

Compound	Deprotonated molecule [M – H] <sup>–</sup>	<i>m/z</i> ( $\Delta$ ppm)	Product ion <i>m/z</i> (rel. abund.)*	Neutral loss(es)
Pinic acid	C <sub>9</sub> H <sub>13</sub> O <sub>4</sub> <sup>–</sup>	185.08193 (–0.002)	141.09194 (100)	CO <sub>2</sub>
			167.07127 (16)	H <sub>2</sub> O
			123.08155 (4)	CH <sub>2</sub> O <sub>3</sub>
Monoperoxyipinic acid isomer I	C <sub>9</sub> H <sub>13</sub> O <sub>5</sub> <sup>–</sup>	201.07706 (1.060)	111.08149 (100)	C <sub>2</sub> H <sub>2</sub> O <sub>4</sub>
			155.07127 (38)	CH <sub>2</sub> O <sub>2</sub>
			139.07639 (37)	CH <sub>2</sub> O <sub>3</sub>
			140.08423 (10)	CHO <sub>3</sub>
			157.08694 (8)	CO <sub>2</sub>
			183.06619 (8)	H <sub>2</sub> O
			127.07643 (5)	C <sub>2</sub> H <sub>2</sub> O <sub>3</sub>
			84.02166 (3)	C <sub>5</sub> H <sub>9</sub> O <sub>3</sub>
			115.00367 (3)	C <sub>5</sub> H <sub>10</sub> O
			129.05568 (3)	C <sub>3</sub> H <sub>4</sub> O <sub>2</sub>
			99.04513 (2)	C <sub>4</sub> H <sub>6</sub> O <sub>3</sub>
			111.04514 (2)	C <sub>3</sub> H <sub>6</sub> O <sub>3</sub>
			121.06583 (2)	CH <sub>4</sub> O <sub>4</sub>
			184.07401 (1)	OH
95.08662 (1)	C <sub>2</sub> H <sub>2</sub> O <sub>5</sub>			
Monoperoxyipinic acid isomer II	C <sub>9</sub> H <sub>13</sub> O <sub>5</sub> <sup>–</sup>	201.07711 (1.293)	183.06605 (100)	H <sub>2</sub> O
			157.08678 (35)	CO <sub>2</sub>
			139.07625 (31)	CH <sub>2</sub> O <sub>3</sub>
			155.07116 (10)	CH <sub>2</sub> O <sub>2</sub>
			111.08142 (5)	C <sub>2</sub> H <sub>2</sub> O <sub>4</sub>
			127.07635 (2)	C <sub>2</sub> H <sub>2</sub> O <sub>3</sub>
			121.06577 (2)	CH <sub>4</sub> O <sub>4</sub>
Diperoxyipinic acid	C <sub>9</sub> H <sub>13</sub> O <sub>6</sub> <sup>–</sup>	217.07232 (2.573)	156.07910 (100)	CHO <sub>3</sub>
			155.07132 (16)	CH <sub>2</sub> O <sub>3</sub>
			111.08152 (13)	C <sub>2</sub> H <sub>2</sub> O <sub>5</sub>
			183.06628 (7)	H <sub>2</sub> O <sub>2</sub>
			171.06625 (3)	CH <sub>2</sub> O <sub>2</sub>
			173.08189 (2)	CO <sub>2</sub>
			199.06122 (1)	H <sub>2</sub> O
			74.00093 (1)	C <sub>7</sub> H <sub>11</sub> O <sub>3</sub>
127.07646 (1)	C <sub>2</sub> H <sub>2</sub> O <sub>4</sub>			