination of t_1 from the first 6 hours of desorption using a monoexponential decay function, and then fitting the curve in the range 10-40 hours to the biexponential decay function using fixed A_1 and t_1.*

Table S2. *Transition temperatures (T*) obtained from DSC measurements of vacuumed and pre-aged samples.*

Sample	Contact time days	*T** °C	*T** °C	*T** °C	*T** °C	*T** °C	T^*_{AV} °C	*SD* °C
Vac 1	0	38.3	39.8	38.3	37.9	38.4	38.5	0.7
	5	41.2	40.5	41.4	41.8	41.6	41.3	0.5
	10	40.5	40.7	40.5	41.8	41.3	40.9	0.6
	16	43.6	41.6	41.3			42.2	1.3
	22	41.4	42.5	41.9	42.1	41.8	41.9	0.4
	29	41.3	42.4	41.4	42.0	42.3	41.9	0.5
Vac 2	0	39.6	39.9	40.0	40.8	40.3	40.1	0.5
	6	39.7	40.3	40.0	41.2	41.1	40.5	0.7
	10	41.8	40.9	41.1	41.2	42.4	41.5	0.6
	16	41.9	42.0	41.2	42.2	41.6	41.8	0.4
	22	41.2	41.2	41.2	43.8	42.4	42.0	1.1
Vac 3	0	38.4	39.4	39.8			39.2	0.7
	7	38.9	40.8	39.7			39.8	0.9
	10	40.0	39.9	40.4			40.1	0.3
	16	41.4	40.9	40.3			40.9	0.5
	22	41.0	39.9	41.7	42.3		41.2	1.1
	29							
re-aged 1	0	43.8	43.4	45.4	44.1	36.7	42.7	3.4
	10	42.0	42.4	39.9	43.4	42.4	42.0	1.3
	16	42.4	43.6	46.3	42.9	42.1	43.4	1.7
	22	42.2	41.6	44.1	44.3		43.0	1.4
	29	42.4	42.1	42.7	43.3	43.4	42.8	0.6
Pre-aged 2	0	42.0	44.0	43.2	42.1		42.8	1.0
	4	40.6	-	40.3	44.4	41.9	41.8	1.9
	10	43.5	42.2	43.4	41.6	42.0	42.5	0.8
	16	42.2	41.7	44.3		44.2	43.1	1.3
	23	41.9	41.2	39.9	43.9	42.8	41.9	1.5

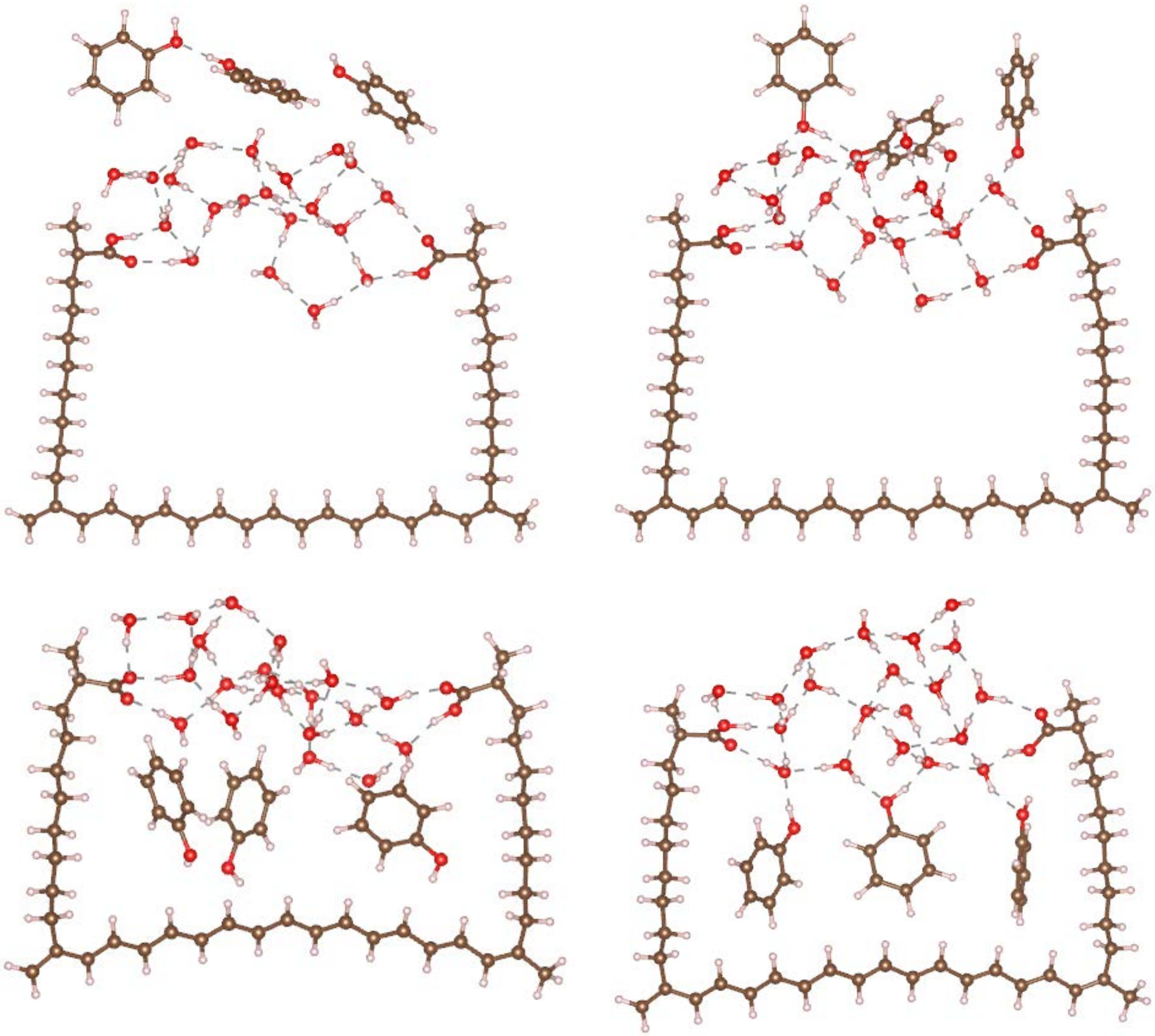

Figure S2. *COSMO optimized geometries of phenol-WaMB-SOM with different mutual position of phenol molecules with respect to the WaMB chain (models 1-4 from left to right) in polar environment (methanol). Atom color scheme: C – brown, O – red, and H – white.*

Table S3. *Fitting parameters obtained from relation between t1 resp t2 and T* for vacuumed and pre-aged samples. The error given for the slope correspond to the standard error of the slope obtained by linear regression. The parameters highlighted in green suggest some relation between the time constant and T*. Criteria were: p <0.05 respective: "standard error of slope is smaller than slope"*

	slope /h °C^{-1}	**Prob.>F**	**Pearson R**	**Corr. R2**
t_1_vac	0.16 ± 0.07	0.0311	0.5394	0.2403
t_2_vac	0.26 ± 0.26	0.3419	0.2543	-0.0021
t_1_pre-aged	0.30 ± 0.18	0.1310	0.5112	0.1690
t_2_pre-aged	0.65 ± 0.94	0.5075	0.2382	-0.0612
t_1_all	0.16 ± 0.04	0.0015	0.5913	0.3226
t_2_all	0.25 ± 0.20	0.2105	0.2540	0.0255