

AMB Express

New azaphilones from *Aspergillus neoglaber*

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S1. UV-VIS spectra for sassafrin E, sassafrin F, and sassafrinamine A.

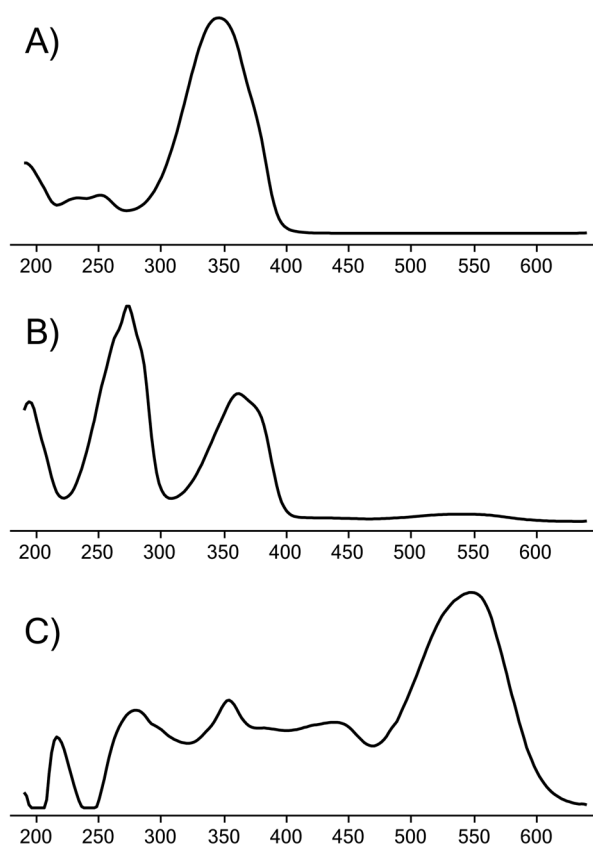
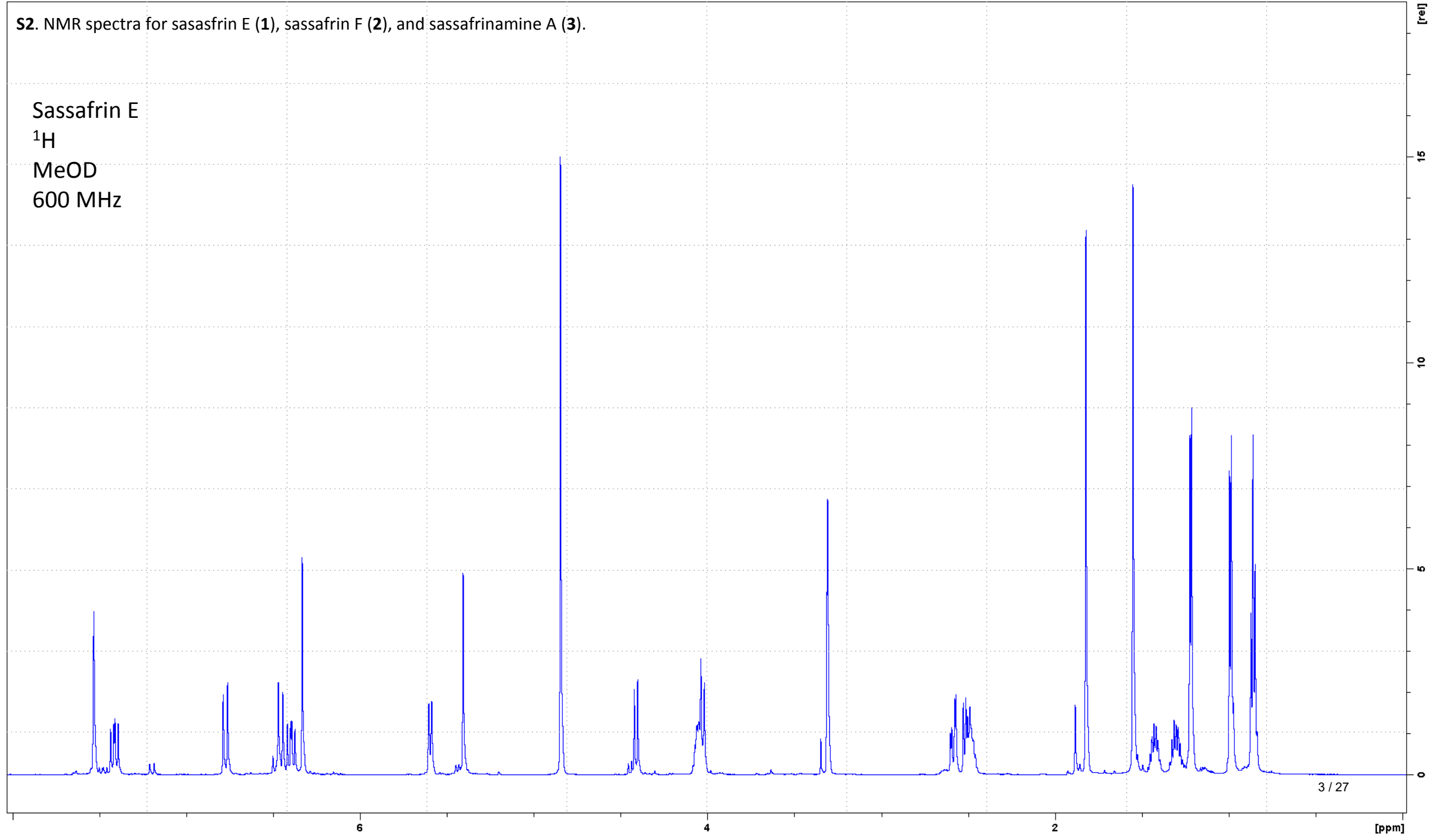


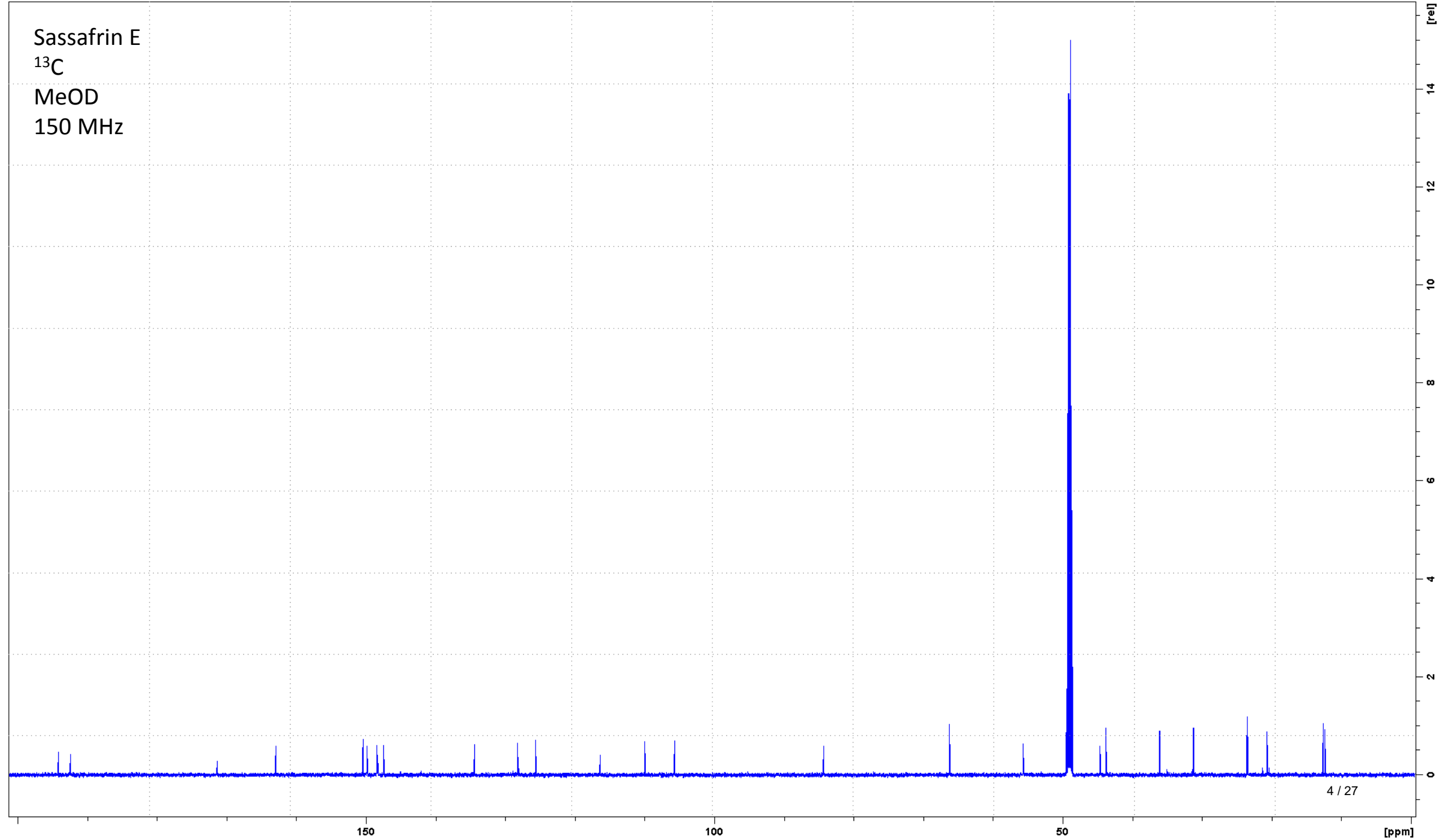
Figure S1. UV-VIS spectra for A) Sassafrin E, B) Sassafrin F, C) Sassafrinamine A. All spectra were recorded during UHPLC analysis in acetonitrile and H₂O, acidified with 20mM formic acid.

S2. NMR spectra for sasasfrin E (1), sassafrin F (2), and sassafrinamine A (3).

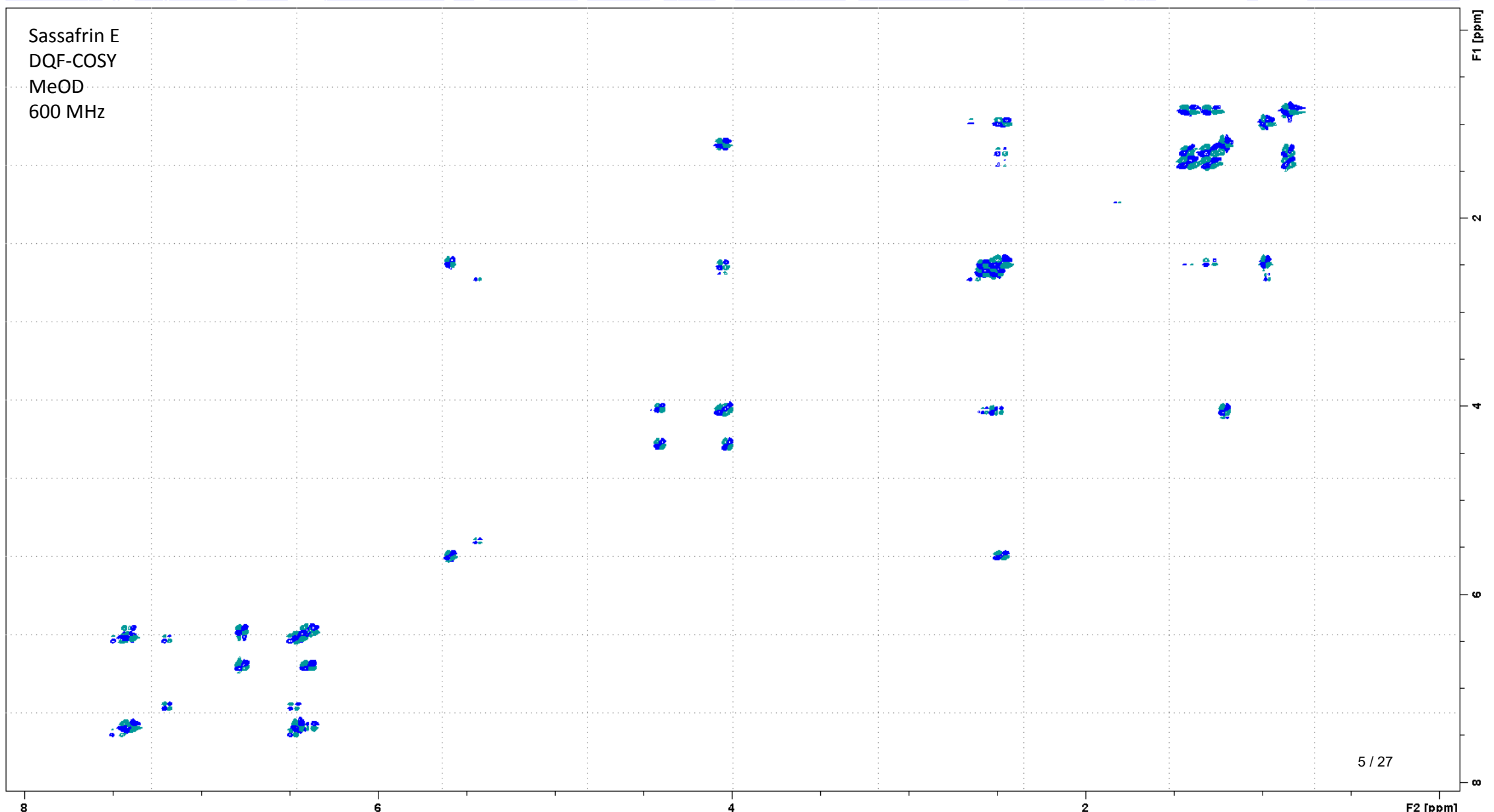
Sassafrin E
 ^1H
MeOD
600 MHz



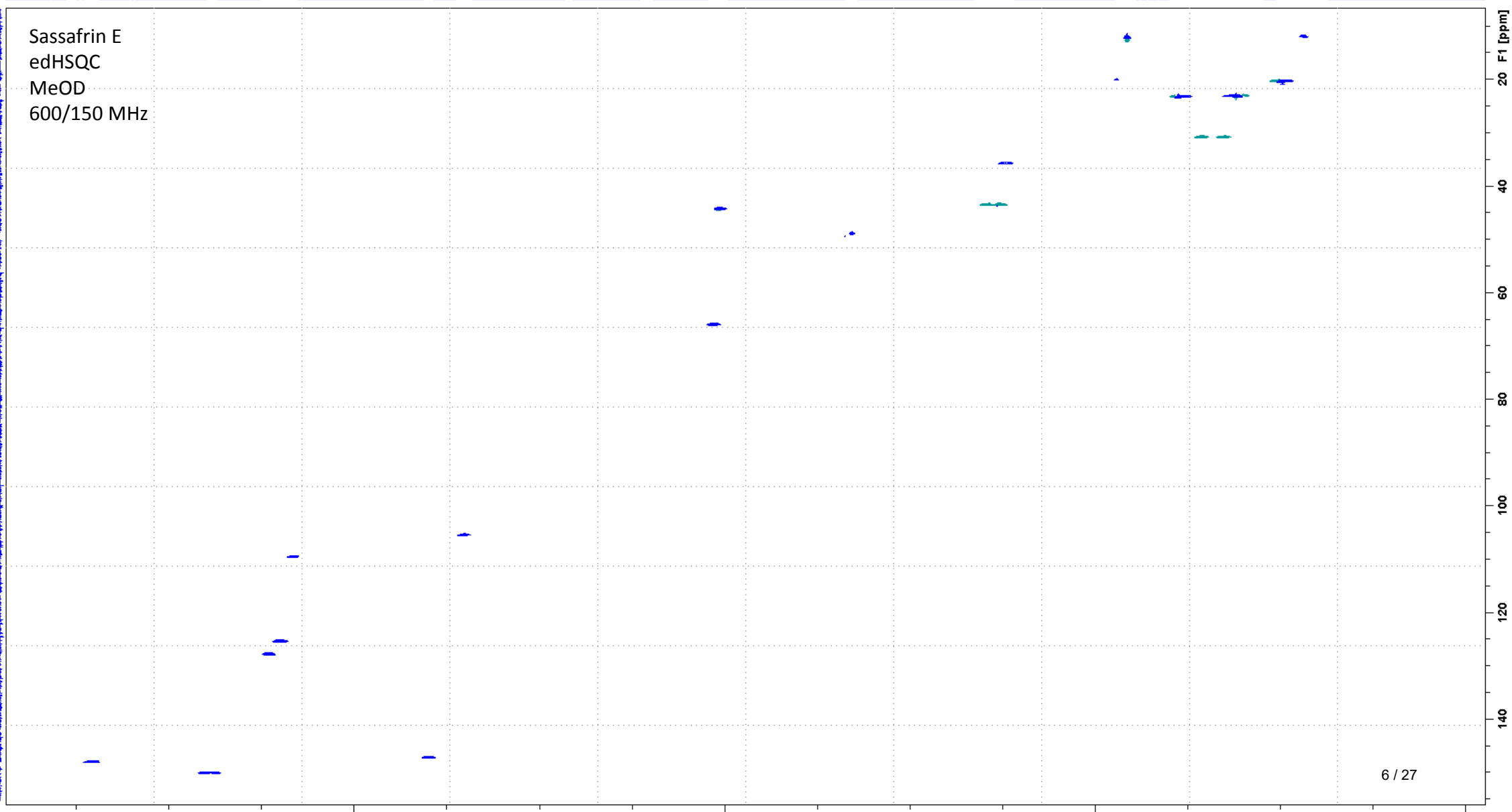
Sassafrin E
 ^{13}C
MeOD
150 MHz



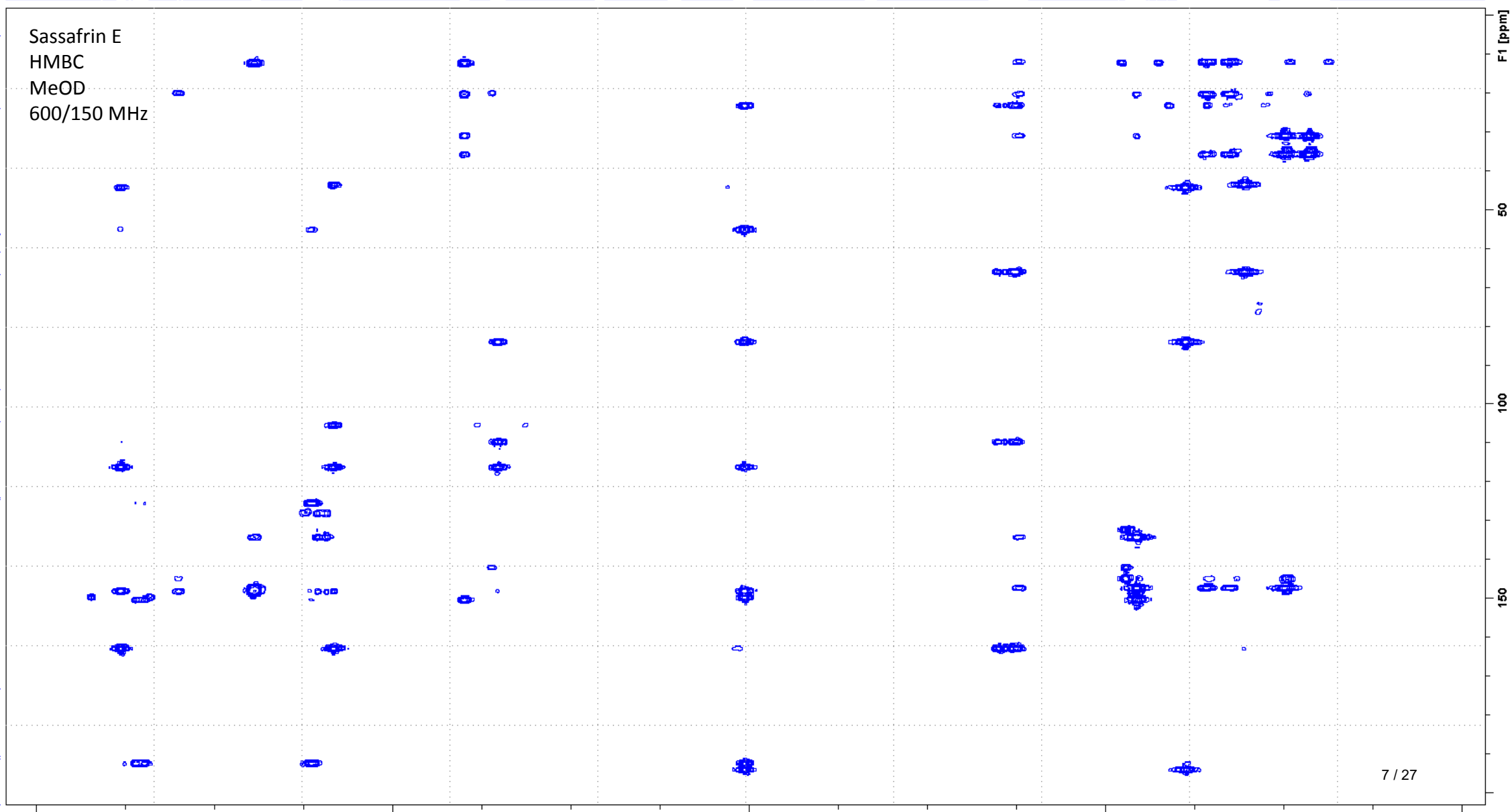
Sassafrin E
DQF-COSY
MeOD
600 MHz



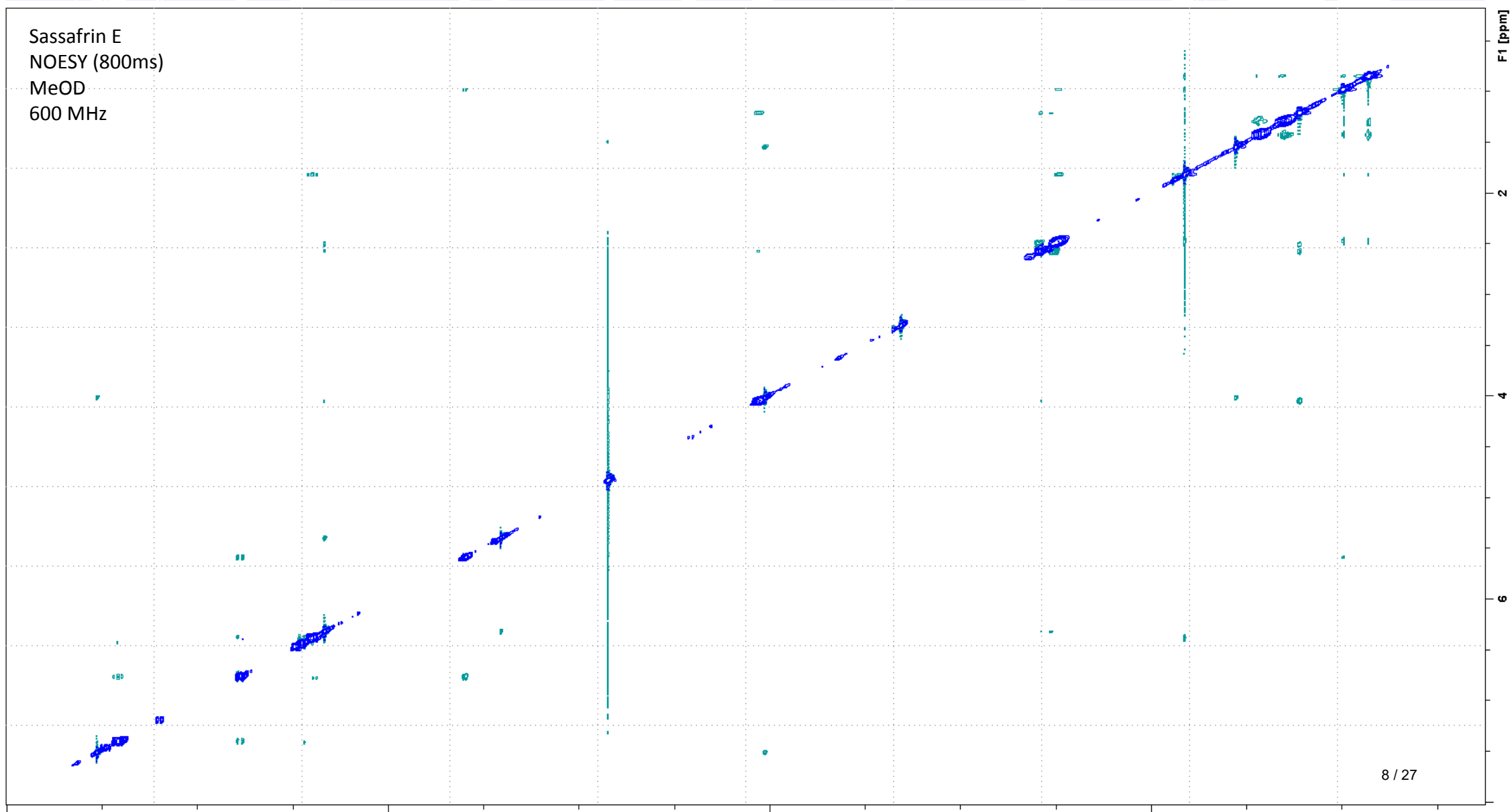
Sassafrin E
edHSQC
MeOD
600/150 MHz



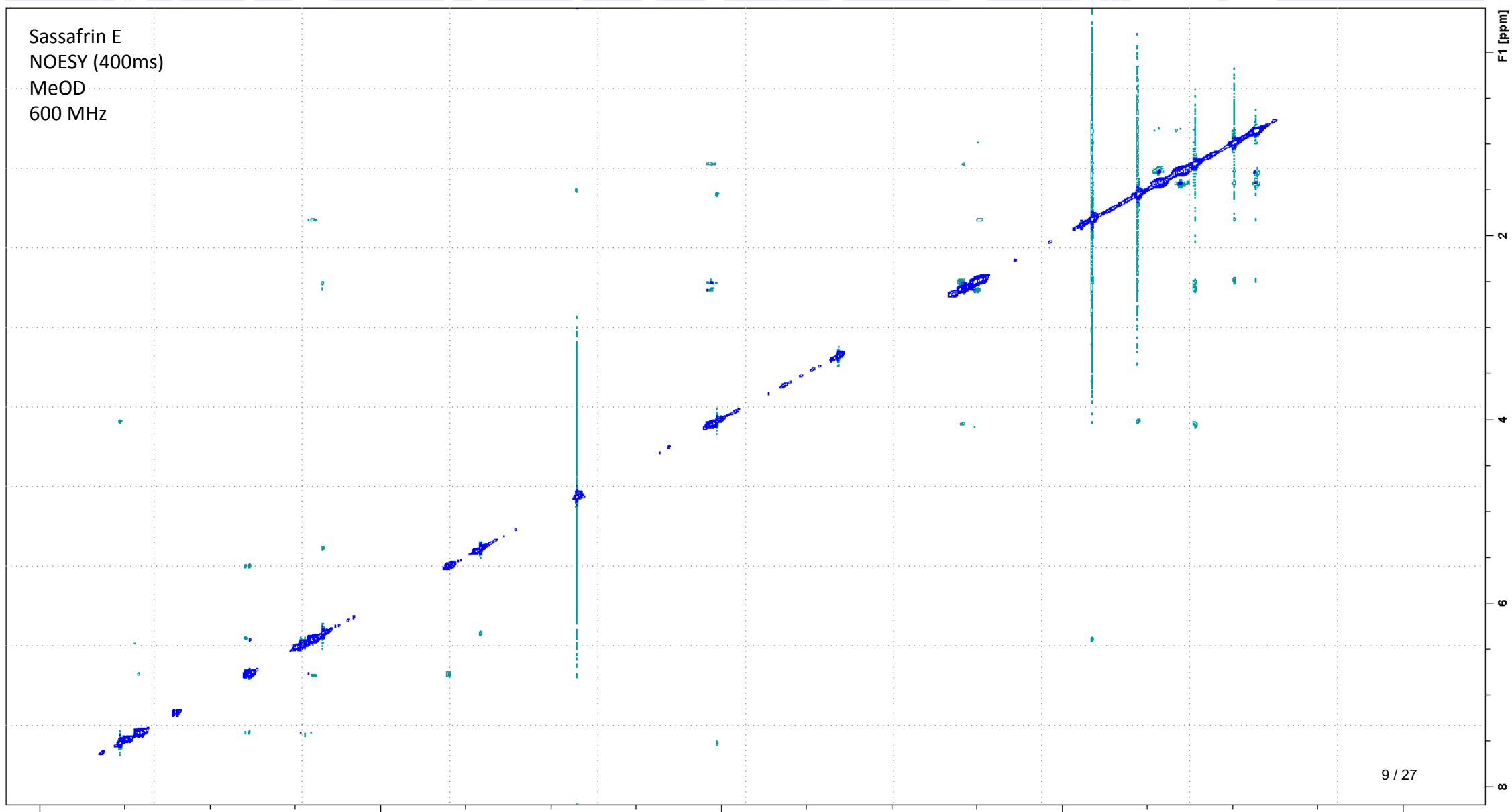
Sassafrin E
HMBC
MeOD
600/150 MHz



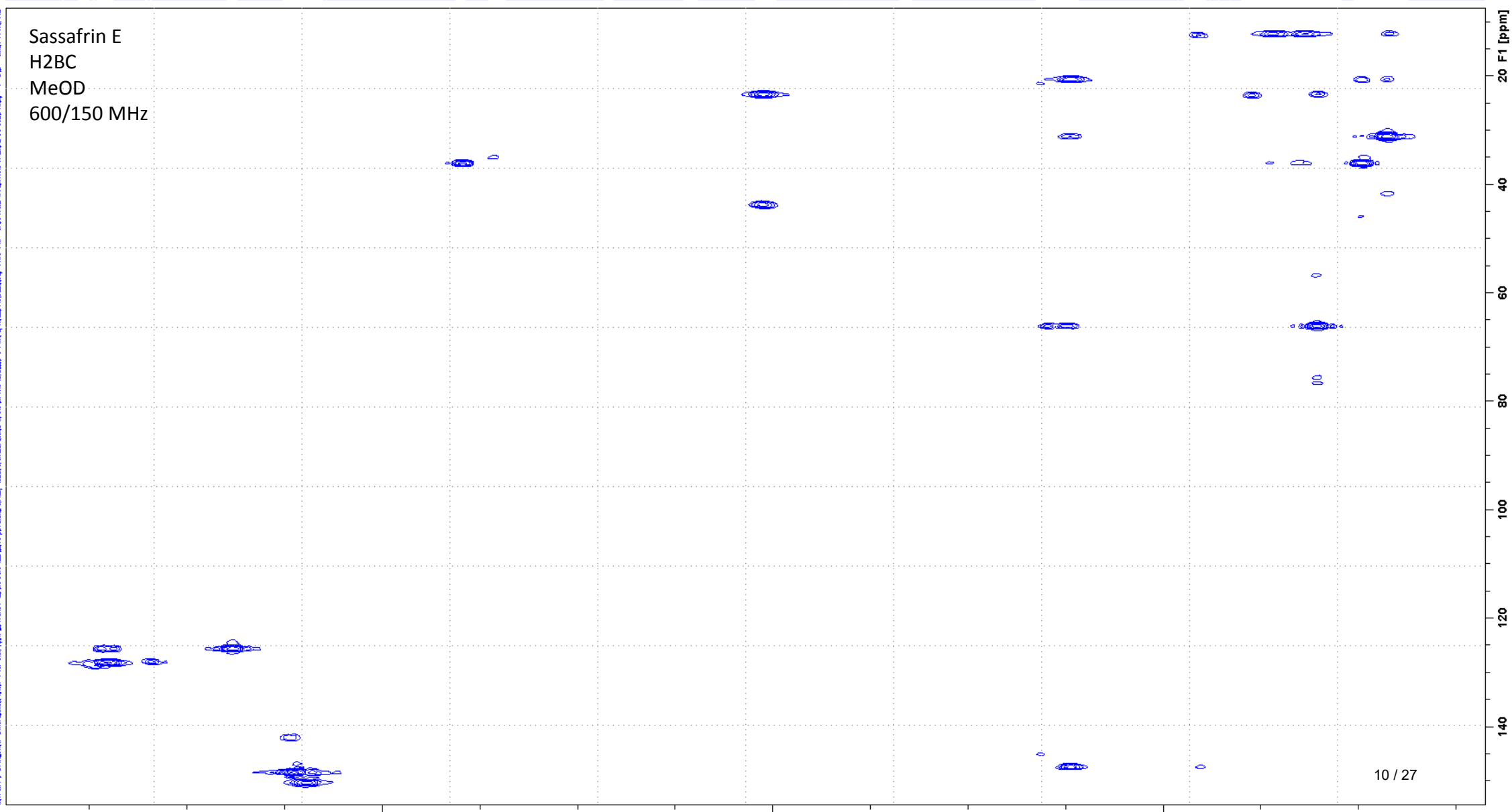
Sassafrin E
NOESY (800ms)
MeOD
600 MHz



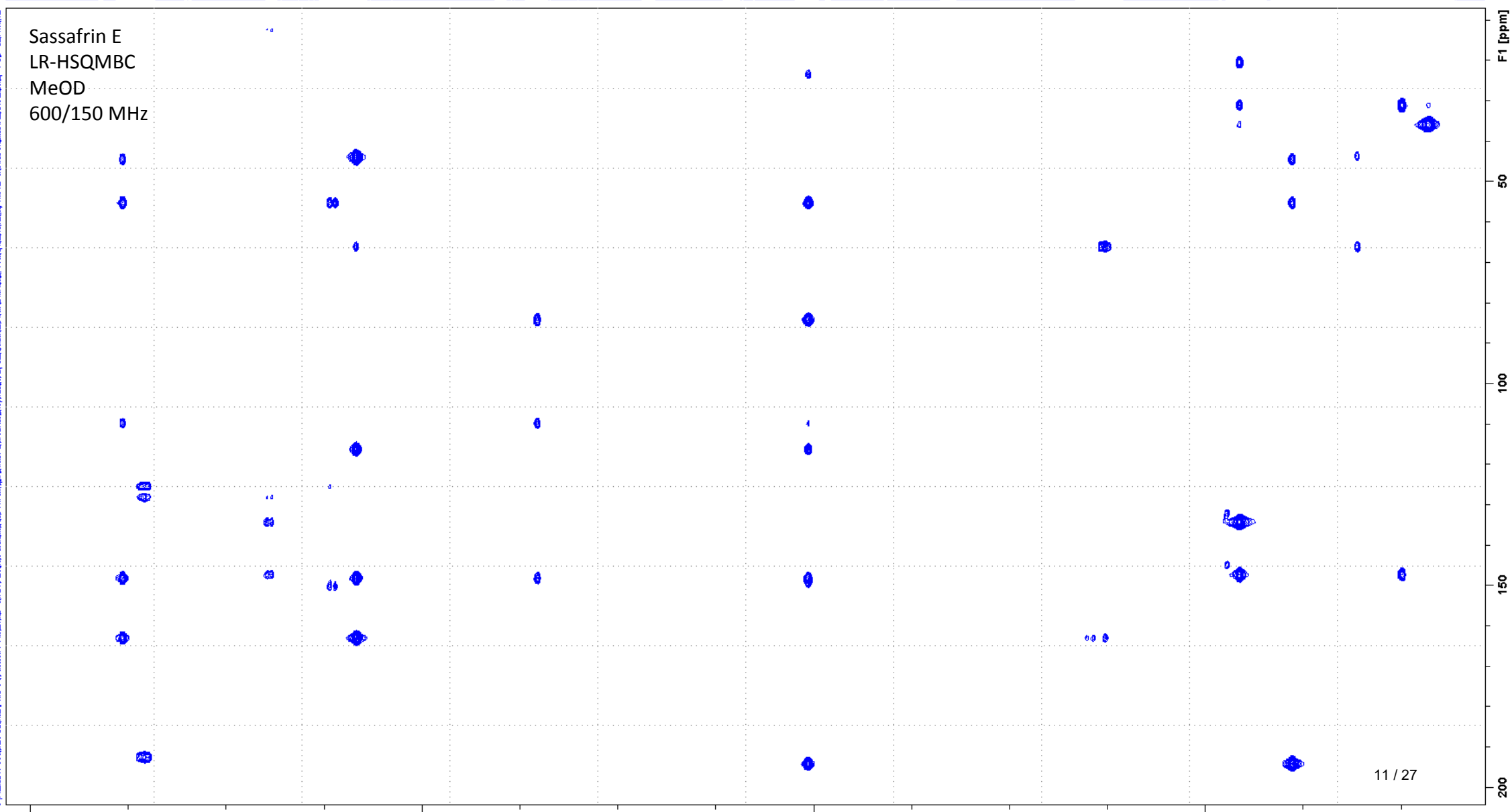
Sassafrin E
NOESY (400ms)
MeOD
600 MHz



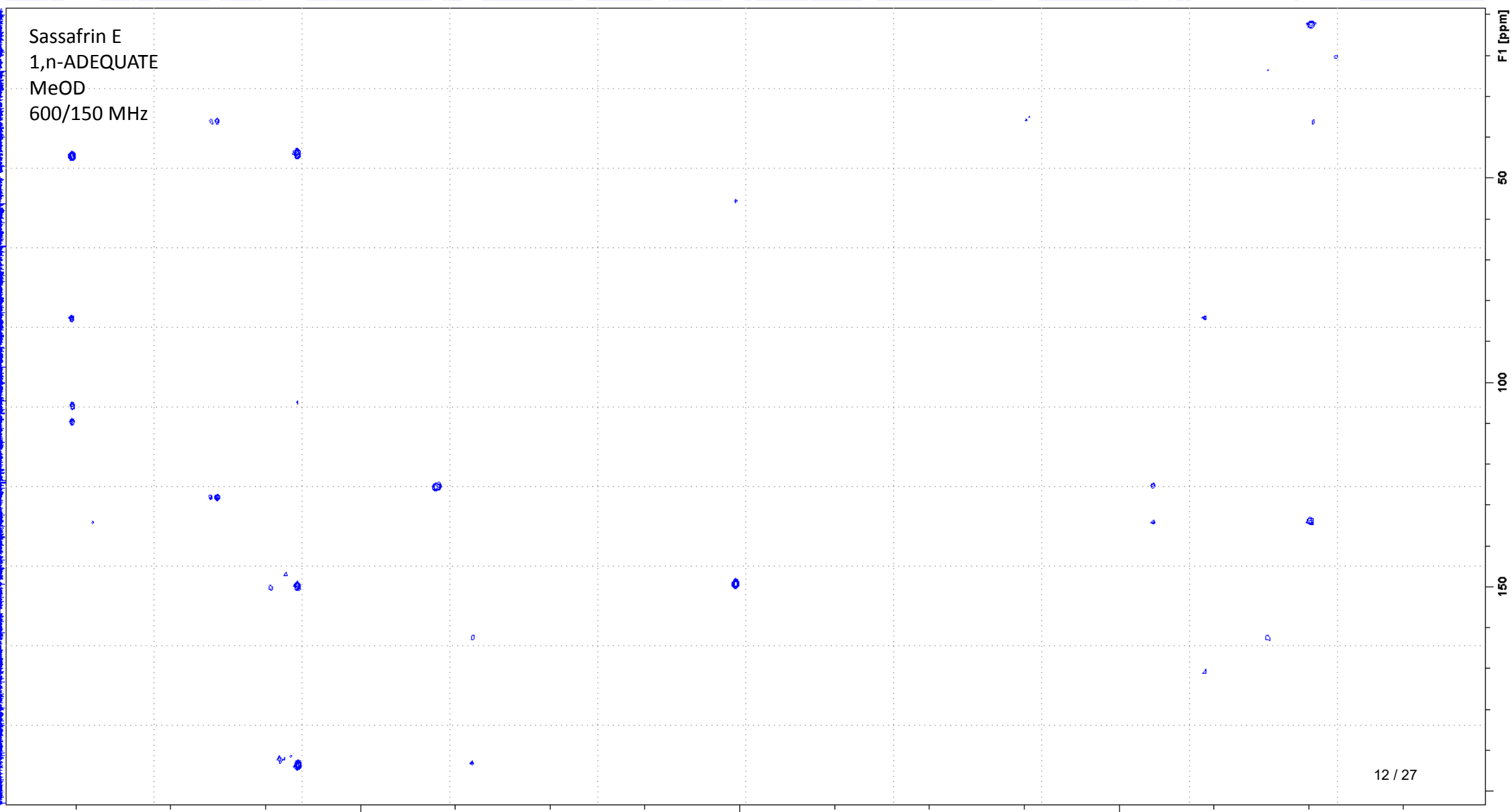
Sassafrin E
H2BC
MeOD
600/150 MHz



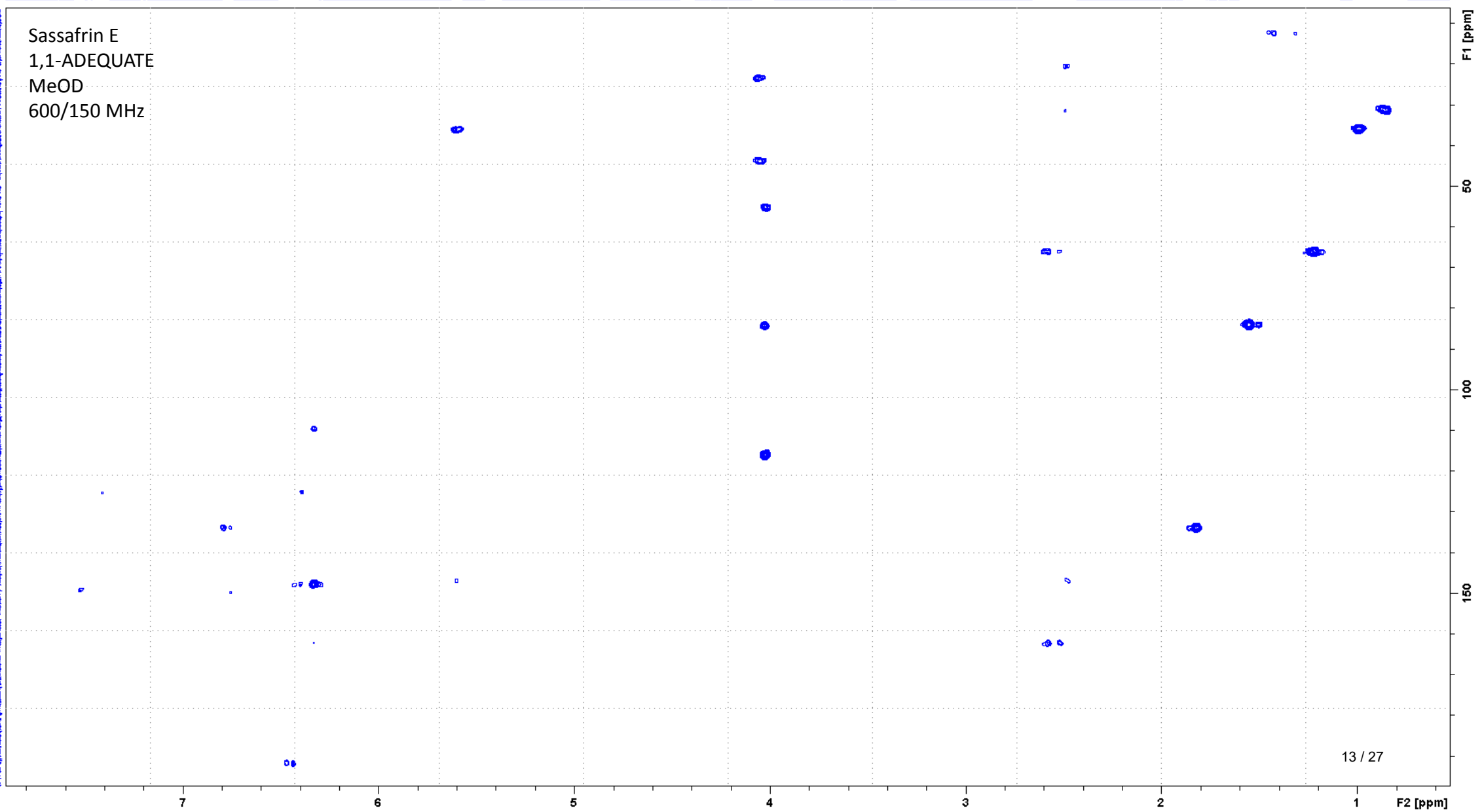
Sassafrin E
LR-HSQMBC
MeOD
600/150 MHz



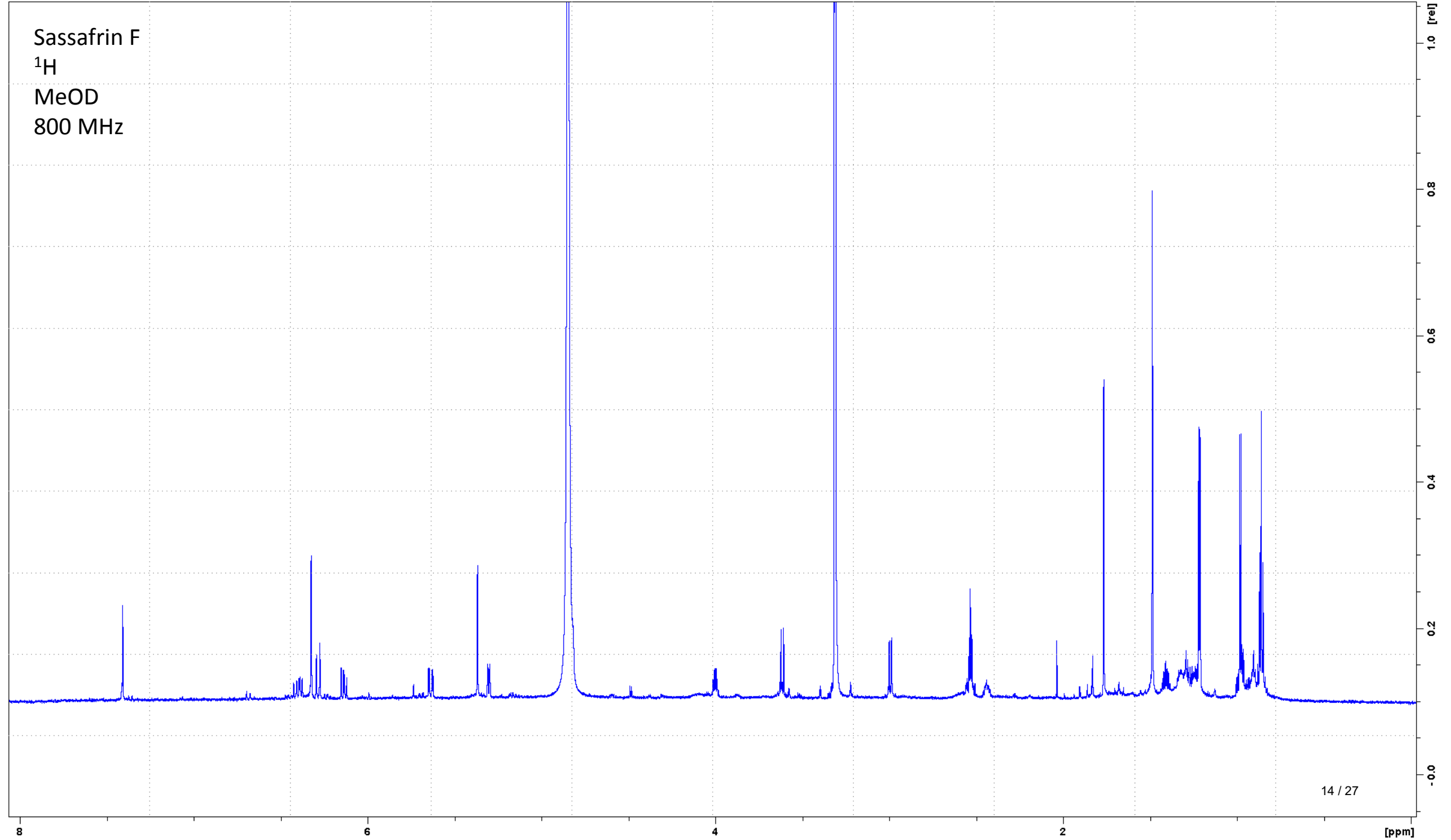
Sassafrin E
1,n-ADEQUATE
MeOD
600/150 MHz

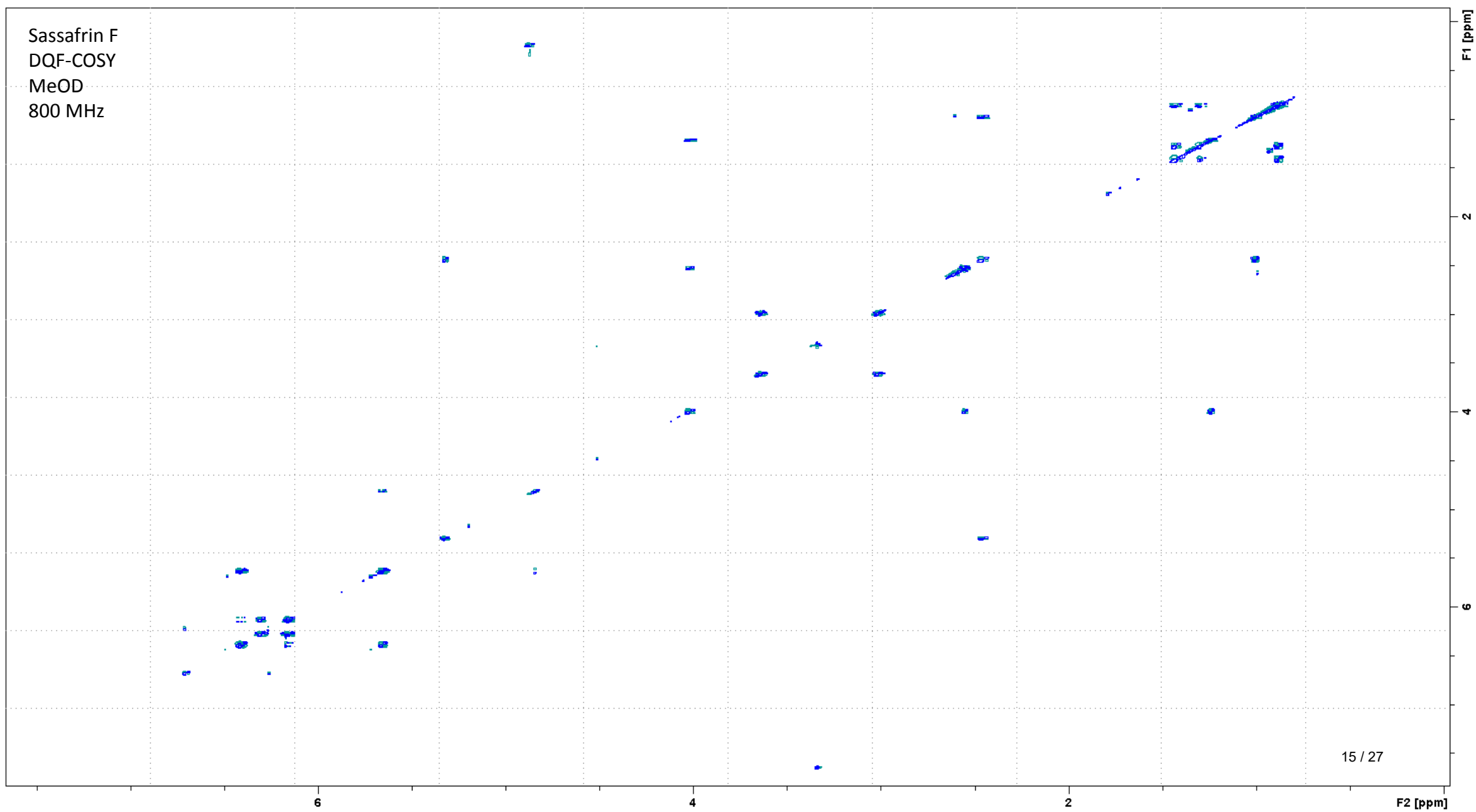
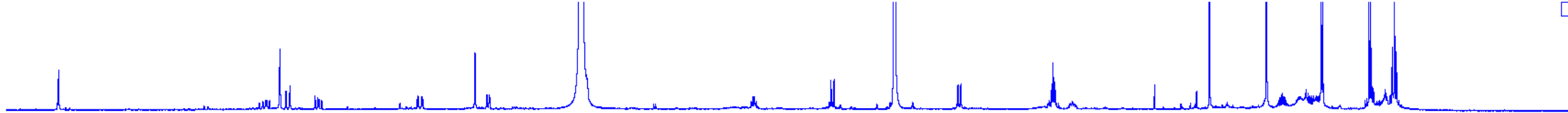


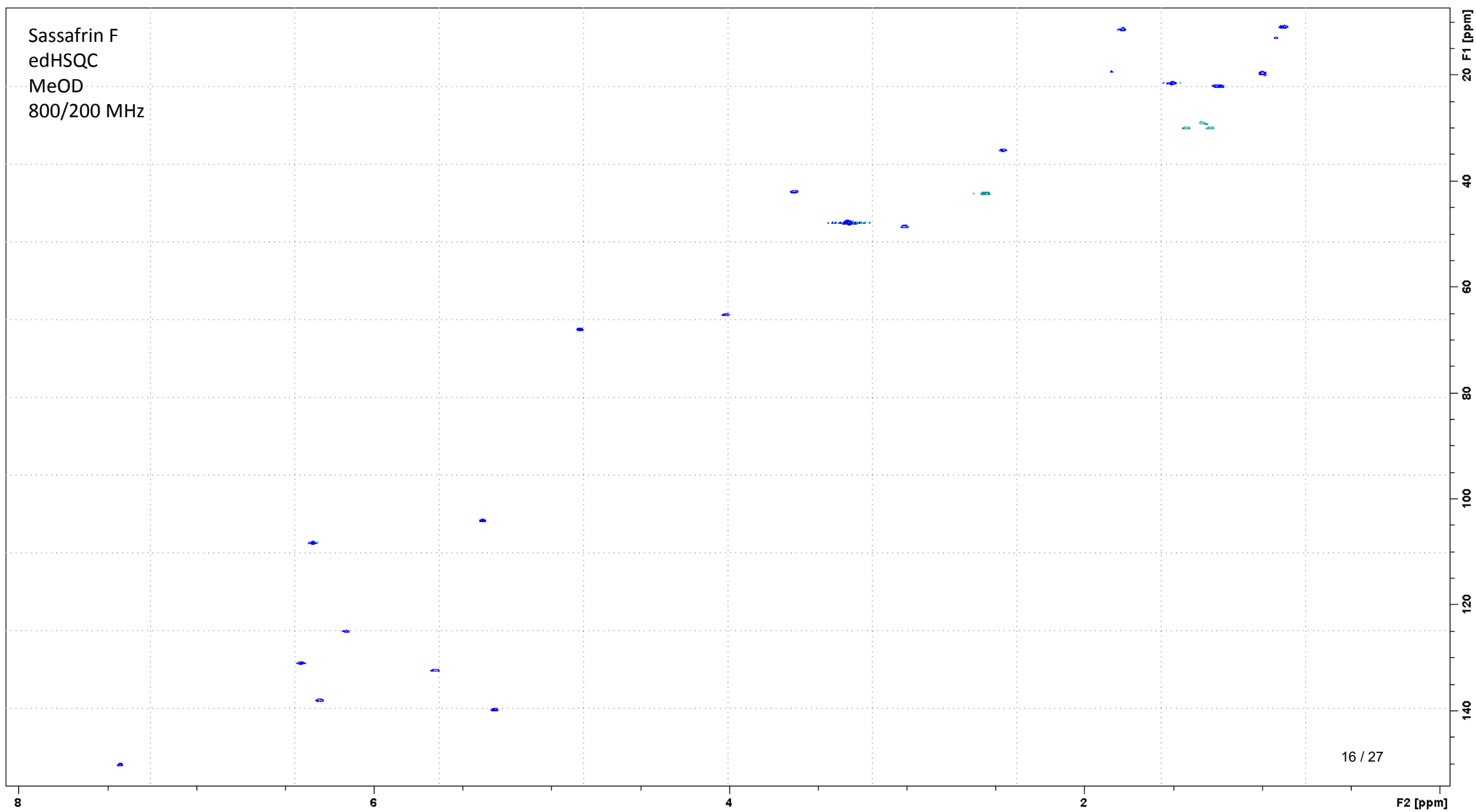
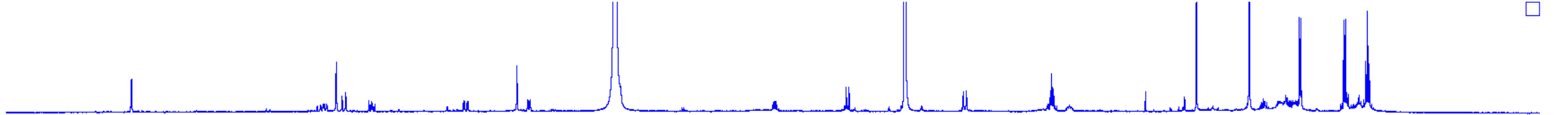
Sassafrin E
1,1-ADEQUATE
MeOD
600/150 MHz

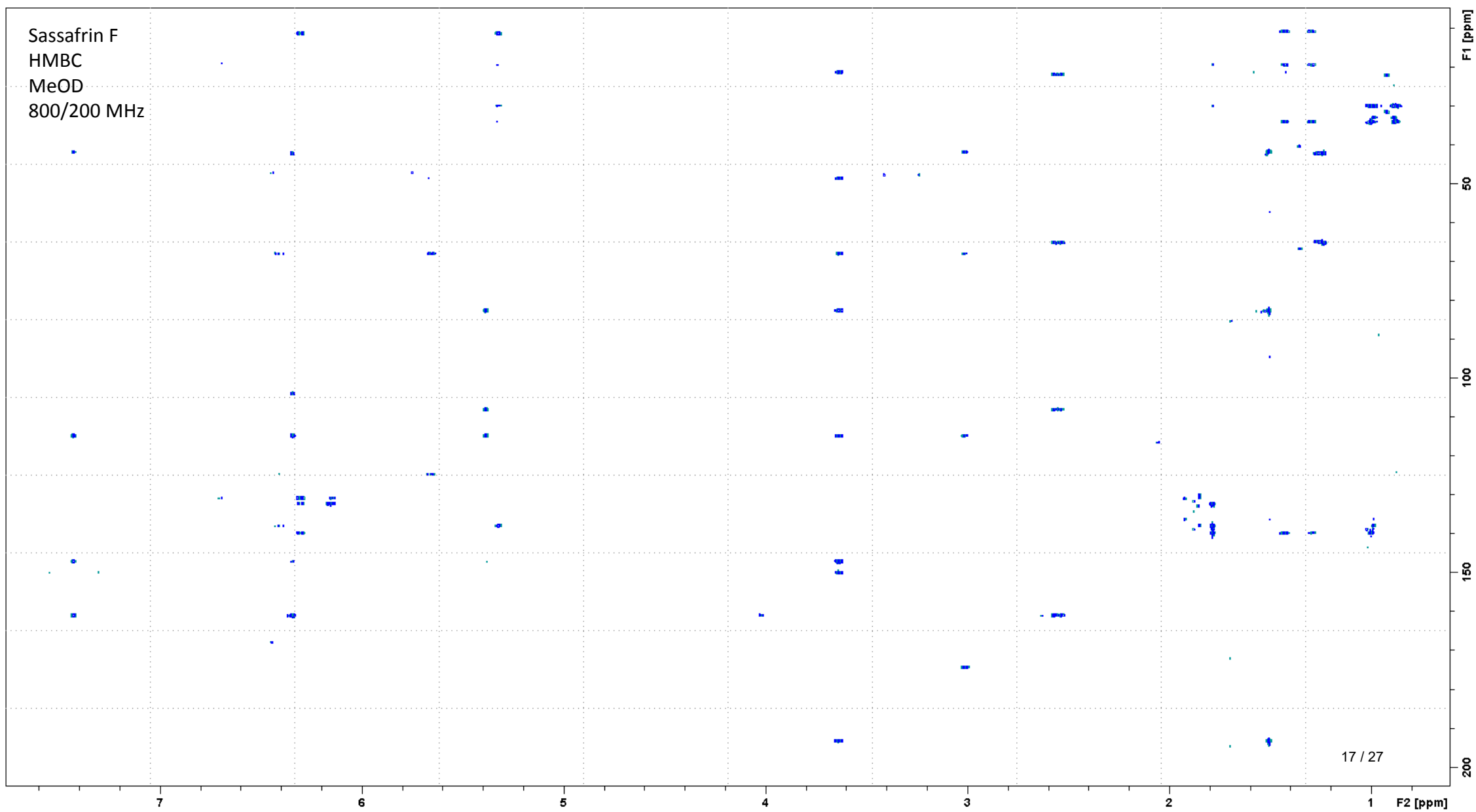
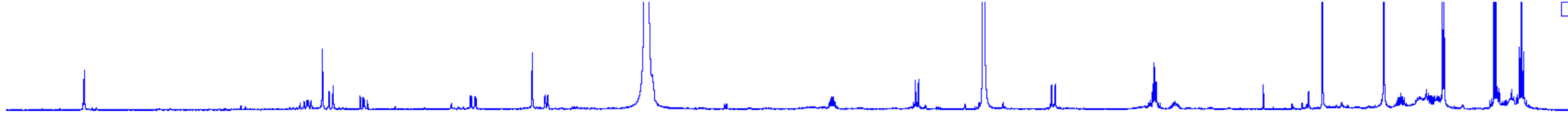


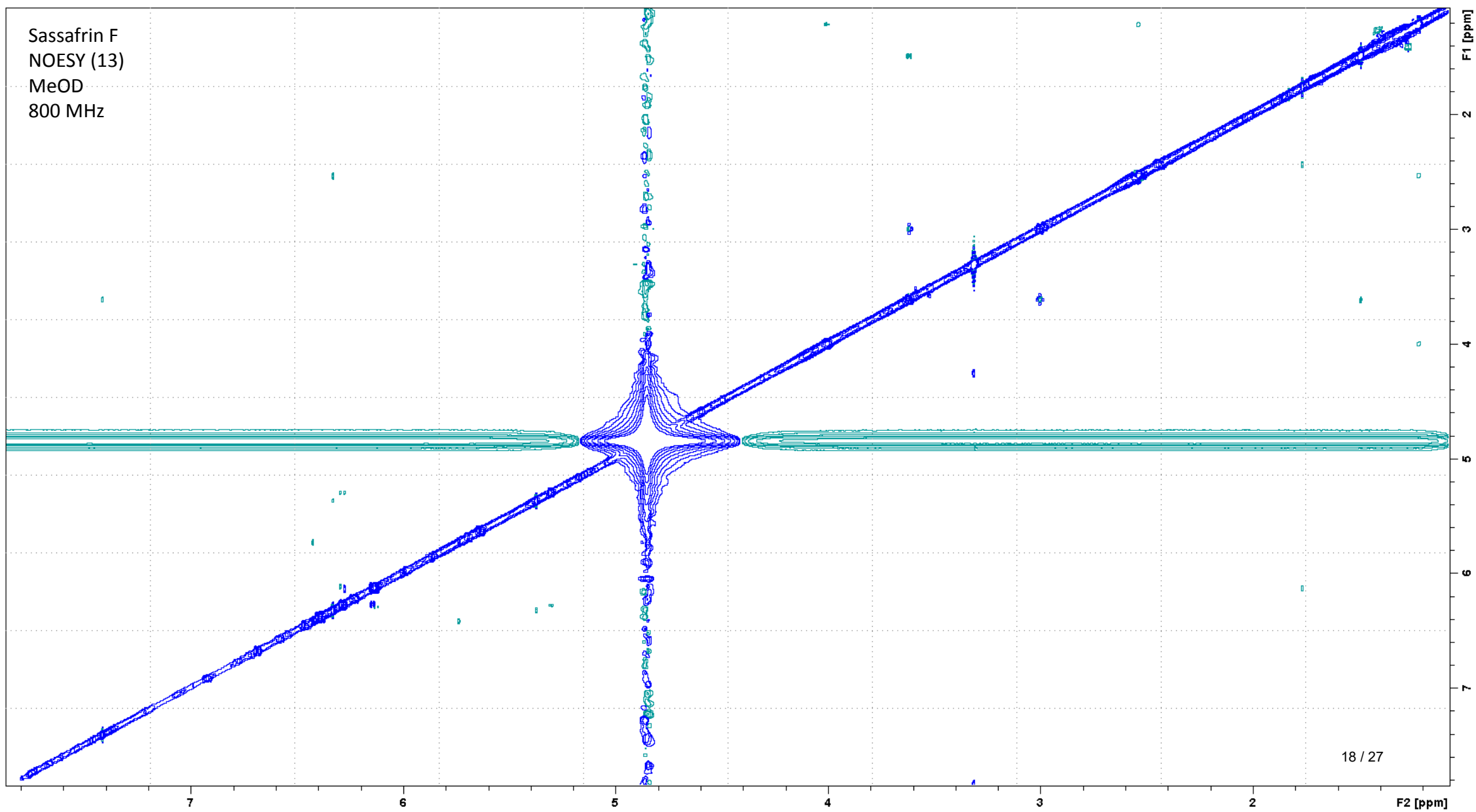
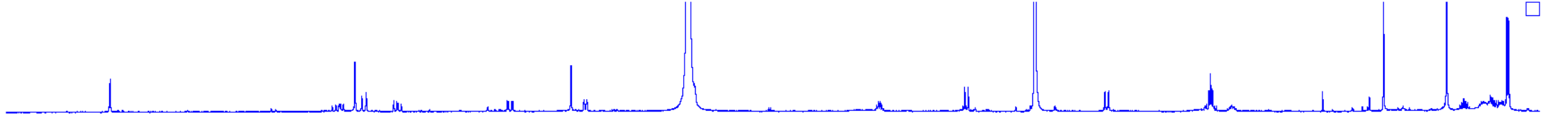
Sassafrin F
 ^1H
MeOD
800 MHz

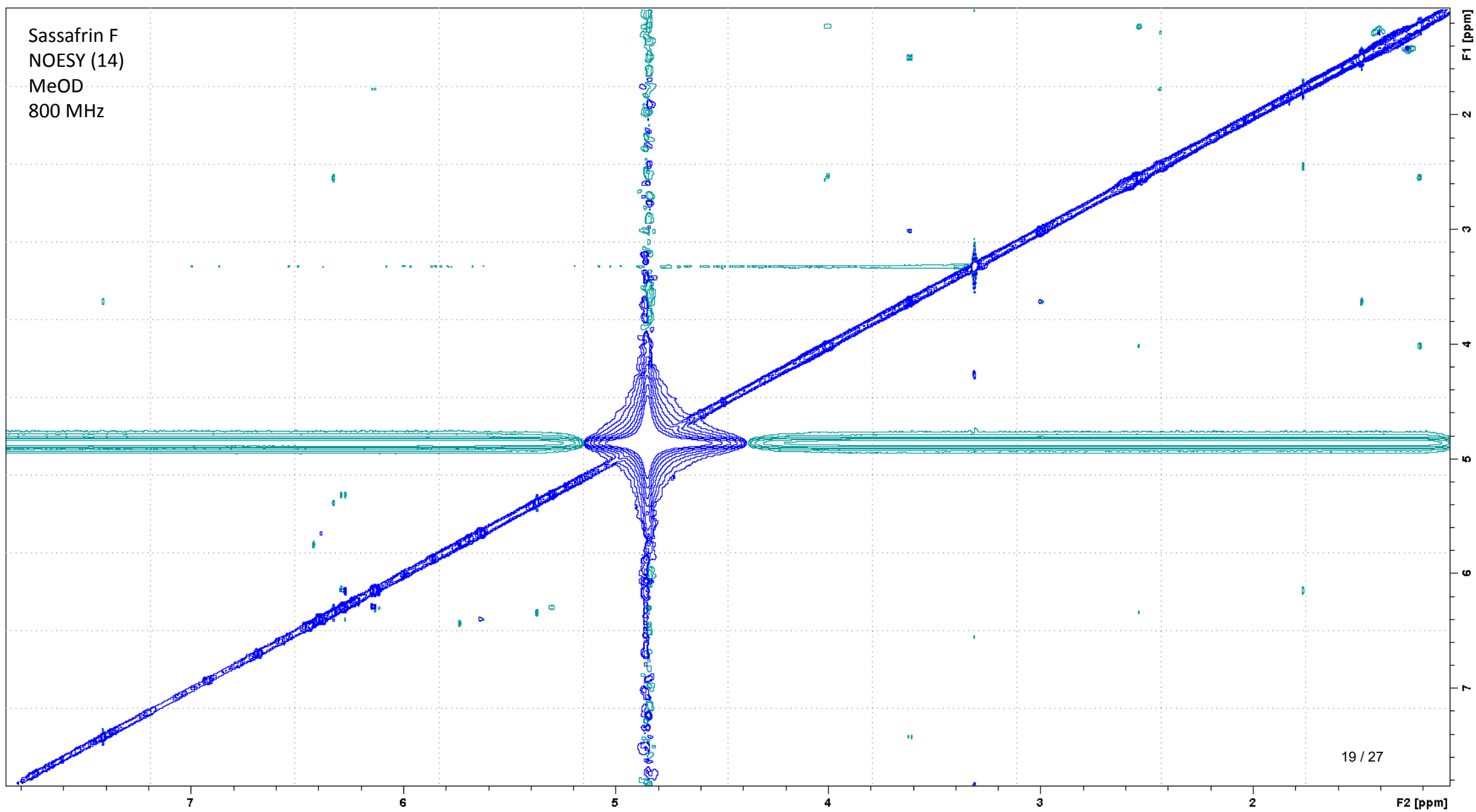
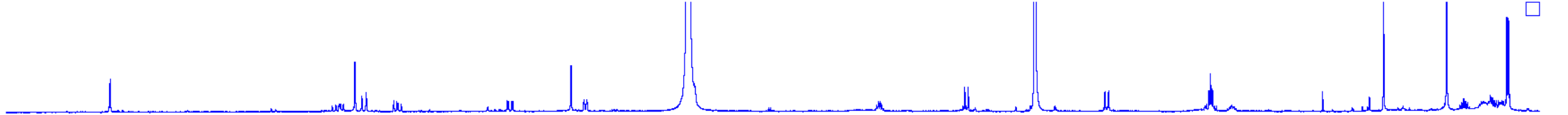










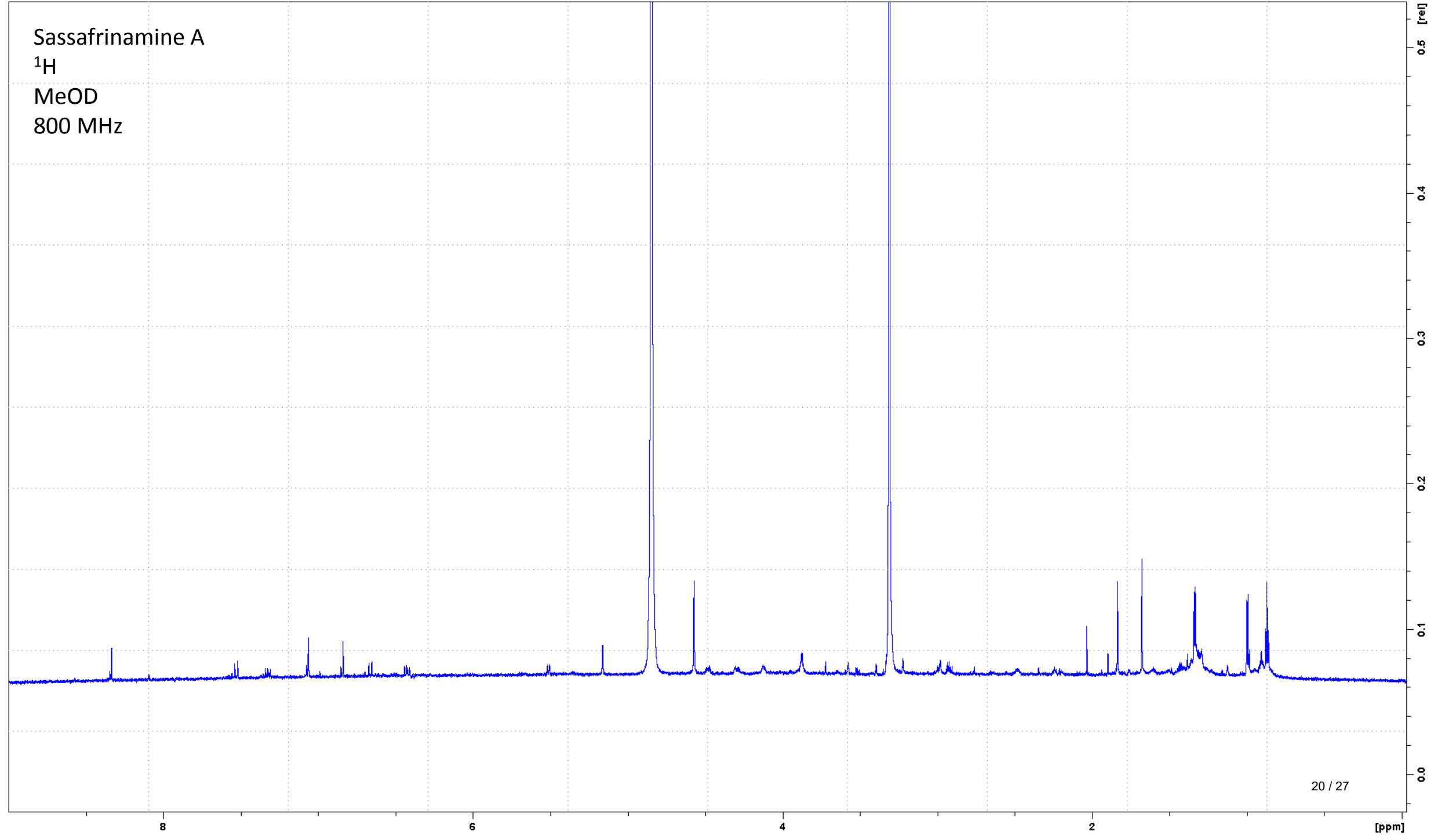


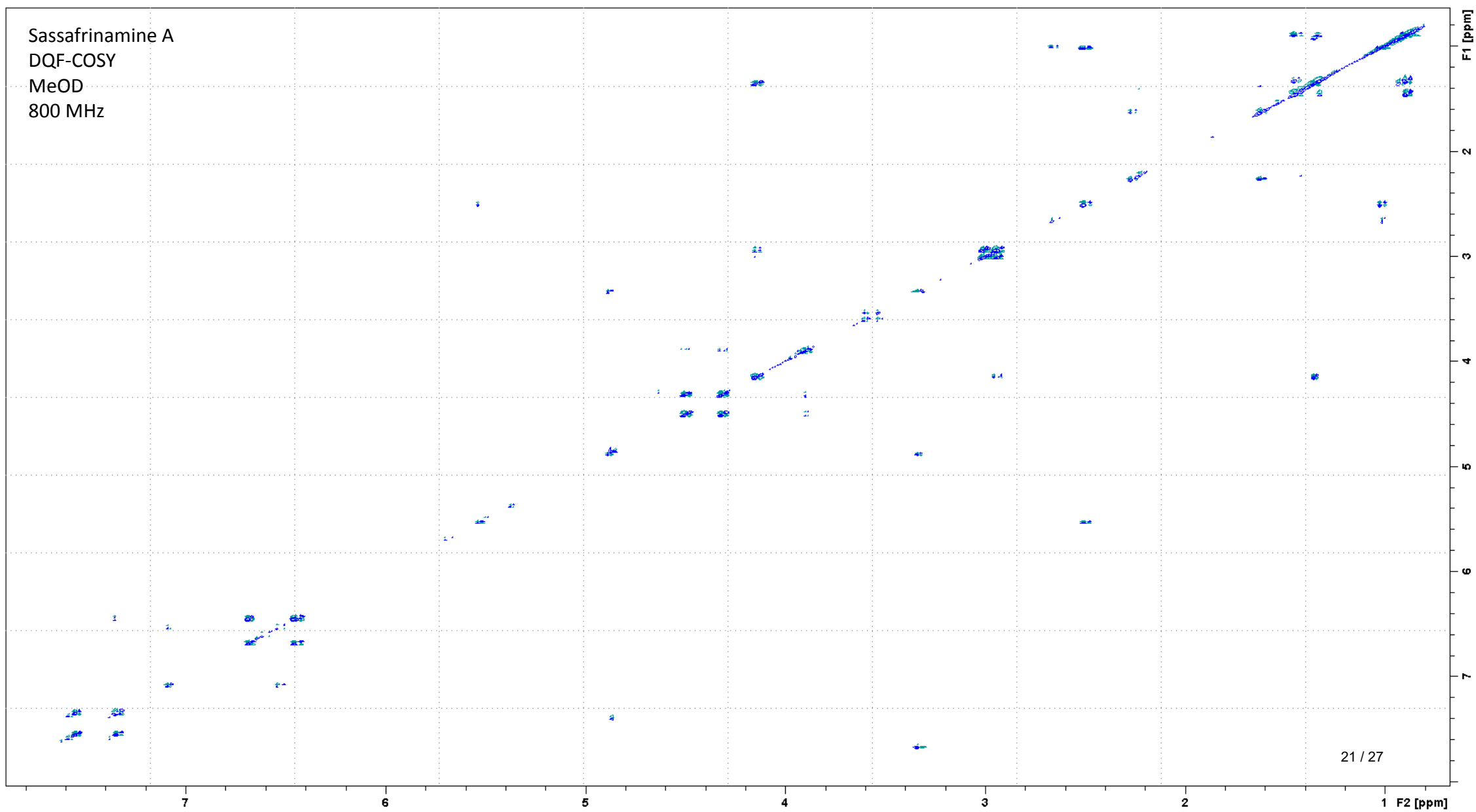
Sassafrinamine A

^1H

MeOD

800 MHz





Sassafrinamine A
edHSQC
MeOD
800/200 MHz

F1 [ppm]

20

40

60

80

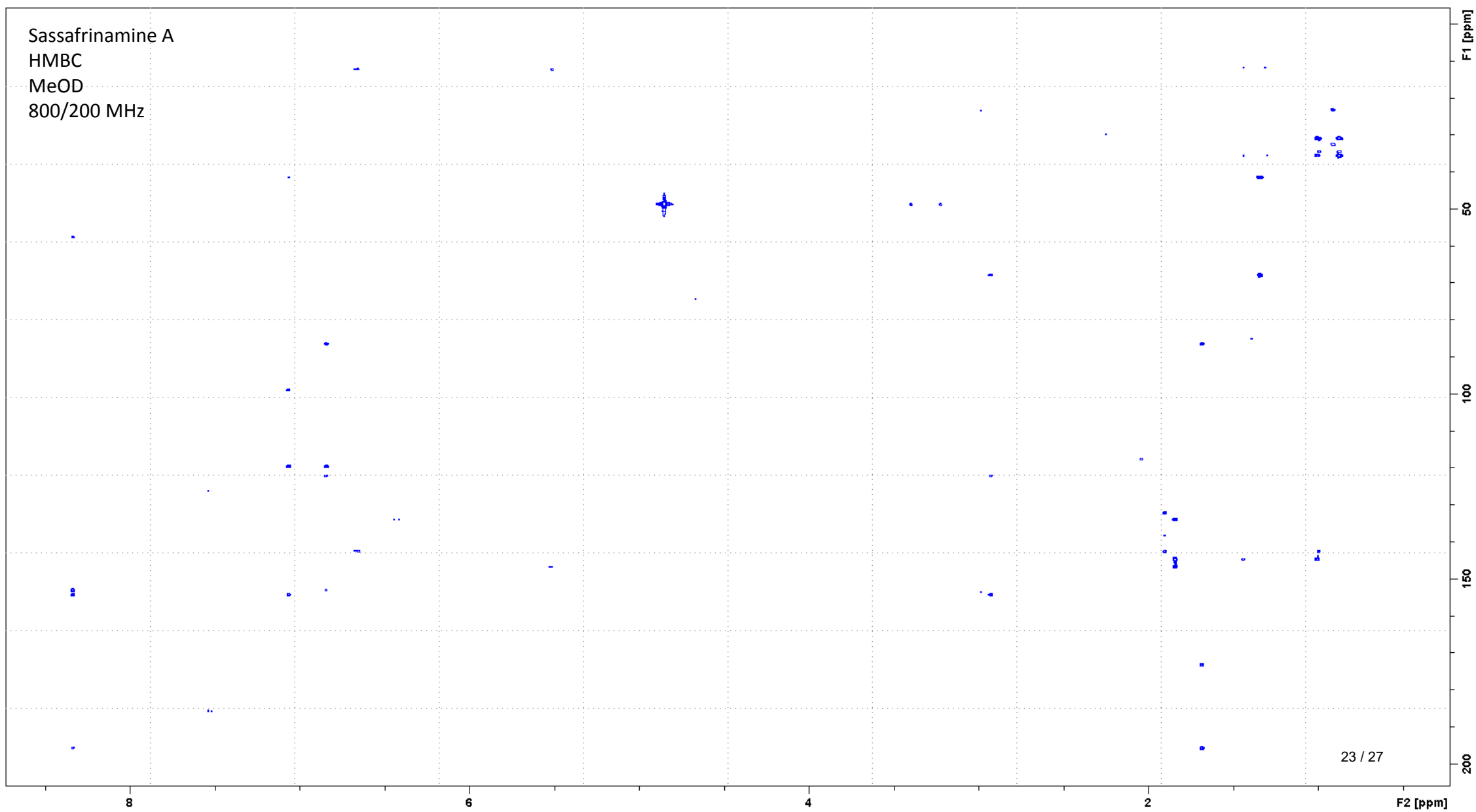
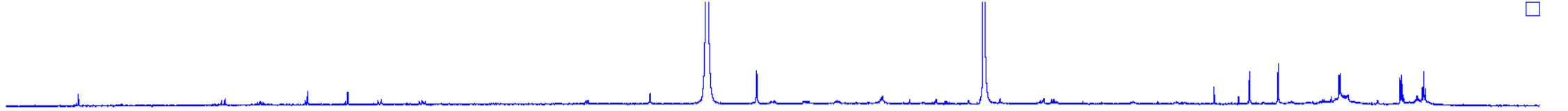
100

120

140

F2 [ppm]

22 / 27



S3. Tandem mass spectra and proposed fragmentation pathway for deuterated sassafrin E.

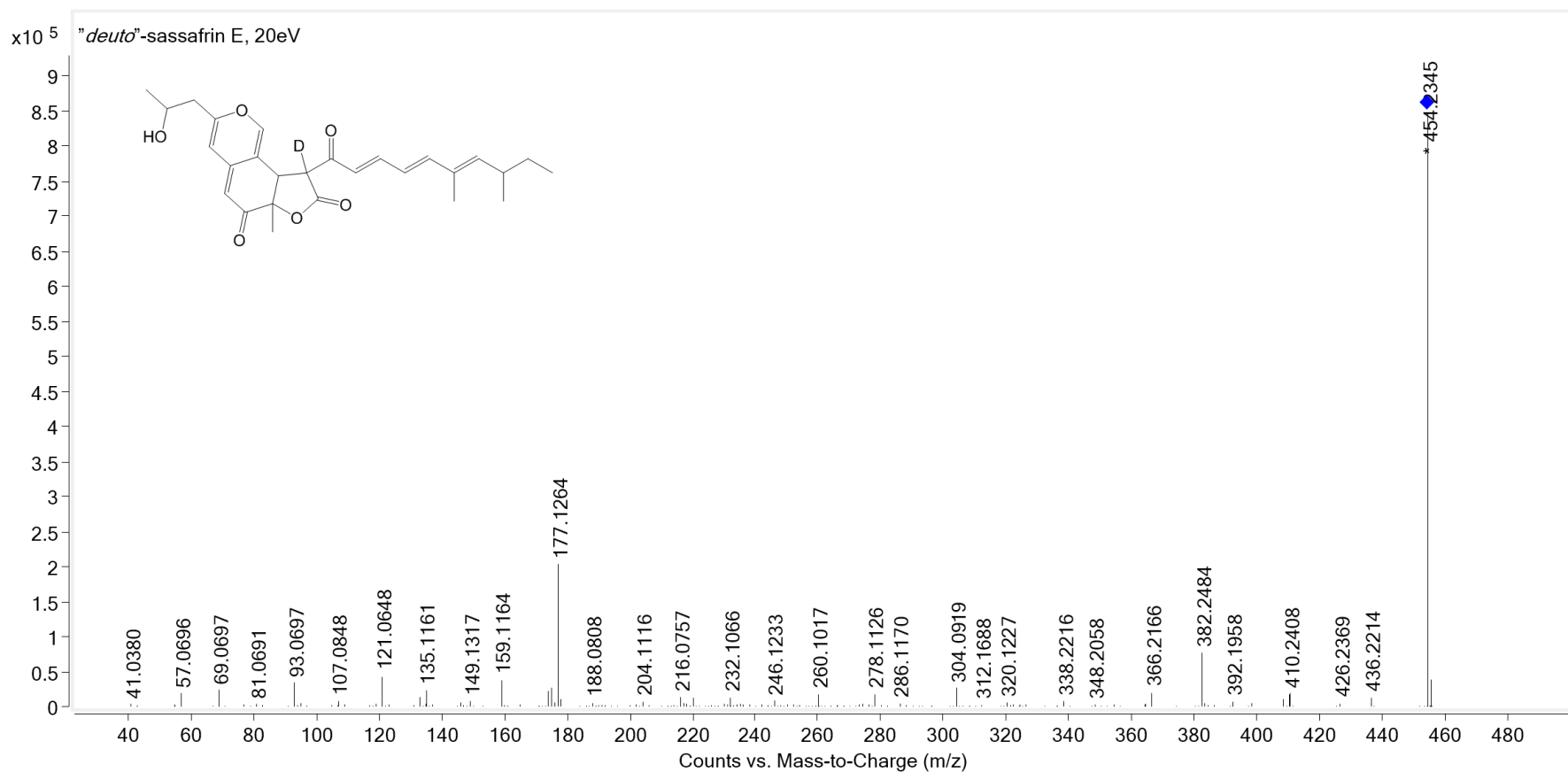


Figure S2. Tandem mass spectrum for deuterated sassafrin E at 20 eV collision energy.

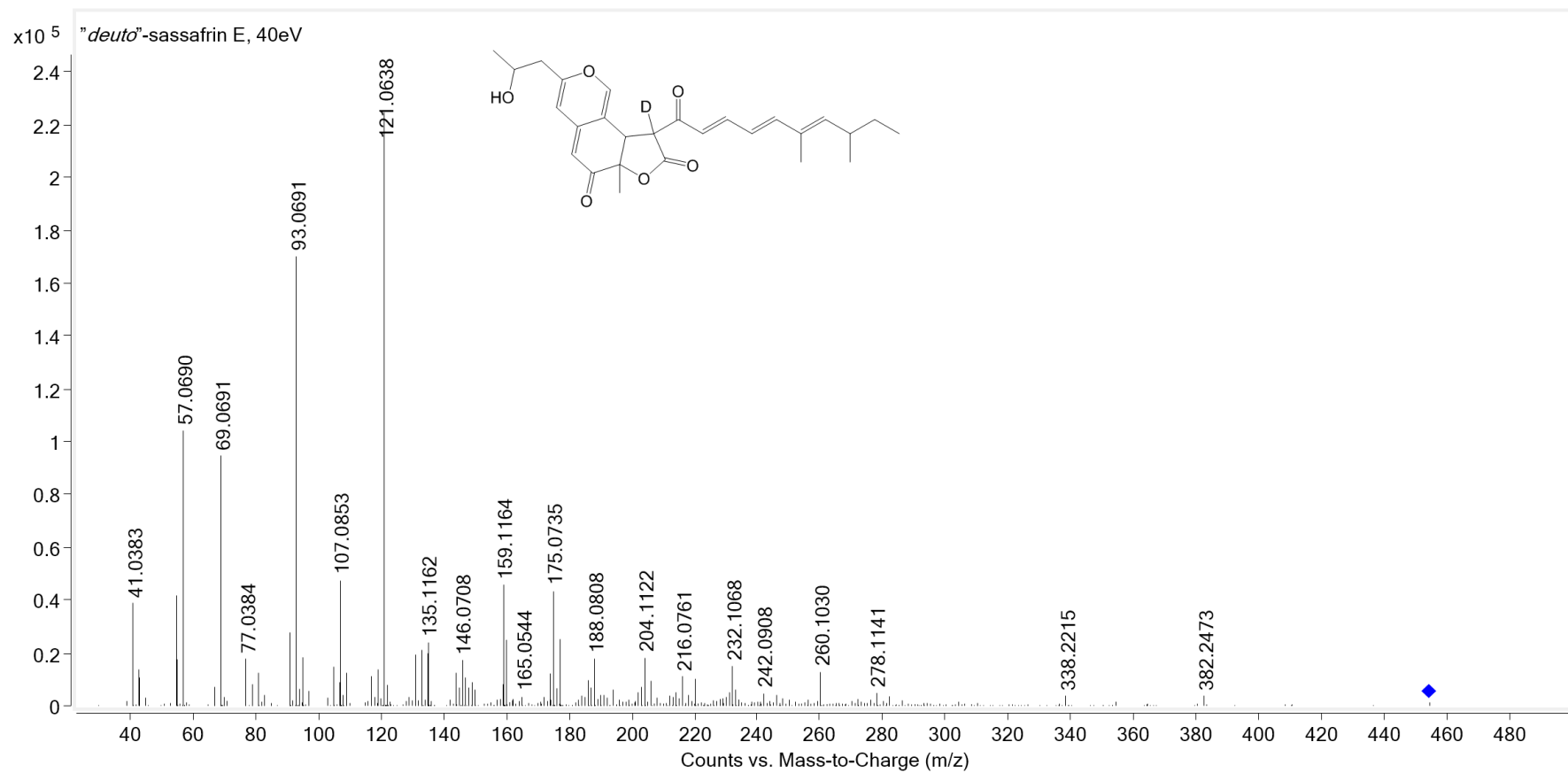


Figure S3. Tandem mass spectrum for deuterated sassafrin E at 40 eV collision energy

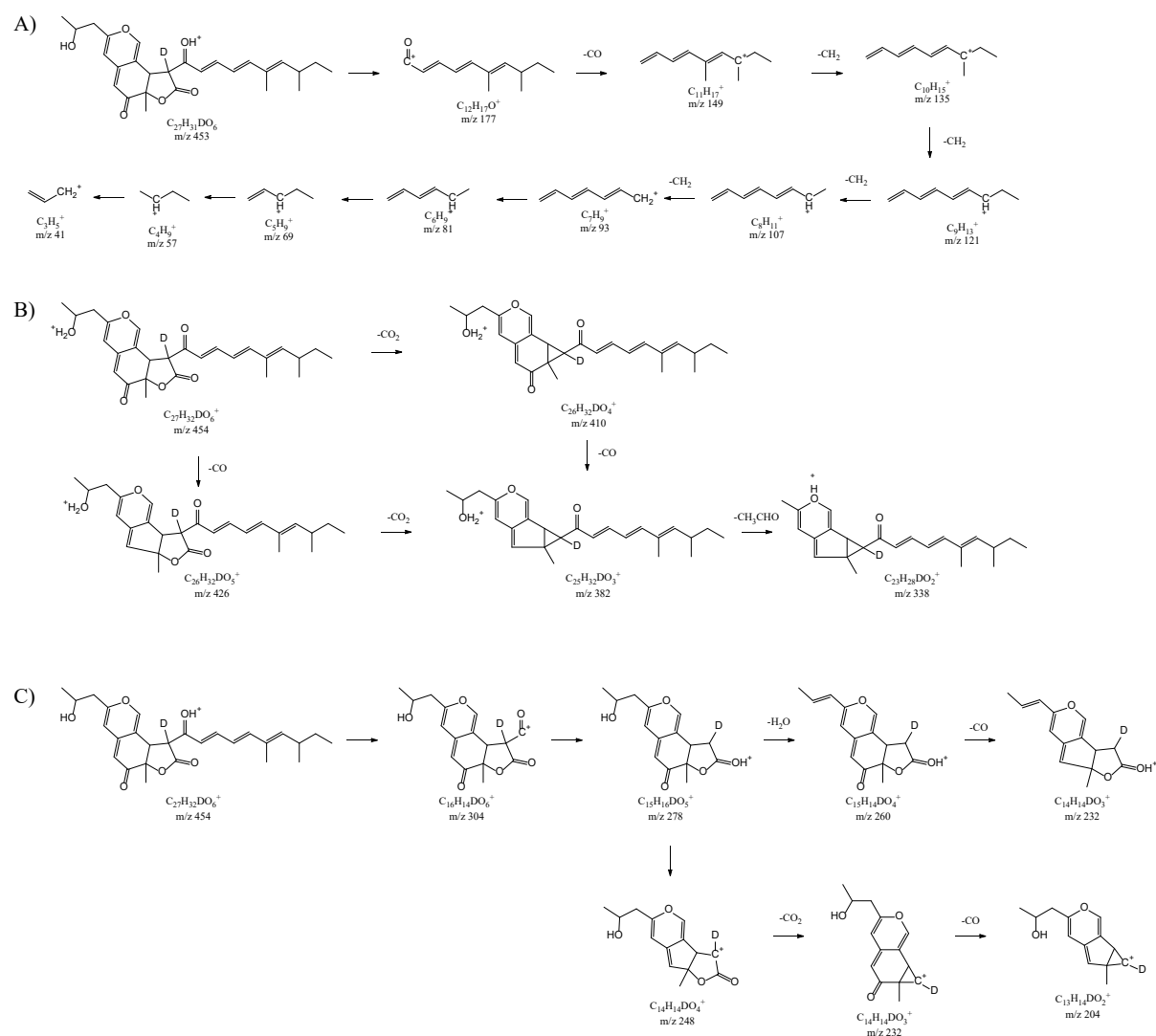


Figure S4. Proposed MS/MS fragmentation pathways for sassafrin E (1), based on deuterium in position H-23.

S4. Dereplication of m/z 453 compound in *Aspergillus neoglaber* compared to *Penicillium echinulatum*.

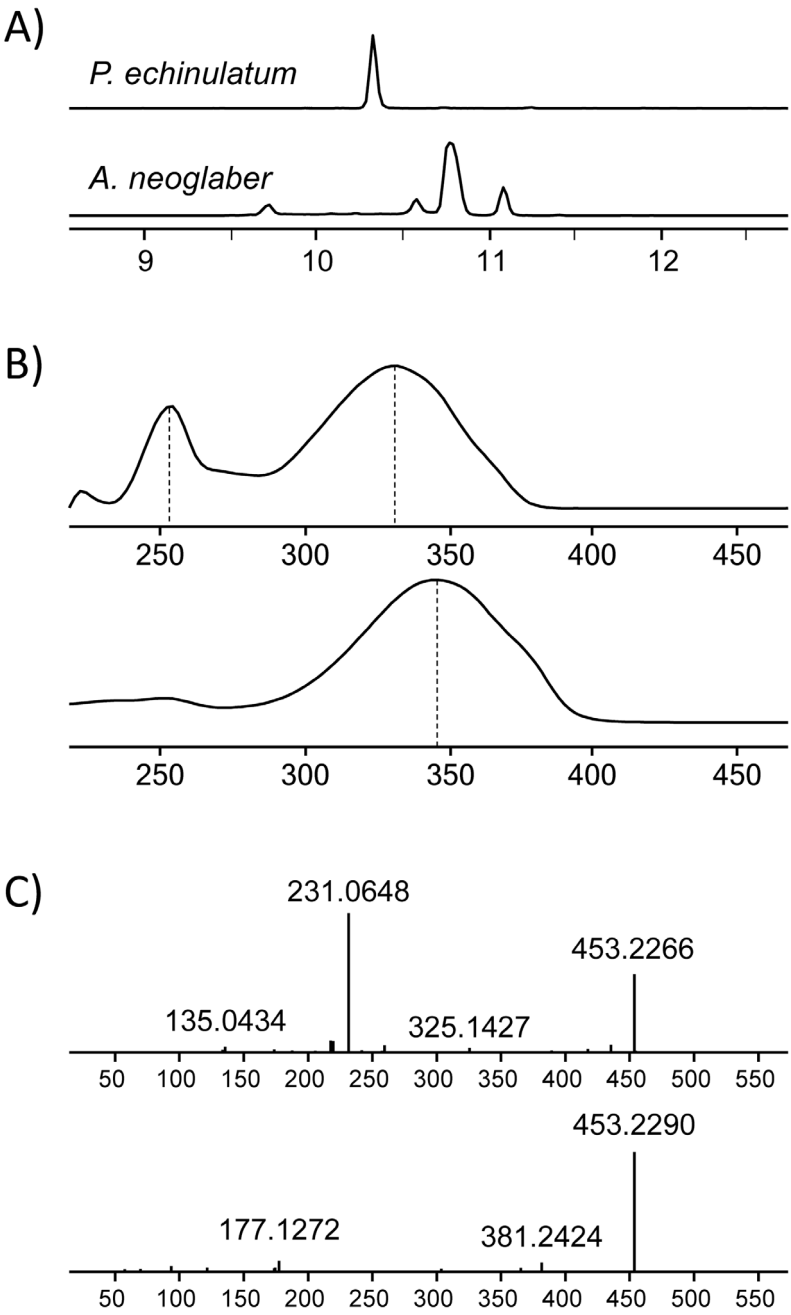


Figure S5. A) Extracted ion chromatogram (m/z 453.2277) for extracts from *P. echinulatum* and *A. neoglaber*. B) UV-VIS spectra for the m/z 453 compounds in *P. echinulatum* (top) and *A. neoglaber* (bottom). C) Tandem mass spectra (20 eV) for the m/z 453 compounds in *P. echinulatum* (top) and *A. neoglaber* (bottom).