Supplementary Information

Pharmacometabolomics for predicting variable busulfan exposure in paediatric haematopoietic stem cell transplantation patients

Bora Kim[1,*], Ji Won Lee[2,*,#], Kyung Taek Hong[2], Kyung-Sang Yu[1], In-Jin Jang[1], Kyung Duk Park[2], Hee Young Shin[2], Hyo Seop Ahn[2], Joo-Youn Cho[1], and Hyoung Jin Kang[2]

[1]Department of Clinical Pharmacology and Therapeutics, Seoul National University College of Medicine and Hospital, Seoul, Korea; [2]Department of Pediatrics, Cancer Research Institute, Seoul National University College of Medicine and Hospital, Seoul, Korea.

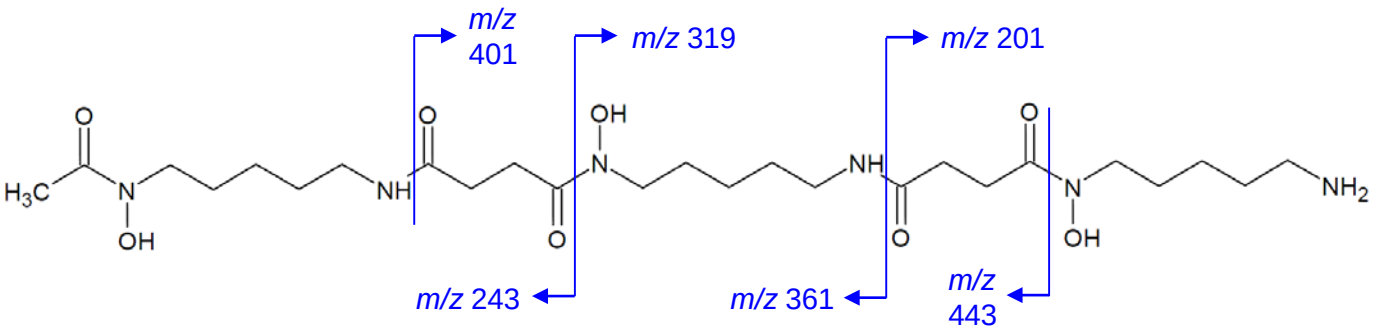
*These authors equally contributed to this work.
[#]Current affiliation: Department of Pediatrics, Samsung Medical Center, Sungkyunkwan University School of Medicine

Corresponding Authors:
Hyoung Jin Kang, E-mail: kanghj@snu.ac.kr Phone: (82)2-2072-3304, Fax: (82)2-743-3455
Joo-Youn Cho, E-mail: joocho@snu.ac.kr Phone: (82)2-2072-3625, Fax: (82)2-743-3455

Supplementary Figures

Supplementary Figure S1. (**A**) Deferoxamine structure and its mass fragmentation. (**B**) MS/MS spectra of urinary deferoxamine (upper) and authentic deferoxamine (lower). The fragments and relative intensities of 16 urinary metabolites were compared with the fragmentation pattern of authentic deferoxamine.

A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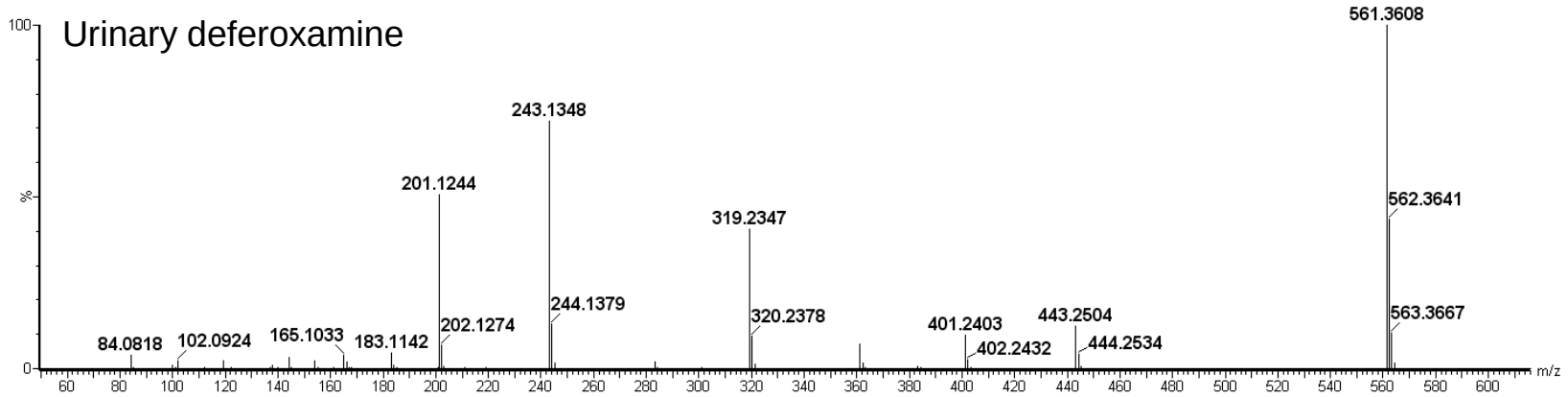
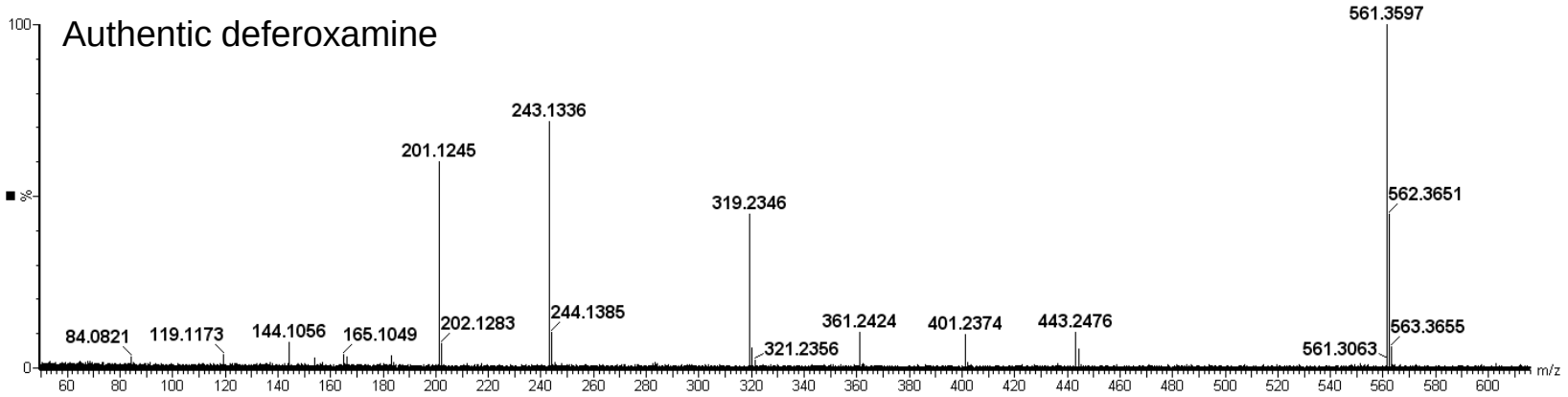
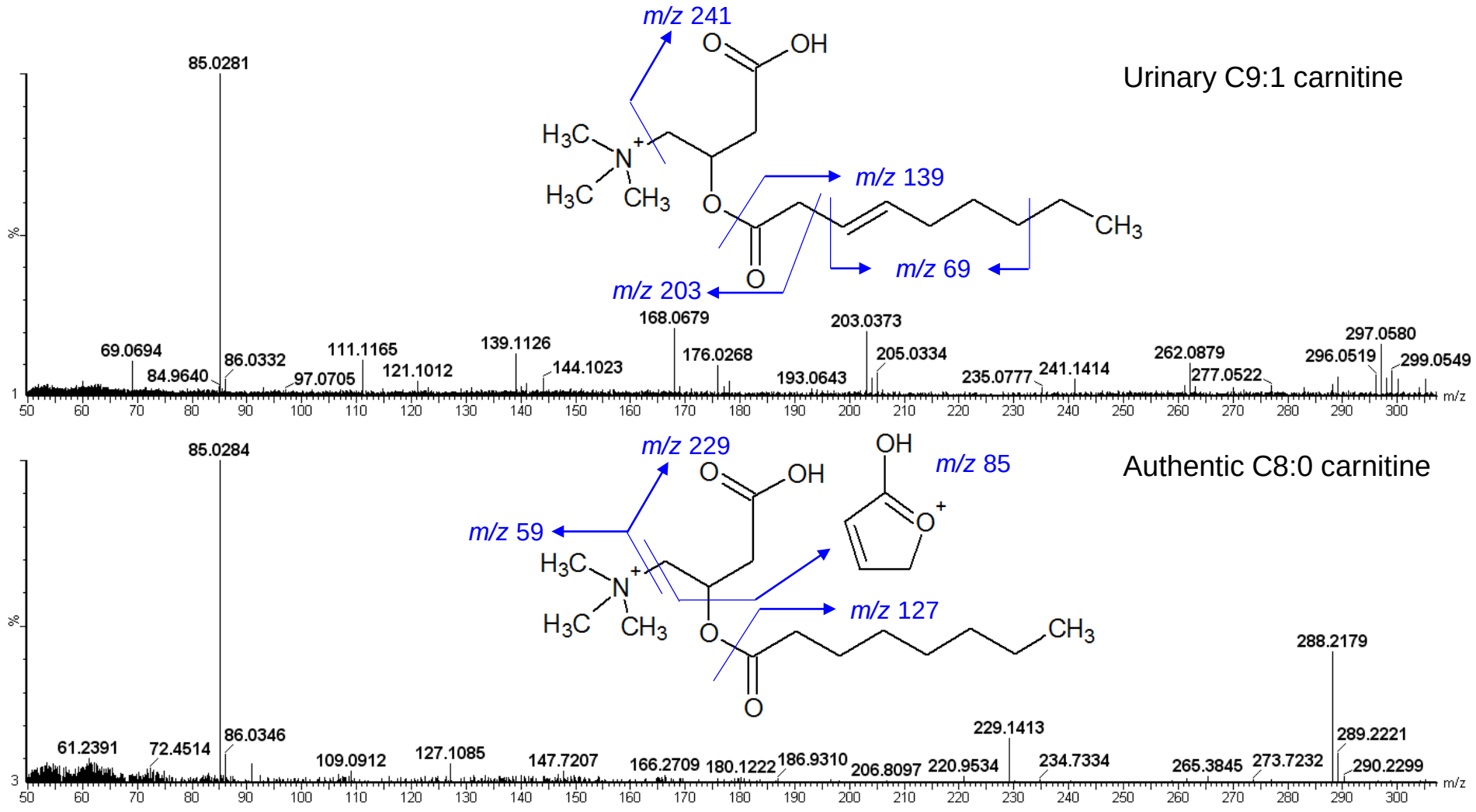
m/z 319
m/z 201
m/z 243
m/z 361
m/z 443

B

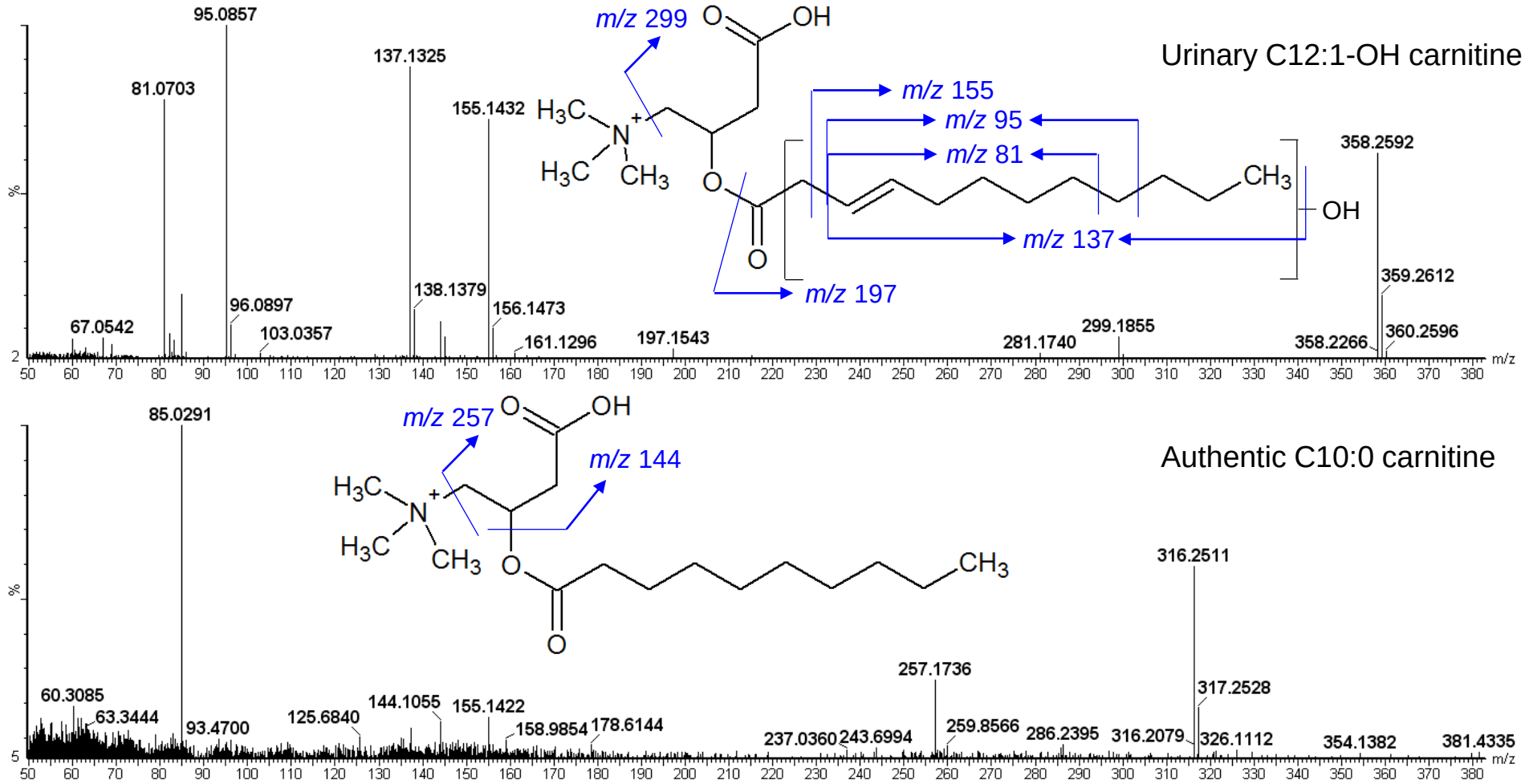

Urinary deferoxamine
561.3608
243.1348
201.1244
319.2347
562.3641
244.1379
320.2378
563.3667
84.0818
102.0924
165.1033
183.1142
202.1274
401.2403
443.2504
402.2432
444.2534
m/z


Authentic deferoxamine
561.3597
243.1336
201.1245
319.2346
562.3651
244.1385
361.2424
401.2374
443.2476
563.3655
84.0821
119.1173
144.1056
165.1049
202.1283
321.2356
561.3063
m/z

Supplementary Figure S2. The fragments of urinary C9:1 carnitine was compared with authentic C8:0 carnitine. MS/MS spectra and each structure of C9:1 carnitine and C8:0 carnitine.



Supplementary Figure S3. The fragments of urinary C12:1-OH carnitine was compared with authentic C10:0 carnitine. MS/MS spectra and each structure of C12:1-OH carnitine and C10:0 carnitine.



Supplementary Figure S4. Phenylacetylglutamine structure and MS/MS spectra of urinary PAGN, [M−H]− adduct, [2M+Na−2H]− adduct, and authentic PAGN.