

Development and optimization of a LC-MS/MS method for the detection of magnolia officinalis extracts in cosmetics: Insights from DFT-assisted sample preparation

Yongqi Yao,^{*a} Guangfeng Zeng,^a Zhiyuan Wang,^a Jianjun Xie,^a Cheng Chen,^b Yingye

Hou,^a Keyin Xiao,^a Cuiling Cai,^a Jie Dong,^a Qing Liu,^{*a} and Longyan Xu^{*a}

^a *Food and Cosmetics Testing Institute, Guangzhou Customs Technology Center, 510423 Guangzhou, People's Republic of China.*

^b *School of Energy Science and Engineering, University of Science and Technology of China, 230026 Hefei, People's Republic of China.*

*Corresponding author:

gziqtcyyq@163.com; 787854418@qq.com (Y.-Q. Yao)

gdciqlq@163.com (Q. Liu)

xlyciq@126.com (L.-Y. Xu)

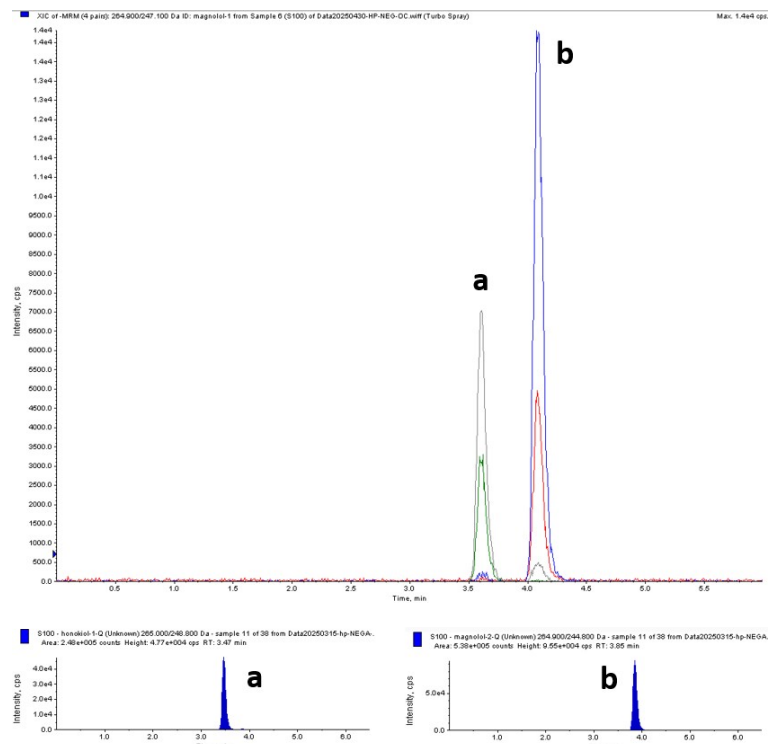


Figure S1. Chromatograms and MRM mass spectra for the 2 *magnolia officinalis* extracts obtained via LC-MS/MS. Analytes: honokiol (a); magnolol (b).

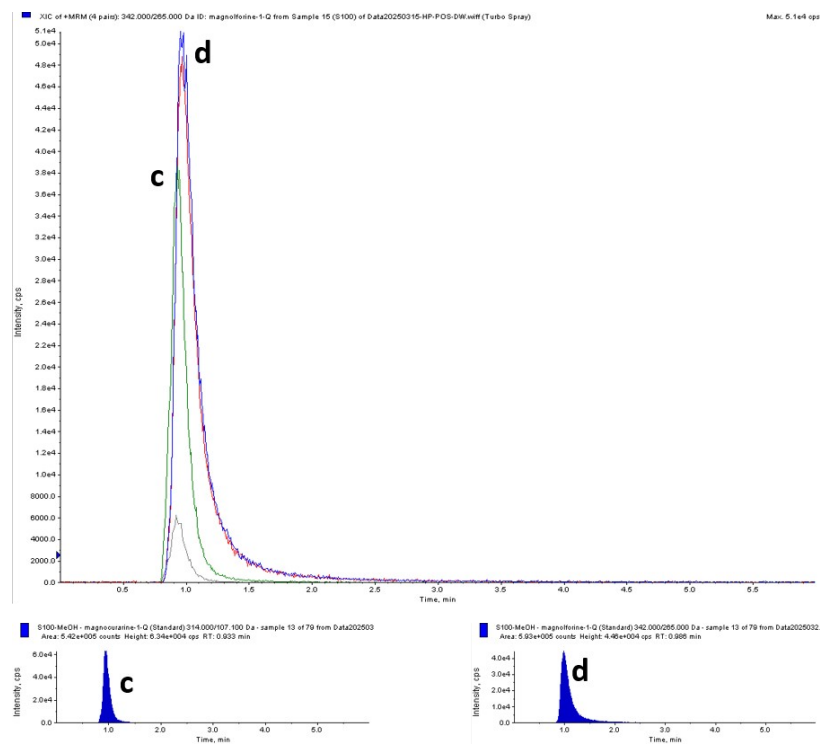


Figure S2. Chromatograms and MRM mass spectra for the 2 *magnolia officinalis* extracts obtained via LC-MS/MS. Analytes: magnocurarine (c); magnoflorine (d).

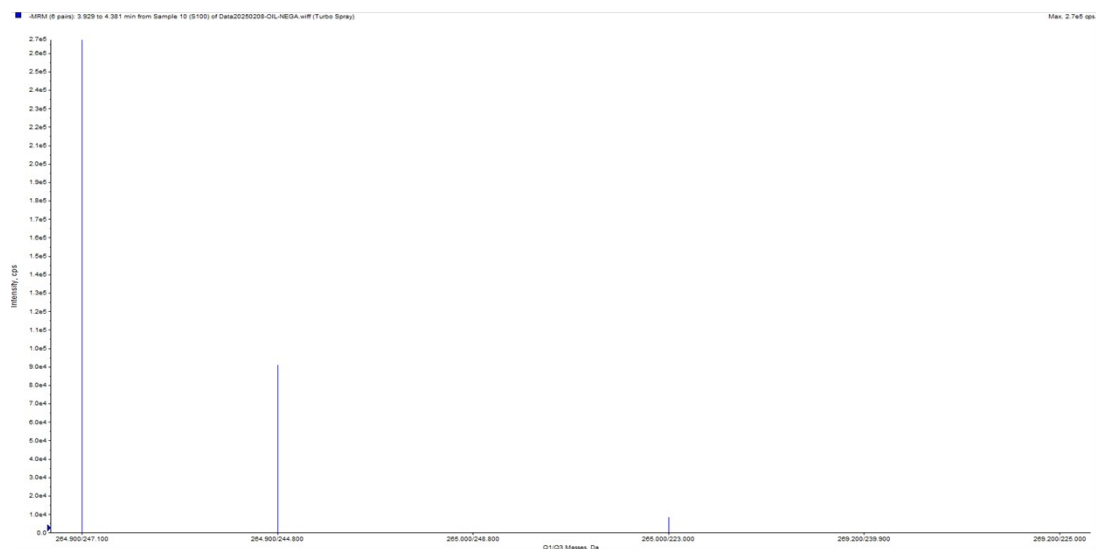


Figure S3. Mass Spectra for magnolol.

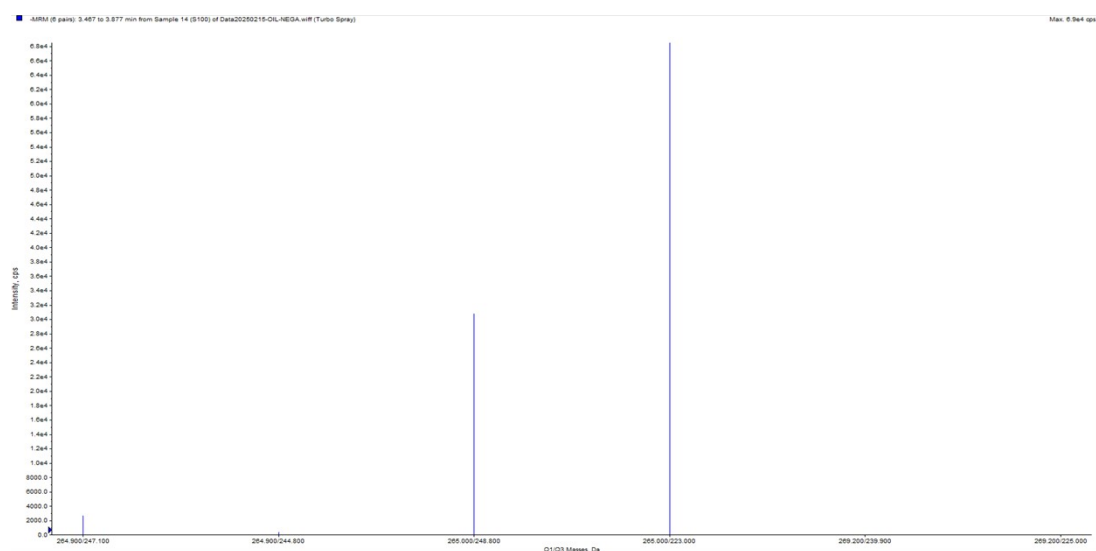


Figure S4. Mass Spectra for honokiol.

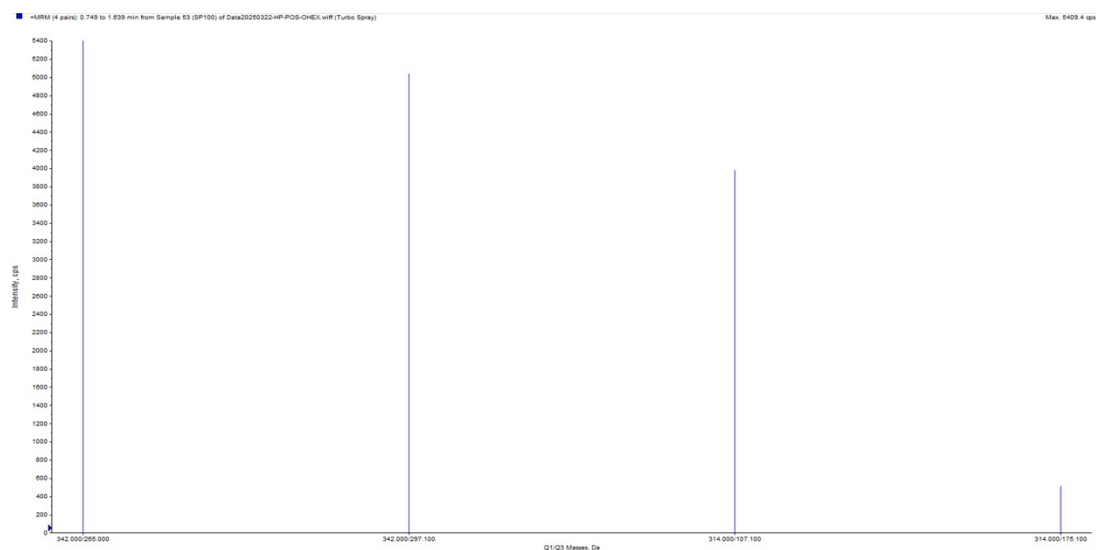


Figure S5. Mass Spectra for magnoflorine.

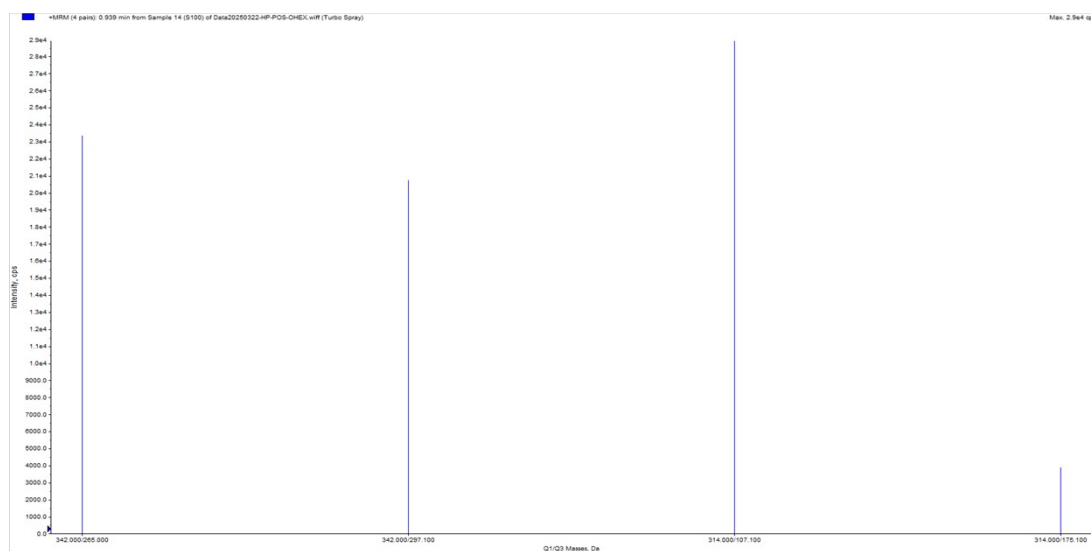


Figure S6. Mass Spectra for magnocurarine.

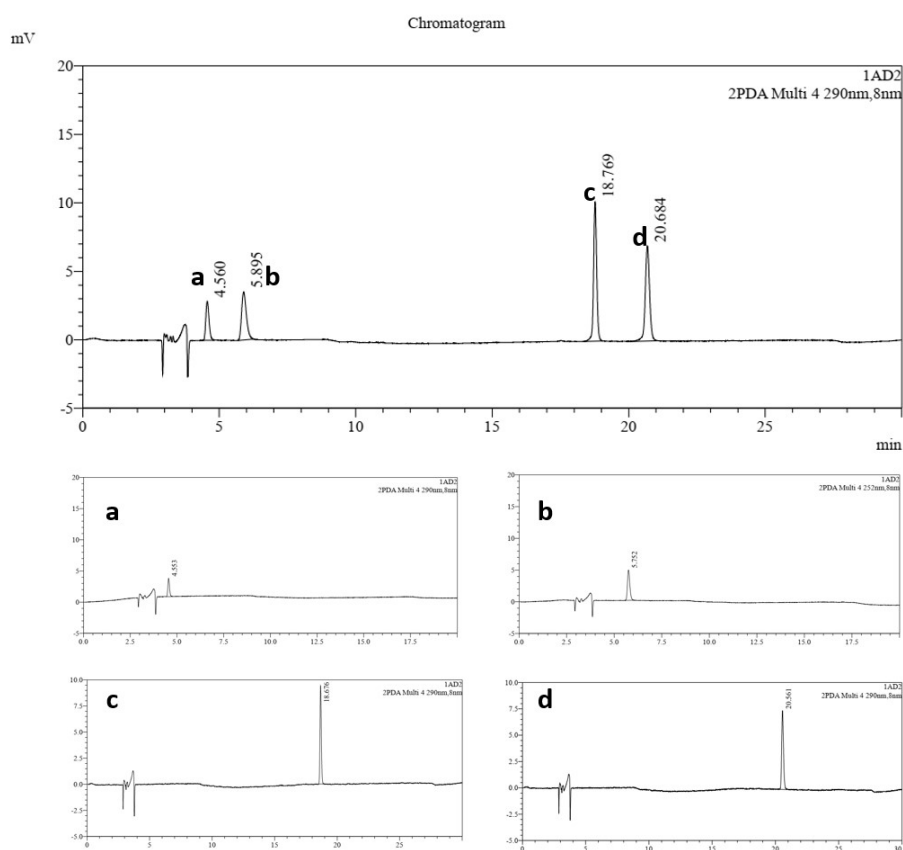


Figure S7. Chromatograms for the 4 magnolia officinalis extracts obtained via UPLC. Analytes: magnocurarine (a); magnoflorine (b); honokiol (c); magnolol (d).

Table S1. Gradient program for mobile phase of 4 magnolia officinalis extracts in UPLC.

Time	Module	Command	Value
5	Pumps	Pump B conc.	20
10	Pumps	Pump B conc.	50
15	Pumps	Pump B conc.	70
25	Pumps	Pump B conc.	70
27	Pumps	Pump B conc.	20
30	Controller	Stop	-

[a] Wavelength = 290 nm. [b] Phase A: 0.1% H₃PO₄, Phase B: Acetonitrile. [c] Flow: 1 mL/min. [d] Inj. volume: 10 µL.

Table S2. Chromatographic parameters and linearity of 4 magnolia officinalis extracts in UPLC.

Magnolia officinalis extracts	Retention time [min]	Linearity		
		Slope	Intercept	R ²
magnocurarine	4.560	2390	-7.09	0.9997
magnoflorine	5.890	4277	172.83	0.9999
honokiol	18.769	8357	-939.33	0.9998
magnolol	20.684	7897	1256.79	0.9997

Table S3. Spiked concentrations of 4 magnolia officinalis extracts in blank commercial cosmetics.

Magnolia Extracts	Cream	Mask	Aqueous	Oil
	Single-Point Recovery Rates [%]			
Magnolol	44.8-136.0	66.0-98.2	41.7-88.6	50.2-97.8
Honokiol	33.9-103.1	23.5-92.7	21.0-93.2	17.7-92.5
Magnocurarine	43.5-73.3	33.8-102.0	39.5-57.7	44.7-114.0
Magnoflorine	58.0-96.1	40.5-84.1	50.6-69.7	51.7-108.2

Table S4. Product information for commercially available cosmetic samples.

Lable in Table 3	Brand	Cosmetics	Country-of-Brand
cream A	Moraz	Dry Hands-Hand craem	Israel
cream B	SANS SOUCIS	AQUA CLEAR SKIN	Germany
cream C	MWM	AC7 Anti-Acne Serum	Korea
cream D	Haa	PHYTOEXTRAC MULTI-ACID REFERSHING SMALL GEL CREAM	China
cream E	comfort zone	HYDRAMEMORY SERUM	Italy
aqueous A	DÉTVFO	SOOTHING MOISTURIZING ESSENCE TONER	China
aqueous B ^[a]	Qiriness	Radiance Activating Treatment Lotion	France
aqueous C	LUCENBASE	Men's Oil Control Refreshing Moisturizing Toner	China
aqueous D	RRMKKE	BALANCING HYDRATING ESSENCE TONER	China
aqueous E ^[a]	MWM	Revitalizing Soothing Essential Tonic	Korea
mask A ^[a]	FULFIL	SPOT CLEARING MASK	China
mask B ^[a]	SUNDUK	Pore Tightening ReBalance Fresh Pack	Korea
mask C	Cible Skin	LE MASQUE POLYACTIFS	France
mask D ^[a]	MINBOSS	Salicylic Acid Anti-Acen Oil Control MASK	China
mask E	comfort zone	SUBLIME SKIN LIFT-MASK	Italy
oil A ^[a]	GOURMESH	INTENSIVPFLEGE ÖL-SERUM	Germany
oil B	LA MER	the renewal oil	America
oil C	Ultra V	IDEBNONE AMPOULE	Korea
oil D ^[a]	Otto Hahn	ASPALATHUS LINEARIS Acne Essence Gel	Germany
oil E	MEDUTHERAPY	Skin Cleansing Essence Ampoule	China
raw material A		Magnolia Officinalis Bark Solution	China
raw material B		Magnolia Officinalis Essential Oil	China
raw material C		Magnolia Officinalis Tree Extract	China

[a] The cosmetic packaging states that magnolia officinalis extract is present as a kind of trace-ingredient. [b] Literally translated from the original Chinese label.