

IDENTIFICATION OF SULPHUR IN NAIL POLISH BY PATTERN
RECOGNITION METHOD OF PORTABLE ENERGY DISPERSIVE X-RAY
FLUORESCENCE SPECTRAL DATA

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Supplemental Material

Table S1. Characteristics of the studied nails polish. The column weight refers to the mass of samples applied in the support surface.

Number	Brand	Type	Color	Weight (g)
1	B	Varnish	Coral	0.0417
2	A	Metallic	Purple	0.0496
3	C	Cream	Yellow	0.0352
4	A	Cream	Red	0.0222
5	A	Ultra Cream	Green	0.0351
6	A	Metallic	Red	0.0386
7	A	Ultra Cream	Blue	0.0628
8	A	Sparkling	Red	0.0366
9	A	Cream	Beige	0.0361
10	A	Ultra Cream	Pink	0.0399
11	A	Metallic	Black - Purple	0.0569
12	A	Metallic	Red	0.0307
13	A	Natural	Champagne	0.0851
14	A	Metallic	Brown	0.0228
15	A	Cream	Beige	0.0388
16	A	Ultra Cream	Pink	0.0481
17	A	Sparkling	Transparent	0.0645
18	A	Cream	Orange	0.0287
19	B	Varnish	Red	0.0258
20	B	Cream	Red	0.0267
21	B	Varnish	Gold	0.0432
22	B	Glitter	Transparent	0.0281
23	B	Sparkling	Champanhe	0.0252
24	F	Metallic	Red	0.0618
25	D	Cream	Pink	0.0334
26	D	Cream	Purple	0.0571
27	D	Cream	Red	0.0321
28	D	Cream	Pink	0.0469

Number	Brand	Type	Color	Weight (g)
29	D	Cream	Purple	0.0296
30	D	Cream	Pink	0.0467
31	C	Cream	Red	0.0421
32	D	Glitter	Transparent	0.0371
33	F	Cream	Red	0.0281
34	F	Cream	Pink	0.0300
35	F	Sparkling	Gold	0.0229
36	F	Cream	White	0.0529
37	E	Sparkling	Carmines	0.0354
38	E	Cream	Red	0.0266
39	E	Cream	Red	0.0541
40	E	Cream	Carmines	0.0432
41	F	Cream	Green	0.0295
42	A	Ultra Cream	Purple	0.0267
43	A	Metallic	Gray	0.0291
44	A	Cream	Red	0.0405
45	A	Metallic	Blue	0.0309
46	A	Cream	Red	0.0202
47	A	Sparkling	Transparent	0.0444
48	B	Cream	Blue	0.0502
49	B	Varnish	Red	0.0402
50	A	Cream	Red	0.0178
51	B	Cream	Black	0.0312
52	F	Cream	Pink	0.0442
53	F	Cream	Red	0.0622
54	F	Cream	Green	0.0402
55	C	Cream	Red	0.0471
56	C	Cream	Black	0.0562
57	F	Magnetic	Gray	0.0326
58	B	Sparkling	Salmon	0.0502
59	A	Matte	Red	0.0442
60	B	Sparkling	Gold	0.0382
61	F	Sparkling	Salmon	0.0462
62	A	Sparkling	Gold	0.0452
63	B	Cream	Red	0.0425
64	F	Cream	Yellow	0.0478
65	E	Sparkling	Green	0.0528
66	E	Cream	Orange	0.0470
67	F	Cream	Purple	0.0480
68	A	Cream	Pink	0.0521
69	D	Cream	Pink	0.0219

Number	Brand	Type	Color	Weight (g)
70	F	Sparkling	Orange	0.0456
71	A	Cream	Brown	0.0430
72	A	Matte	Blue	0.0495
73	B	Varnish	Red	0.0665
74	B	Pearly	Pink	0.0670
75	C	Pearly	Carmines	0.0686
76	A	Cream	Red	0.0416
77	B	Cream	Beige	0.0423
78	D	Pearly	Gold	0.0383
79	B	Cream	Purple	0.0355
80	A	Ultra Cream	Navy blue	0.0511
81	D	Cream	Pink	0.0484
82	C	Cream	Pink	0.0352
83	B	Cream	Purple	0.0281
84	C	Pearly	Brown	0.0512
85	B	Cream	Gray	0.0455
86	A	Metallic	Champagne	0.0400
87	A	Cream	Brown	0.0405
88	B	Varnish	Pink	0.0639
89	E	Cream	Violet	0.0583
90	A	Cream	White	0.0405
91	A	Sparkling	Transparent	0.0469
92	B	Cream	Coral	0.0410
93	B	Varnish	Gray	0.0502
94	F	Cream	Red	0.0400
95	B	Cream	Green	0.0463
96	A	Ultra Cream	Salmon	0.0363
97	B	Varnish	Purple	0.0422
98	E	Cream	Red	0.0515
99	A	Metallic	Pink	0.0433
100	B	Natural	Transparent	0.0625

Table S2. Concentration results for each nail polish samples. Values in mg kg⁻¹ with standard deviation. NI means Not Identified or under quantification limit.

N°	S (x10⁵)	Ca	Ti (x10⁵)	Fe	Cu	Zn	Bi
1	NI	322 ± 46	0.049 ± 0.001	284 ± 12	NI	27 ± 2	NI
2	0.30 ± 0.01	249 ± 94	0.041 ± 0.002	441 ± 31	NI	NI	NI
3	0.34 ± 0.04	841 ± 10	0.014 ± 0.0010	48 ± 9	NI	NI	NI
4	1.24 ± 0.13	475 ± 48	0.0007 ± 0.0003	19 ± 14	NI	18 ± 6	NI
5	0.41 ± 0.03	442 ± 62	0.050 ± 0.001	203 ± 6	NI	NI	NI
6	0.44 ± 0.02	544 ± 56	0.022 ± 0.001	148 ± 10	NI	20 ± 2	NI
7	0.32 ± 0.01	281 ± 44	0.054 ± 0.002	36 ± 2	73 ± 1	NI	NI
8	0.48 ± 0.03	393 ± 24	0.022 ± 0.001	408 ± 10	NI	93 ± 6	NI
9	0.81 ± 0.01	170 ± 57	0.077 ± 0.002	NI	NI	46 ± 1	NI
10	0.37 ± 0.03	445 ± 62	0.022 ± 0.001	47 ± 1	NI	NI	NI
11	0.18 ± 0.01	189 ± 52	0.0322 ± 0.0005	68 ± 1	NI	NI	NI

12	0.56 ± 0.04	837 ± 26	0.0012 ± 0.0003	4050 ± 187	NI	87 ± 6	NI
13	0.29 ± 0.01	83 ± 8	0.0213 ± 0.0005	NI	NI	NI	NI
14	0.67 ± 0.04	671 ± 137	0.036 ± 0.001	3820 ± 105	NI	121 ± 2	NI
15	0.30 ± 0.02	361 ± 75	0.065 ± 0.003	73 ± 8	NI	NI	NI
16	0.23 ± 0.02	278 ± 24	0.015 ± 0.001	11 ± 3	NI	NI	NI
17	0.28 ± 0.01	415 ± 39	0.0030 ± 0.0003	56 ± 6	NI	1348 ± 76	NI
18	0.46 ± 0.03	289 ± 112	0.060 ± 0.003	71 ± 14	623 ± 49	2287 ± 121	NI
19	NI	2156 ± 87	NI	410 ± 36	402 ± 23	191 ± 12	NI
20	NI	1129 ± 69	0.0127 ± 0.0002	2085 ± 43	78 ± 1	79 ± 17	NI
21	NI	311 ± 47	0.030 ± 0.002	149 ± 6	306 ± 28	1578 ± 113	NI
22	0.08 ± 0.01	675 ± 13	0.0004 ± 0.0001	209 ± 2	NI	NI	NI
23	NI	465 ± 141	0.0709 ± 0.0005	668 ± 10	NI	161 ± 7	NI
24	0.34 ± 0.02	371 ± 41	0.0062 ± 0.0001	27 ± 3	NI	4 ± 1	935 ± 11
25	0.91 ± 0.04	373 ± 69	0.030 ± 0.002	45 ± 10	NI	NI	NI
26	0.46 ± 0.02	281 ± 28	0.010 ± 0.001	707 ± 35	NI	NI	NI
27	0.95 ± 0.02	537 ± 41	0.017 ± 0.001	540 ± 36	NI	NI	NI

28	0.54 ± 0.02	248 ± 34	0.039 ± 0.001	172 ± 18	NI	NI	NI
29	0.90 ± 0.01	236 ± 65	0.044 ± 0.001	851 ± 34	NI	NI	NI
30	0.61 ± 0.01	307 ± 39	0.0238 ± 0.0004	38 ± 7	NI	NI	NI
31	0.38 ± 0.01	244 ± 43	0.0036 ± 0.0002	44 ± 8	NI	1801 ± 162	NI
32	NI	143 ± 45	NI	NI	213 ± 1	588 ± 29	NI
33	0.70 ± 0.02	459 ± 18	0.152 ± 0.011	NI	118 ± 81	73 ± 6	NI
34	0.56 ± 0.04	455 ± 4	0.146 ± 0.001	328 ± 14	NI	10 ± 4	NI
35	0.84 ± 0.08	423 ± 193	0.035 ± 0.001	6179 ± 91	NI	NI	NI
36	0.19 ± 0.04	260 ± 8	0.147 ± 0.003	48 ± 9	NI	22 ± 2	NI
37	0.45 ± 0.12	462 ± 68	0.0110 ± 0.0003	10958 ± 539	NI	35 ± 5	NI
38	0.67 ± 0.06	704 ± 14	0.0026 ± 0.0002	377 ± 26	NI	25 ± 4	NI
39	0.42 ± 0.04	434 ± 37	NI	58 ± 3	NI	3 ± 1	NI
40	0.39 ± 0.02	610 ± 39	0.0085 ± 0.0001	2025 ± 61	NI	51 ± 4	NI
41	0.71 ± 0.04	128 ± 30	0.114 ± 0.003	99 ± 14	97 ± 9	27 ± 19	NI
42	0.36 ± 0.03	485 ± 14	0.023 ± 0.001	394 ± 22	NI	NI	NI
43	0.46 ± 0.01	471 ± 101	0.060 ± 0.001	72 ± 6	NI	6 ± 1	NI

44	0.49 ± 0.02	673 ± 46	0.0129 ± 0.0003	NI	NI	55 ± 1	NI
45	0.54 ± 0.01	36 ± 40	0.101 ± 0.003	2702 ± 68	NI	NI	NI
46	1.20 ± 0.07	1480 ± 48	0.0002 ± 0.0001	NI	19 ± 12	71 ± 13	NI
47	0.61 ± 0.04	173 ± 63	0.0029 ± 0.0003	NI	NI	NI	NI
48	NI	259 ± 38	0.031 ± 0.001	1876 ± 62	NI	8 ± 2	NI
49	NI	627 ± 23	NI	688 ± 17	91 ± 5	90 ± 8	NI
50	0.66 ± 0.05	493 ± 55	0.038 ± 0.001	NI	NI	NI	NI
51	NI	NI	0.0027 ± 0.0004	33508 ± 1590	NI	NI	NI
52	0.46 ± 0.02	494 ± 24	0.043 ± 0.001	54 ± 4	NI	42 ± 3	NI
53	0.43 ± 0.04	69 ± 29	0.0093 ± 0.0004	NI	NI	NI	NI
54	0.66 ± 0.04	240 ± 56	0.159 ± 0.004	103 ± 1	337 ± 20	NI	NI
55	0.39 ± 0.04	246 ± 22	0.0030 ± 0.0002	56 ± 10	NI	NI	NI
56	0.36 ± 0.01	301 ± 12	0.0008 ± 0.0001	52 ± 4	24 ± 3	20 ± 2	NI
57	NI	661 ± 527	0.014 ± 0.005	42637 ± 506	NI	17 ± 3	NI
58	0.36 ± 0.01	128 ± 17	0.00013 ± 0.00006	274 ± 217	NI	53 ± 9	824 ± 17
59	0.21 ± 0.02	290 ± 27	0.021 ± 0.001	4908 ± 845	NI	NI	NI

60	0.10 ± 0.01	299 ± 11	0.0137 ± 0.0005	972 ± 54	2184 ± 107	468 ± 12	3884 ± 28
61	0.30 ± 0.03	296 ± 28	0.034 ± 0.002	29 ± 4	NI	NI	1644 ± 17
62	0.18 ± 0.03	416 ± 64	0.035 ± 0.001	185 ± 11	NI	NI	NI
64	0.15 ± 0.01	231 ± 38	0.027 ± 0.001	NI	NI	NI	NI
65	0.41 ± 0.03	300 ± 37	0.0002 ± 0.0001	33 ± 6	59 ± 4	NI	2496 ± 19
66	0.54 ± 0.07	258 ± 37	NI	39 ± 6	NI	NI	NI
67	0.39 ± 0.02	705 ± 16	0.0055 ± 0.0002	23 ± 5	43 ± 3	7 ± 2	NI
68	0.36 ± 0.01	NI	0.052 ± 0.001	NI	NI	NI	NI
69	1.37 ± 0.01	586 ± 115	0.184 ± 0.002	136 ± 5	NI	NI	NI
70	0.36 ± 0.01	918 ± 36	0.0033 ± 0.0002	28 ± 3	NI	NI	NI
71	0.23 ± 0.03	298 ± 54	0.016 ± 0.001	4027 ± 390	NI	33 ± 4	NI
72	0.25 ± 0.01	132 ± 36	0.095 ± 0.005	24 ± 2	43 ± 7	17 ± 6	NI
73	NI	283 ± 41	0.0025 ± 0.0019	6376 ± 122	NI	38 ± 1	NI
74	0.02 ± 0.01	312 ± 44	0.165 ± 0.011	NI	NI	8 ± 5	11283 ± 34
75	0.32 ± 0.01	196 ± 6	NI	51 ± 10	NI	27 ± 1	5688 ± 24
76	0.36 ± 0.02	219 ± 112	0.0134 ± 0.0004	842 ± 15	NI	NI	NI

77	NI	233 ± 13	0.045 ± 0.002	405 ± 21	NI	NI	1910 ± 19
78	0.73 ± 0.03	NI	0.063 ± 0.001	6630 ± 251	NI	3 ± 1	NI
79	NI	800 ± 26	0.018 ± 0.001	1102 ± 42	NI	NI	NI
80	0.28 ± 0.02	256 ± 18	0.0127 ± 0.0002	22 ± 5	182 ± 6	12 ± 4	NI
81	0.61 ± 0.01	368 ± 68	0.033 ± 0.002	46 ± 3	NI	NI	NI
82	0.41 ± 0.01	394 ± 36	0.017 ± 0.001	27 ± 3	NI	NI	NI
83	NI	495 ± 133	0.242 ± 0.002	638 ± 24	NI	47 ± 8	NI
84	0.46 ± 0.01	495 ± 79	0.009 ± 0.001	2503 ± 52	NI	122 ± 13	NI
85	0.01 ± 0.01	259 ± 20	0.045 ± 0.001	12 ± 6	NI	NI	427 ± 11
86	0.38 ± 0.01	151 ± 102	0.080 ± 0.005	254 ± 33	NI	NI	NI
87	0.43 ± 0.01	202 ± 36	0.018 ± 0.001	1845 ± 33	NI	14 ± 4	NI
88	NI	161 ± 16	0.027 ± 0.002	272 ± 222	NI	9 ± 1	NI
89	0.39 ± 0.02	317 ± 25	0.0052 ± 0.0003	41 ± 5	10 ± 2	3 ± 1	NI
90	0.53 ± 0.01	25 ± 54	0.040 ± 0.003	NI	NI	10 ± 3	NI
91	0.30 ± 0.01	167 ± 28	0.048 ± 0.001	149 ± 7	NI	27 ± 6	NI
92	0.02 ± 0.01	236 ± 4	0.130 ± 0.005	22 ± 4	NI	9 ± 3	774 ± 14

93	0.02 ± 0.01	182 ± 45	0.013 ± 0.009	656 ± 476	NI	NI	427 ± 10
94	0.14 ± 0.03	1609 ± 183	0.074 ± 0.004	512 ± 31	NI	16 ± 3	NI
95	NI	128 ± 52	0.053 ± 0.001	1800 ± 37	NI	NI	NI
96	0.52 ± 0.02	211 ± 52	0.064 ± 0.001	1520 ± 25	NI	NI	NI
97	NI	612 ± 35	0.047 ± 0.003	803 ± 64	NI	1.8 ± 0.6	NI
98	0.37 ± 0.07	216 ± 46	0.0073 ± 0.0002	NI	NI	NI	NI
99	0.37 ± 0.02	358 ± 49	0.053 ± 0.001	128 ± 1	NI	NI	NI
100	NI	98 ± 21	0.027 ± 0.001	30 ± 6	NI	29 ± 1	NI

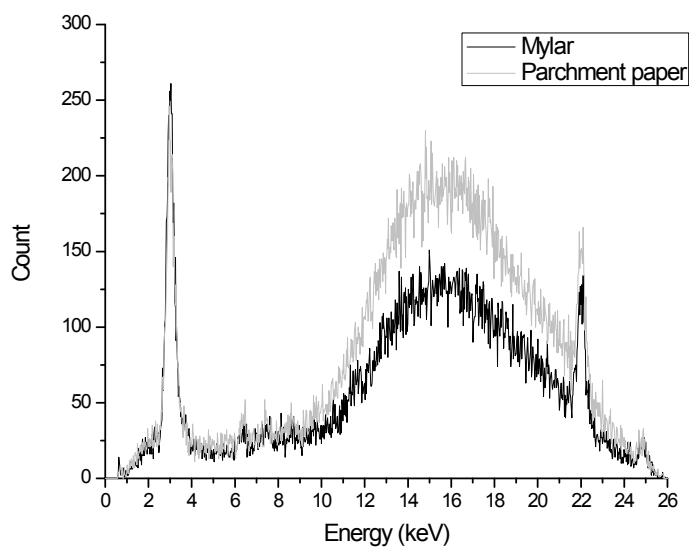


Figure S1. Spectra from mylar film and parchment paper used to spread the nail polish samples.

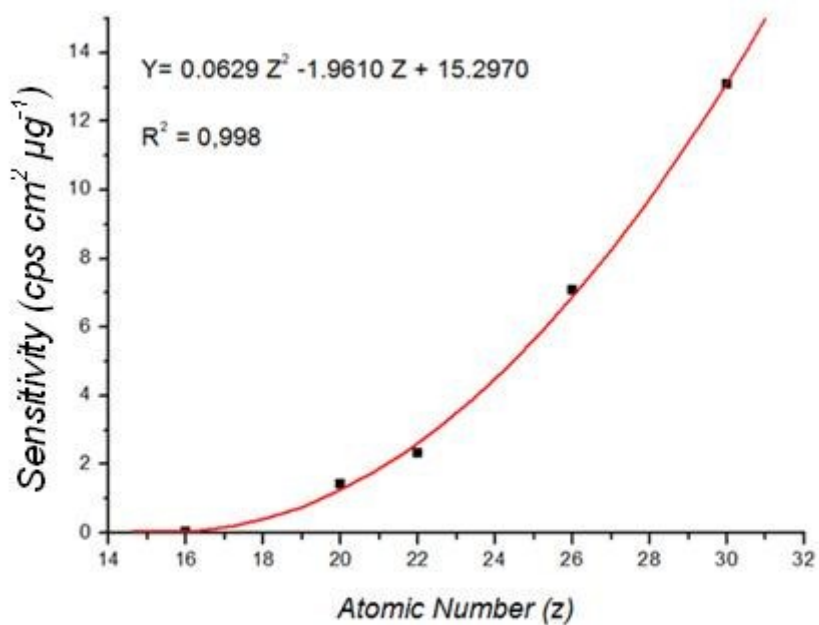


Figure S2. Element Sensitivity for K α line versus atomic number (Z) obtained from MicroMatter membrane standards.