# EPA Method 8270 Semi Volatile Organic Compounds Analysis on a New Benchtop Time-of-Flight Mass Spectrometer

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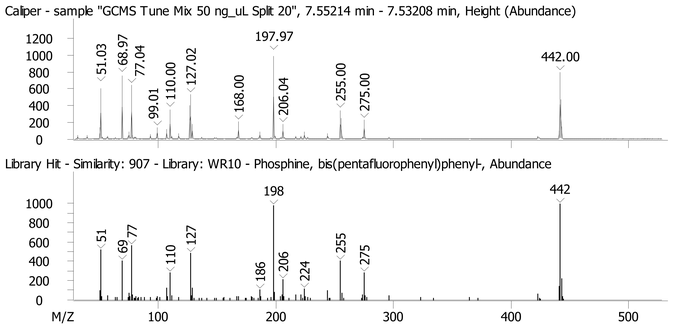
## Instrument Parameters and System Performance Evaluation

**GC-TOFMS (Pegasus® BT) Conditions**

| **Gas Chromatograph** | **LECO L-Pal3 Autosampler with Agilent 7890B GC** |
|---|---|
| Injection: | GC inlet, split 20:1 @ 270 °C |
| Carrier Gas: | He @ 1.4 ml/min, Constant Flow |
| Column: | ZB-SemiVolatiles, 30 m x 0.25 mm ID x 0.25 µm df (Phenomenex, Torrance, CA) |
| Oven Program: | 70 °C (1 min), to 285 °C @ 28 °C/min, to 305 °C @ 3 °C/min, to 320 °C @ 30 °C/min (1 min); Total time: 16.5 min |
| Transfer Line : | 300 °C |
| **Mass Spectrometer** | **LECO Pegasus BT** |
| Ion Source Temperature: | 250 °C |
| Mass Range: | 30-650 m/z |
| Acquisition Rate: | 10 spectra/s |

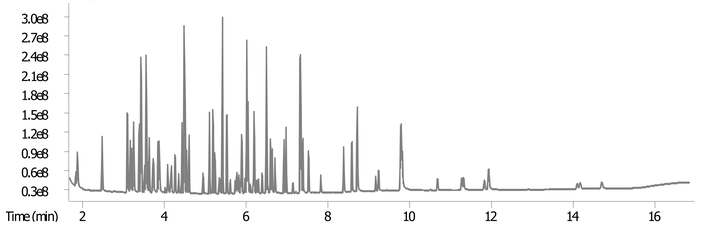
**DFTPP tuning results for 10 replicate injections shows the Pegasus BT routinely passes**

| Mass | Ion Abundance Criteria | Mean | STDEV | Min | Max | Criteria |
|---|---|---|---|---|---|---|
| 51 | 10-80% of Base Peak | 64.5 | 0.25 | 64.1 | 64.9 | PASS |
| 68 | < 2% of mass 69 | 1.93 | 0.04 | 1.87 | 1.98 | PASS |
| 70 | < 2% of mass 69 | 0.38 | 0.01 | 0.37 | 0.40 | PASS |
| 127 | 10-80% of Base Peak | 52.1 | 0.18 | 51.9 | 52.4 | PASS |
| 197 | < 2% of mass 69 | 0.22 | 0.03 | 0.19 | 0.28 | PASS |
| 198 | Base Peak, or > 50% of Mass 442 | | Base Peak | | | PASS |
| 199 | 5-9% of mass 198 | 6.73 | 0.04 | 6.68 | 6.77 | PASS |
| 275 | 10-60% of Base Peak | 23.0 | 0.08 | 22.9 | 23.1 | PASS |
| 365 | > 1% of mass 198 | 1.90 | 0.02 | 1.86 | 1.92 | PASS |
| 441 | Present but < 24% of mass 442 | 13.2 | 0.03 | 13.15 | 13.25 | PASS |
| 442 | Base Peak, or > 50% of mass 198 | 76.5 | 0.3 | 76.1 | 76.9 | PASS |
| 443 | 15-24% of mass 442 | 19.5 | 0.08 | 19.4 | 19.6 | PASS |

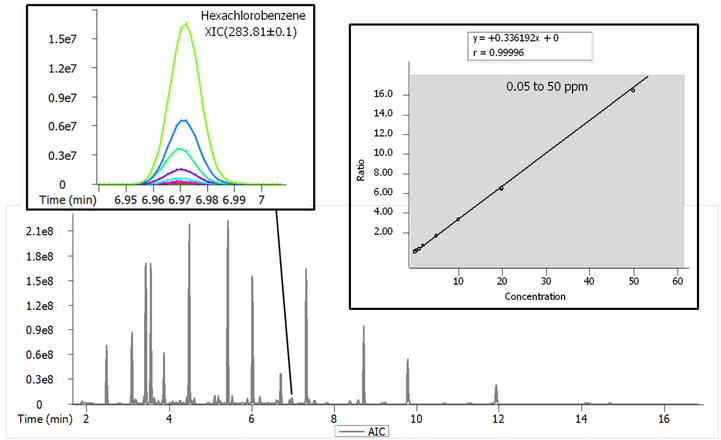


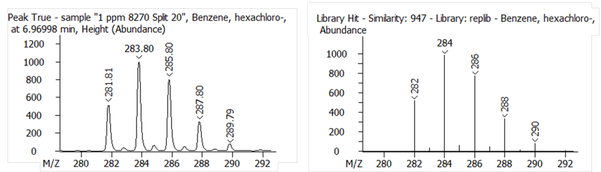

**DFTPP Spectrum from Pegasus BT (Top) and library (Bottom)**

## Quantitation in ChromaTOF® 5.0: Initial Calibration




**Total ion chromatogram (TIC) of a 5 ppm standard containing 90 components.**



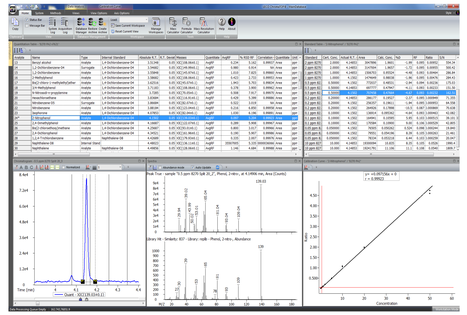




**Extracted ion chromatogram (XIC) of the quant mass for hexachlorobenzene (HCB) from 0.05 to 50 ppm and its corresponding calibration curve, with the Analytical Ion Chromatogram (AIC) of a 1 ppm standard split 20:1 indicating where HCB elutes in the chromatogram, and the profile mass spectrum of the molecular isotope cluster.**

Delivering the Right Results

## Calibration and Quantitation on LECO Pegasus BT

**Quantitation using ChromaTOF 5.0 to evaluate calibration data for 8270 compounds.**



**EPA Method 8270 Calibration Curve Data for 84 Compounds from 0.05 to 50 ppm.**

| Name | Type | R.T. (min) | Avg RF | % RSD RF | r |
|---|---|---|---|---|---|
| N-Nitrosodimethylamine | Analyte | 1.837 | 0.577 | 8.425 | ------ |
| Pyridine* | Analyte | 1.975 | 1.174 | 7.698 | ------ |
| 2-Fluorophenol | Surrogate | 2.475 | 0.367 | 5.14 | ------ |
| Phenol-d6 | Surrogate | 3.090 | 0.581 | 3.92 | ------ |
| Phenol* | Analyte | 3.100 | 0.314 | 7.758 | ------ |
| Aniline | Analyte | 3.163 | 1.304 | 3.669 | ------ |
| Bis(2-chloroethyl) ether | Analyte | 3.198 | 1.025 | 5.732 | ------ |
| 2-Chlorophenol-D4 | Surrogate | 3.242 | 0.373 | 3.895 | ------ |
| 2-Chlorophenol | Analyte | 3.253 | 0.398 | 7.524 | ------ |
| 1,3-Dichlorobenzene | Analyte | 3.380 | 1.032 | 6.147 | ------ |
| 1,4-Dichlorobenzene | Analyte | 3.437 | 1.075 | 7.583 | ------ |
| Benzyl alcohol | Analyte | 3.513 | 0.234 | 5.162 | ------ |
| 1,2-Dichlorobenzene-D4 | Surrogate | 3.547 | 0.98 | 0.914 | ------ |
| 1,2-Dichlorobenzene | Analyte | 3.558 | 1.01 | 7.825 | ------ |
| 2-Methylphenol | Analyte | 3.587 | 0.423 | 2.733 | ------ |
| Bis(2-chloro-1-methylethyl)ether | Analyte | 3.625 | 1.943 | 5.703 | ------ |
| 3/4-Methylphenol | Analyte | 3.712 | 0.378 | 3.9 | ------ |
| N-Nitrosodi-n-propylamine | Analyte | 3.729 | 0.508 | 7.917 | ------ |
| Hexachloroethane | Analyte | 3.837 | 0.429 | 5.399 | ------ |
| Nitrobenzene-D5 | Surrogate | 3.867 | 0.522 | 3.019 | ------ |
| Nitrobenzene | Analyte | 3.882 | 0.216 | 6.85 | ------ |
| Isophorone | Analyte | 4.079 | 1.03 | 6.196 | ------ |
| 2-Nitrophenol | Analyte | 4.150 | 0.098 | 5.204 | ------ |
| 2,4-Dimethylphenol | Analyte | 4.167 | 0.289 | 5.908 | ------ |
| Bis(2-chloroethoxy)methane | Analyte | 4.257 | 0.8 | 3.017 | ------ |
| 2,4-Dichlorophenol | Analyte | 4.345 | 0.19 | 5.907 | ------ |
| 1,2,4-Trichlorobenzene | Analyte | 4.427 | 0.335 | 2.007 | ------ |
| Naphthalene | Analyte | 4.499 | 1.146 | 4.684 | ------ |
| 4-Chloroaniline | Analyte | 4.537 | 0.772 | 7.899 | ------ |
| Hexachlorobutadiene | Analyte | 4.600 | 0.156 | 1.946 | ------ |
| 4-Chloro-3-methylphenol | Analyte | 4.944 | 0.251 | 5.033 | ------ |
| 2-Methylnaphthalene | Analyte | 5.097 | 0.588 | 5.282 | ------ |
| 1-Methylnaphthalene | Analyte | 5.184 | 0.578 | 5.149 | ------ |
| Hexachlorocyclopentadiene | Analyte | 5.232 | 0.326 | 2.02 | ------ |
| 2,4,6-Trichlorophenol | Analyte | 5.337 | 0.089 | 6.534 | ------ |
| 2,4,5-Trichlorophenol | Analyte | 5.364 | 0.101 | 9.49 | ------ |
| 2-Fluorobiphenyl | Surrogate | 5.415 | 1.771 | 3.367 | ------ |
| 2-Chloronaphthalene | Analyte | 5.524 | 1.554 | 3.336 | ------ |
| 2-Nitroaniline | Analyte | 5.607 | 0.127 | 7.753 | ------ |
| 1,4-Dinitrobenzene | Analyte | 5.729 | 0.056 | 7.153 | ------ |
| Dimethyl phthalate | Analyte | 5.767 | 0.552 | 6.982 | ------ |
| 1,3-Dinitrobenzene | Analyte | 5.790 | 0.104 | 7.962 | ------ |

| Name | Type | R.T. (min) | Avg RF | % RSD RF | r |
|---|---|---|---|---|---|
| 2,6-Dinitrotoluene | Analyte | 5.819 | 0.171 | 7.38 | ------ |
| 1,2-Dinitrobenzene | Analyte | 5.864 | 0.072 | 8.875 | ------ |
| Acenaphthylene | Analyte | 5.889 | 2.2 | 7.71 | ------ |
| 3-Nitroaniline | Analyte | 5.965 | 0.173 | 6.112 | ------ |
| Acenaphthene | Analyte | 6.040 | 1.341 | 2.539 | ------ |
| 2,4-Dinitrophenol‡ | Analyte | 6.057 | 0.04 | 10.238 | ------ |
| 4-Nitrophenol | Analyte | 6.095 | 0.112 | 5.813 | ------ |
| 2,4-Dinitrotoluene | Analyte | 6.170 | 0.166 | 7.711 | ------ |
| Dibenzofuran | Analyte | 6.192 | 2.148 | 1.868 | ------ |
| 2,3,5,6-Tetrachlorophenol | Analyte | 6.255 | 0.08 | 10.589 | ------ |
| 2,3,4,6-Tetrachlorophenol | Analyte | 6.292 | 0.089 | 11.549 | ------ |
| Diethyl Phthalate | Analyte | 6.385 | 0.483 | 8.33 | ------ |
| 4-Chlorophenyl phenyl ether | Analyte | 6.490 | 0.671 | 3.345 | ------ |
| Fluorene | Analyte | 6.492 | 1.249 | 6.793 | ------ |
| 4-Nitroaniline | Analyte | 6.497 | 0.186 | 5.994 | ------ |
| 4,6-Dinitro-2-methylphenol | Analyte | 6.525 | 0.052 | 8.015 | ------ |
| Diphenylamine | Analyte | 6.592 | 1.097 | 4.717 | ------ |
| Azobenzene | Analyte | 6.630 | 0.289 | 7.106 | ------ |
| 2,4,6-Tribromophenol | Surrogate | 6.700 | 0.079 | 6.93 | ------ |
| 4-Bromophenyl phenyl ether | Analyte | 6.920 | 0.438 | 8.076 | ------ |
| Hexachlorobenzene | Analyte | 6.970 | 0.336 | 2.276 | ------ |
| Pentachlorophenol* | Analyte | 7.140 | 0.038 | 11.186 | ------ |
| Phenanthrene | Analyte | 7.337 | 1.335 | 4.781 | ------ |
| Anthracene | Analyte | 7.382 | 1.828 | 3.421 | ------ |
| Carbazole | Analyte | 7.519 | 1.436 | 3.42 | ------ |
| Dibutyl phthalate | Analyte | 7.820 | 0.357 | 10.856 | ------ |
| Fluoranthene | Analyte | 8.379 | 1.479 | 1.563 | ------ |
| Pyrene | Analyte | 8.579 | 1.542 | 3.832 | ------ |
| p-Terphenyl-d14 | Surrogate | 8.712 | 0.52 | 8.99 | ------ |
| Benzyl butyl phthalate | Analyte | 9.164 | 0.141 | 9.953 | ------ |
| Bis(2-ethylhexyl) adipate | Analyte | 9.234 | 0.131 | 9.617 | ------ |
| Benz[a]anthracene | Analyte | 9.767 | | | 0.9987 |
| Bis(2-ethylhexyl)phthalate* | Analyte | 9.791 | 0.239 | 10.425 | ------ |
| Chrysene | Analyte | 9.811 | 1.379 | 4.165 | ------ |
| Di-n-octyl phthalate | Analyte | 10.676 | 0.279 | 7.858 | ------ |
| Benzo[b]fluoranthene | Analyte | 11.264 | 1.041 | 6.505 | ------ |
| Benzo[k]fluoranthene | Analyte | 11.309 | 1.114 | 7.535 | ------ |
| Benzo[a]pyrene | Analyte | 11.821 | 0.896 | 7.607 | ------ |
| Indeno[1,2,3-cd]pyrene | Analyte | 14.094 | 0.633 | 8.146 | ------ |
| Dibenz[a,h]anthracene | Analyte | 14.164 | 0.704 | 7.091 | ------ |
| Benzo[ghi]perylene | Analyte | 14.691 | 0.926 | 7.95 | ------ |

*The 0.05 ppm standard was not included in the calibration curve because the %D was greater than 20%. ‡ The detection limit was 0.2 ppm for 2,4-Dinitrophenol.

## Summary

- The Pegasus BT is a powerful instrument for target and non-target analysis in the same data acquisition.
- Pegasus BT meets or exceeds the EPA Method 8270 requirements for instrument performance.
- With TOFMS, all of the masses are collected all the time without compromising sensitivity and without mass spectral skewing, resulting in unsurpassed spectral fidelity for library database searching and identifying analytes with confidence.