Settings on Orbitrap Elite

Method for molecular analysis of Dissolved Organic Matter (DOM)

Supporting file to publication:

" Molecular signals of heterogeneous terrestrial environments identified in dissolved organic matter: A comparative analysis of Orbitrap and ion cyclotron resonance mass spectrometers "

By Carsten Simon, Vanessa-Nina Roth, Thorsten Dittmar and Gerd Gleixner.

# This is no tune file to be directly used in Thermo Tune Plus Software. It rather gives numbers to instrument settings that

# - can be controlled by the user (U),

# - may be tuned (T), or

# - can only be observed (O).

#######################################################################

# General settings

U Spectrum type Profile

U Averaging No

U Profile mode Reduced

U Advanced Signal Processing: On

U FT apodization: On

U FT zero offset: On

# Syringe Pump

U Flow Rate (microliter/min): 7.00

U Syringe Diameter (mm): 3.26

U Syringe Type: Hamilton, 500 microliters

# ESI Source

U Spray Voltage (kV): 2.65

T Spray Current (microA): 0.26

T Sheath Gas Flow Rate: 25.00

T Aux Gas Flow Rate: 0.2

T Sweep Gas Flow Rate: 0.09

U Capillary Temp (Celsius): 274.97

T S-Lens RF Level (%): 70

# Scan settings

U Mass Range Normal

U Resolution 240000

U Scan type Full

U Microscans 1

U Max Inject time (ms): 100

U Source Fragmentation (SID): On

U SID Energy (V): 40.0

U Locking: Off

# Vacuum

O Ion Gauge (E-5 Torr): 1.67

O Convectron Gauge (Torr): 1.49

# FT Vacuum

O FT Penning Gauge (E-10 Torr): 0.49

O FT Pirani Gauge 1 (Torr): 1.59

O FT Pirani Gauge 2 (Torr): 0.00

# Ion Optics

T Multipole 00 Offset (V): 41.02

T Lens 0 (V): 43.19

T Multipole 0 Offset (V): 49.4

T Lens 1 (V): 57.18

O Gate Lens (V): 130.07

T Multipole 1 Offset (V): 53.2

T Multipole RF (Vp-p): 791.86

T Front Lens (V): 50.02

O Front Section Offset (V): 53.07

O Center Section Offset (V): 56.04

O Back Section Offset (V): 51.06

O Back Lens (V): 57.14

# FT Ion Optics

U AGC Target (FT, Full MS) 1.00E+06

U Full Scan Injection Waveforms Yes

O Trap Eject Offset (V): 6.00

O FT Transfer Multipole Offset (V): -3.79

O FT Transfer Multipole Amplitude (Vp-p): 500.00

O FT Gate Lens Offset (V): -3.37

O FT Trap Lens Offset (V): -8.09

O FT Storage Multipole Offset (V): -7.95

O FT Storage Multipole Amplitude (Vp-p): 500.00

O FT Reflect Lens Offset (V): 11.22

O FT Main RF Amplitude (Vp-p): 1370.36

O FT Main RF Current (A): 0.19

O FT Main RF Frequency (kHz): 3033.77

O FT HV Ion Energy (V): -1574.87

O FT HV Lens 2 (V): 0.00

O FT HV Lens 3 (V): 266.09

O FT HV Lens 4 (V): 0.37

O FT HV Lens 6 (V): -668.98

O FT HV Push Voltage (V): -171.33

O FT HV Pull Voltage (V): 250.27

# Main RF

O Main RF Detected (V): 0.00

O RF Detector Temp (Celsius): 58.89

O RF Generator Temp (Celsius): 46.19

# Ion Detection System

O Dynode (kV): 14.93

O Multiplier 1 (V): -1588.74

O Multiplier 2 (V): -1530.63

# FT Analyzer

O FT CE Measure Voltage (V): 3453.68

O FT CE Inject Voltage (V): 2743.66

O FT Deflector Measure Voltage (V): -440.81

O FT Deflector Inject Voltage (V): -16.54

O FT Analyzer Temp. (Celsius): 25.99

O FT Analyzer TEC Voltage: 2.86

O FT Analyzer TEC Current: 0.76

O FT Analyzer TEC Temp. (Celsius): 26.40

O FT CE Electronics Temp. (Celsius): 31.85

O FT CE Electronics TEC Temp. (Celsius): 25.18