

GC-MS Discrimination of Citrulline from Ornithine and Homocitrulline from Lysine by Chemical Derivatization: Evidence of Formation of N^5 -Carboxy-ornithine and N^6 -Carboxy-lysine

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Citation: Baskal, S.; Bollenbach, A.; Tsikas, D. GC-MS Discrimination of Citrulline from Ornithine and Homocitrulline from Lysine by Chemical Derivatization: Evidence of Formation of N^5 -Carboxy-ornithine and N^6 -Carboxy-lysine. *Molecules* **2021**, *26*, 2301. <https://doi.org/10.3390/molecules26082301>

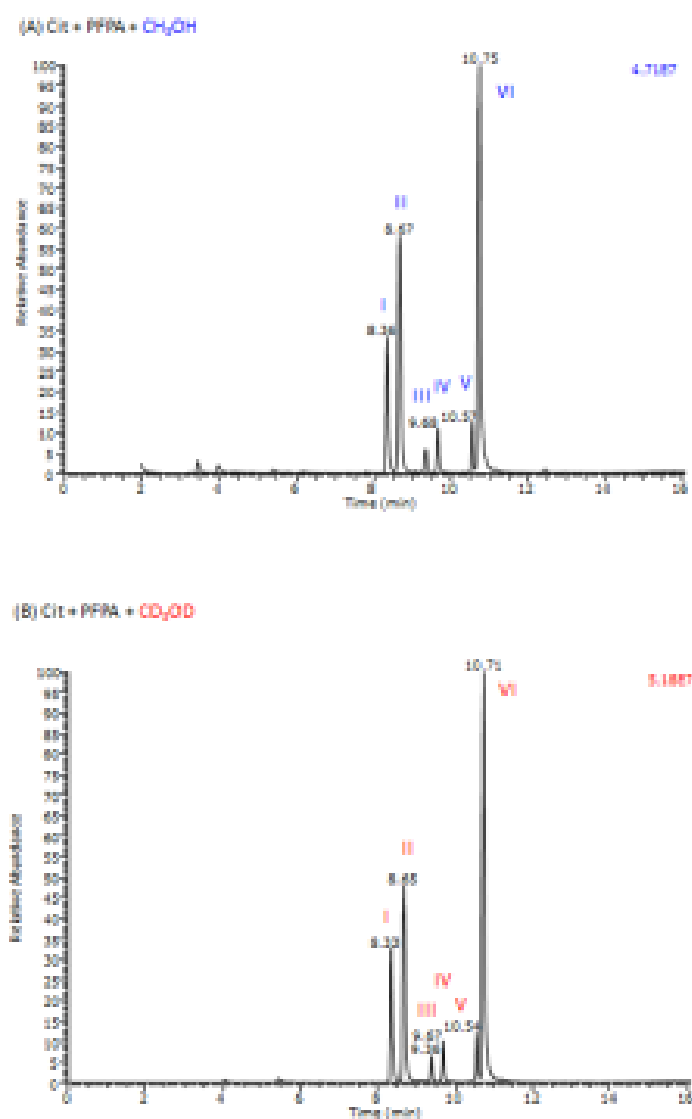
Academic Editor: Paraskevas D. Tzanavaras
Received: 24 March 2021
Accepted: 13 April 2021
Published: date

Publisher's Note: MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.

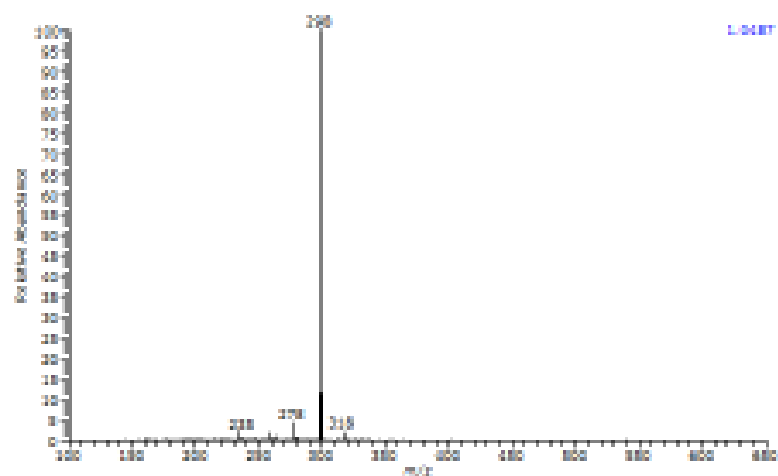


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Figure S1. Separate derivatization of citrulline and homocitrulline (5 nmol each) by procedure B, i.e., first with PFPA/EA and then 2 M HCl/CH₃OH or 2 M HCl/CD₃OD, and structural characterization of their reaction products by GC-MS.



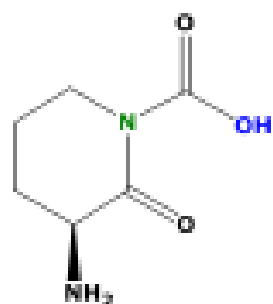
(A1) Cit+ PFPA + CH_3OH : Peak I, $t_R=8.33$ min



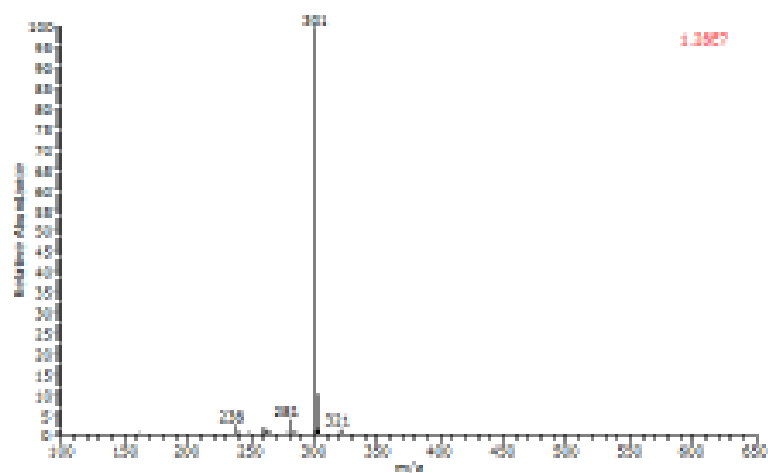
1.3487

Peak I

t_R 8.36/8.33

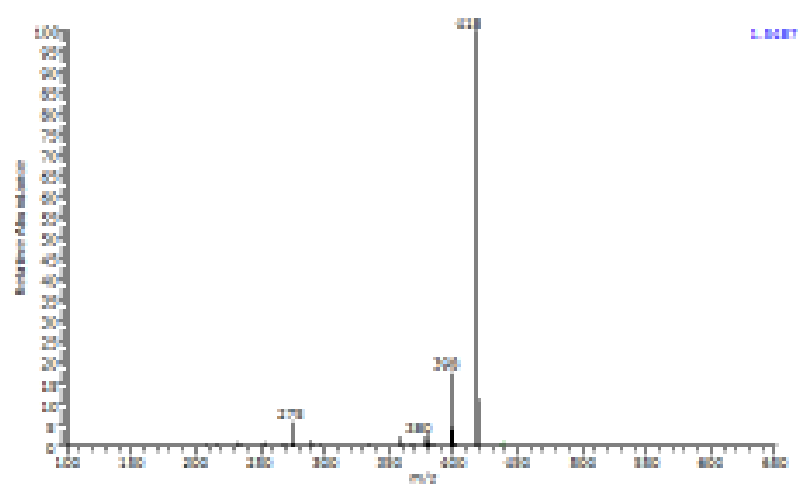


(B1) Cit+ PFPA + CD_3OD : Peak I, $t_R=8.33$ min



1.3507

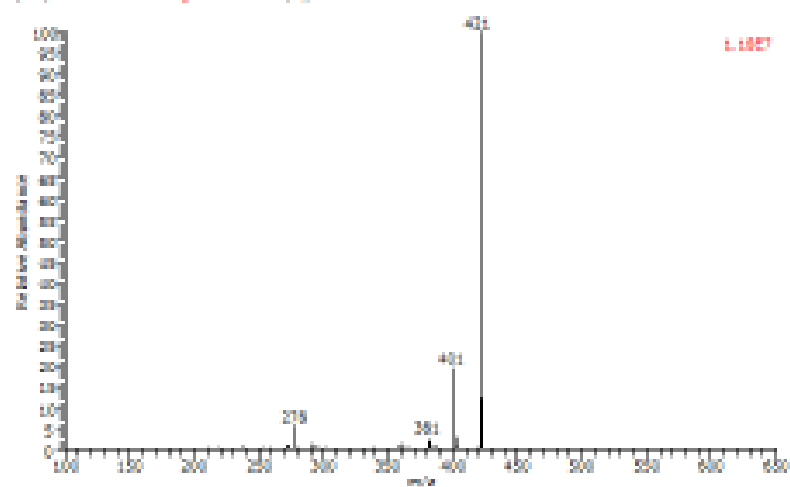
(A2) Cit + PFPs + CH_3OH : Peak II, $t_R=8.87$ min



Peak II

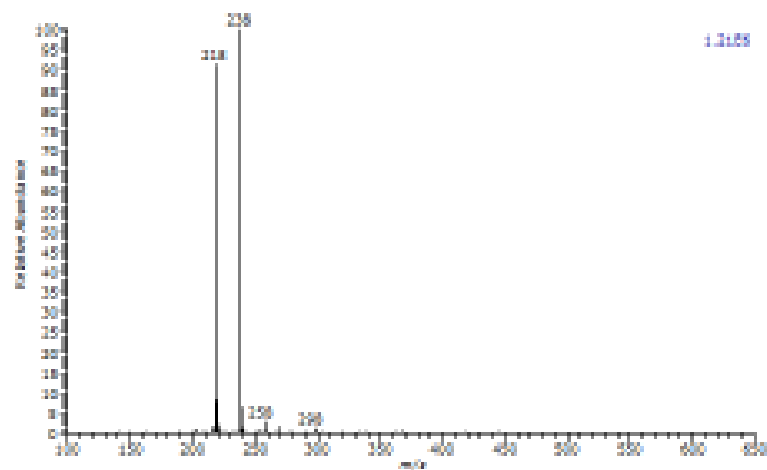
Ornithine from Cit

(B2) Cit + PFPs + CO_2O : Peak II, $t_R=8.63$ min



t_R 8.67/8.63

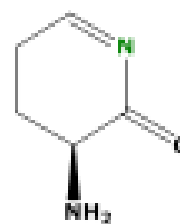
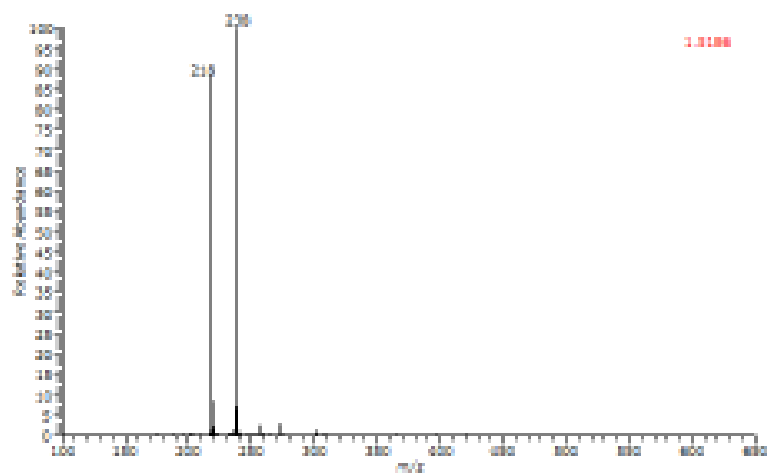
(A3) Cit + PFPA + CH_3OH : Peak III, $t_R=9.36$ min



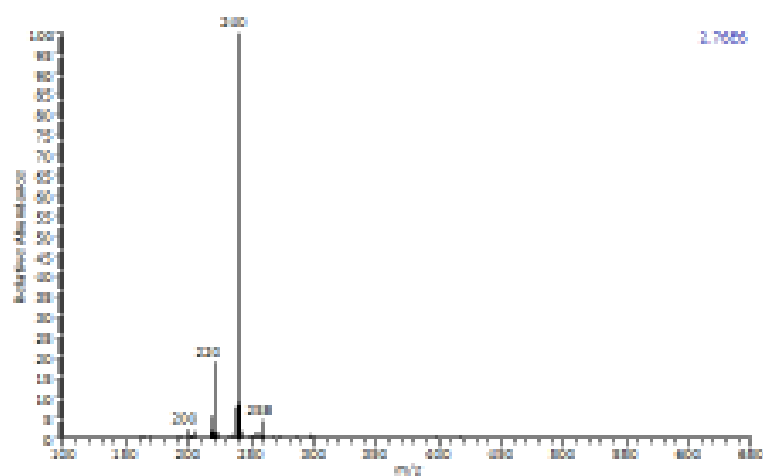
Peak III

t_R 9.36/9.36

(B3) Cit + PFPA + CD_3OD : Peak III, $t_R=9.36$ min



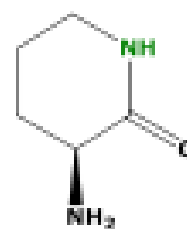
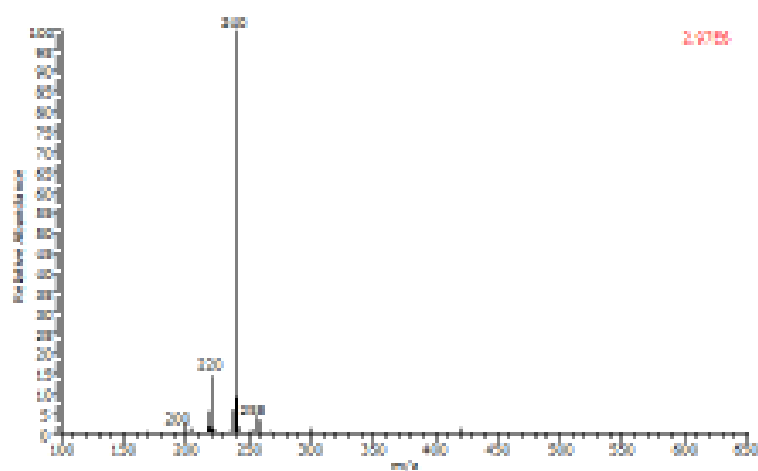
(A4) Cit + PFPA = CH_3OH : Peak IV, $t_R=9.67$ min



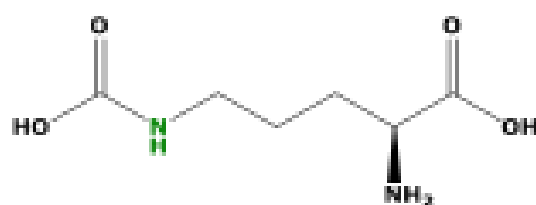
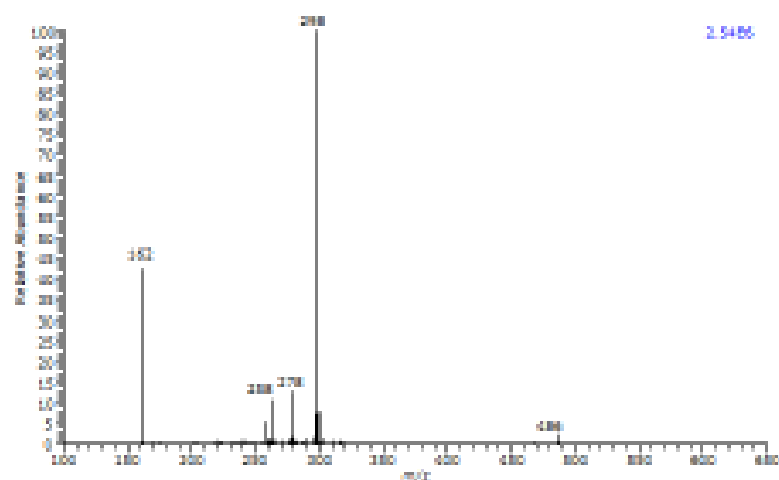
Peak IV

t_R 9.67/9.63

(B4) Cit + PFPA = CD_3OD : Peak IV, $t_R=9.35$ min



(A5) Cit + PFPA + CH_3OH : Peak V, $t_R=10.57$ min

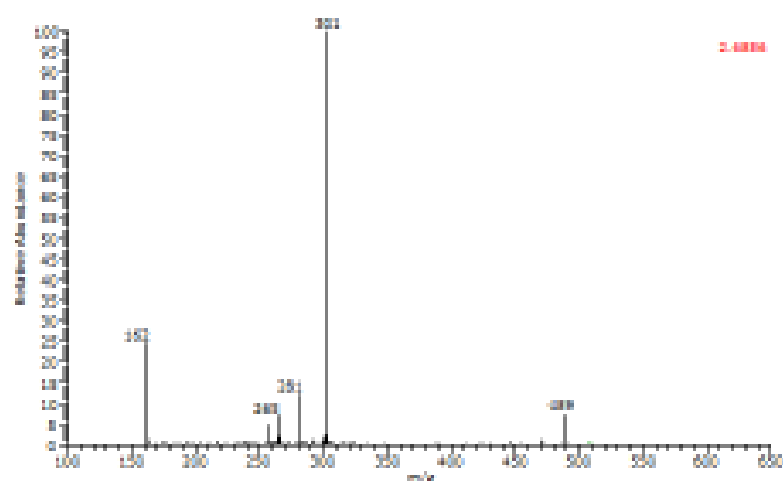


t_R 10.57/10.52

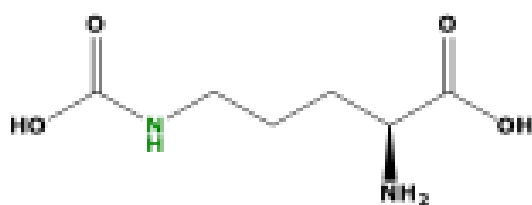
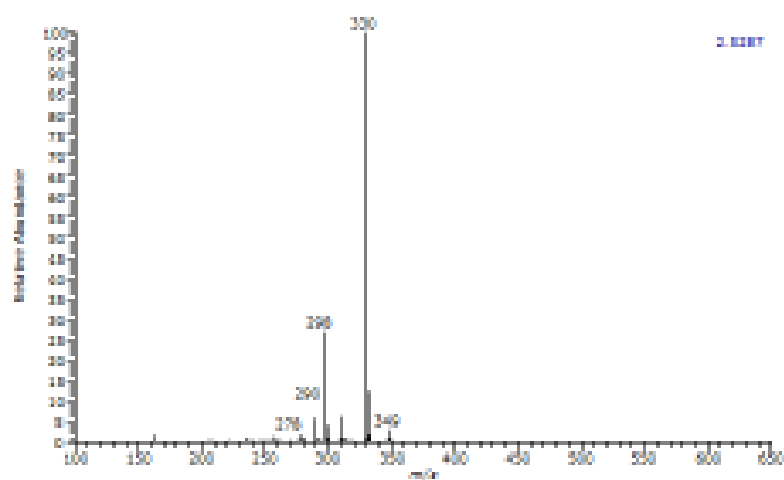
from Cit

*N*⁶-Carboxy-Ornithin

(B5) Cit + PFPA + CD_3OD : Peak V, $t_R=10.54$ min



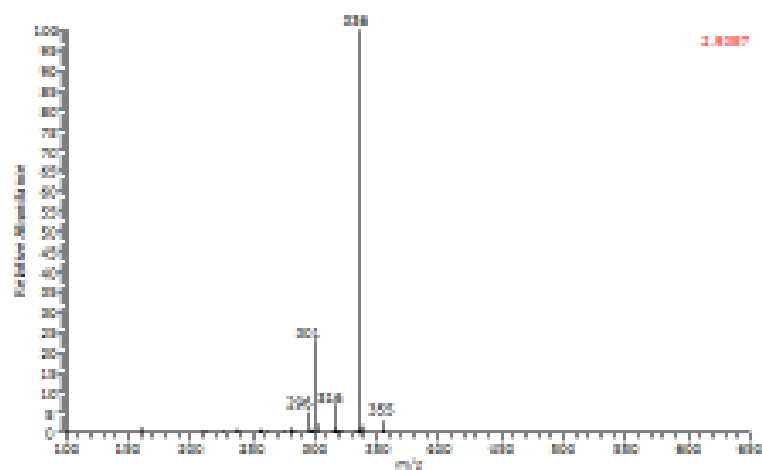
(A6) Cit+ PFPA + CH₃OH: Peak VI, t_R=10.75 min



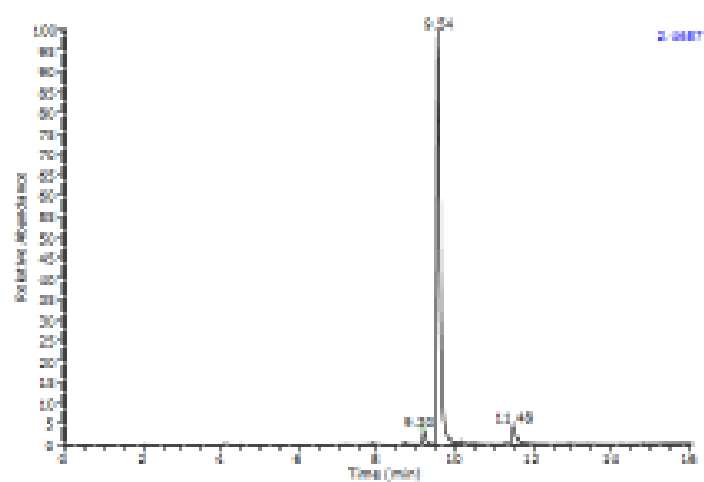
Peak VI

t_R 10.75/10.71

(B6) Cit+ PFPA + CD₃OD: Peak VI, t_R=10.71 min



(D) hCit+ PFPA + CH_3OH

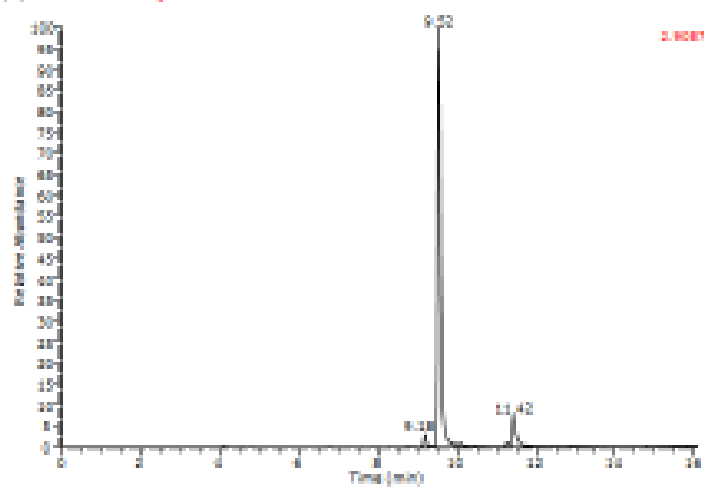


tR 9.54/9.52

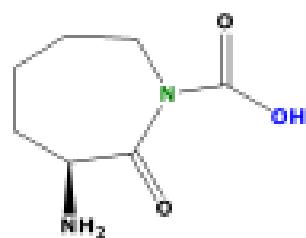
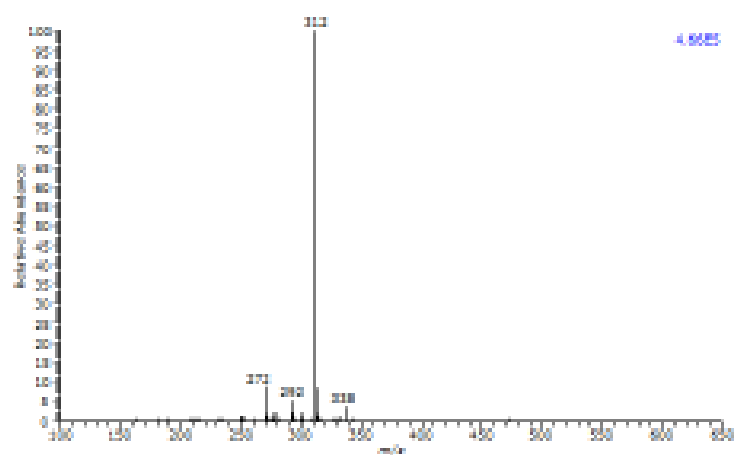
Lysine

from hCit

(E) hCit+ PFPA + CD_3OD



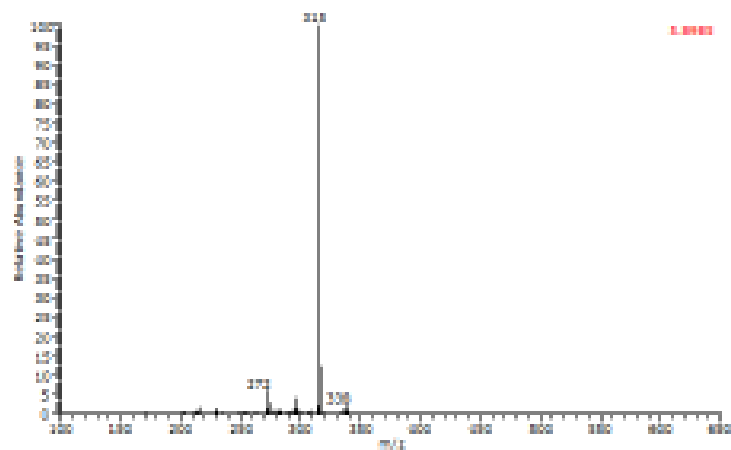
(D1) hCit+ PPA+ CH_3OH : t_R =9.21 min



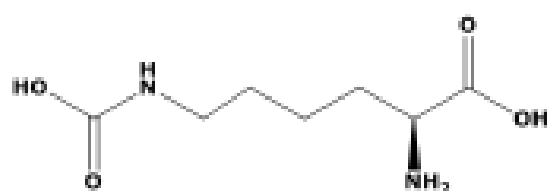
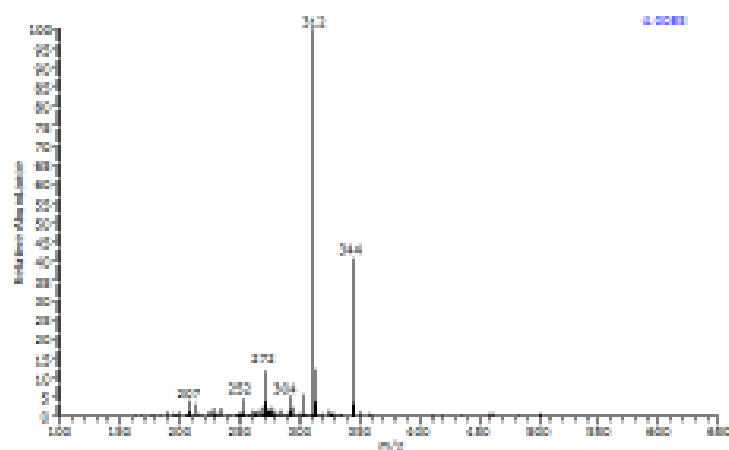
t_R 9.21/9.18

from hCit

(E1) hCit+ PPA+ CD_3OD : t_R =9.18 min



(D3) hCit+ PFPA = CH_2OH : t_R =11.47 min

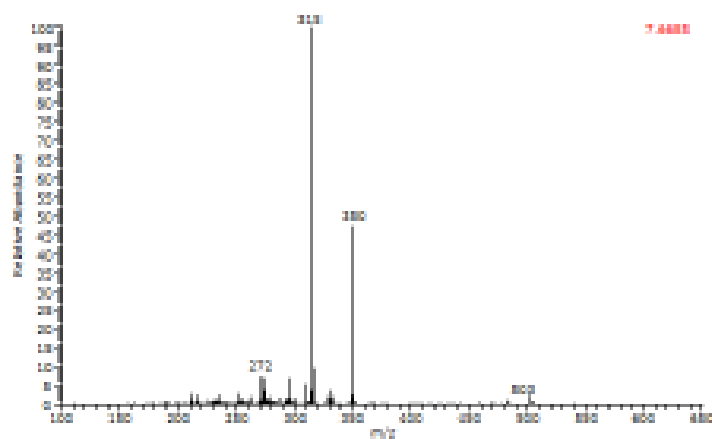


t_R 11.47/11.42

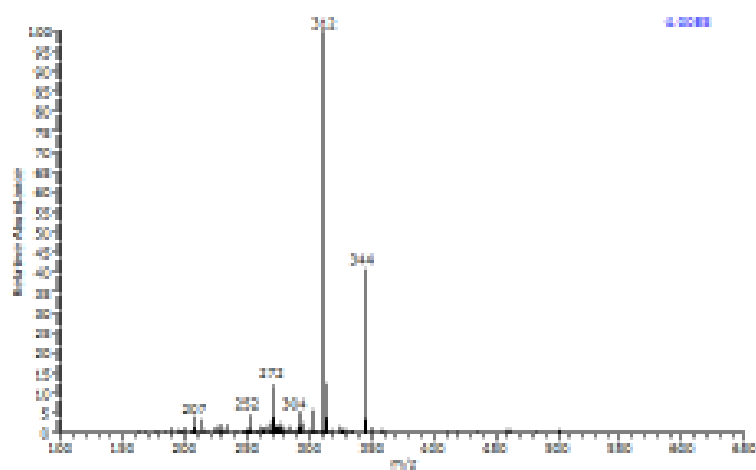
from hCit

***N*⁶-carboxy-L-lysine**

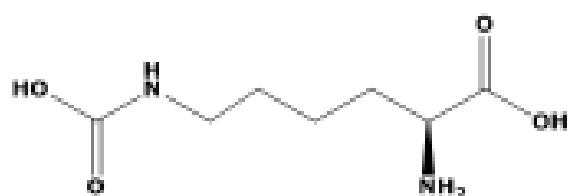
(E5) hCit+ PFPA = CO_2CO : t_R =11.42 min



(D8)hCit+PFPA=CH₂OH: t_R=11.47 min



4.3083

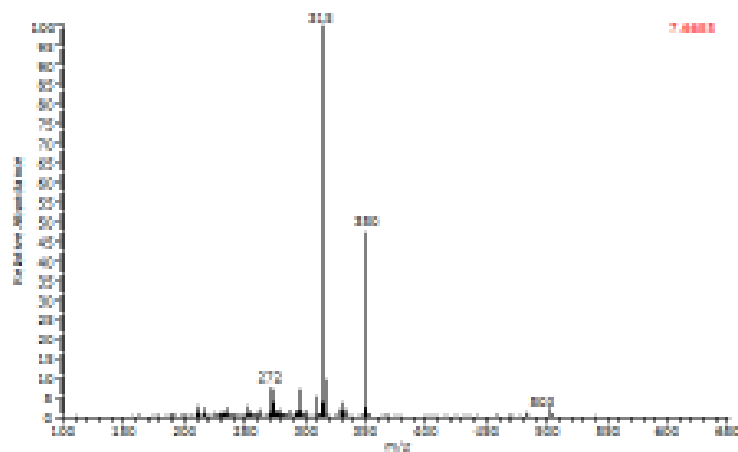


tR 11.47/11.42

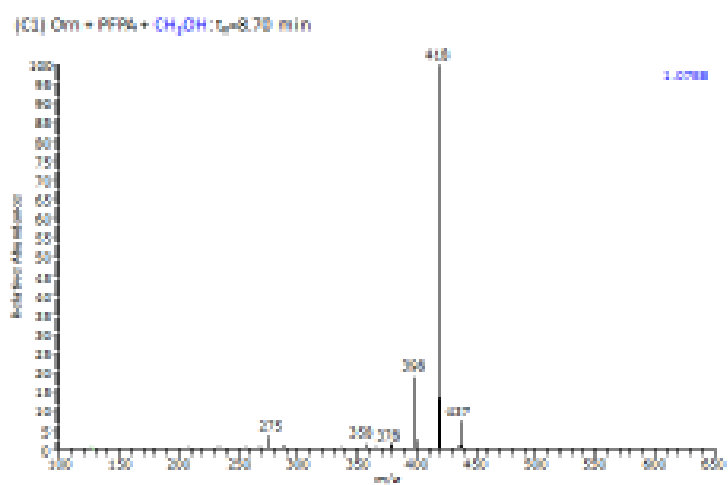
from hCit

N⁶-carboxy-L-lysine

(E3)hCit+PFPA=CO₂OO: t_R=11.42 min



7.8883



Omithine-Standard

t_R 8.67/8.63

