Mass Spectrometry Details

In-house analysis Thermo Fisher LCQ Deca.

ESI source:
Ionization mode: positive
Sheath gas flow rate: 35
Sweep gas flow rate: 0
Spray voltage: 4.5kV
Capillary temperature: 250ºC
Capillary voltage: 3V
Tube lens offset: -30V

Injection control:
AGC settings:
FullMS Target: 5e7

Ion optics:
Multipole 1 Offset: -1.25V
Lens voltage: -16V
Multipole 2 Offset: -11V
Multipole RF Amplitude: 400V
Enhance Lens: -68V

NMSF Atmospheric Solids Analysis Probe (ASAP)

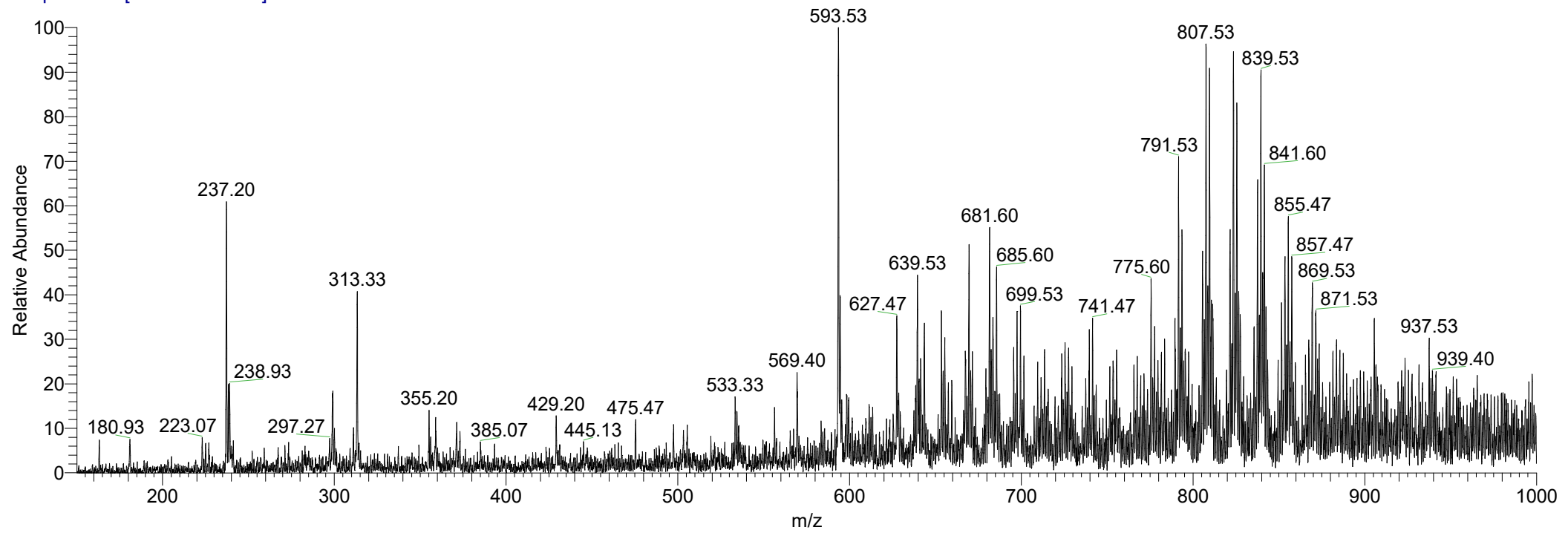
APCI on a Waters Xevo G2-S instrument.

ASAP analyses: Initial characterisation of samples was made by atmospheric pressure chemical ionisation (APCI) mass spectrometry via an atmospheric solids analysis probe (ASAP) on a Waters Xevo G2-S instrument. A small amount of solid sample was transferred to the tip of a glass capillary, which was then placed within the ASAP source and inserted into the instrument. The vaporizer temperature was increased from 50°C to a temperature at which ions were observed and acquired and the discharge current was 4 μA . Data was processed using vendor MassLynx software.

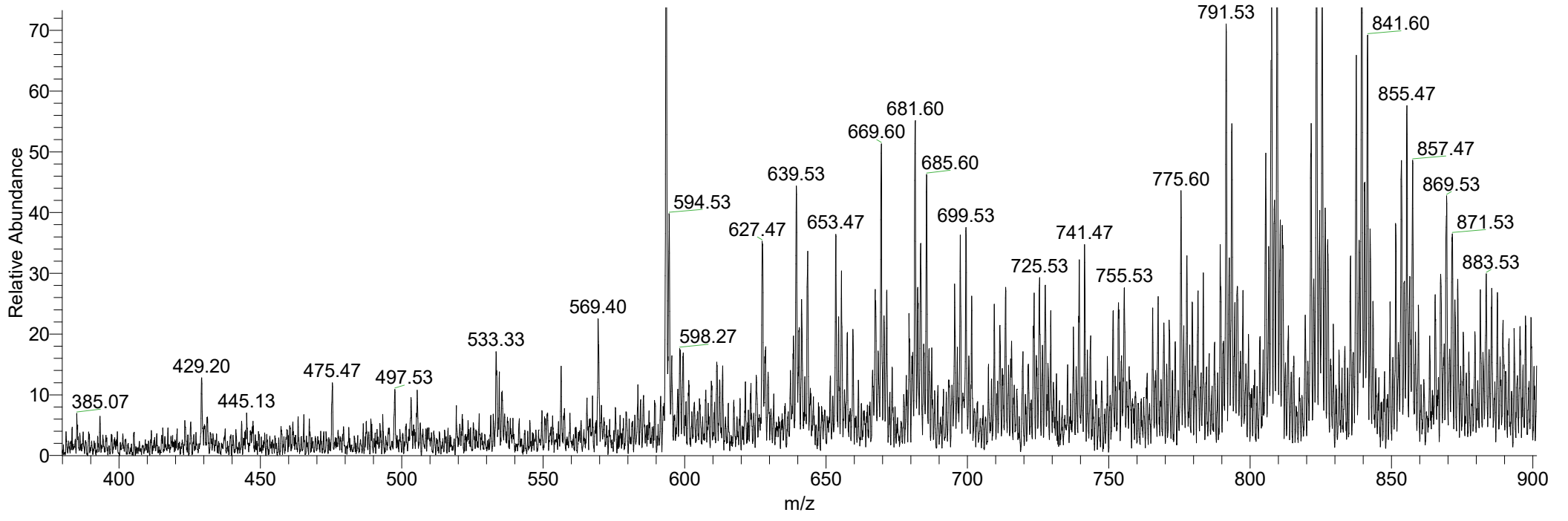
Please also see the header of each spectrum.

E:\dan_evans\RAW FILES\100%\CH1 08/16/18 13:27:31 CH1

CH1 #1-50 RT: 0.01-0.75 AV: 50 NL: 2.38E5
T: + p ESI ms [150.00-1000.00]

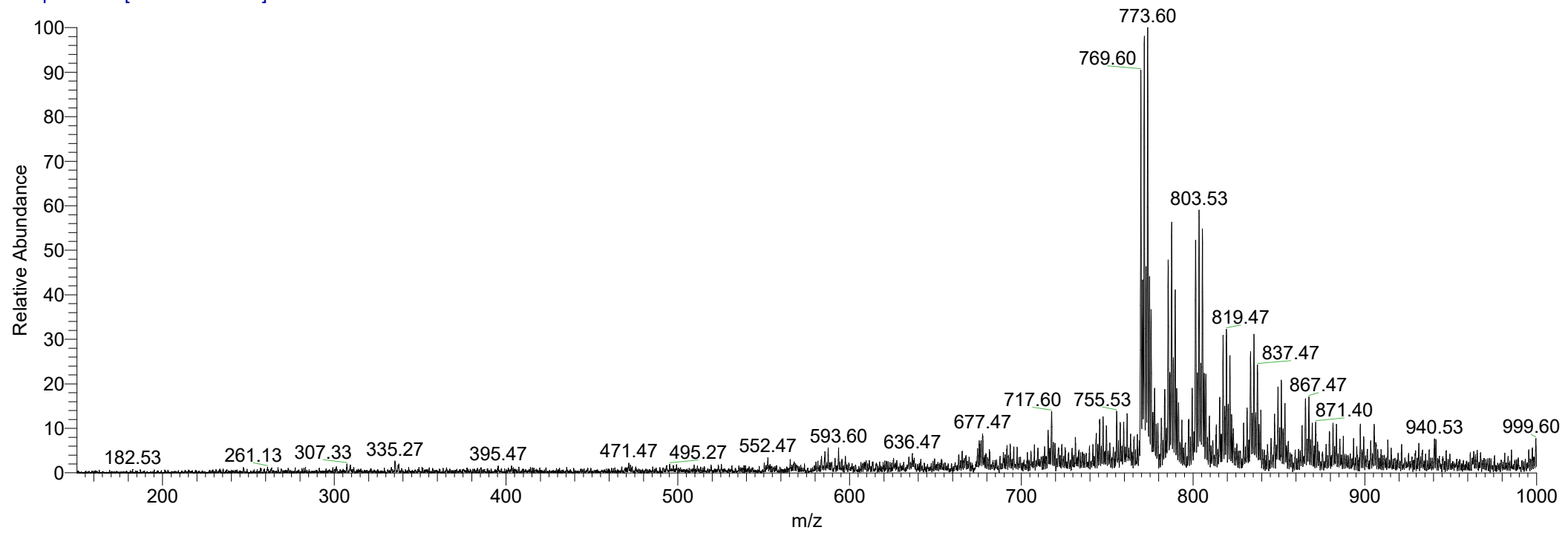


CH1 #1-50 RT: 0.01-0.75 AV: 50 NL: 2.38E5
T: + p ESI ms [150.00-1000.00]

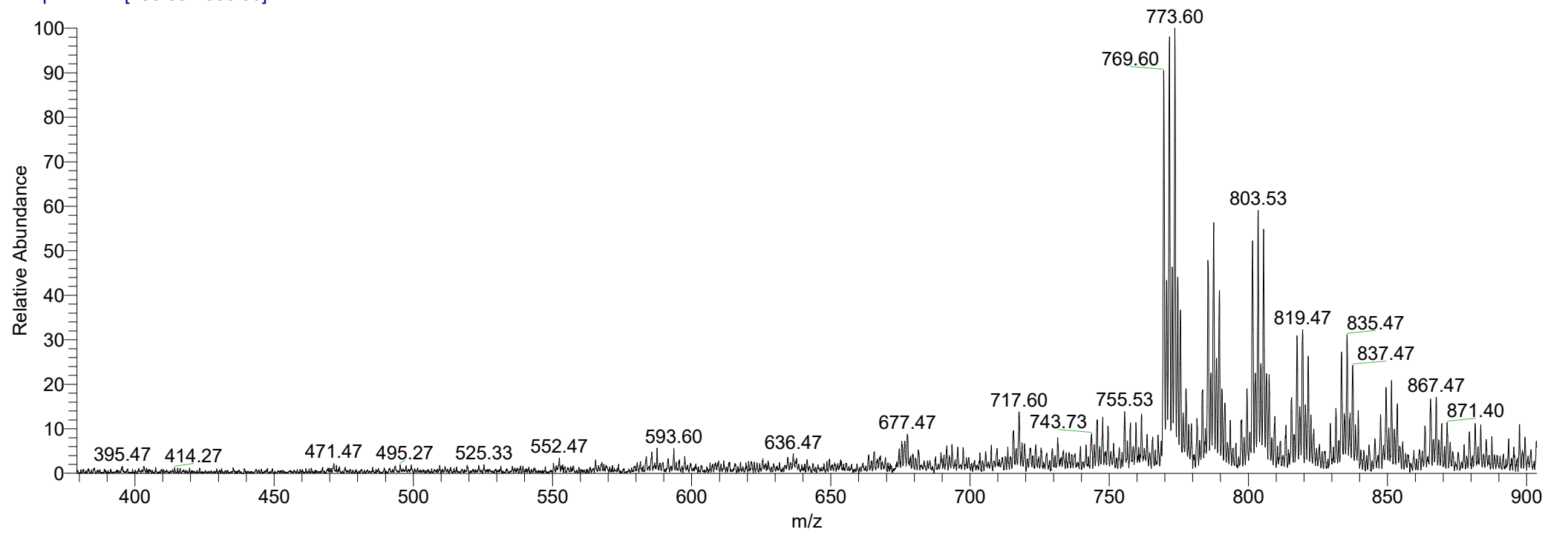


E:\dan_evans\RAW FILES\100%\CH2 08/16/18 13:41:43 CH2

CH2 #1-50 RT: 0.00-0.74 AV: 50 NL: 1.08E6
T: + p ESI ms [150.00-1000.00]

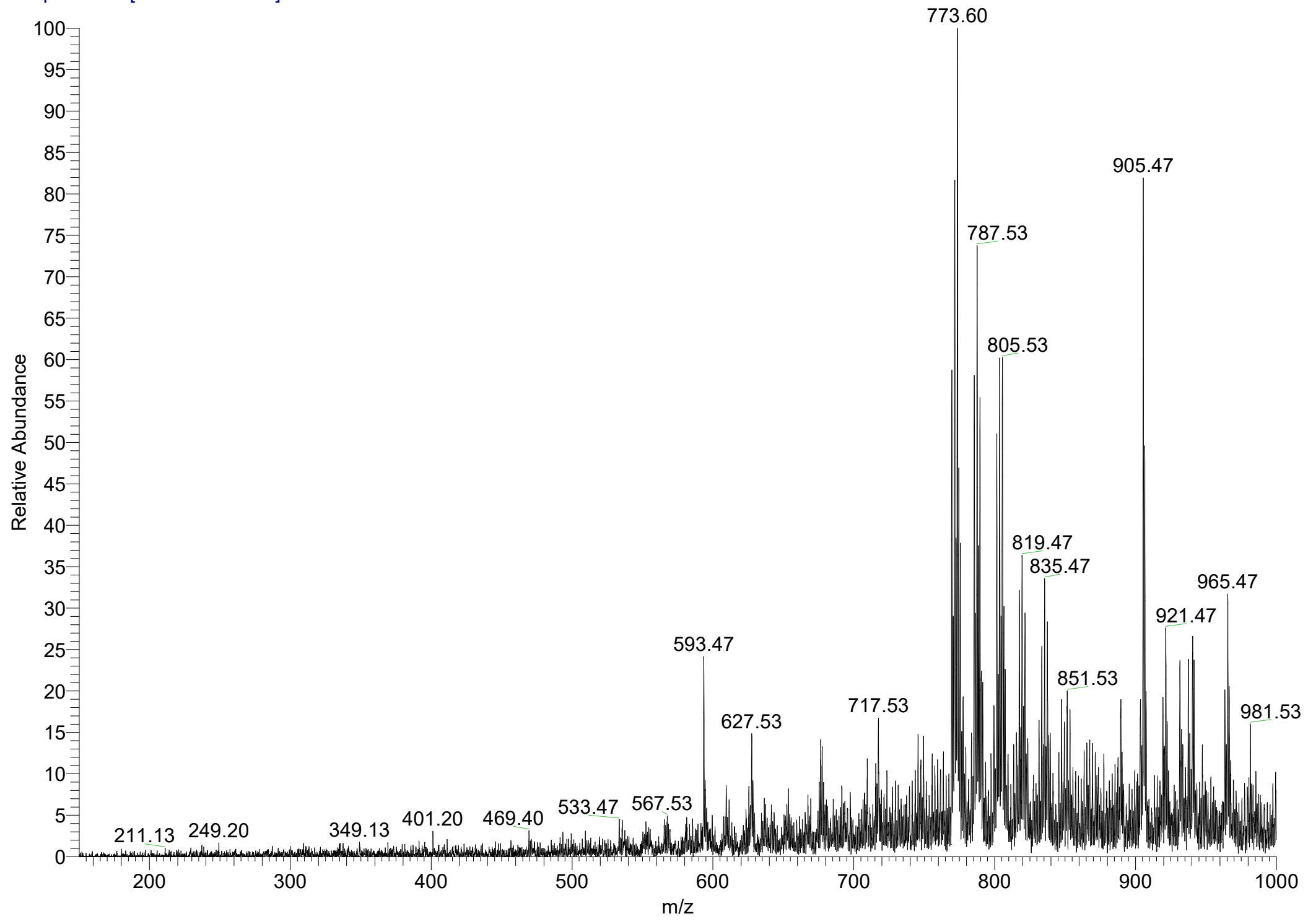


CH2 #1-50 RT: 0.00-0.74 AV: 50 NL: 1.08E6
T: + p ESI ms [150.00-1000.00]



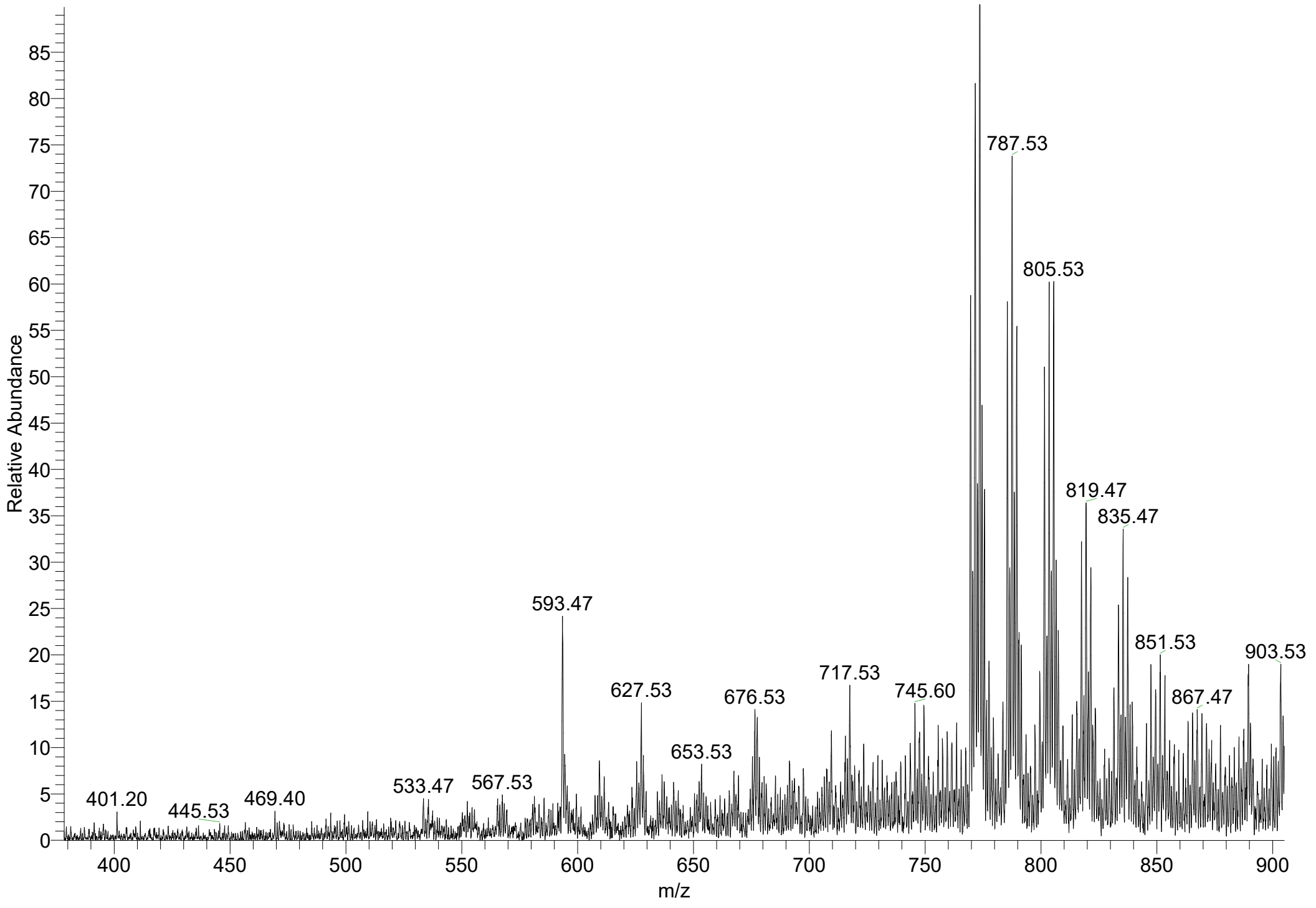
E:\dan_evans\RAW FILES\100%\CH3 08/16/18 13:48:27 CH3

CH3 #1-50 RT: 0.01-0.74 AV: 50 NL: 8.70E5
T: + p ESI ms [150.00-1000.00]



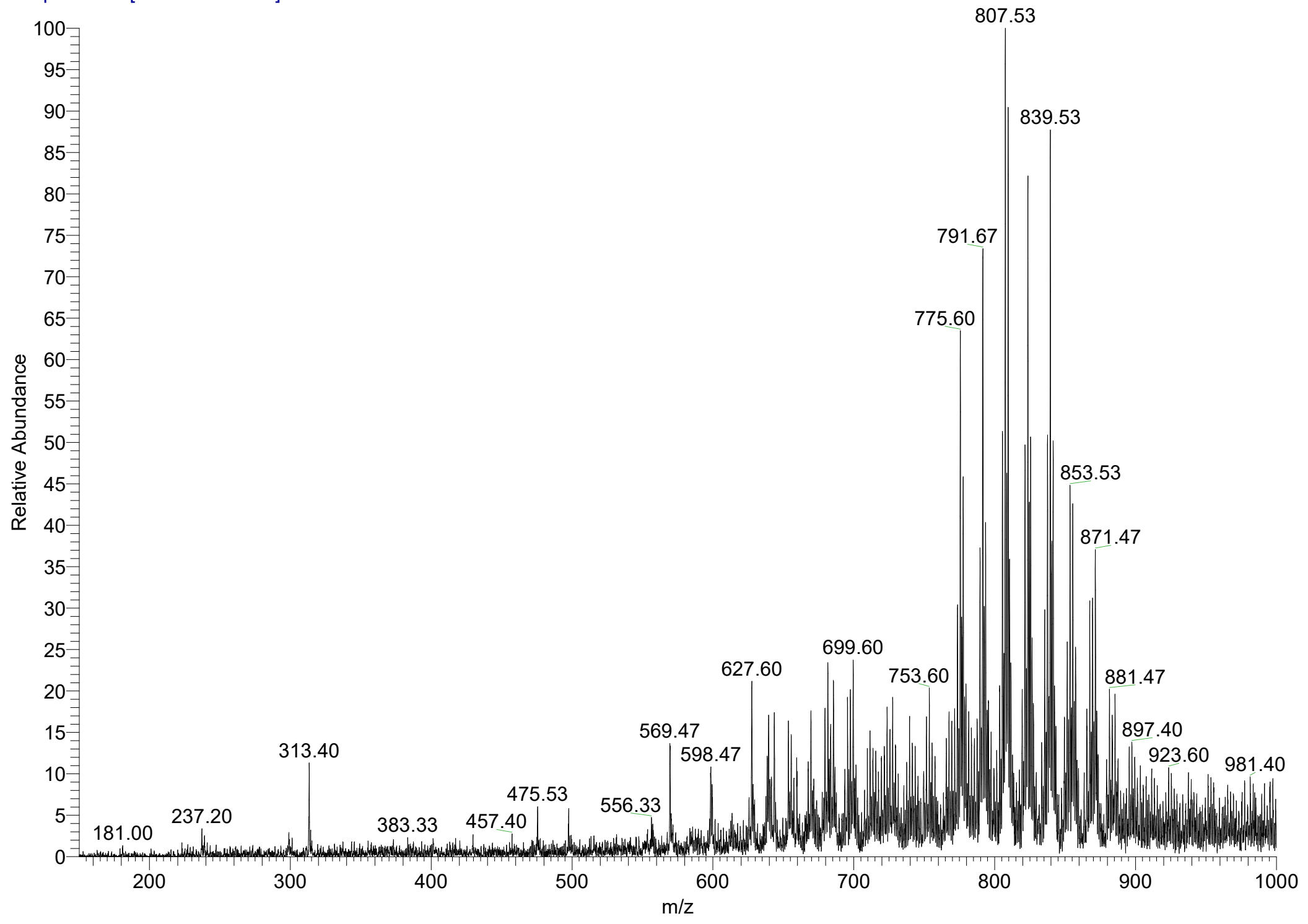
E:\dan_evans\RAW FILES\100%\CH3 08/16/18 13:48:27 CH3

CH3 #1-50 RT: 0.01-0.74 AV: 50 NL: 8.70E5
T: + p ESI ms [150.00-1000.00]



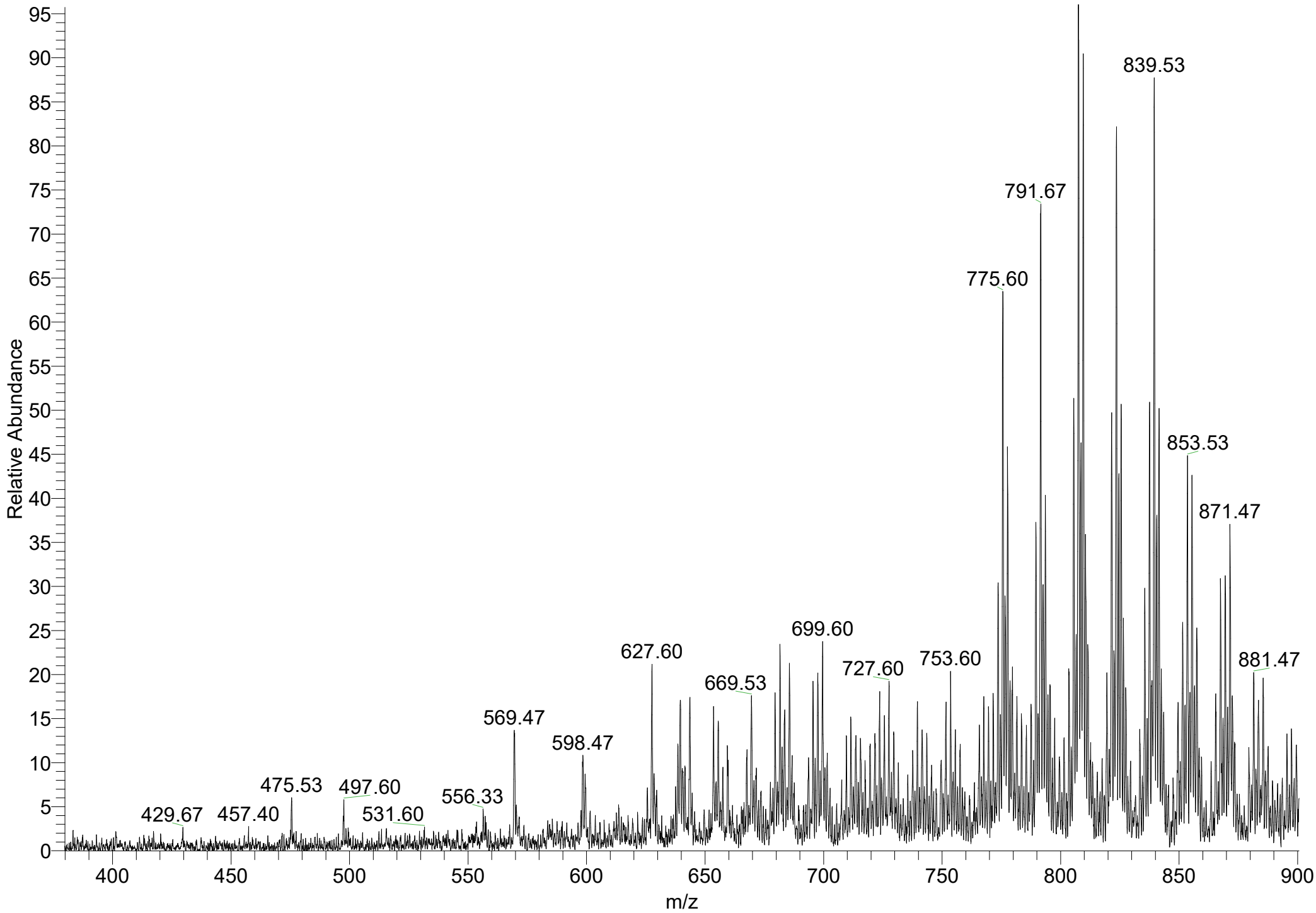
E:\dan_evans\RAW FILES\100%\CH4 08/16/18 13:55:06 CH4

CH4 #1-50 RT: 0.00-0.74 AV: 50 NL: 7.04E5
T: + p ESI ms [150.00-1000.00]



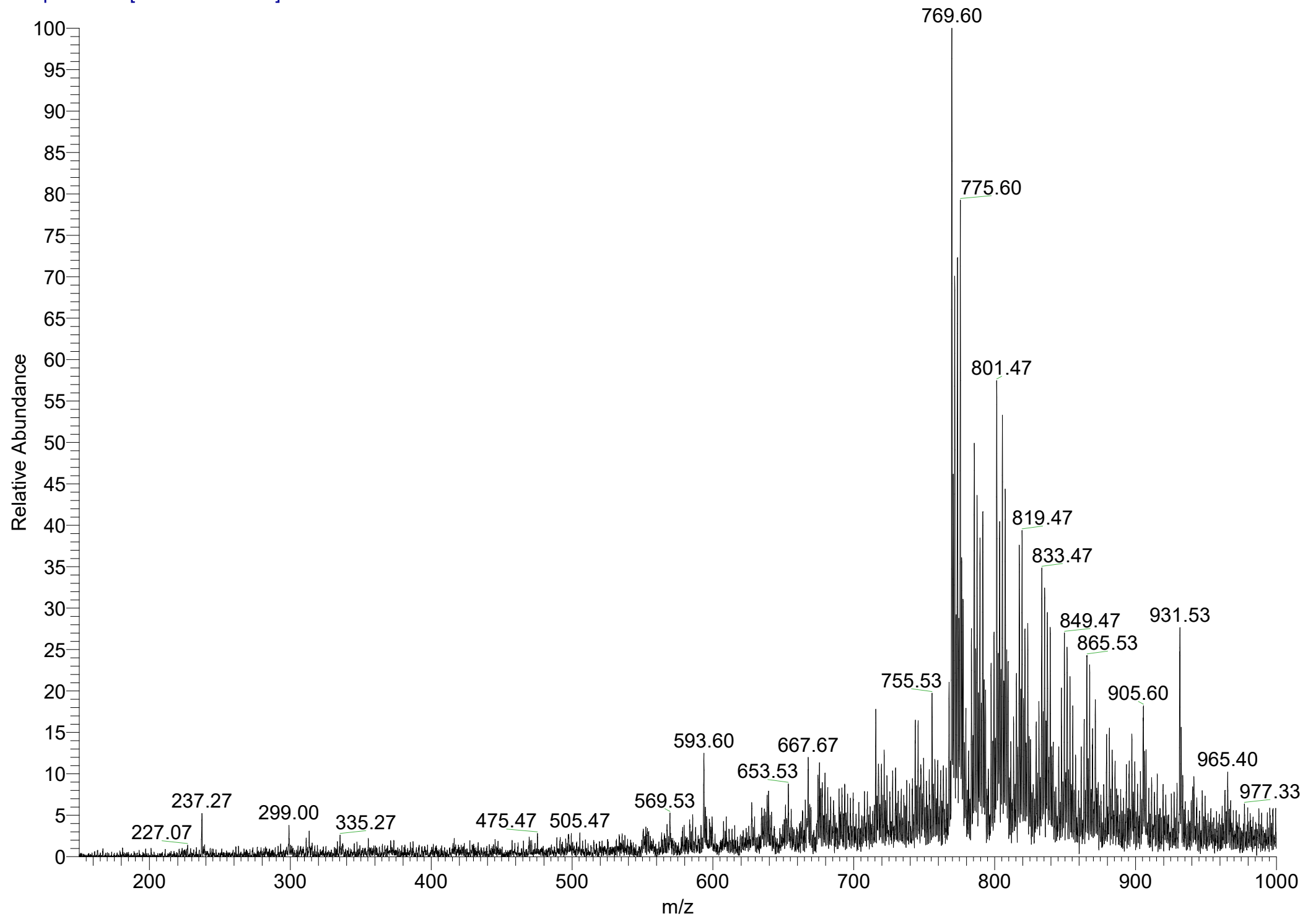
E:\dan_evans\RAW FILES\100%\CH4 08/16/18 13:55:06 CH4

CH4 #1-50 RT: 0.00-0.74 AV: 50 NL: 7.04E5
T: + p ESI ms [150.00-1000.00]



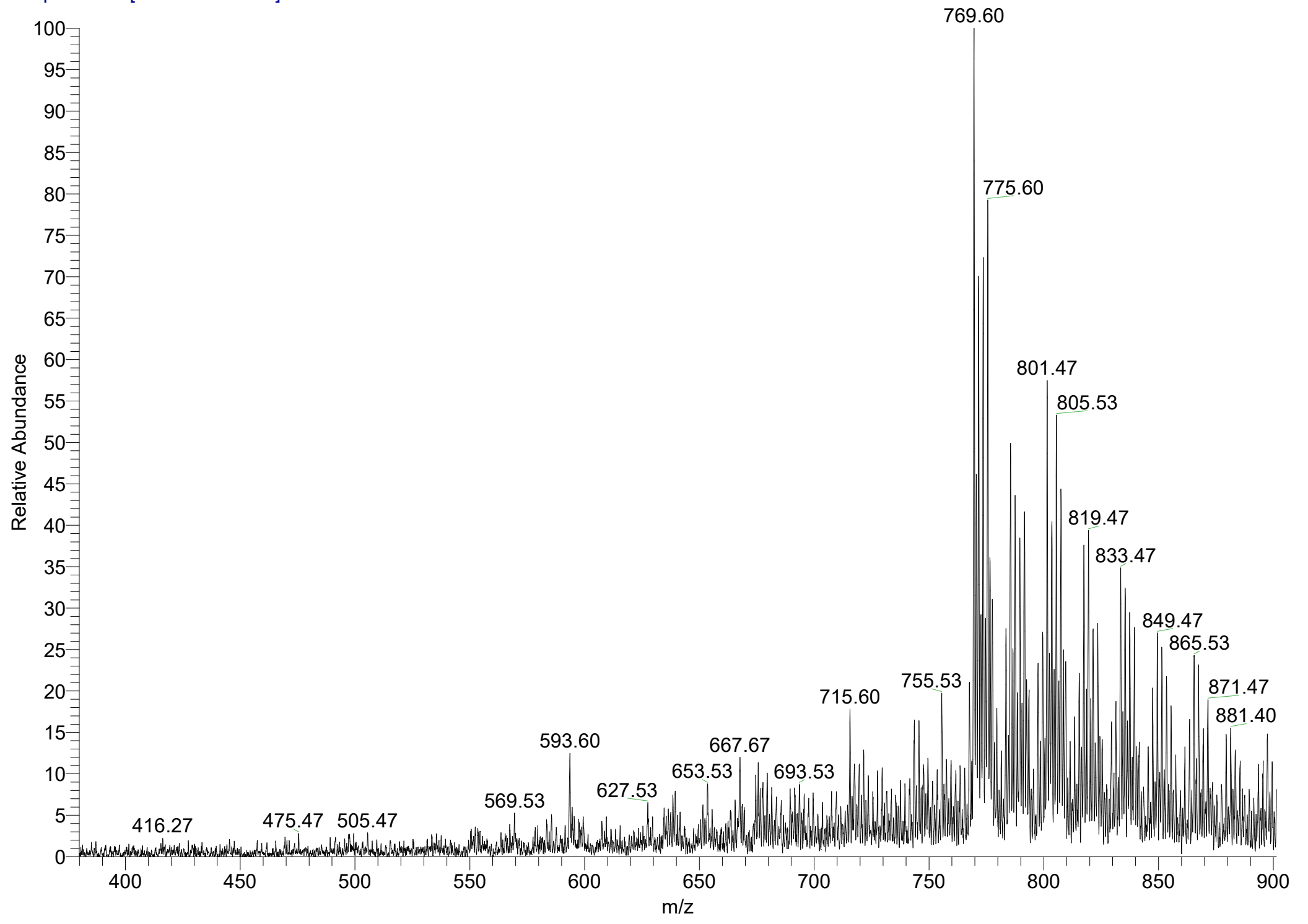
E:\dan_evans\RAW FILES\100%\CH5 08/16/18 14:00:03 CH5

CH5 #1-50 RT: 0.01-0.75 AV: 50 NL: 9.18E5
T: + p ESI ms [150.00-1000.00]



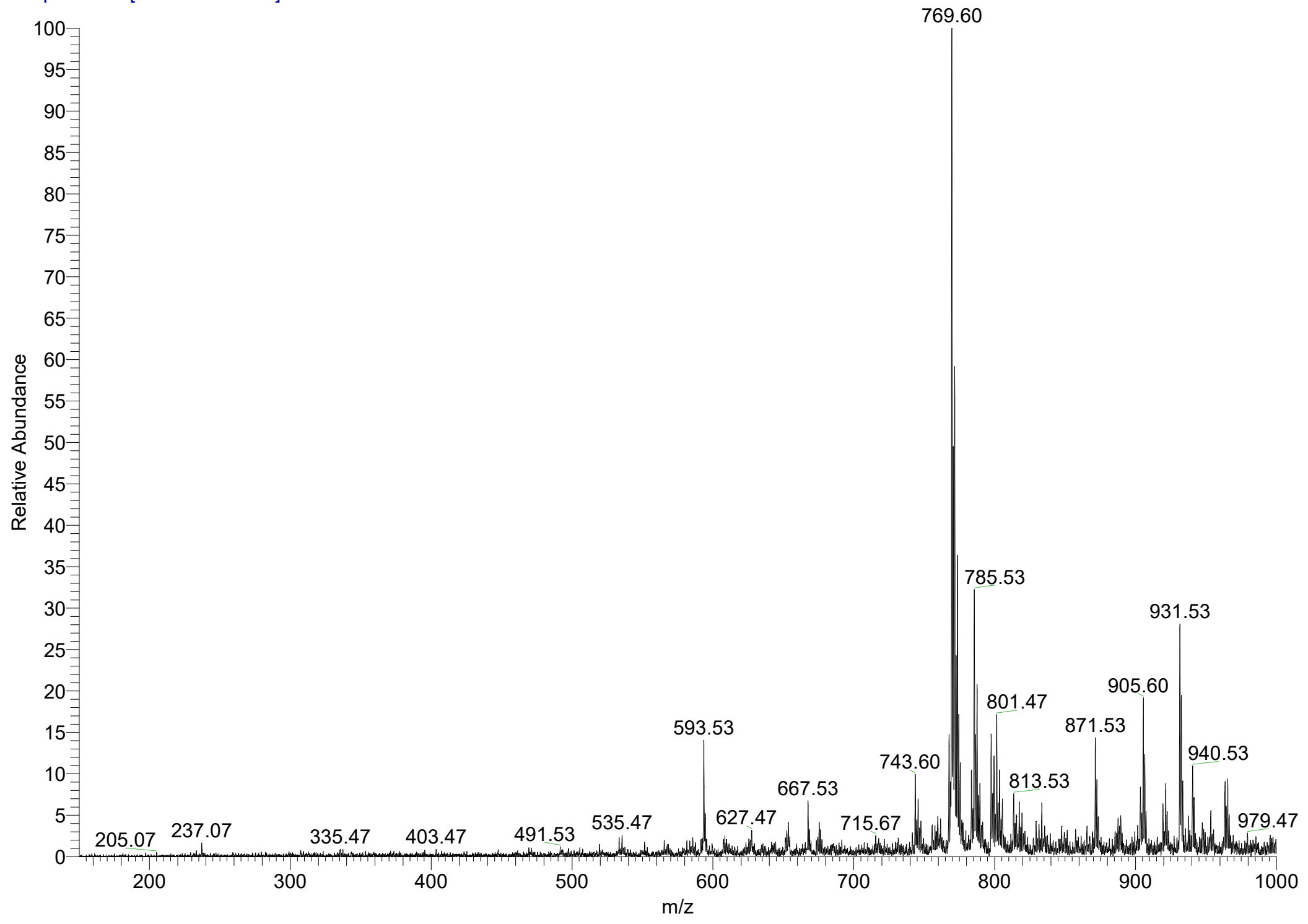
E:\dan_evans\RAW FILES\100%\CH5 08/16/18 14:00:03 CH5

CH5 #1-50 RT: 0.01-0.75 AV: 50 NL: 9.18E5
T: + p ESI ms [150.00-1000.00]



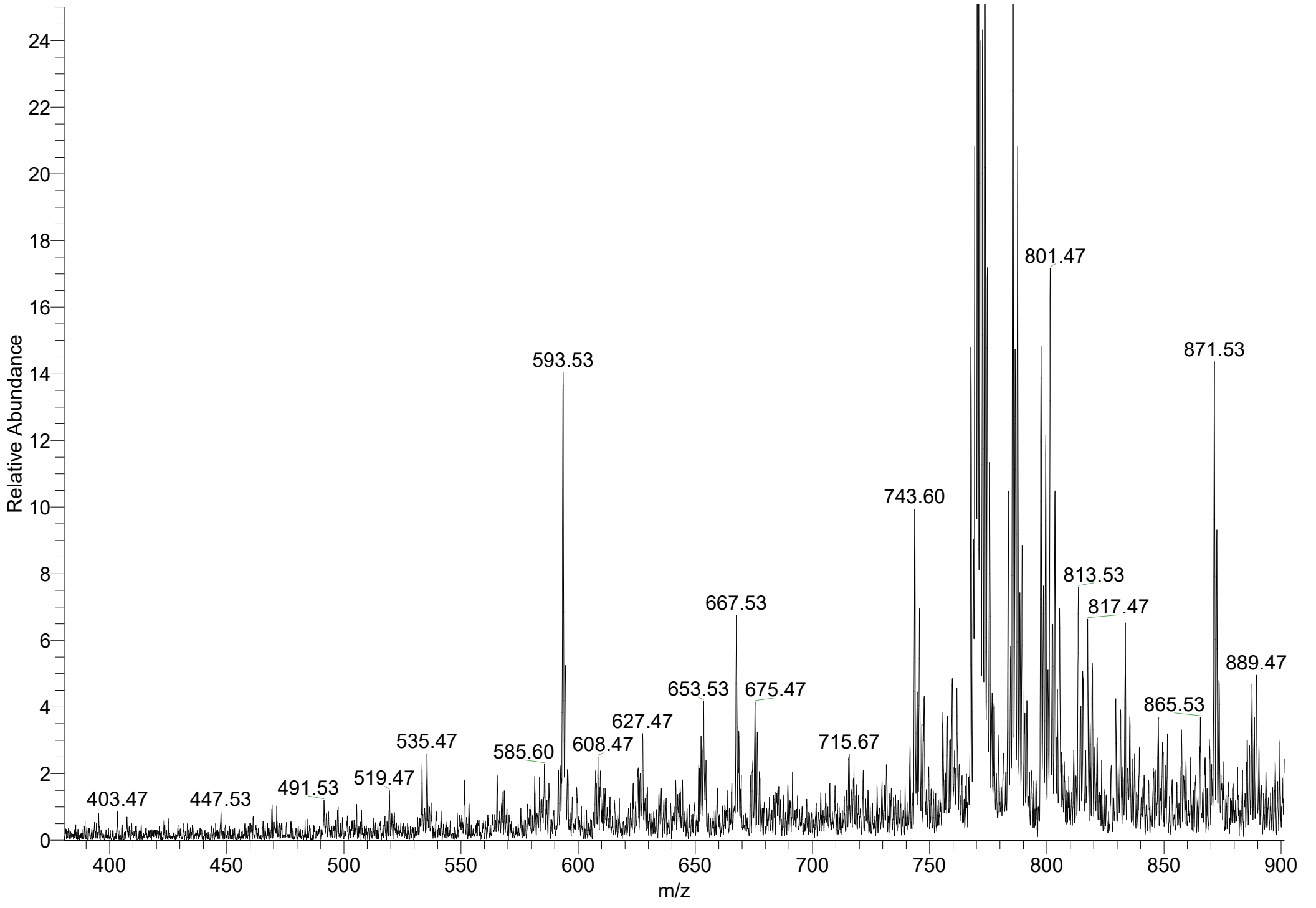
E:\dan_evans\RAW FILES\100%\CH6 08/16/18 14:05:17 CH6

CH6 #1-50 RT: 0.00-0.74 AV: 50 NL: 3.12E6
T: + p ESI ms [150.00-1000.00]



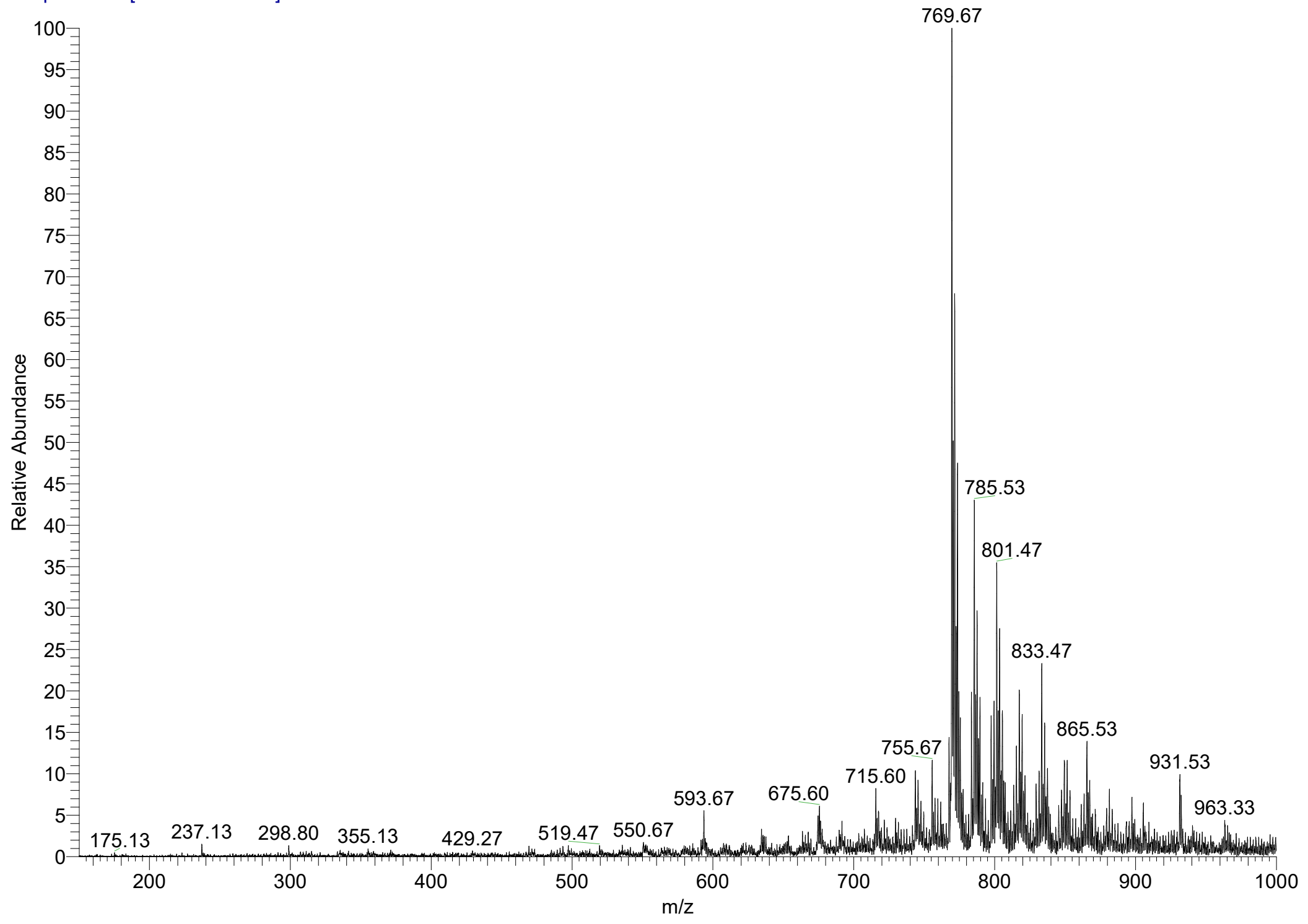
E:\dan_evans\RAW FILES\100%\CH6 08/16/18 14:05:17 CH6

CH6 #1-50 RT: 0.00-0.74 AV: 50 NL: 3.12E6
T: + p ESI ms [150.00-1000.00]



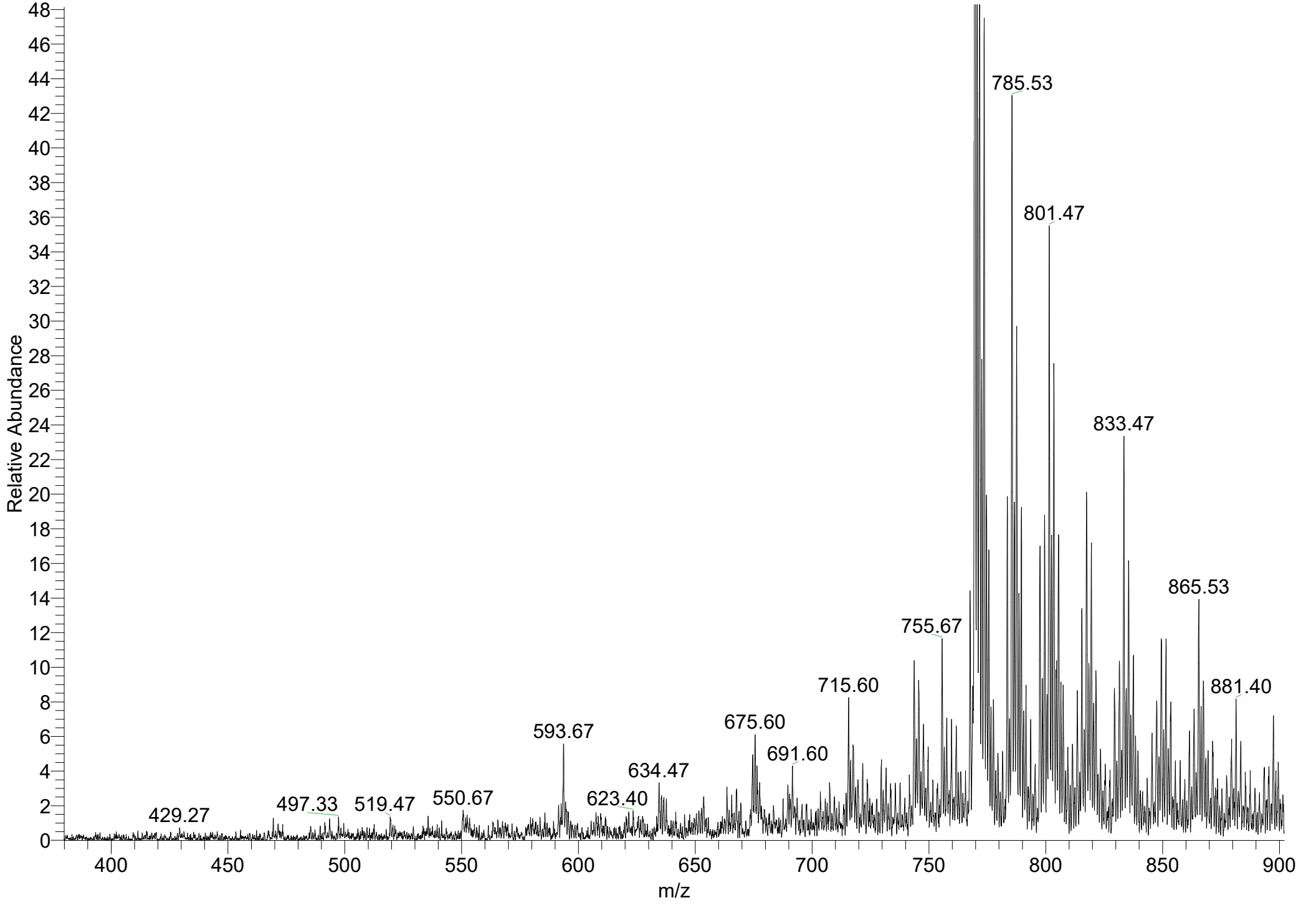
E:\dan_evans\RAW FILES\100%\CH7 08/16/18 14:10:17 CH7

CH7 #1-50 RT: 0.01-0.75 AV: 50 NL: 2.45E6
T: + p ESI ms [150.00-1000.00]



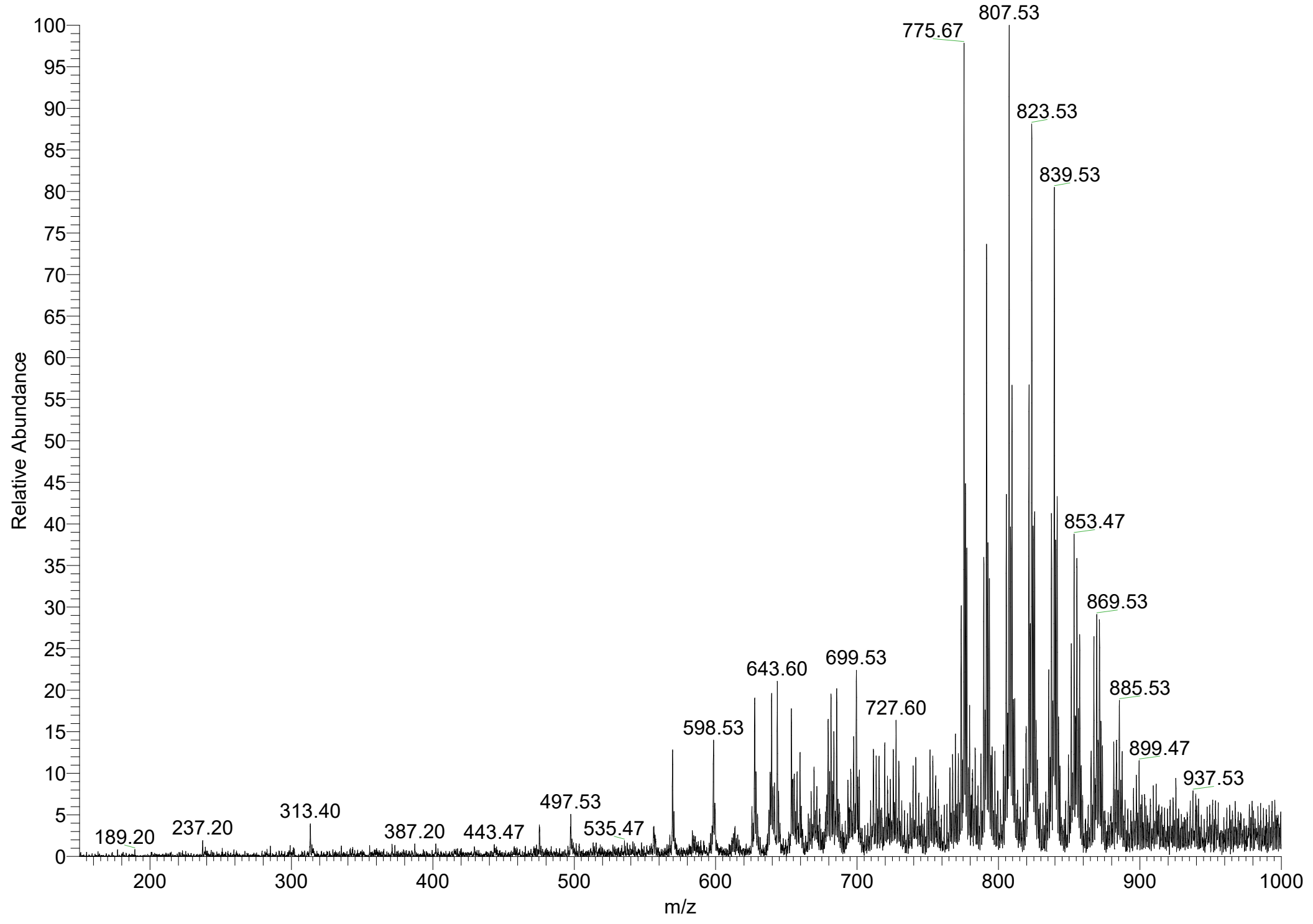
E:\dan_evans\RAW FILES\100%\CH7 08/16/18 14:10:17 CH7

CH7 #1-50 RT: 0.01-0.75 AV: 50 NL: 2.45E6
T: + p ESI ms [150.00-1000.00]



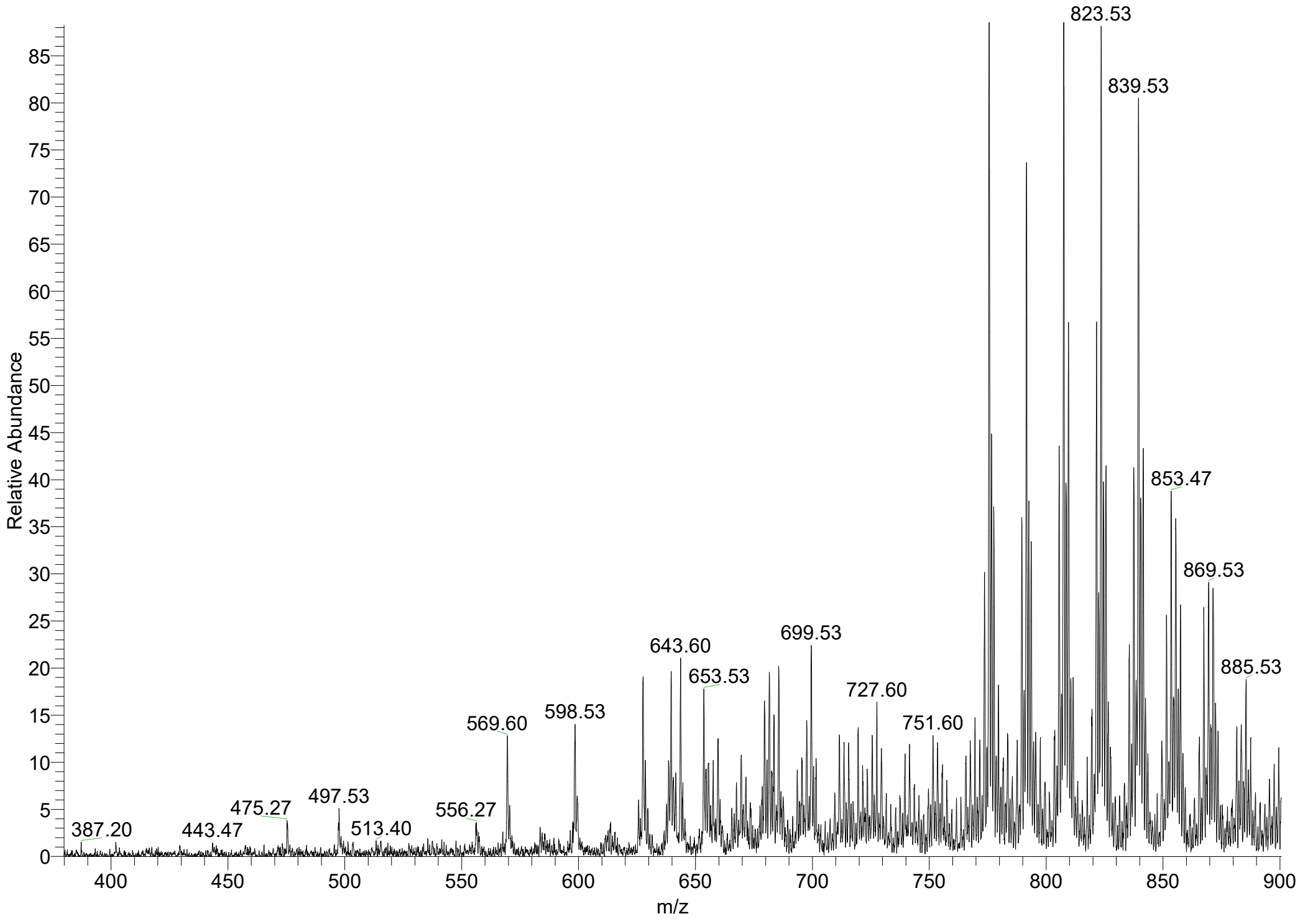
E:\dan_evans\RAW FILES\100%\CH8 08/16/18 14:16:06 CH8

CH8 #1-50 RT: 0.01-0.75 AV: 50 NL: 1.33E6
T: + p ESI ms [150.00-1000.00]



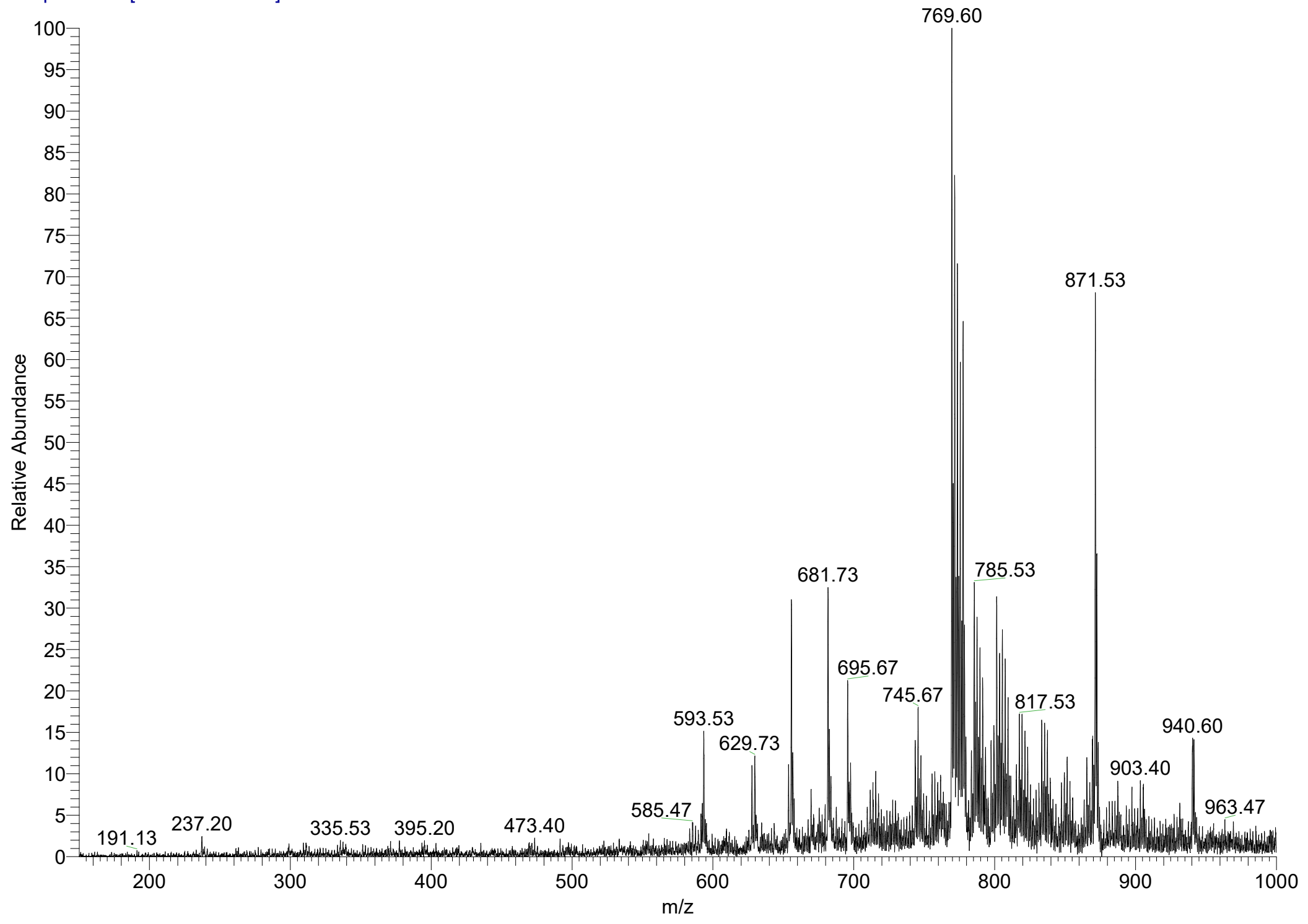
E:\dan_evans\RAW FILES\100%\CH8 08/16/18 14:16:06 CH8

CH8 #1-50 RT: 0.01-0.75 AV: 50 NL: 1.33E6
T: + p ESI ms [150.00-1000.00]



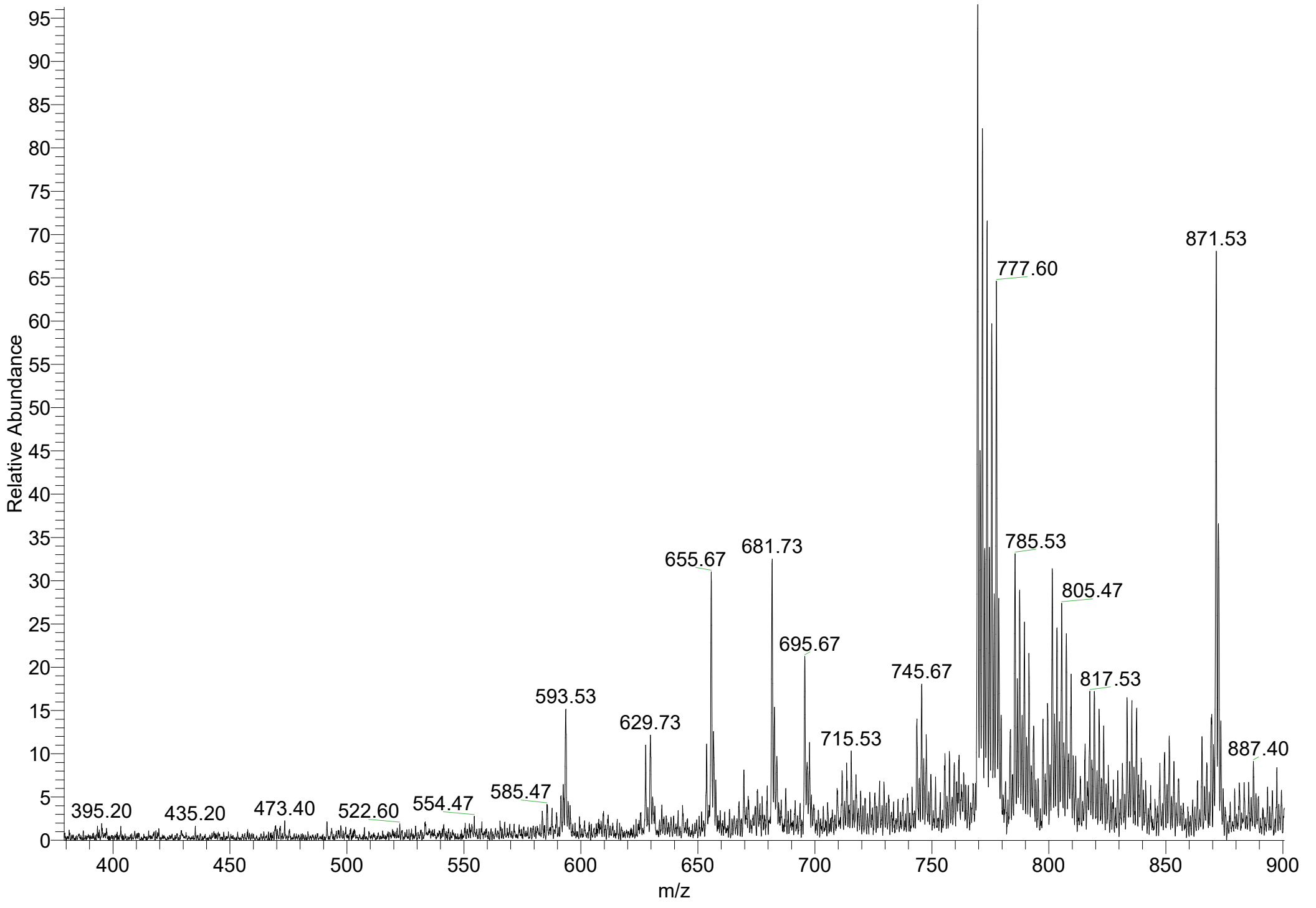
E:\dan_evans\RAW FILES\100%\CH9 08/16/18 14:21:16 CH9

CH9 #1-50 RT: 0.01-0.74 AV: 50 NL: 1.59E6
T: + p ESI ms [150.00-1000.00]



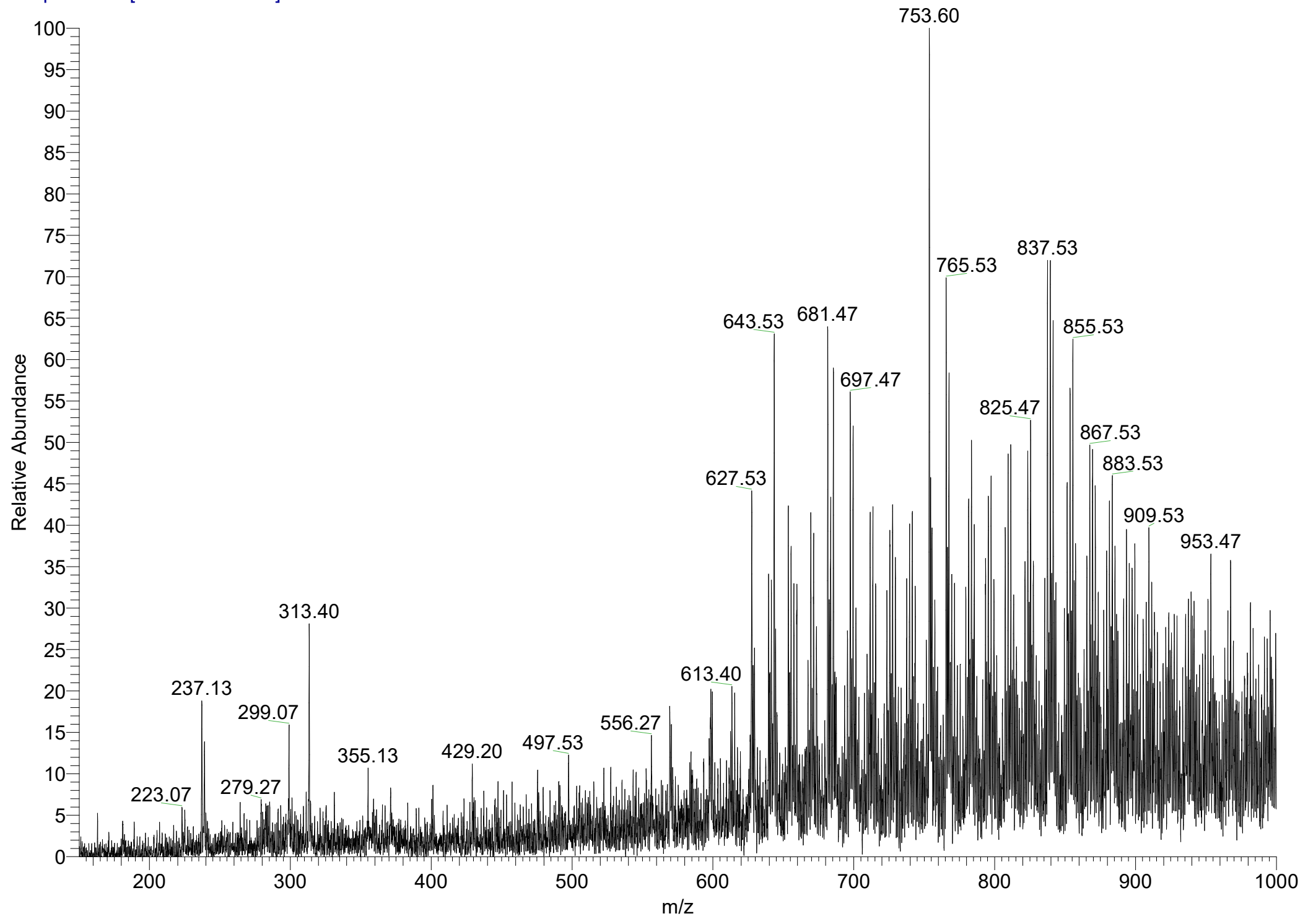
E:\dan_evans\RAW FILES\100%\CH9 08/16/18 14:21:16 CH9

CH9 #1-50 RT: 0.01-0.74 AV: 50 NL: 1.59E6
T: + p ESI ms [150.00-1000.00]



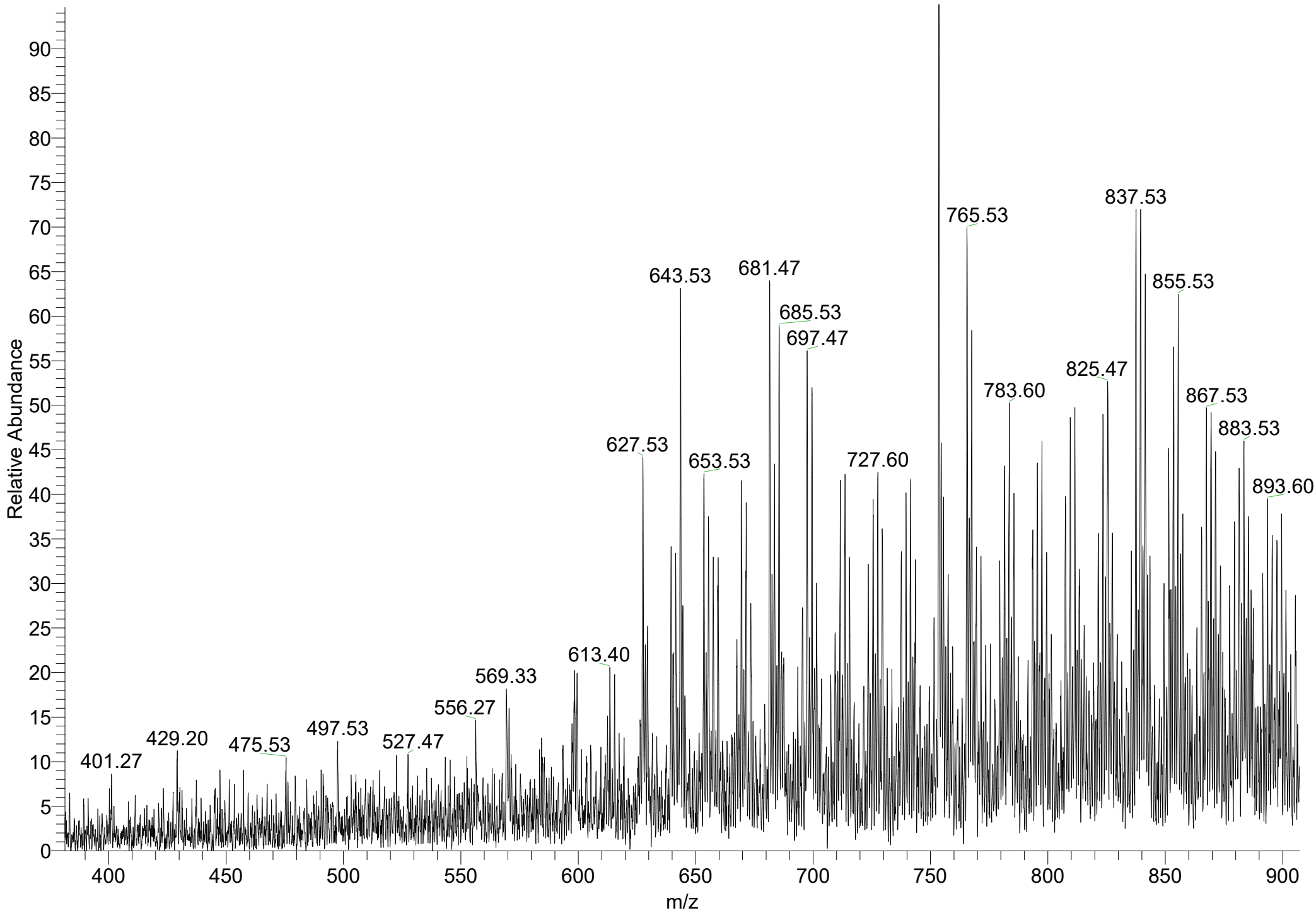
E:\dan_evans\RAW FILES\100%\CH10 08/16/18 14:29:32 CH10

CH10 #1-50 RT: 0.00-0.74 AV: 50 NL: 2.55E5
T: + p ESI ms [150.00-1000.00]



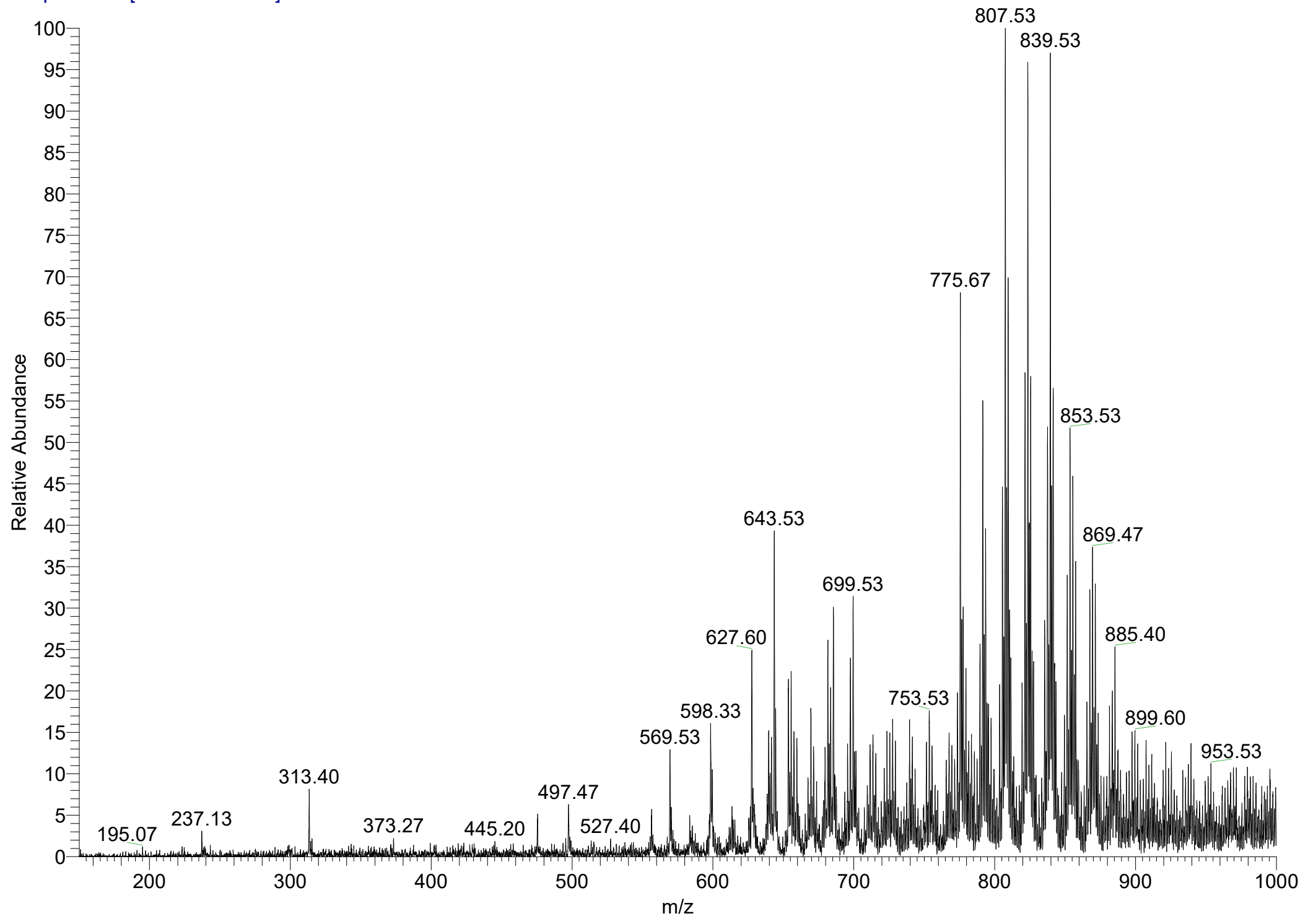
E:\dan_evans\RAW FILES\100%\CH10 08/16/18 14:29:32 CH10

CH10 #1-50 RT: 0.00-0.74 AV: 50 NL: 2.55E5
T: + p ESI ms [150.00-1000.00]



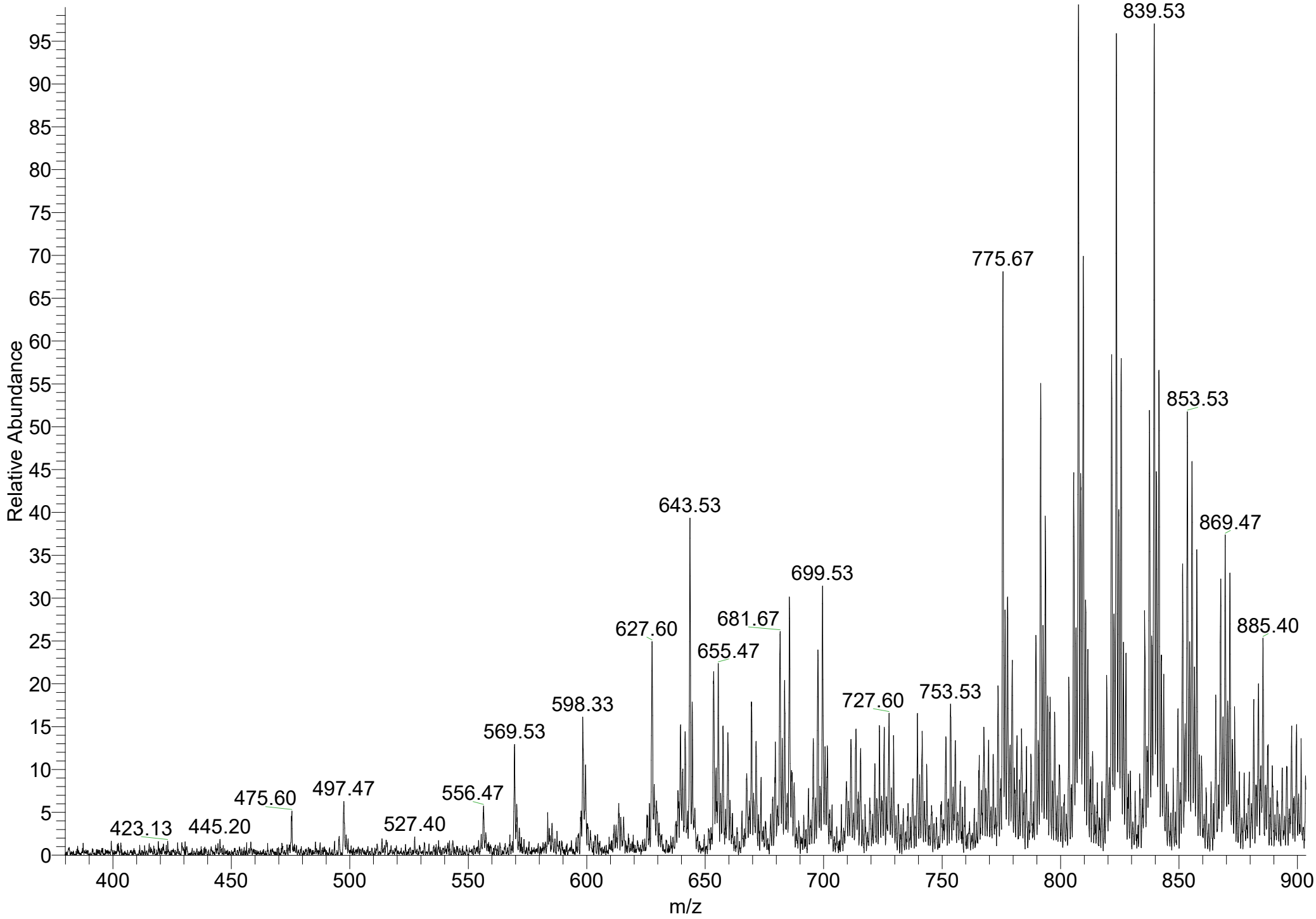
E:\dan_evans\RAW FILES\100%\S1 08/16/18 14:46:51 S1

S1 #1-50 RT: 0.01-0.75 AV: 50 NL: 8.83E5
T: + p ESI ms [150.00-1000.00]



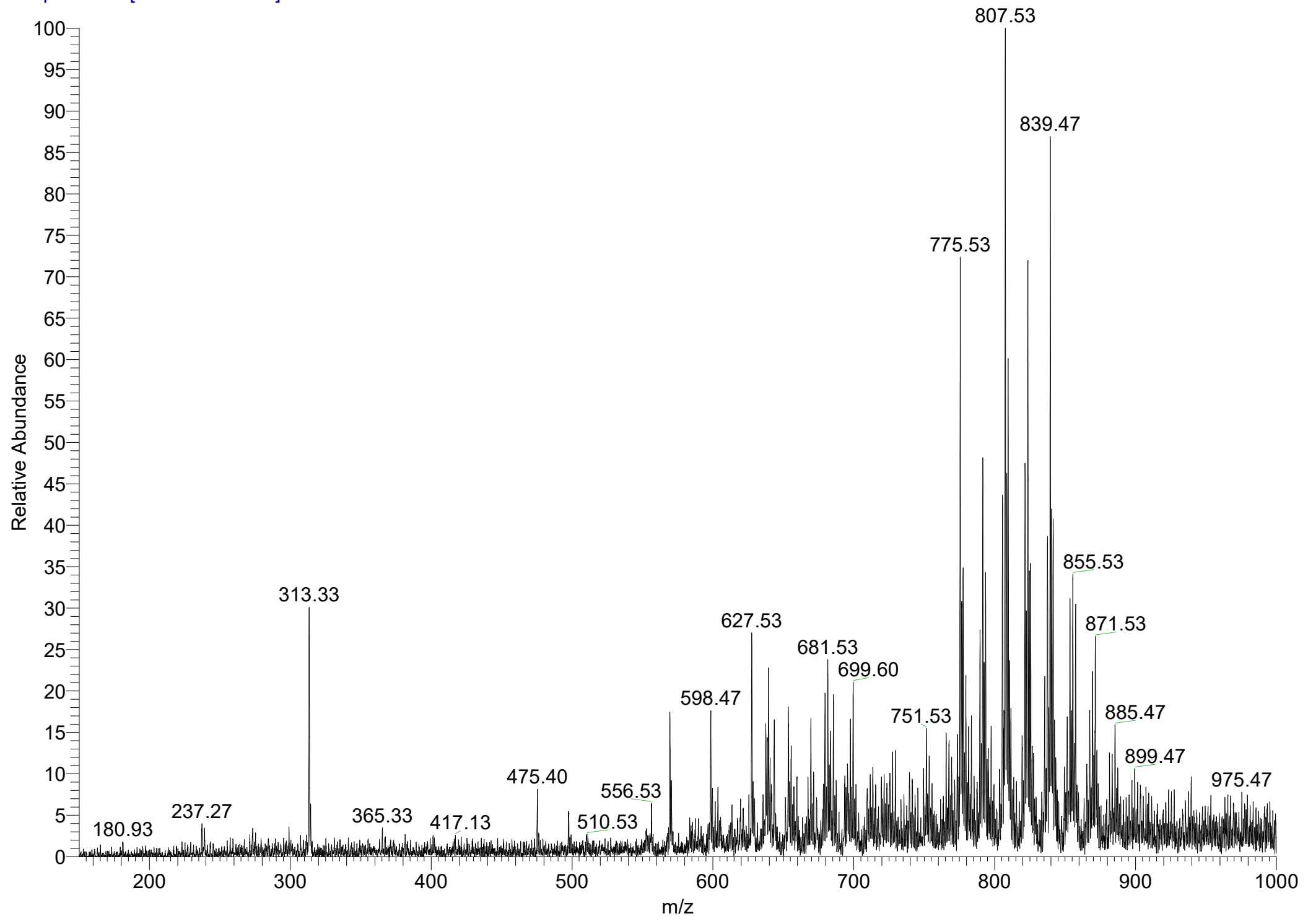
E:\dan_evans\RAW FILES\100%\S1 08/16/18 14:46:51 S1

S1 #1-50 RT: 0.01-0.75 AV: 50 NL: 8.83E5
T: + p ESI ms [150.00-1000.00]



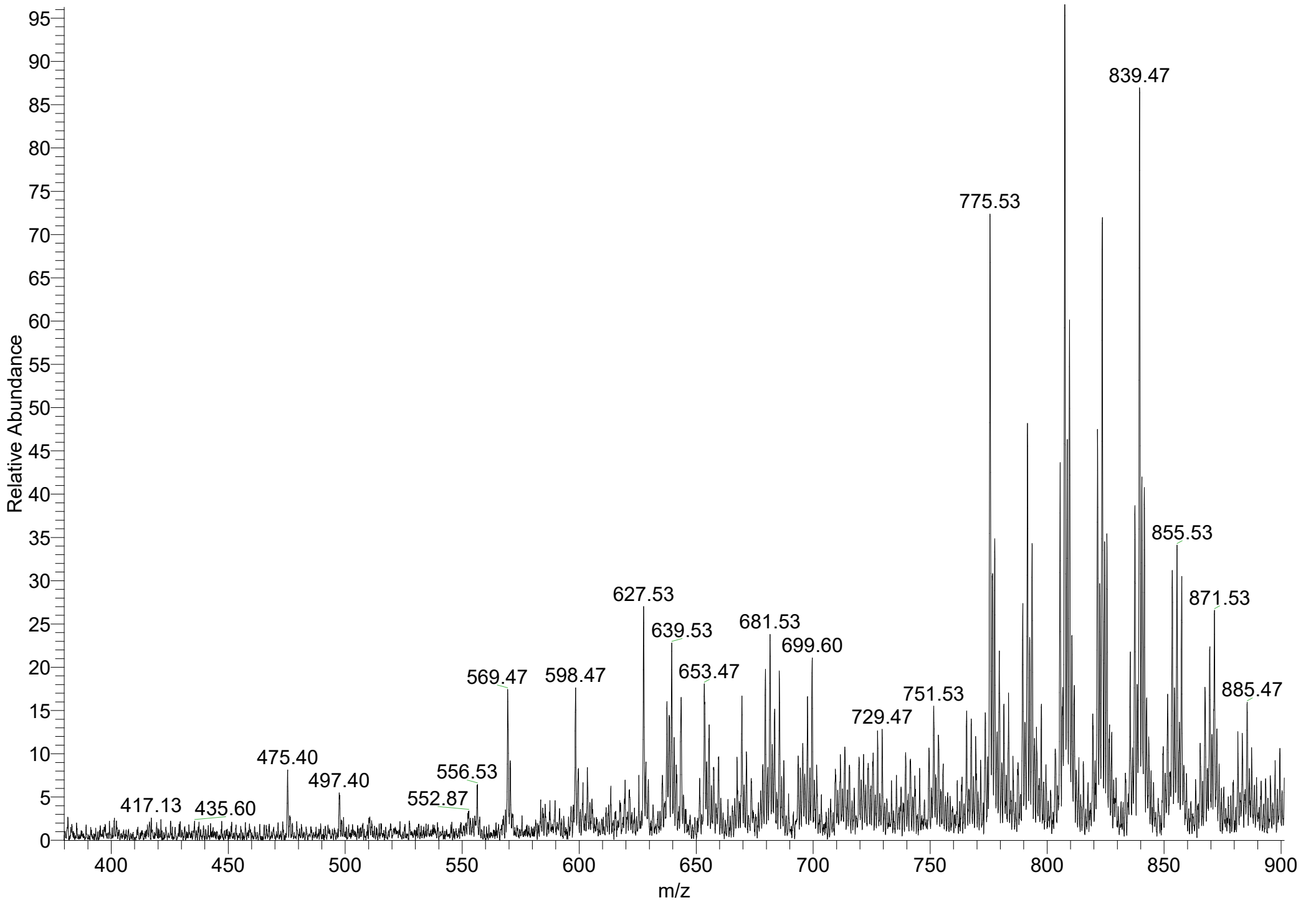
E:\dan_evans\RAW FILES\100%\S2 08/16/18 14:51:59 S2

S2 #1-50 RT: 0.00-0.74 AV: 50 NL: 5.99E5
T: + p ESI ms [150.00-1000.00]



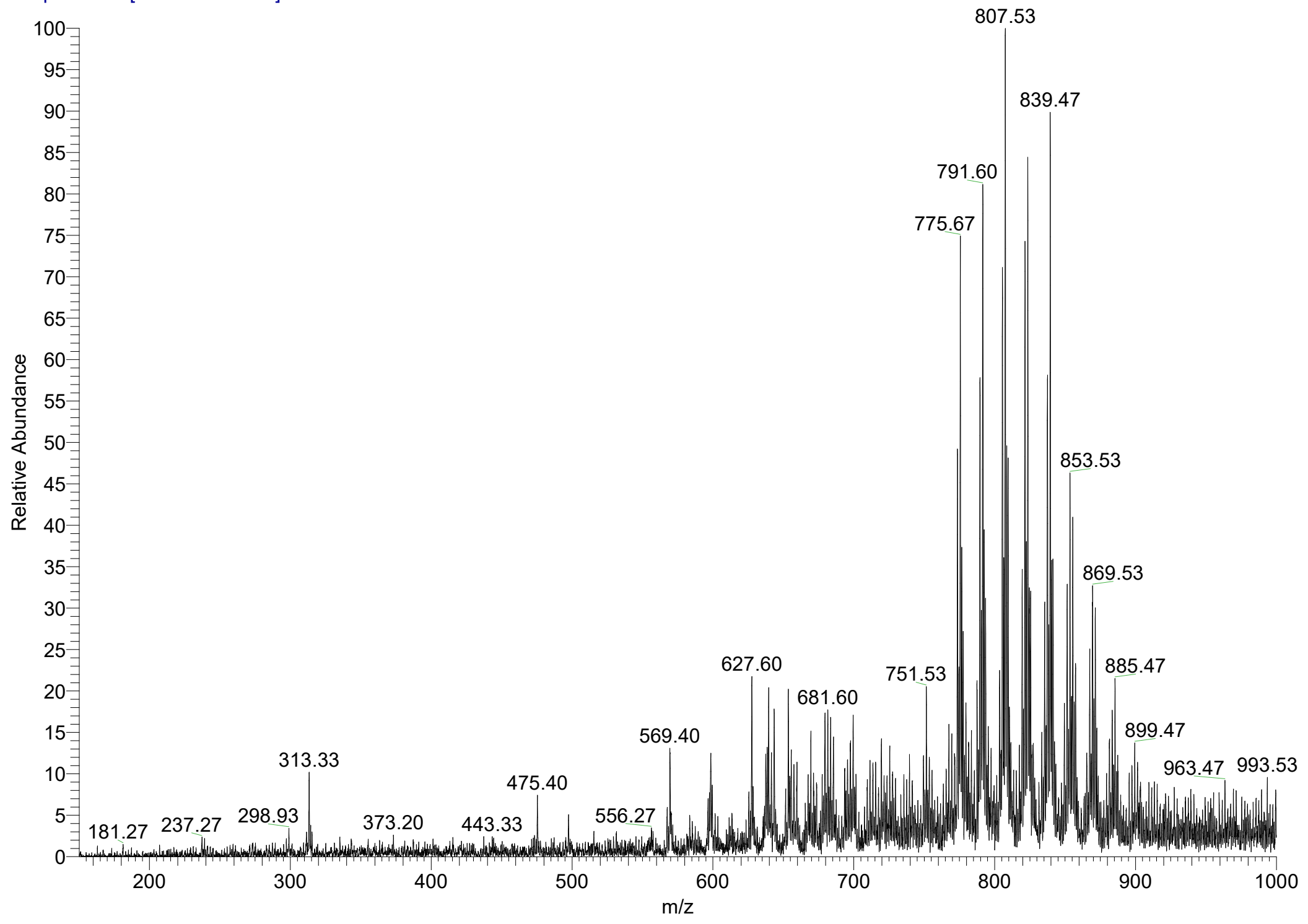
E:\dan_evans\RAW FILES\100%\S2 08/16/18 14:51:59 S2

S2 #1-50 RT: 0.00-0.74 AV: 50 NL: 5.99E5
T: + p ESI ms [150.00-1000.00]



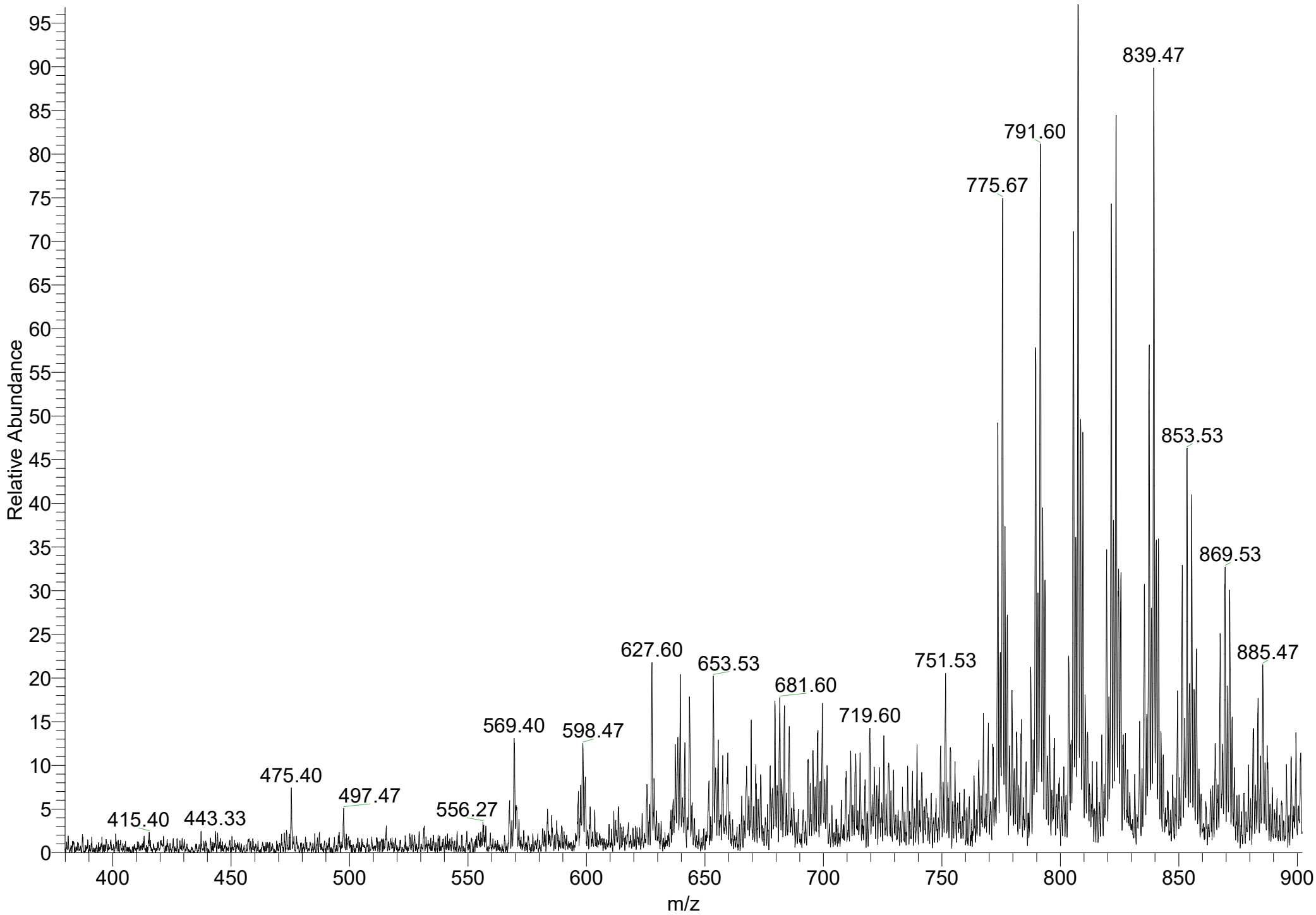
E:\dan_evans\RAW FILES\100%\S3 08/16/18 14:56:45 S3

S3 #1-50 RT: 0.01-0.74 AV: 50 NL: 9.38E5
T: + p ESI ms [150.00-1000.00]



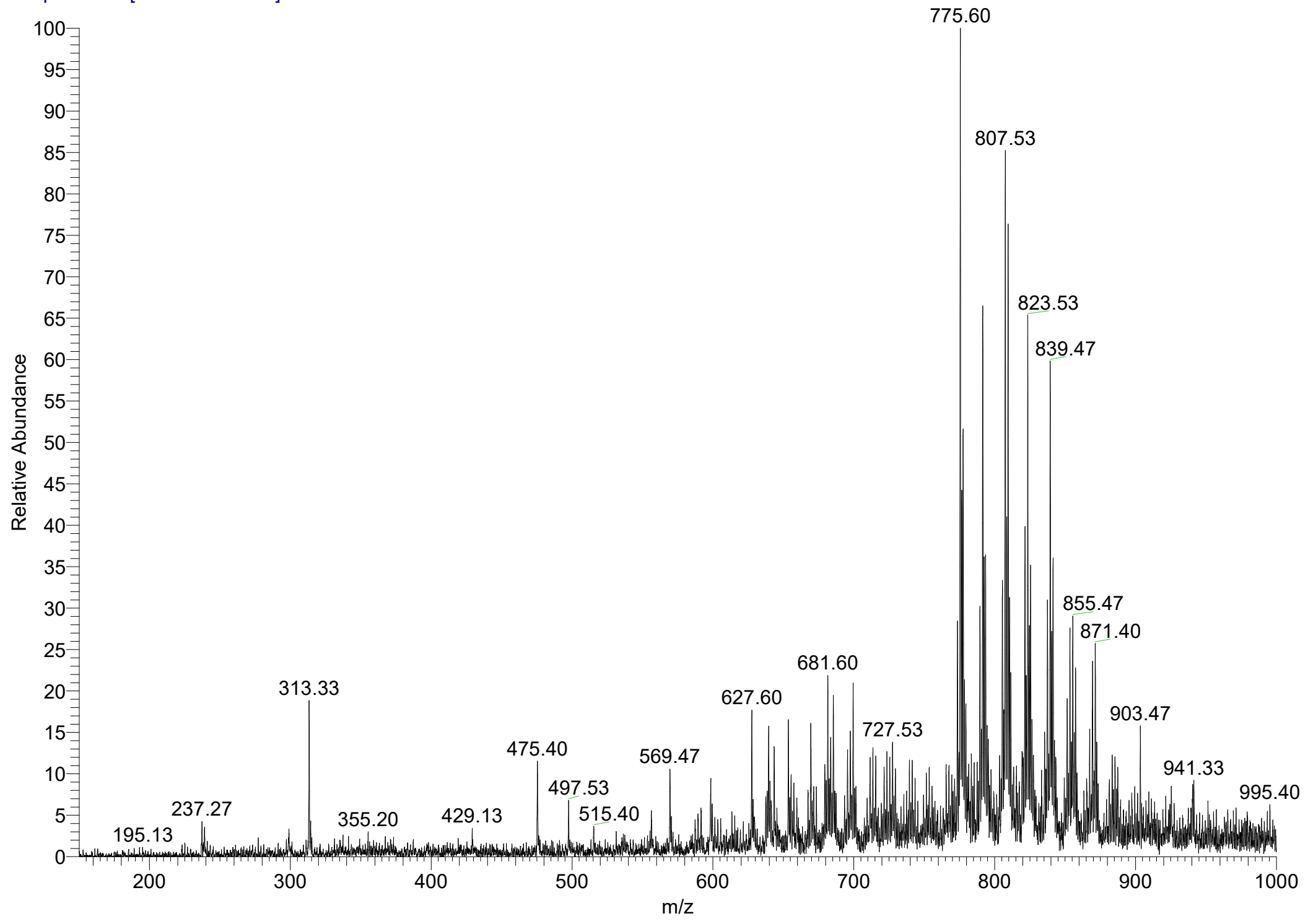
E:\dan_evans\RAW FILES\100%\S3 08/16/18 14:56:45 S3

S3 #1-50 RT: 0.01-0.74 AV: 50 NL: 9.38E5
T: + p ESI ms [150.00-1000.00]



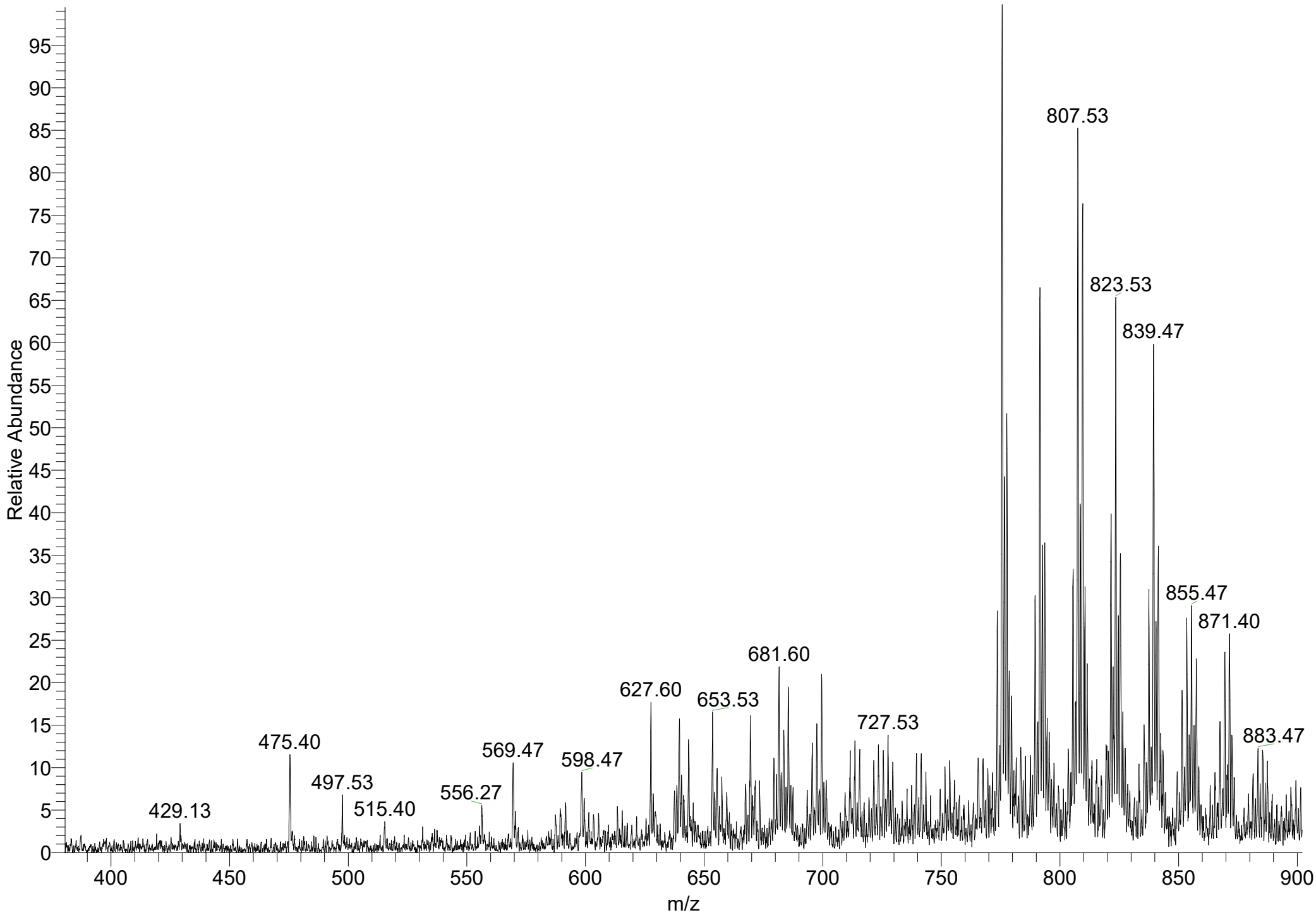
E:\dan_evans\RAW FILES\100%\S4 08/16/18 15:01:35 S4

S4 #1-50 RT: 0.01-0.75 AV: 50 NL: 1.19E6
T: + p ESI ms [150.00-1000.00]



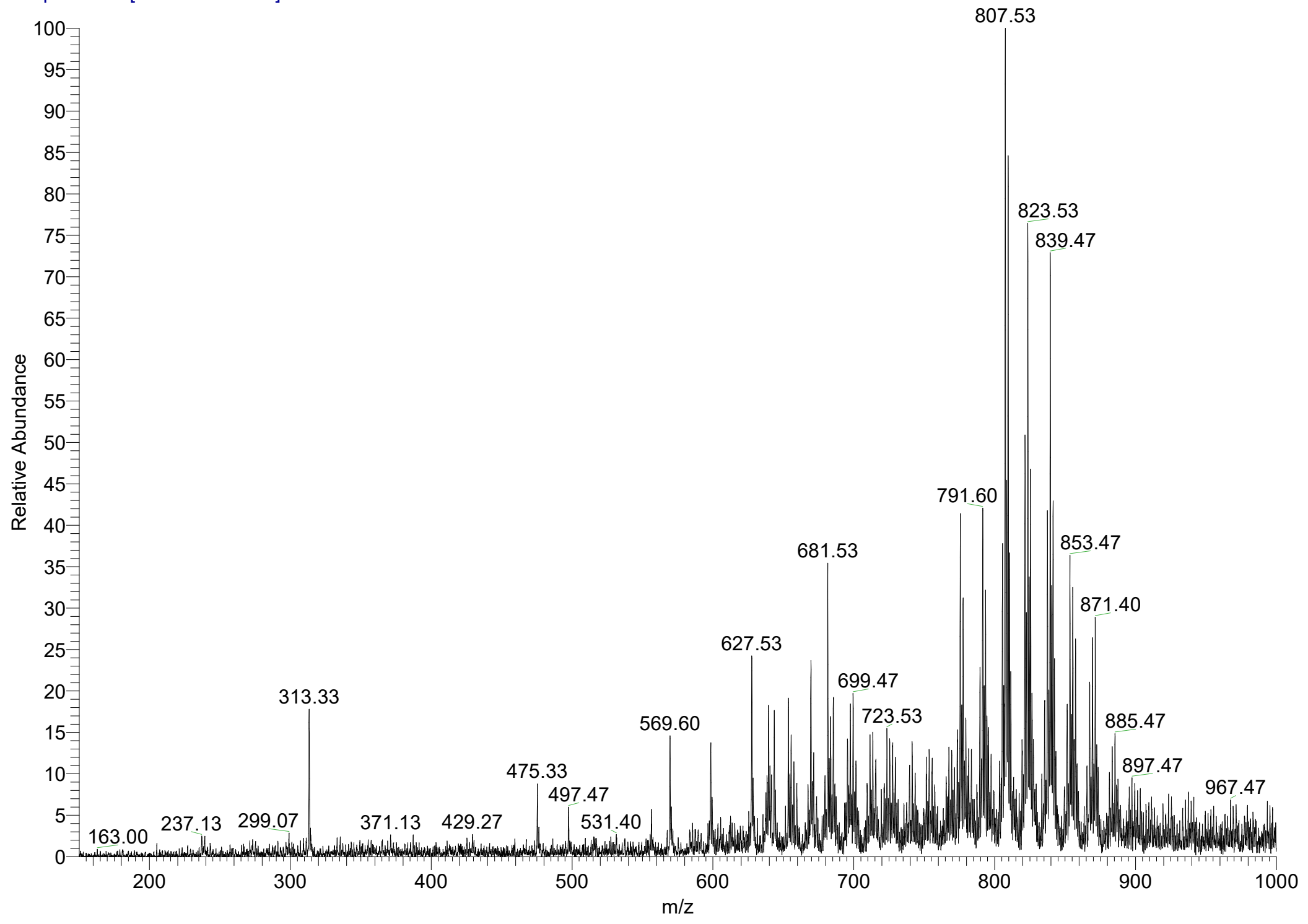
E:\dan_evans\RAW FILES\100%\S4 08/16/18 15:01:35 S4

S4 #1-50 RT: 0.01-0.75 AV: 50 NL: 1.19E6
T: + p ESI ms [150.00-1000.00]



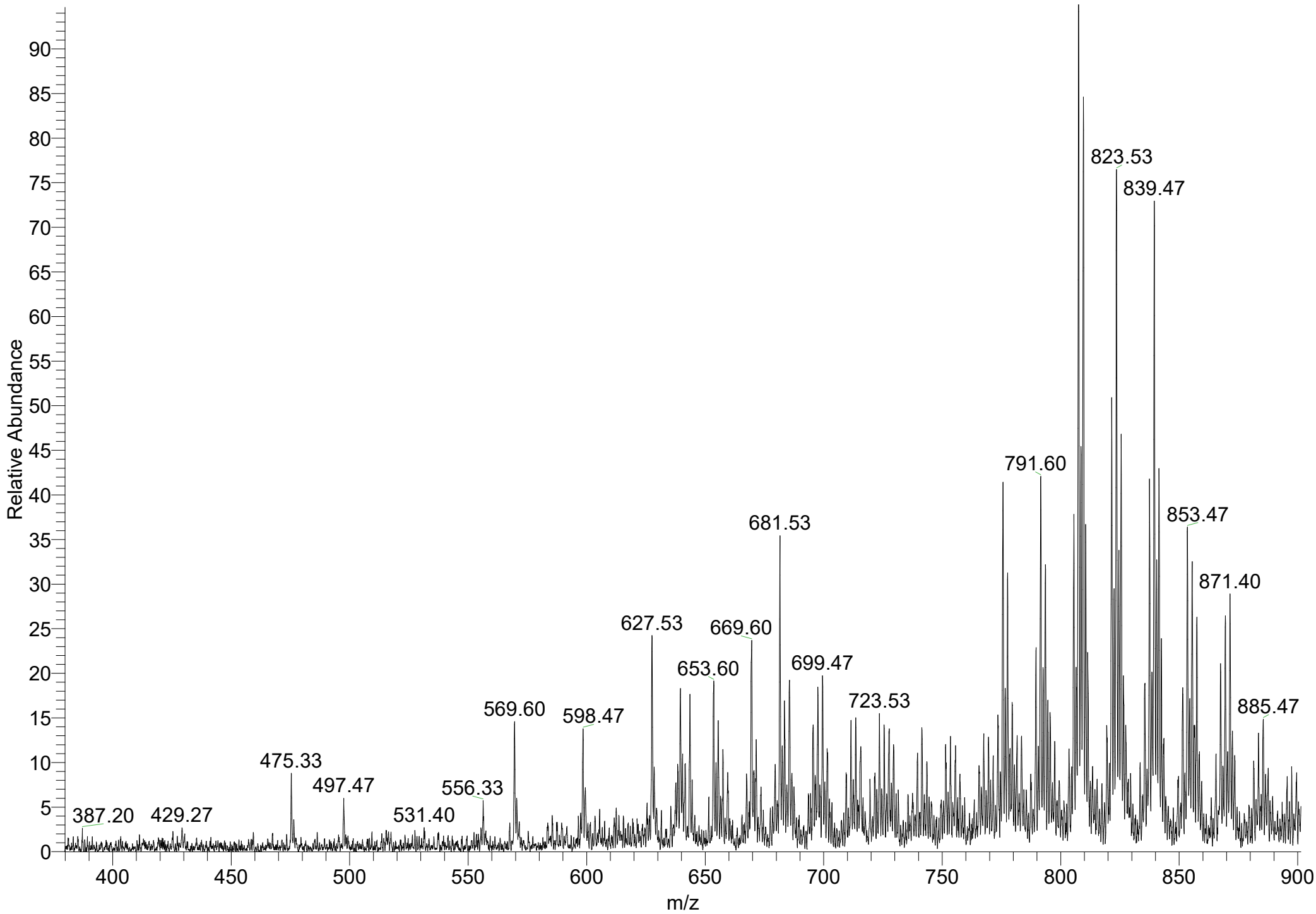
E:\dan_evans\RAW FILES\100%\S5 08/16/18 15:06:39 S5

S5 #1-50 RT: 0.01-0.75 AV: 50 NL: 9.50E5
T: + p ESI ms [150.00-1000.00]



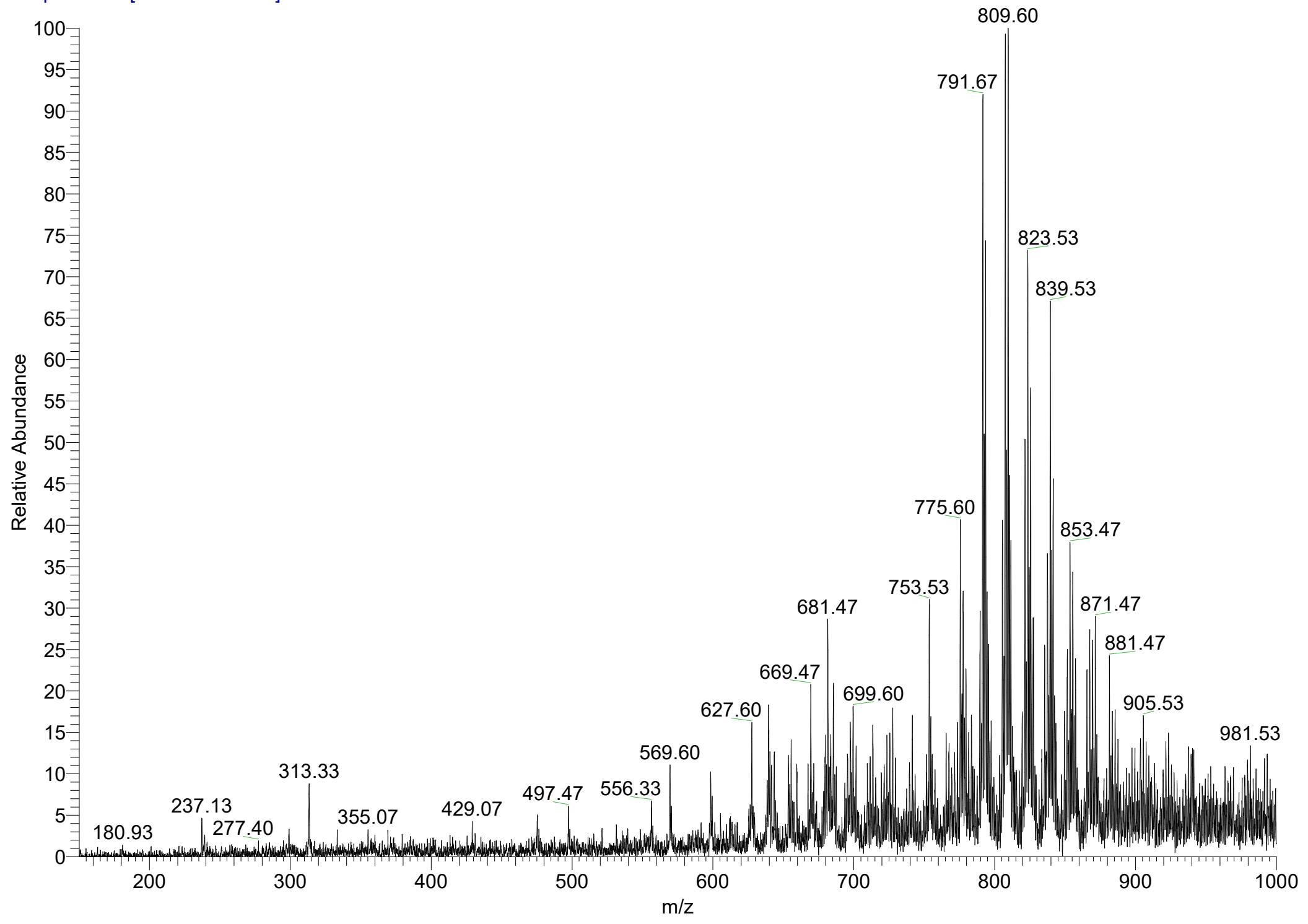
E:\dan_evans\RAW FILES\100%\S5 08/16/18 15:06:39 S5

S5 #1-50 RT: 0.01-0.75 AV: 50 NL: 9.50E5
T: + p ESI ms [150.00-1000.00]



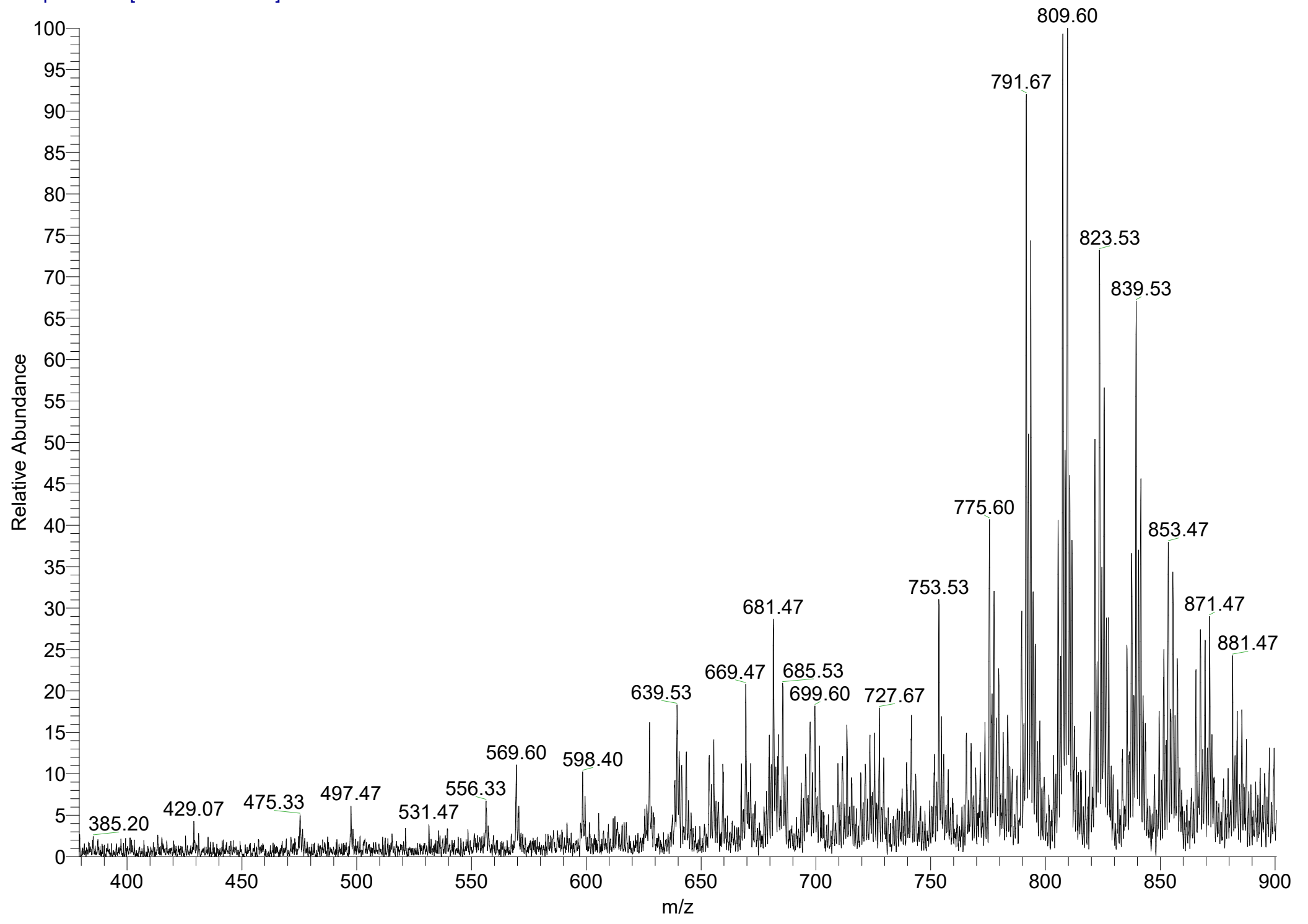
E:\dan_evans\RAW FILES\100%\S6 08/16/18 15:11:09 S6

S6 #1-50 RT: 0.01-0.75 AV: 50 NL: 8.62E5
T: + p ESI ms [150.00-1000.00]



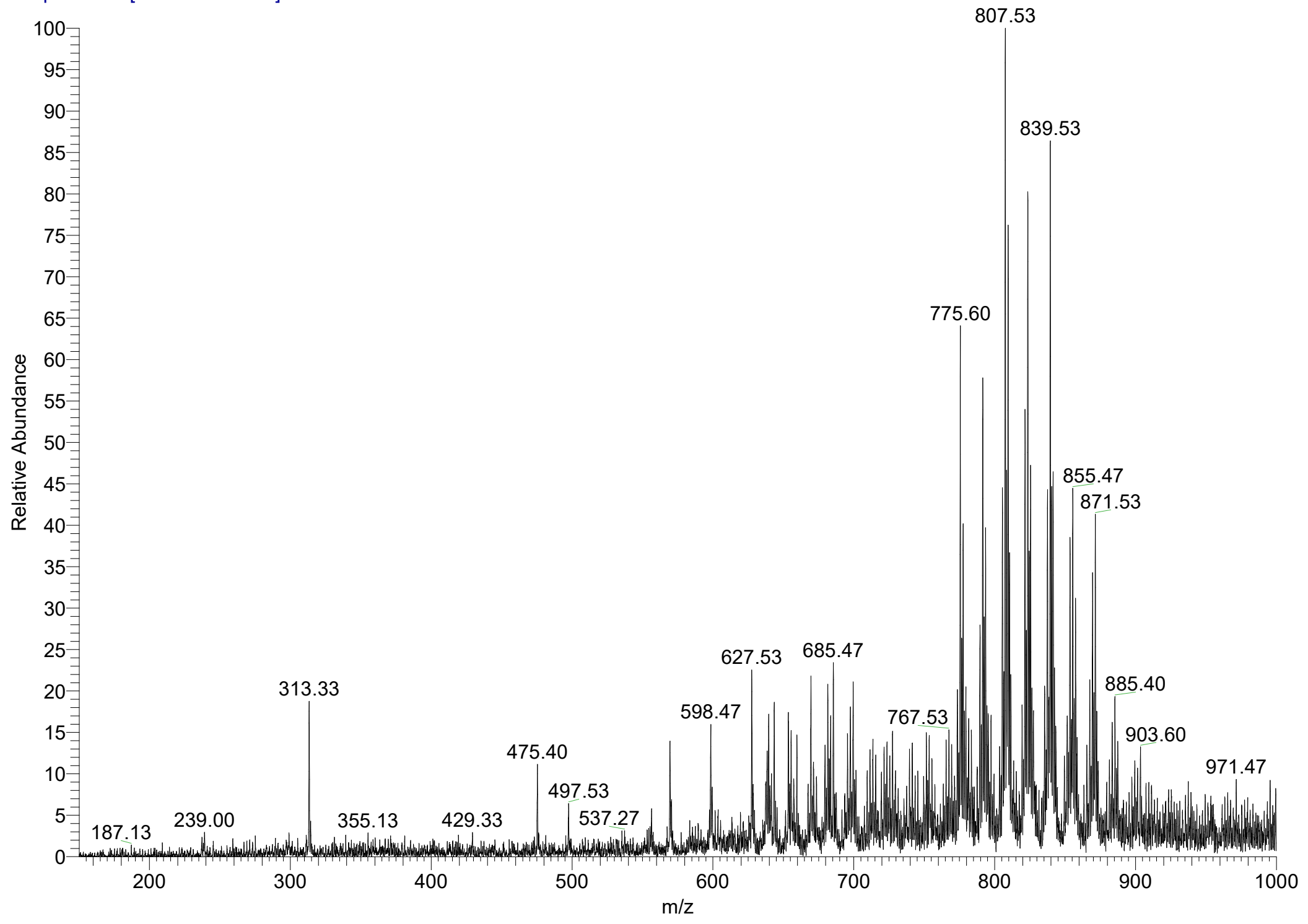
E:\dan_evans\RAW FILES\100%\S6 08/16/18 15:11:09 S6

S6 #1-50 RT: 0.01-0.75 AV: 50 NL: 8.62E5
T: + p ESI ms [150.00-1000.00]



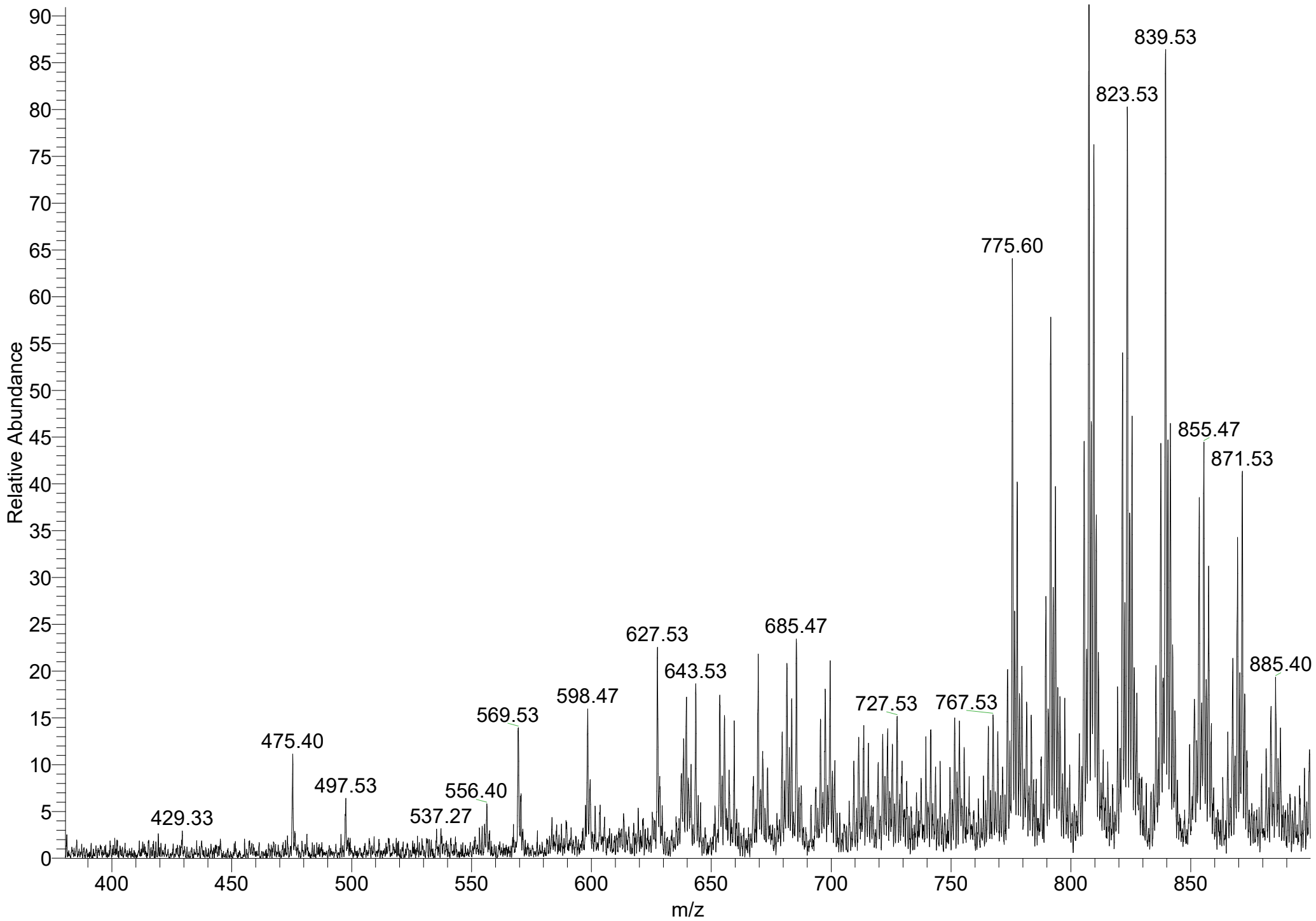
E:\dan_evans\RAW FILES\100%\S7 08/16/18 15:15:28 S7

S7 #1-50 RT: 0.01-0.74 AV: 50 NL: 8.18E5
T: + p ESI ms [150.00-1000.00]



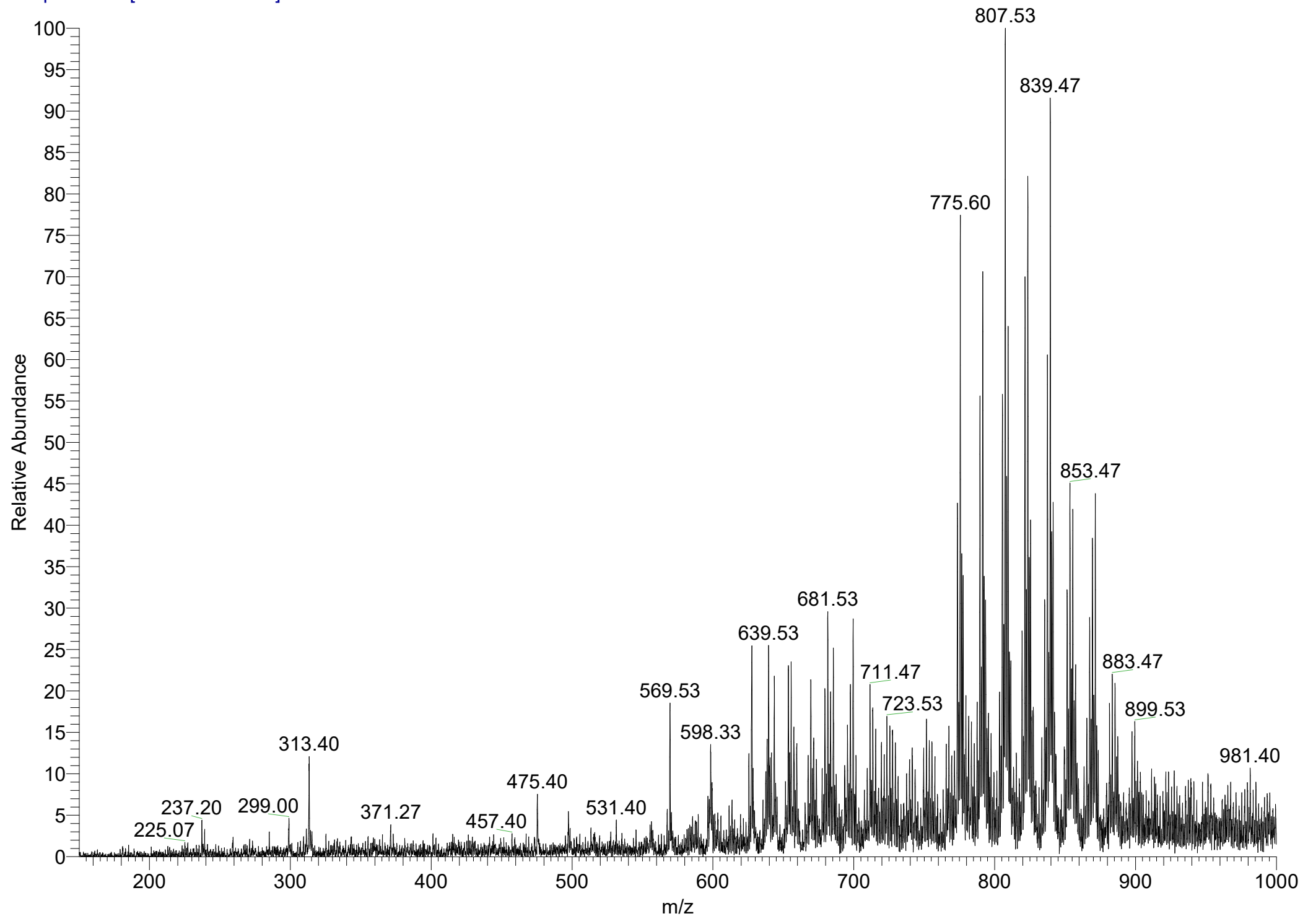
E:\dan_evans\RAW FILES\100%\S7 08/16/18 15:15:28 S7

S7 #1-50 RT: 0.01-0.74 AV: 50 NL: 8.18E5
T: + p ESI ms [150.00-1000.00]



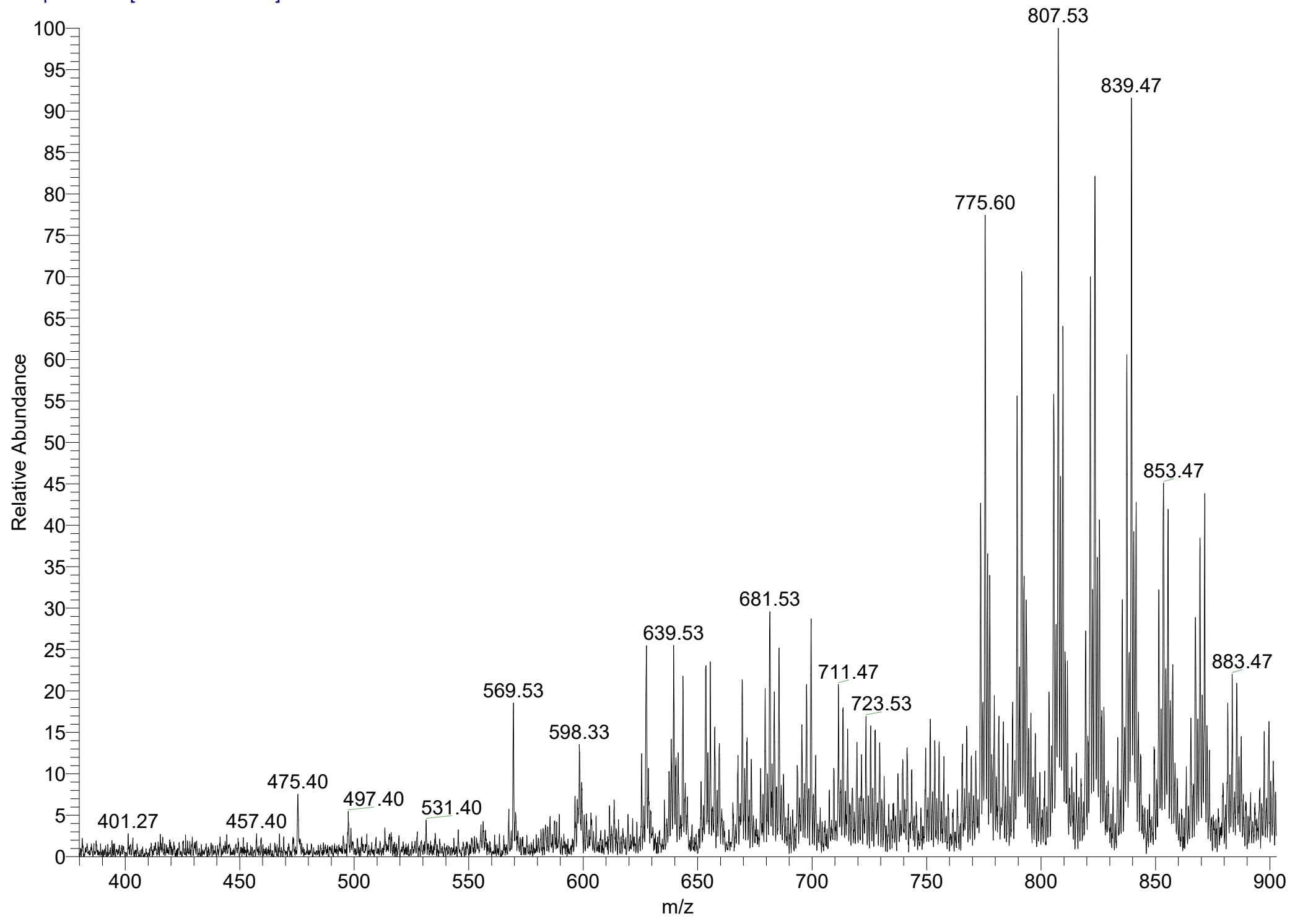
E:\dan_evans\RAW FILES\100%\S8 08/16/18 15:20:05 S8

S8 #1-50 RT: 0.01-0.74 AV: 50 NL: 7.94E5
T: + p ESI ms [150.00-1000.00]



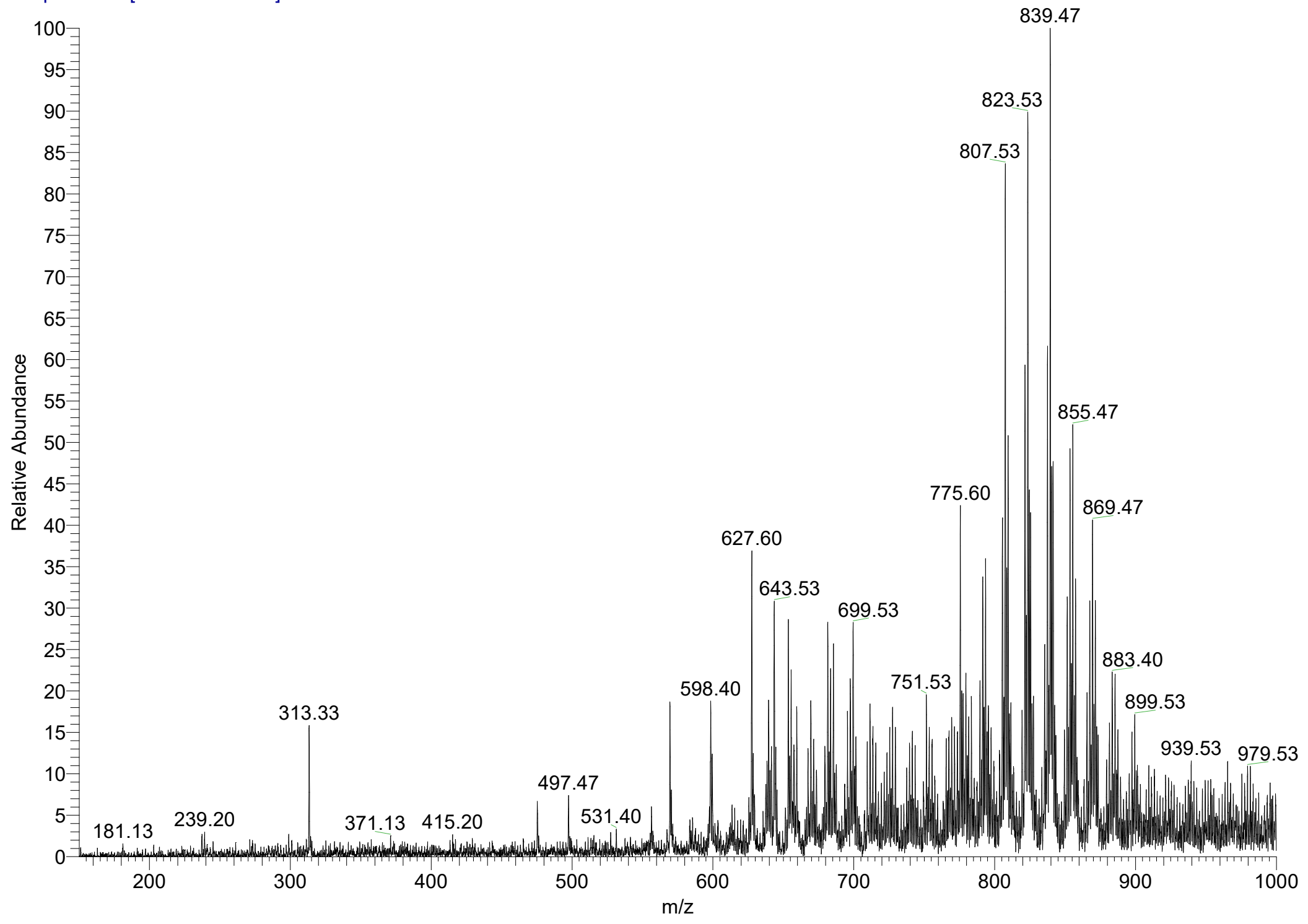
E:\dan_evans\RAW FILES\100%\S8 08/16/18 15:20:05 S8

S8 #1-50 RT: 0.01-0.74 AV: 50 NL: 7.94E5
T: + p ESI ms [150.00-1000.00]



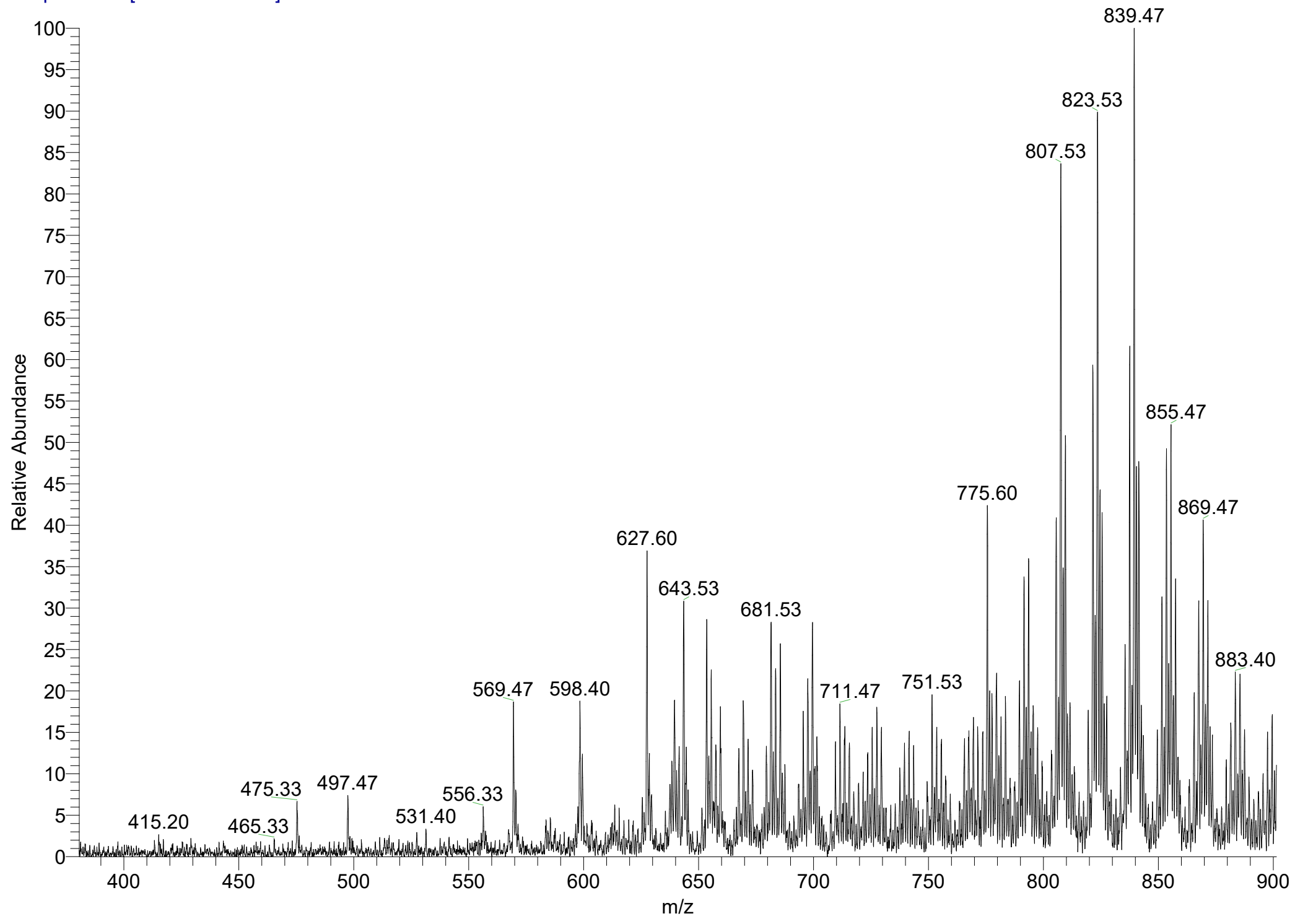
E:\dan_evans\RAW FILES\100%\S9 08/16/18 15:25:28 S9

S9 #1-50 RT: 0.01-0.75 AV: 50 NL: 7.68E5
T: + p ESI ms [150.00-1000.00]



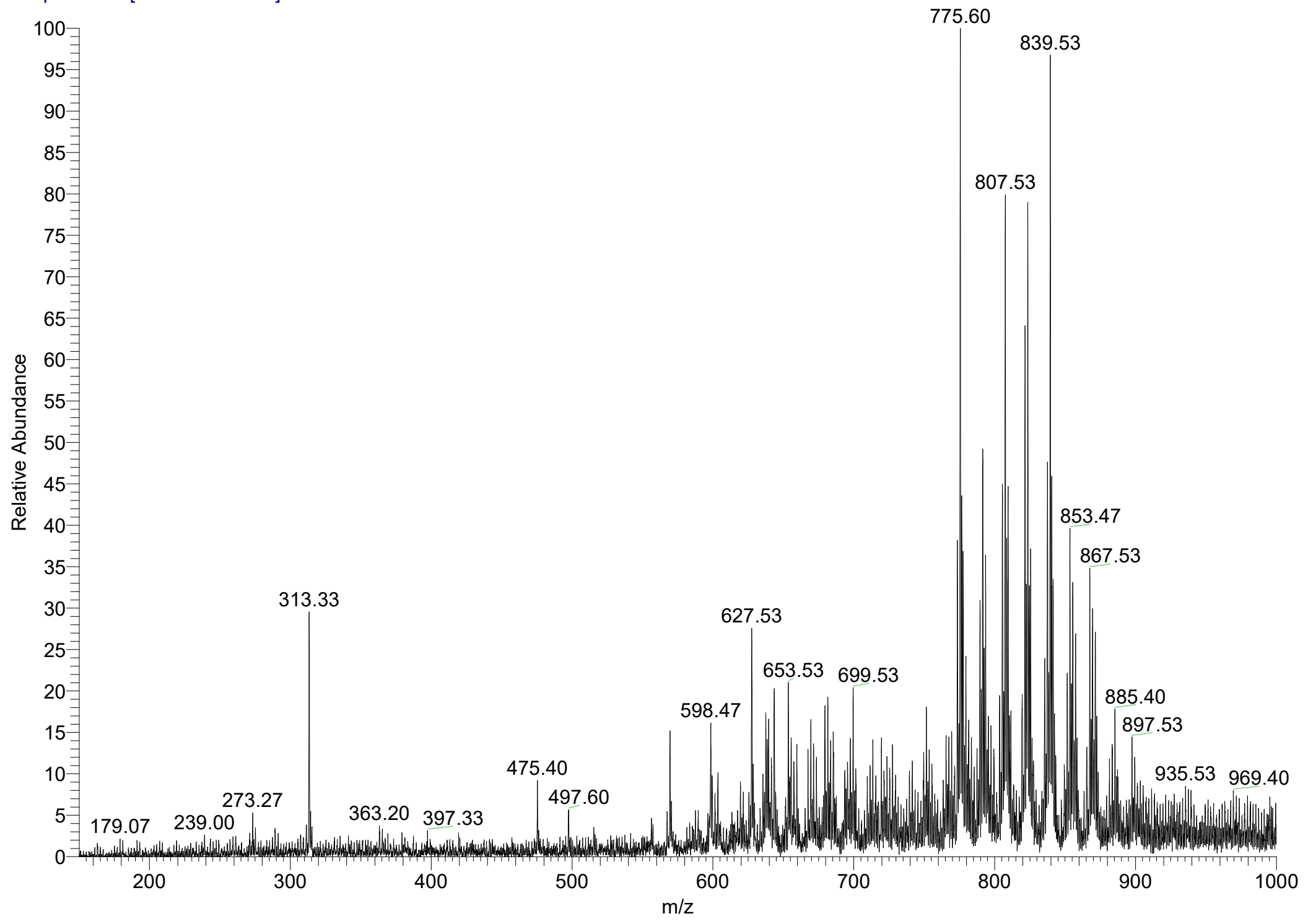
E:\dan_evans\RAW FILES\100%\S9 08/16/18 15:25:28 S9

S9 #1-50 RT: 0.01-0.75 AV: 50 NL: 7.68E5
T: + p ESI ms [150.00-1000.00]



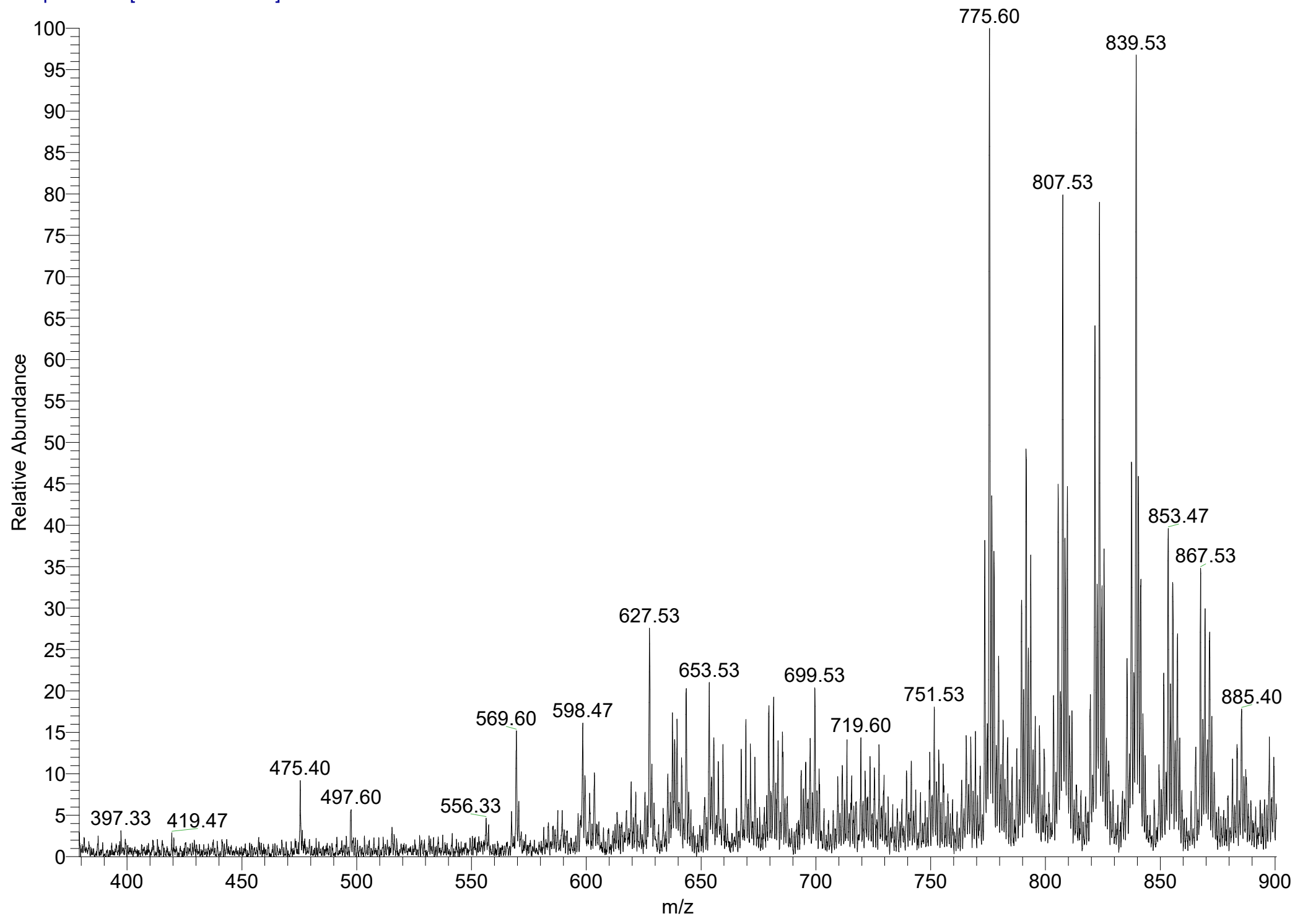
E:\dan_evans\RAW FILES\100%\S10 08/16/18 15:32:02 S10

S10 #1-50 RT: 0.00-0.74 AV: 50 NL: 5.21E5
T: + p ESI ms [150.00-1000.00]



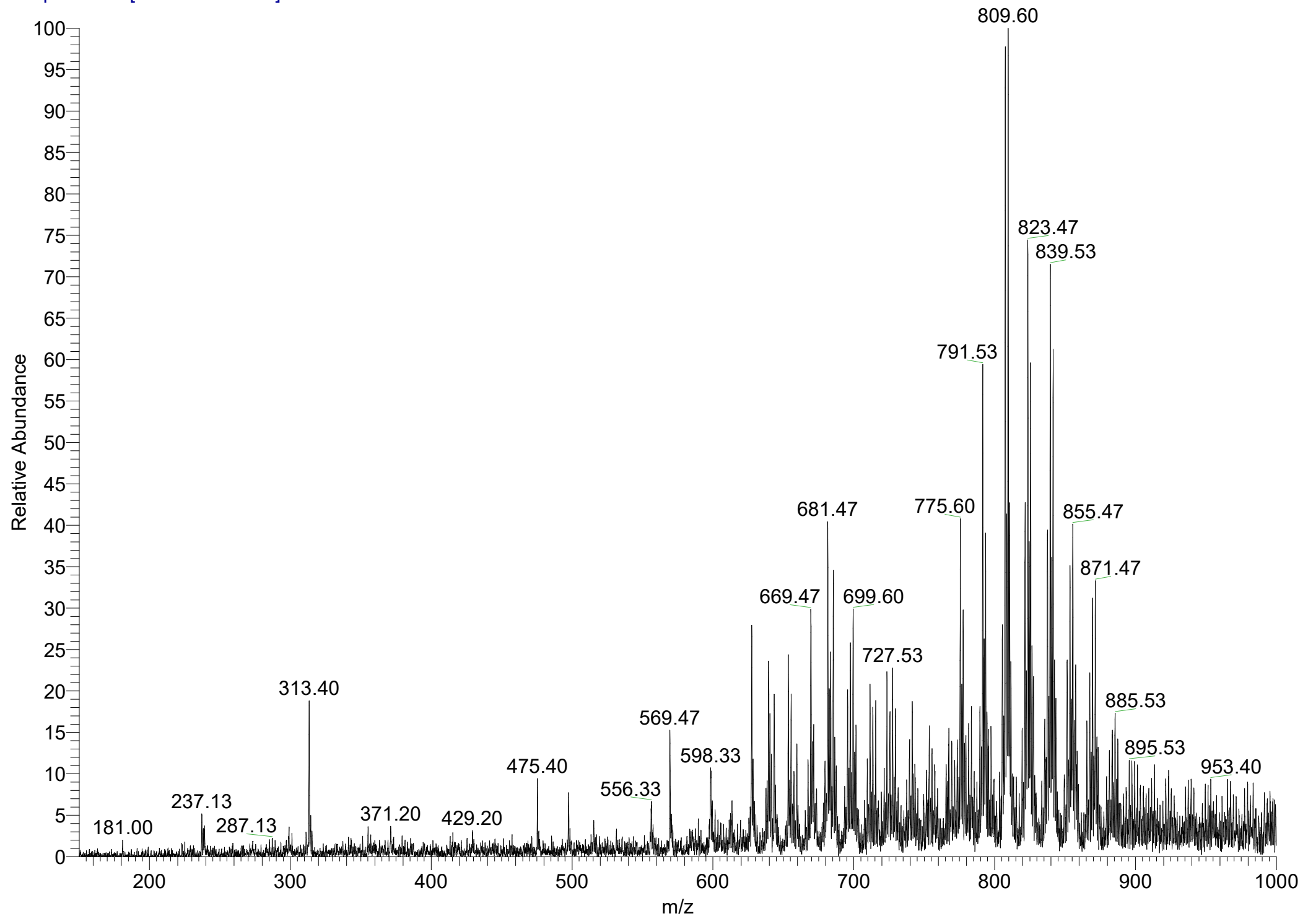
E:\dan_evans\RAW FILES\100%\S10 08/16/18 15:32:02 S10

S10 #1-50 RT: 0.00-0.74 AV: 50 NL: 5.21E5
T: + p ESI ms [150.00-1000.00]



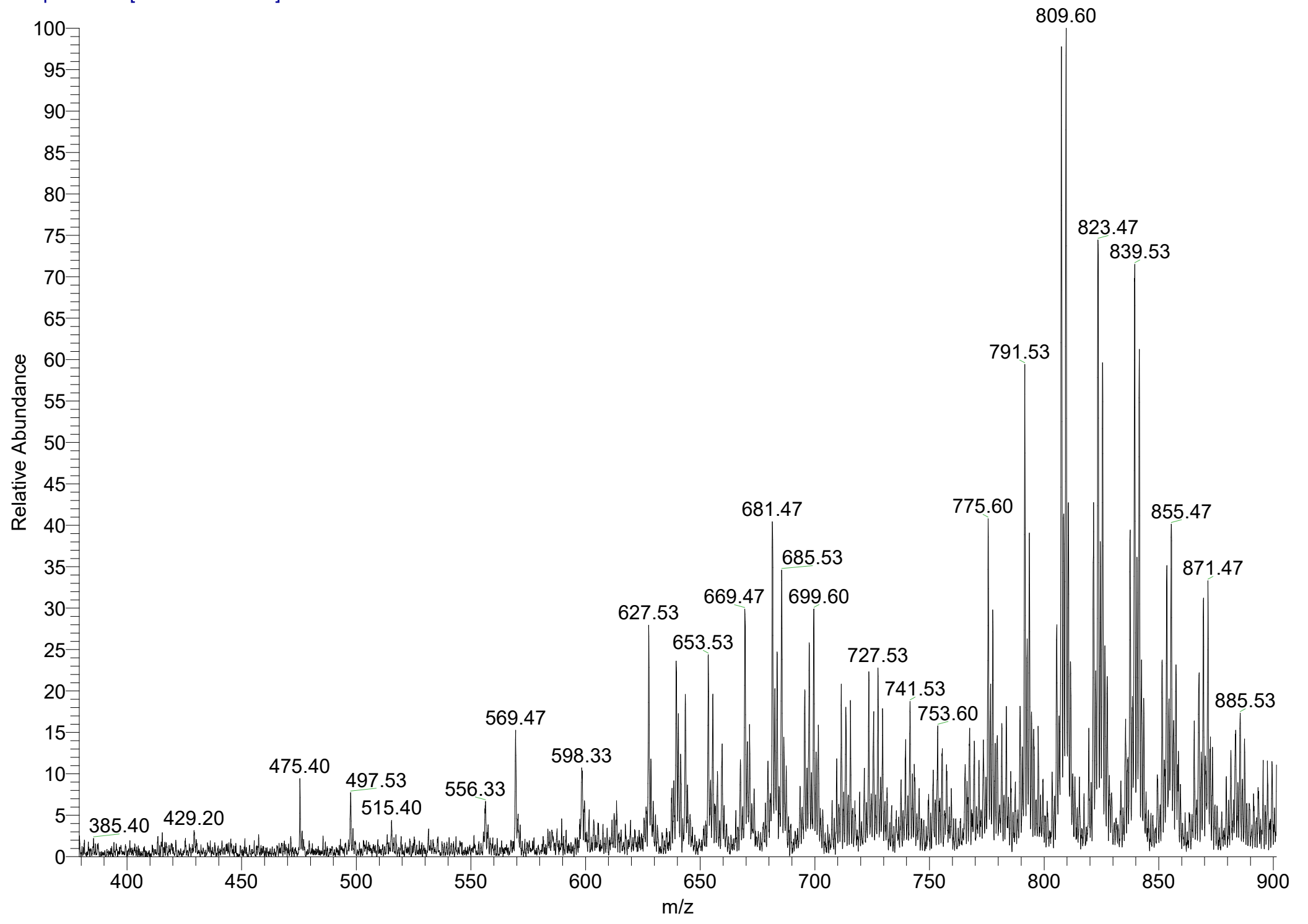
E:\dan_evans\RAW FILES\100%\S11 08/16/18 15:40:55 S11

S11 #1-50 RT: 0.01-0.74 AV: 50 NL: 8.25E5
T: + p ESI ms [150.00-1000.00]



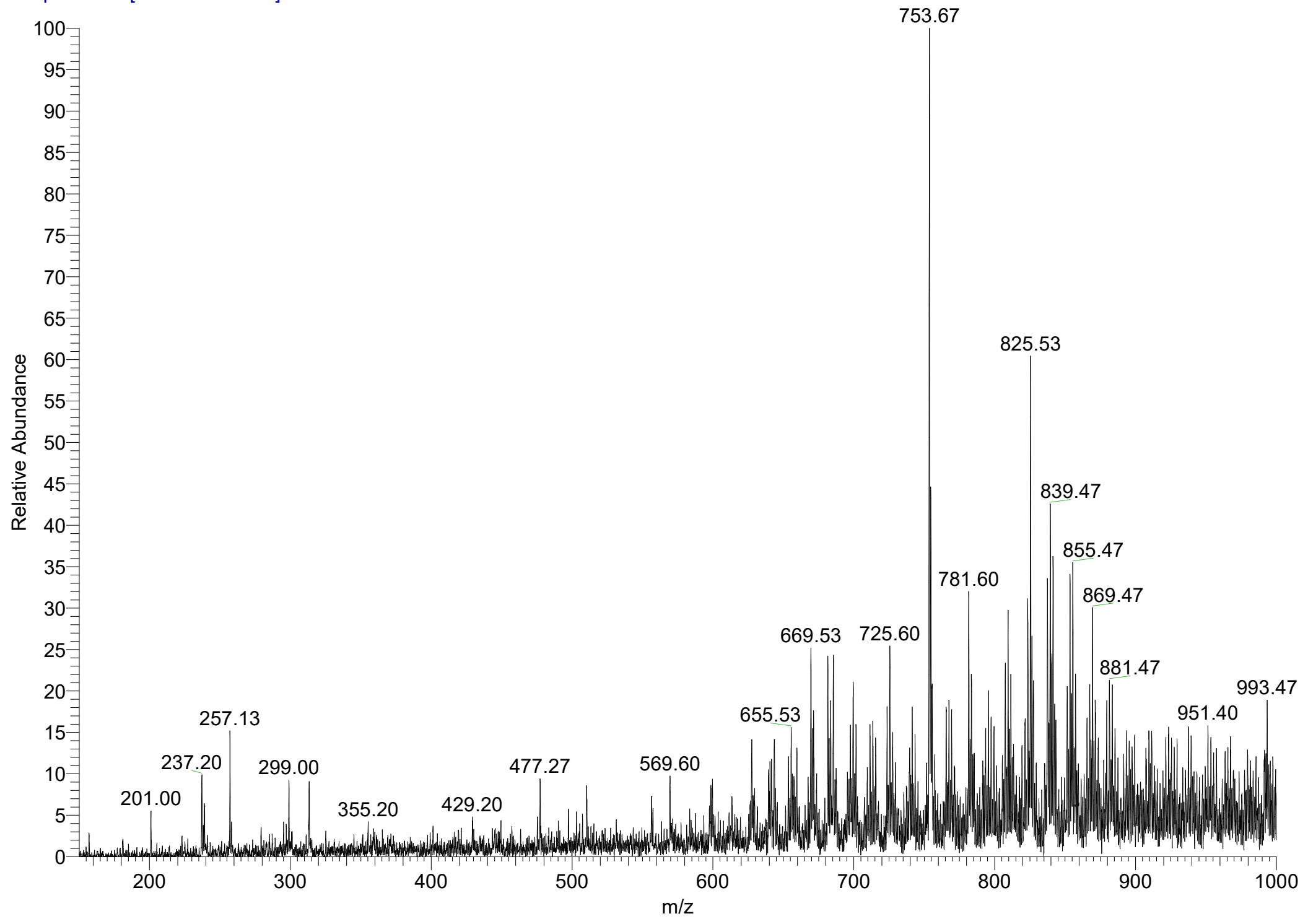
E:\dan_evans\RAW FILES\100%\S11 08/16/18 15:40:55 S11

S11 #1-50 RT: 0.01-0.74 AV: 50 NL: 8.25E5
T: + p ESI ms [150.00-1000.00]



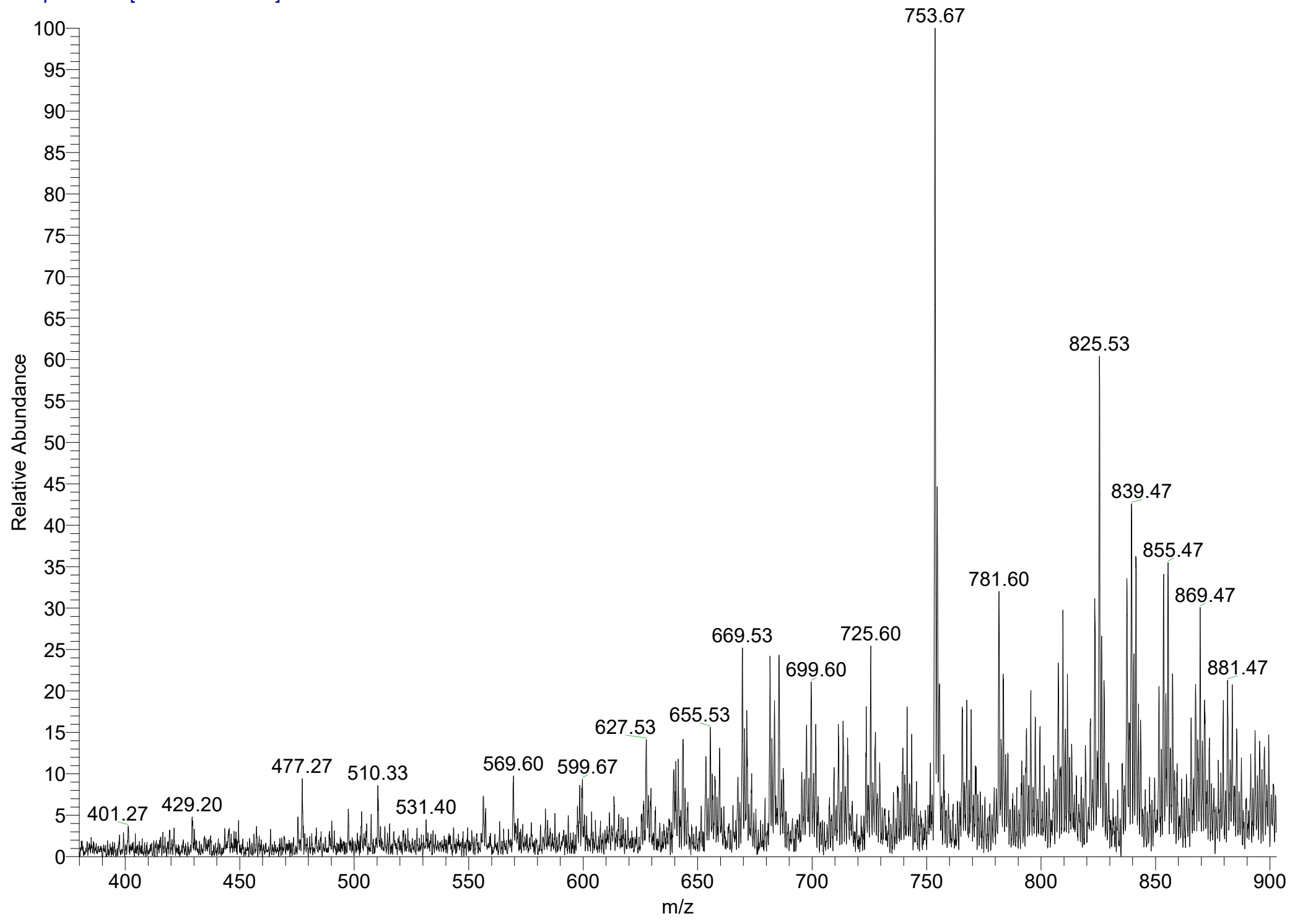
E:\dan_evans\RAW FILES\100%\S12 08/16/18 15:46:27 S12

S12 #1-50 RT: 0.00-0.74 AV: 50 NL: 6.82E5
T: + p ESI ms [150.00-1000.00]



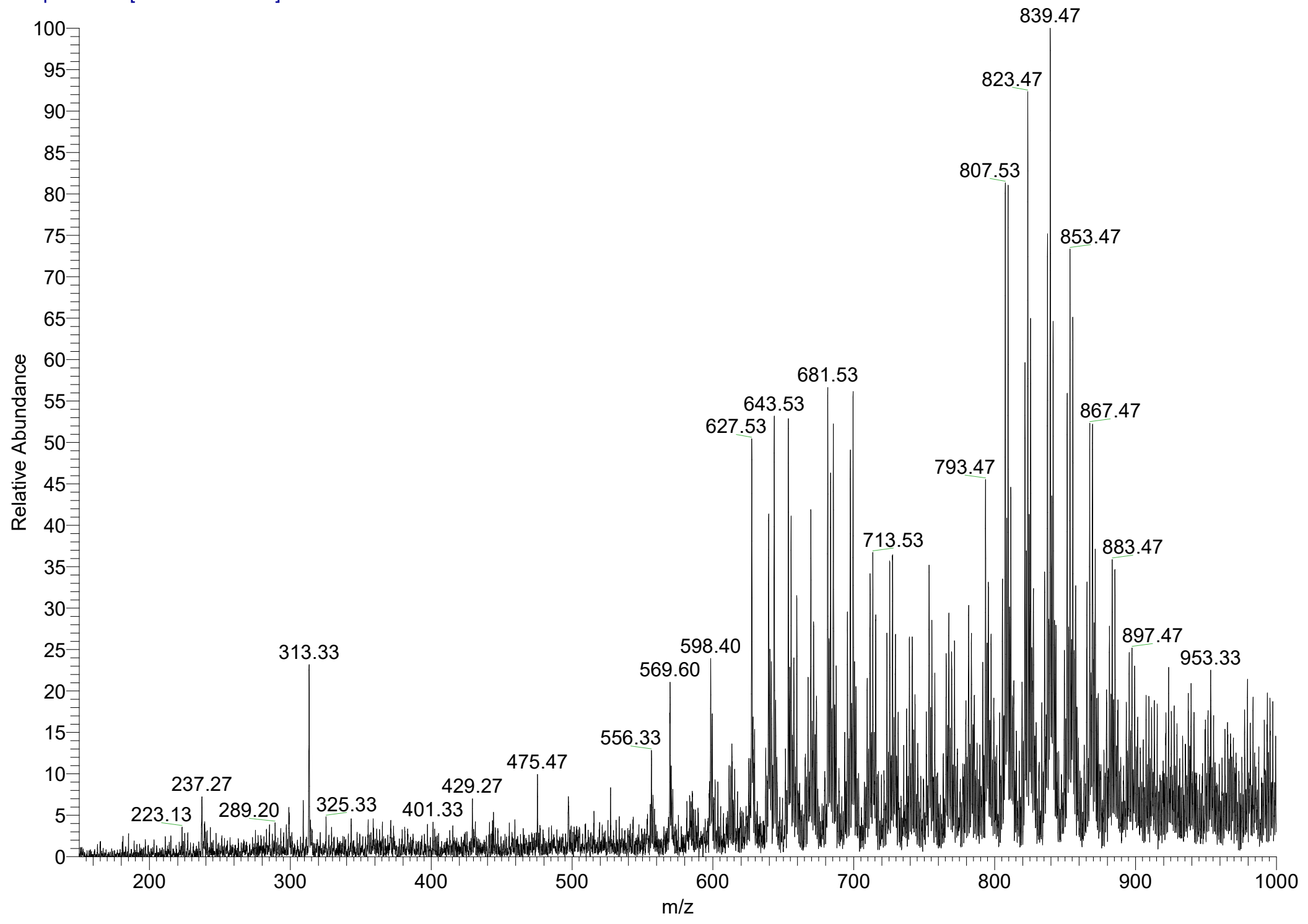
E:\dan_evans\RAW FILES\100%\S12 08/16/18 15:46:27 S12

S12 #1-50 RT: 0.00-0.74 AV: 50 NL: 6.82E5
T: + p ESI ms [150.00-1000.00]



E:\dan_evans\RAW FILES\100%\S13 08/16/18 15:51:07 S13

S13 #1-50 RT: 0.01-0.74 AV: 50 NL: 4.11E5
T: + p ESI ms [150.00-1000.00]



E:\dan_evans\RAW FILES\100%\S13 08/16/18 15:51:07 S13

S13 #1-50 RT: 0.01-0.74 AV: 50 NL: 4.11E5
T: + p ESI ms [150.00-1000.00]