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Allyl isothiocyanate canonical forms

compound	RP ^a	MS spectral data m/z (relative intensity)	identification
1 diallyl sulfide	1118	116 ((M + 2) ⁺ , 1), 114 (M ⁺ , 27), 99 (31), 73 (57), 72 (34), 71 (28), 47 (21), 45 (100), 41 (47)	<i>b, c</i>
2 allyl isothiocyanate ^f	1353	101 ((M + 2) ⁺ , 3), 99 (M ⁺ , 74), 72 (33), 71 (9), 70 (6), 59 (5), 58 (5), 45 (12), 44 (8), 41 (100)	
3 allyl thiocyanate	1440	101 ((M + 2) ⁺ , 3), 99 (M ⁺ , 56), 98 (10), 72 (32), 71 (11), 58 (23), 46 (6), 45 (23), 41 (100)	<i>c</i>
4 diallyl disulfide	1468	148 ((M + 2) ⁺ , 1), 146 (M ⁺ , 10), 113 (12), 105 (12), 81 (19), 79 (11), 71 (12), 47 (12), 45 (45), 41 (100)	<i>b, c</i>
5 3 <i>H</i> -1,2-dithiolene	1513	106 ((M + 2) ⁺ , 5), 105 (13), 104 (M ⁺ , 56), 103 (100), 71 (14), 69 (12), 64 (10), 58 (9), 45 (33)	<i>d</i>
6 diallyl trisulfide	1787	180 ((M + 2) ⁺ , 1), 178 (M ⁺ , 7), 113 (96), 103 (9), 73 (100), 69 (4), 64 (13), 47 (15), 45 (64), 41 (80)	<i>c</i>
7 2-vinyl-4 <i>H</i> -1,3-dithiin	1833	146 ((M + 2) ⁺ , 7), 144 (M ⁺ , 57), 111 (45), 103 (15), 97 (20), 73 (13), 72 (86), 71 (100), 45 (45)	<i>b, c</i>
8 4 <i>H</i> -1,2,3-trithiin	1841	138 ((M + 2) ⁺ , 16), 136 (M ⁺ , 100), 103 (15), 72 (54), 71 (93), 69 (10), 64 (19), 45 (35)	<i>c</i>
9 5-methyl-1,2,3,4-tetrathiane	2005	172 ((M + 2) ⁺ , 18), 170 (M ⁺ , 100), 128 (43), 106 (30), 64 (34), 59 (10), 45 (13), 41 (18)	<i>c</i>
10 diallyl tetrasulfide		210 (M ⁺ , 12), 146 (55), 105 (37), 104 (16), 81 (24), 73 (78), 64 (32), 45 (45), 41 (100)	<i>c</i>



