

# Supporting Information

## Application of the electron spin resonance technique in the characterization of Brazilian oils: correlation with their biodegradation level and polar composition

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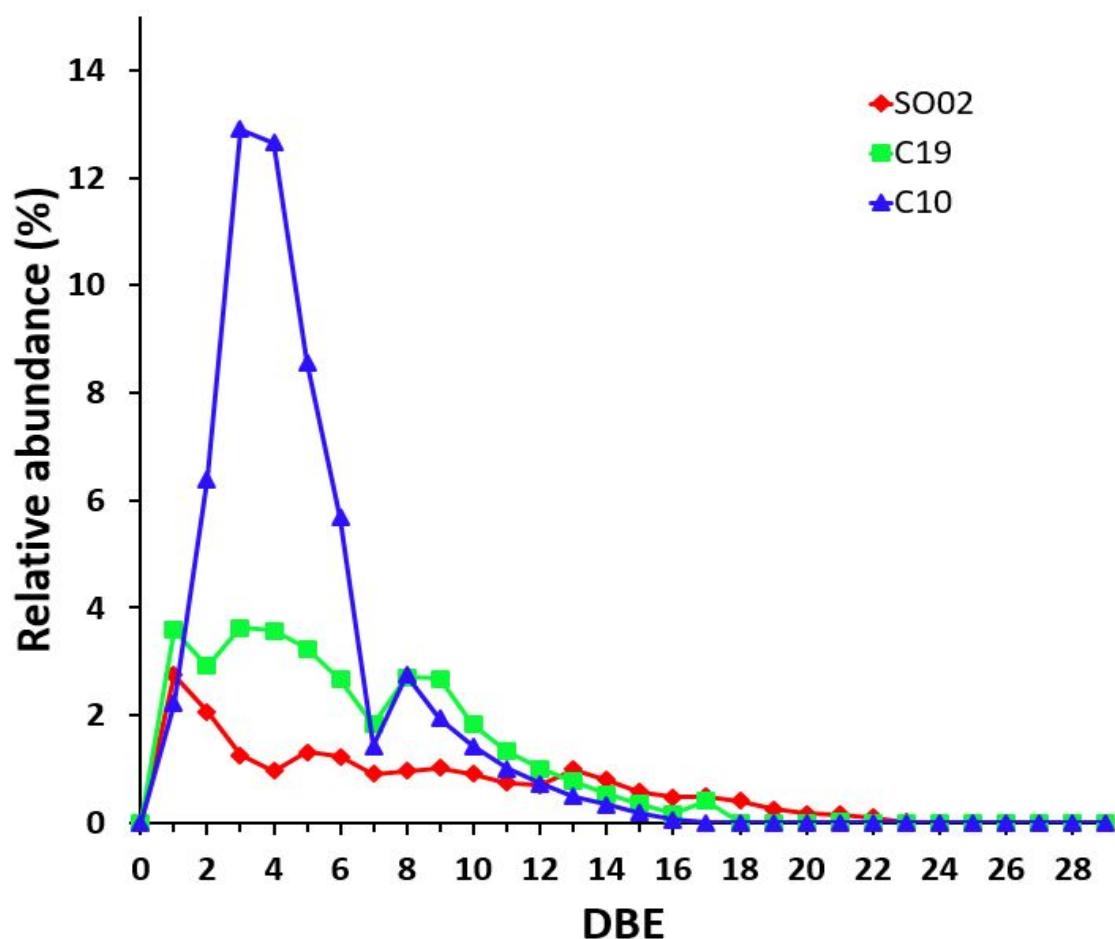
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**Table S1.** Consolidated data referring to the main results of the applied analyses and the biodegradation level of the oil samples: API gravity, total acid number (TAN), GC-FID, elemental CHN analysis, FTIR, ESI(-) FT-ICR MS by measuring the relative abundance of the NO, NO<sub>2</sub>, and O<sub>2</sub> classes, and DBE15 NO, DBE14 NO<sub>2</sub>, and DBE3 O<sub>2</sub> classes, and the quantification of free radicals calculated by ESR of SO02, C19, and C10 oils and their fractions

TECHNIQUES AND OBTAINED PARAMETERS		SAMPLES		
		SO02	C19	C10
<b>Biodegradation Level</b>		<b>very slight</b>	<b>moderate</b>	<b>heavy</b>
<b>API°</b>		43	25	19
<b>TAN (mg KOHg<sup>-1</sup>)</b>		0.17	0.27	2.30
<b>Liquid chromatography</b>	Sat (%)	58.2	39.9	32.5
	Aro (%)	14.0	19.4	23.2
	Res (%)	1.3	13.4	21.2
	Asp (%)	8.8	10.4	12.7
<b>GC-FID</b>	Pr/nC <sub>17</sub>	0.14	1.13	1.41
	Ph/nC <sub>18</sub>	0.06	0.76	0.96
<b>Elemental CHN analysis</b>	N (%)	0.09	0.64	0.51
	H/C	0.155	0.134	0.133
<b>FTIR (band intensity) - Res</b>	C-H (aromatics)	weak	very strong	very strong
	C-O	weak	strong	strong
<b>FTIR (band intensity) - Asp</b>	C-H (aromatics)	weak	weak	very strong
	C-O	weak	weak	strong
<b>ESI(-) FT-ICR MS (class relative abundance)</b>	NO	6.81	8.56	4.89
	NO <sub>2</sub>	2.33	10.45	11.15
	O <sub>2</sub>	19.28	33.08	61.15

<b>ESI(-) FT-ICR MS (DBE relative abundance)</b>	DBE 15 NO	0.45	0.85	0.63
	DBE 14 NO	0.44	9.48	0.41
	DBE 3 O <sub>2</sub>	1.32	3.23	8.56
<b>Free Radical ESR quantification (x10<sup>4</sup> a.u)</b>	Oil	6.19	10.60	9.39
	Res	5.19	11.33	7.12
	Asp	4.96	5.19	8.87

Sat: saturated; Aro: aromatic; Res: resin; Asp: Asphaltene; GC-FID: gas chromatography with flame ionization detector; FTIR: Fourier-transform infrared spectroscopy; ESI(-) FT-ICR MS: Fourier transform ion cyclotron resonance mass spectrometry using electrospray ionization in negative mode; ESR: electron spin resonance.



**Figure S1.** DBE distribution of the O<sub>2</sub> class for the oil samples SO02, C19, and C10.