Analysis of Polyphenolic compounds of *Stryphnodendron adstringens* (Barbatimão) by MALDI-TOF mass spectrometry

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Palavras Chave: *Mass spectrometry, Barbatimão, Fragmentation reactions, Tannin, Proanthocyanidins*

Abstract

This work presents chemical analysis of Barbatimão polyphenolic compounds by MALDI-TOF mass spectrometry.

Introduction

Sthryphnodendron adstringens, known in Brazil as Barbatimão, is a specie used in ulcer and healing skin treatment. The biological activity of this plant is assigned to the phenolic chemicals present in its bark. The chemical analysis of this molecules is complex, once traditional LC-MS using electrospray ionization is ineffective to separate and to ionize the polyphenols. In this work, it was applied MALDI-TOF to analyze fractions rich in tannin obtained from the classical chromatography from crude ethanolic extract of Barbatimão's bark.

Results and Discussion

It was identified four series of tannin (Table 1). The structures was confirmed by successive fragmentations by retro-Diels-Alder reaction[1] followed by the procyanidin (PCY) loss. Figure 1 shows the MALDI-TOF mass spectra and the RDA and the remaining unit fragmentation. The molecule in Figure 1 represents the series 1. The other series have an extra oxygen in the last three units.

Figure 1. MALDI spectra and successive fragmentation loss of 136 Da and 152 Da.

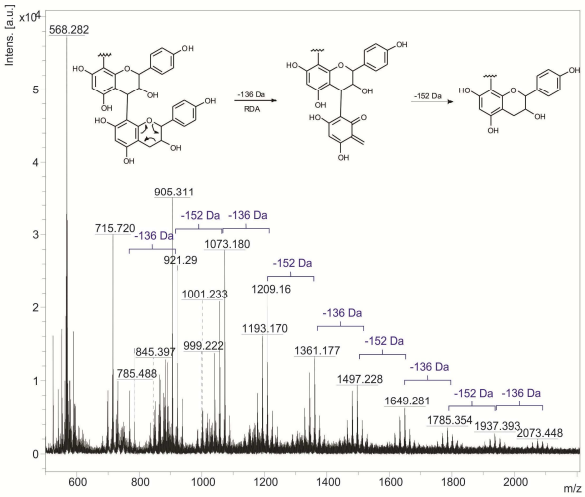

Table 1. Polyphenols identified in Barbatimão.

Series	$[M+Na]^+$	MF	Compound
1	899.1956	$C_{45}H_{38}O_{18}Na$	3PCY
	1041.1980	$C_{53}H_{46}O_{21}Na$	
	1177.2185	$C_{60}H_{50}O_{24}Na$	4PCY
	1329.2093	$C_{68}H_{58}O_{27}Na$	
	1465.2312	$C_{75}H_{62}O_{30}Na$	5PCY
	1617.2280	$C_{83}H_{70}O_{33}Na$	
	1753.2600	$C_{90}H_{74}O_{36}Na$	6PCY
2	905.1964	$C_{45}H_{38}O_{19}Na$	3-Oxo-PCY
	1057.1923	$C_{53}H_{46}O_{22}Na$	
	1193.2191	$C_{60}H_{50}O_{25}Na$	4-Oxo-PCY
	1345.2004	$C_{68}H_{58}O_{28}Na$	
	1481.2207	$C_{75}H_{62}O_{31}Na$	5-Oxo-PCY
	1633.2168	$C_{83}H_{70}O_{34}Na$	
	1769.2432	$C_{90}H_{74}O_{37}Na$	6-Oxo-PCY
3	921.1828	$C_{45}H_{38}O_{20}Na$	3-2Oxo-PCY
	1073.1784	$C_{53}H_{46}O_{23}Na$	
	1209.2045	$C_{60}H_{50}O_{26}Na$	4-2Oxo-PCY
	1361.1947	$C_{68}H_{58}O_{29}Na$	
	1497.2157	$C_{75}H_{62}O_{32}Na$	5-2Oxo-PCY
	1649.2054	$C_{83}H_{70}O_{35}Na$	
	1785.2363	$C_{90}H_{74}O_{38}Na$	6-2Oxo-PCY
4	937.1599	$C_{45}H_{38}O_{21}Na$	3-3Oxo-PCY
	1089.3472	$C_{53}H_{46}O_{24}Na$	
	1225.1906	$C_{60}H_{50}O_{27}Na$	4-3Oxo-PCY
	1377.1858	$C_{68}H_{58}O_{30}Na$	
	1513.1898	$C_{75}H_{62}O_{33}Na$	5-3Oxo-PCY
	1665.1920	$C_{83}H_{70}O_{36}Na$	
	1801.5481	$C_{90}H_{74}O_{39}Na$	6-3Oxo-PCY

This work shows the potential of MALDI to analyze this class of polyphenols. This strategy doesn't require the compounds isolation to identify the units, which can be identify monitoring successive RDA fragmentation followed by the unit loss[2]. In addition, poor chromatography resolution and ionization doesn't exist as in LC-MS using EI ionization, once it can be analyzed in mixture by MALDI.

Conclusions

This work evidences an important use of MALDI-TOF mass spectrometry to develop studies that comprise this class of molecules in phenolic-rich plant species. This technique allowed the identification of 4 series of tannins and the procyanidin unit.

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