

Supplementary table 3. Headspace GC-MS performance metrics, with the authentic standards used in the study.

Abbreviations: LOQ, limit of quantitation (lowest point of calibration curve); RSD, relative standard deviation. Analytes: ACN, allyl cyanide; AITC, allyl isothiocyanate; CS₂, carbon disulfide; Me₂S, dimethyl sulfide; PCN, phenylpropionitrile; PEITC, phenylethyl isothiocyanate. Intraday and interday RSD was calculated from samples 0.005 µL of each authentic standard (3.35E-05 – 8.29E-05 mmol, depending on analyte), diluted with MeCN.

| Analyte | LOQ average, mmol | Average R ² | Intraday RSD | Interday RSD | Example equation |
|-------------------|-------------------|------------------------|--------------|--------------|-------------------------|
| acetone | 5.79E-07 | 0.9958 | 17.80% | 15.76% | y = 7.74E+11 x -9.58E+5 |
| ACN | 1.09E-06 | 0.9846 | 13.29% | 0.54% | y = 1.37E+12 x -5.90E+6 |
| AITC | 1.02E-06 | 0.9515 | 17.10% | 12.78% | y = 2.35E+12 x -1.10E+7 |
| CS ₂ | 6.64E-06 | 0.9725 | 8.43% | 2.76% | y = 5.30E+11 x -2.55E+6 |
| ethyl acetate | 1.82E-06 | 0.9880 | 10.74% | 15.26% | y = 1.13E+12 x -3.33E+6 |
| Me ₂ S | 8.84E-06 | 0.9782 | 18.41% | 40.22% | y = 4.19E+11 x -1.92E+6 |
| methyl acetate | 2.33E-06 | 0.9921 | 15.55% | 32.85% | y = 4.22E+11 x -9.88E+5 |
| methyl formate | 2.95E-06 | 0.9933 | 11.58% | 62.14% | y = 1.42E+11 x -5.87E+5 |
| PCN | 5.96E-07 | 0.9488 | 22.15% | 10.04% | y = 8.83E+12 x -3.07E+7 |
| PEITC | 2.85E-07 | 0.9514 | 25.05% | 9.04% | y = 1.24E+13 x -3.31E+7 |