

Supplementary Materials

Rat Pharmacokinetics and In Vitro Metabolite Identification of KM-819, a Parkinson's Disease Candidate, Using LC-MS/MS and LC-HRMS

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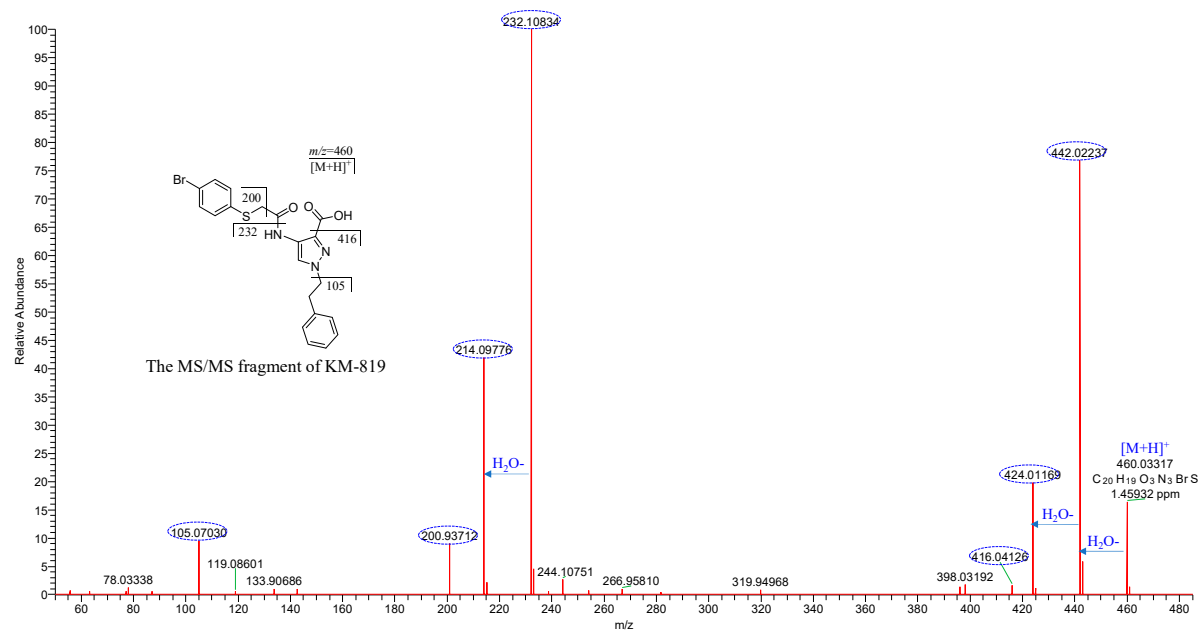
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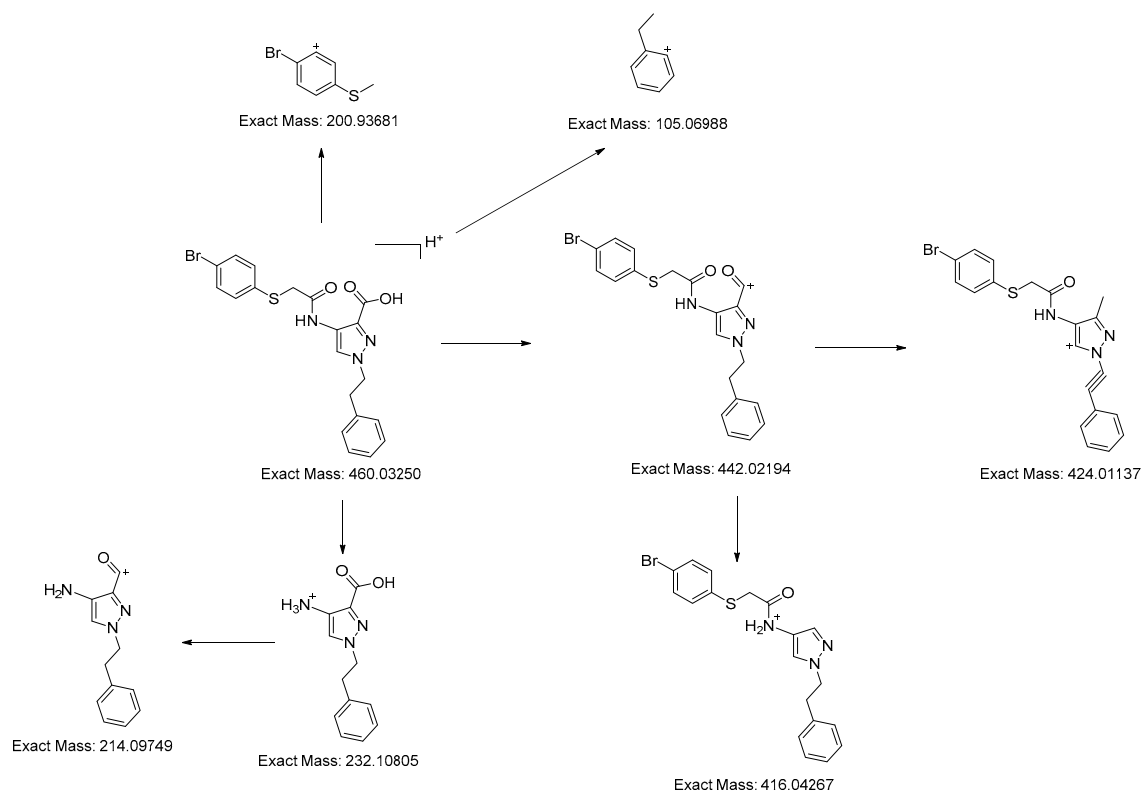
Supplementary Figure S1. (a) MS/MS spectra of KM-819 and (b) putative fragmentation pathways of KM-819

KM-819-STD #9643 RT: 11.60 AV: 1 NL: 1.22E7

F: FTMS + p ESI d Full ms2 460.0327@hcd20.00 [50.0000-485.0000]



(a)

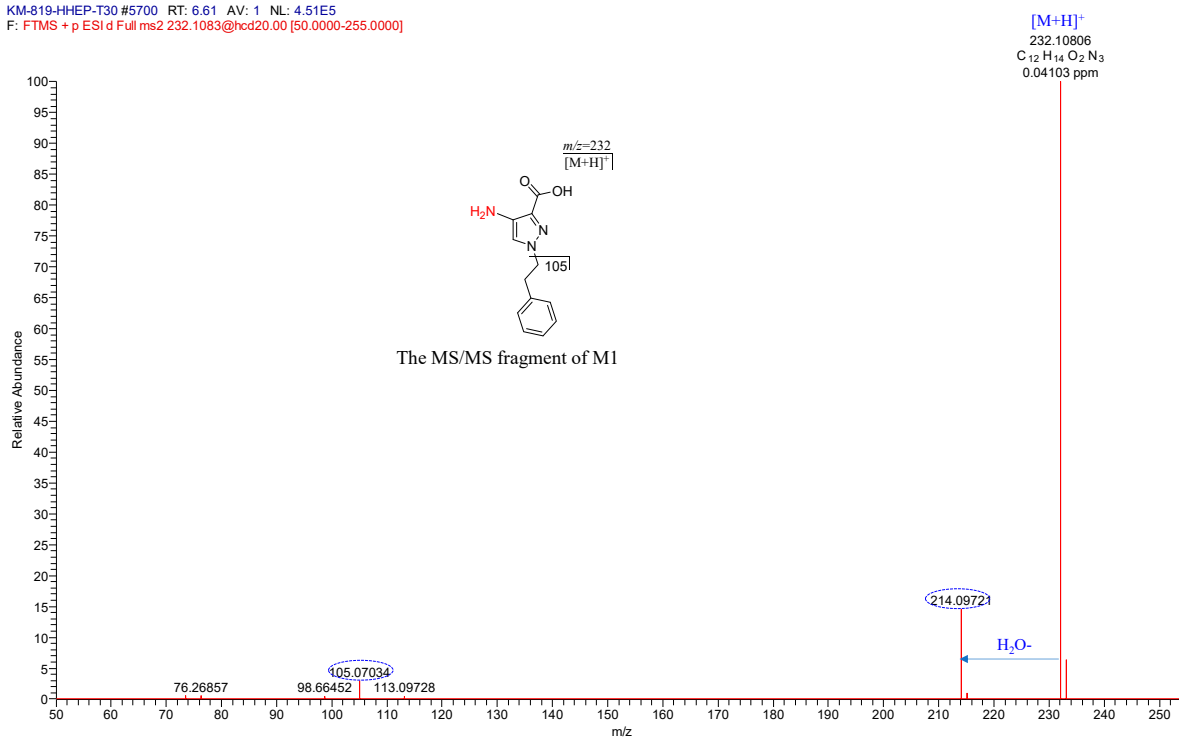


(b)

Supplementary Figure S2. MS/MS spectra of M1, the de-alkylation metabolite of KM-819, and structure elucidation

KM-819-HHEP-T30 #5700 RT: 6.61 AV: 1 NL: 4.51E5

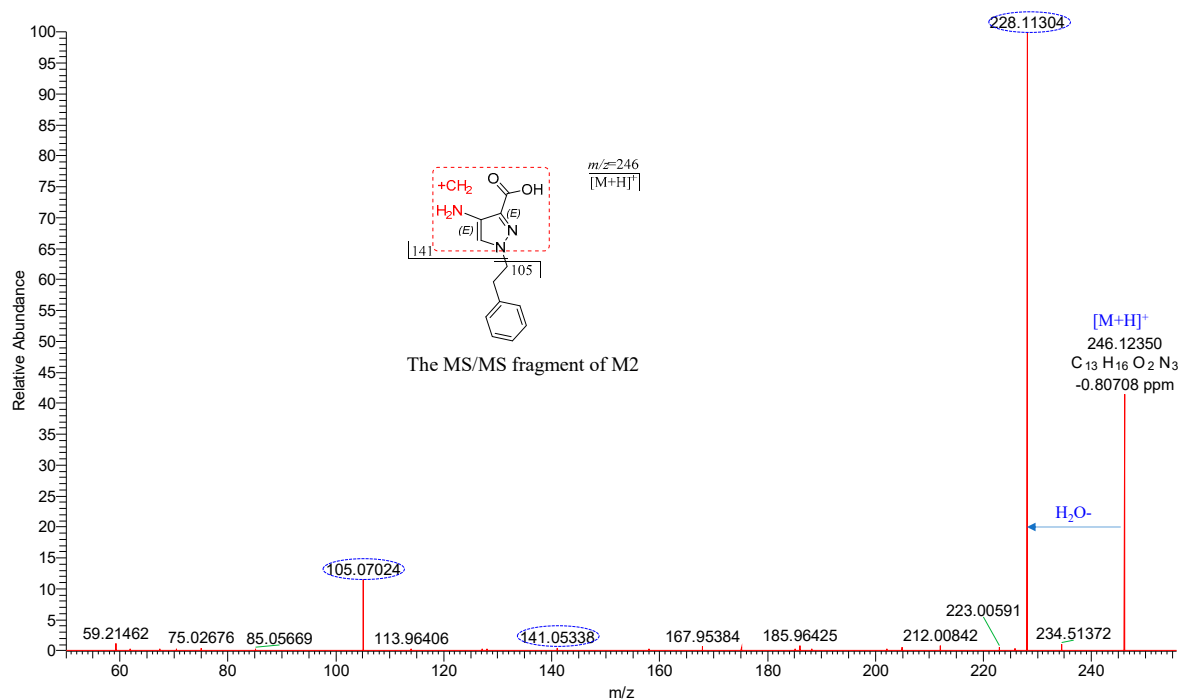
F: FTMS + p ESI d Full ms2 232.1083@hcd20.00 [50.0000-255.0000]



Supplementary Figure S3. MS/MS spectra of M2, the De-alkylated and methylated metabolite of KM-819, and structure elucidation

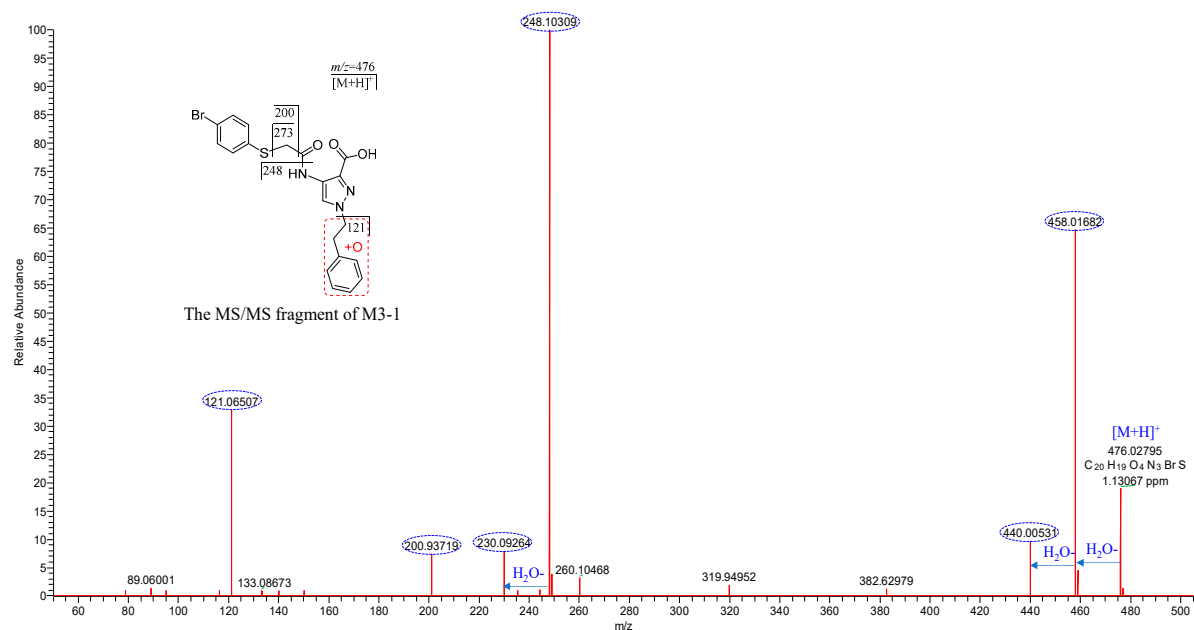
KM-819-DHEP-T30 #7540 RT: 7.59 AV: 1 NL: 7.16E5

F: FTMS + p ESI d Full ms2 246.0216@hcd20.00 [50.0000-270.0000]



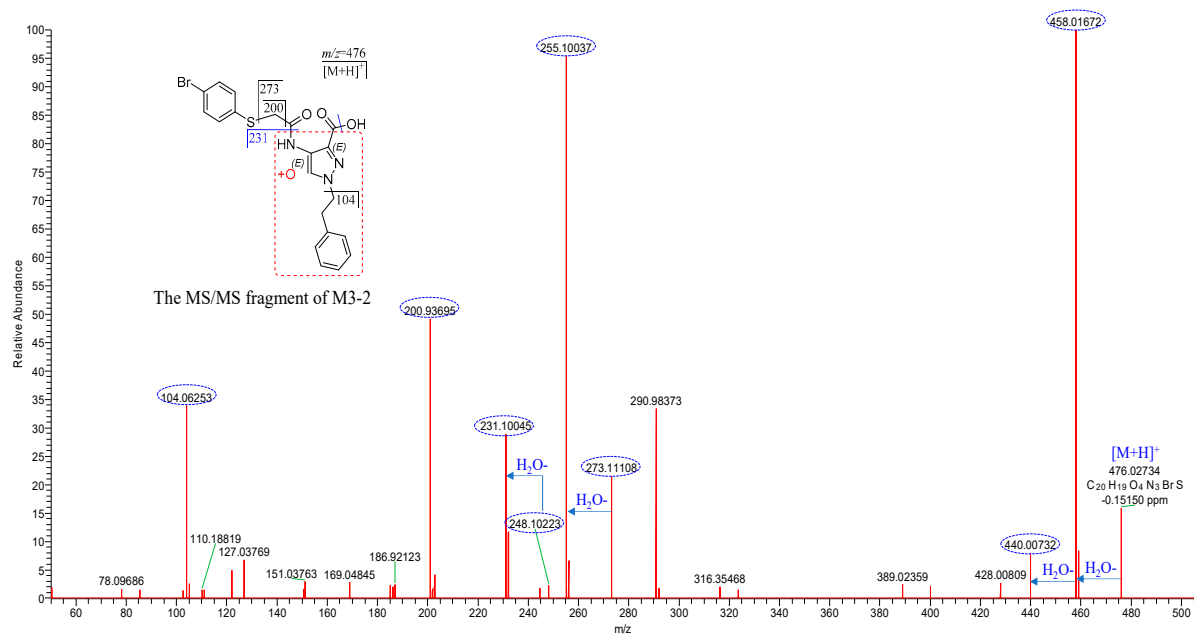
Supplementary Figure S4. MS/MS spectra of (a) M3-1, (b) M3-2, (c) M3-3, (d) M3-4, (e) M3-5, the mono-oxidation metabolite of KM-819, and structure elucidation

KM-819-HHEP-T30 #7249 RT: 8.47 AV: 1 NL: 2.45E5
F: FTMS + p ESI d Full ms2 476.0276@hcd20.00 [50.0000-505.0000]



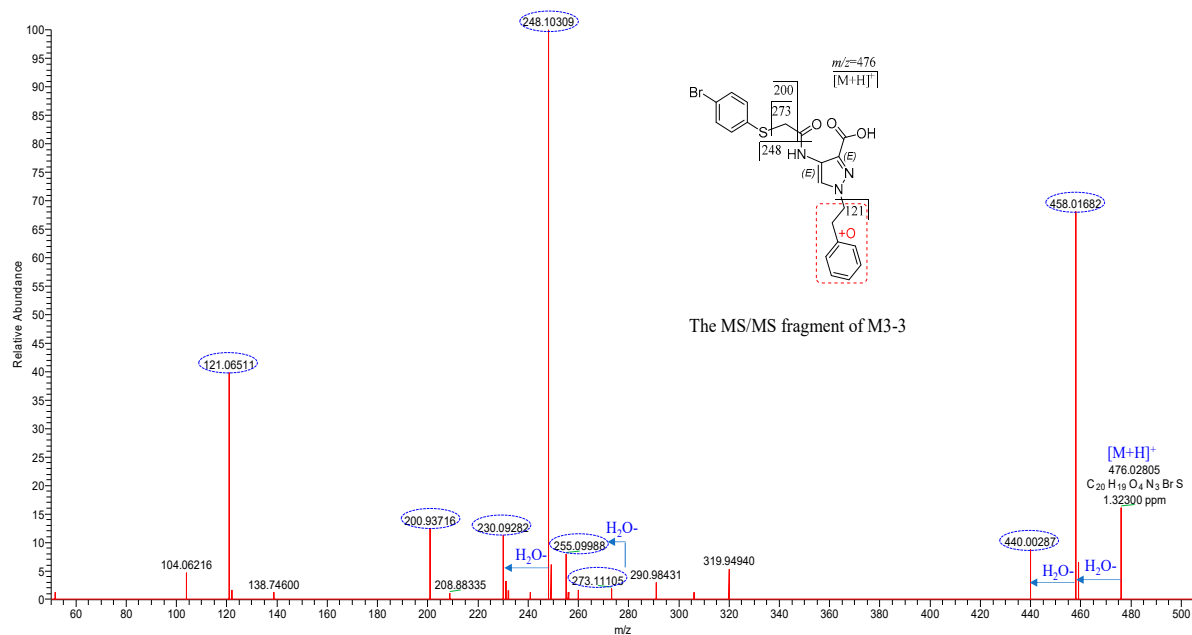
(a)

KM-819-HHEP-T30 #7900 RT: 9.22 AV: 1 NL: 1.45E5
F: FTMS + p ESI d Full ms2 476.0276@hcd20.00 [50.0000-505.0000]



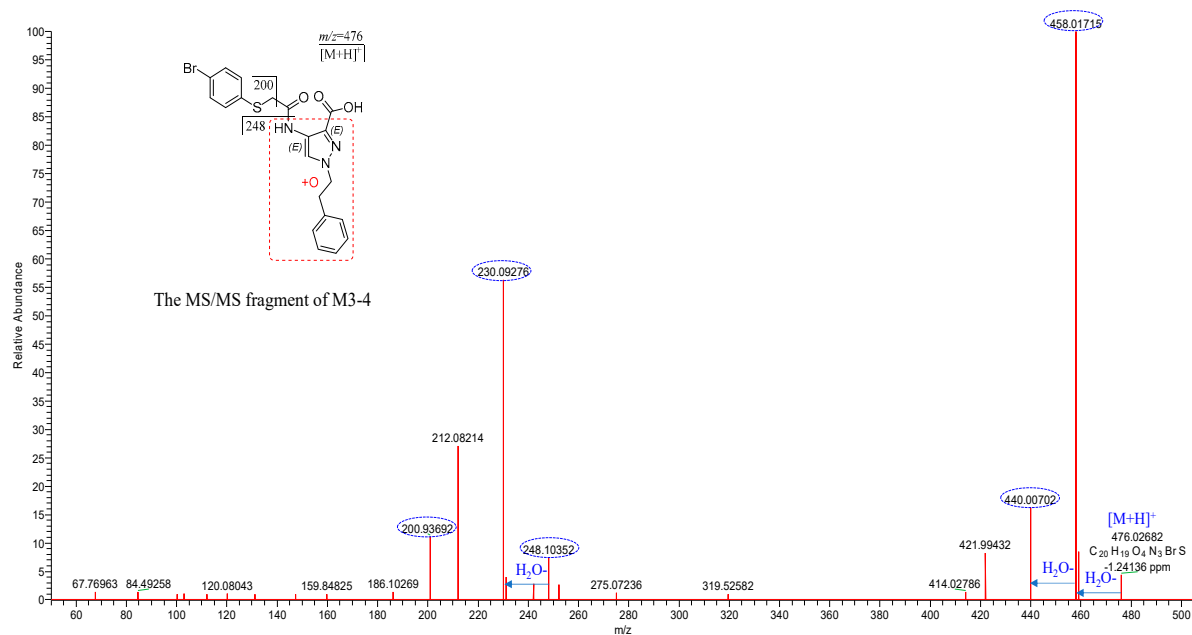
(b)

KM-819-HHEP-T30 #7968 RT: 9.30 AV: 1 NL: 2.03E5
F: FTMS + p ESId Full ms2 476.0276@hcd20.00 [50.0000-505.0000]



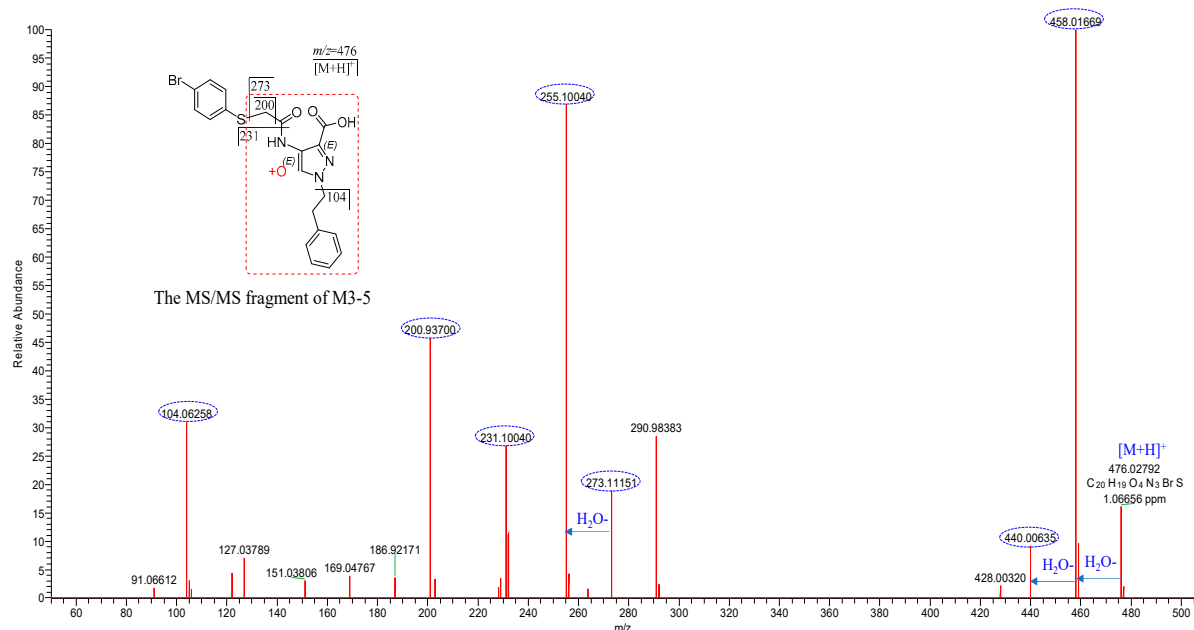
(c)

KM-819-HHEP-T30 #8186 RT: 9.56 AV: 1 NL: 2.24E5
F: FTMS + p ESId Full ms2 476.0276@hcd20.00 [50.0000-505.0000]



(d)

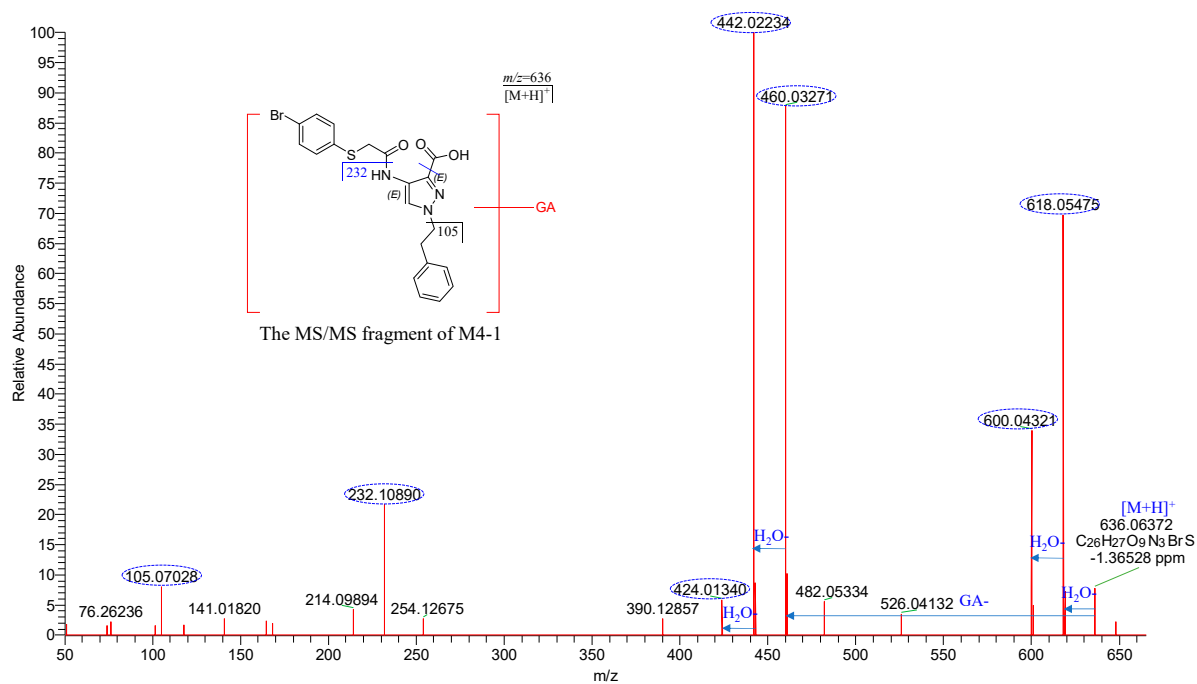
KM-819-HHEP-T30 #8602 RT: 10.05 AV: 1 NL: 1.38E5
F: FTMS + p ESI d Full ms2 476.0276@hcd20.00 [50.0000-505.0000]



(e)

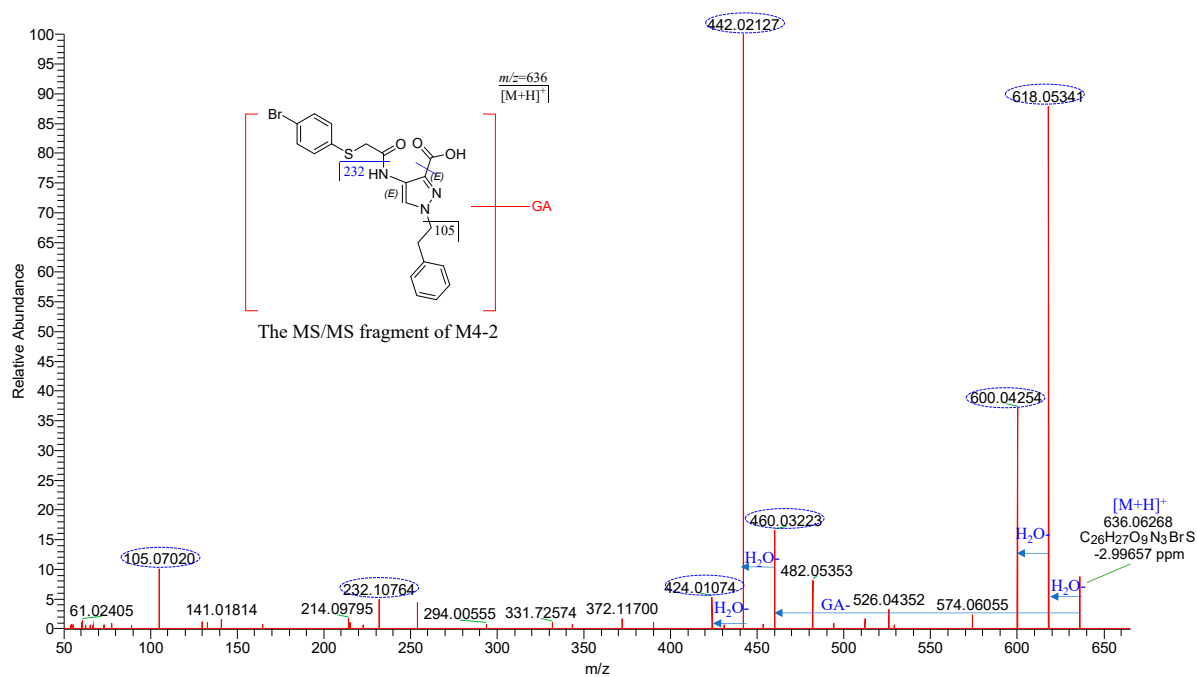
Supplementary Figure S5. MS/MS spectra of (a) M4-1, (b) M4-2, the glucuronidation metabolite of KM-819, and structure elucidation

KM-819-RHEP-T30-IHCD #8845 RT: 10.38 AV: 1 NL: 1.33E5
F: FTMS + p ESI d Full ms2 636.0650@hcd15.00 [50.0000-665.0000]



(a)

KM-819-DHEP-T30-IHCD #10168 RT: 10.54 AV: 1 NL: 3.65E5
 F: FTMS + p ESI d Full ms2 636.0640@hcd15.00 [50.0000-665.0000]



(b)

Supplementary Figure S6. MS/MS spectra of M5, the di-oxidation metabolite of KM-819, and structure elucidation

KM-819-RHEP-T30 #9134 RT: 10.75 AV: 1 NL: 3.52E5
 F: FTMS + p ESI d Full ms2 492.0228@hcd20.00 [50.0000-520.0000]

