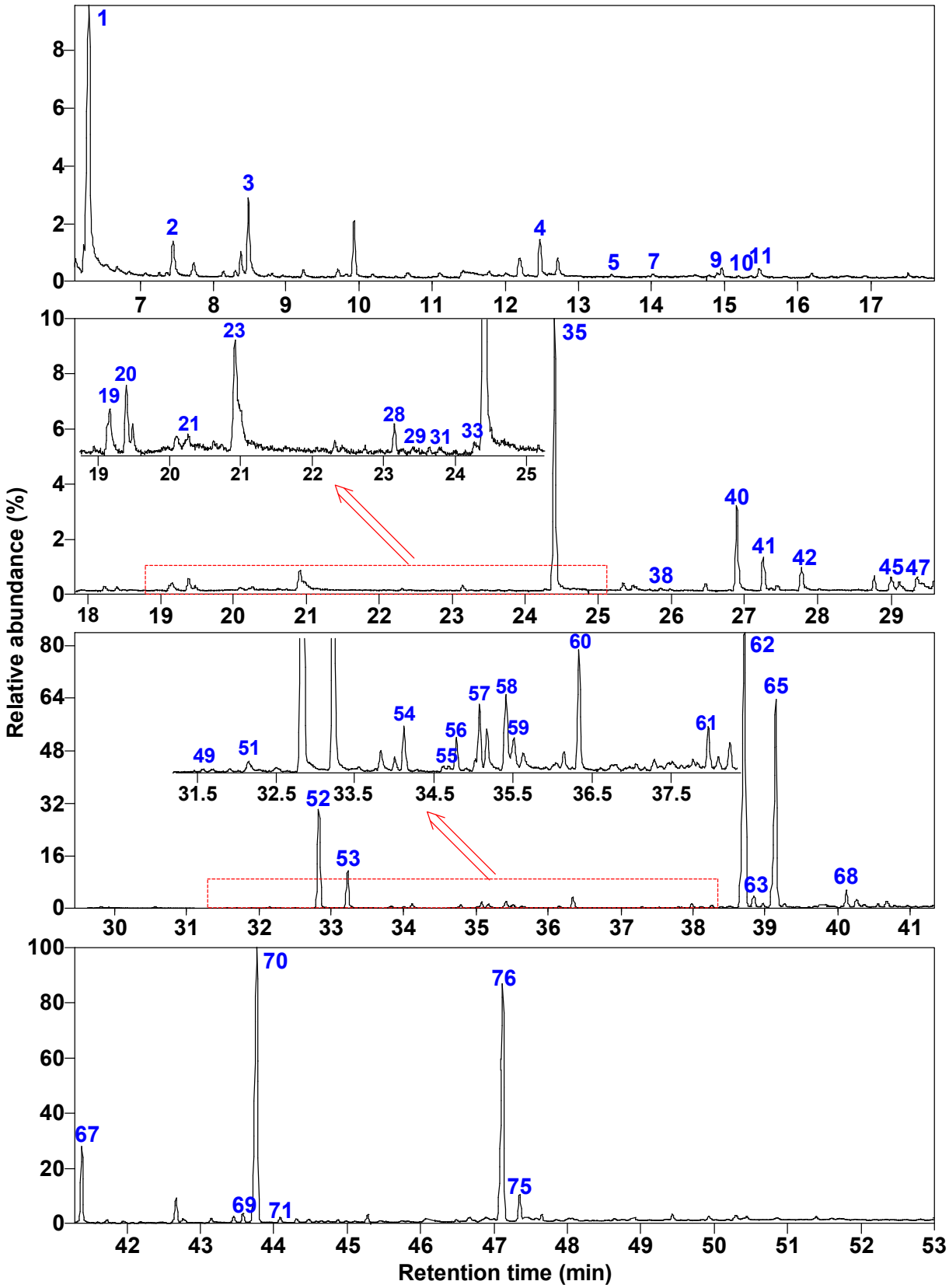


Fig. S1 Total ion chromatogram of MEIEP from RICO of YPC by analysis with GC/MS.

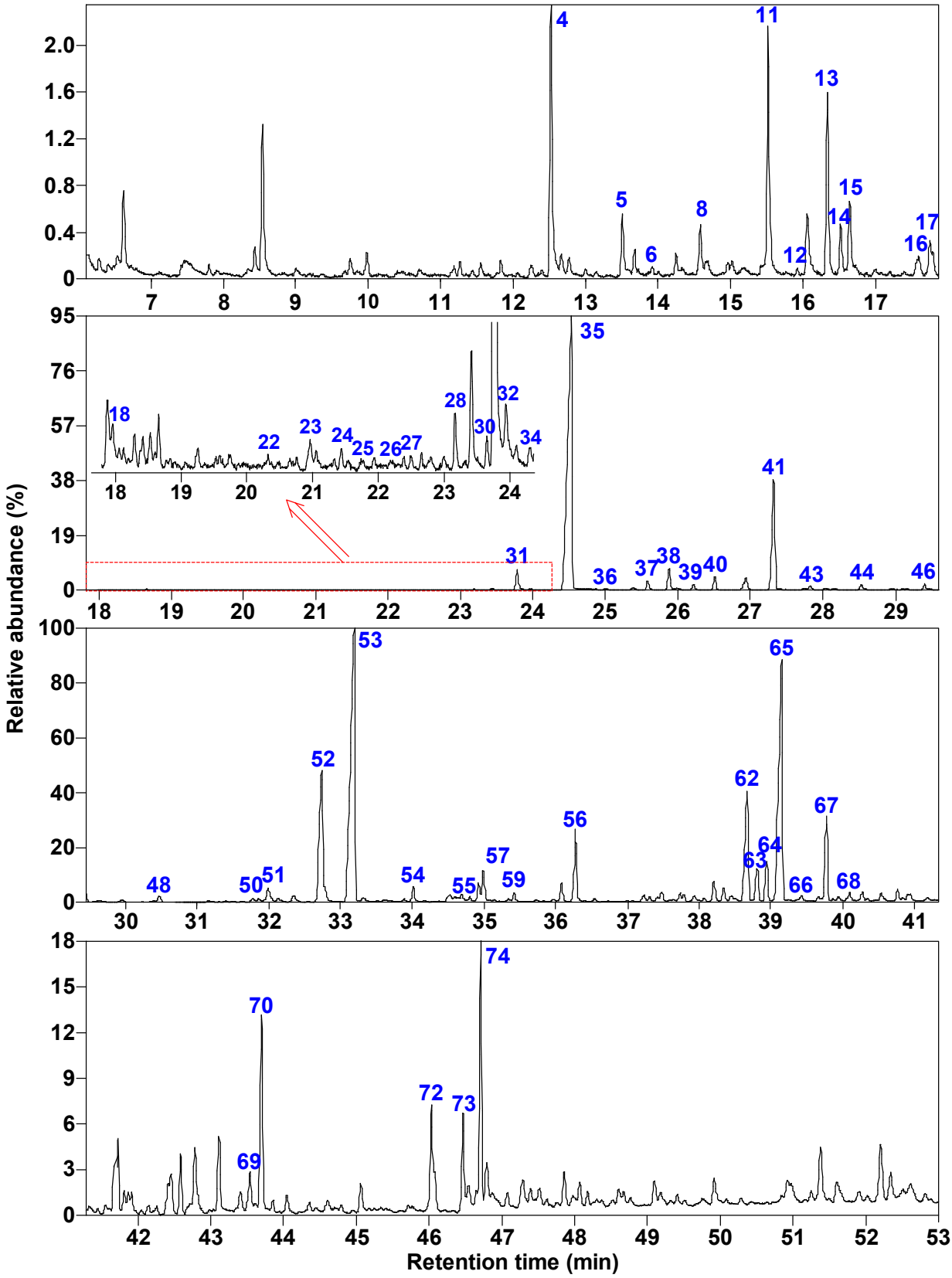


Fig. S2 Total ion chromatogram of MEEP from RICO of YPC by analysis with GC/MS.

Table S1 Relative abundances of CAs from RICO of YPC by analysis with ASAP/TOF-MS

$[M-31]^+/z$	Formula	Corresponding CA	AR in the CA	Isolated into	
				IEP	EP
BCAs				79.77	78.63
105.04176	C_7H_5O	C_6H_5COOH			0.99
119.01268	C_8H_7O	$C_6H_4COOHCH_3$			0.22
163.03994	$C_9H_7O_3$	$C_6H_4(COOH)_2$		2.17	
163.04719	$C_9H_7O_3$	$C_6H_4(COOH)_2$			16.74
177.05532	$C_{10}H_9O_3$	$C_6H_3(COOH)_2CH_3$			8.01
221.04700	$C_{11}H_9O_5$	$C_6H_3(COOH)_3$		10.50	
221.07901	$C_{11}H_9O_5$	$C_6H_3(COOH)_3$			18.31
235.06192	$C_{12}H_{11}O_5$	$C_6H_2(COOH)_3CH_3$			11.01
279.08505	$C_{13}H_{11}O_7$	$C_6H_2(COOH)_4$			18.42
279.08703	$C_{13}H_{11}O_7$	$C_6H_2(COOH)_4$		23.12	
293.06573	$C_{14}H_{13}O_7$	$C_6H(COOH)_4CH_3$		3.57	
293.06714	$C_{14}H_{13}O_7$	$C_6H(COOH)_4CH_3$			3.44
337.06080	$C_{15}H_{13}O_9$	$C_6H(COOH)_5$			1.31
337.07870	$C_{15}H_{13}O_9$	$C_6H(COOH)_5$		22.82	
351.05856	$C_{16}H_{15}O_9$	C_6 $(COOH)_5CH_3$		1.00	
365.05590	$C_{17}H_{17}O_9$	C_6 $(COOH)_5CH_2CH_3$		1.60	
395.06733	$C_{17}H_{15}O_{11}$	$C_6H(COOH)_6$		14.99	
Naphthalenepolycarboxylic acids				2.55	14.33
313.07278	$C_{18}H_{17}O_5$	$C_{10}H_4(COOH)_3(CH_2)_2CH_3$		0.58	
313.02997	$C_{18}H_{17}O_5$	$C_{10}H_4(COOH)_3(CH_2)_2CH_3$			0.15
327.08839	$C_{19}H_{19}O_5$	$C_{10}H_4(COOH)_3(CH_2)_3CH_3$			1.45
353.08996	$C_{16}H_{11}O_5Cl_2$	$C_{10}H_2(COOH)_3CH_3Cl_2$			8.43
371.08206	$C_{20}H_{19}O_7$	$C_{10}H_3(COOH)_4(CH_2)_2CH_3$		0.90	
387.10938	$C_{19}H_{15}O_9$	$C_{10}H_3(COOH)_5$			0.87
413.09099	$C_{23}H_{25}O_7$	$C_{10}H_3(COOH)_4(CH_2)_5CH_3$			1.29
427.10593	$C_{24}H_{27}O_7$	$C_{10}H_3(COOH)_4(CH_2)_6CH_3$			0.25
441.0935	$C_{25}H_{29}O_7$	$C_{10}H_3(COOH)_4(CH_2)_7CH_3$			0.10
445.11598	$C_{21}H_{17}O_{11}$	$C_{10}H_2(COOH)_6$			0.32
457.08681	$C_{24}H_{25}O_9$	$C_{10}H_2(COOH)_5(CH_2)_4CH_3$		0.18	
457.11507	$C_{24}H_{25}O_9$	$C_{10}H_2(COOH)_5(CH_2)_4CH_3$			0.11
471.09806	$C_{25}H_{27}O_9$	$C_{10}H_2(COOH)_5(CH_2)_5CH_3$		0.56	
471.10385	$C_{25}H_{27}O_9$	$C_{10}H_2(COOH)_5(CH_2)_5CH_3$			0.15
487.12781	$C_{24}H_{23}O_{11}$	$C_{10}H(COOH)_6(CH_2)_2CH_3$			0.07
487.12952	$C_{24}H_{23}O_{11}$	$C_{10}H(COOH)_6(CH_2)_2CH_3$		0.06	
503.12265	$C_{23}H_{19}O_{13}$	$C_{10}H(COOH)_7$			0.10
503.12301	$C_{23}H_{19}O_{13}$	$C_{10}H(COOH)_7$		0.10	
515.12297	$C_{26}H_{27}O_{11}$	$C_{10}H(COOH)_6(CH_2)_4CH_3$			0.29
529.1066	$C_{27}H_{29}O_{11}$	$C_{10}H(COOH)_6(CH_2)_5CH_3$		0.11	
529.13577	$C_{27}H_{29}O_{11}$	$C_{10}H(COOH)_6(CH_2)_5CH_3$			0.11

Table S1 Relative abundances of CAs from RICO of YPC by analysis with ASAP/TOF-MS (continued)

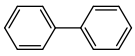
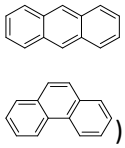
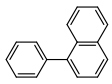
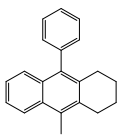
$[M-31]^+/z$	Formula	Corresponding CA	AR in the CA	Isolated into	
				IEP	EP
Naphthalenepolycarboxylic acids				2.55	14.33
543.14089	$C_{28}H_{31}O_{11}$	$C_{10}H(COOH)_6(CH_2)_6CH_3$			0.03
561.12871	$C_{25}H_{21}O_{15}$	$C_{10}(COOH)_8$			0.08
573.12916	$C_{28}H_{29}O_{13}$	$C_{10}(COOH)_7(CH_2)_4CH_3$			0.38
587.14567	$C_{29}H_{31}O_{13}$	$C_{10}(COOH)_7(CH_2)_5CH_3$			0.08
587.77308	$C_{29}H_{31}O_{13}$	$C_{10}(COOH)_7(CH_2)_5CH_3$		0.04	
601.11732	$C_{30}H_{33}O_{13}$	$C_{10}(COOH)_7(CH_2)_6CH_3$		0.01	
Biphenylpolycarboxylic acids				4.71	
325.05992	$C_{19}H_{17}O_5$	$C_{12}H_6(COOH)_3(CH_2CH_3)$		2.31	
383.07065	$C_{21}H_{19}O_7$	$C_{12}H_5(COOH)_4(CH_2CH_3)$		0.56	
413.09171	$C_{21}H_{17}O_9$	$C_{12}H_5(COOH)_5$		1.25	
441.08289	$C_{23}H_{21}O_9$	$C_{12}H_4(COOH)_5(CH_2CH_3)$		0.30	
499.15756	$C_{25}H_{23}O_{11}$	$C_{12}H_3(COOH)_6(CH_2CH_3)$		0.14	
557.16755	$C_{27}H_{25}O_{13}$	$C_{12}H_2(COOH)_7(CH_2CH_3)$		0.14	
Anthracene- and/or phenanthrenepolycarboxylic acids			 ( )		2.91
263.05830	$C_{17}H_{11}O_3$	$C_{14}H_8(COOH)_2$			1.81
321.06534	$C_{19}H_{13}O_5$	$C_{14}H_7(COOH)_3$			1.09
Phenylnaphthalenepolycarboxylic acids				0.96	0.02
563.1304	$C_{30}H_{27}O_{11}$	$C_{16}H_5(COOH)_6(CH_2)_2CH_3$		0.01	
621.14567	$C_{32}H_{29}O_{13}$	$C_{16}H_4(COOH)_7(CH_2)_2CH_3$		0.02	
679.15507	$C_{34}H_{31}O_{15}$	$C_{16}H_3(COOH)_8(CH_2)_2CH_3$			0.01
679.1578	$C_{34}H_{31}O_{15}$	$C_{16}H_3(COOH)_8(CH_2)_2CH_3$		0.13	
737.16166	$C_{36}H_{33}O_{17}$	$C_{16}H_2(COOH)_9(CH_2)_2CH_3$			trace
737.16592	$C_{36}H_{33}O_{17}$	$C_{16}H_2(COOH)_9(CH_2)_2CH_3$		0.51	
765.17183	$C_{38}H_{37}O_{17}$	$C_{16}H_2(COOH)_9(CH_2)_4CH_3$			trace
779.18804	$C_{39}H_{39}O_{17}$	$C_{16}H_2(COOH)_9(CH_2)_5CH_3$			trace
795.17216	$C_{38}H_{35}O_{19}$	$C_{16}H(COOH)_{10}(CH_2)_2CH_3$		0.25	
853.17788	$C_{40}H_{37}O_{21}$	$C_{16}(COOH)_{11}(CH_2)_2CH_3$		0.04	
Methyl(phenyl)tetrahydroanthracenecarboxylic acids				0.06	
647.13719	$C_{34}H_{31}O_{13}$	$C_{21}H_{13}(COOH)_7$		0.02	
705.14392	$C_{36}H_{33}O_{15}$	$C_{21}H_{12}(COOH)_8$		0.02	
763.1505	$C_{38}H_{35}O_{17}$	$C_{21}H_{11}(COOH)_9$		0.01	
821.15782	$C_{40}H_{37}O_{19}$	$C_{21}H_{10}(COOH)_{10}$		trace	

Table S1 Relative abundances of CAs from RICO of YPC by analysis with ASAP/TOF-MS (continued)

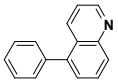
$[M-31]^+/z$	Formula	Corresponding CA	AR in the CA	Isolated into	
				IEP	EP
Isobenzofuran-1,3-dionepolycarboxylic acids				6.85	
175.00456	$C_9H_3O_4$	$C_8H_3O_3COOH$		0.83	
233.01088	$C_{11}H_5O_6$	$C_8H_2O_3(COOH)_2$		3.90	
291.01863	$C_{13}H_7O_8$	$C_8HO_3(COOH)_3$		1.60	
349.02417	$C_{15}H_9O_{10}$	$C_8O_3(COOH)_4$		0.51	
Phenylquinolinepolycarboxylic acids				0.06	
578.15629	$C_{30}H_{28}O_{11}N$	$C_{15}H_4(COOH)_6(CH_2)_3CH_3N$		0.01	
636.16175	$C_{32}H_{30}O_{13}N$	$C_{15}H_3(COOH)_7(CH_2)_3CH_3N$		0.01	
694.168	$C_{34}H_{32}O_{15}N$	$C_{15}H_2(COOH)_8(CH_2)_3CH_3N$		0.02	
752.17776	$C_{36}H_{34}O_{17}N$	$C_{15}H(COOH)_9(CH_2)_3CH_3N$		0.01	
810.18387	$C_{38}H_{36}O_{19}N$	$C_{15}(COOH)_{10}(CH_2)_3CH_3N$		trace	
2-Methylisoindoline-1,3-dionepolycarboxylic acids				5.04	4.11
246.04229	$C_{12}H_8O_5N$	$C_9H_5O_2(COOH)_2N$		1.83	
304.04865	$C_{14}H_{10}O_7N$	$C_9H_4O_2(COOH)_3N$		1.95	
362.05484	$C_{16}H_{12}O_9N$	$C_9H_3O_2(COOH)_4N$		1.26	
246.04135	$C_{12}H_8O_5N$	$C_9H_5O_2(COOH)_2N$			3.82
304.0495	$C_{14}H_{10}O_7N$	$C_9H_4O_2(COOH)_3N$			0.28

Table S2 Relative abundances of CAs from RICO of YPC by analysis with DARTIS/TOF-MS

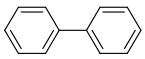
[M+H]+ and/or M+/z	Formula	Corresponding CA	AR in the CA	Isolated into	
				IEP	EP
Pyridinepolycarboxylic acids				13.55	10.81
196.06080	$C_9H_{10}O_4N$	$C_5H_3(COOH)_2N$		2.44	
196.06550	$C_9H_{10}O_4N$	$C_5H_3(COOH)_2N$			1.27
210.07466	$C_{10}H_{12}O_4N$	$C_5H_2(COOH)_2CH_3N$			0.99
210.07522	$C_{10}H_{12}O_4N$	$C_5H_2(COOH)_2CH_3N$		1.32	
224.11858	$C_{11}H_{14}O_4N$	$C_5H_2(COOH)_2CH_2CH_3N$			0.56
254.06546	$C_{11}H_{12}O_6N$	$C_5H_2(COOH)_3N$			1.18
254.06818	$C_{11}H_{12}O_6N$	$C_5H_2(COOH)_3N$		1.27	
268.07660	$C_{12}H_{14}O_6N$	$C_5H(COOH)_3CH_3N$			0.73
268.07923	$C_{12}H_{14}O_6N$	$C_5H(COOH)_3CH_3N$		1.32	
312.16017	$C_{13}H_{14}O_8N$	$C_5H(COOH)_4N$		1.37	
312.17156	$C_{13}H_{14}O_8N$	$C_5H(COOH)_4N$			1.32
326.12433	$C_{14}H_{16}O_8N$	$C_5(COOH)_4CH_3N$			1.52
326.12774	$C_{14}H_{16}O_8N$	$C_5(COOH)_4CH_3N$		1.52	
340.14096	$C_{15}H_{18}O_8N$	$C_5(COOH)_4CH_2CH_3N$		1.37	
340.14909	$C_{15}H_{18}O_8N$	$C_5(COOH)_4CH_2CH_3N$			0.75
354.15916	$C_{16}H_{20}O_8N$	$C_5(COOH)_4(CH_2)_2CH_3N$			1.06
354.16410	$C_{16}H_{20}O_8N$	$C_5(COOH)_4(CH_2)_2CH_3N$		1.78	
368.14957	$C_{17}H_{22}O_8N$	$C_5(COOH)_4(CH_2)_3CH_3N$			0.55
370.15073	$C_{15}H_{16}O_{10}N$	$C_5(COOH)_5N$		1.16	
370.15890	$C_{15}H_{16}O_{10}N$	$C_5(COOH)_5N$			0.86
Biphenylpolycarboxylic acids				10.44	14.33
342.12018	$C_{19}H_{18}O_6$	$C_{12}H_6(COOH)_3CH_3$			0.93
356.13333	$C_{20}H_{20}O_6$	$C_{12}H_6(COOH)_3CH_2CH_3$		2.43	
356.13578	$C_{20}H_{20}O_6$	$C_{12}H_6(COOH)_3CH_2CH_3$			3.90
384.15956	$C_{22}H_{24}O_6$	$C_{12}H_6(COOH)_3(CH_2)_3CH_3$			2.04
384.1649	$C_{22}H_{24}O_6$	$C_{12}H_6(COOH)_3(CH_2)_3CH_3$		1.70	
398.14911	$C_{23}H_{26}O_6$	$C_{12}H_6(COOH)_3(CH_2)_4CH_3$		1.16	
398.16482	$C_{23}H_{26}O_6$	$C_{12}H_6(COOH)_3(CH_2)_4CH_3$			1.41
412.18653	$C_{24}H_{28}O_6$	$C_{12}H_6(COOH)_3(CH_2)_5CH_3$		1.25	
426.17486	$C_{25}H_{30}O_6$	$C_{12}H_6(COOH)_3(CH_2)_6CH_3$		1.38	
426.18031	$C_{25}H_{30}O_6$	$C_{12}H_6(COOH)_3(CH_2)_6CH_3$			2.33
440.13524	$C_{26}H_{32}O_6$	$C_{12}H_6(COOH)_3(CH_2)_7CH_3$		1.48	
440.13635	$C_{26}H_{32}O_6$	$C_{12}H_6(COOH)_3(CH_2)_7CH_3$			2.17
454.15447	$C_{27}H_{34}O_6$	$C_{12}H_6(COOH)_3(CH_2)_8CH_3$			1.56
454.15453	$C_{27}H_{34}O_6$	$C_{12}H_6(COOH)_3(CH_2)_8CH_3$		1.04	

Table S2 Relative abundances of CAs from RICO of YPC by analysis with DARTIS/TOF-MS (continued)

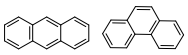
[M+H]+ and/or M+/z	Formula	Corresponding CA	AR in the CA	Isolated into	
				IEP	EP
Anthracene- and/or phenanthrenecarboxylic acids				46.40	40.35
M^+/z					
352.17404	$C_{20}H_{16}O_6$	$C_{14}H_7(COOH)_3$			2.04
352.17497	$C_{20}H_{16}O_6$	$C_{14}H_7(COOH)_3$		1.73	
366.18341	$C_{21}H_{18}O_6$	$C_{14}H_6(COOH)_3CH_3$		1.55	
366.19455	$C_{21}H_{18}O_6$	$C_{14}H_6(COOH)_3CH_3$			0.83
380.16986	$C_{22}H_{20}O_6$	$C_{14}H_6(COOH)_3CH_2CH_3$			1.96
380.17025	$C_{22}H_{20}O_6$	$C_{14}H_6(COOH)_3CH_2CH_3$		6.44	
394.17996	$C_{23}H_{22}O_6$	$C_{14}H_6(COOH)_3(CH_2)_2CH_3$		2.26	
394.18357	$C_{23}H_{22}O_6$	$C_{14}H_6(COOH)_3(CH_2)_2CH_3$			1.38
408.16566	$C_{24}H_{24}O_6$	$C_{14}H_6(COOH)_3(CH_2)_3CH_3$			2.80
408.17105	$C_{24}H_{24}O_6$	$C_{14}H_6(COOH)_3(CH_2)_3CH_3$		2.39	
410.18005	$C_{22}H_{18}O_8$	$C_{14}H_6(COOH)_4$			11.34
410.18065	$C_{22}H_{18}O_8$	$C_{14}H_6(COOH)_4$		11.72	
424.15083	$C_{23}H_{20}O_8$	$C_{14}H_5(COOH)_4CH_3$		1.68	
424.16609	$C_{23}H_{20}O_8$	$C_{14}H_5(COOH)_4CH_3$			1.16
452.18820	$C_{25}H_{24}O_8$	$C_{14}H_5(COOH)_4(CH_2)_2CH_3$		0.99	
452.19789	$C_{25}H_{24}O_8$	$C_{14}H_5(COOH)_4(CH_2)_2CH_3$			0.77
466.16997	$C_{26}H_{26}O_8$	$C_{14}H_5(COOH)_4(CH_2)_3CH_3$			0.73
468.17933	$C_{24}H_{20}O_{10}$	$C_{14}H_5(COOH)_5$		3.04	
468.18174	$C_{24}H_{20}O_{10}$	$C_{14}H_5(COOH)_5$			2.64
480.17804	$C_{27}H_{28}O_8$	$C_{14}H_5(COOH)_4(CH_2)_4CH_3$			0.58
482.17119	$C_{25}H_{22}O_{10}$	$C_{14}H_4(COOH)_5CH_3$			0.65
494.22660	$C_{28}H_{30}O_8$	$C_{14}H_5(COOH)_4(CH_2)_5CH_3$			0.60
$[M+H]^+$/z					
295.16392	$C_{18}H_{15}O_4$	$C_{14}H_8(COOH)_2$			0.58
295.16447	$C_{18}H_{15}O_4$	$C_{14}H_8(COOH)_2$		1.42	
309.18386	$C_{19}H_{17}O_4$	$C_{14}H_7(COOH)_2CH_3$			0.52
353.16810	$C_{20}H_{17}O_6$	$C_{14}H_7(COOH)_3$		4.24	
353.16985	$C_{20}H_{17}O_6$	$C_{14}H_7(COOH)_3$			3.26
367.19103	$C_{21}H_{19}O_6$	$C_{14}H_6(COOH)_3CH_3$		1.32	
367.19200	$C_{21}H_{19}O_6$	$C_{14}H_6(COOH)_3CH_3$			0.72
381.17468	$C_{22}H_{21}O_6$	$C_{14}H_6(COOH)_3CH_2CH_3$		1.68	
381.17533	$C_{22}H_{21}O_6$	$C_{14}H_6(COOH)_3CH_2CH_3$			0.72
411.17801	$C_{22}H_{19}O_8$	$C_{14}H_6(COOH)_4$		4.60	
411.18163	$C_{22}H_{19}O_8$	$C_{14}H_6(COOH)_4$			5.32
425.18603	$C_{23}H_{21}O_8$	$C_{14}H_5(COOH)_4CH_3$			0.65
469.18005	$C_{24}H_{21}O_{10}$	$C_{14}H_5(COOH)_5$			1.07
469.18326	$C_{24}H_{21}O_{10}$	$C_{14}H_5(COOH)_5$		1.33	

Table S2 Relative abundances of CAs from RICO of YPC by analysis with DARTIS/TOF-MS (continued)

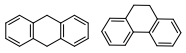
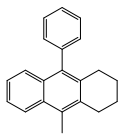
[M+H]+ and/or M+/z	Formula	Corresponding CA	AR in the CA	Isolated into	
				IEP	EP
Dihydroanthracene- and/or dihydrophenanthrenecarboxylic acids				2.16	7.12
M^+/z					
484.16837	$C_{25}H_{24}O_{10}$	$C_{14}H_6(COOH)_5CH_3$		1.15	
484.17211	$C_{25}H_{24}O_{10}$	$C_{14}H_6(COOH)_5CH_3$			1.16
498.15132	$C_{26}H_{26}O_{10}$	$C_{14}H_6(COOH)_5CH_2CH_3$			0.66
504.24794	$C_{24}H_{21}O_{10}Cl$	$C_{14}H_6(COOH)_5Cl$			0.57
512.19282	$C_{27}H_{28}O_{10}$	$C_{14}H_6(COOH)_5(CH_2)_2CH_3$			0.84
518.25183	$C_{25}H_{23}O_{10}Cl$	$C_{14}H_5(COOH)_5CH_3Cl$		1.01	
518.25458	$C_{25}H_{23}O_{10}Cl$	$C_{14}H_5(COOH)_5CH_3Cl$			0.73
532.25877	$C_{26}H_{25}O_{10}Cl$	$C_{14}H_5(COOH)_5CH_2CH_3Cl$			0.56
546.29769	$C_{27}H_{27}O_{10}Cl$	$C_{14}H_5(COOH)_5(CH_2)_2CH_3Cl$			0.81
$[M+H]^+$/z					
581.15829	$C_{27}H_{28}O_{10}Cl_2$	$C_{14}H_4(COOH)_5(CH_2)_2CH_3Cl_2$			0.89
639.16778	$C_{29}H_{30}O_{12}Cl_2$	$C_{14}H_3(COOH)_6(CH_2)_2CH_3Cl_2$			0.89
Methyl(phenyl)tetrahydroanthracenecarboxylic acids					1.92
721.24021	$C_{38}H_{41}O_{14}$	$C_{21}H_{12}(COOH)_7(CH_2)_2CH_3$			1.27
779.24836	$C_{40}H_{43}O_{16}$	$C_{21}H_{11}(COOH)_8(CH_2)_2CH_3$			0.65

Table S3 Relative abundances of other species from RICO of YPC by analysis with DARTIS/TOF-MS

$[M+H]^+$ and/or M^+/z	Formula	Isolated into	
		IEP	EP
Quinolines		22.32	19.97
130.06565	C_9H_8N	7.23	
130.06669	C_9H_8N		7.58
144.08045	$C_{10}H_{10}N$	7.90	
144.08151	$C_{10}H_{10}N$		6.34
158.09696	$C_{11}H_{12}N$		4.70
158.09743	$C_{11}H_{12}N$	5.89	
172.11215	$C_{12}H_{14}N$	1.30	
172.11269	$C_{12}H_{14}N$		0.80
186.11731	$C_{13}H_{16}N$		0.55
2-Methylthiophenes		5.14	5.49
98.09736	C_5H_6S	5.14	
98.09740	C_5H_6S		5.49