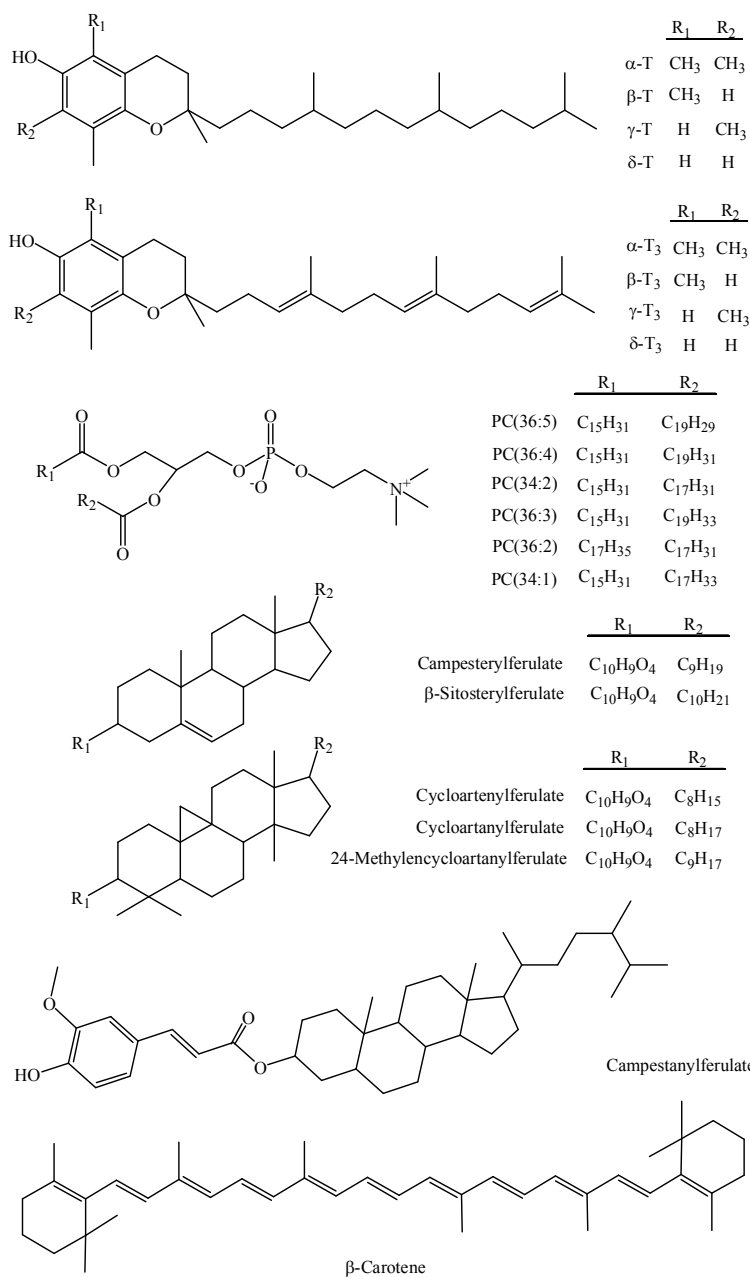
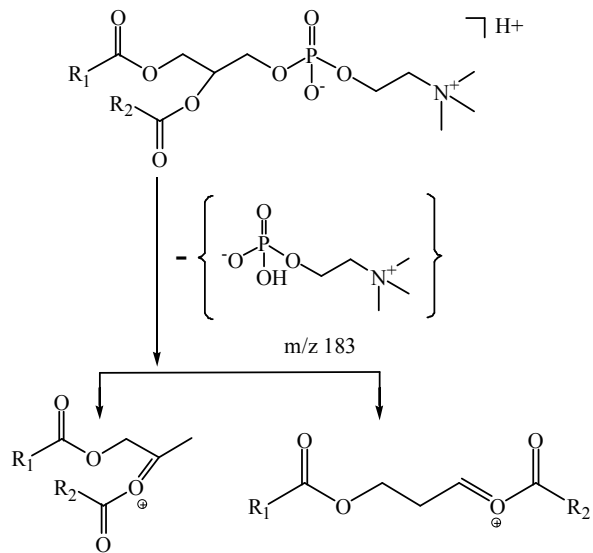
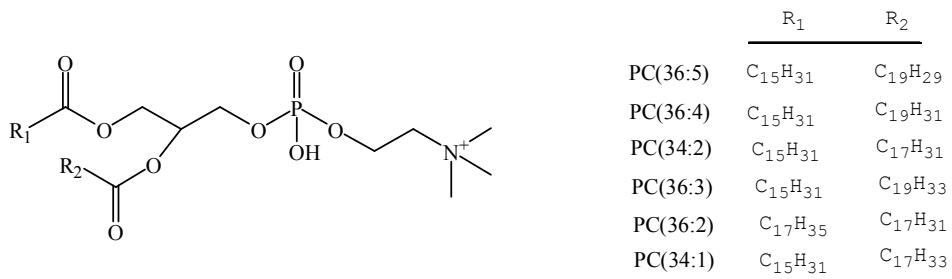


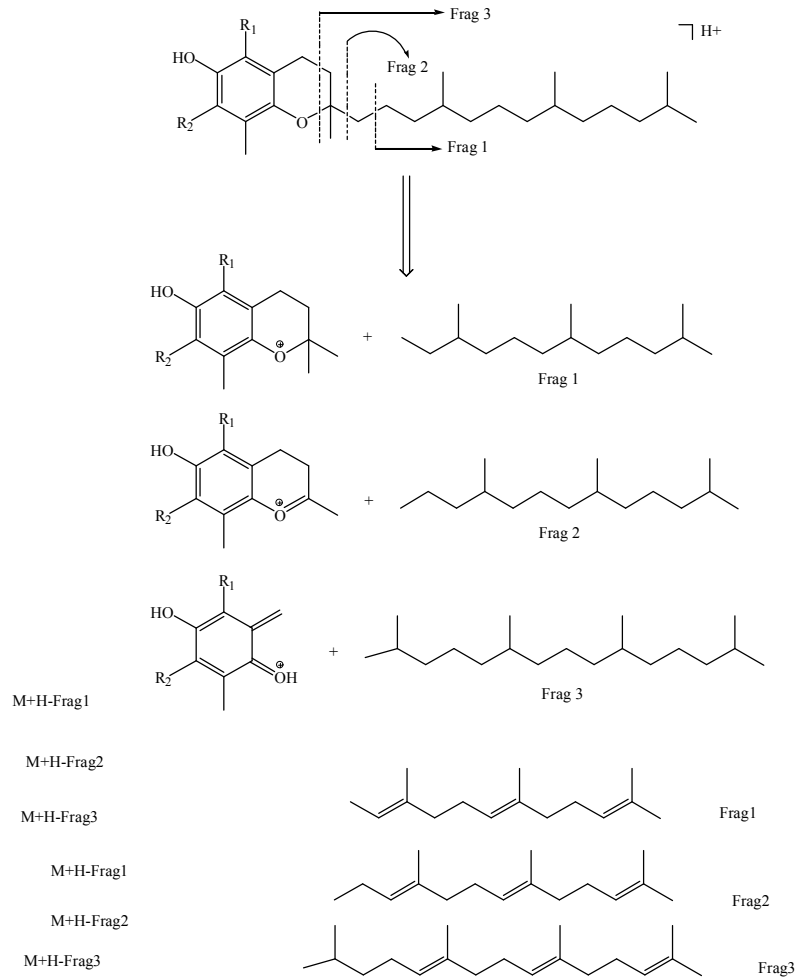
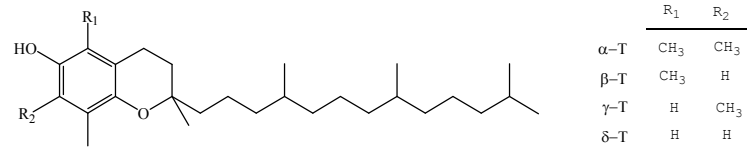
ChemDraw files as follows:



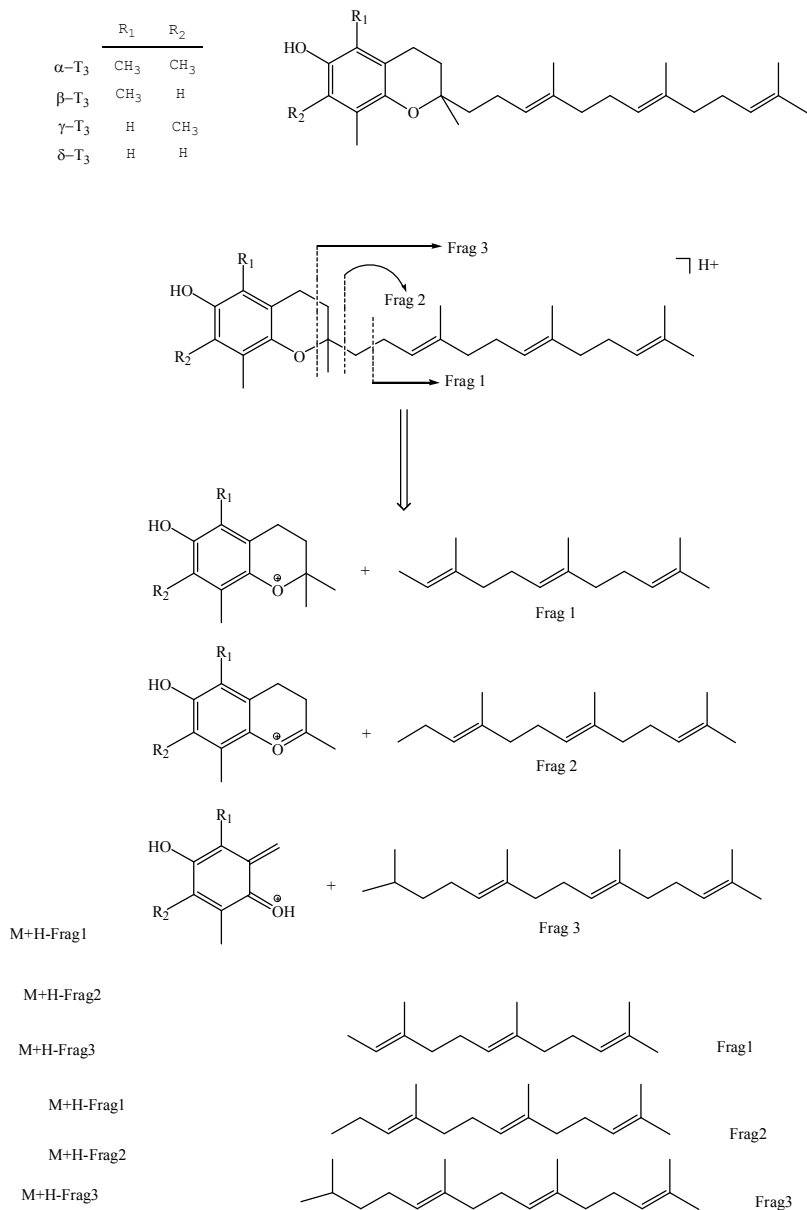
21 nutritional compositions



The fragmentation patterns of phospholipids

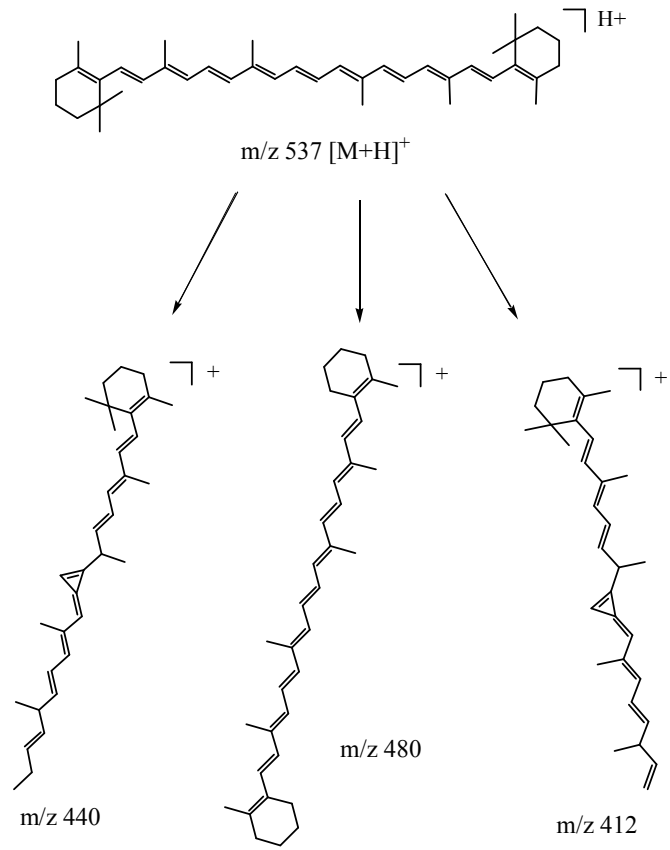


The fragmentation patterns of tocopherols

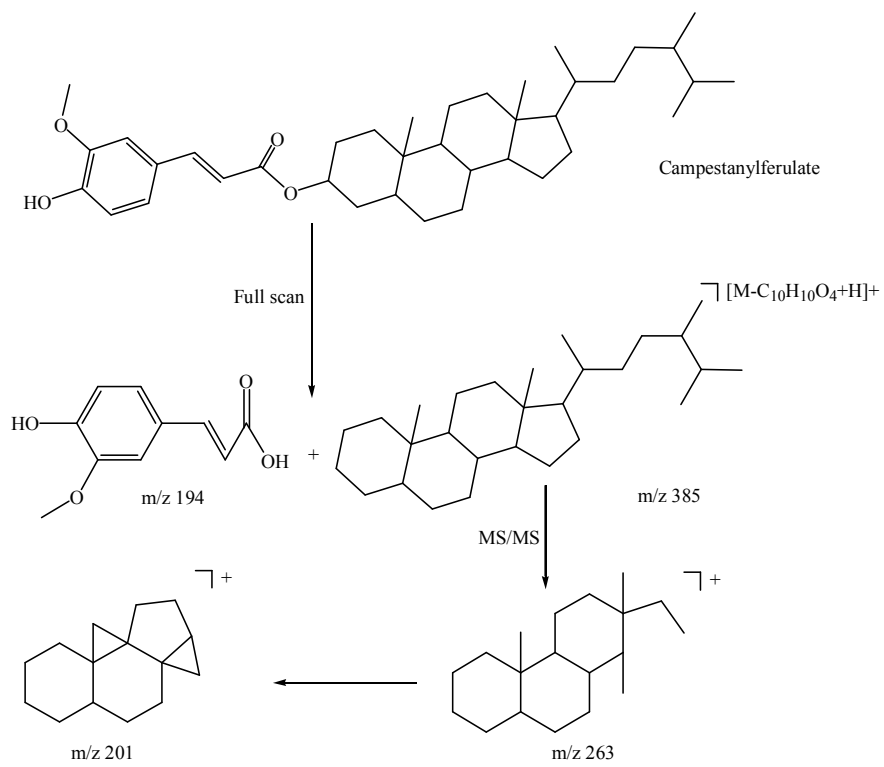
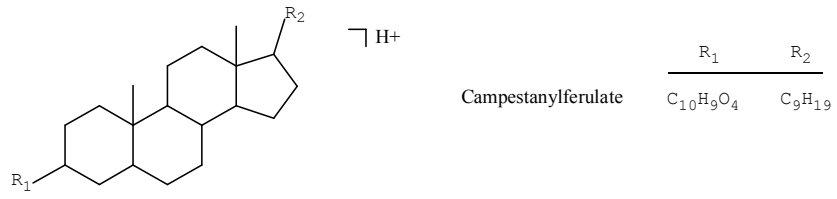


The fragmentation patterns of tocotrienols

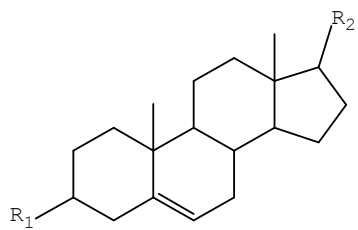
β -Carotene



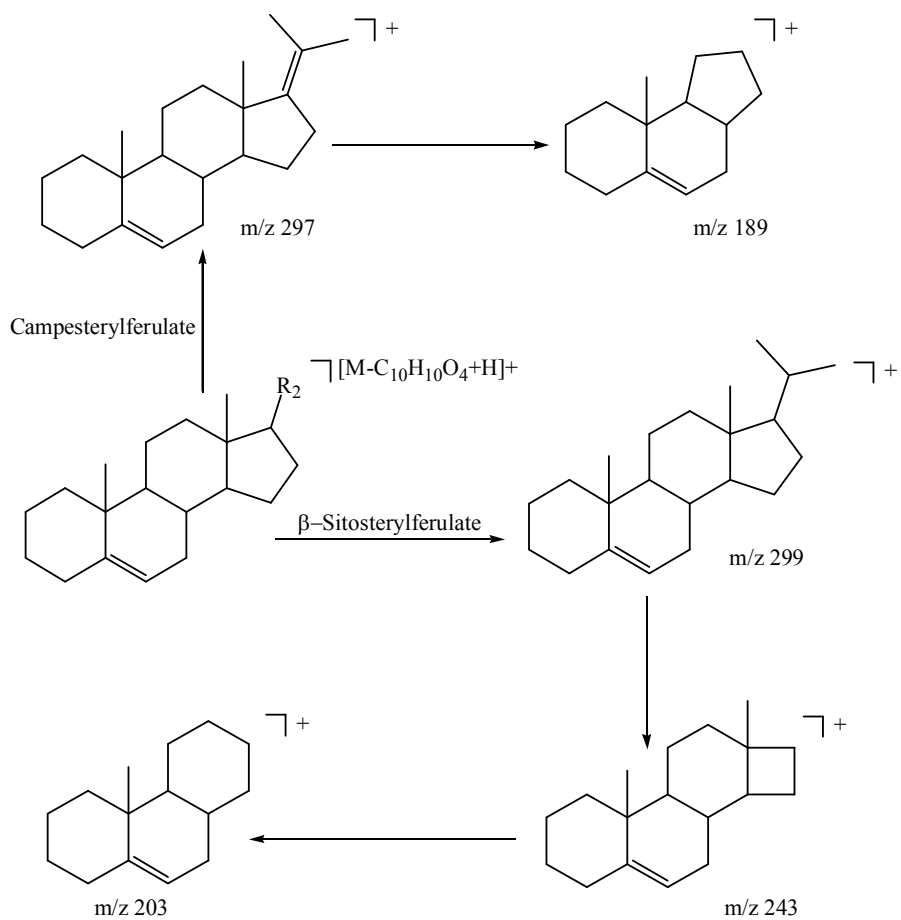
The fragmentation patterns of β -carotene



The fragmentation patterns of γ -oryzanol (1)

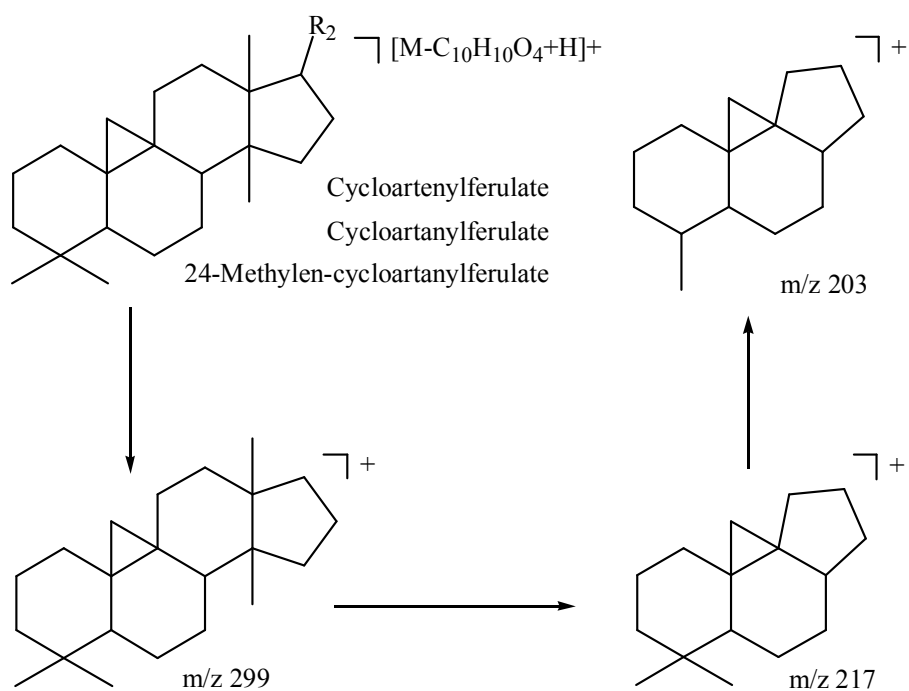


| | R ₁ | R ₂ |
|----------------------|---|---------------------------------|
| Campesterylferulate | C ₁₀ H ₉ O ₄ | C ₉ H ₁₉ |
| β-Sitosterylferulate | C ₁₀ H ₉ O ₄ | C ₁₀ H ₂₁ |



The fragmentation patterns of γ -oryzanols (2)

| R ₁ | R ₂ |
|---|--------------------------------|
| C ₁₀ H ₉ O ₄ | C ₈ H ₁₅ |
| C ₁₀ H ₉ O ₄ | C ₈ H ₁₇ |
| C ₁₀ H ₉ O ₄ | C ₉ H ₁₇ |



The fragmentation patterns of γ -oryzanols (3)

The source files of ChemDraw as follows:



21 nutritional compositions.cdx



The fragmentation patterns of phospholipids.cdx



The fragmentation patterns of tocopherols.cdx



The fragmentation patterns of tocotrienols.cdx



The fragmentation patterns of β -carotene.cdx



The fragmentation patterns of γ -oryzanol(1).cdx



The fragmentation patterns of γ -oryzanols(2).cdx



The fragmentation patterns of γ -oryzanols(3).cdx

Figures A.1-A.3 as follows:

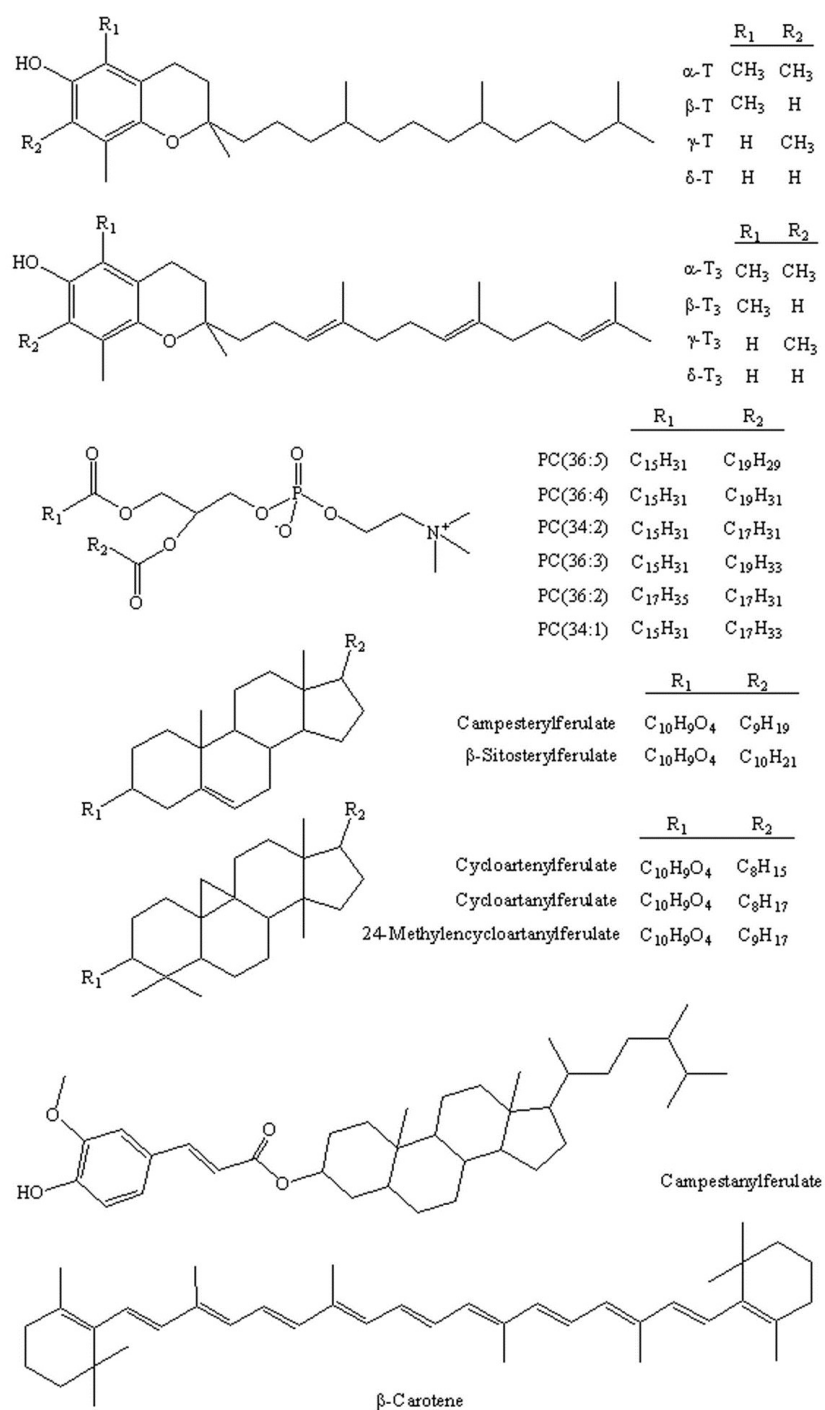


Figure A.1. The basic chemical structures of 21 nutrients in rice.

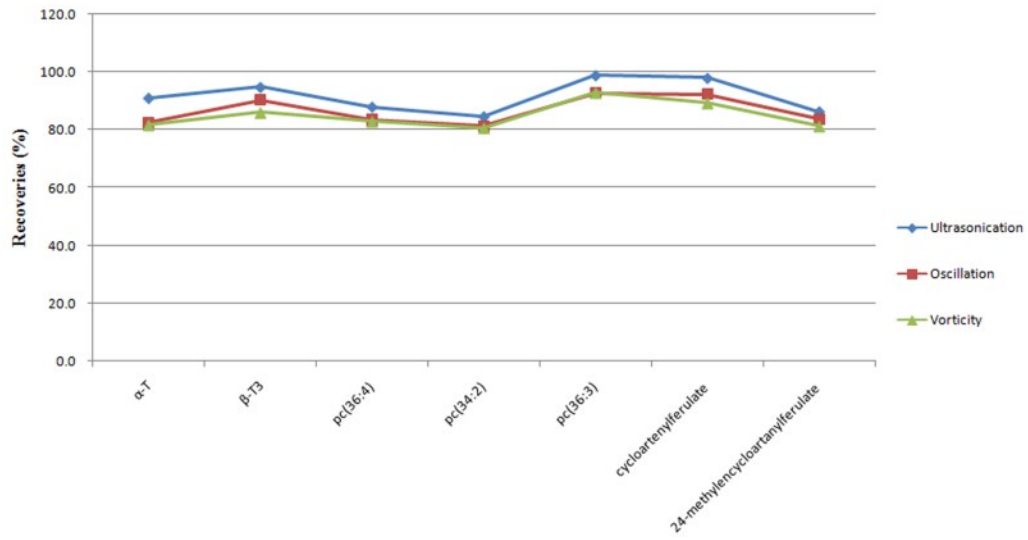


Figure A.2. Recoveries of nutritional compounds extracted by ultrasonication, oscillation and vorticity methods in white rice.

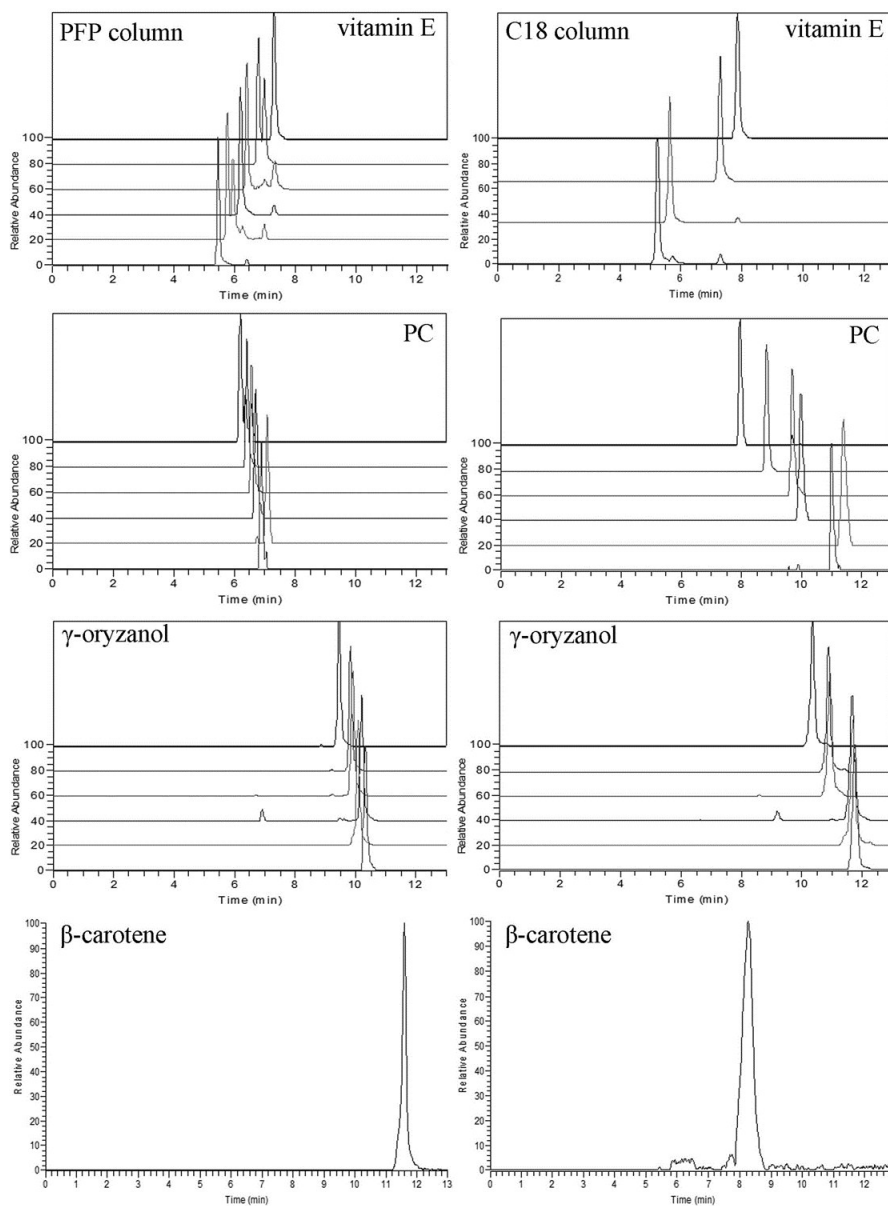


Figure A.3. The separation of chromatographic columns: PFP and C18 columns.

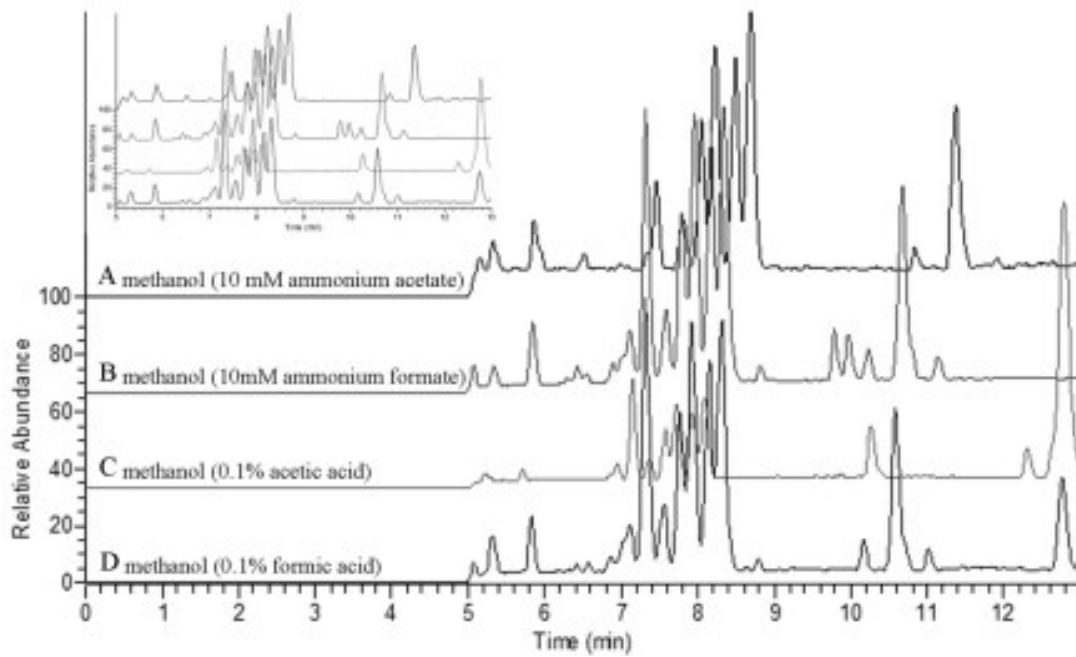


Figure A.4. The optimization of elution system (A: methanol-10 mM ammonium acetate, B: methanol-10mM ammonium formate, C: methanol-0.1% acetic acid, D: methanol-0.1% formic acid).

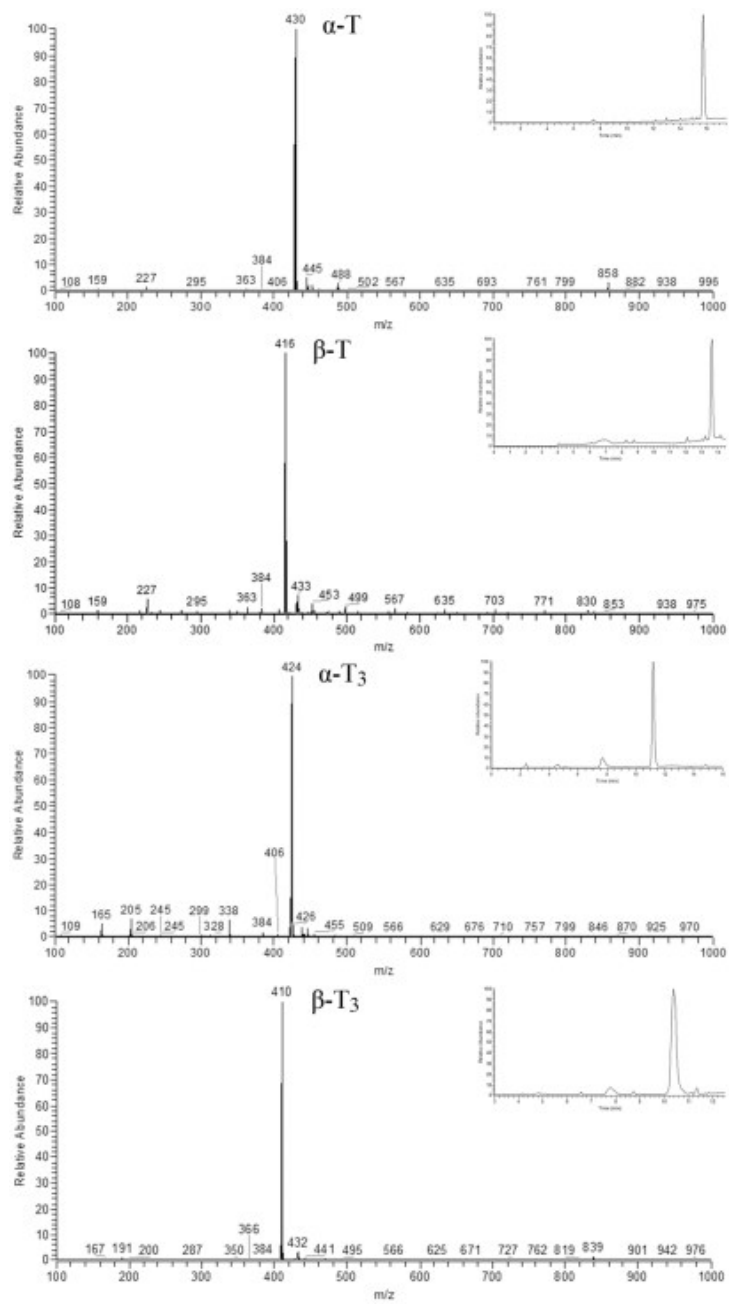


Figure A.5. The molecular peaks of vitamin E with non-ionization in the ESI source.

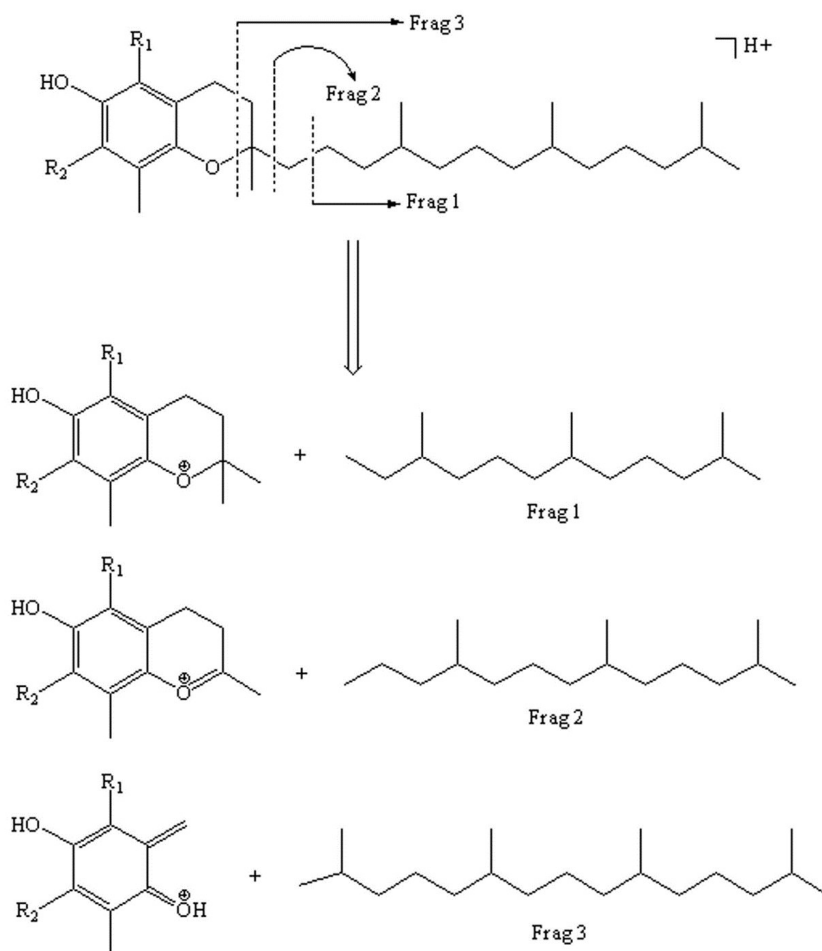
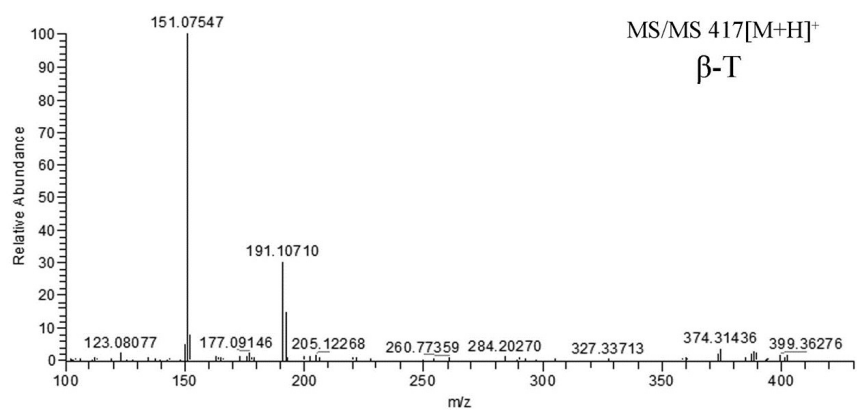


Figure A.6. The fragmentation patterns of tocopherols.

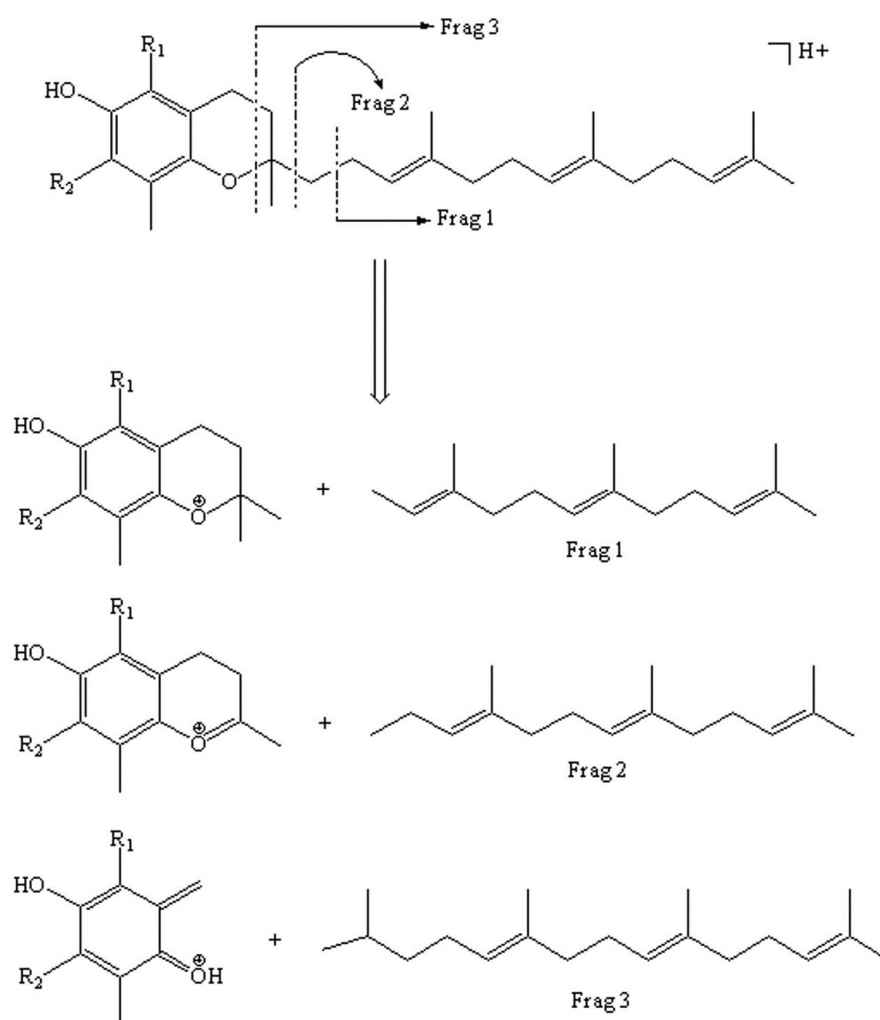
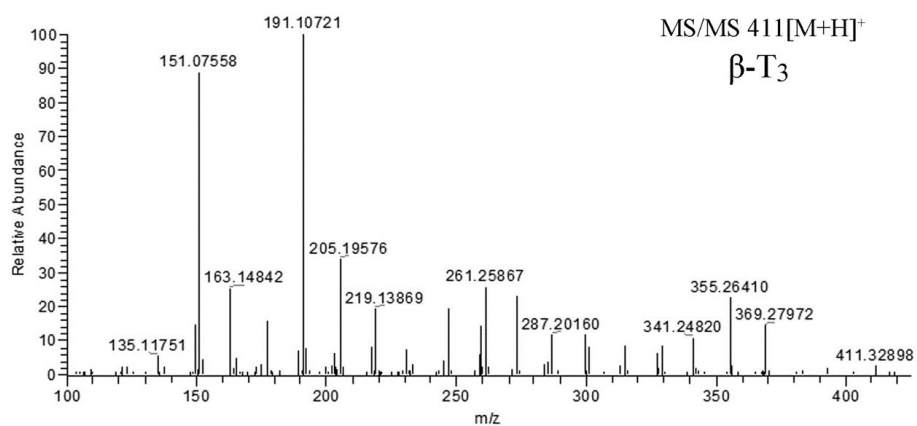


Figure A.7. The fragmentation patterns of tocotrienols.

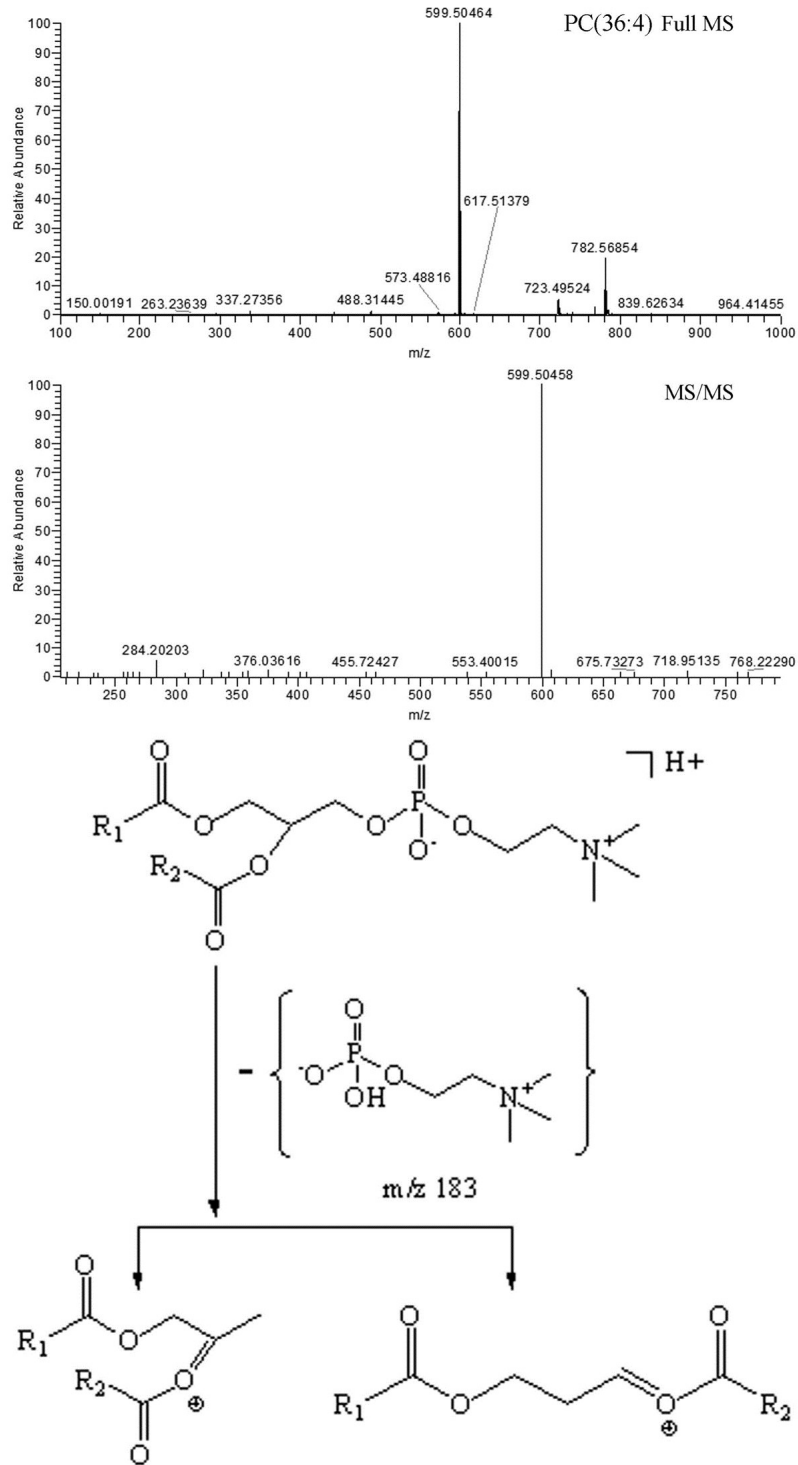


Figure A.8. The fragmentation patterns of phospholipids.

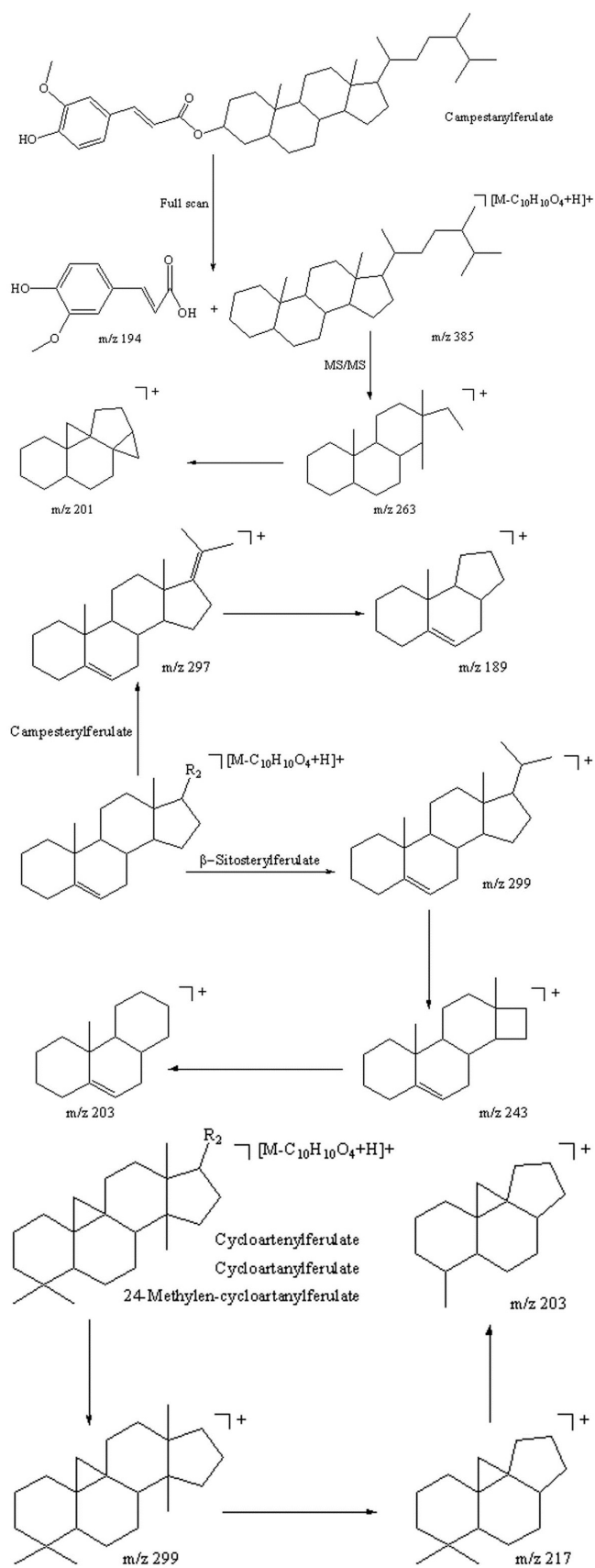


Figure A.9. The fragmentation patterns of γ -oryzanols.

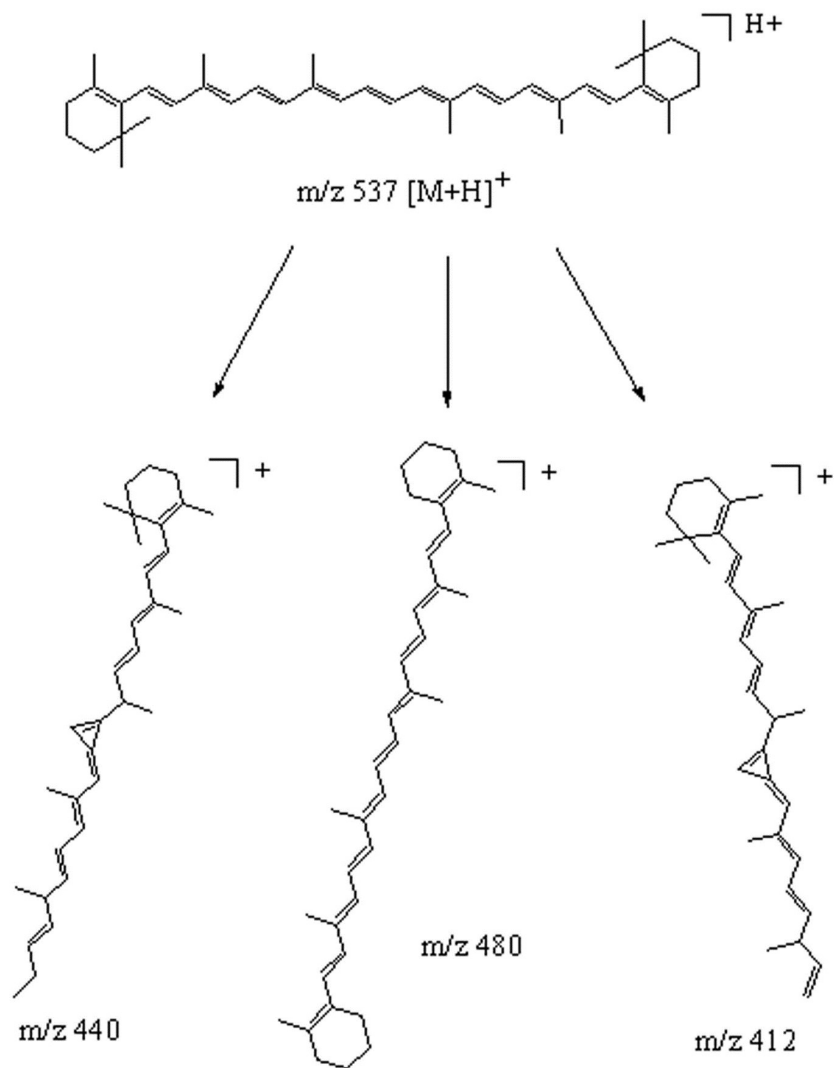
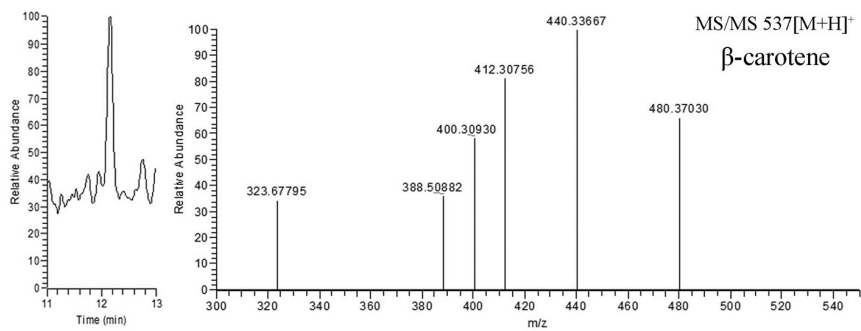


Figure A.10. The fragmentation patterns of β-carotene.

Table A.1-A.3 as follows:

Table A.1 Identification of 21 components using UHPLC-LTQ-Orbitrap MS.

| NO. | Tr (min) | Ion mode | Measured mass (m/z) | Calculated mass (m/z) | Mass error (ppm) | Fragment ion information (MS/MS) | Molecular formula | Compounds |
|-----|----------|--|---------------------|-----------------------|------------------|----------------------------------|---|---|
| 1 | 7.54 | [M+H] ⁺ | 431.38901 | 431.38836 | 1.5 | MS: 205(98%),165(100%) | C ₂₉ H ₅₀ O ₂ | α-T |
| 2 | 7.20 | [M+H] ⁺ | 417.37314 | 417.37271 | 1.0 | MS: 191(30%),151(100%) | C ₂₈ H ₄₈ O ₂ | β-T |
| 3 | 6.99 | [M+H] ⁺ | 417.37268 | 417.37271 | -0.1 | MS: 191(26%),151(100%) | C ₂₈ H ₄₈ O ₂ | r-T |
| 4 | 6.58 | [M+H] ⁺ | 403.35754 | 403.35706 | 1.2 | MS: 191(100%),177(64%),163(70%) | C ₂₇ H ₄₆ O ₂ | δ-T |
| 5 | 6.37 | [M+H] ⁺ | 425.34219 | 425.34141 | 1.8 | MS: 199(100%),151(62%) | C ₂₉ H ₄₄ O ₂ | α-T3 |
| 6 | 6.12 | [M+H] ⁺ | 411.32599 | 411.32576 | 0.6 | MS: 205(34%),191(100%),151(89%) | C ₂₈ H ₄₂ O ₂ | β-T3 |
| 7 | 5.92 | [M+H] ⁺ | 411.32553 | 411.32576 | -0.6 | MS: 205(36%),191(100%),151(96%) | C ₂₈ H ₄₂ O ₂ | r-T3 |
| 8 | 5.6 | [M+H] ⁺ | 397.31000 | 397.31011 | -0.3 | MS: 201(100%),187(69%) | C ₂₇ H ₄₀ O ₂ | δ-T3 |
| 9 | 6.46 | [M+H] ⁺ | 780.55267 | 780.55378 | -1.4 | MS: 597(100%) | C ₄₄ H ₇₈ O ₈ NP | PC(36:5) |
| 10 | 6.71 | [M+H] ⁺ | 782.56976 | 782.56943 | 0.4 | MS: 599(100%) | C ₄₄ H ₈₀ O ₈ NP | PC(36:4) |
| 11 | 6.89 | [M+H] ⁺ | 758.56946 | 758.56943 | 0.0 | MS: 575(100%) | C ₄₂ H ₈₀ O ₈ NP | PC(34:2) |
| 12 | 7.03 | [M+H] ⁺ | 784.58569 | 784.58508 | 0.8 | MS: 601(100%) | C ₄₄ H ₈₂ O ₈ NP | PC(36:3) |
| 13 | 7.45 | [M+H] ⁺ | 786.60077 | 786.60073 | 0.1 | MS: 603(100%) | C ₄₄ H ₈₄ O ₈ NP | PC(36:2) |
| 14 | 7.24 | [M+H] ⁺ | 760.58508 | 760.58508 | 0.0 | MS: 577(100%) | C ₄₂ H ₈₂ O ₈ NP | PC(34:1) |
| 15 | 9.85 | [M- C ₁₀ H ₁₀ O ₄ +H] ⁺ | 409.38351 | 409.38288 | 1.5 | MS: 299(57%),217(100%),203(57%) | C ₄₀ H ₄₈ O ₄ | cycloartenyl ferulate 24- methylency cloartanylfe |
| 16 | 10.25 | [M- C ₁₀ H ₁₀ O ₄ +H] ⁺ | 423.39978 | 423.39853 | 3.0 | MS: 299(100%),217(83%) | C ₄₁ H ₆₀ O ₄ | ulate campesteryl |
| 17 | 10.35 | [M- C ₁₀ H ₁₀ O ₄ +H] ⁺ | 383.36765 | 383.36723 | 1.1 | MS: 297(59%),189(100%) | C ₃₈ H ₅₆ O ₄ | ferulate β- sitosterylfer |
| 18 | 10.66 | [M- C ₁₀ H ₁₀ O ₄ +H] ⁺ | 397.38303 | 397.38288 | 0.4 | MS: 299(35%),243(100%),203(52%) | C ₃₉ H ₅₈ O ₄ | ulate cycloartanyl |
| 19 | 10.51 | [M- C ₁₀ H ₁₀ O ₄ +H] ⁺ | 411.39905 | 411.39853 | 1.3 | MS: 299(68%),217(100%),203(96%) | C ₄₀ H ₆₀ O ₄ | ferulate campestanlyl |
| 20 | 10.79 | [M- C ₁₀ H ₁₀ O ₄ +H] ⁺ | 385.38300 | 385.38288 | 0.3 | MS: 263(69%),201(100%) | C ₃₈ H ₅₈ O ₄ | ferulate |
| 21 | 12.12 | [M+H] ⁺ | 537.44653 | 537.44548 | 2.0 | MS: 480(65%),440(100%),412(80%) | C ₄₀ H ₅₆ | β-carotene |

Table A.2 Recoveries yielded

| Compounds | R% (n=3) | | | | | |
|---------------------------------|------------|--------------|-------------|------------|--------------|-------------|
| | White rice | | | Brown rice | | |
| | High level | Medium level | Lower level | High level | Medium level | Lower level |
| α -T | 90.7 | 91.0 | 90.7 | 99.2 | 91.1 | 99.4 |
| β -T | 94.9 | 97.7 | 81.4 | 91.9 | 97.9 | 96.4 |
| γ -T | 92.0 | 98.8 | 89.7 | 94.8 | 98.8 | 92.2 |
| δ -T | 92.1 | 97.1 | 99.4 | 87.7 | 98.2 | 97.2 |
| α -T3 | 82.5 | 95.7 | 83.7 | 84.9 | 95.8 | 94.1 |
| β -T3 | 97.6 | 94.9 | 98.4 | 93.4 | 96.9 | 89.8 |
| γ -T3 | 82.8 | 90.8 | 97.7 | 84.8 | 94.1 | 94.5 |
| δ -T3 | 88.8 | 91.4 | 92.0 | 86.1 | 92.4 | 93.2 |
| PC(36:5) | 86.6 | 83.3 | 99.9 | 95.8 | 96.8 | 98.8 |
| PC(36:4) | 98.2 | 87.6 | 96.1 | 96.1 | 90.9 | 84.9 |
| PC(34:2) | 80.6 | 83.7 | 94.7 | 84.3 | 84.5 | 97.8 |
| PC(36:3) | 92.9 | 98.7 | 87.1 | 96.7 | 98.7 | 90.0 |
| PC(36:2) | 90.0 | 96.1 | 91.7 | 85.6 | 83.6 | 99.1 |
| PC(34:1) | 109.6 | 104 | 105.3 | 106.7 | 103 | 101.9 |
| cycloartenylferulate | 94.6 | 97.7 | 99.5 | 93.7 | 93.1 | 95.0 |
| 24-methylencycloartanylferulate | 97.0 | 85.9 | 85.9 | 97.1 | 87.6 | 95.8 |
| campesterylferulate | 95.2 | 98.1 | 93.5 | 87.4 | 89.2 | 98.3 |
| β -sitosterylferulate | 90.9 | 86.5 | 94.3 | 92.5 | 97.7 | 96.2 |
| cycloartanylferulate | 90.3 | 97.7 | 93.7 | 91.5 | 94.8 | 92.2 |
| campestanylferulate | 93.2 | 87.6 | 86.2 | 95.4 | 90.4 | 97.5 |
| β -carotene | 86.3 | 97.3 | 83.2 | 99.0 | 81.1 | 83.5 |

Table A.3 Classification results of the discriminant analysis.

| | | Single | Predicted Group Membership | | | | | |
|----------|-------|---------|----------------------------|-------|-------|-------|-------|-------|
| | | Linkage | 1 | 2 | 3 | 4 | 5 | Total |
| Original | Count | 1 | 6 | 0 | 0 | 0 | 0 | 6 |
| | | 2 | 0 | 6 | 0 | 0 | 0 | 6 |
| | | 3 | 0 | 0 | 6 | 0 | 0 | 6 |
| | | 4 | 0 | 0 | 0 | 6 | 0 | 6 |
| | | 5 | 0 | 0 | 0 | 0 | 6 | 6 |
| | (%a) | 1 | 100.0 | .0 | .0 | .0 | .0 | 100.0 |
| | | 2 | .0 | 100.0 | .0 | .0 | .0 | 100.0 |
| | | 3 | .0 | .0 | 100.0 | .0 | .0 | 100.0 |
| | | 4 | .0 | .0 | .0 | 100.0 | .0 | 100.0 |
| | | 5 | .0 | .0 | .0 | .0 | 100.0 | 100.0 |

^a 100.0% of original grouped cases correctly classified.