

Supplementary Materials of “Synthesis and Structural Identification of a Biaryl Ether-Linked Zearalenone Dimer” by Julia Keller, Luisa Hantschke, Hajo Haase and Matthias Koch.

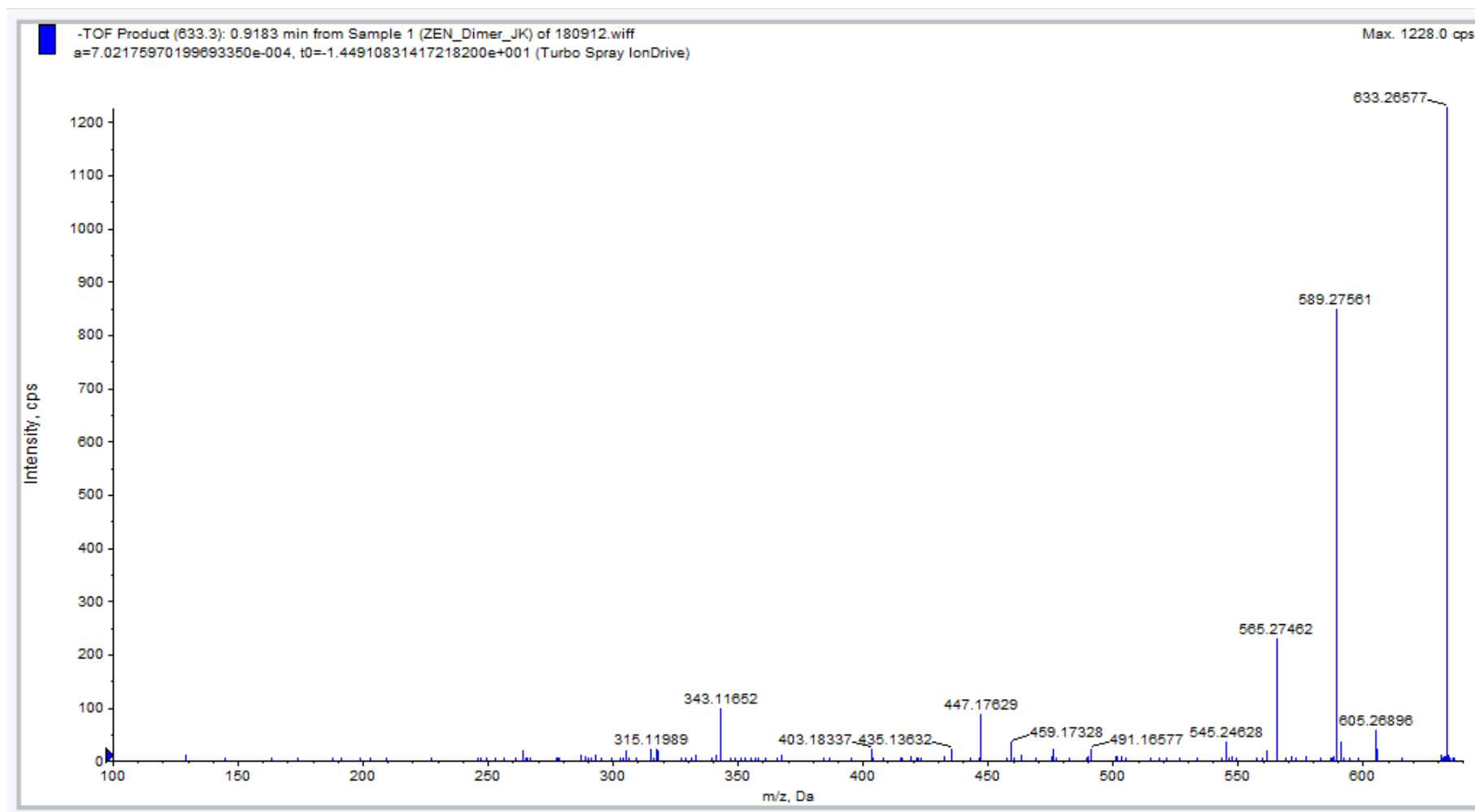


Fig. S1 MS/MS fragmentation spectrum of the ZEN-dimer obtained with Q-TOF in negative ionization mode.

Keller, BAM, ZEN-Dimer

File: H BAM 023942 W

Pulse Sequence: PROTON

Solvent: cd3od

Temp. 29.0 C / 302.1 K

Data from MR-400 "WallE"

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 7225.4 Hz

16 repetitions

OBSERVE H1, 399.8564448 MHz

DATA PROCESSING

Line broadening 0.1 Hz

FT size 262144

Total time 1 min, 20 sec

Datum: Jul 10 2018

Operator: U. Franke

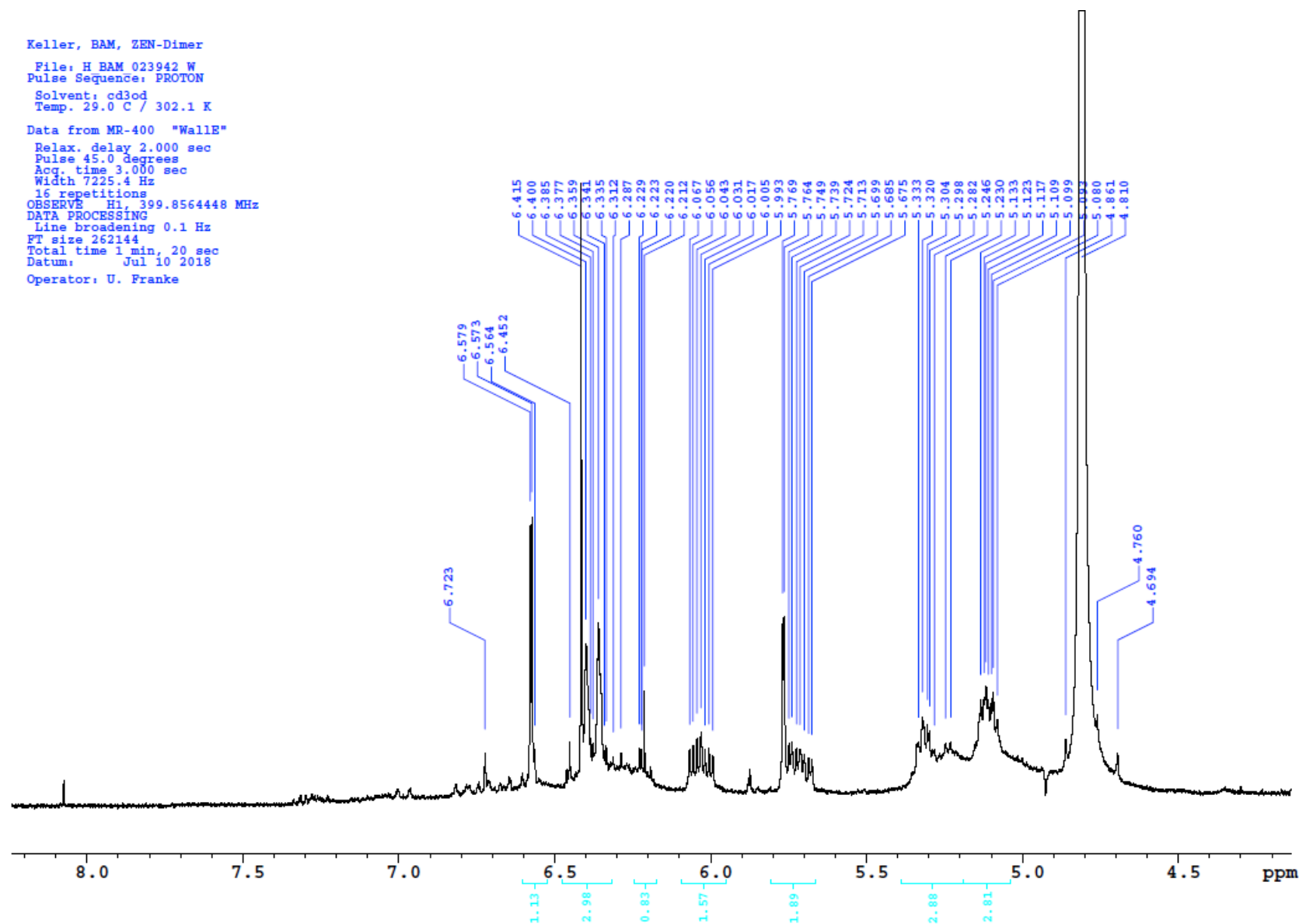


Fig. S2 ¹H-NMR spectrum of the 16-O-15'-biaryl ether-linked zearelenone dimer

Keller, BAM, SEW-Dimer
 File: C_BAM_007635.W
 Pulse Sequence: CARBON
 Solvent: cd3od
 Temp. 29.0 C / 302.1 K
 Data from MR-400 "WALLE"
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.285 sec
 Width 25510.2 Hz
 10000 repetitions
 OBSERVE C13, 100.5438413 MHz
 DECOUPLE H1, 399.8584467 MHz
 Power 45 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 65536
 Total time 6 hr, 20 min, 46 sec
 Datum: Jul 10 2018
 Operator: U. Franke

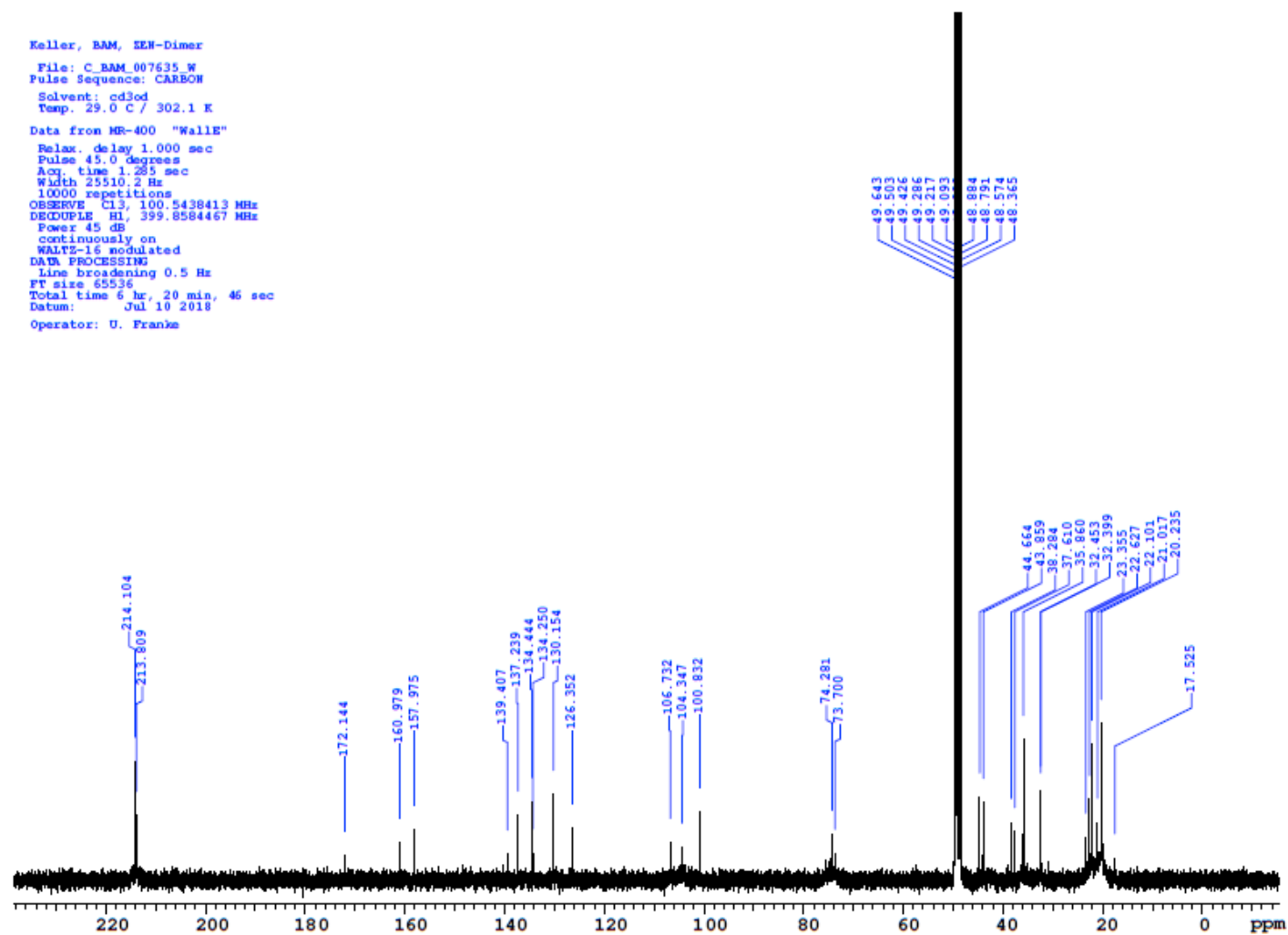


Fig. S3 ^{13}C -NMR spectrum of the 16-O-15'-biaryl ether-linked zearealenone dimer

Keller, BAM, ZEN-Dimer
 File: 2D_BAM_001134.W
 Pulse Sequence: gCOSY
 Solvent: cd3od
 Temp: 29.0 C / 302.1 K
 Data from MR-400 "Walle"
 Relax. delay 1.000 sec
 Acq. time 0.150 sec
 Width: 7225.4 Hz
 2D Width 7225.4 Hz
 4 repetitions
 200 increments
 OBSERVE H1, 399.8564429 MHz
 DATA PROCESSING
 Sg. sine bell 0.071 sec
 F1 DATA PROCESSING
 Sg. sine bell 0.028 sec
 FT size 2048 x 2048
 Total time 16 min, 30 sec
 Datum: Jul 4 2018
 Operator: U. Franke

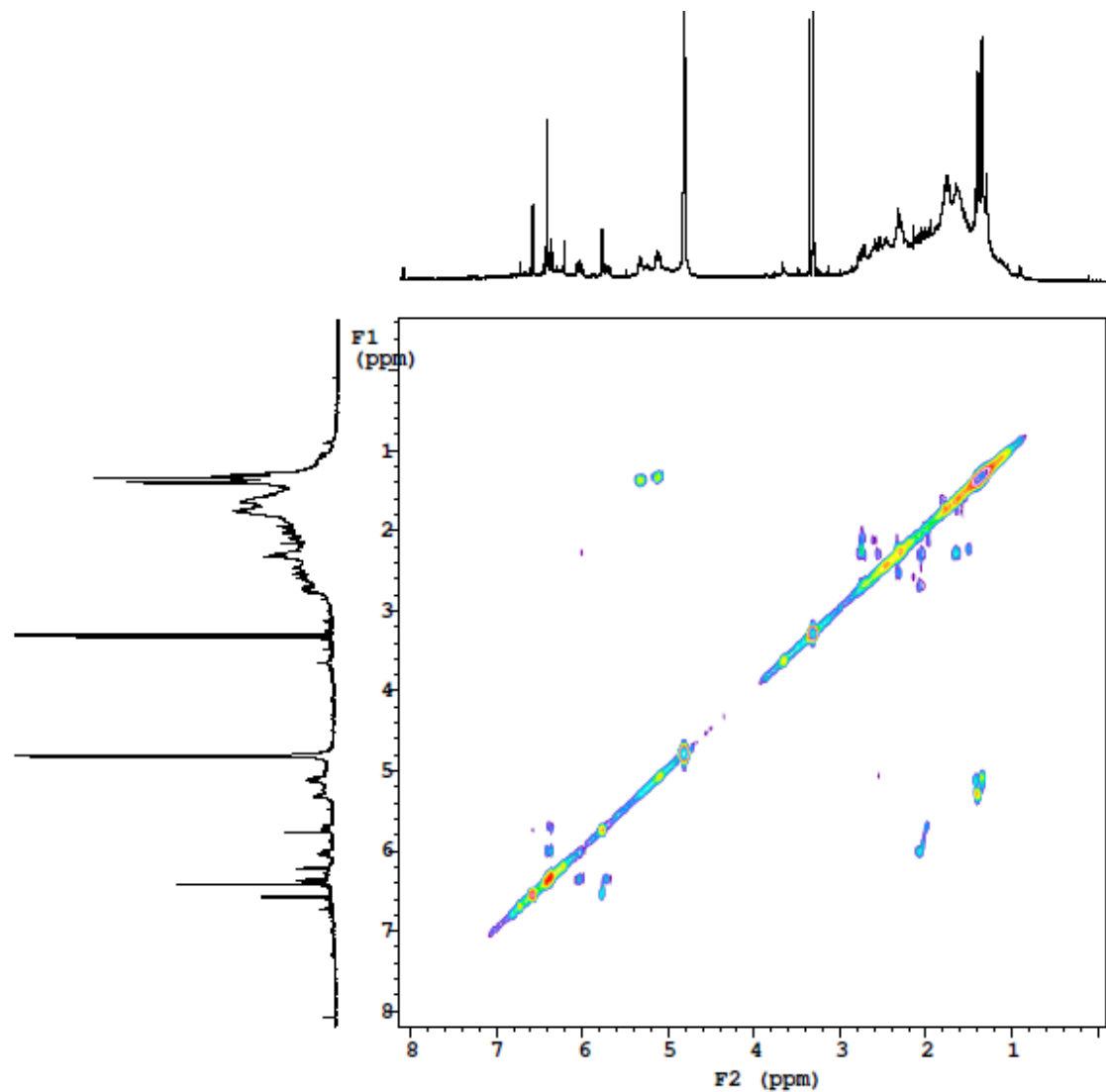


Fig. S4 COSY spectrum of the 16-O-15'-biaryl ether-linked zearelenone dimer

Keller, BAM, ZEN-Dimer

File: 2D_BAM_001141.W

Pulse Sequence: ghmbscad

Solvent: cd3od

Temp. 29.0 C / 302.1 K

Data from MR-400 "Walle"

Relax. delay 1.000 sec

Acq. time 0.150 sec

Width 7225.4 Hz

2D Width 24132.7 Hz

16 repetitions

2 x 256 increments

OBSERVE H1, 399.8564452 MHz

DATA PROCESSING

Sq. sine bell 0.071 sec

F1 DATA PROCESSING

Gauss apodization 0.010 sec

FT size 2048 x 2048

Total time 2 hr, 49 min, 35 sec

Datum: Jul 10 2018

Operator: U. Franke

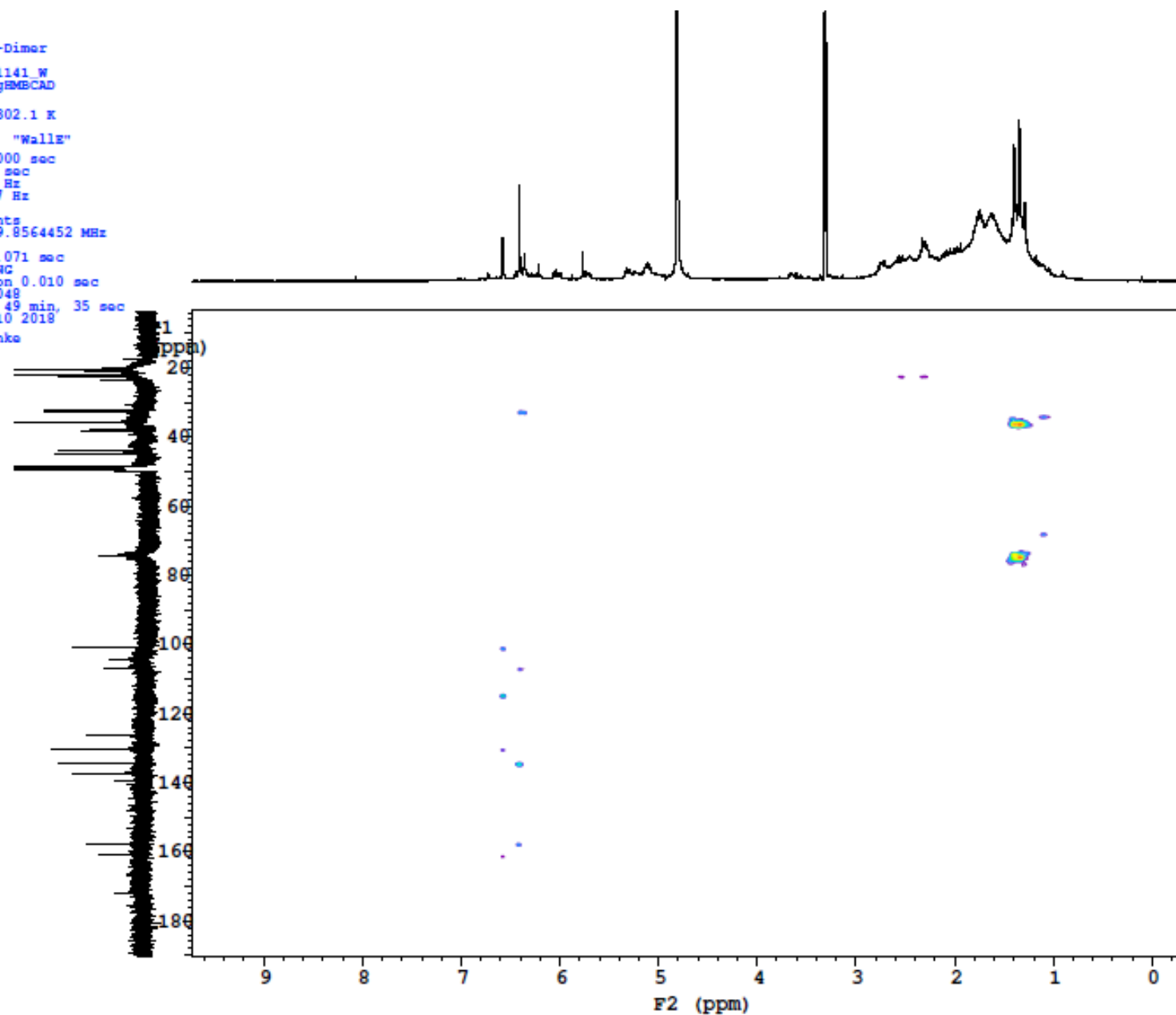


Fig. S5 HMBC spectrum of the 16-O-15'-biaryl ether-linked zearalenone dimer

Keller, BAM, ZEN-Dimer

File: 2D BAM 001143 W
Pulse Sequence: HSQCAD

Solvent: cd3od
Temp. 29.0 C / 302.1 K

Data from MR-400 "WallE"

Relax. delay 1.000 sec
Acq. time 0.150 sec
Width 7225.4 Hz
2D Width 20110.6 Hz
8 repetitions
2 x 200 increments
OBSERVE H1, 399.8564452 MHz
DECOUPLE C13, 100.5530326 MHz
Power 36 dB
on during acquisition
off during delay
W40 ATB2 modulated

DATA PROCESSING

Gauss apodization 0.065 sec
F1 DATA PROCESSING
Gauss apodization 0.009 sec
FT size 2048 x 2048
Total time 1 hr, 4 min, 35 sec
Datum: Jul 10 2018

Operator: U. Franke

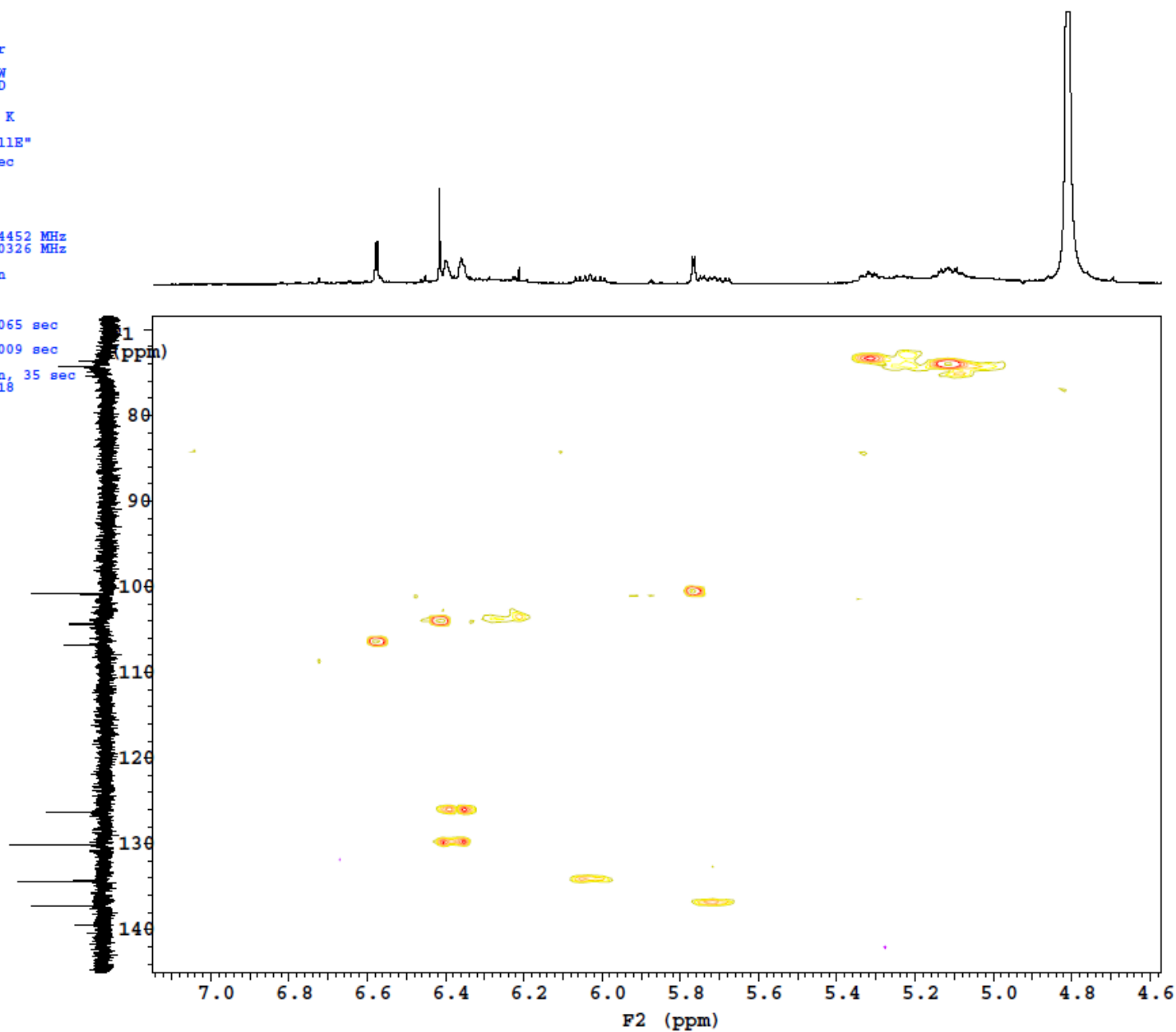


Fig. S6 HSQC spectrum of the 16-O-15'-biaryl ether-linked zearelenone dimer

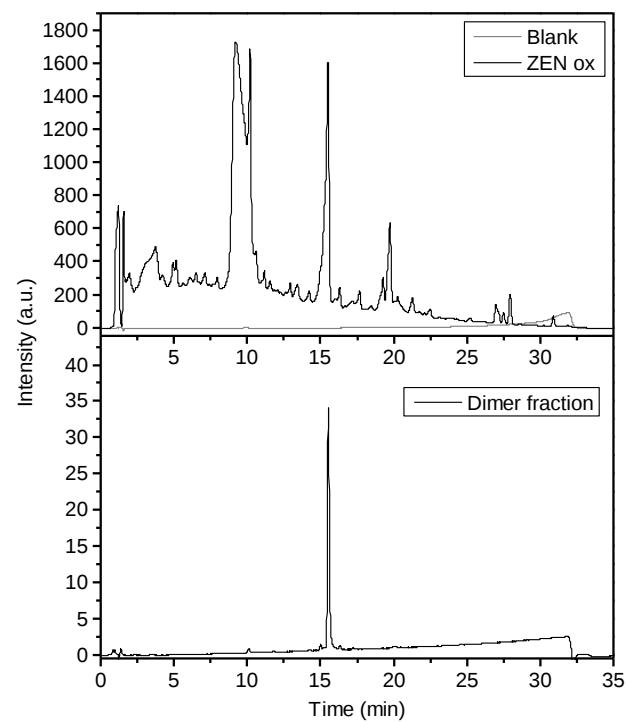


Fig. S7 HPLC-DAD chromatograms ($\lambda=254$ nm) of the zearelenone dimer reaction mixture before fractionation (top) and after fractionation (bottom)