



Impact of heat treatment on database recall and metabolomic fingerprints used for timber identification employing direct analysis in real time time-of-flight mass spectrometry

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Received: 26 February 2025 / Accepted: 30 April 2025 / Published online: 5 June 2025
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Abstract

Illegal logging is a profitable transnational crime, prompting the development of global reference databases to support tools for identifying wood species and harvest location. While these tools are effective for raw timber, they have not been systematically evaluated for manufactured wood products which undergo high temperature, pressure, and steam treatments. Although it is known that these treatments alter wood's chemical composition, no chemical technique has demonstrated its ability to generalize measurements from raw wood to its manufactured form. This paper examines the impact of heat treatments and plywood manufacturing on metabolomic fingerprints and database recall for timber species identification. Processes included plywood manufacturing of *Betula pendula* and lab-based heat treatments (72 °C to 250 °C) for *Cedrela odorata* and *Dalbergia nigra* (both CITES-listed), as well as *Diospyros crassiflora* and *Araucaria cunninghamii*. The database recall for *D. crassiflora* and *D. nigra*, both dark woods, were largely unaffected by temperature whereas the database recall decreased with increasing temperatures for *C. odorata* (species-level database recall dropping below 30% after 24 h at 200 °C and continuing to decline with longer treatments) and *A. cunninghamii* (species-level database recall dropping below 10% after 24 h at 150 °C and continuing to decline with longer treatments) and due to manufacturing processes of the *B. pendula* plywood (manufacturer, using a single tree for each plywood batch. The logs were soaked and pressed at 120–135 °C). The findings underscore the need for (1) complementary identification methods for manufactured wood products and (2) further research into how manufacturing processes impact the effectiveness of identification and traceability methods under development.

Introduction

The illegal timber trade has garnered global attention, with both government agencies and private sectors alike involved in the fight against illegal trade and deforestation. To tackle the presence of illegal wood found in trade, many methods have been developed for wood identification and harvest location determination based on wood anatomy, genetics and chemistry. Each of these techniques depend on global reference databases that can be used to determine or validate the harvest location or identity of the wood sample from an opaque supply chain (Low et al. 2022). These databases are often constructed from raw or minimally treated wood. However, the interception of illegal timber can occur at any point in the supply chain, including after processing which can include heat treatments of more than 71 °C (200 °F), as in the case of plywood to extreme chemical, thermal, or enzymatic modifications (Radics et al. 2017; Ali et al. 2021).

According to a 2016 UNODC report, plywood accounts for the largest share of international trade and the highest percentage of illegal production among the three primary wood products: roundwood, lumber, and plywood (Gan et al. 2016). Generally, plywood manufacturing is composed of nine steps with several heat-based steps with temperatures reaching 93 °C using hot water baths, steam heat, hot water spray, or a combination of the three. Drying temperatures can reach 150 °C to 200 °C and press temperatures can be 132 °C to 165 °C (EPA 2002). These heat treatments alter the chemical composition of wood by degrading cellulose, hemicellulose, lignin, and extractives. Extractives, which consist primarily of secondary metabolites formed from the metabolism of primary compounds during heartwood formation, are commonly used for species identification in various chemical analysis methods. However, their response to manufacturing processes can significantly influence the applicability and reliability of downstream identification techniques.

For example, in *Acacia* treated at 210 °C to 230 °C for 2 h to 6 h, lignin and extractives initially increase with temperature but decrease over time, while hemicellulose and hydroxyl groups consistently decline (Esteves et al. 2008; Tuong and Li 2011). *Eucalyptus* shows similar trends for autoclave and oven treatments of 2 h to 24 h at 170 °C to 200 °C, with the authors reporting extractive content rising in the form of increasing water and ethanol extractives due to polysaccharide degradation then falling during continued treatment (Esteves et al. 2008). The rates of these chemical changes can also be impacted by wood properties and dimensions. Choong and Skaar (1972) observed that moisture diffusivity in wood increases with thickness, and surface emissivity is inversely proportional to thickness. This relationship suggests that thinner wood sections, such as veneers, may allow for faster migration and potential depletion of extractives during thermal processing. Since extractives often contain key metabolomic markers used for species classification, their loss during manufacturing could diminish the reliability of chemical fingerprint-based identification methods.

Lumber is typically kiln-dried at temperatures ranging from 110 to 200 °F (43 °C to 71 °C), depending on factors such as wood species, thickness, and ultimately the desired moisture content (Wengert 2010; Yin and Liu 2021). For

instance, conventional kilns often begin drying at temperatures between 100 and 130 °F (38 °C to 54 °C) when the lumber's moisture content is above 50%. As drying progresses and moisture content decreases, temperatures may be gradually increased to facilitate further drying. Drying schedules are controlled to ensure that the wood reaches the target moisture content without causing defects such as cracking or warping (Hermawan et al. 2024). The specific temperatures and durations used can vary based on the type of wood and its intended use.

The chemical changes (e.g., reduction in extractives, degradation of chemical profile) in wood present methodological questions to all chemistry-based species or harvest location identification methods including infrared spectroscopy, stable isotope ratio analysis, metabolomic profiling, x-ray fluorescence, trace element analysis et cetera. In addition to chemical methods, genetic methods also require additional considerations for method development and applicability of raw timber to processed counterparts. For instance, ancient DNA and related methods have shown promise in extraction from heat treated products but efficiency remains a barrier (Jiao et al. 2020).

Direct Analysis in Real Time Time-of-Flight Mass Spectrometry (DART-TOFMS) collects the untargeted metabolomic fingerprint, also called chemical profile or chemical fingerprint in literature, of wood and is a well-established tool for species identification (Brunswick et al. 2021; Cody et al. 2012; Evans et al. 2017; Lancaster and Espinoza 2012; McClure et al. 2015; Paredes-Villanueva et al. 2018; Price et al. 2021b) with support for origin verification or screening (Deklerck et al. 2020b; Finch et al. 2017; Price et al. 2021a). The Forensic Spectra of Trees (ForeST©) Database held by the National Fish and Wildlife Forensics Laboratory (Ashland, OR, USA) contains the untargeted metabolomic fingerprints generated by DART-TOFMS of protected and commercially relevant wood species. While original recommendations for database use were limited to JEOL-line DART-TOFMS, cross-platform applicability has been demonstrated recently, increasing database accessibility (Lancaster et al. 2024). In the species determination of an unknown wood sample the recommended use of the ForeST© database occurs in three steps, generally:

1. Search for candidate species, “hits”, in the database based on the spectrum of the “unknown” sample.
2. Visually compare the unknown to the candidate species.
3. Develop a classification model using the candidate species reference spectra and apply the unknown.

With respect to the first step, the selection of correct hits (true positives or candidates species to develop the classification models downstream) from spurious hits (false positives rejected for downstream classification) and for the complex wood spectra can be weighted based on “prior probability factors” described by Stein (2012) may include: (1) Expert opinion from a chemist familiar with the analyte; (2) Frequency of the compound in analyses of similar mixtures; and (3) The number of citations (e.g., replicates in the database) for the compound. To account for these factors in the ForeST© (v2021) framework, expert review of the hit list and

spectral data enhances confidence in positive identifications, while replicate spectra increase the number of supporting “citations.” A detailed walkthrough and underlying assumptions for using the database are provided in the GTTN Data Analysis Guide (Deklerck et al. 2020a). While an intermediate validation study (Price et al. 2022) of the complete method for tropical hardwoods demonstrated accuracy of species identification for genera in Fabaceae ($n = 7$) and Meliaceae ($n = 3$), previous studies have relied on limited models rather than untargeted database searches that would be more reflective of regulatory scenarios.

This study examines how the veneer and plywood manufacturing process for birch, along with lab-based heating experiments (from 72 to 250 °C) and autoclaving, affect database recall for three high-value hardwoods and one softwood. The species studied include the CITES-listed *Cedrela odorata* and *Dalbergia nigra*, as well as commercially significant *Diospyros crassiflora* and *Araucaria cunninghamii*. The lab-based heating experiments utilizing a muffle furnace and autoclave serve as proxies to some manufacturing kiln processes. Notably, our study applied time and temperature conditions that exceeded those typically used in standard commercial kiln drying, and did not monitor moisture content to explore the stability of the metabolomic fingerprint under extreme thermal conditions. The investigation uses (1) cosine similarity and heatmap evaluation to show chemical change in the metabolomic fingerprints and (2) an untargeted search of the ForeST© metabolomic fingerprint database, meaning that species identification is based on a database search with no pre-set limitations or species filters. Database or library recall, the fraction of accurate instances among all those retrieved from the search of the database, addresses the first step of species identification and has broader implications in the downstream analysis. We evaluate the database recall at each taxonomic level (species, genus, and family) in relation to temperature, time, and surface area. In the context of wood materials, surface area refers to the exposed outer surface of the wood that interacts with the surrounding environment—be it during chemical extraction, thermal treatment, or analytical techniques like direct analysis mass spectrometry. Wood slivers, chips, fiber, and veneer sheets have a greater *proportion* of the cellular matrix exposed, meaning more cell walls, extractives, and compounds relative to the total are accessible at the surface as compared to larger dimension wood.

Materials and methods

Lab-based heat treatment

Chemically validated reference samples of *Cedrela odorata*, *Diospyros crassiflora*, *Dalbergia nigra*, and *Araucaria cunninghamii* were obtained from the US Fish and Wildlife Forensics Laboratory xylarium. Each sample was subsampled into three groups: (1) 21 blocks of approximately 1 cm³ for temperature-by-time experiments, (2) five slivers for control spectra, and (3) an additional 20 slivers allocated for autoclave treatments. For each temperature and time combination, five pseudoreplicate slivers were analyzed, except for the autoclave condition, which used three pseudoreplicates. This sampling scheme is summarized in the block diagram (Table 1).

Table 1 Block diagram summary of lab-based heat treatments. Each time-block uses a unique subsection of the original reference specimen

Treatment	Control	Muffle Furnace								Autoclave
Sample type during heat treatment	n/a	Wood Block "cubes"				Slivers				Cubes
Temperature	n/a	72 °C, 100 °C, 150 °C, 200 °C, or 250 °C				72 °C				121 °C
Time (hours)	n/a	2	8	24	48	2	8	24	48	0.5
Pseudoreplicate slivers	5	5	5	5	5	5	5	5	5	3

Wood slivers generally measure 1–2 mm thick, 2–5 mm wide, and 1–2 cm long. Chemical validation was performed by confirming that the metabolomic fingerprint aligned with established species-level signatures sourced from several sources including academic institutions, private collections, commercial suppliers.

Temperature x Time Study: Subsampled blocks were put in a muffle furnace (Thermolyne 1300, Thermo Scientific) for 2, 8, 24, or 48 h and then each block was subsampled (i.e., a sliver was cut from the block) 5 times for analysis by DART-TOFMS. This process was repeated on fresh wood blocks for every temperature (72 °C, 100 °C, 150 °C, 200 °C, and 250 °C). One block per species was placed in an autoclave (Tuttnauer Model 5596) at 121 °C and 15 psi for 30 min and 5 slivers were subsampled for DART-TOFMS analysis.

Surface Area Study: From the same reference samples used above, an excess of 20 slivers per species were heated at 72 °C in the muffle furnace. At each time point (2 h, 8 h, 24 h, and 48 h), five slivers per species were removed for DART-TOFMS analysis (4 times × 5 slivers = 20 spectra/species).

Plywood

One *Betula pendula* log was sourced from Latvia and another from Estonia. Each log was assigned a unique number and traced through the manufacturing process, with subsamples collected at each stage. Plywood production was carried out by a private manufacturer, using a single tree for each plywood batch. The logs were soaked in water at 40 °C for 24 h, then peeled and separated. The wet veneer was matched to the corresponding log number to maintain traceability. Plywood samples were then pressed using two different adhesives: a phenol-based adhesive ("Prefere") at 135 °C and a melamine-based adhesive ("Melfemo") at 125 °C. Each log yielded a plywood sample with phenol-based adhesive, a plywood sample with melamine-based adhesive, a veneer, and a stem disk sample containing both heartwood and sapwood. From each sample, ten slivers were collected for DART-TOFMS analysis. The outermost layer of the plywood samples was carefully subsampled to avoid including the adhesive layers between the plies. Additionally, a separate subsample containing adhesive was analyzed and compared to the wood spectra to confirm that adhesive components were not contributing to the plywood spectral profiles (data not shown).

Mass spectrometry

Positive ion-mode mass spectra were collected using a time-of-flight mass spectrometer (AccuTOF 4G, JEOL, USA, INC., Peabody, MA, USA) attached to a DART ion source (IonSense Inc., Saugus, MA, USA) using helium at 350 °C as the ionizing gas. The mass spectrometer parameters were set at: electrode 1, 150 V; electrode 2 voltage 250 V; Orifice 1, 120 °C and 30 V; ring lens, orifice 2, 5 V; ion guide RF voltage 600 V, focus lens −120 V. Dataset was acquired by scanning mass-to-charge ratio (m/z) 90–1000 at a sampling interval of 0.25 ns and recording interval at 0.80 s with a manufacturer stated resolving power of > 6000 full-width at half maximum. Total ion chromatograms were calibrated with polyethylene glycol 600 (Sigma-Aldrich, St. Louis, MO, USA), averaging 3–5 s of scans, and then exported to centroided text files.

Computational analysis

A frequency plot m/z and relative intensities, or heatmap, of lab-based heat treatment spectra and a heatmap for plywood spectra was compiled using Mass Mountaineer (version 6.07.6.0, RBC Software, Peabody, MA., USA): Mass Mountaineer was used to align m/z and export mass spectra as a csv-files with a 20 millimass unit (mmu; 0.001 Da) threshold (heatmaps available in SI). Rstudio (2023.06.0 + 421 "Mountain Hydrangea") was used for statistical analysis including cosine similarity calculations and pairwise significance tests. See Supplementary Information 1 (SI1) for additional figures and SI2 for complete R code and relevant citations with package versions (Hadley 2016; Kassambara 2021; Ooms 2023; Wickham 2023; Wickham et al. 2019; Wickham and Seidel 2023; Zhu et al. 2019). Pairwise similarity was visualized using Microsoft® Excel® for Microsoft 365 MSO (Version 2407 Build 16.0.17830.20166) (Fig. 4).

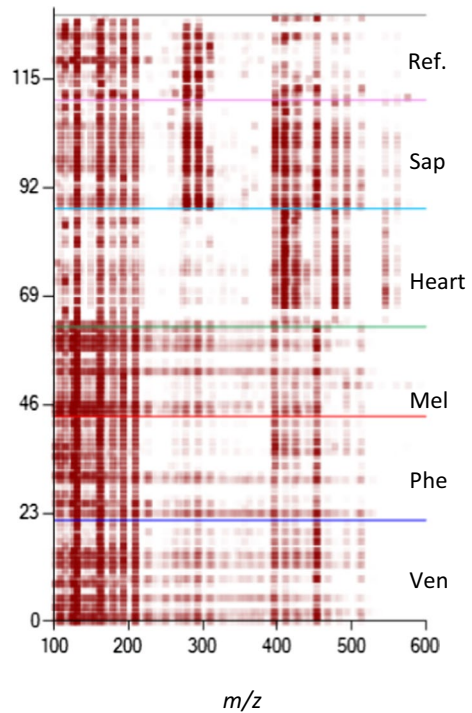
To calculate the database recall, each mass spectrum was searched against the ForeST© library Angiosperms v2021 database with 14,664 reference spectra for hardwoods and ForeST© library Gymnosperms v2020 with 1500 reference spectra for the softwoods, using “forward” search and a 5 mmu mass tolerance. The top 15 hits from each search were recorded. The recall of the database search was calculated by comparing the correct species, genus, and family to the 15 hits.

Results and discussion

Plywood

The spectra of *Betula pendula* from the georeferenced logs were compared to the reference database (Fig. 1). The spectra of the "raw" sapwood closely matched the reference database, consistent with the sapwood spectra achieving the highest recall in the database. The spectra of the melamine-based adhesive plywood, phenol-based

Fig. 1 Heatmap of the *Betula pendula* reference spectra (Ref), raw sapwood (Sap), raw heartwood (Heart), melamine-based adhesive plywood (Mel), phenol-based adhesive plywood (Phe), and veneer (Ven)



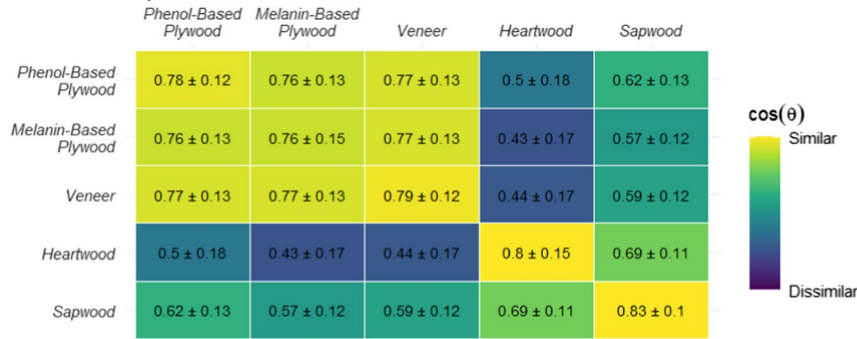
adhesive plywood, and veneer were similar to each other, as reflected by the cosine similarity scores (Fig. 2A). Cosine similarity is a common method for demonstrating spectral similarity in metabolomics and is widely used tool to evaluate near-identical spectra (Huber et al. 2021; Stein and Scott 1994). These scores indicated consistent intra- and inter-group similarities, along with a consistent dissimilarity to the heartwood and sapwood spectra.

The database recall (Fig. 2B) for sapwood was ~57% and fell to 30.7% (Mel.), 39.1% (Phe), and 41.8% (Veneer). The veneer may have a slightly higher recall rate as it undergoes fewer manufacturing steps compared to the layered plywood. Notably, the heartwood recall was on par with the phenol adhesive and veneer. This is possibly due to the database containing sapwood reference spectra and not heartwood.

Lab-based heat treatments

The heatmap of spectra for each species at different temperatures and times shows qualitative changes in metabolomic fingerprints due to heat treatments (Fig. 3). For the lab-based treatments, notable changes are observed in the 250 °C treatments across all species, with some species showing changes at lower temperatures. At 24 h at 200 °C, *C. odorata* shows loss of the original high-intensity signals starting at m/z 194 (highlighted in heatmap). Degradation and new compound appearance can

A Cosine Similarity Score Matrix



B Database Recall Summary Statistics

Type	Species (%)			Genus (%)			Family (%)	
	μ	±	σ	μ	±	σ	μ	σ
Sapwood	57.4	±	6.4	57.4	±	6.4	66.7	10
Heartwood	44.5	±	7.2	44.5	±	7.2	46.7	9.2
Melanin Adhesive Plywood	30.7	±	13.3	30.7	±	13.3	36.2	9
Phenol Adhesive Plywood	39.1	±	10.2	39.1	±	10.2	42.4	9.9
Veneer	41.8	±	7.5	41.8	±	7.5	43	9.2

Bold* *Paired t-test to show significant difference at 95 % confidence interval from sapwood.

Fig. 2 (A) Cosine similarities of the raw and manufactured birch plywood products. (B) Mean (μ) and standard deviation (σ) for the database recall of the first 15 hits of *Betula pendula* plywood ($n = 10$ replicates from 2 logs), Betulaceae, from an untargeted database search of > 14,000 reference spectra

be most easily observed for *A. cunninghamii* (SI1 Fig. 1). In *A. cunninghamii*, there is a shift in intensity from mid-range masses around m/z 411 to lower masses and at 250 °C, m/z 163 signal is lost, and at 24 h at 250 °C, m/z 149 becomes a prominent peak. At 250 °C the *Dalbergia* genus-significant ion m/z 375 caviunin (Kite et al. 2010), and mid-range *D. crassiflora* m/z decrease in relative intensity and the intensity shifts from mid to lower mass ranges. This pattern likely reflects the degradation of volatile extractives and the appearance of new compounds due to cell wall breakdown and chemical changes during heat treatment (Esteves and Pereira 2009).

The heatmap highlights considerable variation in metabolomic fingerprints even within a single individual. For example, in *A. cunninghamii* treated at both 72 °C and 150 °C, the m/z 229 signal shows notable variability. This may result from sample inhomogeneity or inconsistencies in ionization-zone introduction, rather than from the heat treatment itself. Although wood is a structured, three-dimensional material, thin slivers analyzed via ambient ionization often expose different cell types and irregular surfaces, leading to uncontrollable variability in the ionization process. Previous studies have shown that spatial variation in metabolite distribution correlates with anatomical features (Mai and Zhang 2023); vessels and parenchyma tend to yield more diverse ion signals compared to fibers (Deklerck et al. 2022) as well as between early wood and latewood (Kim and Daniel 2016). Our findings support that natural variation in metabolomic fingerprints within a single tree can be

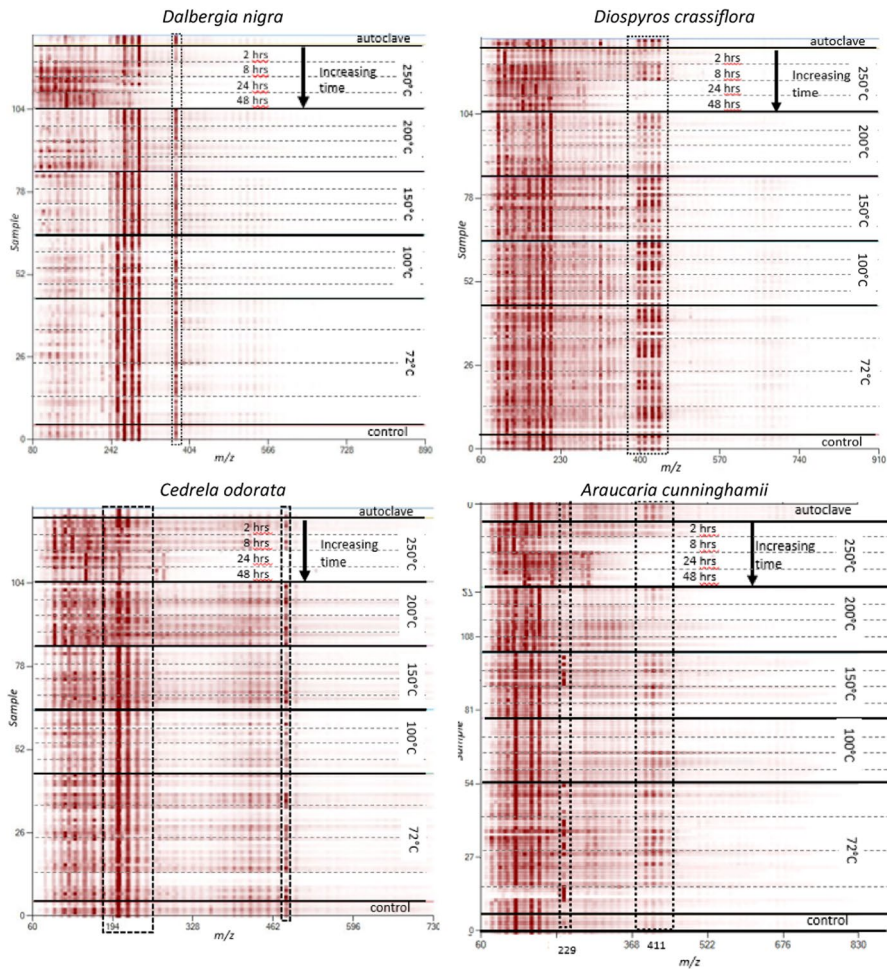


Fig. 3 Heat map representation of lab-based heat treatment spectra. Each row represents a reference spectrum, and each column is the relative intensity (m/z) with color as an indication of the intensity of the ion. Heating time (48, 24, 8, 2 h) is organized down the y axis. Control ($n=5$), 72 °C ($n=40$; 20 from cube and 20 from slivers with $n=5$ per time period), 100–250 °C ($n=20$; 5 replicate $\times$ 4 times), autoclave ($n=3$)

substantial. However, this intra-sample or intra-species variability is generally not greater than the inter-species differences used in classification, as demonstrated by successful species-level discrimination of *A. cunninghamii* in Evans et al. (2017).

These sources of variation, spatial heterogeneity and ionization dynamics, should be embraced when designing reference databases. Pseudoreplication of rare specimens can help capture the natural variability within a species, especially when limited reference material is available. Ideally, such replication is complemented by broad sampling across individuals, as is done in the ForeST© Database. Importantly, replicate analysis of a single individual can also help contextualize intra-species

variation, reducing the risk of misclassifying such variability as analytical or sampling error.

Cosine similarity

The cosine similarity of all spectra demonstrated a degradation in the metabolomic fingerprint as the heat treatments increased in length and temperature. The degradation of the metabolomic fingerprint had varying degrees of impact on the database recall. The trends observed in the heat map evaluation are reflected in the changes to the cosine similarity. Cosine similarity for all results ranged from ~1, indicating the average spectra for each treatment are very similar, to approaching 0, indicating the spectra are distinct from another. Detailed heatmap representation of the average cosine similarity (CS) values are in SI1 Figs. S2–S5. Except for outlier results from *Araucaria* at 8 h and 48 h at 72 °C, all species show a consistent pattern of decline in the average CS of the control to each subsequent heat treatment (Fig. 4). The most significant CS decline tended to start at 8 h at 200 °C, earlier than is visually noted in the heatmap Fig. 3.

Database recall

Table 2 shows the overall mean and standard deviation for each treatment by temperature and time, with graphical representation in the box and whiskers plot

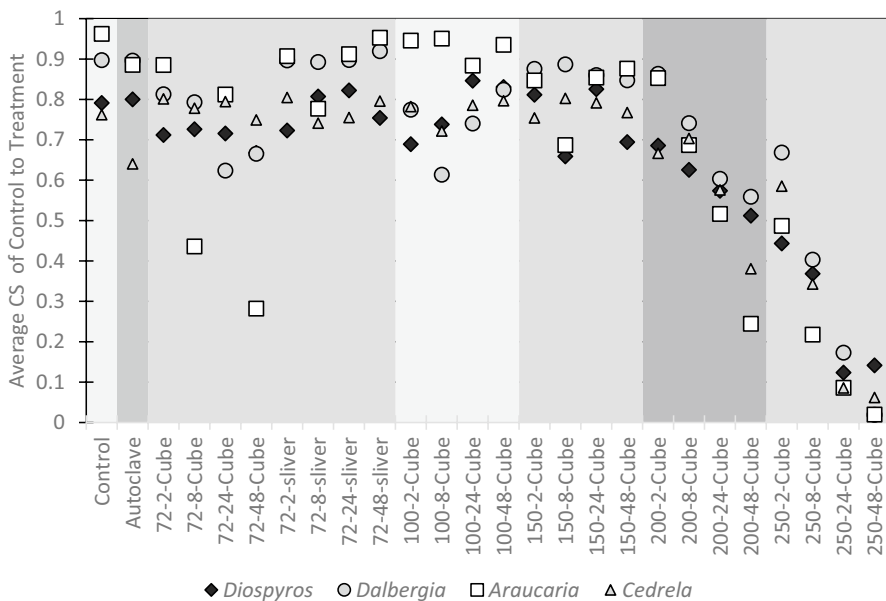


Fig. 4 Average cosine similarity of the control ($n = 5$), for each muffle furnace heat treatment ($n = 5$), and autoclave ($n = 3$). Labels are formatted Temperature (°C) – Time (hours) – Type (sliver or cube)

Table 2 Mean (μ) and standard deviation (σ) ($n = 5$ for all muffle furnace treatments and $n = 3$ for autoclave) for the database recall of the first 15 hits for each species. **Bold and highlighted cells** denote paired t -test that show significant difference at 95% confidence interval from the control

Type	Temp	Time (h)	<i>Diospyros crassiflora</i>						<i>Cedrela odonata</i>						<i>Araucaria cunninghamii</i>											
			Species (%)		Genus (%)		Family (%)		Species (%)		Genus (%)		Family (%)		Species (%)		Genus (%)		Family (%)							
			μ	σ	μ	σ	μ	σ	μ	σ	μ	σ	μ	σ	μ	σ	μ	σ	μ	σ	μ	σ				
Cube	Control	0	77	± 15	100	± 0	100	± 0	45	± 42	91	± 13	91	± 13	35	± 7	52	± 11	75	± 9	0	± 0	20	± 14	32	± 10
		0.5	87	± 12	100	± 0	100	± 0	76	± 25	100	± 0	100	± 0	27	± 7	53	± 7	62	± 10	8.9	± 10	27	± 12	40	± 12
	72	2	72	± 23	100	± 0	100	± 0	45	± 32	87	± 19	87	± 19	12	± 7	24	± 10	39	± 15	12	± 9	29	± 13	47	± 21
		8	88	± 9	100	± 0	100	± 0	69	± 17	100	± 0	100	± 0	16	± 6	27*	± 12	39	± 12	23	± 10	84	± 13	88	± 7
	24	78	± 30	100	± 0	100	± 0	47	± 17	100	± 0	98	± 3	24	± 5	40	± 9	50	± 9	7	± 8	30	± 21	50	± 25	
100	48	48	81	± 24	100	± 0	100	± 0	57	± 35	97	± 6	97	± 6	15	± 14	31	± 11	37	± 21	21	± 14	73	± 28	7	± 25
		2	80	± 19	100	± 0	100	± 0	48	± 24	99	± 3	99	± 3	23	± 14	43	± 21	57	± 23	8	± 9	21	± 15	35	± 21
	8	8	79	± 26	100	± 0	100	± 0	53	± 17	100	± 0	100	± 0	15	± 10	37	± 17	49	± 22	5	± 9	15	± 15	19	± 21
		24	76	± 43	100	± 0	100	± 0	39	± 39	100	± 0	100	± 0	25	± 6	43	± 20	60	± 13	15	± 9	27	± 16	39	± 22
	48	92	± 6	100	± 0	100	± 0	56	± 33	99	± 3	99	± 3	31	± 17	43	± 18	57	± 23	15	± 6	36	± 8	55*	± 11	
150	2	2	89	± 10	100	± 0	100	± 0	40	± 35	97	± 6	97	± 6	19	± 12	36	± 14	49	± 22	16	± 6	51	± 28	67	± 19
		8	91	± 6	100	± 0	100	± 0	49	± 15	97	± 4	97	± 4	29	± 8	39	± 13	59	± 10	19	± 10	55	± 26	63	± 27
	24	24	79	± 12	100	± 0	100	± 0	32	± 34	95	± 12	95	± 12	31	± 8	44	± 16	60	± 14	9	± 6	20	± 11	28	± 19
		48	77	± 11	100	± 0	100	± 0	39	± 30	97	± 4	97	± 4	31	± 9	49	± 13	61	± 18	5	± 3	15	± 6	17	± 6
	200	2	87	± 7	100	± 0	100	± 0	65	± 33	99	± 3	99	± 3	32	± 6	43	± 9	68	± 22	5	± 3	16	± 9	25	± 22
200	8	8	93	± 8	100	± 0	100	± 0	32	± 44	95	± 9	95	± 9	19	± 9	36	± 15	55	± 24	4	± 4	16	± 9	21	± 15
		24	68	± 24	93	± 8	96	± 9	16	± 32	92	± 11	92	± 11	15	± 12	29	± 19	53	± 21	1	± 3	9	± 9	15	± 7
	48	51	± 28	76	± 26	88	± 20	7	± 7	97	± 4	97	± 4	1	± 3	8	± 11	47	± 40	1	± 3	12	± 7	19	± 10	

Table 2 (continued)

Type	Temp	Time (h)	<i>Dalbergia nigra</i>						<i>Diospyros crassiflora</i>						<i>Cedrela odonata</i>						<i>Araucaria cunninghamii</i>					
			Species (%)		Genus (%)		Family (%)		Species (%)		Genus (%)		Family (%)		Species (%)		Genus (%)		Family (%)		Species (%)		Genus (%)		Family (%)	
			μ	$\pm \sigma$	μ	$\pm \sigma$	μ	$\pm \sigma$	μ	$\pm \sigma$	μ	$\pm \sigma$	μ	$\pm \sigma$	μ	$\pm \sigma$	μ	$\pm \sigma$	μ	$\pm \sigma$	μ	$\pm \sigma$	μ	$\pm \sigma$	μ	$\pm \sigma$
250		2	84	± 4	100	± 0	100	± 0	1	± 3	64	± 37	64	± 37	16	± 17	23	± 23	32	± 27	1	± 3	9	± 9	16	± 6
		8	22	± 21	44	± 40	59	± 54	16	± 17	99	± 3	99	± 3	5	± 9	16	± 12	27	± 23	1	± 3	12	± 6	15	± 7
		24	5	± 12	13	± 30	49	± 32	0	± 0	41	± 23	41	± 23	0	± 0	7	± 5	9	± 6	0	± 0	9.3	± 6	17	± 8
		48	0	± 0	0	± 0	24	± 6	0	± 0	36	± 19	36	± 11	0	± 0	5	± 3	5	± 3	0	± 0	5.3	± 6	21	± 17
Silver		2	83	± 6	100	± 0	100	± 0	13	± 21	92	± 11	92	± 11	29	± 6	47	± 8	65	± 21	5	± 6	28	± 24	36	± 30
		8	84	± 4	100	± 0	100	± 0	19	± 12	95	± 6	95	± 6	27	± 12	47	± 13	64	± 18	12	± 3	48	± 13	67	± 17
		24	84	± 8	100	± 0	100	± 0	68	± 21	100	± 0	100	± 0	35	± 6	48	± 15	70	± 9	10	± 9	33	± 19	47	± 30
		48	81	± 9	100	± 0	100	± 0	43	± 34	97	± 6	97	± 6	41	± 3	53	± 13	71	± 19	4	± 9	21	± 23	35	± 29

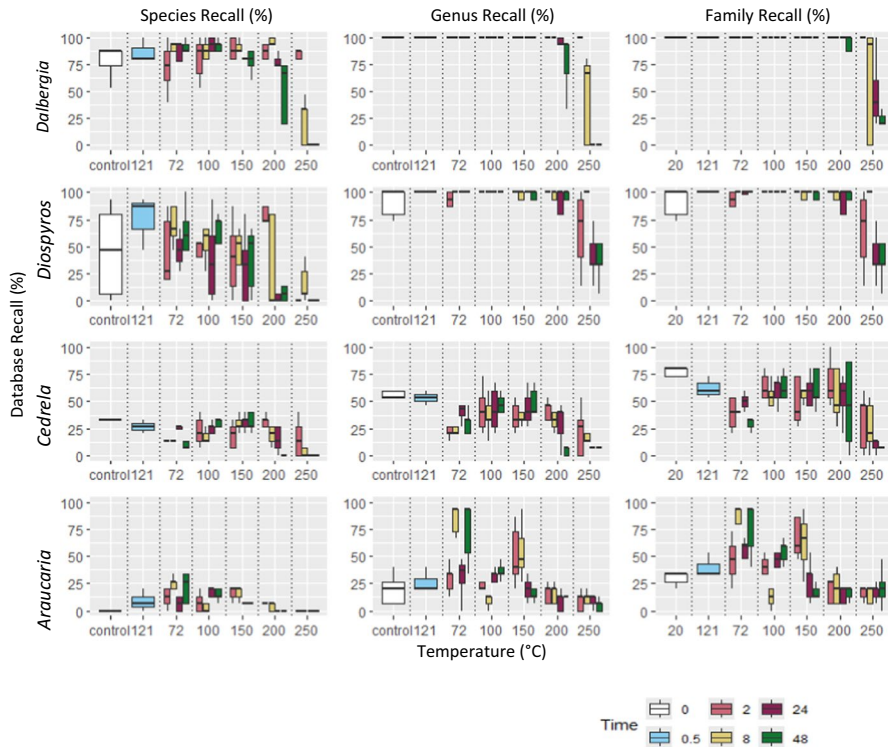


Fig. 5 Box and whiskers plot for recall of the database search for species, genus, and family, column 1–3 respectively, of *Dalbergia nigra*, *Diospyros crassiflora*, *Cedrela odorata*, and *Araucaria cunninghamii* (rows 1–4, respectively), excluding sliver samples

Fig. 5. In Table 2, the bold and highlighted boxes denote paired t-test that show significant difference at 95% confidence interval from the control, pre-treatment spectra.

***Dalbergia nigra*:** The metabolomic fingerprint remained stable up to 250 °C for 2 h before a significant drop in species-match recall (Fig. 5; row 1). Genus and family matches were accurate until treatments of 24 h at 250 °C where recall fell below 39% for genus and 58% for family matches. This drop corresponds to significant differences in genus-level recall for treatments at 200 °C and 250 °C over 2–48 h. Control and autoclave recalls were consistent with all temperature treatments except those more extreme than 24 h at 200 °C. Thus, heat treatments used in conventional manufacturing (e.g., below 200 °C and without chemical impregnation) have a minimal impact on the metabolomic fingerprint of *Dalbergia*.

***Diospyros crassiflora*:** The database recall for genus and family are the same which could be due to *Diospyros* being the only Ebenaceae genus in ForeST© 2021. Recall for both genus and family dropped significantly after 8 h at 200 °C and 8 h at 250 °C for species matches (Fig. 5; row 2). Rank sum analysis indicated that temperature treatments caused the largest differences in genus-level

recall, especially at 250 °C. For all treatments except at 250 °C, recall for genus and family matches was 90%. At 250 °C, recall fell to 60% for both taxonomic levels. Control and autoclave recall was consistent with other temperature treatments, except for 250 °C. Therefore, the chemical profile of dark *Diospyros*, whether autoclaved or heated up to 200 °C, is unlikely to adversely affect species-level database recall.

***Cedrela odorata*:** Genus matches for heat-treated samples ranged from 35 to 52%, dropping below 30% after 24 h at 200 °C and continuing to decline with longer treatments (Fig. 5; row 3). Control and autoclaved samples had higher genus-level recall at 52% and 53%, respectively, compared to the dry-heated samples. The data indicates that *C. odorata* can withstand up to 8 h at 200 °C while still providing a usable metabolic fingerprint for database searches at the genus level. However, average recall decreased from 52 to 36% from the control to 8 h at 200 °C, with the number of reported families and genera doubling, reflecting less precise and less accurate searches.

***Araucaria cunninghamii*:** Due to abnormal 0% species recall, genus-level comparisons are more reliable for evaluating the impact of heat treatments. The highest recall for *A. cunninghamii* was similar to the lowest recall for *C. odorata*. *Dalbergia nigra* treated for 48 h at 250 °C had higher recall than the best quality *A. cunninghamii* spectra where the highest recall was achieved at 8 h at 72 °C, with hits from ten genera and three families.

To determine whether the low species recall was due to the specific *A. cunninghamii* sample used for generating pseudoreplicate spectra or if it was characteristic of the taxa, we confirmed that the source sample was representative of the species and tested database recall of representative samples for *A. araucana* and *A. angustifolia* (SI1 Fig. 6). The *A. araucana* samples showed higher recall, achieving 100% at the family level and 90–100% at the genus level. In contrast, the recall for *A. angustifolia* was similar to that of *A. cunninghamii*. The improved recall for *A. araucana* is likely due to its more distinctive chemical profile, which may be attributed to higher intensity and/or a greater number of extractives in its heartwood.

Surface area consideration:

The impact of low-temperature heat on the chemistry of high-surface-area, sliver-sized wood was examined by comparing the impact of heat for slivers versus cubes at 72 °C (Fig. S7). The species match recall between slivers and cubes showed no significant difference except for *C. odorata* ($p \leq 0.001$), where slivers had higher recall. This suggests that the low heat treatments did not negatively affect the chemical profile of high-surface-area wood slivers. Although slivers treated at this low temperature cannot serve as proxies for veneer sheets, which experience higher temperatures and pressures, they represent the dimensions of slivers used to generate much of the ForeST© reference spectra.

The higher recall of the *D. crassiflora* and *D. nigra* compared to *A. cunninghamii* and *C. odorata* emphasizes the need to investigate the impact of heat treatment on identification methods. Historically used for furniture and instrument making, *Dalbergia* species can still be found in trade though as whole woods products, as in the

Hongmu furniture trade. Zhang et al. (2019) also evaluated Hongmu species *Pterocarpus santalinus* and *P. tinctorius* for chemical modifications in response to heat (120 °C for 10 day and 70 °C for 20 days) noting changes to the metabolomic fingerprint without losing species-differentiating features. In contrast, *Araucaria* species are commonly used for plywood which undergo the intensive heating/drying/pressing processes.

Diospyros crassiflora and *Dalbergia nigra* are both dense, dark woods—basic specific gravity ≥ 0.75 g/cm³ (Wheeler 2011). *Araucaria cunninghamii* and *Cedrela odorata* in comparison are lighter, less dense woods, basic specific gravity 0.48–0.60 and 0.40–0.75 g/cm³, respectively (Wheeler 2011). The recall rate differences are possibly due to (1) the higher number of extractives in their heartwood, (2) better retention of characteristic molecules, or (3) sampling bias in the database.

Database recall discrepancies can be influenced by sampling bias – unequal or unbalanced representations of spectra representing natural variation which can bias results. Within the database, *Dalbergia* has hundreds of spectra, including 95 from *D. nigra*. *Diospyros* has extensive representation with hundreds of spectra, including 54 from *D. crassiflora*. In contrast, *A. cunninghamii* is represented by only 30 individuals, alongside approximately 100 specimens from other species in the genus. *Cedrela odorata* has data from over 110 individuals and several hundred other specimens within the genus. *Dalbergia nigra* with the larger representation in the database would likely represent more variation than a species with fewer representatives. Despite lower genus-level recall of *Cedrela* in this study (52%), compared to *Dalbergia*, this does not imply low identification accuracy in practice. For example, studies by Evans et al. (2017) on *Araucaria* and Paredes et al. (2018) on *Cedrela* confirm that DART-TOFMS remains reliable for identifying species in these genera. In contrast to *A. cunninghamii*, *B. pendula* had fewer representatives in the database (19 individuals), and no other species in the genus represented, and still had higher recall. Notably, database recall of the *B. pendula* sample was distinctively from sapwood and the ForeST© Database references, based on heatmap analysis (Fig. 1) were also sapwood – while Price et al 2022 demonstrated how sapwood can have spurious results in the ForeST© Database, the *B. pendula* example here demonstrates a clear match for sapwood. Further, the diagnostic peaks (higher m/z) were maintained for both heartwood and sapwood with similar relative intensities. Peaks associated with being dominant in sapwood, m/z 131.050, 163.075, 179.070, were more intense in the sapwood, veneer, and manufactured plywood spectra.

Interpretations of database recall rates benefit from an understanding of the underlying variation in recall of species independently. For example, the *A. cunninghamii* recall results, especially in contrast to the *D. nigra*, could present methodological implications for identification downstream of the database search result if one is expecting similar recall. The impact of the variable database recall is ameliorated by the downstream steps used in classification. To explicitly account for database recall, and as a standard practice in many analytical identification schemes, running a known reference sample of the candidate species simultaneous to the unknown would assist in determining recall probability for the database. This systematic evaluation of database recall for the candidate species in an unknown identification would demonstrate the “probability of obtaining

the measured properties of the questioned-source specimen had it come from the known source” which is the most appropriate measure for assessing validity of an identification (Morrison et al. 2017).

The database recall for *A. cunninghamii* demonstrates prior probability tools for interpreting recall. For all treatments below 72 °C (n = 40 spectra; 675 hits), *A. cunninghamii* had a recall of 41% for true positives and false positives included *Pinus* (17%), *Agathis* (12%), and 10 other genera (30%). While lower spectral uniqueness of *A. cunninghamii* resulted in low database recall, the prior probability for positive *A. cunninghamii* identification is improved due to the ratio of hits. To further increase probability of accurate identification, the spectra are compared head to tail matches (SI1 Fig. 8 and Fig. 9) and multivariate models are generated for classification or prediction. This methodology is well established in the use of mass spectral libraries (Stein 2012).

The variable database recall for treated timber and sapwood *B. pendula* illustrates the complex application of mass spectral reference libraries in timber. Jankowska et al. (2020) offer a maxim that can be appreciated by all forensic scientists working with wood: “Wood, as a complex structure, is a material for which it is difficult to formulate general conclusions.” This paper supports the claim enthusiastically.

Many practitioners of chemical identification using DART-TOFMS advocate for incorporating additional wood characteristics—such as fluorescence, anatomy, and density—to enhance identification accuracy (Carmona et al. 2020; Deklerck et al. 2021; Price et al. 2021a, 2021b). Depending on the degree of wood manipulation, different tools may be needed to enhance identification or add prior probability to database searches – for instance wood anatomy can often achieve genus-level identification (Gasson et al. 2021). Each identification technique has strengths and weaknesses, and only a synergistic approach will yield the highest accuracy in species identification. Untargeted database searches can benefit from traditional wood anatomy, helping refine results based on anatomical traits. These refinements can range from broad distinctions like gymnosperms vs. angiosperms to more specific genera-level limiters.

The elevated temperatures used in this study more closely resemble torrefaction processes, where biomass (including wood) is heated to 250 °C to 300 °C for 10 to 20 min in an oxygen-free environment (Radics et al 2017). However, torrefied wood has not yet been the focus of metabolomic investigations using DART-TOFMS. A limitation of this study is that spectra were generated using only a single reference sample per species, except for the *B. pendula* plywood, which does not account for potential variations in a species’ response to heat. Differences in tree density, influenced by environmental factors, could lead to varying levels of chemical retention. Additionally, the data was collected by a single analyst using one instrument at specific time intervals and so some batch effects may be observed in the data. Nevertheless, the trend of increasingly altered metabolomic fingerprints with more extreme treatments likely outweighs any potential systematic errors. Moreover, while exact manufacturing conditions couldn’t be replicated in-house, the high heat, steam, and pressure typical of plywood processing are realistically expected to affect metabolomic fingerprints as shown with the *B. pendula* veneer and plywood.

Conclusion

This paper evaluated the effectiveness of database searches for identifying the taxa of kiln- and autoclaved-heated wood, using the processes as proxies for some common manufacturing practices. At low temperatures, in-lab muffle furnace heated wood being most similar to kiln dried wood and the high-humidity of autoclaving being adjacent to plywood manufacturing practices. Plywood manufacturing, which often involves illegal wood, uses processes like hot water baths, steam heat, or hot water spray. In a real-life example, *Betula pendula* plywood was also investigated – tracing the same tree from raw wood through the veneer and plywood process. Based on these manufacturing conditions and existing research on wood's chemical changes, this study suggests that manufactured products like plywood have reduced database recall, *depending on the species*, which has the potential to complicate identification efforts.

Currently, no large-scale species or origin identification techniques (whether chemical, genetic, isotopic, etc.) have proven effective or otherwise for use of raw wood *to its manufactured forms* and work is required as a community of practice to establish the bounds and limitations. The complexity of global supply chains and manufacturing processes, which can alter wood's chemical and genetic profiles, highlights the challenges in monitoring illegal wood. To improve the effectiveness of global reference databases in combating illegal timber trade, the impact of manufacturing on wood composition should be systematically studied for each identification method, whether genetic, chemical, or image-based, especially when legality frameworks require genus or species-level taxonomy and high-resolution geographic inference.

Supplementary Information The online version contains supplementary material available at <https://doi.org/10.1007/s00226-025-01666-2>.

Acknowledgements The authors thank the enumerable contributions from collaborating institutions and individuals, past and present, that have made the ForeST© Database possible.

Author Contributions CAL: Conceptualization, Investigation, Methodology, Formal analysis, Visualization, Software, Writing—Original Draft, Editing. PJM and ERP Investigation, Data collection, Writing – Review & Editing. VD: Conceptualization, Writing—Review & Editing.

Funding CL was covered in part by Defra International Climate Finance Programme [Project 29084].

Data Availability Data is provided within the manuscript or supplementary information files.

Declarations

Conflicts of Interest Statement The authors declare that they have no competing financial interests. The findings and conclusions in this article are those of the authors and do not necessarily represent the views of the U.S. Fish and Wildlife Service or the U.S. Forest Service, the Royal Botanical Gardens, Kew, Meise Botanic Garden, or World Forest ID. The authors declare no competing interests.

Compliance with Ethical Standards This article does not contain any studies with human and/or animal participants performed by any of the authors.

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