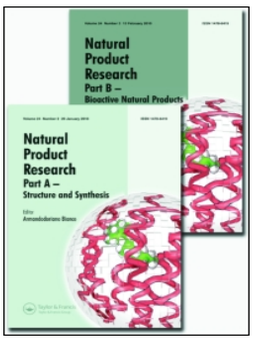

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SHORT COMMUNICATION

Phenolic profile and antioxidant activity from non-toxic Mexican *Jatropha curcas* L. shell methanolic extracts

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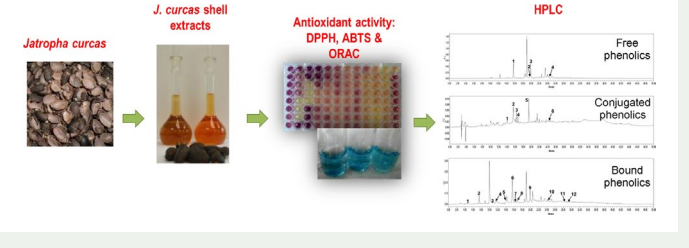
ABSTRACT

Jatropha curcas seed shells are the by-product obtained during oil extraction process. Recently, its chemical composition has gained attention since its potential applications. The aim of this study was to identify phenolic compounds profile from a non-toxic *J. curcas* shell from Mexico, besides, evaluate *J. curcas* shell methanolic extract (*Jc*SME) antioxidant activity. Free, conjugate and bound phenolics were fractionated and quantified (606.7, 193.32 and 909.59 µg/g shell, respectively) and 13 individual phenolic compounds were detected by HPLC. The radical-scavenging activity of *Jc*SME was similar to Trolox and ascorbic acid by DPPH assay while by ABTS assay it was similar to BHT. Effective antioxidant capacity by ORAC was found (426.44 ± 53.39 µmol Trolox equivalents/g shell). The Mexican non-toxic *J. curcas* shell is rich in phenolic compounds with high antioxidant activity; hence, it could be considerate as a good source of natural antioxidants.

Abbreviations: SFP, soluble free phenolics; SCP, soluble conjugated phenolics; BP, bound phenolics; % ARA, antiradical activity percentage; IC_{50}, concentration required to cause a 50% of radical inhibition; BHT, butylated hydroxytoluene; TE, Trolox equivalents; *Jc*SME, *Jatropha curcas* shell methanolic extract



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1. Introduction

Jatropha curcas seeds consist of an inner kernel with high oil content (suitable to produce biodiesel) and an outer shell that constitutes about 35–40% of the seed weight (Makkar & Becker 2009). On the other hand, phenolic compounds have been extensively investigated because they exhibited a diverse range of bioactivities such as antioxidative. These compounds in plants may exist in free, soluble conjugated and insoluble-bound forms; free forms are present within the plant cell vacuoles, whereas soluble esters or conjugates are esterified to sugars and other low-molecular-mass components, and insoluble bound forms are covalently linked to cell wall structural components (Wang et al. 2015). It has been reported that species such as *Jatropha isabellei* Müll contains bioactive compounds such as phenolic acids, flavonoids, and tannins and extracts from the plant have shown notable antioxidant activity (Fröhlich et al. 2013). Recently, Li et al. (2014) isolated two new lignans and other compounds with important antioxidative activity from *J. curcas* seeds. Moreover, Fu et al. (2014) reported total phenolic content and antioxidant activities from *J. curcas* seed shells collected in China and its potential as a source of natural antioxidants. Currently, in Mexico non-toxic *J. curcas* materials have been evaluated for the biofuel production, but information regarding the phenolic compounds profile of seed shell and their potential biological activities are not available. Therefore, this research was conducted to evaluate the phenolic compound profile and the antioxidant activity from non-toxic *J. curcas* shell methanolic extract (*Jc*SME) cultivated in Mexico, in order to provide information that would indicate a value-added of this by-product as a source of antioxidant compounds.

2. Results and discussion

2.1. Phenolic compounds profile of J. curcas shell

Different phenolic compound profiles were detected among SFP, SCP and BP fractions by HPLC (Figures S1 and S2), the phenolic analytical fractionation was opted since the extract characterization from *Jc*SME is poor (data not shown). The majority of phenolic compounds in *J. curcas* shell (Table 1) were present in the bound form (53.01%) and were released upon alkaline hydrolysis. Distribution of percentage of soluble and bound phenolic compounds in non-toxic *J. curcas* shell was similar to those reported for different millet grains (Chandrasekara & Shahidi 2011). Thirteen phenolic compounds were identified in the *J. curcas* shell and quercetin, *ρ*-coumaric, *o*-coumaric, myricetin and rutin were the main individual phenolics. Twelve compounds were identified in the BF fraction: rutin, *ρ*-coumaric, quercetin, protocatechuic, were the main individual phenolic compounds in this fraction, in addition to *o*-coumaric, gallic, *ρ*-hydroxybenzoic, caffeic, sinapic and ferulic acid, as well as apigenin and kaempferol. In the SCP fraction, quercetin, myricetin, rutin, sinapic and ferulic acid were found, while quercetin, myricetin, *ρ*-coumaric and *o*-coumaric in SFP. Quercetin and *ρ*-coumaric acid were found in the three fractions. Quercetin and *ρ*-coumaric acid have been detected in soybean seed coat (Kim et al. 2006). Important biological activities have been reported of phenolic compounds found in higher concentrations in non-toxic *J. curcas* shell. For example, quercetin is a well-known antioxidant flavonoid that prevents oxidant injury and cell death by several mechanisms (Gupta et al. 2015).

To the best of our knowledge, there are no previous reports indicating the phenolic compounds profile from non-toxic *J. curcas* shell. Oskoueian et al. (2011) identified gallic

Table 1. Soluble free, soluble conjugate and bound phenolic content (μg/g shell) in non-toxic Mexican *J. curcas* shell, determined by HPLC.

Fraction	Phenolic compound	Concentration (μg/g shell)
Soluble free phenolics (35.63%)	*p*-coumaric acid	155.64 ± 10.55
	o-coumaric acid	177.06 ± 3.79
	Myricetin	132.68 ± 7.35
	Quercetin	141.30 ± 11.93
	Total	606.70 ± 4.95
Soluble conjugated phenolics (11.35%)	*p*-coumaric acid	1.95 ± 0.81
	Sinapic acid	22.59 ± 3.87
	Ferulic acid	16.57 ± 1.15
	Rutin	34.64 ± 0.25
	Myricetin	63.58 ± 5.74
	Quercetin	53.96 ± 2.11
	Total	193.32 ± 8.11
Bound phenolics (53.01%)	Gallic acid	49.34 ± 10.74
	Protocatechuic acid	120.23 ± 1.92
	p-hydroxybenzoic acid	65.53 ± 11.81
	Caffeic acid	48.96 ± 0.71
	p-coumaric acid	128.19 ± 6.07
	o-coumaric acid	64.11 ± 2.36
	Sinapic acid	47.28 ± 8.47
	Ferulic acid	53.29 ± 6.08
	Rutin	154.44 ± 17.95
	Quercetin	122.49 ± 6.77
	Apigenin	22.56 ± 7.20
	Kaempferol	26.12 ± 6.00
	Total	902.59 ± 60.62
Total identified by HPLC		1702.62 ± 73.68

acid, pyrogallol, rutin, myricetin and daidzein in kernel meal extract while Namuli et al. (2011) reported different phenolic acids and flavonoids in various plant parts, both in toxic *J. curcas* plants.

2.2. Antioxidant activity

The free radical scavenging activity of the *Jc*SME and synthetic antioxidants of reference are presented in Figure S3. In all cases, % ARA (DPPH and ABTS methods) increased in a dose-dependent manner (Figure S3(A) and (C)). For determination of IC_{50} value, the natural logarithm of antioxidant or extract concentration was plotted vs. % ARA (Figure S3(B) and (D)). The IC_{50} values of *JcSME* were 0.1374 mg/mL for DPPH and 0.1496 mg/mL for ABTS. Lower IC_{50} values indicated higher antioxidant activity. Regarding to their antioxidant activity, synthetic antioxidants and extract had the following descending order: ascorbic acid (0.0845 mg/mL) > Trolox (0.1211 mg/mL) > *JcSME* > BTH (0.2896 mg/mL). In the case of DPPH test, no significant differences were detected ($p > 0.05$) between ascorbic acid, Trolox and *Jc*SME while BHT presented an IC_{50} significantly different ($p \leq 0.05$) than the others antioxidants, including *Jc*SME. According to these results, the *J. curcas* shell extract showed strong antiradical activity, and it was comparable to synthetic antioxidants ascorbic acid and Trolox and higher than BHT. Regarding to ABTS methodology, analysis of variance showed no significant differences ($p > 0.05$) between IC_{50} of *Jc*SME and BHT (0.1880 mg/mL) while ascorbic acid and Trolox showed significantly higher ($p \leq 0.05$) antioxidant activity (0.0746 and 0.0764 mg/mL, respectively). Hence, *Jc*SME showed high antiradical activity and it was similar to BHT. A high antioxidant capacity of *Jc*SME was determined using ORAC method (426.44 μmol TE/g

of shell) that was better than those reported for different legumes seeds such as lentils, black soybeans, and common beans (Xu et al. 2007) and for some millet grains (Chandrasekara & Shahidi 2011). In general, the results obtained by three antioxidant methodologies for non-toxic Mexican *J. curcas* were similar to ethanolic extracts of *J. curcas* cultivated in China (Fu et al. 2014).

3. Conclusion

Overall, our results demonstrated that the non-toxic *J. curcas* shell is rich in bioactive phenolic compounds with high antioxidant activity, hence it could be considerate as a good source of natural antioxidants with potential for application in the industry in general, as well as for the development of nutraceuticals with high added value. The results encourage future *in vivo* antioxidant assays as well as complementary evaluations of biological activities. To the best of our knowledge, this is the first report of characterization of phenolic compounds profile and evaluation of antioxidant activity of non-toxic Mexican *J. curcas* shell extracts.

Supplementary material

Supplementary material relating to this paper is available online, alongside Figures S1–S3.

Disclosure statement

No potential conflict of interest was reported by the authors.

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