Application Note

Extractables and Leachables

Agilent

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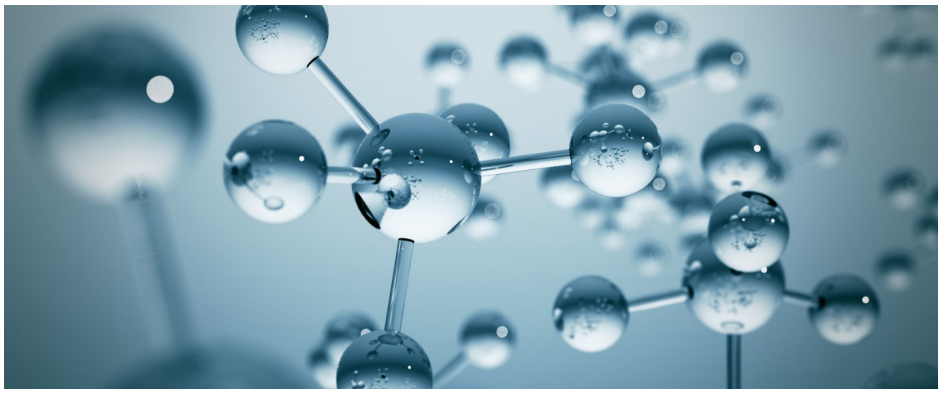
Analysis of Volatile Compounds Identified in Rubber Gasket Extracts Using GC/MSD and High-Resolution GC/Q-TOF



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Abstract

Chemicals that are part of polymeric container closure systems (CCS) and drug delivery systems have the potential to migrate into drug products during manufacturing, storage, transport, and delivery, and must be identified in the final products to ensure their safety.

This application note presents a rubber gasket extractables study using a unit mass resolution gas chromatography/mass selective detector (GC/MSD) and a high-resolution gas chromatography/quadrupole time-of-flight (GC/Q-TOF) mass spectrometer to establish a process for identifying GC-amenable extractables and leachable (E&L) compounds.

Introduction

Elastomeric gaskets, plungers, and O-rings are common sources of leachable compounds in the manufacturing, storage, and delivery of drug products. E&Ls derived from elastomeric components may impact the stability and efficacy of small and large molecule drug products[1], and therefore need to be characterized thoroughly. Exposure to some E&L chemicals, such as phthalates and nitrosamines, even at low levels, may cause safety concerns.[2] Chemicals derived from the elastomer manufacturing process typically include accelerators, activators, antioxidants, fillers, plasticizers (including phthalates), mold release agents, and other additives[3] that may leach into the final product. Some additives present in elastomer packaging materials may also contain polycyclic aromatic hydrocarbons (PAHs)[4] and aliphatic hydrocarbons.

GC/MS is a commonly used technique for analyzing volatile and semivolatile organic compounds in the E&L space. This study demonstrates the capabilities of GC/MSD to identify GC-amenable compounds present in a solvent extract of a rubber gasket by leveraging chromatographic deconvolution in combination with retention index (RI)-based filtering. Adding a high-resolution accurate mass GC/Q-TOF into the E&L workflow provided a higher number of identified chemicals. It also increased confidence in compound identification and enabled structure elucidation of unknown compounds.

The study was performed in the Network Workstation configuration using Agilent OpenLab Electronic Content Management (ECM) XT as the data repository. This configuration enabled tools that facilitate compliance with various national and EU electronic record regulations, including audit trails, user authentication, role-based permission controls, and remote data storage.[5]

Experimental

Sample preparation

Rubber syringe gaskets were extracted using tetrahydrofuran (THF) solvent at room temperature for six months. An aliquot of the extracts, along with solvent blanks, were analyzed using GC/MSD and GC/Q-TOF systems.

Data acquisition

The GC/MS analysis was performed using an Agilent 5977C GC/MSD and an Agilent 7250 GC/Q-TOF system in electron ionization (EI) mode. The GC/Q-TOF was also used in low-energy EI mode to help identify molecular ions of unknowns.

Injection conditions were optimized for a broad range of E&L compound boiling points. Using pulsed splitless injection mode and delaying the purge flow to the split vent for 1 to 2 minutes maximized the response for both low- and high-boiling compounds (Figure 1).

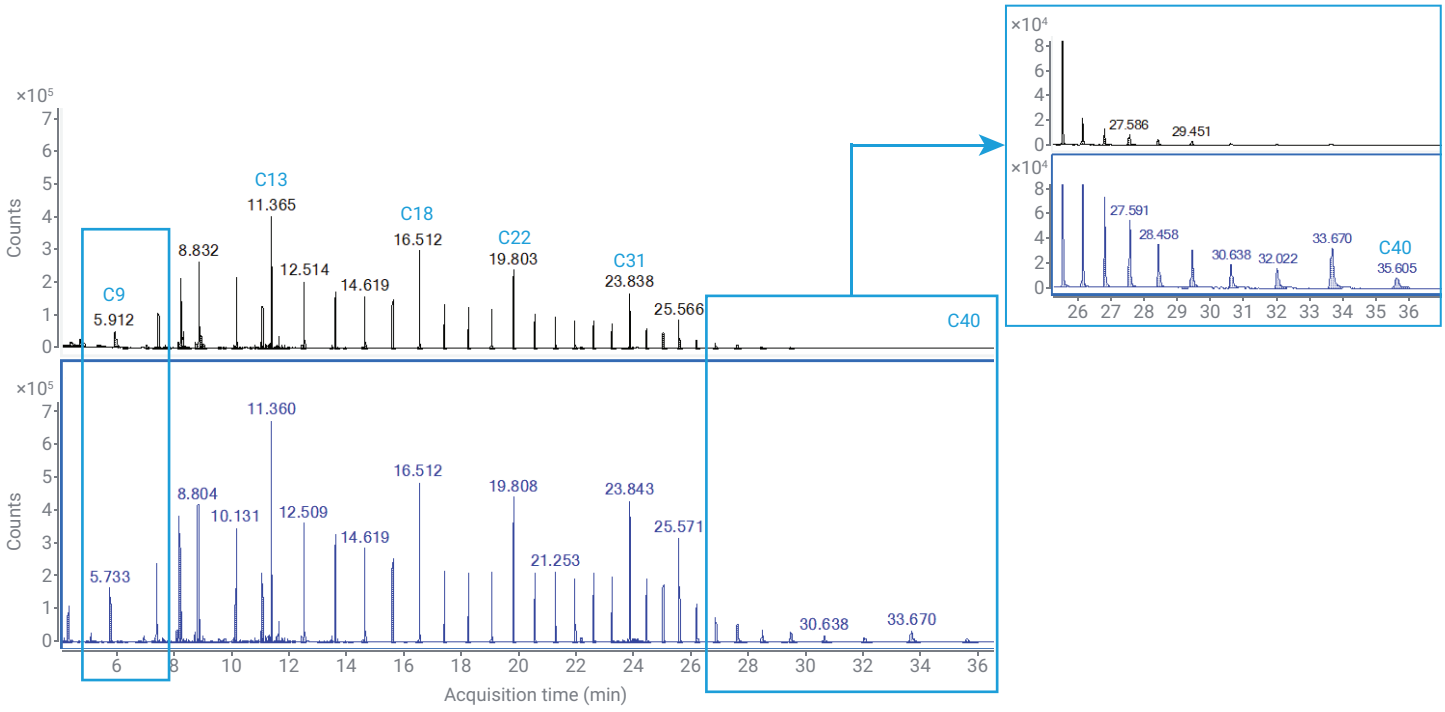

Figure 1. EIC (*m/z* 57) of a C5 to C40 *n*-alkane standard analyzed under the starting (top) and optimized (bottom) conditions.

Initially, both 30 m × 0.25 mm, 0.25 µm and 20 m × 0.18 mm, 0.18 µm Agilent J&W DB-5ms Ultra Inert columns were evaluated for their chromatographic separation capabilities of the complex E&L extracts, as well as sensitivity after optimization of the carrier gas flow for each column dimension. While the 20 m column provided sharper peaks and greater sensitivity for trace-level compounds, the 30 m column offered better separation, with a higher number of components reliably identified. The 30 m column was therefore selected.

All data were acquired in full spectrum acquisition mode using the new Agilent J&W DB-5Q nonpolar low bleed column and the DB-5ms Ultra Inert GC column. The acquisition software operated under a unified compliance environment using OpenLab ECM XT. The typical data acquisition parameters are shown in Table 1.

Table 1. Data acquisition parameters.

Parameter	Value
MS	Agilent 7250 GC/Q-TOF; Agilent 5977C GC/MSD
GC	Agilent 8890 GC
Column	Agilent J&W DB-5Q, 30 m × 0.25 mm, 0.25 µm (p/n 122-5532Q)
Inlet	Multimode inlet, 4 mm Ultra Inert inlet liner, single taper with wool
Injection Volume	1 µL
Injection Mode	Pulsed splitless (1 min purge, pulse at 40 psi for 1.1 min)
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 (Q-TOF)/300 °C (MSD)
Electron Energy	70 eV (standard EI MSD, Q-TOF); 15, 12, and 10 eV (low-energy EI, Q-TOF)
Emission Current	5 µA (standard EI, Q-TOF); 0.3 µA (low-energy EI, Q-TOF), 35 µA MSD
Spectral Acquisition Rate	5 Hz (Q-TOF), 2 Hz (MSD)
Mass Range	*m/z* 50 to 1,000 (Q-TOF), 45 to 450 (MSD)

Data processing

The chromatographic deconvolution and library search were performed in the Agilent MassHunter Unknowns Analysis 12.1 Update 2. The NIST23 library was used to perform the initial compound identification. Structural elucidation was performed using the Agilent Molecular Structure Correlator (MSC) software 8.2.

Retention time (RT) locking was used to ensure consistent RTs between the GC/MSD and GC/Q-TOF systems. It also allowed for both RI and RT matching.

Results and discussion

Advantages of using the new Agilent low-bleed DB-5Q column for E&L applications

A beta version of the new Agilent DB-5Q column was evaluated in terms of suitability for E&L studies. Many compounds of interest, including phthalates, antioxidants, UV-absorbers, and stabilizers have high boiling points. The detection of these compounds is therefore more susceptible to interference from column bleed, which is more evident at high oven temperatures. Two different sets of DB-5Q and DB-5ms UI columns were compared and a significantly lower column bleed at high oven temperatures was observed for the DB-5Q columns, compared to the DB-5ms UI. One representative example is shown in Figure 2A. The data were acquired on the GC/Q-TOF using an emission current of 0.3 µA, resulting in similar perfluorotributylamine (PFTBA) abundances. The oven was kept at 325 ˚C while PFTBA and background spectra were recorded.

A few high-boiling compounds, such as antioxidants and UV-absorbers, were also analyzed on the two columns for comparison. The DB-5Q column produced less column bleed background in these conditions, as evident from the TIC of the UV absorbers (Figure 2B), and a spectrum of the antioxidant Irgafos 168, extracted without background subtraction (Figure 2C).

It is typical for E&L extracts to contain a significant proportion of water; therefore, the DB-5Q column performance was tested before and after 130 injections of E&L extracts with various solvents, including ethanol:water (1:1) and THF. Octafluoronaphthalene (OFN) was injected at 1 pg onto the column before and after 130 extract injections. Peak shape, response, and spectrum integrity were all maintained after injecting water-containing extracts (Figure 3).

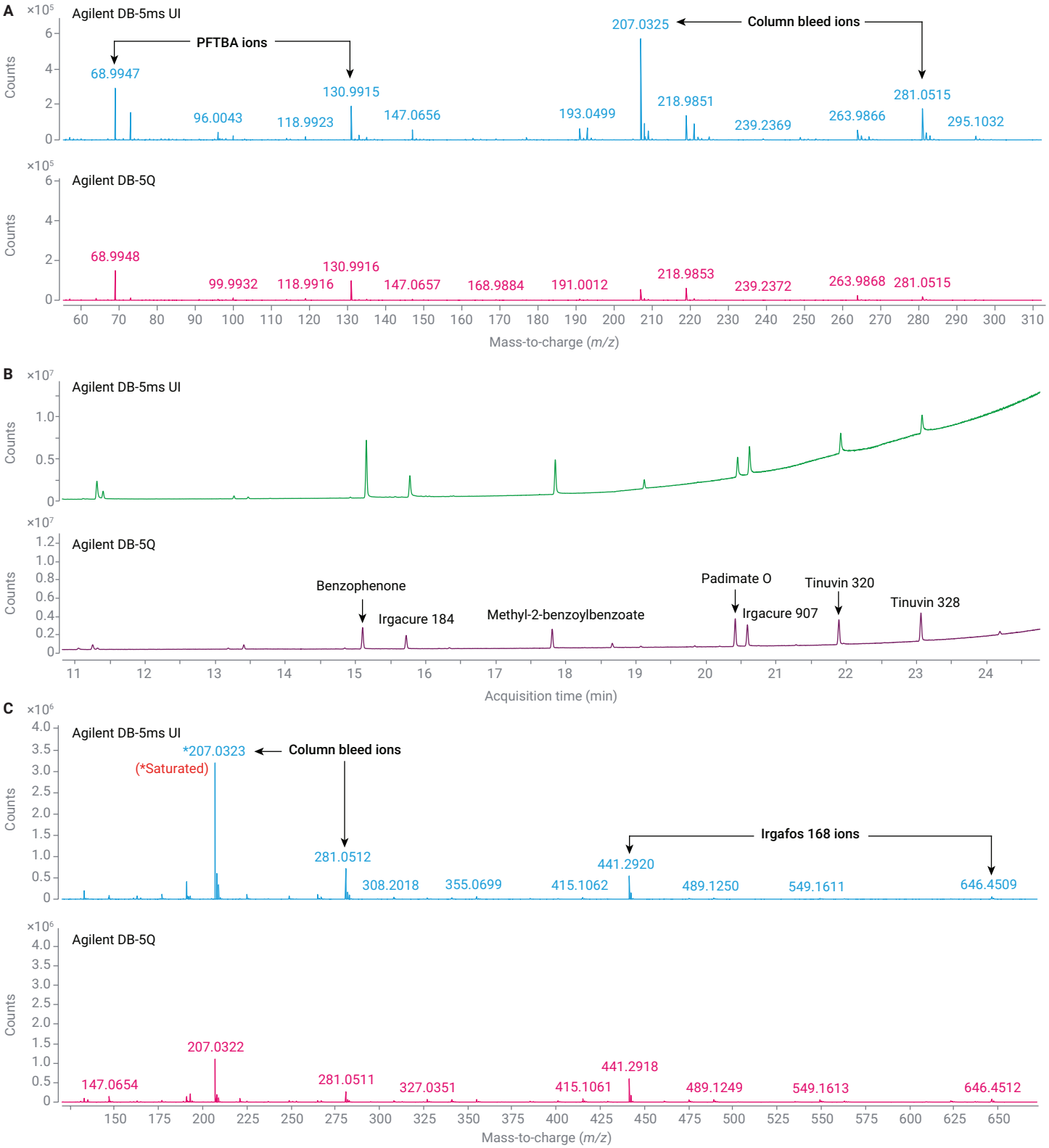

Figure 2. Agilent DB-5ms and DB-5Q column bleed comparison on the GC/Q-TOF. (A) Background and PFTBA spectra collected at oven temperature 325 °C and emission current 0.3 µA. (B) TIC of UV absorbers. (C) Raw spectra of an antioxidant Irgafos 168 without background subtraction (high boiling compound with an RI of 3,398 and an RT of 27.6 minutes).

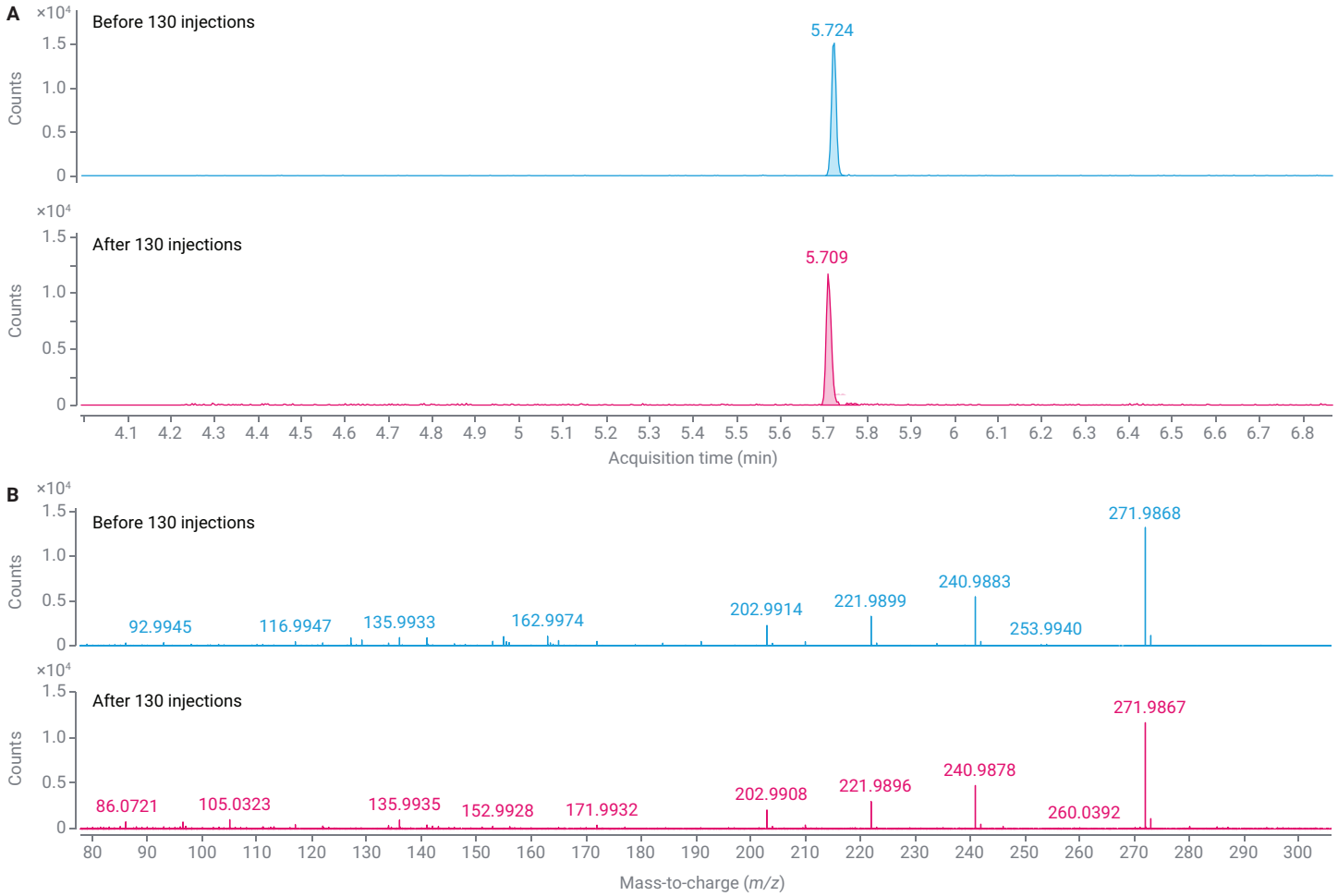

Figure 3. (A) OFN EIC for *m/z* 271.9867 ± 20 ppm and (B) OFN spectrum. OFN was injected at 1 pg onto an Agilent DB-5Q column before and after 130 injections. All injections were performed in splitless mode.

The consistency of RTs and RIs between the DB-5Q and the standard DB-5ms UI column was also evaluated. The RT values for *n*-alkanes in a range of C7 to C39, analyzed using an RT-locked method, were found to be very close when comparing the two columns (Figure 4A). The RIs for 70 compounds of various chemical classes and boiling points had a remarkable consistency between the DB-5Q and DB-5ms columns (with an average delta RI of 0.97 RI units) and were comparable to NIST experimental RI values for the semistandard nonpolar column phase (Figure 4B).

For additional information about the new ultralow bleed 5Q columns, see a separate technical note.[6]

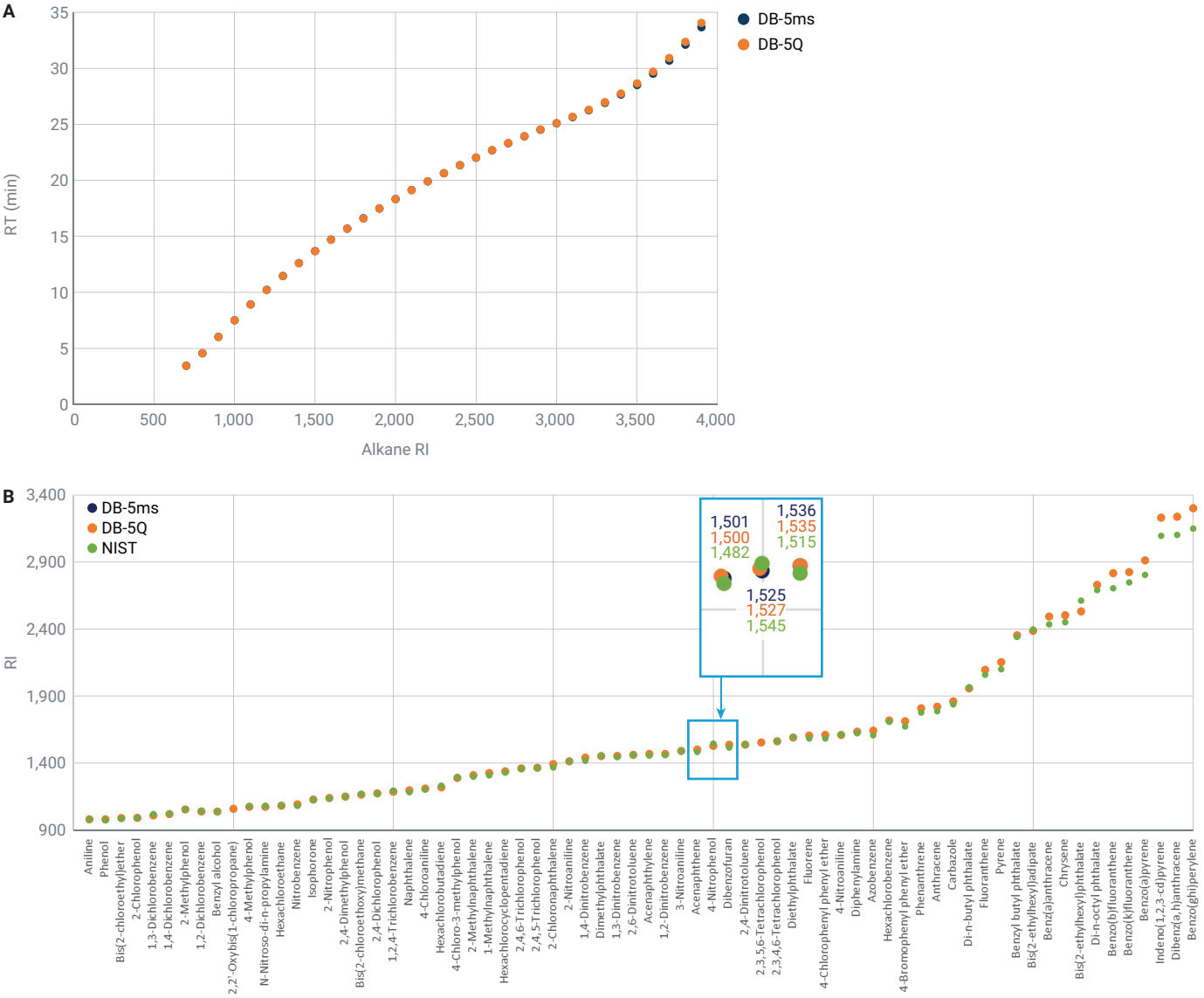

Figure 4. A comparison of RTs and RIs between the Agilent DB-5ms UI column and Agilent DB-5Q column. (A) *n*-Alkane RTs on the DB-5ms UI (blue) and DB-5Q (orange) columns. (B) RI consistency for 70 compounds between the DB-5ms (dark blue) and DB-5Q (orange) columns. NIST23 experimental RIs are shown in green.

Identification of semivolatile compounds in rubber gasket extract using GC/MSD and GC/Q-TOF

Over 100 compounds were initially identified in the sample using the GC/MSD by searching deconvoluted spectra against the NIST23 library and filtering the results based on RIs. Figure 5 shows an example of an identified compound, eicosyl acetate, in the presence of coeluting components with a high library match score (LMS) and excellent RI matching.

To take advantage of the accurate mass, high sensitivity in full spectrum acquisition mode, and MS/MS capabilities beneficial for identification of unknowns, the same rubber gasket extracts were also analyzed using the GC/Q-TOF. Over 80 compounds were identified in common between the GC/MSD and GC/Q-TOF, a few of which are shown in Table 2.

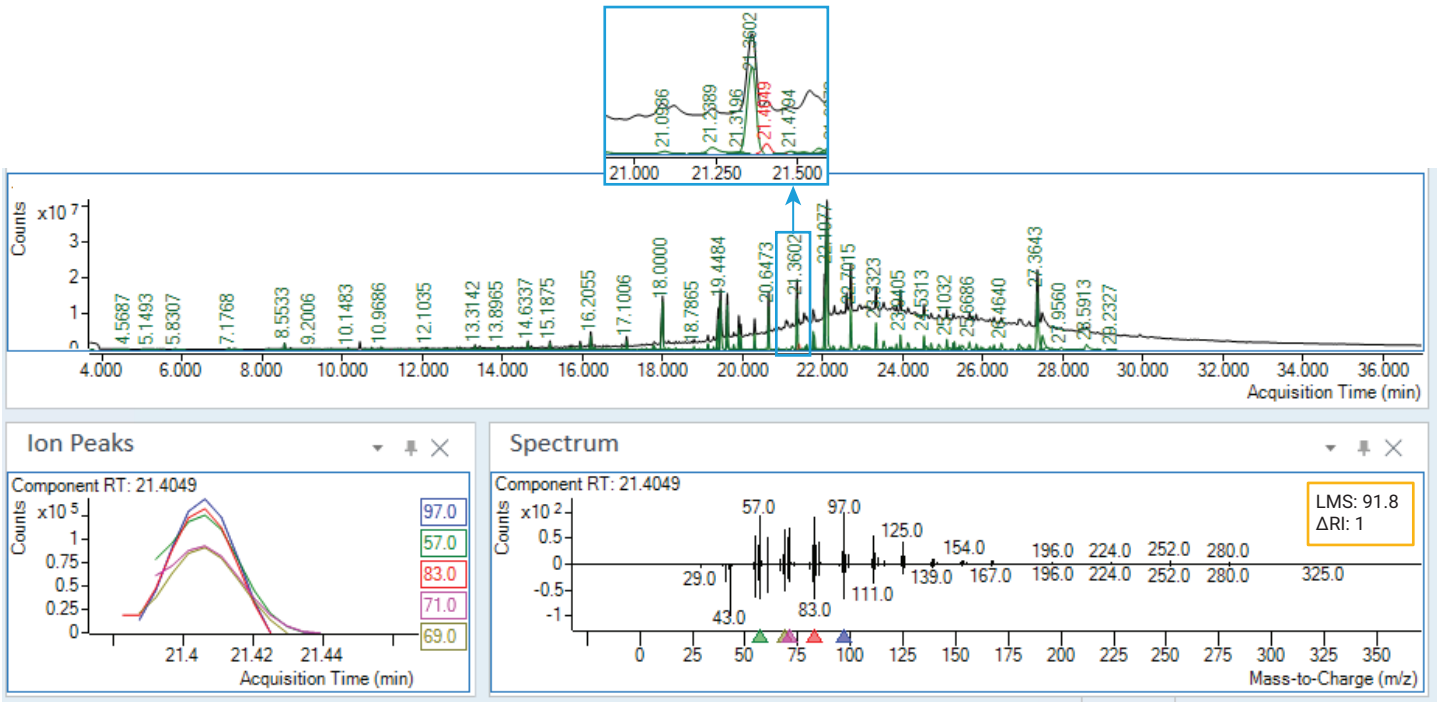

Figure 5. TIC of a rubber gasket sample and deconvoluted spectrum for eicosyl acetate with an LMS of 91.8 and RI delta of 1.

Table 2. Common compounds identified by both GC/MSD and GC/Q-TOF using a library match factor cutoff of 70.

RT	Compound Name	Formula	CAS No.
4.48	Butanoic acid	$C_4H_8O_2$	107-92-6
5.11	Dipropyl acetal	$C_8H_{18}O_2$	105-82-8
5.68	N-Ethylacetamide	C_4H_9NO	625-50-3
5.75	Pentanoic acid	$C_5H_{10}O_2$	109-52-4
7.13	Hexanoic acid	$C_6H_{12}O_2$	142-62-1
7.15	Glycerin	$C_3H_8O_3$	56-81-5
7.22	Phenol	C_6H_6O	108-95-2
8.04	2-Acetyl-5-methylfuran	$C_7H_8O_2$	1193-79-9
8.44	Heptanoic acid	$C_7H_{14}O_2$	111-14-8
8.53	Isovaleraldehyde dipropyl acetal	$C_{11}H_{24}O_2$	1000431-60-3
8.54	Acetophenone	C_8H_8O	98-86-2
8.55	*p*-Cresol	C_7H_8O	106-44-5
8.60	4-Methylbenzaldehyde	C_8H_8O	104-87-0
8.79	(1-Methoxypropyl)benzene	$C_{10}H_{14}O$	59588-12-4
9.23	Triacetonamine	$C_9H_{17}NO$	826-36-8
9.63	Benzoic acid	$C_7H_6O_2$	65-85-0
9.72	Octanoic acid	$C_8H_{16}O_2$	124-07-2
10.95	Nonanoic acid	$C_9H_{18}O_2$	112-05-0
11.69	2,3-Dihydro-1H-pyrrolizin-1-one	C_7H_7NO	17266-64-7
12.74	Diphenyl ether	$C_{12}H_{10}O$	101-84-8
12.85	*n*-tert-Butylphenetole	$C_{12}H_{18}O$	17269-94-2
12.93	Longifolene	$C_{15}H_{24}$	475-20-7
13.18	Dimethyl phthalate	$C_{10}H_{10}O_4$	131-11-3
13.41	Ethyl 3-phenylpropenoate	$C_{11}H_{12}O_2$	103-36-6
13.42	1-Dodecanol	$C_{12}H_{26}O$	112-53-8
13.76	2,4-Di-tert-butylphenol	$C_{14}H_{22}O$	96-76-4
13.78	Butylated hydroxytoluene	$C_{15}H_{24}O$	128-37-0
14.38	(3-Decyl)benzene	$C_{16}H_{26}$	4621-36-7
14.54	Pentyl salicylate	$C_{12}H_{16}O_3$	2050-08-0
14.63	Diethyl phthalate	$C_{12}H_{14}O_4$	84-66-2
14.79	*p*-tert-Octylphenol	$C_{14}H_{22}O$	140-66-9
15.12	Tributyl phosphate	$C_{12}H_{27}O_4P$	126-73-8
15.39	(1-Ethylnonyl)benzene	$C_{17}H_{28}$	4536-87-2
15.56	*n*-Hexyl salicylate	$C_{13}H_{18}O_3$	6259-76-3
15.62	3-Pentadecanone	$C_{15}H_{30}O$	18787-66-1
15.74	4-(1,1-Dimethylheptyl)phenol	$C_{15}H_{24}O$	30784-30-6
15.82	4-(7-Methyloctyl)phenol	$C_{15}H_{24}O$	24518-48-7
15.93	1-Phenyl-1,3,3-trimethylindane	$C_{18}H_{20}$	3910-35-8
16.20	Tetradecanoic acid	$C_{14}H_{28}O_2$	544-63-8
16.30	3,5-di-tert-Butyl-4-hydroxybenzaldehyde	$C_{15}H_{22}O_2$	1620-98-0
16.67	2,6,10,14-Tetramethylhexadecane (Phytane)	$C_{20}H_{42}$	638-36-8
16.74	3,5-di-tert-Butyl-4-hydroxyacetophenone	$C_{16}H_{24}O_2$	14035-33-7
16.81	Isopropyl myristate	$C_{17}H_{34}O_2$	110-27-0
16.98	2,4-Diphenyl-4-methyl-2(E)-pentene	$C_{18}H_{20}$	22768-22-5
17.59	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	$C_{17}H_{24}O_3$	82304-66-3
17.60	Farnesyl acetone	$C_{18}H_{30}O$	1117-52-8
17.98	Dibutyl phthalate	$C_{16}H_{22}O_4$	84-74-2
17.99	*n*-Hexadecanoic acid	$C_{16}H_{32}O_2$	57-10-3
18.34	18-Norabieta-8,11,13-triene	$C_{19}H_{28}$	1000197-14-1
18.71	N,N-Dimethyltetradecanamide	$C_{16}H_{33}NO$	3015-65-4
19.38	Linoleic acid	$C_{18}H_{32}O_2$	60-33-3
19.60	Octadecanoic acid	$C_{18}H_{36}O_2$	57-11-4
19.80	*n*-Pentadecylcyclohexane	$C_{21}H_{42}$	6006-95-7
20.31	N,N-Dimethylpalmitamide	$C_{18}H_{37}NO$	3886-91-7
21.40	Eicosyl acetate	$C_{22}H_{44}O_2$	822-24-2
21.46	Antioxidant 2246	$C_{23}H_{32}O_2$	119-47-1
21.56	N,N-Dimethyllinoleamide	$C_{20}H_{37}NO$	2501-33-9
21.60	N,N-Dimethyloleamide	$C_{20}H_{39}NO$	2664-42-8
21.74	Dehydroabietic acid	$C_{20}H_{28}O_2$	1740-19-8
22.09	Antioxidant 425	$C_{25}H_{36}O_2$	88-24-4
23.02	Squalane	$C_{30}H_{62}$	111-01-3
23.83	13-Docosenamide, (Z)-	$C_{22}H_{43}NO$	112-84-5
26.81	Chondrillasterol	$C_{29}H_{48}O$	481-17-4
27.37	(24Z)-Ethylidenecholesterol	$C_{29}H_{48}O$	481-14-1

To gain higher confidence in E&L compound identification, the accurate mass information was used to either confirm or reject the compound ID with assistance of the ExactMass tool of the MassHunter Unknowns Analysis software. The ExactMass tool automatically assigns fragment ions with formulas that are a subset of the molecular formula of the top library hit, when possible. The library hit can be considered a false positive when most specific fragments do not match the compound formula within a small mass error. Figure 6 provides two such examples.

Due to the higher sensitivity in full spectrum acquisition mode and higher data acquisition rate of the GC/Q-TOF, compared to the GC/MSD, a few additional compounds have been identified by GC/Q-TOF (Table 3). These compounds included catalysts, solvents, vulcanization accelerators, plasticizers, antioxidants, and UV stabilizers used in rubber manufacturing. The compound identification was confirmed using accurate mass and RI information.

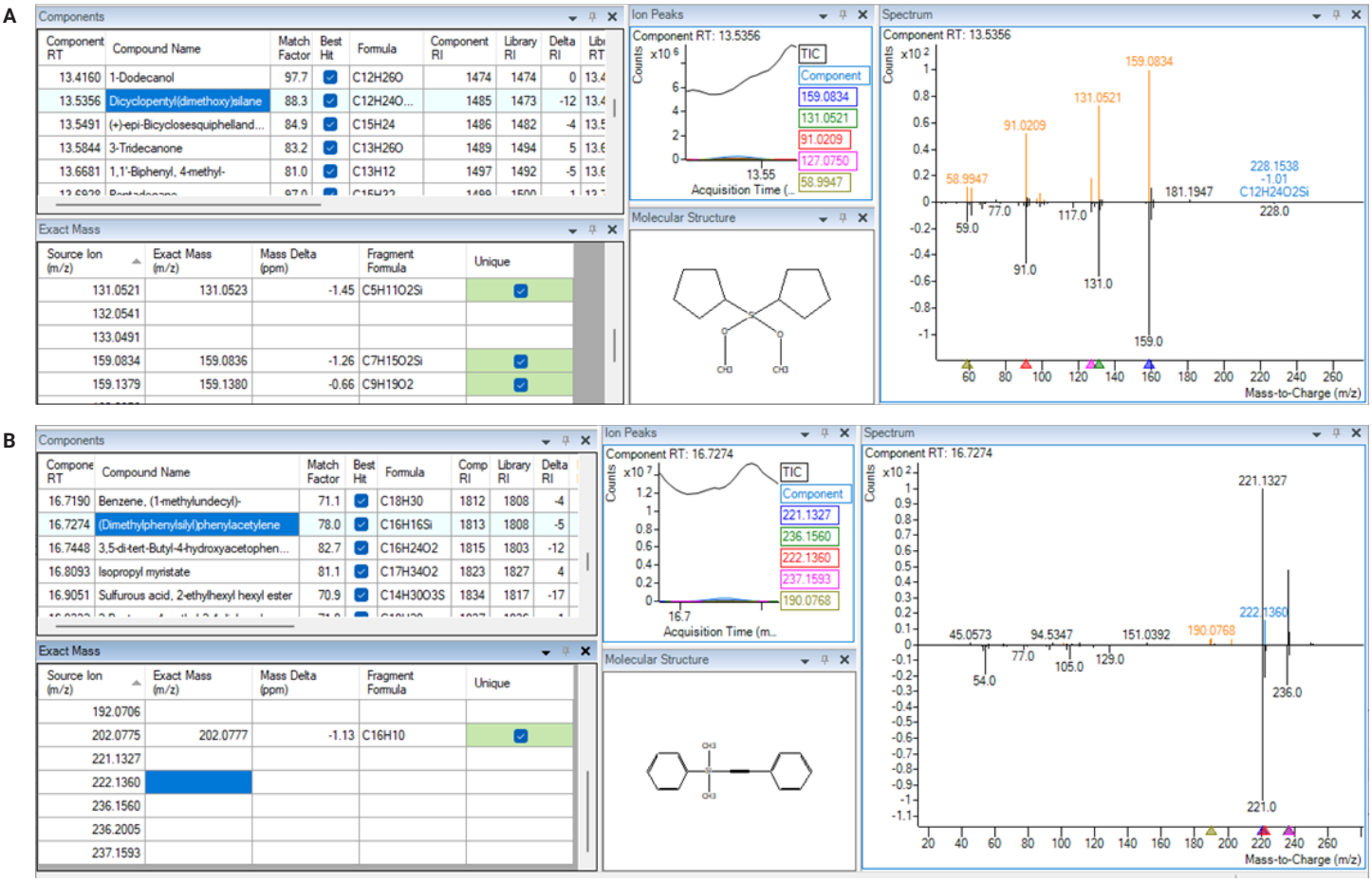

Figure 6. Confirmation of compound ID using accurate mass. Fragment formulas are assigned based on accurate mass and the molecular formula of the library hit. The mass error of each prominent fragment ion is then calculated and displayed in the ExactMass table. (A) A confirmed compound identified uniquely by GC/Q-TOF. (B) A false positive, as determined when processing the GC/Q-TOF data based on accurate mass. However, the same compound ID was incorrectly assigned to this spectrum based on the GC/MSD unit mass data with a high library match score of 89.

Table 3. Compounds identified uniquely by GC/Q-TOF.

RT	Compound Name	Match Factor	Formula	Delta RI	CAS No.
4.17	Methyl isobutyl ketone	92.8	$C_6H_{12}O$	−29.7	108-10-1
4.61	Acetylacetone	87.7	$C_5H_8O_2$	−19.7	123-54-6
4.63	Dimethylformamide	99.1	C_3H_7NO	−21.2	68-12-2
4.86	Hexanal	96.7	$C_6H_{12}O$	−18.9	66-25-1
5.03	Furfural	80.0	$C_5H_4O_2$	1.1	98-01-1
5.80	*o*-Xylene	96.5	C_8H_{10}	3.3	95-47-6
5.93	2,6-Lutidine (2,6-dimethylpyridine)	82.0	C_7H_9N	−14.1	108-48-5
6.02	2-Heptanone	94.6	$C_7H_{14}O$	−9.3	110-43-0
6.21	Heptanal	94.6	$C_7H_{14}O$	−11.7	111-71-7
6.66	3-Hepten-2-one	79.6	$C_7H_{12}O$	−6.2	1119-44-4
6.91	Piperidine, 2,2,6,6-tetramethyl-	91.0	$C_9H_{19}N$	−19.8	768-66-1
7.10	Benzaldehyde	90.9	C_7H_6O	−10.8	100-52-7
7.36	α-Methylstyrene	95.6	C_9H_{10}	−4.2	98-83-9
7.63	Octanal	89.1	$C_8H_{16}O$	−5.5	124-13-0
7.96	2-Ethylhexanol	92.6	$C_8H_{18}O$	−1.7	104-76-7
8.11	N-Methyl-α-pyrrolidone	84.7	C_5H_9NO	1.4	872-50-4
8.16	2-(2-Hydroxypropoxy)-1-propanol	82.7	$C_6H_{14}O_3$	0.1	106-62-7
9.01	Nonanal	96.3	$C_9H_{18}O$	−3.0	124-19-6
10.08	2,4-Dimethylthiophenol	89.1	$C_8H_{10}S$	19.0	13616-82-5
10.29	Benzene, 1,3-dibromo-	91.2	$C_6H_4Br_2$	14.1	108-36-1
10.70	Benzothiazole	92.2	C_7H_5NS	−9.3	95-16-9
11.44	*m*-tert-Butylphenol	72.0	$C_{10}H_{14}O$	−2.2	585-34-2
12.35	3-Hydroxy-2,2,4-trimethylpentyl 2-methylpropanoate**	73.2	$C_{12}H_{24}O_3$	−3.7	77-68-9
12.57	*p*-tert-Pentylphenol	74.3	$C_{11}H_{16}O$	3.2	80-46-6
13.27	BHT-quinol	84.6	$C_{15}H_{24}O_2$	14.2	10396-80-2
13.54	Dicyclopentyl(dimethoxy)silane	88.3	$C_{12}H_{24}O_2Si$	−11.9	126990-35-0
13.58	3-Tridecanone	83.2	$C_{13}H_{26}O$	4.6	1534-26-5
13.98	Ethyl 4-ethoxybenzoate	82.8	$C_{11}H_{14}O_3$	−5.7	23676-09-7
14.77	(2-Decyl)benzene	88.2	$C_{16}H_{26}$	10.0	4537-13-7
15.06	(1-Butylheptyl)benzene	83.8	$C_{17}H_{28}$	−4.1	4537-15-9
15.08	Fenuron	73.1	$C_9H_{12}N_2O$	−5.2	101-42-8
15.15	Benzophenone	93.4	$C_{13}H_{10}O$	−10.0	119-61-9
15.55	2,4-Ditert-butyl-6-nitrophenol	78.7	$C_{14}H_{21}NO_3$	1.7	20039-94-5
15.89	4-(1,1-Dimethylheptyl)phenol	83.2	$C_{15}H_{24}O$	−25.9	30784-30-6
16.69	Anthracene	86.4	$C_{14}H_{10}$	−23.5	120-12-7
17.17	Diisobutyl phthalate	88.5	$C_{16}H_{22}O_4$	5.0	84-69-5
17.70	Methyl hexadecanoate	74.6	$C_{17}H_{34}O_2$	1.3	112-39-0
19.01	*p*-Tolyl disulfide	73.8	$C_{14}H_{14}S_2$	3.4	103-19-5
21.05	Methyl dehydroabietate	79.9	$C_{21}H_{30}O_2$	−17.2	1235-74-1
22.26	Bis(2-ethylhexyl) phthalate (DEHP)	69.6	$C_{24}H_{38}O_4$	0.0	1000377-93-5
25.72	Tinuvin 770	87.1	$C_{28}H_{52}N_2O_4$	130.4*	52829-07-9

* Only predicted RI is available
** Component of texanol

Identification of unknown compounds in the rubber gasket extract

A few unknowns have been selected for further identification. A typical structure elucidation workflow of unknown compounds requires identification of the molecular ion as the first step. This is challenging when using a standard EI, as the abundance of molecular ions in EI is rarely preserved. Low-energy EI (LE-EI) is a type of soft ionization that could help increase the relative abundance of molecular ions and thus their tentative identification. This technique is enabled by the LE-EI capable source of the 7250 GC/Q-TOF and is complementary to chemical ionization (CI). This technique does not require a reagent gas or a source change and uses the same tune file as a standard EI. Based on LE-EI results, molecular ions of the unknown compounds were proposed and listed in Table 4.

Table 4. Molecular ion formulas of unknowns tentatively identified in the LE-EI experiments.

RT (min)	Tentative *m/z* of Molecular Ion	Formula
5.59	98.0362	$C_5H_6O_2$
6.37	142.0988	$C_8H_{14}O_2$
7.82	155.1067	$C_9H_{15}O_2$
8.44	143.1067	$C_8H_{15}O_2$
10.72	154.0988	$C_9H_{14}O_2$
11.93	166.0988	$C_{10}H_{14}O_2$
12.10	150.1039	$C_{10}H_{14}O$
13.31	182.0937	$C_{10}H_{14}O_3$
13.89	206.1301	$C_{13}H_{18}O_2$
15.19	250.1927	$C_{16}H_{26}O_2$

An example of how LE-EI can be used for identification or confirmation of molecular ions is shown in Figure 7, where a gradual increase of tentative molecular ion relative abundance at lower electron energies is observed.

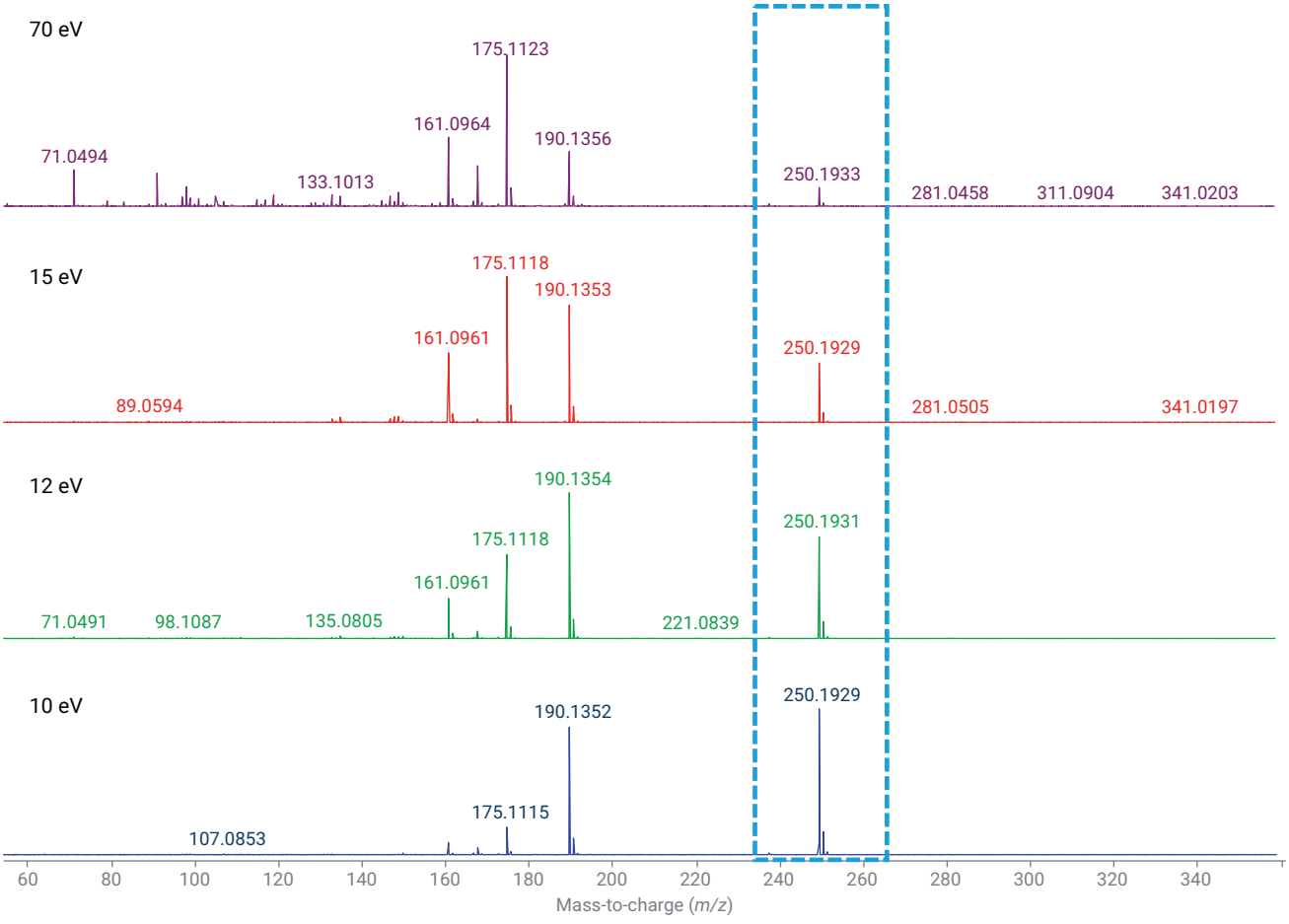

Figure 7. An example of using LE-EI to identify or confirm molecular ions. The lower the electron energy, the higher the relative abundance of the molecular ion. The tentative molecular ion is outlined in the rectangle.

Tentative molecular ions identified using LE-EI were selected as precursors in MS/MS experiments (Figure 8) to further perform structure elucidation. The target MS/MS was performed by alternating the MS/MS and full spectrum acquisition modes. The accurate *m/z* of the precursors were entered in the Acquisition software to facilitate correct recognition of the *m/z* of the molecular ion in the downstream data processing. The collision energy (CE) was optimized for each compound to yield optimal fragmentation, preserving an abundance of high- and mid-range *m/z* ions in the spectrum, when possible.

The structure elucidation was carried out in the MSC software. The molecular formulas were automatically assigned based on the accurate mass ions from the full spectrum data that matched the *m/z* of the precursor at the same RT. All possible structures for each tentative molecular formula were extracted from the ChemSpider database and evaluated based on fragmentation patterns. A proposed structure for one of the unknowns is shown in Figure 9.

This structure could potentially correspond to a degradation product of an antioxidant.

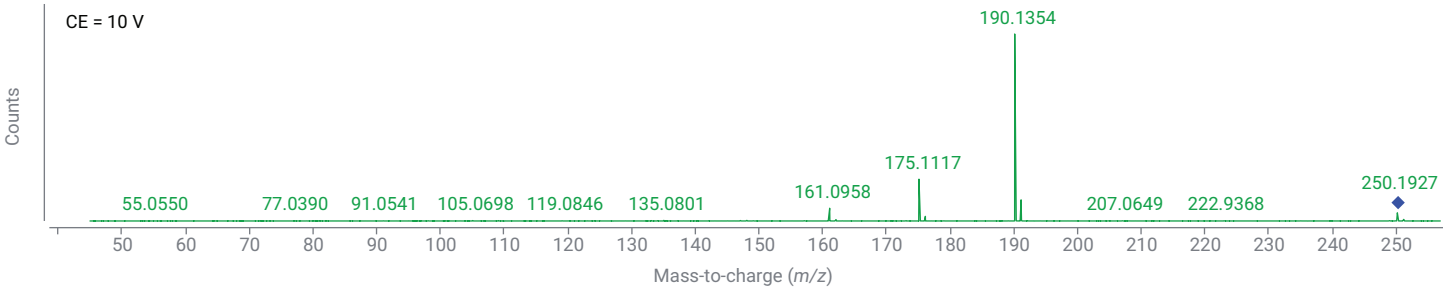

Figure 8. The MS/MS spectrum of one of the unknowns, using a tentative molecular ion as a precursor.

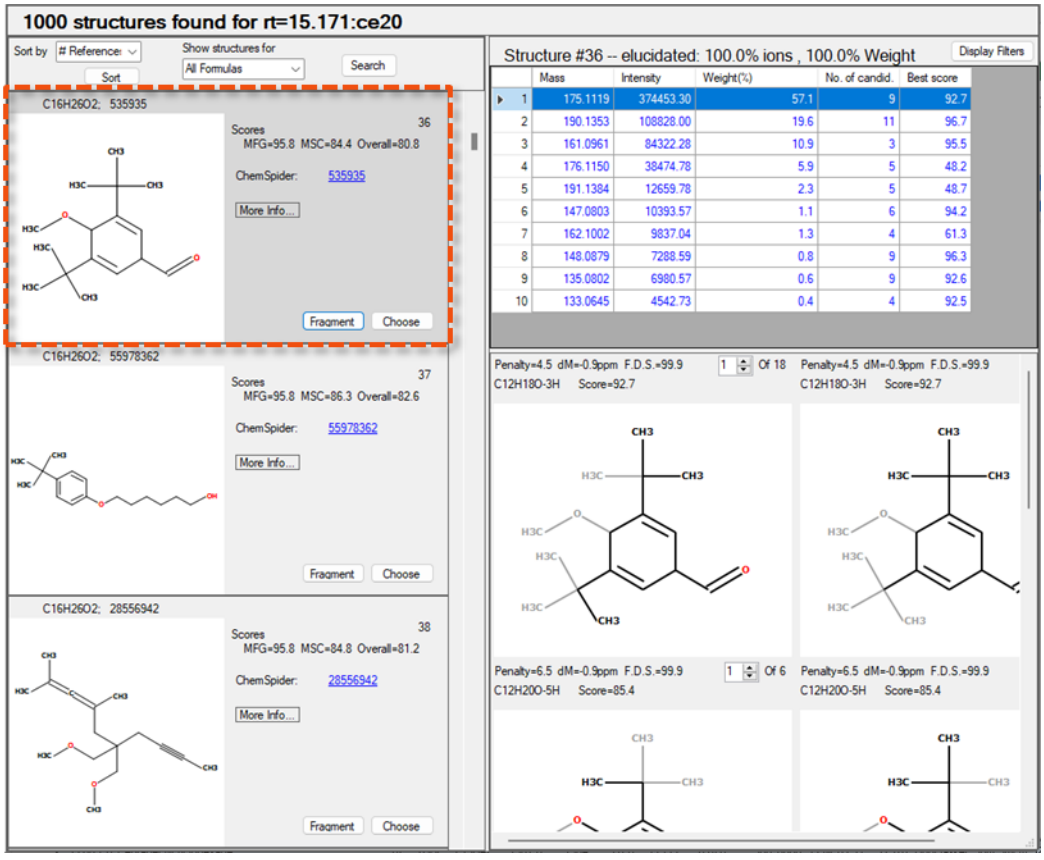

Figure 9. A proposed structure for one of the unknown compounds in rubber gasket extract using MSC.

Conclusion

The GC/MSD is an effective and accessible tool for the analysis of volatile and semivolatile compounds in complex E&L extracts. The established workflow includes deconvolution and an RI-based library search with the data acquisition performed in a compliant environment.

The high-resolution Agilent 7250 GC/Q-TOF enabled the identification of additional components with increased confidence, as well as structure elucidation of the unknown compounds.

Furthermore, using the novel ultra-low bleed Agilent J&W DB-5Q GC column resulted in a significant decrease in background, which helps in the identification of late-eluting compounds.

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