

# Supplementary Information

## Comprehensive Two-Dimensional Gas Chromatography Coupled to Time of Flight Mass Spectrometry: New Biomarker Parameter Proposition for the Characterization of Biodegraded Oil

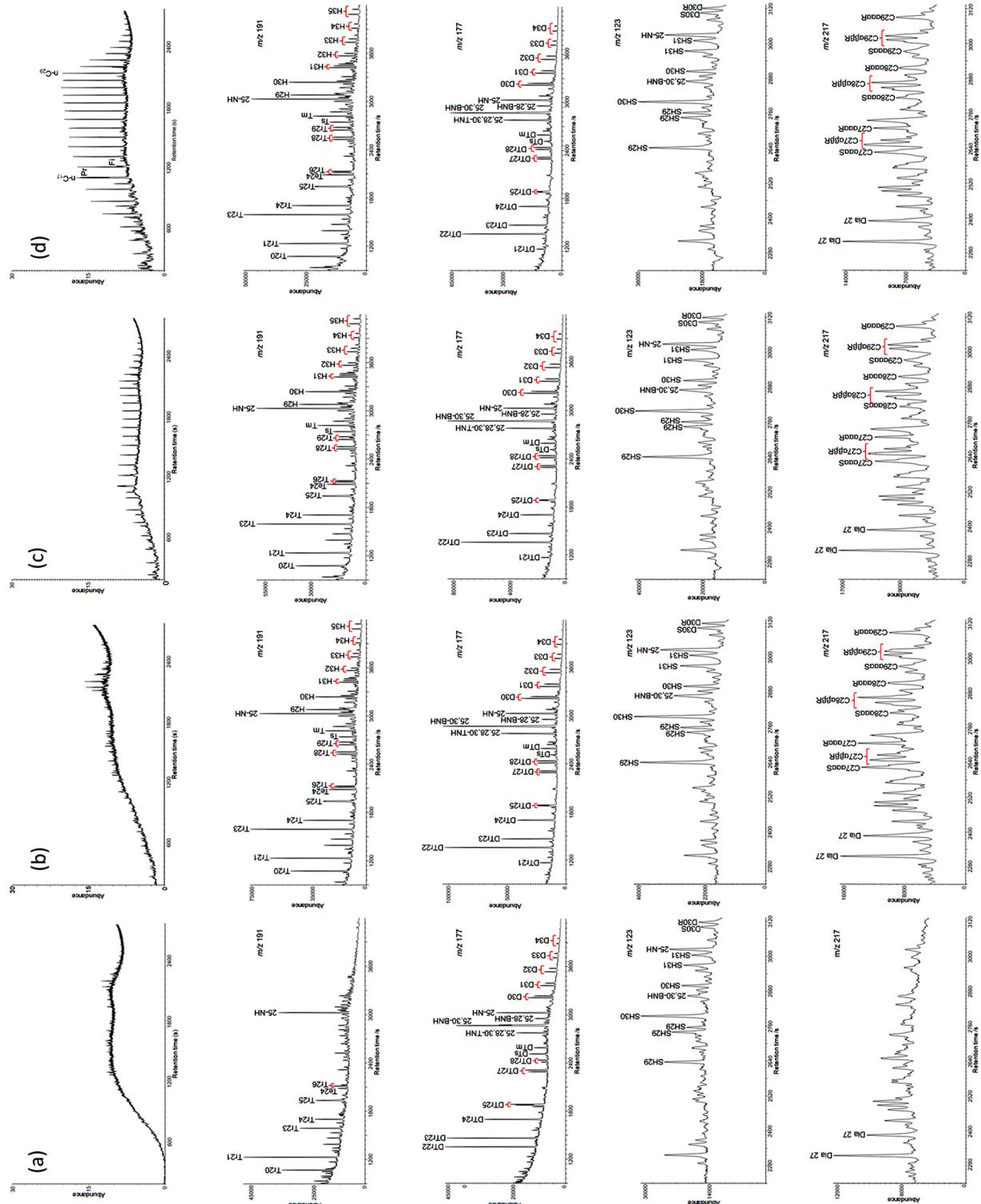
**Renata F. Soares,\*<sup>a</sup> Ricardo Pereira,<sup>a</sup> Raphael S. F. Silva,<sup>a</sup> Leonardo Mogollon<sup>b</sup> and Débora A. Azevedo\*<sup>a</sup>**

<sup>a</sup>Instituto de Química, Universidade Federal do Rio de Janeiro,  
 Ilha do Fundão, 21941-909 Rio de Janeiro-RJ, Brazil

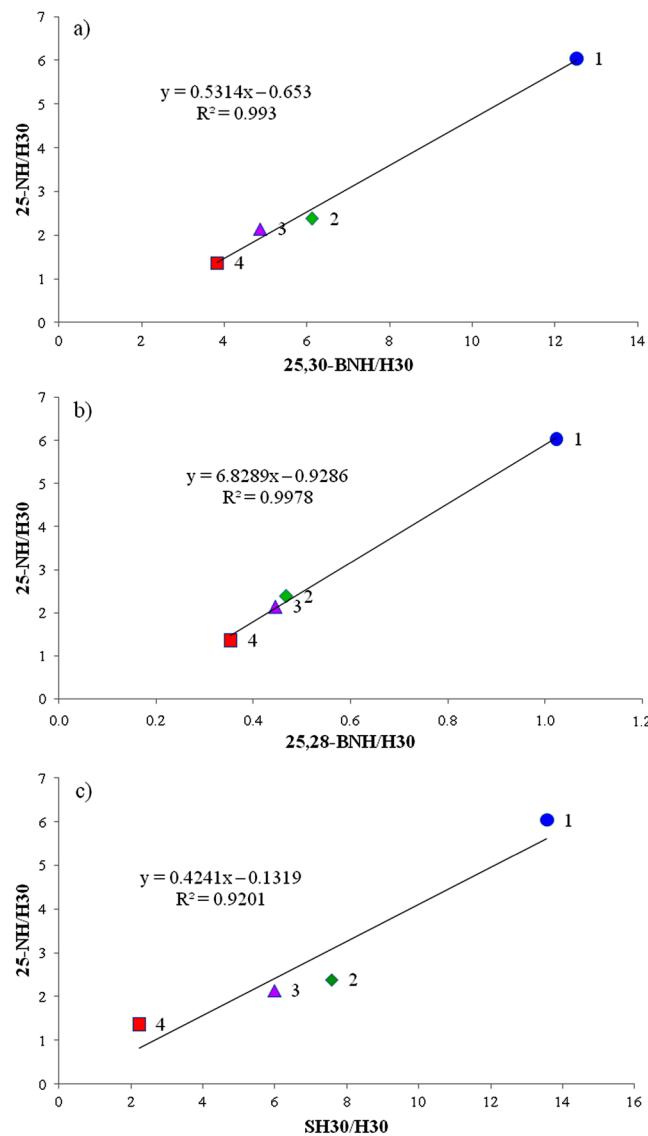
<sup>b</sup>Instituto Colombiano del Petróleo, ECOPETROL S. A., Bucaramanga, Colombia

**Table S1.** Table of abbreviations

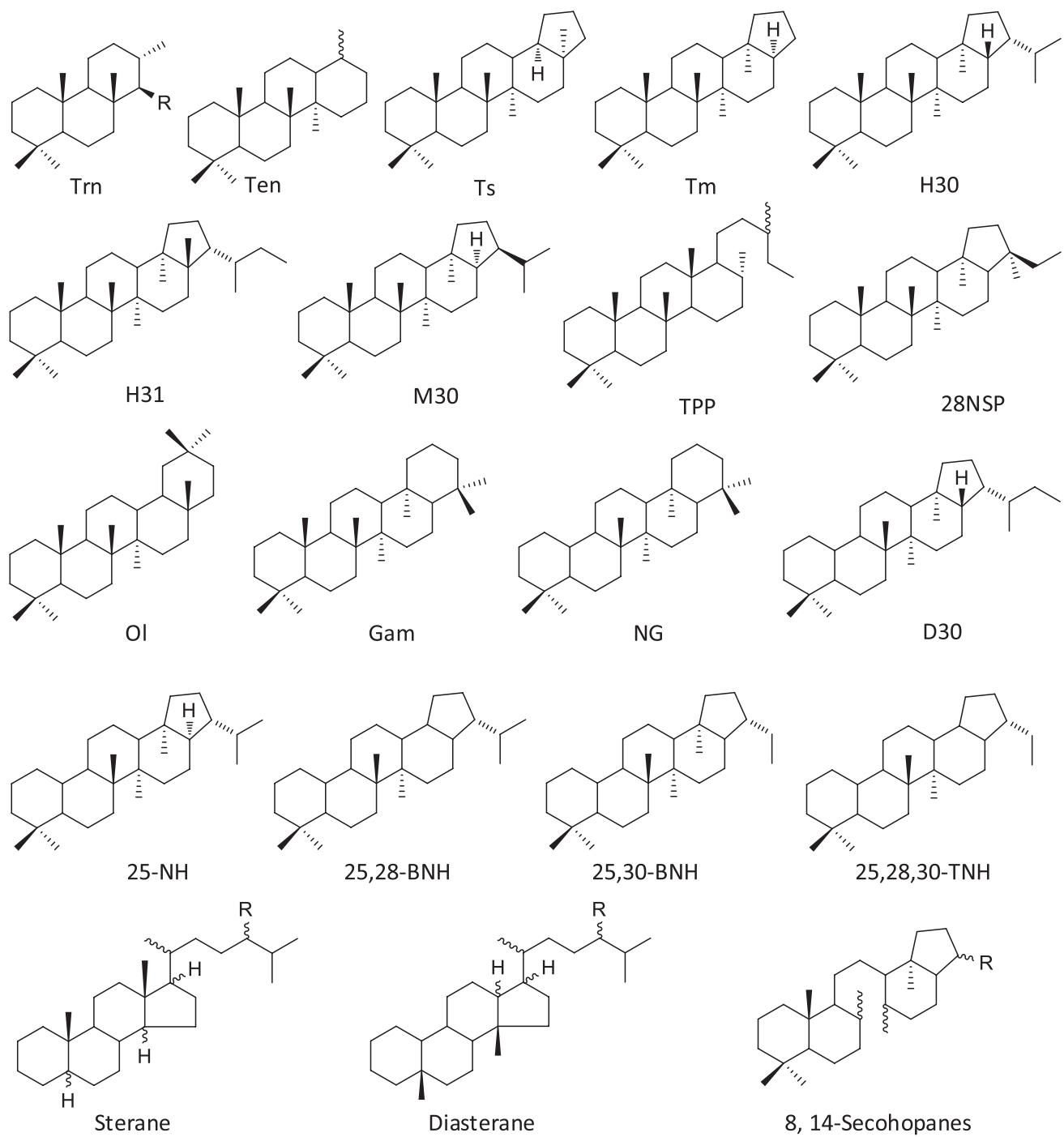
Trn	C <sub>n</sub> tricyclic terpane	D33	17α(H),21β(H)-25-nor-30,31,32,33-tetrakishomohopane (22S + 22R)
Ten	C <sub>n</sub> tetracyclic terpane	D34	17α(H),21β(H)-25-nor-30,31,32,33,34-pentakishomohopane (22S + 22R)
Ts	18α(H),21β(H)-22,29,30-tris-nor-neohopane	M29	17B(H),21A(H)-30-nor-hopane
Tm	17α(H),21β(H)-22,29,30-tris-nor-hopane	M30	C <sub>30</sub> 17B(H),21A(H)-hopane
DTs	demethylated Ts; 18α(H),21β(H)-22,25,29,30-tetra-nor-neohopane	NH30	17α(H),30-nor-29-homohopane
DTm	demethylated Tm; 17α(H), 21β(H)-22,25,29,30-tetra-nor-hopane	29NSP	C <sub>29</sub> 28-nor-spergulane
H28	17a(H),18a(H),21b(H)-28,30-bis-nor-hopane	NG	nor-gammacerane
H29	17A(H),21B(H)-30-nor-hopane	25-NH	C <sub>29</sub> 17α(H),21β(H)-25-nor-hopane
C29Ts	18α(H),21β(H)-30-nor-neohopane	TPP	tetracyclic polyprenoid
H30	C <sub>30</sub> 17a(H),21b(H)-30-hopane	Gam	gammacerane
H31	17α(H),21β(H)-30-homohopane (22S + 22R)	OL	oleanane
H32	17α(H),21β(H)-30,31-bishomohopane (22S + 22R)	25,28-BNH	17α(H),18α(H),21β(H)-25,28-bis-nor-hopane
H33	17α(H),21β(H)-30,31,32-trishomohopane (22S + 22R)	25,30-BNH	17α(H),18α(H),21β(H)- 25,30-bis-nor-hopane
H34	17α(H),21β(H)-30,31,32,33-tetrakishomohopane (22S + 22R)	25,28,30-TNH	17α(H),18α(H),21β(H)-25,28,30-tris-nor-hopane
H35	17α(H),21β(H)-30,31,32,33,34-pentakishomohopane (22S + 22R)	SH	secohopane
D30	17α(H),21β(H)-25-nor-30-homohopane (22S + 22R)	St	sterane
D31	17α(H),21β(H)-25-nor-30,31-bishomohopane (22S + 22R)	C <sub>n</sub> ααα(Σ+P)	C <sub>n</sub> sterane ααα (C <sub>27</sub> -C <sub>30</sub> ) (S + R)
D32	17α(H),21β(H)-25-nor-30,31,32-trishomohopane (22S + 22R)	C <sub>n</sub> αββ(Σ+P)	C <sub>n</sub> sterane αββ (C <sub>27</sub> -C <sub>30</sub> ) (S + R)
		Dia 27	C <sub>27</sub> diasterane



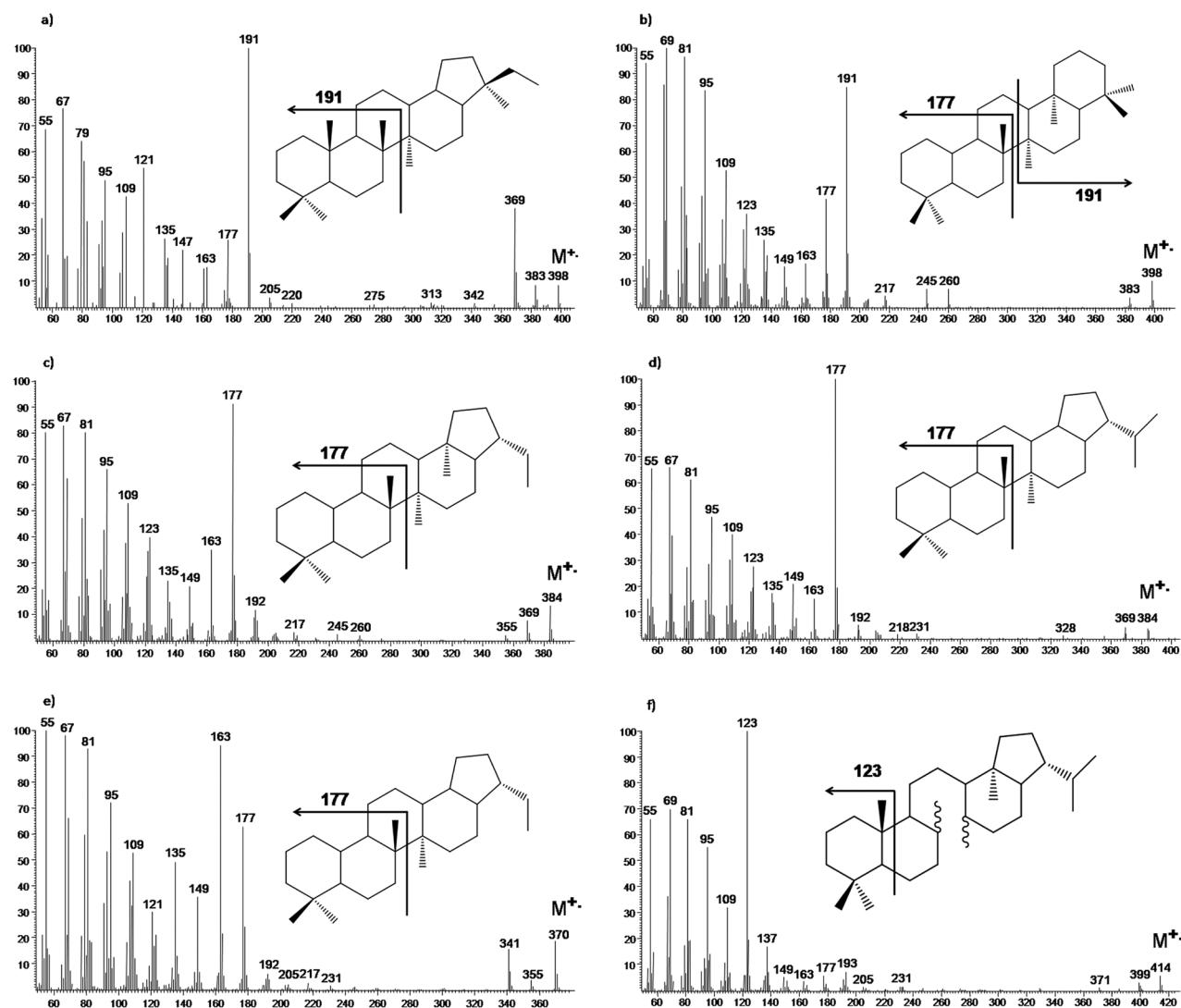
**Figure S1.** Whole oil chromatogram (GC-FID), and saturated hydrocarbon fraction GC-MS  $m/z$  191 chromatogram,  $m/z$  177 chromatogram,  $m/z$  123 chromatogram and  $m/z$  217 chromatogram, respectively, from (a) Oil #1, (b) Oil #2, (c) Oil #3 and (d) Oil #4.



**Figure S2.** Correlation graphics between: (a) 25,30-BNH/H30 and 25-NH/H30, (b) 25,28-BNH/H30 and 25-NH/H30, (c) SH30/H30 and 25-NH/H30.



**Figure S3.** Selected structures of cited compounds.



**Figure S4.** Mass spectra of: (a)  $C_{29}$  28-nor-spergulane, (b) nor-gammacerane, (c) 25,30-bis-nor-hopane (25,30-BNH), (d) 25,28-bis-nor-hopane (25,28-BNH), (e) 25,28,30-tris-nor-hopane (25,28,30-TNH) and (f)  $C_{30}$  8,14-secohopane with the fragmentation which leads to the diagnostic ion.