

New Capillary Gas Chromatography Column Optimized for the Analysis of Semivolatiles

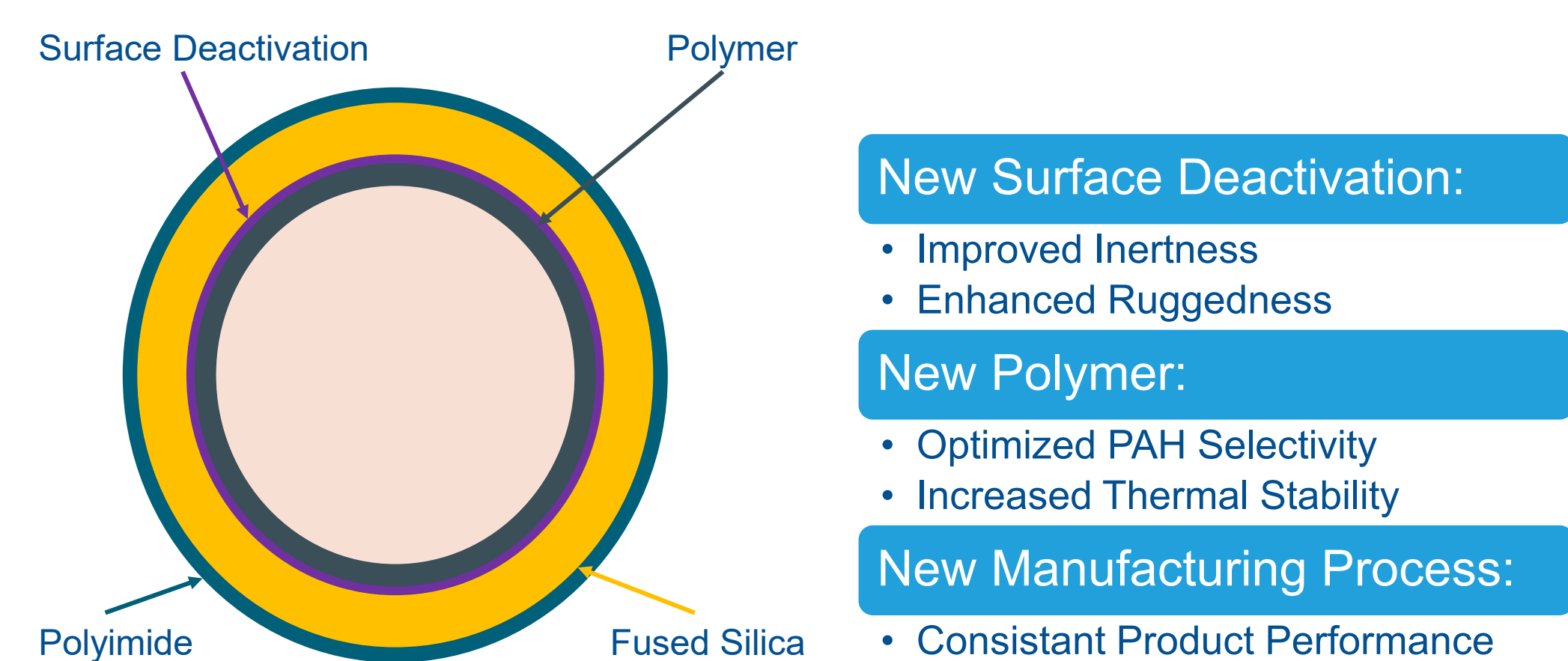
Jessi Collier, Jana Hepner, Kristi Sellers, Whitney Dudek-Salisbury, Scott Adams, Jaap de Zeeuw, & Chris English.
Restek Corporation, 110 Benner Circle, Bellefonte, PA 16823, United States

Outline

The US Environmental Protection Agency developed a method for the analysis of Semivolatiles using GC-MS/MS. This allows the determination of on-column amounts of target compounds to be detected at orders of magnitude lower concentrations than conventional single quadrupole mass spectrometers. New column requirements include enhanced robustness, thermal stability, improved PAH selectivity and extended lifetime following highly contaminated extracts.

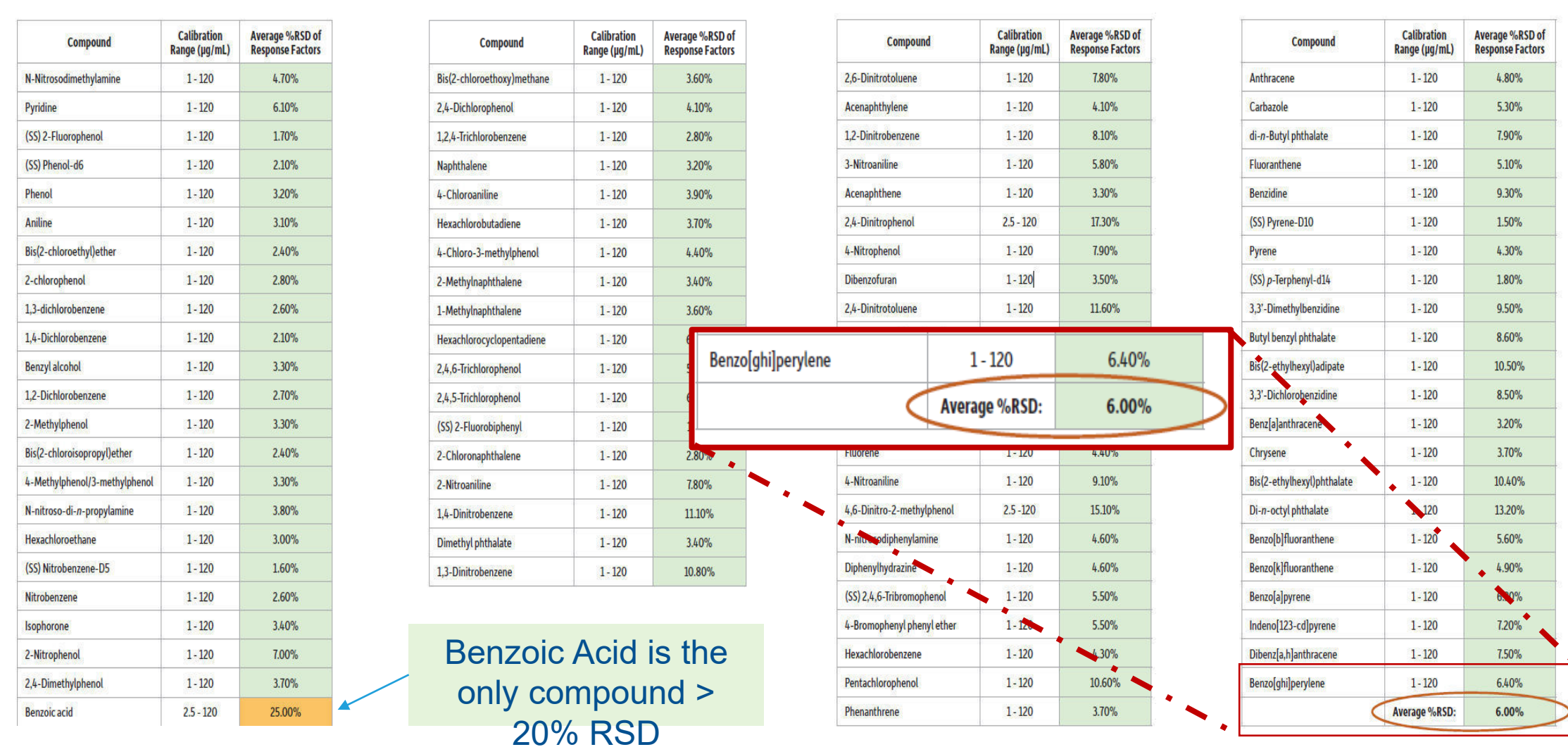
This poster will show specific weaknesses of a general purpose 5-type columns for the analysis of environmental samples and the advantages of this new column for use with tandem mass spectrometers.

Enhanced SVOC Performance



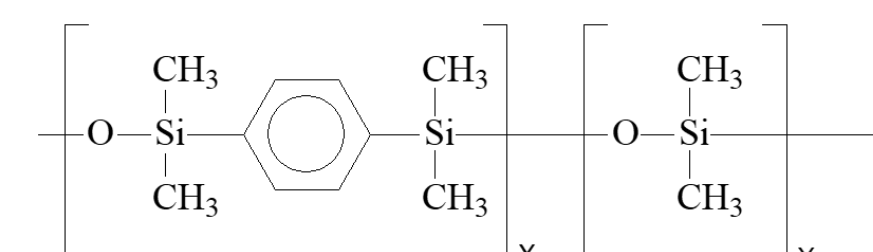
Inertness = Linear Calibrations

Average %RSDs for 6 Rxi-SVOCms columns (16623) calibrated from 1 ng/μL to 120 ng/μL



New Polymer

The polymer used for the Rxi-SVOCms has a silphenylene backbone, like the Rxi-5SII MS



Application specific formulation changes optimized the PAH separations and improved thermal stability

New maximum temperature of 340C

Designed to be a drop-in replacement for the DB-5ms and DB-5ms UI

Similar phase chemistries

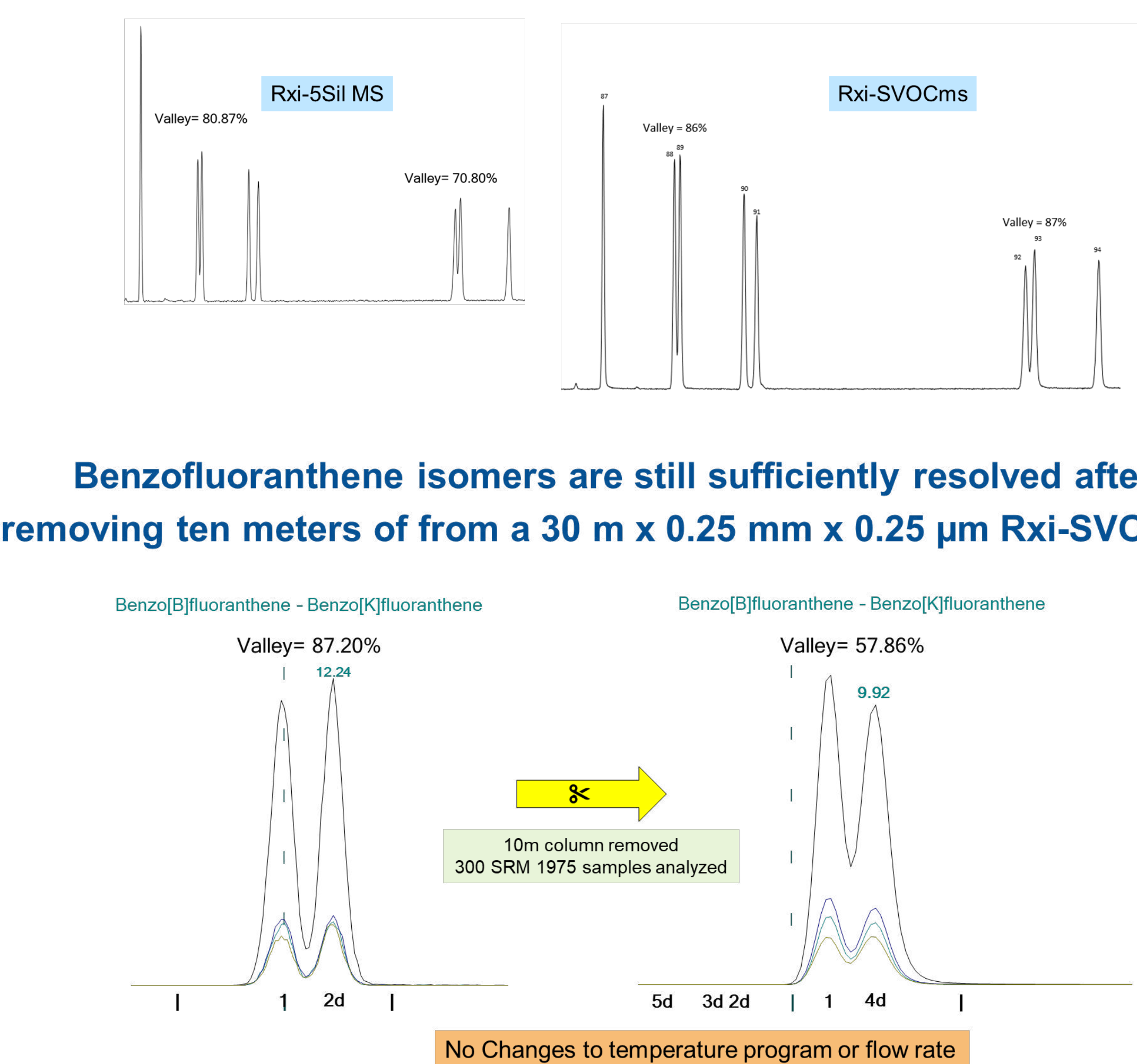
DB-UI 8270D for Semivolatiles
ZB-5ms Semivolatiles
SLB-5ms Semivolatiles

Other Silphenylene type phases

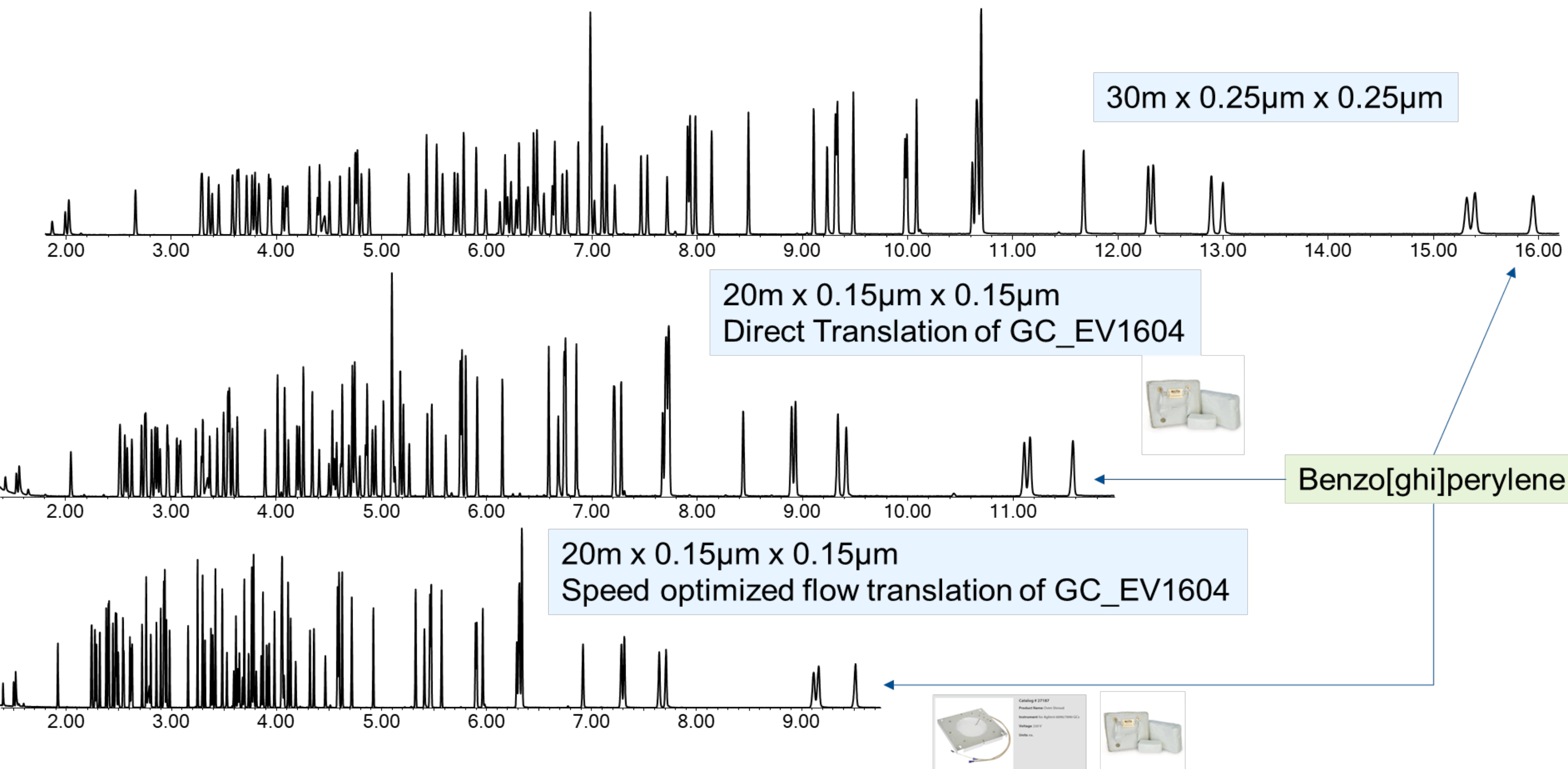
Rxi-5SII MS
DB-5ms
DB-5ms UI
VF-ms
BFX-5
ZB-5ms
CP-SII 8 CB LBMS
Optima-5ms
PE-5ms
SLB-5ms

Optimized PAH Selectivity

Improved Benzo[fluoranthene] and Indeno[123-cd]pyrene – Dibenz[a]anthracene Separations on the Rxi-SVOCms



Fast GC Method Translation Preserves Elution Profiles

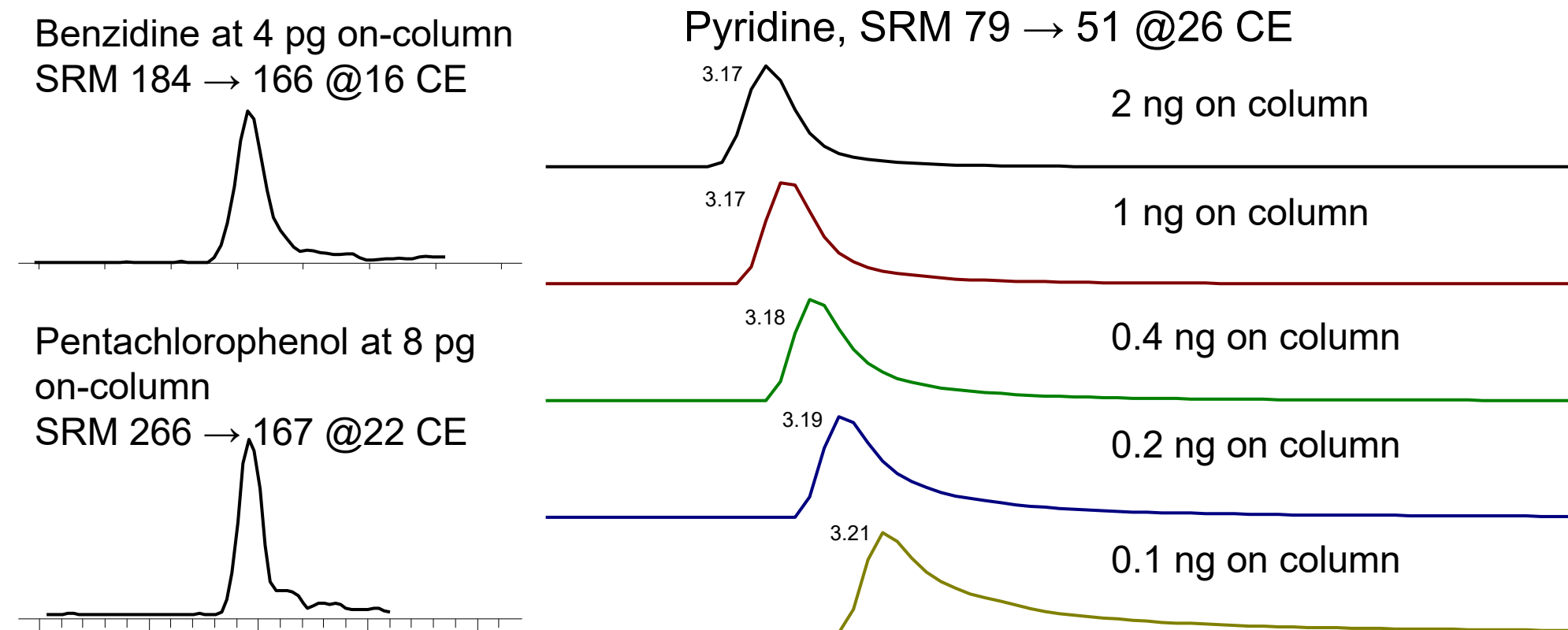
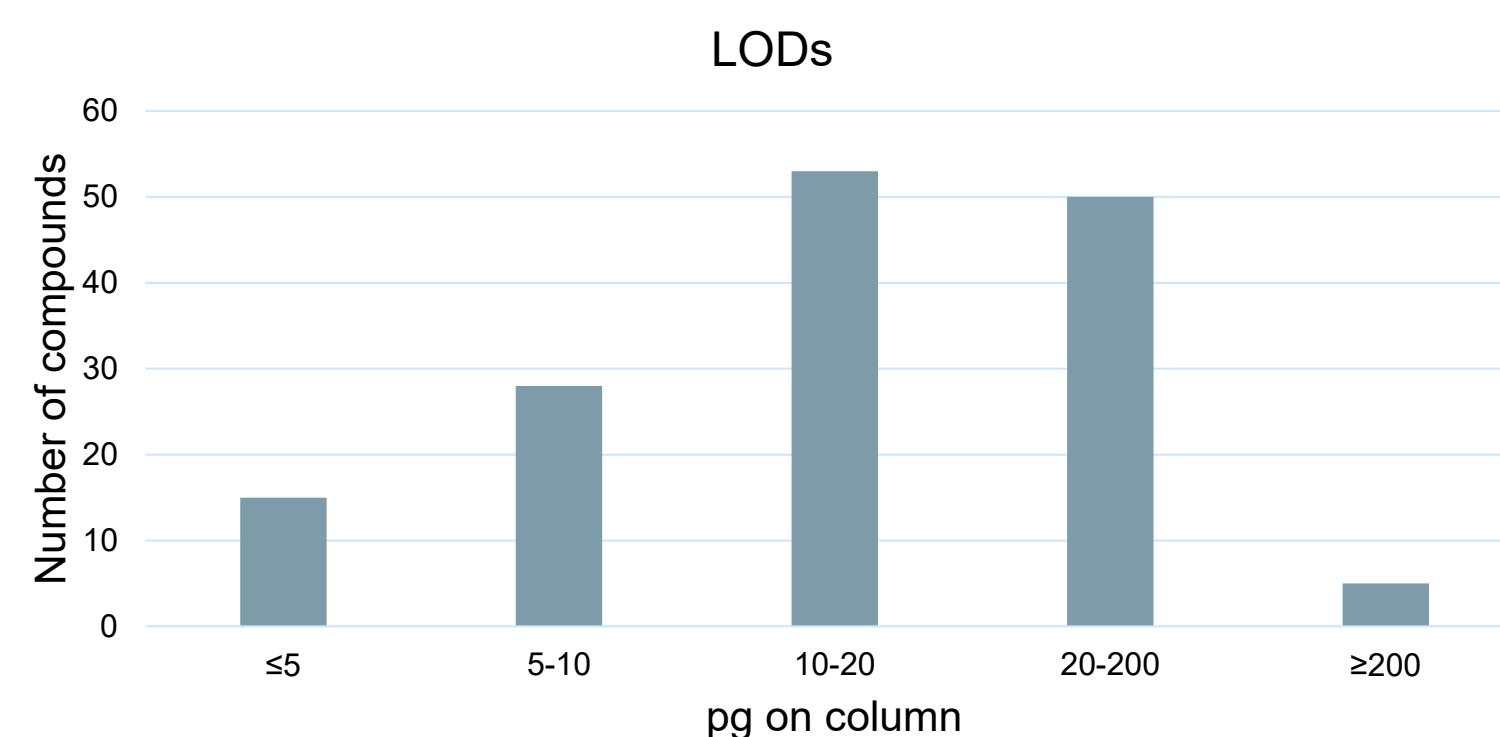


EPA 8270E GC-MSMS analysis with 150+ compounds

Exceptionally low LODs – more than 60% of compounds were below 20 pg on column.

Good performance at the lowest levels for benzidine and pentachlorophenol.

Compounds such as pyridine or acrylamide showed retention time shift



Name	Quant Ion							Qual Ions							Name	Quant Ion							Qual Ions							Name	Quant Ion							Qual Ions							
	RT	Prc	Prd	CE	Prc	Prd	CE	Prc	Prd	CE	Prc	Prd	CE	RT		Prc	Prd	CE	Prc	Prd	CE	Prc	Prd	CE	RT	Prc	Prd	CE	Prc		Prd	CE	RT	Prc	Prd	CE	Prc	Prd	CE						
1,4-Dioxane	2.79	88	28	14	58	28	6	88	57	8	1,4-Phenylenediamine	9.77	108	80	20	83	12	108	81	10	Hexachlorobenzene	14.37	288	216	26	249	214	12	284	249	14														
N-Nitrosodimethylamine	3.08	74	42	16	74	43	12	74	44	6	4-Chloro-3-methylphenol	10.04	142	77	26	107	77	12	142	107	12	Dimethoate	14.51	125	47	14	83	63	8	125	79	8													
Pyridine	3.20	79	51	26	52	26	18	79	52	12	Isosafrole I	10.16	162	104	12	131	103	8	162	131	12	Atrazine	14.70	215	58	10	200	122	8	215	200	8													
Ethyl methacrylate	3.62	99	43	14	69	41	6	99	53	12	2-Methylnaphthalene	10.28	141	89	30	115	89	16	141	115	16	Pentachlorophenol	14.77	270	169	22	228	165	14	266	167	12													
2-Picolone	3.96	93	65	18	66	39	18	93	66	12	1-Methylnaphthalene	10.46	141	89	30	115	89	14	141	115	16	4-Aminobiphenyl	14.79	169	141	22	168	141	8	168	167	10													
N-Nitrosomethylethylamine	4.12	88	42	16	88	43	8	88	71	6	Hexachloropentadiene	10.59	272	237	12	237	119	20	237	143	22	Pentachloronitrobenzene	14.81	295	237	14	237	143	20	295	265	8													
Methyl methanesulfonate	4.52	80	48	28	65	48	18	80	65	8	1,2,4,5-Tetrachlorobenzene	10.61	216	108	36	179	143	8	216	181	14	Propylamine	15.00	254	191	16	173	145	14	254	226	10													
2-Fluorophenol	4.73	112	63	22	92	63	14	112	92	6	Isosafrole II	10.73	162	104	12	131	103	10	162	131	12	Octadecane	15.10	99	41	14	85	43	6	99	57	6													
Acrylamide	4.80	71	44	22	55	27	6	71	55	6	2,3-Dichloroaniline	10.83	163	90	18	161	90	16	161	99	18	Phenanthrene-d10	15.10	188	160	20	184	154	32	184	156	22													
N-Nitrosodiethylamine	5.05	102	44	10	102	56	12	102	85	6	2,4,6-Trichlorophenol	10.83	196	97	24	132	97	10	160	97	16	Phenanthrene	15.16	178	151	32	176	150	20	178	152	20													
Ethyl methanesulfonate	5.51	109	45	10	79	48	34	109	79	6	2,4,5-Trichlorophenol	10.88	196	97	24	132	97	10	196	132	12	Dinoseb	15.22	240	117	24	163	116	14	240	211	8													
Benzaldehyde	6.01	105	51	26	77	51	14	105	77	10	2-Fluorobiphenyl	10.99	172	151	22	172	170	22	172	171	12	Disulfoton	15.22	97	65	16	88	60	6	97	79	12													
Phenol	6.13	94	39	30	94	65	16	94	66	10	Isosafrole	11.16	162	77	31	131	103	10	162	127	16	Anthrane	15.26	178	151	32	177	151	18	178	152	18													
Phenol-d6	6.14	99	69	18	71	42	16	99	71	8	2-Chloronaphthalene	11.20	162	77	31	127	77	16	162	127	16	Carbazole	15.60	167	139	24	166	140	14	167	166	12													
Aniline	6.17	93	65	20	66	39	18	93	66	10	Biphenyl	11.20	153	126	32	154	115	24	154	152	22	Methyl Parathion	15.95	263	79	24	125	47	12	263	109	10													
Pentachloroethane	6.26	167	95	32	117	82	30	167	132	14	1-Chloronaphthalene	11.25	162	77	31	127	77	16	162	127	16	n-Butyl phthalate	16.41	149	65	20	149	93	14	149	121	12													
bis-(2-Chloroethyl)ether	6.28	93	27	22	63	27	10	93	63	6	o-Nitroaniline	11.41	138	65	22	108	80	8	138	92	12	4-Nitroquinoline-N-oxide	16.69	190	77	20	101	75	10	190	160	8													
2-Chlorophenol	6.35	128	63	24	64	38	12	128	64	14	Diphenyl ether	11.42	170	141	16	141	115	14	170	142	10	Ethyl Parathion	16.73	291	81	26	109	81	10	291	109	10													
Decane	6.49	85	41	12	71	43	6	85	43	6	1,4-Naphthoquinone	11.56	158	102	14	102	76	12	158	130	8	Methapyrilene	16.90	190	97	14	97	53	16	190	157	8													
1,3-Dichlorobenzene	6.61	146	75	24	111	75	12	146	111	12	1,2-Dinitrobenzene	11.70	168	75	20	122	75	12	168	122	8	Isodrin	17.19	261	191	28	193	123	28	261	226	16													
1,4-Dichlorobenzene-d4	6.71	150	76	38	150	78	26	150	115	14	1,3-Dinitrobenzene	11.83	168	75	22	76	50	10	168	122	8	Fluoranthene	17.47	202	152	30	200	174	22	202	176	26													
1,4-Dichlorobenzene	6.74	146	75	24	111	75	12	146	111	14	Diphenyl phthalate	11.83	163	77	20	163	92	24	163	133	8	Benzidine	17.80	184	130	26	184	156	18	184	166	16													
Benzyl alcohol	6.94	108	77	22	79	51	20	108	79	12	1,6-Dinitrotoluene	11.91	165	63	20	148	90	10	165	148	8	Pyrene-d10	17.84	212	208	36	212	210	20																
1,2-Dichlorobenzene	6.98	146	111	12	111	50	36	111	75	10	Acenaphthylene	11.98	152	76	36	152	102	26	152	126	24	Pyrene	17.88	200	149	34	200	150	26	200	174	24													
Indene	7.12	116	89	28	115	63	26	115	89	16	1,4-Dinitrobenzene	11.99	168	51	14	76	63	6	168	63	26	p-Terphenyl-d14	18.30	244	226	18	244	240	22	244	242	14													
2-Methylphenol	7.14	108	77	24	79	51	20	108	80	8	3-Nitroaniline	12.21	138	65	20	92	65	8	138	92	12	Aramite 1	18.39	319	123	10	175	107	14	319	185	6													
2,2'-oxybis(1-chloropropane)	7.20	121	45	6	77	51	12	121	77	8	Acenaphthene-d10	12.24	164	160	32	162	160	18	164	162	14	Aramite 2	18.49	319	107	36	185	63	12	319	185	6													
N-Nitrosopyrrolidine	7.34	100	43	8	100	55	6	100	68	8	Acenaphthene	12.32	153	77	38	153	126	36	154	127	34	p-Dimethylaminoazobenzene	18.57	225	120	10	120	77	16	225	148	6													
Acetophenone	7.37	105	51	26	77	51	14	105	77	12	2,4-Dinitrophenol	12.41	184	107	10	154	79	12	184	154	6	Chlorobenzilate	18.71	251	111	30	139	111	12	251	139	12													
3- and 4-Methylphenol	7.41	107	51	26	70	43	6	107	77	12	4-Nitrophenol	12.57	139	81	14	109	81	8	139	109	6	Famfur	19.17	218	109	14	125	47	14	218	79	12													
N-Nitrosomorpholine	7.42	116	56	10	86	56	6	116	86	6	Pentachlorobenzene	12.60	250	142	38	215	179	10	250	215	16	3,3'-Dimethylbenzidine	19.21	212	180	22	211	195	16	212	196	8													
o-Toluidine	7.44	107	77	26	106	77	16	106	79	8	2,4-Dinitrotoluene	12.66	165	63	22	89	63	12	165	119	6	Kepon	19.24	272	127	13	237	119	24	272	143	22													
Hexachloroethane	7.56	201	131	30	117	82	24	201	166	12	Dibenzofuran	12.66	168	139	22	139	63	30	139	89	18	Benzy] butyl phthalate	19.31	206	149	8	149	65	20	206	121	10													
Nitrobenzene-d5	7.63	128	54	28	82	54	12	128	82	12	1-Naphthylamine	12.81	143	115	22	115	89	16	143	116	10	Bis(2-ethylhexyl) adipate	19.55	129	55	14	111	83	6	129	83	8													
Nitrobenzene	7.68	123	51	30	77	51	12	123	77	10	2,3,5,6-Tetrachlorophenol	12.83	234	133	26	232	131	26	232	168	12	2-Acetylaminofluorene	19.69	223	180	26	181	152	34	223	181	10													
N-Nitrosopiperidine	7.94	114	41	10	114	84	6	114	97	6	2,3,4,6-Tetrachlorophenol	12.91	234	131	24	232	133	26	232	168	12	Benz[a]anthracene	20.23	228	202	24	226	199	36	226	200	34													
Isophorone	8.12	138	82	8	82	39	12	54	6	2-Naphthylamine	12.97	143	115	24	115	89	16	143	116	10	Chrysene-d12	20.23	240	121	22	240	236	30	240	238	14														
2-Nitrophenol	8.25	139	81	12	109	81	8	139	109	6	Diethyl Phthalate	13.21	177	149	8	149	65	20	149	93	12	3,3'-Dichlorobenzidine	20.25	252	154	26	252	181	24	252	182	10													
4,4-Dimethylphenol	8.36	122	77	26	107	77	14	122	107</																																				