ANALYSIS OF BIOCIDES USING UPLC®

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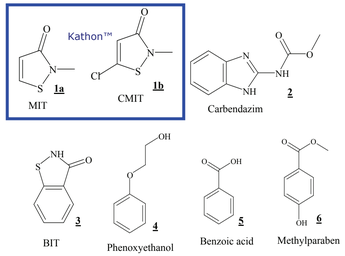
Solution for Biocide Analysis

Experiment:

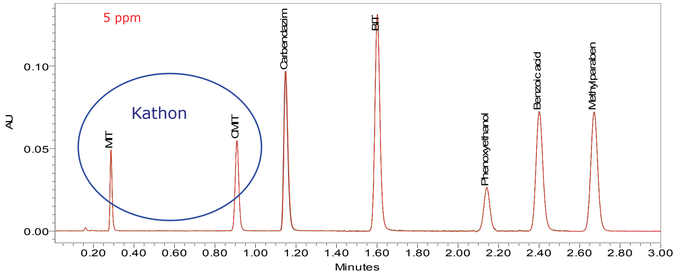
3-minute analysis of a blend of common biocides



Instrument and Operation Conditions

LC:	ACQUITY UPLC® with PDA
Software:	Empower™
Column:	ACQUITY UPLC BEH C_{18} 2.1 mm x 50 mm
Weak Wash:	95:5 H_2O/CH_3CN (600 µL)
Strong Wash:	50:50 H_2O/CH_3CN (600 µL)
Mobile Phase A:	0.05v% of TFA in H_2O
Mobile Phase B:	0.05v% of TFA in CH_3CN
Linear Gradient:	5% B to 15% B in 2.9 min
Flow Rate:	1 mL/min
Sampling Rate:	20 pt/s
Injection Volume:	5 µL
Column Temperature:	30 °C
PDA:	210-500 nm
PDA Filter Response:	0.1 sec

Overlay 9 Replicate Injections: PDA Timed Chromatograms



UPLC® RT Reproducibility

Table 1.
Component Summary For Retention Time

	MIT (min)	CMIT (min)	Carbendazim (min)	BIT (min)	Phenoxyethanol (min)	Benzoic acid (min)	Methylparaben (min)
1	0.286	0.908	1.147	1.600	2.141	2.400	2.671
2	0.286	0.908	1.147	1.601	2.141	2.401	2.672
3	0.287	0.908	1.147	1.601	2.141	2.400	2.671
4	0.286	0.908	1.148	1.602	2.142	2.401	2.672
5	0.286	0.908	1.148	1.601	2.141	2.400	2.671
6	0.286	0.908	1.149	1.602	2.142	2.401	2.672
7	0.287	0.908	1.148	1.601	2.141	2.400	2.671
8	0.286	0.908	1.150	1.602	2.142	2.401	2.672
9	0.287	0.909	1.150	1.602	2.142	2.401	2.672
Mean	0.286	0.908	1.148	1.601	2.142	2.401	2.672
Std. Dev.	0.001	0.000	0.001	0.001	0.001	0.001	0.001
% RSD	0.19	0.04	0.10	0.03	0.03	0.02	0.02

UPLC® Area Reproducibility

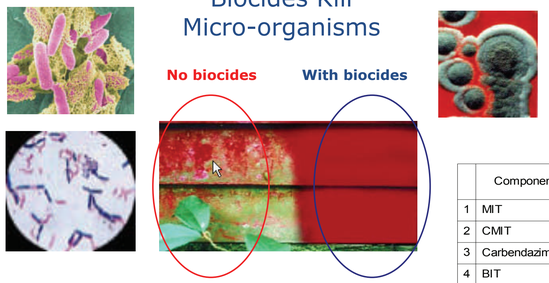
Table 2.
Component Summary For Area

	MIT	CMIT	Carbendazim	BIT	Phenoxyethanol	Benzoic acid	Methylparaben
1	34745	68748	134846	227719	57857	172510	173458
2	34730	68894	134698	228692	57882	173440	172053
3	34684	69423	134511	227840	57682	170783	172192
4	34741	69168	135187	228238	57388	173125	172113
5	34761	68952	134533	228331	58008	170433	172156
6	34673	69132	134817	228461	57802	170579	171725
7	34753	68903	135014	228616	57863	172557	171723
8	34781	68736	135018	227710	57845	170954	171833
9	34782	69050	134694	228489	57809	172072	172143
Mean	34739	69001	134813	228233	57793	171828	172155
Std. Dev.	38	219	229	383	174	1157	523
% RSD	0.1	0.3	0.2	0.2	0.3	0.7	0.3

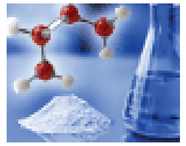
What Do They Have in Common?

Protected by Biocides!

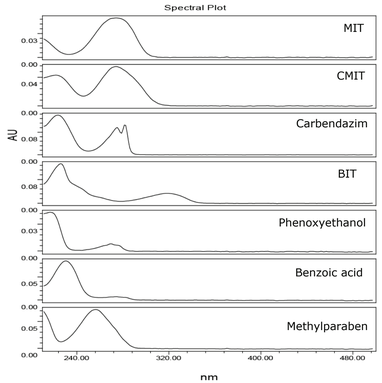
Biocides Kill Micro-organisms



Needs for Biocide Analysis



Meet Regulatory Mandates to Protect



UV Spectra

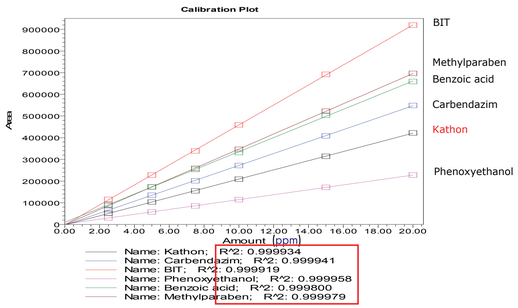
Extracted from PDA Chromatograms for Library & Peak Purity:

- Confirm peak identity
- Assure non-coelution of spectrally dissimilar components

PDA library matching results table

	Component	Match1 Spect. Name	Match1 Angle	Match1 Threshold	Purity1 Angle	Purity1 Threshold
1	MIT	2-methyl-4-isothiazolin-3-one	0.488	1.585	0.705	1.035
2	CMIT	5-chloro-2-methyl-4-isothiazoline-3-one	0.293	1.465	0.694	0.842
3	Carbendazim	carbendazim	0.169	1.239	0.320	0.546
4	BIT	1,2-benzisothiazol-3-one	0.181	1.277	0.371	0.616
5	Phenoxyethanol	2-phenoxyethanol	0.820	2.663	2.062	2.449
6	Benzoic acid	benzoic acid	0.217	1.387	0.508	0.703
7	Methylparaben	methylparaben	0.288	1.385	0.465	0.726

UV/PDA Calibration Curves



Conclusions

ACQUITY UPLC® System rapidly and accurately analyzes biocides

- Separate 7 components in 3 minutes
  - Baseline resolution
- Excellent reproducibility
- Great sensitivity

Empower™ data automation, from collection to reporting

- Peak purity & identification
- Calibration & quantification
- Custom calculations
- Automate report generation

Ideal solution for:
QC, product development, and problem-solving

References

1. P. J. Lee, A. J. Di Gioia, *ACQUITY UPLC PDA ANALYSIS OF BIOCIDES (PART 1), Waters Corporation*, Application Note 720001832EN, **2006**.
2. P. J. Lee, A. J. Di Gioia, *ACQUITY UPLC PDA ANALYSIS OF BIOCIDES (PART 2): PASS OR FAIL CUSTOM CALCULATION, Waters Corporation*, Application Note 720001833EN, **2006**.
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