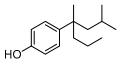
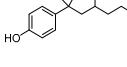
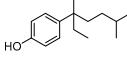
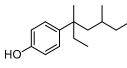
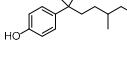
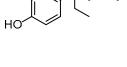
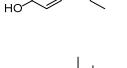
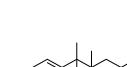
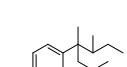
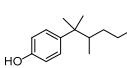
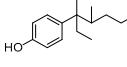
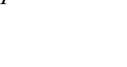


Supporting Information:

Table S1. Names, structures, side chain lengths and substituents of 4-NP isomers.

	Structures	Nomenclature	The length of side chain	α substitute	β substitute
NP ₁		4-[1,3-dimethyl-1-n-propylbutyl]phenol	4	Me, Pr	Et
NP ₂		4-[1,1,3-trimethylhexyl]phenol	6	Me, Me	None
NP ₃		4-[1-ethyl-1,4-dimethylpentyl]phenol	5	Me, Et	Me
NP ₄		4-[1-ethyl-1,3-dimethylpentyl]phenol	5	Me, Et	Me
NP ₅		4-[1,1,4-trimethylhexyl]phenol	6	Me, Me	None
NP ₆		4-[1-ethyl-1,3-dimethylpentyl]phenol	5	Me, Et	Me
NP ₇		4-[2-ethyl-1,1-dimethylpentyl]phenol	5	Me, Me	Et
NP ₈		4-[1,2-dimethyl-1-n-propylbutyl]phenol	4	Me, Pr	Me, Et
NP ₉		4-[1-ethyl-1,2-dimethylpentyl]phenol	5	Me, Et	Me, Me
NP ₁₀		4-[1,2-dimethyl-1-n-propylbutyl]phenol	4	Me, Pr	Me, Et
NP ₁₁		4-[1,1,2-trimethylhexyl]phenol	6	Me, Me	Me
NP ₁₂		4-[1-ethyl-1,2-dimethylpentyl]phenol	5	Me, Et	Me, Me

a: Me represents methyl; Et represents ethyl; Pr represents propyl; i-Pr represents isopropyl.

Table S2. The physicochemical properties of the soils

	China soil	Florida soil
pH	7.88	6.20
CEC (cmol/kg)	6.88	4.20
TOM (%)	4.77	15.37

Note: TOM indicates total organic matter. CEC: Cation exchange capacity.

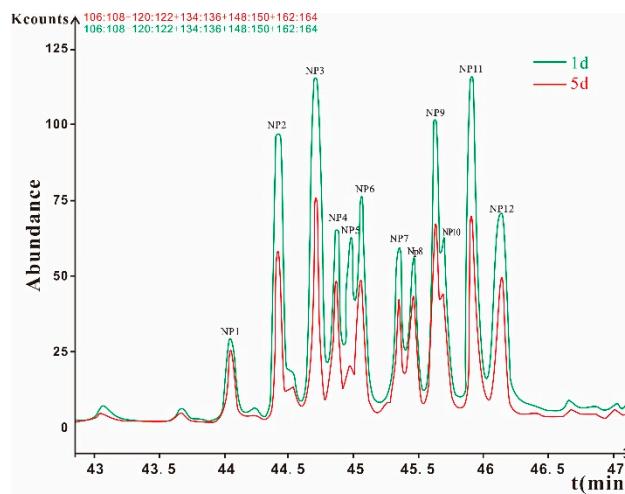


Fig. S1. Spectra of NP isomers during degradation in CN soil on the 1st and 5th day

Table S3. Molecular connection index of NP isomers

	NP1	NP2	NP3	NP4	NP5	NP6	NP7	NP8	NP9	NP10	NP11	NP12
$^1\chi^v$	6.273	6.452	6.633	6.339	6.254	6.339	6.32	6.21	6.58	6.21	6.28	6.58
$^2\chi^v$	4.347	5.009	5.94	4.564	5.2	4.564	5.58	5.023	6.193	5.023	5.026	6.193
$^4\chi^v_{pc}$	4.036	4.487	5.54	3.937	3.48	3.937	4.62	4.12	5.12	4.12	3.22	5.12

Table S4. Steric hindrance and I_{dwbar} of NP isomers

	NP1	NP2	NP3	NP4	NP5	NP6	NP7	NP8	NP9	NP10	NP11	NP12
Steric	1.496	1.456	1.481	1.488	1.448	1.488	1.488	1.517	1.510	1.517	1.477	1.510
I_{dwbar}	6.718	6.686	6.700	6.709	6.679	6.709	6.710	6.724	6.714	6.724	6.688	6.714