

Supplementary Material

Table S1. Schedule Change of volatile substance content during storage period of ‘Ruixue’ apples (μg/kg)

Compound	Content (μg/kg)					
	0 d	30 d	60 d	90 d	120 d	150 d
Butanoic acid, propyl ester	-	37.641±2.75	169.848±10.45	106.734±8.09	122.217±8.34	181.196±6.35
Butanoic acid, 2-methyl-, propyl ester	12.384±0.53	17.508±1.05	45.741±3.89	24.084±2.12	24.531±2.45	35.298±2.67
Butanoic acid, butyl ester	39.408±1.98	199.765±9.89	649.924±30.56	297.675±16.89	432.294±20.24	497.244±25.13
Butanoic acid, 2-methylbutyl ester	22.822±1.34	53.804±2.19	95.473±4.45	54.521±1.94	77.201±5.23	69.996±4.37
Acetic acid, hexyl ester	13.905±0.56	74.378±2.75	257.919±10.72	91.221±5.19	22.811±1.93	54.044±4.37
Butanoic acid, 2-methyl-, 2-methylbutyl ester	61.778±4.95	59.348±2.56	58.430±2.87	31.726±3.22	27.002±1.05	33.146±1.64
Butanoic acid, pentyl ester	17.588±0.56	69.941±3.82	144.401±10.30	84.155±4.74	125.896±9.04	160.138±12.05
Butanoic acid, 2-methyl-, pentyl ester	74.402±5.90	90.778±6.07	99.04±4.96	68.079±2.89	33.673±0.45	80.405±2.72
Propanoic acid, hexyl ester	91.156±6.16	144.670±9.11	476.165±45.09	300.508±23.18	208.574±15.21	263.932±17.38
Hexanoic acid, butyl ester	37.100±2.67	472.599±18.02	790.549±59.40	626.144±42.61	489.860±39.02	-
Butanoic acid, hexyl ester	172.956±10.41	964.571±79.90	1697.36±104.4	1571.19±102.5	1811.85±99.34	3033.50±210.2
Butanoic acid, 2-methyl-, hexyl ester	1230.16±98.94	2139.61±156.5	2361.48±112.7	2650.63±145.8	2047.45±134.2	3269.33±211.9
Hexanoic acid, 2-methylbutyl ester	25.740±1.78	112.423±10.13	194.504±12.45	-	-	-
Hexanoic acid, pentyl ester	-	161.167±10.17	245.505±5.94	-	262.17±16.27	-
Hexanoic acid, hexyl ester	130.478±9.06	1140.33±67.90	1602.41±92.91	358.557±29.45	2058.35±153.9	462.706±27.81
Hexyl tiglate	52.665±3.19	10.823±0.78	39.226±1.70	77.418±5.39	66.459±5.41	108.992±29.08
Octanoic acid, hexyl ester	-	36.419±1.41	55.455±4.18	121.261±10.12	82.820±5.06	128.180±8.23
Butanoic acid, ethyl ester	-	-	35.690±3.75	25.546±1.49	31.015±1.58	51.056±5.03
Propanoic acid, butyl ester	-	-	92.674±4.29	28.561±2.16	20.694±4.28	24.695±1.95
Propanoic acid, hexyl ester	-	27.170±1.74	-	-	-	-
Propanoic acid, pentyl ester	-	13.638±0.83	53.644±3.47	-	-	-
Butanoic acid, 2-methylpropyl ester	-	-	-	-	19.755±1.05	23.329±0.95
Hexanoic acid, propyl	-	-	73.457±2.75	66.754±6.64	69.340±4.38	116.089±10.9
6-Octen-1-ol, 3,7-dimethyl-, formate	-	20.458±0.73	35.590±2.96	31.278±1.28	-	-

Compound

Content (μg/kg)

	0 d	30 d	60 d	90 d	120 d	150 d
Hexadecane, 1,1-bis(dodecyloxy)-	-	-	23.433 ± 0.69	-	-	-
Hexanal	106.327 ± 5.62	268.722 ± 10.73	713.606 ± 57.81	483.448 ± 39.20	620.856 ± 48.88	793.972 ± 66.31
2-Hexenal, (E)-	-	38.902 ± 1.51	66.199 ± 3.36	-	31.822 ± 3.09	27.121 ± 1.72
2-Hexenal	1022.57 ± 78.19	1570.15 ± 139.9	2553.39 ± 185.3	1423.94 ± 109.9	1432.23 ± 103.3	1303.29 ± 99.41
Octanal	-	-	19.185 ± 0.94	174.30 ± 13.56	202.631 ± 19.58	137.563 ± 13.31
2-Heptenal, (Z)-	-	28.503 ± 2.05	36.425 ± 2.19	34.972 ± 3.08	22.061 ± 1.07	-
Nonanal	56.753 ± 5.48	54.291 ± 4.93	151.055 ± 55.04	36.867 ± 2.27	55.073 ± 3.88	44.798 ± 2.75
2-Octenal, (E)-	20.442 ± 0.79	34.678 ± 1.20	61.586 ± 4.17	43.260 ± 3.61	45.861 ± 3.36	24.010 ± 1.38
2,4-Heptadienal, (E,E)-	-	23.660 ± 0.54	-	-	-	-
Decanal	39.688 ± 2.67	44.529 ± 3.27	118.928 ± 69.41	54.168 ± 3.69	50.501 ± 3.48	-
2-Nonenal, (Z)-	24.379 ± 0.62	63.101 ± 3.55	106.472 ± 68.11	55.941 ± 4.01	68.254 ± 6.17	92.525 ± 5.99
1-Butanol, 2-methyl-	-	103.433 ± 9.43	251.317 ± 21.39	295.571 ± 21.14	193.477 ± 16.74	251.074 ± 16.15
1-Pentanol	-	-	23.216 ± 0.47	33.259 ± 12.21	24.754 ± 15.49	30.755 ± 3.99
2-Heptenal, (Z)-	40.829 ± 2.11	382.891 ± 12.67	781.407 ± 45.85	996.576 ± 33.72	936.723 ± 58.83	1093.42 ± 99.31
13-Heptadecyn-1-ol	11.942 ± 0.69	-	20.435 ± 0.57	-	-	-
5-Hepten-2-ol, 6-methyl-	-	-	-	260.248 ± 19.88	155.724 ± 13.11	450.005 ± 39.98
1-Butanol	-	82.988 ± 65.03	208.871 ± 11.23	239.291 ± 11.59	142.188 ± 11.84	184.115 ± 8.41
1-Octen-3-one	12.164 ± 0.99	11.889 ± 0.34	39.745 ± 1.27	18.338 ± 0.23	16.871 ± 0.64	15.414 ± 0.34
5-Hepten-2-one, 6-methyl-	22.796 ± 1.91	139.391 ± 8.10	180.899 ± 1.14	329.364 ± 14.62	298.578 ± 26.33	119.949 ± 9.37
Tetradecane	-	11.289 ± 0.44	-	-	-	17.206 ± 0.58
p-Xylene	12.268 ± 0.26	37.326 ± 1.55	-	-	51.977 ±	16.365 ±
cis- α -Farnesene	15.868 ± 0.82	98.499 ± 4.99	59.267 ± 2.01	86.118 ± 5.34	81.745 ± 7.19	66.770 ± 4.74
trans- α -Bergamotene	388.427 ± 29.35	541.361 ± 36.11	1301.80 ± 87.59	269.162 ± 19.19	2051.86 ± 176.7	-
α -Farnesene	914.003 ± 59.37	8219.12 ± 452.5	2563.11 ± 115.1	613.205 ± 49.33	2283.07 ± 167.3	10303.4 ± 893
Estragole	19.868 ± 0.36		31.899 ± 1.33	-	-	-
cis-Thujopsene	18.987 ± 1.87	-	72.968 ± 4.59	126.281 ± 9.79	89.621 ± 6.40	92.208 ± 8.19
Butanoic acid, 2-methyl-, heptyl ester	-	14.609 ± 0.94	19.642 ± 0.96	19.071 ± 1.18	22.349 ± 1.54	37.618 ± 2.66

Note: Values are means \pm standard error of three biological replicates; - no such substance has been detected.

Table S2. Predicted properties of different carboxylesterases characterized in plants and of the intracellular locus of the proteins on websites.

Gene name	Gene name	Chromosome	Size/aa	Length of CDS/kp	Subcellular localization	<i>pI</i>	Protein W
<i>MdCXE3</i>	MD02G1275900	2	1011	698	cytoplasm	5.04	83705.47
<i>MdCXE5</i>	MD02G1276600	2	1002	656	cytoplasm	5.05	83055.26
<i>MdCXE6</i>	MD03G1273300	3	1041	560	cytoplasm	5.04	85577.45
<i>MdCXE9</i>	MD05G1076400	5	975	782	cytoplasm	5.08	80633.09
<i>MdCXE10</i>	MD05G1078900	5	999	680	cytoplasm	5.08	82941.45
<i>MdCXE12</i>	MD05G1191100	5	960	588	endoplasmic reticulum	5.08	78325.40
<i>MdCXE17</i>	MD08G1226300	8	1094	552	endoplasmic reticulum	5.02	91200.72
<i>MdCXE20</i>	MD10G1068500	10	1023	549	cytoplasm	5.01	85350.25
<i>MdCXE23</i>	MD10G1091200	10	1116	560	endoplasmic reticulum	5.05	92593.40
<i>MdCXE25</i>	MD10G1091900	10	939	527	endoplasmic reticulum	5.08	77709.78

Table S3. Apple genome names corresponding to 42 MdCXE members

Name	Apple ID	Name	Apple ID	Name	Apple ID
<i>MdCXE1</i>	MD02G1198400	<i>MdCXE2</i>	MD02G1198500	<i>MdCXE3</i>	MD02G1275900
<i>MdCXE4</i>	MD02G1276300	<i>MdCXE5</i>	MD02G1276600	<i>MdCXE6</i>	MD03G1273300
<i>MdCXE7</i>	MD04G1212400	<i>MdCXE8</i>	MD05G1060700	<i>MdCXE9</i>	MD05G1076400
<i>MdCXE10</i>	MD05G1078900	<i>MdCXE11</i>	MD05G1191000	<i>MdCXE12</i>	MD05G1191100
<i>MdCXE13</i>	MD06G1052300	<i>MdCXE14</i>	MD07G1043400	<i>MdCXE15</i>	MD07G1046000
<i>MdCXE16</i>	MD08G1104000	<i>MdCXE17</i>	MD08G1226300	<i>MdCXE18</i>	MD09G1017600
<i>MdCXE19</i>	MD09G1086100	<i>MdCXE20</i>	MD10G1068500	<i>MdCXE21</i>	MD10G1091000
<i>MdCXE22</i>	MD10G1091100	<i>MdCXE23</i>	MD10G1091200	<i>MdCXE24</i>	MD10G1091600
<i>MdCXE25</i>	MD10G1091900	<i>MdCXE26</i>	MD11G1176900	<i>MdCXE27</i>	MD11G1191000
<i>MdCXE28</i>	MD11G1296000	<i>MdCXE29</i>	MD12G1046500	<i>MdCXE30</i>	MD12G1227200
<i>MdCXE31</i>	MD13G1108800	<i>MdCXE32</i>	MD13G1187400	<i>MdCXE33</i>	MD13G1187500
<i>MdCXE34</i>	MD13G1187900	<i>MdCXE35</i>	MD14G1045500	<i>MdCXE36</i>	MD15G1085200
<i>MdCXE37</i>	MD15G1124600	<i>MdCXE38</i>	MD16G1045600	<i>MdCXE39</i>	MD16G1188100
<i>MdCXE40</i>	MD16G1188500	<i>MdCXE41</i>	MD17G1018400	<i>MdCXE42</i>	MD00G1203100

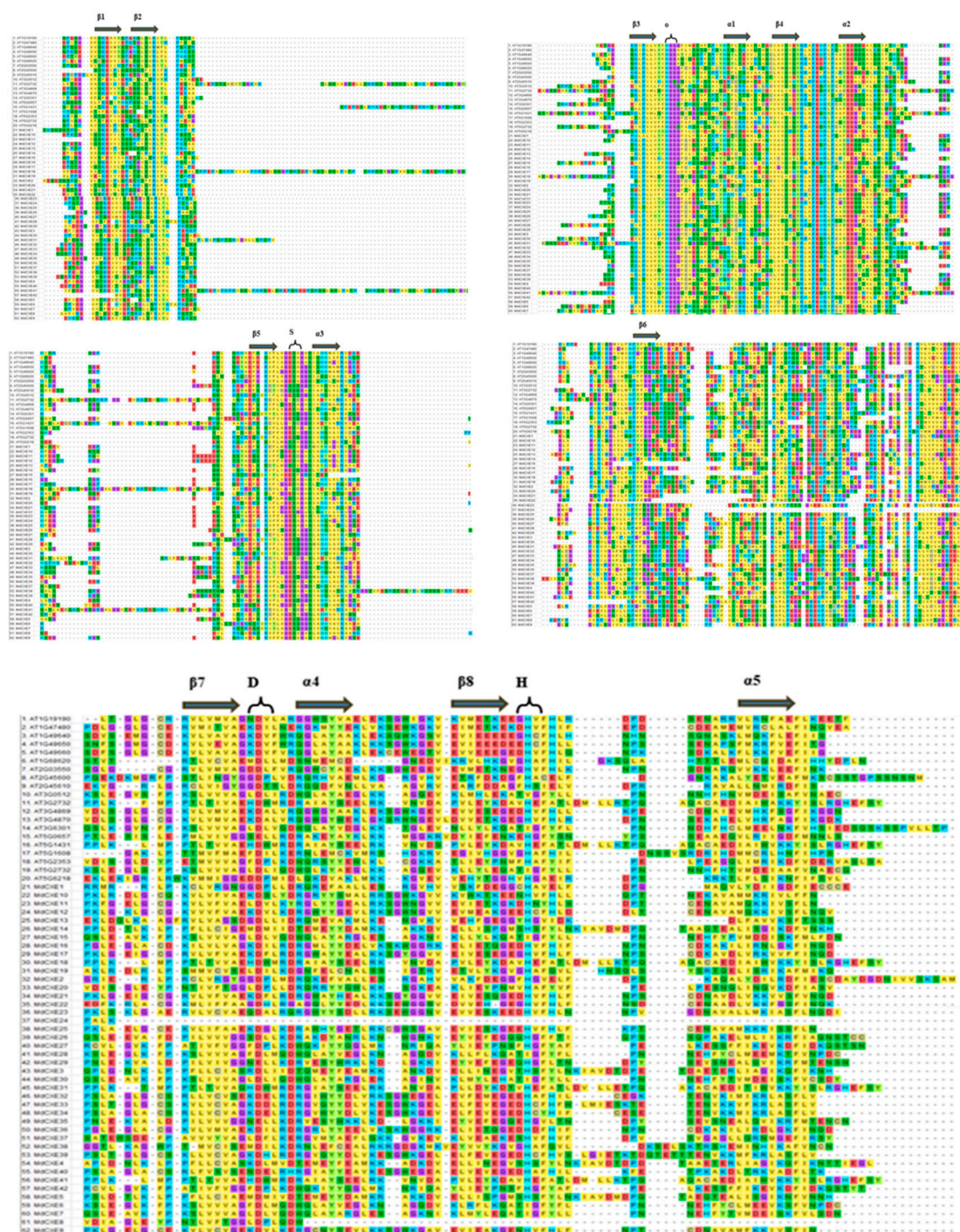


Figure S1. Multiple sequence alignment of CXE gene family in apple and *Arabidopsis thaliana*. The *MdCXEs* α/β hydrolase predicted domain is highlighted in(➡). Putative residues constituting the catalytic triad (Ser/Thr, Asp, and His) are denoted is marked.