

Supplementary materials

Title

Fragmentation of dicarboxylic and tricarboxylic acids in the Krebs cycle using GC-EI-MS and GC-EI-MS/MS.

Authors

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Supplementary materials 2 MS spectra of EI-fragments of TBDMS derivatives

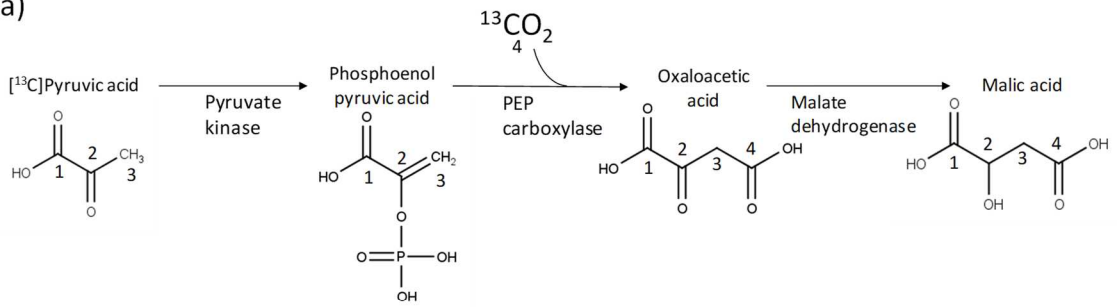
Supplementary materials 3 MS/MS spectra of CID-fragments of TMS derivatives

Supplementary materials 4 MS/MS spectra of CID-fragments of TBDMS derivatives

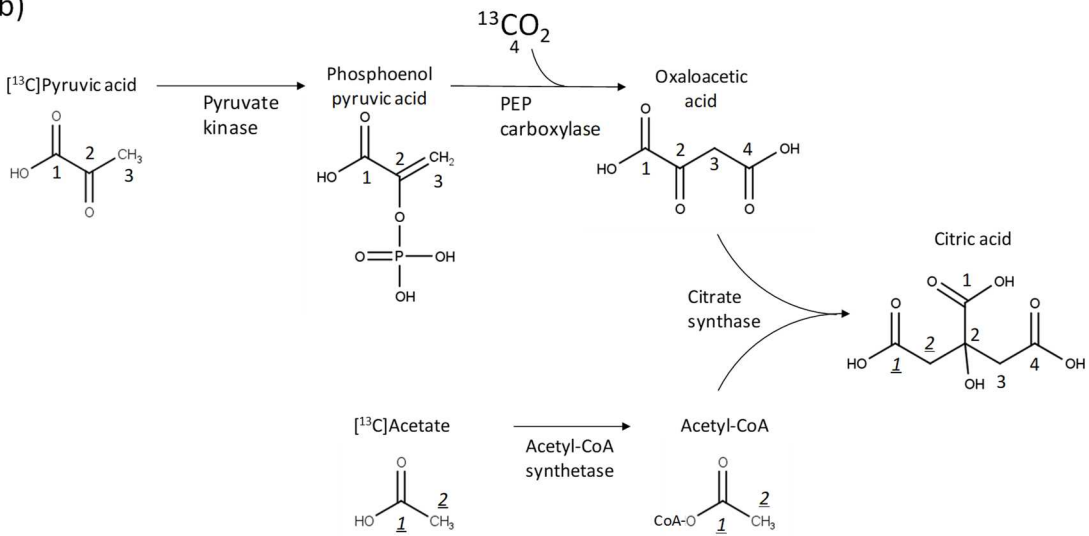
Supplementary figure 1

Carbon transition of enzyme reactions *in vitro* of (a) malic and (b) citric acid.

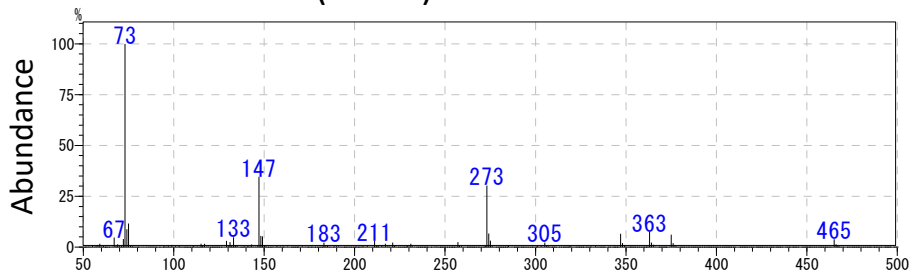
(a)



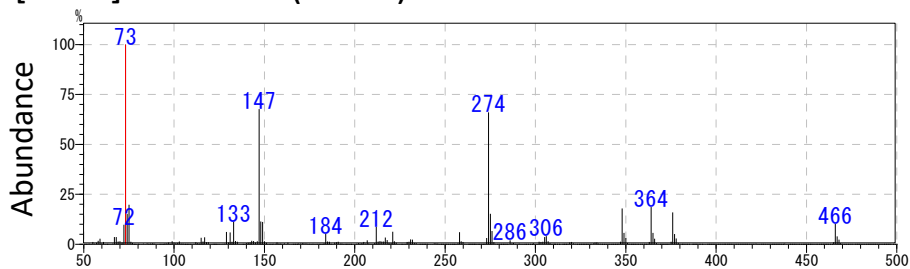
(b)



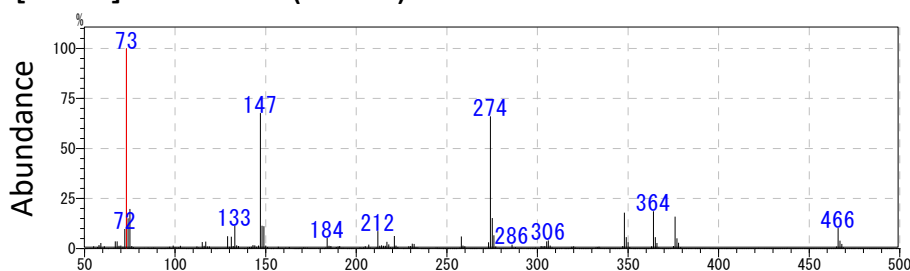
Natural citric acid (4TMS)



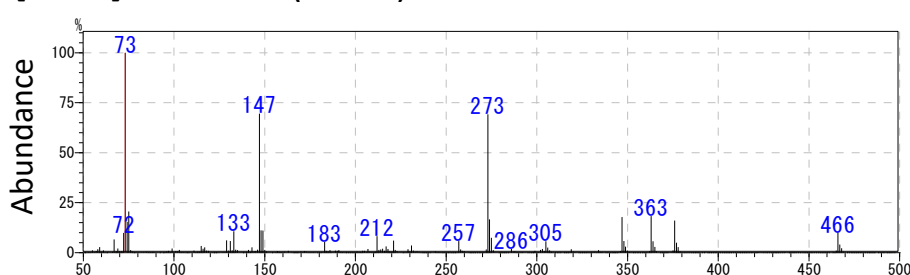
[1-¹³C]citric acid (4TMS)



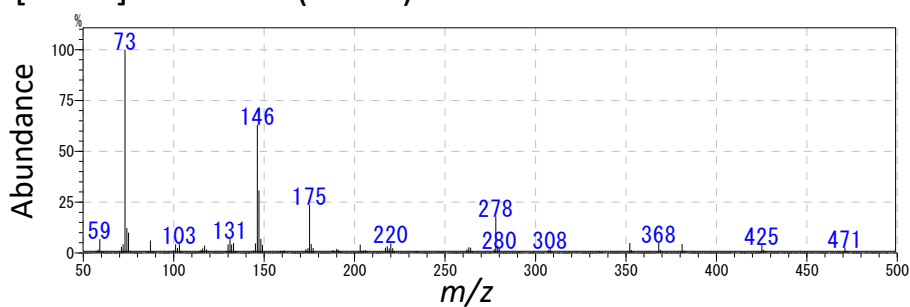
[5-¹³C]citric acid (4TMS)



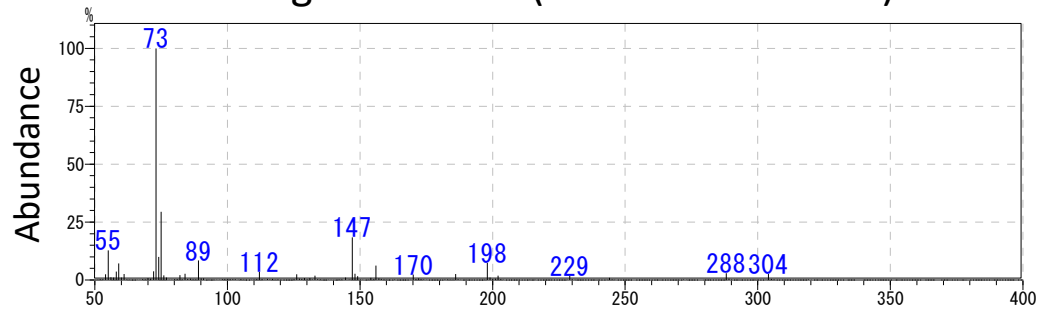
[6-¹³C]citric acid (4TMS)



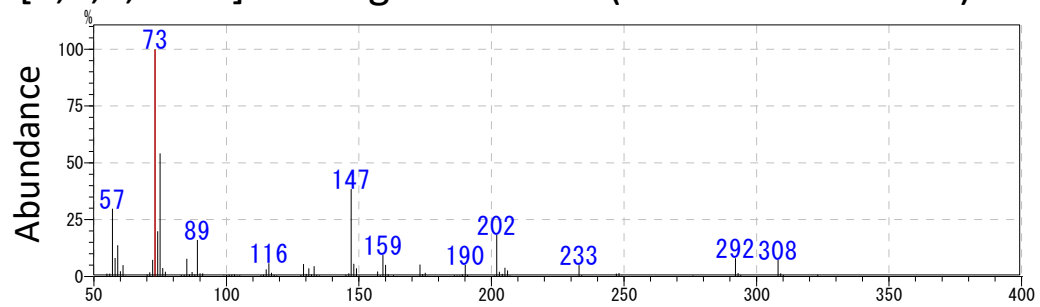
[U-¹³C]citric acid (4TMS)



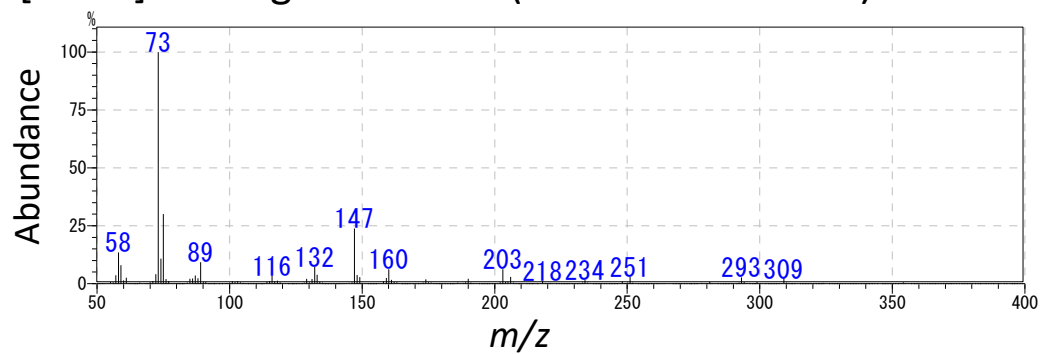
Natural α -ketoglutaric acid (1MEOX and 2TMS)



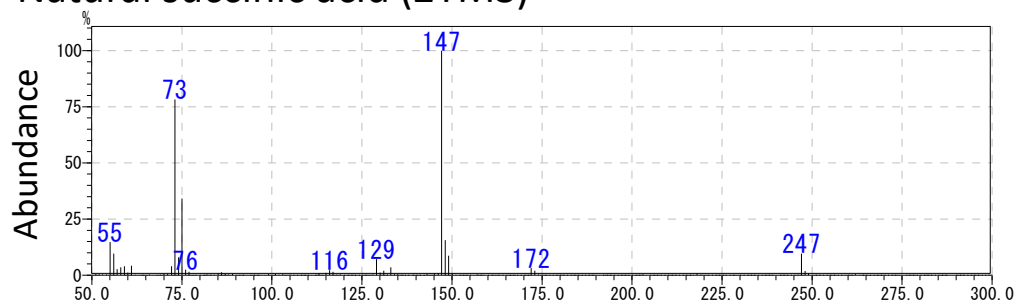
[1,2,3,4- ^{13}C] α -ketoglutaric acid (1MEOX and 2TMS)



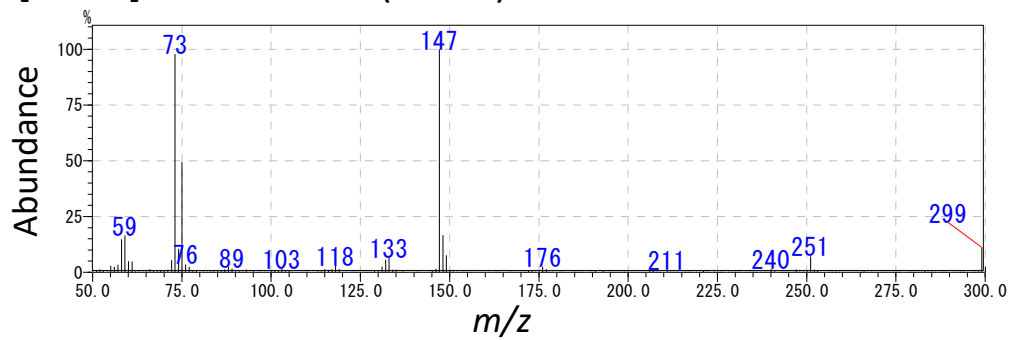
[U- ^{13}C] α -ketoglutaric acid (1MEOX and 2TMS)



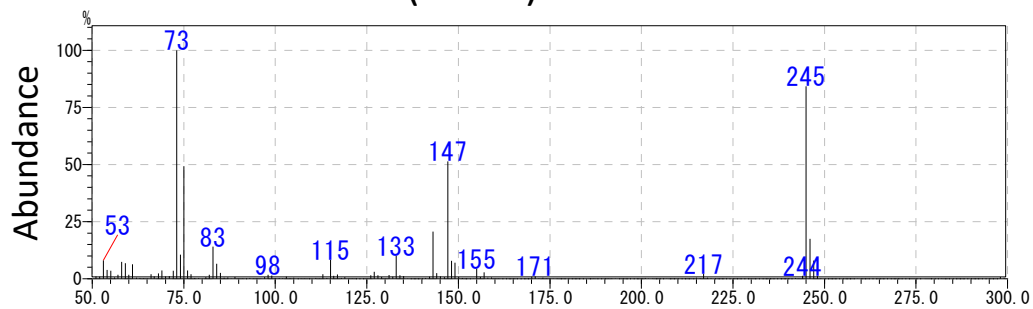
Natural succinic acid (2TMS)



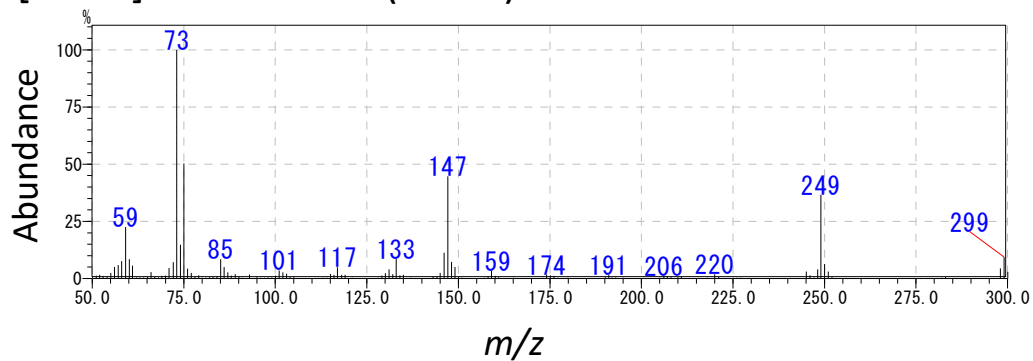
[U-¹³C]succinic acid (2TMS)



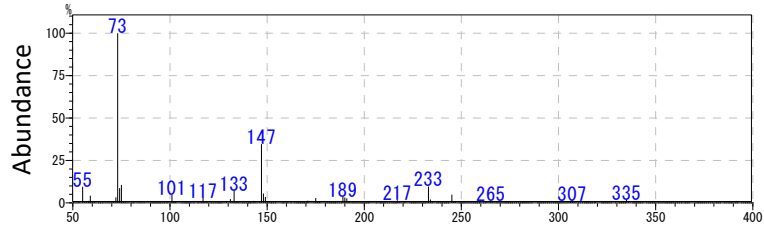
Natural fumaric acid (2TMS)



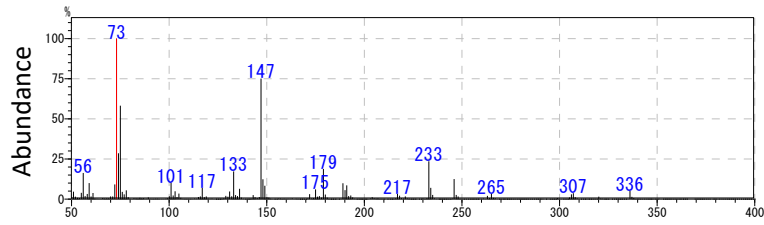
[U-¹³C]fumaric acid (2TMS)



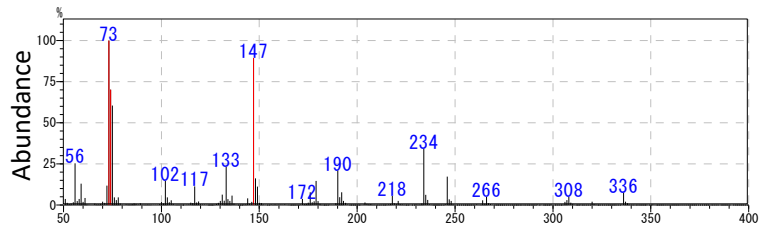
Natural malic acid (3TMS)



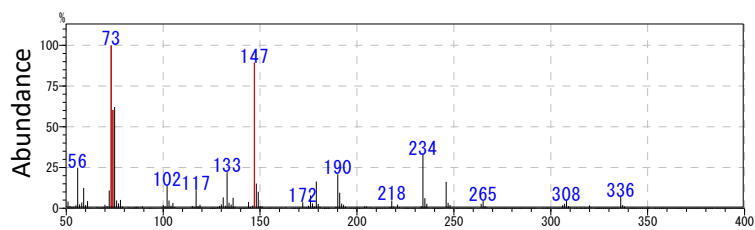
[1-¹³C]malic acid (3TMS)



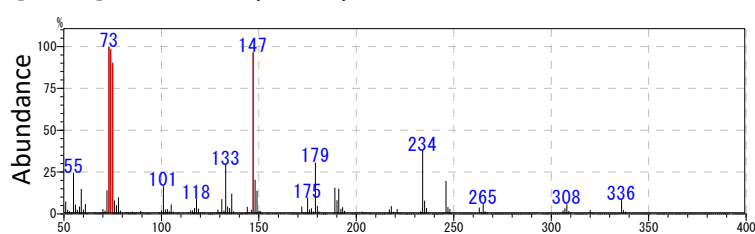
[2-¹³C]malic acid (3TMS)



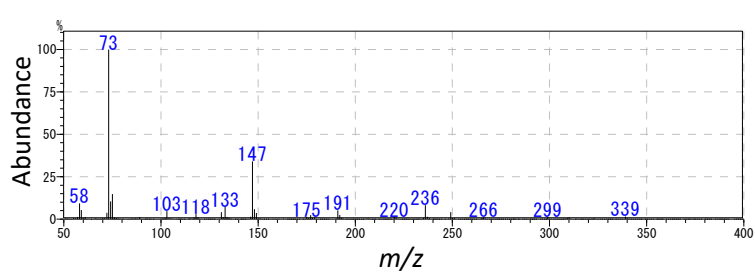
[3-¹³C]malic acid (3TMS)



[4-¹³C]malic acid (3TMS)

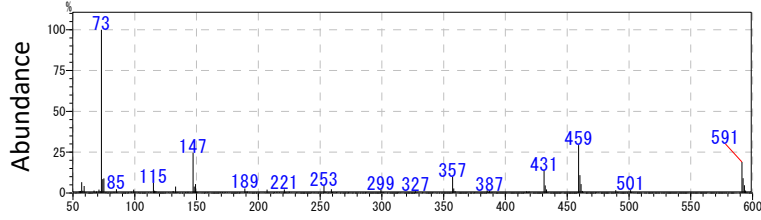


[U-¹³C]malic acid (3TMS)

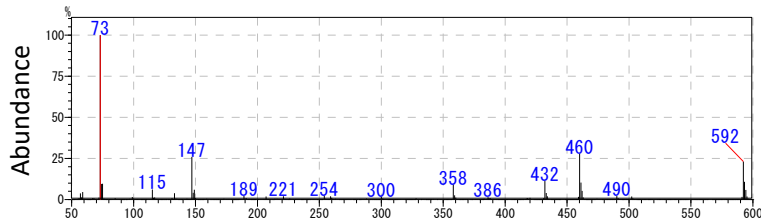


Supplementary materials 2 MS spectra of EI-fragments of TBDMS derivatives

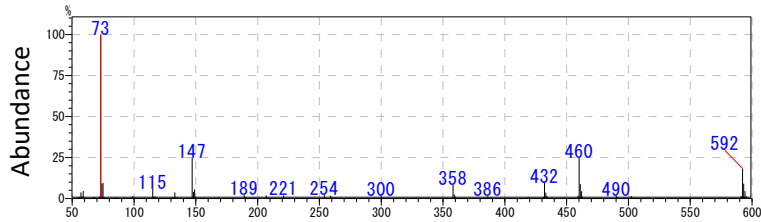
Natural citrate (4TBDMS)



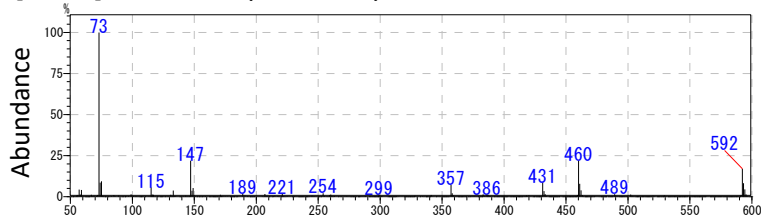
[1-¹³C]citric acid (4TBDMS)



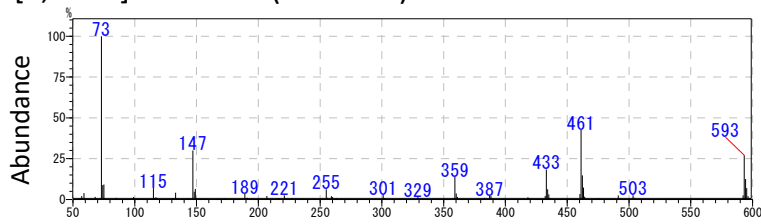
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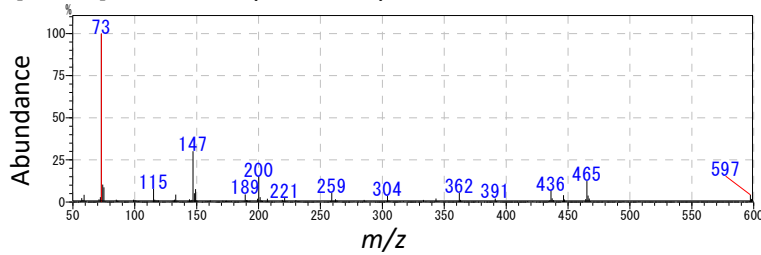
[6-¹³C]citric acid (4TBDMS)



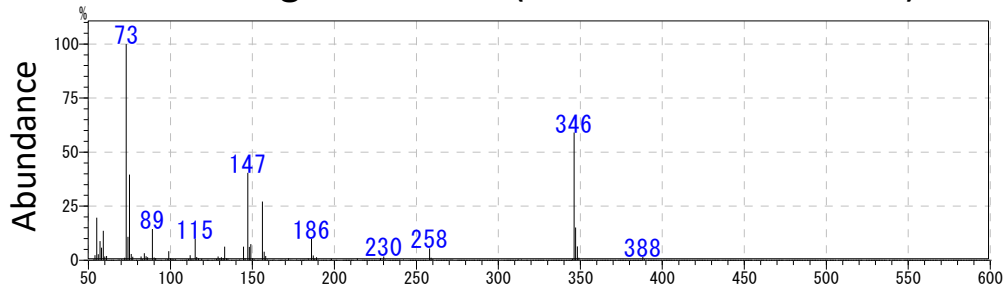
[1,5-¹³C]citric acid (4TBDMS)



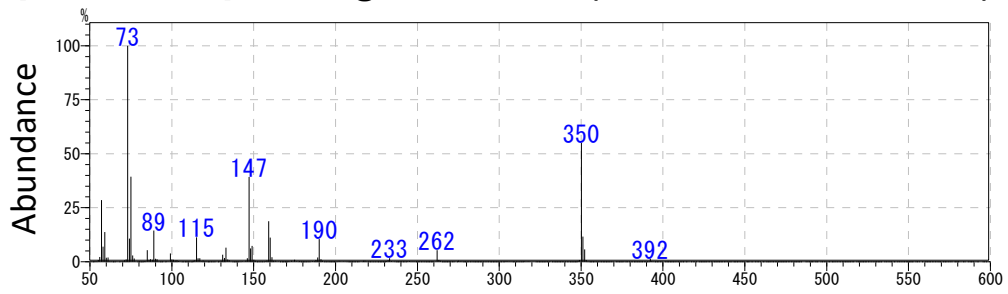
[U-¹³C]citric acid (4TBDMS)



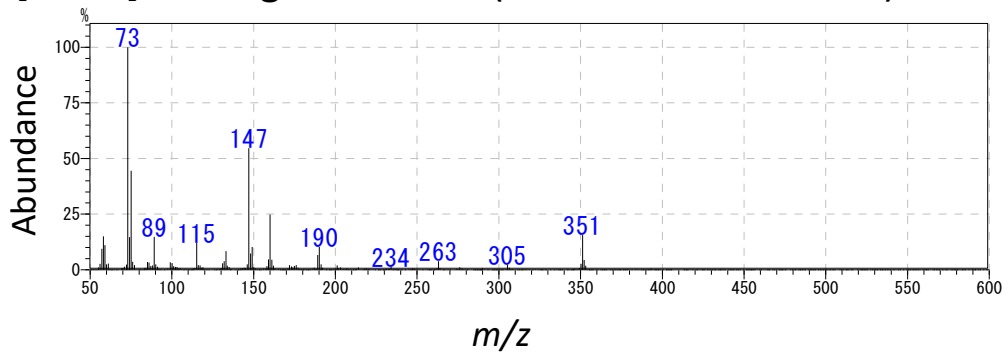
Natural α -ketoglutaric acid (1MEOX and 2TBDMS)



[1,2,3,4- ^{13}C] α -ketoglutaric acid (1MEOX and 2TBDMS)

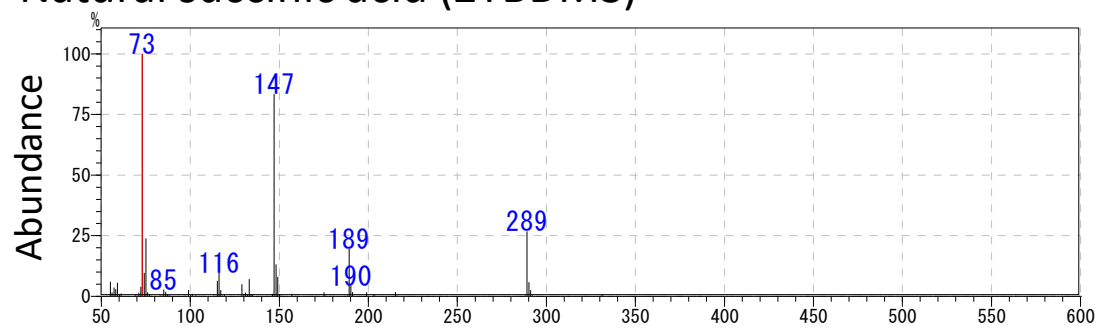


[U- ^{13}C] α -ketoglutaric acid (1MEOX and 2TBDMS)

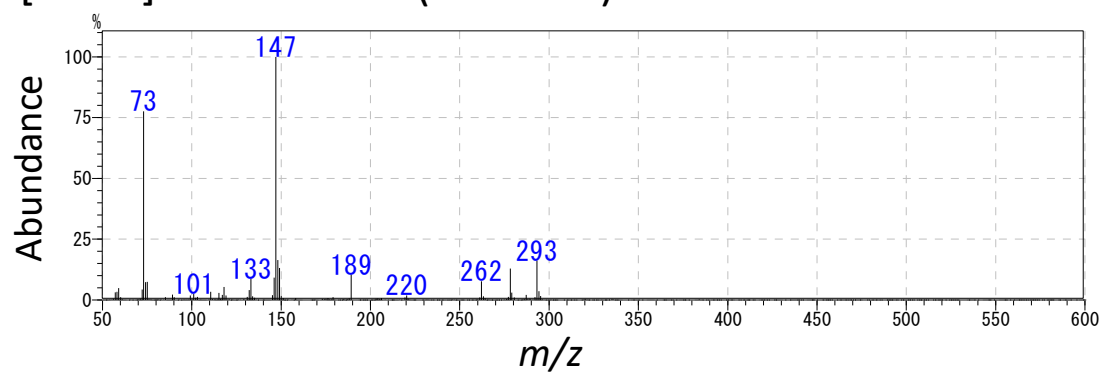


m/z

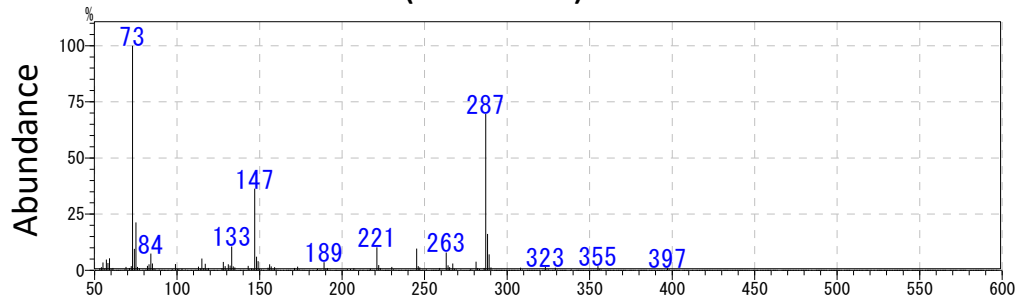
Natural succinic acid (2TBDMS)



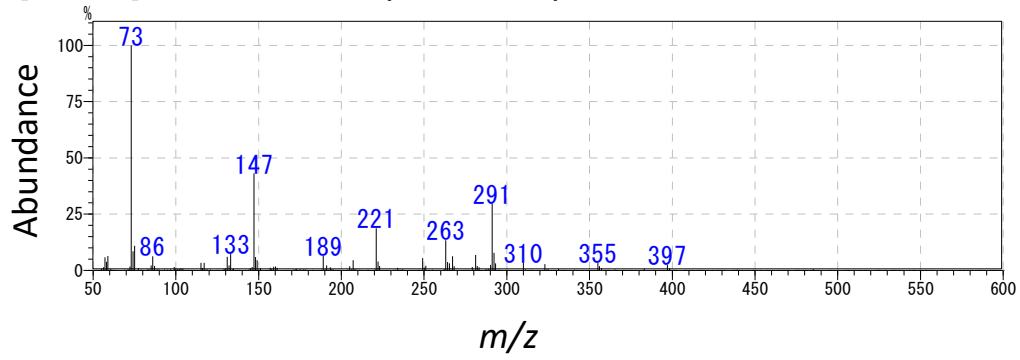
[U-¹³C]succinic acid (2TBDMS)



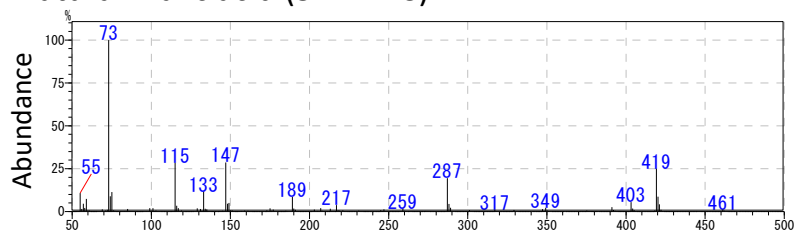
Natural fumaric acid (2TBDMS)



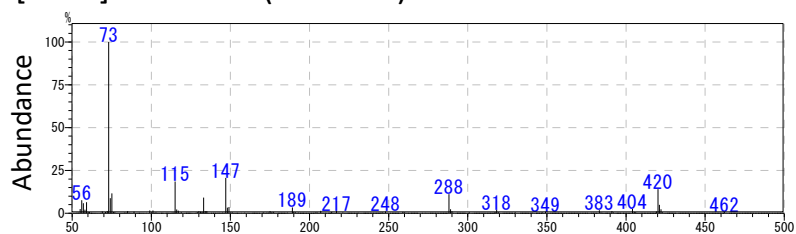
[U-¹³C]fumaric acid (2TBDMS)



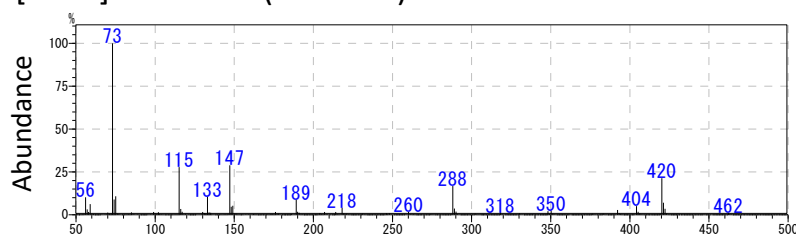
Natural malic acid (3TBDMS)



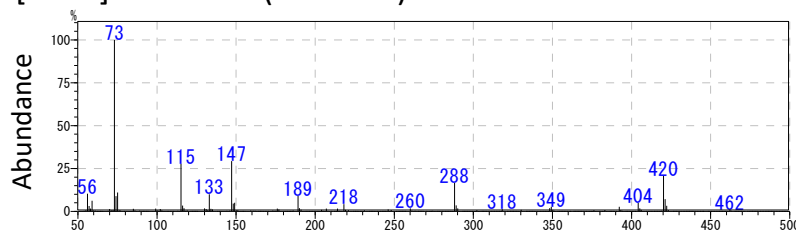
[1-¹³C]malic acid (3TBDMS)



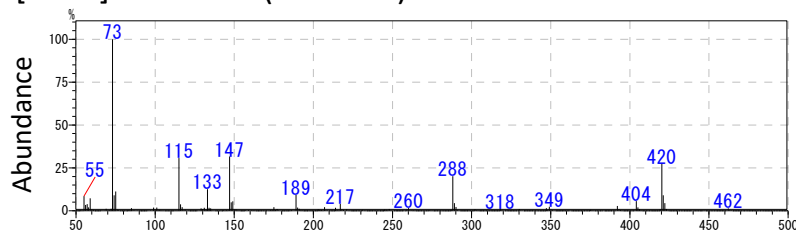
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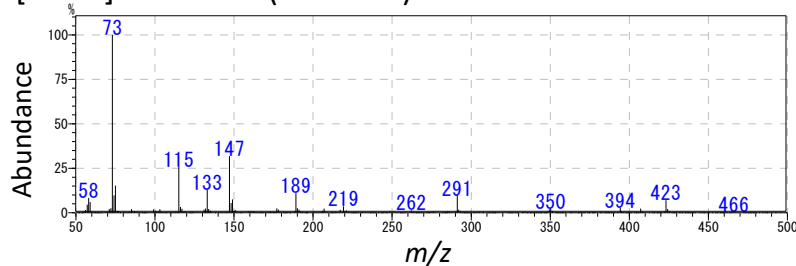
[3-¹³C]malic acid (3TBDMS)



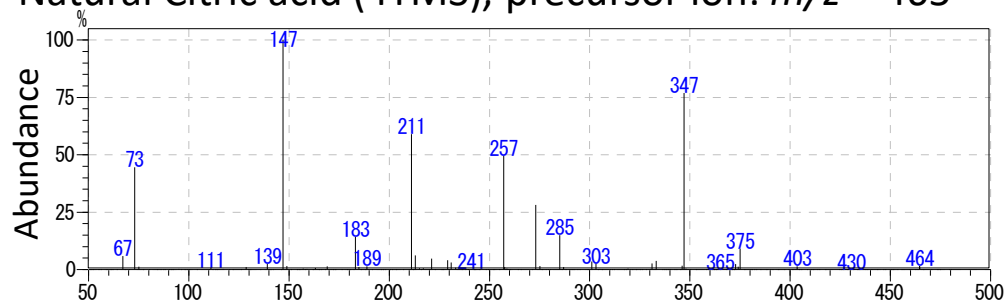
[4-¹³C]malic acid (3TBDMS)



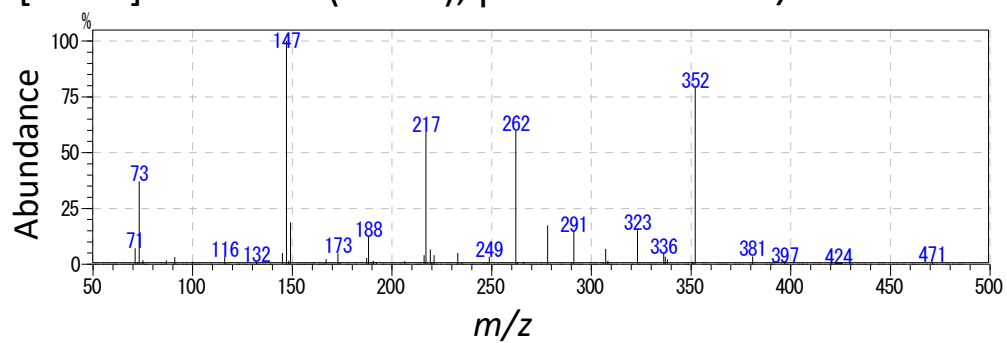
[U-¹³C]malic acid (3TBDMS)



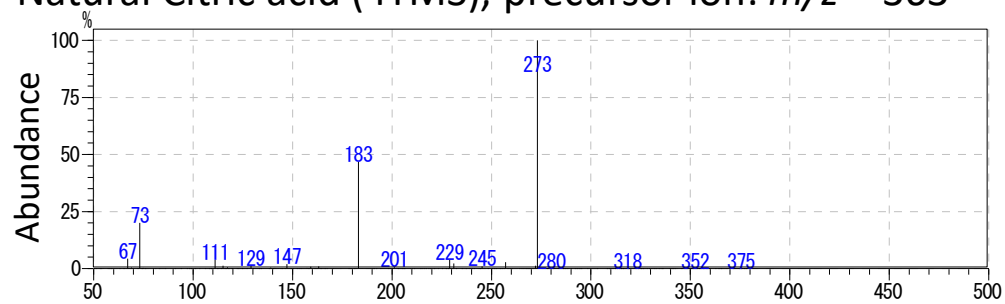
Natural Citric acid (4TMS), precursor ion: $m/z = 465$



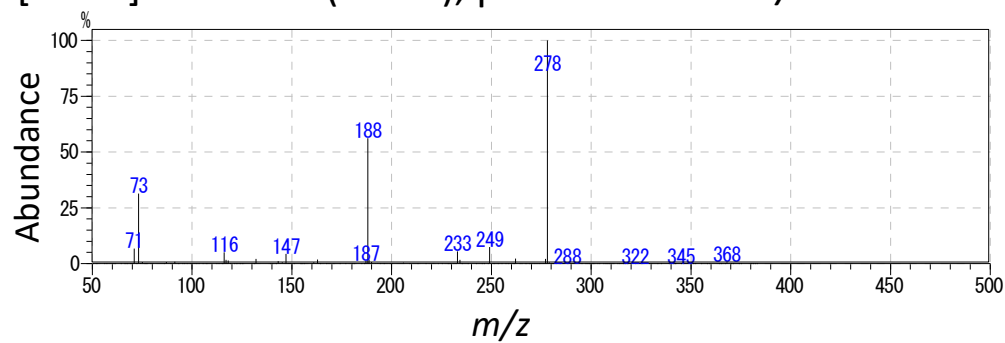
[U- ^{13}C]citric acid (4TMS), precursor ion: $m/z = 471$



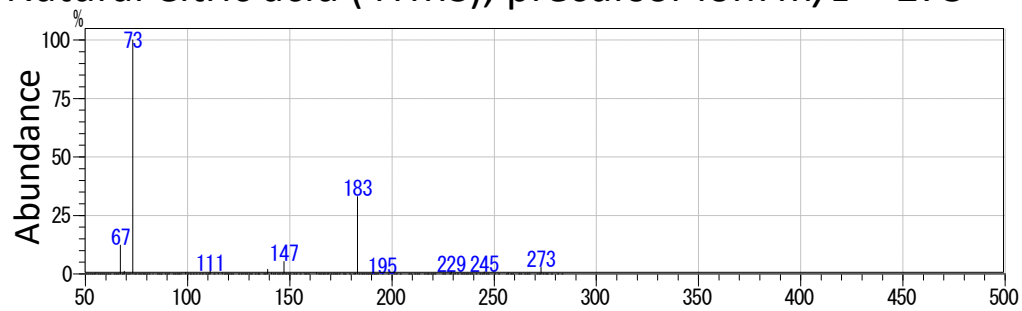
Natural Citric acid (4TMS), precursor ion: $m/z = 363$



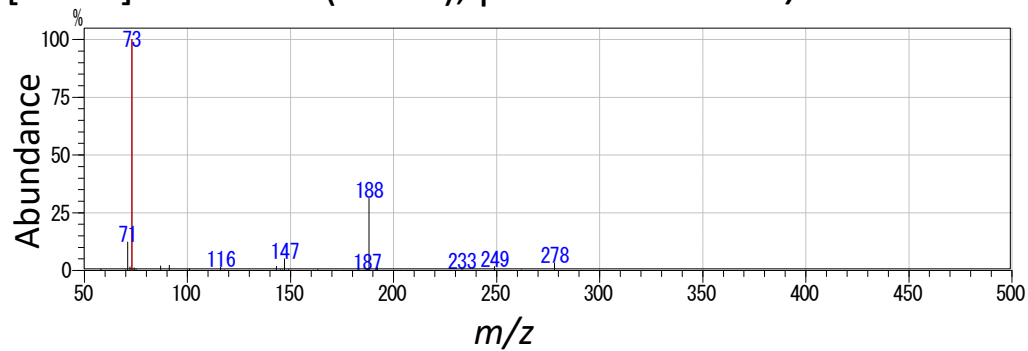
[U- ^{13}C]citric acid (4TMS), precursor ion: $m/z = 368$



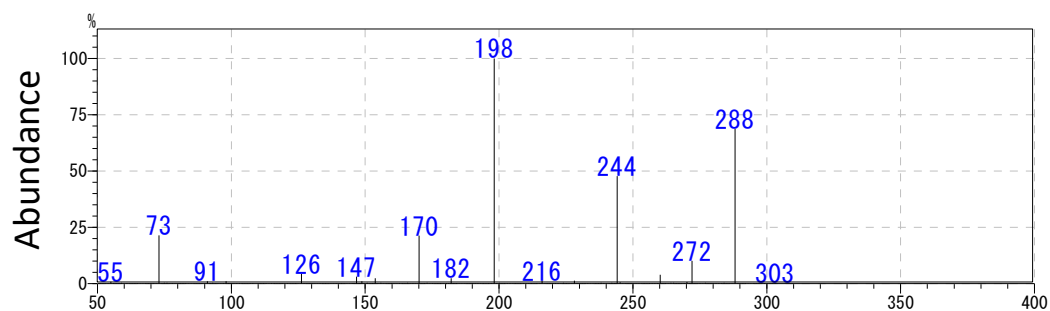
Natural Citric acid (4TMS), precursor ion: $m/z = 273$



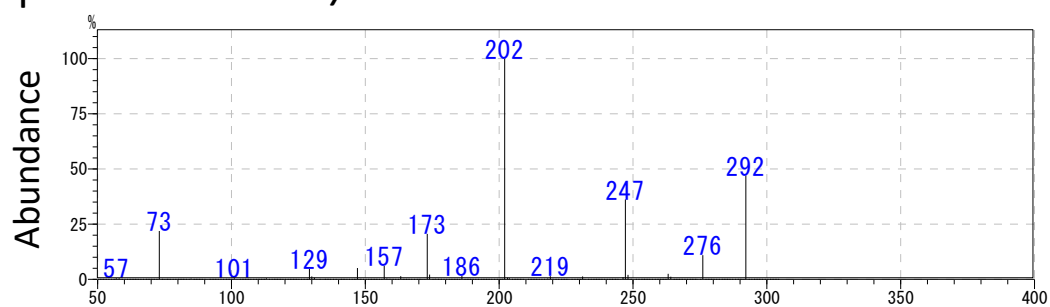
[U- ^{13}C]citric acid (4TMS), precursor ion: $m/z = 278$



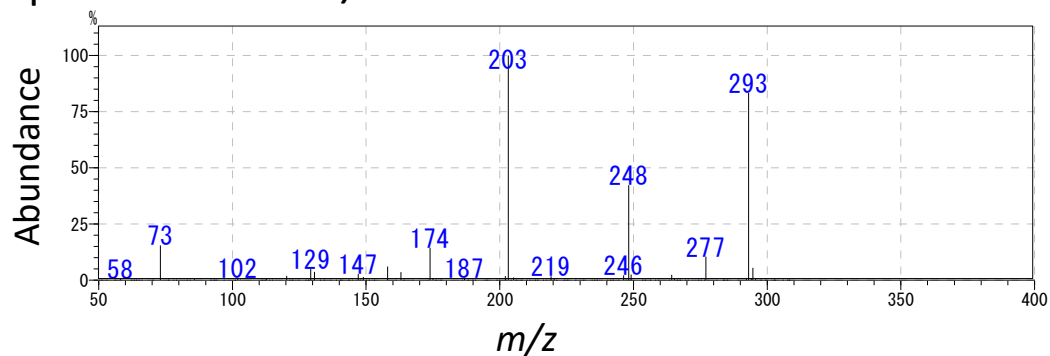
Natural α -ketoglutaric acid (1MEOX and 2TMS),
precursor ion: $m/z = 288$



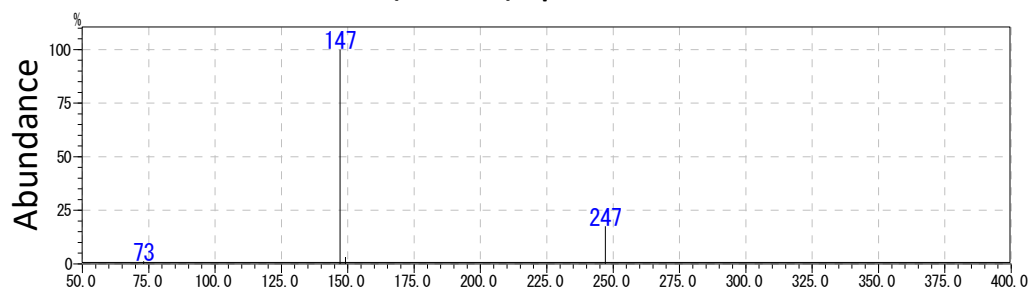
[1,2,3,4- ^{13}C] α -ketoglutaric acid (1MEOX and 2TMS),
precursor ion: $m/z = 292$



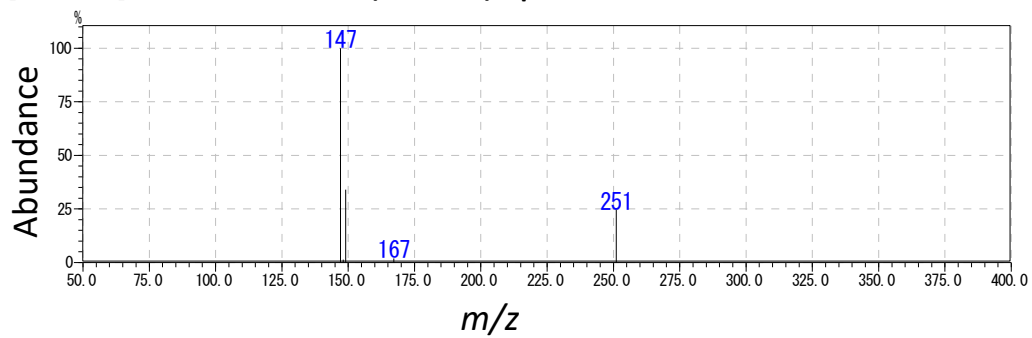
[U- ^{13}C] α -ketoglutaric acid (1MEOX and 2TMS),
precursor ion: $m/z = 293$



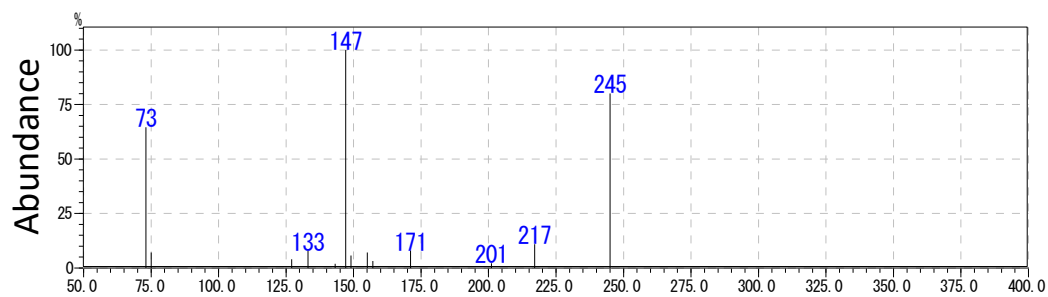
Natural succinic acid (2TMS), precursor ion: $m/z = 247$



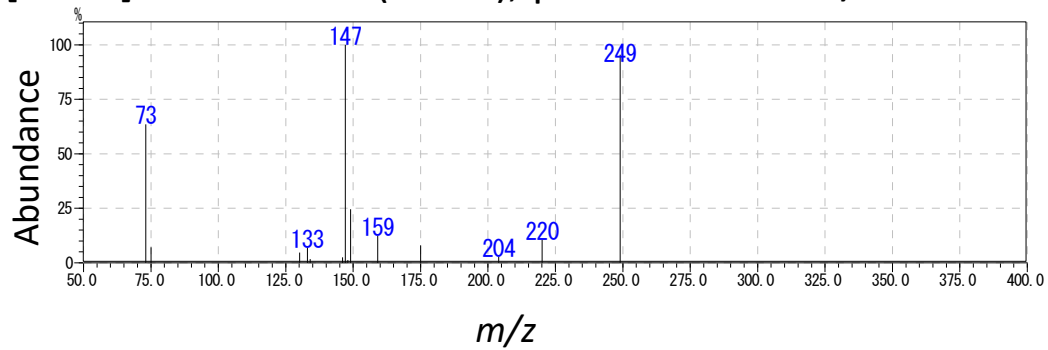
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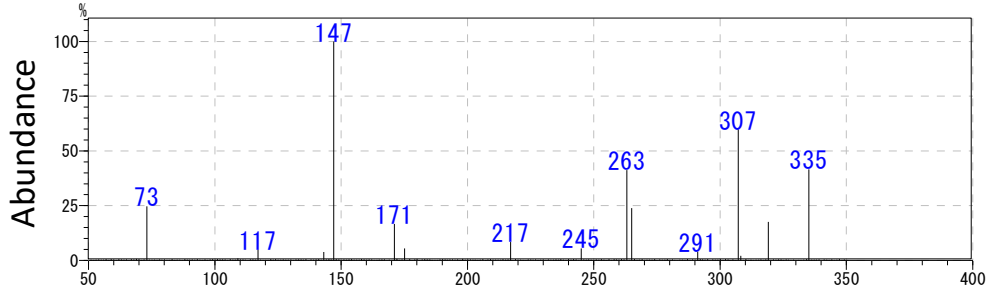
Natural fumaric acid (2TMS), precursor ion: $m/z = 245$



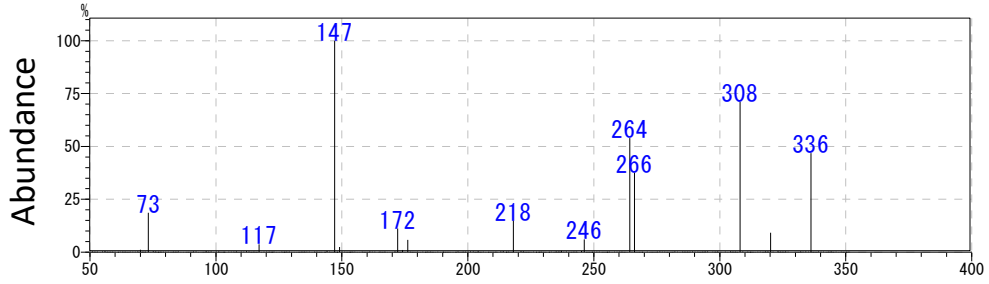
[U- ^{13}C]fumaric acid (4TMS), precursor ion: $m/z = 249$



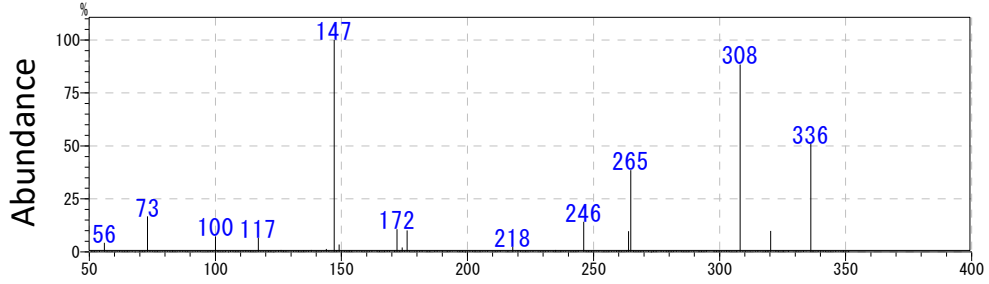
Natural malic acid (3TMS), precursor ion: $m/z = 335$



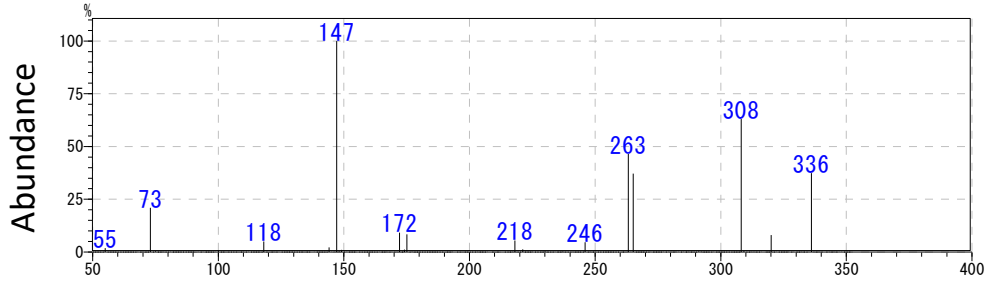
[2- ^{13}C]malic acid (3TMS), precursor ion: $m/z = 336$



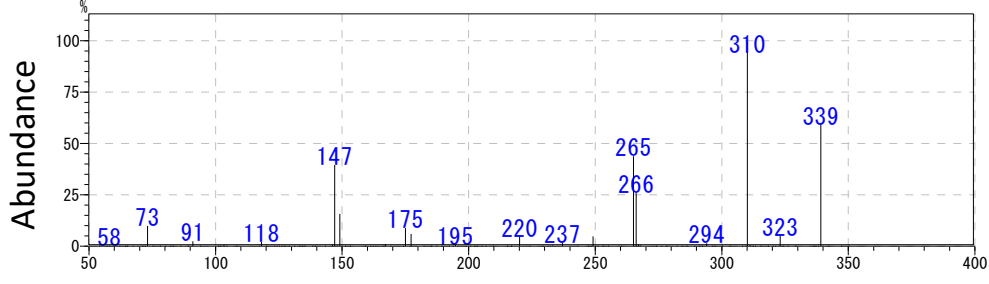
[3- ^{13}C]malic acid (3TMS), precursor ion: $m/z = 336$



[4- ^{13}C]malic acid (3TMS), precursor ion: $m/z = 336$

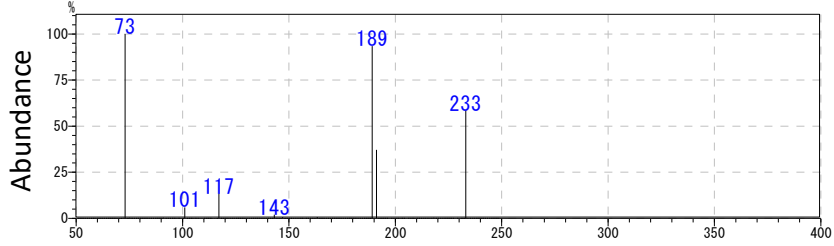


[U- ^{13}C]malic acid (3TMS), precursor ion: $m/z = 339$

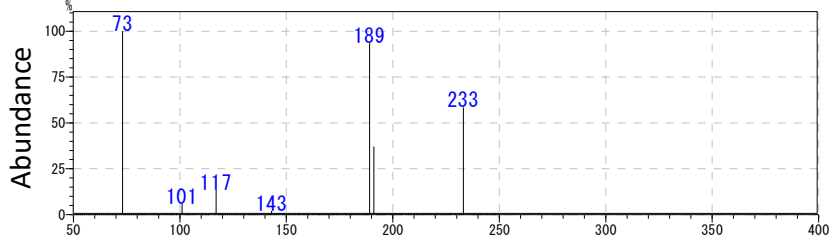


m/z

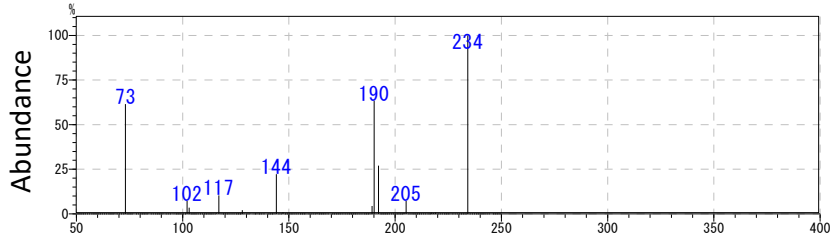
Natural malic acid (3TMS), precursor ion: $m/z = 233$



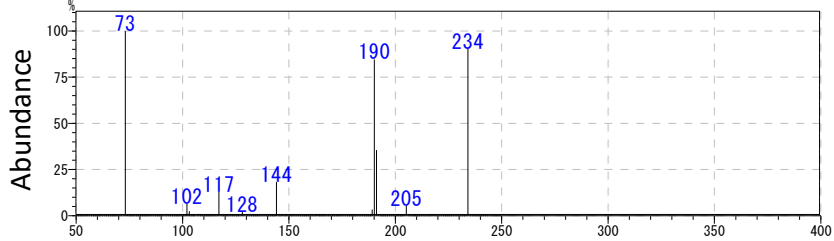
[1- ^{13}C]malic acid (3TMS), precursor ion: $m/z = 233$



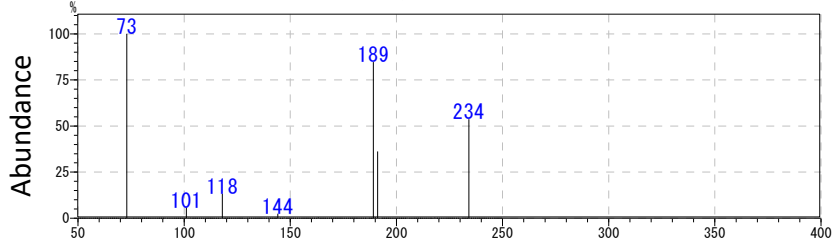
[2- ^{13}C]malic acid (3TMS), precursor ion: $m/z = 234$



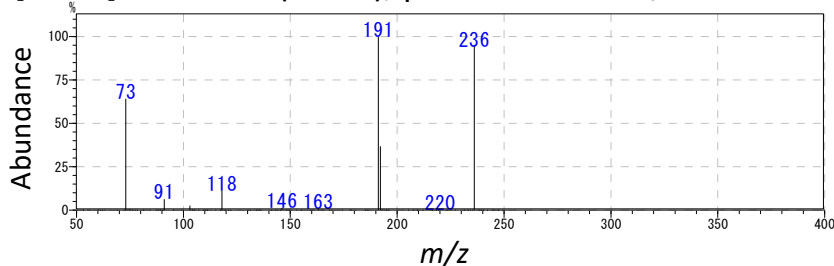
[3- ^{13}C]malic acid (3TMS), precursor ion: $m/z = 234$



[4- ^{13}C]malic acid (3TMS), precursor ion: $m/z = 234$

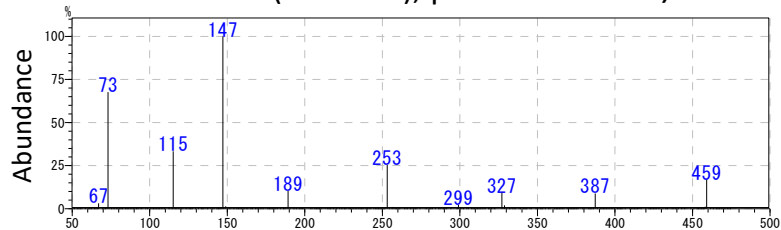


[U- ^{13}C]malic acid (3TMS), precursor ion: $m/z = 236$

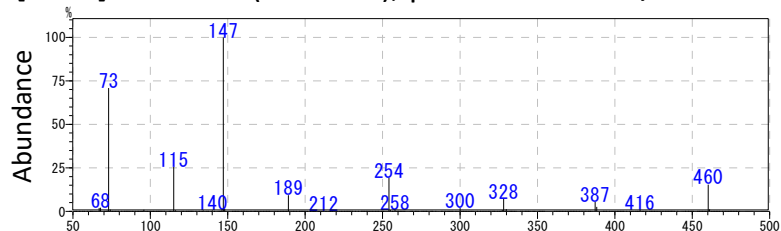


Supplementary materials 4 MS/MS spectra of CID-fragments of TBDMS derivatives

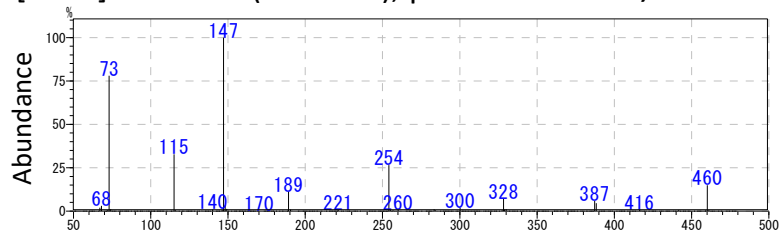
Natural citric acid (4TBDMS), precursor ion: $m/z = 459$



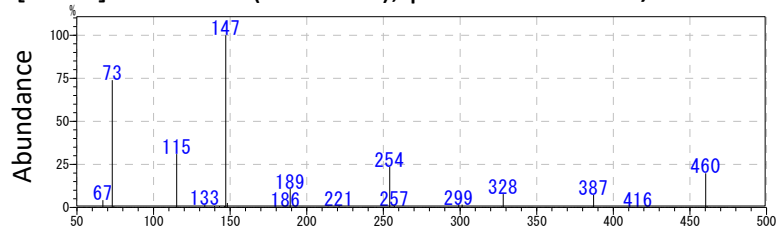
[1-¹³C]citric acid (4TBDMS), precursor ion: $m/z = 460$



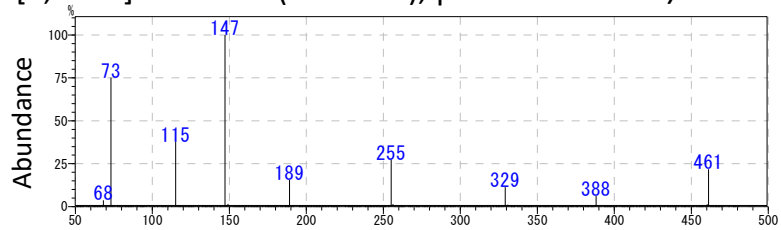
[5-¹³C]citric acid (4TBDMS), precursor ion: $m/z = 460$



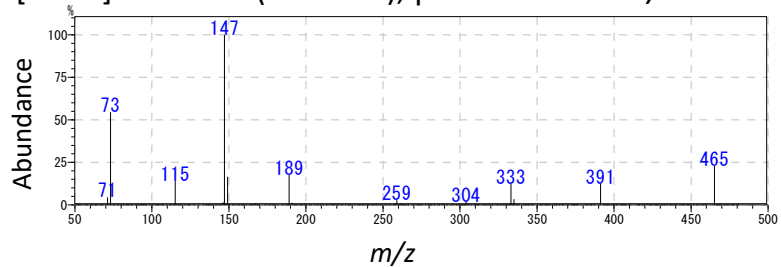
[6-¹³C]citric acid (4TBDMS), precursor ion: $m/z = 460$



[1,5-¹³C]citric acid (4TBDMS), precursor ion: $m/z = 461$

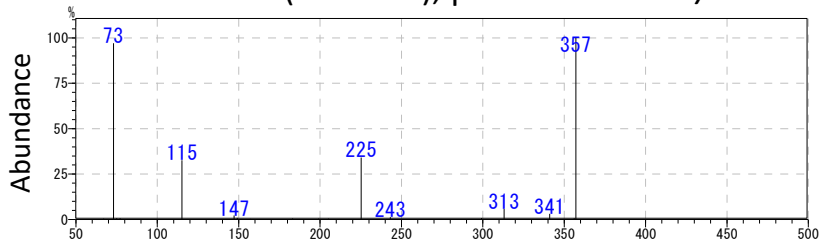


[U-¹³C]citric acid (4TBDMS), precursor ion: $m/z = 465$

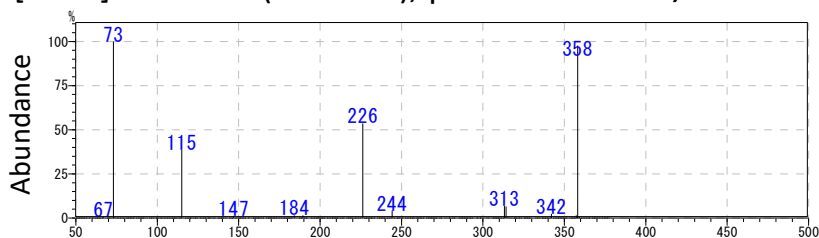


m/z

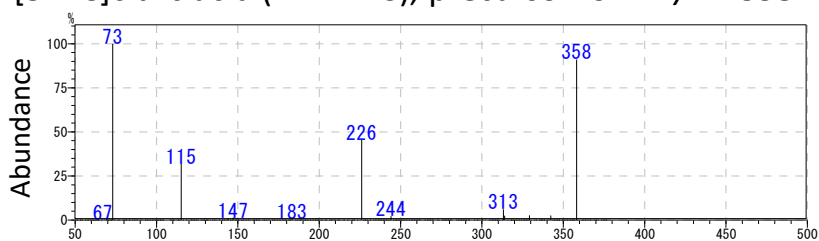
Natural citric acid (4TBDMS), precursor ion: $m/z = 357$



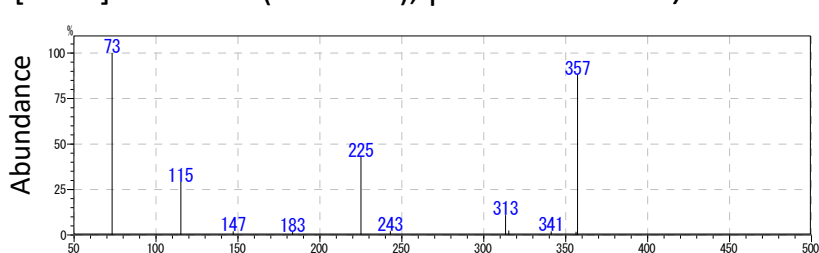
[1-¹³C]citric acid (4TBDMS), precursor ion: $m/z = 358$



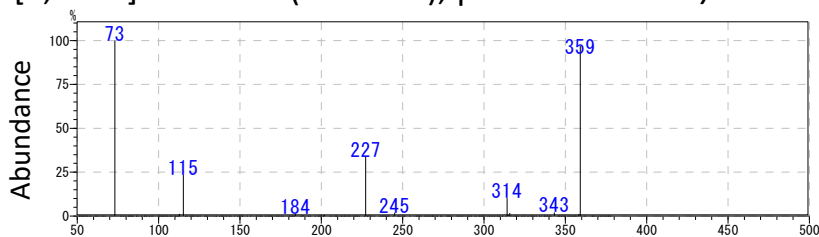
[5-¹³C]citric acid (4TBDMS), precursor ion: $m/z = 358$



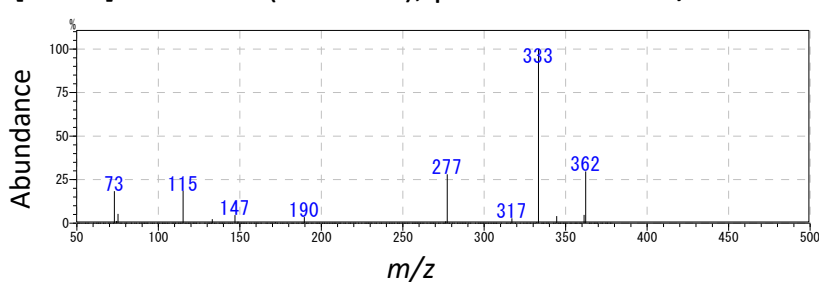
[6-¹³C]citric acid (4TBDMS), precursor ion: $m/z = 357$



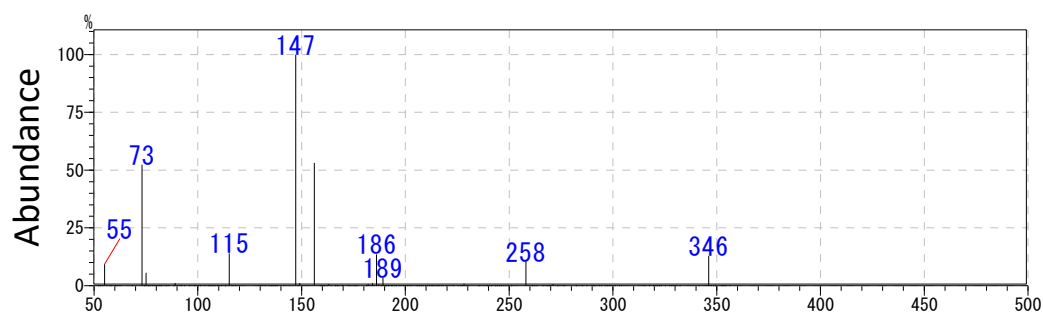
[1,5-¹³C]citric acid (4TBDMS), precursor ion: $m/z = 359$



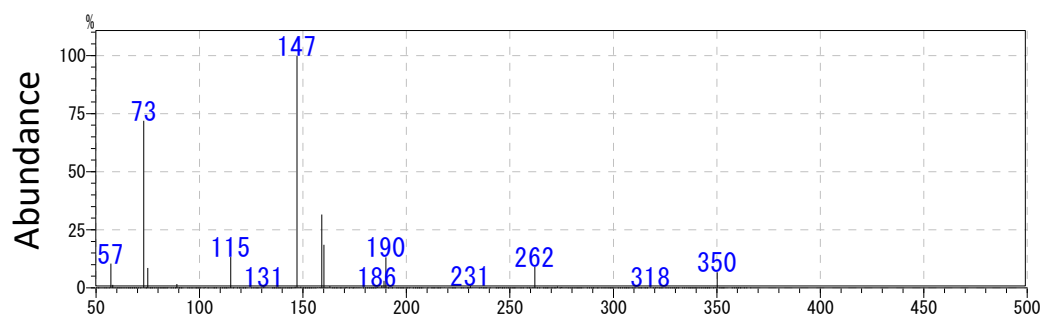
[U-¹³C]citric acid (4TBDMS), precursor ion: $m/z = 362$



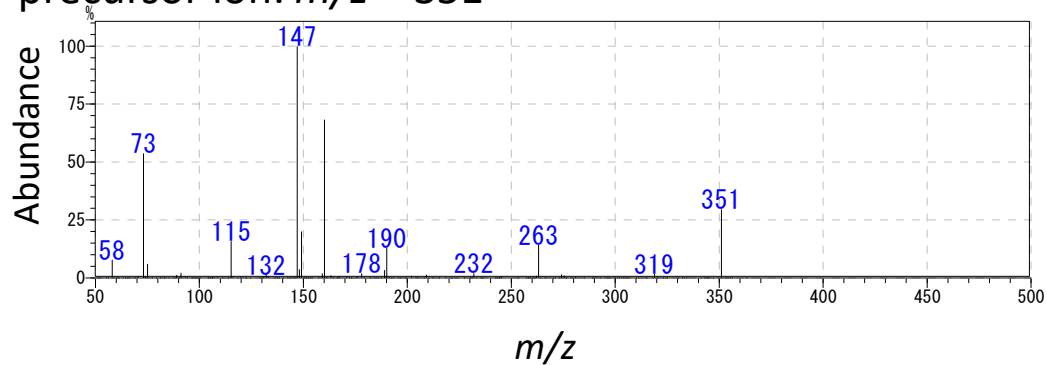
Natural α -ketoglutaric acid (1MEOX and +2TBDMS),
precursor ion: $m/z = 346$



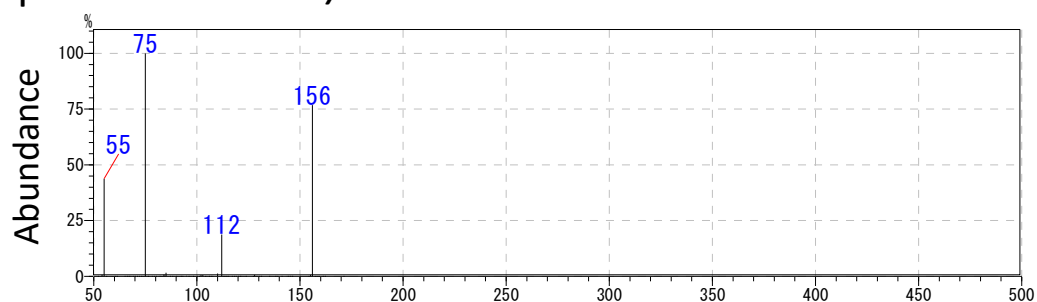
[1,2,3,4- ^{13}C] α -ketoglutaric acid (1MEOX and 2TBDMS),
precursor ion: $m/z = 350$



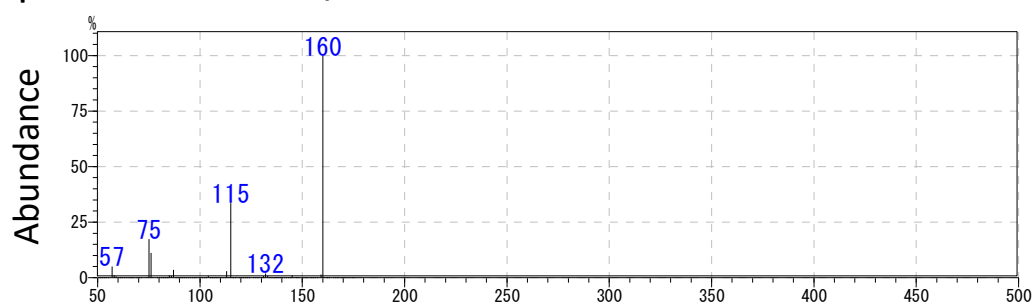
[U- ^{13}C] α -ketoglutaric acid (1MEOX and 2TBDMS),
precursor ion: $m/z = 351$



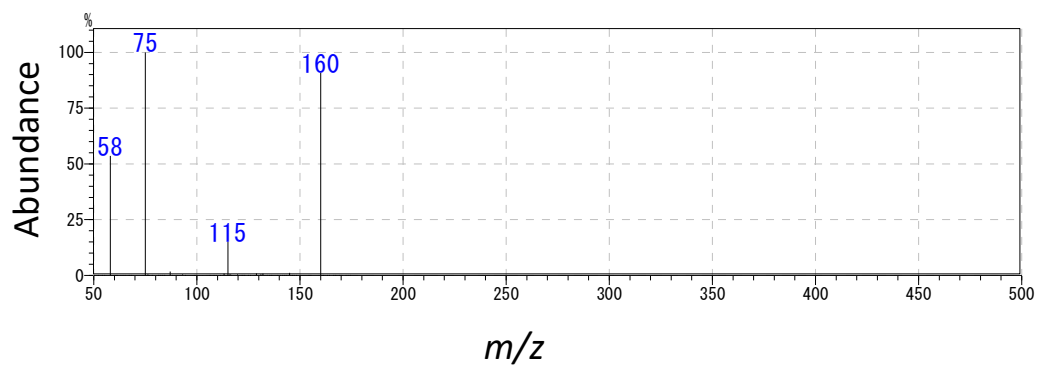
Natural α -ketoglutaric acid (1MEOX and 2TBDMS),
precursor ion: $m/z = 156$



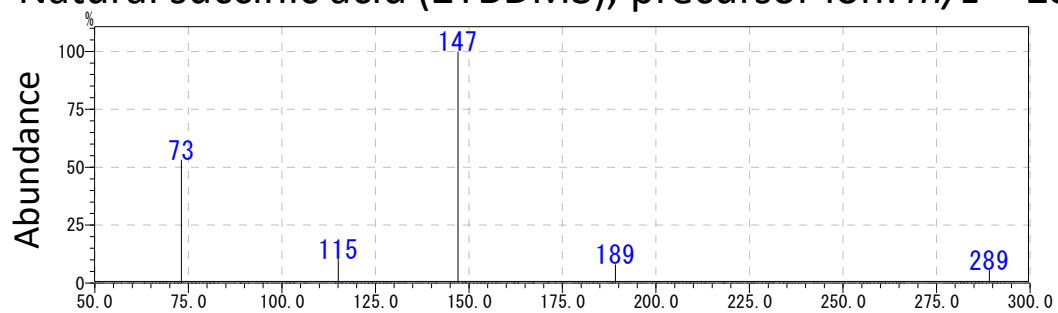
[1,2,3,4- ^{13}C] α -ketoglutaric acid (1MEOX and 2TBDMS),
precursor ion: $m/z = 160$



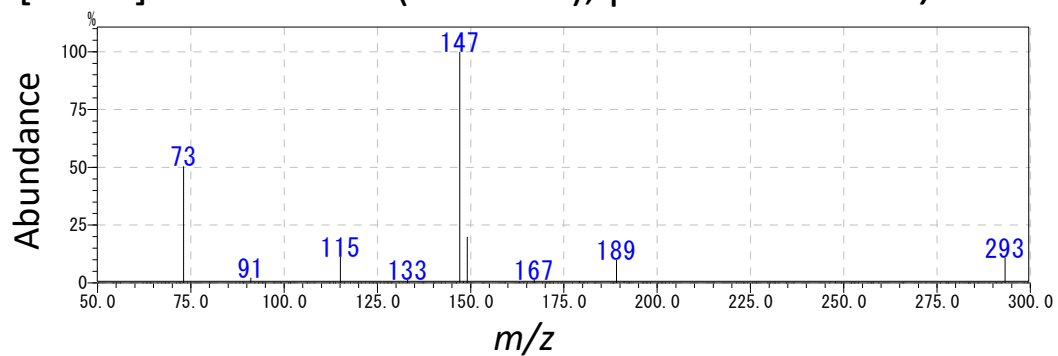
[U- ^{13}C] α -ketoglutaric acid (1MEOX and 2TBDMS),
precursor ion: $m/z = 160$



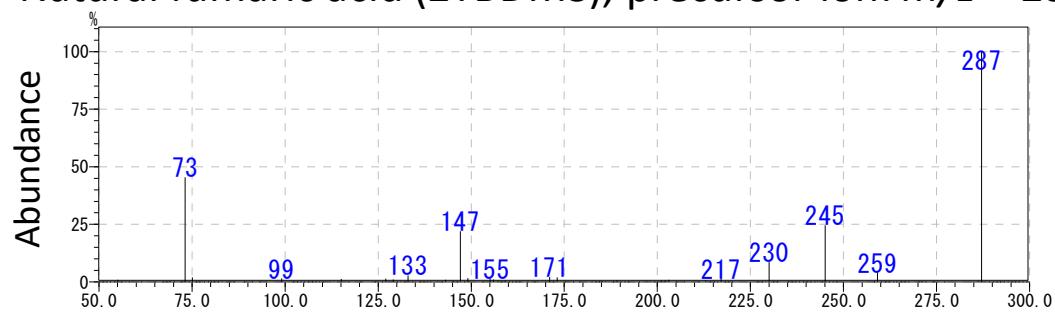
Natural succinic acid (2TBDMS), precursor ion: $m/z = 289$



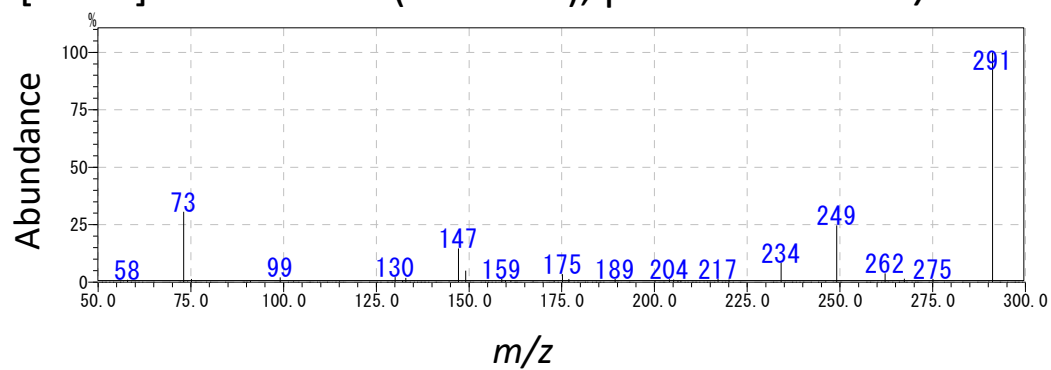
[U- ^{13}C]succinic acid (2TBDMS), precursor ion: $m/z = 293$



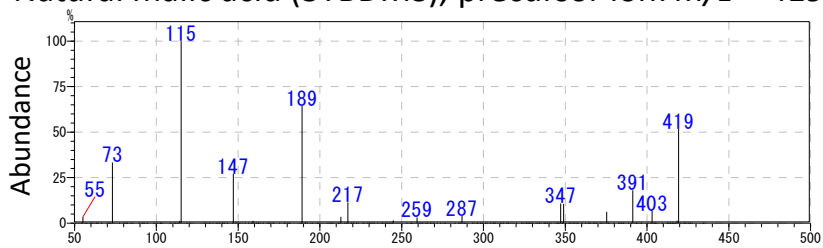
Natural fumaric acid (2TBDMS), precursor ion: $m/z = 287$



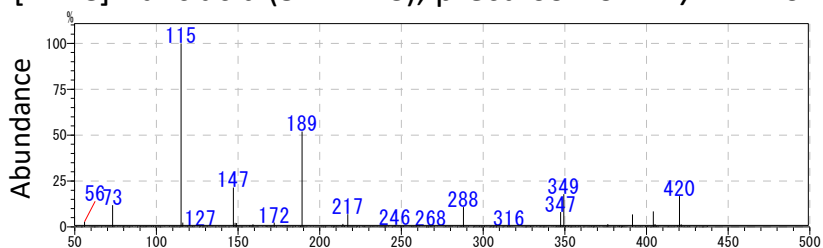
[U- ^{13}C]fumaric acid (2TBDMS), precursor ion: $m/z = 291$



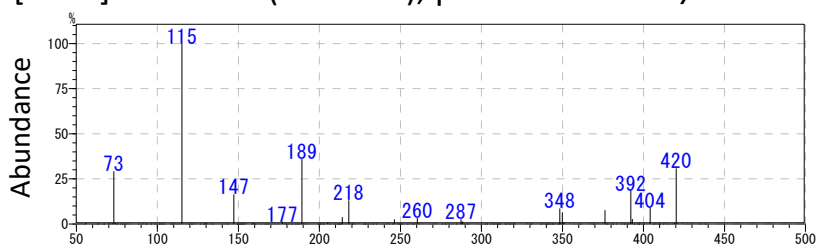
Natural malic acid (3TBDMS), precursor ion: $m/z = 419$



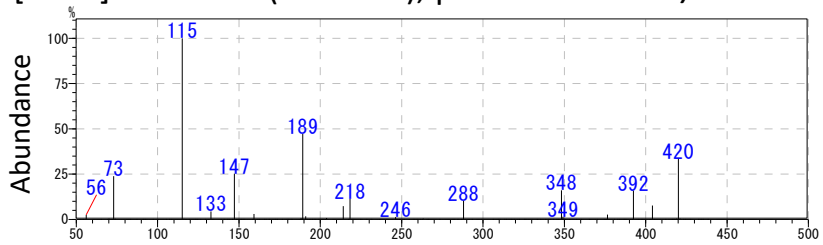
[1- ^{13}C]malic acid (3TBDMS), precursor ion: $m/z = 420$



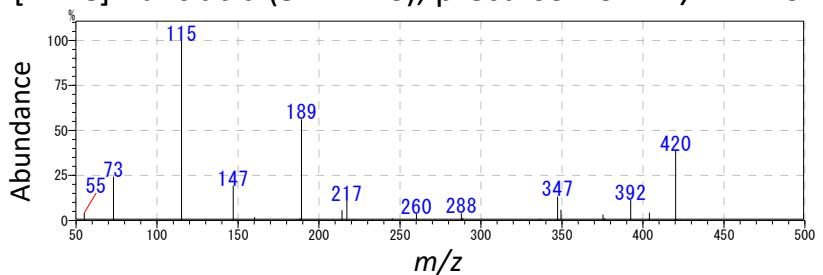
[2- ^{13}C]malic acid (3TBDMS), precursor ion: $m/z = 420$



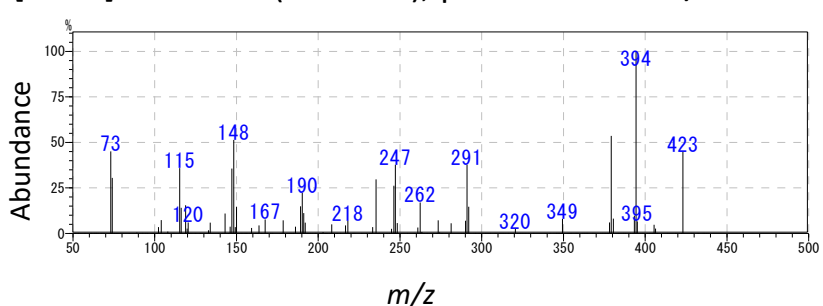
[3- ^{13}C]malic acid (3TBDMS), precursor ion: $m/z = 420$



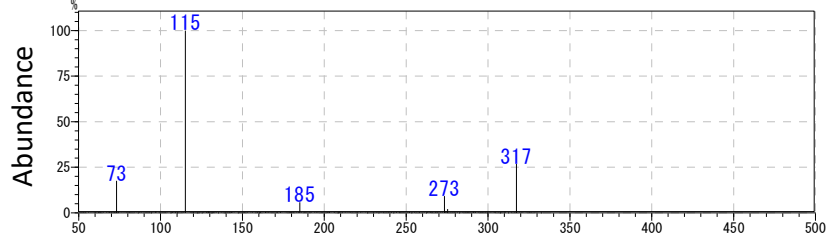
[4- ^{13}C]malic acid (3TBDMS), precursor ion: $m/z = 420$



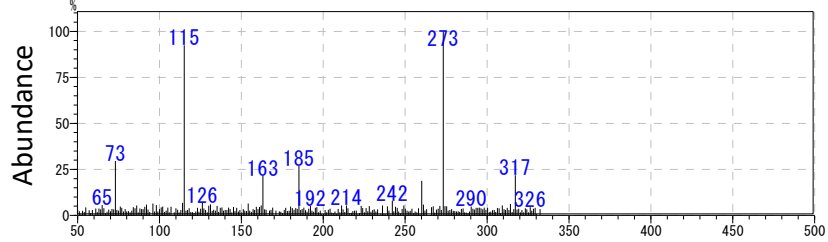
[U- ^{13}C]malic acid (3TBDMS), precursor ion: $m/z = 423$



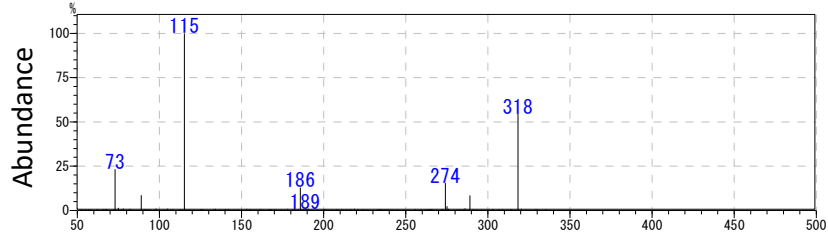
Natural malic acid (3TBDMS), precursor ion: $m/z = 317$



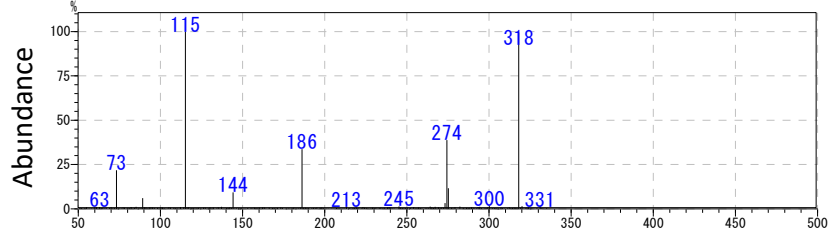
[1-¹³C]malic acid (3TBDMS), precursor ion: $m/z = 317$



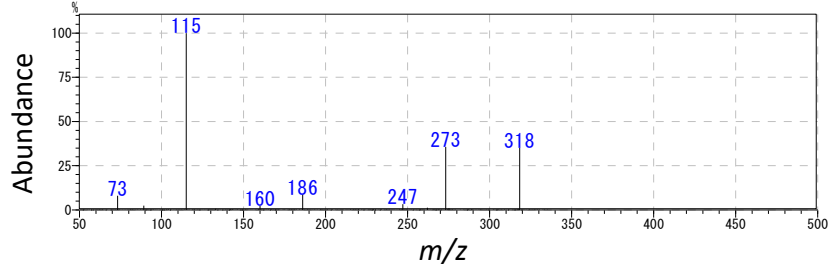
[2-¹³C]malic acid (3TBDMS), precursor ion: $m/z = 318$



[3-¹³C]malic acid (3TBDMS), precursor ion: $m/z = 318$



[4-¹³C]malic acid (3TBDMS), precursor ion: $m/z = 318$



[U-¹³C]malic acid (3TBDMS), precursor ion: $m/z = 320$

