

**Synthesis and optical properties of heptamethine cyanine dyes containing a phenyl ring at
the *meso*-position.**

Andrew Levitz[#], Fahad Marmarchi[#], and Maged Henary^{*}

Department of Chemistry, Georgia State University, Atlanta, GA 30302, USA

^{*}To whom correspondence should be addressed. [#]These authors contributed equally to this work.

***Corresponding Author:**

Maged Henary, Ph.D.

100 Piedmont Ave. #315

Atlanta, GA 30303

Office: 404-413-5566; Fax: 404-413-5505

Email: mhenary1@gsu.edu

Supplemental Information

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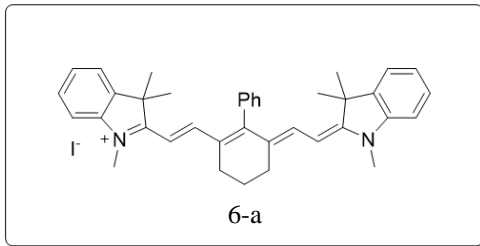
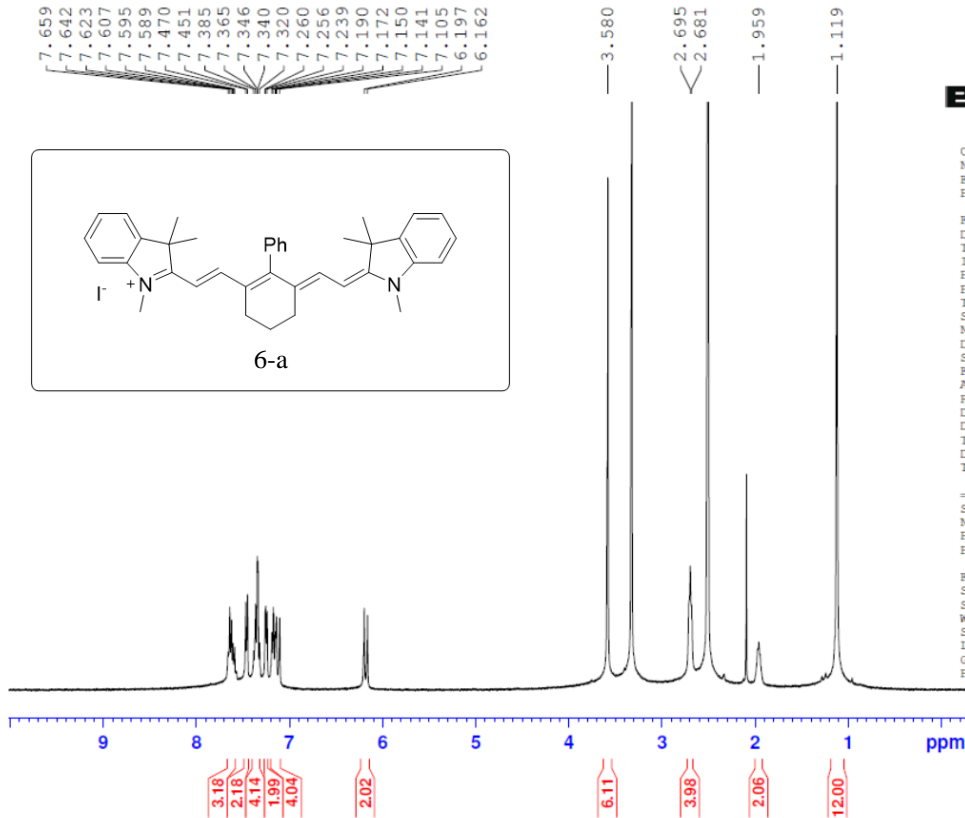
¹H and ¹³C NMR spectra of the dyes synthesized in this study

Absorbance and fluorescence spectra of the of the dyes synthesized in this study

Beer-Lambert plots of the of the dyes synthesized in this study

HSA binding spectra of 6k

Mass spectra of the dyes synthesized in this study



AL_167_DMSO_1H

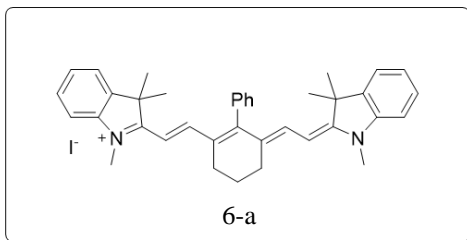
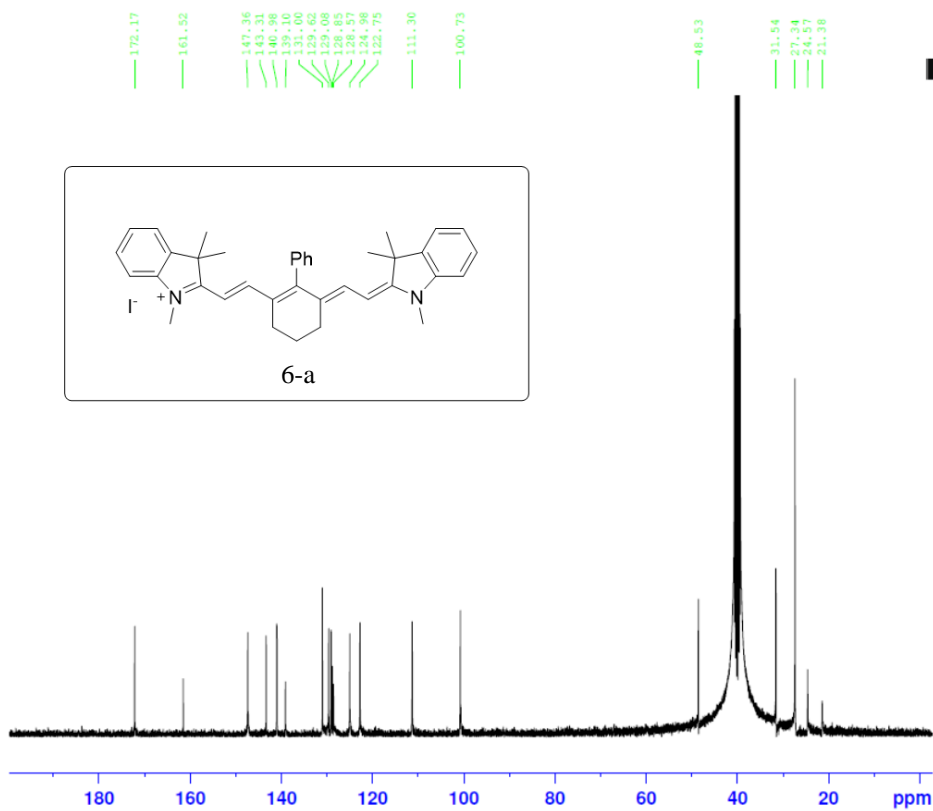
BRUKER

Current Data Parameters
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 PROCNO 1

F2 - Acquisition Parameters
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 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 19
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 203
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 SF01 400.1424710 MHz
 NUC1 1H
 P1 13.55 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1400000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



AL_167_DMSO_13C

BRUKER

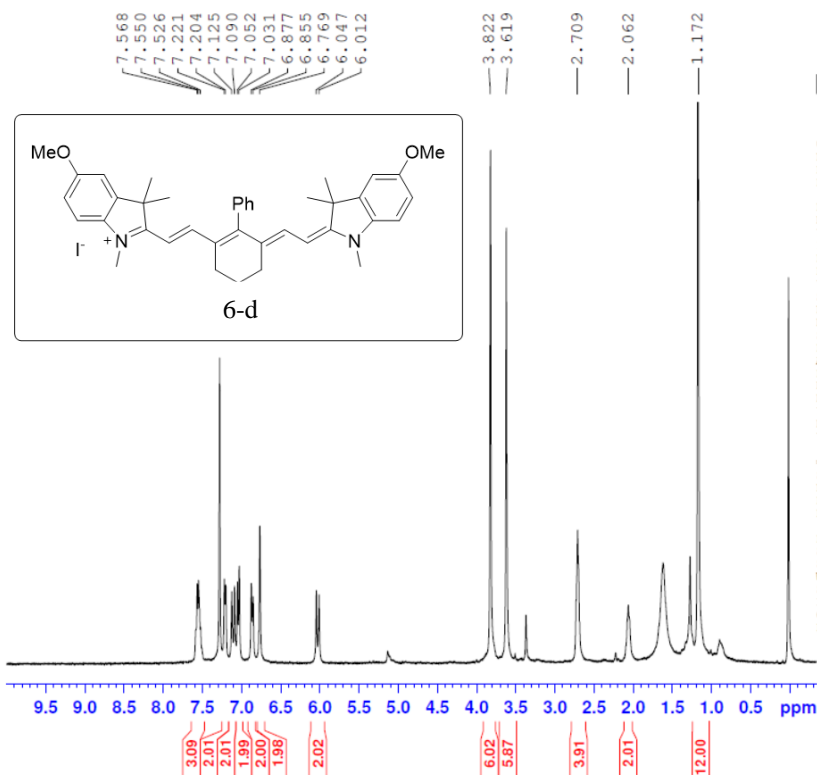
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 PULPROG jmod
 TD 65536
 SOLVENT DMSO
 NS 11153
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 298.0 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.00000000 sec
 D20 0.00689655 sec
 TD0 1

==== CHANNEL f1 =====
 SF01 100.6253446 MHz
 NUC1 13C
 P1 9.00 usec
 P2 18.00 usec
 PLW1 62.00000000 W

==== CHANNEL f2 =====
 SF02 400.1416006 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 16.00000000 W
 PLW12 0.36267000 W

F2 - Processing parameters
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 SF 100.6152830 MHz
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 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



AL_190_CDC13_1H

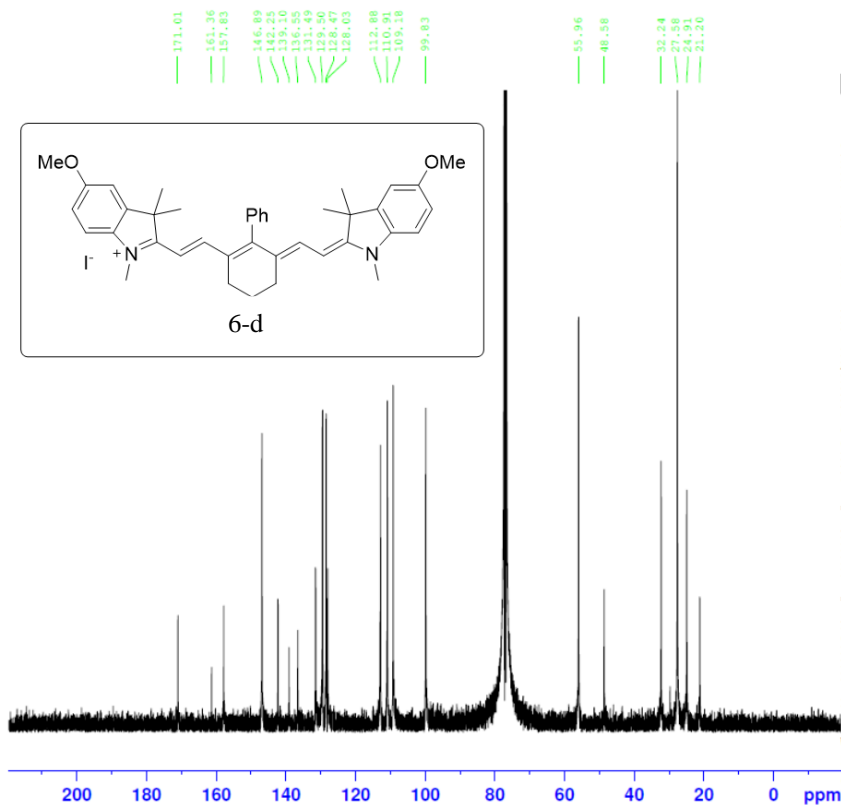


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 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
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 Time 14.12
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 27
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 203
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 SF01 400.1424710 MHz
 NUC1 1H
 P1 13.55 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1400000 MHz
 WDW EM
 SSB 0
 LB 0 0.30 Hz
 GB 0
 PC 1.00



AL_190_CDC13_13C



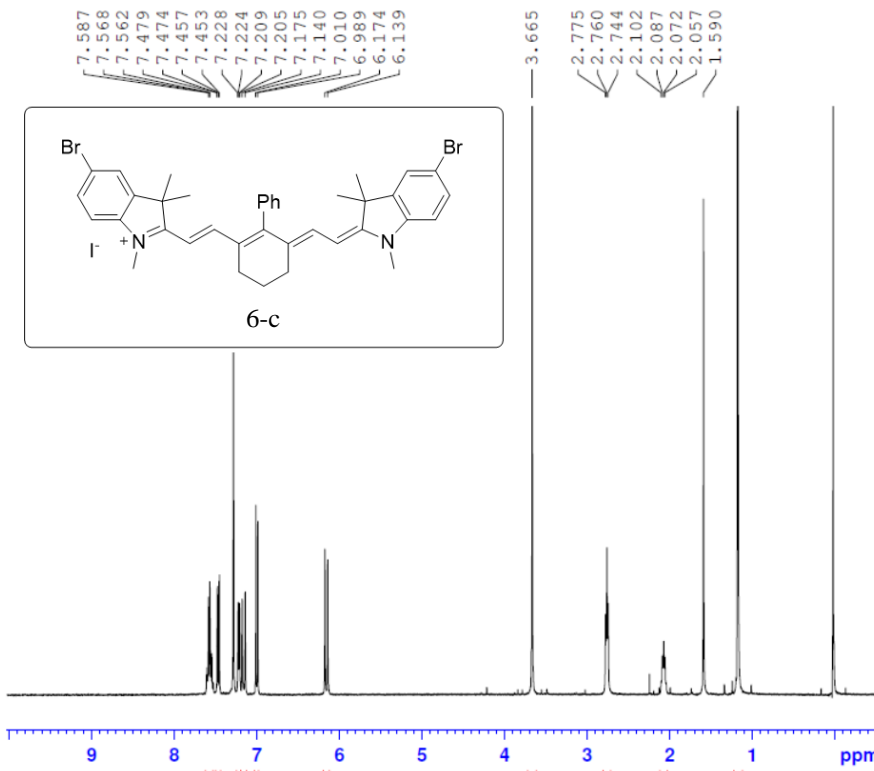
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 EXPNO 1
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F2 - Acquisition Parameters
 Date_ 20160424
 Time 23.29
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG jmod
 TD 65536
 SOLVENT CDC13
 NS 10074
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 298.1 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.00000000 sec
 D20 0.00689655 sec
 TD0 1

==== CHANNEL f1 =====
 SF01 100.6253446 MHz
 NUC1 13C
 P1 9.00 usec
 P2 18.00 usec
 PLW1 62.00000000 W

==== CHANNEL f2 =====
 SF02 400.1416006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 16.00000000 W
 PLW12 0.36267000 W

F2 - Processing parameters
 SI 32768
 SF 100.6152830 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



AL_181_CDC13_1H

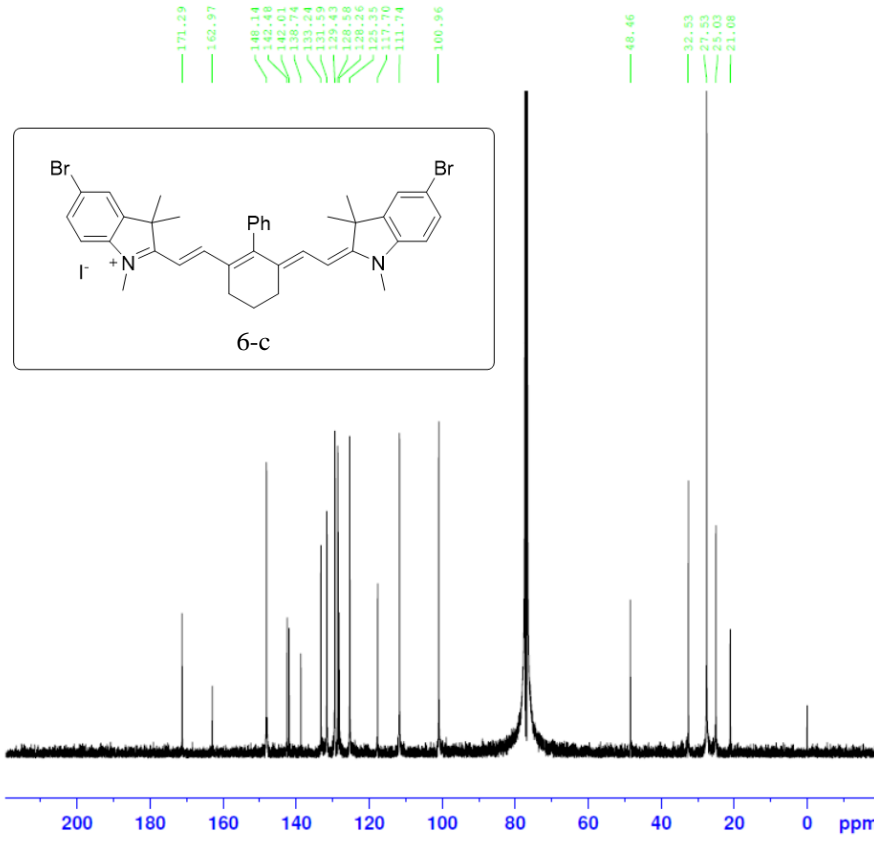


Current Data Parameters
 NAME AL_181_cdc13_1H
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160301
 Time 13.45
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 ID 65536
 SOLVENT CDCl3
 NS 9
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 203
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1424710 MHz
 NUC1 1H
 P1 13.55 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1400000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



AL_181_CDC13_13C



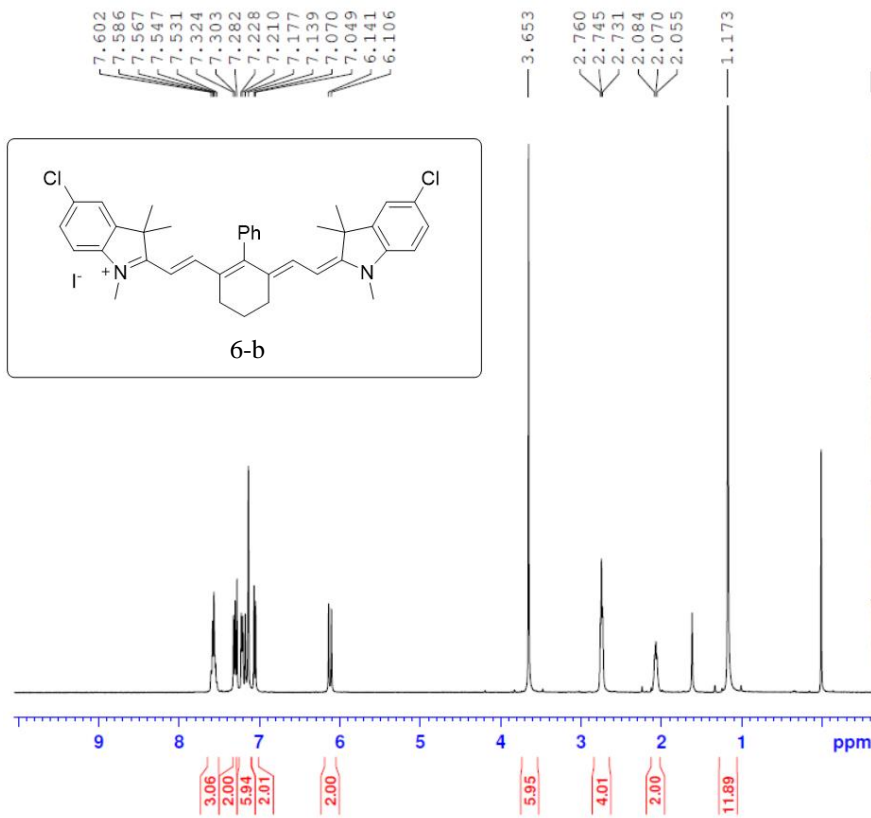
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 Date_ 20160306
 Time 22.44
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG jmod
 TD 65536
 SOLVENT CDCl3
 NS 11500
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 298.1 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.00000000 sec
 D20 0.00689655 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 100.6253446 MHz
 NUC1 13C
 P1 9.00 usec
 P2 18.00 usec
 PLW1 62.00000000 W

===== CHANNEL f2 =====
 SFO2 400.1416006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 16.00000000 W
 PLW12 0.36267000 W

F2 - Processing parameters
 SI 32768
 SF 100.6152830 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



AL_188_CDC13_1H

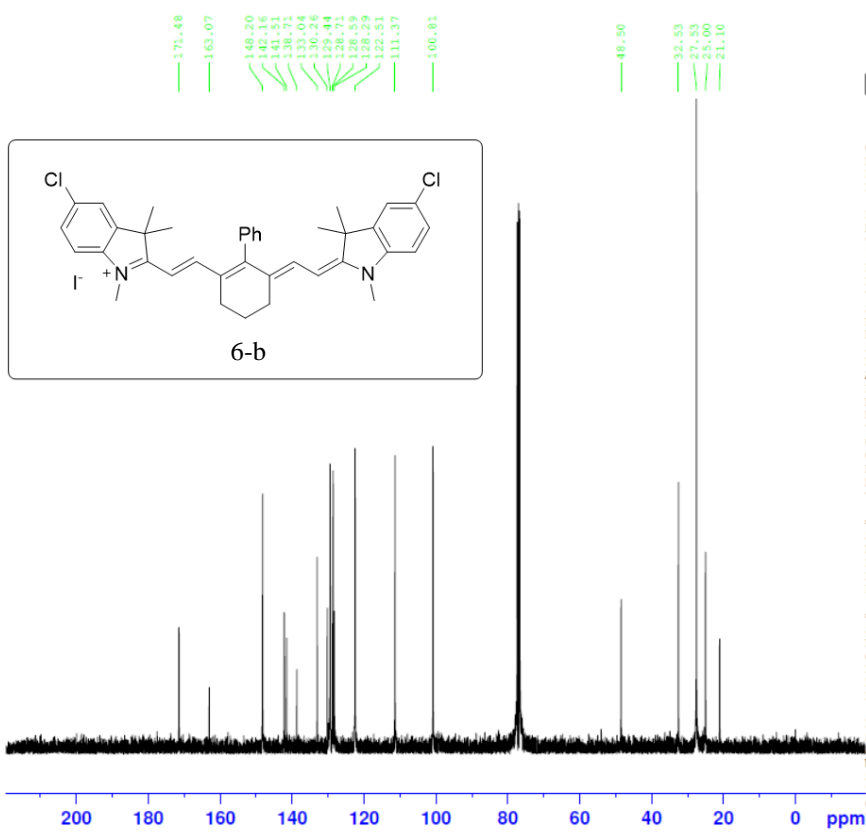
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Current Data Parameters
 NAME AL_188_CDC13_1H
 EXPNO 2
 PROCNO 2

F2 - Acquisition Parameters
 Date_ 20160404
 Time_ 15.09
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 161
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 =====
 SFO1 400.1424710 MHz
 NUC1 1H
 P1 13.55 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1400000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



AL_188_CDC13_13C

BRUKER

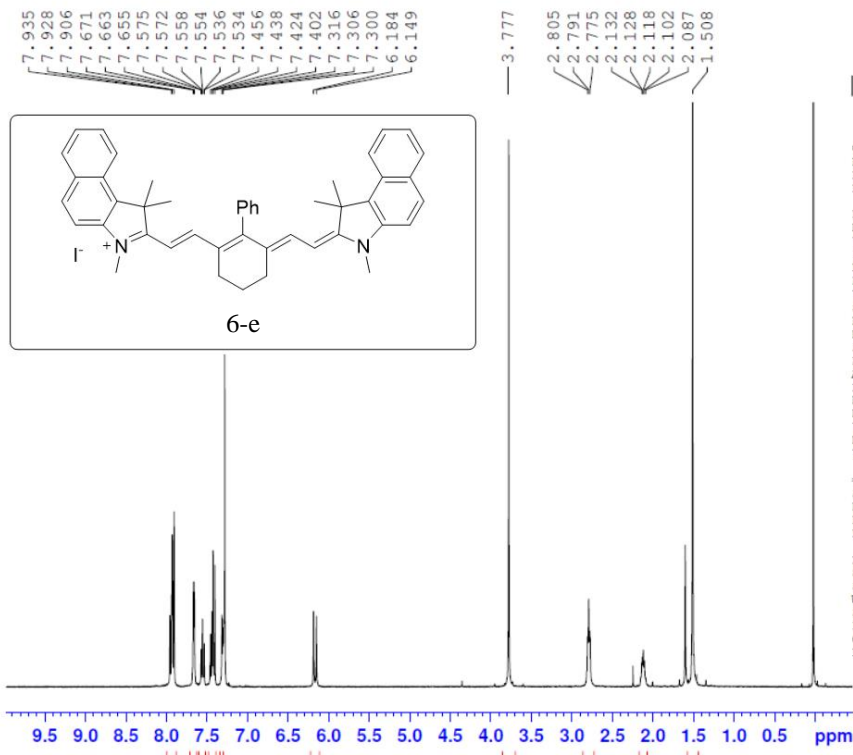
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 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160404
 Time_ 15.39
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG jmod
 TD 65536
 SOLVENT CDC13
 NS 679
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 298.2 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.00000000 sec
 D20 0.00689655 sec
 TDO 1

==== CHANNEL f1 =====
 SFO1 100.6253446 MHz
 NUC1 13C
 P1 9.00 usec
 P2 18.00 usec
 PLW1 62.00000000 W

==== CHANNEL f2 =====
 SFO2 400.1416006 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 16.00000000 W
 PLW12 0.36267000 W

F2 - Processing parameters
 SI 32768
 SF 100.6152830 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



AL_184_CDC13_1H

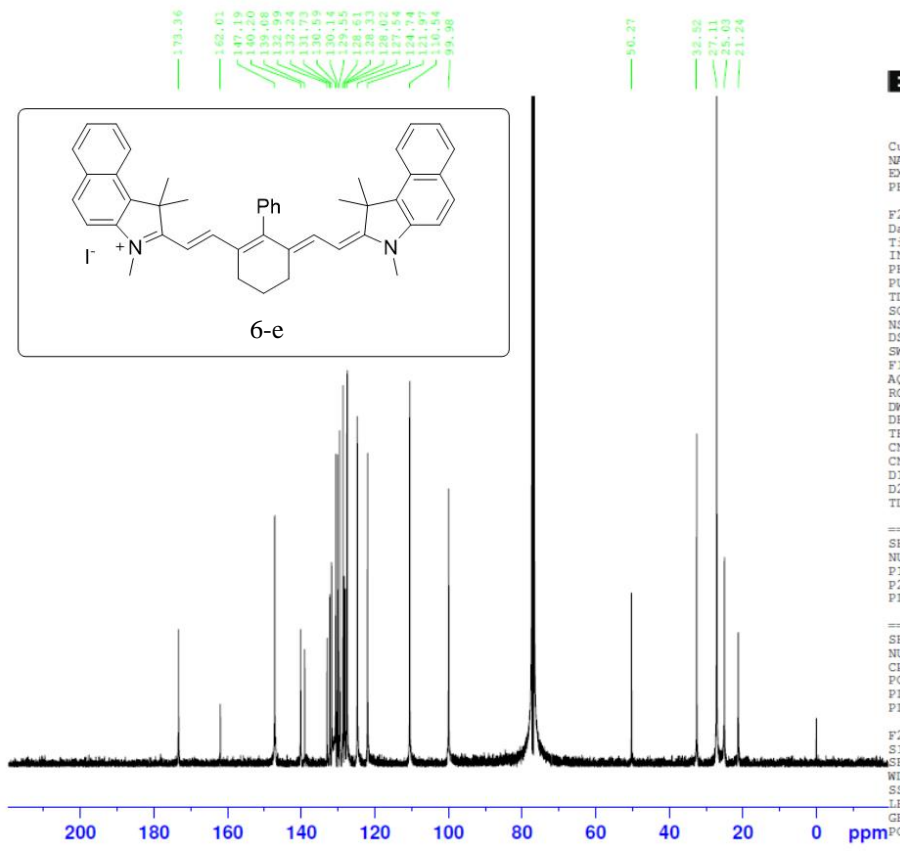


Current Data Parameters
 NAME AL_184_CDC13_1H
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160304
 Time 14:18
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 7
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 203
 EW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1424710 MHz
 NUC1 1H
 P1 13.55 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1400000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



AL_184_CDC13_13C



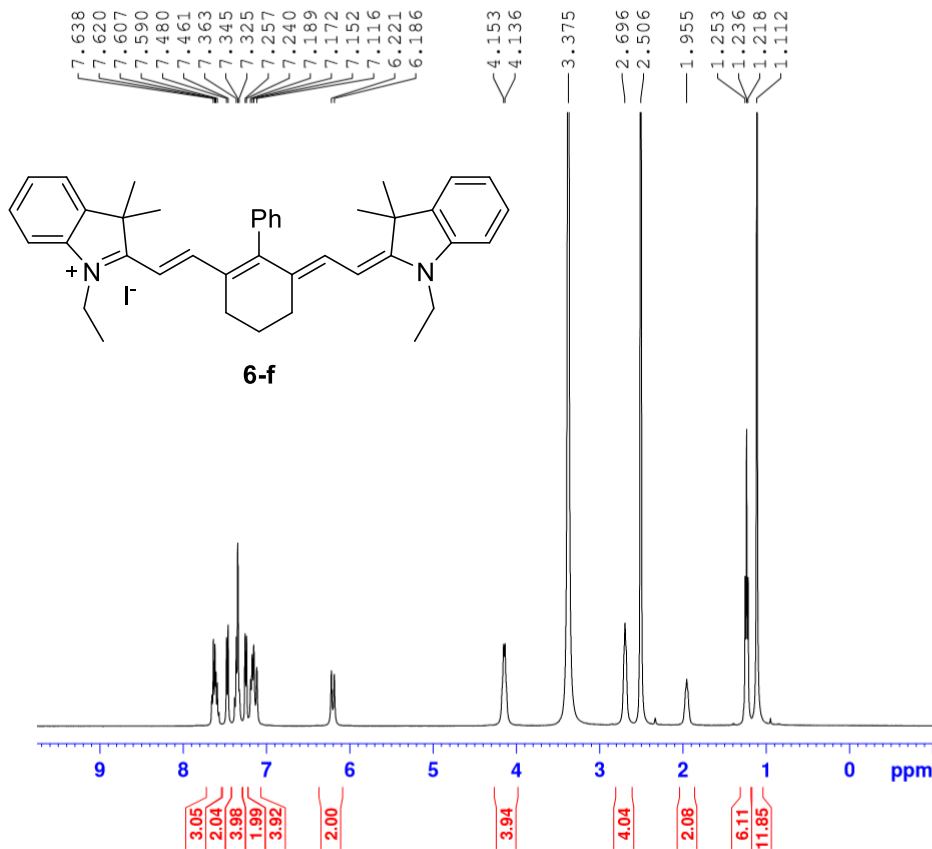
Current Data Parameters
 NAME AL_184_CDC13_13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160306
 Time 0:09
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG jmod
 TD 65536
 SOLVENT CDC13
 NS 12500
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 298.2 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.00000000 sec
 D20 0.00689655 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 100.6253446 MHz
 NUC1 13C
 P1 9.00 usec
 P2 18.00 usec
 PLW1 62.00000000 W

===== CHANNEL f2 =====
 SFO2 400.1416006 MHz
 NUC2 1H
 CPDPRG2 waitz16
 PCPD2 90.00 usec
 PLW2 16.00000000 W
 PLW12 0.36267000 W

F2 - Processing parameters
 SI 32768
 SF 100.6152830 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

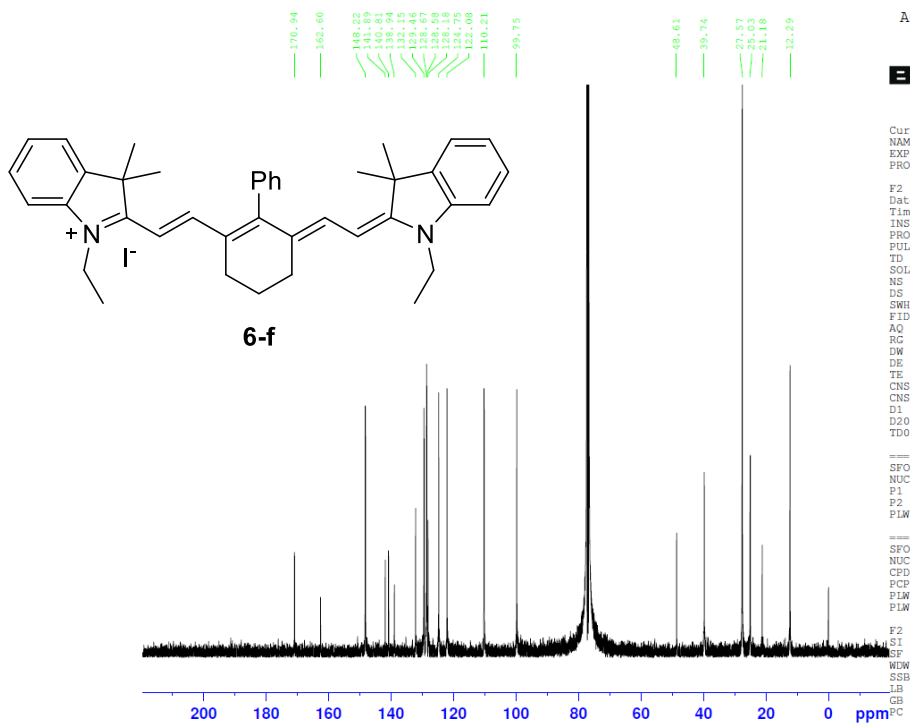


Current Data Parameters
 NAME Ph-AC5-DMSO-1H
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20171218
 Time 13.21
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 64
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 101
 DW 62.400 usec
 DE 6.50 usec
 TE 295.6 K
 D1 1.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1424710 MHz
 NUC1 1H
 P1 13.55 usec
 PLW1 16.0000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1400000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



AC_5_CDC13_13C



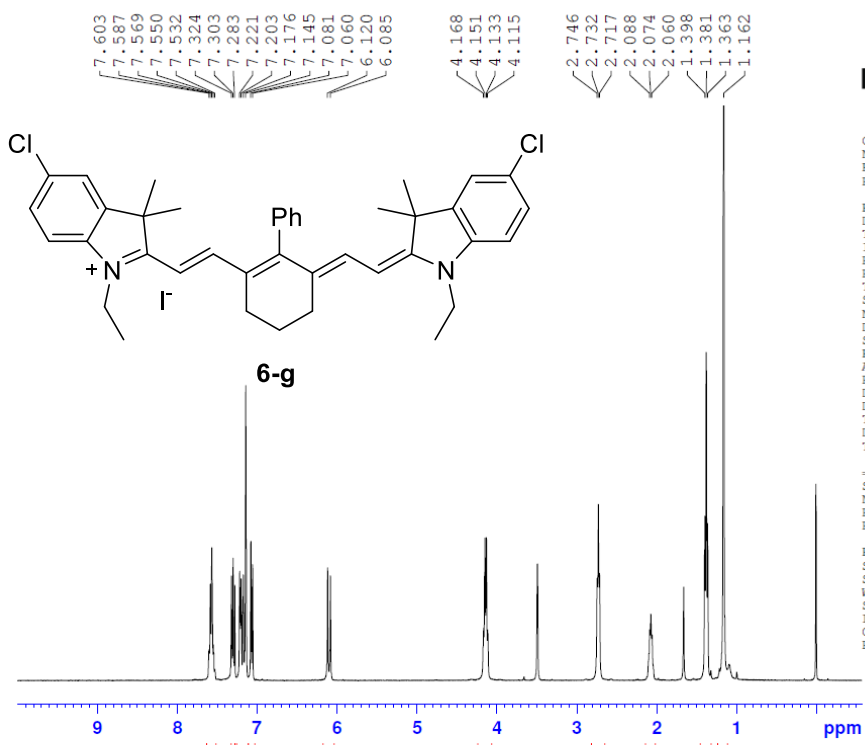
Current Data Parameters
 NAME AC_5_CDC13_13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160428
 Time 23.28
 INSTRUM spect
 PROBHD 5 mm PABBO HB-
 PULPROG jmod
 TD 65536
 SOLVENT CDCl3
 NS 8750
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RC 203
 DW 20.800 usec
 DE 6.50 usec
 TE 298.3 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.0000000 sec
 D20 0.00689655 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 100.6253446 MHz
 NUC1 13C
 P1 9.00 usec
 P2 18.00 usec
 PLW1 62.0000000 W

===== CHANNEL f2 =====
 SFO2 400.1416006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 16.0000000 W
 PLW12 0.36267000 W

F2 - Processing parameters
 SI 32768
 SF 100.6152830 MHz
 WDW EM
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 LB 1.00 Hz
 GB 0
 PC 1.40



AC_7_CDC13_1H

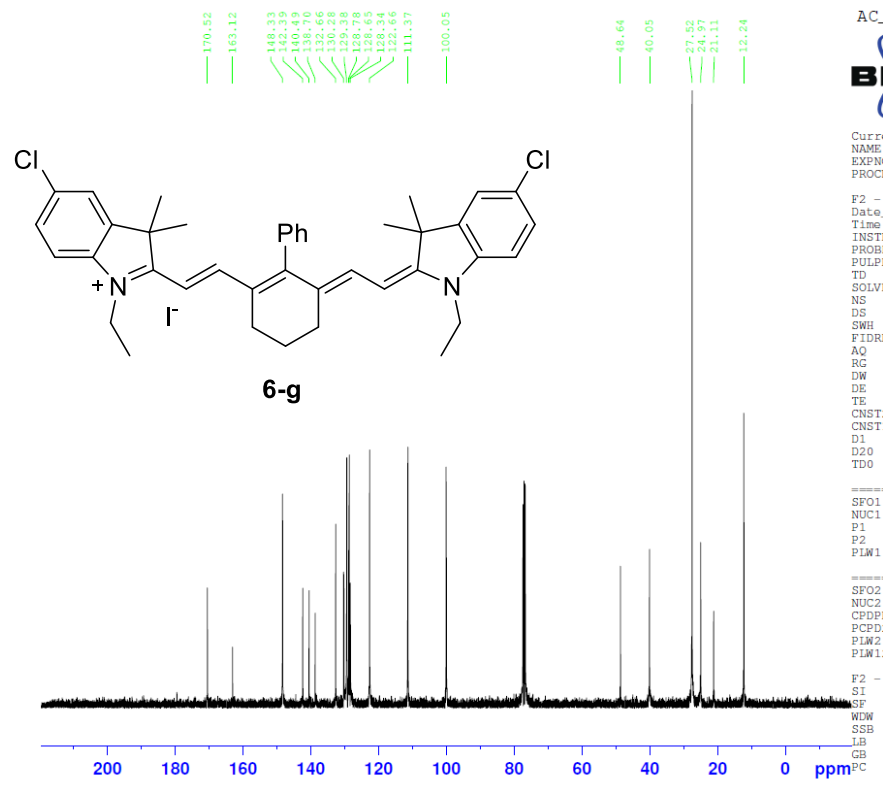
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Current Data Parameters
 NAME AC_7_CDC13_1H
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160329
 Time 15.06
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 6
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 128
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 =====
 SFO1 400.1424710 MHz
 NUC1 1H
 P1 13.55 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1400000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



AC_7_CDC13_13C

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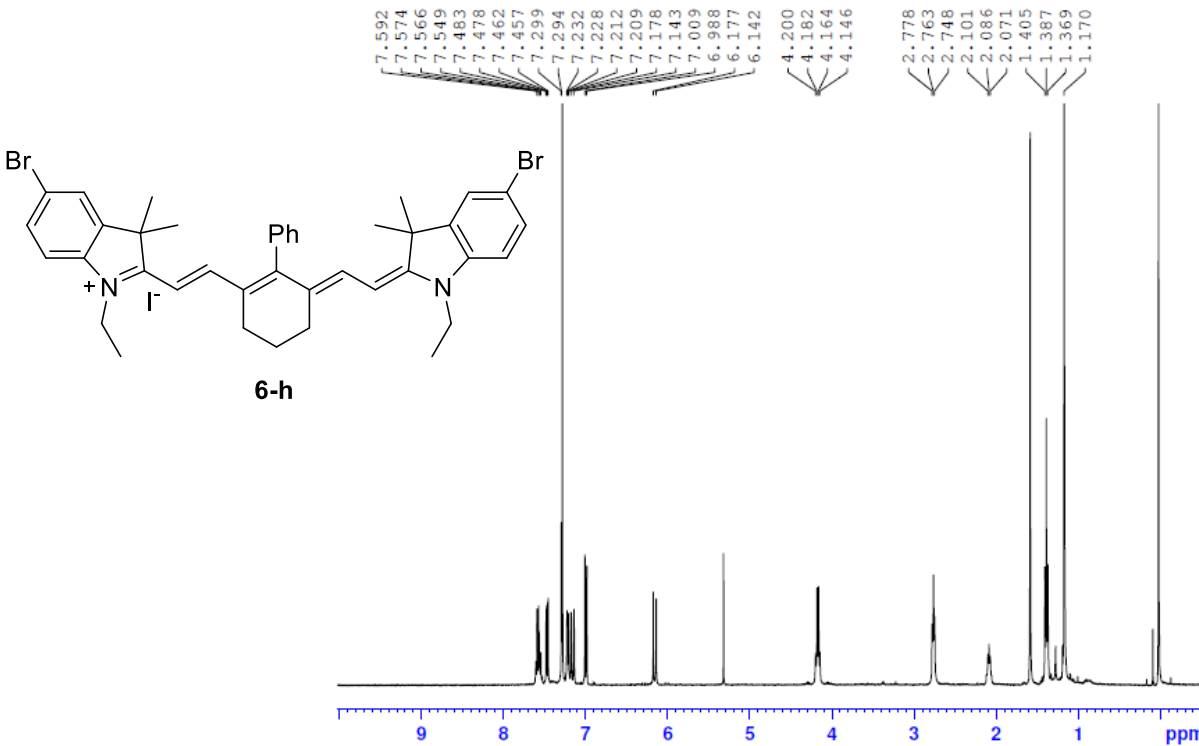
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 PULPROG jmod
 TD 65536
 SOLVENT CDC13
 NS 690
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 298.2 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.00000000 sec
 D20 0.00689655 sec
 TDO 1

==== CHANNEL f1 =====
 SFO1 100.6253446 MHz
 NUC1 13C
 P1 9.00 usec
 P2 18.00 usec
 PLW1 62.00000000 W

==== CHANNEL f2 =====
 SFO2 400.1416006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 16.00000000 W
 PLW12 0.36267000 W

F2 - Processing parameters
 SI 32768
 SF 100.6152830 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



AC_5_CDC13_1H

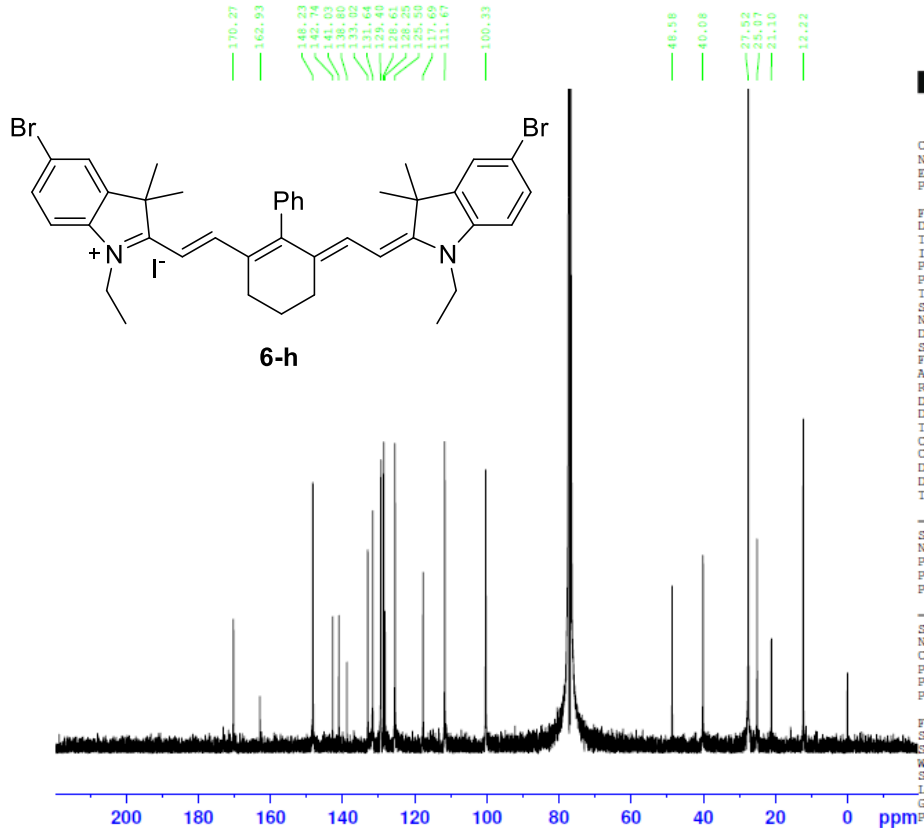
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Current Data Parameters
 NAME AC_5_CDC13_1H
 EXPNO 1
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F2 - Acquisition Parameters
 Date_ 20160301
 Time 13.51
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 ID 65536
 SOLVENT CDC13
 NS 14
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 203
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 ID0 1

CHANNEL f1
 SFO1 400.1424710 MHz
 NUC1 1H
 P1 13.55 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1400000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



AC_5_CDC13_13C

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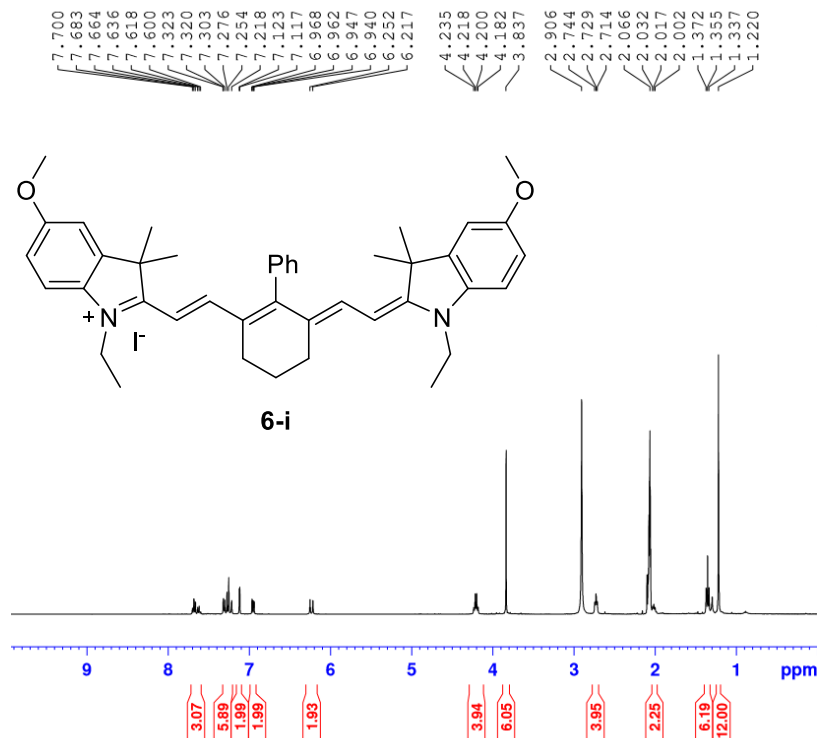
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 Date_ 20160515
 Time 23.51
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG jmod
 ID 65536
 SOLVENT CDC13
 NS 10237
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 298.2 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.00000000 sec
 D20 0.00689655 sec
 ID0 1

CHANNEL f1
 SFO1 100.6253446 MHz
 NUC1 13C
 P1 9.00 usec
 P2 18.00 usec
 PLW1 62.00000000 W

CHANNEL f2
 SFO2 400.1416006 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 16.00000000 W
 PLW12 0.36267000 W

F2 - Processing parameters
 SI 32768
 SF 100.6152830 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

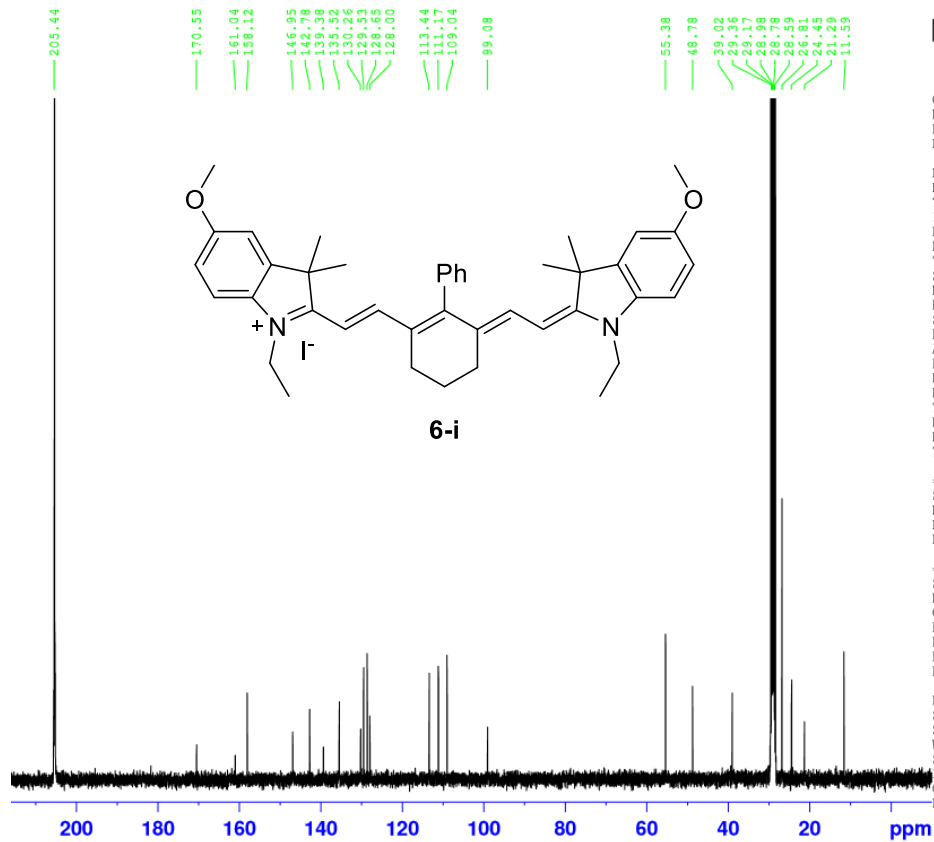


Current Data Parameters
 NAME Ph-AC8-acetone-1H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180112
 Time 16.57
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT Acetone
 NS 3
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 114
 DW 62.400 usec
 DE 6.50 usec
 TE 295.5 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 400.1424710 MHz
 NUC1 1H
 P1 13.55 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1400000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME Ph-AC8-acetone-13C
 EXPNO 2
 PROCNO 1

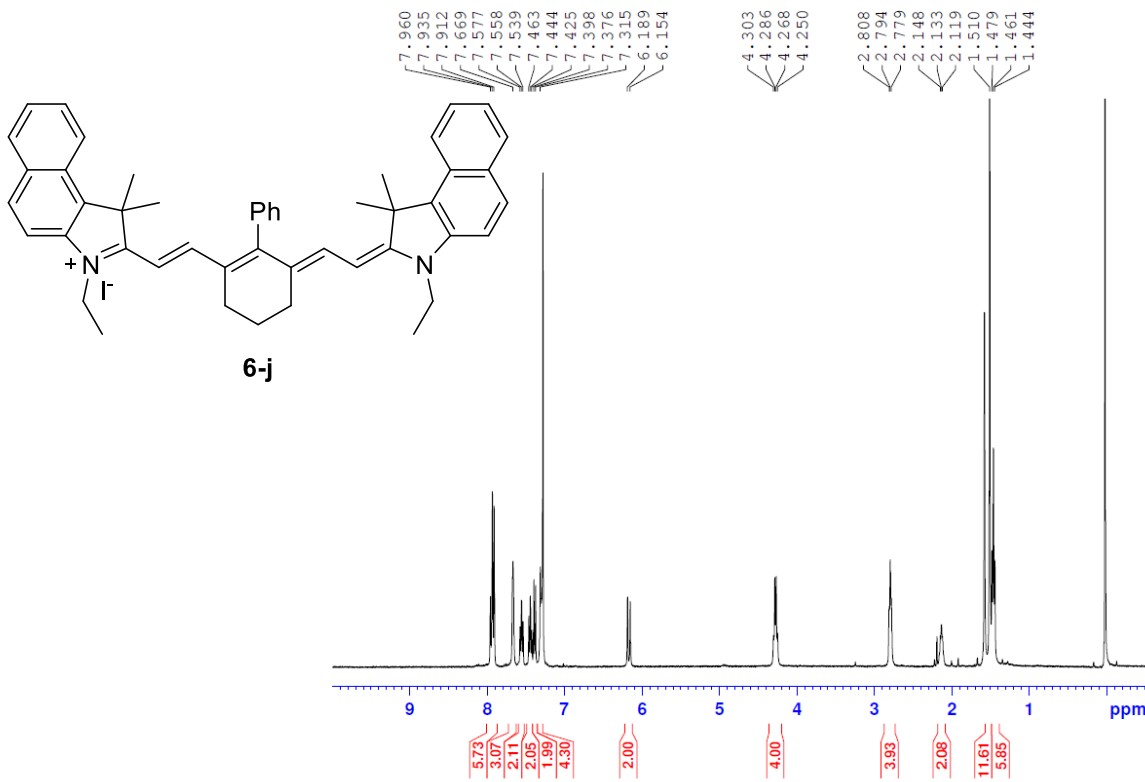
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 Date_ 20180116
 Time 13.52
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 2055
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 295.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 100.6253441 MHz
 NUC1 13C
 P1 9.25 usec
 PLW1 62.00000000 W

==== CHANNEL f2 =====
 SFO2 400.1416006 MHz
 NUC2 1H
 CPDPRG12 waltz16
 PCDD2 90.00 usec
 PLW2 16.00000000 W
 PLW12 0.36267000 W
 PLW13 0.29376000 W

F2 - Processing parameters
 SI 32768
 SF 100.6152830 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Signal seen at δ 205.44 ppm corresponds to the carbonyl group of acetone- d_6



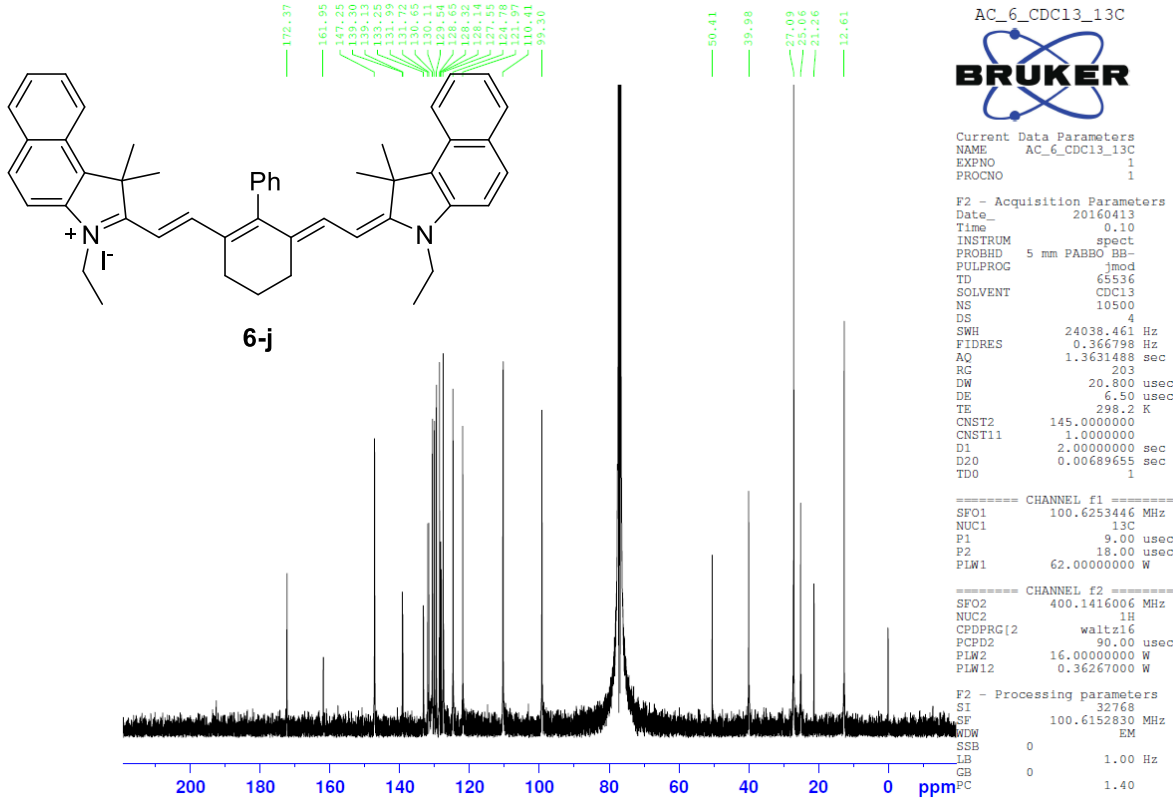
BRUKER

Current Data Parameters
 NAME AC_6_CDC13_1H
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160410
 Time 22.42
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 20
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 203
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 =====
 SFO1 400.1424710 MHz
 NUC1 1H
 P1 13.55 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1400000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



BRUKER

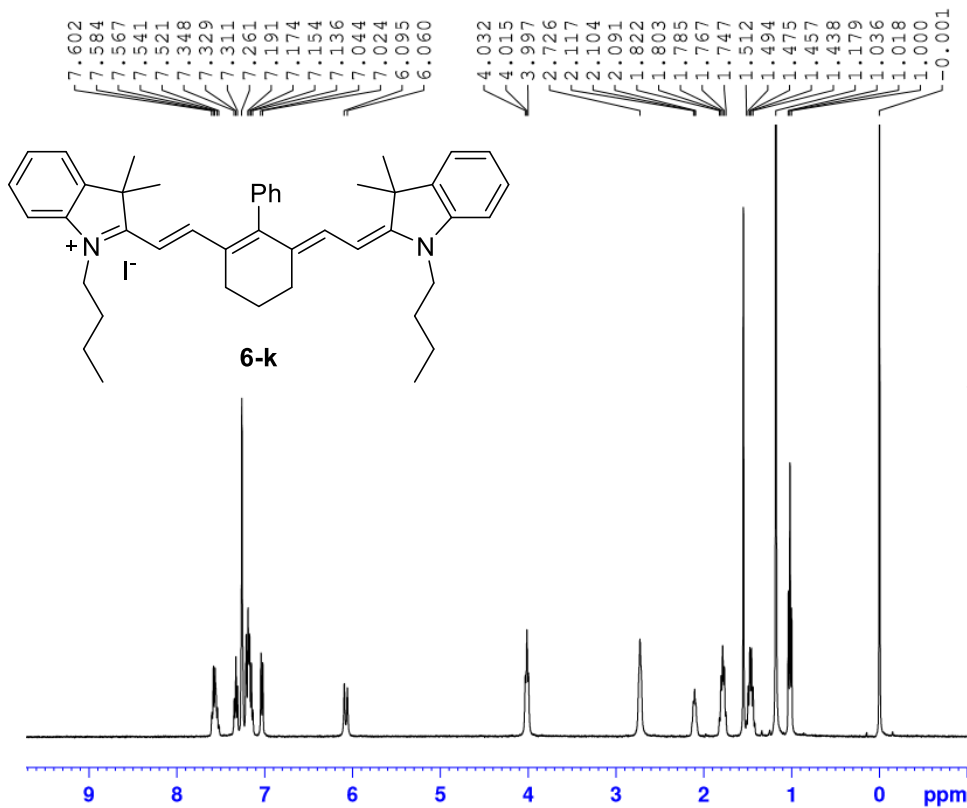
Current Data Parameters
 NAME AC_6_CDC13_13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160413
 Time 0.10
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG jmod
 TD 65536
 SOLVENT CDC13
 NS 10500
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 298.2 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.00000000 sec
 D20 0.00689655 sec
 TDO 1

==== CHANNEL f1 =====
 SFO1 100.6253446 MHz
 NUC1 13C
 P1 9.00 usec
 P2 18.00 usec
 PLW1 62.00000000 W

==== CHANNEL f2 =====
 SFO2 400.1416006 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 16.00000000 W
 PLW12 0.36267000 W

F2 - Processing parameters
 SI 32768
 SF 100.6152830 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

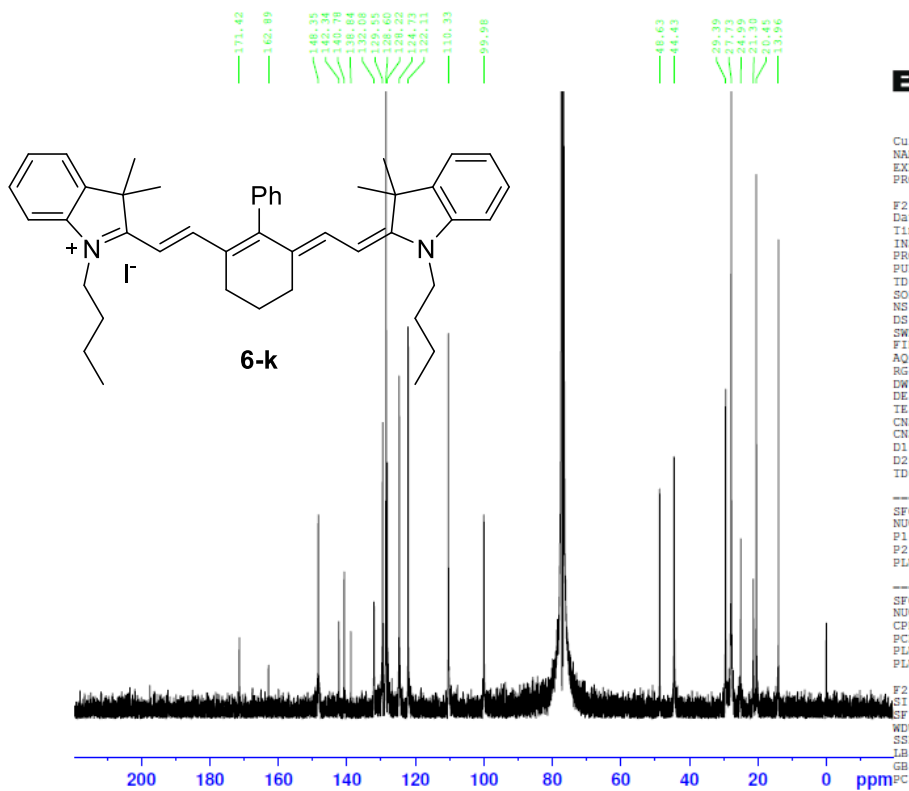


Current Data Parameters
 NAME FM_4_CDC13_1H
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160315
 Time 13.41
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 12
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.089465 sec
 RG 203
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1424710 MHz
 NUC1 1H
 P1 13.55 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1400085 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



FM_4_CDC13_13C

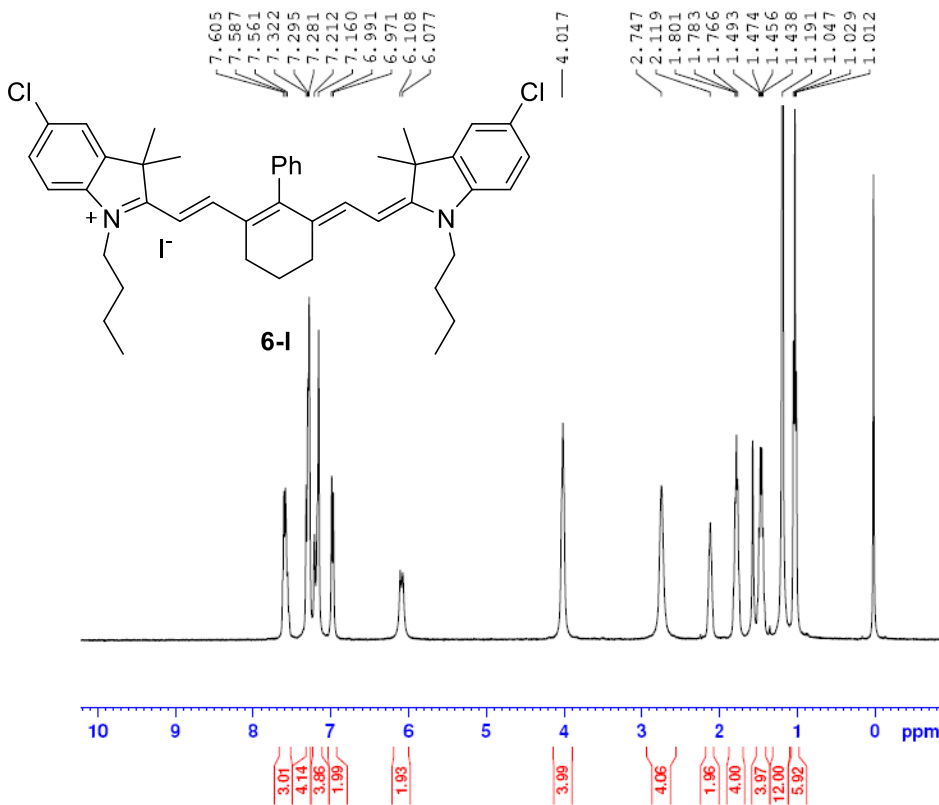
Current Data Parameters
 NAME FM_4_CDC13_13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160504
 Time 0.41
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG jmod
 TD 65536
 SOLVENT CDC13
 NS 9573
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 298.2 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.00000000 sec
 D20 0.00689655 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 100.6253446 MHz
 NUC1 13C
 P1 9.00 usec
 P2 18.00 usec
 PLW1 62.00000000 W

===== CHANNEL f2 =====
 SFO2 400.1416006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 16.00000000 W
 PLW12 0.36267000 W

F2 - Processing parameters
 SI 32768
 SF 100.6152830 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



FM_C1Dye_CDC13_1H



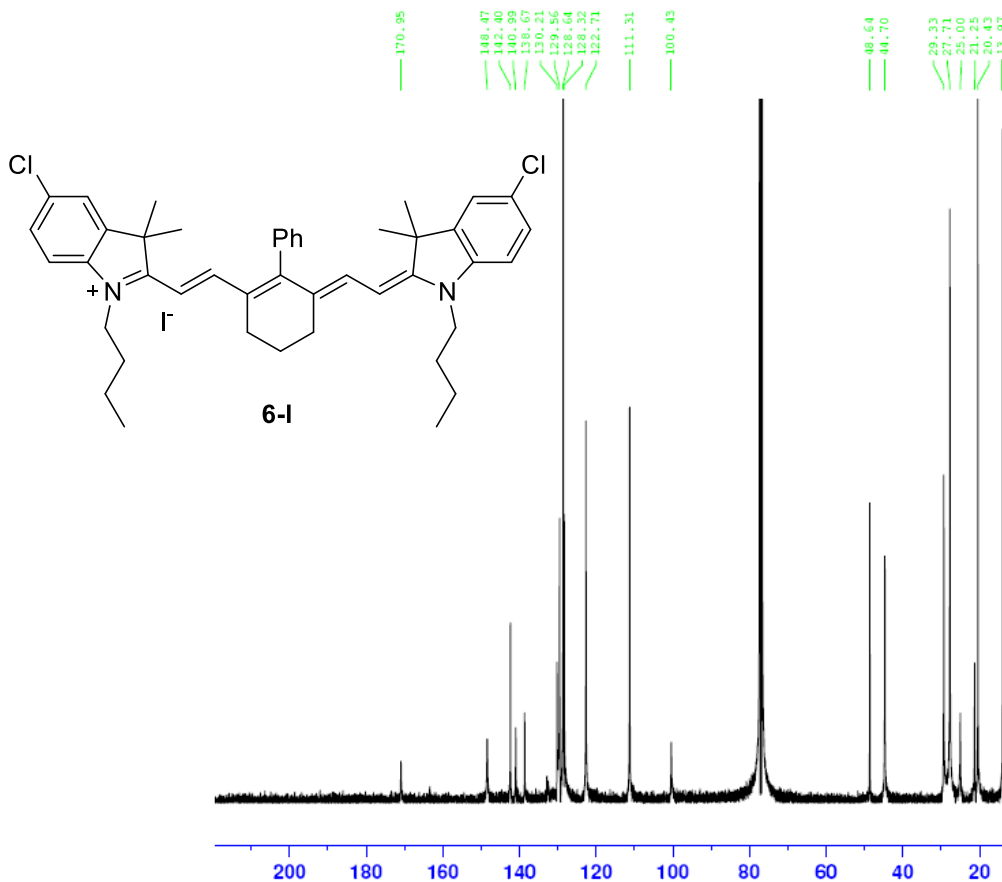
Current Data Parameters
 NAME FM_C1Dye_CDC13_1H
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160328
 Time 15:19
 INSTRUM spect
 PROBHD 5 mm FAPBO BB-
 PULPROG zg30
 ID 65536
 SOLVENT CDCl3
 NS 13
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 161
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

CHANNEL f1
 SFO1 400.1424710 MHz
 NUC1 1H
 F1 13.55 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1400000 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

10 9 8 7 6 5 4 3 2 1 0 ppm



FM_C1Dye_CDC13_13C



Current Data Parameters
 NAME FM_C1Dye_CDC13_13C
 EXPNO 1
 PROCNO 1

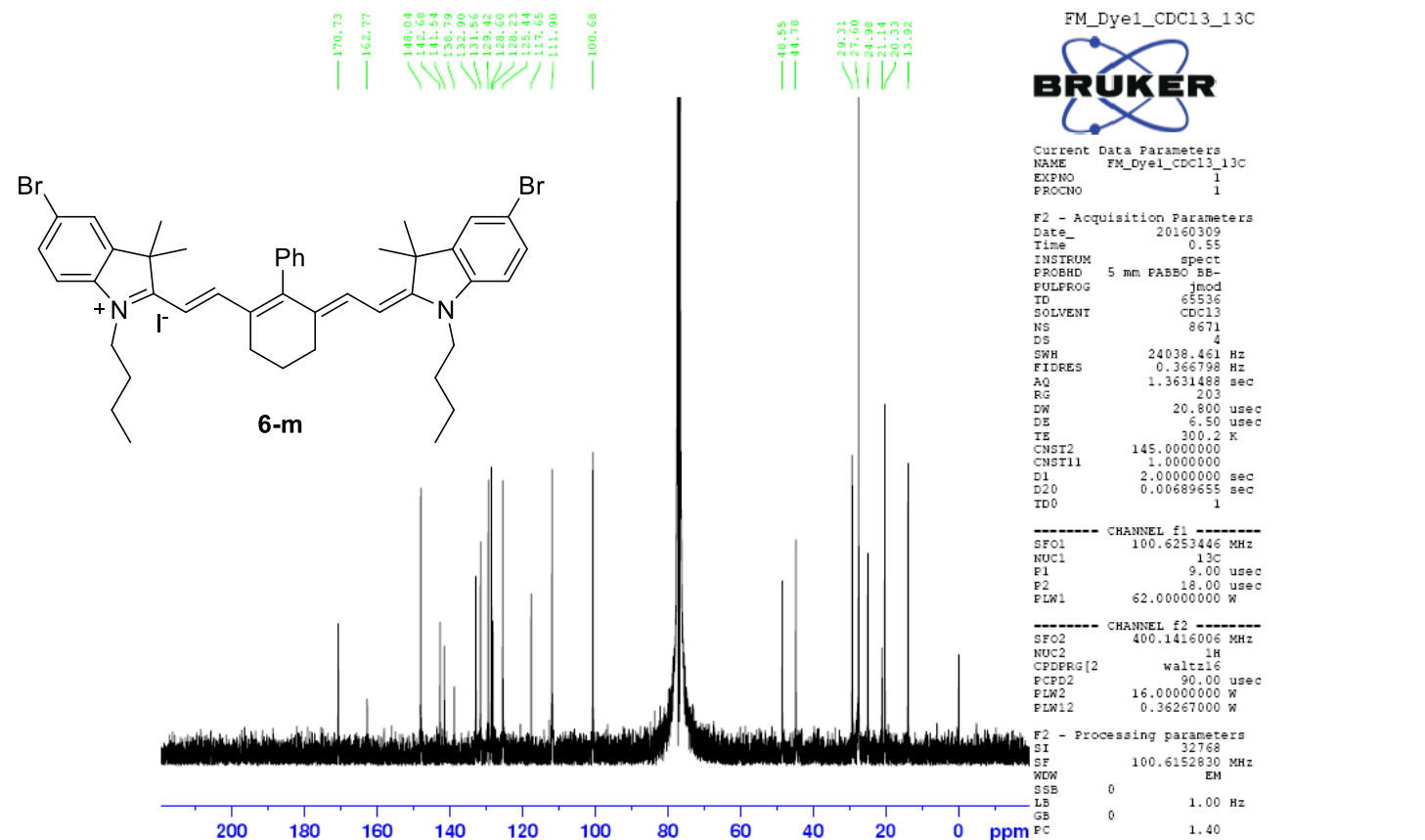
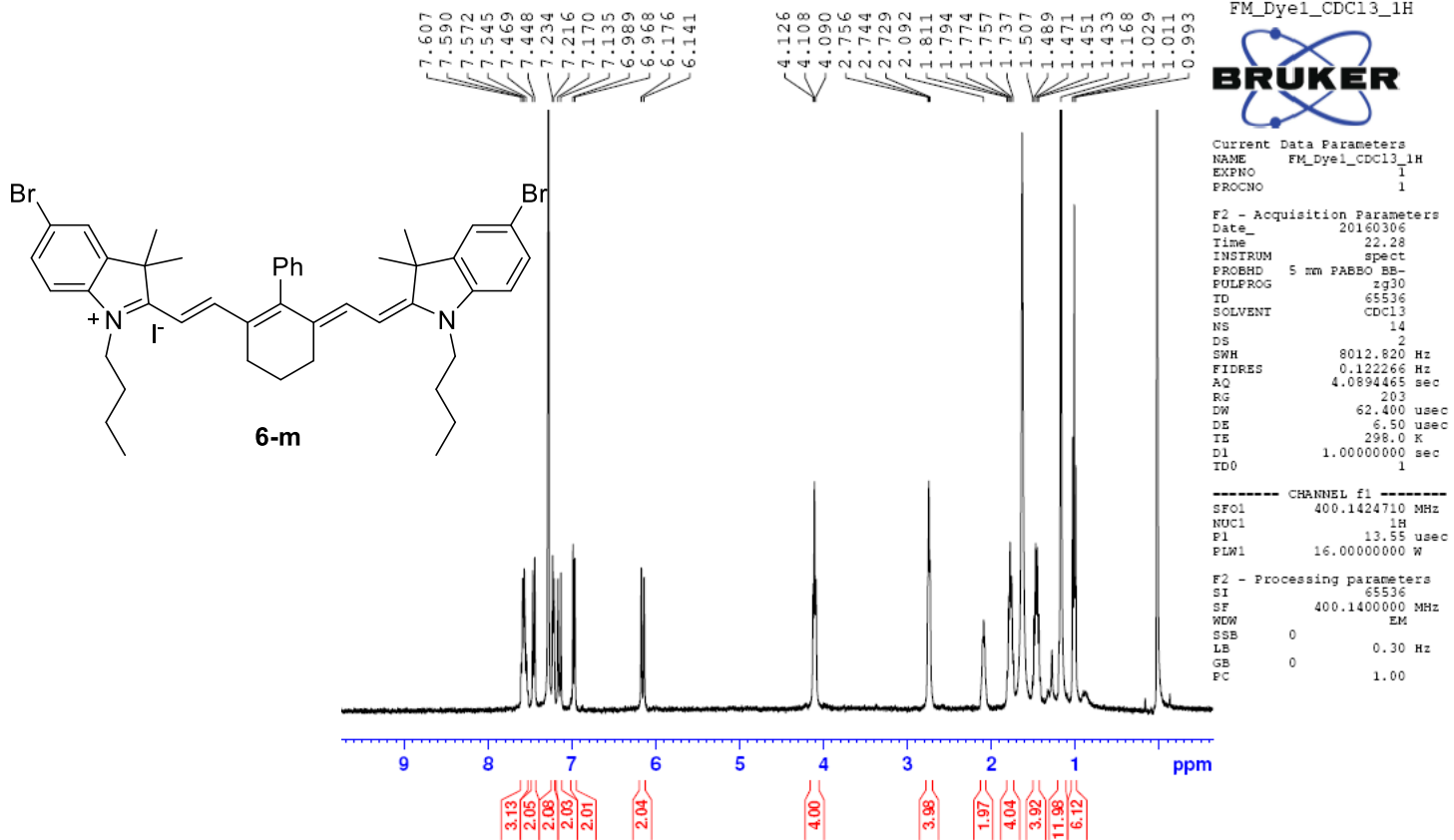
F2 - Acquisition Parameters
 Date_ 20160401
 Time 0:24
 INSTRUM spect
 PROBHD 5 mm FAPBO BB-
 PULPROG jmod
 ID 65536
 SOLVENT CDCl3
 NS 10206
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 298.2 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.00000000 sec
 D20 0.00689655 sec
 TD0 1

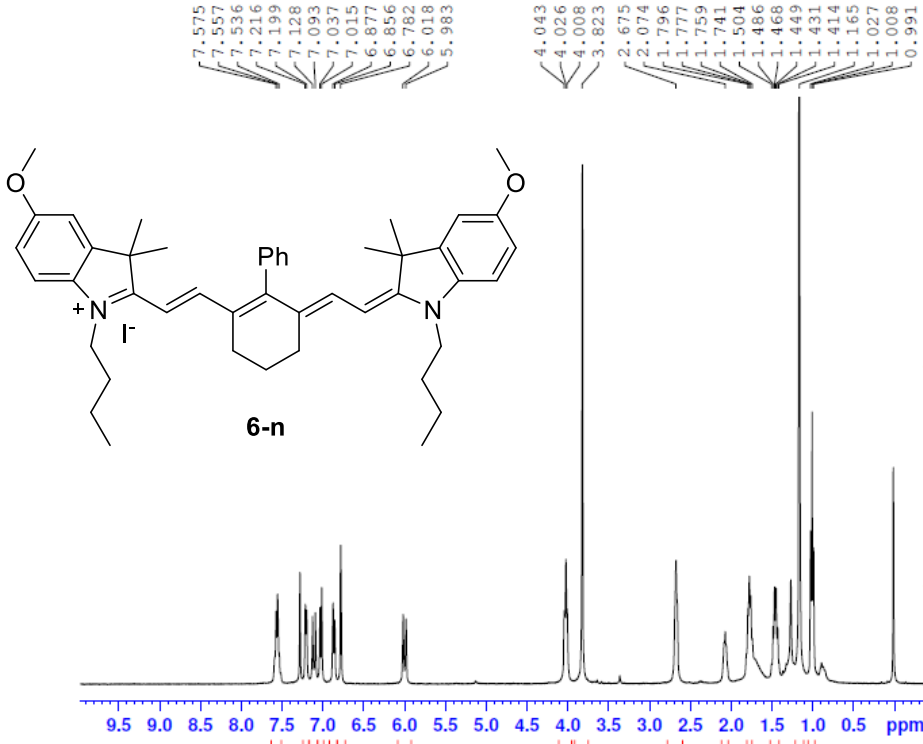
CHANNEL f1
 SFO1 100.6253446 MHz
 NUC1 13C
 F1 9.00 usec
 P2 18.00 usec
 PLW1 62.00000000 W

CHANNEL f2
 SFO2 400.1416006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 FCPD2 90.00 usec
 PLW2 16.00000000 W
 PLW12 0.36267000 W

F2 - Processing parameters
 SI 32768
 SF 100.6152830 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

200 180 160 140 120 100 80 60 40 20 0 ppm





FM_14_CDC13_1H

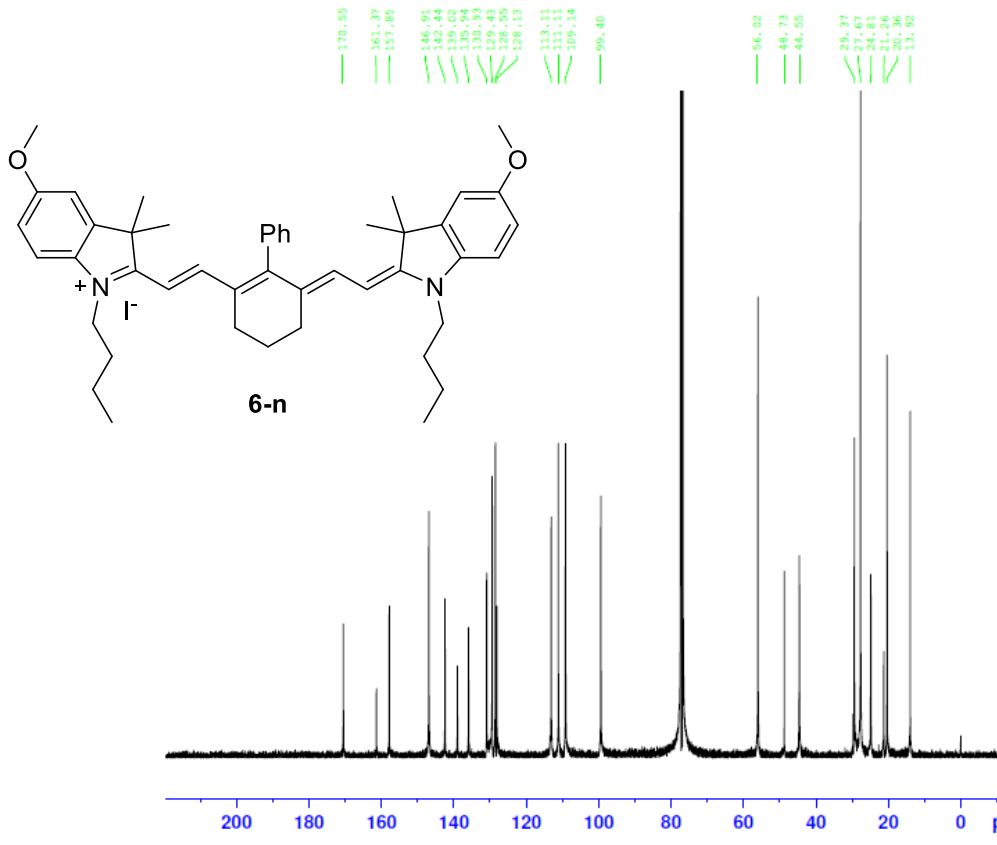
BRUKER

Current Data Parameters
 NAME FM_14_CDC13_1H
 EXPNO 3
 PROCNO 3

F2 - Acquisition Parameters
 Date_ 20160414
 Time 13.55
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 ID 65536
 SOLVENT CDC13
 NS 11
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 144
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1

CHANNEL f1
 SFO1 400.1424710 MHz
 NUC1 1H
 P1 13.55 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1400000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



FM_14_CDC13_13C

BRUKER

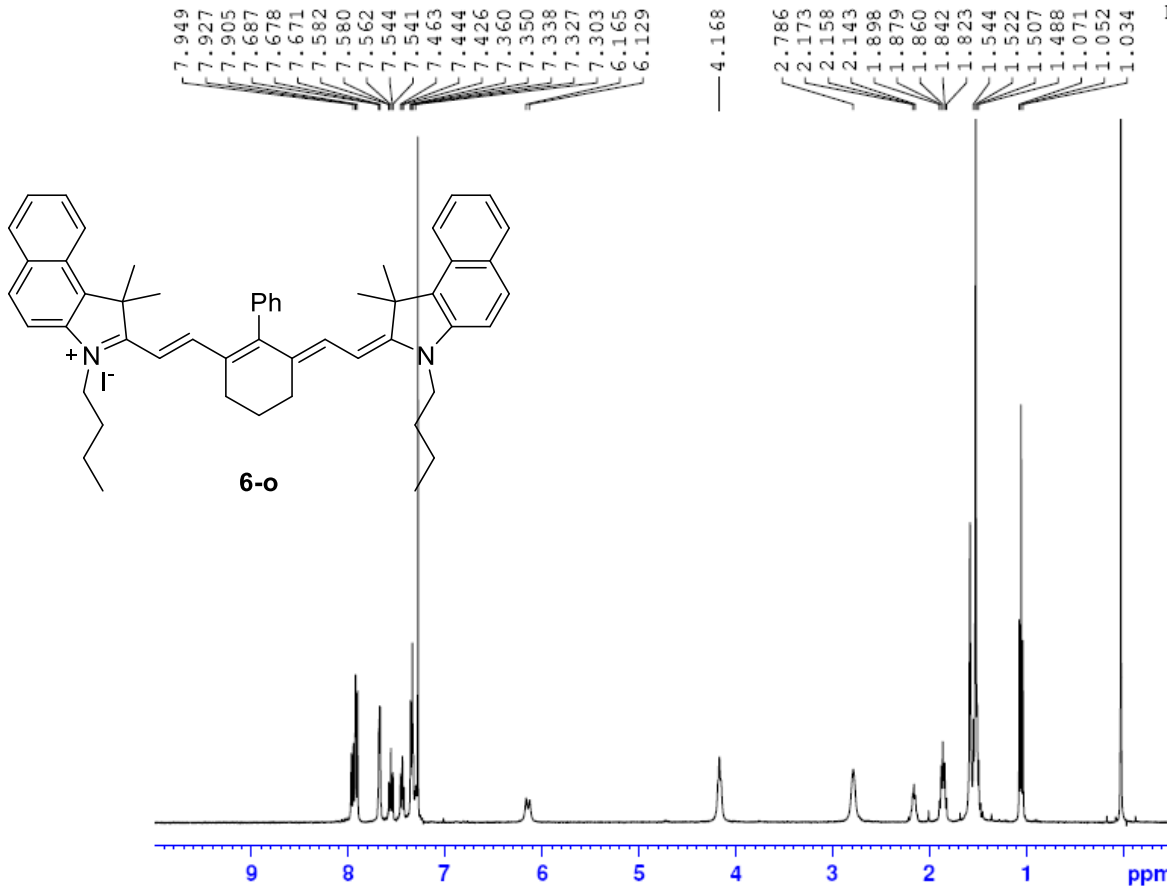
Current Data Parameters
 NAME FM_14_CDC13_13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160425
 Time 23.59
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG jmod
 ID 65536
 SOLVENT CDC13
 NS 10899
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 298.3 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.0000000 sec
 D20 0.00689655 sec
 TDO 1

CHANNEL f1
 SFO1 100.6253446 MHz
 NUC1 13C
 P1 9.00 usec
 P2 18.00 usec
 PLW1 62.00000000 W

CHANNEL f2
 SFO2 400.1416006 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 FCPD2 90.00 usec
 PLW2 16.00000000 W
 PLW12 0.36267000 W

F2 - Processing parameters
 SI 32768
 SF 100.6152830 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



FM_BenzEdey_CDC13_1H

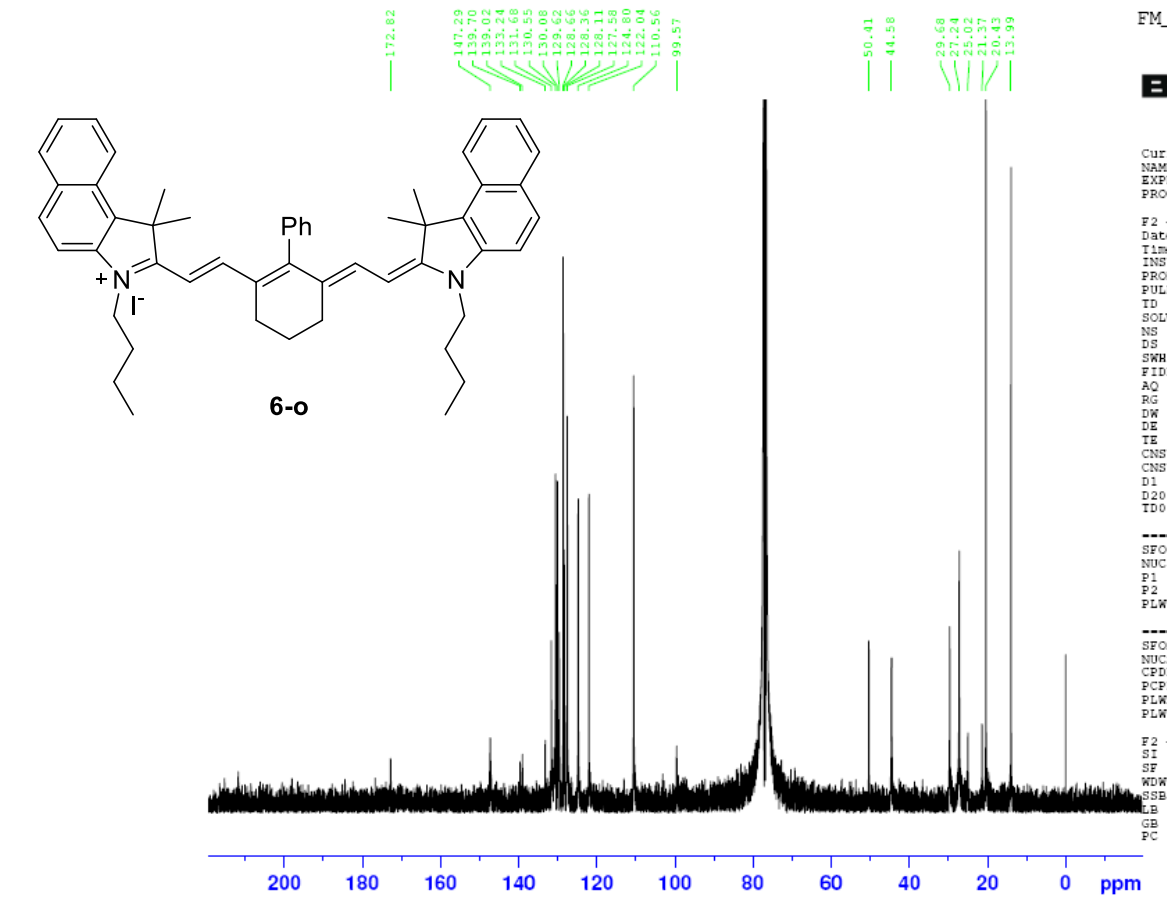


Current Data Parameters
 NAME FM_BenzEdey_CDC13_1H
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160401
 Time 16.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 ID 65536
 SOLVENT CDCl3
 NS 15
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 203
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.0000000 sec
 ID0 1

----- CHANNEL f1 -----
 SFO1 400.1424710 MHz
 NUC1 1H
 P1 13.55 usec
 PLW1 16.0000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1400000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



FM_BenzEdey_CDC13_13C



Current Data Parameters
 NAME FM_BenzEdey_CDC13_13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160402
 Time 2.09
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG jmod
 ID 65536
 SOLVENT CDCl3
 NS 8831
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 298.2 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.0000000 sec
 D20 0.00689655 sec
 ID0 1

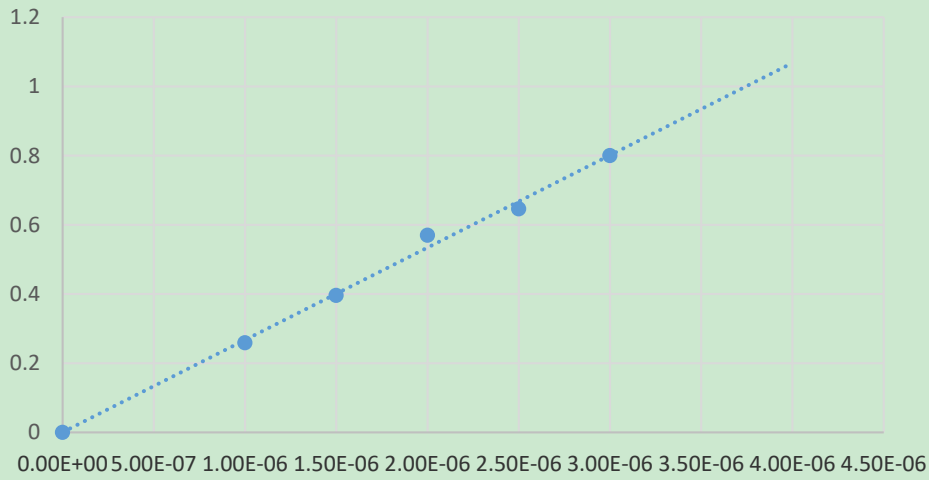
----- CHANNEL f1 -----
 SFO1 100.6253446 MHz
 NUC1 13C
 P1 9.00 usec
 P2 18.00 usec
 PLW1 62.0000000 W

----- CHANNEL f2 -----
 SFO2 400.1416006 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 16.0000000 W
 PLW12 0.36267000 W

F2 - Processing parameters
 SI 32768
 SF 100.6152830 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

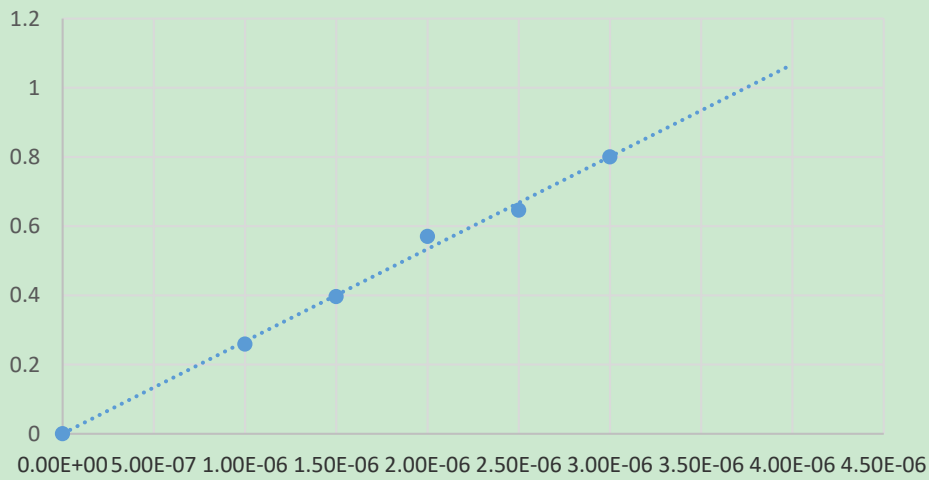
$y = 266800x + 0.0005$
 $R^2 = 0.9956$

6-aT1 ABS

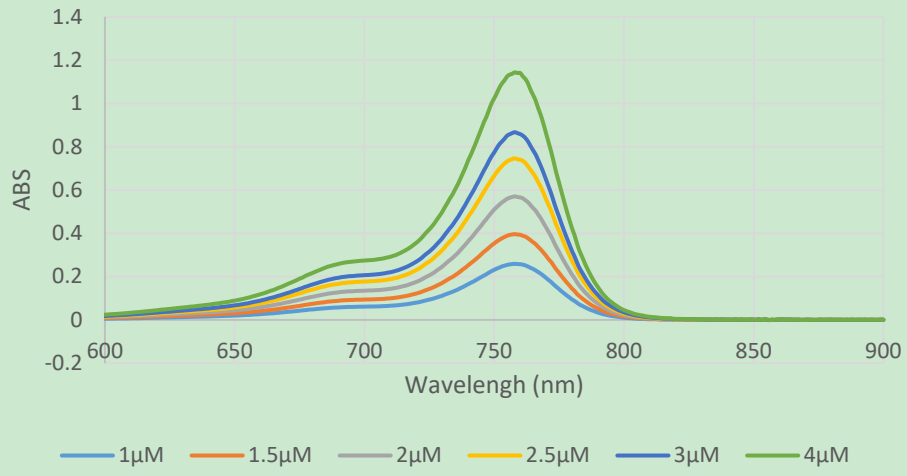


$y = 266800x + 0.0005$
 $R^2 = 0.9956$

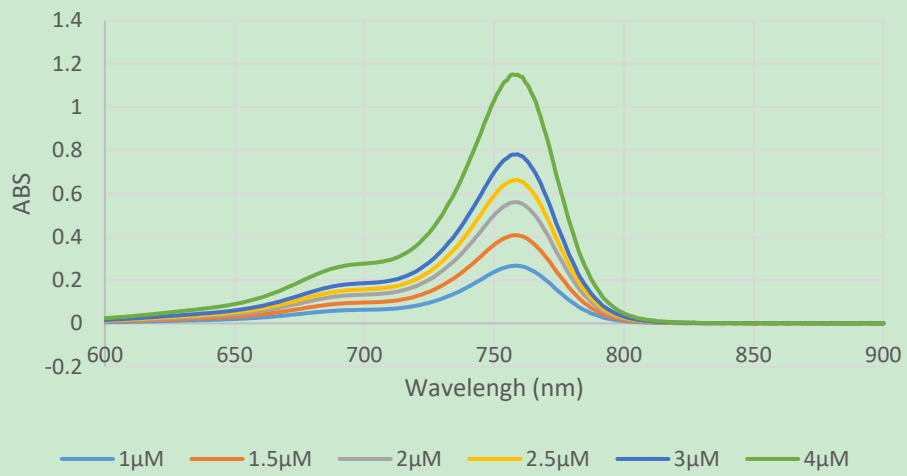
6-aT1 ABS

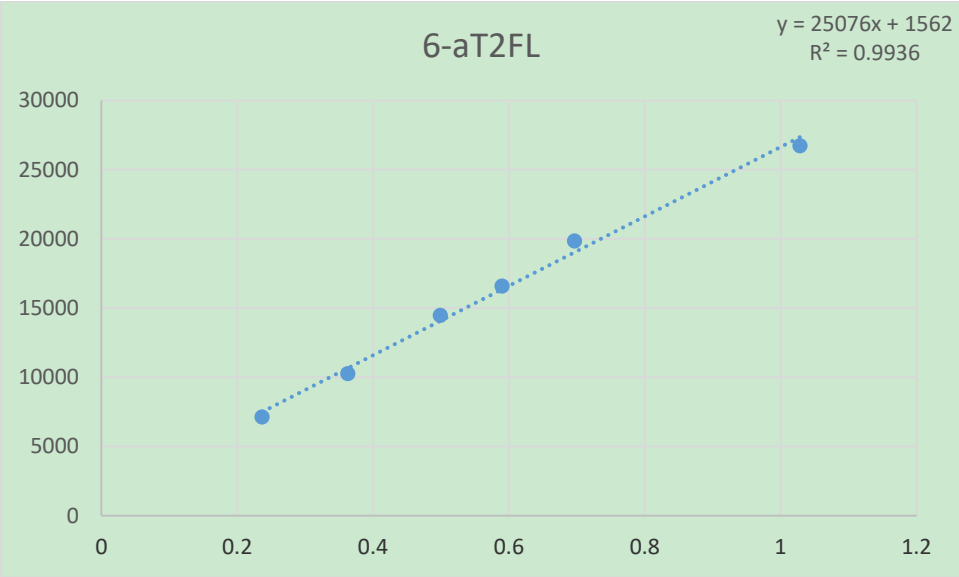
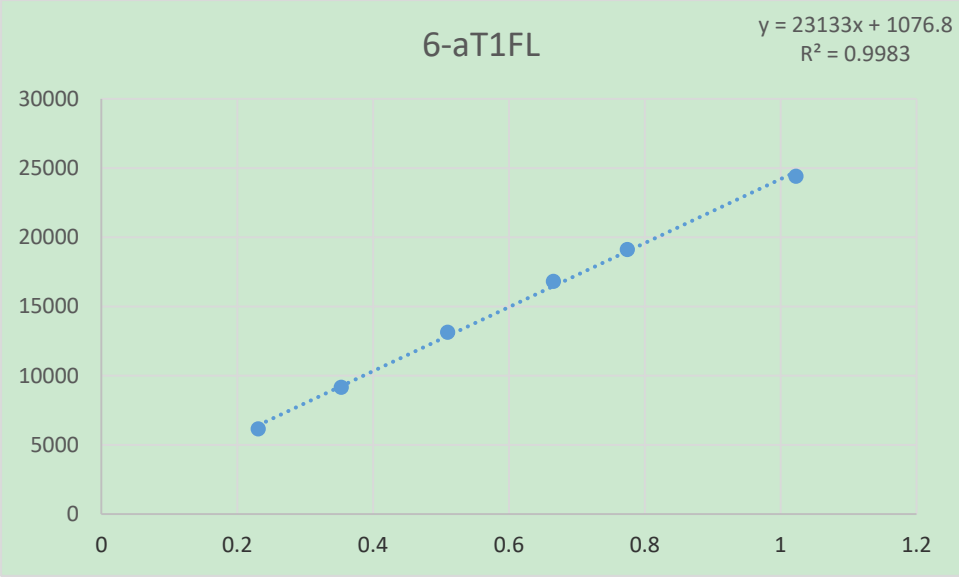


6-aT1 ABS

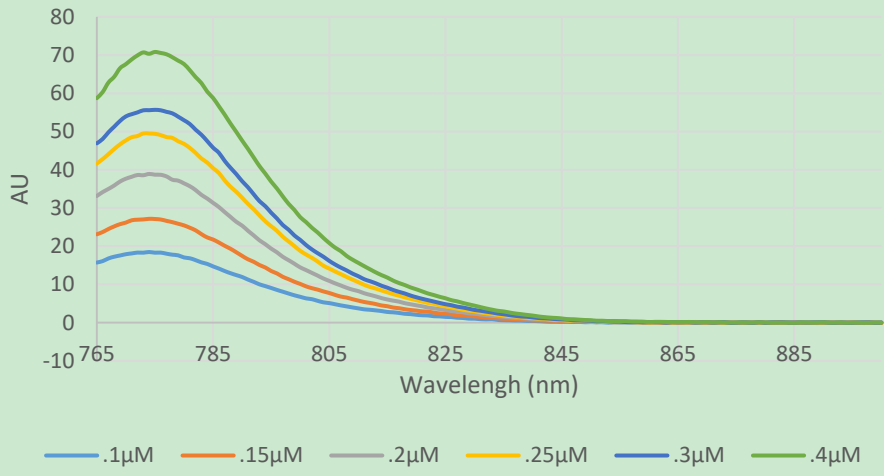


6-aT2 ABS

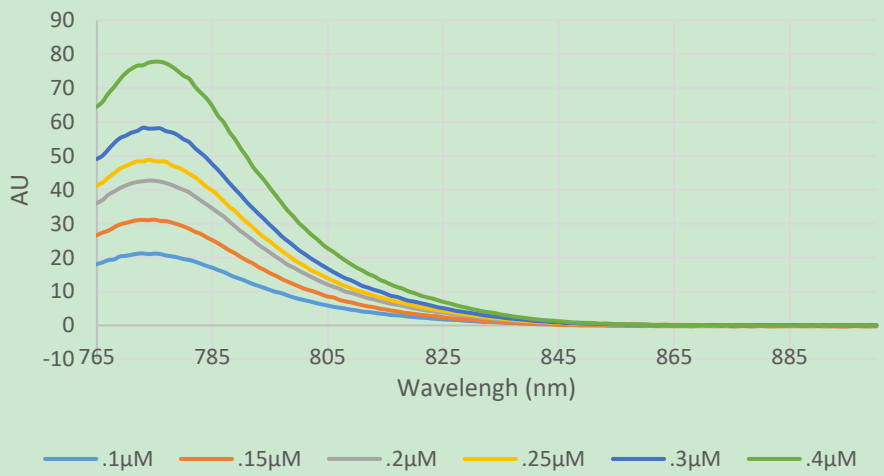




6-aT1 FL

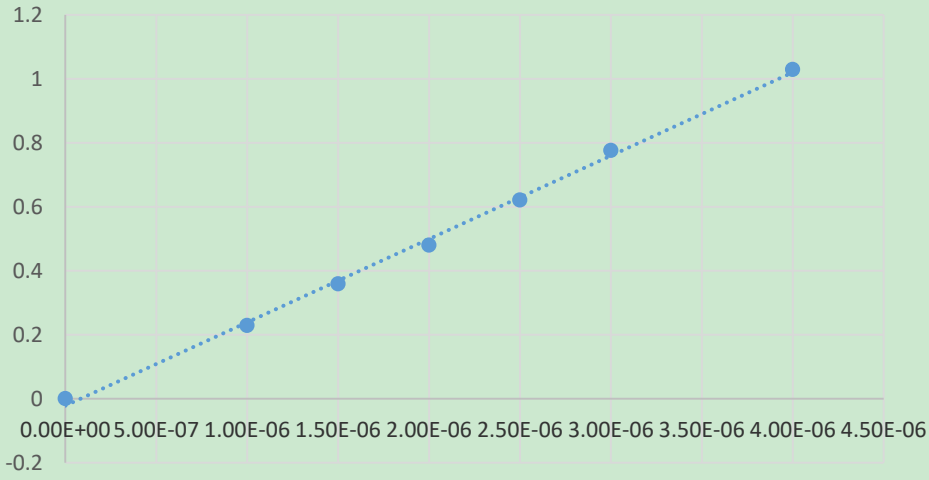


6-aT2 FL



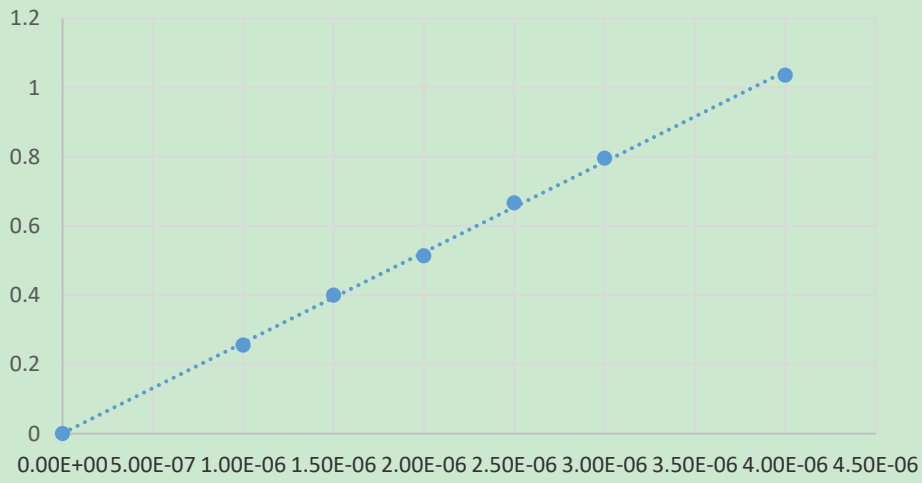
6-bT1 abs

$y = 260571x - 0.022$
 $R^2 = 0.998$

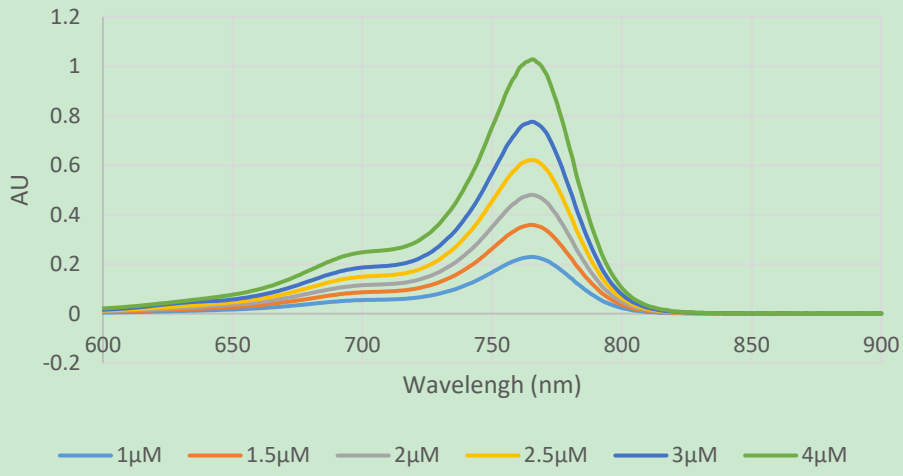


6-bT2 abs

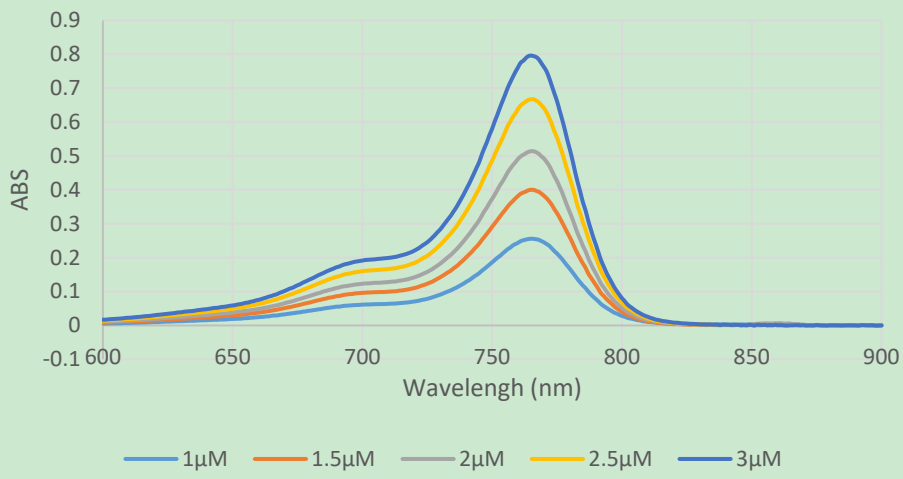
$y = 261476x + 0.0012$
 $R^2 = 0.9992$

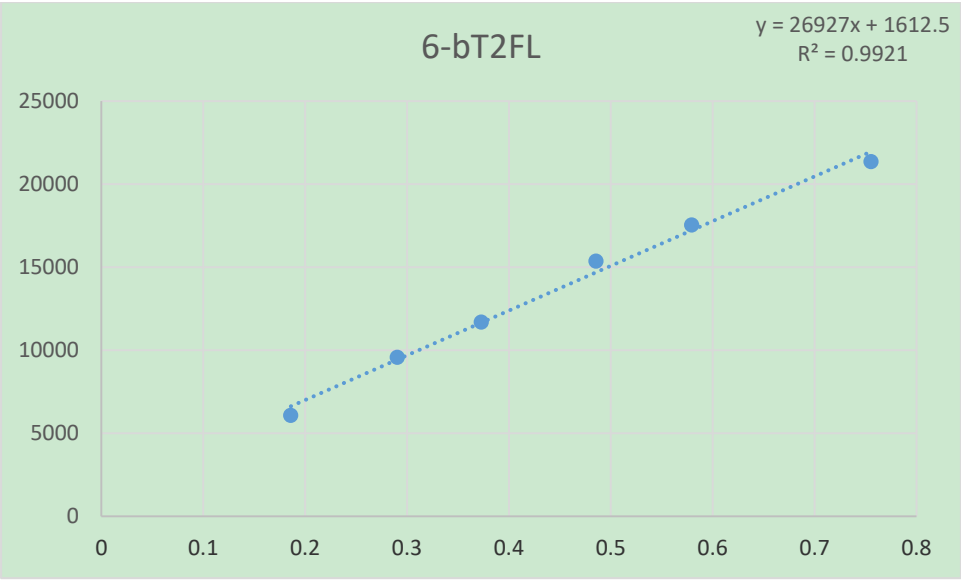
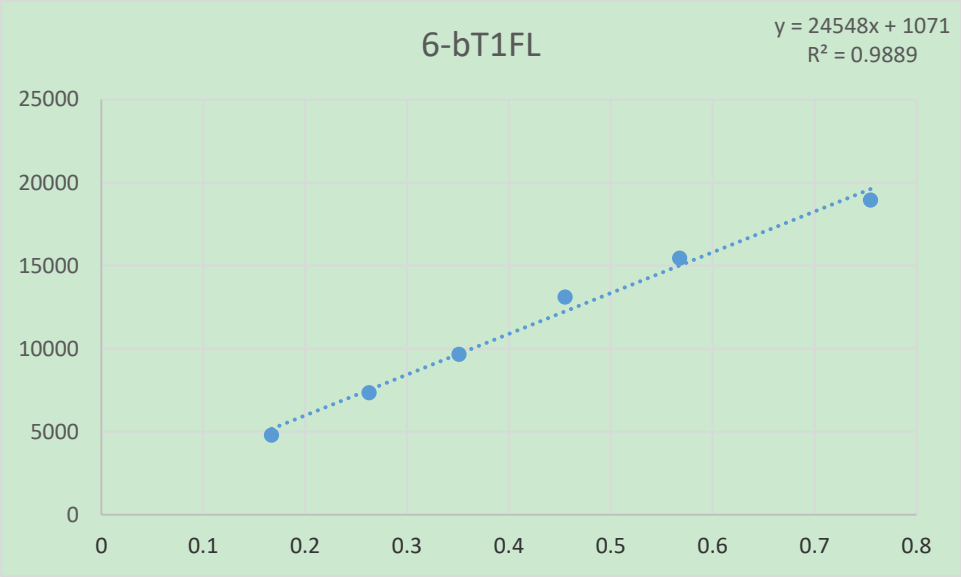


6-bT1 ABS

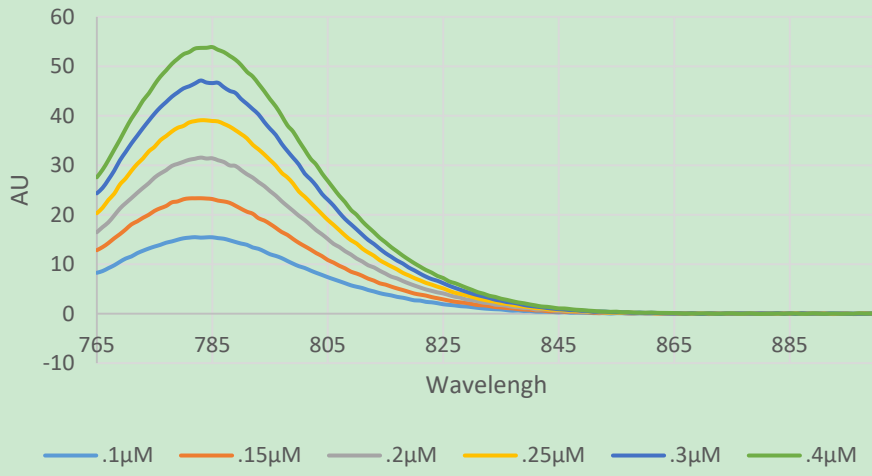


6-bT2 ABS

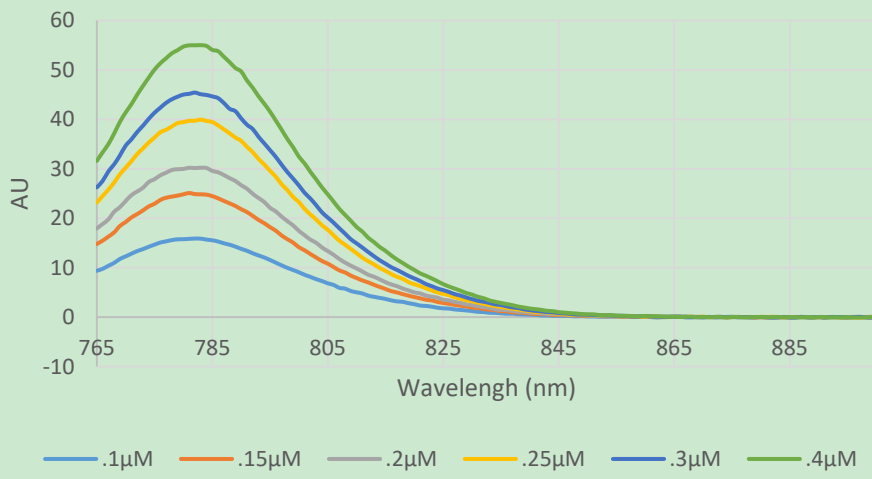




6-bT2 FL

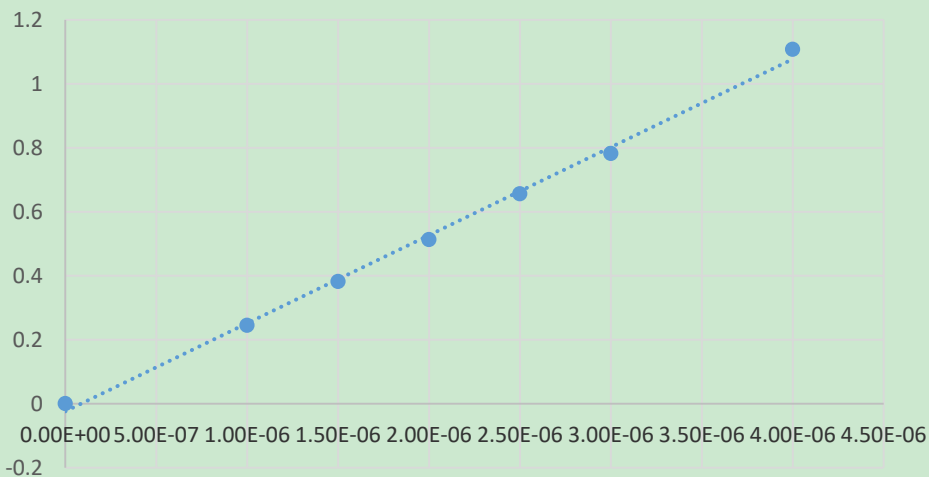


6-bT2 FL



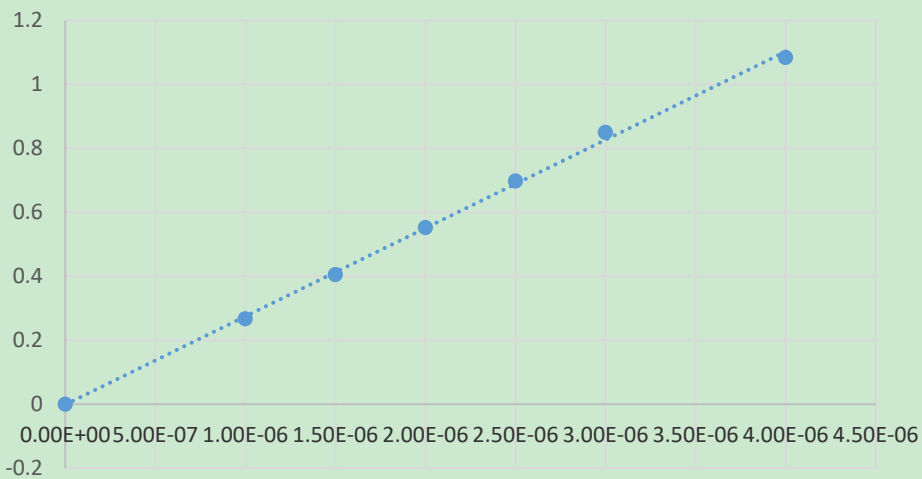
6-c T1 ABS

$y = 275238x - 0.0239$
 $R^2 = 0.9972$

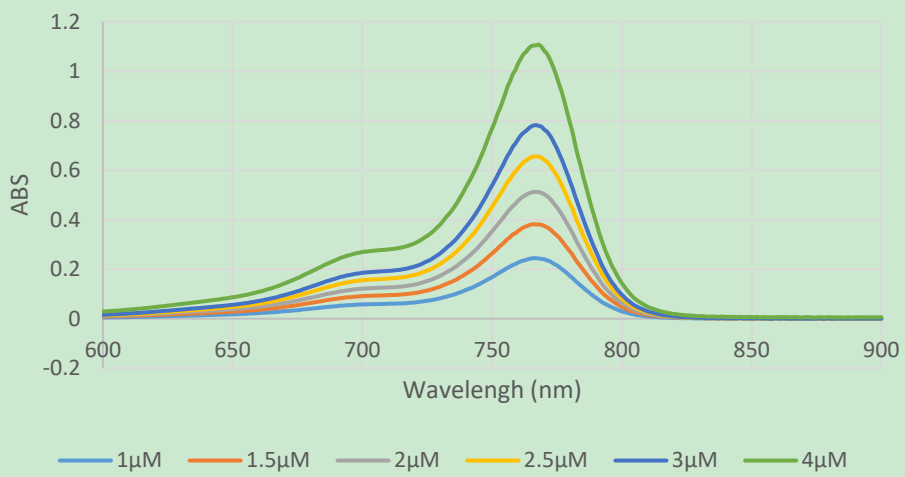


6-c T2 ABS

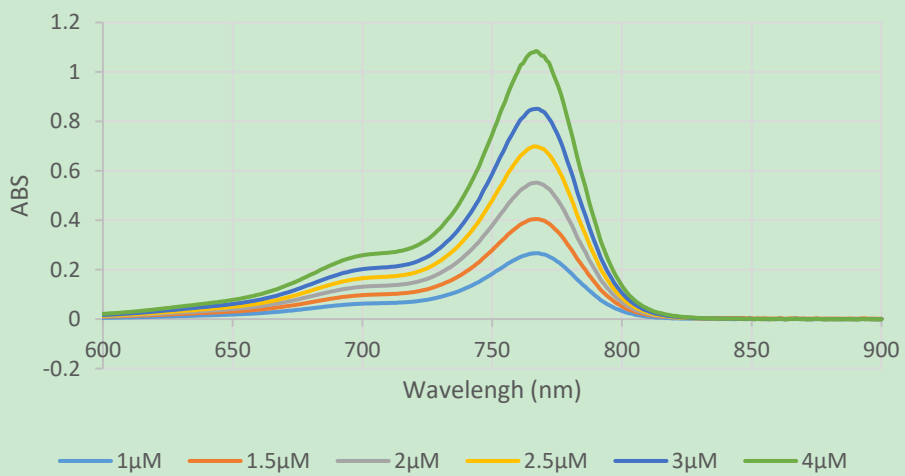
$y = 275952x - 0.001$
 $R^2 = 0.9986$

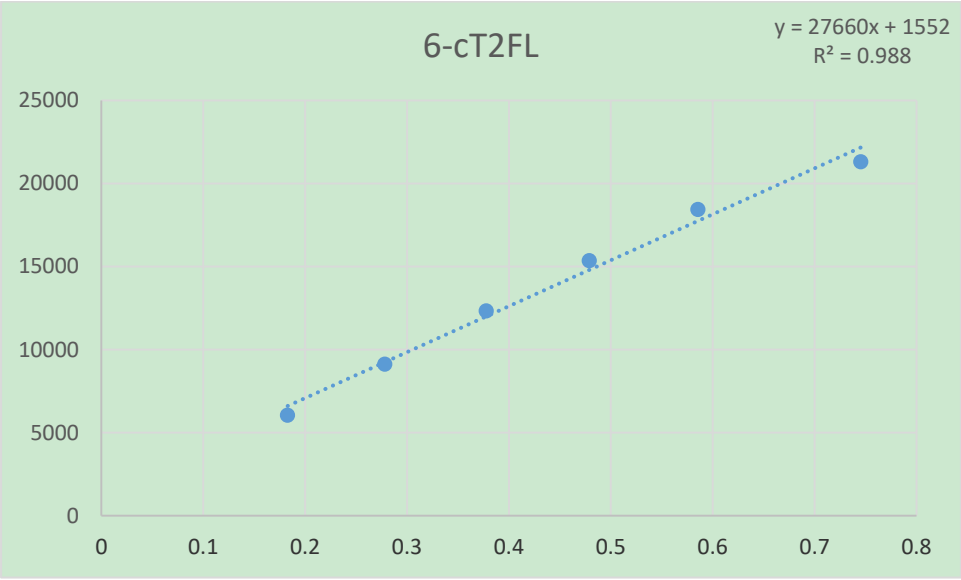
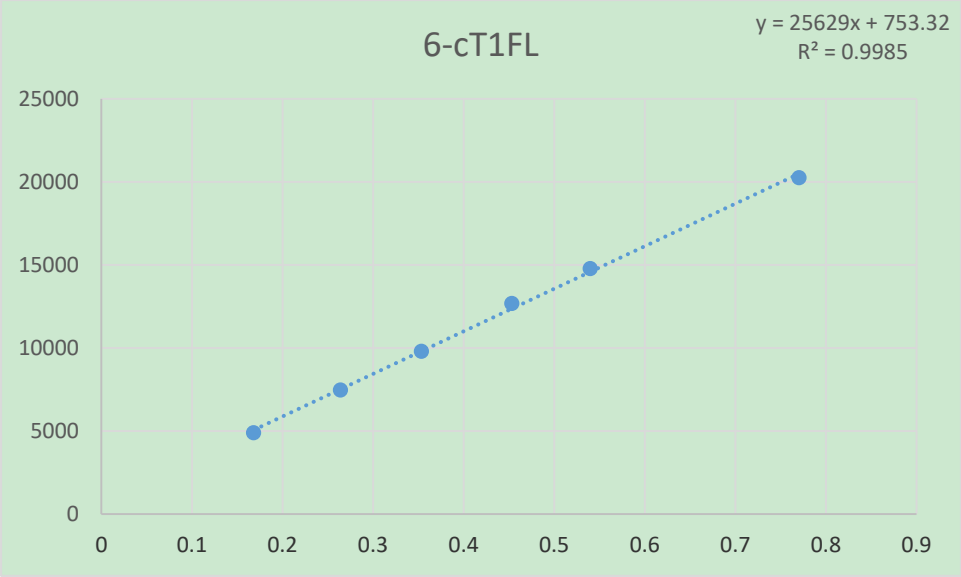


6-cT1 ABS

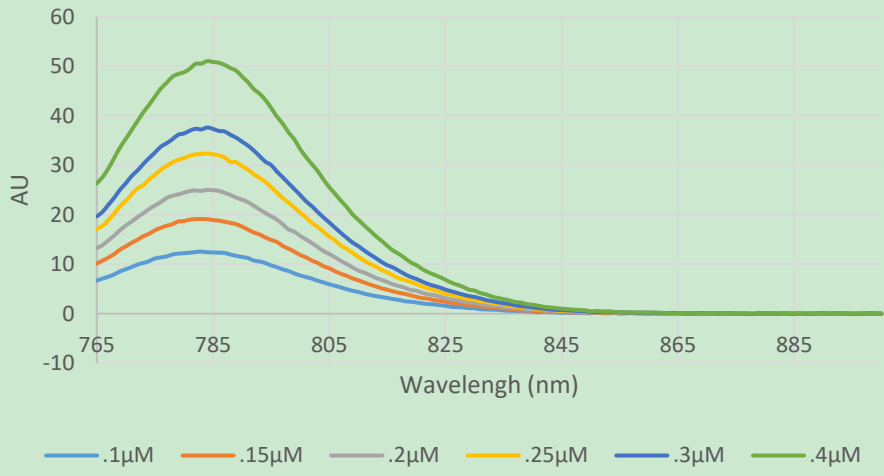


6-cT2 ABS

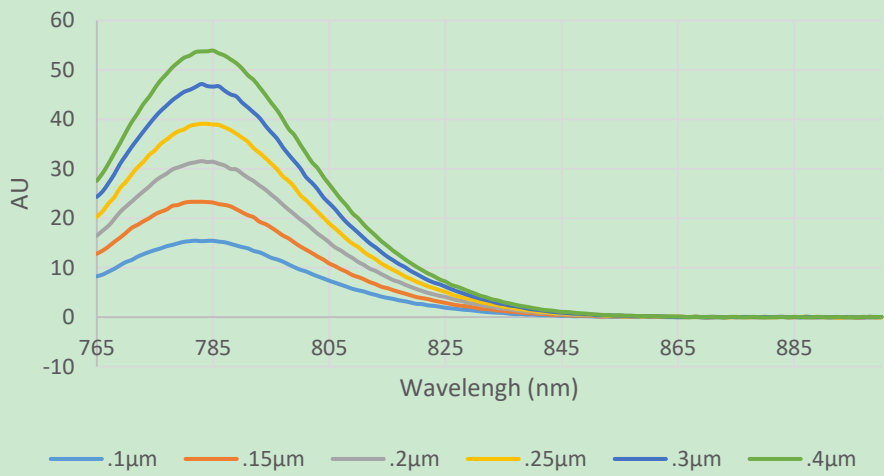




6-cT1 FL

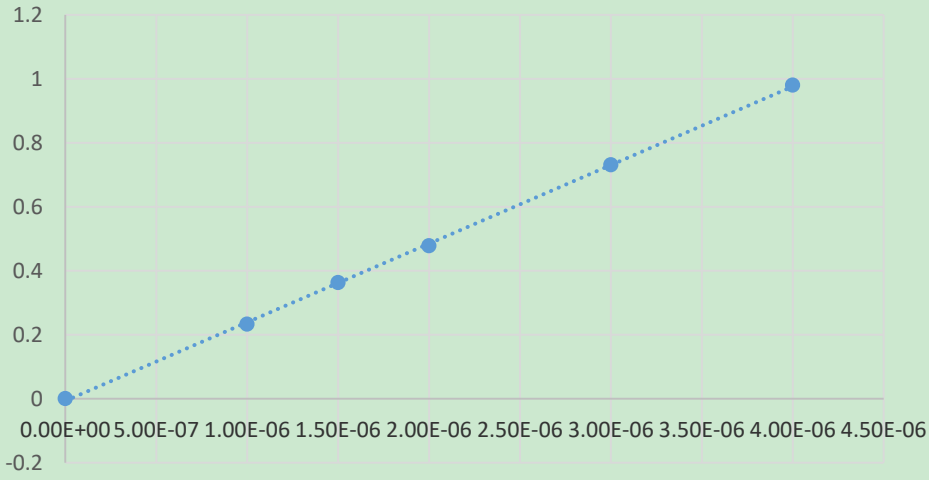


6-c T2 FL



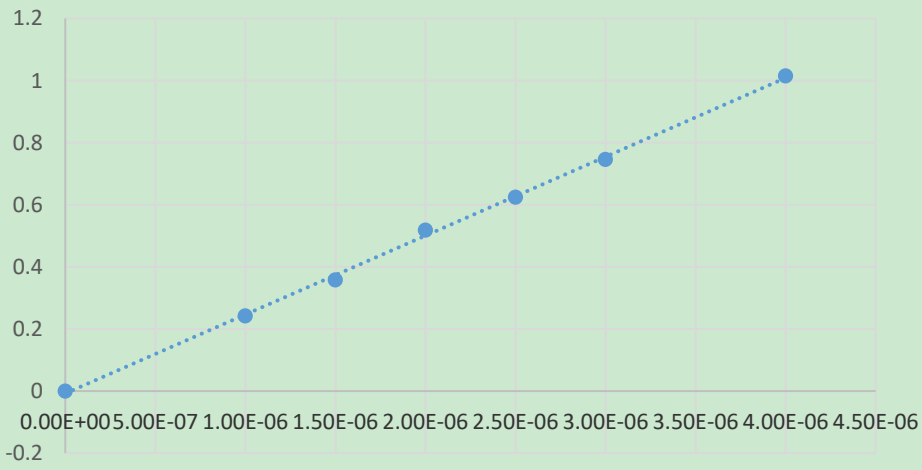
6-dT1 abs

$y = 245739x - 0.0068$
 $R^2 = 0.9998$

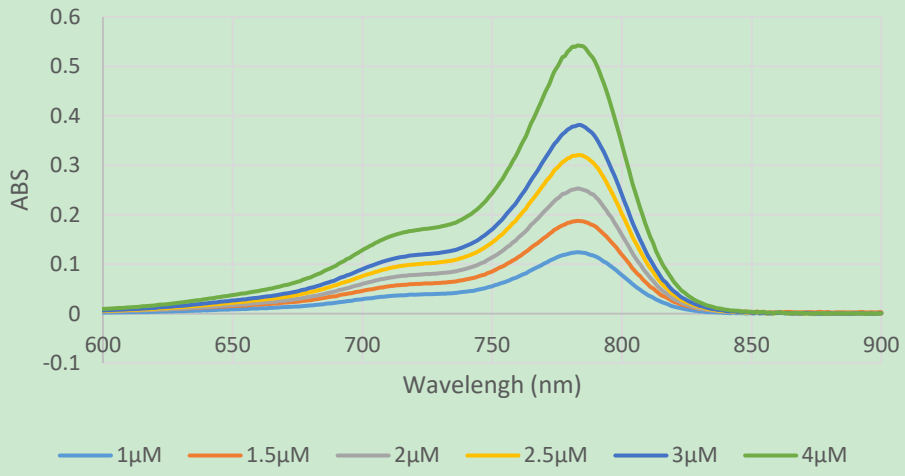


6-d t2 abs

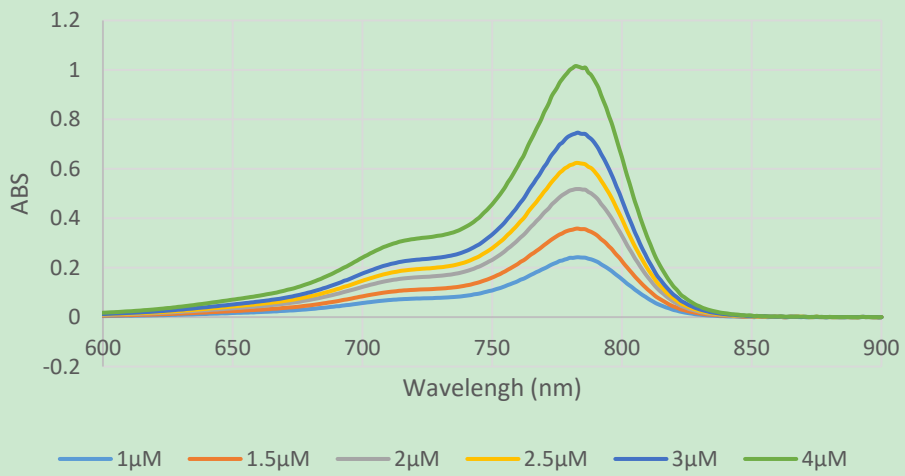
$y = 254000x - 0.0076$
 $R^2 = 0.9989$

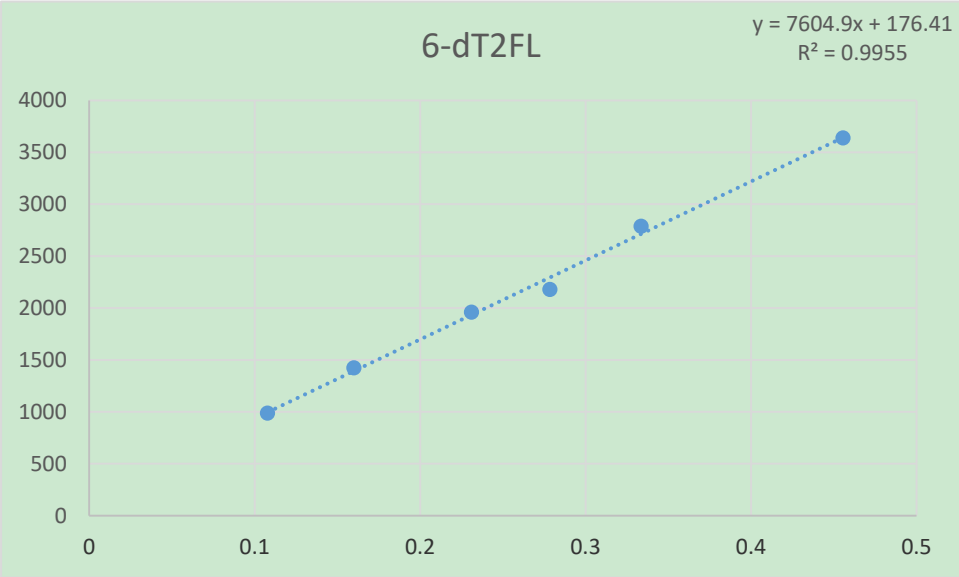
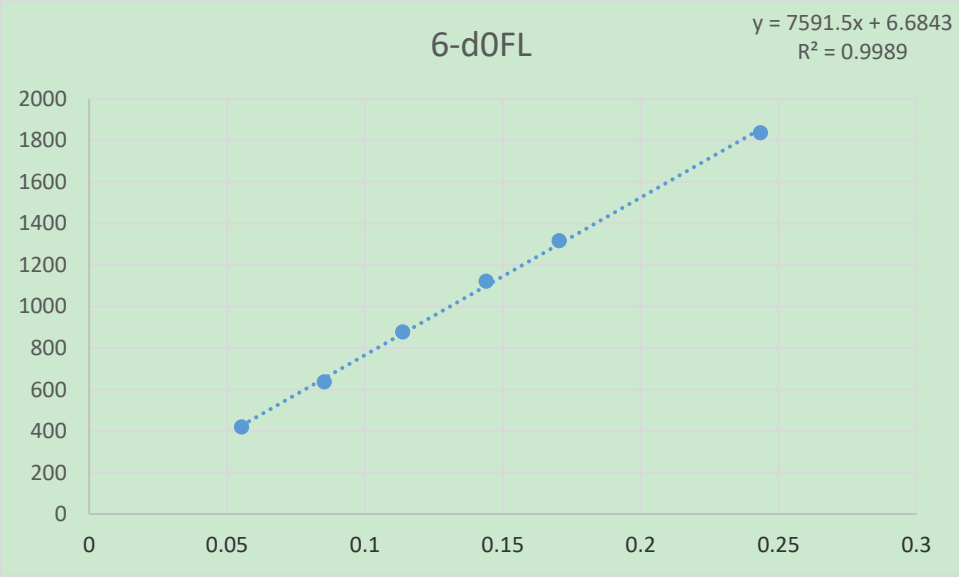


6-d T1 ABS

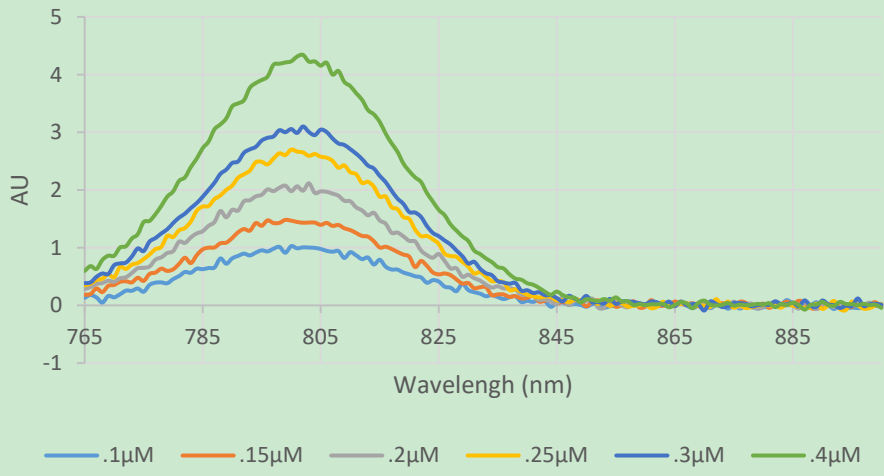


6-d T2 ABS

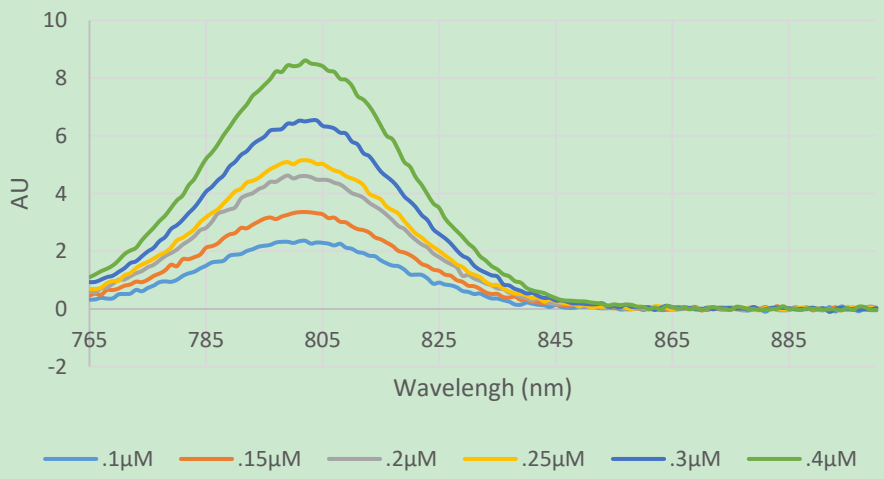




6-dT1 FL

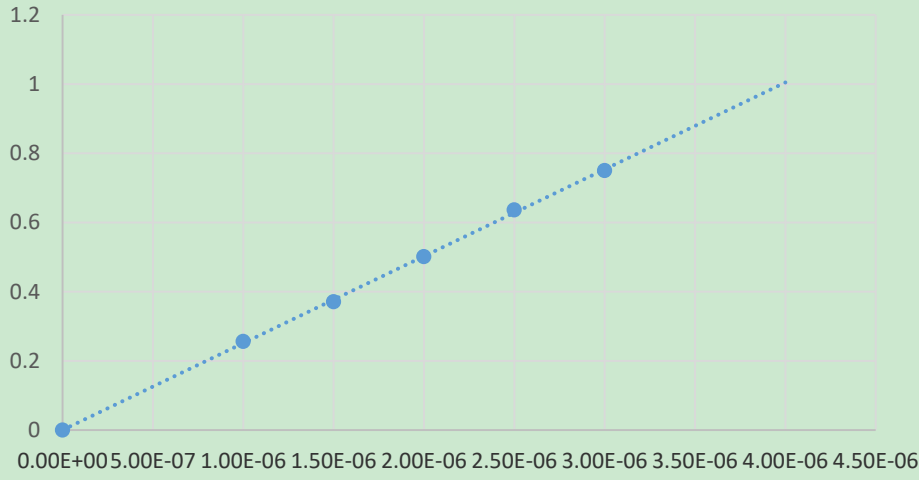


6-dT2 FL



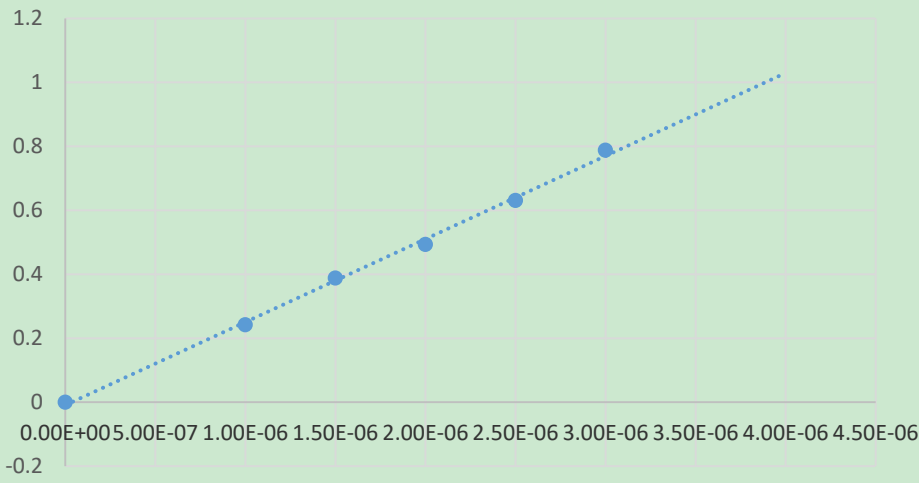
6-eT1 abs

$y = 251057x + 0.0006$
 $R^2 = 0.9996$

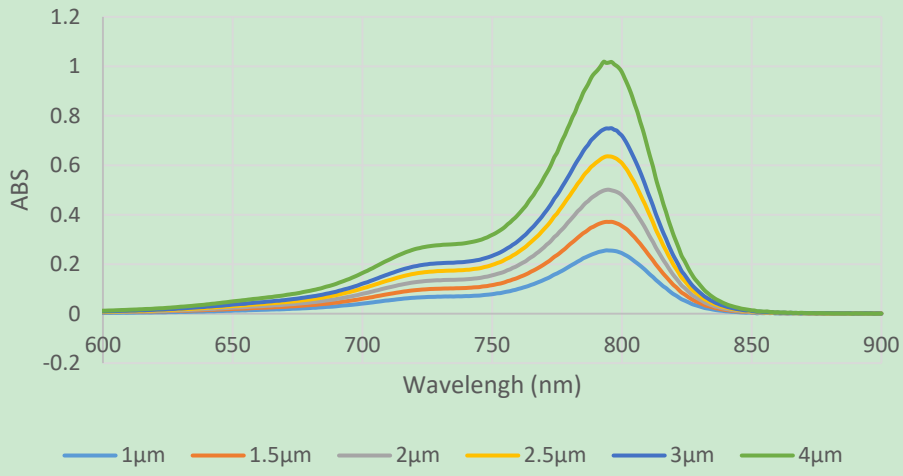


6-eT2 abs

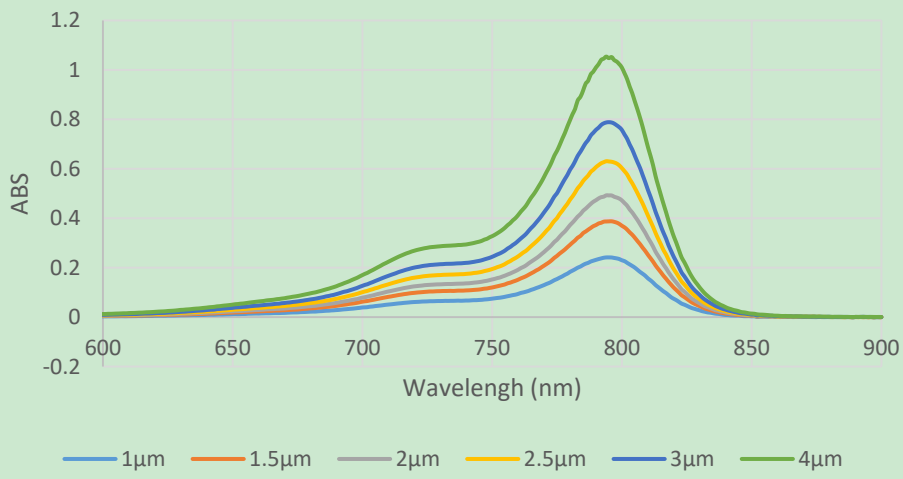
$y = 259686x - 0.0091$
 $R^2 = 0.9977$

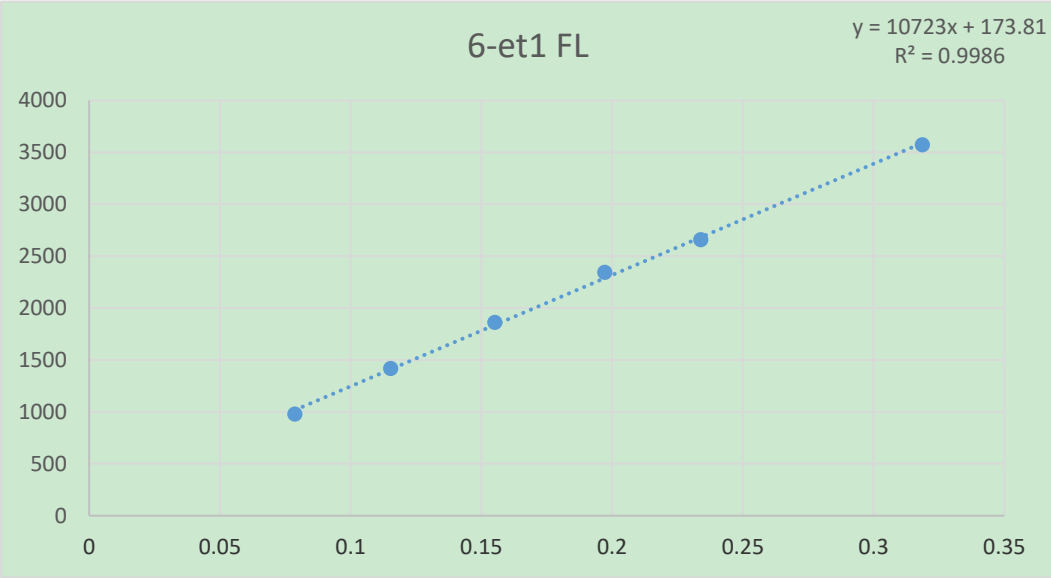
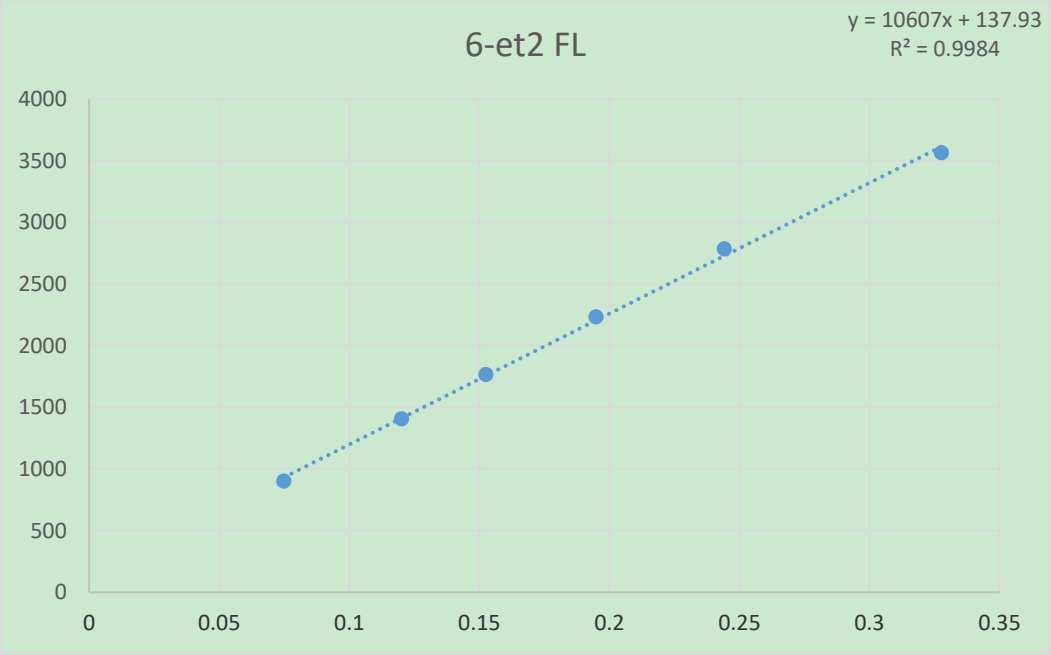


6-eT1 ABS

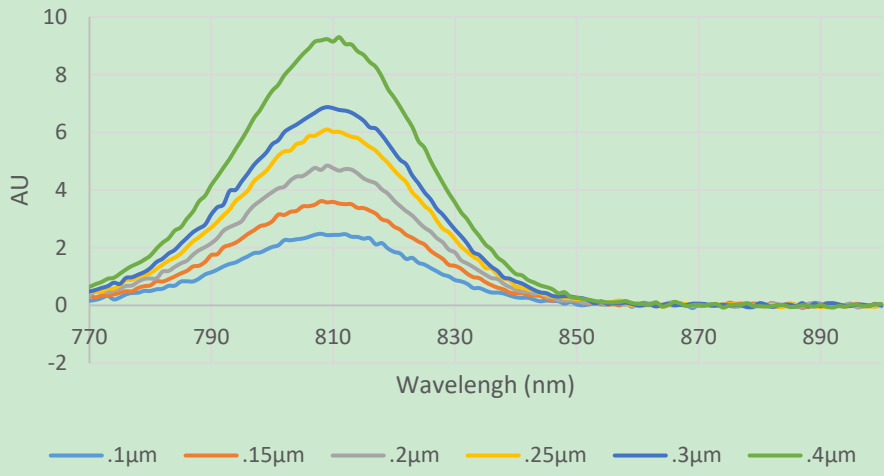


6-eT2 ABS

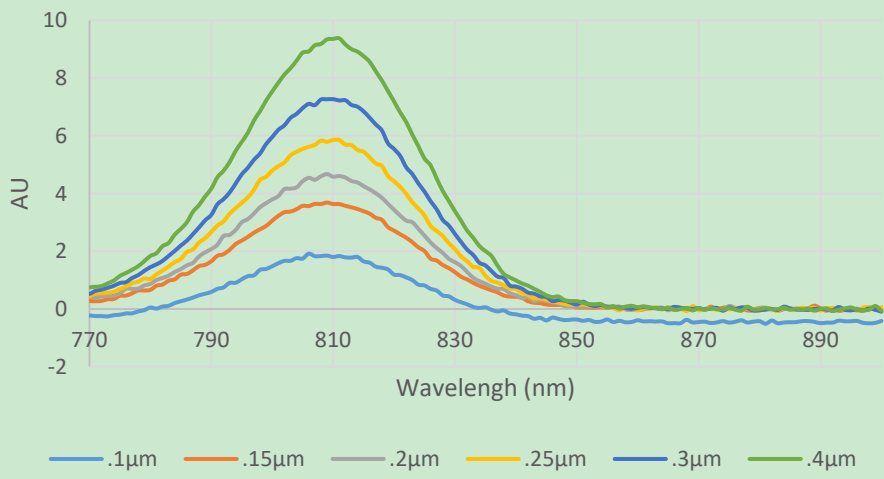


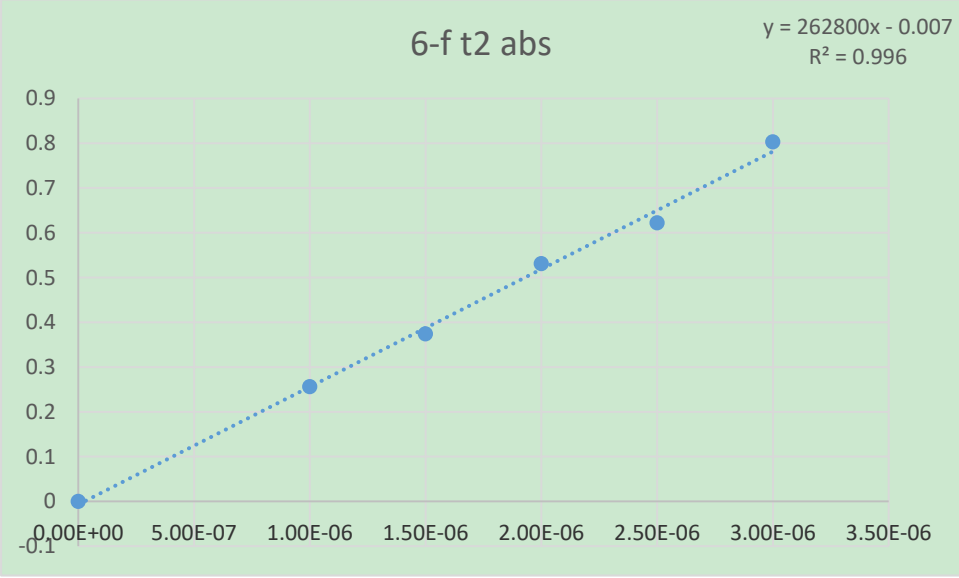
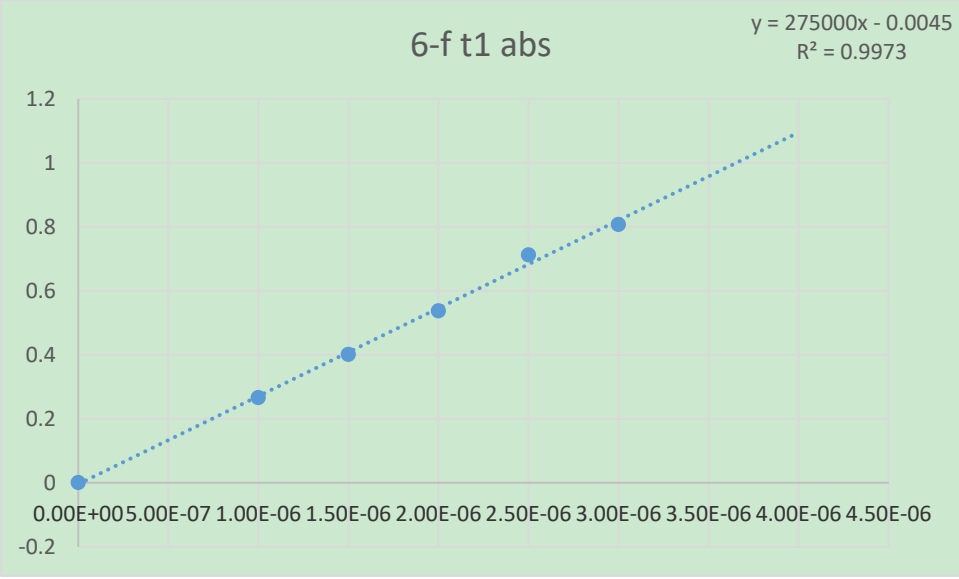


6-eT1 FL

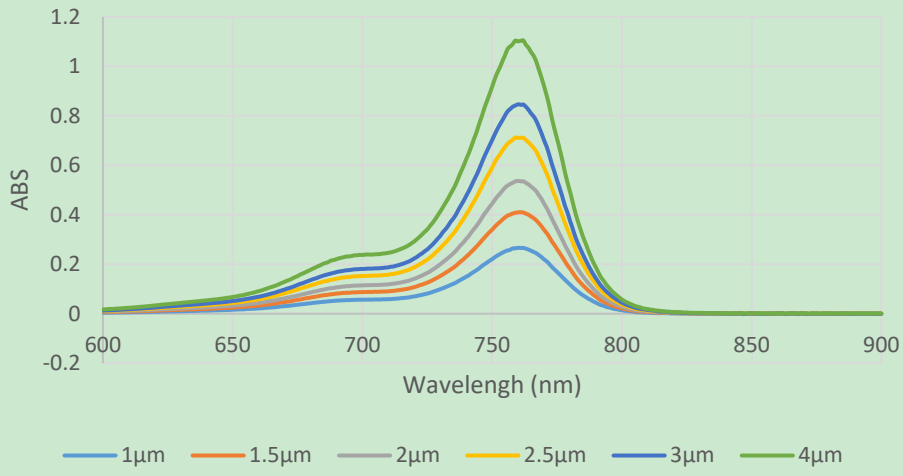


6-eFL

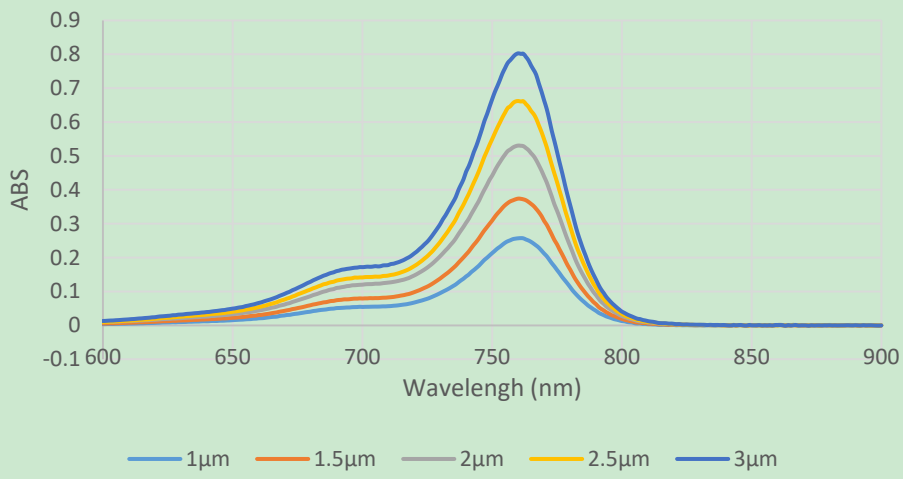


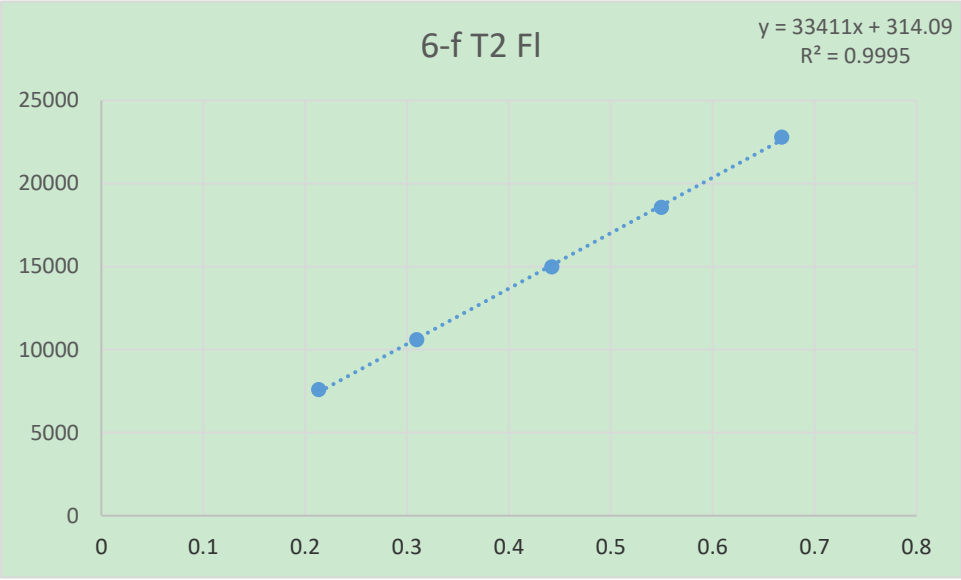
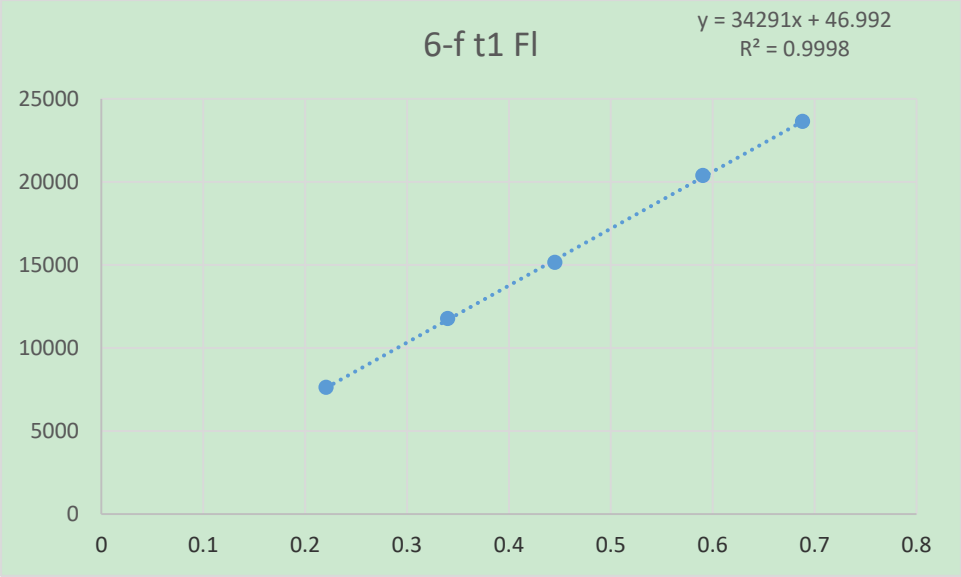


6-f T1 ABS

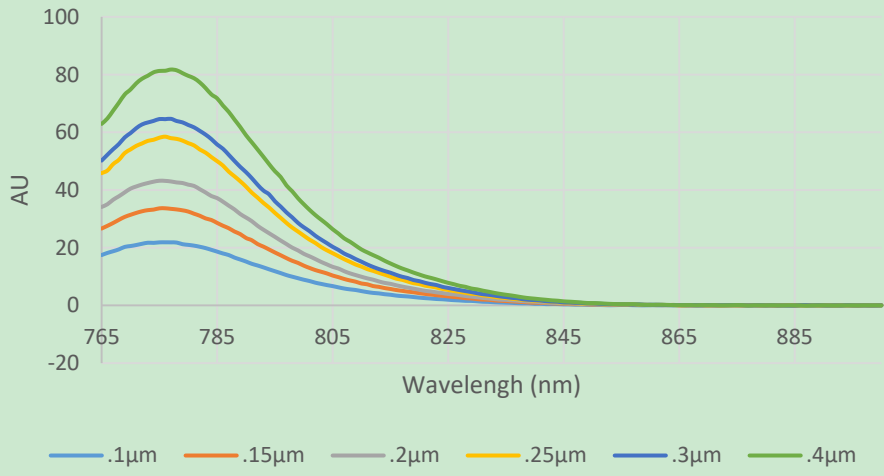


6-f T2 ABS

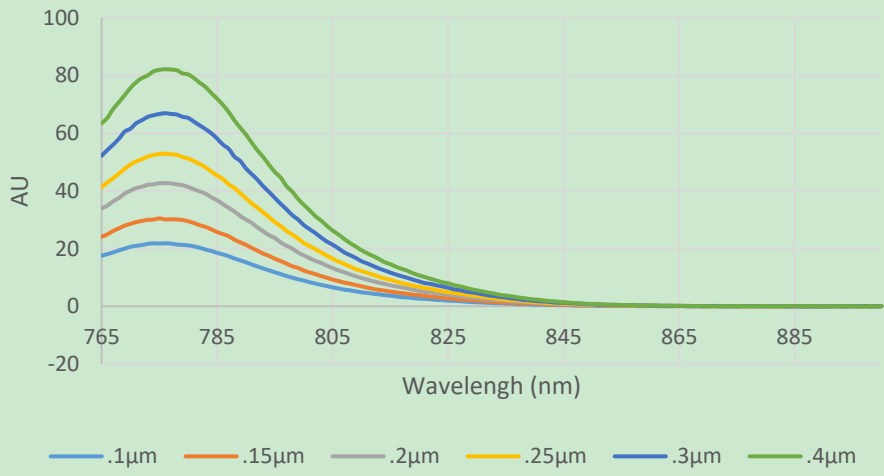


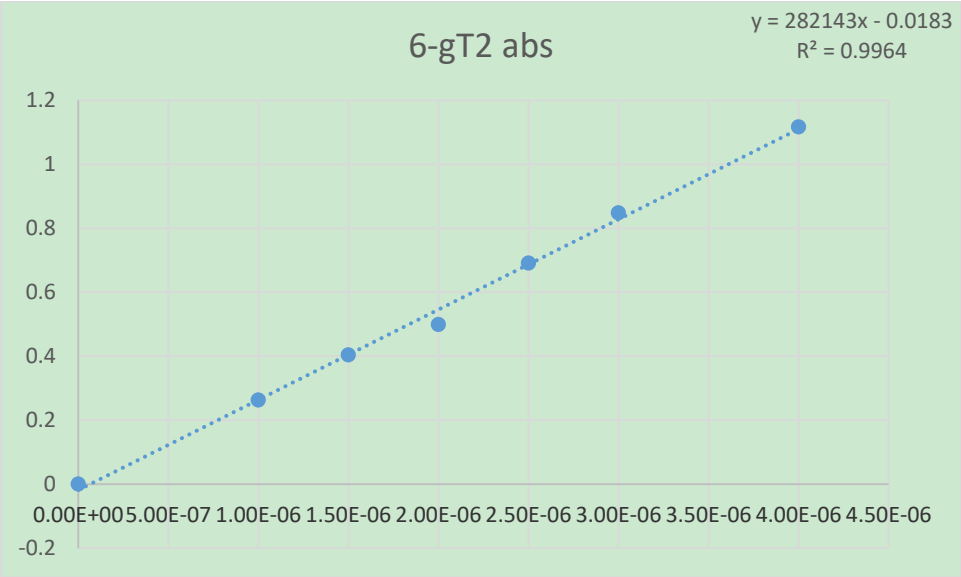
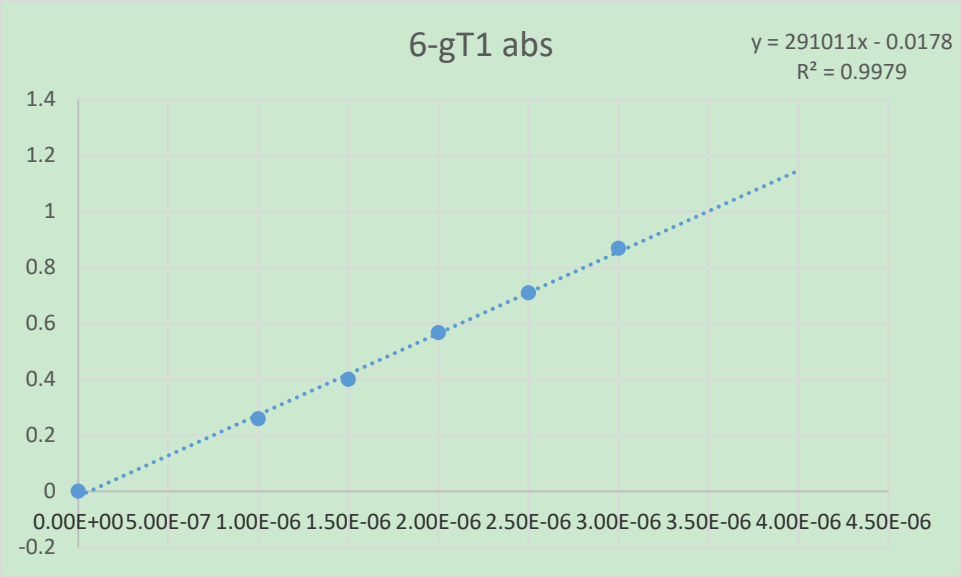


6-f T1 FL

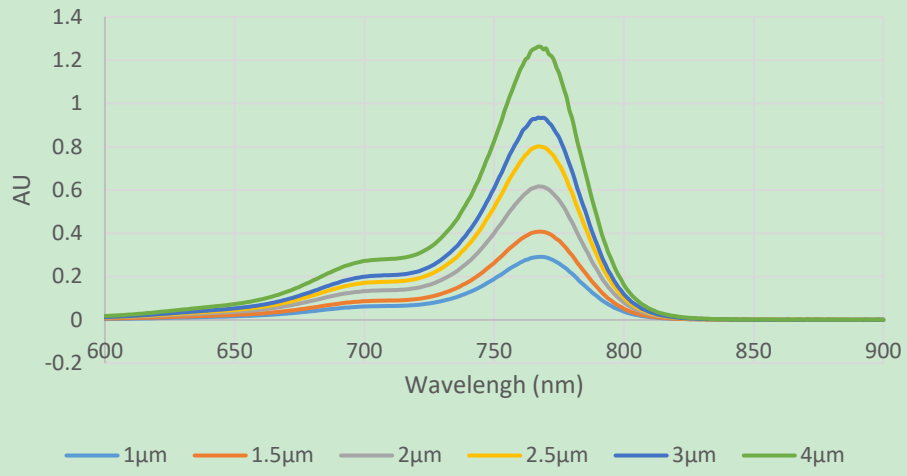


6-f T2 FL

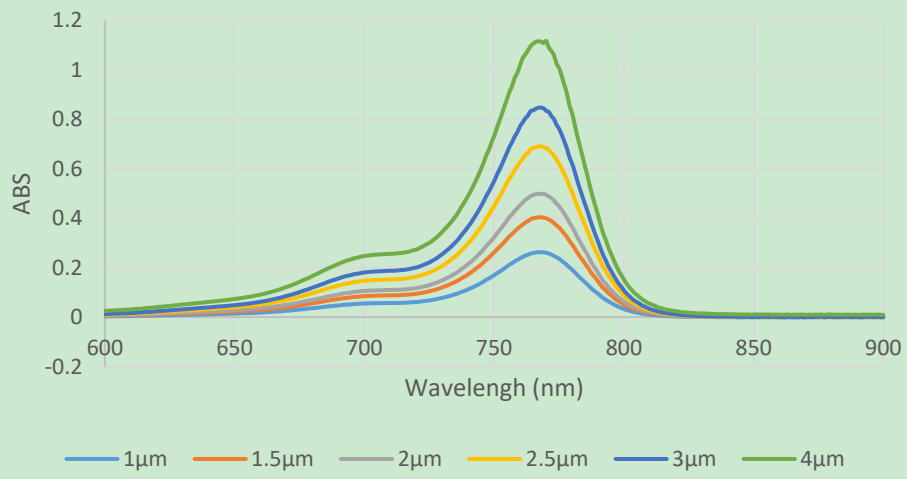


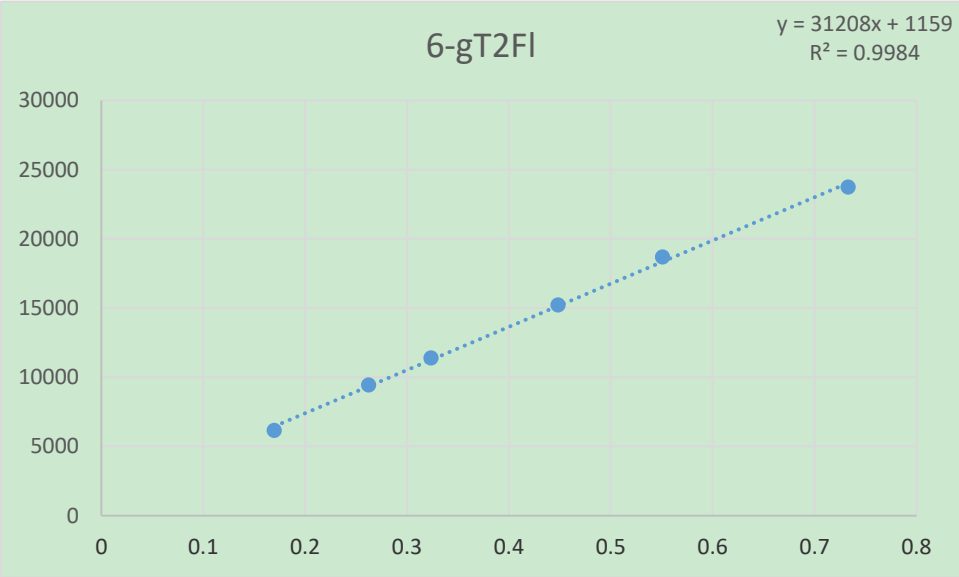
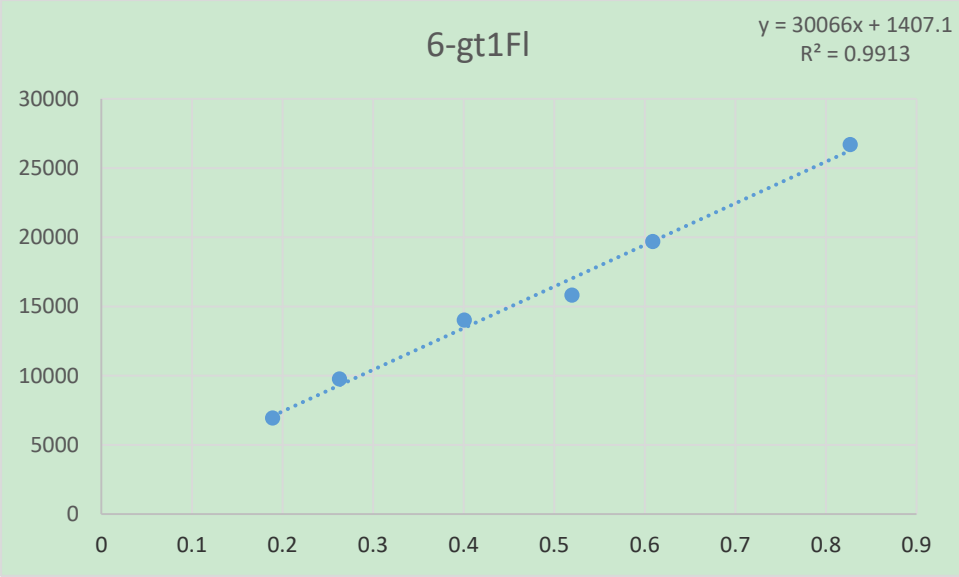


6-gT1 ABS

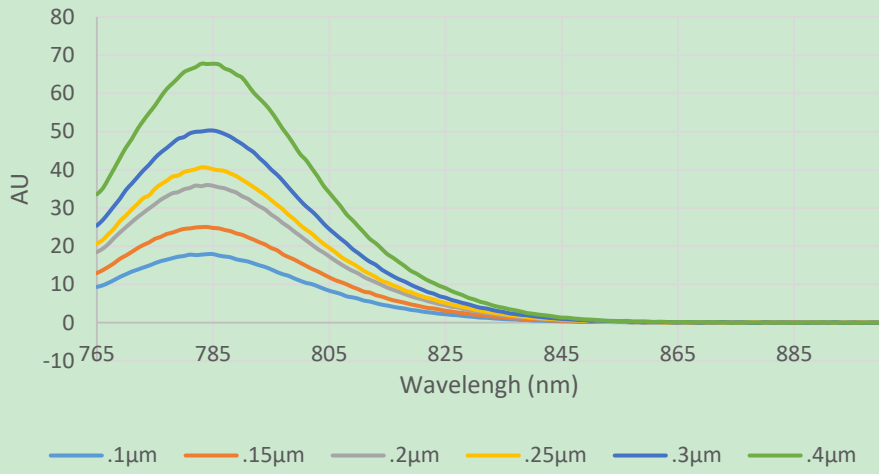


6-gT2 ABS

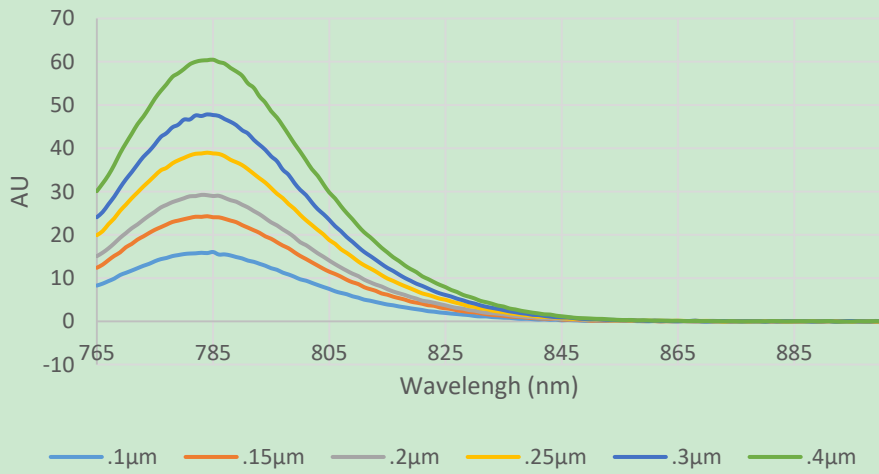


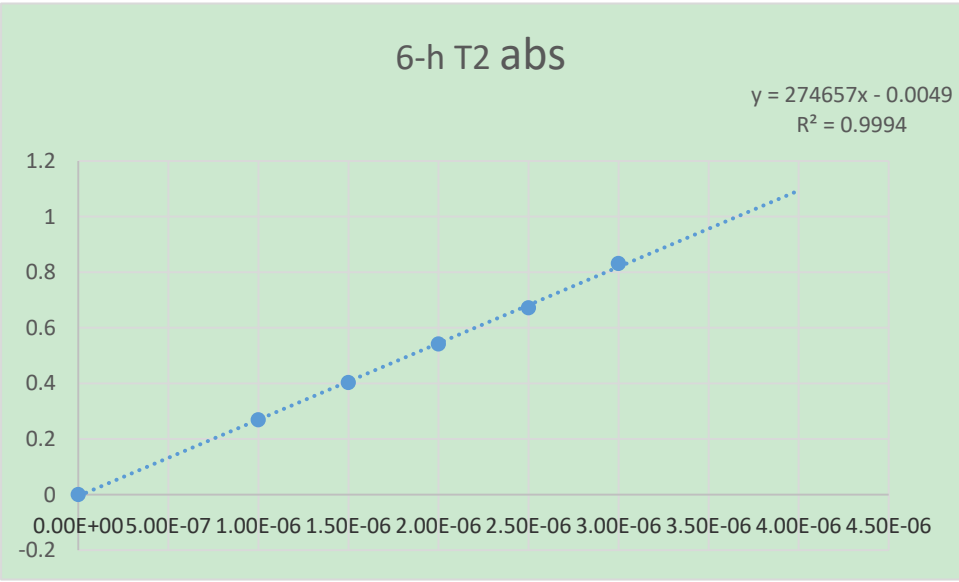
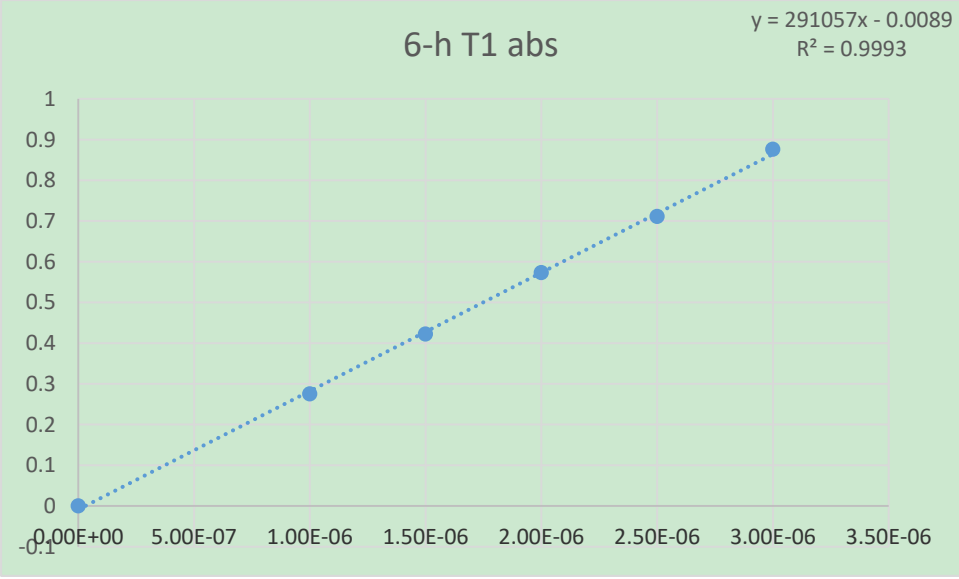


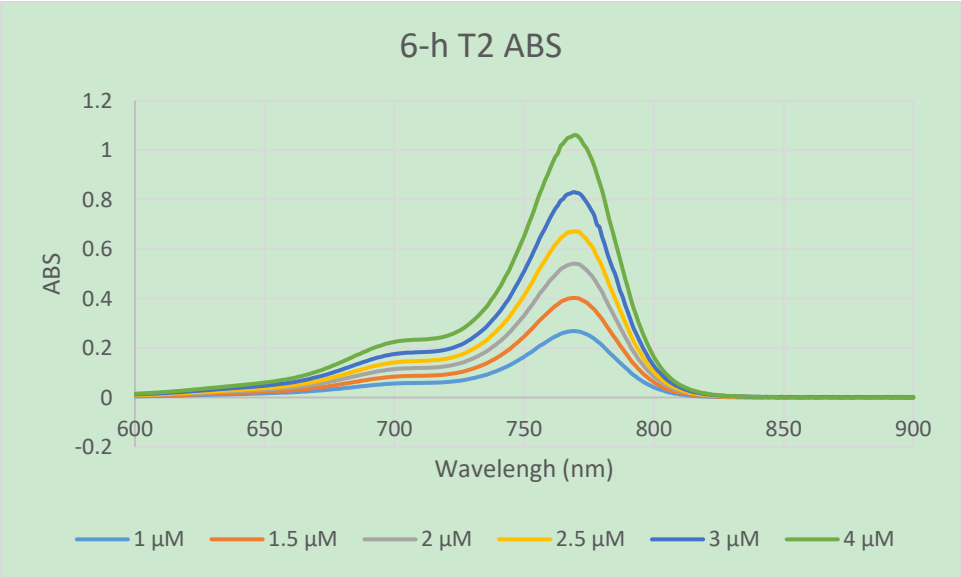
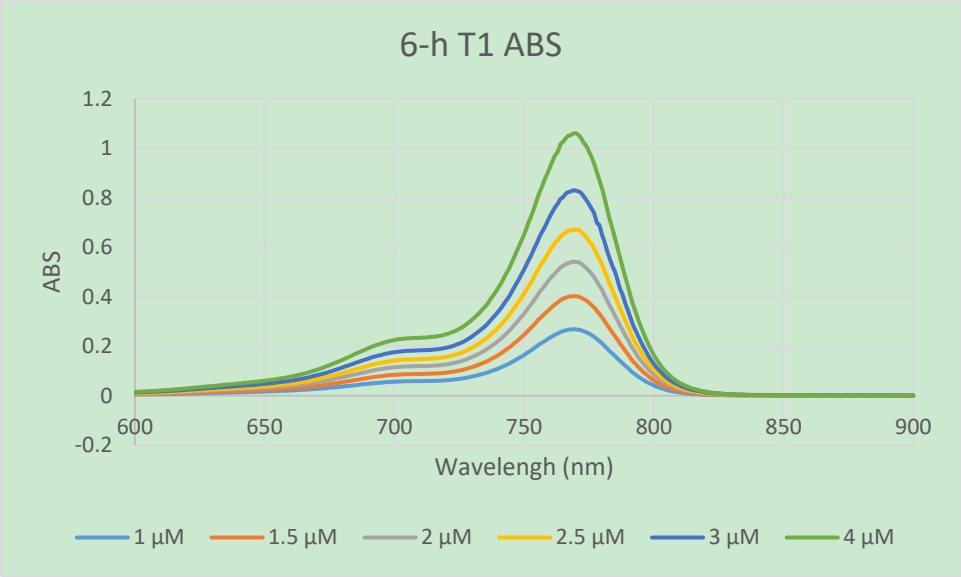
6-gT1 FL

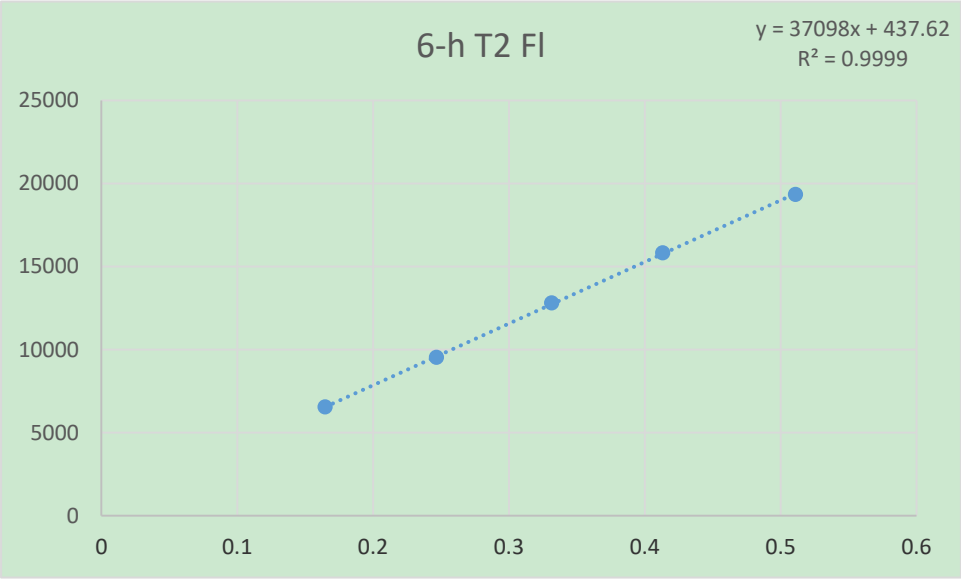
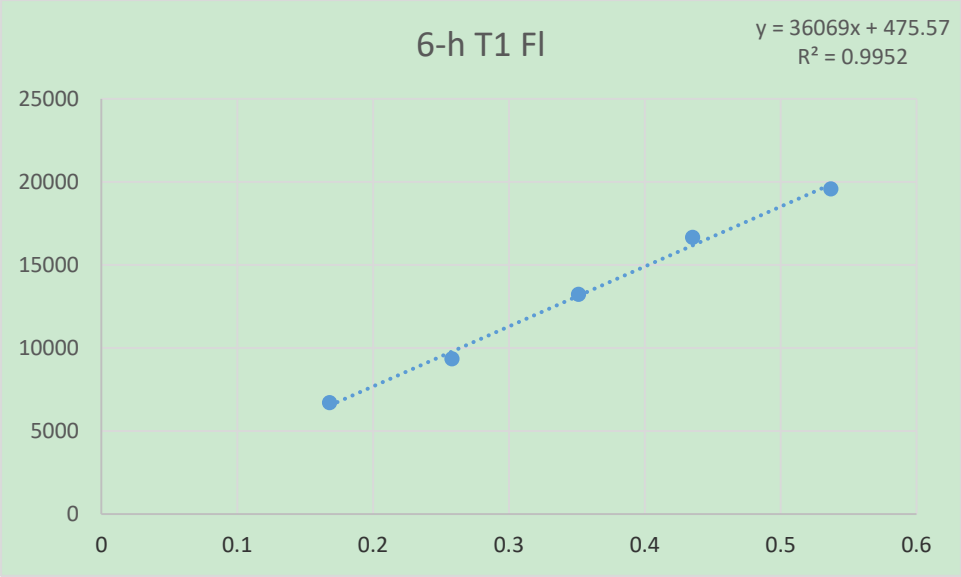


6-gT2 FL

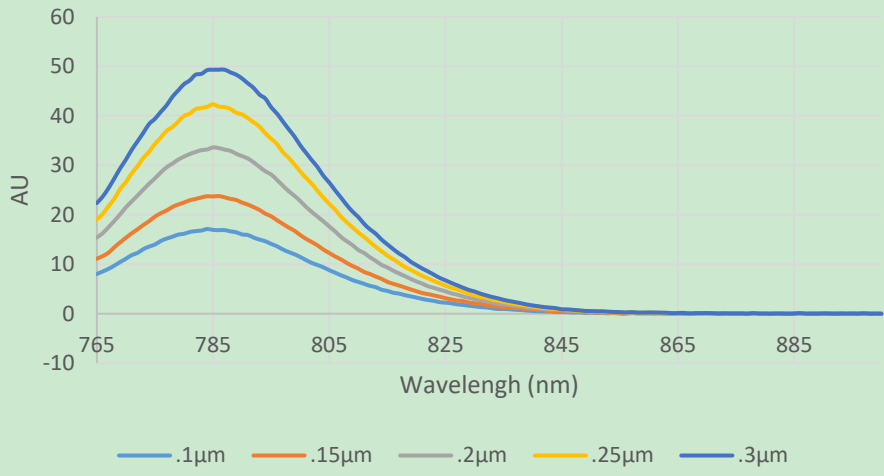




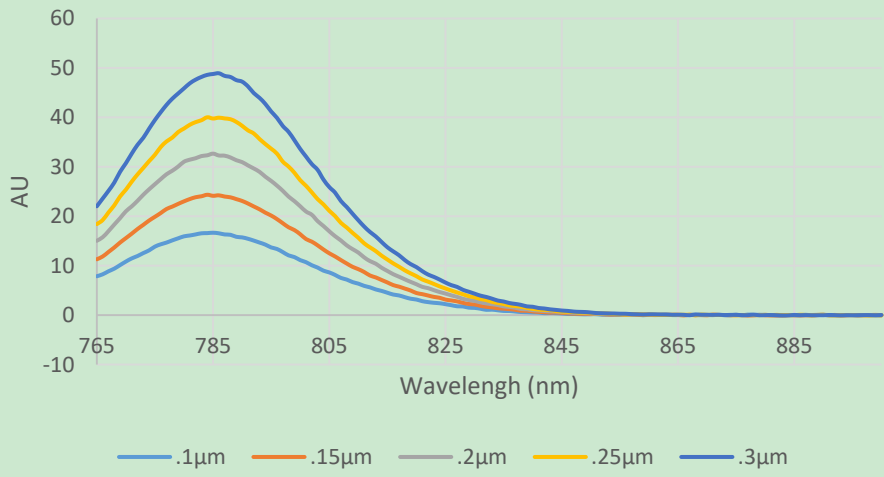




6-h T1 FL

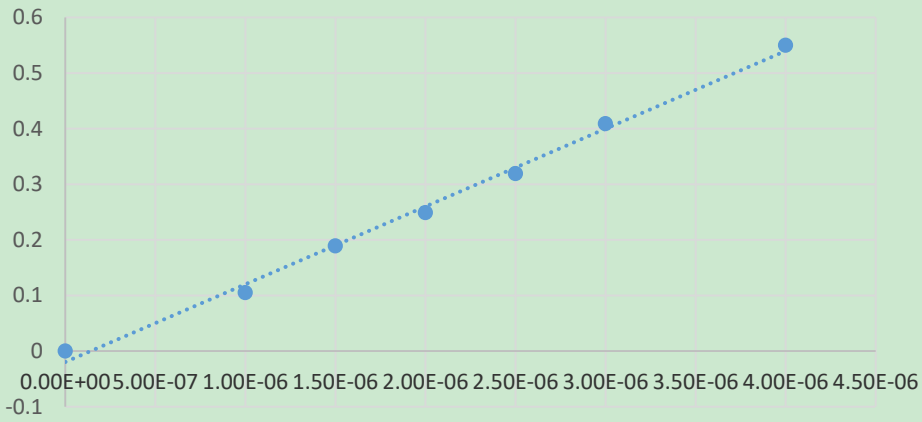


6-h T2 FL



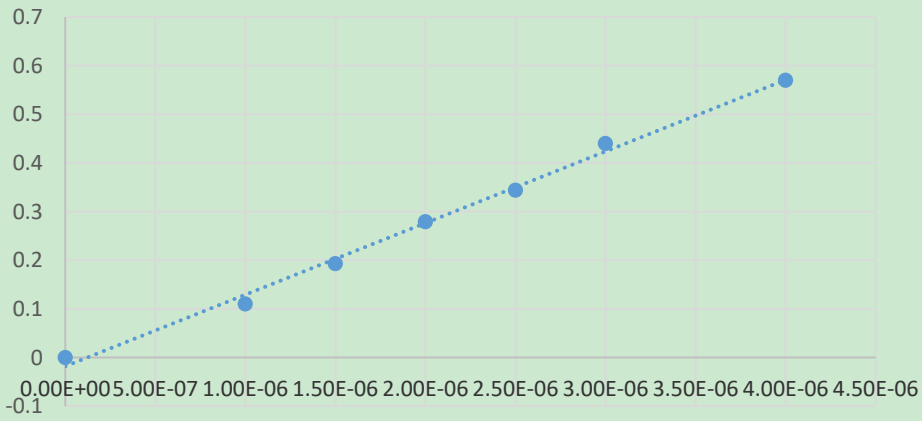
6-i T1 abs

$$y = 139905x - 0.0197$$
$$R^2 = 0.9949$$

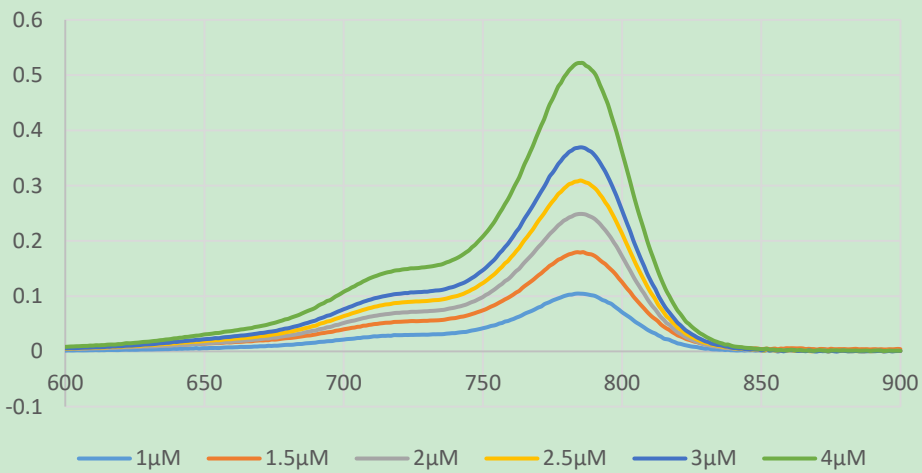


6-i T2 abs

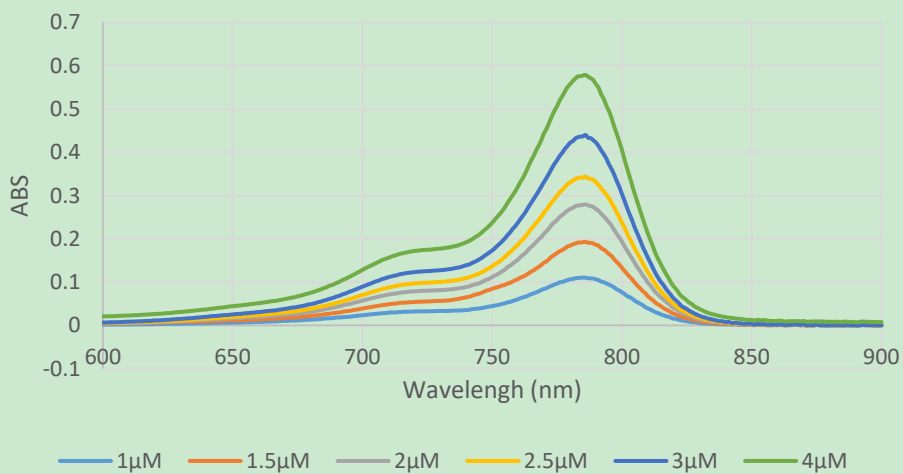
$$y = 147190x - 0.0178$$
$$R^2 = 0.9952$$

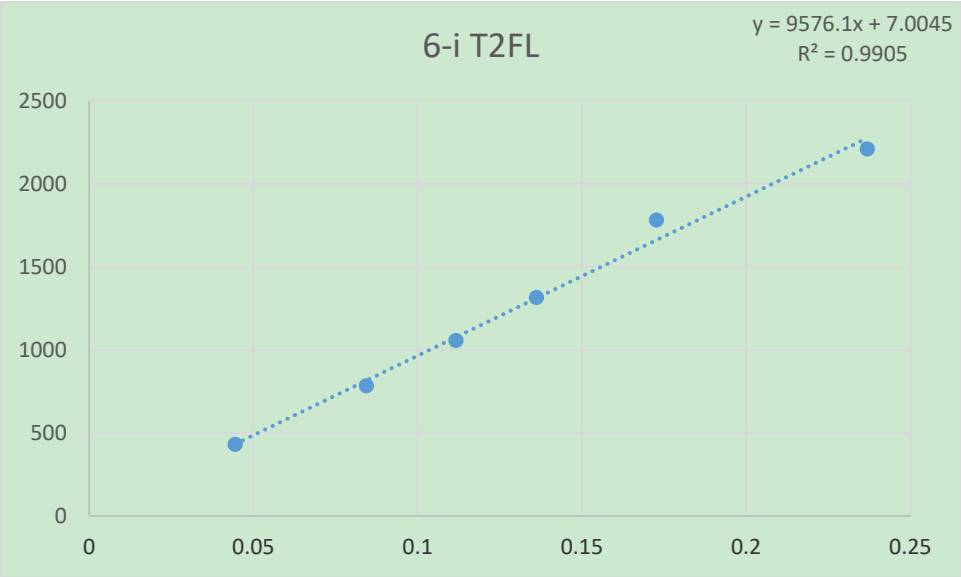
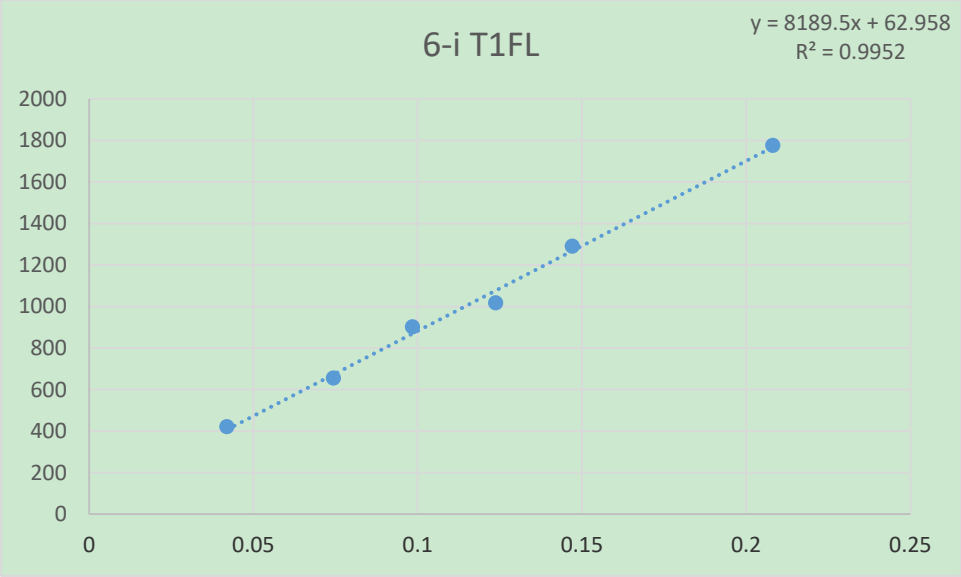


6-i T1 ABS

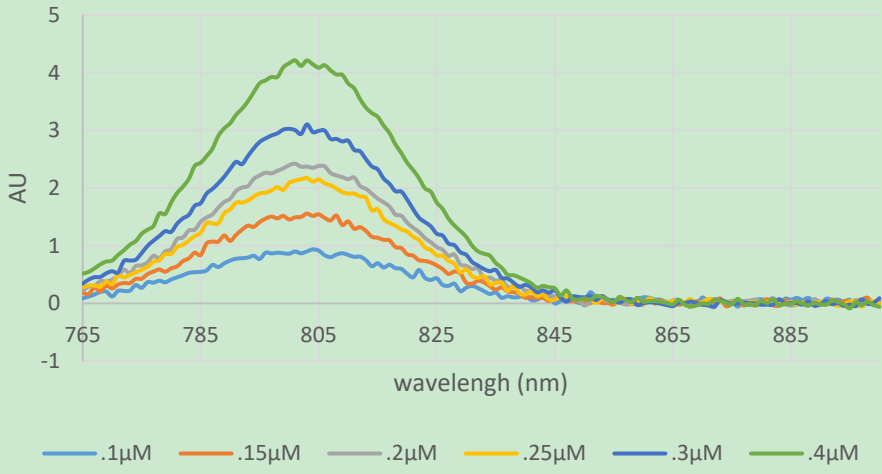


6-i T2 ABS

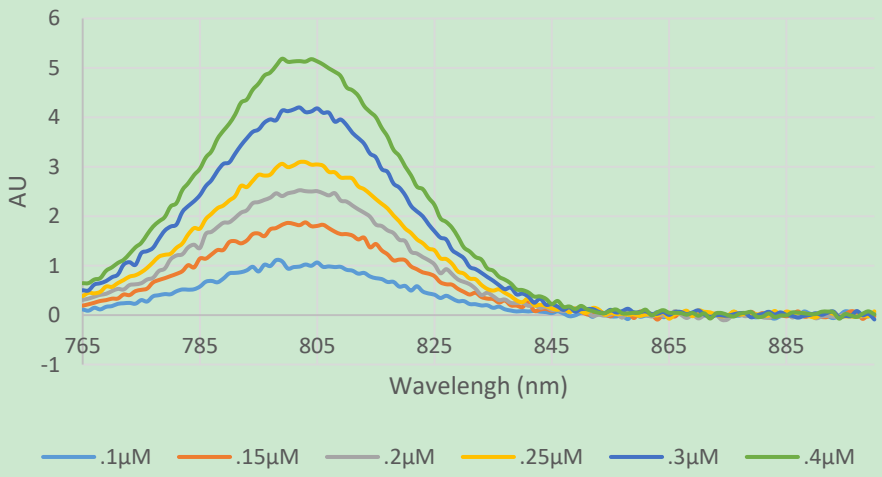


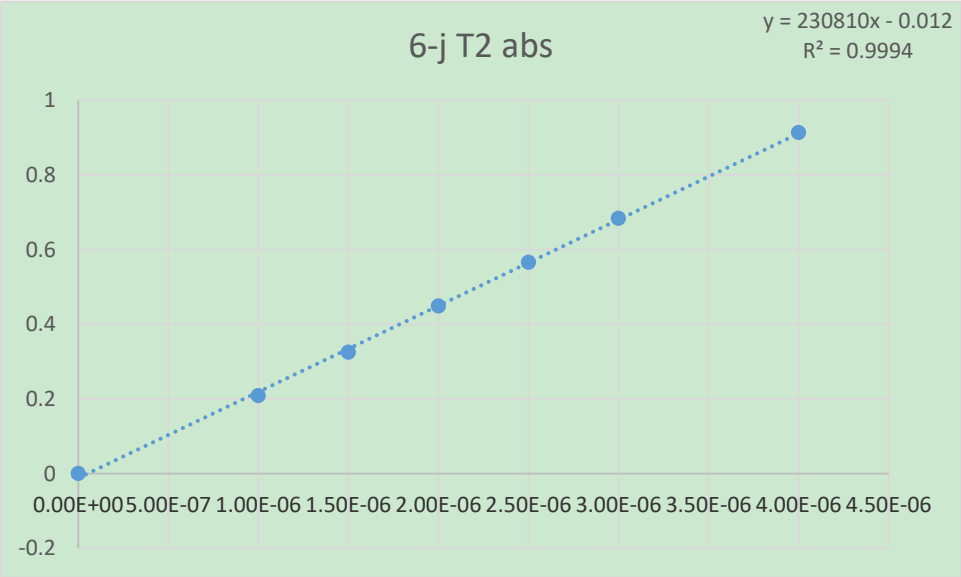
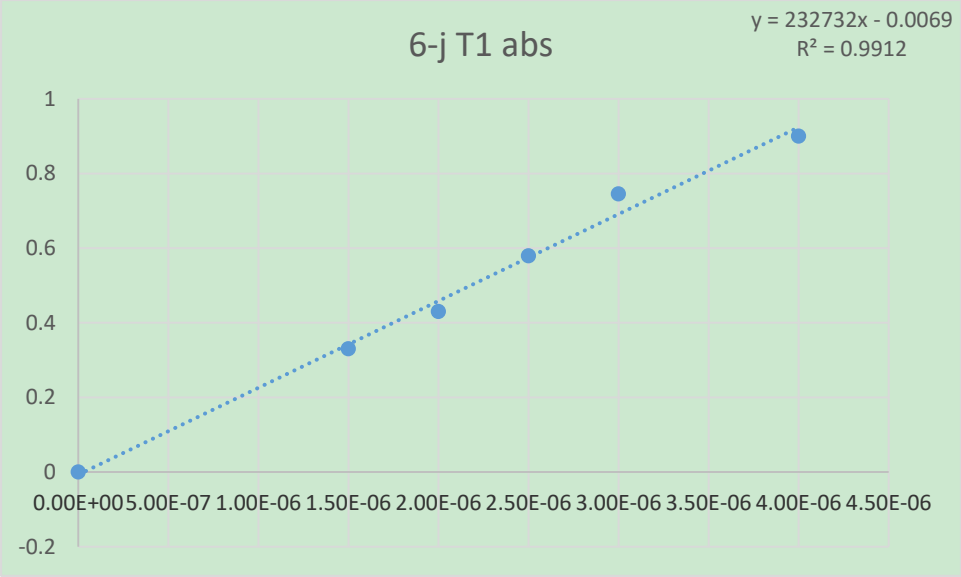


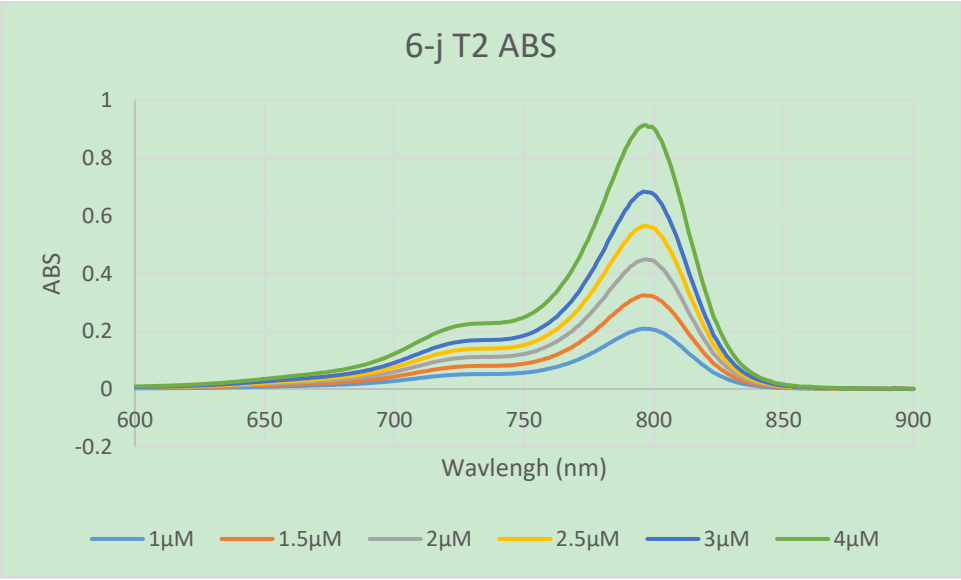
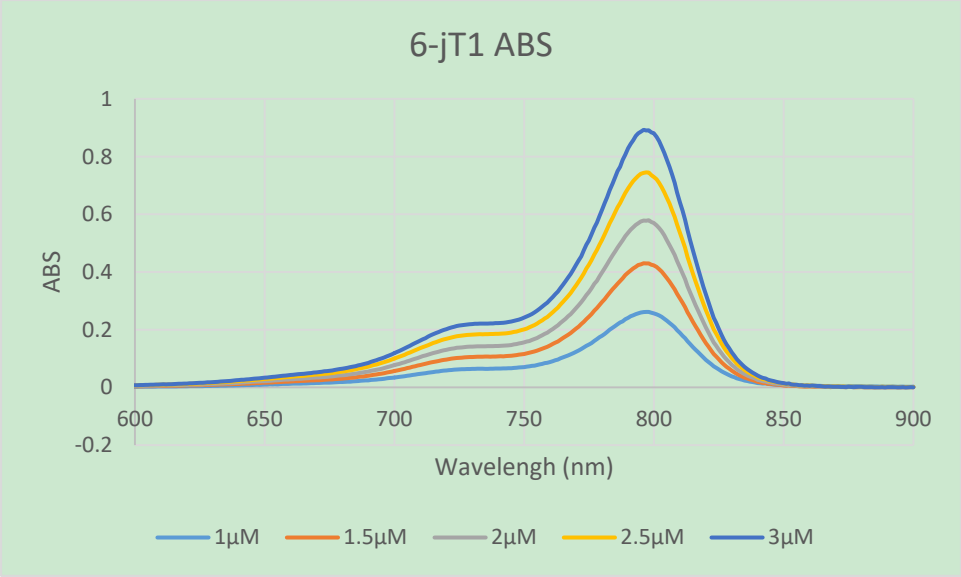
6-i T1 FL

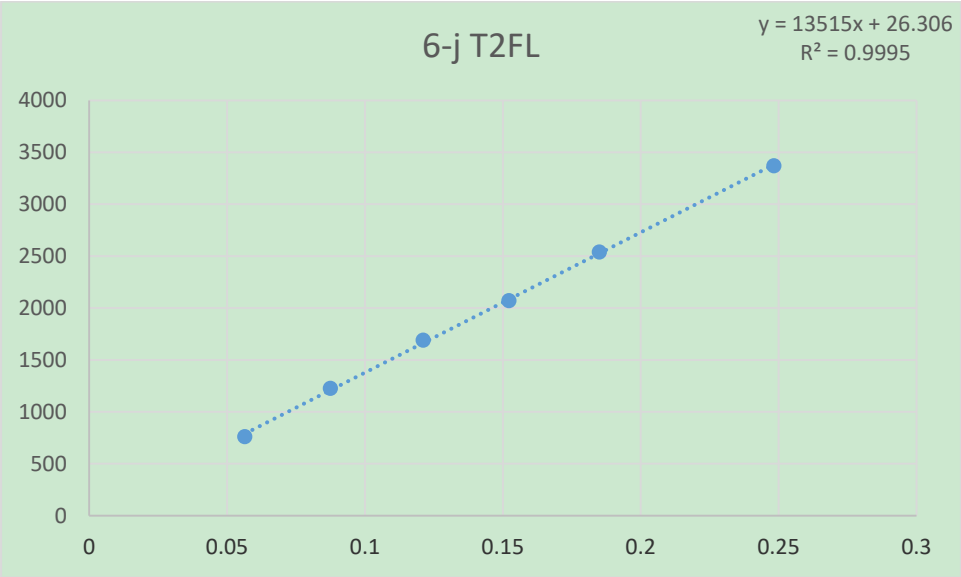
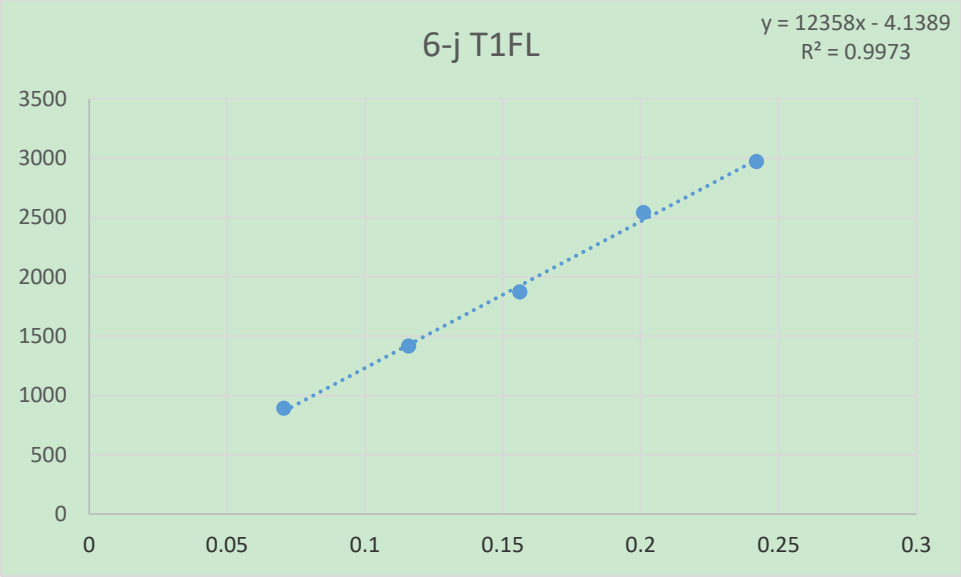


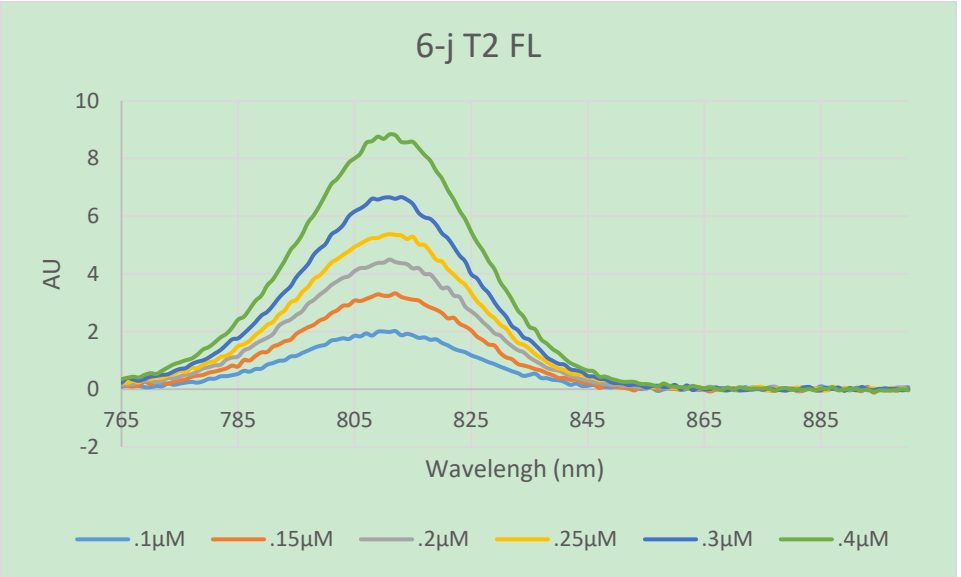
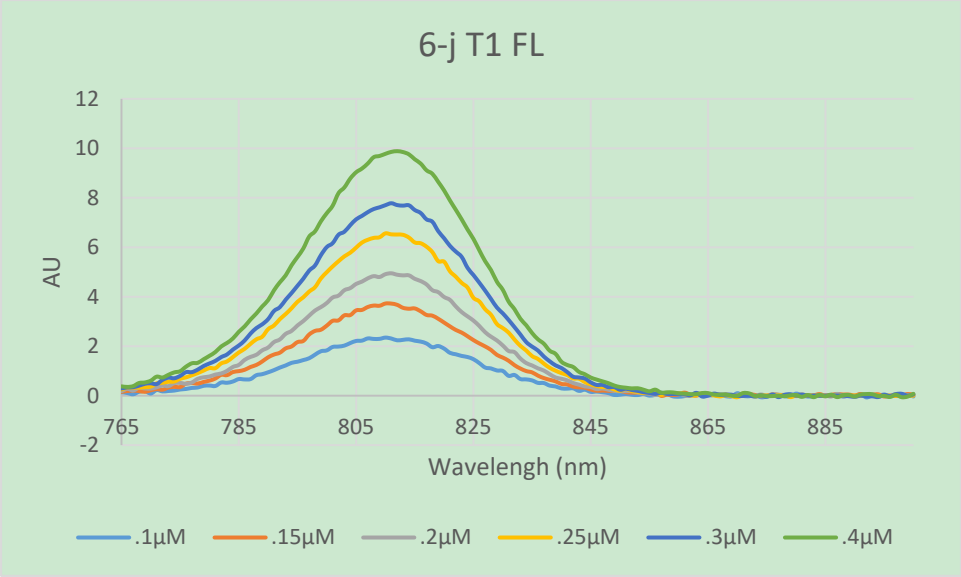
6-i T2 FL





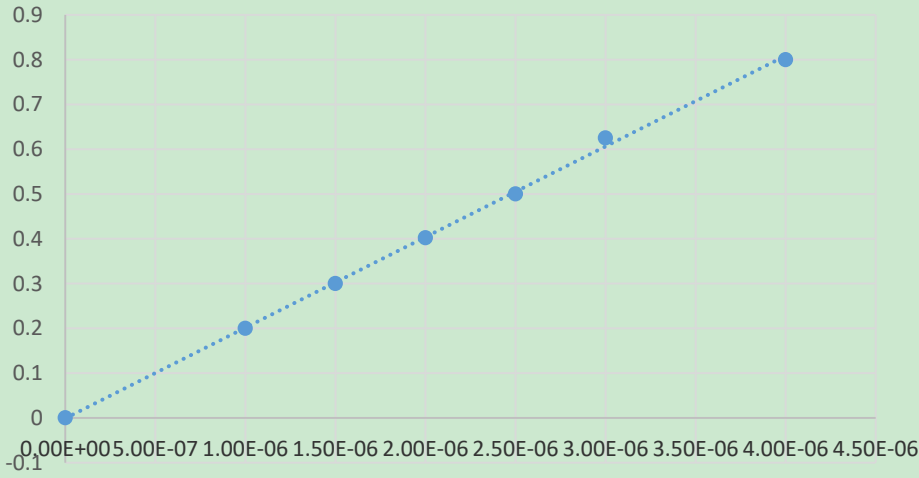






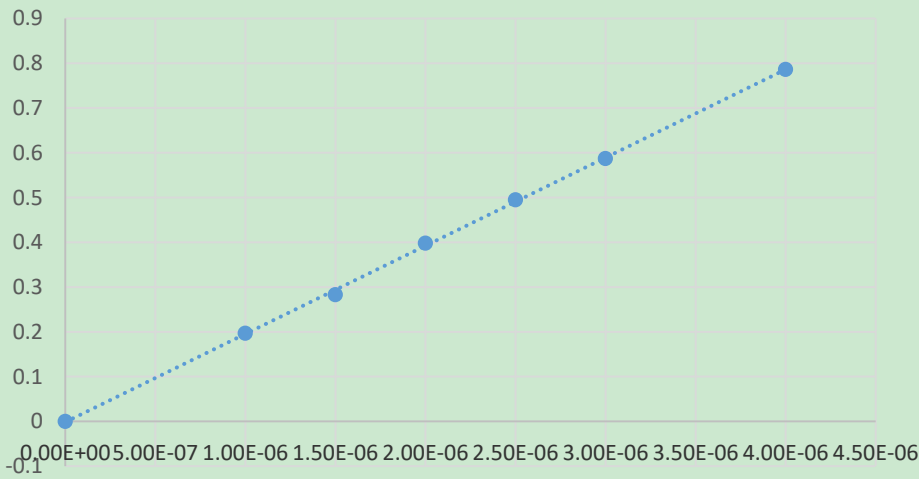
6-k T1 abs

$$y = 202381x - 0.0009$$
$$R^2 = 0.9989$$

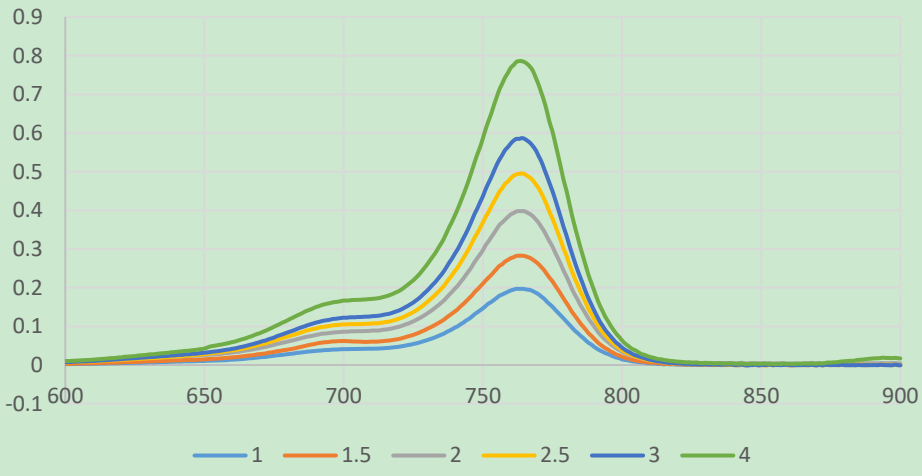


6-k T2 abs

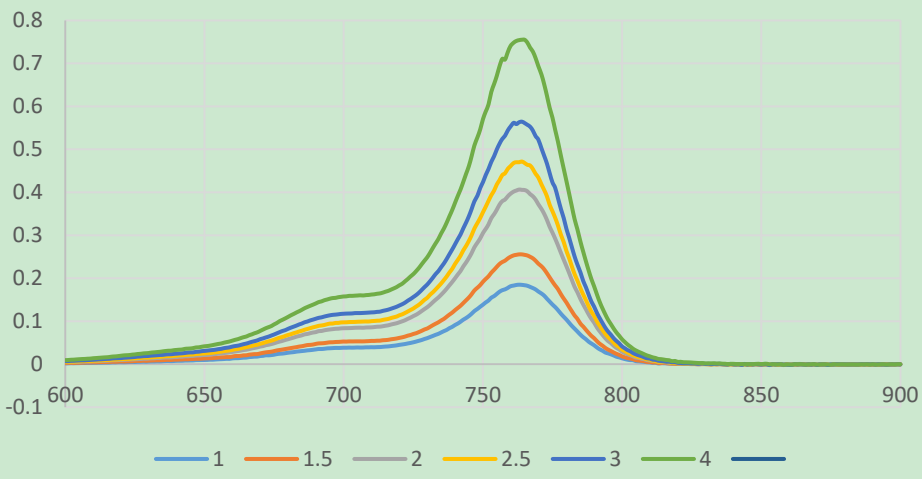
$$y = 196952x - 0.0016$$
$$R^2 = 0.9996$$

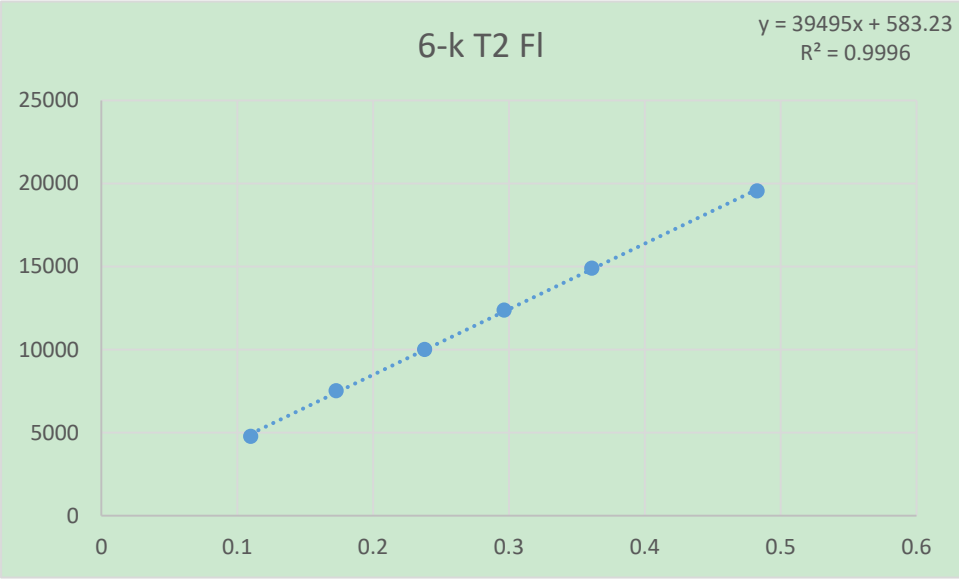
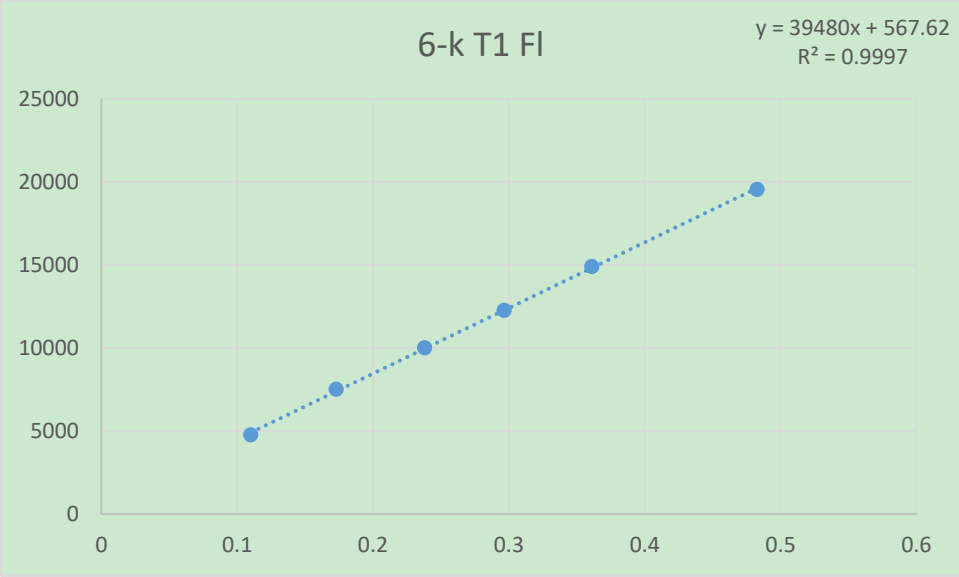


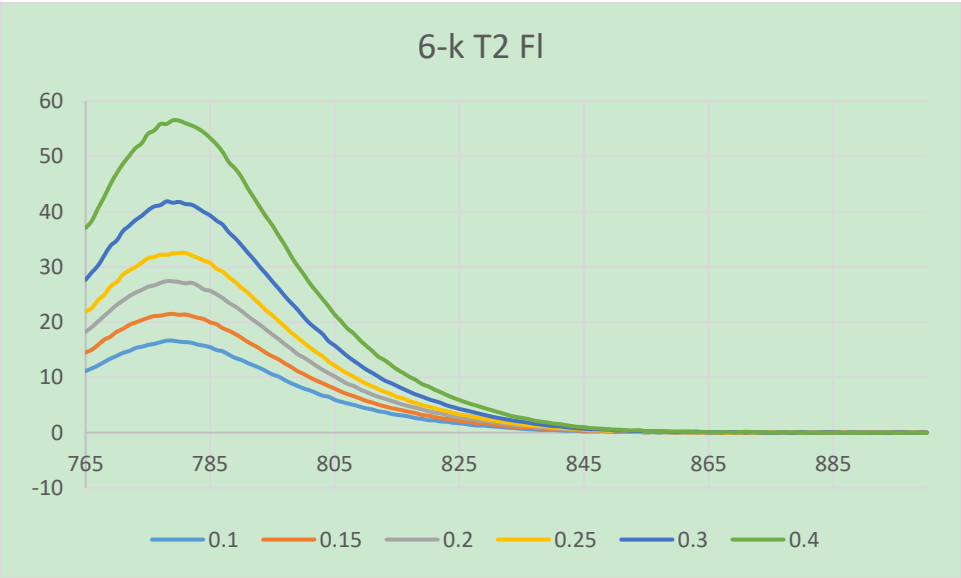
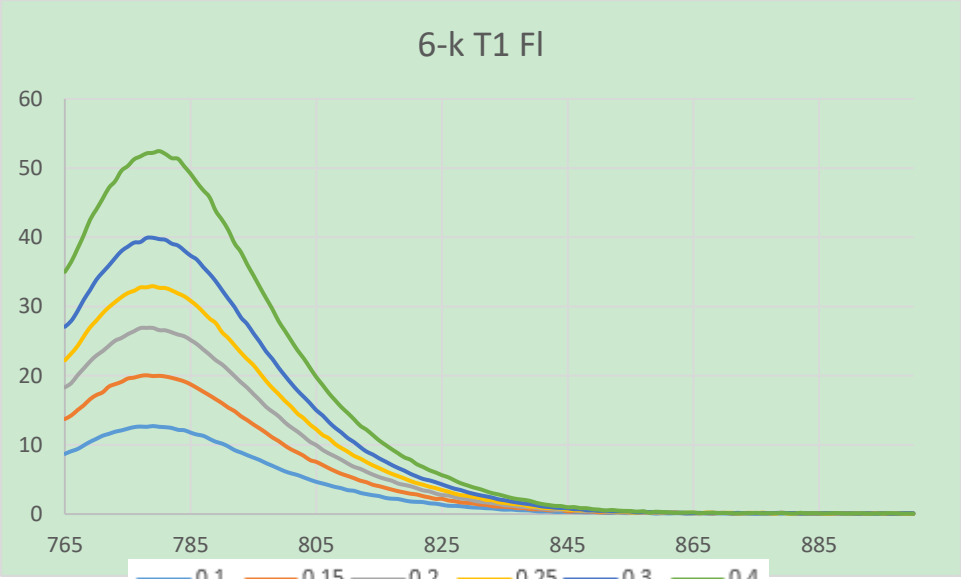
6-k T1 ABS



6-k T2 ABS

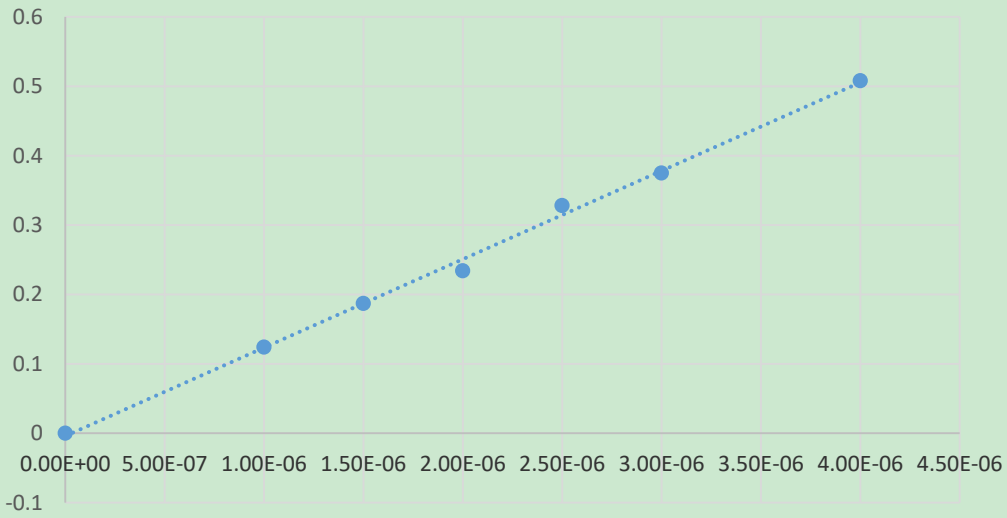






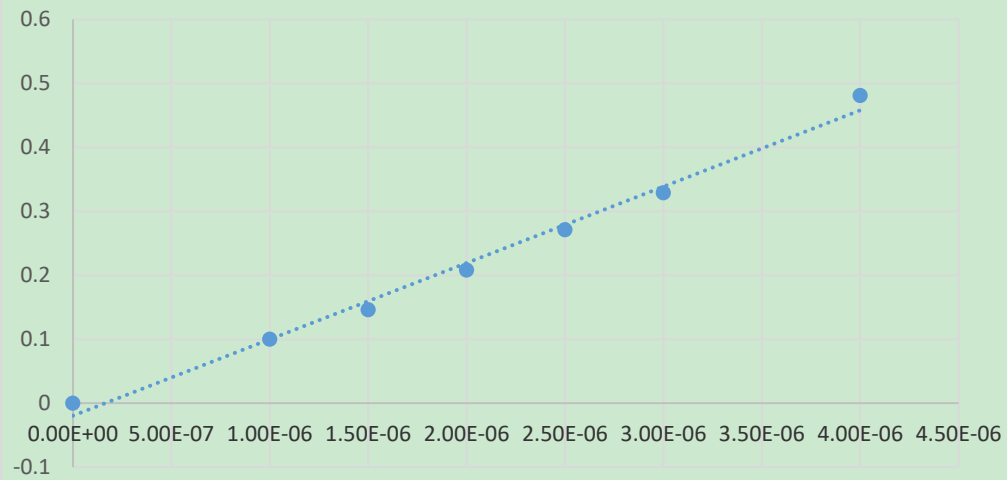
$y = 127381x - 0.0039$
 $R^2 = 0.9971$

6-I T1 ABS

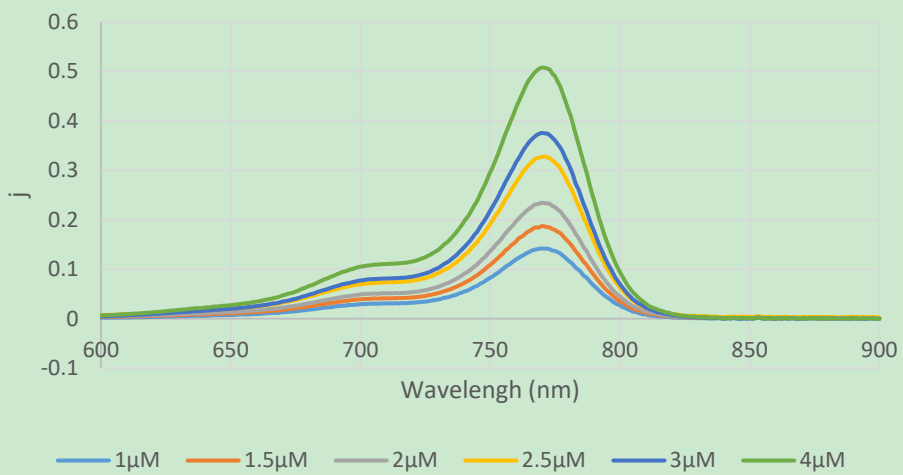


$y = 119381x - 0.0195$
 $R^2 = 0.9909$

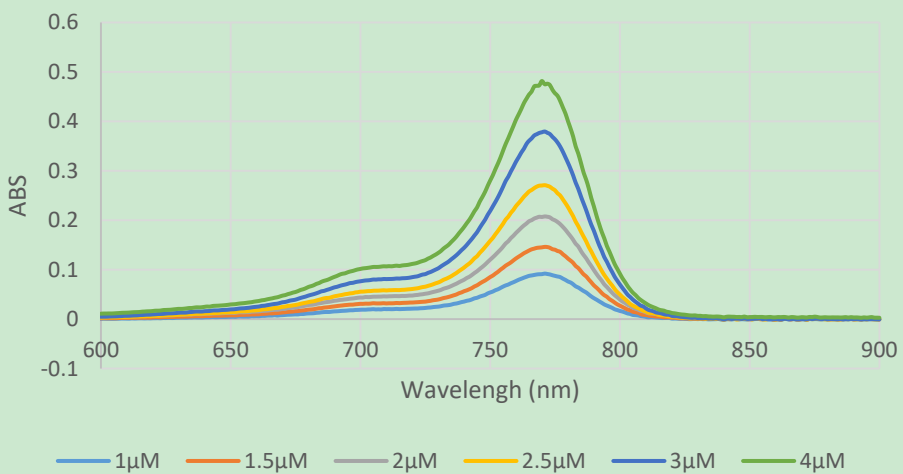
6-I T2 ABS



6-I T1 ABS

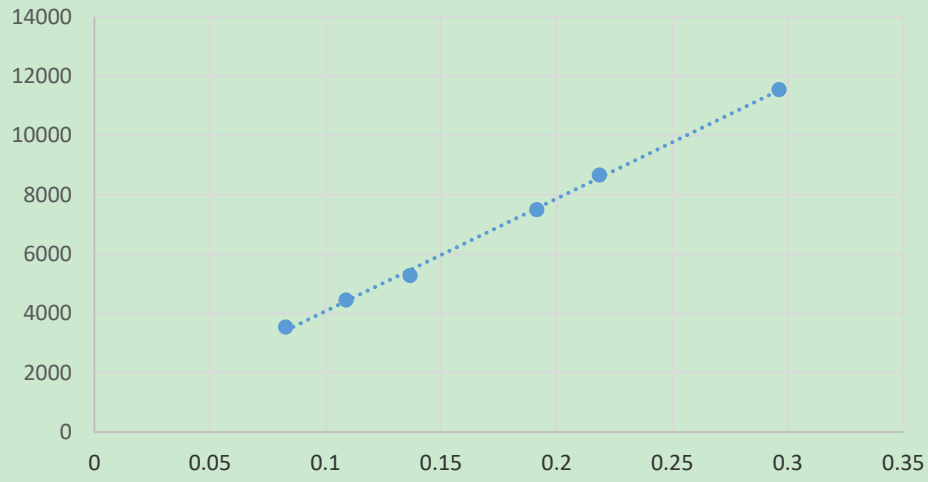


6-I T2 ABS



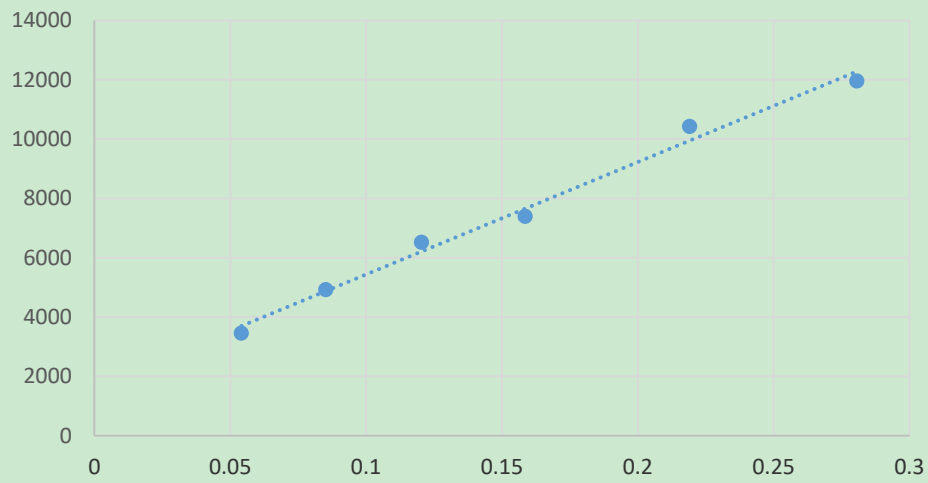
$y = 37939x + 285.28$
 $R^2 = 0.9987$

6-I T1 FL

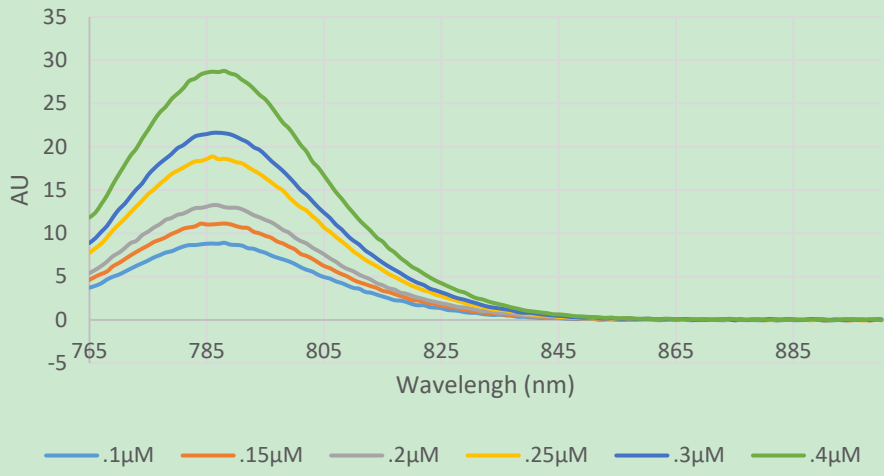


$y = 37870x + 1649.4$
 $R^2 = 0.9893$

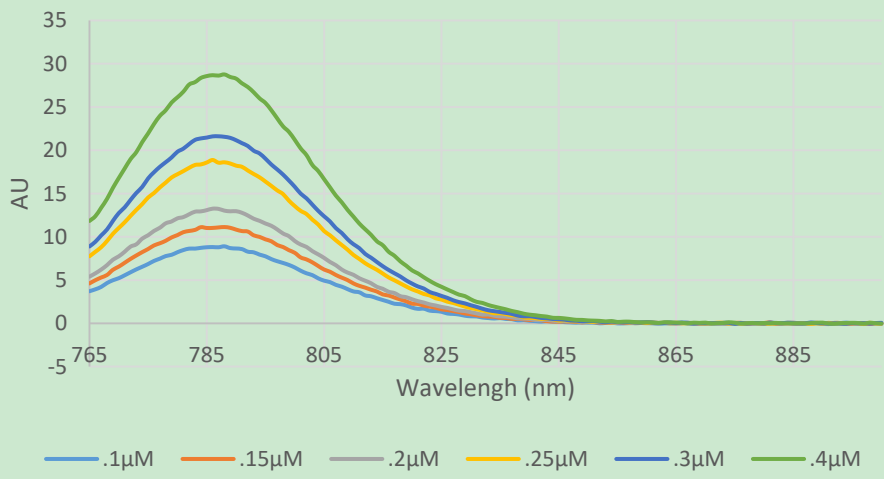
6-I T2 FL



6-I T1 FL

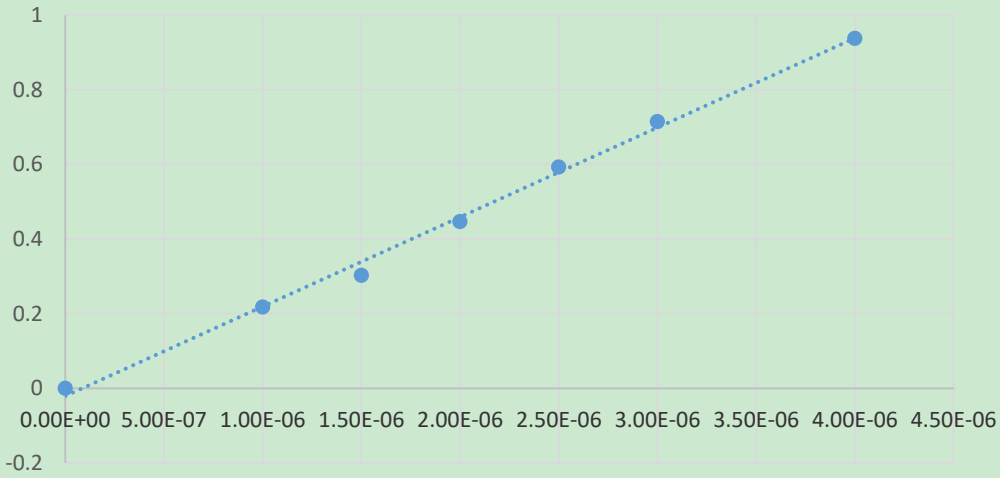


6-I T2 FL



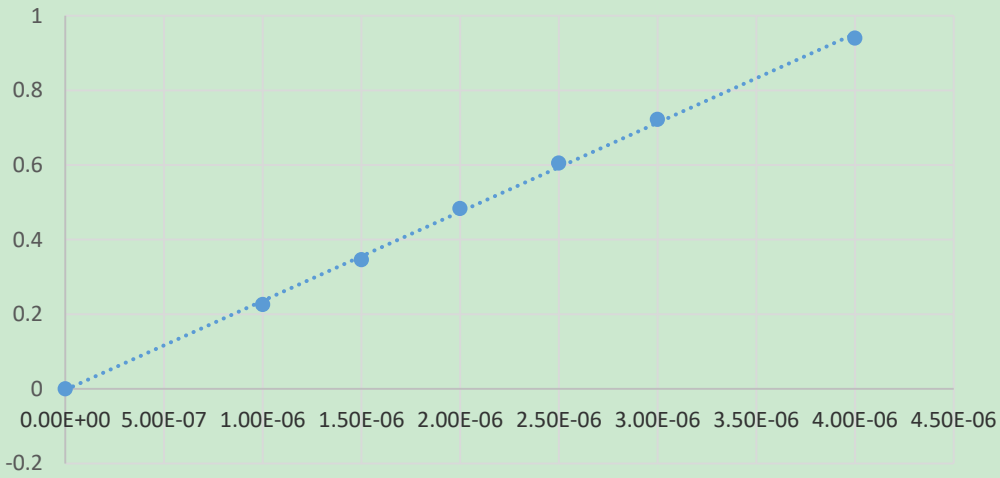
$y = 239810x - 0.0205$
 $R^2 = 0.9961$

6-m T1 ABS

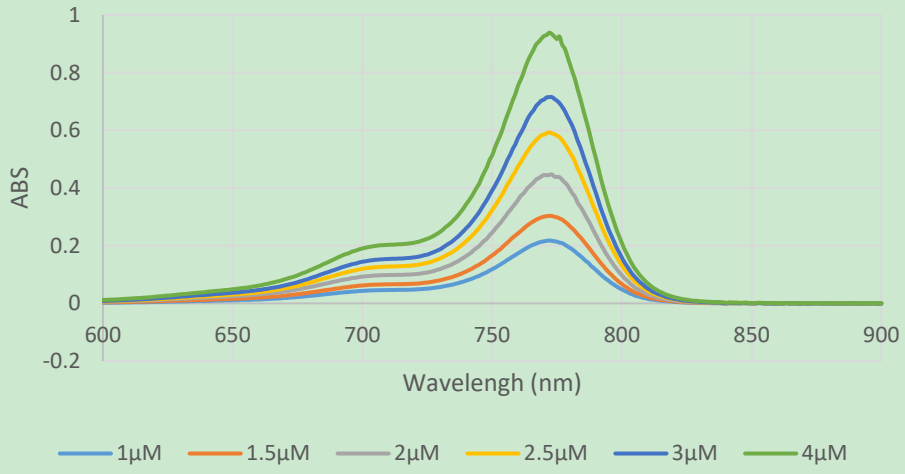


$y = 238619x - 0.0027$
 $R^2 = 0.999$

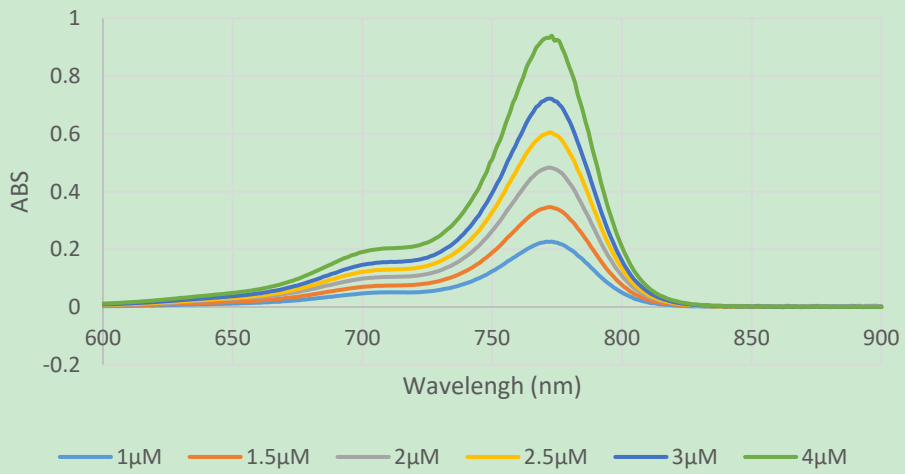
6-m T2 ABS



6-m T1 ABS

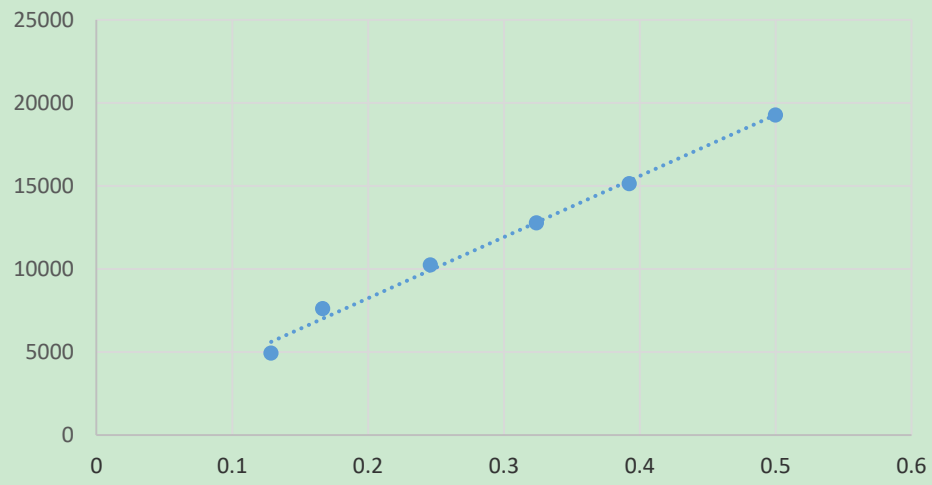


6-m T2 ABS



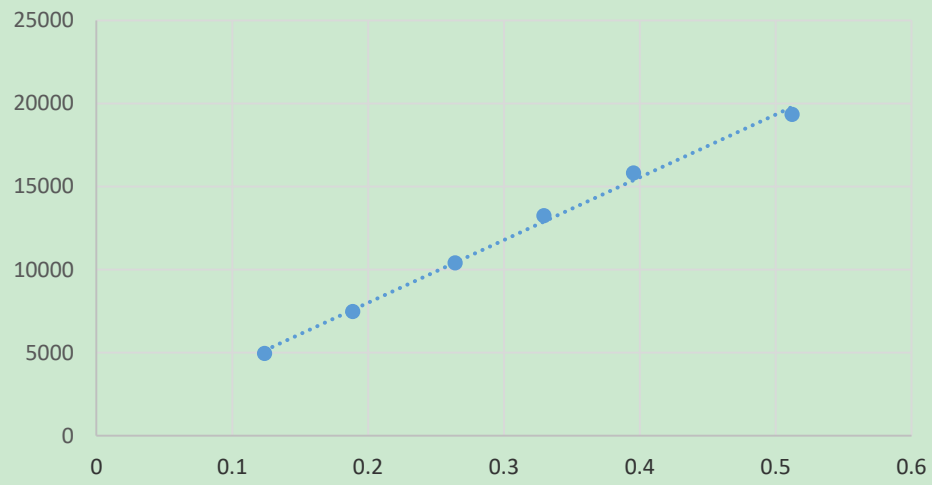
$y = 36806x + 877.1$
 $R^2 = 0.9929$

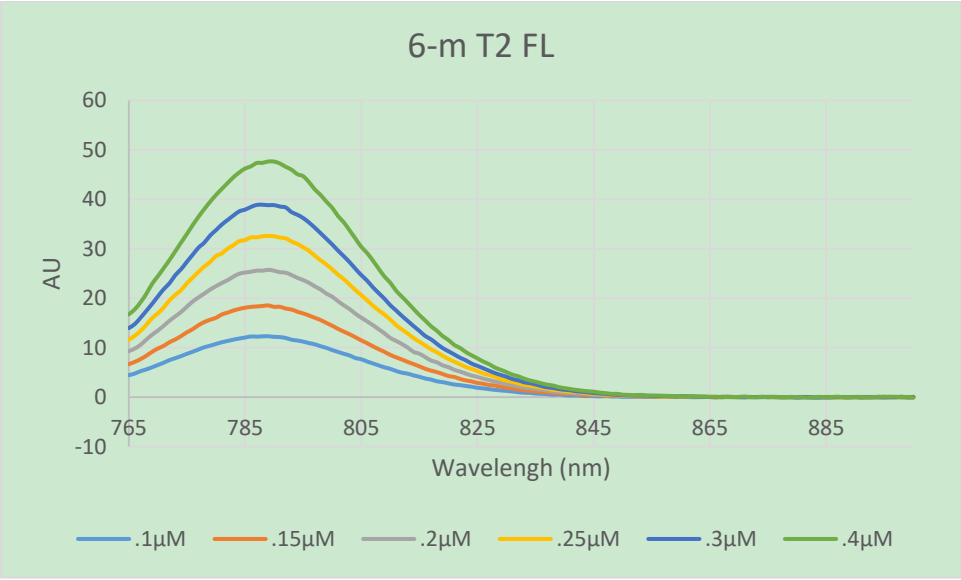
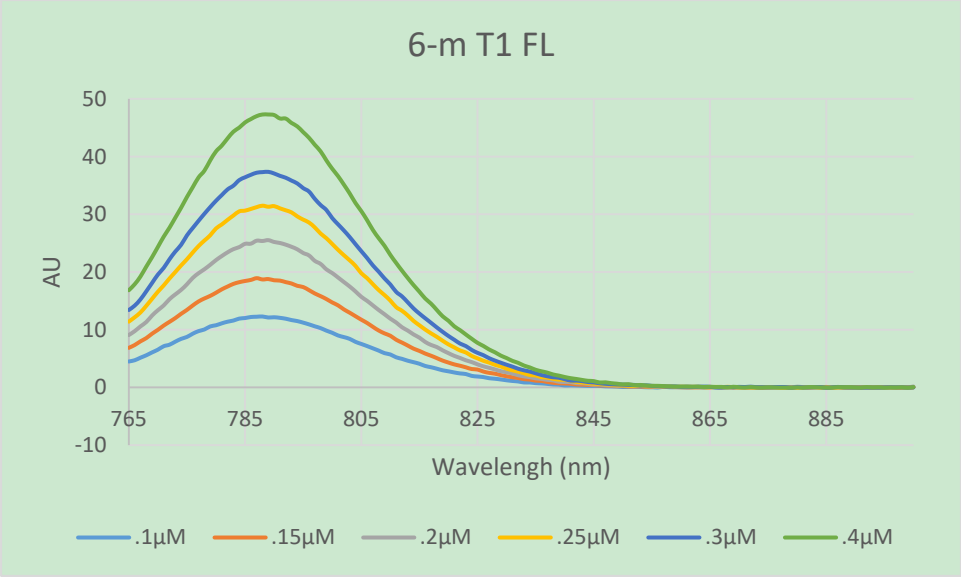
6-m T1 FI



$y = 37767x + 447.91$
 $R^2 = 0.9961$

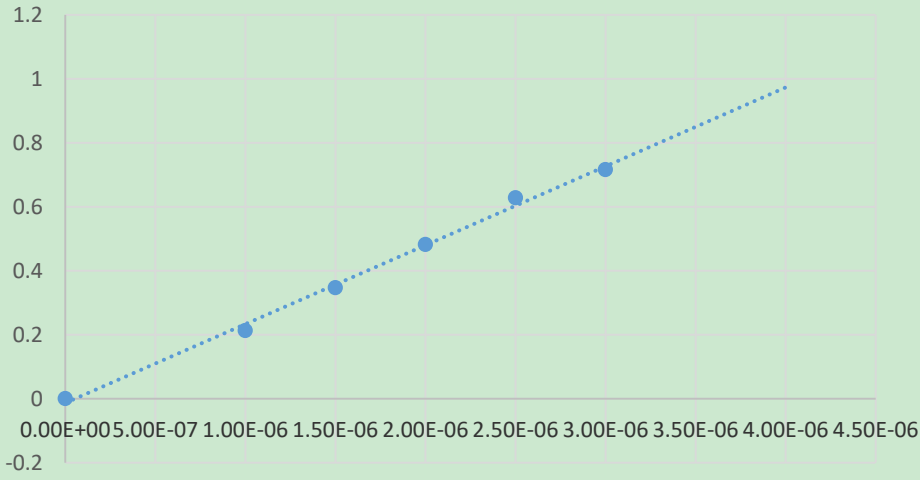
6-m T2 FL





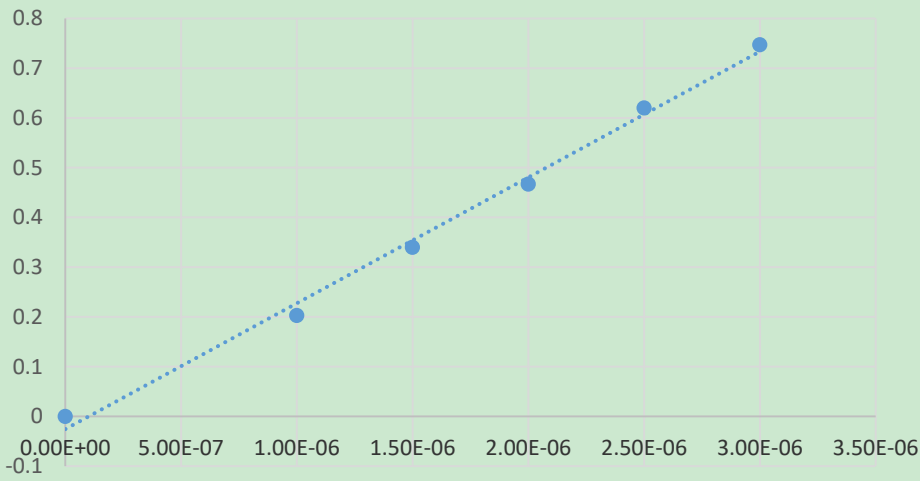
$y = 246657x - 0.0134$
 $R^2 = 0.996$

6-nT1 ABS

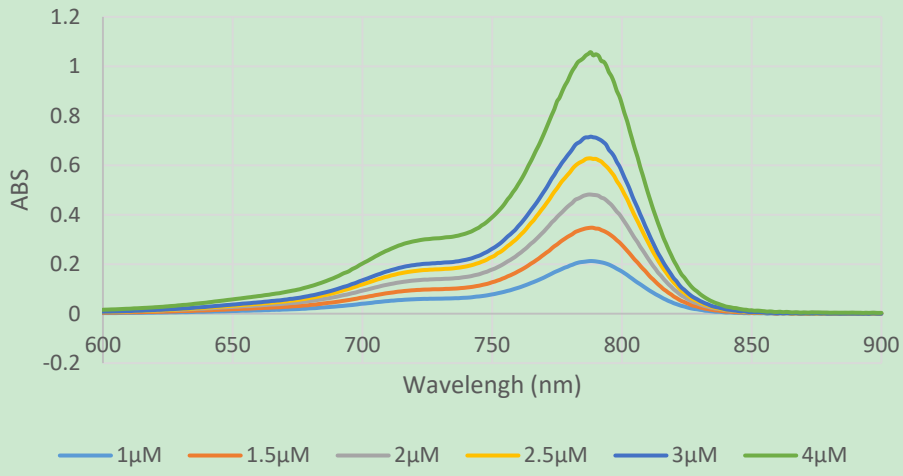


$y = 253086x - 0.0256$
 $R^2 = 0.9947$

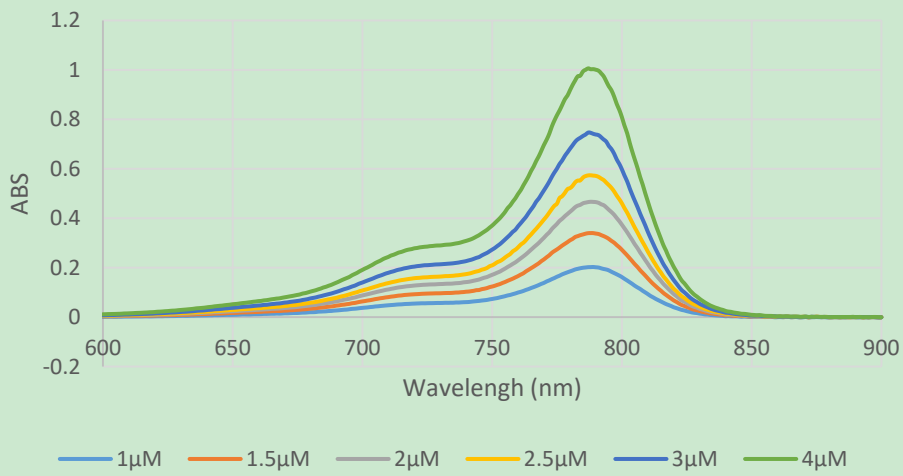
6-nT2 ABS



6-nT1 ABS

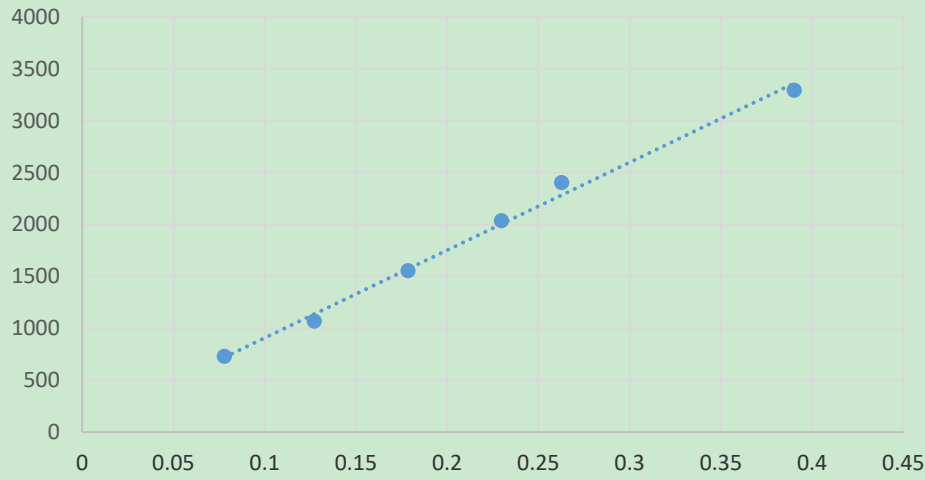


6-nT2 ABS



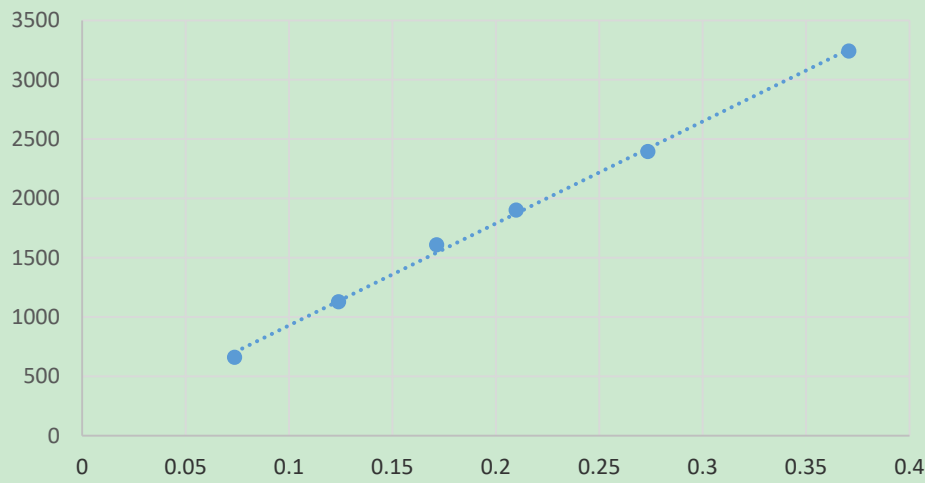
$y = 8449.2x + 62.987$
 $R^2 = 0.9943$

6-nT1 FL

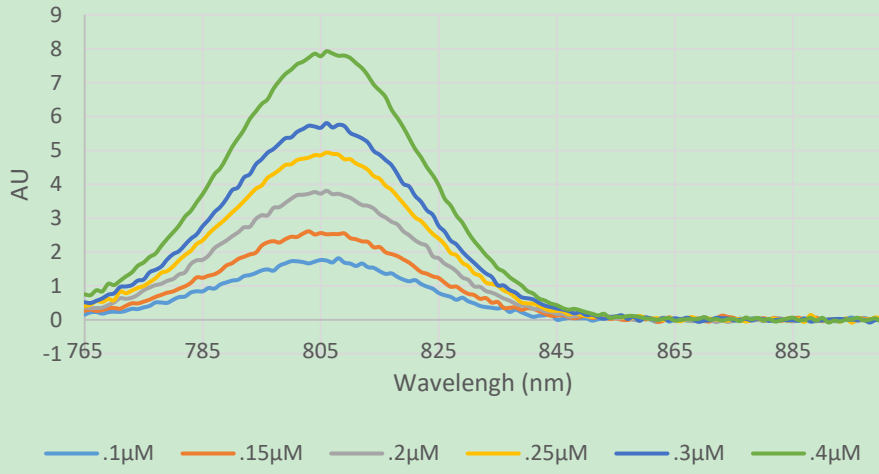


$y = 8592.7x + 69.994$
 $R^2 = 0.9981$

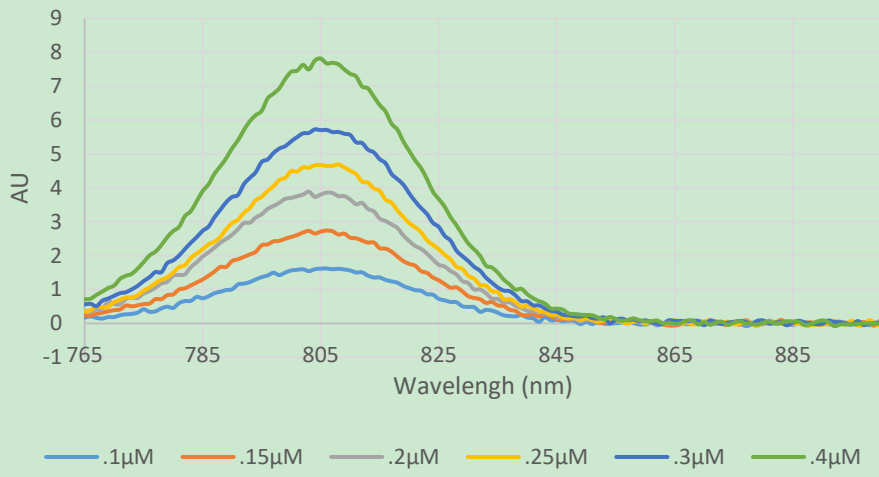
6-nT2 FL



6-NT1 FL

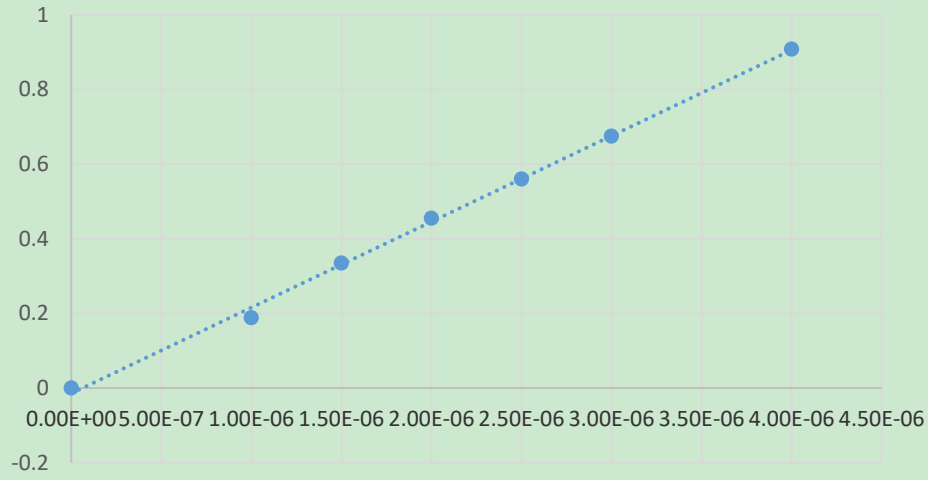


6-NT2 FL



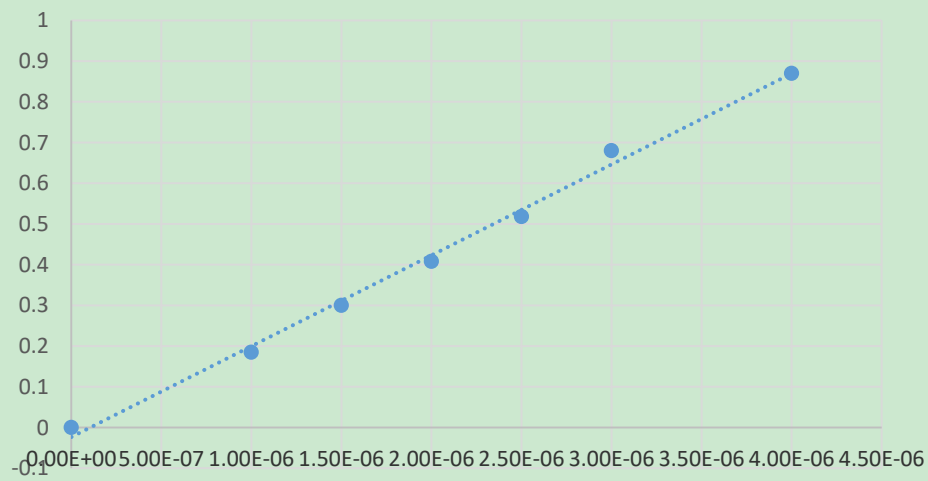
$y = 230048x - 0.0142$
 $R^2 = 0.9981$

6-oT1 ABS

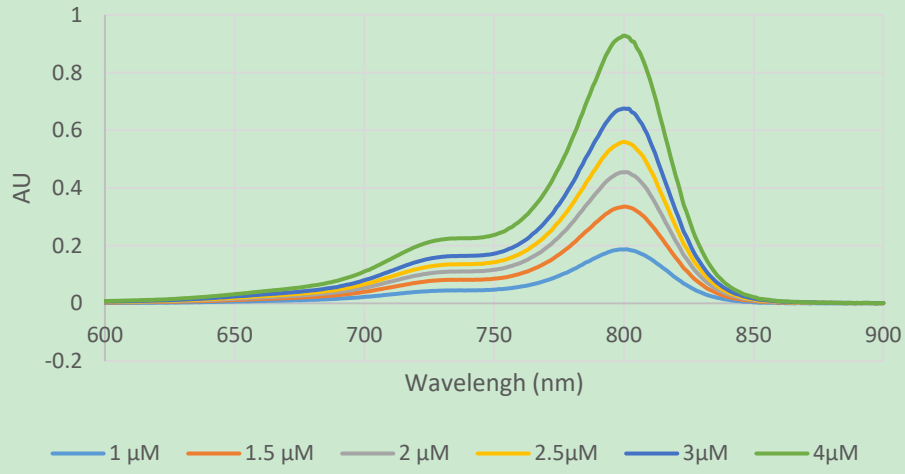


$y = 223238x - 0.0235$
 $R^2 = 0.9952$

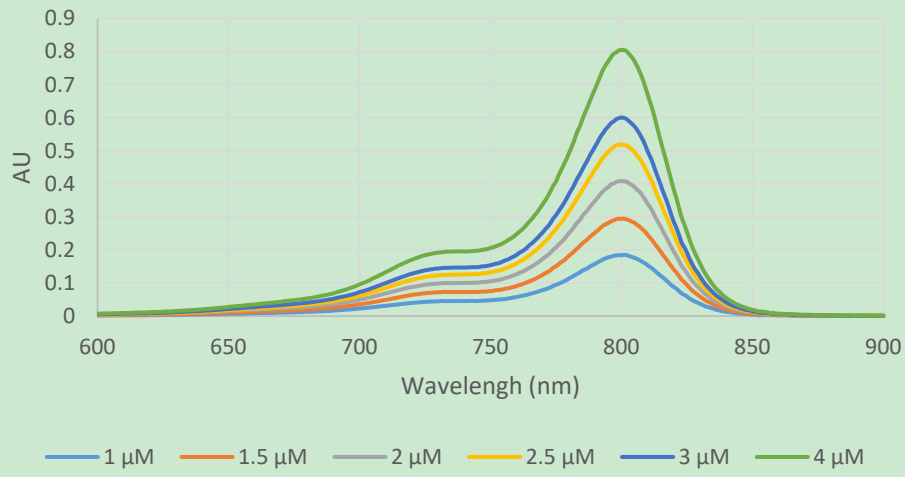
6-oT2 ABS



6-oT1 ABS

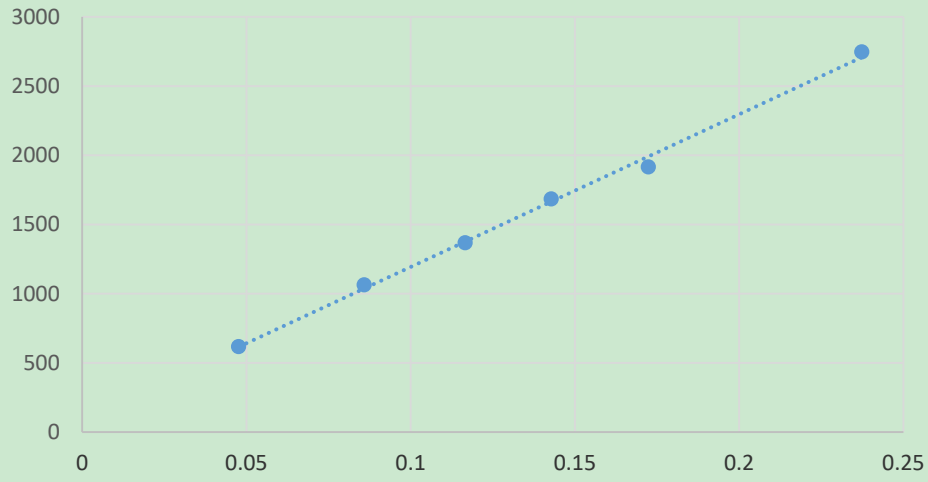


6-oT2 ABS



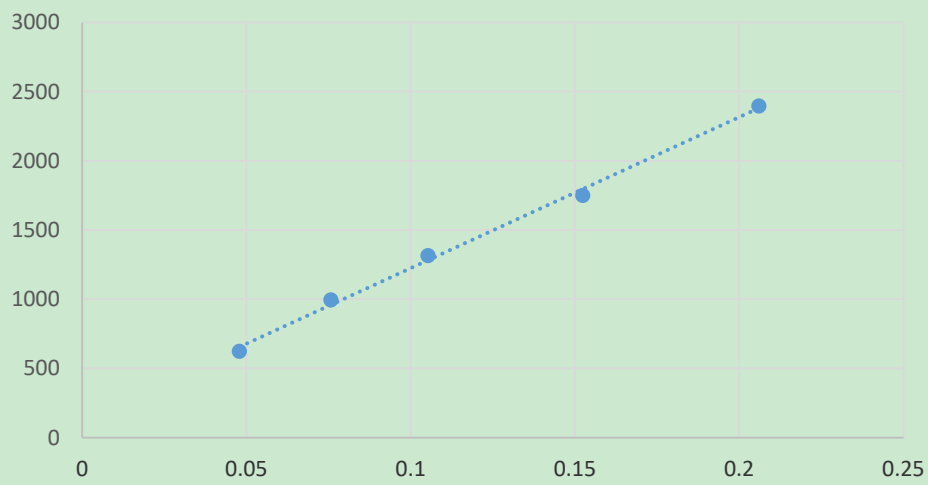
$y = 11029x + 90.3$
 $R^2 = 0.997$

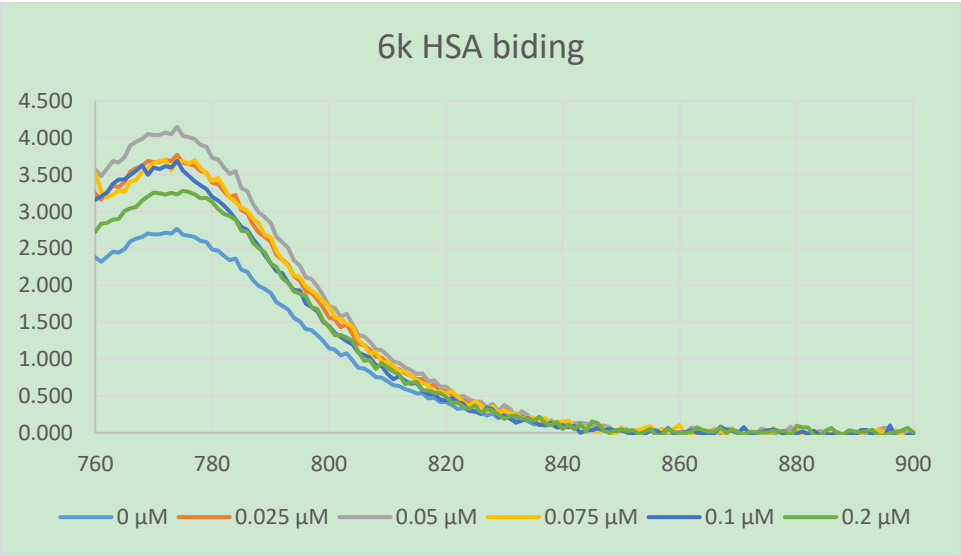
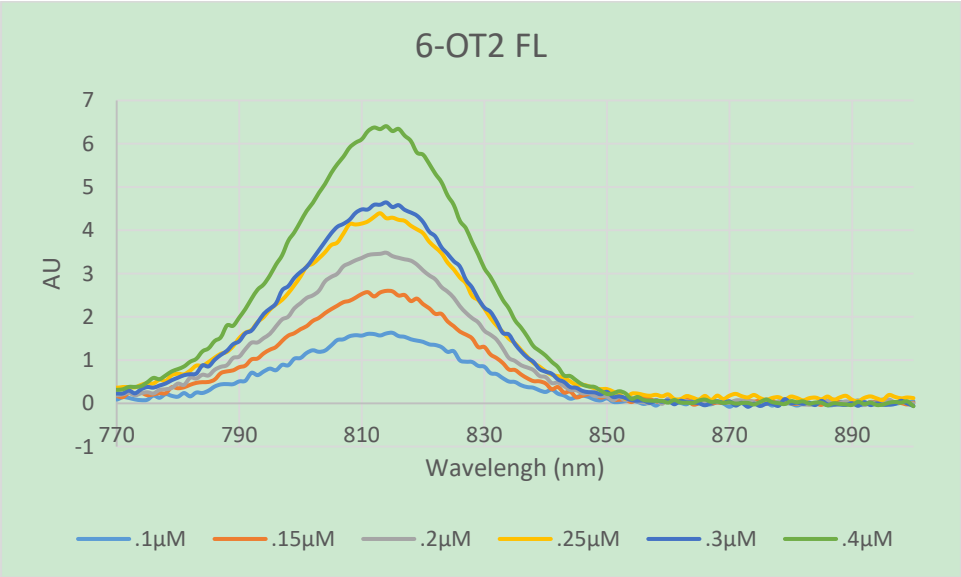
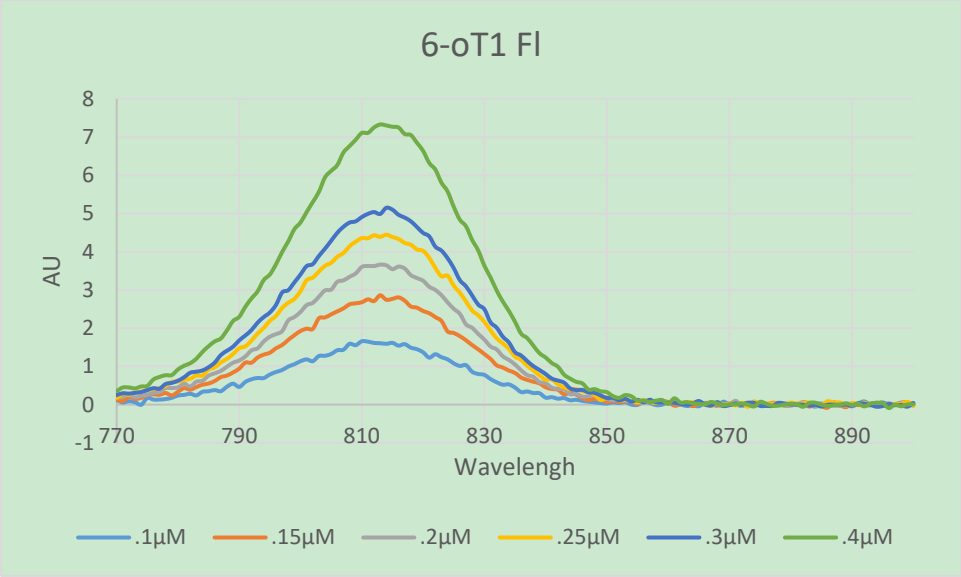
6-oT1FL



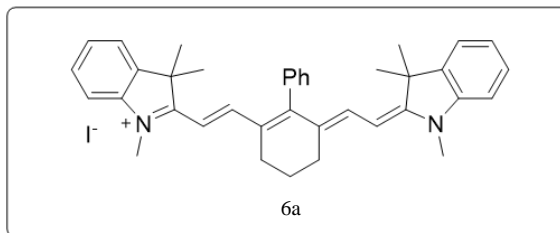
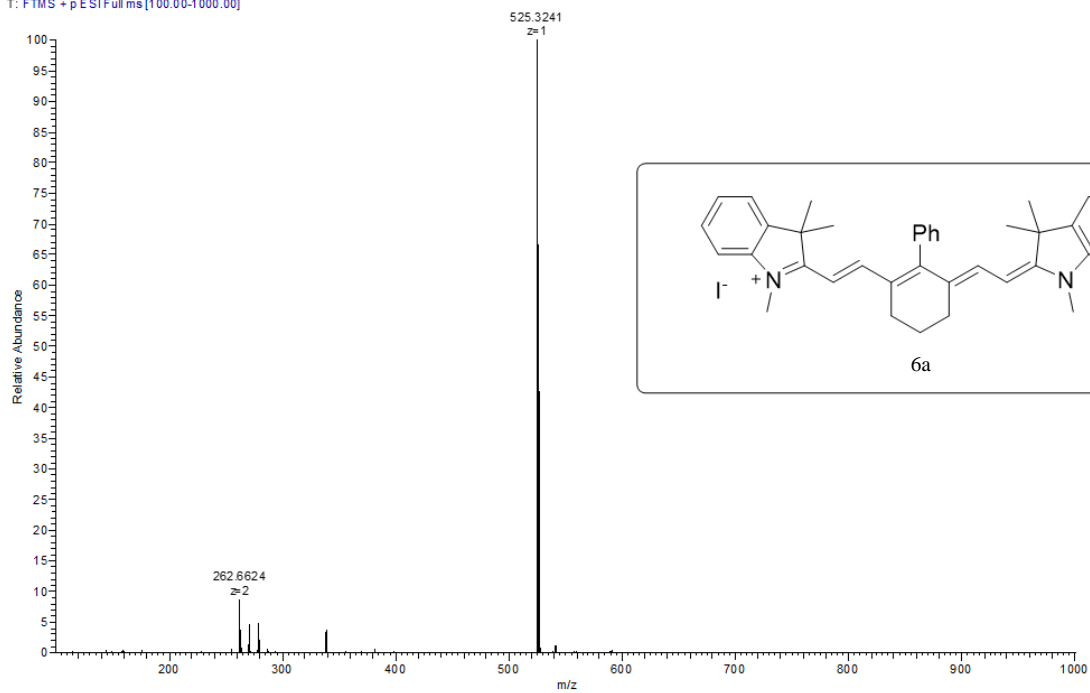
$y = 10908x + 133.91$
 $R^2 = 0.997$

6-oT2FL

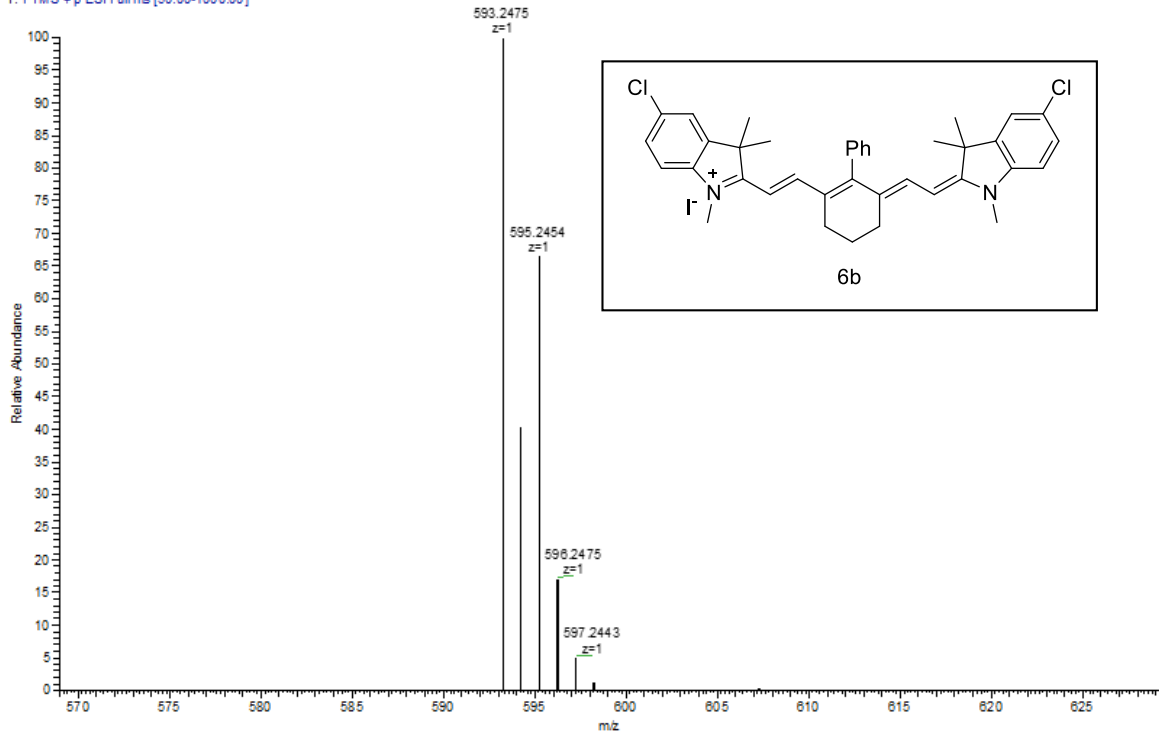




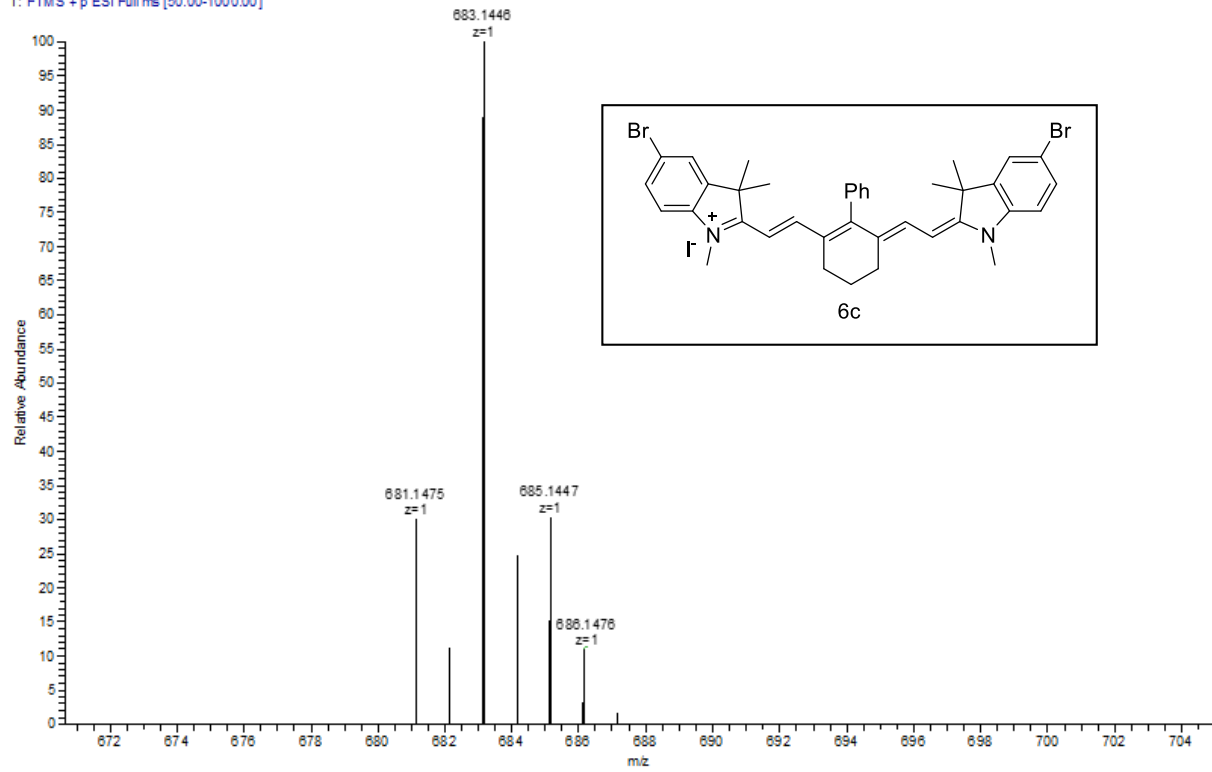
ANDY_AC_167_ESIPOS_HENARY_032917 #129-138 RT: 1.82-1.95 AV: 10 NL: 2.13E8
T: FTMS + p ESI Full ms [100.00-1000.00]



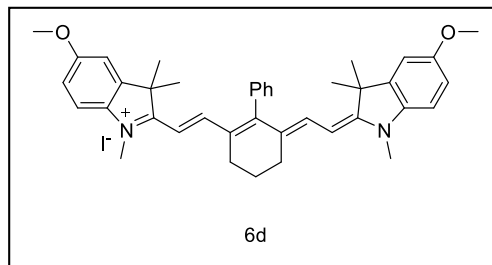
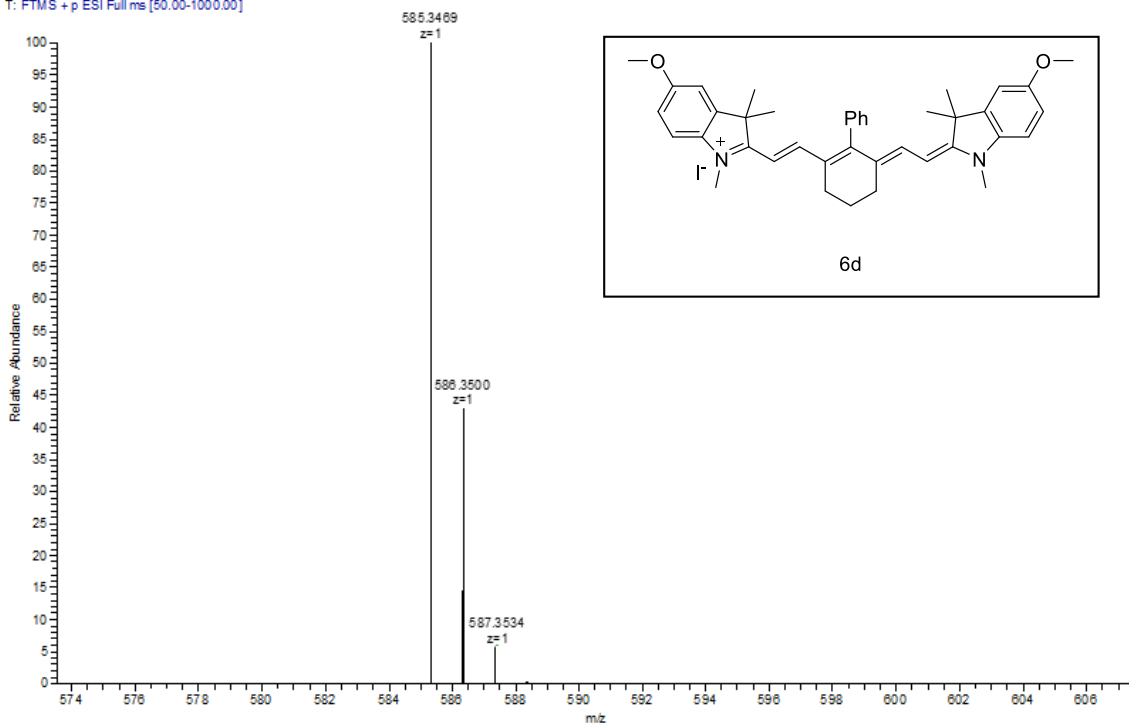
FM_AL188CLM_e_ESIPOS_HENARY_121417#144-147 RT: 2.05-2.09 AV: 4 NL: 3.64E7
T: FTMS + p ESI Full ms [50.00-1000.00]



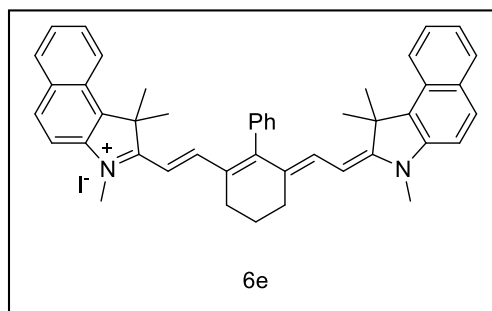
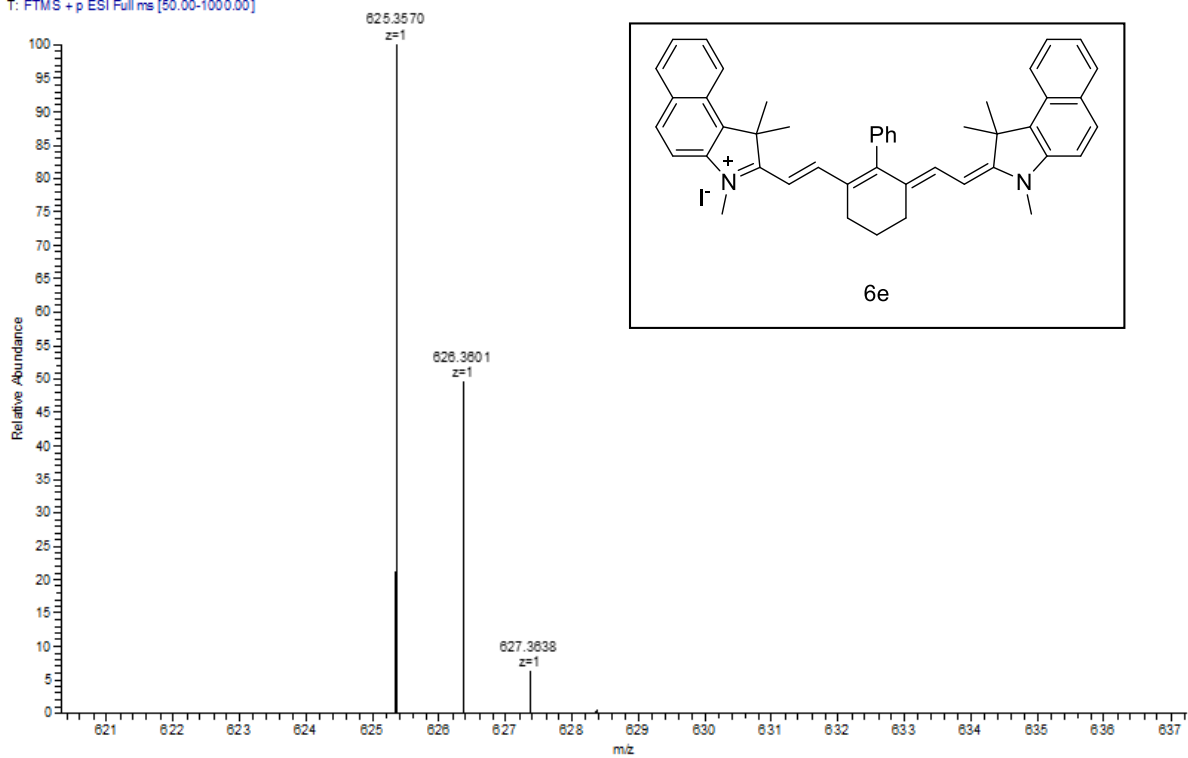
FM_AL1818M_e_ESIPOS_HENARY_121417#145-147 RT: 2.06-2.09 AV: 3 NL: 2.82E7
T: FTMS + p ESI Full ms [50.00-1000.00]



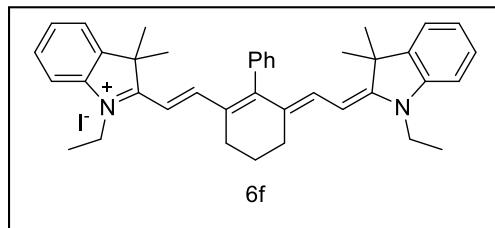
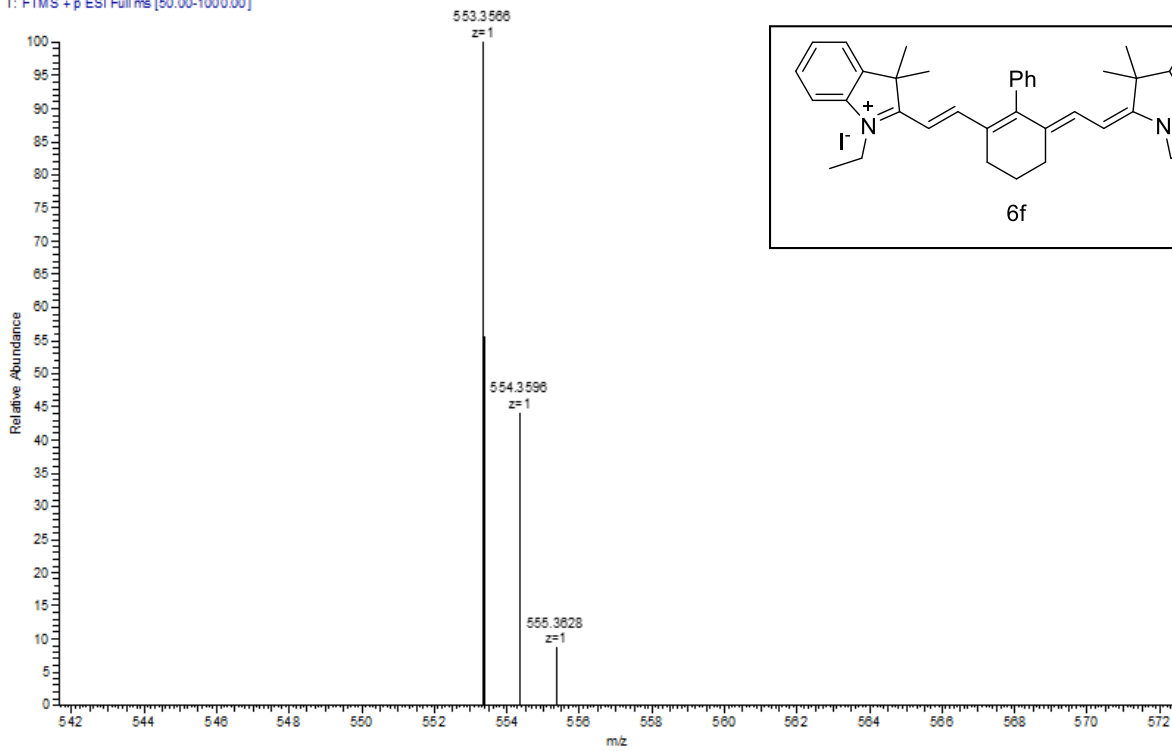
FM_AL190MeOMe_ESIPOS_HENARY_121417 #146-151 RT: 2.08-2.14 AV: 6 NL: 2.46E8
T: FTMS + p ESI Full ms [50.00-1000.00]



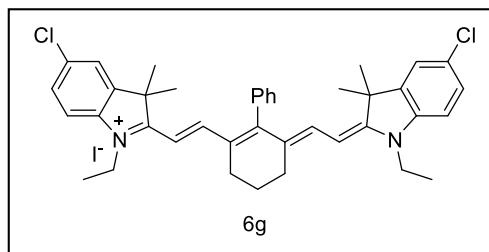
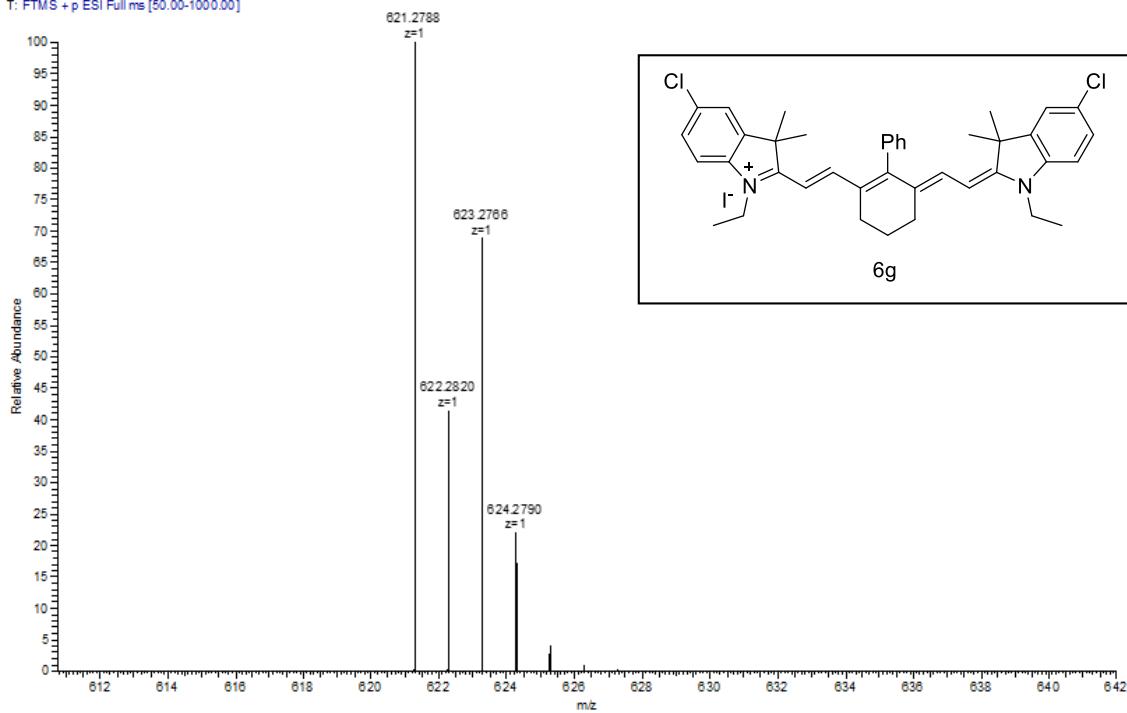
FM_AL184BEMe_ESIPOS_HENARY_121417 #145-150 RT: 2.06-2.13 AV: 6 NL: 1.32E8
T: FTMS + p ESI Full ms [50.00-1000.00]



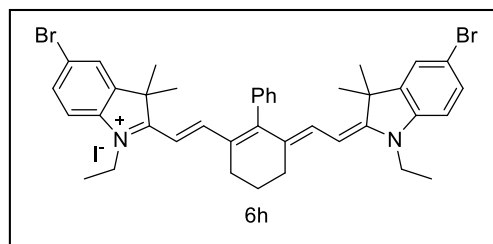
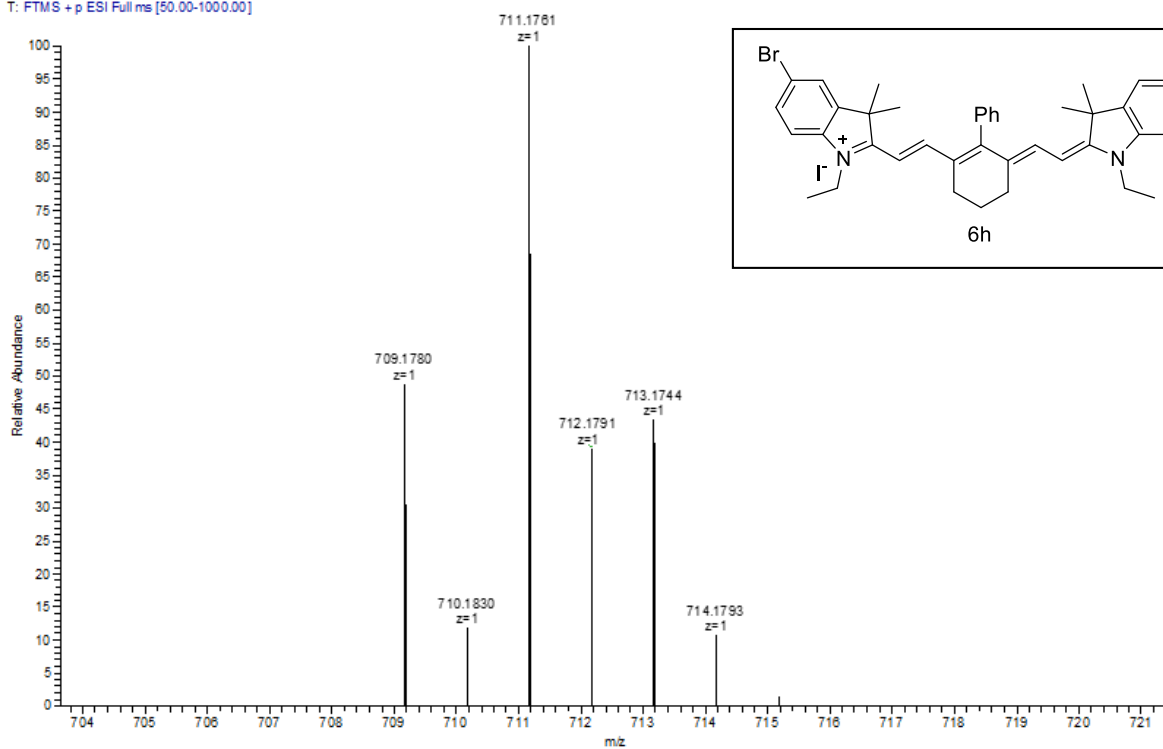
FM_AL5HET_ESIPOS_HENARY_121417 #147-150 RT: 2.09-2.13 AV: 4 NL: 4.27E8
T: FTMS + p ESI Full ms [50.00-1000.00]



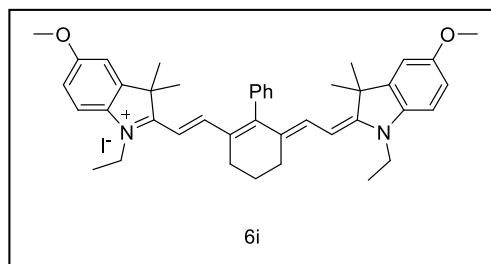
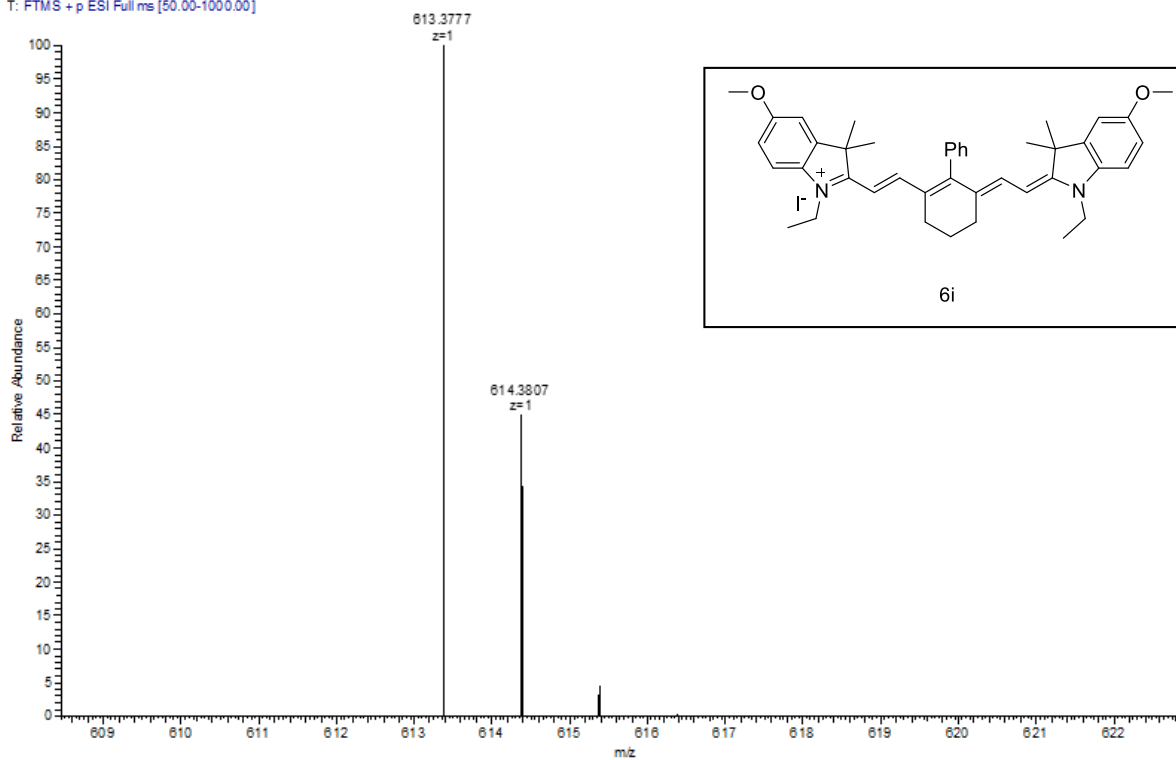
FM_AL7CLET_ESIPOS_HENARY_121417 #142-146 RT: 2.02-2.07 AV: 5 NL: 4.69E7
T: FTMS + p ESI Full ms [50.00-1000.00]



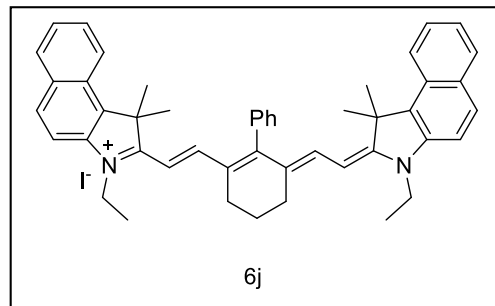
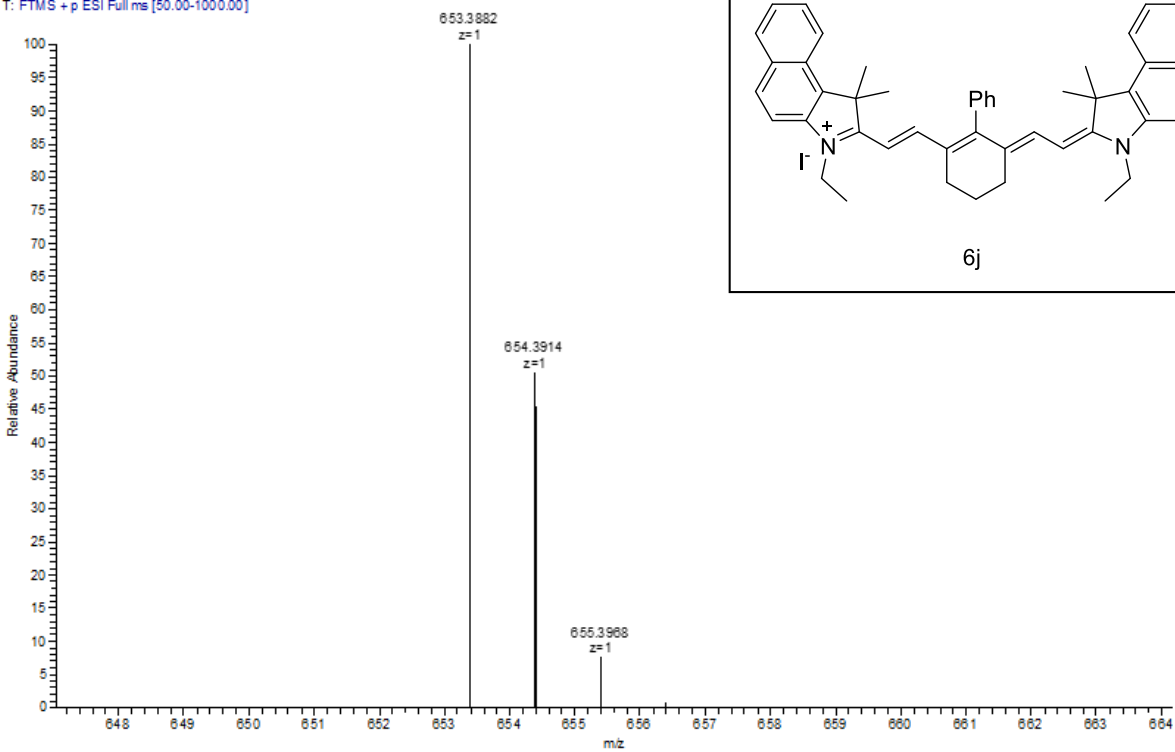
FM_AL4BrET_ESIPOS_HENARY_121417 #145-148 RT: 2.06-2.10 AV: 4 NL: 424E7
T: FTMS + p ESI Full ms [50.00-1000.00]



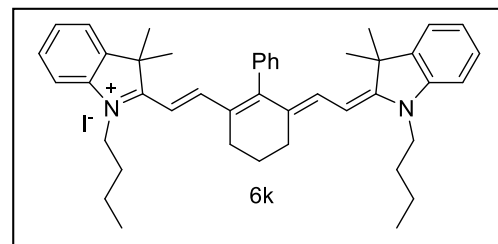
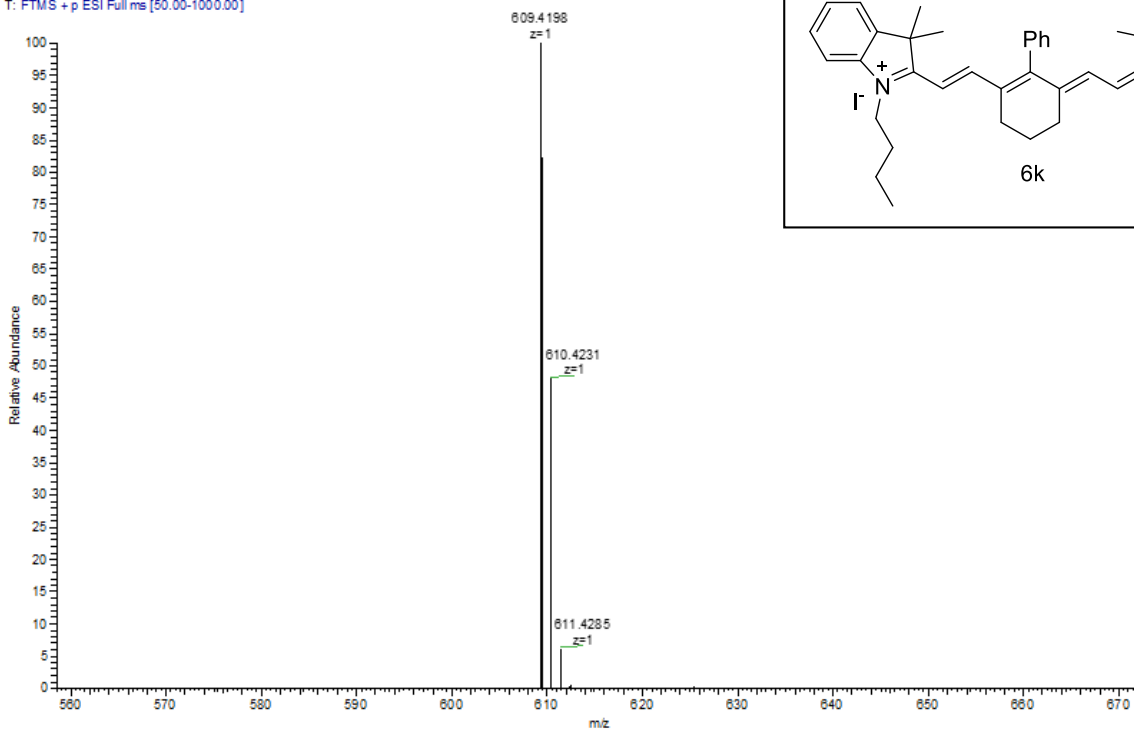
FM_AL8MeOET_ESIPOS_HENARY_121417 #139-146 RT: 1.97-2.07 AV: 8 NL: 1.84E8
T: FTMS + p ESI Full ms [50.00-1000.00]



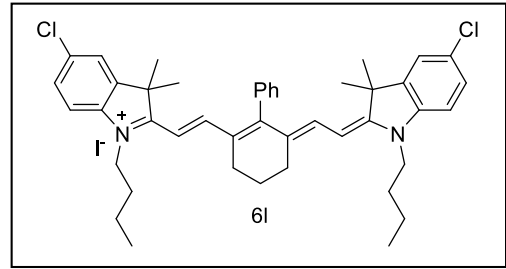
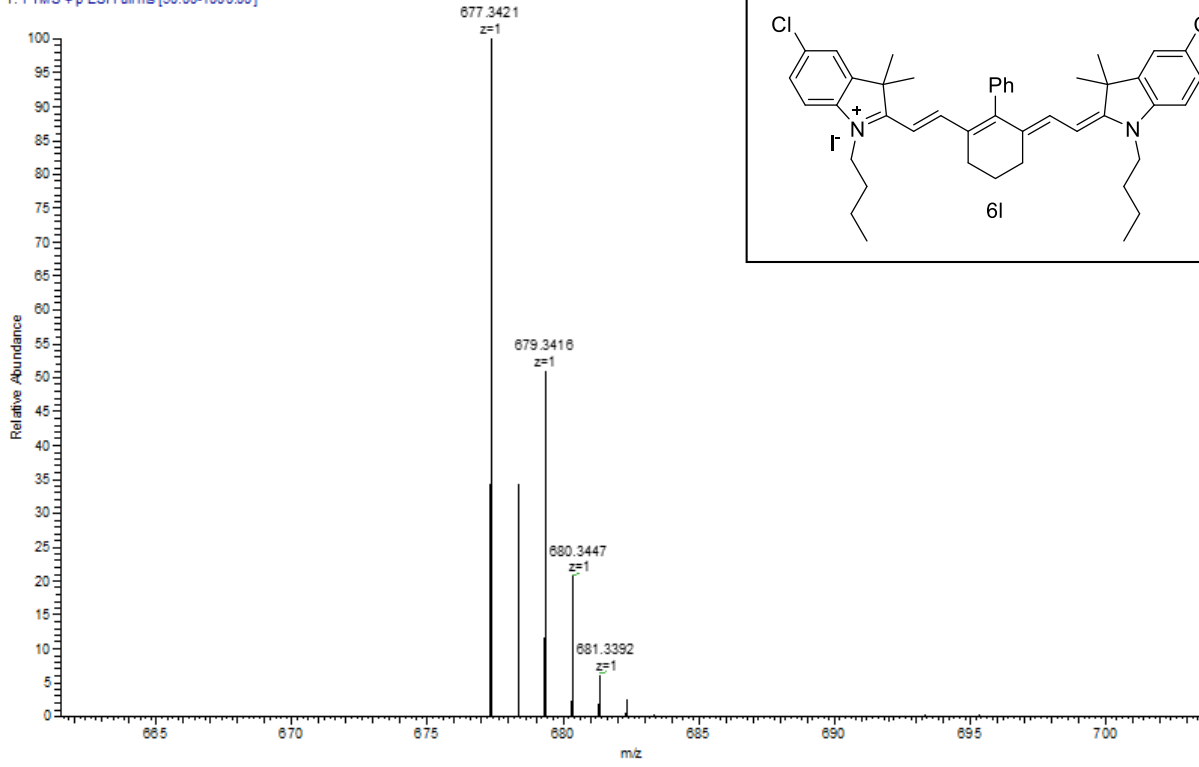
FM_AL8BEET_ESIPOS_HENARY_121417 #147-150 RT: 2.09-2.13 AV: 4 NL: 8.98E7
T: FTMS + p ESI Full ms [50.00-1000.00]



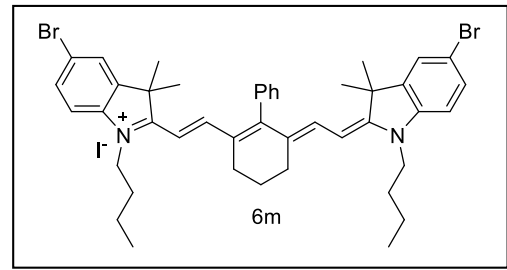
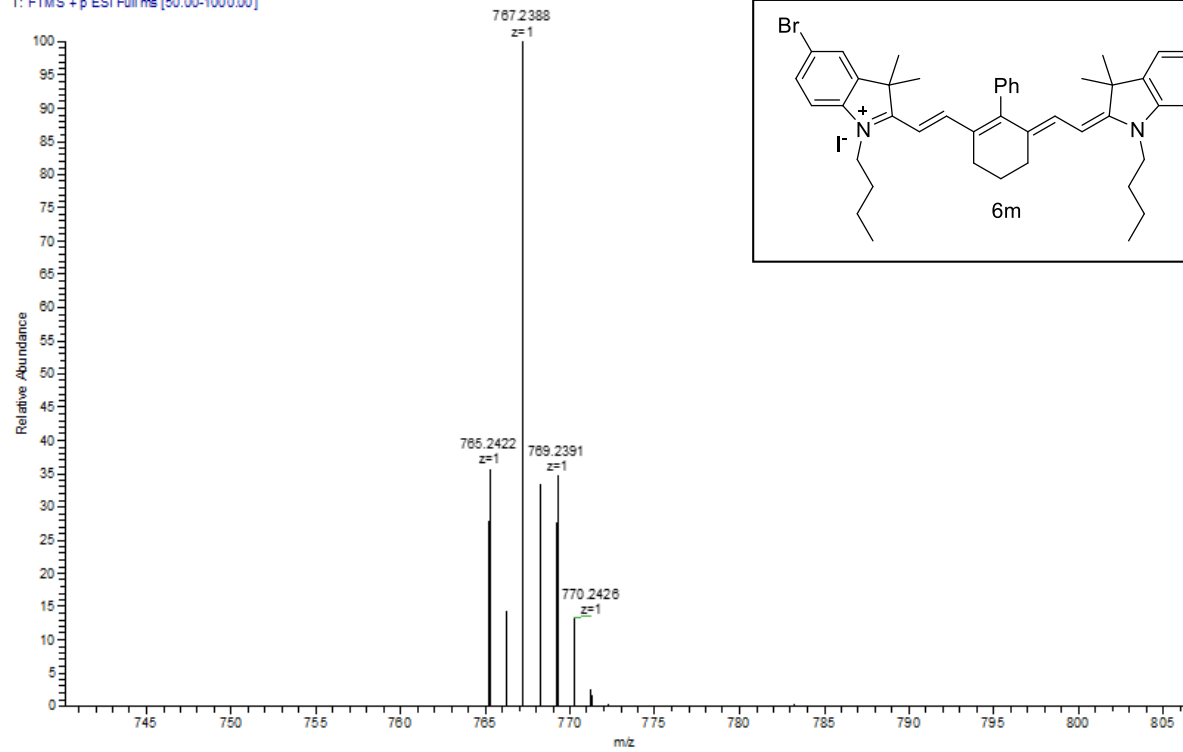
FM_FM8HBu_ESIPOS_HENARY_121417 #152-156 RT: 2.16-2.21 AV: 5 NL: 1.13E8
T: FTMS + p ESI Full ms [50.00-1000.00]



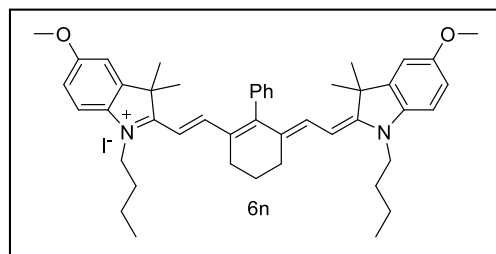
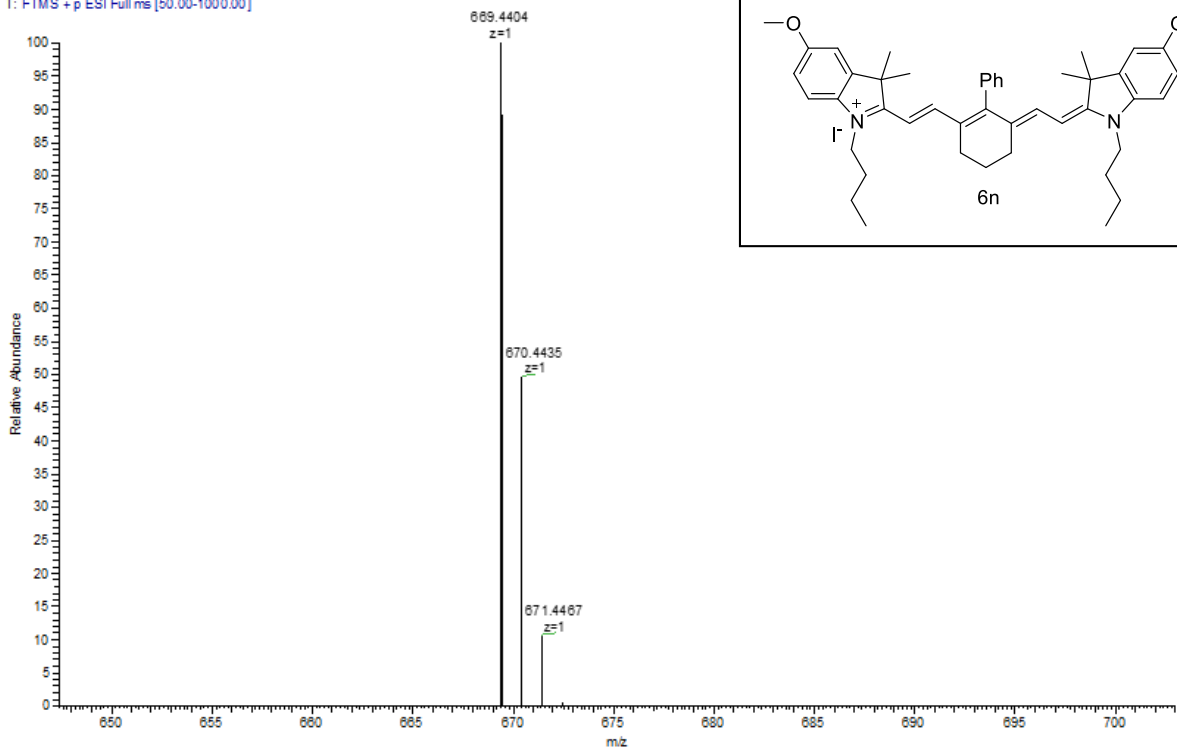
FM_FM11C1Bu_ESIPOS_HENARY_121417#175-179 RT: 2.49-2.55 AV: 5 NL: 1.53E7
T: FTMS +p ESI Full ms [50.00-1000.00]



FM_5BrBu_ESIPOS_HENARY_121417#185-191 RT: 2.62-2.70 AV: 7 NL: 1.88E7
T: FTMS +p ESI Full ms [50.00-1000.00]



FM_14MeOBu_ESIPOS_HENARY_121417 #147-151 RT: 2.09-2.14 AV: 5 NL: 2.25E8
T: FTMS + p ESI Full ms [50.00-1000.00]



FM_9BEbu_ESIPOS_HENARY_121417 #142 RT: 2.02 AV: 1 NL: 1.23E7
T: FTMS + p ESI Full ms [50.00-1000.00]

