Quantitative trace analysis of fullerenes in river sediment from Spain and soils from Saudi Arabia

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Table S1. SRM transitions and some instrumental parameters

|	Compound	Empirical formula	Cone Energy	Precursor Ion	Collision Energy	Product Ion
Unfuncionalized fullerenes	C_{60} fullerene	C_{60}	250	720	50	720
				721	50	721
	C_{70} fullerene	C_{70}	250	840	50	840
				841	50	841
	C_{76} fullerene	C_{76}	250	912	50	912
				913	50	913
	C_{78} fullerene	C_{78}	250	936	50	936
				937	50	937
	C_{84} fullerene	C_{84}	250	1008	50	1008
				1009	50	1009
Funcionalized fullerenes	PCBM	$C_{72}H_{14}O_2$	125	910	70	720
				911	70	721
	ThPCBM	$C_{70}H_{12}O_2S$	125	916	60	720
				917	60	721
	NMFP	$C_{63}H_7N$	150	777	40	720
				778	40	721
Isotopically-labelled fullerenes	$^{13}C_{60}$	$^{13}C_{12}{}^{12}C_{48}$	250	740	50	740
				741	50	741

PCBM: [6,6]-phenyl C_{61} butyric acid methyl ester,; ThPCBM: [6,6]-Thienyl C_{61} butyric acid methyl ester; NMFP: *N*-methyl fulleropyrrolidine

Fig. S1. Location of Llobregat River / Riera de Rubí samples
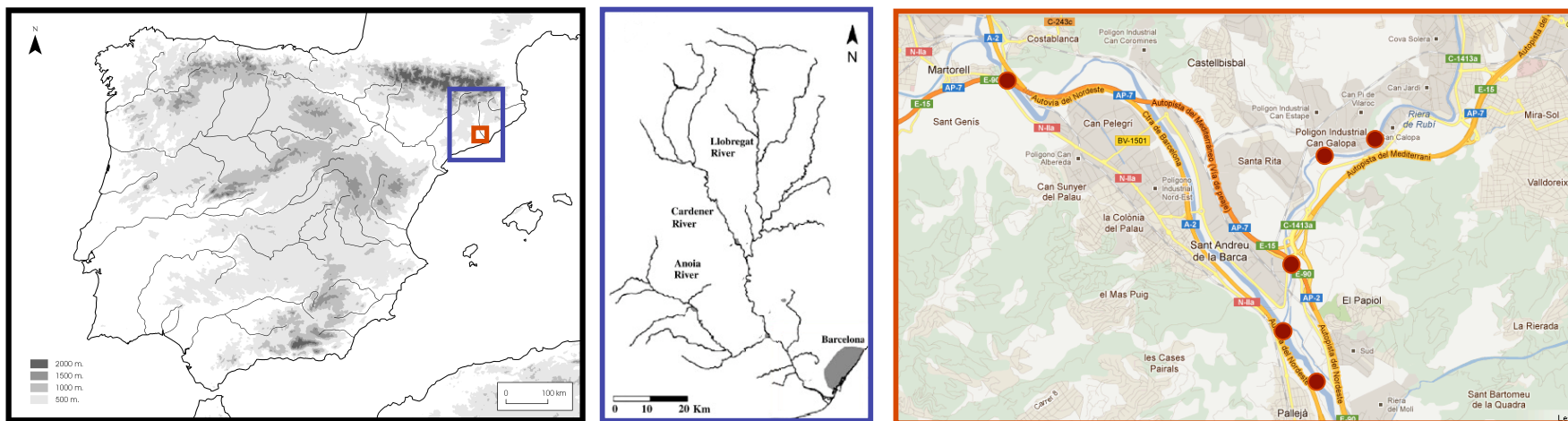
	River	Town	Observation	Latitude	Longitude
1	Llobregat	Pallejà	After Riera de Rubí-Llobregat confluence	41.4261	2.00363
2	Riera de Rubí	Rubí (Can Galopa Ind. Park)	Before WWTP	41.4638	2.01515
3	Riera de Rubí	Rubí (Can Galopa Ind. Park) - Castellbisbal (Sta.Rita Ind.Park)	After WWTP	41.45649	2.00147
4	Llobregat	El Papiol	Riera de Rubí-Llobregat confluence	41.4361	1.99582
5	Riera de Rubí	Castellbisbal (North-East Ind.	Stagnant section of the river.	41.4456	1.99640
6	Llobregat	Martorell (Pont del Diable)	Before Riera de Rubí-Llobregat	41.4783	1.96454

Fig. S2. Location of soil samples from Saudi Arabia
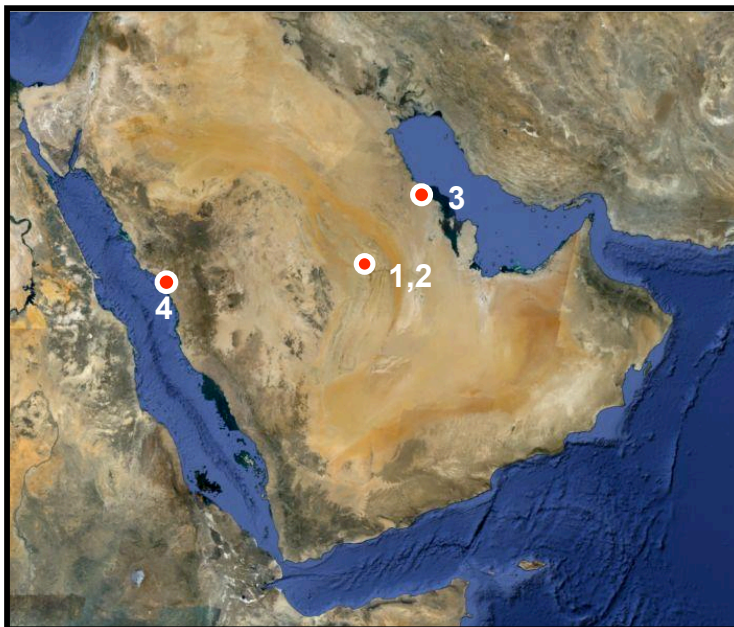
	City	Number of samples		
		Urban Area	Industrial Area	Total
1	Riyadh	13	4	17
2	Diriyah	7	8	15
3	Jubail	5	8	13
4	Yanbu' al	13	0	13

Fig. S3. ASE optimization

Recovery of C60 (%)

Temperature (°C)

Solvent: Tol, Tol:Hex, Tol:MeOH, Hex

Recovery of ThPCBM (%)

Temperature (°C)

Solvent: Tol, Tol:Hex, Tol:MeOH, Hex

Recovery of PCBM (%)

Temperature (°C)

Solvent: Tol, Tol:Hex, Tol:MeOH, Hex

Recovery of CPTAE (%)

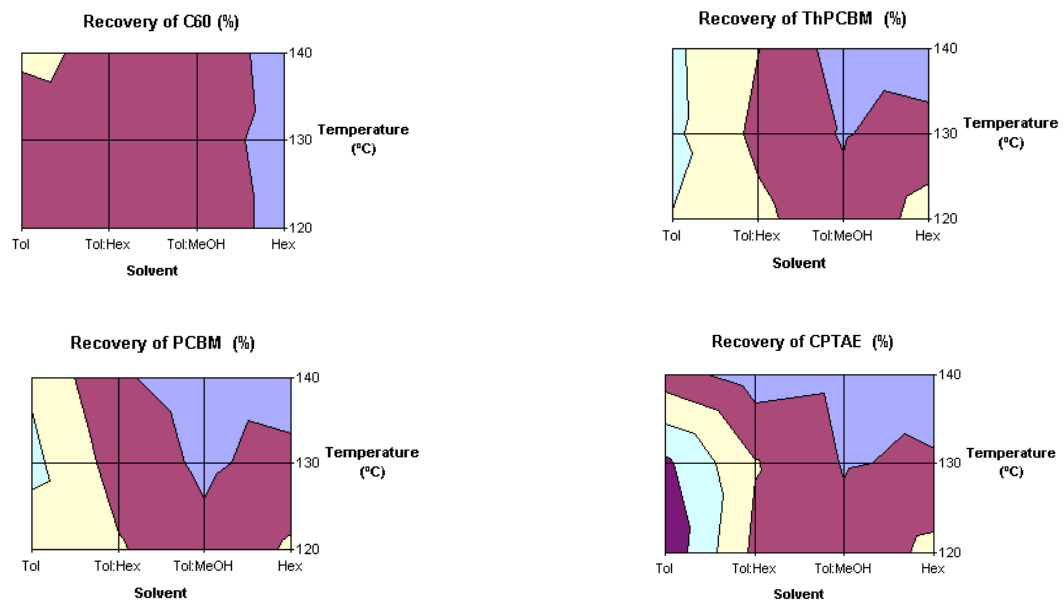Temperature (°C)

Solvent: Tol, Tol:Hex, Tol:MeOH, Hex
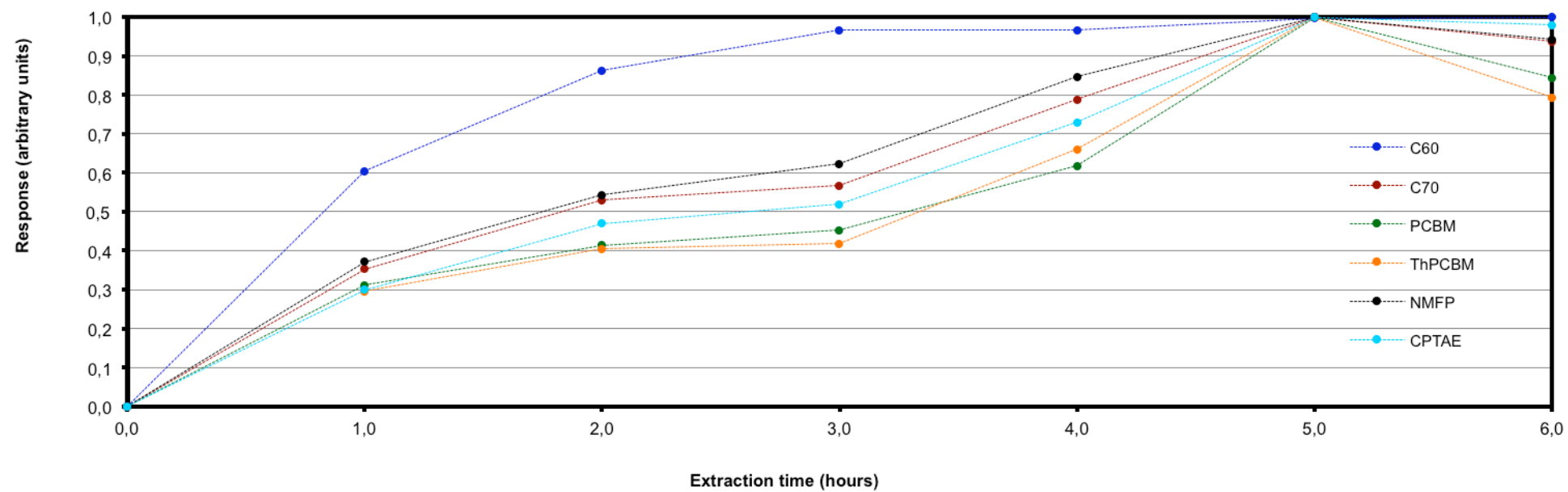
Fig. S4. Optimization of the UASE extraction time

Fig. S5. Optimization of the extractant volume/number of extractions