

Supplements

*p*H Effect and Chemical Mechanisms of Antioxidant Higenamine

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Suppl. 1 The structures of ABTS^{•+}, PTIO[•], and DPPH[•]

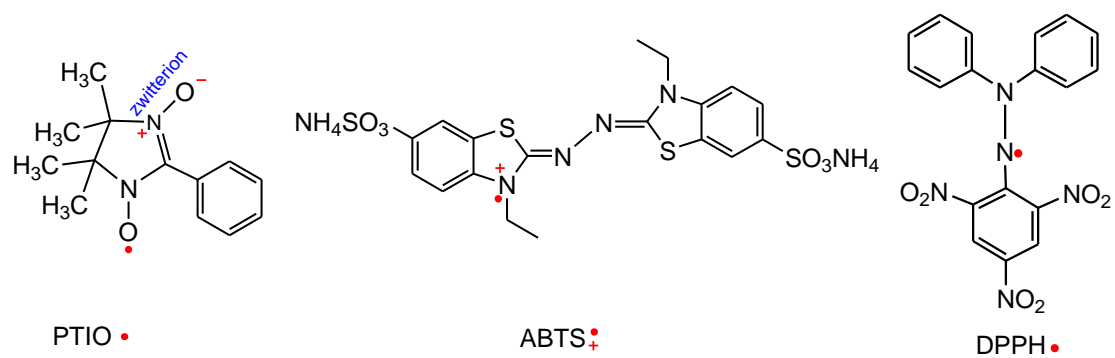


Fig. S1 The structures of ABTS^{•+}, PTIO[•], and DPPH[•].

Suppl. 2 The experimental results of DPPH• scavenging assay

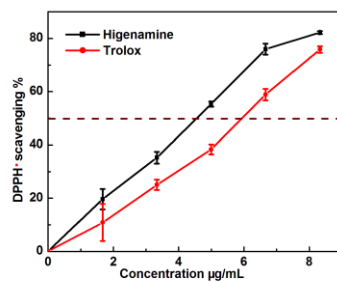


Fig. S2 The dose response curves of DPPH• scavenging assay; Each value is expressed as mean \pm SD, n = 3

Table S1 The comparison of IC₅₀ values of higenamine and Trolox in free radical assays.

	higenamine	Trolox
DPPH• scavenging assay µg/mL	4.6 \pm 0.5	5.3 \pm 0.1
DPPH• scavenging assay µM	<u>17.1\pm0.2</u>	<u>23.3\pm0.3</u>

The data underlined were cited in Fig. 2 in the main text.

Suppl. 3 The original data of UPLC-ESI-Q-TOF-MS/MS analysis

Higenamine standard

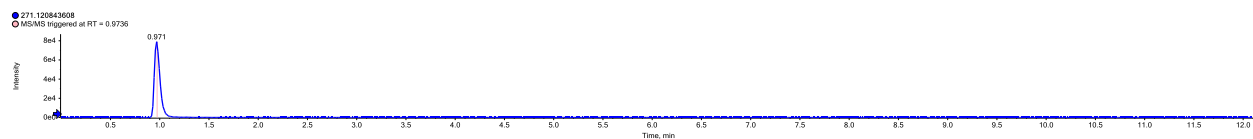


Fig. S3 UPLC chromatography diagram of higenamine standard

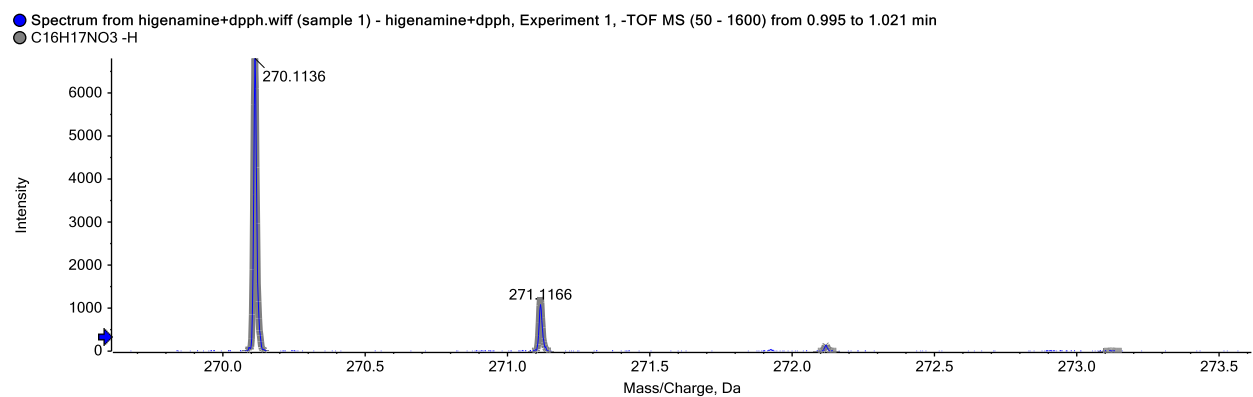


Fig. S4 MS spectra of higenamine standard

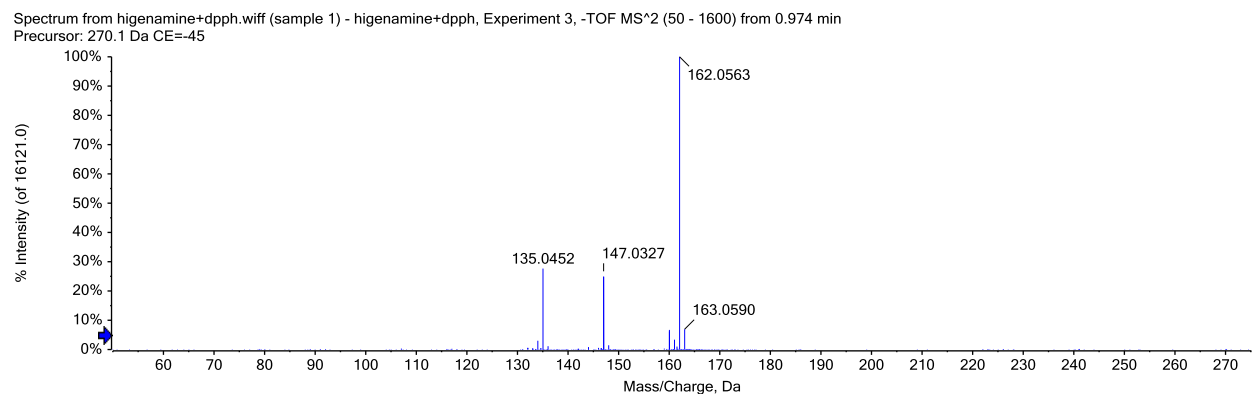


Fig. S5 MS/MS spectra of higenamine standard

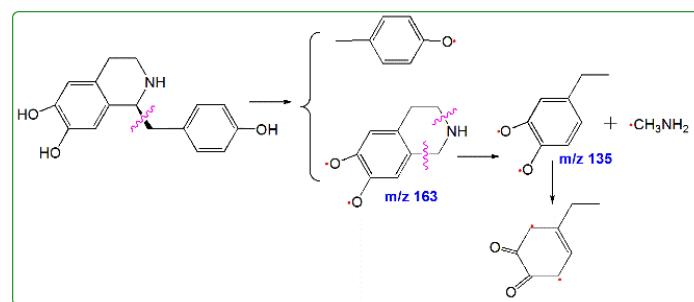


Fig. S6 The possible fragments of higenamine standard

DPPH• standard

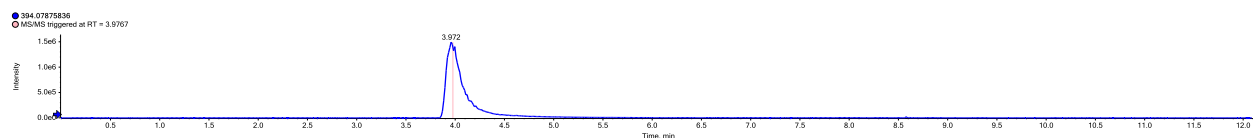


Fig. S7 UPLC chromatography diagram of DPPH• standard

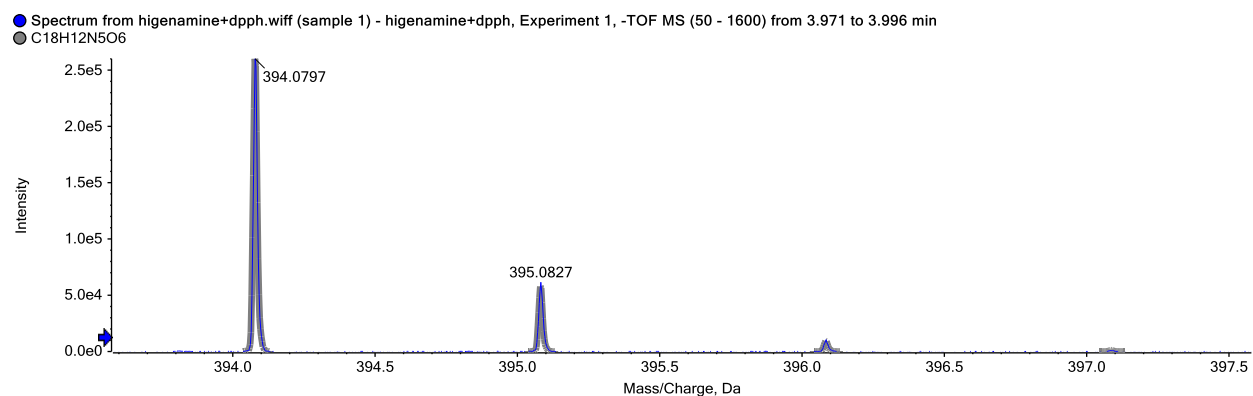


Fig. S8 MS spectra of DPPH• standard

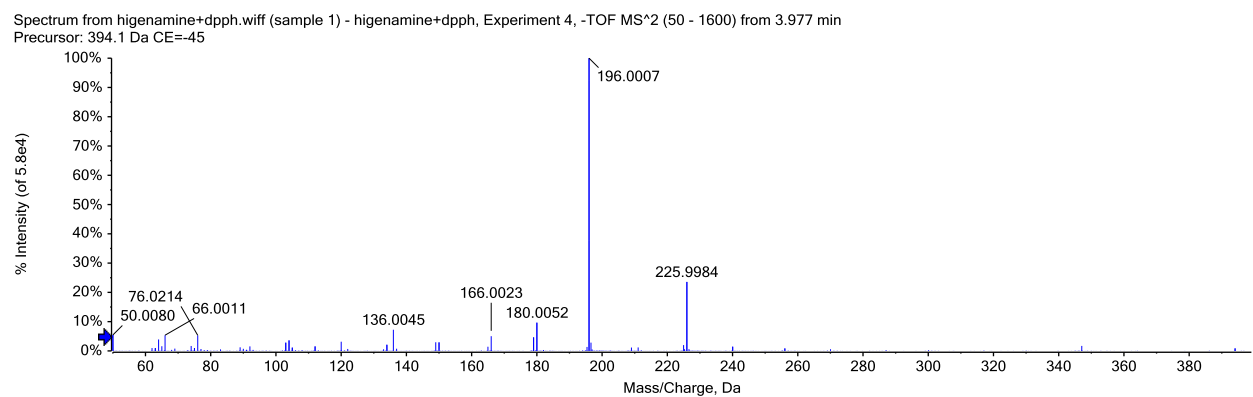


Fig. S9 MS/MS spectra of DPPH• standard

Higenamine-Higenamine ($C_{32}H_{34}N_2O_6-H$)

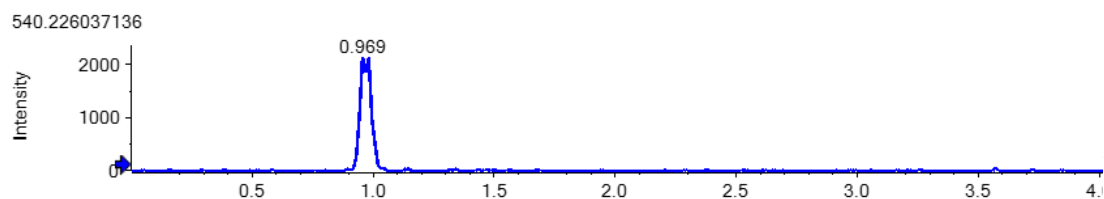


Fig. S10 UPLC chromatography diagram of higenamine-higenamine dimer

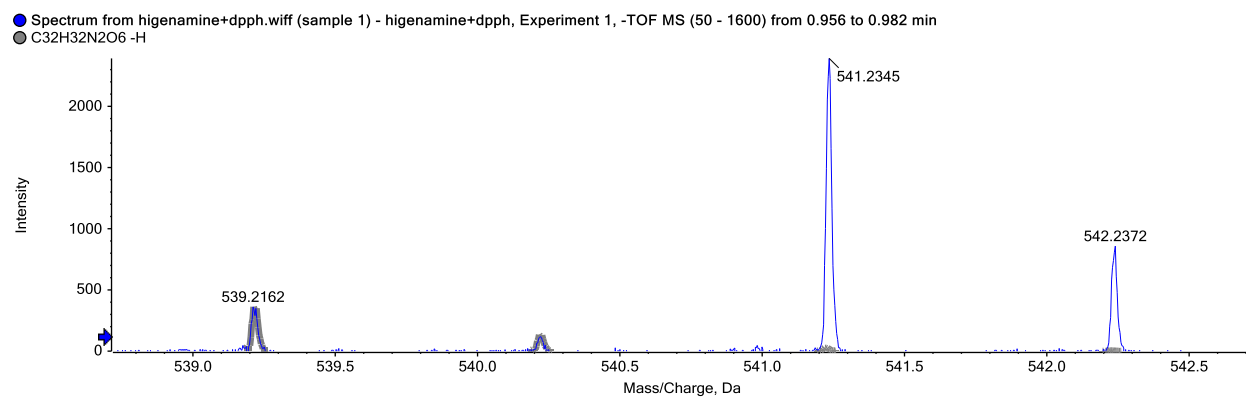


Fig. S11 MS spectra of higenamine-higenamine dimer

Higenamine-DPPH ($C_{34}H_{28}N_6O_9-H$)

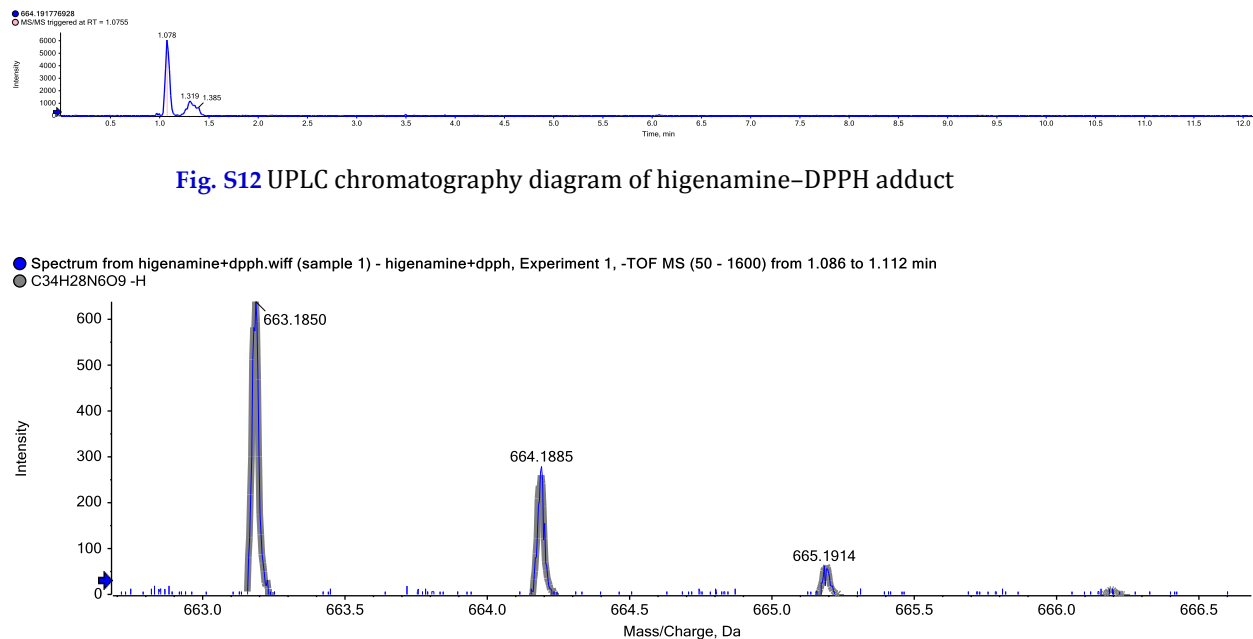


Fig. S13 MS spectra of higenamine-DPPH adduct

Spectrum from higenamine+dpvh.wiff (sample 1) - higenamine+dpvh, Experiment 2, -TOF MS² (50 - 1600) from 1.075 min
Precursor: 663.2 Da CE=-45

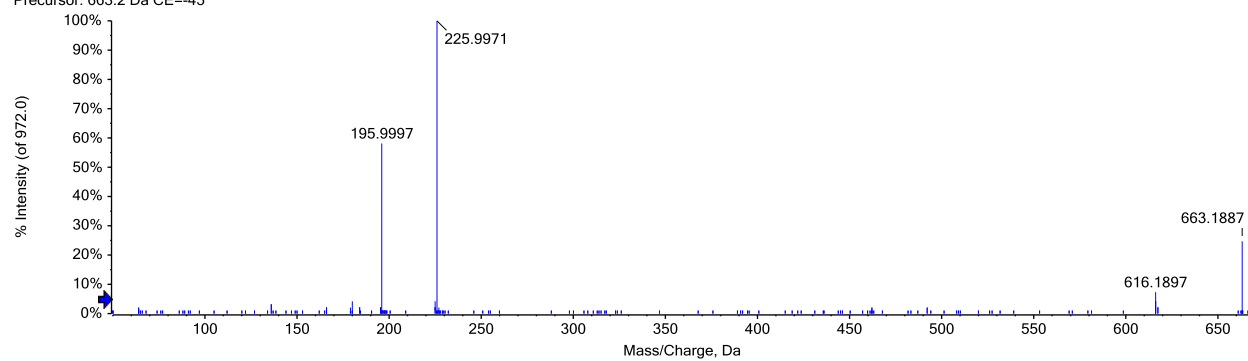


Fig. S14 MS/MS spectra of higenamine-DPPH adduct

Suppl. 4 The experimental results of PTIO• assay

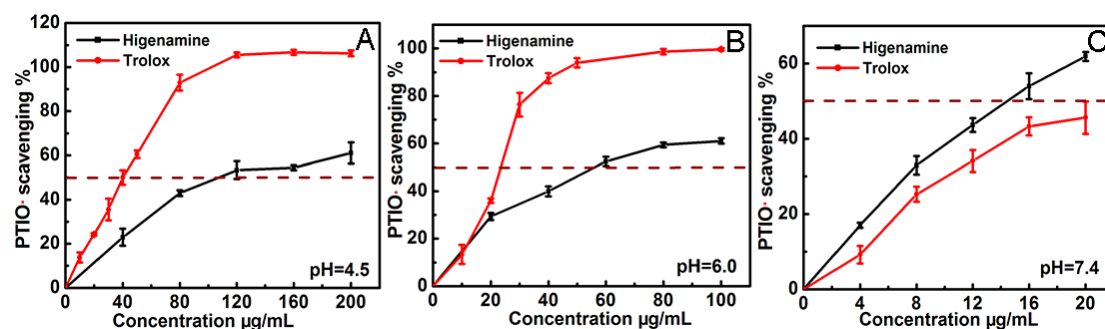


Fig. S15 A The dose response curves of PTIO• (pH 4.5) assays; B The dose response curves of PTIO• (pH 6.0) assays; C The dose response curves of PTIO• (pH 7.4) assays; Each value is expressed as mean \pm SD, n = 3

Table S2 The comparison of IC₅₀ values of higenamine and Trolox in PTIO•-scavenging.

	higenamine	Trolox
PTIO•-scavenging (pH 4.5) µg/mL	104.8 \pm 6.5	41.1 \pm 2.3
PTIO•-scavenging (pH 4.5) µM	<u>386.5 \pm 24.1</u>	<u>164.2 \pm 9.1</u>
PTIO•-scavenging (pH 6.0) µg/mL	53.4 \pm 2.6	25.1 \pm 0.7
PTIO•-scavenging (pH 6.0) µM	<u>196.6 \pm 9.4</u>	<u>100.1 \pm 2.8</u>
PTIO•-scavenging (pH 7.4) µg/mL	14.9 \pm 0.4	20.3 \pm 1.4
PTIO•-scavenging (pH 7.4) µM	<u>55.0 \pm 1.7</u>	<u>81.0 \pm 5.6</u>

The data underlined were cited in Fig. 4 or Table 1 in the main text.

Suppl. 5 The experimental results of Fe³⁺-reducing and Cu²⁺-reducing assays

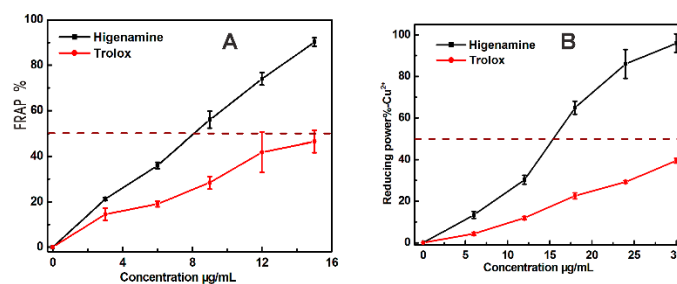


Fig. S16 A The dose response curves of Fe³⁺-reducing assay (FPRP); B The dose response curves of Cu²⁺-reducing assays; Each value is expressed as mean ± SD, n = 3

Table S3 The comparison of IC₅₀ values of higenamine and Trolox in Metal-reducing assay.

	higenamine	Trolox
Fe ³⁺ -reducing assay (FRAP) µg/mL	8.1±0.1	15.8±2.0
Fe ³⁺ -reducing assay (FRAP) µM	<u>30.0±0.3</u>	<u>63.1±8.0</u>
Cu ²⁺ -reducing assay µg/mL	15.5±0.2	35.5±1.1
Cu ²⁺ -reducing assay µM	<u>57.0±1.0</u>	<u>154.8±2.0</u>

The data underlined were cited in Table 1 in the main text.

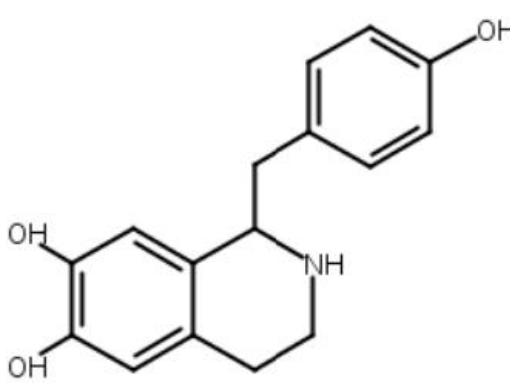
Suppl. 6 The analysis certificate of higenamine



四川省维克奇生物科技有限公司
Sichuan Weikeqi Biological Technology Co., Ltd.

质检报告

Quality Test Report

产品名称	去甲乌药碱				
Product Name	Higenamine				
数量	26.98g				
Amount	26.98g				
批号	wkq16060301				
Batch Number	wkq16060301				
报告日期	2016.06.03				
Report Date	2016.06.03				
生产日期	2016.05.24				
Manufacture Date	2016.05.24				
分子式	C ₁₆ H ₁₇ NO ₃	分子量	271.314	CAS 号	5843-65-2
项目		规定		结果	
Characters		Provisions		Results	
性状		白色粉末		符合	
Characteristics		White powder		Complies	
纯度 Purity (HPLC)		≥98%		98.36%	
Analyst:		Checker:		Q.C. director	
检验员:		复核员:		负责人	

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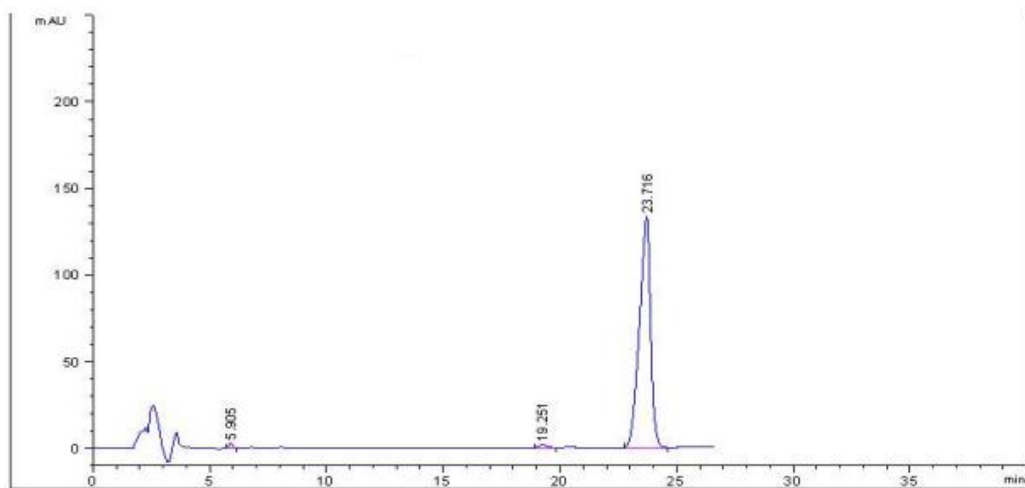


维克奇生物

四川省维克奇生物科技有限公司

Sichuan Weikeqi Biological Technology Co., Ltd.

去甲乌药碱液相图谱



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	5.905	BB	0.1586	30.17862	2.88027	0.6748
2	19.251	BB	0.3695	42.97988	1.79607	0.9610
3	23.716	BB	0.4928	4399.30713	133.28027	98.3642

总量 : 4472.46563 137.95661

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