Supporting information

The first application of ¹H NMR spectroscopy for the assessment of the authenticity of perfumes

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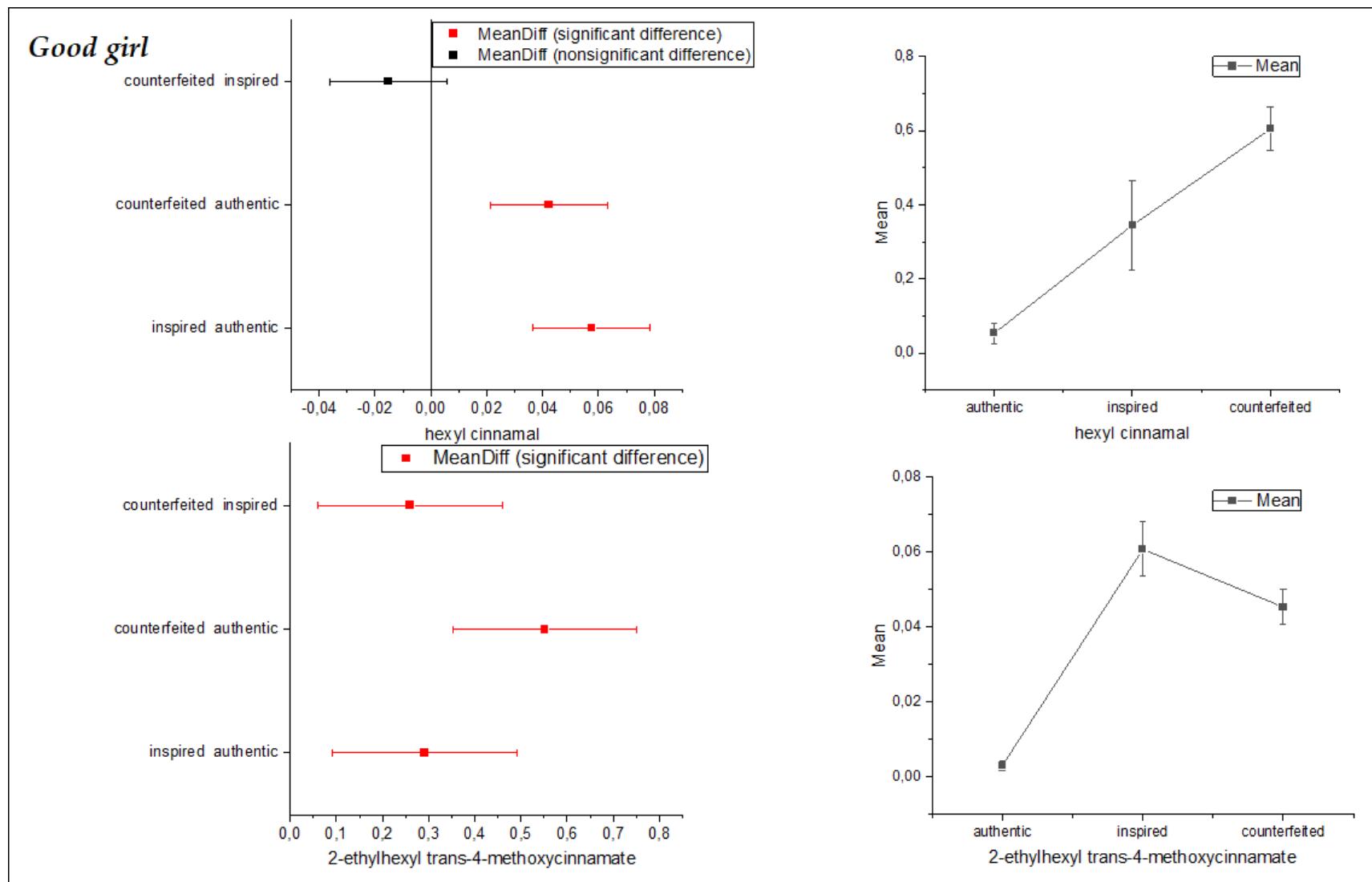
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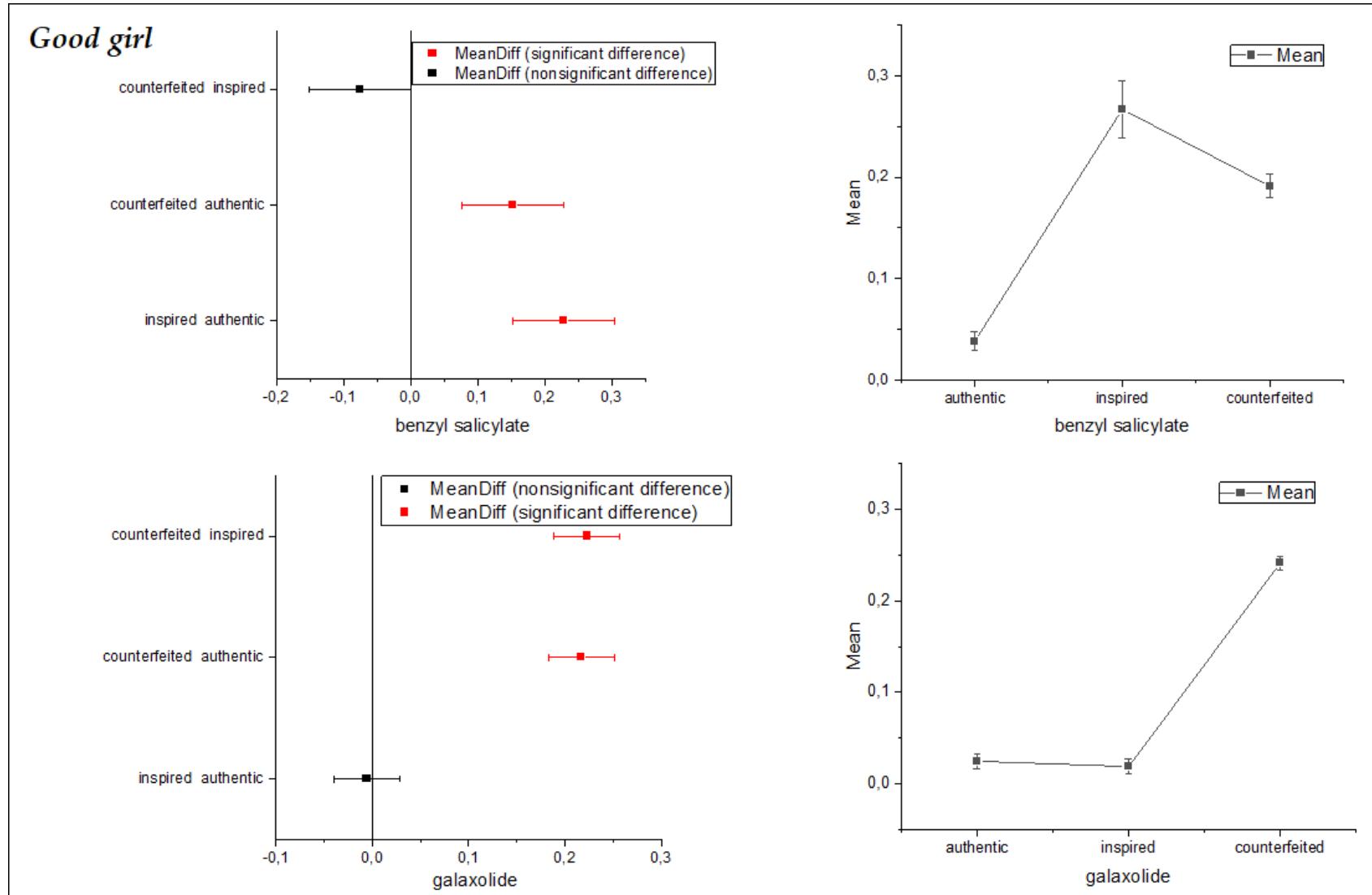
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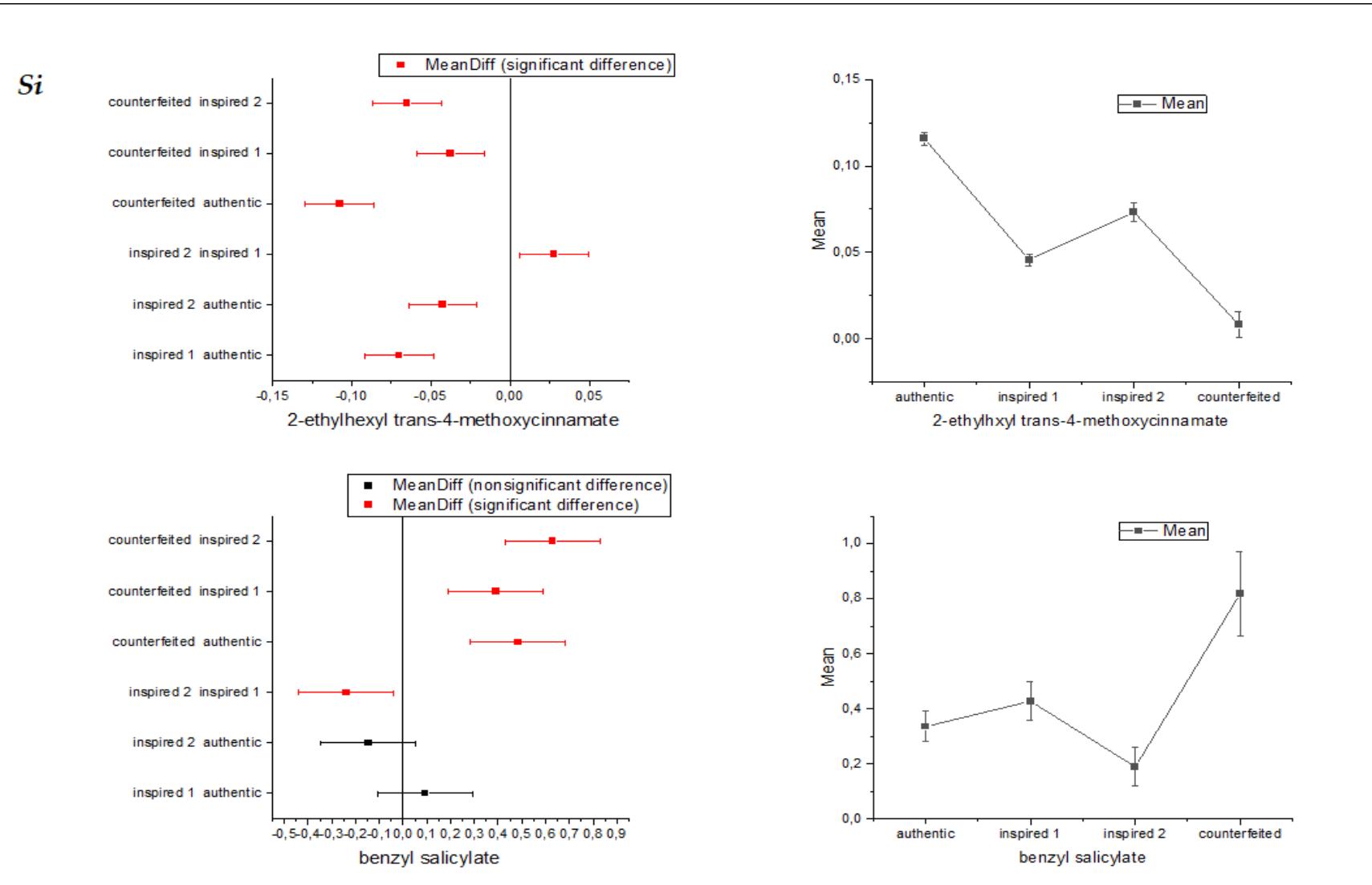
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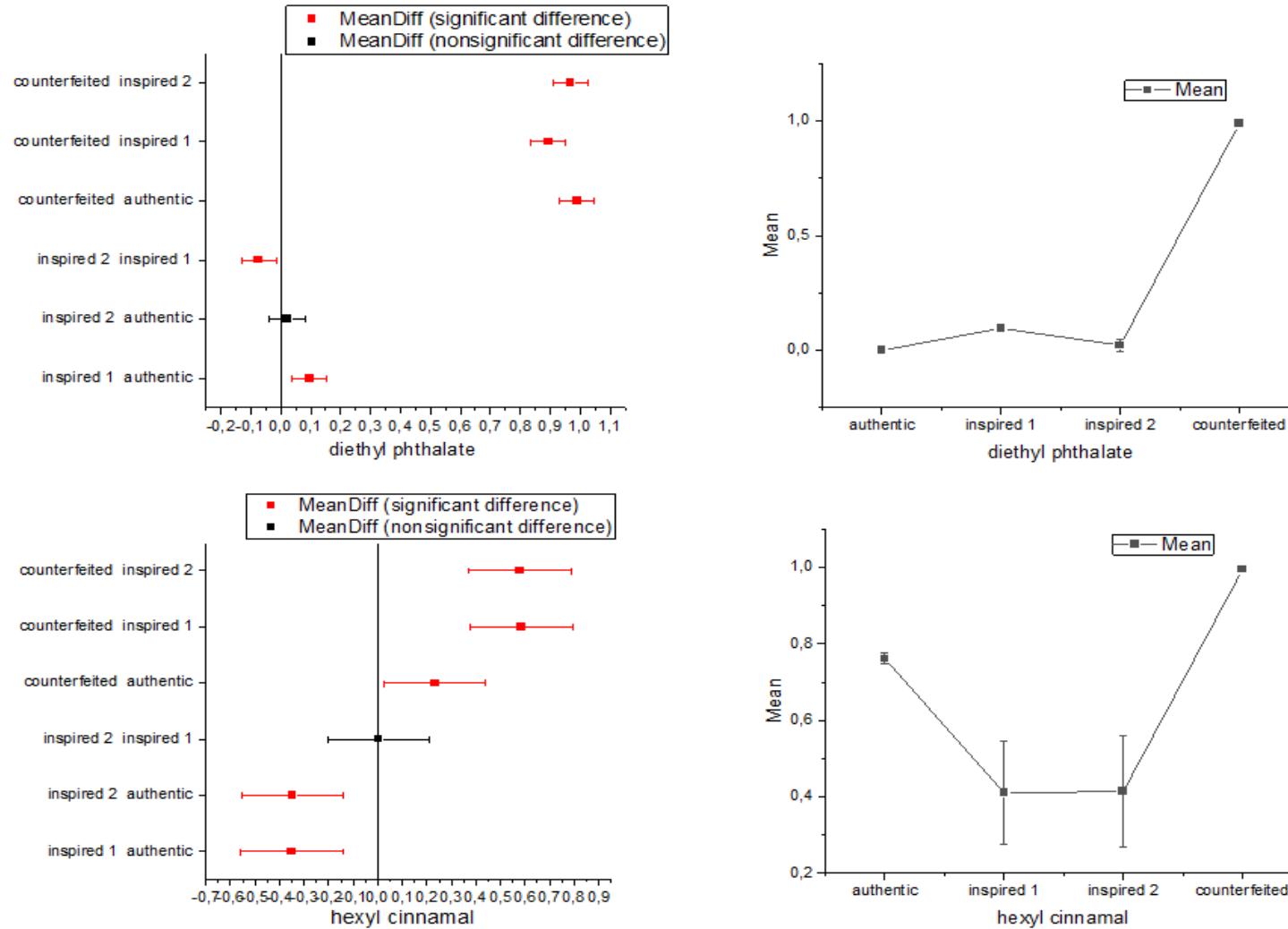
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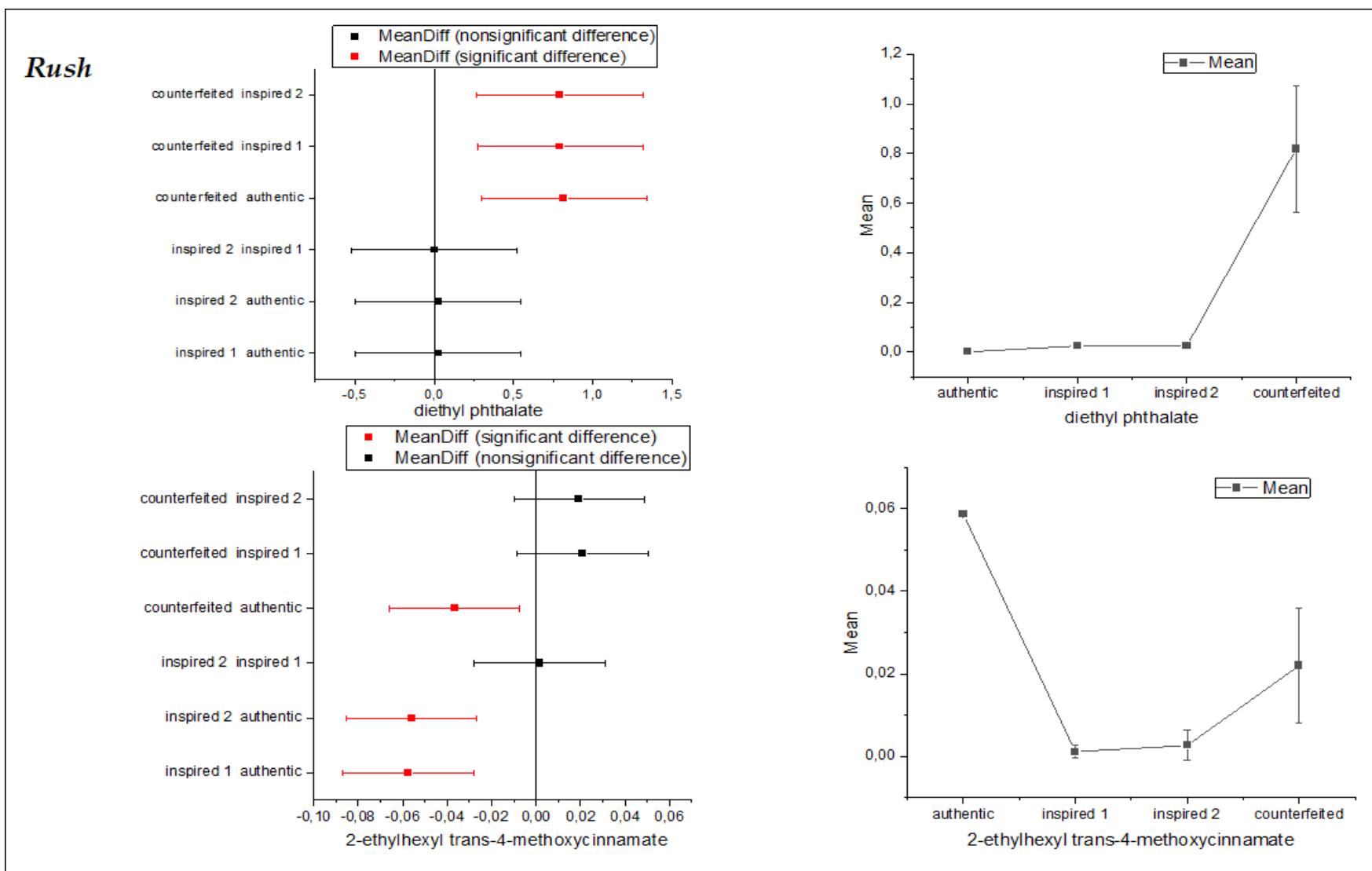
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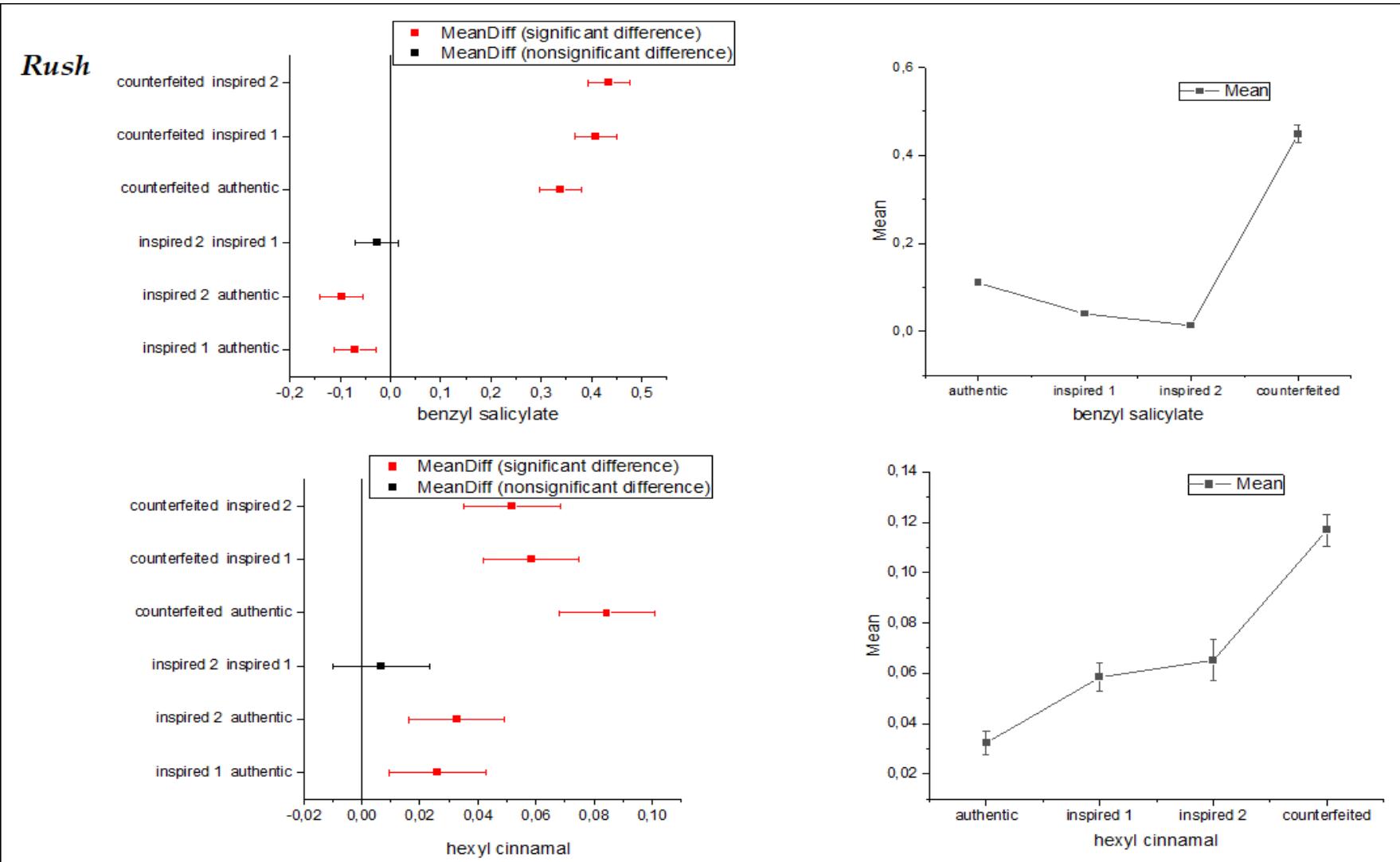
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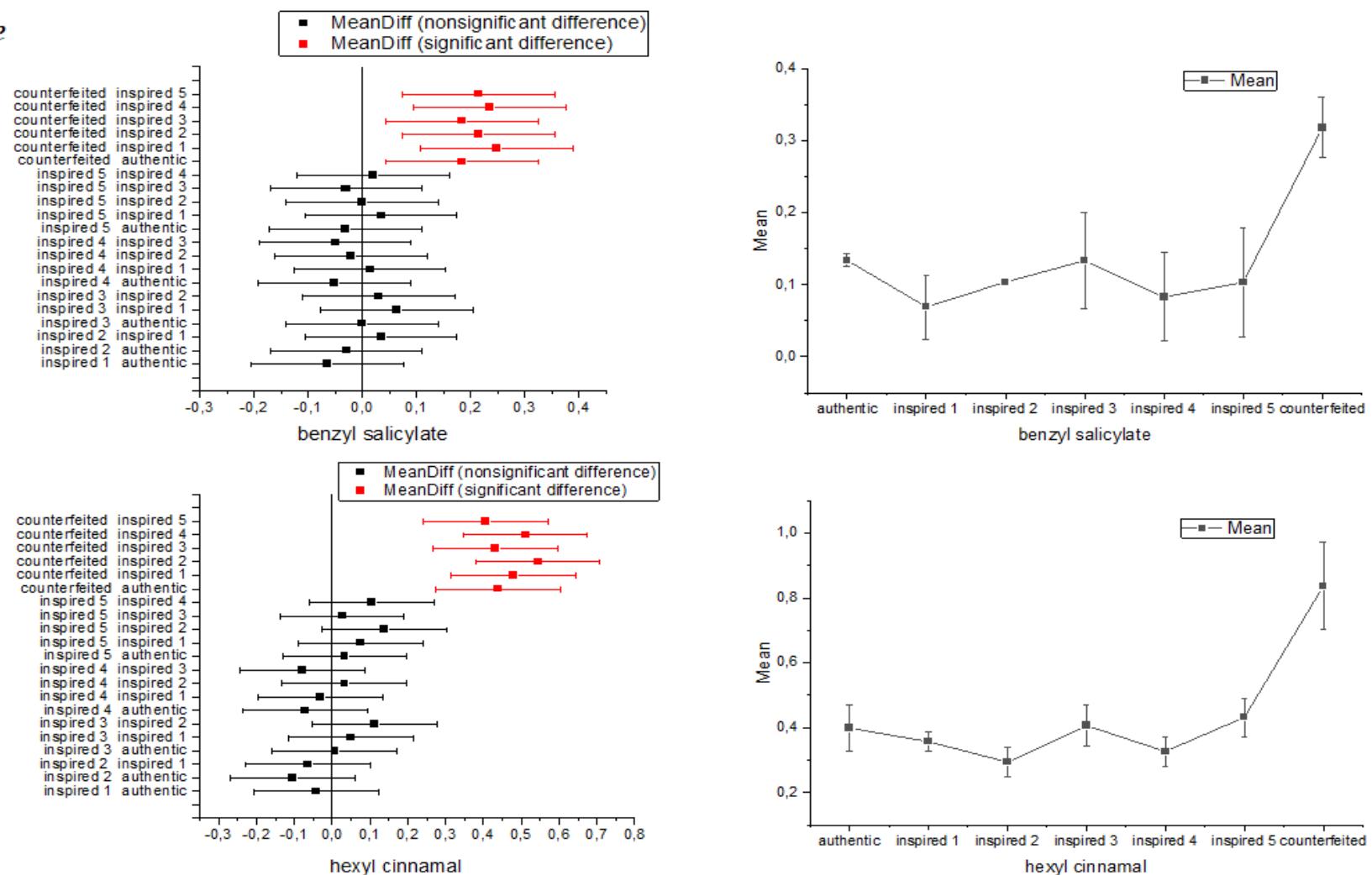
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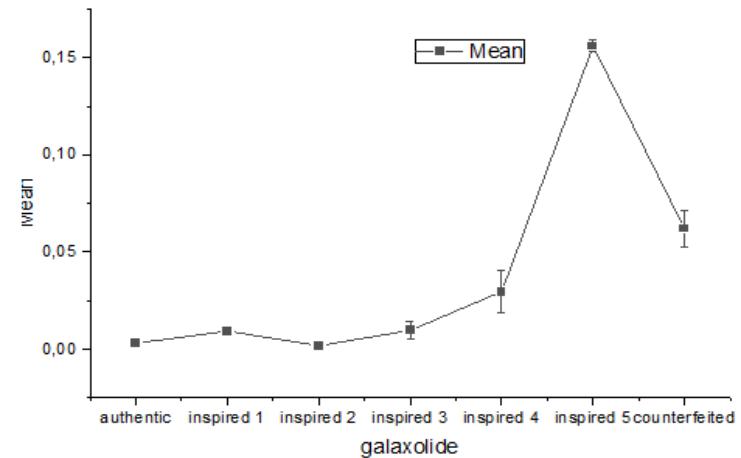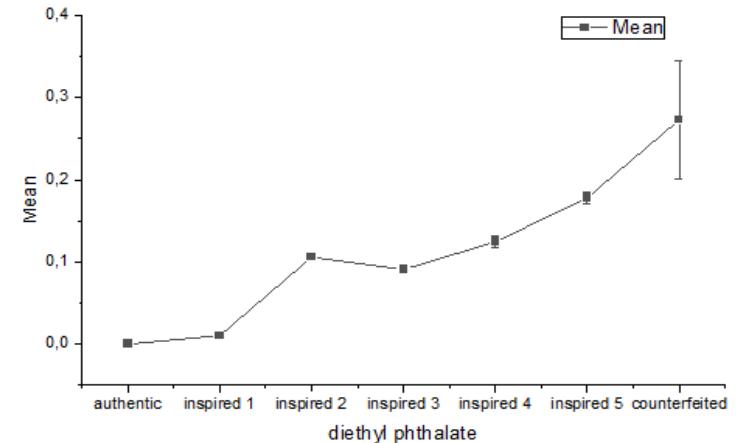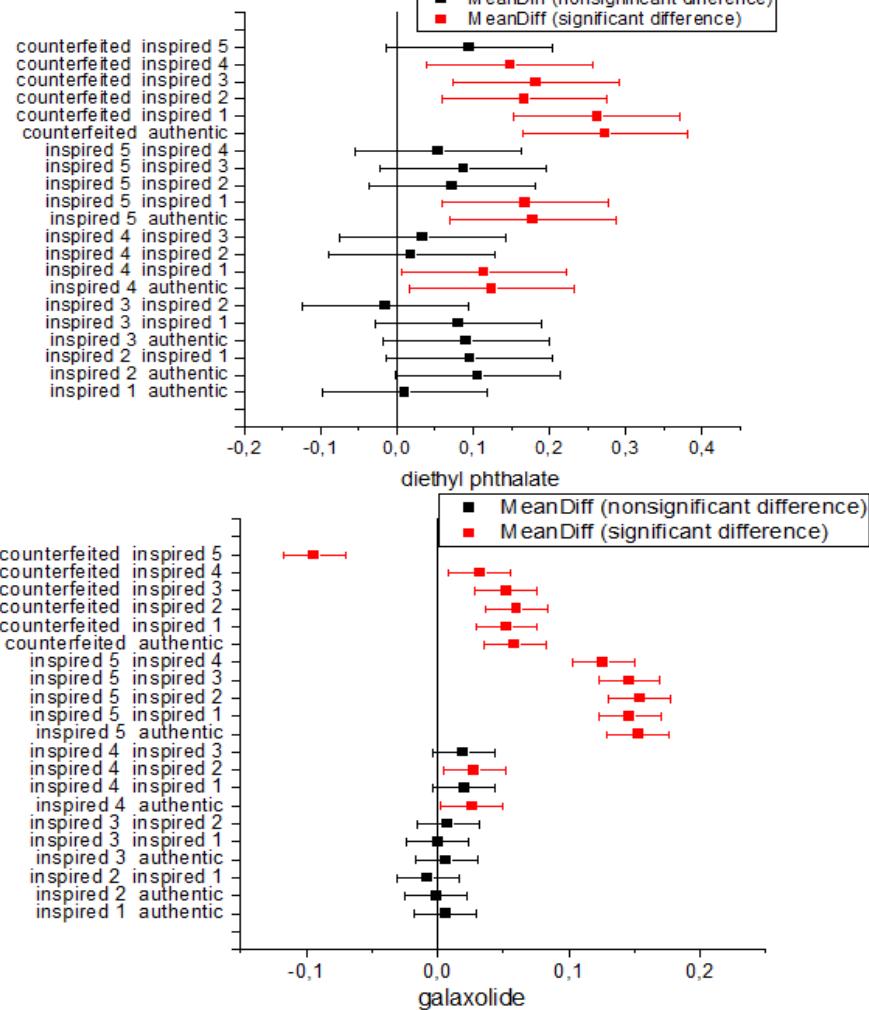
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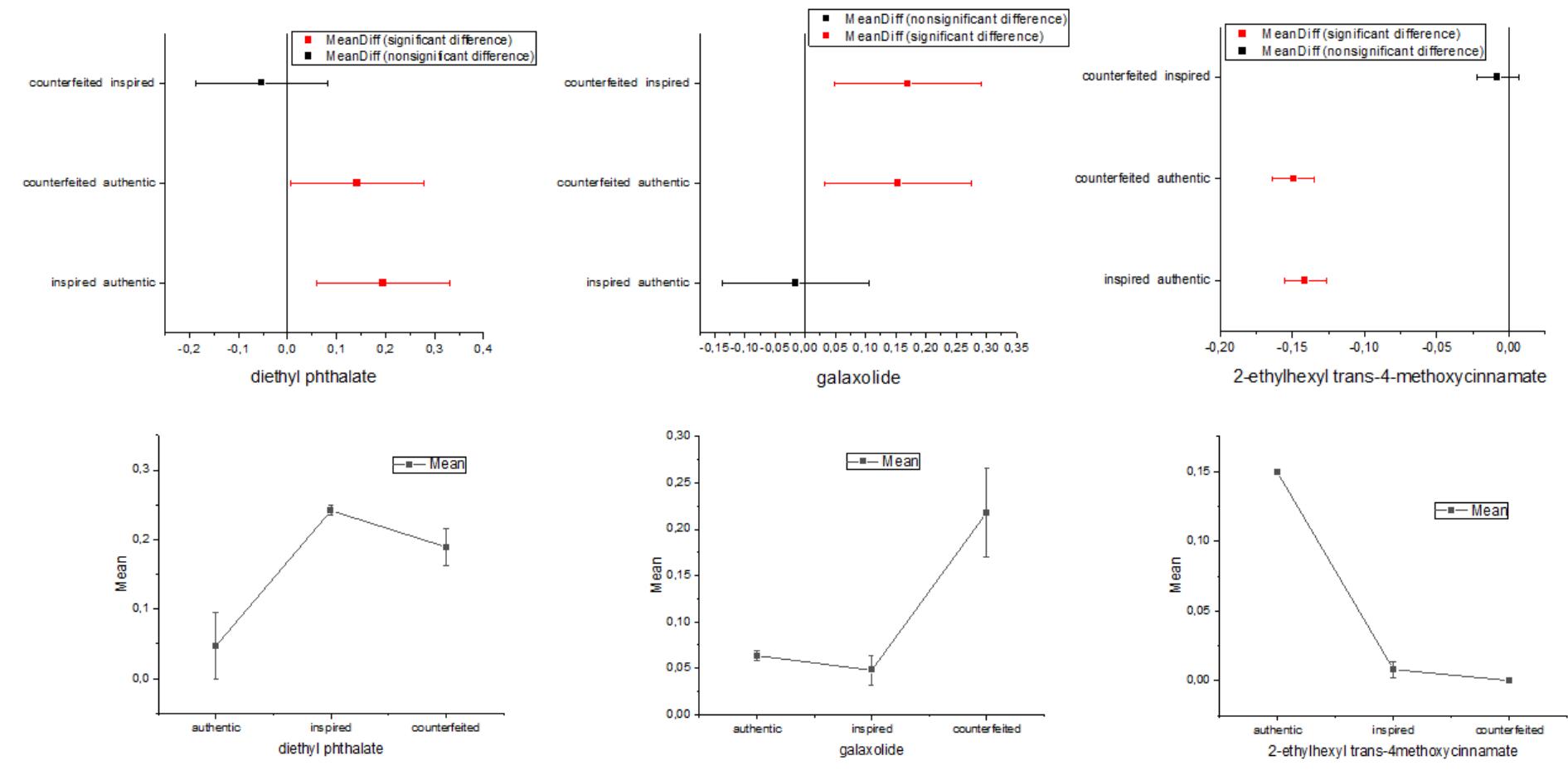
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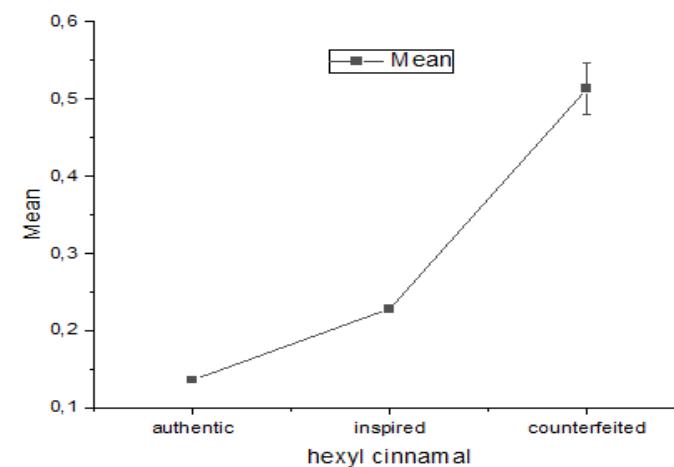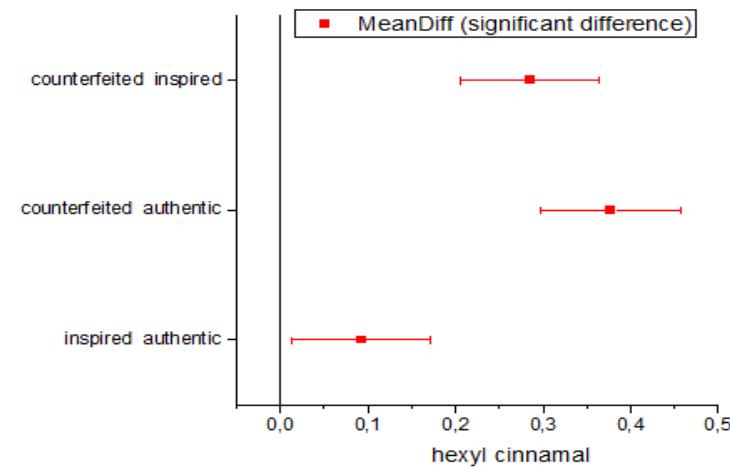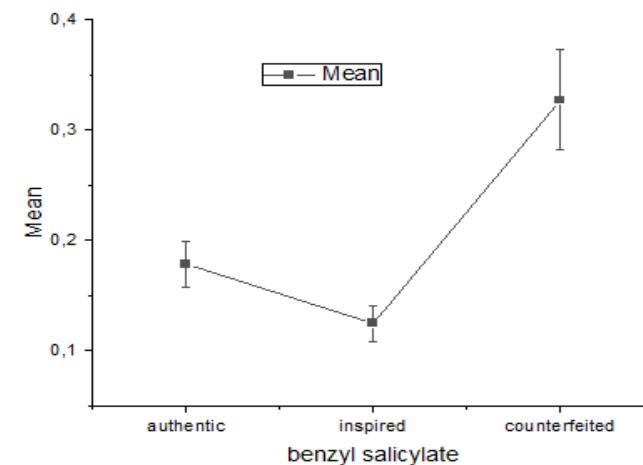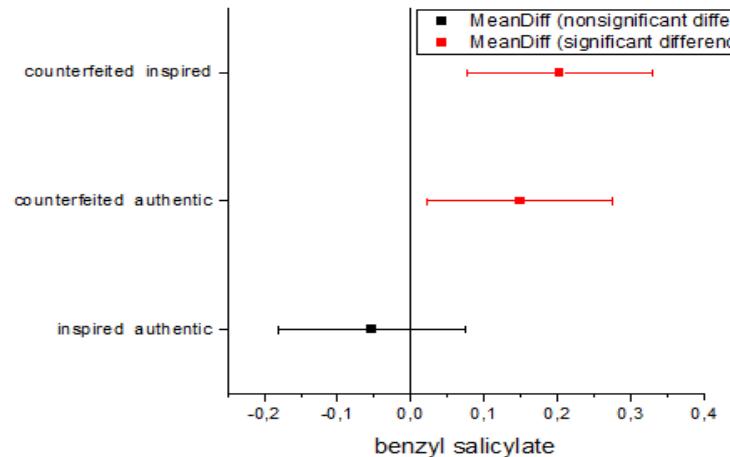
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2. Representative ^{1}H NMR spectra of the authentic, inspired and counterfeited samples.
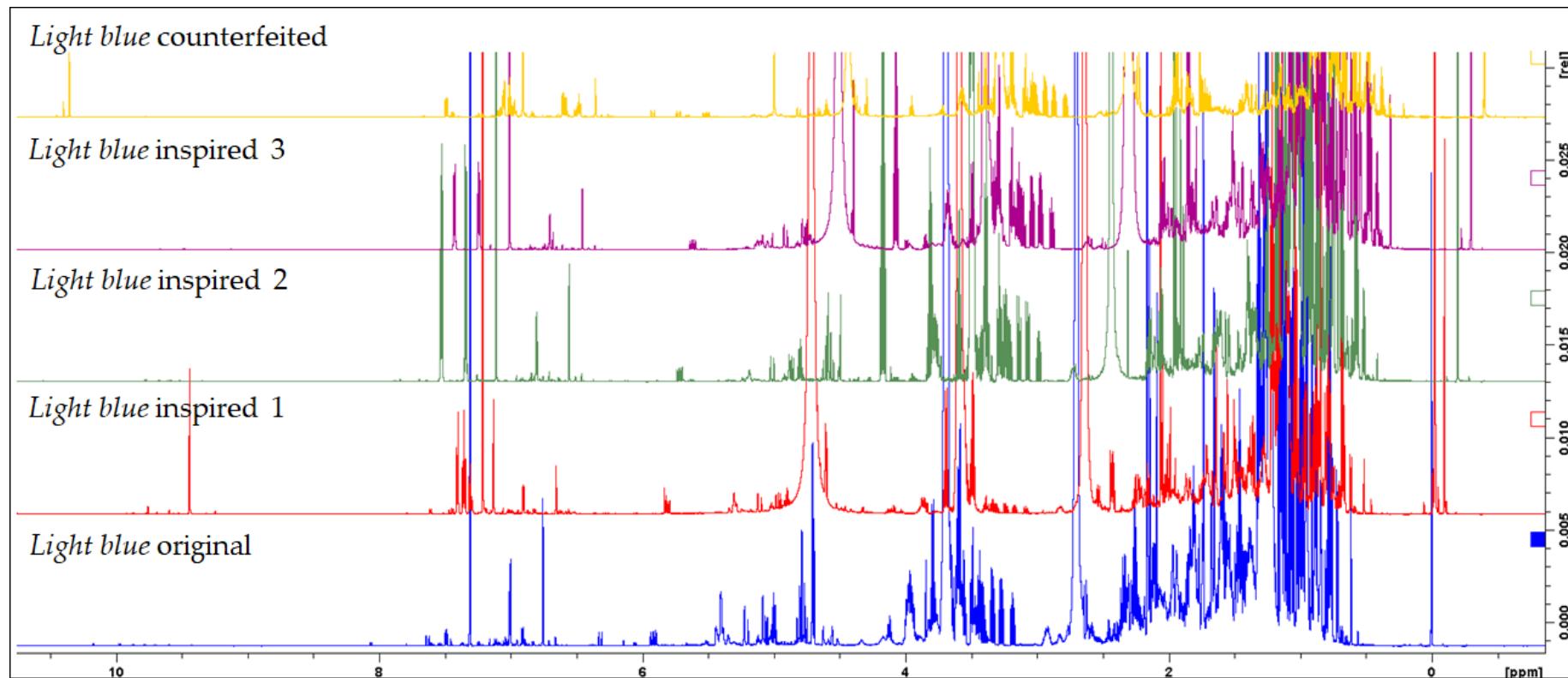
Figure S12 ^{1}H NMR spectra of authentic, inspired and counterfeited samples of *Light blue* in spectral region from 0 to 11 ppm.
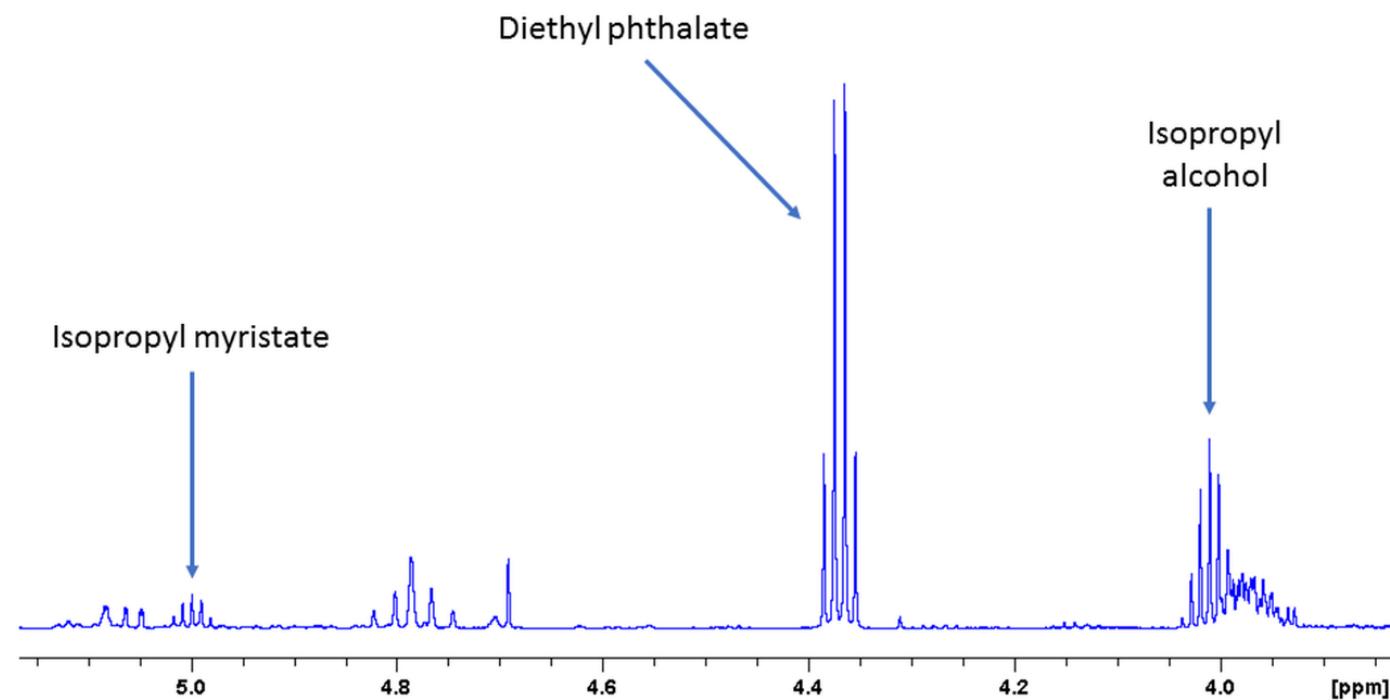
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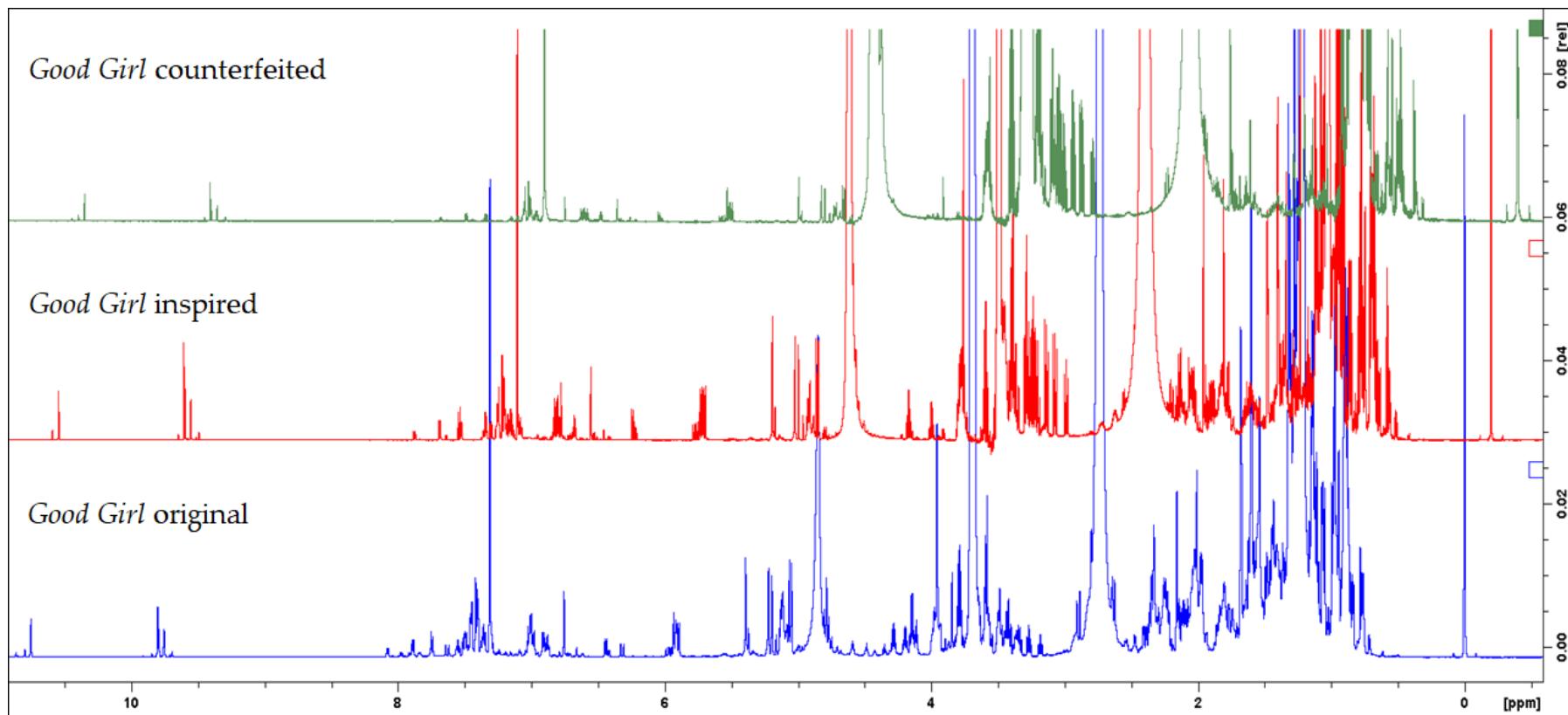
Figure S14 ^{1}H NMR spectra of authentic, inspired and counterfeited samples of *Good girl* in spectral region from 0 to 11 ppm.
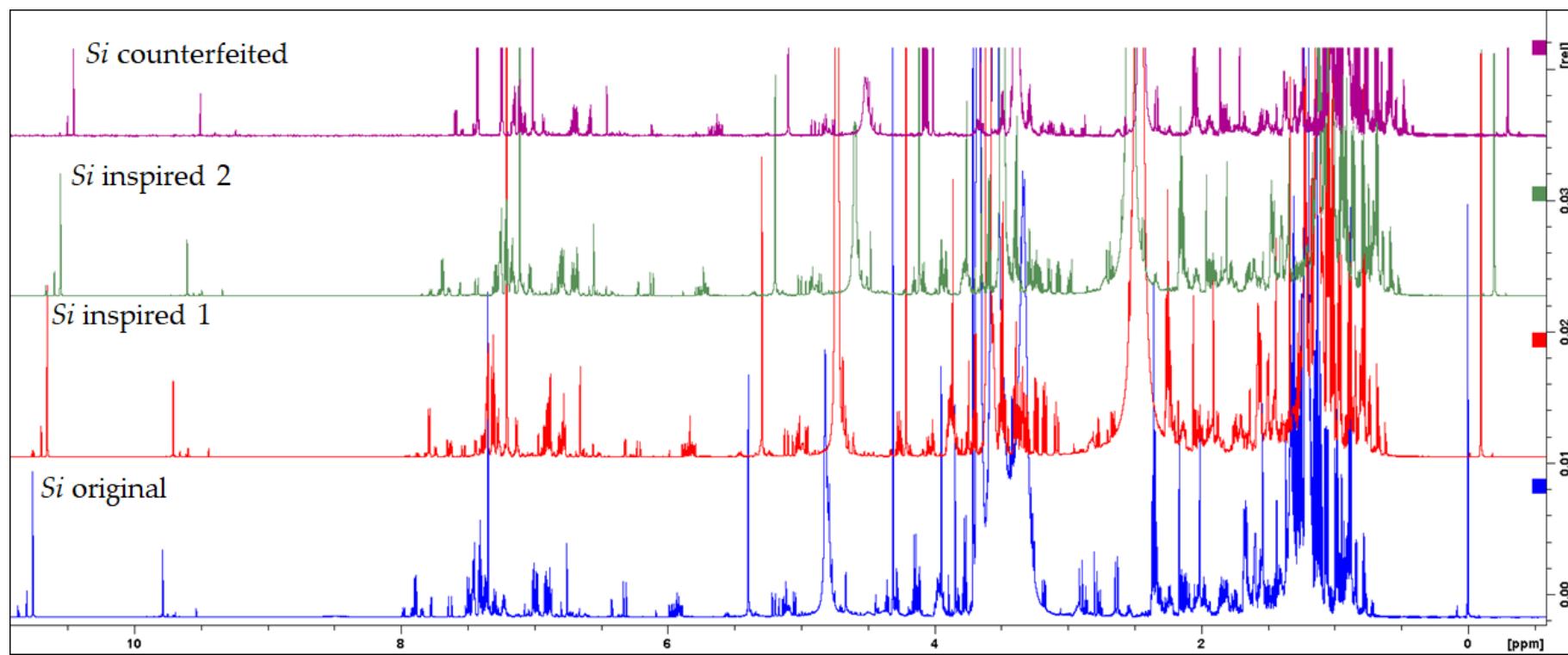
Figure S15 ¹H NMR spectra of authentic, inspired and counterfeited samples of *Si* in spectral region from 0 to 11 ppm.
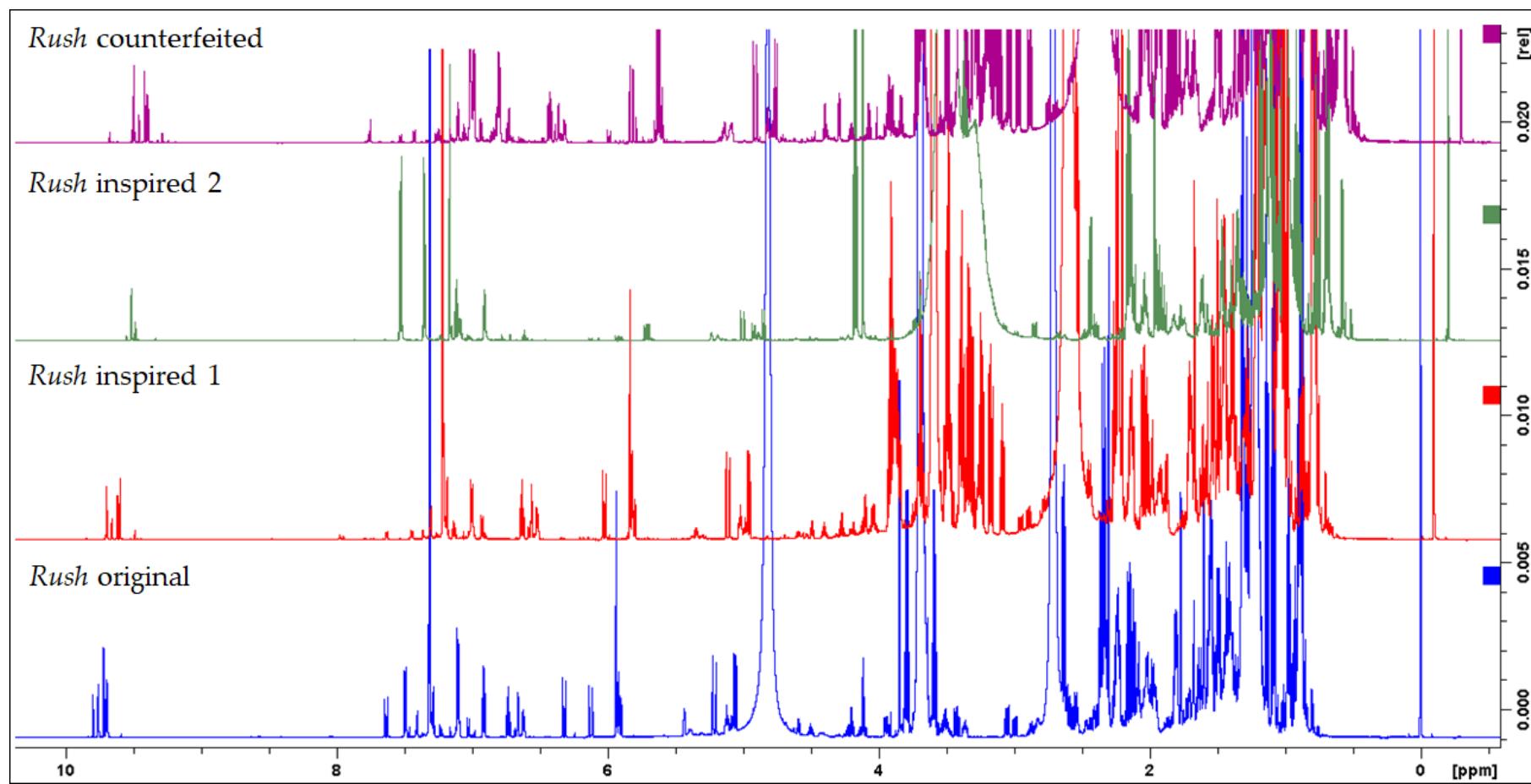
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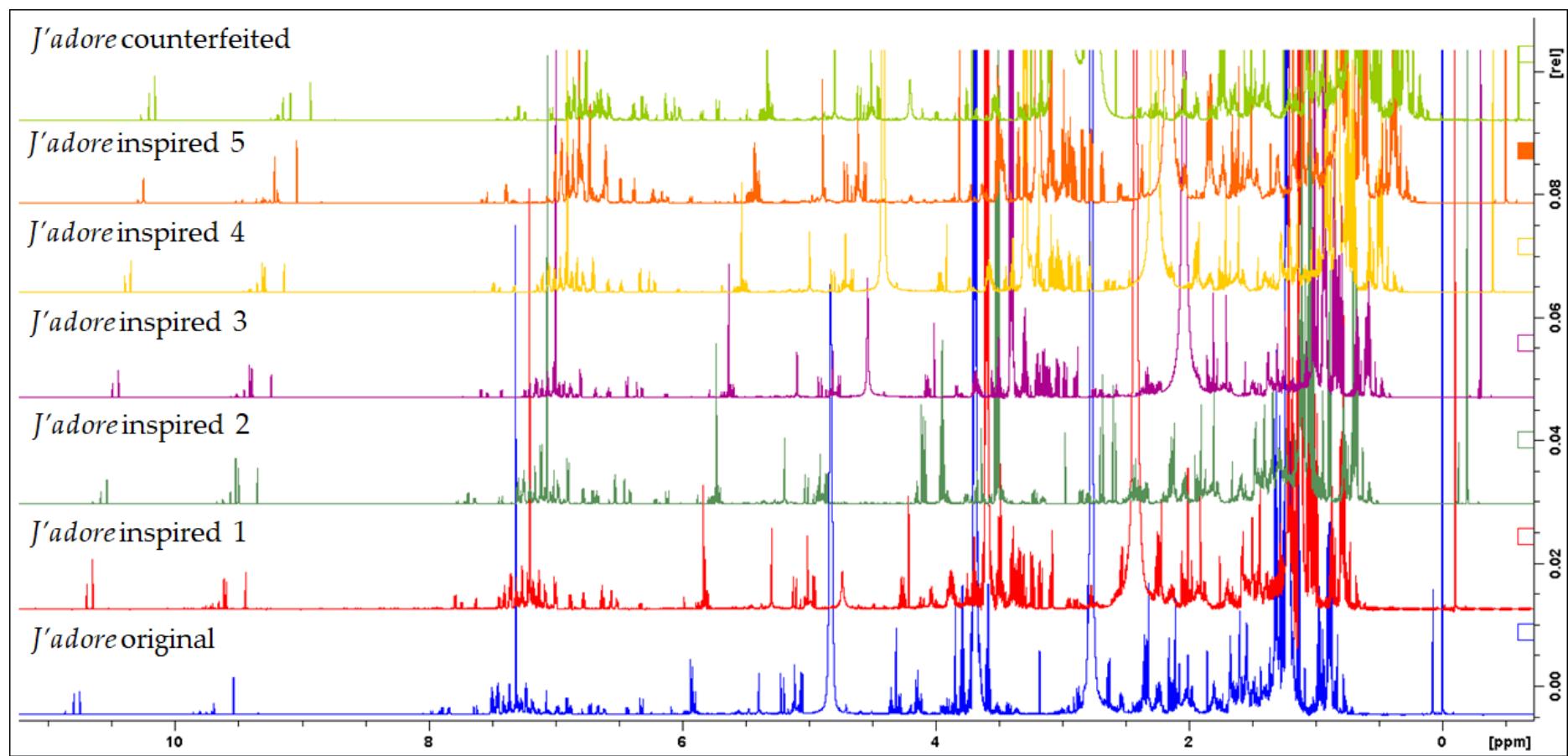
Figure S17 ^{1}H NMR spectra of authentic, inspired and counterfeited samples of *J'adore* in spectral region from 0 to 11 ppm.

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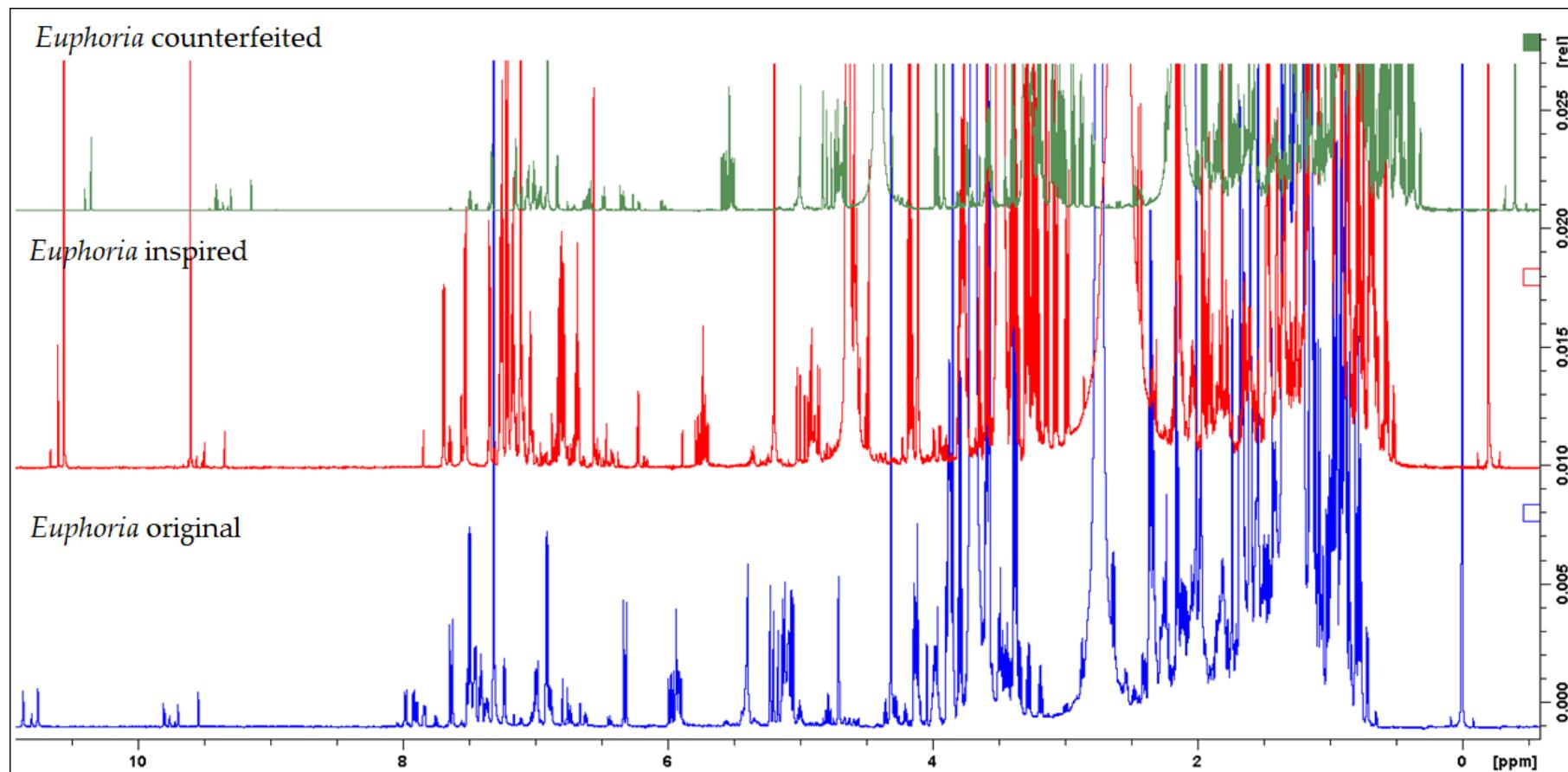
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3. Table with main compounds assigned in ^{1}H NMR spectra of perfume samples

**Table S1.** The main compounds assigned in ^{1}H NMR spectra of perfume samples, their diagnostic ^{1}H signals, chemical shifts δ_H and multiplicities.

LP	Compound	Functional group	Chemical shift [ppm] (multiplet)
1	α-Hexyl cinnamaldehyde*	-C(O)$\underline{H}$	9.53 (s)
		2xH$_{Ar}$	7.47 (d)
		2xH$_{Ar}$	7.42 (t)
		H$_{Ar}$	7.38 (t)
		CH=	7.17 (s)
2	Benzyl alcohol	5xH$_{Ar}$	7.20 -7.40(m)
		-C$\underline{H}_2$-	4.54 (d)
3	Cinnamaldehyde	-C(O)$\underline{H}$	9.69 (d)
		H$_{Ar}$	6.72 (dd)
		H$_{Ar}$	7.57 (m)
		H$_{Ar}$	7.44 (m)
4	β-pinene*	=CH$_2$	4.55 (m) and 4.62 (m)
5	Benzaldehyde	-C(O)$\underline{H}$	10.02 (s)
		2xH$_{Ar}$	7.86 (d)
		H$_{Ar}$	7.60 (t)
		2xH$_{Ar}$	7.51 (t)
6	Benzyl benzoate	-CH$_2$-	5.35 (s)
		2xH$_{Ar}$	8.07 (d)
		H$_{Ar}$	7.55 (t)
		2xH$_{Ar}$	7.41 (t)
		2xH$_{Ar}$	7.3-7.5 (m)

LP	Compound	Functional group	Chemical shift [ppm] (multiplet)
7	Ethylene brasylate*	-CH$_2$-	4.31 (s)
8	Citral	-C(O)H	9.87 (d)
		=CH	5.81 (d)
9	Citronellal	-C(O)H	9.75 (t)
		-CH=	5.11 (m)
10	Methyl dihydrojasmonate*	-CH$_3$	3.63 (s)
11	Ethylvanillin	-C(O)H	9.85 (s)
		-OCH$_2$-	4.15 (q)
12	Vanillin	-C(O)H	9.83 (s)
13	Eugenol	-OCH$_3$	3.84 (s)
14	Diethyl phthalate*	-CH$_3$	1.37 (t)
		-CH$_2$-	4.37 (q)
		H$_{Ar}$	7.72 (dd)
		H$_{Ar}$	7.53 (dd)
15	Galaxolide*	H$_{Ar}$	6.76 (s)
		H$_{Ar}$	7.00 (s)
16	γ-Terpinene*	=CH-	5.43 (br.s)
		-CH$_2$-	2.60 (br.s)
17	Geraniol	-CH$_2$-	5.20 (dt)
18	Coumarin	=CH-	6.42 (d)
		C(O)O-	
19	Lilial	-C(O)H	9.67 (d)
		-(CH$_3$)$_3$	1.39 (s)
20	Linalool*	H$_2$C=CH-	5.92 (m)

LP	Compound	Functional group	Chemical shift [ppm] (multiplet)
		$H_2C=CH-$	5.04 (dd) and 5.21 (dd)
21	Limonene*	$=CH_2$	4.71 (s)
		$=CH-$	5.40 (br.s)
22	Isopropyl myristate*	$-CH-$	5.00 (sp)
		$-(CH_3)_2$	1.23 (d)
23	Benzyl salicylate	$-CH_2-$	5.39 (s)
		H_{Ar}	6.88 (t)
		H_{Ar}	6.97 (d)
		H_{Ar}	7.32-7.5 (m)
		H_{Ar}	7.85 (d)
		$-OH$	10.75 (s)
24	Cyclohexene*	$-CH_2-$	5.66 (br.s)
25	Isopropyl alcohol	$-CH-$	4.07 (sp)
		$-(CH_3)_2$	1.21 (d)
26	Isokurkumenol*	$=CH-$	5.59 (br.s)
27	γ-Muurolene*	$-CH-C\underline{H}=$	5.50 (d)
		$=CH_2$	4.58 (m)
		$(CH_3)_2$	0.78 (d) and 0.90 (d)
28	1,1'-Oxydi-2-propanol*	$2x-CH_2-$	3.32 (dd) and 3.46 (dd)
		$2xCH$	3.95 – 4.05 (m)
		$2x\ CH_3$	1.15 (d)
29	α-Cedrene*	$CH-C\underline{H}_3$	0.84 (d)
		$-C\underline{H}-CH=$	2.17 (m)
		$-CH-C\underline{H}=$	5.22 (br.s)
30	Thujopsene*	$=C\underline{H}-CH_2-$	4.99 (m)

LP	Compound	Functional group	Chemical shift [ppm] (multiplet)
		=CH-C$\underline{H}_2$-	1.40 (m) and 1.78 (m)
		=C-CH$_3$	1.80 (br.s)
31	2,6-di-*tert*-butyl-4-methylphenol*	2xH$_{Ar}$	7.13 (s)
		-OH	5.14 (s)
		-CH$_3$	2.42 (s)
32	Cedrol*	C$\underline{H}_3$-C-OH	1.32 (br.s)
33	Methyl jasmonate*	-C$\underline{H}$=CH-	5.25 (m)
		-CH=CH-	5.46 (m)
		-OCH$_3$	3.69 (s)
34	Pyrrolo[3,2,1-*jk*]carbazole*	=CH	6.91 (d)
35	2-Methylbenzofuran*	2xH$_{Ar}$	7.26 (m)
		=CH	6.41 (td)
		-CH$_3$	2.50 (d)
36	(Z)-Ocimenone*	-CH$_3$	2.00 (d)
		=CH$_2$	5.53 (dd) and 5.64 (dd)
		=CH	6.17 (dq)
		=CH	6.40 (dd)
37	Ambrox*	-CH$_3$	1.08 (s)
38	Ketone musk*	(CH$_3$)$_3$	1.50 (s)
		C(O)-CH$_3$	2.45 (s)
39	2-ethylhexyl trans-4-methoxycinnamate	=CH	7.63 (d, J=16 Hz)
		2xH$_{Ar}$	7.47 (d)
		=CH	6.31 (d, J=16 Hz)
		2xH$_{Ar}$	6.88 (d)

LP	Compound	Functional group	Chemical shift [ppm] (multiplet)
		$-OCH_3$	3.71 (s)

*Compounds detected by means of GC/MS for original *Light Blue*, its substitutes and counterfeit version by Borowiecka *et al*.

**4.** PCA analysis conducted for full spectrum bucket tables.
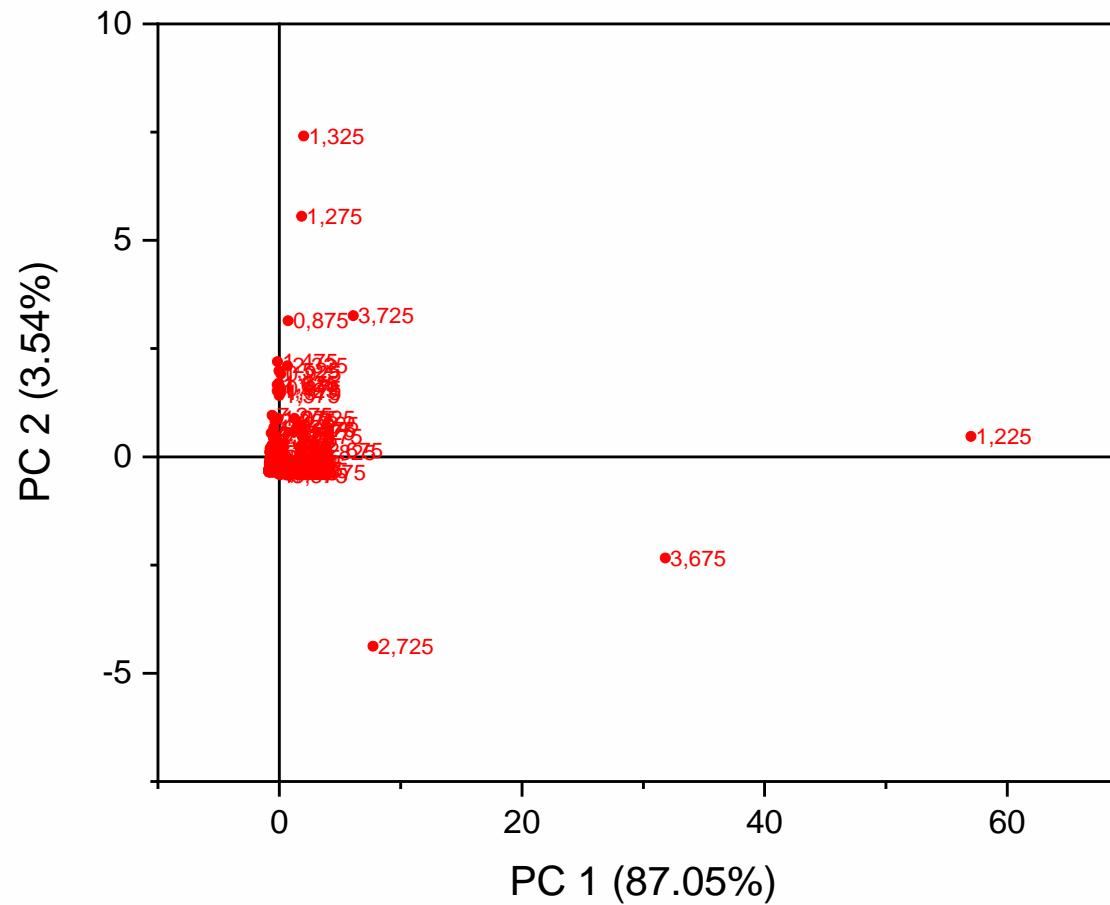
Figure S19 PCA loading plot generated from the ¹H NMR spectra from the authentic perfume and counterfeited and inspired samples for the range of chemical shifts from 0 to 10 ppm.

**5.** Comparison of the bucket tables from NMR spectra for two authentic samples.

Equation	y = a + b*x
Plot	Light blue
Weight	No Weighting
Intercept	-1,71561E-4 ± 7,870
Slope	1,0005 ± 5,59281E-
Residual Sum of Sq	6,77356E-5
Pearson's r	0,99998
R-Square (COD)	0,99997
Adj. R-Square	0,99997
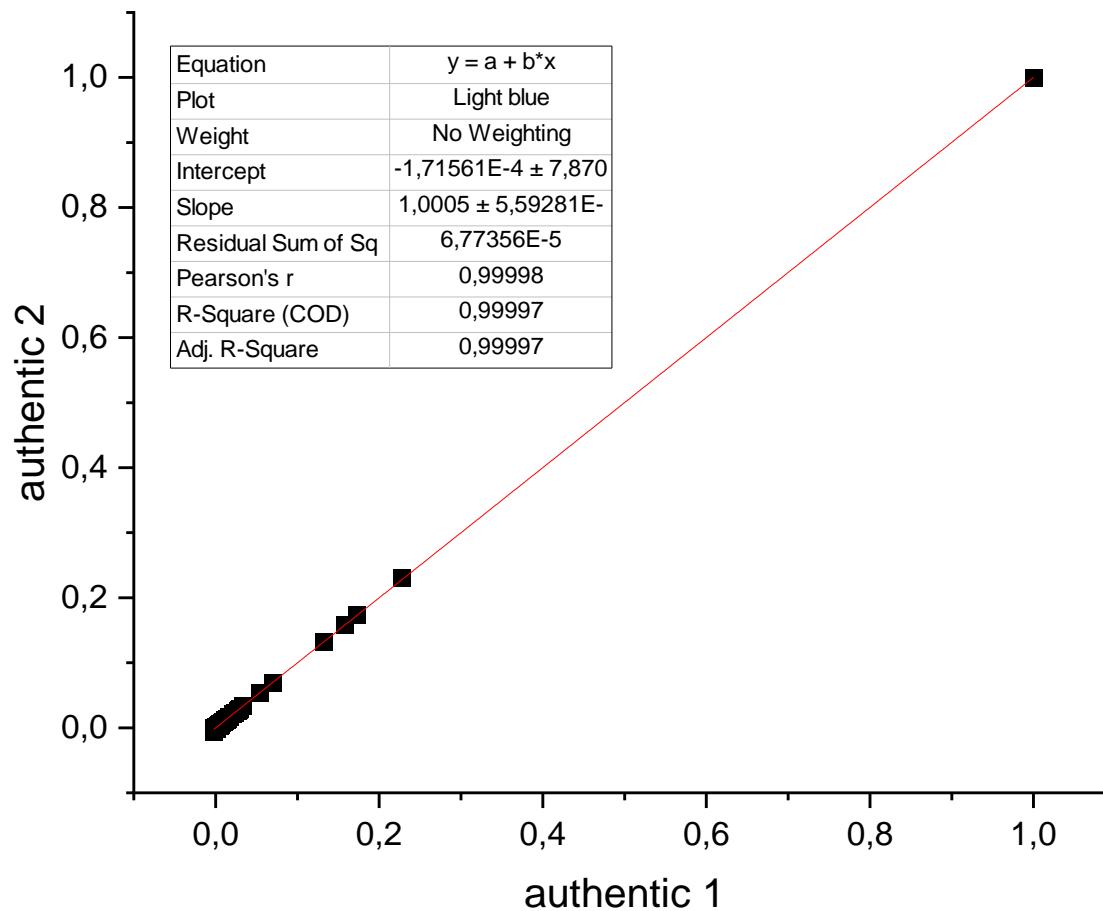
Figure S20 The comparison of the buckets from NMR spectra for two authentic samples of *Light blue*.

| Equation	y = a + b*x
Plot	J'adore
Weight	No Weighting
Intercept	0,00126 ± 0,00389
Slope	0,95385 ± 0,0188
Residual Sum of Squares	0,02596
Pearson's r	0,99118
R-Square (COD)	0,98244
Adj. R-Square	0,98206
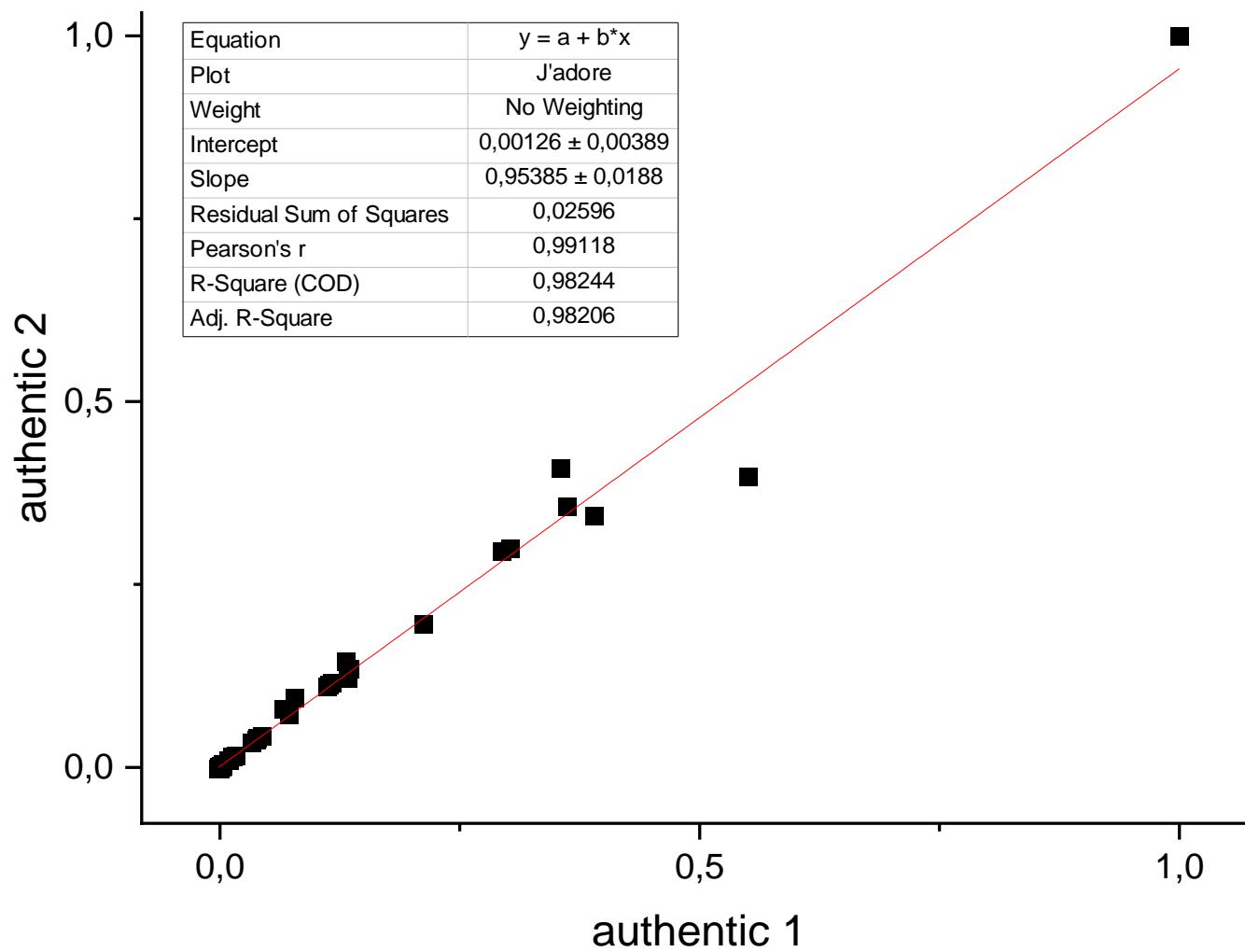
Figure S21 The comparison of the buckets from NMR spectra for two authentic samples of *J'adore*.