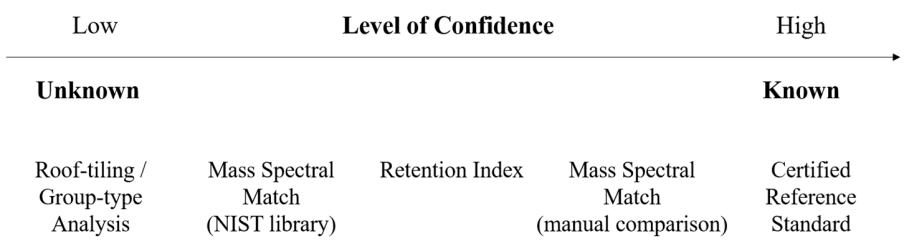
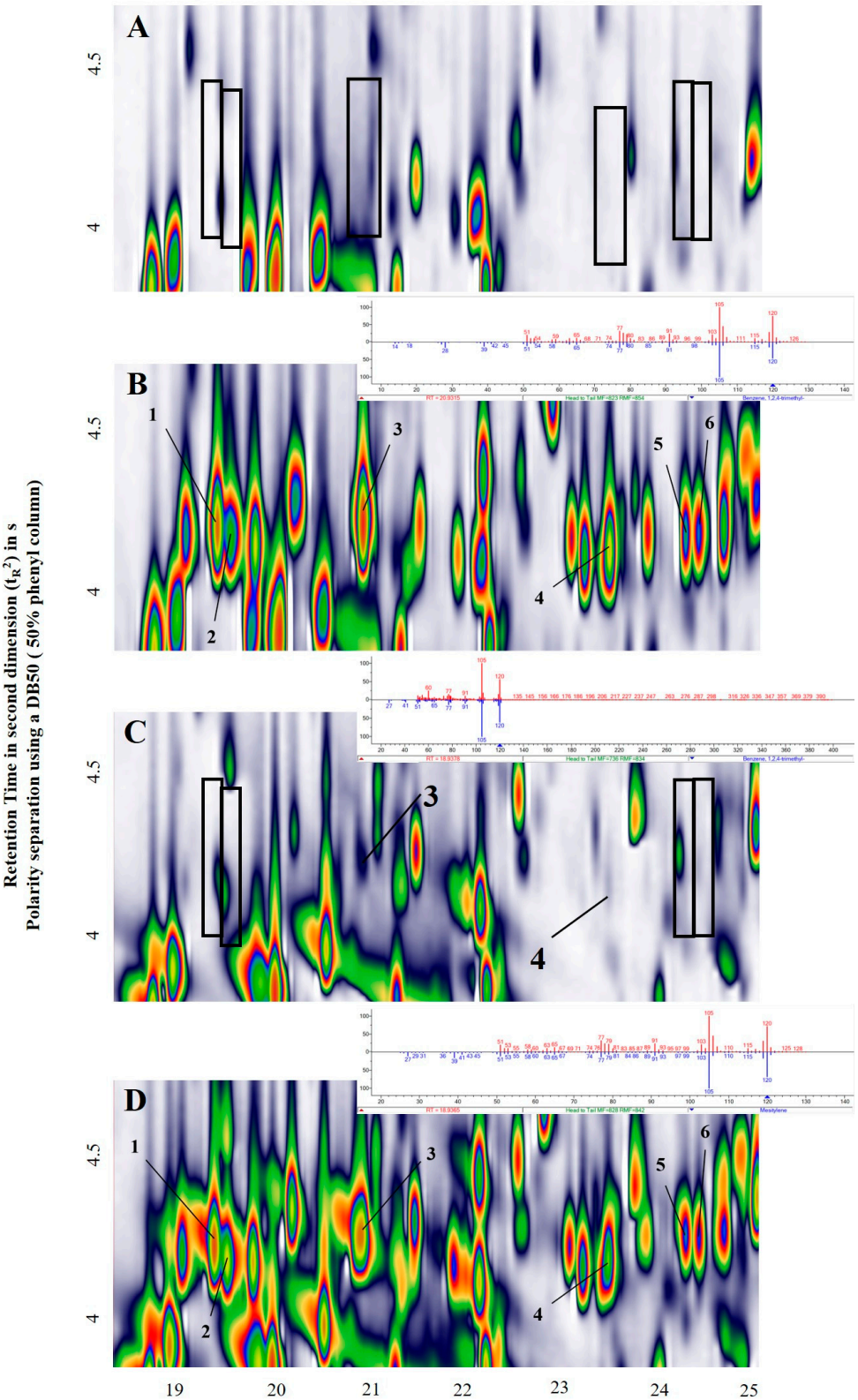
Compound Identification Strategy



Group	Compound	Identification Confidence
n-Alkanes	C_7 to C_{28}	Certified Reference Standard
Cyclohexanes	methyl- to decylcyclohexane	Mass Spectral Match (manual comparison)
Alkylated Aromatics	benzene, toluene, ethylbenzene, p- and m-xylene, o-xylene, propylbenzene, 3-ethyltoluene, 1,3,5-trimethylbenzene, 2-ethyltoluene, 4-ethyltoluene, 1,2,4-trimethylbenzene, 1,2,3-trimethylbenzene, 1-ethyl-2,3-dimethylbenzene, 1,2,4,5-tetramethylbenzene, 1,2,3,5-tetramethylbenzene, 1,2,3,4-tetramethylbenzene	Certified Reference Standard
	isopropylbenzene, propylbenzene, 1,3-diethylbenzene, 3- & 4-propyltoluene, 1,4-diethylbenzene, n-butylbenzene, 1-ethyl-3,5-dimethylbenzene, 1-ethyl-2,5-dimethylbenzene, 1-ethyl-3,4-dimethylbenzene, 1-ethyl-2,4-dimethylbenzene, isobutylbenzene, sec-butylbenzene, 3-, 4-, and 2-isopropyltoluene, 1,2,-dimethylbenzene, 2-propyltoluene, 1-ethyl-2,6-dimethylbenzene, isopentylbenzene, 1-tert-butyl-2-methylbenzene, pentylbenzene, 1,3,5-trimethylbenzene, 1,2,4-trimethylbenzene, hexylbenzene	Mass Spectral Match (manual comparison)
Indanes	indane	Certified Reference Standard
	1-methylindane, 5-methylindane, 2-methylindane, 4,7-dimethylindane and dimethylindane isomers	Mass Spectral Match (manual comparison)
Condensed Ring Aromatics	naphthalene, 2-methylnaphthalene, 1-methylnaphthalene, 2-ethylnaphthalene, 1-ethylnaphthalene, acenaphthylene, acenaphthene, fluorene, phenanthrene, anthracene, fluoranthene, pyrene, benz(a)anthracene	Certified Reference Standard

	2,6- and 1,3- and 1,7-dimethylnaphthalene, 1,6-dimethylnaphthalene, 1,4-dimethylnaphthalene, 1,2-dimethylnaphthalene, 1,8-dimethylnaphthalene, 2,3-dimethylnaphthalene, 2,3,5-trimethylnaphthalene, trimethylnaphthalene isomers	Mass Spectral Match (manual comparison)
Other	2,6-dimethyloctane, 2,2-dimethyl-3-octene, 1,1,2-trimethyl-3-(2-methylpropyl)-cyclopropane	Retention Index

Figure S1. Analyte identification strategy and corresponding identification confidence for target compounds in this study.


A
B
C
D
1
2
3
4
5
6
4.5
4
19
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25
Retention Time in second dimension (t_R^2) in s
Polarity separation using a DB50 (50% phenyl column)
Retention Time in first dimension (t_R^1) in mins
Boiling point separation using a DB5 (5% phenyl column)

Figure S2. Chromatogram area showing statistically significant target compounds from chemometric analysis with wood matrix blank (A), spiked wood matrix (B), NBC-2GB (C), and DB-2GB (D). Compound annotations (where compounds are present) refer to 3-Ethyltoluene (1), 4-Ethyltoluene (2), 1,2,4-Trimethylbenzene (3), 1-Ethyl-3,5-Dimethylbenzene (4), 1-Ethyl-2,5-Dimethylbenzene (5), and 1-Ethyl-2,4-Dimethylbenzene (6). With the exception of the matrix blank, where none of the target compounds were present, each chromatogram also displays the mass spectral comparison for 1,2,4-Trimethylbenzene (3) between the obtained spectrum (red, top) and the library spectrum (blue, bottom).