

CHARACTERIZATION DATA FOR

Rational design of bioavailable photosensitizers for manipulation and imaging of biological systems

Thomas C Binns^{1,2,3}, Anthony X Ayala¹, Jonathan B Grimm¹, Ariana N Tkachuk¹, Guillaume A Castillon⁴, Sebastien Phan⁴, Lixia Zhang¹, Timothy A Brown¹, Zhe Liu¹, Stephen R Adams⁵, Mark H Ellisman⁴, Minoru Koyama¹, and Luke D Lavis^{1,6,*}

¹Janelia Research Campus; Howard Hughes Medical Institute; Ashburn, VA, 20147; USA

²Graduate School; University of Arkansas for Medical Sciences; Little Rock, AR, 72205; USA

³College of Medicine; University of Arkansas for Medical Sciences; Little Rock, AR, 72205; USA

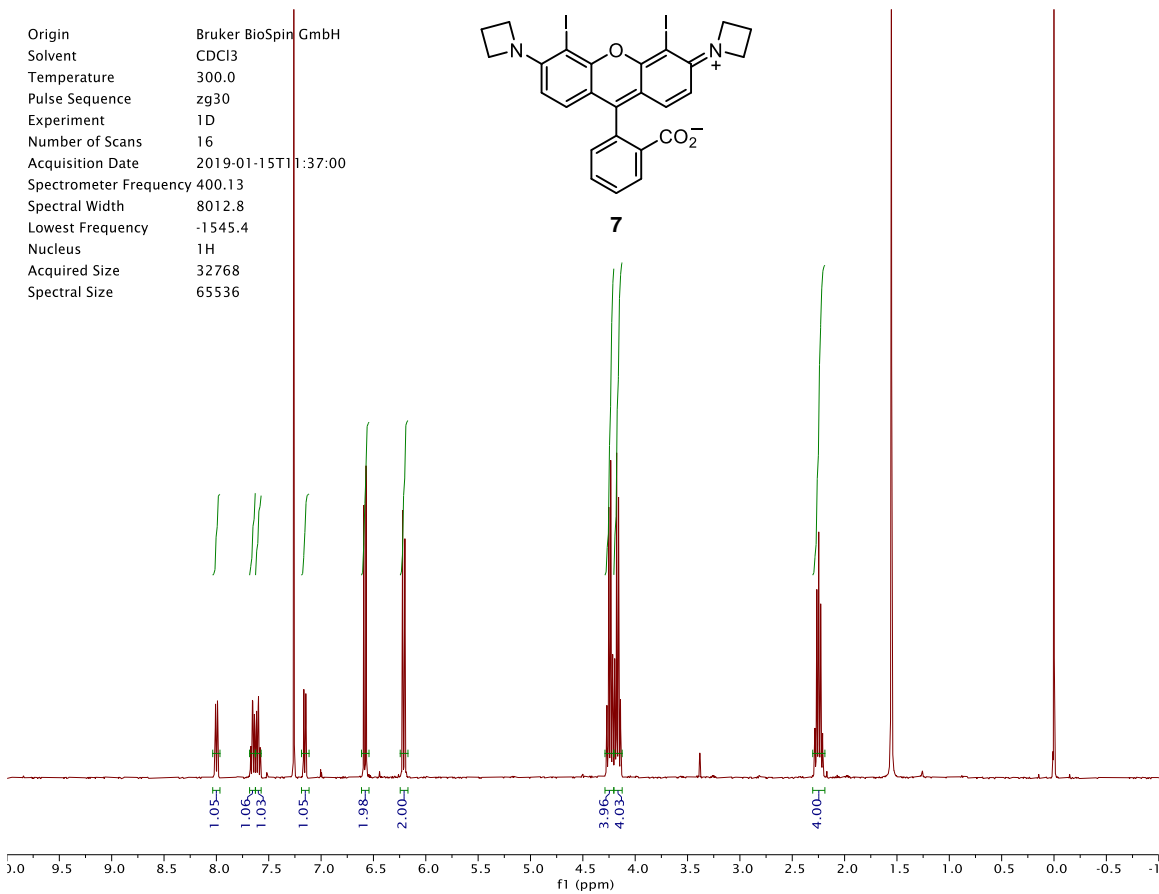
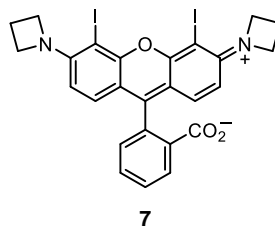
⁴Department of Neurosciences; University of California San Diego; La Jolla, CA, 92093; USA

⁵Department of Pharmacology; University of California San Diego; La Jolla, CA, 92093; USA

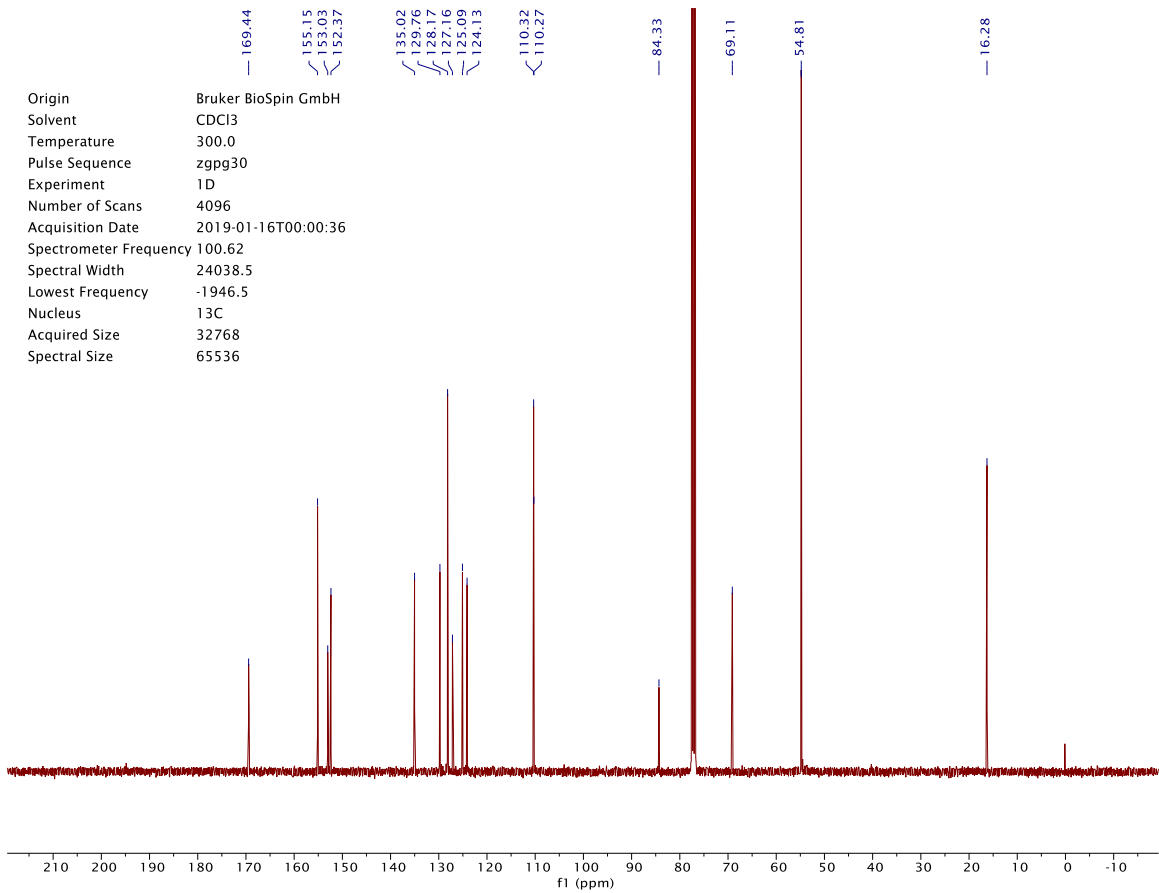
⁶Lead Contact

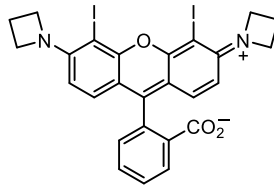
*Corresponding author email: lavisl@janelia.hhmi.org

Origin Bruker BioSpin GmbH
 Solvent CDCl3
 Temperature 300.0
 Pulse Sequence zg30
 Experiment 1D
 Number of Scans 16
 Acquisition Date 2019-01-15T11:37:00
 Spectrometer Frequency 400.13
 Spectral Width 8012.8
 Lowest Frequency -1545.4
 Nucleus 1H
 Acquired Size 32768
 Spectral Size 65536



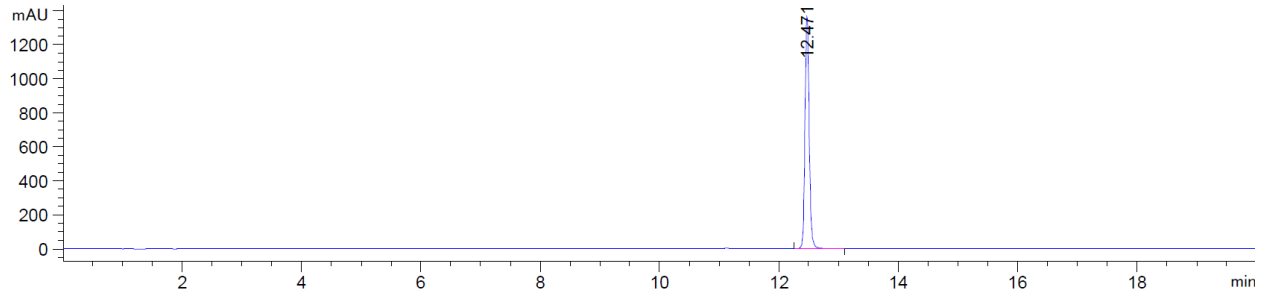
Origin Bruker BioSpin GmbH
 Solvent CDCl3
 Temperature 300.0
 Pulse Sequence zgpg30
 Experiment 1D
 Number of Scans 4096
 Acquisition Date 2019-01-16T00:00:36
 Spectrometer Frequency 100.62
 Spectral Width 24038.5
 Lowest Frequency -1946.5
 Nucleus 13C
 Acquired Size 32768
 Spectral Size 65536



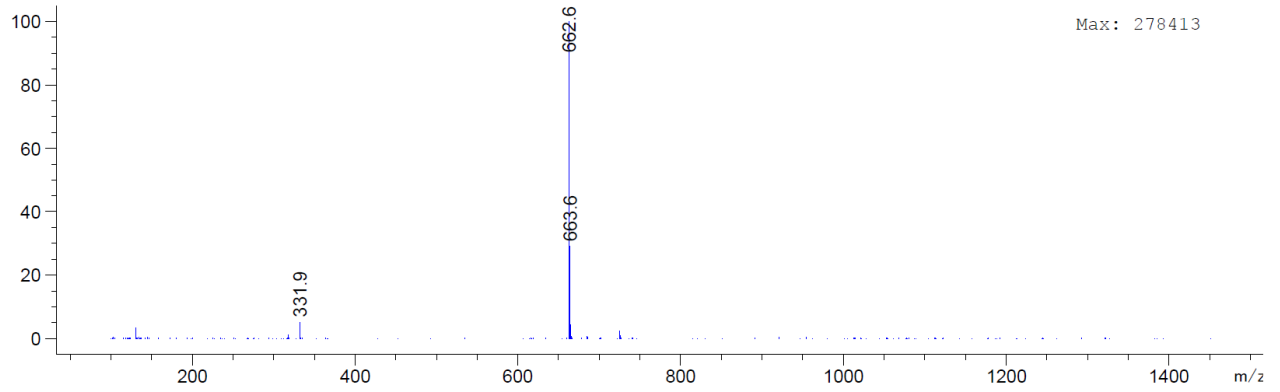


7

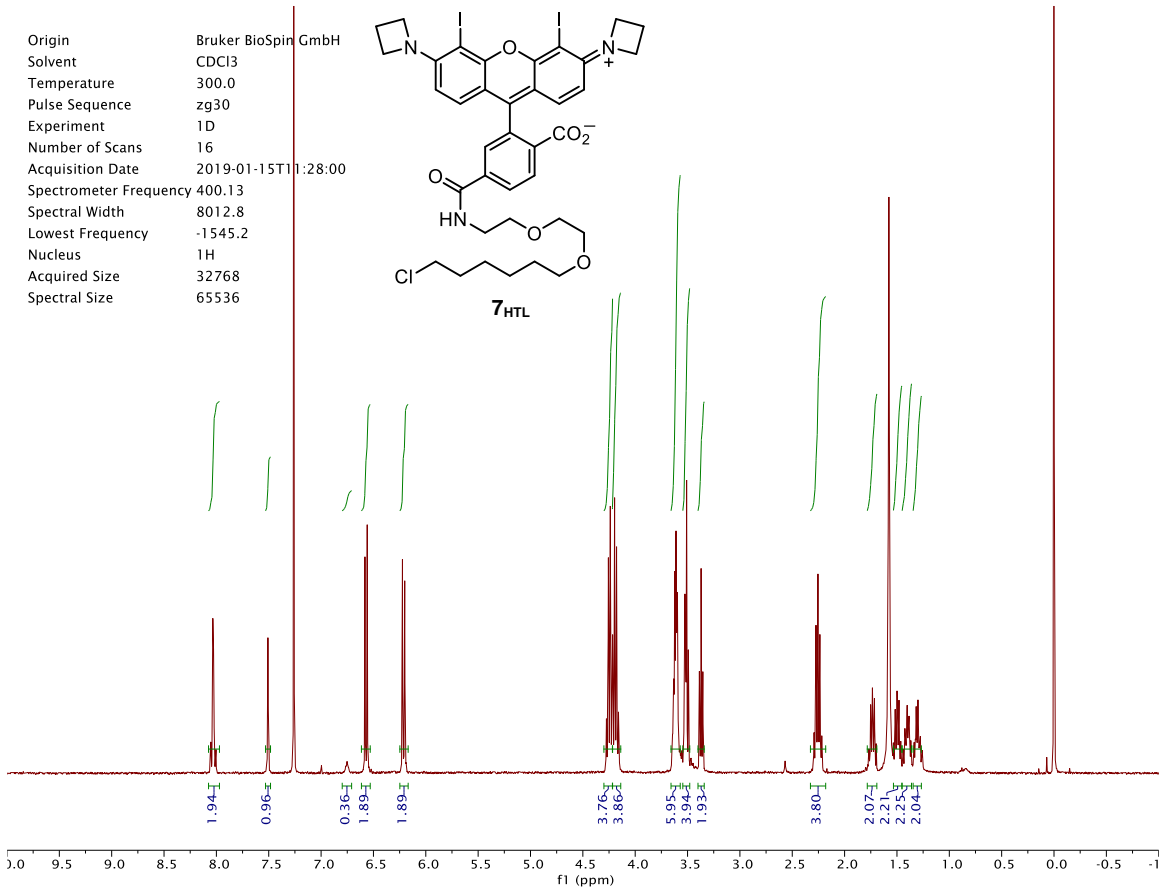
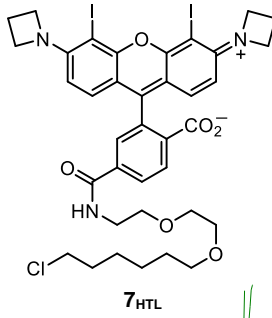
DAD1 C, Sig=575.4 Ref=off (2019_01\DAIY_SEQUENCE_LC 2019-01-11 14-51-07\2019_010000002.D)



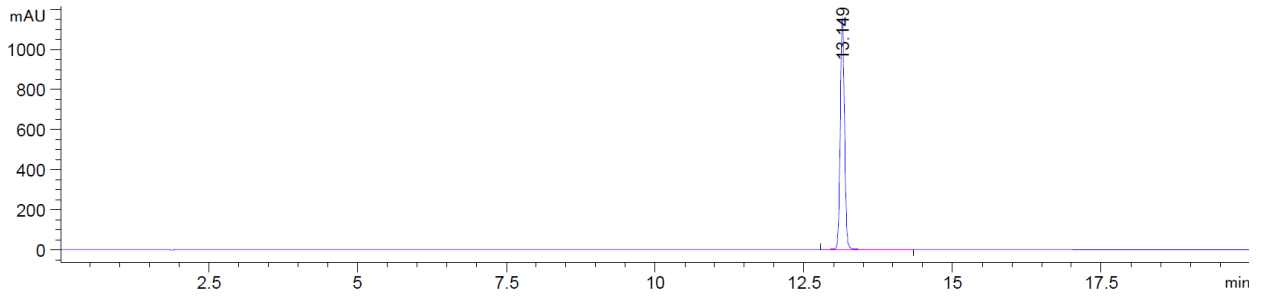
*MSD2 SPC, time=12.479:12.552 of C:\CHEM321\DATA\2019_01\DAIY_SEQUENCE_LC 2019-01-11 14-51-07\2019_010000002.D ES-



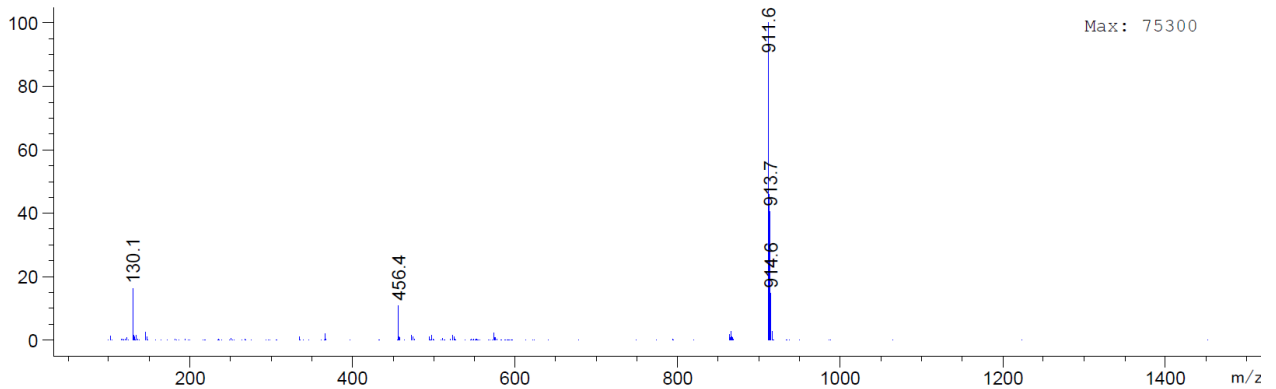
Origin: Bruker BioSpin GmbH
 Solvent: CDCl3
 Temperature: 300.0
 Pulse Sequence: zg30
 Experiment: 1D
 Number of Scans: 16
 Acquisition Date: 2019-01-15T11:28:00
 Spectrometer Frequency: 400.13
 Spectral Width: 8012.8
 Lowest Frequency: -1545.2
 Nucleus: 1H
 Acquired Size: 32768
 Spectral Size: 65536



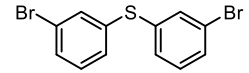
DAD1 C, Sig=575.4 Ref=off (2019_01\DAIY_SEQUENCE_LC 2019-01-11 11-10-29\2019_010000002.D)



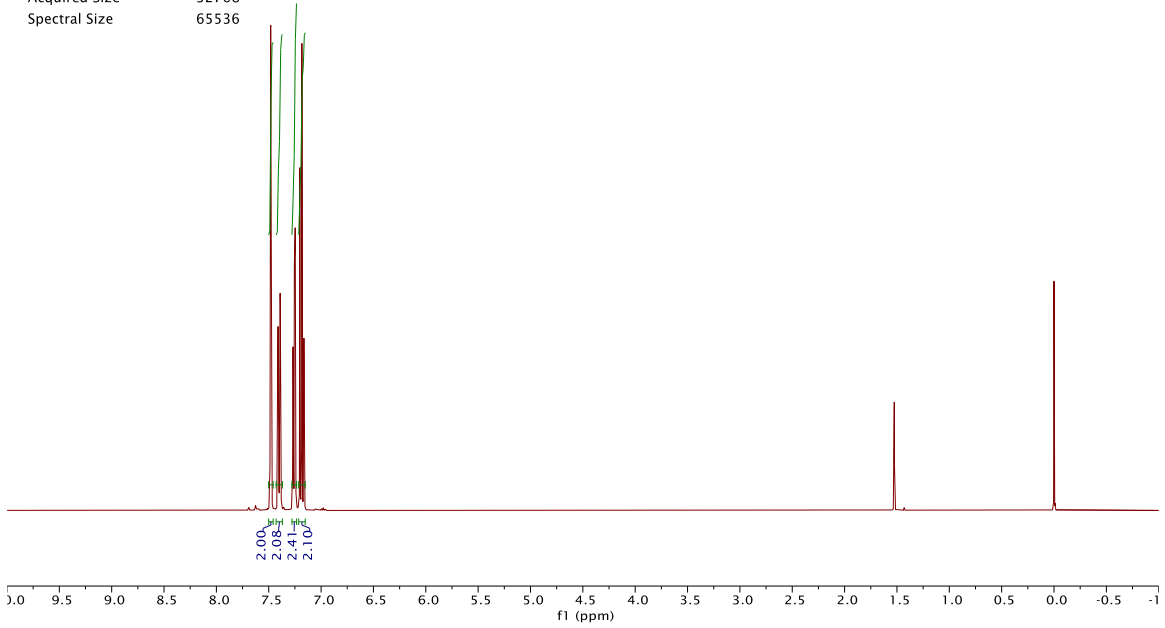
*MSD2 SPC, time=13.151:13.242 of C:\CHEM321\DATA\2019_01\DAIY_SEQUENCE_LC 2019-01-11 11-10-29\2019_010000002.D ES-



Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 300.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Acquisition Date 2018-03-19T19:06:00
Spectrometer Frequency 400.13
Spectral Width 8012.8
Lowest Frequency -1547.3
Nucleus 1H
Acquired Size 32768
Spectral Size 65536

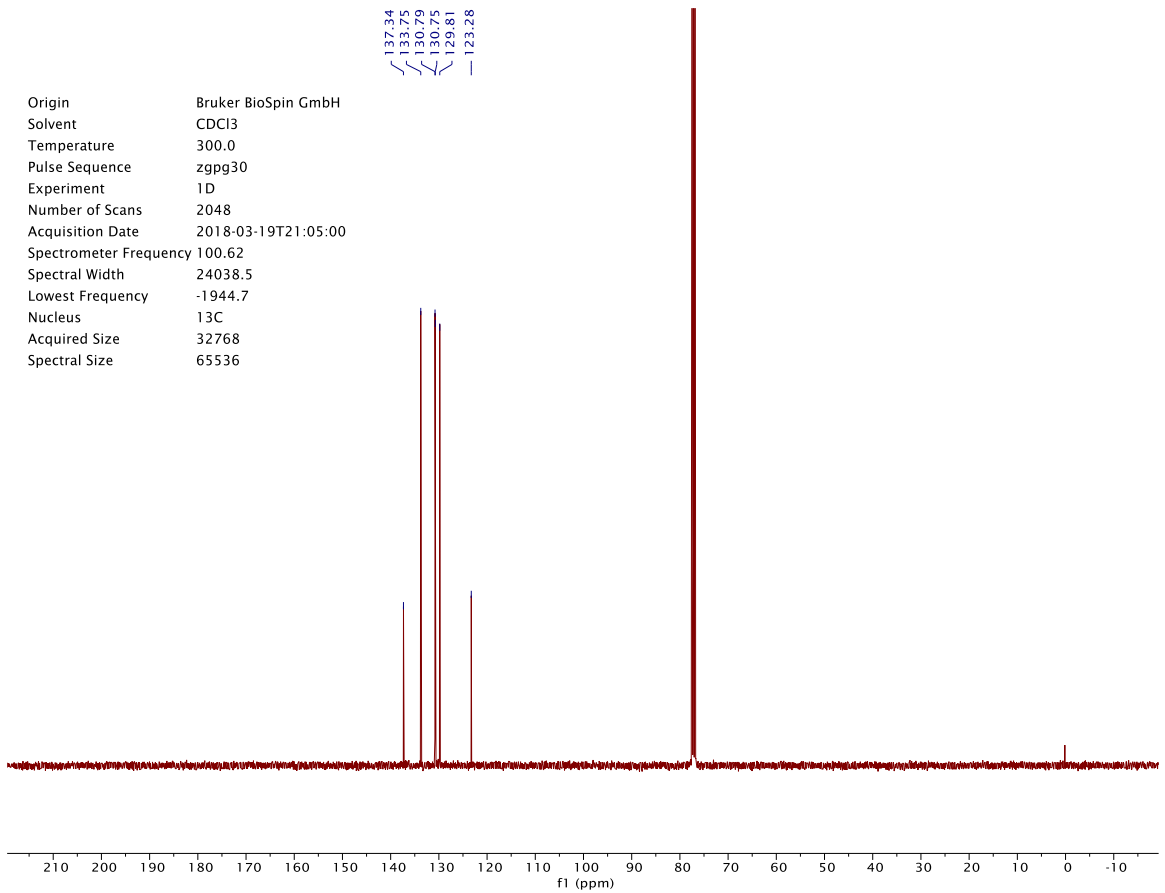


16

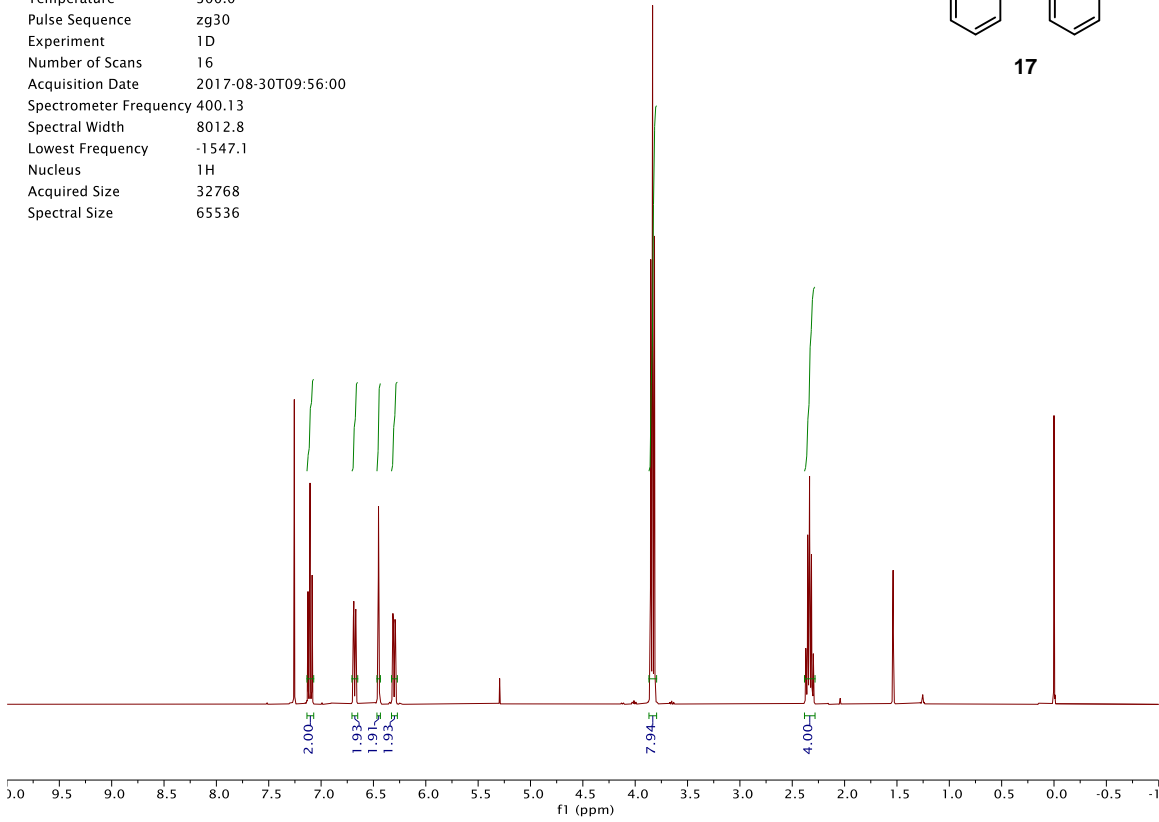
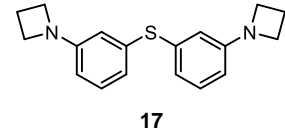


Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 300.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 2048
Acquisition Date 2018-03-19T21:05:00
Spectrometer Frequency 100.62
Spectral Width 24038.5
Lowest Frequency -1944.7
Nucleus 13C
Acquired Size 32768
Spectral Size 65536

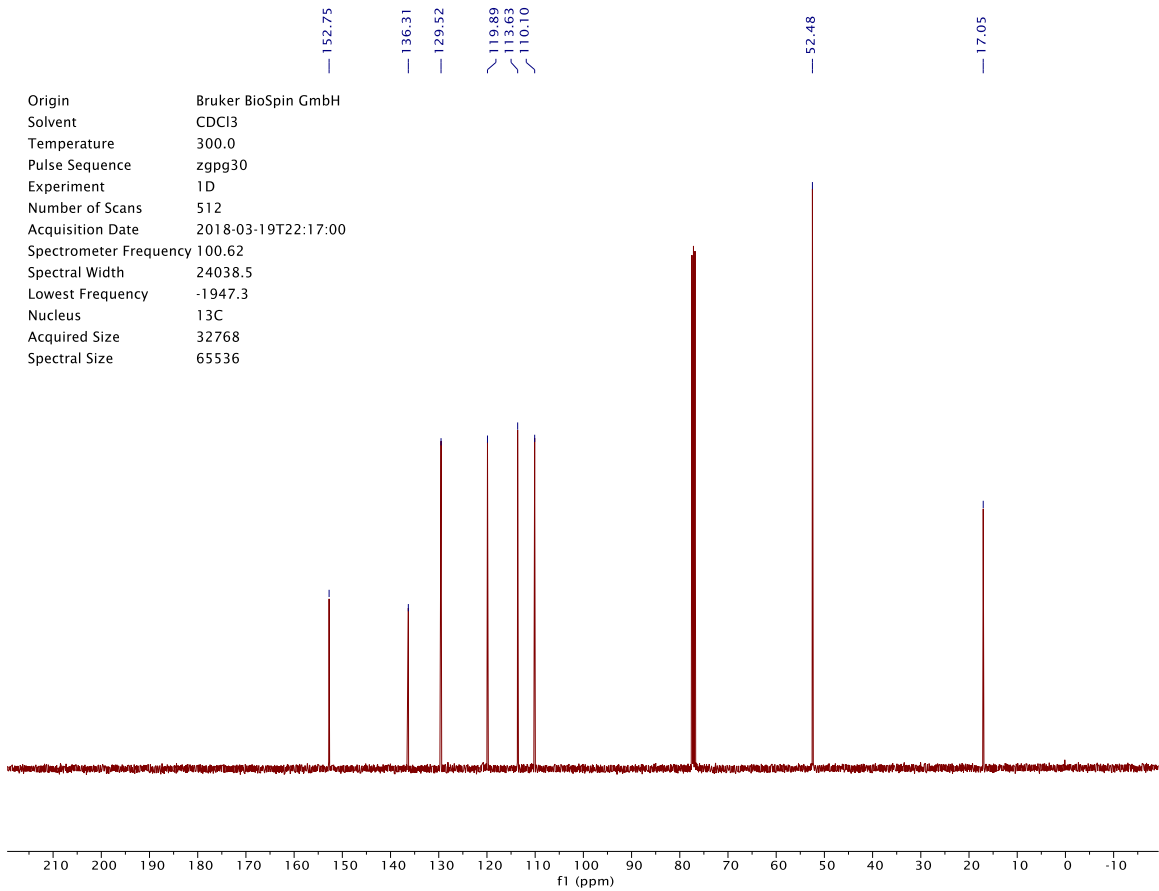
137.34
133.75
130.79
130.75
129.81
123.28



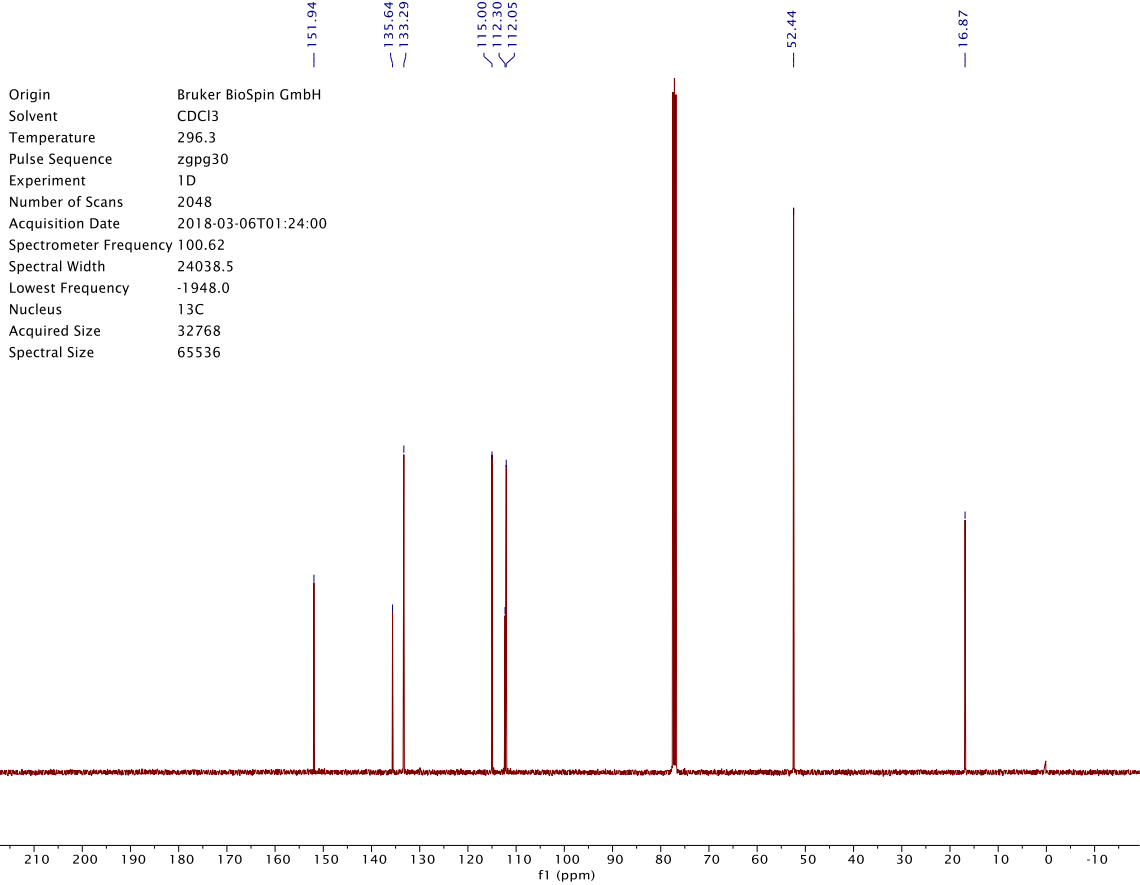
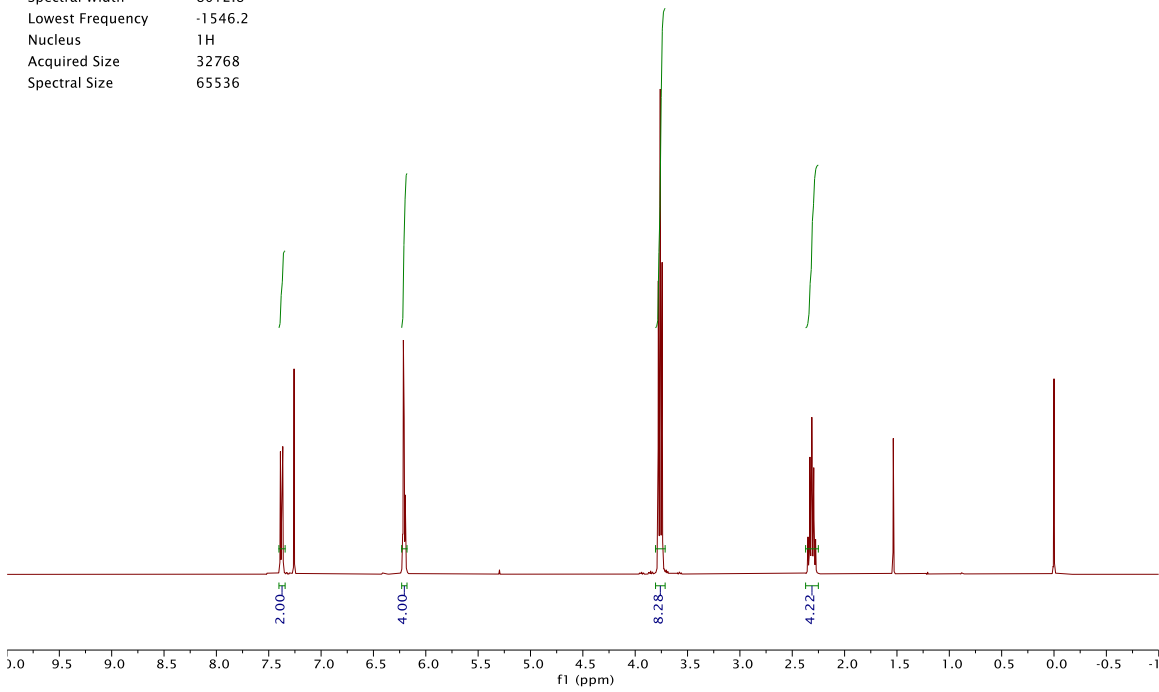
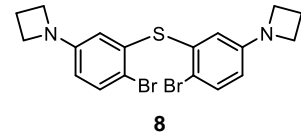
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 300.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Acquisition Date 2017-08-30T09:56:00
Spectrometer Frequency 400.13
Spectral Width 8012.8
Lowest Frequency -1547.1
Nucleus 1H
Acquired Size 32768
Spectral Size 65536



Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 300.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Acquisition Date 2018-03-19T22:17:00
Spectrometer Frequency 100.62
Spectral Width 24038.5
Lowest Frequency -1947.3
Nucleus 13C
Acquired Size 32768
Spectral Size 65536

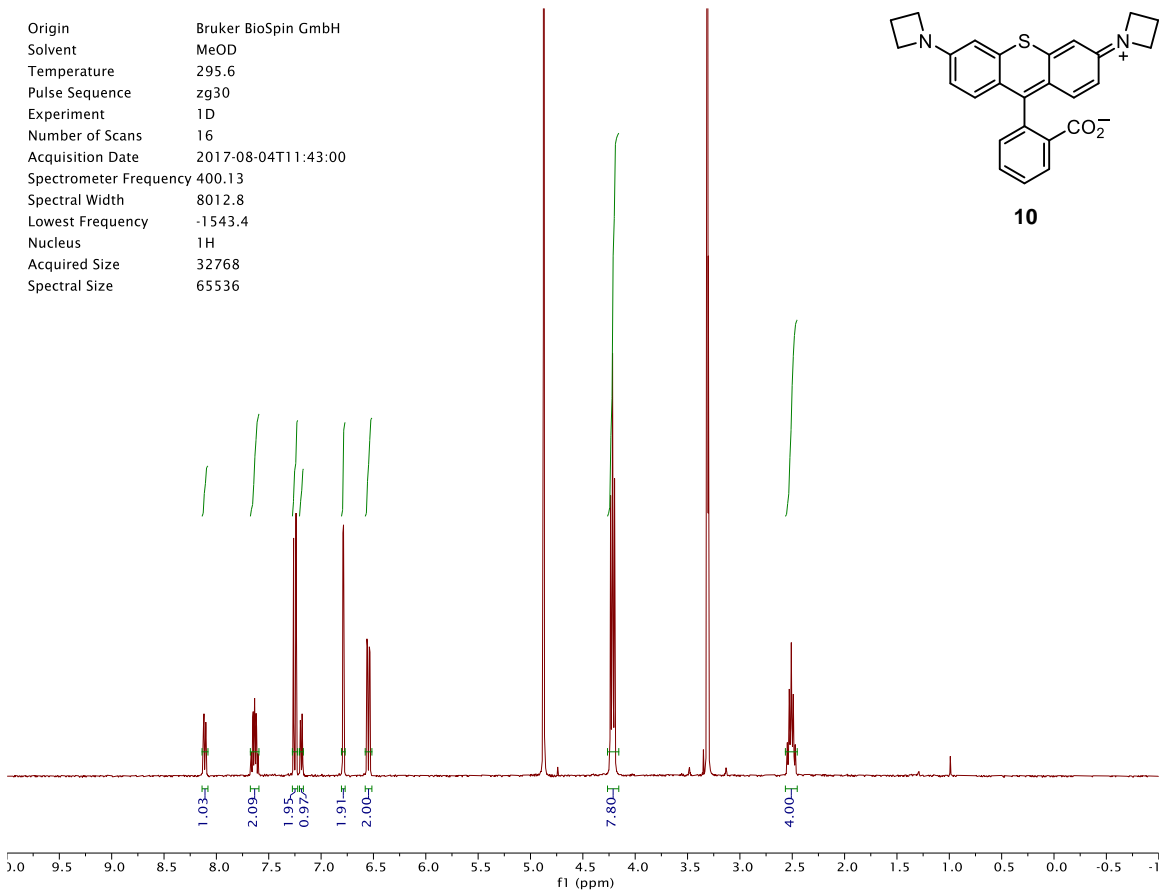
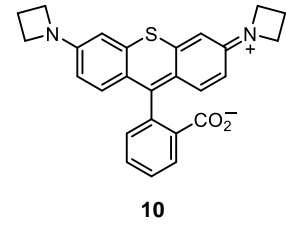


Origin Bruker BioSpin GmbH
 Solvent CDCl3
 Temperature 300.0
 Pulse Sequence zg30
 Experiment 1D
 Number of Scans 16
 Acquisition Date 2017-08-31T15:09:00
 Spectrometer Frequency 400.13
 Spectral Width 8012.8
 Lowest Frequency -1546.2
 Nucleus 1H
 Acquired Size 32768
 Spectral Size 65536

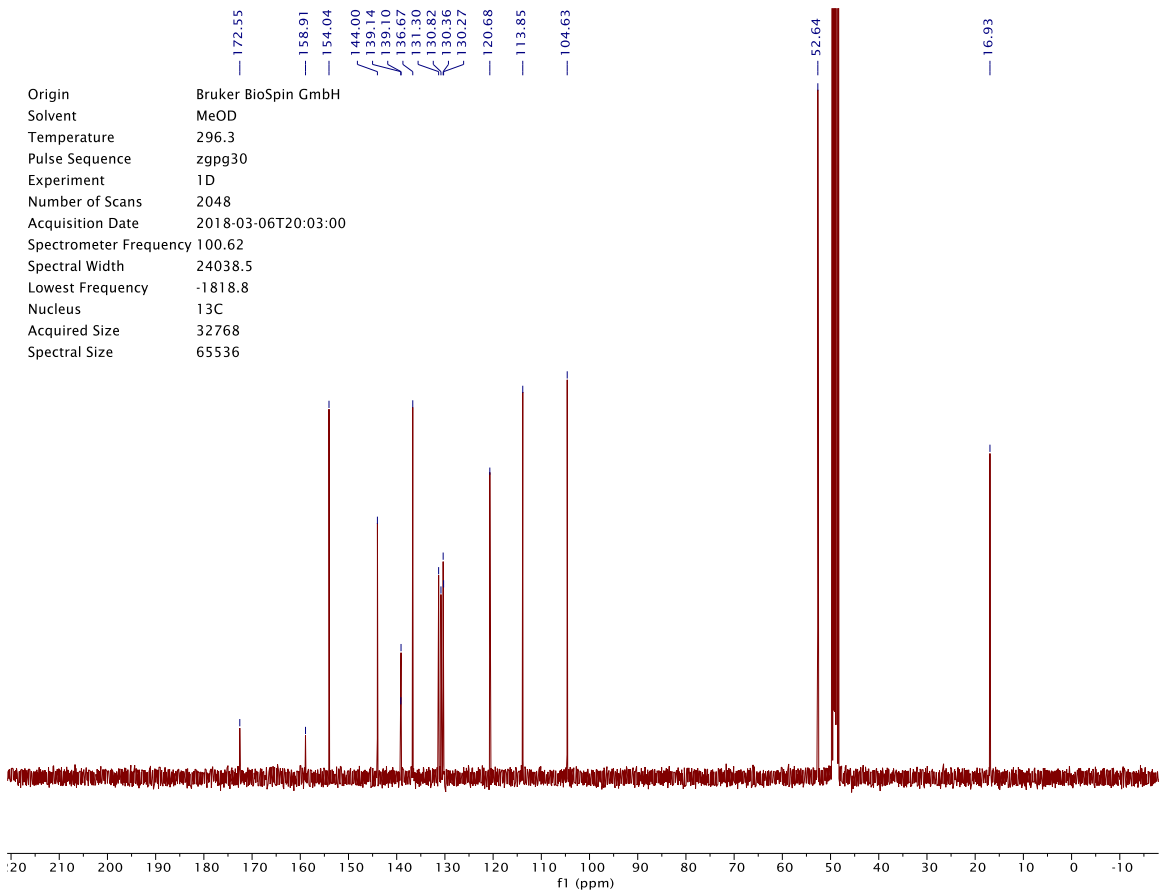


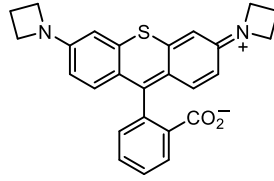
Origin Bruker BioSpin GmbH
 Solvent CDCl3
 Temperature 296.3
 Pulse Sequence zgpg30
 Experiment 1D
 Number of Scans 2048
 Acquisition Date 2018-03-06T01:24:00
 Spectrometer Frequency 100.62
 Spectral Width 24038.5
 Lowest Frequency -1948.0
 Nucleus 13C
 Acquired Size 32768
 Spectral Size 65536

Origin Bruker BioSpin GmbH
 Solvent MeOD
 Temperature 295.6
 Pulse Sequence zg30
 Experiment 1D
 Number of Scans 16
 Acquisition Date 2017-08-04T11:43:00
 Spectrometer Frequency 400.13
 Spectral Width 8012.8
 Lowest Frequency -1543.4
 Nucleus ¹H
 Acquired Size 32768
 Spectral Size 65536

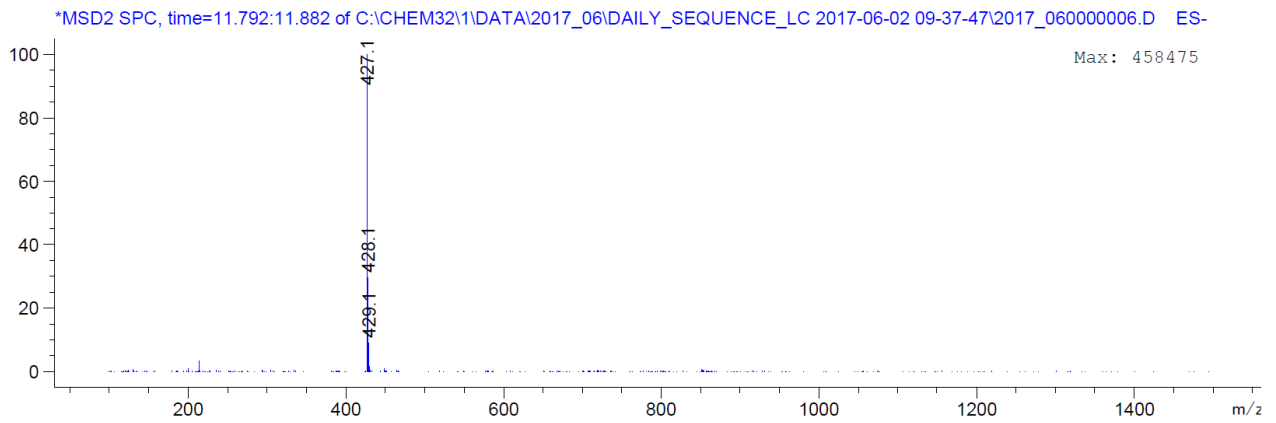
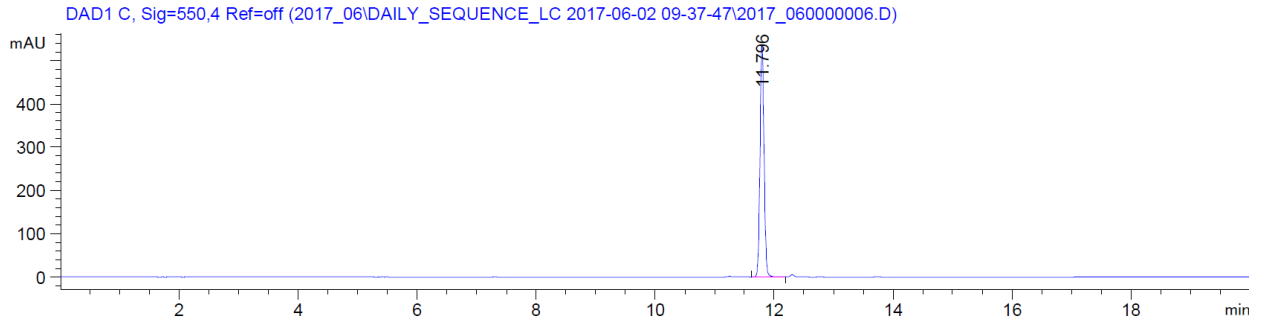


Origin Bruker BioSpin GmbH
 Solvent MeOD
 Temperature 296.3
 Pulse Sequence zgpg30
 Experiment 1D
 Number of Scans 2048
 Acquisition Date 2018-03-06T20:03:00
 Spectrometer Frequency 100.62
 Spectral Width 24038.5
 Lowest Frequency -1818.8
 Nucleus ¹³C
 Acquired Size 32768
 Spectral Size 65536

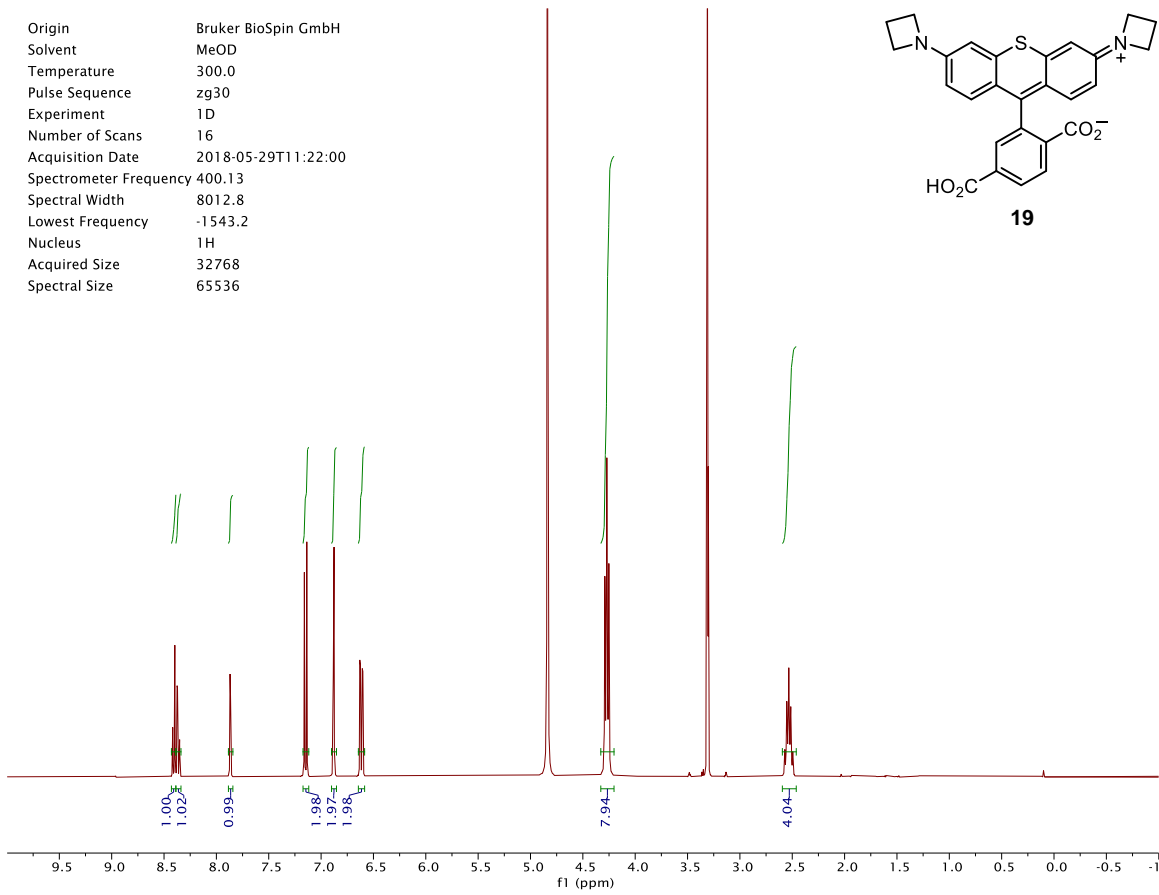
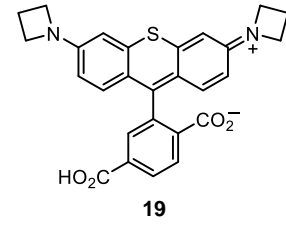




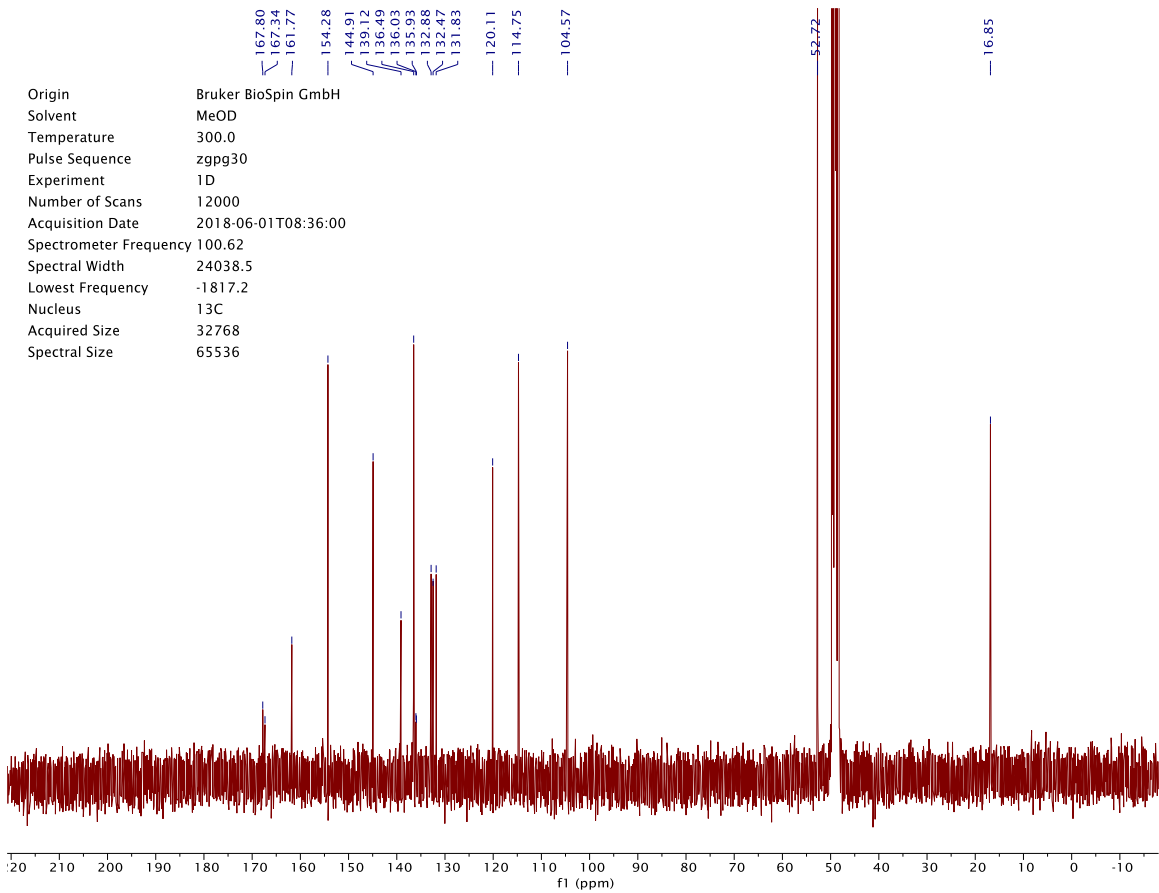
10

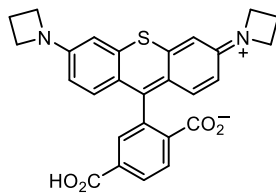


Origin Bruker BioSpin GmbH
 Solvent MeOD
 Temperature 300.0
 Pulse Sequence zg30
 Experiment 1D
 Number of Scans 16
 Acquisition Date 2018-05-29T11:22:00
 Spectrometer Frequency 400.13
 Spectral Width 8012.8
 Lowest Frequency -1543.2
 Nucleus ¹H
 Acquired Size 32768
 Spectral Size 65536



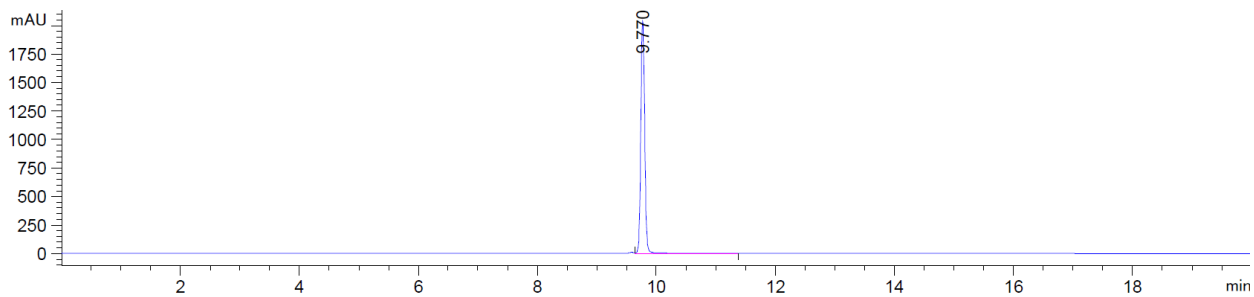
Origin Bruker BioSpin GmbH
 Solvent MeOD
 Temperature 300.0
 Pulse Sequence zgpg30
 Experiment 1D
 Number of Scans 12000
 Acquisition Date 2018-06-01T08:36:00
 Spectrometer Frequency 100.62
 Spectral Width 24038.5
 Lowest Frequency -1817.2
 Nucleus ¹³C
 Acquired Size 32768
 Spectral Size 65536



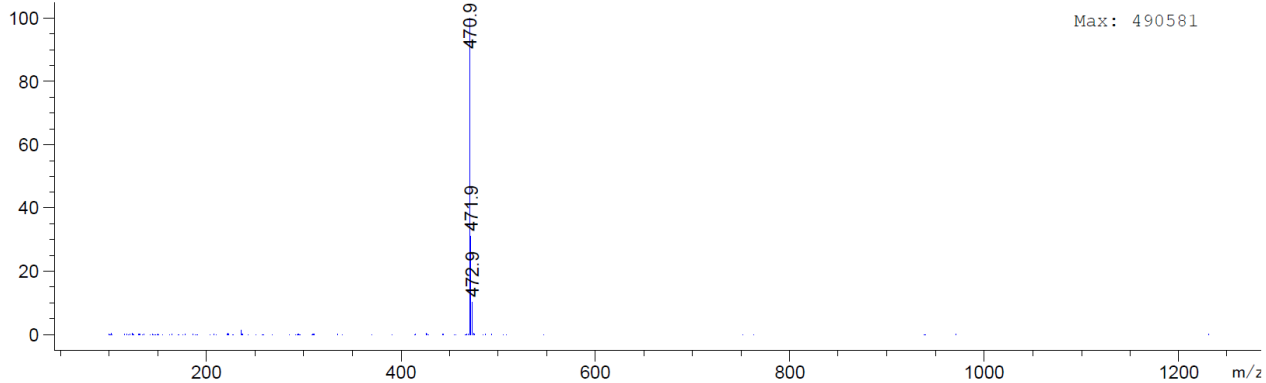


19

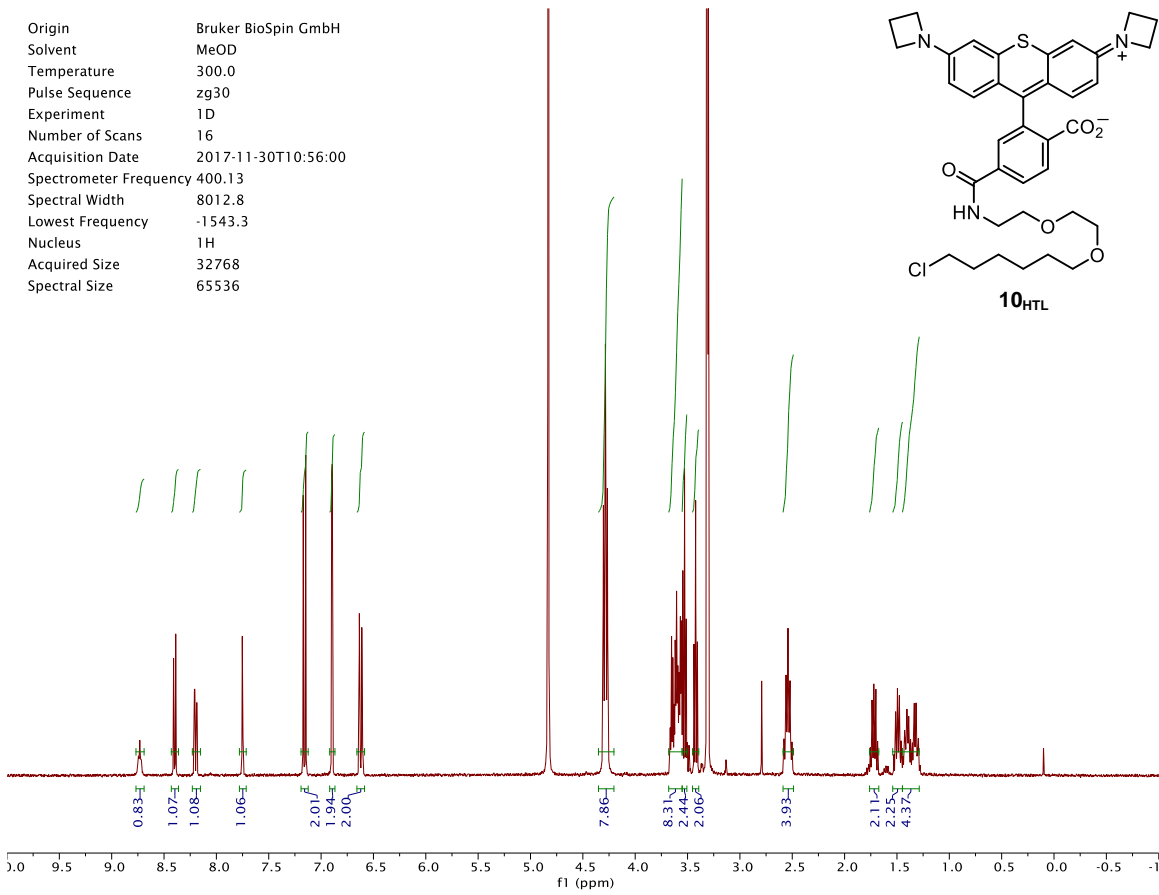
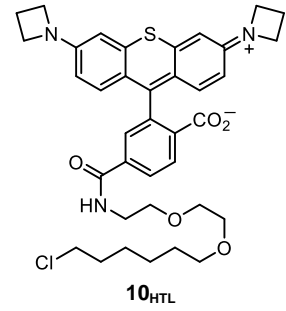
DAD1 C, Sig=575.4 Ref=off (2018_05\DAI..._SEQUENCE_LC 2018-05-25 13-19-21\2018_050000002.D)



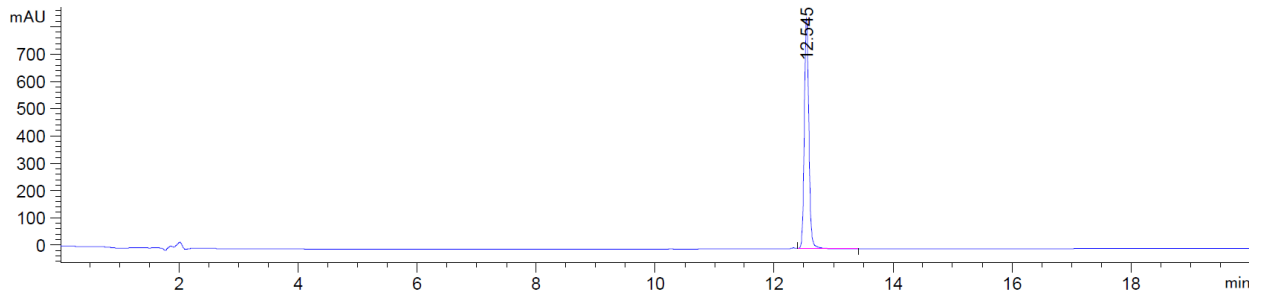
*MSD2 SPC, time=9.771:9.862 of C:\CHEM32\1\DATA\2018_05\DAI..._SEQUENCE_LC 2018-05-25 13-19-21\2018_050000002.D ES-AP



Origin Bruker BioSpin GmbH
 Solvent MeOD
 Temperature 300.0
 Pulse Sequence zg30
 Experiment 1D
 Number of Scans 16
 Acquisition Date 2017-11-30T10:56:00
 Spectrometer Frequency 400.13
 Spectral Width 8012.8
 Lowest Frequency -1543.3
 Nucleus ¹H
 Acquired Size 32768
 Spectral Size 65536



DAD1 C, Sig=575.4 Ref=off (2017_11\DAIY_SEQUENCE_LC 2017-11-27 16-18-22\2017_11000001.D)



*MSD2 SPC, time=12.646:12.736 of C:\CHEM321\DATA\2017_11\DAIY_SEQUENCE_LC 2017-11-27 16-18-22\2017_11000001.D ES-

