Supplementary information for

Catechin as a new improving agent for photo-Fenton-like system at near-neutral pH for the removal of inderal

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The supplementary materials (SM) contain complementary data concerning the adopted analytical methods and procedures, 9 figures and 2 tables.

Figure A.1 − The UV-vis spectra and the molecular structure of Inderal

Figure A.2 − The calibration curves for the detection of inderal (a) , phenol (b) and Fe(III) (c)

Figure A.3 − The photodegradation of inderal by Fe(III)-nordihydroguaiaretic acid(a) and Fe(III)- pyrocatechol violet complexes(b) at different pH values. Reaction conditions included the following: [Fe(III)]= 50 μmol/L, [nordihydroguaiaretic acid]= 200 μmol/L, [pyrocatechol violet]= 200 μmol/L, [inderal]=10 μmol/L.

Figure A.4 − The UV-vis spectra of Fe(III), catechin, a mixture of Fe(III) and catechin at **(a)** pH=6.0 and **(b)** pH=3.0. ([Fe(III)]=20 μmol/L, [catechin]=200 μmol/L)

Figure A.5 − The determination of Fe(III)-catechin conditional stability constant by

continuous variation methods at pH 6.0.

Figure A.6 − (a) Determination of •OH (μmol/L) in different pH conditions and reduction rate of Fe(III) in photo/dark reaction (b). Reaction conditions included the following: [Fe(III)]= 50 μmol/L, [catechin]= 200 μmol/L, [inderal]=10 μmol/L, pH = 6.0.

Figure A.7 − HPLC chromatograms and (+)-ESI-MS spectra of inderal and its photodegradation products.

Figure A.8 − The total ions chromatogram of GC-MS and comparison of mass spectra between photoproducts and standard compounds.

Table A.1 The molecular structure of catechin, nordihydroguaiaretic acid, pyrocatecholviolet, 2-chloro-3′,4′-dihydroxyacetophenone, 2,3-dihydroxybenzoic acid

Table A.2 Inderal and its major photolysis products in the Fe(III)-catechin system by GS-MS analysis.

1. The UV-vis spectra and the molecular structure of inderal

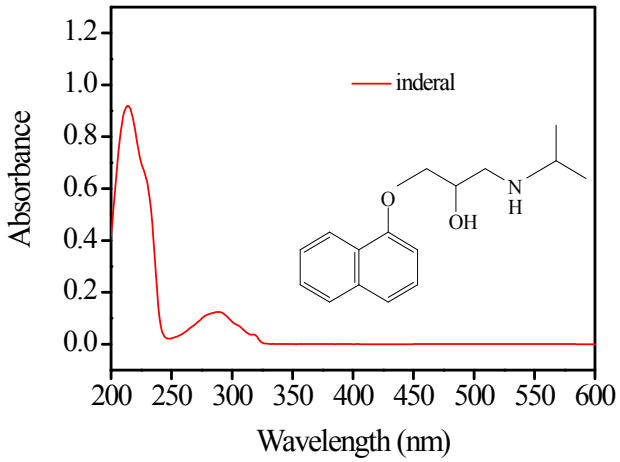
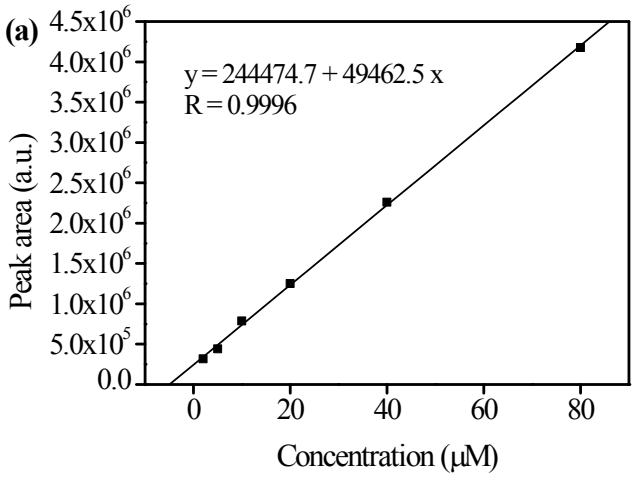
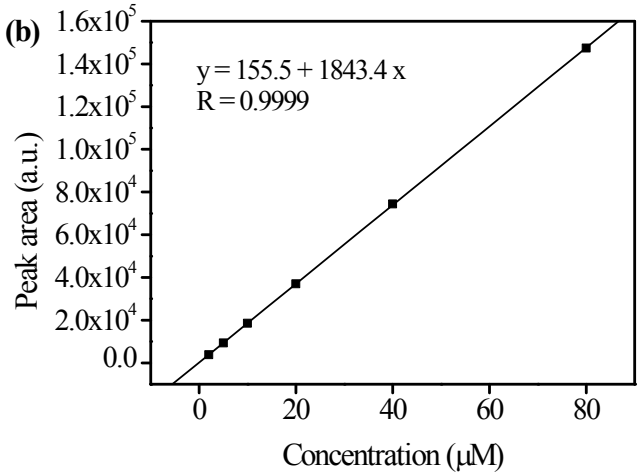


Figure A.1 − The UV-vis spectra and the molecular structure of Inderal

2. Calibration curve





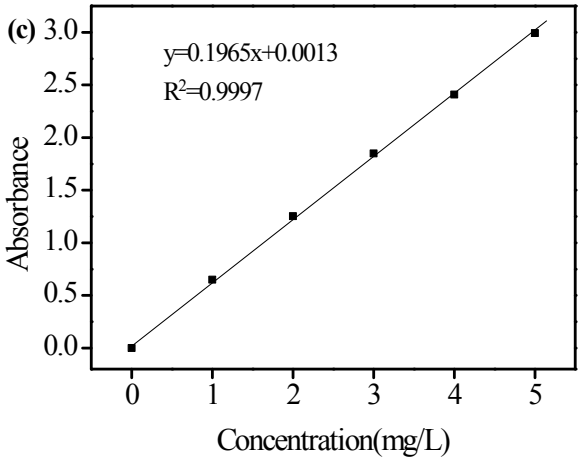


Figure A.2 − The calibration curves for the detection of inderal (a) , phenol (b) and Fe(III) (c)

3. The photodegradation of inderal by Fe(III)-nordihydroguaiaretic acid and Fe(III)-pyrocatechol violet complexes at different pH values

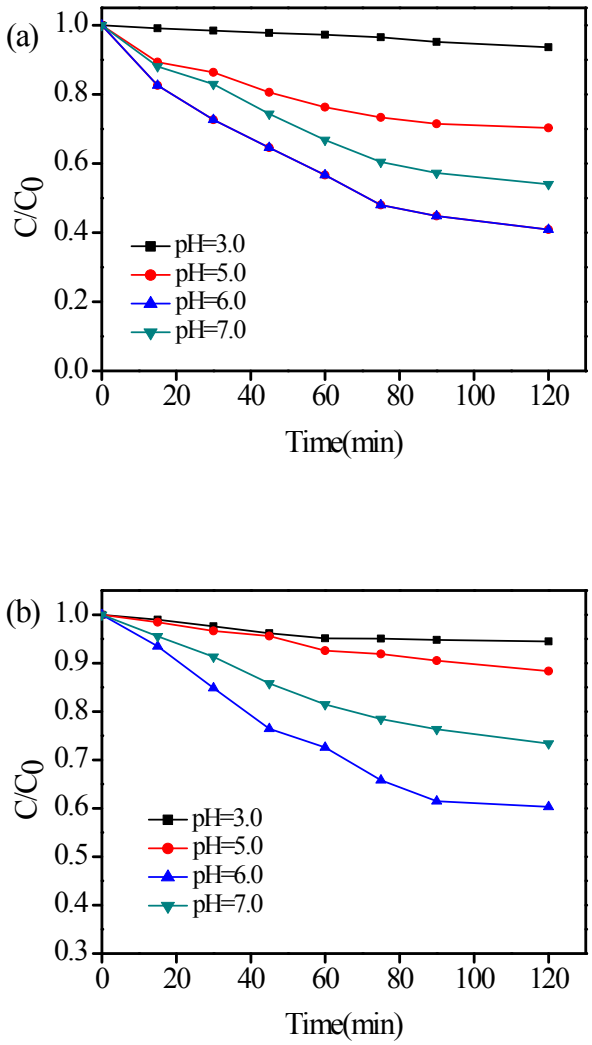
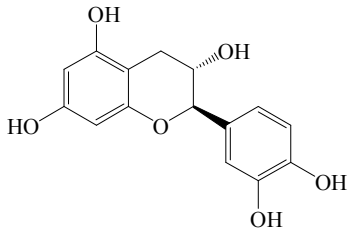
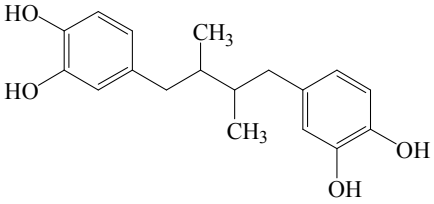
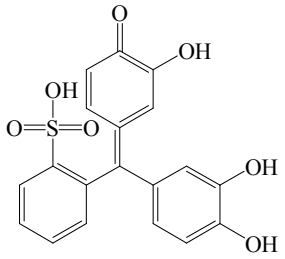
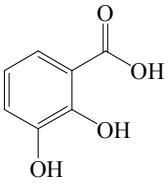
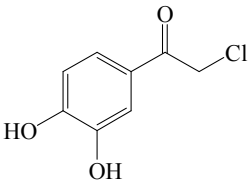


Figure A.3 − The photodegradation of inderal by Fe(III)-nordihydroguaiaretic acid(a) and Fe(III)- pyrocatechol violet complexes(b) at different pH values. Reaction conditions included the following: [Fe(III)]= 50 μmol/L, [nordihydroguaiaretic acid]= 200 μmol/L, [pyrocatechol violet]= 200 μmol/L, [inderal]=10 μmol/L.

4.The molecular structure of five Fe(III) ligands

Table A.1 The molecular structure of catechin, nordihydroguaiaretic acid, pyrocatecholviolet, 2-chloro-3′,4′-dihydroxyacetophenone, 2,3-dihydroxybenzoic acid

Name	Molecular structure
catechin	
nordihydroguaiaretic acid	
pyrocatechol violet	
2,3-dihydroxybenzoic acid	
2-chloro-3′,4′-dihydroxyacetophenone	

5. The UV-vis spectra of Fe(III)-catechin complexes at different pH

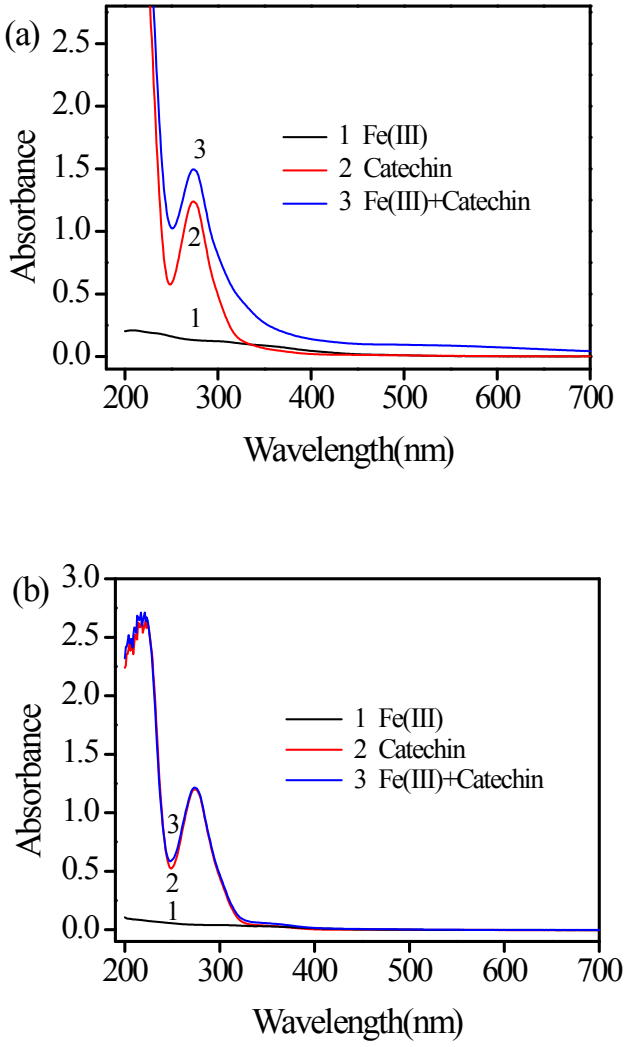


Figure A.4 − The UV-vis spectra of Fe(III), catechin, a mixture of Fe(III) and catechin at **(a)** pH=6.0 and **(b)** pH=3.0. ([Fe(III)]=20 μmol/L, [catechin]=200 μmol/L)

6. The determination of Fe(III)-catechin conditional stability constant

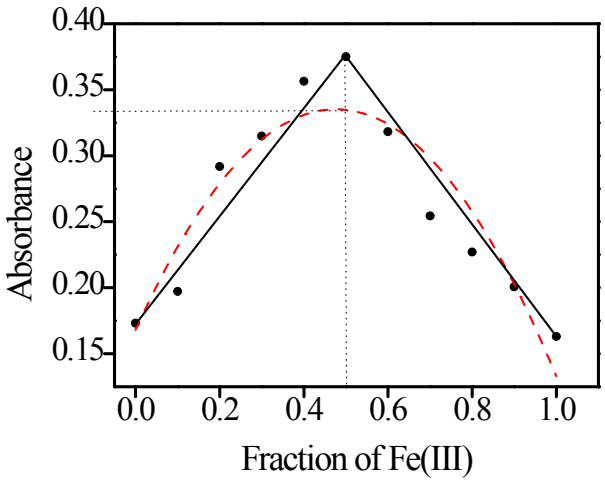
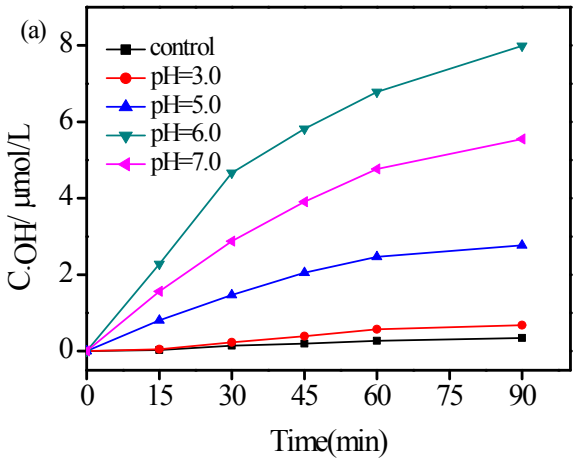


Figure A.5 − The determination of Fe(III)-catechin conditional stability constant by continuous variation methods at pH 6.0

7. The determination of •OH and Fe(II)



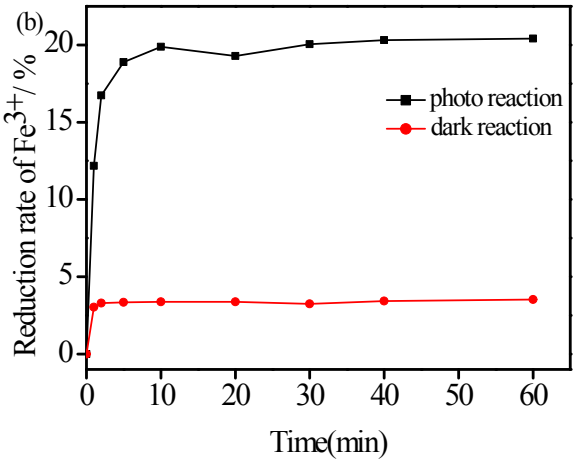
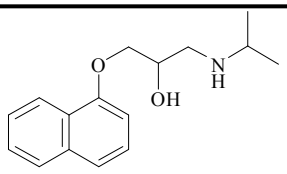
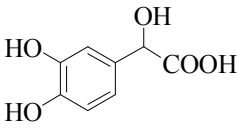
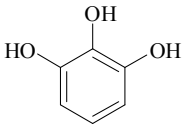
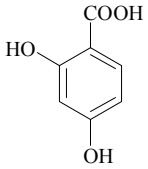
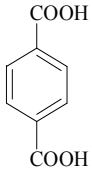
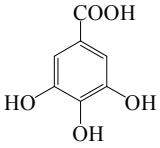
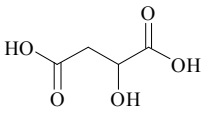
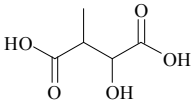
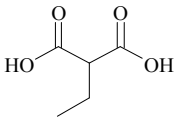
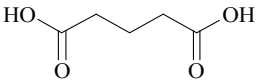
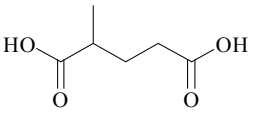
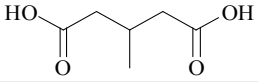


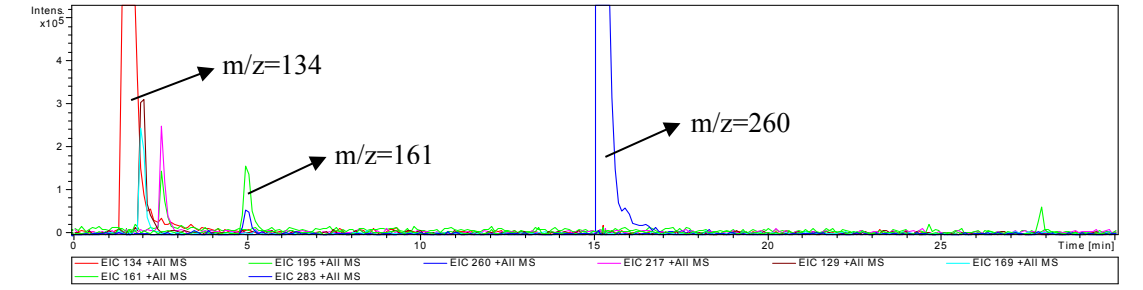
Figure A.6 − (a) Determination of •OH (μmol/L) in different pH conditions and reduction rate of Fe(III) in photo/dark reaction (b). Reaction conditions included the following: [Fe(III)]= 50 μmol/L, [catechin]= 200 μmol/L, [inderal]=10 μmol/L, pH = 6.0.

8. The main intermediates and the mass spectra of photodegradation products

Table A.2 Inderal and its major photolysis products in the Fe(III)-catechin system by GS-MS analysis.

Retention time (min)	Name	Molecular structure
54.96	inderal	

53.88	3,4-dihydroxymandelic acid	
36.18	pyrogallol	
40.63	protocatechuic acid	
44.51	p-phthalic acid	
49.82	gallic acid	
24.51	malic acid	
25.56	2-methyl-3-hydroxylsuccinic acid	
25.56	ethylmalonic acid	
30.46	glutaric acid	
30.88	2-methylglutaric acid	
31.48	3-methylglutaric acid	



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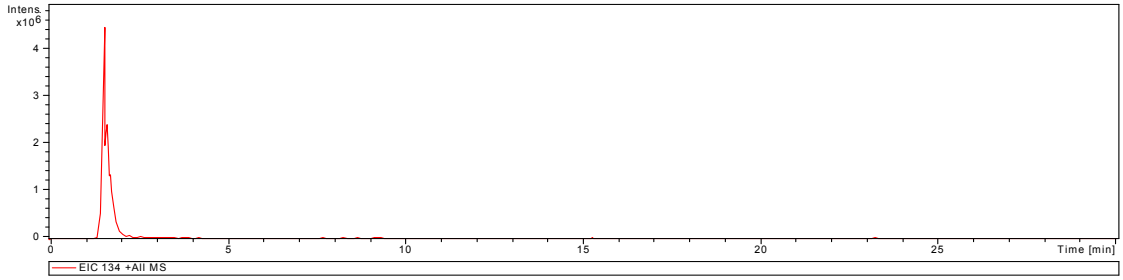

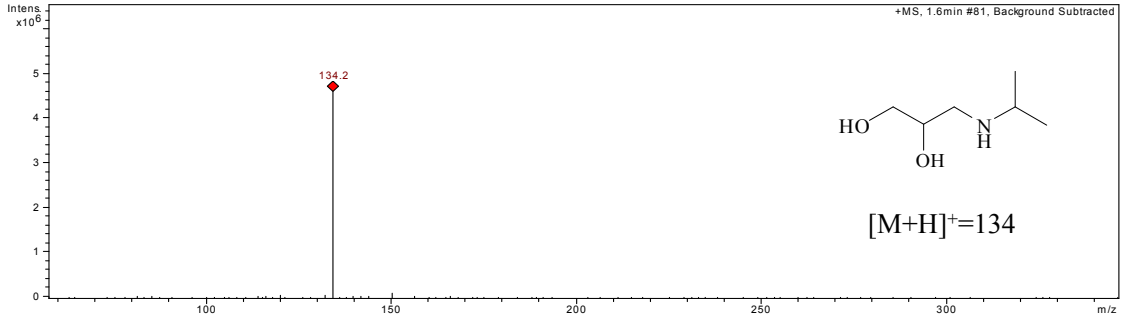

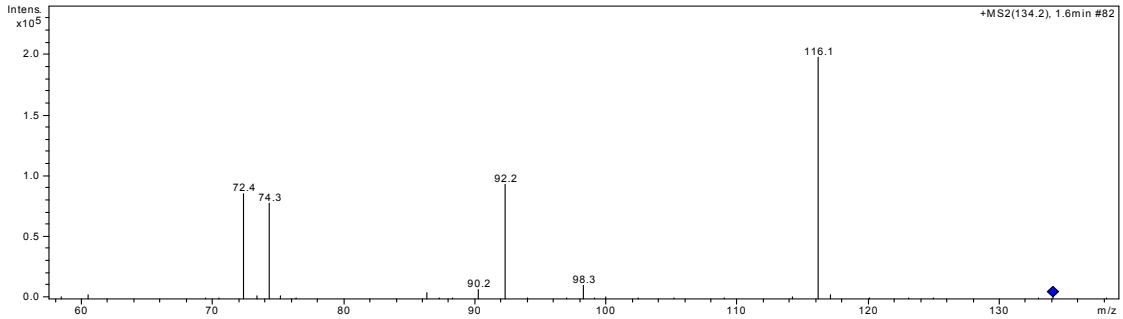

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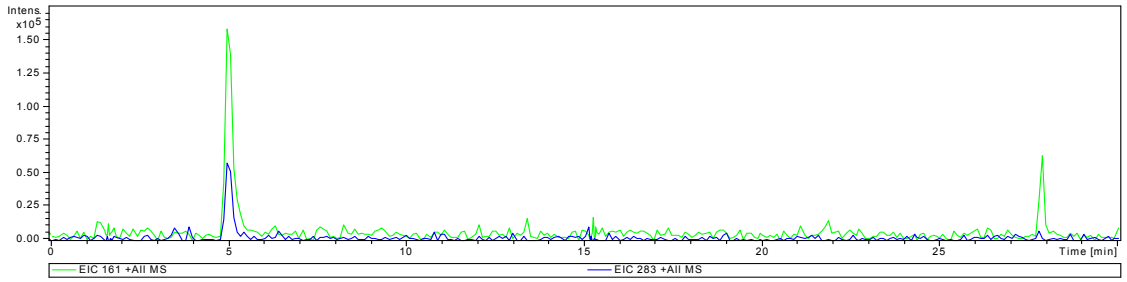
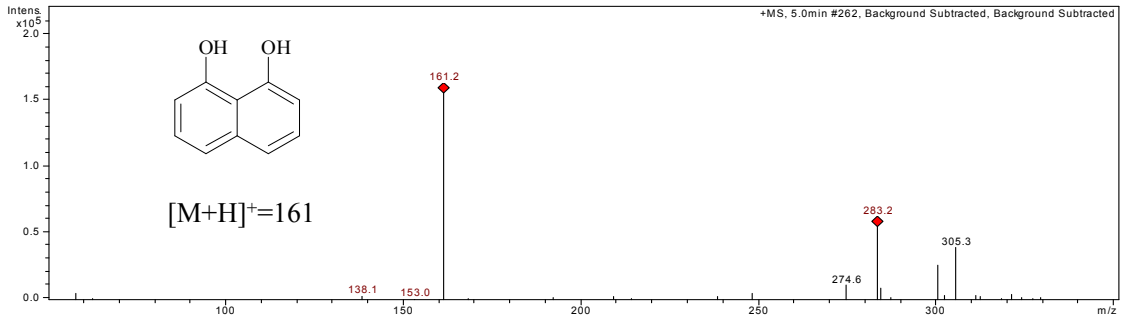




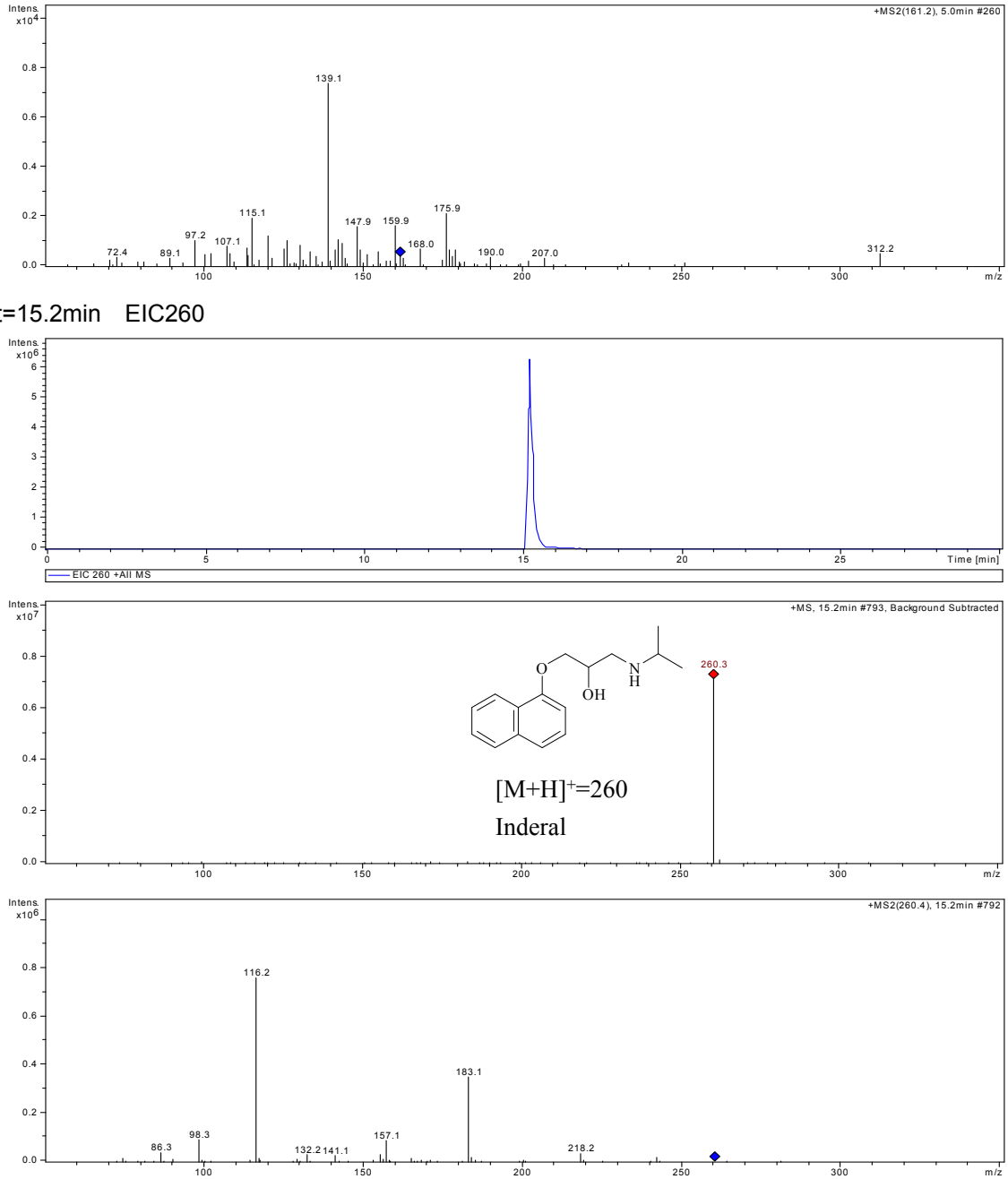
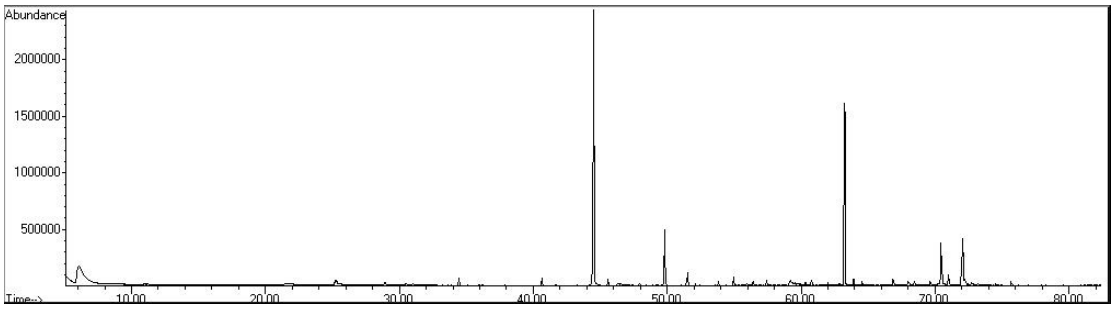
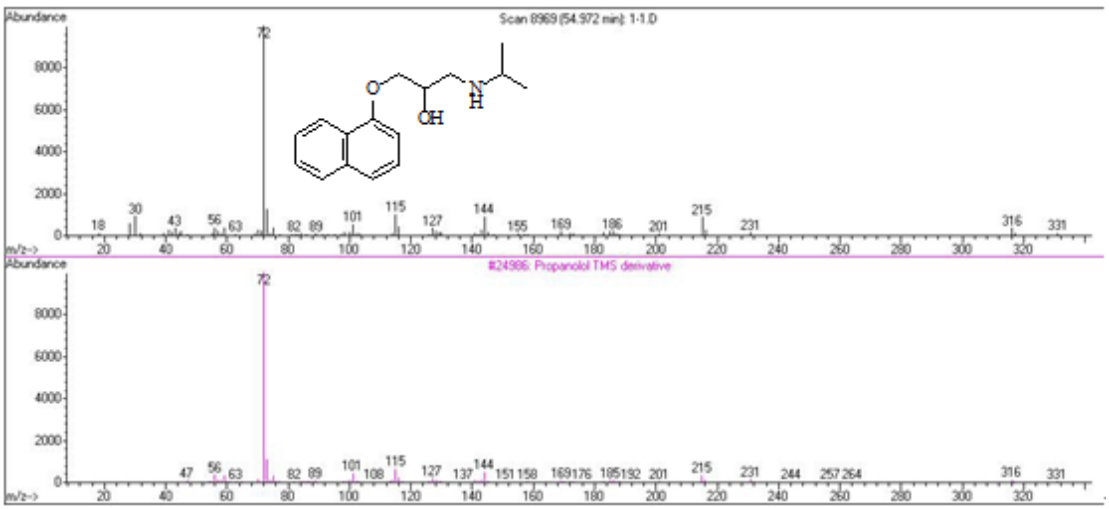


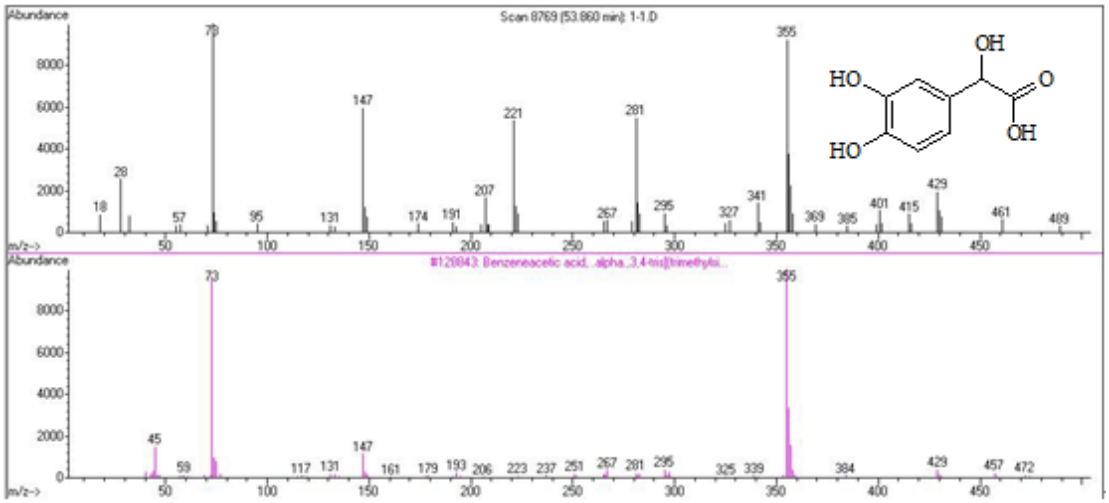
Figure A.7 − HPLC chromatograms and (+)-ESI-MS spectra of inderal and its photodegradation products.



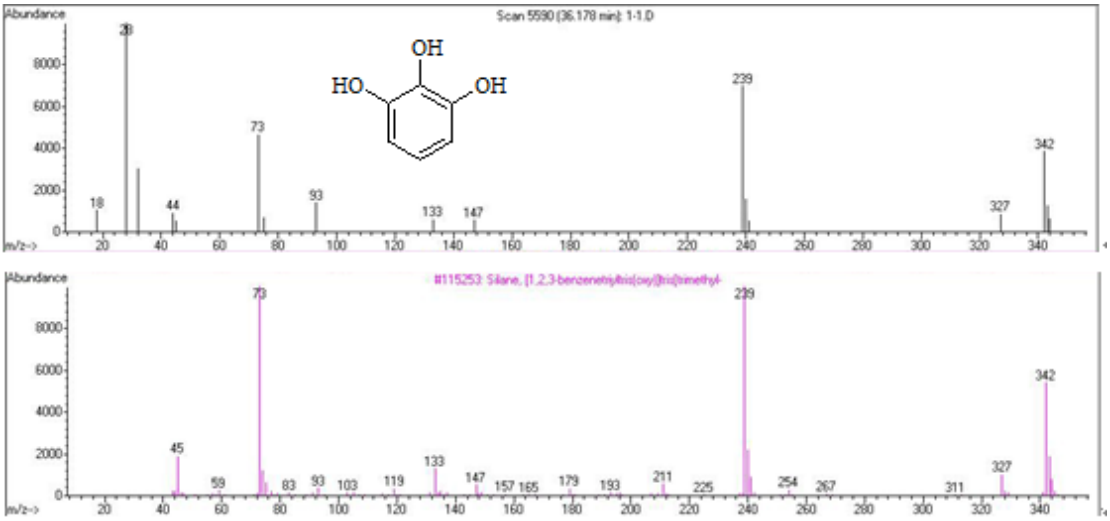
The total chromatogram of GC-MS



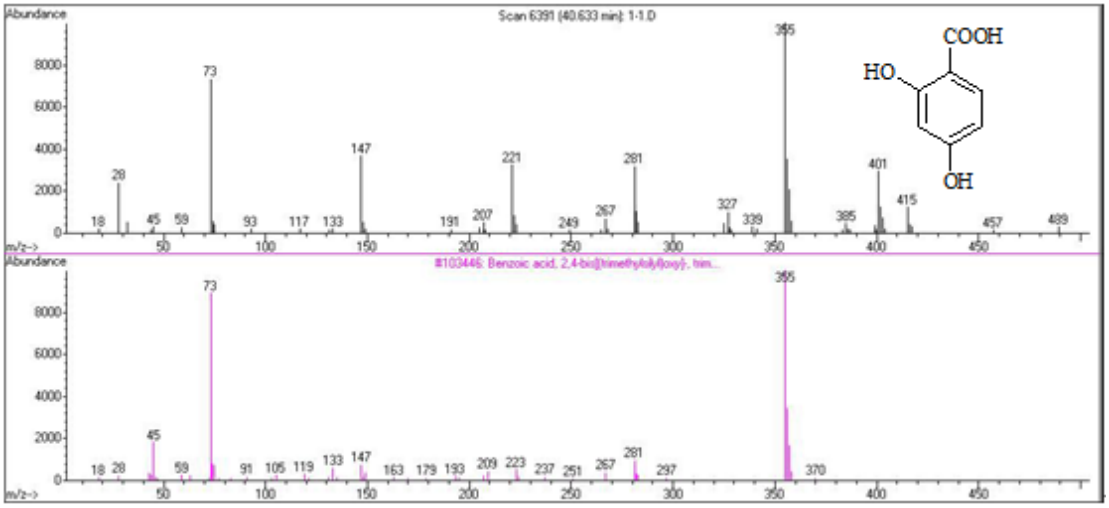
inderal



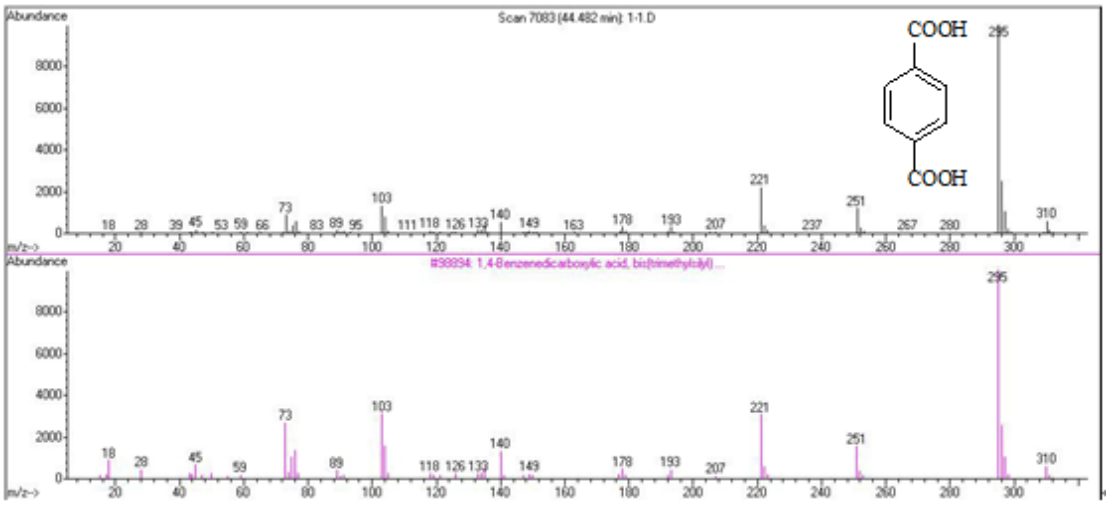
3,4-dihydroxy mandelic acid



pyrogallol



protocatechuic acid



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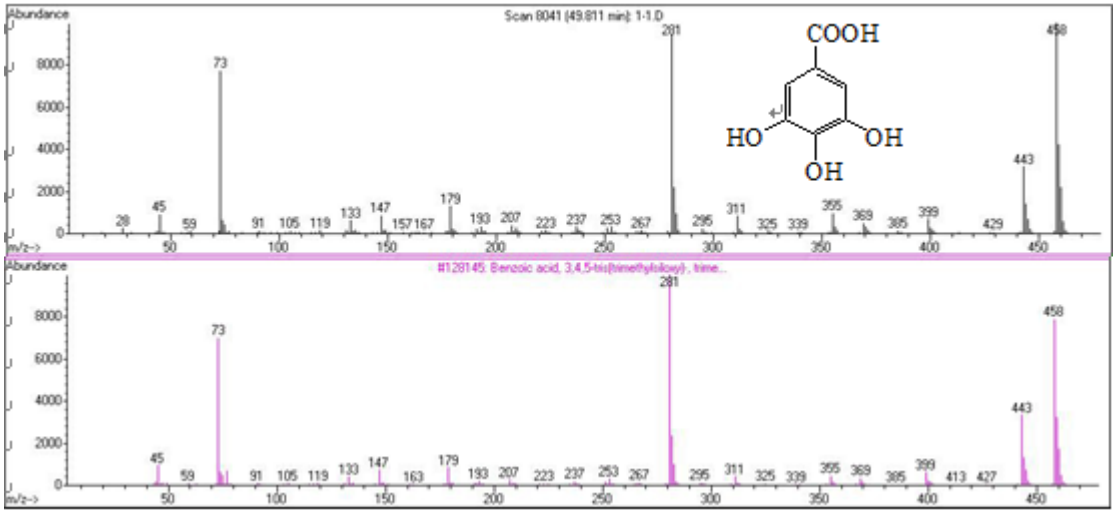
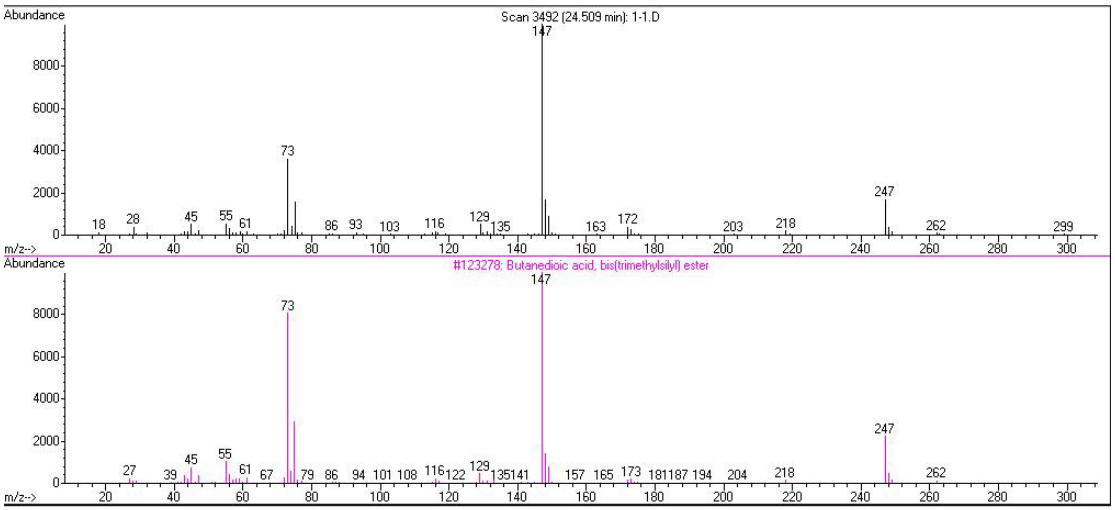
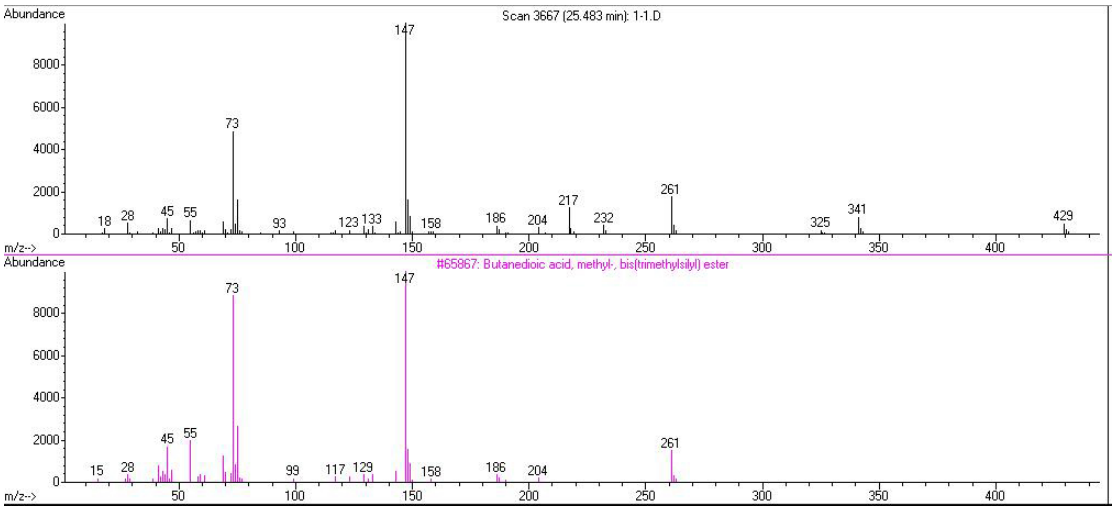


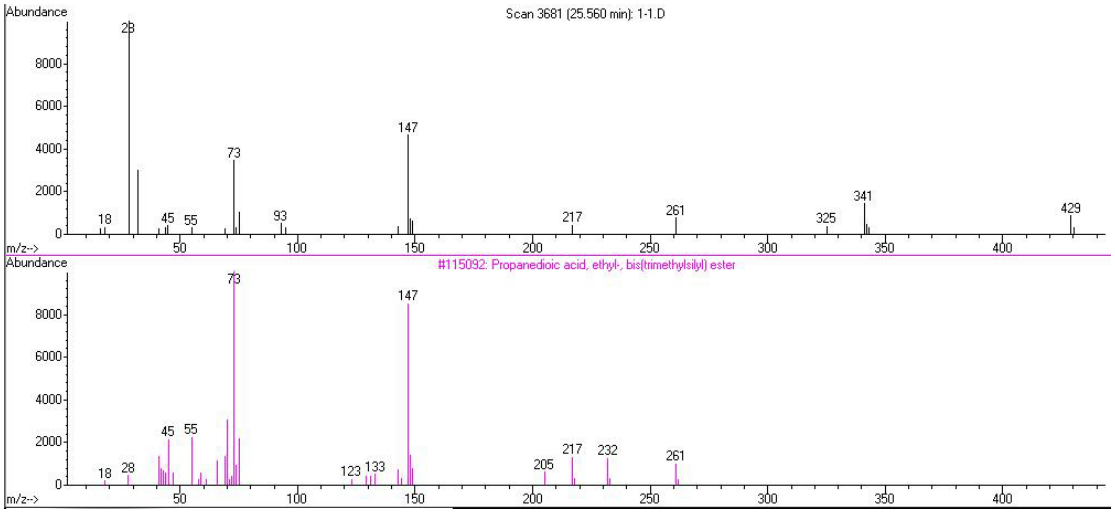
gallic acid



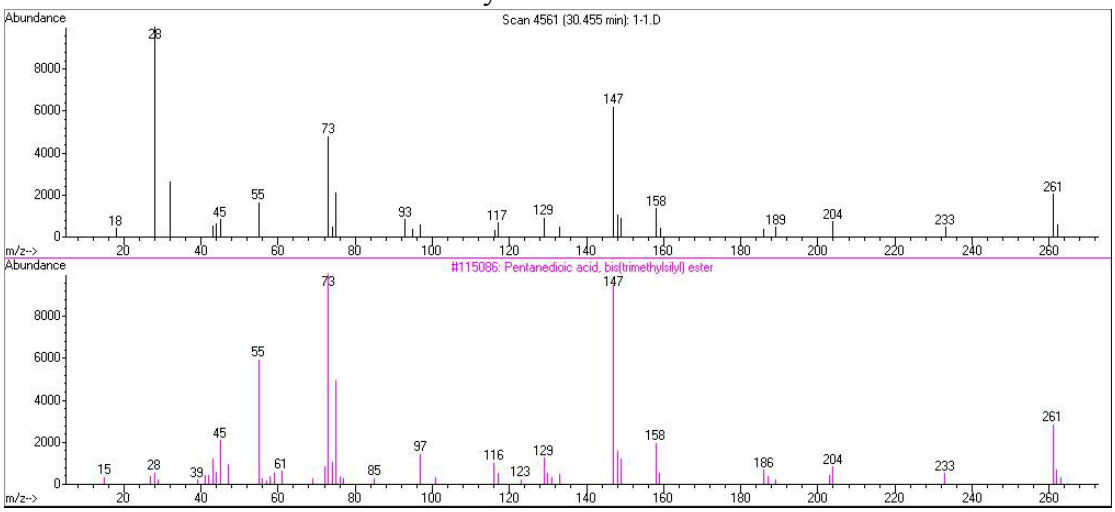
malic acid



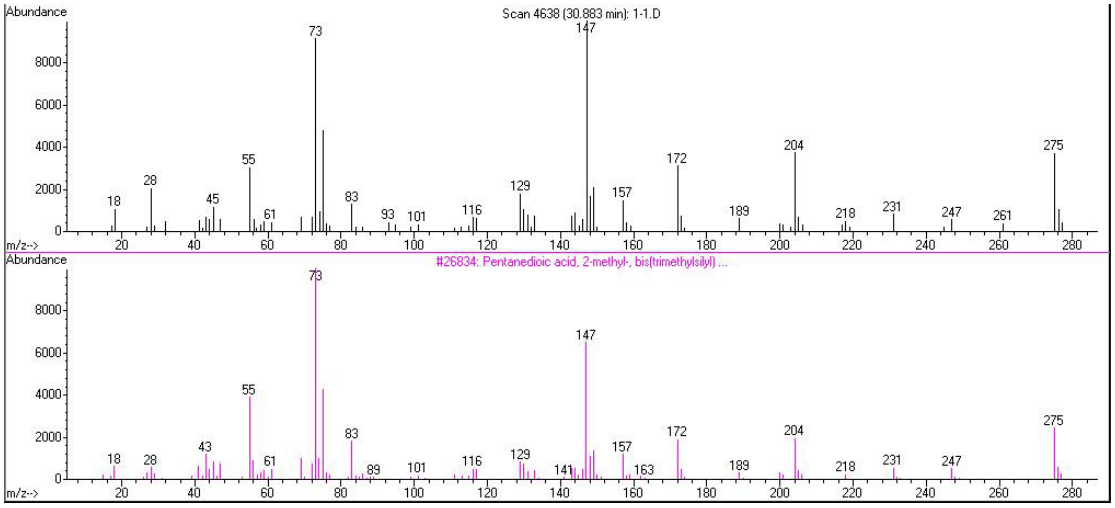
2-methyl-3-hydroxylsuccinic acid



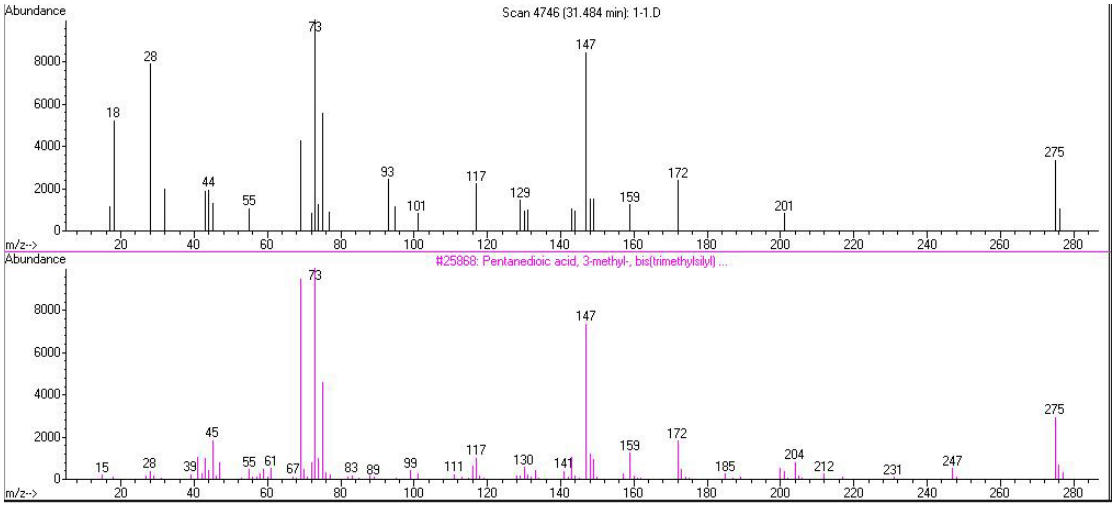
ethylmalonic acid



glutaric acid



2-methylglutaric acid



3-methylglutaric acid

Figure A.8 − The total ions chromatogram of GC-MS and comprison of mass spectra between photoproducts and standard compounds.