

USER NOTES:

Within each class, the compounds are ordered by retention time.

The following terms are used to specify the type of mass spectral identification:

- **Authentic MS RT:** matched to both the spectrum and retention time of an authentic material.
- **Authentic MS:** matched to the spectrum of an authentic material; compound is an isomer with a different retention time.
- **Reference Database MS:** matched to a spectrum in the NIST 2008 electron impact database.
- **Literature MS:** matched to a spectrum reported in the literature.
- **Manual - Congener Group:** manually identified and belonging to a family of observed congeners. At least one congener within the family was identified with Authentic MS RT criteria.
- **Manual:** spectrum identified through manual interpretation.
- **Unknown:** spectrum could not be identified.

Fragment Ions:

- The blue m/z values printed within the spectrum generally indicate the most abundant ion in the cluster.
- The m/z values within the identity table generally refer to the monoisotopic fragment ion.
- The marks printed above the spectrum indicate peaks described in the identity table: red for those belonging to named fragments and grey for interferences due to coeluting compounds.

Chemical Formulas: If there is only one element, the number is placed first (3Br is three bromines). If there are two or more elements, the number is placed second (Br3Cl is three bromines and one chlorine).

The retention times of the identified PCBs are described in the metadata, but the spectra are not included because of space considerations. Fifty-five PCB congeners were identified and they are commonly observed contaminants with known mass spectra.

INSTRUMENTAL METHOD:

The literature reference includes a description of the study goals, sample, extraction method, direct sample introduction method, GC×GC/TOF-MS method, the purpose and basic design of the software, and results. The instrumental method is repeated below:

A Pegasus 4D (LECO, St. Joseph, MI, USA) GC×GC/TOF-MS was used with a Restek (Bellefonte, PA, USA) Siltek deactivated column (5 m length, 0.25 mm i.d.) attached to the inlet as a guard column, a Restek Rtx5Sil-MS (15 m length, 0.25 mm i.d., 0.25 µm film thickness) as the first dimension of separation, and a J&W Scientific (Folsom, CA, USA) DB-17MS (2 m length, 0.18 mm, 0.18 µm thickness) as the second dimension of separation.

Ultrahigh-purity helium (Airgas, Radnor, PA, USA) was used as the carrier gas. The primary oven temperature was held at 60 °C for 7.5 min, then ramped at 10 °C/min to 300 °C and held for 20 min. The secondary oven temperature was programmed to be 20 °C higher than the primary oven. For GC×GC, the modulation period was set to 3.5 sec, with a 0.9 sec hot pulse duration and a 35 °C modulator temperature offset vs. the primary oven temperature. The MS transfer line and the ion source temperatures were at 270 °C and 250 °C, respectively. The electron energy was -80 eV and the detector voltage was 1850 V. The data acquisition rate was 100 spectra/sec.