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Supplementary material

Studying the degradation of bulk PTFE into microparticles via SP ICP-MS: A systematically developed method for the detection of F-containing particles

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Table S1: Doehlert experimental design for optimisation of the (A) plasma, and (B) bandpass

Exp.	Matrix Code		Experimental Conditions			
			(A) Plasma		(B) Bandpass	
	Variable 1	Variable 2	Sample Depth (mm)	Nebulizer Flow (mL min^{-1})	Q1 Mass Gain (V)	Q1 Mass Offset (V)
1	0	0	4.5	1.40	10	130
2	0	1	4.5	1.50	10	150
3	0.866	0.5	6.0	1.45	20	140
4	0	-1	4.5	1.30	10	110
5	-0.866	-0.5	3.0	1.35	0	120
6	-0.866	0.5	3.0	1.45	0	140
7	0.866	-0.5	6.0	1.35	20	120
CP	0	0	4.5	1.40	10	130
CP	0	0	4.5	1.40	10	130
CP	0	0	4.5	1.40	10	130

Table S2: Central Composite experimental design for optimization of extract 2 and deflect of ion optics.

Exp.	Matrix Code		Experimental Conditions	
	Variable 1	Variable 2	Extract 2 (V)	Deflect (V)
1	-1	-1	-5	-5
2	-1	1	-5	5
3	1	-1	5	-5
4	1	1	5	5
5	-1.41421	0	-7	0
6	1.41421	0	7	0
7	0	-1.41421	0	-7
8	0	1.41421	0	7
9 (CP)	0	0	0	0
10 (CP)	0	0	0	0

Figure S1: Colorimetric map obtained from the Central Composite experimental design (2 factors: 10 exp) for ion optics optmisation. Selected conditions are marked as a white circle.

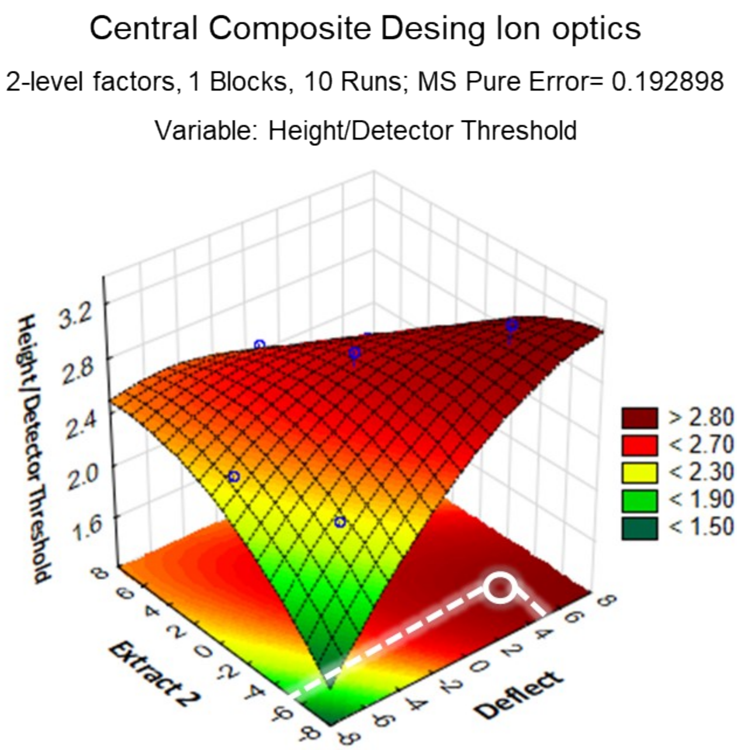

Table S3: Factorial design 2^5 executed to discriminate between significant and non-significant factors that can affect the CRC performance

Exp.	Matrix Code					Experimental Conditions				
	Var 1	Var 2	Var 3	Var 4	Var 5	Oct Bias	Energy Discrimination	He Flow	H_2 Flow	O_2 Flow
1	-1	-1	-1	-1	-1	-8	-5	0	0	5
2	1	-1	-1	-1	-1	-2	-5	0	0	5
3	-1	1	-1	-1	-1	-8	2	0	0	5
4	1	1	-1	-1	-1	-2	2	0	0	5
5	-1	-1	1	-1	-1	-8	-5	2	0	5
6	1	-1	1	-1	-1	-2	-5	2	0	5
7	-1	1	1	-1	-1	-8	2	2	0	5
8	1	1	1	-1	-1	-2	2	2	0	5
9	-1	-1	-1	1	-1	-8	-5	0	2	5
10	1	-1	-1	1	-1	-2	-5	0	2	5
11	-1	1	-1	1	-1	-8	2	0	2	5
12	1	1	-1	1	24	-2	2	0	2	5
13	-1	-1	1	1	-1	-8	-5	2	2	5
14	1	-1	1	1	-1	-2	-5	2	2	5
15	-1	1	1	1	-1	-8	2	2	2	5
16	1	1	1	1	-1	-2	2	2	2	5
17	-1	-1	-1	-1	1	-8	-5	0	0	30
18	1	-1	-1	-1	1	-2	-5	0	0	30
19	-1	1	-1	-1	1	-8	2	0	0	30
20	1	1	-1	-1	1	-2	2	0	0	30
21	-1	-1	1	-1	1	-8	-5	2	0	30
22	1	-1	1	-1	1	-2	-5	2	0	30
23	-1	1	1	-1	1	-8	2	2	0	30
24	1	1	1	-1	1	-2	2	2	0	30
25	-1	-1	-1	1	1	-8	-5	0	2	30
26	1	-1	-1	1	1	-2	-5	0	2	30
27	-1	1	-1	1	1	-8	2	0	2	30
28	1	1	-1	1	1	-2	2	0	2	30
29	-1	-1	1	1	1	-8	-5	2	2	30
30	1	-1	1	1	1	-2	-5	2	2	30
31	-1	1	1	1	1	-8	2	2	2	30
32	1	1	1	1	1	-2	2	2	2	30

Figure S2: Pareto chart for the factorial design 2^5 showing the significant factors that affect the CRC performance.

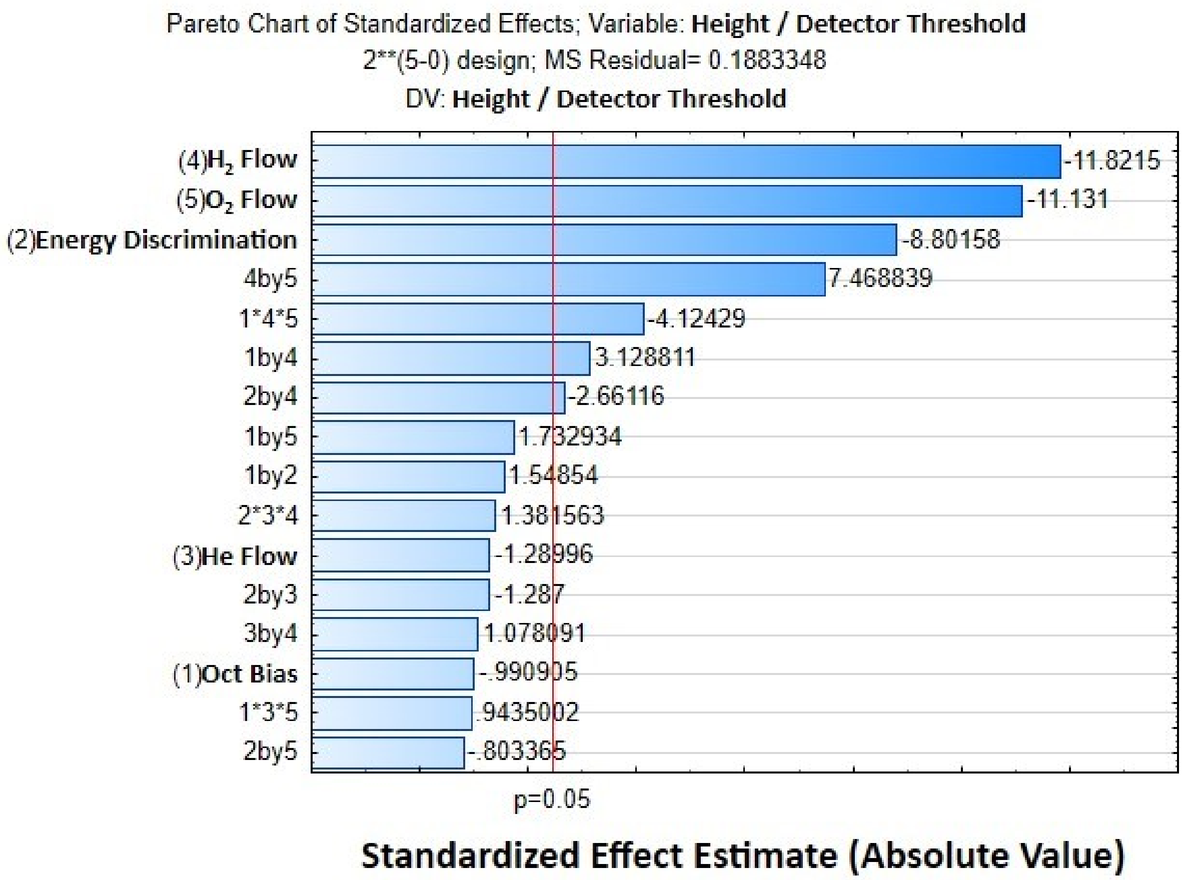

Table S4: Box-Behnken experimental design for optimization of H_2 flow, O_2 flow, and energy discrimination of CRC.

Exp.	Matrix Code			Experimental Conditions		
	Var 1	Var 2	Var 3	H_2 Flow	O_2 Flow	Energy Discrimination
1	-1	-1	0	0	5	-10
2	1	-1	0	1	5	-10
3	-1	1	0	0	15	-10
4	1	1	0	1	15	-10
5	-1	0	-1	0	10	-15
6	1	0	-1	1	10	-15
7	-1	0	1	0	10	-5
8	1	0	1	1	10	-5
9	0	-1	-1	0.5	5	-15
10	0	1	-1	0.5	15	-15
11	0	-1	1	0.5	5	-5
12	0	1	1	0.5	15	-5
13	0	0	0	0.5	10	-10
14	0	0	0	0.5	10	-10
15	0	0	0	0.5	10	-10

Figure S3. Box-Behnken Designs (3 factors: 15 exp) for CRC optimisations: A) O_2 flow vs H_2 flow, B) Energy discrimination vs H_2 flow and C) Energy discrimination vs O_2 flow. Optimised values are shown at the bottom of the figures, respectively.