

Supplemental data: Mass spectrometry

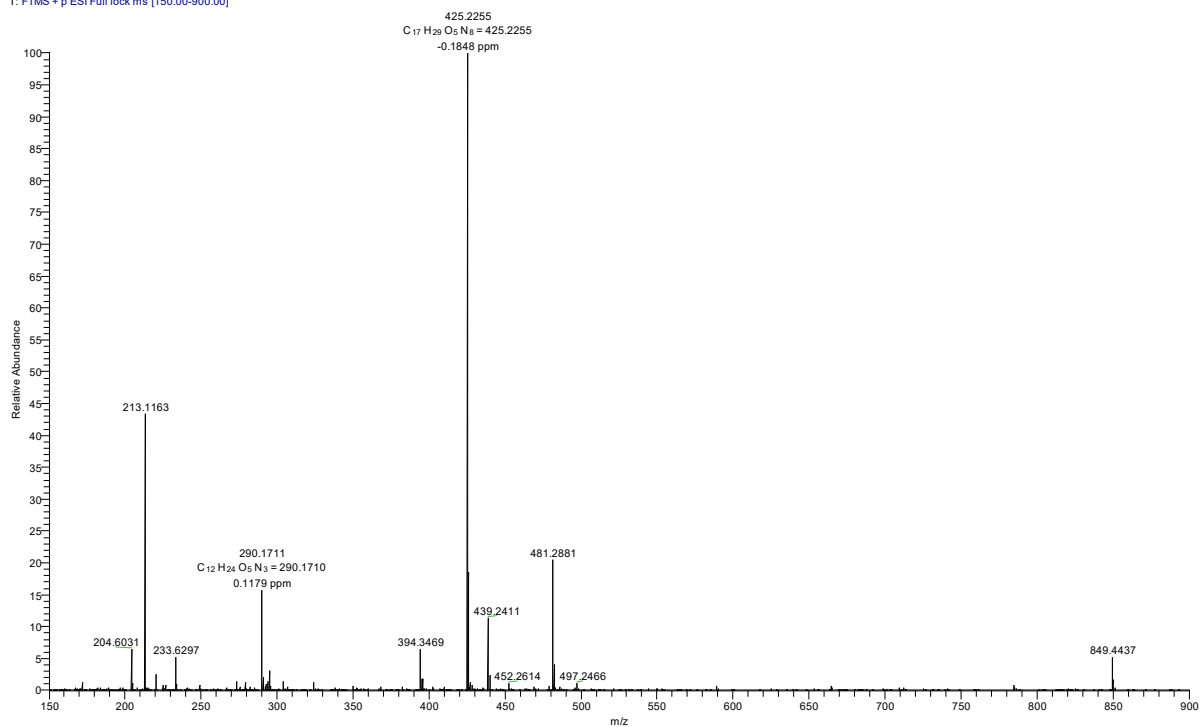
Compound 1a

D:\data_2019\juphr92shr1

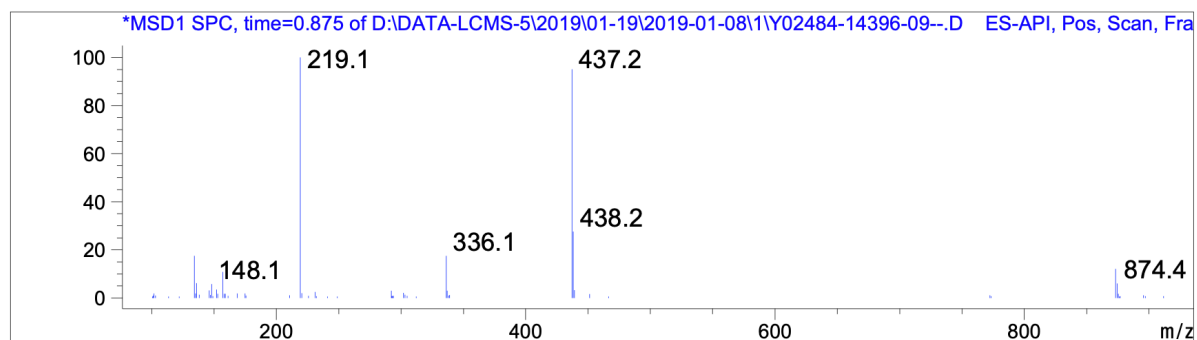
1/24/2019 9:18:42 AM

nbl344

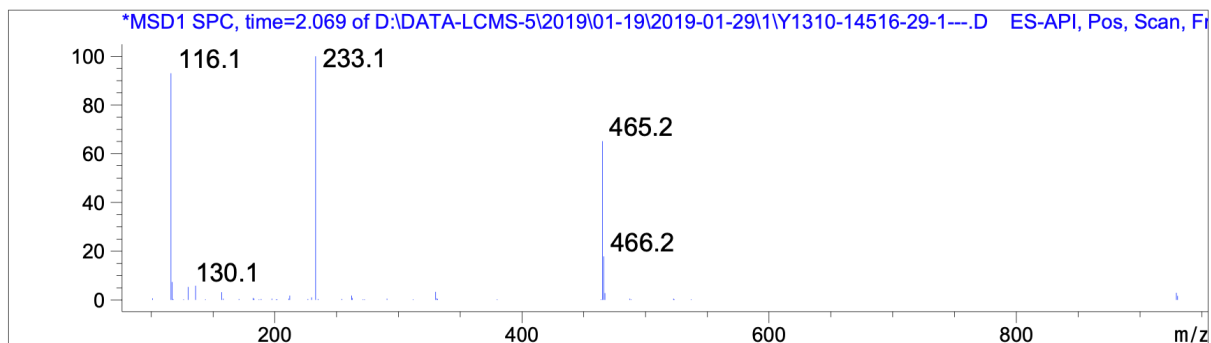
juphr92shr1 #1 RT: 0.02 AV: 1 NL: 1.45E7
T: FTMS + p ESI Full lock ms [150.00-900.00]



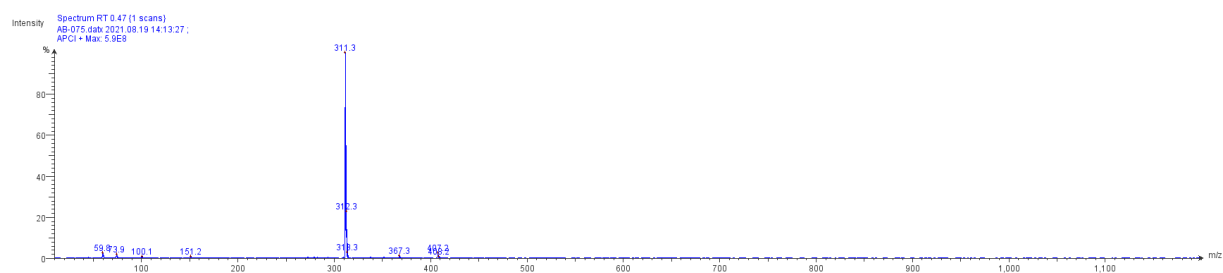
Compound 2b



Compound 1c



Compound 2a



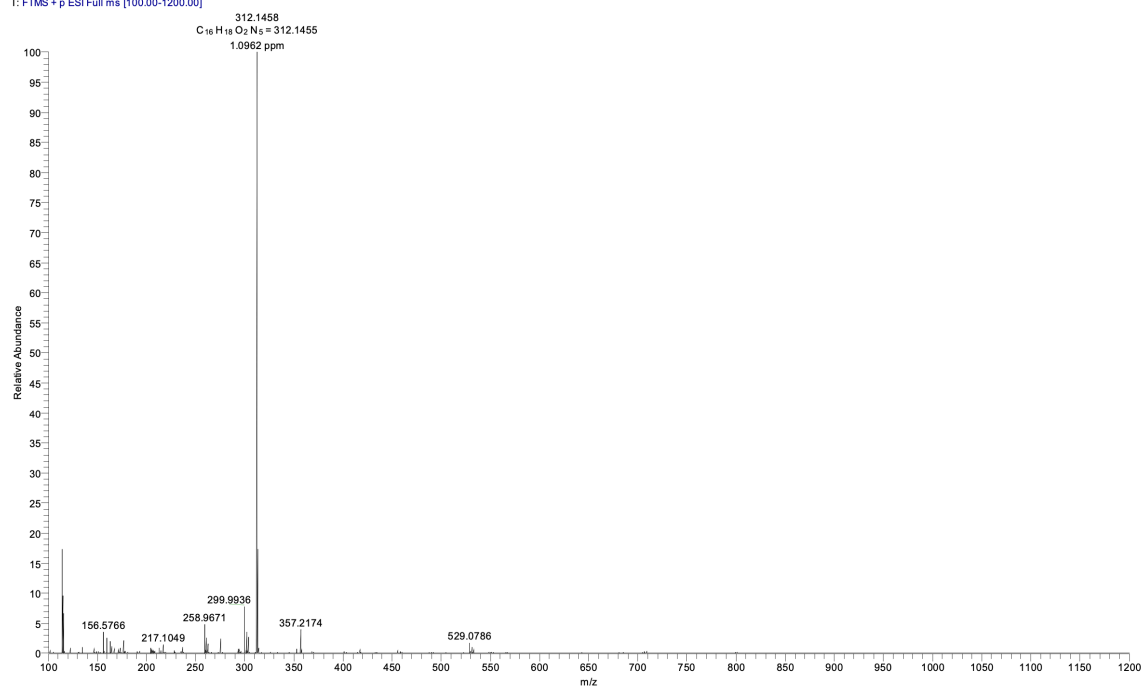
Compound 2b

D:\data_2023\juphu29shr1

6/22/2023 11:16:39 AM

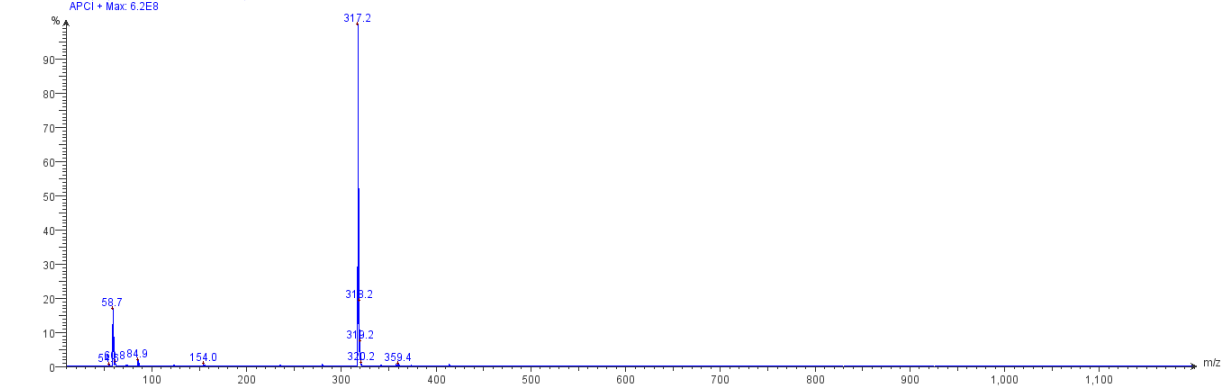
ab077

juphu29shr1 #1 RT: 0.02 Av: 1 NL: 1.37E8
T: FTMS + p ESI Full ms [100.00-1200.00]

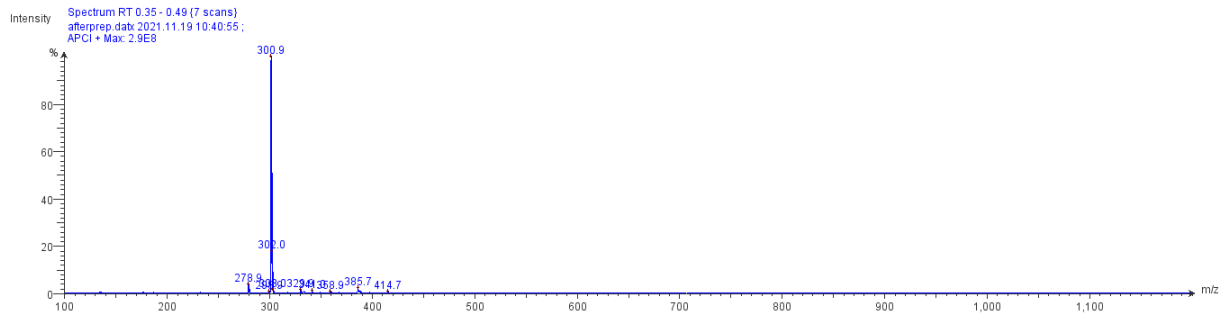


Compound 2c

Intensity Spectrum RT 0.14 - 0.27 (6 scans)
afterprep date: 2021.09.24 12:19:14 ;
APCI • Max: 6.2E8



Compound 2d



Compound 2e

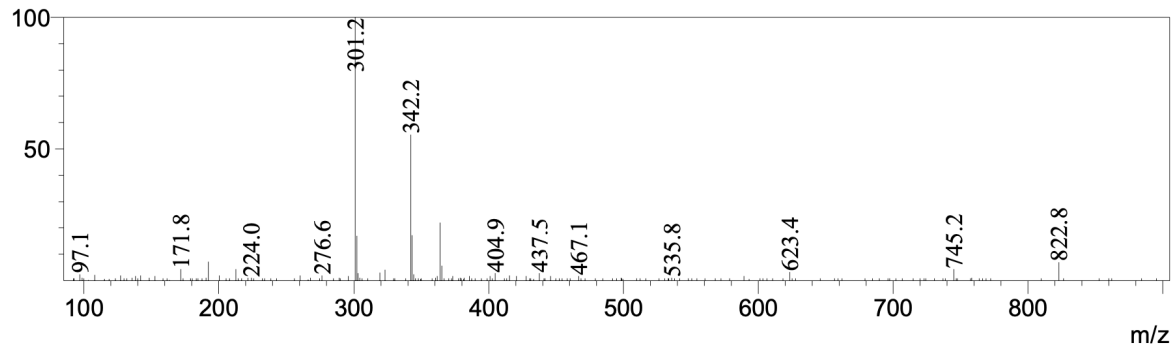
Mass Spectrum

Line#: 1

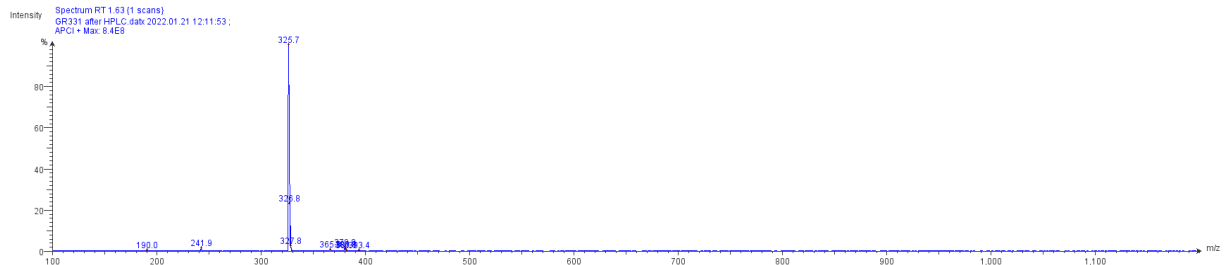
Acquisition Mode: Scan (Positive)

R.Time: 0.942(Scan#:146) Spectrum Mode: Averaged 0.935-0.948(145-147)

BasePeak: 301.2(39633)



Compound 2f



Compound 2g

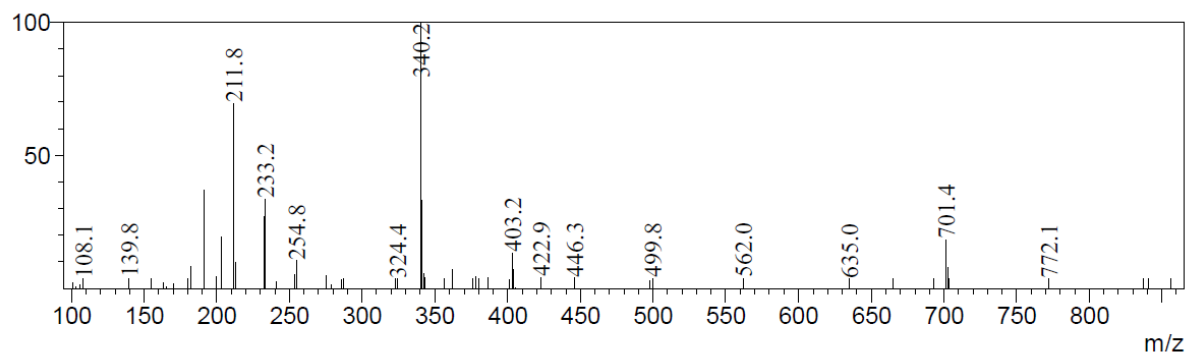
Mass Spectrum

Line#: 1

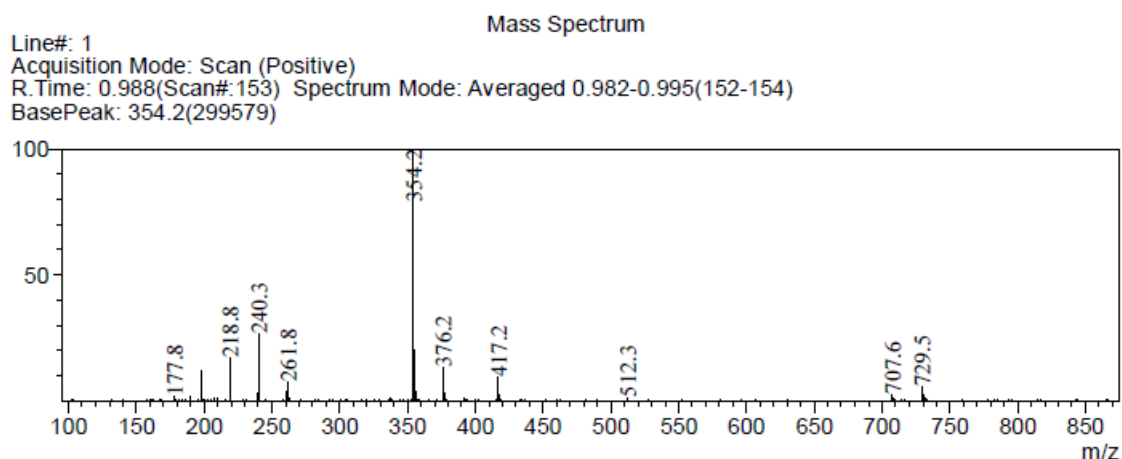
Acquisition Mode: Scan (Positive)

R.Time: 0.928(Scan#:144) Spectrum Mode: Single 0.928(144) Background: 0.895-0.982(139-152)

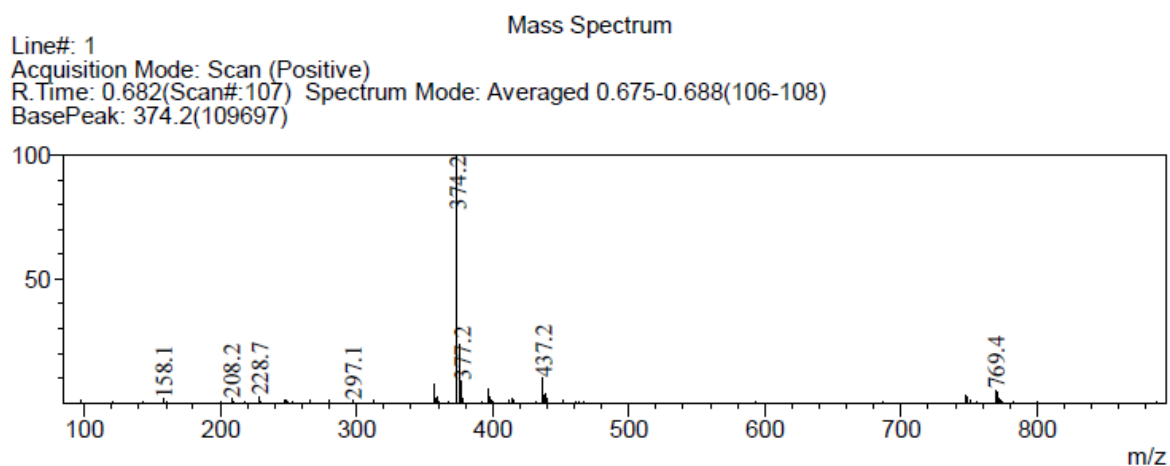
BasePeak: 340.2(26794)



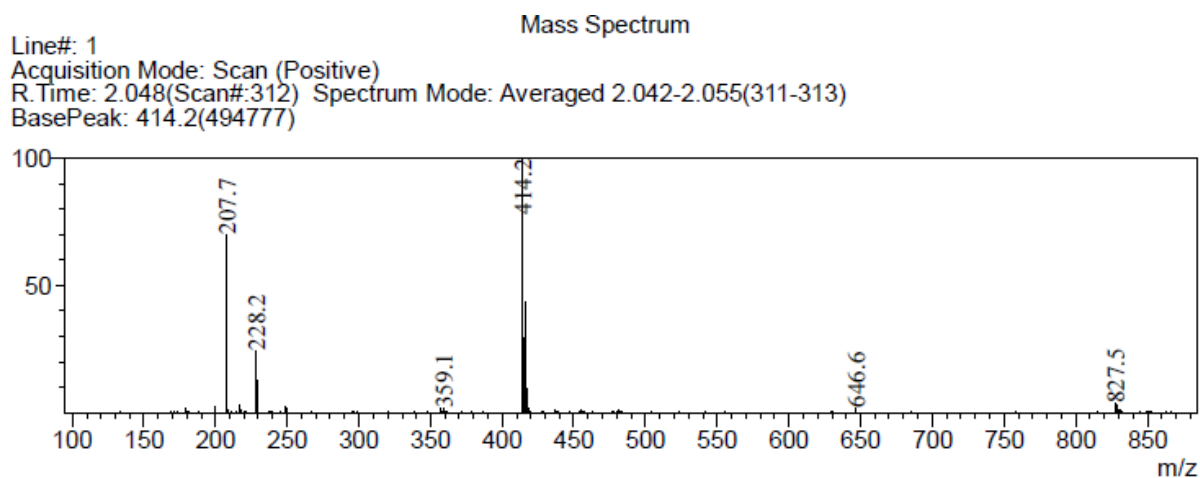
Compound 2h



Compound 3a



Compound 3b



Compound 4/KMI169

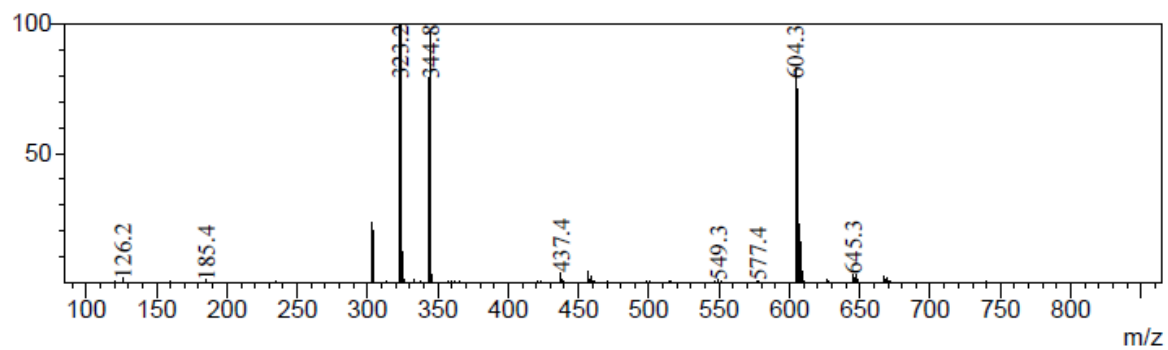
Mass Spectrum

Line#: 1

Acquisition Mode: Scan (Positive)

R.Time: 1.188(Scan#:182-184) Spectrum Mode: Averaged 1.182-1.195(182-184)

BasePeak: 323.2(152487)



Compound KMI169Ctrl

Mass Spectrum

Line#: 1

Acquisition Mode: Scan (Positive)

R.Time: 0.733(Scan#:226-228) Spectrum Mode: Averaged 0.730-0.737(226-228)

BasePeak: 316.9(555571)

