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Combined LC/MS and GC/MS Approach for Analysis of Extractables and Leachables in Complex Matrices Using High Resolution Mass Spectrometry

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Introduction

A challenge of extractable and leachable applications is that extracts from polymeric materials may contain compounds of a wide diversity (based on volatility, molecular weight, and chemical classes). Therefore, both LC/MS and GC/MS techniques are generally used for comprehensive coverage. The study's goal was to develop analytical methods and workflows for acquisition and efficient processing of the complex E&L data with a focus on a non-targeted approach.

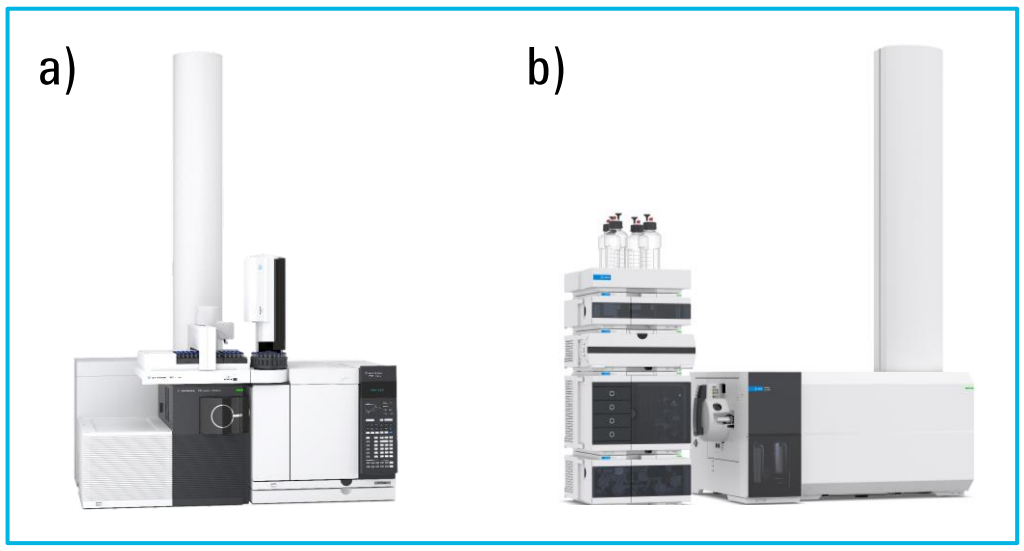

Figure 1.a) 7250 GC/Q-TOF and b) Revident LC/Q-TOF

Experimental

Rubber syringe gaskets were extracted using tetrahydrofuran (THF) solvent at room temperature for six months. Catheters from four different brands composed of different polymeric base materials were extracted with 20 mL of EtOH:H_2O (1:1) at 37 ºC over a three-week period. An aliquot of each extract was analyzed using both the GC/Q-TOF and LC/Q-TOF systems. GC/MS analysis was performed using the 8890 GC coupled to the 7250 Q-TOF. For GC/MS, chromatographic deconvolution and library search were performed in the MassHunter Unknowns Analysis 12.1. The NIST23 library was used to perform initial compound identification. All data collection was performed utilizing MassHunter Acquisition Network Workstation configuration, which integrates with OpenLab ECM XT, facilitating centralized management and high integrity data storage and access.

The LC/MS analysis was preformed using the 1290 Infinity II LC coupled to the Revident LC/Q-TOF. More detailed instrumental parameters are displayed in Tables 1 and 2. Statistical analysis for the catheter data was performed using Mass Profiler Professional (MPP) software (version 15.1).

Experimental

Table 1. GC/Q-TOF method parameters

Parameter	Value
MS	Agilent 7250 GC/Q-TOF
GC	Agilent 8890 GC
Column	Agilent DB-5Q*, 30 m, 0.25 mm, 0.25 µm
Inlet	MMI, 4 mm Ultra Inert liner, single taper with wool
Injection volume	1 µL
Injection mode	Splitless
Inlet temperature program	65 °C for 0.01 min, 300 °C/min to 280 °C
Oven temperature program	45 °C for 2 min; 12 °C/min to 325 °C, 11 min hold
Carrier gas	Helium
Column flow	1 mL/min constant flow
Transfer line temperature	325 °C
Quadrupole temperature	150 °C
Source temperature	200 °C
Electron energy	70 eV
Emission current	5 µA
Spectral acquisition rate	5 Hz
Mass range	50 to 1000 *m/z*

* - available in August 2024

Table 2. LC/Q-TOF method parameters

Parameter	Value
LC	Agilent 1290 Infinity II
MS	Agilent Revident LC/Q-TOF
Column	Agilent PS AQ-C18 2.1 x 100 mm Column
Column temperature	40 °C
Injection volume	1 µL
Flow rate	0.35 mL/min
Mobile Phase A	Water w/2.5mM NH_4Formate 0.05% FA
Mobile Phase B	Methanol w/2.5 mM NH_4Formate 0.05% FA
LC gradient	2% B for 1.0 min; to 100% B at 16.0; hold 100% B to 28.0 min; to 2% at 28.1 min post time 5 min
MS source	Dual AJS ESI
MS mode	Auto MS/MS
Polarity	Positive
Collison energy	20; 40
MS range	40-1700 *m/z*
Acquisition rate	4 spectra/sec for MS; 6 spectra/sec for MS/MS
Drying Gas temperature	250 °C
Drying gas	11 L/min
Nebulizer pressure	35 psi
Sheath gas temperature	300 °C
Capillary Voltage	3500 V

DB-5Q Column Performance at High Oven Temperatures

The new Agilent DB-5Q column (available starting August 2024) has demonstrated significant decrease in column bleed at 325 ºC (Figure 2).

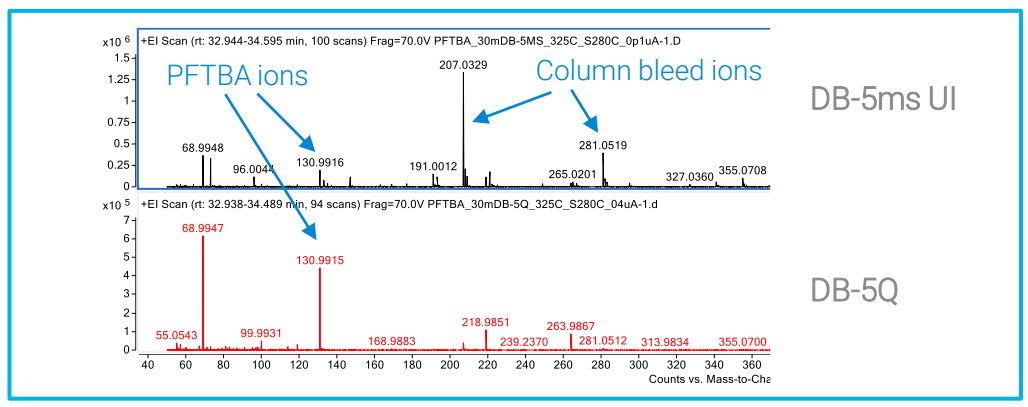

Figure 2. DB-5ms (top) and DB-5Q (bottom) columns comparison. PFTBA (normalized for abundance) run at 325 ºC oven temperature.

E&L Compounds Identified in Rubber Gasket Extracts

Table 3 shows the compounds identified in rubber gasket extract using GC/Q-TOF. Nonaromatic and aromatic hydrocarbons are uniquely detected by GC/MS since in most cases they won't ionize using electrospray ionization. Figure 3 shows the separation of phthalates.

Table 3. List of E&L compounds identified in the rubber gasket extract by GC/Q-TOF after blank subtraction.

Aromatic Hydrocarbons

RT	Compound Name	Match Factor	Formula	Delta RI	CAS#
5.80	o-Xylene	96.5	C8H10	3.3	95-47-6
7.36	α-Methylstyrene	95.6	C9H10	-4.2	98-83-9
14.38	(3-Decyl)benzene	74.7	C16H26	0.5	4621-36-7
14.77	(2-Decyl)benzene	88.2	C16H26	10.0	4537-13-7
15.06	(1-Butylheptyl)benzene	83.8	C17H28	-4.1	4537-15-9
15.39	(1-Ethylnonyl)benzene	85.8	C17H28	-0.5	4536-87-2
15.93	1-Phenyl-1,3,3-trimethylindane	96.3	C18H20	-12.8	3910-35-8
16.64	2,4-Diphenyl-4-methyl-1-pentene	89.8	C18H20	3.0	1000111-58-0
16.69	Anthracene	88.2	C14H10	-23.5	120-12-7
16.98	2,4-Diphenyl-4-methyl-2(E)-pentene	90.8	C18H20	-6.0	22768-22-5
18.29	18-Norabieta-8,11,13-triene	74.2	C19H28	-26.6	1000197-14-1

Nonaromatic Hydrocarbons

RT	Compound Name	Match Factor	Formula	Delta RI	CAS#
12.93	Longifolene	91.9	C15H24	-23.1	475-20-7
14.42	3-Methylpentadecane	93.3	C16H34	-1.7	2882-96-4
16.67	2,6,10,14-Tetramethylhexadecane (Phytane)	97.3	C20H42	-5.2	638-36-8
18.15	n-Tridecylcyclohexane	80.3	C19H38	-11.0	6006-33-3
18.79	2,3-Dimethylnonadecane	85.5	C21H44	-8.8	75163-99-4
18.85	2-Methyleicosane	90.2	C21H44	-1.5	1560-84-5
19.80	n-Pentadecylcyclohexane	83.9	C21H42	-3.6	6006-95-7
21.09	2-Methyltricosane	89.2	C24H50	-1.8	1928-30-9
21.79	2-Methyltetracosane	79.2	C25H52	-3.2	1560-78-7
23.02	Squalane	84.7	C30H62	2.7	111-01-3

Aromatic Oxygenates

RT	Compound Name	Match Factor	Formula	Delta RI	CAS#
7.10	Benzaldehyde	90.9	C7H6O	-10.8	100-52-7
7.22	Phenol	99.1	C6H6O	0.8	108-95-2
8.54	Acetophenone	95.5	C8H8O	-7.0	98-86-2
8.55	p-Cresol	81.7	C7H8O	3.2	106-44-5
8.60	4-Methylbenzaldehyde	96.5	C8H8O	2.0	104-87-0
8.79	(1-Methoxypropyl)benzene	94.4	C10H14O	22.0	59588-12-4
9.63	Benzoic acid	92.8	C7H6O2	18.3	65-85-0
11.44	m-tert-Butylphenol	72.0	C10H14O	-2.2	585-34-2
12.57	p-tert-Pentylphenol	74.3	C11H16O	3.2	80-46-6
12.74	Diphenyl ether	90.7	C12H10O	-7.3	101-84-8
12.85	p-tert-Butylphenetole	93.4	C12H18O	-4.0	17269-94-2
13.18	Dimethyl phthalate	93.1	C10H10O4	2.0	131-11-3
13.41	Ethyl 3-phenylpropenoate	97.5	C11H12O2	-9.1	103-36-6
13.76	2,4-Di-tert-butylphenol	85.6	C14H22O	7.6	96-76-4
13.78	Butylated Hydroxytoluene	72.2	C15H24O	5.5	128-37-0
13.98	Ethyl 4-ethoxybenzoate	82.8	C11H14O3	-5.7	23676-09-7
14.54	Pentyl salicylate	86.7	C12H16O3	-4.1	2050-08-0
14.63	Diethyl Phthalate	95.7	C12H14O4	2.3	84-66-2
14.79	p-tert-Octylphenol	83.9	C14H22O	-5.7	140-66-9
15.08	Fenuron	73.1	C9H12N2O	-5.2	101-42-8
15.15	Benzophenone	93.4	C13H10O	-10.0	119-61-9
15.55	2,4-Ditert-butyl-6-nitrophenol	78.7	C14H21NO3	1.7	20039-94-5
15.56	n-Hexyl salicylate	88.8	C13H18O3	-5.4	6259-76-3
15.74	4-(1,1-Dimethylheptyl)phenol	94.8	C15H24O	-9.4	30784-30-6
15.82	4-(7-Methyloctyl)phenol	93.6	C15H24O	5.2	24518-48-7
15.89	4-(1,1-Dimethylheptyl)phenol	83.2	C15H24O	-25.9	30784-30-6
16.30	3,5-di-tert-Butyl-4-hydroxybenzaldehyde	86.9	C15H22O2	4.8	1620-98-0
16.74	3,5-di-tert-Butyl-4-hydroxyacetophenone	82.7	C16H24O2	-12.3	14035-33-7
17.09	N-Phenylheptanamide	86.8	C13H19NO	-28.1	56051-98-0
17.17	Diisobutyl phthalate	88.5	C16H22O4	5.0	84-69-5
17.98	Dibutyl phthalate	84.1	C16H22O4	6.2	84-74-2
21.05	Methyl dehydroabietate	79.9	C21H30O2	-17.2	1235-74-1
21.46	2,2'-Methylenebis[4-Methyl-6-tert-butylphenol] (Antioxidant 2246)	90.5	C23H32O2	-3.8	119-47-1
21.74	Dehydroabietic acid	91.9	C20H28O2	-0.3	1740-19-8
22.09	2,2'-Methylenebis(6-tert-butyl-4-ethylphenol) (Cyanox 425)	93.3	C25H36O2	19.6	88-24-4
22.26	Bis(2-ethylhexyl) phthalate (DEHP)	73.7	C24H38O4	0.0	117-81-7
29.28	Tris(2,4-di-tert-butylphenyl) phosphate	78.5	C42H63O4P	6.0	95906-11-9

Nonaromatic Oxygenates

RT	Compound Name	Match Factor	Formula	Delta RI	CAS#
4.17	Methyl Isobutyl Ketone	92.8	C6H12O	-29.7	108-10-1
4.48	Butanoic acid	90.5	C4H8O2	10.9	107-92-6
4.61	Acetylacetone	87.7	C5H8O2	-19.7	123-54-6
4.63	Dimethylformamide	99.1	C3H7NO	-21.2	68-12-2
4.86	Hexanal	96.7	C6H12O	-18.9	66-25-1
5.03	Furfural	80.0	C5H4O2	1.1	98-01-1
5.11	Dipropyl acetal	86.9	C8H18O2	22.5	105-82-8
5.68	N-Ethylacetamide	93.2	C4H9NO	0.2	625-50-3
5.75	Pentanoic acid	96.6	C5H10O2	19.5	109-52-4
6.02	2-Heptanone	94.6	C7H14O	-9.3	110-43-0
6.21	Heptanal	94.6	C7H14O	-11.7	111-71-7
6.66	3-Hepten-2-one	79.6	C7H12O	-6.2	1119-44-4
7.13	Hexanoic acid	92.5	C6H12O2	15.6	142-62-1
7.15	Glycerin	85.6	C3H8O3	-26.1	56-81-5
7.33	Butanal diisopropyl acetal	87.9	C10H22O2	-17.7	1000431-62-3
7.36	6-Methyl-5-heptene-2-one	83.2	C8H14O	-3.6	110-93-0
7.63	Octanal	89.1	C8H16O	-5.5	124-13-0
7.96	2-Ethylhexanol	92.6	C8H18O	-1.7	104-76-7
8.04	2-Acetyl-5-methylfuran	93.7	C7H8O2	1.3	1193-79-9
8.11	N-Methyl-α-pyrrolidone	84.7	C5H9NO	1.4	872-50-4
8.16	2-(2-Hydroxypropoxy)-1-propanol	82.7	C6H14O3	0.1	106-62-7
8.44	Heptanoic acid	91.4	C7H14O2	12.2	111-14-8
8.53	Isovaleraldehyde dipropyl acetal	86.2	C11H24O2	38.8	1000431-60-3
9.01	Nonanal	96.3	C9H18O	-3.0	124-19-6
9.23	2,2,6,6-Tetramethyl-4-piperidone (Triacetonamine)	91.2	C9H17NO	13.2	826-36-8
9.72	Octanoic acid	91.9	C8H16O2	19.2	124-07-2
10.95	Nonanoic acid	95.7	C9H18O2	14.4	112-05-0
11.69	2,3-Dihydro-1H-pyrrolizin-1-one	93.7	C7H7NO	-15.2	17266-64-7
12.35	3-Hydroxy-2,2,4-trimethylpentyl 2-methylpropanoate (component of Texanol)	73.2	C12H24O3	-3.7	77-68-9
13.27	BHT-OH	84.6	C15H24O2	14.2	10396-80-2
13.42	1-Dodecanol	97.7	C12H26O	0.1	112-53-8
13.58	3-Tridecanone	83.2	C13H26O	4.6	1534-26-5
15.62	3-Pentadecanone	88.9	C15H30O	6.0	18787-66-1
16.20	Tetradecanoic acid	89.0	C14H28O2	11.8	544-63-8
16.81	Isopropyl myristate	81.1	C17H34O2	4.4	110-27-0
17.59	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	89.3	C17H24O3	11.5	82304-66-3
17.60	Farnesyl acetone	82.9	C18H30O	4.4	1117-52-8
17.70	Methyl hexadecanoate	74.6	C17H34O2	1.3	112-39-0
17.99	n-Hexadecanoic acid	91.7	C16H32O2	8.5	57-10-3
18.71	N,N-Dimethyltetradecanamide	84.2	C16H33NO	-4.0	3015-65-4
19.38	Linoleic acid	93.7	C18H32O2	-0.4	60-33-3
19.60	Octadecanoic acid	85.7	C18H36O2	10.7	57-11-4
20.31	N,N-Dimethylpalmitamide	87.2	C18H37NO	0.9	3886-91-7
21.40	Eicosyl acetate	80.1	C22H44O2	-0.3	822-24-2
21.56	N,N-Dimethyllinoleamide	83.9	C20H37NO	-6.2	2501-33-9
21.60	N,N-Dimethyloleamide	90.8	C20H39NO	-5.1	2664-42-8
23.83	13-Docosenamide, (Z)-	81.4	C22H43NO	7.5	112-84-5
25.72	Tinuvin 770*	87.1	C28H52N2O4	130.4	52829-07-9
26.81	Chondrillasterol	81.1	C29H48O	16.3	481-17-4
27.37	(24Z)-Ethylidenecholesterol (Isofucosterol)	83.0	C29H48O	-19.0	481-14-1
27.73	Dihydrochondrillasterol	84.0	C29H50O	3.6	18525-35-4

*- Only predicted RI is available

Other

RT	Compound Name	Match Factor	Formula	Delta RI	CAS#
5.93	2,6-Lutidine (2,6-Dimethylpyridine)	82.5	C7H9N	-14.1	108-48-5
6.91	2,2,6,6-Tetramethylpiperidine	91.0	C9H19N	-19.8	768-66-1
10.08	2,4-Dimethylthiophenol	89.1	C8H10S	19.0	13616-82-5
10.29	1,3-Dibromobenzene	91.2	C6H4Br2	14.1	108-36-1
10.70	Benzothiazole	92.2	C7H5NS	-9.3	95-16-9
13.54	Dicyclopentyl(dimethoxy)silane	88.3	C12H24O2Si	-11.9	126990-35-0
15.12	Tributyl phosphate	76.7	C12H27O4P	5.6	126-73-8
19.01	p-Tolyl disulfide	73.8	C14H14S2	3.4	103-19-5

The top hits identified by the LC/Q-TOF using positive ion Data Dependent Acquisition (DDA) MSMS are listed in Table 4. The data was processed using MassHunter Qualitative Analysis Molecular Feature Extraction (MFE) unsupervised data mining tool. Compound identification was performed using Formula Generation tool that considers isotope fidelity, and the new Agilent E&L Personal Compound Database Library (PCDL).

Table 4. Top hits identified in rubber gasket extract by the LC/Q-TOF.

RT	Name	Formula	Area	Compound Classes
8.262	Tripropylene glycol diacrylate	C15H24O6	1647945	Acrylate
9.828	Tinuvin 7709	C28H52N2O4	2095866	HALS Additive
11.483	Diethyl phthalate	C12H14O4	3932233	Phthalate
11.701	3,5-Di-tert-butylbenzaldehyde	C15H22O	7832178	Breakdown Product
12.464	Ethyl 703	C17H29NO	1151185	Amide
13.058	Palmitoleoyl ethanolamide	C18H35NO2	1924000	Ethanolamide
13.058	Linoleic acid	C18H32O2	1820832	Fatty Acid
14.433	Dibutyl Phthalate	C16H22O4	1246480	Phthalate
14.574	Triisobutyl phosphate	C12H27O4P	777580	Phosphate
15.424	Irganox 3052	C26H34O3	1609956	Antioxidant
15.973	Palmitamide	C16H33NO	5137453	Amide
16.443	Ethyl 712	C28H42O2	1361382	Bisphenol Compound
16.536	Octadecanamide	C18H37NO	12462242	Amide
16.623	Cyanox 425	C25H36O2	14751385	Antioxidant
16.623	Bis(3,5-dimethyl-4-hydroxyphenyl)methane	C17H20O2	4892589	Antioxidant
16.623	Bisphenol G	C21H28O2	1738538	Bisphenol Compound
16.699	N-Hexadecylmethacrylamide	C20H39NO	17394128	Amide
16.744	3-hydroxypropyl octadecanoate	C21H42O3	2059940	Stearic Acid Ester
16.935	Isodecyl phosphite	C30H63O3P	1118256	Phosphite
17.085	Cyanox MTDP	C34H66O4S	1038890	Antioxidant
17.826	Ionox 330 (Irganox 330)	C54H78O3	892923	Antioxidant
18.029	Irgafos TNPP	C45H69O4P	774026	Phosphate
18.416	lauryl stearyl thiodipropionate	C36H70O4S	1201643	Antioxidant
18.467	Dioleoylglycerol	C39H72O5	2911053	Glycerol Ester
19.013	Octyl decyl phthalate	C26H42O4	1531185	Phthalate
19.034	Erucamide	C22H43NO	1615261	Amide
20.158	Trimyristin	C45H86O6	1797089	Glycerol Ester
22.597	Tripalmitin	C51H98O6	1474030	Glycerol Ester
23.672	Glyceryl trioleate	C57H104O6	5409572	Glycerol Ester

Identification of E&L Compounds in Catheter Extracts

The EtOH:H2O catheter extracts have been analyzed using both the GC/Q-TOF and LC/Q-TOF systems. The GC/Q-TOF used retention indices (RIs) match as well as the fragment ion's accurate mass fit to the molecular formula (enabled by ExactMass Tool of Unknowns Analysis software, Figure 4) to increase confidence in compound library matches.

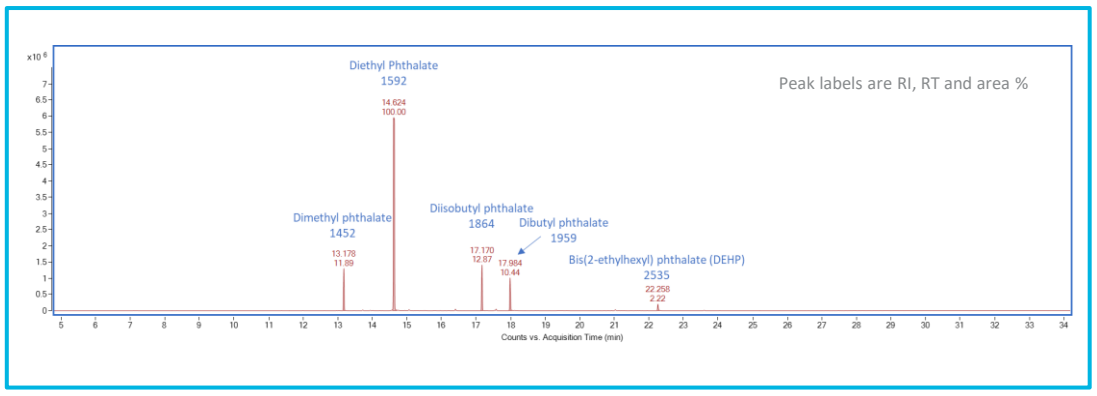

Figure 3. Separation of phthalates using GC/Q-TOF, including di-isobutyl and dibutyl phthalates isomers.

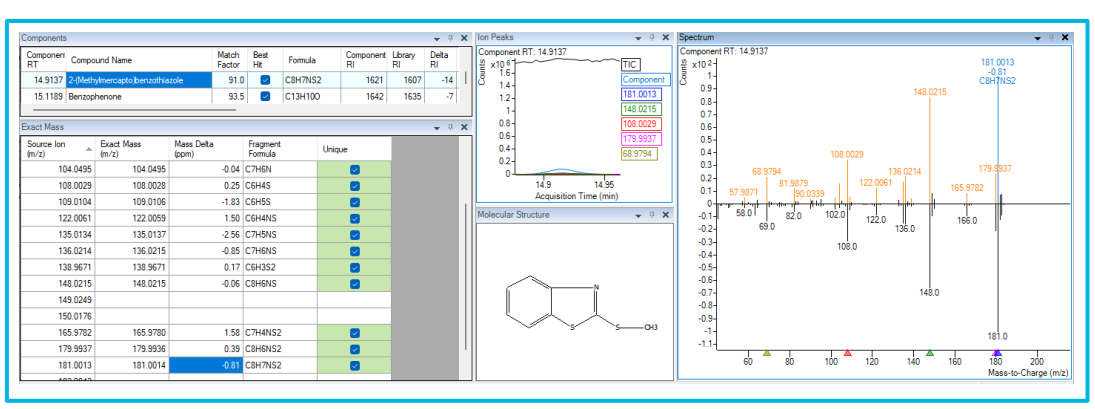

Figure 4. ExactMass tool of Unknowns Analysis helps to confirm compound ID. Accurate mass is used to assign formulas and calculate mass error of each prominent fragment ion based on the molecular formula of NIST library hit (displayed in the table in the lower left corner).

Difference in Extractable Profiles between Four Types of Catheters

GC/Q-TOF data were imported to MPP in a form of CEF files to perform statistical analysis. Principal component analysis (PCA) plot showed a clear clustering between different catheter types (Figure 5). One example showing variation in extractables profiles between two catheter types (B and P) is displayed in Figure 6.

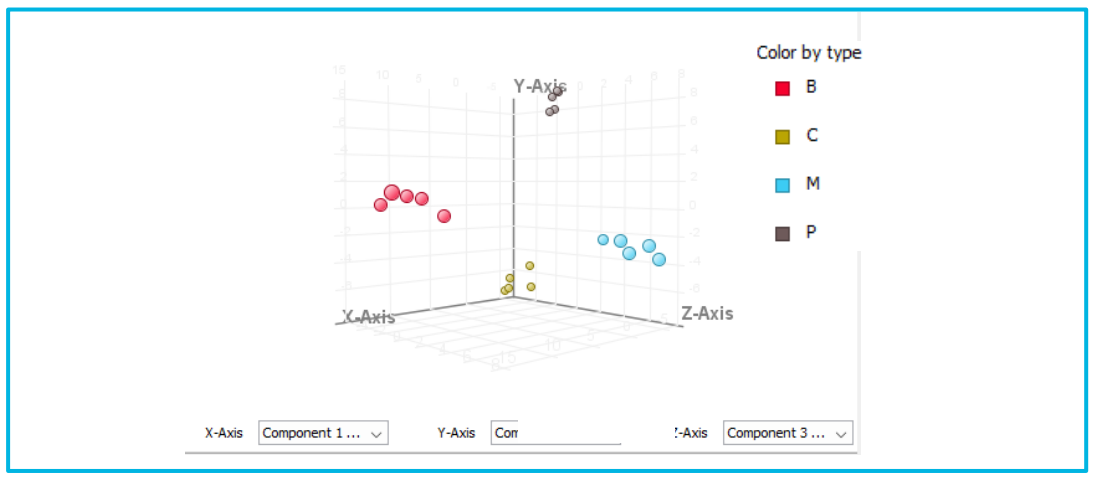

Figure 5. PCA plot showing separation of clusters of different types of catheters.

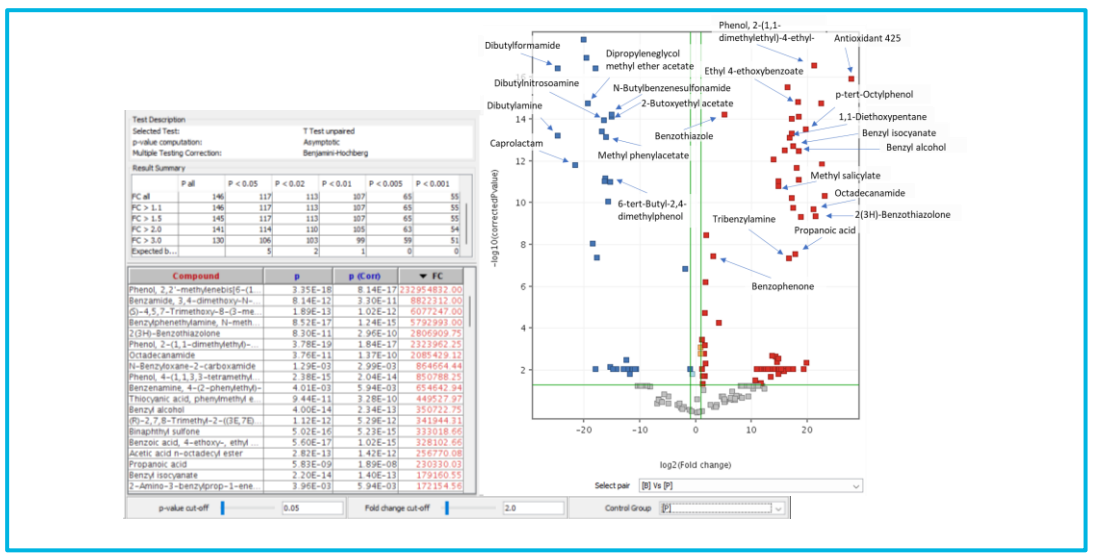

Figure 6. Volcano plot showing log of fold change *vs* log of p-Value for catheter B *vs* P.

Compounds Identified in Catheter Samples

Both LC/Q-TOF and GC/Q-TOF data have been converted to generic format and processed together in MPP. Venn diagrams shown in Figures 7 and 8 reveal coverage of extractables profiles by LC and GC and differences between the catheter extracts, respectively.

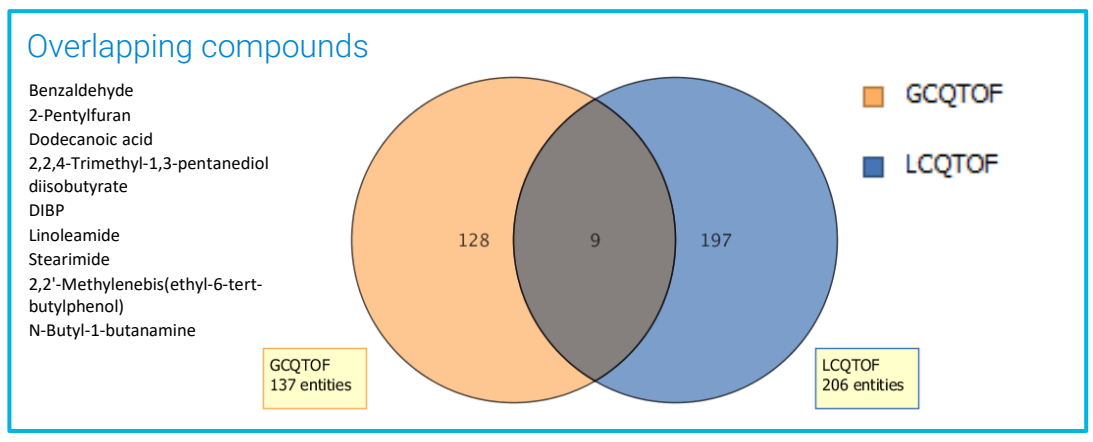

Figure 7. Coverage of extractables space by GC/Q-TOF and LC/Q-TOF.

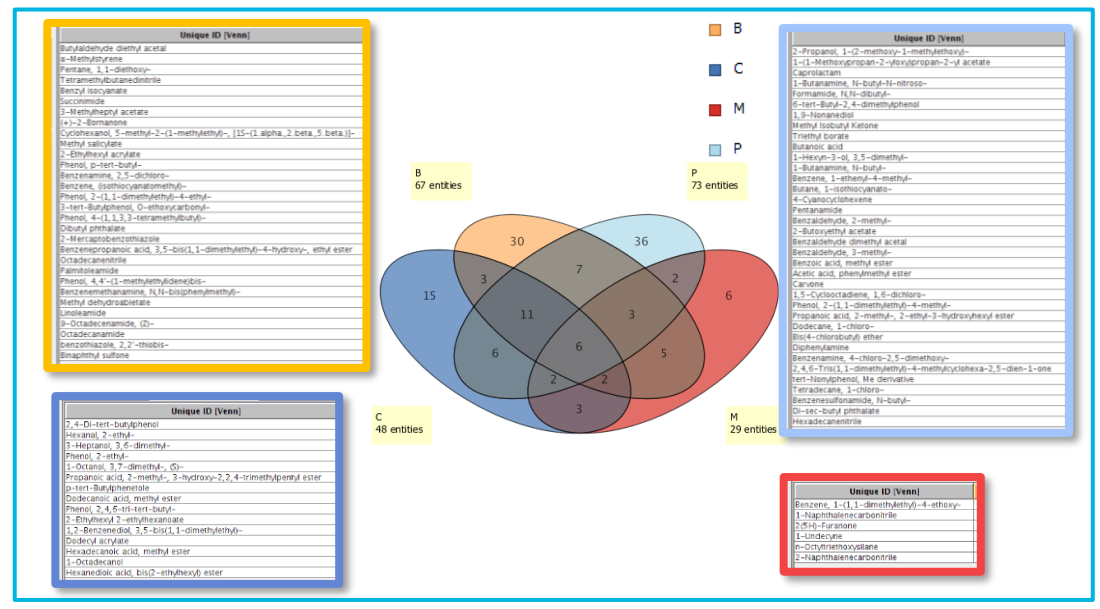

Figure 8. Venn diagram showing the overlap of extracted compounds that were detected by the GC/Q-TOF. Listed are unique compounds identified in each type of catheter.

Table 5 provides a list of E&L compounds detected by the GC/Q-TOF in catheter samples that showed up in at least two catheter types. The compounds listed were identified with a minimum library match of 75, fragment annotation confirmation and an RI matching within 30 RI units.

Table 5. E&L compounds detected by the GC/Q-TOF that were found in common in at least two types of catheters.

RT	Compound Name	Match Factor	Formula	RI	Library RI	Delta RI	CAS#	B	C	M	P
3.93	Toluene	88.6	C7H8	743.0	764	21.0	108-88-3			x	x
7.04	Benzaldehyde	96.2	C7H6O	968.8	962	-6.8	100-52-7	x		x	x
7.37	Benzonitrile	76.7	C7H5N	990.8	984	-6.8	100-47-0	x		x	
7.91	2-Ethylhexanol	96.2	C8H18O	1028.2	1030	1.8	104-76-7	x	x	x	x
8.49	Acetophenone	82.3	C8H8O	1069.2	1066	-3.2	98-86-2	x	x		
8.96	Nonanal	89.2	C9H18O	1103.1	1104	0.9	124-19-6	x	x		x
9.88	Benzoic acid, ethyl ester	85.2	C9H10O2	1173.0	1171	-2.0	93-89-0	x	x		x
10.16	Naphthalene	99.0	C10H8	1194.1	1182	-12.1	91-20-3	x	x	x	x
10.67	Benzothiazole	98.3	C7H5NS	1235.3	1228	-7.3	95-16-9	x		x	x
10.84	1,3-Di-tert-butylbenzene	79.8	C14H22	1249.3	1249	-0.3	1014-60-4	x			x
11.54	2-Methylnaphthalene	91.1	C11H10	1306.8	1297	-9.8	91-57-6		x		x
11.73	1-Methylnaphthalene	90.0	C11H10	1323	1307	-16	90-12-0	x	x	x	
12.54	p-tert-Pentylphenol	80.6	C11H16O	1394.3	1400	5.7	80-46-6	x	x		
12.64	2,4,7,9-Tetramethyl-5-decyn-4,7-diol (Surfynol 104)	93.0	C14H26O2	1402.9	1407	4.1	126-86-3	x	x	x	x
12.82	Phenol, 2-(1,1-dimethylethyl)-4-ethyl-	97.4	C12H18O	1419.7	1439	19.3	96-70-8	x		x	
13.16	Dimethyl phthalate	81.7	C10H10O4	1450.4	1454	3.6	131-11-3	x	x		
13.24	2,6-Di-tert-butyl-4-hydroxy-4-methyl-2,5-cyclohexadienone	88.6	C15H24O2	1457.6	1475	17.4	10396-80-2	x	x		x
13.38	1-Dodecanol	93.7	C12H26O	1470.8	1474	3.2	112-53-8	x	x		x
13.39	Phthalimide	87.3	C8H5NO2	1471.5	1450	-21.5	85-41-6	x		x	x
13.74	Butylated Hydroxytoluene	97.0	C15H24O	1503.5	1513	9.5	128-37-0	x	x		x
13.94	o-Hydroxybiphenyl	84.7	C12H10O	1523.4	1507	-16.4	90-43-7	x			x
13.95	Ethyl 4-ethoxybenzoate	93.9	C11H14O3	1524.6	1522	-2.6	23676-09-7	x	x	x	
14.22	Dodecanoic acid	94.8	C12H24O2	1551.6	1567	15.4	143-07-7	x			x
14.58	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate (Kodaflex txib)	85.4	C16H30O4	1587.3	1588	0.7	6846-50-0	x	x		x
14.59	Diethyl Phthalate	84.8	C12H14O4	1588.0	1594	6.0	84-66-2	x	x	x	x
14.92	2-(Methylmercapto)benzothiazole	89.1	C8H7NS2	1621.4	1607	-14.4	615-22-5	x			x
15.12	Benzophenone	93.7	C13H10O	1642.1	1635	-7.1	119-61-9	x	x		x
15.31	2,2',5,5'-Tetramethyl-1,1'-biphenyl	82.3	C16H18	1662.1	1663	0.9	3075-84-1	x	x		
15.47	2(3H)-Benzothiazolone	97.8	C7H5NOS	1678.7	1676	-2.7	934-34-9	x		x	
15.85	4,6-di-tert-Butylresorcinol	84.6	C14H22O2	1718.5	1746	27.5	5374-06-1	x	x		x
15.97	2,6-Diisopropylnaphthalene	85.7	C16H20	1731.2	1728	-3.2	24157-81-1	x		x	
16.52	2,5-Di-tert-butylhydroquinone	78.2	C14H22O2	1790.4	1784	-6.4	88-58-4	x	x	x	x
17.14	Diisobutyl phthalate	87.2	C16H22O4	1860.5	1869	8.5	84-69-5	x	x	x	
17.96	Dibutyl phthalate	88.5	C16H22O4	1955.4	1965	9.6	84-74-2	x	x		x
17.97	2,5-Di-tert-pentylhydroquinone	75.8	C16H26O2	1957.1	1970	12.9	79-74-3	x	x	x	x
19.71	Hexadecanamide	92.8	C16H33NO	2175.3	2184	8.7	629-54-9	x			x
21.03	Linoleamide	95.3	C18H33NO	2355.5	2348	-7.5	3999-01-7	x			x
22.04	2,2'-Methylenebis(6-tert-butyl-4-ethylphenol) (Antioxidant 425)	96.2	C25H36O2	2501.1	2529	27.9	88-24-4	x		x	

Conclusions

- A combined high-resolution GC/MS and LC/MS approach for the analysis of extractables and leachables was developed using rubber gasket samples and different types of catheters.
- Both GC/MS and LC/MS techniques were necessary to cover a comprehensive list of E&L compounds.

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