

Mass spectral studies of N-Oxides of CWC related aminoethanols by GC/MS after silylation[†]

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SUPPLEMENTARY INFORMATION

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Table S1. HRMS data for the ions detected in the EIMS of compounds **1-13**.

Compound No.	ion (<i>m/z</i>)	Elemental composition	Observed mass (<i>m/z</i>)	Calculated mass (<i>m/z</i>)	Error (ppm)
1	366	C ₁₄ H ₃₆ NO ₄ Si ₃	366.1946	366.1952	-1.68
	278	C ₁₁ H ₂₈ NO ₃ Si ₂	278.1608	278.1619	3.87
	262	C ₁₁ H ₂₈ NO ₂ Si ₂	262.1673	262.1688	-5.95
	89	C ₃ H ₉ O ₂ Si	89.04315	89.04227	9.95
	73	C ₃ H ₉ Si	73.0469	73.0474	-5.98
2	279	C ₁₁ H ₂₉ NO ₃ Si ₂	279.1686	279.1689	1.20
	264	C ₁₀ H ₂₆ NO ₃ Si ₂	264.1451	264.1439	-4.75
	176	C ₇ H ₁₈ NO ₂ Si	176.1107	176.1099	-4.21
	160	C ₇ H ₁₈ NOSi	160.1158	160.1167	5.52
	73	C ₃ H ₉ Si	73.0479	73.0473	7.66
3	293	C ₁₂ H ₃₁ NO ₃ Si ₂	293.1838	293.1842	-1.63
	278	C ₁₁ H ₂₈ NO ₃ Si ₂	278.1615	278.1608	2.76
	73	C ₃ H ₉ Si	73.0468	73.0474	-7.25
4	177	C ₇ H ₁₉ NO ₂ Si	177.1185	177.1183	-1.45
	162	C ₆ H ₁₆ NO ₂ Si	162.0950	162.0940	-6.19
	89	C ₃ H ₉ O ₂ Si	89.0423	89.0418	-5.58
	88	C ₄ H ₁₀ N ₂ O	88.0771	88.0762	9.87
	72	C ₄ H ₁₀ N	72.0821	72.0813	11.09
5	191	C ₈ H ₂₁ NO ₂ Si	191.1338	191.1339	-1.19
	176	C ₇ H ₁₈ NO ₂ Si	176.1107	176.1101	-3.01
	160	C ₈ H ₂₀ O ₂ Si	160.1286	160.1283	1.81
	146	C ₆ H ₁₆ NOSi	146.0989	146.1001	-7.95
	86	C ₅ H ₁₂ N	86.0962	86.0970	-9.40
	72	C ₄ H ₁₀ N	72.0832	72.0813	9.01
6	58	C ₃ H ₇ N	58.0546	58.0549	-5.37
	205	C ₉ H ₂₃ NO ₂ Si	205.1498	205.1497	-0.65
	190	C ₈ H ₂₀ NO ₂ Si	190.1263	190.1280	8.53
	176	C ₇ H ₁₈ NO ₂ Si	176.1107	176.1109	1.50
	86	C ₅ H ₁₂ N	86.0970	86.0972	2.40
	116	C ₄ H ₁₀ NOSi	116.0529	116.0532	-2.47
	100	C ₆ H ₁₄ N	100.1121	100.1126	-5.01
	160	C ₇ H ₁₆ NO ₂ Si	160.0936	160.0920	-5.01
	130	C ₅ H ₁₂ NOSi	130.0681	130.0688	-5.49
	148	C ₅ H ₁₄ NO ₂ Si	148.0811	148.0794	11.70
	174	C ₈ H ₂₀ NOSi	174.1294	174.1314	-11.60
7	146	C ₆ H ₁₆ NOSi	146.1000	146.1001	-0.75
	205	C ₉ H ₂₃ NO ₂ Si	205.1498	205.1489	-4.32
	190	C ₈ H ₂₀ NO ₂ Si	190.1263	190.1270	3.61
	130	C ₅ H ₁₂ NOSi	130.0690	130.0688	1.60
	86	C ₅ H ₁₂ N	86.0969	86.0964	-6.26
	116	C ₄ H ₁₀ NOSi	116.0528	116.0532	-3.60
	100	C ₆ H ₁₄ N	100.1128	100.1126	1.68
	148	C ₆ H ₁₄ NOSi	148.0808	148.0794	9.49
	174	C ₈ H ₂₀ NOSi	174.1300	174.1314	-8.08
	146	C ₆ H ₁₆ NOSi	146.1013	146.1001	8.25
8	160	C ₇ H ₁₈ NOSi	160.1147	160.1158	-6.70
	205	C ₉ H ₂₃ NO ₂ Si	205.1498	205.1497	-0.77
	190	C ₈ H ₂₀ NO ₂ Si	190.1263	190.1276	6.40
	116	C ₄ H ₁₀ NOSi	116.0532	116.0524	-6.99

	100	C ₆ H ₁₄ N	100.1130	100.1126	3.92
	86	C ₅ H ₁₂ N	86.0977	86.0970	8.30
	174	C ₈ H ₂₀ NOSi	174.1334	174.1314	11.56
	146	C ₆ H ₁₆ NOSi	146.0991	146.1001	-6.95
	144	C ₆ H ₁₄ NOSi	144.0858	144.0845	9.37
9	219	C ₁₀ H ₂₅ NO ₂ Si	219.1612	219.1655	-4.53
	204	C ₉ H ₂₂ NO ₂ Si	204.1399	204.1420	-10.34
	190	C ₈ H ₂₀ NO ₂ Si	190.1253	190.1263	-5.59
	100	C ₆ H ₁₄ N	100.112	100.1126	-3.27
	130	C ₆ H ₁₆ NO	130.1217	130.1232	-11.45
	114	C ₇ H ₁₆ N	114.1293	114.1283	9.37
10	219	C ₁₀ H ₂₅ NO ₂ Si	219.1991	219.1655	3.01
	204	C ₉ H ₂₂ NO ₂ Si	204.1424	204.1420	2.25
	100	C ₆ H ₁₄ N	100.1118	100.1126	-8.34
	130	C ₆ H ₁₆ NO	130.1224	130.1232	-6.30
	114	C ₇ H ₁₆ N	114.1296	114.1283	11.74
11	233	C ₁₁ H ₂₇ NO ₂ Si	233.1821	233.1811	4.36
	218	C ₁₀ H ₂₄ NO ₂ Si	218.1589	218.1576	5.88
	204	C ₉ H ₂₂ NO ₂ Si	204.1401	204.1420	-9.17
	130	C ₉ H ₁₈ N	130.0664	130.0657	5.53
	128	C ₈ H ₁₈ N	128.1451	128.1439	9.44
	114	C ₇ H ₁₆ N	114.1276	114.1283	-5.96
12	233	C ₁₁ H ₂₇ NO ₂ Si	233.1829	233.1811	7.59
	218	C ₁₀ H ₂₄ NO ₂ Si	218.1580	218.1576	1.60
	204	C ₉ H ₂₂ NO ₂ Si	204.1423	204.1420	1.70
	114	C ₇ H ₁₆ N	114.1279	114.1283	-3.68
13	233	C ₁₁ H ₂₇ NO ₂ Si	233.1810	233.1811	-0.55
	218	C ₁₀ H ₂₄ NO ₂ Si	218.1587	218.1576	4.80
	204	C ₉ H ₂₂ NO ₂ Si	204.1428	204.1420	3.79
	114	C ₇ H ₁₆ N	114.1290	114.1283	6.45

Table S2. HRMS data for the ions detected in the CIMS of compound 5.

Ion	(<i>m/z</i>)	Elemental composition	Observed mass (<i>m/z</i>)	Calculated mass (<i>m/z</i>)	Error (ppm)
[M+H]⁺	206	C ₉ H ₂₄ NO ₂ Si	206.1586	206.1576	4.8
[MH-O]⁺	190	C ₉ H ₂₄ NOSi	190.1637	190.1627	5.3
[MH-(O-CH₃)]⁺	174	C ₈ H ₂₀ NOSi	174.1322	174.1314	4.6

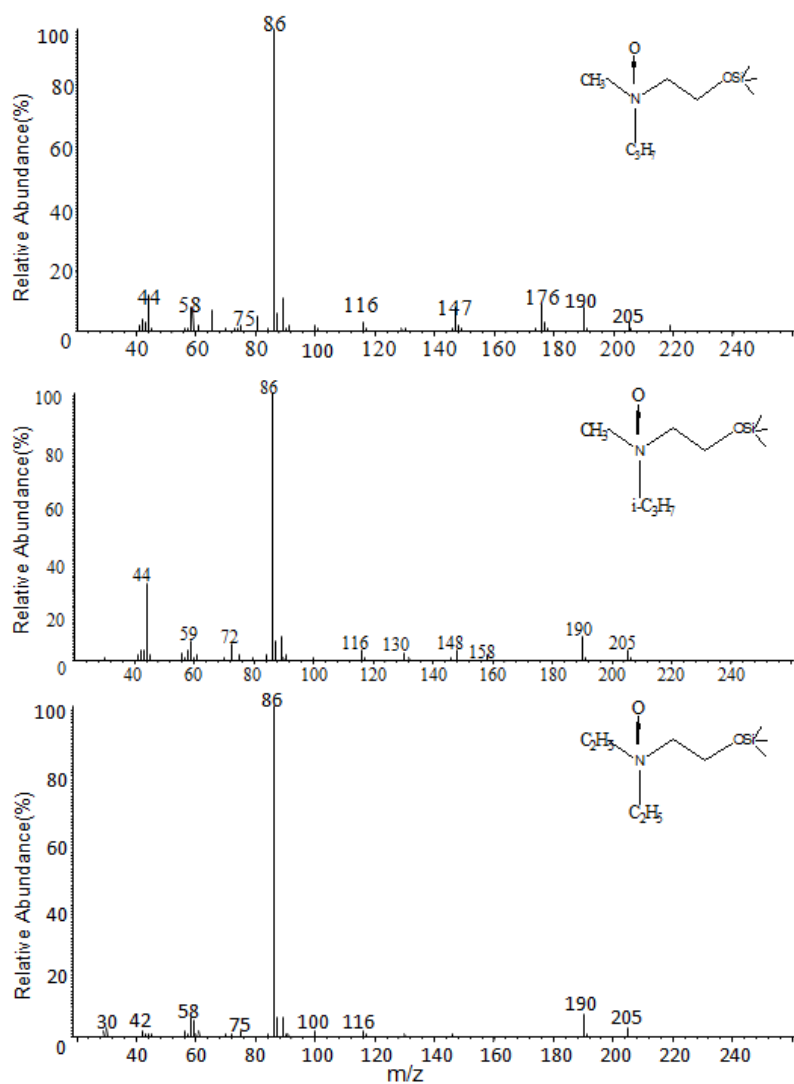


Figure S1. EI mass spectra of compounds 11, 12 and 13.

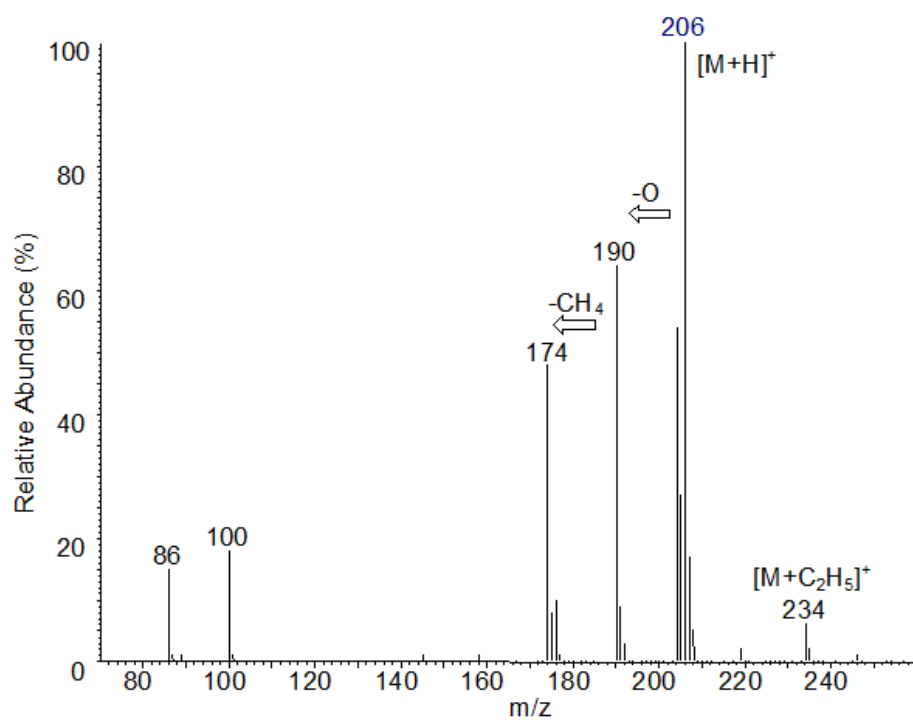


Figure S2. Methane/CI mass spectrum of compound 7.

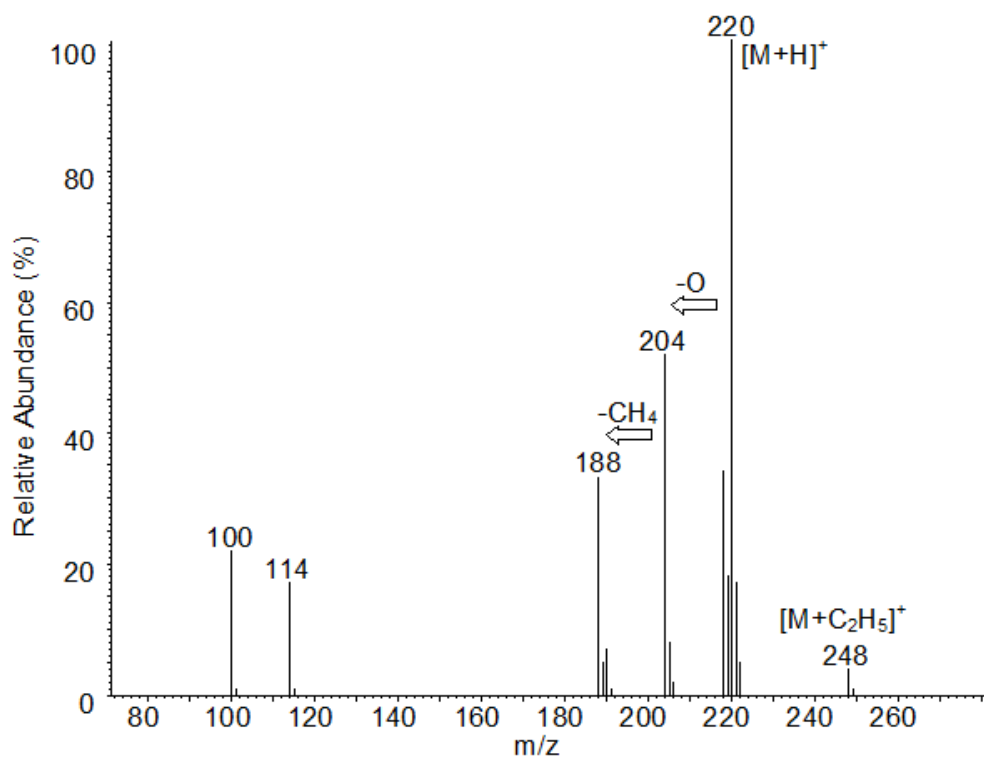


Figure S3. Methane/CI mass spectrum of compound 9.

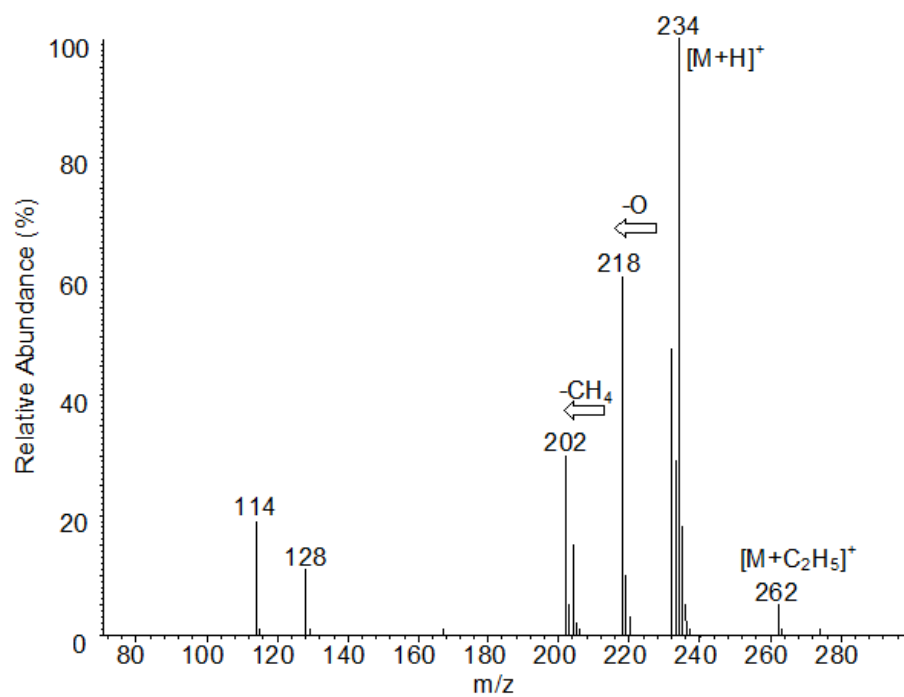


Figure S4. Methane/CI mass spectrum of compound **11**.

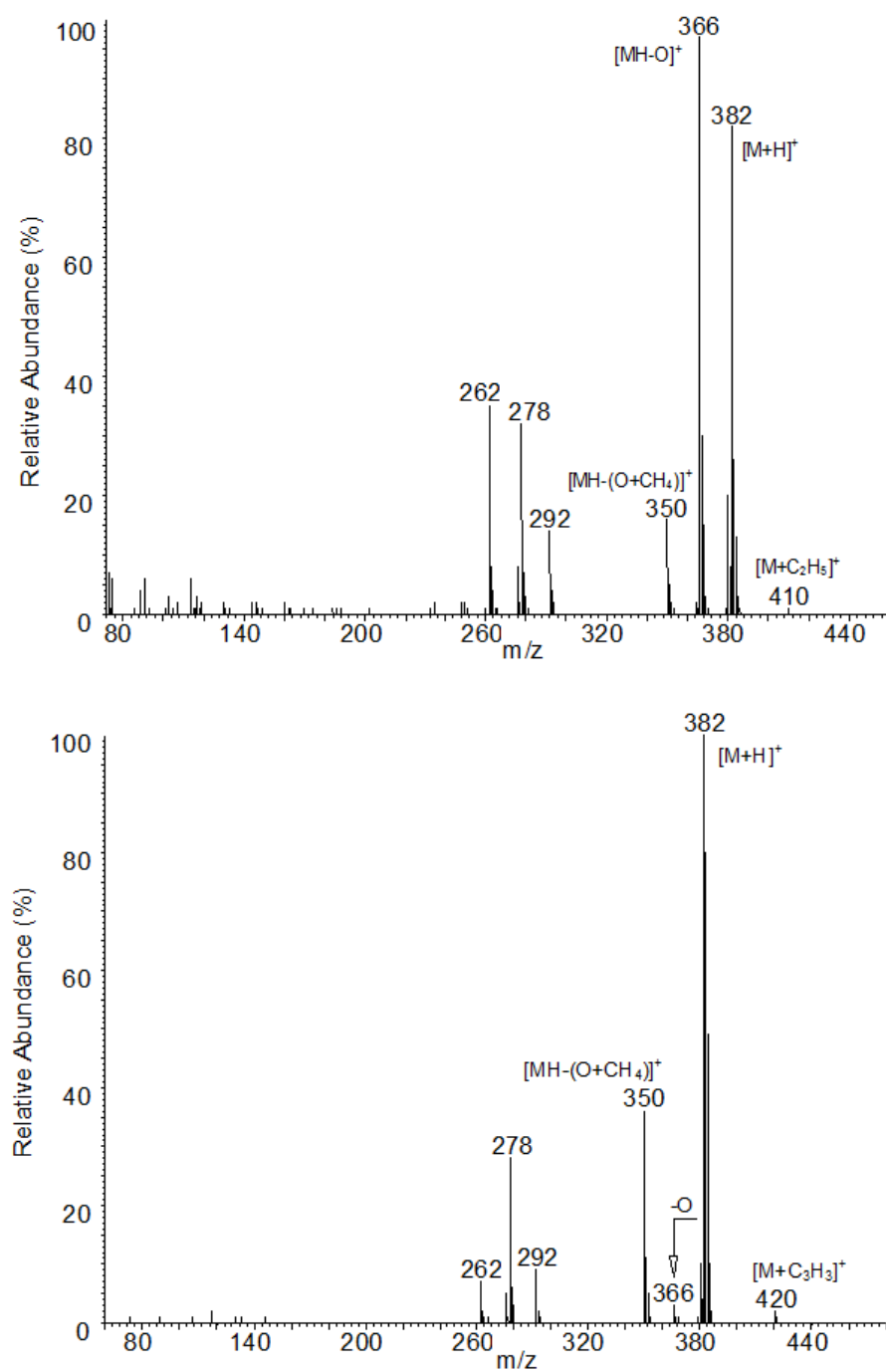


Figure S5. Methane/CI mass spectrum (top) and isobutane/CI mass spectrum (bottom) of compound **1**.