

Supplementary data

Ultrafine particles issued from gasoline-fuels and biofuel surrogates combustion: a comparative study of the physicochemical and *in vitro* toxicological effects

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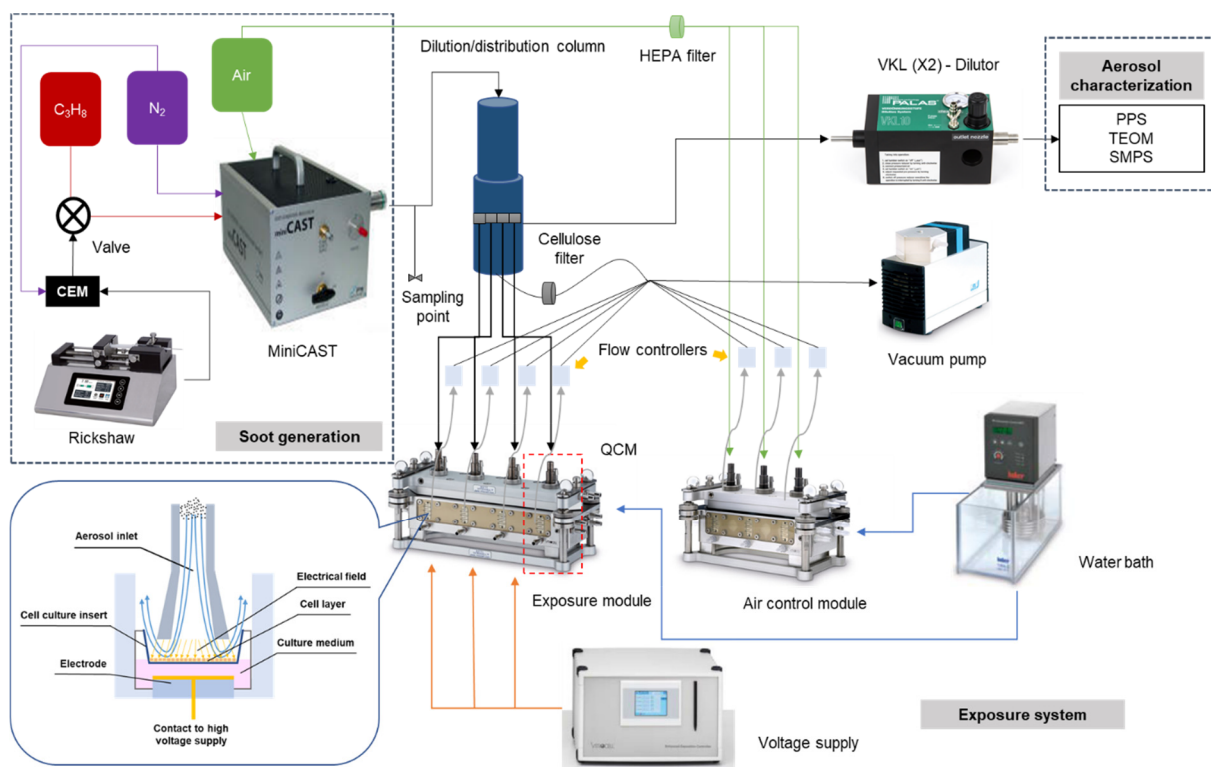


Figure S1: Aerosol exposure system. Adapted from (Juarez-Facio et al., 2022)

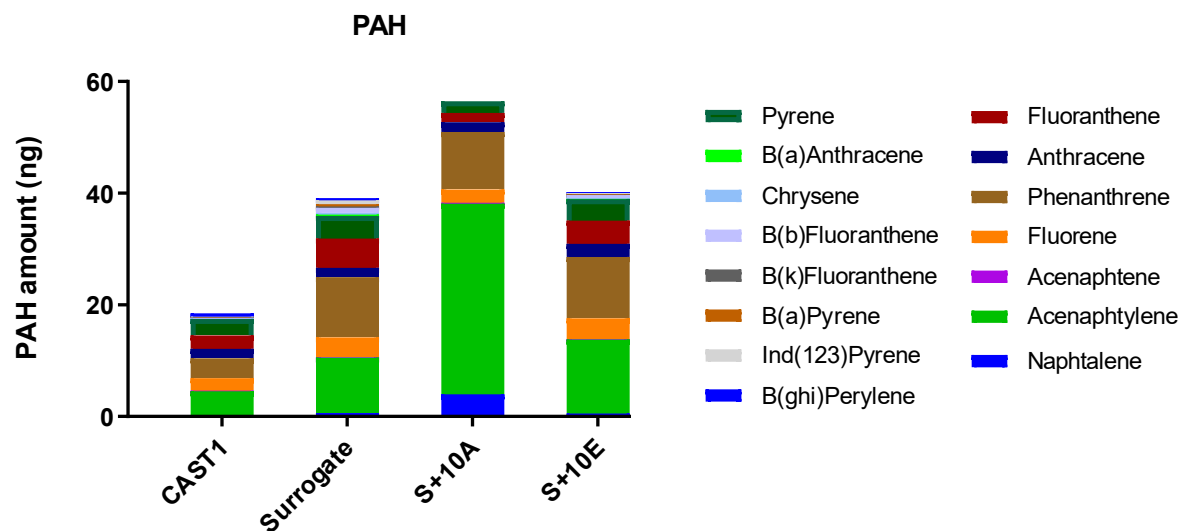


Figure S2: Amount of the different PAH and oxy-PAH in the four studied aerosols.

32 **Table S1:** LDI+ FTICR MS method parameters

MALDI			Acquisition		
	Plate Offset (V)	100		Low m/z	98.27
	Deflector Plate (V)	200		High m/z	1200
	Laser power (%)	18		Size	4M
	Laser Shots	100		Average scans	30
	Frequency (Hz)	1000		Accumulation (s)	x
	Laser Focus	Medium		FID (s)	1.258 35
Ion Transfer			Analyzer		
Source optics	Capillary Exit (V)	150	Para Cell	Transfer Exit Lens (V)	-20
	Deflector Plate (V)	200		Analysis Entrance (V)	-10
	Funnel 1 (V)	150		Side Kick (V)	0
	Skimmer 1 (V)	25		Side Kick Offset (V)	-1.5
	Funnel RF Amplitude (Vpp)	60		Front Trap Plate (V)	1.7
Octopole	Frequency (MHz)	5		Back Trap Plate (V)	1.7
	RF Amplitude (Vpp)	350	Back Trap Plate Quench (V)	-30	
Quadrupole	Q1 Mass(m/z)	120		Sweep Excitation Power (%)	35
Collision Cell	Collision Voltage (V)	0.5	Shimming DC Bias	0°	1.513
	DC Extract Bias (V)	0.5		90°	1.51
	RF Frequency (MHz)	2		180°	1.487
	Collision RF Amplitude (Vpp)	1200		270°	1.49
Transfer Optics	Time of Flight (ms)	0.8	Gated Injection DC Bias	0°	2.3
	Frequency (MHz)	6		90°	1.5
	RF Amplitude (Vpp)	200		180°	0.7
				270°	1.5

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35 **Table S2:** Internal recalibration ions for LDI+ FTICR MS analysis

Ion	m/z	Ion	m/z
C19H11	239.08553	C42H18	522.14030
C20H12	252.09335	C45H19	559.14813
C21H13	265.10118	C46H20	572.15595
C22H12	276.09335	C48H20	596.15595
C23H13	289.10118	C50H20	620.15595
C25H13	313.10118	C52H20	644.15595
C26H14	326.10900	C53H21	657.16378
C28H14	350.10900	C55H21	681.16378
C29H15	363.11683	C58H22	718.17160
C31H15	387.11683	C60H24	744.18725
C33H15	411.11683	C62H24	768.18725
C34H16	424.12465		
C37H17	461.13248		
C40H18	498.14030		

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37 **Table S3:** Estimated concentrations for the compounds detected on the gas phase, sampled
 38 with and without filter (/: not detected).

		CAST1		Surrogate		S+10A		S+10E		Limit of quantification
	Compounds	Molar % (with filter)	Molar % (without filter)	Molar % (with filter)	Molar % (with filter)	Molar % (with filter)	Molar % (without filter)	Molar % (with filter)	Molar % (without filter)	Molar %
TCD	Dihydrogen H ₂	/	/	0,034	0,03	0,03	0,031	0,035	0,033	0.008
	Methane CH ₄	/	/	0,027	0,029	0,029	0,03	0,035	0,036	0.035
MS	Carbon dioxide CO ₂	1,0085	0,8539	0,6305	0,6559	0,6559	0,6059	0,5827	0,6379	0.0044
	Ethylene C ₂ H ₄	/	/	0,0159	0,0183	0,0183	0,0164	0,0227	0,0254	0.0005
	Acetylene C ₂ H ₂	/	/	0,0104	0,0119	0,0119	0,0105	0,0135	0,0160	0.0119
	Ethane C ₂ H ₆	/	/	0,0007	0,0008	0,0008	0,0005	0,0008	0,0010	0.0196
	Propene C ₃ H ₆	/	/	0,0045	0,0035	0,0035	0,0031	0,0039	0,0041	0.0003
	Propane C ₃ H ₈	0,0005	0,0002	/	/	/	/	/	/	0.0003
	Propadiene C ₃ H ₄	/	/	0,0012	0,001	0,001	0,0009	0,0011	0,0011	0.0003
	Propyne C ₃ H ₄	/	/	0,0022	0,002	0,002	0,0017	0,0021	0,0023	0.0003
	Acetaldehyde C ₂ H ₄ O	/	/	/	/	/	/	0,0001	0,0001	0.0003
	Isobutene C ₄ H ₈	/	/	0,0013	0,001	0,001	0,0008	0,0011	0,0011	0.0003
	1-buten-3-yne C ₄ H ₄	/	/	0,0007	0,0009	0,0009	0,0006	0,0009	0,0010	0.0003
	1,3 butadiene C ₄ H ₆	/	/	0,0022	0,0022	0,0022	0,0019	0,0025	0,0027	0.0003
	1,3 butadiyne C ₄ H ₂	/	/	/	/	/	/	0,0002	0,0002	0.0003
	Cyclopentadiene C ₅ H ₆	/	/	0,0011	0,0023	0,0023	0,0016	0,0017	0,0022	0.0003
	Benzene C ₆ H ₆	/	/	0,00004	0,00004	0,00004	0,00004	0,00004	0,00004	0.00002
	Toluene C ₇ H ₈	/	/	0,00004	0,00004	0,00004	0,00004	0,00004	0,00006	0.00002

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