

Supporting Information

Monolith dip-it: a bifunctional device for improving the sensitivity of direct analysis in real time mass spectrometry

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Table SI Results comparison before and after monolith dip-it extraction in positive mode

Name	Formula	[M+H] ⁺	C (μg/mL)	T (°C)	S/N(before)	S/N(after)
Sudan I	C ₁₆ H ₁₂ N ₂ O	249.102	0.1	350	<1	61.9
Sudan II	C ₁₈ H ₁₆ N ₂ O	277.1335	0.1	350	<1	31.0
Sudan III	C ₂₂ H ₁₆ N ₄ O	353.1397	0.1	350	<1	25.1
Sudan IV	C ₂₄ H ₂₀ N ₄ O	381.171	0.1	350	<1	21.9
Sudan Red 7B	C ₂₄ H ₂₁ N ₅	380.187	0.1	400	<1	18
Rhodamine B	C ₂₈ H ₃₁ ClN ₂ O ₃	443.2335	1	400	<1	65.9
6,9-Dichloro-2-methoxyacridine	C ₁₄ H ₉ Cl ₂ NO	278.01	1	400	25.9	76.2
Acridine	C ₁₃ H ₉ N	180.0808	1	400	52.5	594.4
2-Aminoanthraquinone	C ₁₄ H ₉ NO ₂	224.0706	1	400	<1	4.9
4-Amino-3,5-dimethyl-1,2,4-triazole	C ₄ H ₈ N ₄	113.0822	1	350	1.3	413.3
minoacrinine	C ₁₃ H ₁₀ N ₂	195.0917	1	400	<1	291.3
Simazine	C ₇ H ₁₂ ClN ₅	202.0854	0.1	400	<1	13.6
Propazine	C ₉ H ₁₆ ClN ₅	230.1167	0.1	350	<1	31.3
Prometon	C ₁₀ H ₁₉ N ₅ O	226.1662	0.1	400	1.5	40.9
Gesatamine	C ₉ H ₁₇ N ₅ O	212.1506	0.1	400	3.2	50.5
Melamine	C ₃ H ₆ N ₆	127.0727	1	400	9.7	254
Dodecanamine	C ₁₂ H ₂₇ N	186.2216	1	350	1.5	269.1
Quinine	C ₂₀ H ₂₄ N ₂ O ₂	325.1919	1	350	<1	12.3
Sulfadoxine	C ₁₂ H ₁₄ N ₄ O ₄ S	311.0809	1	400	<1	168.3
Amitriptyline	C ₂₀ H ₂₃ N	278.1903	1	350	<1	50.7
Methyltestosterone	C ₂₀ H ₃₀ O ₂	303.2319	1	350	<1	28.8
Sulfadiazine	C ₁₀ H ₁₀ N ₄ O ₂ S	251.0597	1	350	<1	15.2
Guanosine	C ₁₀ H ₁₃ N ₅ O ₅	284.0989	1	350	<1	12.2
Sulfamerazine	C ₁₁ H ₁₂ N ₄ O ₂ S	265.0754	1	400	<1	72.6
Uridine	C ₉ H ₁₂ N ₂ O ₆	245.0768	1	350	1.9	2.7

Table S2 Results comparison before and after monolith dip-it extraction in negative mode

Name	Formula	[M-H] ⁻	C (μg/mL)	T (°C)	S/N(before)	S/N(after)
p-Chlorobenzoic acid	C ₇ H ₅ ClO ₂	155.5592	1	350	7.1	76.1
Erucic acid	C ₂₂ H ₄₂ O ₂	338.3185	1	350	<1	5.4
2, 5-Dihydroxybenzoic acid	C ₇ H ₆ O ₄	154.0266	1	400	3.4	14.1
Nalidixic acid	C ₁₂ H ₁₂ N ₂ O ₃	232.0848	1	350	1.9	43.9
Cholic acid	C ₂₄ H ₄₀ O ₅	408.2876	1	350	<1	6.4
Arachidic acid	C ₂₀ H ₄₀ O ₂	312.3028	1	350	<1	4.5
m-Hydroxybenzoic acid	C ₇ H ₆ O ₃	138.0317	1	350	<1	11.1
α-Naphthoic acid	C ₁₁ H ₈ O ₂	172.0524	1	350	2.9	34.3
Aurintricarboxylic Acid	C ₂₂ H ₁₄ O ₉	422.0638	1	350	<1	25.1
Carbazole	C ₁₂ H ₉ N	167.0735	1	350	1.5	24.5
Tetradecanoic acid	C ₁₄ H ₂₈ O ₂	228.2089	1	350	1	96.2
3-Indolebutyric acid	C ₁₂ H ₁₃ NO ₂	203.0946	1	350	<1	14.8
Vanillic acid	C ₈ H ₈ O ₄	168.0423	1	350	2.1	33.5
N-Phenylanthranilic acid	C ₁₃ H ₁₁ NO ₂	213.079	1	350	2.1	10.1
5-Sulfosalicylic acid	C ₇ H ₁₀ O ₈ S	254.0096	1	350	<1	32.9

Table S3 Comparison of the mass spectrometry based methods used for determination of Sudan dyes

Analyte	Real samples	Sample preparation	Detection	LODs	Precision (%RSD)	Ref.
Sudan I	Chili foods	Ethanol extraction	LC-APCI-MS	3000 ng/g	< 3	1
Sudan I ~IV	Chili and curry food	DMSO extraction	LC-ESI-MS	1.5~5.5 ng/mL	< 8.2	2
Sudan I ~IV	Paprika paste	Acetone extraction	GC-MS	0.3~7.7 ng/g	10.2~16	3
Sudan I ~IV	Chili products	Silica solid-phase extraction	ESI-MS	1.1~4.3 ng/g	< 8.6	4
Sudan I ~IV	Chili products	Acetone extraction	LC-ESI-MS	3~11 ng/g	1~13	5
Sudan I ~IV	Chili powders	Acetonitrile extraction	LC-ESI-MS	5~50 ng/g	1.7~13.6	6
Sudan I ~IV	Spices powders.	Acetone extraction	TLC-MS	108.9~98 0.4 ng/g	1.48~2.50	7
Sudan I ~IV	Food samples	QuEChERS extraction	LC-ESI-MS	1.50~4.04 ng/g	1.42~5.30	8
Sudan I ~IV	Cosmetics and foodstuffs	No	Paper spray-MS	5~20 ng/g	No	9
Sudan I ~IV	Chili powder tomato sauce	Hexane extraction	LC-APPI-MS	5~18 ng/mL	< 8	10
Sudan I ~IV	Chili powder	Hexane extraction	DART-MS	80~100 ng/mL	6~25	11
Sudan I ~IV	Chili oil and powder	Carbon nanotube film microextraction	DCBI-MS	1.4~21 ng/g	9.9~19.2	12
Sudan I ~IV	Chili powder	Hexane extraction	DART-MS	5~10 ng/mL	8.5~13.8	This work

Notes and references

1. F. Tateo and M. Bononi, *J. Agric. Food Chem.*, 2004, **52**, 655-658.
2. M. Ma, X. B. Luo, B. Chen, S. P. Sub and S. Z. Yao, *J. Chromatogr. A*, 2006, **1103**, 170-176.
3. U. S. Erdemir, B. Izgi and S. Gucer, *Anal. Methods*, 2013, **5**, 1790-1798.
4. M.-M. Zheng, J.-H. Wu, Y.-Q. Feng and F.-H. Huang, *Anal. Methods*, 2011, **3**, 1851-1858.
5. F. Calbiani, M. Careri, L. Elviri, A. Mangia, L. Pistarà and I. Zagnoni, *J. Chromatogr. A*, 2004, **1042**, 123-130.
6. C.-F. Tsai, C.-H. Kuo and D. Y.-C. Shih, *J. Food Drug Anal.*, 2015, **23**, 453-462.

7. R. Rani, S. Medhe and M. Srivastava, *J. Food Meas. Charact.*, 2015, **9**, 186-194.
8. M. M. A. Omar, A. A. Elbashir and O. J. Schmitz, *Food Chem.*, 2015, **176**, 342-349.
9. Q. Ma, H. Bai, W. Li, C. Wang, X. Li, R. G. Cooks and Z. Ouyang, *Anal. Chim. Acta*, 2016, **912**, 65-73.
10. M. R. V. S. Murty, N. Sridhara Chary, S. Prabhakar, N. Prasada Raju and M. Vairamani, *Food Chem.*, 2009, **115**, 1556-1562.
11. Z. Li, Y.-W. Zhang, Y.-D. Zhang, Y. Bai and H.-W. Liu, *Anal. Methods*, 2015, **7**, 86-90.
12. D. Chen, Y.-Q. Huang, X.-M. He, Z.-G. Shi and Y.-Q. Feng, *Analyst*, 2015, **140**, 1731-1738.