

## SUPPLEMENTARY INFORMATION

### Flavourings, nicotine content, and elemental composition as indicators of regulatory compliance in nicotine pouches and heated tobacco products

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Table S1: Nicotine pouches (NPs) sample designations and their brand (reported as NP-X and B-X, respectively, where X represents the sample or brand number), reported nicotine content, reported mass of NPs, and reported compounds.

Sample designation (Brand)	Reported nicotine content [mg/NP]	Reported mass of NP [g]	Reported compounds on the labelling
NP-1 (B-1)	16.4	1	Salt, cellulose, xanthan gum, water, NaHCO <sub>3</sub> , natural aromatic oils, propylene glycol (PG)
NP-2 (B-1)	12.3	0.75	Salt, cellulose, xanthan gum, water, NaHCO <sub>3</sub> , natural aromatic oils, (PG)
NP-3 (B-1)	12.3	0.75	Salt, cellulose, xanthan gum, water, NaHCO <sub>3</sub> , natural aromatic oils, (PG)
NP-4 (B-1)	12.3	0.75	Salt, cellulose, xanthan gum, water, NaHCO <sub>3</sub> , natural aromatic oils, (PG)
NP-5 (B-2)	4	0.42	Cellulose, water, NaCl, aromas, xylitol, nicotine, PG, sucralose, NaHCO <sub>3</sub>
NP-6 (B-2)	4	0.42	Cellulose, water, NaCl, aromas, xylitol, nicotine, PG, sucralose, NaHCO <sub>3</sub>
NP-7 (B-2)	6	0.42	Cellulose, water, NaCl, aromas, xylitol, nicotine, PG, sucralose, NaHCO <sub>3</sub>
NP-8 (B-2)	10	0.7	Cellulose, water, NaCl, aromas, xylitol, nicotine, sodium alginate, sucralose, NaHCO <sub>3</sub>
NP-9 (B-2)	8	0.7	Cellulose, water, NaCl, aromas, xylitol, nicotine, sodium alginate, sucralose, NaHCO <sub>3</sub>
NP-10 (B-2)	10.9	0.7	Cellulose, water, NaCl, aromas, xylitol, nicotine, sodium alginate, NH <sub>4</sub> Cl, NaHCO <sub>3</sub> , acesulfame potassium
NP-11 (B-2)	10	0.7	Cellulose, water, NaCl, aromas, xylitol, nicotine, sodium alginate, sucralose, NaHCO <sub>3</sub>
NP-12 (B-2)	14	0.7	Cellulose, water, nicotine polacrilex, NaCl, aromas, xylitol, nicotine, NaOH, sucralose, NaHCO <sub>3</sub>

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<b>NP-13 (B-2)</b>	17	0.7	Cellulose, water, nicotine polacrilex, NaCl, aromas, xylitol, nicotine, NaOH, sucralose, NH <sub>4</sub> Cl, NaHCO <sub>3</sub> , acesulfame potassium
<b>NP-14 (B-2)</b>	14	0.7	Cellulose, water, nicotine polacrilex, NaCl, aromas, xylitol, nicotine, NaOH, sucralose, NH <sub>4</sub> Cl, NaHCO <sub>3</sub> , acesulfame potassium
<b>NP-15 (B-3)</b>	9	0.7	Cellulose, water, plant fibers, glycerol (GLY), NaCl, nicotine, aromas, tartaric acid, Na <sub>2</sub> CO <sub>3</sub> , CaCl <sub>2</sub> , acesulfame potassium
<b>NP-16 (B-3)</b>	11	0.7	Cellulose, water, GLY, PG, NaCl, nicotine, aromas, tartaric acid, Na <sub>2</sub> CO <sub>3</sub> , CaCl <sub>2</sub> , acesulfame potassium
<b>NP-17 (B-3)</b>	11	0.7	Cellulose, water, GLY, PG, NaCl, nicotine, aromas, tartaric acid, Na <sub>2</sub> CO <sub>3</sub> , CaCl <sub>2</sub> , acesulfame potassium, ethanol
<b>NP-18 (B-3)</b>	11	0.7	Cellulose, water, GLY, PG, NaCl, nicotine, aromas, tartaric acid, Na <sub>2</sub> CO <sub>3</sub> , CaCl <sub>2</sub> , acesulfame potassium, ethanol
<b>NP-19 (B-4)</b>	8.25	0.5	Cellulose, water, K <sub>2</sub> CO <sub>3</sub> , PG, aromas, nicotine, food preservative
<b>NP-20 (B-4)</b>	8.25	0.5	Cellulose, water, K <sub>2</sub> CO <sub>3</sub> , PG, aromas, nicotine, food preservative
<b>NP-21 (B-4)</b>	13.2	0.8	Cellulose, water, K <sub>2</sub> CO <sub>3</sub> , PG, aromas, nicotine, food preservative
<b>NP-22 (B-4)</b>	8.25	0.5	Cellulose, water, K <sub>2</sub> CO <sub>3</sub> , PG, aromas, nicotine, food preservative
<b>NP-23 (B-5)</b>	12	0.8	Cellulose, water, plant fibers, GLY, PG, NaCl, nicotine, aromas, tartaric acid, Na <sub>2</sub> CO <sub>3</sub> , CaCl <sub>2</sub> , acesulfame potassium, ethanol
<b>NP-24 (B-5)</b>	12	0.8	Cellulose, water, plant fibers, GLY, PG, NaCl, nicotine, aromas, tartaric acid, Na <sub>2</sub> CO <sub>3</sub> , CaCl <sub>2</sub> , acesulfame potassium, ethanol
<b>NP-25 (B-5)</b>	16.5	1.05	Cellulose, water, plant fibers, GLY, PG, NaCl, nicotine, aromas, tartaric acid, Na <sub>2</sub> CO <sub>3</sub> , CaCl <sub>2</sub> , acesulfame potassium, ethanol, triacetin
<b>NP-26 (B-5)</b>	15.5	1	Cellulose, water, plant fibers, GLY, salt, nicotine, aromas, NaHCO <sub>3</sub> , tartaric acid, CaCl <sub>2</sub> , acesulfame potassium

Table S2: Average NP mass, deviation from the reported mass on the labelling, average NP moisture content, and average pouch mass  $\pm$  respective standard deviation (s) from three replicates.

<b>Sample designation</b>	<b>Average NP mass <math>\pm</math> s [mg]</b>	<b>Deviation from the reported mass [%]</b>	<b>Average NP moisture content <math>\pm</math> s [%]</b>	<b>Average pouch mass <math>\pm</math> s [mg]</b>
NP-1	1021.9 $\pm$ 23.5	2.2	55.1 $\pm$ 1.9	27.2 $\pm$ 2.0
NP-2	734.1 $\pm$ 19.2	-1.6	53.6 $\pm$ 0.8	21.4 $\pm$ 0.7
NP-3	731.7 $\pm$ 24.9	-1.8	53.3 $\pm$ 0.5	18.1 $\pm$ 1.2
NP-4	695.7 $\pm$ 30.4	-5.4	52.1 $\pm$ 0.8	22.9 $\pm$ 2.6
NP-5	407.6 $\pm$ 42.6	-1.2	40.6 $\pm$ 1.0	50.9 $\pm$ 2.1
NP-6	400.7 $\pm$ 14.7	-1.9	35.1 $\pm$ 1.9	44.9 $\pm$ 1.9
NP-7	442.5 $\pm$ 33.8	2.3	34.9 $\pm$ 0.5	45.6 $\pm$ 1.9
NP-8	679.9 $\pm$ 59.4	-2.0	46.1 $\pm$ 3.2	57.0 $\pm$ 2.2
NP-9	701.7 $\pm$ 104.5	0.2	44.9 $\pm$ 0.7	65.6 $\pm$ 2.5
NP-10	630.9 $\pm$ 176.6	-6.9	43.9 $\pm$ 0.4	68.1 $\pm$ 3.6
NP-11	681.1 $\pm$ 3.2	-1.9	50.6 $\pm$ 0.6	60.8 $\pm$ 6.2
NP-12	679.9 $\pm$ 53.4	-2.0	47.0 $\pm$ 2.1	55.4 $\pm$ 1.0
NP-13	725.8 $\pm$ 35.8	2.6	46.0 $\pm$ 1.4	74.2 $\pm$ 1.4
NP-14	690.5 $\pm$ 12.3	-0.9	41.5 $\pm$ 0.5	72.6 $\pm$ 1.0
NP-15	623.1 $\pm$ 17.2	-7.7	36.0 $\pm$ 1.1	66.8 $\pm$ 1.8
NP-16	718.5 $\pm$ 18.9	1.9	51.3 $\pm$ 0.6	62.2 $\pm$ 3.5
NP-17	638.5 $\pm$ 11.5	-6.1	44.5 $\pm$ 0.6	54.2 $\pm$ 0.8
NP-18	604.6 $\pm$ 7.7	-9.5	41.1 $\pm$ 0.8	57.4 $\pm$ 2.2
NP-19	493.2 $\pm$ 4.0	-0.7	37.3 $\pm$ 0.8	55.3 $\pm$ 2.4
NP-20	474.8 $\pm$ 4.3	-2.5	39.1 $\pm$ 1.0	49.6 $\pm$ 1.4
NP-21	812.3 $\pm$ 16.2	1.2	47.9 $\pm$ 0.9	70.3 $\pm$ 2.5
NP-22	488.1 $\pm$ 1.6	-1.2	38.7 $\pm$ 0.3	58.1 $\pm$ 0.9
NP-23	816.5 $\pm$ 58.8	1.7	40.5 $\pm$ 0.4	57.3 $\pm$ 1.4
NP-24	819.2 $\pm$ 22.6	1.9	40.4 $\pm$ 0.3	49.0 $\pm$ 2.1
NP-25	991.5 $\pm$ 23.9	-5.9	39.5 $\pm$ 0.3	58.2 $\pm$ 1.5
NP-26	961.6 $\pm$ 11.6	-3.8	40.1 $\pm$ 0.3	66.3 $\pm$ 4.1

Table S3: Heatsticks (HSs) sample designations and their brand (reported as HS-X and B-X, respectively), HS mass, heatstick filler (HSF) mass, filter mass, paper mass, polyactic acid filter mass, and susceptor mass  $\pm$  respective s.

Sample designation (Brand)	Average HS mass $\pm$ s [mg]	Average HSF mass $\pm$ s [mg]	Average filter mass $\pm$ s [mg]	Average paper mass $\pm$ s [mg]	Average polyactic acid filter mass $\pm$ s [mg]	Average susceptor mass $\pm$ s [mg]
HS-1 (B-6)	703.1 $\pm$ 8.3	238.2 $\pm$ 10.7	100.1 $\pm$ 1.8	137.9 $\pm$ 7.3	227.1 $\pm$ 6.1	/
HS-2 (B-6)	709.2 $\pm$ 3.7	248.9 $\pm$ 4.4	99.9 $\pm$ 2.1	131.0 $\pm$ 1.8	228.5 $\pm$ 4.0	/
HS-3 (B-6)	710.2 $\pm$ 0.9	243.3 $\pm$ 5.0	107.1 $\pm$ 2.8	131.5 $\pm$ 0.4	226.9 $\pm$ 4.1	/
HS-4 (B-6)	713.0 $\pm$ 6.7	251.6 $\pm$ 1.7	99.0 $\pm$ 3.2	130.5 $\pm$ 1.1	230.3 $\pm$ 7.5	/
HS-5 (B-6)	705.4 $\pm$ 2.0	246.7 $\pm$ 2.8	96.9 $\pm$ 0.9	133.6 $\pm$ 7.4	227.1 $\pm$ 8.5	/
HS-6 (B-7)	716.2 $\pm$ 2.6	245.4 $\pm$ 2.5	107.6 $\pm$ 2.9	135.5 $\pm$ 1.3	226.2 $\pm$ 4.5	/
HS-7 (B-7)	718.9 $\pm$ 2.3	249.8 $\pm$ 2.9	108.3 $\pm$ 1.3	131.9 $\pm$ 0.8	228.0 $\pm$ 2.0	/
HS-8 (B-7)	721.2 $\pm$ 5.1	252.4 $\pm$ 4.3	108.4 $\pm$ 2.2	132.4 $\pm$ 1.3	226.2 $\pm$ 4.5	/
HS-9 (B-7)	720.6 $\pm$ 1.3	251.6 $\pm$ 0.6	108.1 $\pm$ 1.0	135.9 $\pm$ 0.7	224.3 $\pm$ 3.0	/
HS-10 (B-8)	597.3 $\pm$ 3.2	252.0 $\pm$ 2.0	210.4 $\pm$ 4.7	112.5 $\pm$ 2.4	/	20.3 $\pm$ 0.1
HS-11 (B-8)	606.0 $\pm$ 9.0	266.3 $\pm$ 11.0	206.1 $\pm$ 0.9	111.6 $\pm$ 2.8	/	20.7 $\pm$ 0.8
HS-12 (B-8)	599.9 $\pm$ 5.5	261.6 $\pm$ 7.6	206.7 $\pm$ 1.9	110.7 $\pm$ 0.9	/	20.2 $\pm$ 0.3
HS-13 (B-8)	591.8 $\pm$ 6.6	247.5 $\pm$ 5.1	208.3 $\pm$ 4.6	113.8 $\pm$ 3.0	/	20.9 $\pm$ 0.2
HS-14 (B-8)	583.1 $\pm$ 2.2	247.5 $\pm$ 2.9	204.7 $\pm$ 2.7	110.6 $\pm$ 1.6	/	19.8 $\pm$ 0.2
HS-15 (B-8)	585.2 $\pm$ 5.1	245.8 $\pm$ 5.7	202.2 $\pm$ 8.1	116.1 $\pm$ 4.9	/	20.0 $\pm$ 0.2
HS-16 (B-8)	595.6 $\pm$ 3.7	252.5 $\pm$ 2.7	207.2 $\pm$ 6.2	114.7 $\pm$ 1.9	/	20.5 $\pm$ 0.2

Table S4: Inductively coupled plasma-mass spectrometry operating conditions for the analysis of 18 elements in HSs and NPs.

<b>Interface</b>	Cu sampler and skimmer cone
<b>Sampling depth of the ICP-MS torch</b>	5.0 mm
<b>Cooling chamber temperature</b>	5 °C
<b>Radiofrequency power</b>	1.20 kW
<b>Ar plasma gas flow</b>	9.0 L/min
<b>Ar auxilliary gas flow</b>	1.10 L/min
<b>Ar carrier gas flow</b>	0.70 L/min
<b>He collision cell flow</b>	6.0 mL/min
<b>Collision cell voltage</b>	-21 V
<b>Collision cell energy filter</b>	7.0 V

Table S5: Weighted linear regression parameters and the sum of the absolute values of the relative errors ( $\sum|RE|$ ) for the unweighted and weighted models.  $A_{\text{nicotine}}$  represents the area under the chromatographic peak for nicotine, while  $A_{\text{quinoline}}$  represents the area under the chromatographic peak for quinoline.

<b>Model</b>	<b>Weighting factor (<math>w_i</math>)</b>	<b>Model slope</b> [ $(A_{\text{nicotine}} \cdot L) / (A_{\text{quinoline}} \cdot \text{mg})$ ]	<b>Model intercept</b> [ $A_{\text{nicotine}} / A_{\text{quinoline}}$ ]	<b>Model correlation coefficient</b>	<b><math>\sum RE </math> [%]</b>
<b>1 (unweighted model)</b>	1	0.0069	-0.0609	0.9981	53.6
<b>2</b>	$1/x_i^{0.5}$	0.0069	-0.0460	0.9986	36.3
<b>3</b>	$1/x_i$	0.0068	-0.0380	0.9987	27.1
<b>4</b>	$1/x_i^2$	0.0067	-0.0327	0.9981	22.2
<b>5</b>	$1/y_i^{0.5}$	0.0068	-0.0436	0.9986	33.5
<b>6</b>	$1/y_i$	0.0068	-0.0359	0.9987	24.8
<b>7</b>	$1/y_i^2$	0.0066	-0.0320	0.9979	21.9

Table S6: Average nicotine content  $\pm s$  in HSs expressed in both mg/g of HSF and in mg/HS.

	<b>Average nicotine content <math>\pm s</math></b> <b>[mg/g of HSF]</b>	<b>Average nicotine content <math>\pm s</math></b> <b>[mg/HS]</b>
<b>HS-1</b>	13.2 $\pm$ 0.1	3.1 $\pm$ 0.1
<b>HS-2</b>	14.0 $\pm$ 0.1	3.5 $\pm$ 0.1
<b>HS-3</b>	13.4 $\pm$ 0.1	3.3 $\pm$ 0.1
<b>HS-4</b>	15.5 $\pm$ 0.1	3.9 $\pm$ 0.1
<b>HS-5</b>	12.6 $\pm$ 0.1	3.1 $\pm$ 0.1
<b>HS-6</b>	14.2 $\pm$ 0.1	3.5 $\pm$ 0.1
<b>HS-7</b>	15.7 $\pm$ 0.5	3.9 $\pm$ 0.1
<b>HS-8</b>	16.4 $\pm$ 0.1	4.1 $\pm$ 0.1
<b>HS-9</b>	14.0 $\pm$ 0.1	3.5 $\pm$ 0.1
<b>HS-10</b>	15.5 $\pm$ 0.3	3.9 $\pm$ 0.1
<b>HS-11</b>	15.4 $\pm$ 0.2	4.1 $\pm$ 0.1
<b>HS-12</b>	15.3 $\pm$ 0.1	4.0 $\pm$ 0.1
<b>HS-13</b>	14.8 $\pm$ 0.1	3.7 $\pm$ 0.1
<b>HS-14</b>	14.5 $\pm$ 0.1	3.6 $\pm$ 0.1
<b>HS-15</b>	15.2 $\pm$ 0.1	3.7 $\pm$ 0.1
<b>HS-16</b>	16.6 $\pm$ 0.1	4.2 $\pm$ 0.1

Table S7: Average nicotine content  $\pm$  s in NPs, expressed in both mg/g of NPF and in mg/NP with deviation from the declared nicotine content.

	Average nicotine content $\pm$ s [mg/g of NPF]	Average nicotine content $\pm$ s [mg/NP]	Declared nicotine content [mg/NP]	Deviation from the declared nicotine content [%]
NP-1	11.9 $\pm$ 0.1	10.7 $\pm$ 0.1	16.4	-34.6
NP-2	16.2 $\pm$ 0.1	9.1 $\pm$ 0.1	12.3	-25.9
NP-3	12.7 $\pm$ 0.1	9.0 $\pm$ 0.1	12.3	-27.2
NP-4	16.8 $\pm$ 0.1	9.0 $\pm$ 0.1	12.3	-26.8
NP-5	7.6 $\pm$ 0.2	3.2 $\pm$ 0.1	4	-20.0
NP-6	8.4 $\pm$ 0.1	2.6 $\pm$ 0.1	4	-34.1
NP-7	12.3 $\pm$ 0.1	5.1 $\pm$ 0.1	6	-14.4
NP-8	14.7 $\pm$ 0.1	8.3 $\pm$ 0.1	10	-17.1
NP-9	12.3 $\pm$ 0.3	4.6 $\pm$ 0.1	8	-42.9
NP-10	12.9 $\pm$ 0.1	7.8 $\pm$ 0.1	10.9	-28.1
NP-11	14.5 $\pm$ 0.1	6.9 $\pm$ 0.1	10	-30.8
NP-12	19.5 $\pm$ 0.1	9.1 $\pm$ 0.1	14	-34.8
NP-13	20.0 $\pm$ 0.1	10.9 $\pm$ 0.1	17	-35.9
NP-14	15.6 $\pm$ 0.3	8.3 $\pm$ 0.1	14	-40.5
NP-15	13.1 $\pm$ 0.1	6.6 $\pm$ 0.1	9	-26.7
NP-16	8.8 $\pm$ 0.3	5.2 $\pm$ 0.1	11	-52.9
NP-17	17.8 $\pm$ 0.1	9.3 $\pm$ 0.1	11	-15.2
NP-18	14.1 $\pm$ 0.2	6.8 $\pm$ 0.1	11	-38.1
NP-19	12.9 $\pm$ 0.1	5.6 $\pm$ 0.1	8.25	-32.3
NP-20	10.8 $\pm$ 0.1	4.2 $\pm$ 0.1	8.25	-48.8
NP-21	14.2 $\pm$ 0.1	10.6 $\pm$ 0.1	13.2	-19.4
NP-22	9.5 $\pm$ 0.2	4.2 $\pm$ 0.1	8.25	-49.6
NP-23	14.7 $\pm$ 0.2	10.6 $\pm$ 0.1	12	-11.4
NP-24	15.0 $\pm$ 0.1	11.1 $\pm$ 0.1	12	-7.3
NP-25	17.8 $\pm$ 0.1	15.1 $\pm$ 0.1	16.5	-8.5
NP-26	15.5 $\pm$ 0.2	11.7 $\pm$ 0.2	15.5	-24.8

Table S8: ICP-MS validation parameters for 18 elements in HSs (CC in brackets indicates the use of a collision cell, while NCC stands for no collision cell), including the limit of detection (LOD), limit of quantification (LOQ), the linear concentration range, the square of the calibration coefficient ( $R^2$ ), accuracy (represented as recovery, Re), and precision (represented as the relative standard deviation, RSD).  $I_{HM}$  represents the intensity of the measured elements, while  $I_{IS}$  represents the intensity of the internal standard.

Measured element isotope	LOD [ng/L]	LOQ / [ng/L]	Determined linear concentration range [ $\mu$ g/L]	Slope / [ $(I_{HM} \cdot L) / (I_{IS} \cdot \mu$ g)]	Intercept [ $I_{HM}/I_{IS}$ ]	$R^2$	Re [%]	RSD [%]
<sup>27</sup> Al (CC)	137	456	0.5–400.0	0.1700	-0.0917	0.9997	88.5	1.2
<sup>75</sup> As (CC)	2	8	LOQ–30.0	3.1740	-0.0876	0.9999	102.1	0.3
<sup>137</sup> Ba (CC)	65	217	LOQ–60.0	0.4739	0.0161	0.9999	97.5	1.6
<sup>114</sup> Cd (NCC)	34	114	LOQ–30.0	0.8328	0.0481	0.9999	98.6	2.2
<sup>59</sup> Co (CC)	1	3	LOQ–30.0	36.2771	0.1563	1.0000	97.3	1.9
<sup>52</sup> Cr (CC)	2	6	LOQ–30.0	21.5125	0.8420	0.9999	97.8	2.0

<sup>65</sup> Cu (CC)	93	309	0.5–30.0	15.8204	-2.5067	0.9999	95.4	1.8
<sup>56</sup> Fe (CC)	26	86	5.0–300.0	18.4174	14.9390	0.9999	95.5	1.0
<sup>69</sup> Ga (CC)	3	10	LOQ–30.0	12.4596	0.0534	0.9999	96.6	1.6
<sup>55</sup> Mn (CC)	2	5	0.5–60.0	9.5439	0.3996	0.9999	96.3	1.3
<sup>98</sup> Mo (CC)	11	37	LOQ–30.0	2.0762	0.3576	0.9998	102.9	1.1
<sup>60</sup> Ni (CC)	2	7	LOQ–30.0	10.8297	0.3674	0.9999	96.9	2.5
<sup>207</sup> Pb (NCC)	72	239	LOQ–30.0	1.1265	0.1047	0.9997	98.1	2.2
<sup>118</sup> Sn (NCC)	113	376	LOQ–30.0	0.8901	0.0809	0.9998	101.6	1.0
<sup>88</sup> Sr (CC)	3	9	LOQ–60.0	12.5138	-0.4029	1.0000	96.0	1.7
<sup>47</sup> Ti (CC)	17	55	LOQ–60.0	0.3047	0.0539	0.9999	96.2	0.7
<sup>205</sup> Tl (NCC)	36	121	LOQ–30.0	3.6841	0.5110	0.9997	94.1	2.7
<sup>68</sup> Zn (CC)	21	72	5.0–50.0	5.0834	-2.1202	0.9998	86.2	3.8

Table S9: ICP-MS validation parameters for 18 elements in NPs (CC in brackets indicates the use of a collision cell, while NCC stands for no collision cell), including LOD, LOQ, the linear concentration range, R<sup>2</sup>, accuracy (represented as Re), and precision (represented as RSD).

Measured element isotope	LOD / [ng/L]	LOQ / [ng/L]	Determined linear concentration range / [µg/L]	Slope / [(I <sub>HM</sub> · L) / (I <sub>IS</sub> · µg)]	Intercept [I <sub>HM</sub> /I <sub>IS</sub> ]	R <sup>2</sup>	Re [%]	RSD [%]
<sup>27</sup> Al (CC)	252	839	5.0–60.0	0.1764	-0.0086	0.9996	90.5	1.1
<sup>75</sup> As (CC)	1	5	LOQ–30.0	2.9077	-0.0660	1.0000	101.9	1.2
<sup>137</sup> Ba (CC)	197	657	LOQ–30.0	0.4808	0.0186	1.0000	94.9	0.7
<sup>114</sup> Cd (NCC)	30	99	LOQ–30.0	0.7874	0.1054	0.9999	95.3	0.6
<sup>59</sup> Co (CC)	1	3	LOQ–25.0	35.0840	-0.8046	0.9999	89.8	0.9
<sup>52</sup> Cr (CC)	2	5	LOQ–30.0	23.5292	0.4932	0.9999	89.3	0.4
<sup>65</sup> Cu (CC)	129	431	LOQ–30.0	15.9876	-8.1033	1.0000	88.2	0.7
<sup>56</sup> Fe (CC)	42	140	5.0–50.0	20.8520	2.4233	0.9974	102.5	6.9
<sup>69</sup> Ga (CC)	5	17	LOQ–30.0	12.4535	-0.5050	1.0000	95.2	1.1
<sup>55</sup> Mn (CC)	2	6	LOQ–30.0	10.4222	0.4824	0.9999	92.3	0.7
<sup>98</sup> Mo (CC)	7	23	LOQ–30.0	2.1111	0.1543	1.0000	93.7	1.6
<sup>60</sup> Ni (CC)	4	12	LOQ–30.0	10.5972	0.0949	1.0000	89.2	0.9
<sup>207</sup> Pb (NCC)	181	603	LOQ–30.0	1.1571	0.0053	1.0000	92.5	1.1
<sup>118</sup> Sn (NCC)	122	408	LOQ–30.0	0.8788	0.0672	0.9999	94.4	1.5
<sup>88</sup> Sr (CC)	4	12	LOQ–30.0	11.3637	-0.2935	0.9999	96.1	1.3
<sup>47</sup> Ti (CC)	18	58	LOQ–30.0	0.3217	0.0311	0.9996	96.9	1.0
<sup>205</sup> Tl (NCC)	24	82	LOQ–30.0	3.7866	0.3486	0.9999	94.9	0.6
<sup>68</sup> Zn (CC)	69	228	5.0–60.0	4.4560	3.6320	0.9985	92.8	1.2

Table S10: Elemental content in HSs as measured by ICP-MS, reported as an average of three replicates  $\pm$  s.

	Al		As		Ba		Cd		Co		Cr		Cu	
	$\mu\text{g/g}$	$\mu\text{g/HS}$	$\mu\text{g/g}$	$\mu\text{g/HS}$	$\mu\text{g/g}$	$\mu\text{g/HS}$	$\mu\text{g/g}$	$\mu\text{g/HS}$	$\mu\text{g/g}$	$\mu\text{g/HS}$	$\mu\text{g/g}$	$\mu\text{g/HS}$	$\mu\text{g/g}$	$\mu\text{g/HS}$
<b>HS-1</b>	905.05	215.58	0.34	0.08	63.36	15.09	0.49	0.12	0.89	0.21	2.28	0.54	9.18	2.19
	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$
	0.11	0.03	0.02	0.00	0.57	0.13	0.00	0.00	0.02	0.01	0.00	0.00	0.13	0.03
<b>HS-2</b>	782.12	194.67	0.34	0.08	68.36	17.02	0.33	0.08	0.73	0.18	1.10	0.27	8.82	2.20
	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$
	10.59	2.64	0.10	0.02	0.61	0.15	0.00	0.00	0.02	0.00	0.11	0.03	0.61	0.15
<b>HS-3</b>	978.23	238.00	0.29	0.07	79.24	19.28	0.57	0.14	0.99	0.24	2.48	0.60	9.59	2.33
	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$
	61.02	14.85	0.03	0.01	4.45	1.08	0.00	0.00	0.06	0.01	0.38	0.09	0.40	0.10
<b>HS-4</b>	696.14	175.15	0.30	0.08	52.15	13.12	0.38	0.10	0.77	0.19	1.92	0.48	8.81	2.22
	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$
	7.44	1.87	0.01	0.00	0.32	0.08	0.00	0.00	0.01	0.00	0.20	0.05	0.06	0.02
<b>HS-5</b>	988.05	243.75	0.29	0.07	66.63	16.44	0.40	0.10	0.91	0.22	2.17	0.54	8.55	2.11
	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$
	42.22	10.41	0.02	0.01	2.99	0.74	0.02	0.01	0.03	0.01	0.10	0.03	0.31	0.08
<b>HS-6</b>	846.99	207.85	0.31	0.08	74.11	18.19	0.47	0.12	0.87	0.21	1.32	0.32	8.95	2.20
	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$
	33.54	8.23	0.01	0.00	3.02	0.74	0.02	0.01	0.04	0.01	0.03	0.01	0.38	0.09
<b>HS-7</b>	698.95	174.60	0.26	0.06	76.55	19.12	0.24	0.06	0.75	0.19	0.88	0.22	7.69	1.92
	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$
	0.73	0.18	0.01	0.00	0.39	0.10	0.00	0.00	0.01	0.00	0.03	0.01	0.00	0.00
<b>HS-8</b>	804.68	203.10	0.30	0.08	63.34	15.99	0.50	0.13	0.70	0.18	1.20	0.30	8.76	2.21
	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$
	25.91	6.54	0.00	0.00	0.90	0.23	0.01	0.00	0.01	0.00	0.08	0.02	0.04	0.01
<b>HS-9</b>	811.36	204.14	0.32	0.08	72.88	18.34	0.43	0.11	0.86	0.22	1.42	0.36	9.02	2.27
	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$
	29.33	7.38	0.01	0.00	0.04	0.01	0.02	0.00	0.03	0.01	0.23	0.06	0.23	0.06
<b>HS-10</b>	959.76	241.86	0.39	0.10	61.21	15.42	0.49	0.12	0.90	0.23	3.25	0.82	8.36	2.11
	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$	$\pm$
	23.43	5.90	0.02	0.00	0.82	0.21	0.01	0.00	0.00	0.00	0.28	0.07	0.05	0.01

<b>HS-11</b>	922.17	245.57	0.38	0.10	59.38	15.81	0.45	0.12	0.93	0.25	2.89	0.77	8.15	2.17
	± 15.97	± 4.25	± 0.01	± 0.00	± 0.62	± 0.17	± 0.01	± 0.00	± 0.03	± 0.01	± 0.11	± 0.03	± 0.17	± 0.04
<b>HS-12</b>	908.40	237.64	0.39	0.10	60.79	15.90	0.44	0.12	0.92	0.24	3.25	0.85	8.32	2.18
	± 5.70	± 1.49	± 0.02	± 0.00	± 0.09	± 0.02	± 0.00	± 0.00	± 0.00	± 0.00	± 0.72	± 0.19	± 0.09	± 0.02
<b>HS-13</b>	870.18	215.37	0.33	0.08	61.26	15.16	0.36	0.09	0.91	0.22	2.81	0.70	8.48	2.10
	± 6.75	± 1.67	± 0.00	± 0.00	± 0.14	± 0.03	± 0.00	± 0.00	± 0.01	± 0.00	± 0.04	± 0.01	± 0.08	± 0.02
<b>HS-14</b>	941.02	232.90	0.32	0.08	68.41	16.93	0.41	0.10	0.93	0.23	2.47	0.61	9.25	2.29
	± 56.13	± 13.89	± 0.01	± 0.00	± 0.27	± 0.07	± 0.01	± 0.00	± 0.01	± 0.00	± 0.22	± 0.05	± 0.23	± 0.06
<b>HS-15</b>	890.50	218.88	0.32	0.08	62.64	15.40	0.41	0.10	0.86	0.21	2.68	0.66	8.14	2.00
	± 1.55	± 0.38	± 0.01	± 0.00	± 0.31	± 0.08	± 0.00	± 0.00	± 0.02	± 0.00	± 0.03	± 0.01	± 0.16	± 0.04
<b>HS-16</b>	817.77	206.49	0.35	0.09	57.15	14.43			0.88	0.22	2.81	0.71	9.41	2.38
	± 4.49	± 1.13	± 0.01	± 0.00	± 0.41	± 0.10	<LOQ	<LOQ	± 0.02	± 0.01	± 0.16	± 0.04	± 0.04	± 0.01
	<b>Fe</b>		<b>Ga</b>		<b>Mn</b>		<b>Mo</b>		<b>Ni</b>		<b>Pb</b>		<b>Sn</b>	
	µg/g	µg/HS	µg/g	µg/HS	µg/g	µg/HS	µg/g	µg/HS	µg/g	µg/HS	µg/g	µg/HS	µg/g	µg/HS
<b>HS-1</b>	596.69	142.13	32.97	7.85	152.34	36.29			3.00	0.71			<LOD	<LOD
	± 15.50	± 3.69	± 0.60	± 0.14	± 1.05	± 0.25	<LOQ	<LOQ	± 0.28	± 0.07	<LOQ	<LOQ	<LOD	<LOD
<b>HS-2</b>	461.43	114.85	35.93	8.94	154.26	38.39			1.60	0.40			<LOD	<LOD
	± 7.96	± 1.98	± 0.21	± 0.05	± 0.97	± 0.24	<LOD	<LOD	± 0.19	± 0.05	<LOD	<LOD	<LOD	<LOD
<b>HS-3</b>	671.41	163.35	40.95	9.96	176.62	42.97			2.65	0.64			<LOD	<LOD
	± 2.41	± 0.59	± 2.44	± 0.59	± 10.19	± 2.48	<LOQ	<LOQ	± 0.09	± 0.02	<LOQ	<LOQ	<LOD	<LOD
<b>HS-4</b>	415.41	104.52	27.25	6.86	118.89	29.91			2.23	0.56			<LOD	<LOD
	± 1.29	± 0.33	± 0.27	± 0.07	± 0.67	± 0.17	<LOQ	<LOQ	± 0.13	± 0.03	<LOQ	<LOQ	<LOD	<LOD
<b>HS-5</b>	619.14	152.74	35.43	8.74	144.72	35.70	0.16	0.04	2.01	0.50	<LOQ	<LOQ	<LOD	<LOD

	± 54.00	± 13.32	± 0.05	± 0.01	± 6.86	± 1.69	± 0.01	± 0.00	± 0.03	± 0.01				
<b>HS-6</b>	469.28 ± 1.12	115.16 ± 0.28	38.22 ± 1.44	9.38 ± 0.35	163.74 ± 6.64	40.18 ± 1.63	<LOQ	<LOQ	1.76 ± 0.13	0.43 ± 0.03	<LOQ	<LOQ	<LOD	<LOD
<b>HS-7</b>	419.67 ± 0.15	104.83 ± 0.04	39.75 ± 0.00	9.93 ± 0.00	148.07 ± 0.42	36.99 ± 0.10	0.18 ± 0.01	0.05 ± 0.00	1.13 ± 0.01	0.28 ± 0.00	<LOQ	<LOQ	<LOD	<LOD
<b>HS-8</b>	470.44 ± 2.51	118.74 ± 0.63	32.94 ± 0.51	8.31 ± 0.13	143.66 ± 1.96	36.26 ± 0.49	<LOD	<LOD	1.38 ± 0.06	0.35 ± 0.02	<LOQ	<LOQ	<LOD	<LOD
<b>HS-9</b>	462.71 ± 28.07	116.42 ± 7.06	37.12 ± 0.65	9.34 ± 0.16	160.58 ± 2.09	40.40 ± 0.52	<LOD	<LOD	2.74 ± 0.89	0.69 ± 0.22	<LOQ	<LOQ	<LOD	<LOD
<b>HS-10</b>	642.84 ± 13.06	162.00 ± 3.29	31.60 ± 0.50	7.96 ± 0.13	142.46 ± 2.04	35.90 ± 0.51	<LOQ	<LOQ	3.92 ± 0.13	0.99 ± 0.03	<LOQ	<LOQ	<LOD	<LOD
<b>HS-11</b>	621.44 ± 31.92	165.49 ± 8.50	30.78 ± 0.20	8.20 ± 0.05	138.10 ± 0.04	36.78 ± 0.01	<LOD	<LOD	3.87 ± 0.11	1.03 ± 0.03	<LOQ	<LOQ	<LOD	<LOD
<b>HS-12</b>	630.14 ± 7.30	164.84 ± 1.91	31.15 ± 0.15	8.15 ± 0.04	143.31 ± 1.20	37.49 ± 0.31	<LOD	<LOD	3.94 ± 0.59	1.03 ± 0.15	<LOQ	<LOQ	<LOD	<LOD
<b>HS-13</b>	586.90 ± 0.35	145.26 ± 0.09	31.18 ± 0.32	7.72 ± 0.08	140.64 ± 0.50	34.81 ± 0.12	0.16 ± 0.03	0.04 ± 0.01	3.49 ± 0.20	0.86 ± 0.05	<LOQ	<LOQ	<LOD	<LOD
<b>HS-14</b>	606.00 ± 33.38	149.99 ± 8.26	34.69 ± 0.01	8.59 ± 0.00	147.90 ± 0.04	36.61 ± 0.01	0.18 ± 0.02	0.04 ± 0.01	2.86 ± 0.34	0.71 ± 0.08	<LOQ	<LOQ	<LOD	<LOD
<b>HS-15</b>	604.00 ± 50.80	148.46 ± 12.49	31.31 ± 0.36	7.70 ± 0.09	134.47 ± 0.70	33.05 ± 0.17	0.23 ± 0.03	0.06 ± 0.01	3.59 ± 0.12	0.88 ± 0.03	<LOQ	<LOQ	<LOD	<LOD
<b>HS-16</b>	507.50	128.14	28.10	7.10	125.97	31.81	<LOD	<LOD	3.59	0.91	<LOD	<LOD	<LOD	<LOD

	± 52.67	± 13.30	± 0.49	± 0.12	± 0.87	± 0.22			± 0.80	± 0.20				
	<b>Sr</b>		<b>Ti</b>		<b>Tl</b>		<b>Zn</b>							
	µg/g	µg/HS	µg/g	µg/HS	µg/g	µg/HS	µg/g	µg/HS						
<b>HS-1</b>	90.16 ± 0.73	21.48 ± 0.17	52.42 ± 2.08	12.49 ± 0.50	<LOD	<LOD	23.96 ± 0.24	5.71 ± 0.06						
<b>HS-2</b>	89.62 ± 0.90	22.31 ± 0.22	52.47 ± 0.05	13.06 ± 0.01	<LOD	<LOD	23.48 ± 2.67	5.85 ± 0.66						
<b>HS-3</b>	95.53 ± 0.11	23.24 ± 0.03	68.96 ± 4.48	16.78 ± 1.09	<LOD	<LOD	27.81 ± 3.20	6.77 ± 0.78						
<b>HS-4</b>	76.89 ± 0.94	19.34 ± 0.24	40.45 ± 0.07	10.18 ± 0.02	<LOD	<LOD	23.28 ± 2.92	5.86 ± 0.73						
<b>HS-5</b>	88.48 ± 0.19	21.83 ± 0.05	66.96 ± 1.77	16.52 ± 0.44	<LOD	<LOD	23.28 ± 0.65	5.74 ± 0.16						
<b>HS-6</b>	88.48 ± 2.45	21.71 ± 0.60	48.46 ± 2.03	11.89 ± 0.50	<LOD	<LOD	23.75 ± 1.54	5.83 ± 0.38						
<b>HS-7</b>	93.71 ± 0.62	23.41 ± 0.16	42.01 ± 0.91	10.49 ± 0.23	<LOD	<LOD	21.88 ± 0.53	5.46 ± 0.13						
<b>HS-8</b>	96.80 ± 1.48	24.43 ± 0.37	43.02 ± 1.35	10.86 ± 0.34	<LOD	<LOD	21.49 ± 1.50	5.42 ± 0.38						
<b>HS-9</b>	86.06 ± 0.02	21.65 ± 0.01	46.46 ± 1.25	11.69 ± 0.31	<LOD	<LOD	22.28 ± 1.01	5.61 ± 0.25						
<b>HS-10</b>	88.84 ±	22.39 ±	53.25 ±	13.42 ±	<LOD	<LOD	21.02 ±	5.30 ±						



					0.02	0.01					0.14	0.04		
<b>NP-4</b>	*	*	<LOD	<LOD	0.83 ± 0.03	0.26 ± 0.01	<LOD	<LOD	<LOD	<LOD	0.49 ± 0.16	0.15 ± 0.05	<LOD	<LOD
<b>NP-5</b>	*	*	<LOD	<LOD	<LOQ	<LOQ	<LOD	<LOD	<LOD	<LOD	0.70 ± 0.07	0.13 ± 0.01	<LOD	<LOD
<b>NP-6</b>	<LOQ	<LOQ	<LOD	<LOD	<LOQ	<LOQ	<LOD	<LOD	<LOD	<LOD	0.52 ± 0.00	0.11 ± 0.00	<LOD	<LOD
<b>NP-7</b>	<LOQ	<LOQ	<LOD	<LOD	<LOQ	<LOQ	<LOD	<LOD	<LOD	<LOD	0.21 ± 0.03	0.05 ± 0.01	<LOD	<LOD
<b>NP-8</b>	*	*	<LOD	<LOD	0.63 ± 0.01	0.19 ± 0.00	<LOD	<LOD	<LOD	<LOD	0.22 ± 0.04	0.07 ± 0.01	<LOD	<LOD
<b>NP-9</b>	*	*	<LOD	<LOD	0.55 ± 0.01	0.18 ± 0.00	<LOD	<LOD	<LOD	<LOD	0.32 ± 0.24	0.10 ± 0.08	<LOD	<LOD
<b>NP-10</b>	<LOQ	<LOQ	<LOD	<LOD	0.71 ± 0.02	0.20 ± 0.01	<LOD	<LOD	<LOD	<LOD	0.34 ± 0.05	0.10 ± 0.01	<LOD	<LOD
<b>NP-11</b>	*	*	<LOD	<LOD	<LOQ	<LOQ	<LOD	<LOD	<LOD	<LOD	0.29 ± 0.00	0.08 ± 0.00	<LOD	<LOD
<b>NP-12</b>	<LOQ	<LOQ	<LOD	<LOD	<LOQ	<LOQ	<LOD	<LOD	<LOD	<LOD	0.41 ± 0.00	0.12 ± 0.00	<LOD	<LOD
<b>NP-13</b>	*	*	<LOD	<LOD	0.46 ± 0.02	0.15 ± 0.01	<LOD	<LOD	<LOD	<LOD	0.41 ± 0.02	0.13 ± 0.01	<LOD	<LOD
<b>NP-14</b>	*	*	<LOD	<LOD	<LOQ	<LOQ	<LOD	<LOD	<LOD	<LOD	0.33 ±	0.11 ±	<LOD	<LOD

												0.03	0.01		
<b>NP-15</b>	23.61 ± 0.96	7.84 ± 0.32	<LOD	<LOD	1.84 ± 0.07	0.61 ± 0.02	<LOD	<LOD	<LOD	<LOD	<LOD	0.23 ± 0.05	0.08 ± 0.02	<LOD	<LOD
<b>NP-16</b>	*	*	<LOD	<LOD	<LOQ	<LOQ	<LOD	<LOD	<LOD	<LOD	<LOD	0.18 ± 0.07	0.05 ± 0.02	<LOD	<LOD
<b>NP-17</b>	*	*	<LOD	<LOD	<LOQ	<LOQ	<LOD	<LOD	<LOD	<LOD	<LOD	0.14 ± 0.00	0.04 ± 0.00	<LOD	<LOD
<b>NP-18</b>	<LOQ	<LOQ	<LOD	<LOD	<LOQ	<LOQ	<LOD	<LOD	<LOD	<LOD	<LOD	0.22 ± 0.06	0.07 ± 0.02	<LOD	<LOD
<b>NP-19</b>	*	*	<LOD	<LOD	2.51 ± 0.02	0.64 ± 0.01	<LOD	<LOD	<LOD	<LOD	<LOD	0.43 ± 0.04	0.11 ± 0.01	<LOD	<LOD
<b>NP-20</b>	*	*	<LOD	<LOD	4.49 ± 0.12	1.08 ± 0.03	<LOD	<LOD	<LOD	<LOD	<LOD	0.51 ± 0.15	0.12 ± 0.04	<LOD	<LOD
<b>NP-21</b>	*	*	<LOD	<LOD	9.20 ± 0.28	3.25 ± 0.10	<LOD	<LOD	<LOD	<LOD	<LOD	0.42 ± 0.14	0.15 ± 0.05	<LOD	<LOD
<b>NP-22</b>	*	*	<LOD	<LOD	4.67 ± 0.05	1.13 ± 0.01	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
<b>NP-23</b>	21.80 ± 0.90	9.34 ± 0.38	<LOD	<LOD	<LOQ	<LOQ	<LOD	<LOD	<LOD	<LOD	<LOD	*	*	1.48 ± 0.25	0.64 ± 0.11
<b>NP-24</b>	29.11 ± 0.12	12.77 ± 0.05	<LOD	<LOD	<LOQ	<LOQ	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	2.87 ± 0.08	1.26 ± 0.04
<b>NP-25</b>	26.37 ±	14.29 ±	<LOD	<LOD	<LOQ	<LOQ	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	2.44 ±	1.32 ±

	1.52	0.83											0.37	0.20
<b>NP-26</b>	32.08	16.35	<LOD	<LOD	3.15	1.60	<LOD	<LOD	<LOD	<LOD	0.04	0.02	1.32	0.67
	± 0.02	± 0.01			± 0.02	± 0.01					± 0.00	± 0.00	± 0.02	± 0.01
	<b>Fe</b>		<b>Ga</b>		<b>Mn</b>		<b>Mo</b>		<b>Ni</b>		<b>Pb</b>		<b>Sn</b>	
	µg/g	µg/NP	µg/g	µg/NP	µg/g	µg/NP	µg/g	µg/NP	µg/g	µg/NP	µg/g	µg/NP	µg/g	µg/NP
<b>NP-1</b>	19.99	8.63	0.30	0.13	0.15	0.07	<LOQ	<LOQ	0.42	0.18	<LOD	<LOD	<LOD	<LOD
	± 10.50	± 4.53	± 0.01	± 0.00	± 0.00	± 0.00			± 0.03	± 0.01				
<b>NP-2</b>	14.39	4.60	0.38	0.12	0.14	0.04	<LOD	<LOD	0.65	0.21	<LOD	<LOD	<LOD	<LOD
	± 2.31	± 0.74	± 0.03	± 0.01	± 0.01	± 0.00			± 0.03	± 0.01				
<b>NP-3</b>	*	*	0.36	0.12	0.16	0.05	<LOD	<LOD	0.53	0.17	<LOD	<LOD	<LOD	<LOD
			± 0.01	± 0.00	± 0.03	± 0.01			± 0.18	± 0.06				
<b>NP-4</b>	*	*	0.44	0.14	0.11	0.03	<LOD	<LOD	0.35	0.11	<LOD	<LOD	<LOD	<LOD
			± 0.02	± 0.01	± 0.02	± 0.01			± 0.02	± 0.01				
<b>NP-5</b>	*	*	0.13	0.03	0.10	0.02	<LOD	<LOD	2.90	0.55	<LOD	<LOD	<LOD	<LOD
			± 0.00	± 0.00	± 0.00	± 0.00			± 0.12	± 0.02				
<b>NP-6</b>	*	*	0.21	0.04	0.07	0.01	<LOD	<LOD	0.17	0.04	<LOD	<LOD	<LOD	<LOD
			± 0.02	± 0.00	± 0.02	± 0.00			± 0.06	± 0.01				
<b>NP-7</b>	11.23	2.72	0.14	0.04	0.06	0.02	<LOD	<LOD	0.15	0.04	<LOD	<LOD	<LOD	<LOD
	± 0.89	± 0.21	± 0.01	± 0.00	± 0.03	± 0.01			± 0.00	± 0.00				
<b>NP-8</b>	10.74	3.32	0.32	0.10	0.06	0.02	<LOD	<LOD	0.13	0.04	<LOD	<LOD	<LOD	<LOD
	± 3.55	± 1.10	± 0.02	± 0.00	± 0.00	± 0.00			± 0.02	± 0.01				
<b>NP-9</b>	*	*	0.27	0.09	0.07	0.02	<LOD	<LOD	0.28	0.09	<LOD	<LOD	<LOD	<LOD
			± 0.01	± 0.00	± 0.02	± 0.01			± 0.00	± 0.00				

<b>NP-10</b>	13.36 ± 5.54	3.82 ± 1.58	0.37 ± 0.01	0.11 ± 0.00	0.08 ± 0.01	0.02 ± 0.00	<LOD	<LOD	0.17 ± 0.04	0.05 ± 0.01	<LOD	<LOD	<LOD	<LOD
<b>NP-11</b>	*	*	0.28 ± 0.00	0.08 ± 0.00	0.08 ± 0.00	0.02 ± 0.00	<LOD	<LOD	0.49 ± 0.08	0.13 ± 0.02	<LOD	<LOD	<LOD	<LOD
<b>NP-12</b>	12.26 ± 0.25	3.74 ± 0.07	0.13 ± 0.02	0.04 ± 0.01	0.10 ± 0.06	0.03 ± 0.02	<LOD	<LOD	0.34 ± 0.19	0.10 ± 0.06	<LOD	<LOD	<LOD	<LOD
<b>NP-13</b>	*	*	0.23 ± 0.01	0.07 ± 0.00	0.10 ± 0.01	0.03 ± 0.00	<LOQ	<LOQ	0.52 ± 0.41	0.17 ± 0.13	<LOD	<LOD	<LOD	<LOD
<b>NP-14</b>	*	*	0.15 ± 0.02	0.05 ± 0.01	0.07 ± 0.02	0.02 ± 0.01	<LOQ	<LOQ	0.33 ± 0.24	0.11 ± 0.08	<LOD	<LOD	<LOD	<LOD
<b>NP-15</b>	*	*	0.94 ± 0.02	0.31 ± 0.01	0.84 ± 0.06	0.28 ± 0.02	<LOD	<LOD	0.13 ± 0.04	0.04 ± 0.01	<LOD	<LOD	<LOD	<LOD
<b>NP-16</b>	*	*	0.14 ± 0.01	0.04 ± 0.00	0.11 ± 0.00	0.03 ± 0.00	<LOD	<LOD	0.15 ± 0.07	0.04 ± 0.02	<LOD	<LOD	<LOD	<LOD
<b>NP-17</b>	*	*	0.11 ± 0.00	0.03 ± 0.00	0.10 ± 0.00	0.03 ± 0.00	<LOD	<LOD	0.16 ± 0.02	0.05 ± 0.01	<LOD	<LOD	<LOD	<LOD
<b>NP-18</b>	*	*	0.14 ± 0.01	0.04 ± 0.00	0.08 ± 0.03	0.02 ± 0.01	<LOD	<LOD	0.20 ± 0.10	0.06 ± 0.03	<LOD	<LOD	<LOD	<LOD
<b>NP-19</b>	*	*	1.26 ± 0.01	0.32 ± 0.00	0.23 ± 0.08	0.06 ± 0.02	<LOD	<LOD	0.28 ± 0.14	0.07 ± 0.04	<LOD	<LOD	<LOD	<LOD
<b>NP-20</b>	15.46 ± 1.62	3.71 ± 0.39	2.31 ± 0.05	0.55 ± 0.01	0.29 ± 0.01	0.07 ± 0.00	<LOD	<LOD	0.35 ± 0.05	0.08 ± 0.01	<LOD	<LOD	<LOD	<LOD

<b>NP-21</b>	13.02 ± 2.00	4.60 ± 0.70	4.67 ± 0.17	1.65 ± 0.06	0.74 ± 0.02	0.26 ± 0.01	<LOD	<LOD	0.21 ± 0.00	0.07 ± 0.00	<LOD	<LOD	<LOD	<LOD
<b>NP-22</b>	*	*	2.65 ± 0.08	0.64 ± 0.02	0.34 ± 0.04	0.08 ± 0.01	<LOD	<LOD	<LOQ	<LOQ	<LOD	<LOD	<LOD	<LOD
<b>NP-23</b>	*	*	0.82 ± 0.01	0.35 ± 0.00	1.20 ± 0.07	0.51 ± 0.03	<LOD	<LOD	0.26 ± 0.19	0.11 ± 0.08	<LOD	<LOD	<LOD	<LOD
<b>NP-24</b>	14.17 ± 4.48	6.22 ± 1.97	1.39 ± 0.00	0.61 ± 0.00	0.82 ± 0.07	0.36 ± 0.03	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
<b>NP-25</b>	23.89 ± 1.42	12.94 ± 0.77	1.32 ± 0.04	0.71 ± 0.02	0.88 ± 0.09	0.48 ± 0.05	<LOD	<LOD	0.12 ± 0.11	0.07 ± 0.06	<LOD	<LOD	<LOD	<LOD
<b>NP-26</b>	17.39 ± 4.98	8.87 ± 2.54	1.78 ± 0.02	0.90 ± 0.01	0.93 ± 0.07	0.48 ± 0.03	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD

	<b>Sr</b>		<b>Ti</b>		<b>Tl</b>		<b>Zn</b>	
	µg/g	µg/NP	µg/g	µg/NP	µg/g	µg/NP	µg/g	µg/NP
<b>NP-1</b>	1.64 ± 0.11	0.71 ± 0.05	1.04 ± 0.26	0.45 ± 0.11	<LOD	<LOD	*	*
<b>NP-2</b>	1.66 ± 0.08	0.53 ± 0.03	2.43 ± 0.17	0.78 ± 0.05	<LOD	<LOD	*	*
<b>NP-3</b>	1.39 ± 0.05	0.45 ± 0.02	1.12 ± 0.05	0.36 ± 0.02	<LOD	<LOD	*	*
<b>NP-4</b>	1.54 ± 0.02	0.48 ± 0.01	0.68 ± 0.05	0.21 ± 0.02	<LOD	<LOD	*	*
<b>NP-5</b>	0.13	0.03	0.70	0.13	<LOD	<LOD	*	*

	± 0.04	± 0.01	± 0.41	± 0.08				
<b>NP-6</b>	0.17 ± 0.01	0.04 ± 0.00	0.50 ± 0.13	0.11 ± 0.03	<LOD	<LOD	*	*
<b>NP-7</b>	0.32 ± 0.01	0.08 ± 0.00	0.36 ± 0.06	0.09 ± 0.01	<LOD	<LOD	*	*
<b>NP-8</b>	0.74 ± 0.01	0.23 ± 0.00	1.04 ± 0.07	0.32 ± 0.02	<LOD	<LOD	*	*
<b>NP-9</b>	0.95 ± 0.02	0.30 ± 0.01	0.44 ± 0.15	0.14 ± 0.05	<LOD	<LOD	*	*
<b>NP-10</b>	1.06 ± 0.01	0.30 ± 0.00	<LOQ	<LOQ	<LOD	<LOD	*	*
<b>NP-11</b>	0.83 ± 0.02	0.23 ± 0.00	9.45 ± 0.01	2.60 ± 0.00	<LOD	<LOD	*	*
<b>NP-12</b>	0.13 ± 0.04	0.04 ± 0.01	0.32 ± 0.08	0.10 ± 0.02	<LOD	<LOD	*	*
<b>NP-13</b>	0.37 ± 0.01	0.12 ± 0.00	0.32 ± 0.07	0.10 ± 0.02	<LOD	<LOD	*	*
<b>NP-14</b>	0.11 ± 0.00	0.04 ± 0.00	0.21 ± 0.02	0.07 ± 0.01	<LOD	<LOD	*	*
<b>NP-15</b>	1.74 ± 0.08	0.58 ± 0.03	1.08 ± 0.02	0.36 ± 0.01	<LOD	<LOD	*	*
<b>NP-16</b>	2.05	0.59	0.83	0.24	<LOD	<LOD	*	*

	± 0.11	± 0.03	± 0.13	± 0.04				
<b>NP-17</b>	1.53 ± 0.15	0.46 ± 0.04	0.33 ± 0.07	0.10 ± 0.02	<LOD	<LOD	*	*
<b>NP-18</b>	0.91 ± 0.02	0.27 ± 0.01	<LOQ	<LOQ	<LOD	<LOD	*	*
<b>NP-19</b>	2.39 ± 0.01	0.61 ± 0.00	1.18 ± 0.20	0.30 ± 0.05	<LOD	<LOD	*	*
<b>NP-20</b>	4.74 ± 0.00	1.14 ± 0.00	0.84 ± 0.15	0.20 ± 0.04	<LOD	<LOD	*	*
<b>NP-21</b>	3.28 ± 0.08	1.16 ± 0.03	0.60 ± 0.16	0.21 ± 0.05	<LOD	<LOD	*	*
<b>NP-22</b>	4.70 ± 0.03	1.13 ± 0.01	0.45 ± 0.18	0.11 ± 0.04	<LOD	<LOD	<LOD	<LOD
<b>NP-23</b>	2.38 ± 0.08	1.02 ± 0.03	0.83 ± 0.09	0.36 ± 0.04	<LOD	<LOD	<LOD	<LOD
<b>NP-24</b>	2.42 ± 0.09	1.06 ± 0.04	0.70 ± 0.02	0.31 ± 0.01	<LOD	<LOD	<LOD	<LOD
<b>NP-25</b>	2.33 ± 0.03	1.26 ± 0.02	0.84 ± 0.23	0.46 ± 0.12	<LOD	<LOD	<LOD	<LOD
<b>NP-26</b>	2.71 ± 0.02	1.38 ± 0.01	1.82 ± 0.51	0.93 ± 0.26	<LOD	<LOD	<LOQ	<LOQ

\*Elemental content above LOQ, but below the first calibration point of the linear concentration range.

Compound number	Compound name	HS-1	HS-2	HS-3	HS-4	HS-5	HS-6	HS-7	HS-8	HS-9	HS-10	HS-11	HS-12	HS-13	HS-14	HS-15	HS-16	Number of samples where specific compound was identified
1	acetic acid	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	16
2	propylene glycol	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	16
3	propylene glycol 1-acetate	White	Green	Green	Green	Green	Green	Green	Green	Green	White	Green	Green	Green	Green	Green	Green	14
4	glycerol	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	16
5	benzyl alcohol	Green	White	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	White	White	Green	Green	13
6	1,2,3-propanetriol, 1-acetate	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	16
7	2,3-dihydro-3,5-dihydroxy-6-methyl-4H-pyran-4-one	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	White	15
8	benzyl acetate	Green	White	White	White	White	White	White	White	White	White	White	White	White	White	White	White	1
9	menthol	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	16
10	5-ethyl-1,3-dioxane-5-methanol	White	White	White	White	White	White	White	White	White	White	White	Green	White	White	White	White	5
11	dodecane	Green	Green	White	Green	Green	Green	Green	Green	Green	Green	Green	White	Green	Green	Green	Green	13
12	<i>cis</i> -4- <i>tert</i> -butylcyclohexanol	White	White	White	White	White	White	White	White	White	White	White	Green	White	White	White	White	3
13	<i>trans</i> -4- <i>tert</i> -butylcyclohexanol	White	White	White	White	White	White	White	White	White	White	White	Green	White	White	White	White	9
14	glycerol 1,2-diacetate	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	16
15	nonanoic acid	White	White	White	White	White	White	White	White	White	White	White	White	White	White	White	White	1
16	triacetin	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	16
17	nicotine	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	16
18	hexadecane	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	16
19	vanillin	White	White	White	White	White	White	White	White	White	White	White	Green	White	White	White	White	1
20	geranyl acetone	Green	White	Green	White	Green	White	White	White	White	Green	White	White	White	White	White	White	4
21	ethyl vanillin	White	White	White	White	White	White	White	White	White	White	White	Green	White	White	White	White	1
22	nicotyrine	White	White	Green	White	White	White	White	White	White	White	White	White	White	White	White	White	1
23	$\delta$ -decalactone	White	White	White	White	White	White	White	White	Green	White	White	White	White	White	White	White	1
24	heptadecane	White	Green	White	Green	Green	White	White	White	White	White	Green	White	Green	White	Green	Green	7
25	neophytadiene	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	Green	16
Number of compounds identified in each sample		15	14	15	15	16	15	15	16	17	18	16	18	15	13	14	17	

Figure S1: Identified compounds in 16 HSs by non-targeted gas chromatography mass spectrometry (GC-MS) analysis. Green cells indicate samples in which specific compounds were identified, while white cells indicate that the compound was not identified in that sample.

Compound number	Compound name	HS-1	HS-2	HS-3	HS-4	HS-5	HS-6	HS-7	HS-8	HS-9	HS-10	HS-11	HS-12	HS-13	HS-14	HS-15	HS-16
1	acetic acid	0.12	0.13	0.16	0.11	0.11	0.17	0.23	0.12	0.16	0.18	0.23	0.22	0.32	0.36	0.30	0.20
2	propylene glycol	0.55	1.46	1.16	1.82	1.67	1.09	1.29	1.46	1.70	0.60	1.85	1.72	1.73	1.60	1.72	1.35
3	propylene glycol 1-acetate		0.12	0.12	0.13	0.14	0.10	0.14	0.11	0.11		0.19	0.14	0.15	0.15	0.15	0.11
4	glycerol	10.19	11.19	10.49	12.49	12.52	12.62	12.18	12.95	14.63	13.30	16.64	13.82	14.82	16.11	15.53	13.51
5	benzyl alcohol	8.53		0.54	1.67	1.92	0.72	0.20	0.13	0.12	7.36	0.11	2.23	1.30			0.20
6	1,2,3-propanetriol, 1-acetate	1.94	2.31	4.22	2.10	2.71	3.06	3.24	3.31	2.85	2.77	3.67	2.79	3.67	4.11	4.05	3.71
7	2,3-dihydro-3,5-dihydroxy-6-methyl-4H-pyran-4-one	0.19	0.22	0.71	0.18	0.20	0.29	0.20	0.25	0.25	0.20	0.23	0.19	0.25	0.21	0.20	
8	benzyl acetate	0.58															
9	menthol	2.03	18.48	0.94	1.32	0.74	4.88	20.41	0.44	1.17	0.52	0.46	0.29	0.58	0.44	0.68	0.28
10	5-ethyl-1,3-dioxane-5-methanol								0.12	0.11	0.17		0.26				0.14
11	dodecane	0.24	0.30		0.34	0.32	0.34	0.17	0.30	0.35	0.18	0.21		0.21	0.19		0.16
12	cis-4-tert-butylcyclohexanol										0.11		0.13				0.12
13	trans-4-tert-butylcyclohexanol						0.39	0.24	0.38	0.37	0.51	0.41	0.58			0.31	0.37
14	glycerol 1,2-diacetate	4.29	2.22	3.60	3.64	4.01	3.41	1.32	3.85	3.26	3.15	3.10	3.53	1.73	1.64	1.98	3.99
15	nonanoic acid										0.15						
16	triacetin	21.74	8.51	7.96	12.63	14.67	11.07	3.17	11.47	12.87	12.48	13.11	13.64	5.90	5.22	6.30	13.79
17	nicotine	40.38	45.80	57.89	51.89	48.90	51.46	48.40	52.55	52.44	47.25	50.21	49.40	57.56	58.04	58.37	50.11
18	hexadecane	0.47	0.42	0.36	0.66	0.58	0.41	0.32	0.32	0.51	0.34	0.53	0.39	0.48	0.38	0.47	0.32
19	vanillin												0.40				
20	geranyl acetone	0.33		0.84		0.18					0.19						
21	ethyl vanillin												0.39				
22	nicotyrine			1.01													
23	δ-decalactone									0.35							
24	heptadecane		0.22		0.48	0.37						0.47		0.46		0.56	0.32
25	neophytadiene	8.42	8.62	10.00	10.54	10.95	9.98	8.49	12.24	8.75	10.52	8.58	9.86	10.85	11.55	9.38	11.32
	Total area of identified chromatographic peaks	4.21·10 <sup>7</sup>	4.34·10 <sup>7</sup>	3.75·10 <sup>7</sup>	3.90·10 <sup>7</sup>	3.70·10 <sup>7</sup>	3.60·10 <sup>7</sup>	4.18·10 <sup>7</sup>	3.68·10 <sup>7</sup>	3.30·10 <sup>7</sup>	3.73·10 <sup>7</sup>	3.44·10 <sup>7</sup>	3.46·10 <sup>7</sup>	3.48·10 <sup>7</sup>	3.32·10 <sup>7</sup>	3.40·10 <sup>7</sup>	3.82·10 <sup>7</sup>

Figure S2: Relative areas normalized to 100% of individual chromatographic peaks based on the total area of identified chromatographic peaks for every HS.

Compound number	Compound name	NP-1	NP-2	NP-3	NP-4	NP-5	NP-6	NP-7	NP-8	NP-9	NP-10	NP-11	NP-12	NP-13	NP-14	NP-15	NP-16	NP-17	NP-18	NP-19	NP-20	NP-21	NP-22	NP-23	NP-24	NP-25	NP-26	Number of samples where specific compound was identified	
1	acetaldehyde																											6	
2	ethanol																												25
3	acetonitrile																												13
4	2-methyl-2-propanol																												5
5	2-propen-1-ol																												1
6	ethenyl acetate																												1
7	hexane																												1
8	ethyl acetate																												1
9	2-methyl-1-propanol																												2
10	1-butanol																												21
11	3-methyl-1-butanol																												3
12	2-methyl-1-butanol																												2
13	propylene glycol																												18
14	1-pentanol																												1
15	isobutyl acetate																												2
16	ethyl butanoate																												8
17	butyl acetate																												6
18	2,4-dimethyl-heptane																												1
19	ethyl 2-methylbutanoate																												8
20	ethyl 3-methylbutanoate																												2
21	cis -3-hexen-1-ol																												11
22	trans -2-hexen-1-ol																												2
23	1-hexanol																												4
24	3-methyl-1-butyl acetate																												2
25	2-methyl-1-butyl acetate																												2
26	2,5-diethyltetrahydrofuran																												1
27	pentyl acetate																												1
28	α-thujene																												2
29	α-pinene																												8
30	camphene																												3
31	benzaldehyde																												8
32	2,6,6-trimethyl-2-vinyltetrahydropyran																												1
33	sabinene																												6
34	2,2,4-trimethyl-1,3-dioxolane																												1
35	β-pinene																												11
36	sulcatone																												2
37	3-octanone																												1
38	p-menth-3-ene																												1
39	β-myrcene																												8
40	butyl butanoate																												1
41	3-octanol																												10
42	ethyl hexanoate																												6
43	2,6-dimethyl-3-heptanone																												1
44	cis -3-hexenyl acetate																												7
45	α-phellandrene																												3

Figure S3: Identified compounds in 26 NPs by non-targeted GC-MS analysis (compound numbers 1–45). Green cells indicate samples in which specific compounds were identified, while white cells indicate that the compound was not identified in that sample.

Compound number	Compound name	NP-1	NP-2	NP-3	NP-4	NP-5	NP-6	NP-7	NP-8	NP-9	NP-10	NP-11	NP-12	NP-13	NP-14	NP-15	NP-16	NP-17	NP-18	NP-19	NP-20	NP-21	NP-22	NP-23	NP-24	NP-25	NP-26	Number of samples where specific compound was identified	
46	3-carene																											4	
47	hexyl acetate																												8
48	2-ethyl-1-butanol																												1
49	1,4-cineole																												2
50	$\alpha$ -terpinene																												6
51	<i>o</i> -cymene																												8
52	2-ethyl-1-hexanol																												2
53	D-limonene																												19
54	benzyl alcohol																												6
55	eucalyptol																												12
56	2,2-dimethyl-5-(1-methyl-1-propenyl)-tetrahydrofuran																												1
57	<i>cis</i> - $\beta$ -ocimene																												2
58	2,6-dimethyl-5-heptenal																												1
59	3-ethyl-3-methylheptane																												10
60	isopentyl butanoate																												1
61	$\gamma$ -terpinene																												10
62	2,2,4-trimethyl-hexane																												1
63	acetophenone																												1
64	1-octanol																												1
65	sabinene hydrate																												7
66	2-propenyl hexanoate																												2
67	4-carene																												5
68	pentyl butanoate																												1
69	ethyl heptanoate																												5
70	linalool																												10
71	$\alpha$ -methyl-benzeneacetaldehyde																												1
72	( <i>e</i> )-4-methyl-2-(1-pentenyl)-1,3-dioxolane																												1
73	isopentyl isopentanoate																												4
74	<i>trans</i> -rose oxide																												2
75	3-octanyl acetate																												2
76	fenchol																												2
77	ethyl-3-hydroxyhexanoate																												1
78	<i>trans</i> -limonene oxide																												1
79	1-terpineol																												1
80	isopulegol																												4
81	$\beta$ -terpineol																												2
82	<i>p</i> -menthan-3-one																												21
83	benzyl acetate																												3
84	menthofurane																												5
85	isoborneol																												1
86	ethyl benzoate																												1
87	(1 <i>s</i> ,2 <i>r</i> ,5 <i>r</i> )-(+)-isomenthol																												8
88	borneol																												1
89	ethyl 2,4-dimethyl-1,3-dioxolane-2-acetate																												2
90	terpinen-4-ol																												6

Figure S4: Identified compounds in 26 NPs by non-targeted GC-MS analysis (compound numbers 46–90). Green cells indicate samples in which specific compounds were identified, while white cells indicate that the compound was not identified in that sample.

Compound number	Compound name	NP-1	NP-2	NP-3	NP-4	NP-5	NP-6	NP-7	NP-8	NP-9	NP-10	NP-11	NP-12	NP-13	NP-14	NP-15	NP-16	NP-17	NP-18	NP-19	NP-20	NP-21	NP-22	NP-23	NP-24	NP-25	NP-26	Number of samples where specific compound was identified
91	menthol	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	25
92	3-hexenyl butanoate																				1							1
93	$\alpha$ -methylbenzyl acetate																				1							1
94	hexyl butanoate																				1							1
95	dihydroterpineol			1	1																							2
96	$\alpha$ -terpineol			1	1						1					1						1		1				6
97	<i>trans</i> -dihydrocarvone	1	1					1								1											1	5
98	$\gamma$ -terpineol										1											1		1				3
99	<i>cis</i> -carveol															1								1				1
100	benzaldehyde diethyl acetal																							1				1
101	3-phenylpropanol																					1						1
102	<i>cis</i> -3-hexenyl pentanoate				1																							1
103	pulegone	1		1	1						1			1	1	1											1	8
104	D-carvone	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	24
105	ethyl 2-octenoate																				1							1
106	linalyl acetate																		1									1
107	4-methoxy-benzaldehyde																					1		1				2
108	piperitone	1	1	1	1			1	1		1					1											1	9
109	4-methyl-2-phenyl-1,3-dioxolane																				1							1
110	2-hydroxy-3-isopropyl-6-methyl-2-cyclohexen-1-one											1																1
111	citral											1										1						2
112	cinnamaldehyde																											1
113	dodecane, 4,6-dimethyl						1	1								1					1	1	1	1	1	1	1	12
114	bornyl acetate										1			1	1	1												3
115	anethole															1												1
116	menthyl acetate	1		1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	16
117	2,4-dimethyl-1,3-dioxolane-2-propionate																											1
118	2-hydroxypiperitone											1																1
119	$\alpha,\alpha$ -dimethylphenethyl acetate																1											1
120	dihydrocarvyl acetate	1	1						1							1											1	6
121	piperonal																					1						1
122	$\delta$ -elemene				1																							1
123	butyl 2-ethyl hexanoate																				1							1
124	nicotine	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	26
125	eugenol																					1						1
126	nerol acetate																					1			1			2
127	<i>trans</i> -carveyl acetate	1	1																		1							3
128	$\alpha$ -copaene				1																							1
129	<i>cis</i> -3-hexenyl hexanoate																				1		1					2
130	$\beta$ -damascenone											1												1				2
131	hexyl hexanoate																				1	1						2
132	methyl cinnamate															1						1						2
133	$\beta$ -bourbonene	1	1	1	1			1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	8
134	$\beta$ -elemene				1																						1	2
135	ethyl decanoate																							1				1

Figure S5: Identified compounds in all 26 NPs by non-targeted GC-MS analysis (compound numbers 91–135). Green cells indicate samples in which specific compounds were identified, while white cells indicate that the compound was not identified in that sample.

Compound number	Compound name	NP-1	NP-2	NP-3	NP-4	NP-5	NP-6	NP-7	NP-8	NP-9	NP-10	NP-11	NP-12	NP-13	NP-14	NP-15	NP-16	NP-17	NP-18	NP-19	NP-20	NP-21	NP-22	NP-23	NP-24	NP-25	NP-26	Number of samples where specific compound was identified	
136	diphenyl ether																											1	
137	$\beta$ -damascone																												7
138	p-methoxybenzyl acetate																												2
139	$\alpha$ -ionone																												2
140	$\beta$ -caryophyllene																												14
141	3-allylcyclohexyl propionate																												1
142	trans- $\alpha$ -bergamotene																												4
143	$\beta$ -copaene																												2
144	cinnamyl acetate																												1
145	$\beta$ -farnesene																												6
146	$\alpha$ -caryophyllene																												2
147	5-hexyldihydro-2(3h)-furanone																												3
148	ethyl cinnamate																												1
149	$\beta$ -ionone																												9
150	$\alpha$ -curcumene																												1
151	heneisocane																												12
152	germacrene D																												5
153	2-phenylethyl-3-methyl butanoate																												1
154	$\alpha$ -zingiberene																												1
155	$\beta$ -selinene																												1
156	$\alpha$ -farnesene																												2
157	bicyclgermacrene																												1
158	$\alpha$ -gualene																												1
159	$\beta$ -bisabolene																												3
160	$\beta$ -cadinene																												2
161	$\beta$ -sesquiphellandrene																												1
162	5-heptyldihydro-2(3h)-furanone																												3
163	N-ethyl-p-menthane-3-carboxamide																												3
Number of compounds identified in each sample		43	36	32	56	15	20	19	23	14	19	24	12	23	15	27	23	20	12	57	62	32	43	26	18	30	10		

Figure S6: Identified compounds in all 26 NPs by non-targeted GC-MS analysis (compound numbers 136–163). Green cells indicate samples in which specific compounds were identified, while white cells indicate that the compound was not identified in that sample.

Compound number	Compound name	NP-1	NP-2	NP-3	NP-4	NP-5	NP-6	NP-7	NP-8	NP-9	NP-10	NP-11	NP-12	NP-13	NP-14	NP-15	NP-16	NP-17	NP-18	NP-19	NP-20	NP-21	NP-22	NP-23	NP-24	NP-25	NP-26	
1	acetaldehyde	0.06	0.09	0.05	0.03															0.04		0.11						
2	ethanol	9.32	11.35	6.27	4.63	7.10	1.23	0.46	0.76	8.16	0.91		0.64	0.27	0.33	0.37	2.10	0.19	0.24	0.44	0.99	15.11	13.24	9.77	9.64	6.95	5.61	
3	acetonitrile	0.28	0.35		0.12	0.41	0.27	0.10	0.30					0.09		0.13	1.63	0.07			1.11					0.11		
4	2-methyl-2-propanol	0.07	0.08		0.03								0.10	0.06														
5	2-propen-1-ol																				0.03							
6	ethenyl acetate																								0.02			
7	hexane				0.02																							
8	ethyl acetate																							0.04				
9	2-methyl-1-propanol																					0.10	0.28					
10	1-butanol					1.26	0.66	0.45	0.38	1.70	0.14	0.35	0.53	0.09	0.14	0.04	0.50	0.04			0.10	0.23	0.74	0.16	0.10	0.14	0.17	0.18
11	3-methyl-1-butanol				0.01																0.12			0.36				
12	2-methyl-1-butanol																				0.03			0.08				
13	propylene glycol		0.04	0.04	0.05	0.85	1.23	0.69	0.36	0.88		0.22	3.06	0.08	0.04		0.24	0.40			0.04		0.05	0.22	0.34			
14	1-pentanol																				1.92							
15	isobutyl acetate																					0.40	0.15					
16	ethyl butanoate	0.05	0.05						0.08	0.51											1.02		2.03	2.99	0.06			
17	butyl acetate	0.02	0.03		0.01																0.03	1.37	0.35					
18	2,4-dimethyl-heptane			0.01																								
19	ethyl 2-methylbutanoate	0.03	0.02		0.01					0.14											0.40		1.73	3.84	0.04			
20	ethyl 3-methylbutanoate																				1.38				0.12			
21	cis-3-hexen-1-ol					1.53	0.31		0.39	1.97		3.16	0.84				2.37				0.94	1.98	13.65		0.06			
22	trans-2-hexen-1-ol																						3.18		0.05			
23	1-hexanol																1.38				2.70		11.33	3.38				
24	3-methyl-1-butyl acetate																				1.57			3.15				
25	2-methyl-1-butyl acetate																				0.53			0.91				
26	2,5-pentyl acetate				0.01																							
27	α-thujene				0.12																	0.01						
28	α-pinene	0.10	0.07	0.13	2.49									0.06							0.56	0.31				0.24		
30	camphene				0.06									0.05									0.04					
31	benzaldehyde	0.02	0.03		0.01																							
32	2,6,6-trimethyl-2-vinylnorbornane																											
33	sabinene	0.11	0.13	0.05	2.84																	0.04						
34	2,2,4-trimethyl-1,3-β-pinene	0.31	0.23	0.28	4.03						0.03						0.26				0.02	2.77		0.42		0.03		
36	sulcatone											0.11											0.07					
37	3-octanone		0.11																									
38	p-menth-3-ene				0.04																							
39	β-myrcene	0.32	0.72	0.03	0.39																							
40	butyl butanoate																					0.17	1.22		0.20		0.04	
41	3-octanol	0.26	0.24	0.12	0.08		0.21	0.20	0.32					0.02		1.43						0.02					0.40	
42	ethyl hexanoate											1.75										6.51	0.02	9.23	0.16	0.08		
43	2,6-dimethyl-3-cis-3-hexenyl acetate				0.03																							
44	cis-3-hexenyl acetate								0.37			0.83					1.52				1.82	0.13	0.07		0.08			
45	α-phellandrene				0.21																	0.13				0.04		

Figure S7: Relative areas normalized to 100% of individual chromatographic peaks based on the total area of identified chromatographic peaks for every NP (compound numbers 1–45).



91	menthol	19.52	0.23	42.89	25.40	2.67	26.38	26.90	33.26	0.68	67.03	41.48	0.59	60.95	64.61	23.45	0.42	57.49	87.35	0.09	0.19		0.25	70.57	58.72	68.72	81.78		
92	3-hexenyl butanoate																				3.98								
93	α-methylbenzyl acetate																				1.04								
94	hexyl butanoate																				14.01								
95	dihydroterpineol			0.07	0.03																								
96	α-terpineol			0.08	0.11							2.75					0.18					3.35		2.42					
97	trans-dihydrocarvone	0.42	0.86					0.28								1.69											0.18		
98	γ-terpineol											0.90										0.26		0.23					
99	cis-carveol															0.20													
100	benzaldehyde diethyl																												
101	3-phenylpropanol																					0.11							
102	cis-3-hexenyl pentanoate				0.03																								
103	pulegone	0.14		0.35	0.40						0.07			0.08	0.05	0.22											0.06		
104	D-carvone	35.61	55.37	0.14	0.20	1.02	13.03	13.15	17.88	0.61	0.07	0.19	0.24	0.06	0.04	34.65	0.25	0.09	0.09	0.28	0.44	0.15	1.83		0.11	4.51			
105	ethyl 2-octenoate																				0.41								
106	linalyl acetate																	0.53											
107	4-methoxy-benzaldehyde																					0.98		0.38					
108	piperitone	0.09	0.08	0.10	0.17			0.08	0.14		0.03					0.13											0.04		
109	4-methyl-2-phenyl-1,3-dioxolane																				0.67								
110	2-hydroxy-3-isopropyl-6-methyl-2-cyclohexen-1-													0.09															
111	citral																												
112	cinnamaldehyde																					0.14							
113	dodecane, 4,6-dimethyl						0.28	0.18													0.07	0.14	0.10		0.05	0.06	0.19	0.15	
114	bornyl acetate													0.25			0.23	0.19											
115	anethole																												
116	menthyl acetate	2.58		4.51	3.92	0.28	0.18	0.17	0.24		2.58			2.41	2.17	1.60				0.07	0.04			0.09	0.07		0.54		
117	2,4-dimethyl-1,3-dioxolane-2-propionate																				0.24								
118	2-hydroxypiperitone												0.07																
119	α,α-dimethylphenethyl acetate																					0.21							
120	dihydrocarvyl acetate	0.07	0.07						0.07								0.46				0.04						0.04		
121	piperonal																												
122	δ-elemene				0.61																		0.35						
123	butyl 2-ethyl hexanoate																												
124	nicotine	12.52	19.71	14.18	8.76	80.34	53.40	55.61	43.10	80.45	12.56	39.51	92.56	18.16	21.46	27.32	84.74	35.77	7.07	7.13			6.36	24.87	21.56	17.38	10.04	14.18	11.88
125	eugenol																					0.93							
126	nerol acetate																					0.37			0.15				
127	trans-carveyl acetate	0.05	0.02																			0.11							
128	α-copaene				0.71																								
129	cis-3-hexenyl hexanoate																					3.25		0.04					
130	β-damascenone												0.16														0.19		
131	hexyl hexanoate																					9.47	0.09						
132	methyl cinnamate															0.11								2.19					
133	β-bourbonene	0.29	0.40	0.02	0.07		0.16	0.14	0.44																			0.09	
134	β-elemene				0.19																							0.02	
135	ethyl decanoate																								0.15				

Figure S9: Relative areas normalized to 100% of individual chromatographic peaks based on the total area of identified chromatographic peaks for every NP (compound numbers 91–135).



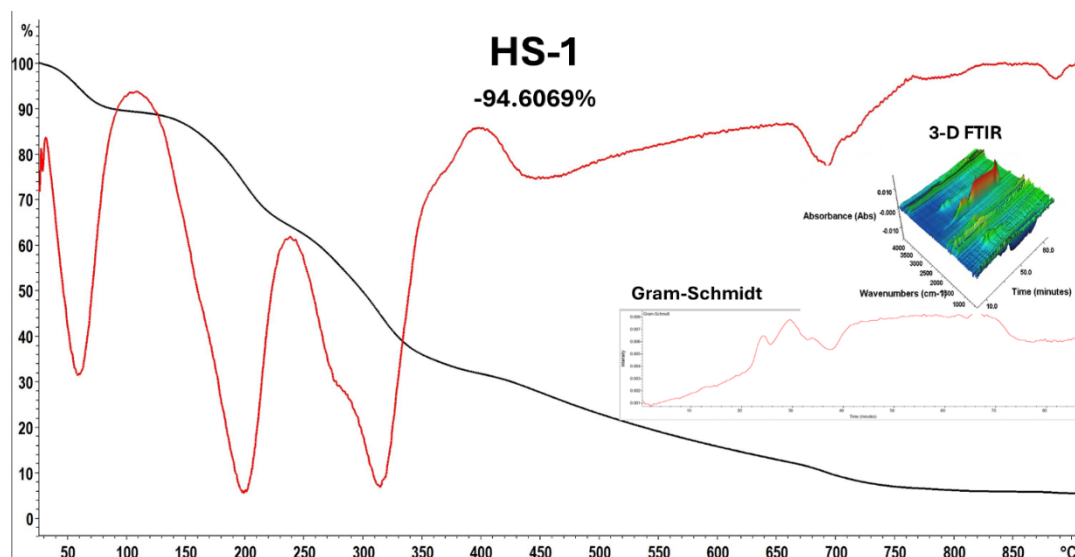


Figure S11: Thermogravimetric analysis (TGA) of HS-1, with the black curve representing mass loss, the red curve representing the derivative curve (DTG), the Gram-Schmidt curve, and 3-dimensional (3-D) FTIR.

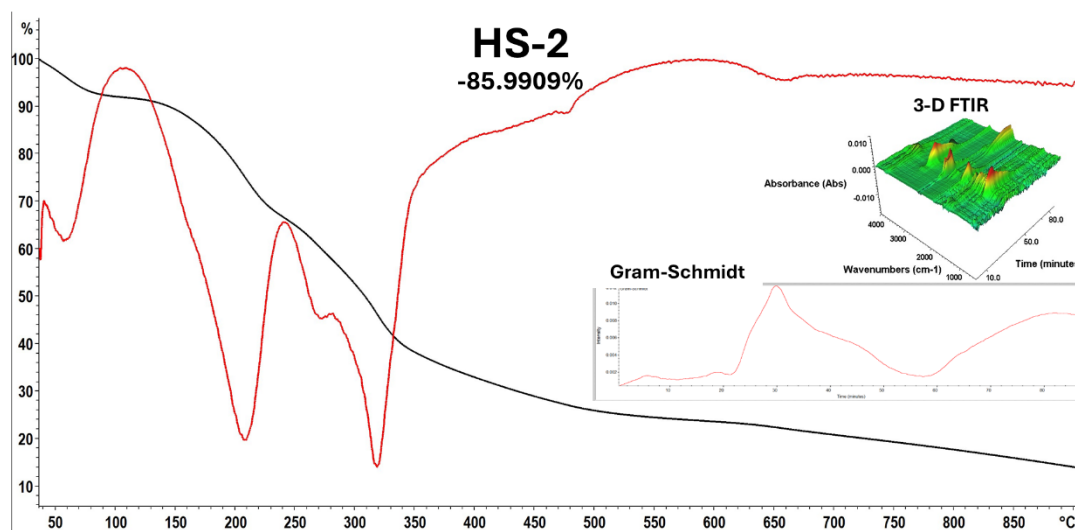


Figure S12: Thermogravimetric analysis (TGA) of HS-2, with the black curve representing mass loss, the red curve representing the derivative curve (DTG), the Gram-Schmidt curve, and 3-dimensional (3-D) FTIR.

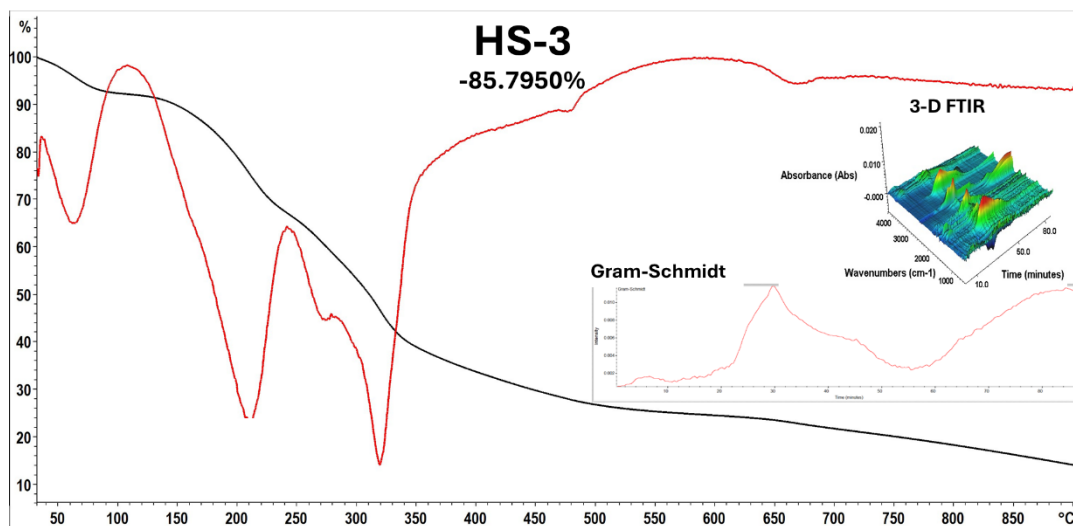


Figure S13: Thermogravimetric analysis (TGA) of HS-3, with the black curve representing mass loss, the red curve representing the derivative curve (DTG), the Gram-Schmidt curve, and 3-dimensional (3-D) FTIR.

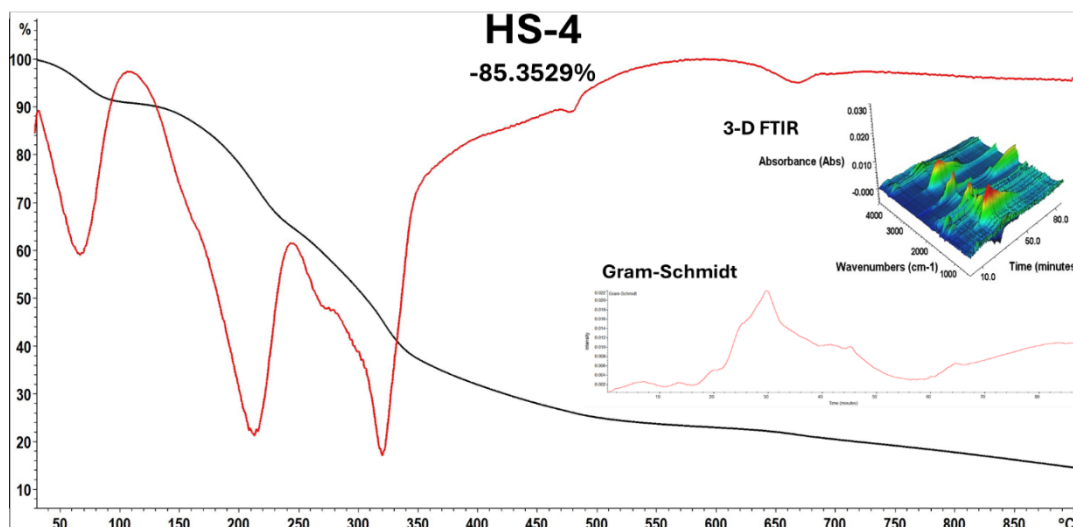


Figure S14: TGA of HS-4, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

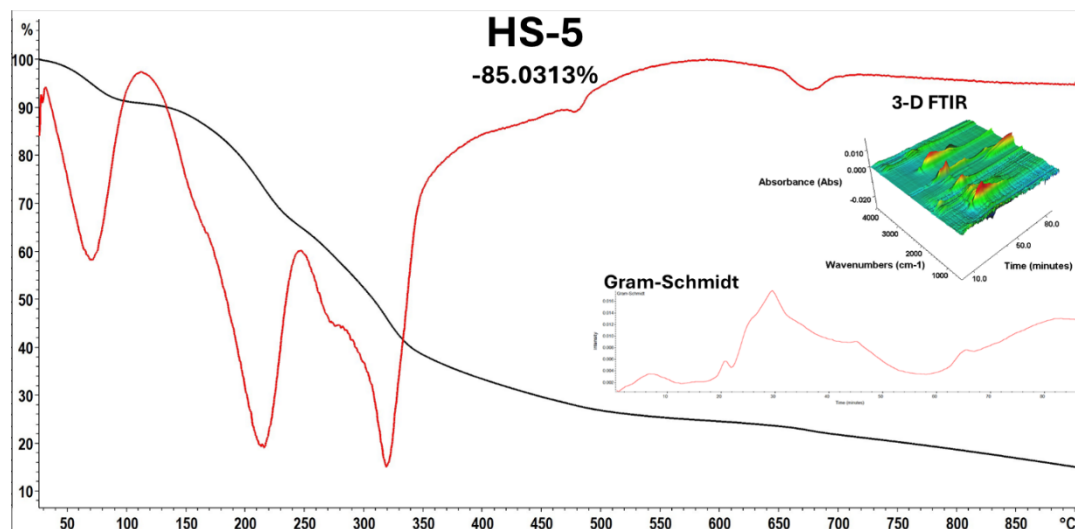


Figure S15: TGA of HS-5, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

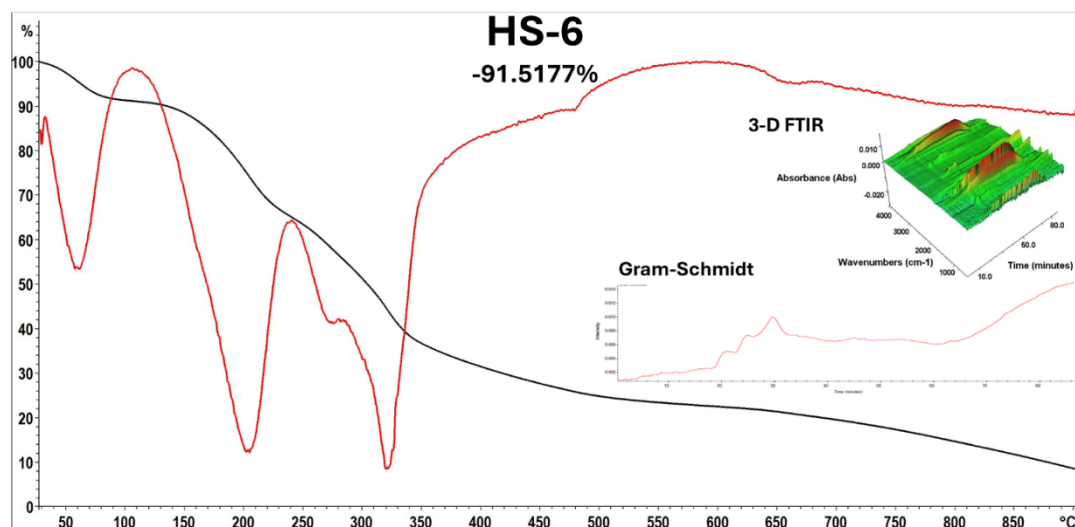


Figure S16: TGA of HS-6, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

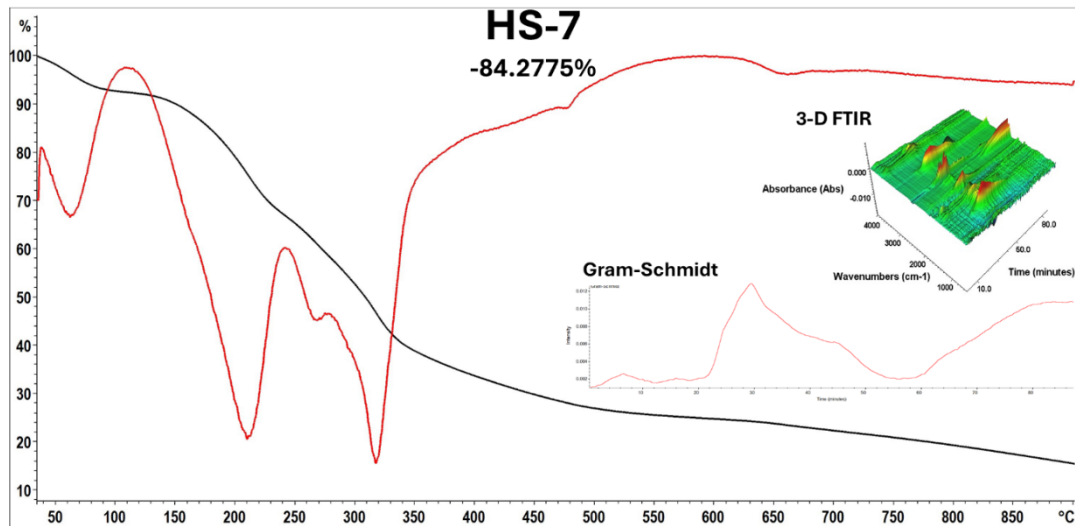


Figure S17: TGA of HS-7, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

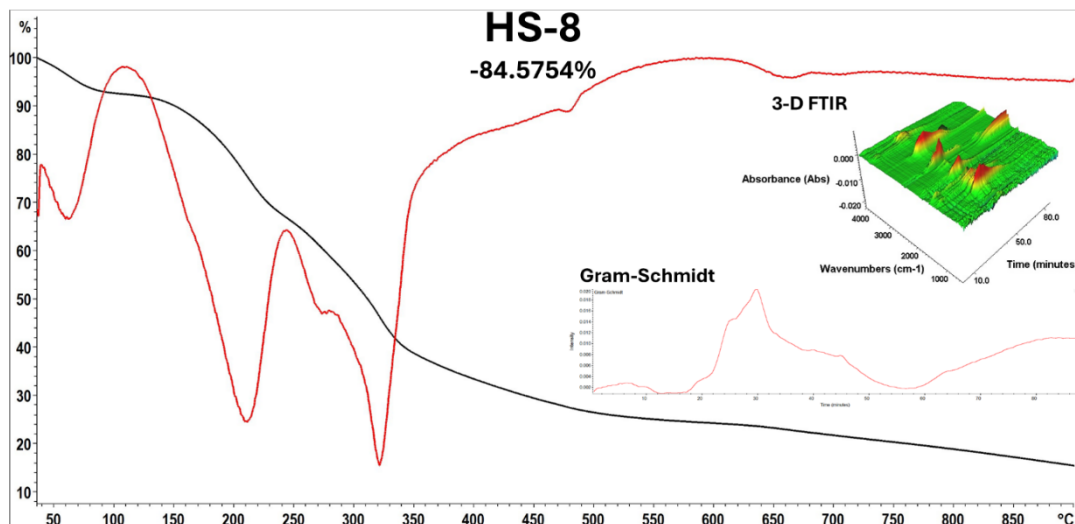


Figure S18: TGA of HS-8, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

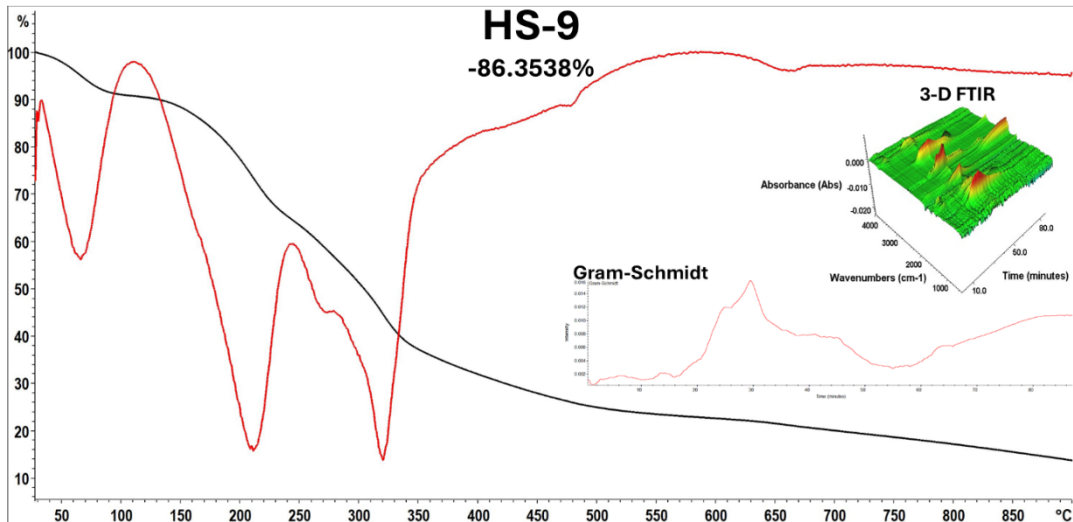


Figure S19: TGA of HS-9, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

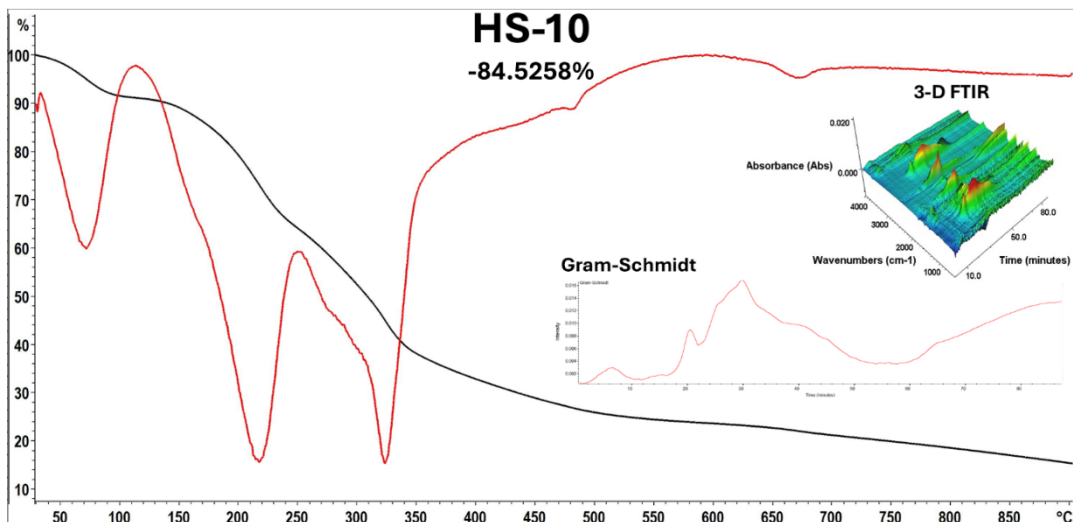


Figure S20: TGA of HS-10, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

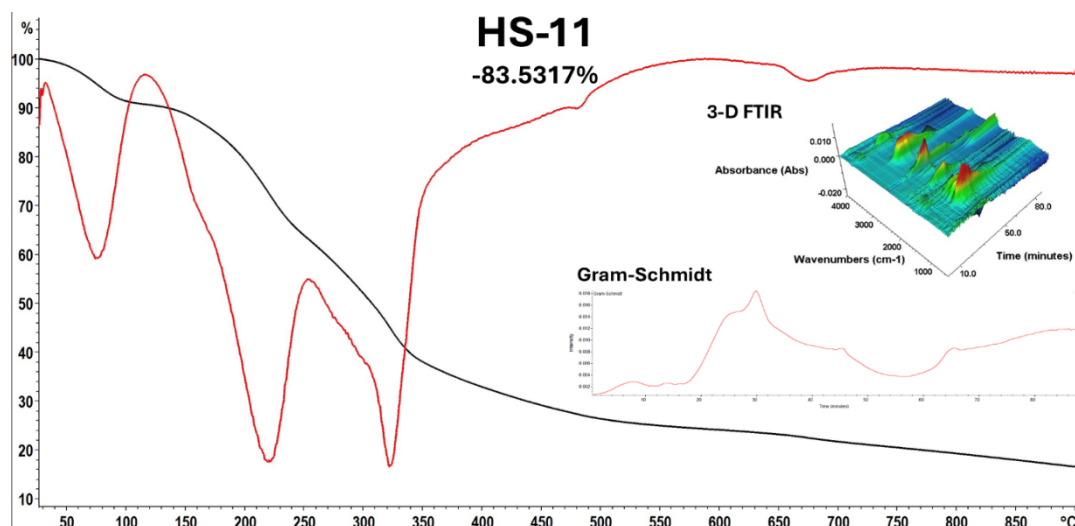


Figure S21: TGA of HS-11, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

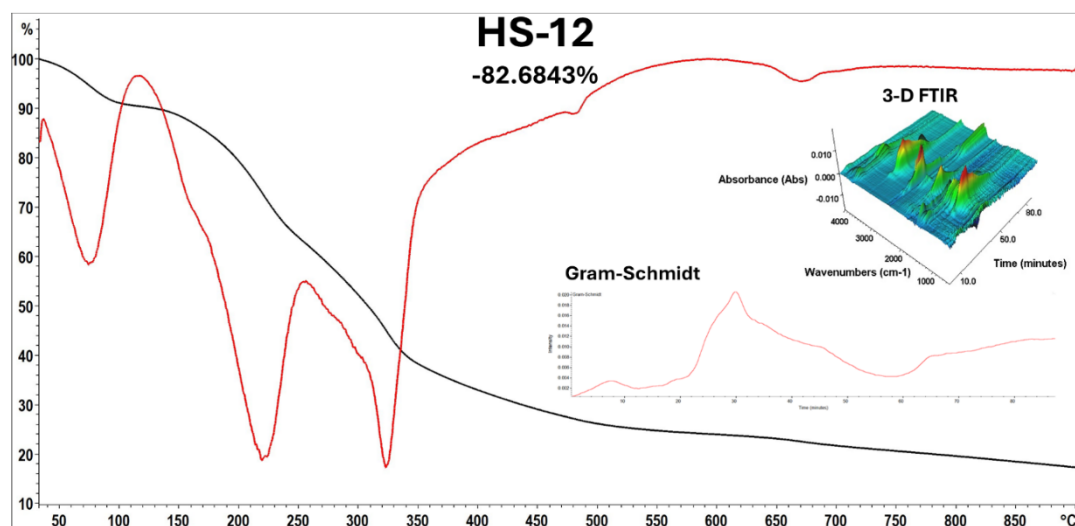


Figure S22: TGA of HS-12, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

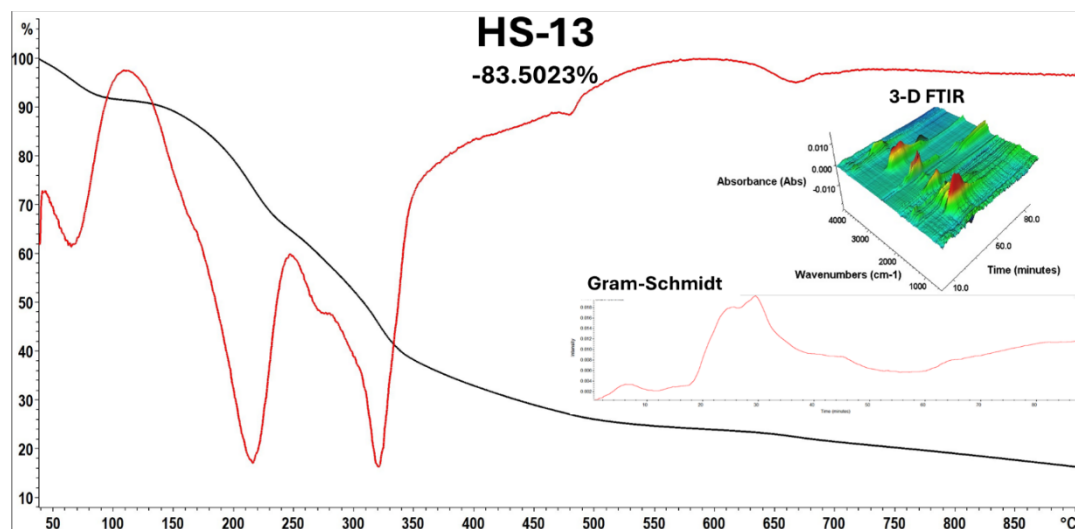


Figure S23: TGA of HS-13, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

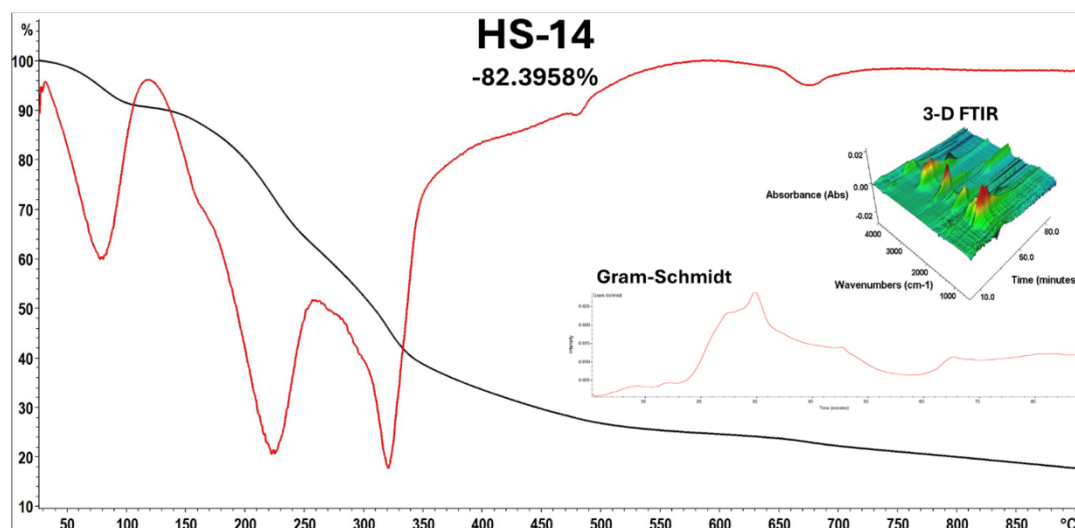


Figure S24: TGA of HS-14, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

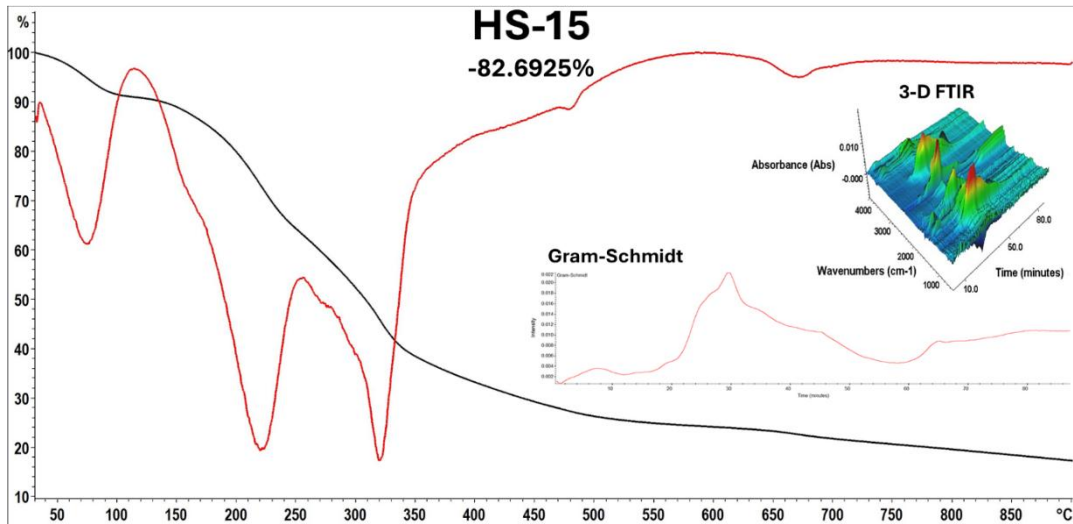


Figure S25: TGA of HS-15, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

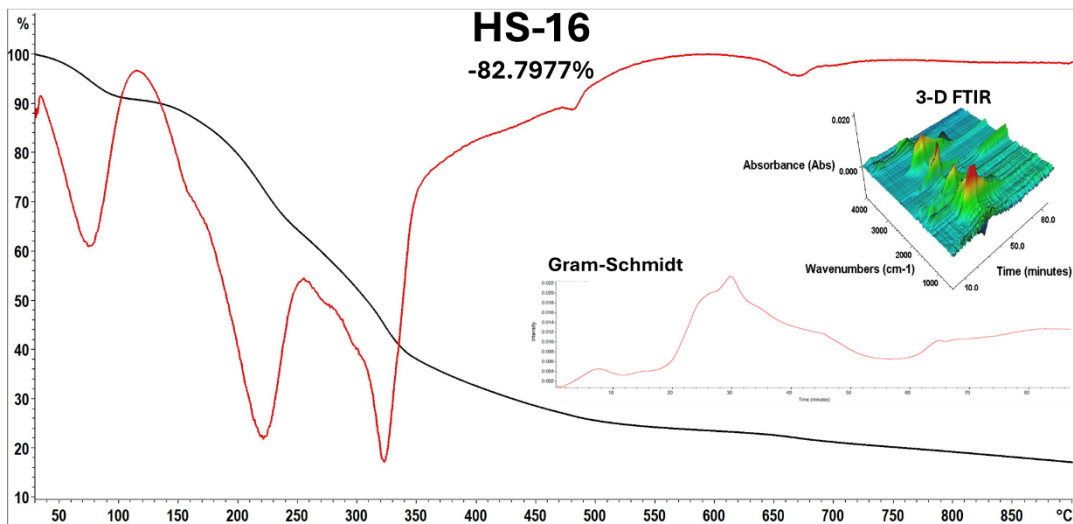


Figure S26: TGA of HS-16, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

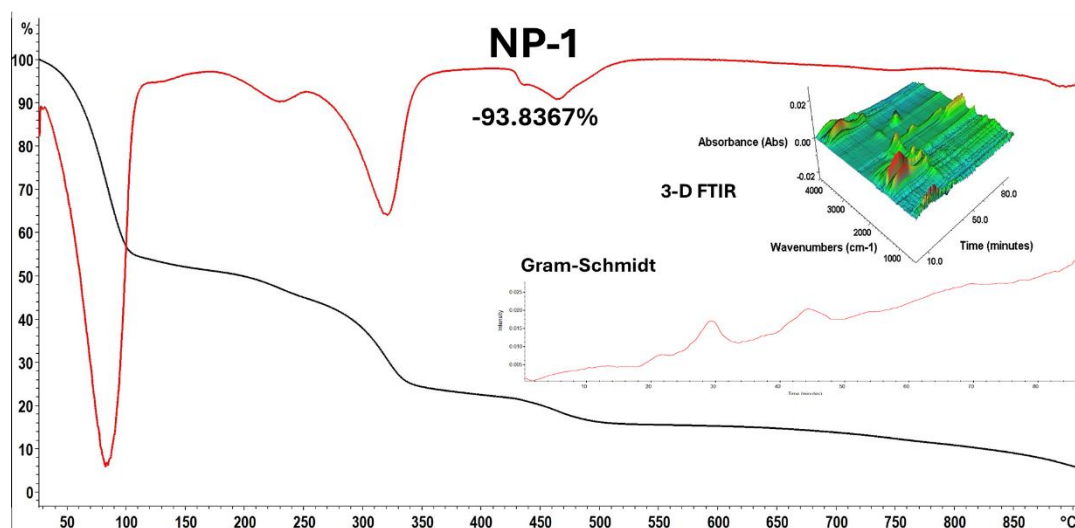


Figure S27: TGA of NP-1, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

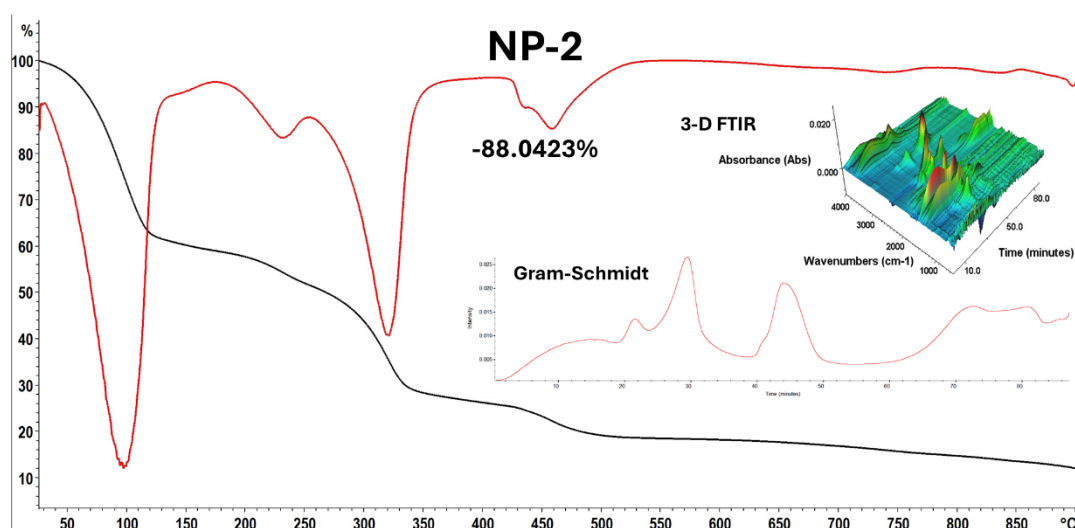


Figure S28: TGA of NP-2, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

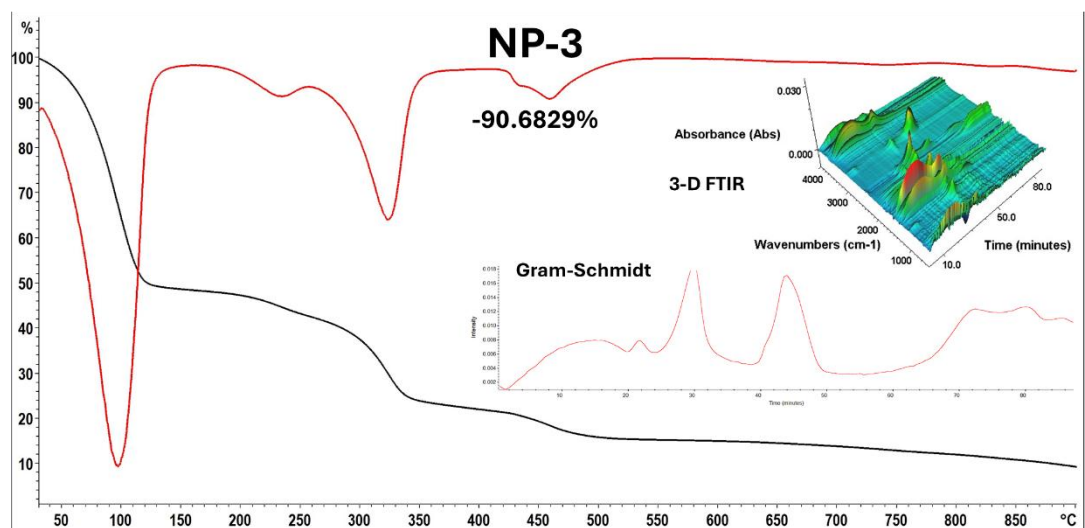


Figure S29: TGA of NP-3, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

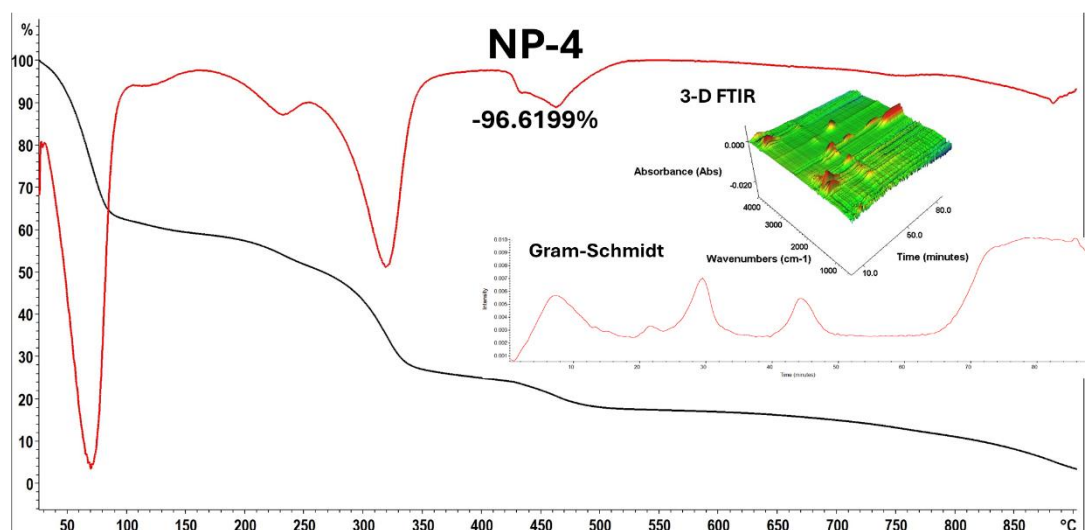


Figure S30: TGA of NP-4, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

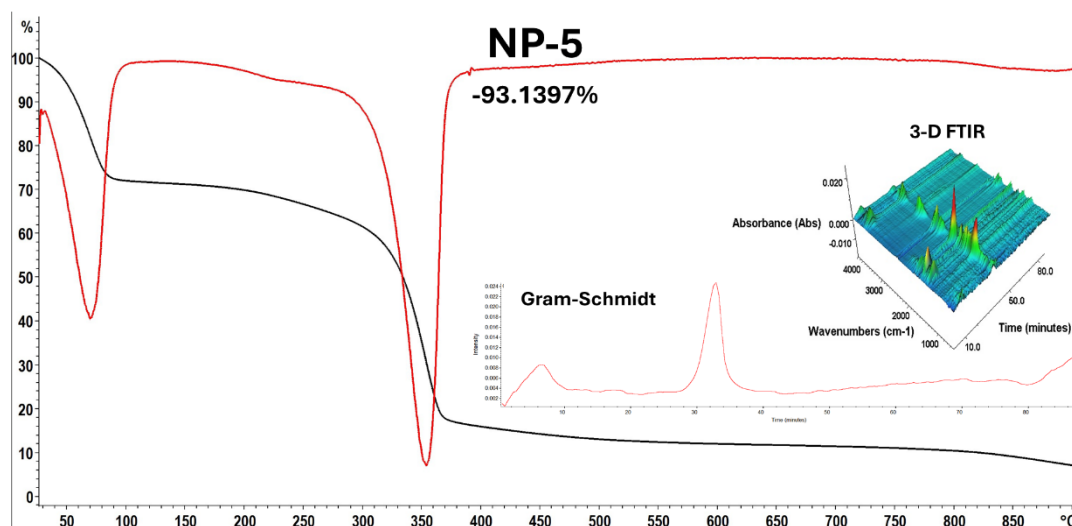


Figure S31: TGA of NP-5, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

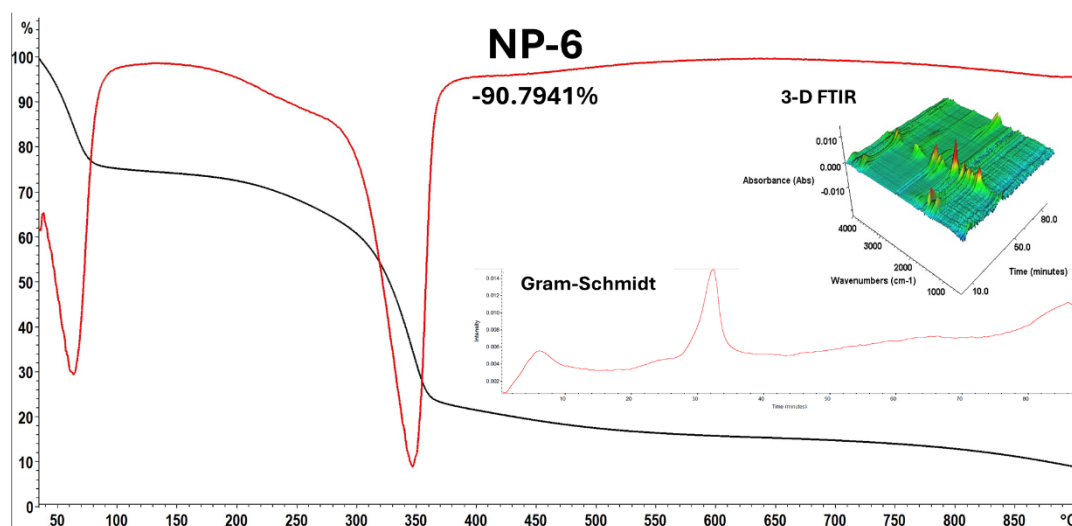


Figure S32: TGA of NP-6, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

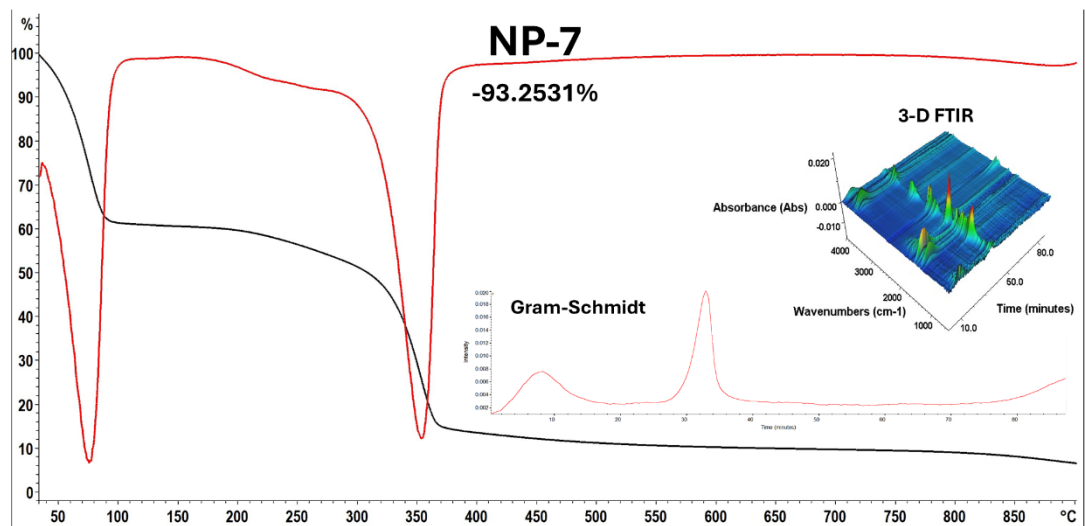


Figure S33: TGA of NP-7, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

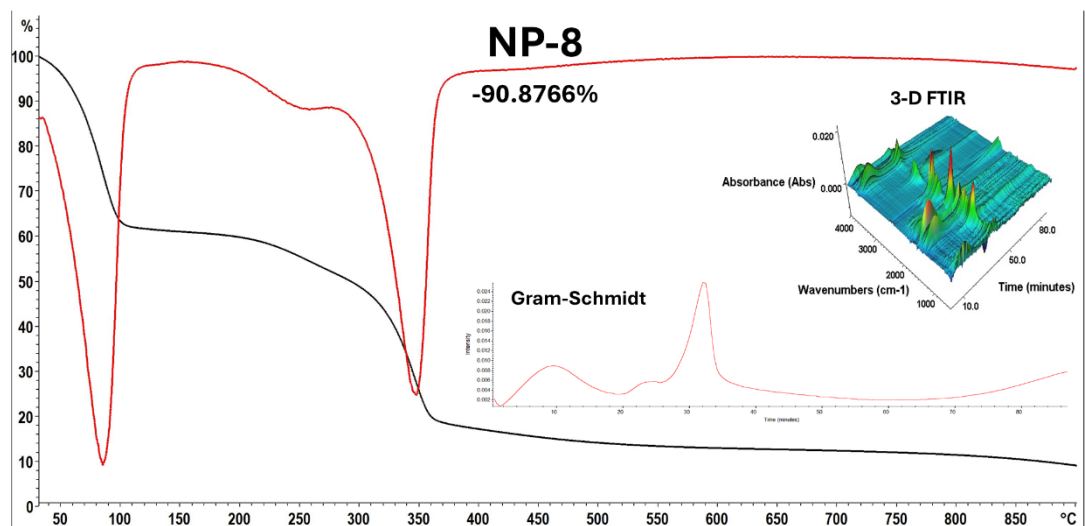


Figure S34: TGA of NP-8, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

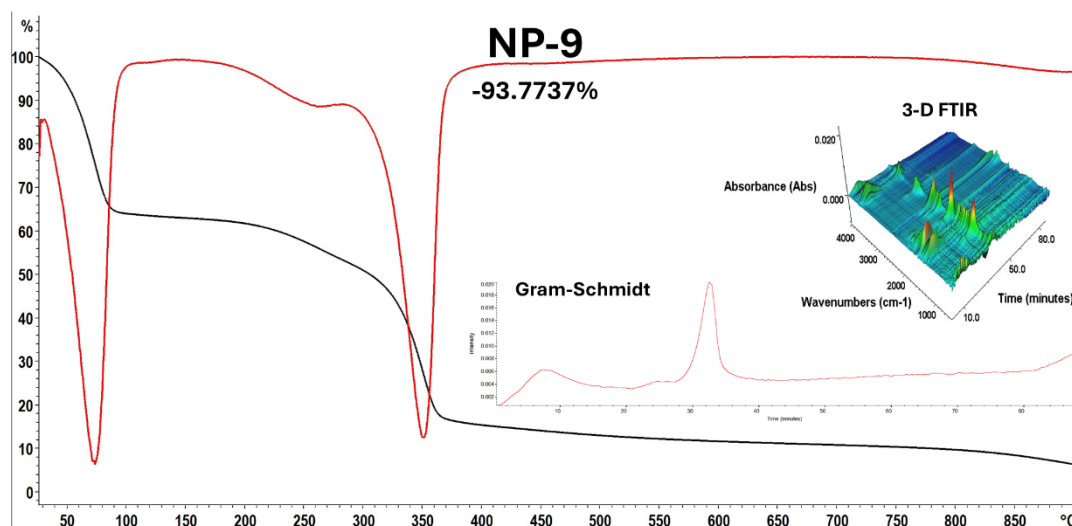


Figure S35: TGA of NP-9, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

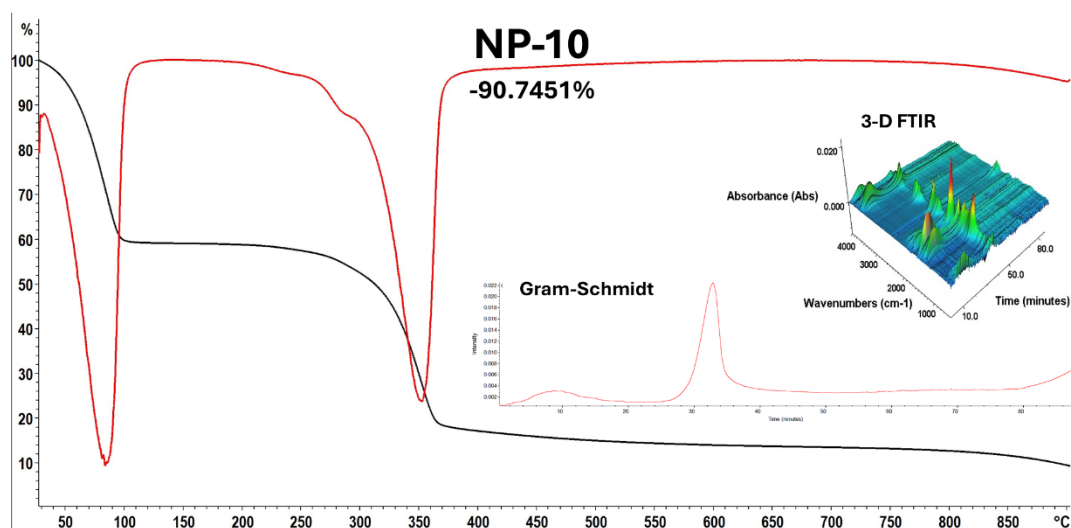


Figure S36: TGA of NP-10, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

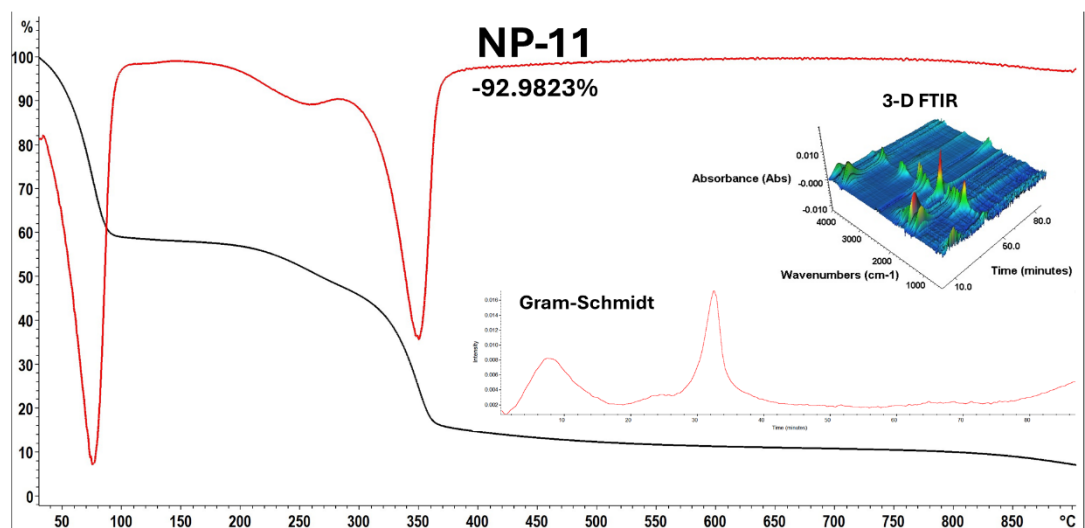


Figure S37: TGA of NP-11, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

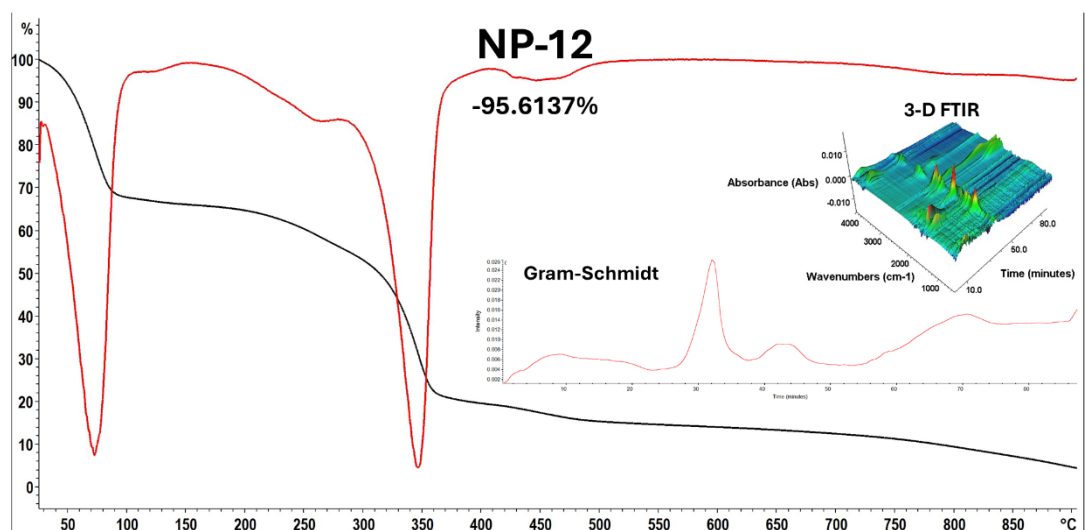


Figure S38: TGA of NP-12, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

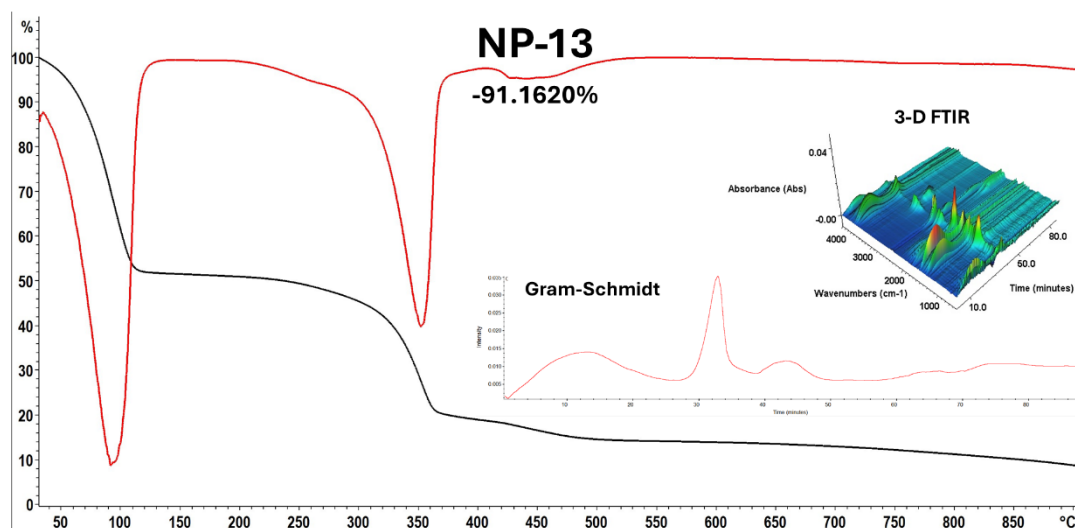


Figure S39: TGA of NP-13, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

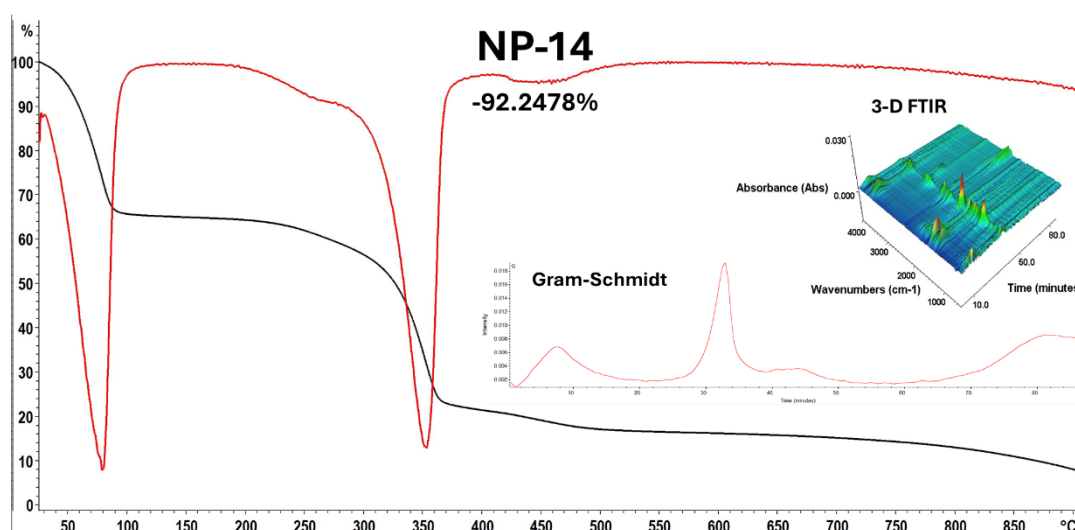


Figure S40: TGA of NP-14, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

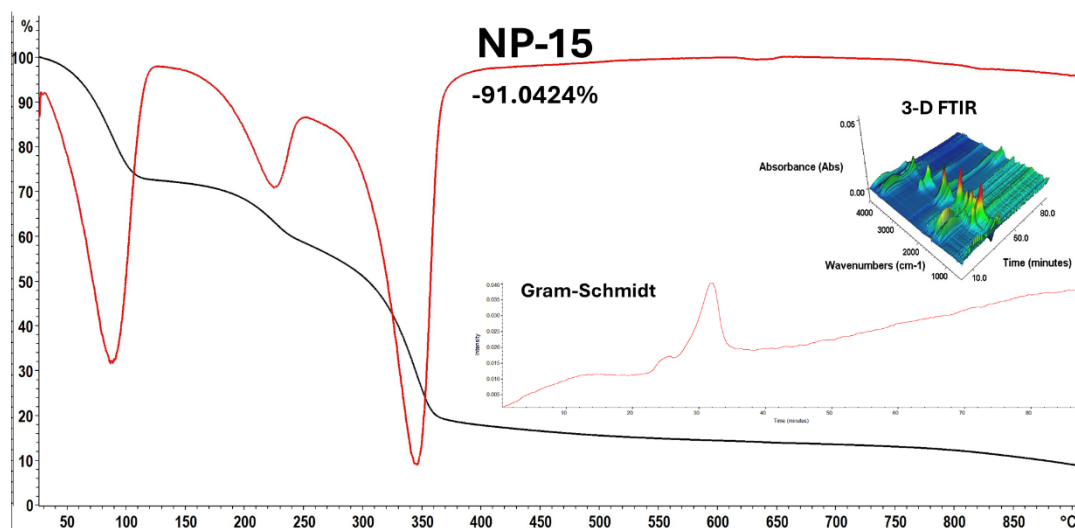


Figure S41: TGA of NP-15, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

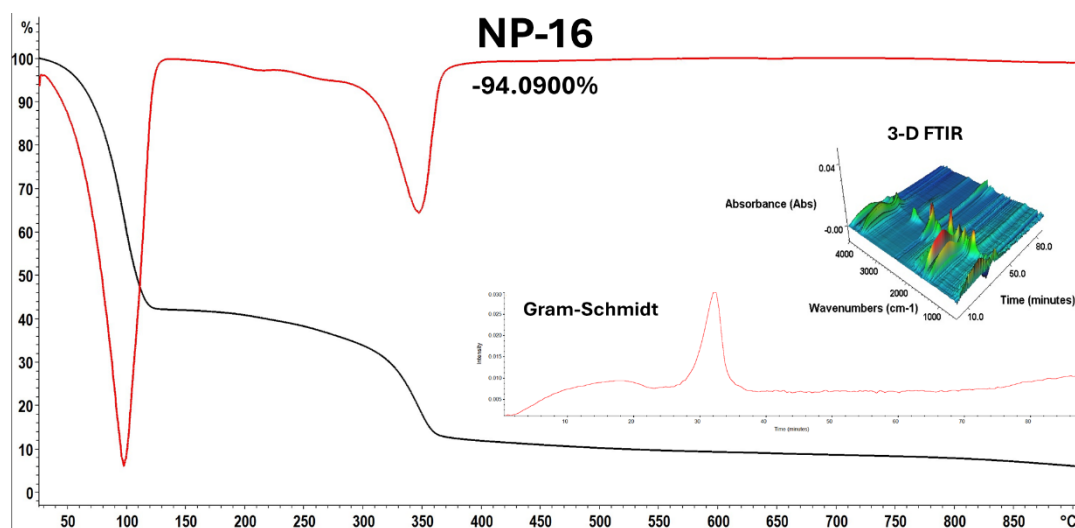


Figure S42: TGA of NP-16, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

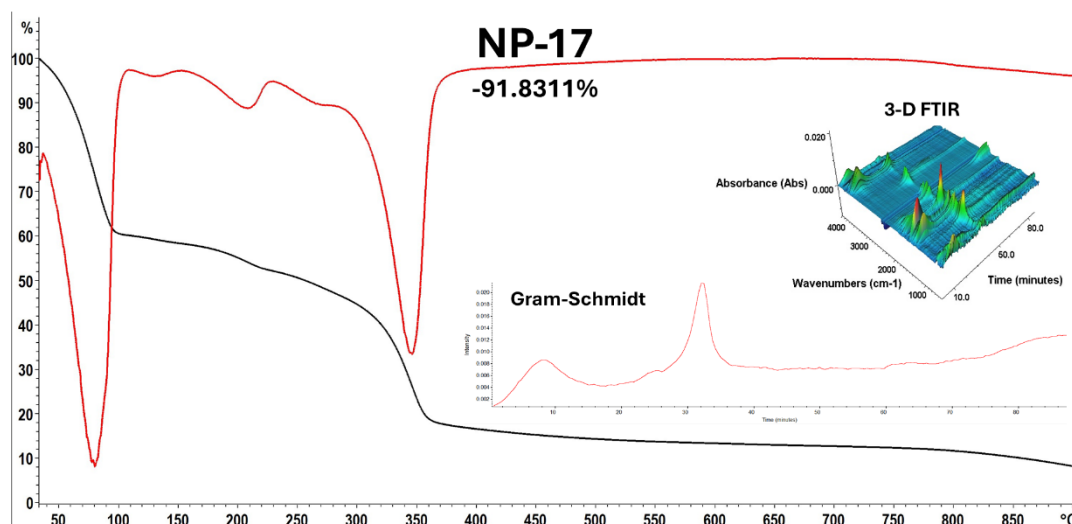


Figure S43: TGA of NP-17, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

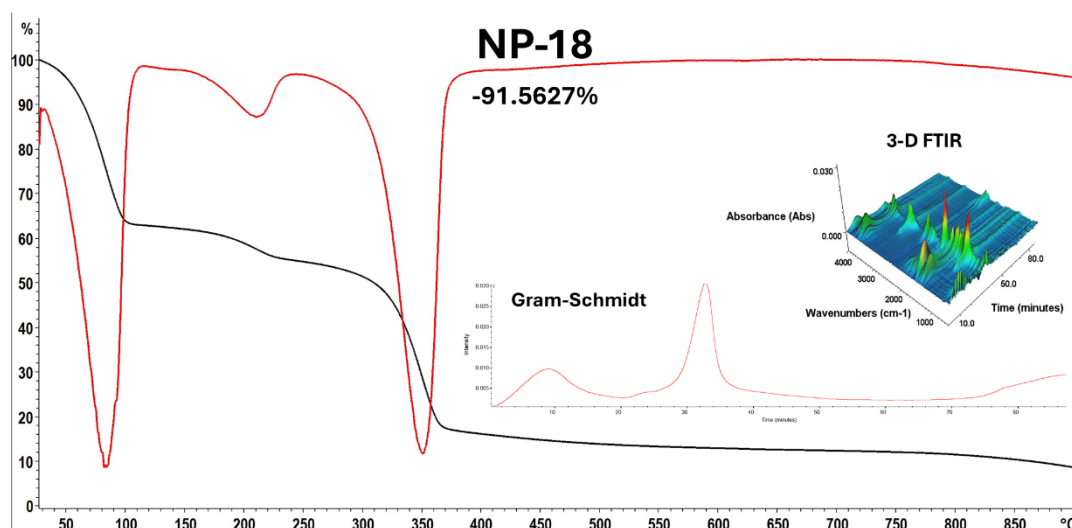


Figure S44: TGA of NP-18, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

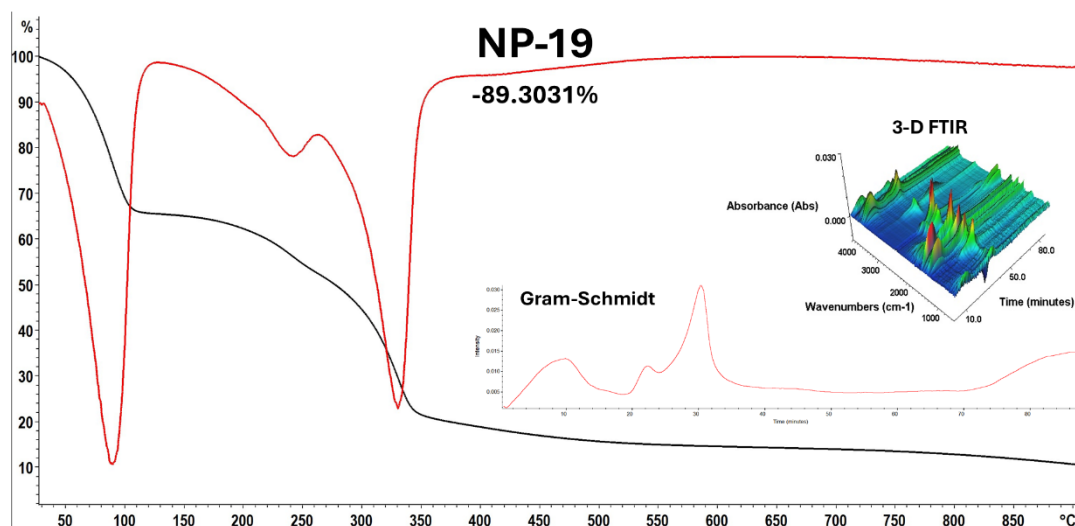


Figure S45: TGA of NP-19, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

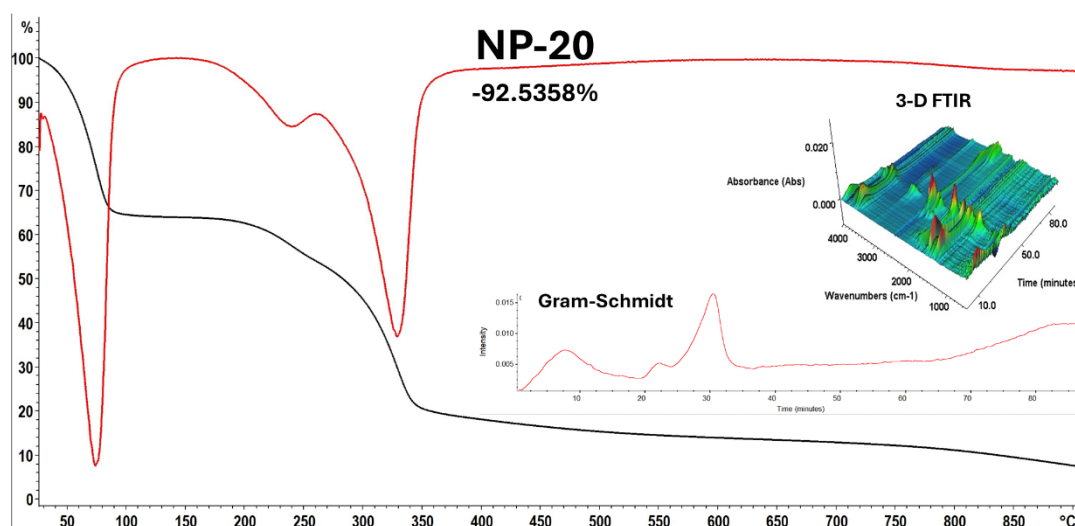


Figure S46: TGA of NP-20, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

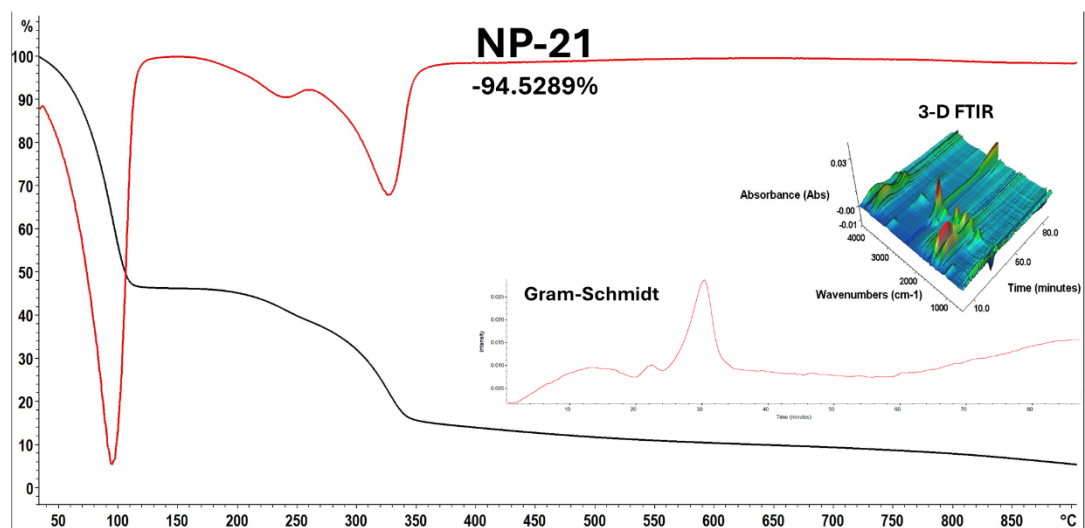


Figure S47: TGA of NP-21, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

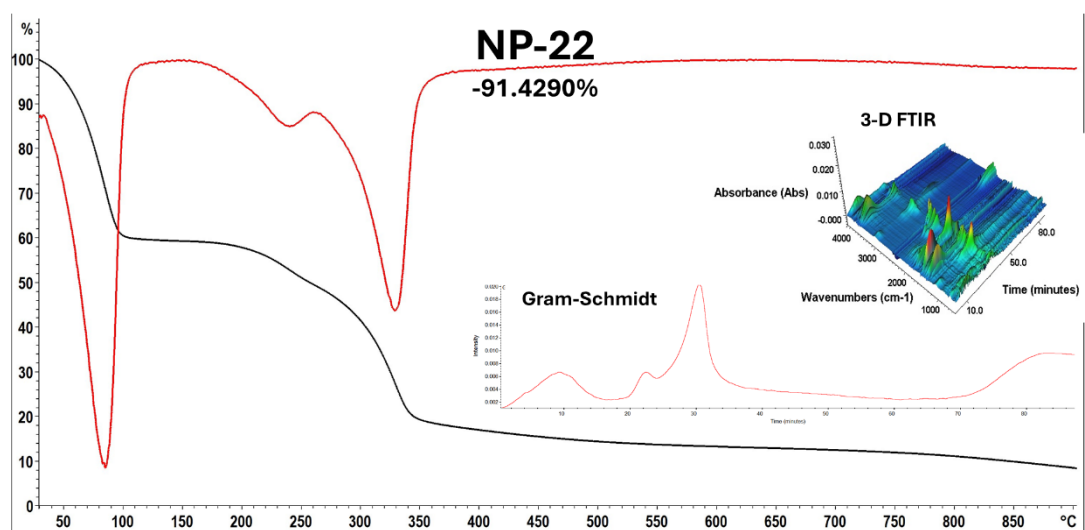


Figure S48: TGA of NP-22, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

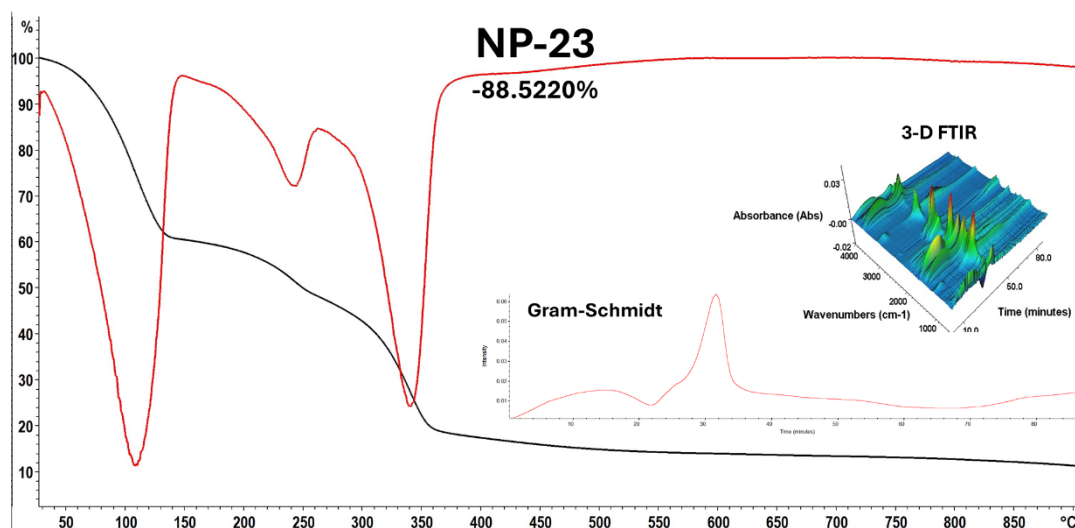


Figure S49: TGA of NP-23, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

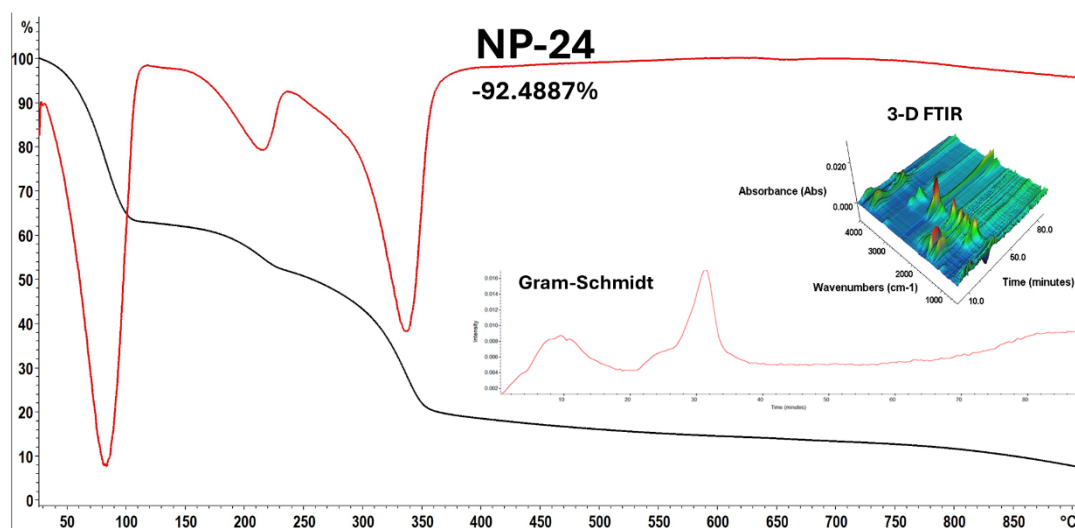


Figure S50: TGA of NP-24, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

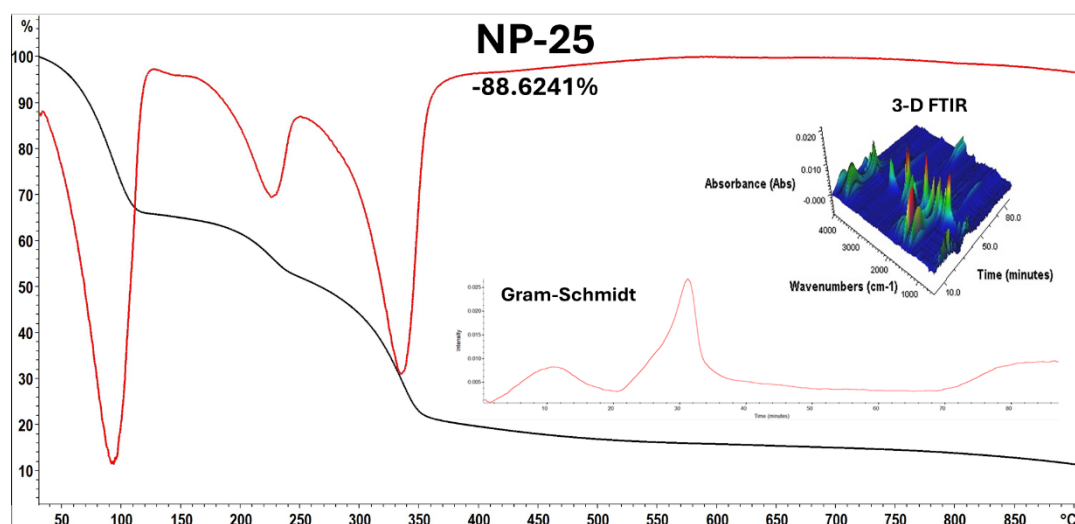


Figure S51: TGA of NP-25, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.

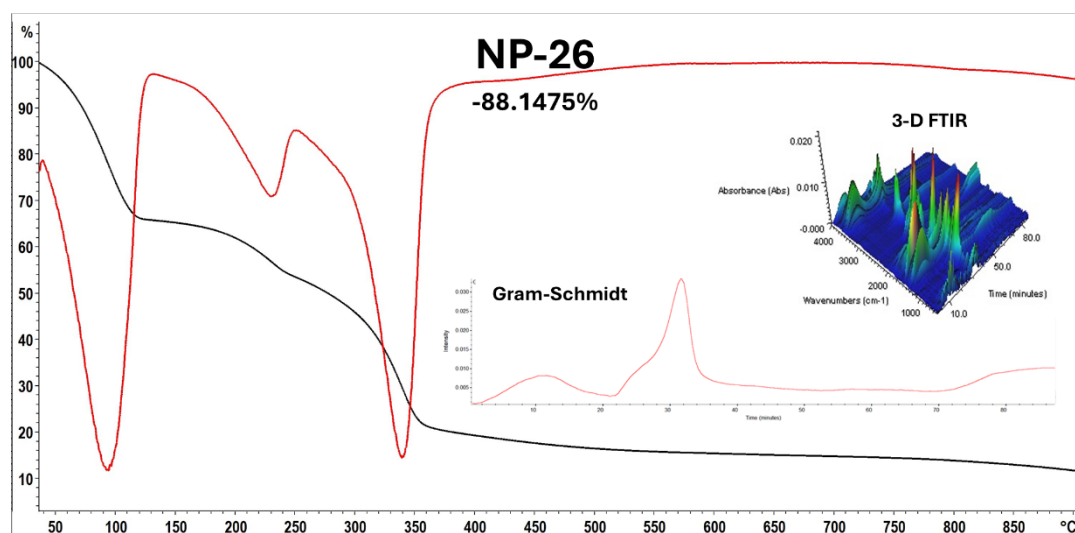


Figure S52: TGA of NP-26, with the black curve representing mass loss, the red curve representing the DTG, the Gram-Schmidt curve, and 3-D FTIR.