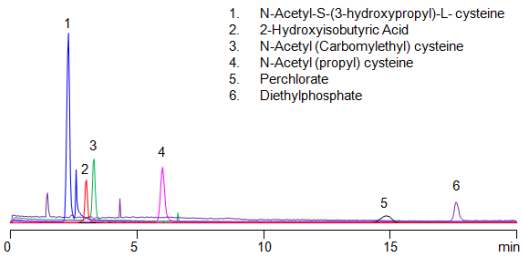
# HPLC-MS Method for Separation of Metabolites and Biomarkers on Newcrom B Column

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|---|---|
| **Column**: | Newcrom B |
| **Column size:** | 4.6 × 150 mm, 5 µm, 100A |
| **Column part number:** | NB-46.150.0510 |
| **Mobile phase:** | Gradient MeCN – 5-50%, 20 min |
| **Buffer:** | Ammonium acetate pH 4.0 –10-25 mM, 20 min |
| **Flow rate:** | 1.0 mL/min |
| **Detection:** | ESI- and ESI+ |

| # | Compound | Expected m/z | Observed m/z | ESI Mode |
|---|---|---|---|---|
| 1 | 3HPMA | 220 | 182 | *Positive* |
| 2 | 2HIB | 103 | 103 | Negative |
| 3 | NAE | 233 | 235 | *Positive* |
| 4 | NAPR | 204 | 206 | *Positive* |
| 5 | PERC | 99 | 99 | Negative |
| 6 | DPP | 248 | 249 | Negative |

Separation type: Liquid Chromatography Mixed-mode

Metabolites and biomarkers are key terms in the fields of biochemistry, pharmacology, and medicine.

N-Acetyl-S-(3-hydroxypropyl)-L-cysteine (3HPMA) is a common metabolite of the herbicide and pollutant Acrolein. 2-Hydroxyisobutyric Acid (2HIB) is a neuro and adrenal toxin that is a common metabolite of the fuel additives Methyl tert-butyl ether (MTBE) and Ethyl tert-butyl ether (ETBE). N-Acetyl(Carbomylethyl)cysteine (NAE) is a metabolite of Acrylamide which can act as a neuro toxin in cases of long term exposure. N-Acetyl(propyl)cysteine (NAPR) is a metabolite of the popular industrial organic solvent 1-bromopropane (1-BP). Perchlorate (PERC) inhibits thyroid activity and can be used to treat hyperthyroidism, but can be toxic in large amounts or in regularly-functioning thyroids. Diphenylphosphate (DPP) is a metabolite of the popular flame retardant triphenyl phosphate (TPHP). These acidic toxin metabolites can be retained, separated, and analyzed on a mixed-mode Newcrom B column with a mobile phase consisting of water, Acetonitrile (MeCN), and Ammonium Acetate (AmAc). This analytical method can be detected with high resolution and peak symmetry with many evaporative detection methods, including Evaporative Light Scattering Detection (ELSD), Charged Aerosol Detector (CAD), and Electrospray Ionization (ESI) for Mass Spectrometry (MS).

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## Method Parameters

| | |
|---|---|
| **Column** | Newcrom B, 4.6 x 150 mm, 5 µm, 100 Å, dual ended |
| **Mobile Phase** | Gradient MeCN/H2O – 5-50%, 20 min |
| **Buffer** | Gradient Ammonium acetate pH 4.0 –10-25 mM, 20 min |
| **Flow Rate** | 1.0 mL/min |
| **Detection** | ESI- and ESI |

Quelle: https://sielc.com/hplc-determination-of-biomarkers