LC-MS Traces

Scheme 8 – Borylation Reaction with Pre-heated catalyst solution
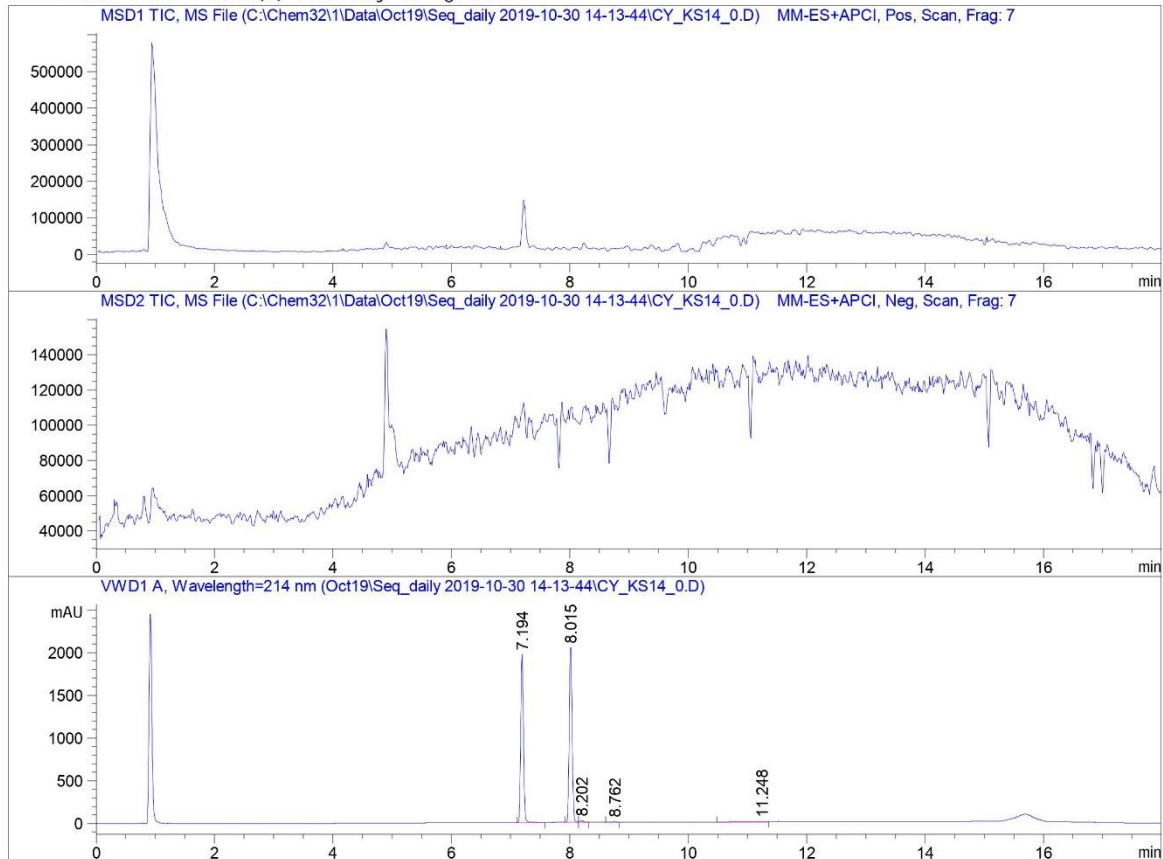
Compound	Retention time (RT)
Bromobenzene	8.01 min
1,3,5-trimethoxybenzene (Internal standard)	7.19 min
Phenylboronic acid pinacol ester	8.76 min

The product (phenylboronic acid pinacol ester) is unstable in the aqueous LC-MS sample solution, will degrade to phenylboronic acid derivatives (RT = 4.99 min).

```
=================================================================
Acq. Operator   : SYSTEM                      Seq. Line :   1
Acq. Instrument : 6130B LCMS                  Location  :   3
Injection Date  : 30-Oct-19 2:16:08 PM             Inj  :   1
                                            Inj Volume : 10.000 µl
Method          : C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\PORO_AMMACE_214_70.M (
                  Sequence Method)
Last changed    : 30-Oct-19 2:13:44 PM by SYSTEM
Method Info     : method for Poroshell 120 4.6 x75 x2.7um
```

Additional Info : Peak(s) manually integrated


```
=================================================================
                    Area Percent Report
=================================================================

Sorted By          :      Signal
Multiplier         :      1.0000
Dilution           :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Data File C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\CY_KS14_0.D
Sample Name: CY_KS14_0

    Signal 1: MSD1 TIC, MS File

    Signal 2: MSD2 TIC, MS File

    Signal 3: VWD1 A, Wavelength=214 nm

Peak RetTime Type Width   Area   Height   Area
  #   [min]   [min]   [mAU*s]   [mAU]   %
----|-------|----|-------|----------|----------|--------|
   1   7.194 BB   0.0501 6223.38770 1963.34949 46.8536
   2   8.015 BV   0.0531 6781.76807 2054.18188 51.0574
   3   8.202 VB   0.0520   65.65144   19.66779   0.4943
   4   8.762 VB   0.0487   17.86457   5.63215   0.1345
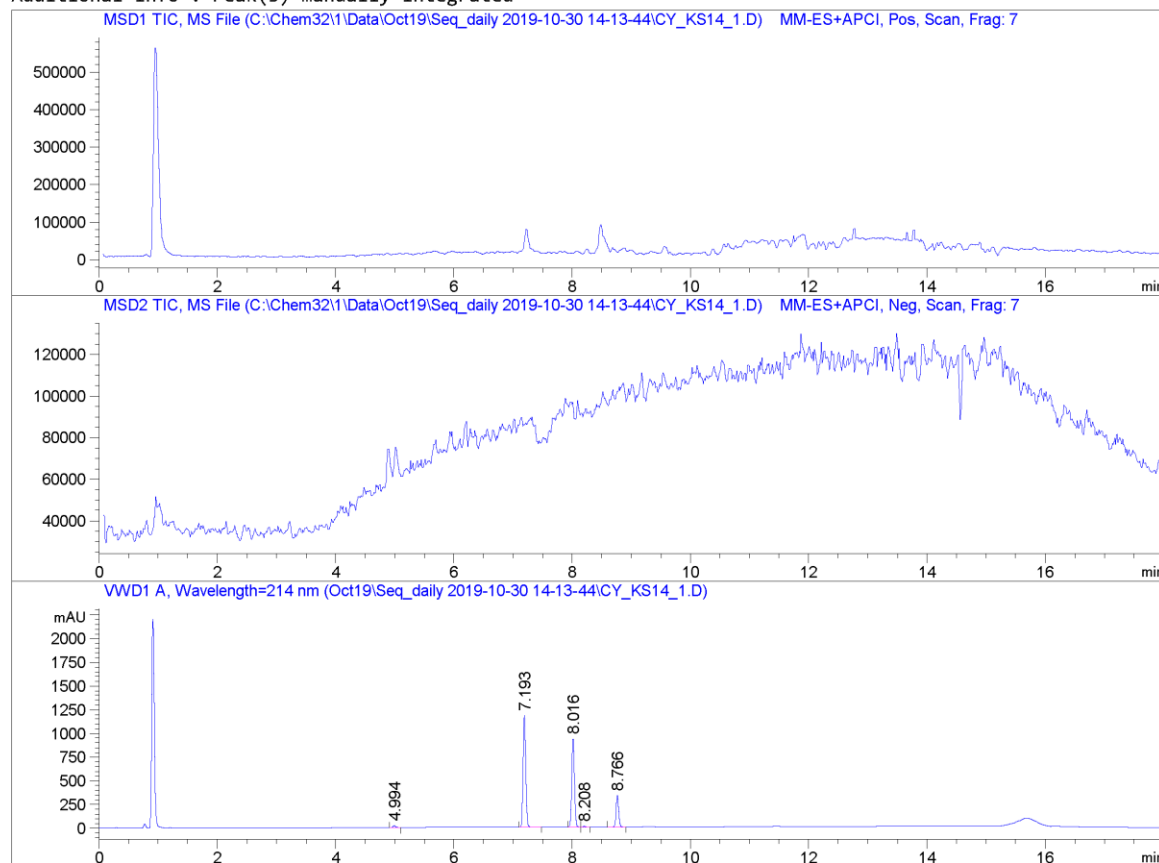   5 11.248 BV   0.4156 193.95953   5.83337   1.4602

Totals :   1.32826e4 4048.66468

===
                        *** End of Report ***

Data File C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\CY_KS14_1.D
Sample Name: CY_KS14_1

```
==================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   2
Acq. Instrument : 6130B LCMS                    Location :   4
Injection Date  : 30-Oct-19 2:35:44 PM              Inj :   1
                                            Inj Volume : 10.000 µl
Method          : C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\PORO_AMMACE_214_70.M (
                  Sequence Method)
Last changed    : 30-Oct-19 2:13:44 PM by SYSTEM
Method Info     : method for Poroshell 120 4.6 x75 x2.7um
```

Additional Info : Peak(s) manually integrated


```
==================================================================
                    Area Percent Report
==================================================================
```

Sorted By   :   Signal
Multiplier   :   1.0000
Dilution   :   1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: MSD1 TIC, MS File

Signal 2: MSD2 TIC, MS File

Signal 3: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.994	BV	0.0516	80.66749	24.44972	1.0405
2	7.193	BB	0.0491	3653.05273	1182.64063	47.1208
3	8.016	BV	0.0490	2987.28027	932.23676	38.5330
4	8.208	VB	0.0493	27.77909	8.60116	0.3583
5	8.766	BV	0.0485	1003.74170	331.11255	12.9473

Totals :   7752.52128 2479.04081

==
                          *** End of Report ***

Data File C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\CY_KS14_2.D
Sample Name: CY_KS14_2

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   3
Acq. Instrument : 6130B LCMS                     Location :   5
Injection Date  : 30-Oct-19 2:55:22 PM               Inj :   1
                                            Inj Volume : 10.000 µl
Method          : C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\PORO_AMMACE_214_70.M (
                  Sequence Method)
Last changed    : 30-Oct-19 2:13:44 PM by SYSTEM
Method Info     : method for Poroshell 120 4.6 x75 x2.7um
```

Additional Info : Peak(s) manually integrated


```
==================================================================
                     Area Percent Report
==================================================================

Sorted By            :      Signal
Multiplier           :      1.0000
Dilution             :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: MSD1 TIC, MS File

Signal 2: MSD2 TIC, MS File

Signal 3: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.004	BV	0.0525	177.51767	52.54781	1.6828
2	5.205	VV	0.1368	27.16753	2.75659	0.2575
3	7.203	MM	0.0538	4897.29492	1517.53845	46.4239
4	8.027	BV	0.0505	3152.93237	984.83838	29.8882
5	8.219	VV	0.0505	32.03975	9.60901	0.3037
6	8.775	VV	0.0483	2262.11768	749.22552	21.4438

Totals :   1.05491e4 3316.51577

===
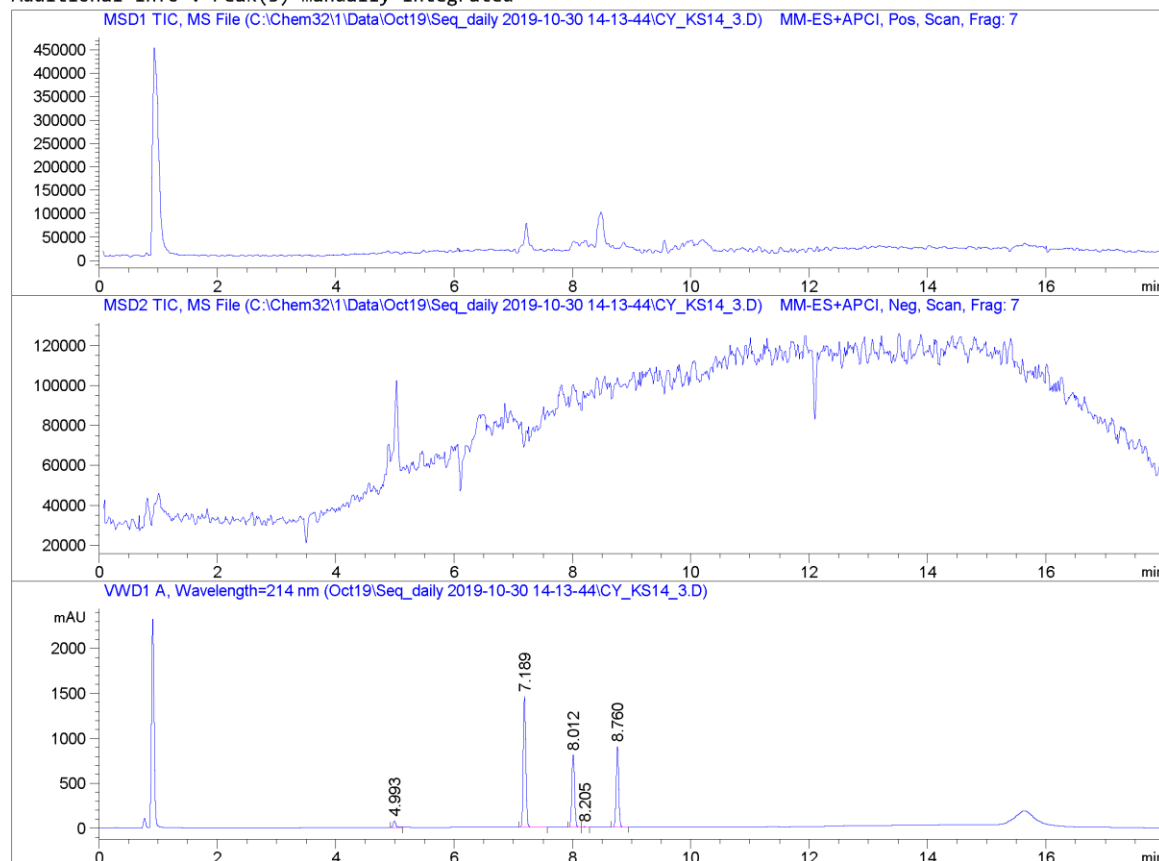*** End of Report ***

Data File C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\CY_KS14_3.D
Sample Name: CY_KS14_3

```
==================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   4
Acq. Instrument : 6130B LCMS                    Location :   6
Injection Date  : 30-Oct-19 3:14:59 PM               Inj :   1
                                            Inj Volume : 10.000 µl
Method          : C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\PORO_AMMACE_214_70.M (
                  Sequence Method)
Last changed    : 30-Oct-19 2:13:44 PM by SYSTEM
Method Info     : method for Poroshell 120 4.6 x75 x2.7um
```

Additional Info : Peak(s) manually integrated


```
==================================================================
                    Area Percent Report
==================================================================

Sorted By            :     Signal
Multiplier           :     1.0000
Dilution             :     1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Data File C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\CY_KS14_3.D
Sample Name: CY_KS14_3

    Signal 1: MSD1 TIC, MS File

    Signal 2: MSD2 TIC, MS File

    Signal 3: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.993	BB	0.0483	227.84889	72.53455	2.2765
2	7.189	BB	0.0491	4497.90479	1458.06519	44.9406
3	8.012	BV	0.0503	2568.38086	805.21124	25.6618
4	8.205	VV	0.0492	23.02415	7.15427	0.2300
5	8.760	BB	0.0467	2691.40649	896.15845	26.8910

Totals :   1.00086e4   3239.12370

    ===
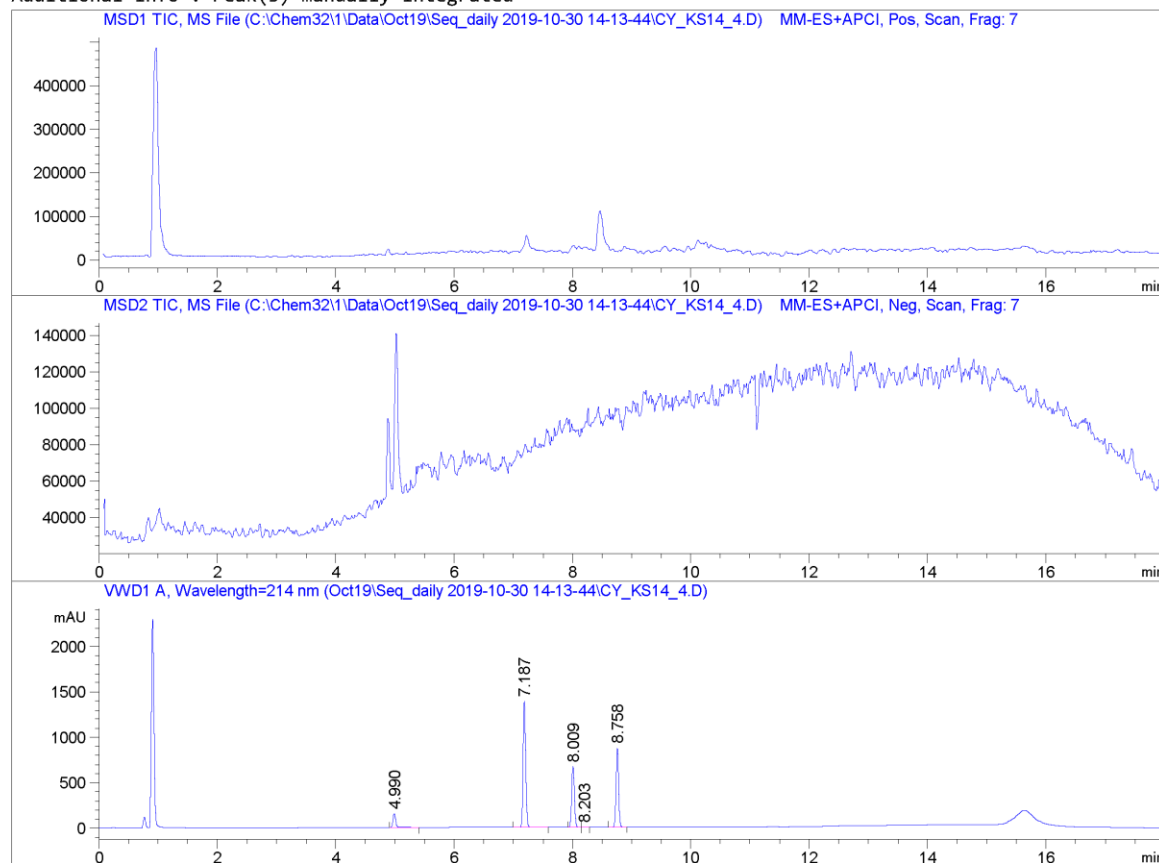   *** End of Report ***

Data File C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\CY_KS14_4.D
Sample Name: CY_KS14_4

```
==================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   7
Acq. Instrument : 6130B LCMS                    Location :   7
Injection Date  : 30-Oct-19 4:13:49 PM               Inj :   1
                                           Inj Volume : 10.000 µl
Method          : C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\PORO_AMMACE_214_70.M (
                  Sequence Method)
Last changed    : 30-Oct-19 2:13:44 PM by SYSTEM
Method Info     : method for Poroshell 120 4.6 x75 x2.7um
```

Additional Info : Peak(s) manually integrated


```
==================================================================
                    Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: MSD1 TIC, MS File

Signal 2: MSD2 TIC, MS File

Signal 3: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.990	BV	0.0539	545.89813	156.04333	5.6577
2	7.187	VB	0.0478	4312.30762	1390.62122	44.6927
3	8.009	BV	0.0505	2135.04932	666.66504	22.1276
4	8.203	VB	0.0483	16.28915	5.17811	0.1688
5	8.758	BV	0.0470	2639.24146	871.17480	27.3531

Totals :   9648.78567 3089.68250

===
                         *** End of Report ***

Data File C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\CY_KS14_5.D
Sample Name: CY_KS14_5

==
Acq. Operator   : SYSTEM   Seq. Line :   8
Acq. Instrument : 6130B LCMS   Location :   8
Injection Date : 30-Oct-19 4:33:30 PM   Inj :   1
                                            Inj Volume : 10.000 µl
Method   : C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\PORO_AMMACE_214_70.M (
                  Sequence Method)
Last changed   : 30-Oct-19 2:13:44 PM by SYSTEM
Method Info   : method for Poroshell 120 4.6 x75 x2.7um

Additional Info : Peak(s) manually integrated

==
                    Area Percent Report
==
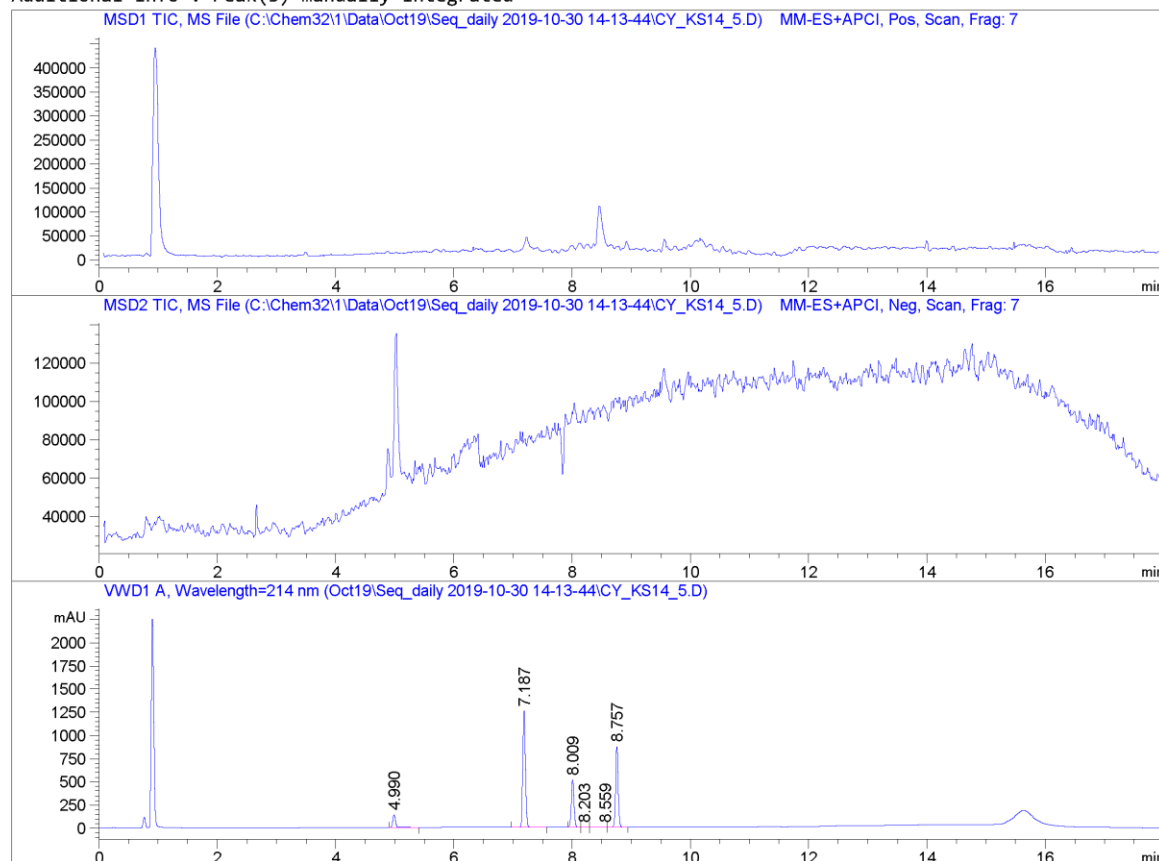
Sorted By   :   Signal
Multiplier   :   1.0000
Dilution   :   1.0000
Use Multiplier & Dilution Factor with ISTDs

Data File C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\CY_KS14_5.D
Sample Name: CY_KS14_5

    Signal 1: MSD1 TIC, MS File

    Signal 2: MSD2 TIC, MS File

    Signal 3: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.990	BV	0.0543	503.34460	142.38148	5.7382
2	7.187	VB	0.0493	3898.15112	1256.08765	44.4397
3	8.009	BV	0.0506	1642.58325	511.23456	18.7258
4	8.203	VV	0.0623	21.99875	5.06778	0.2508
5	8.559	VV	0.1649	26.70543	2.03338	0.3044
6	8.757	VV	0.0475	2678.99780	872.28619	30.5411

Totals :   8771.78096 2789.09105

===
                    *** End of Report ***

Data File C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\CY_KS14_6.D
Sample Name: CY_KS14_6

```
=================================================================
Acq. Operator   : SYSTEM                        Seq. Line :  13
Acq. Instrument : 6130B LCMS                     Location :   9
Injection Date  : 30-Oct-19 6:12:34 PM               Inj :   1
                                            Inj Volume : 10.000 µl
Method          : C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\PORO_AMMACE_214_70.M (
                  Sequence Method)
Last changed    : 30-Oct-19 2:13:44 PM by SYSTEM
Method Info     : method for Poroshell 120 4.6 x75 x2.7um
```

Additional Info : Peak(s) manually integrated


```
=================================================================
                     Area Percent Report
=================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```
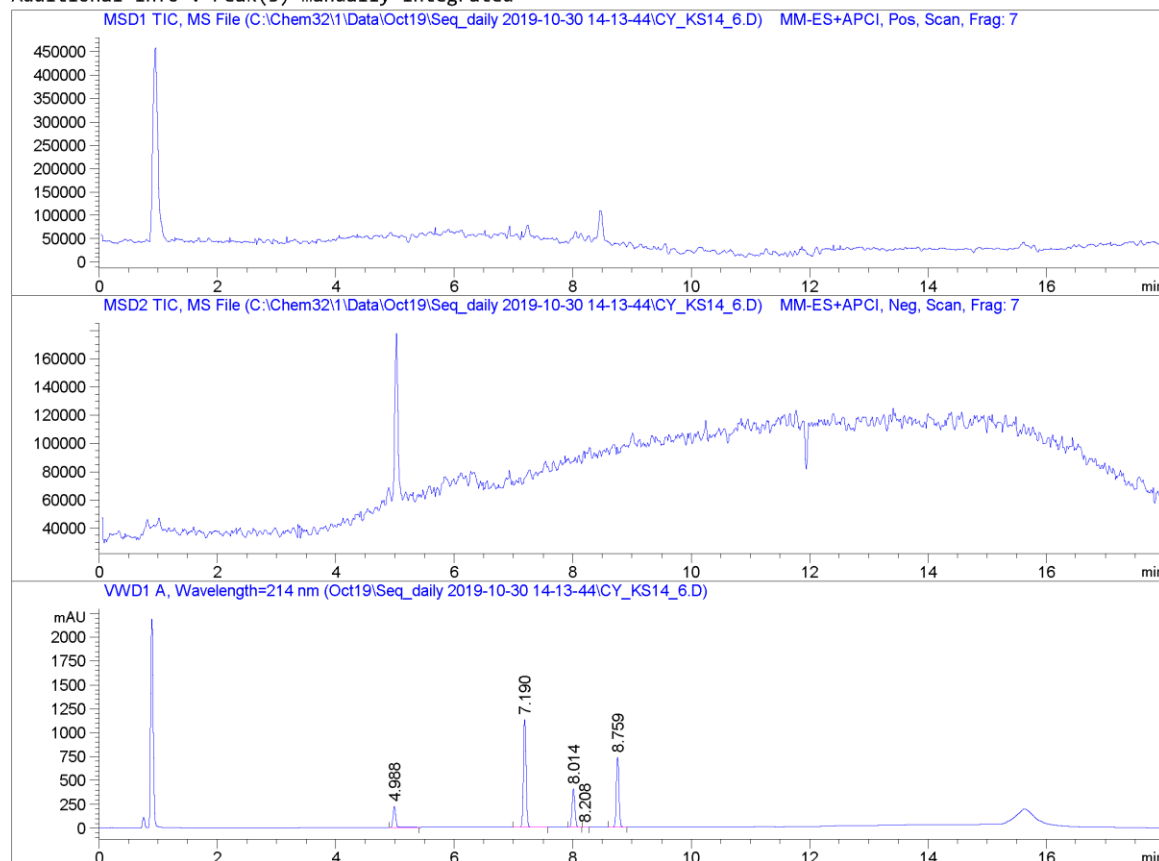
Data File C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\CY_KS14_6.D
Sample Name: CY_KS14_6

    Signal 1: MSD1 TIC, MS File

    Signal 2: MSD2 TIC, MS File

    Signal 3: VWD1 A, Wavelength=214 nm

Peak RetTime Type Width   Area   Height   Area
 #   [min]   [min]   [mAU*s]   [mAU]   %
----|-------|----|-------|----------|----------|--------|
   1   4.988 BV   0.0510 759.91699 225.23894   9.7251
   2   7.190 VB   0.0479 3522.59814 1134.93628 45.0806
   3   8.014 BV   0.0506 1295.47021 403.38464 16.5788
   4   8.208 VB   0.0482   8.28321   2.64713   0.1060
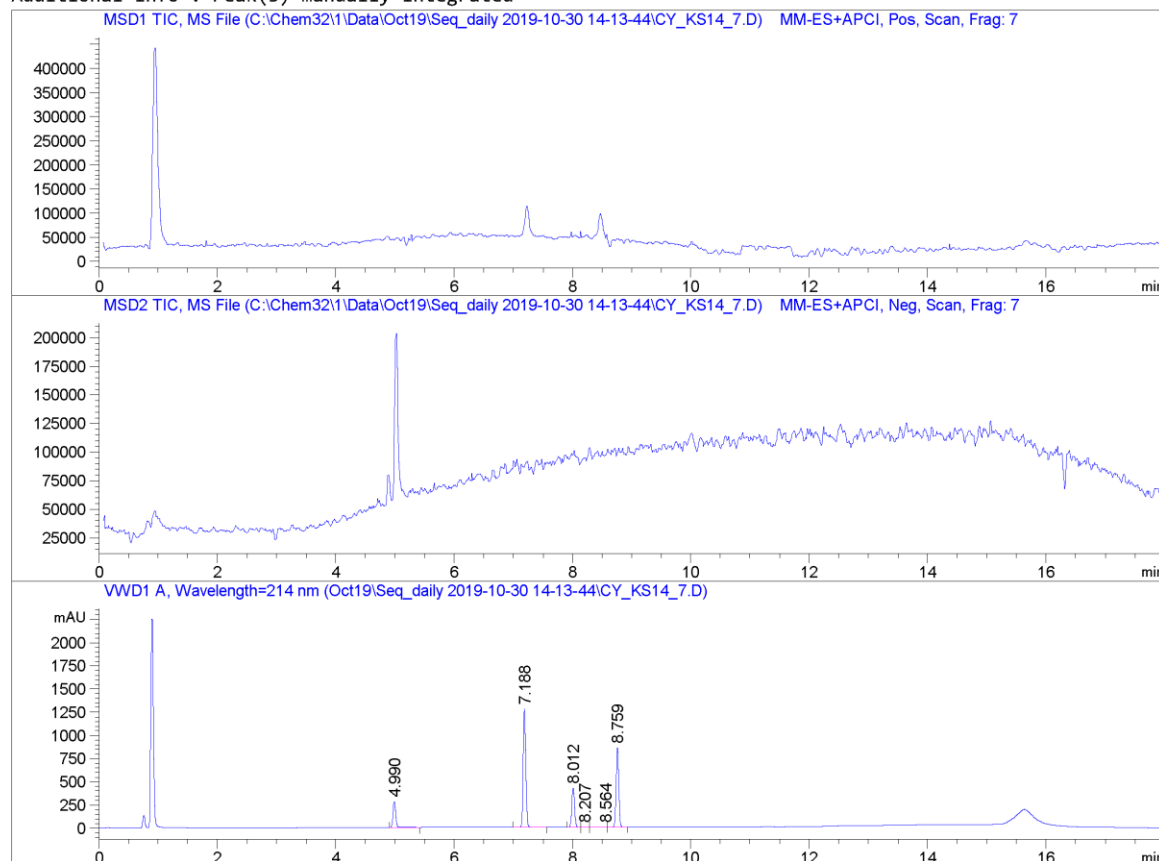   5   8.759 BV   0.0471 2227.73560 732.49530 28.5095

Totals :   7814.00416 2498.70229

===
                       *** End of Report ***

Data File C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\CY_KS14_7.D
Sample Name: CY_KS14_7

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :  14
Acq. Instrument : 6130B LCMS                     Location :   10
Injection Date  : 30-Oct-19 6:32:27 PM                Inj :   1
                                            Inj Volume : 10.000 µl
Method          : C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\PORO_AMMACE_214_70.M (
                  Sequence Method)
Last changed    : 30-Oct-19 2:13:44 PM by SYSTEM
Method Info     : method for Poroshell 120 4.6 x75 x2.7um
```

Additional Info : Peak(s) manually integrated


```
==================================================================
                    Area Percent Report
==================================================================

Sorted By            :       Signal
Multiplier           :       1.0000
Dilution             :       1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Data File C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\CY_KS14_7.D
Sample Name: CY_KS14_7

Signal 1: MSD1 TIC, MS File

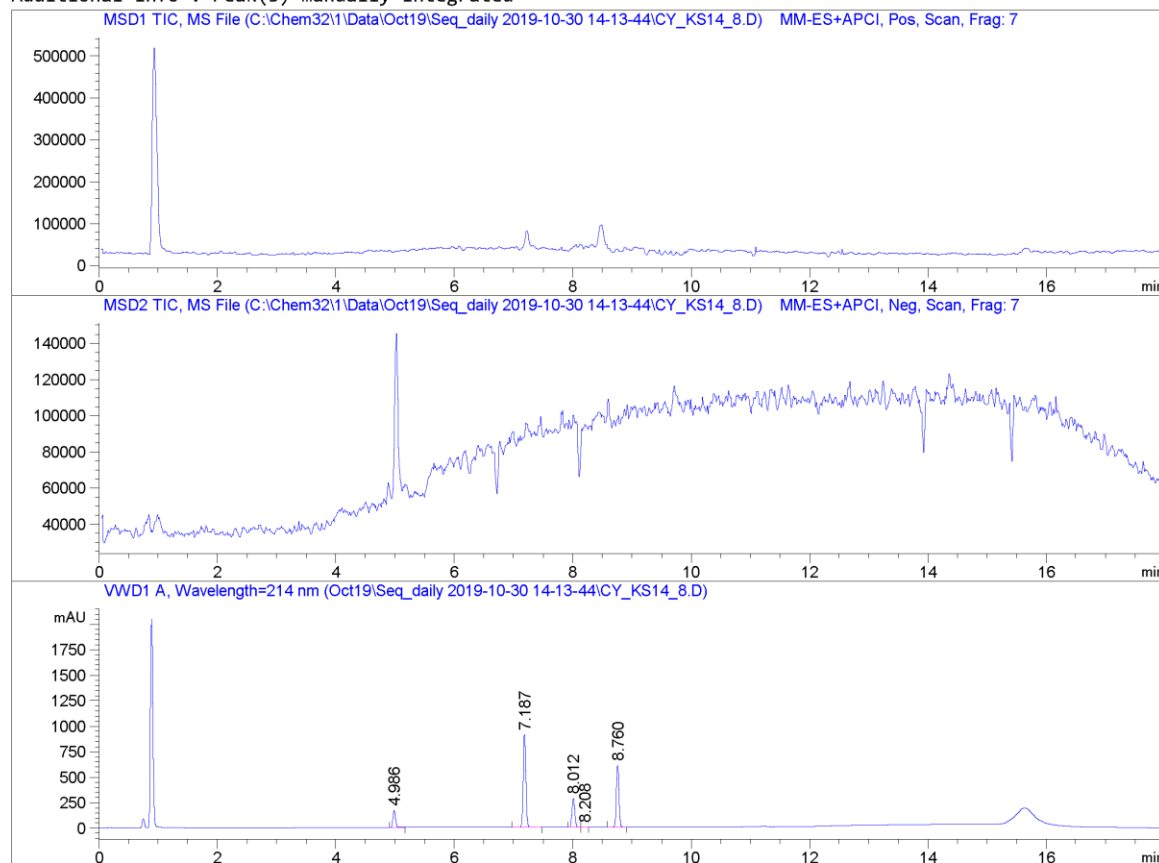Signal 2: MSD2 TIC, MS File

Signal 3: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.990	BV	0.0522	946.99036	282.44565	10.5391
2	7.188	VB	0.0494	3980.46729	1280.17542	44.2987
3	8.012	BV	0.0507	1362.33289	422.85211	15.1614
4	8.207	VV	0.0662	17.51275	3.74745	0.1949
5	8.564	VV	0.1722	29.81522	2.16684	0.3318
6	8.759	VV	0.0476	2648.39087	859.23358	29.4740

Totals :   8985.50937 2850.62104

==
*** End of Report ***

Data File C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\CY_KS14_8.D
Sample Name: CY_KS14_8

```
==================================================================
Acq. Operator   : SYSTEM                    Seq. Line :  16
Acq. Instrument : 6130B LCMS                Location :   11
Injection Date  : 30-Oct-19 7:12:17 PM          Inj :   1
                                         Inj Volume : 10.000 µl
Method          : C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\PORO_AMMACE_214_70.M (
                  Sequence Method)
Last changed    : 30-Oct-19 2:13:44 PM by SYSTEM
Method Info     : method for Poroshell 120 4.6 x75 x2.7um
```

Additional Info : Peak(s) manually integrated


```
==================================================================
                    Area Percent Report
==================================================================

Sorted By          :      Signal
Multiplier         :      1.0000
Dilution           :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: MSD1 TIC, MS File

Signal 2: MSD2 TIC, MS File

Signal 3: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.986	BB	0.0482	531.78156	169.91632	8.7217
2	7.187	VB	0.0475	2791.81250	908.80664	45.7881
3	8.012	BV	0.0504	911.70233	285.12402	14.9527
4	8.208	VB	0.0467	5.94825	1.89950	0.0976
5	8.760	VV	0.0473	1856.00537	607.69055	30.4400

Totals :   6097.25001 1973.43703

===
*** End of Report ***

Data File C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\CY_KS14_9.D
Sample Name: CY_KS14_9

```
==================================================================
Acq. Operator   : SYSTEM                      Seq. Line :  17
Acq. Instrument : 6130B LCMS                  Location :   12
Injection Date  : 30-Oct-19 7:31:53 PM             Inj :   1
                                         Inj Volume : 10.000 µl
Method          : C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\PORO_AMMACE_214_70.M (
                  Sequence Method)
Last changed    : 30-Oct-19 2:13:44 PM by SYSTEM
Method Info     : method for Poroshell 120 4.6 x75 x2.7um
```

Additional Info : Peak(s) manually integrated


```
==================================================================
                    Area Percent Report
==================================================================

Sorted By            :      Signal
Multiplier           :      1.0000
Dilution             :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```
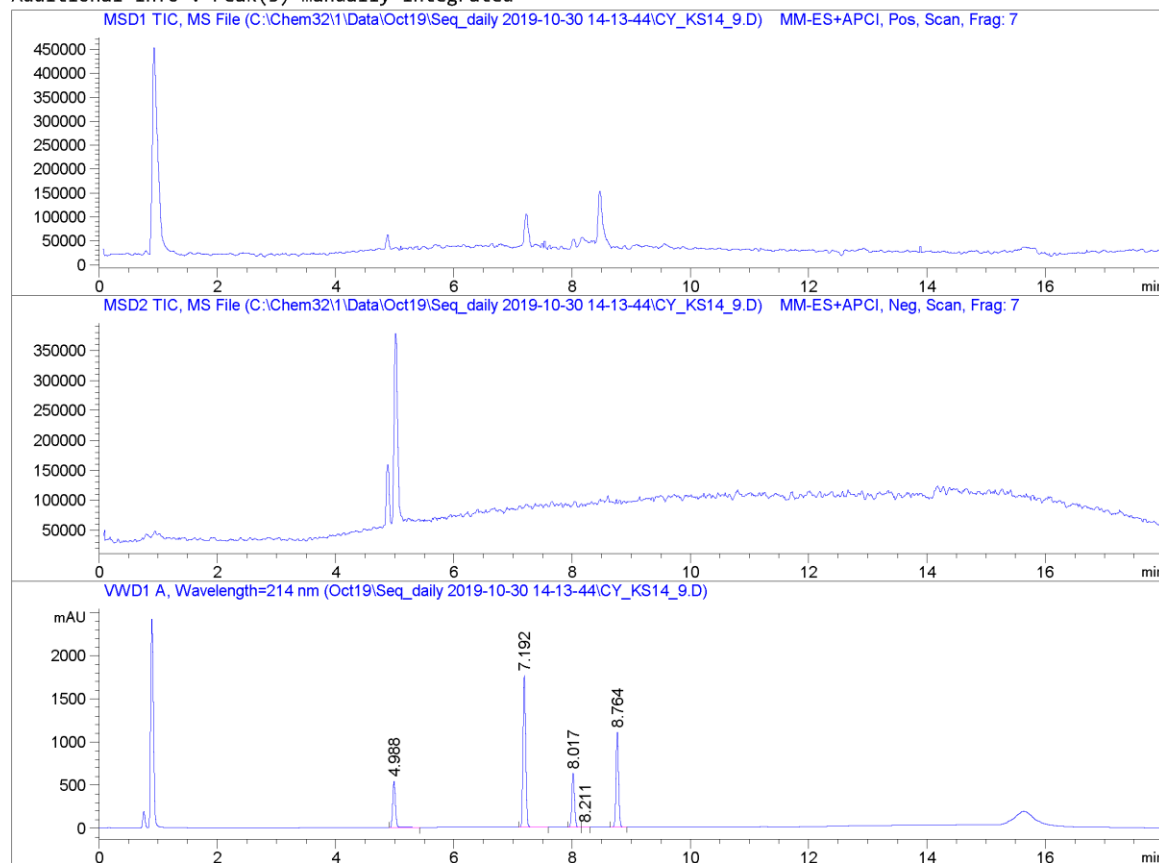
Signal 1: MSD1 TIC, MS File

Signal 2: MSD2 TIC, MS File

Signal 3: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.988	BV	0.0497	1769.19775	541.99048	14.0423
2	7.192	BB	0.0480	5491.95947	1760.93274	43.5903
3	8.017	BV	0.0505	1991.66907	622.03577	15.8081
4	8.211	VB	0.0484	12.36854	3.78086	0.0982
5	8.764	BV	0.0470	3333.84448	1101.54578	26.4611

Totals :   1.25990e4 4030.28562

==
                        *** End of Report ***

Data File C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\CY_KS14_10.D
Sample Name: CY_KS14_10

```
==================================================================
Acq. Operator   : SYSTEM                      Seq. Line :  34
Acq. Instrument : 6130B LCMS                  Location :   13
Injection Date  : 31-Oct-19 1:05:49 AM             Inj :   1
                                           Inj Volume : 10.000 µl
Method          : C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\PORO_AMMACE_214_70.M (
                  Sequence Method)
Last changed    : 30-Oct-19 2:13:44 PM by SYSTEM
Method Info     : method for Poroshell 120 4.6 x75 x2.7um
```

Additional Info : Peak(s) manually integrated


```
==================================================================
                  Area Percent Report
==================================================================

Sorted By           :     Signal
Multiplier          :     1.0000
Dilution            :     1.0000
Use Multiplier & Dilution Factor with ISTDs
```
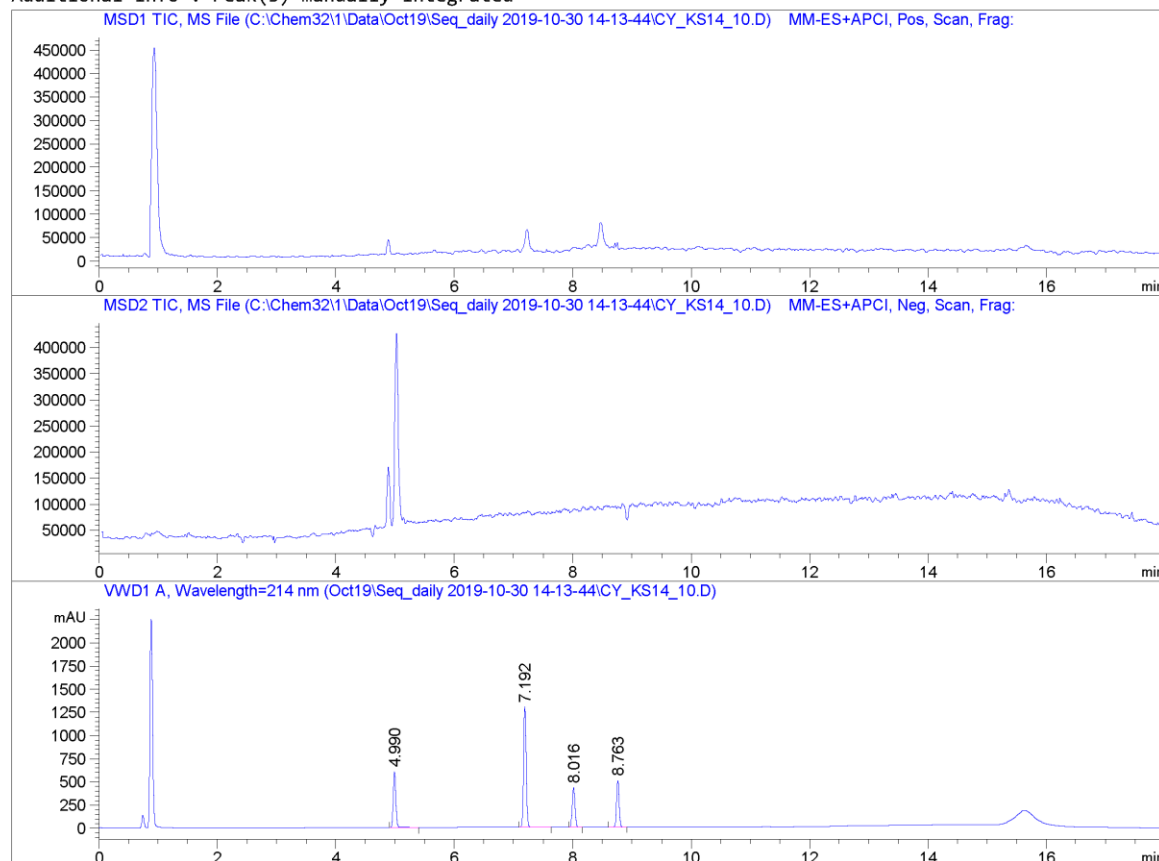
Data File C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\CY_KS14_10.D
Sample Name: CY_KS14_10

Signal 1: MSD1 TIC, MS File

Signal 2: MSD2 TIC, MS File

Signal 3: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.990	BV	0.0480	1890.69495	607.55341	21.5464
2	7.192	BB	0.0489	3999.90137	1302.51331	45.5830
3	8.016	BV	0.0487	1360.69885	428.00900	15.5066
4	8.763	BV	0.0469	1523.68726	504.91229	17.3640

Totals :   8774.98242 2842.98801

===
*** End of Report ***

Data File C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\CY_KS14_11.D
Sample Name: CY_KS14_11

```
==================================================================
Acq. Operator   : SYSTEM                      Seq. Line :  35
Acq. Instrument : 6130B LCMS                   Location :  14
Injection Date  : 31-Oct-19 1:25:24 AM              Inj :   1
                                             Inj Volume : 10.000 µl
Method          : C:\Chem32\1\Data\Oct19\Seq_daily 2019-10-30 14-13-44\PORO_AMMACE_214_70.M (
                  Sequence Method)
Last changed    : 30-Oct-19 2:13:44 PM by SYSTEM
Method Info     : method for Poroshell 120 4.6 x75 x2.7um
```

Additional Info : Peak(s) manually integrated


```
==================================================================
                    Area Percent Report
==================================================================

Sorted By           :      Signal
Multiplier          :      1.0000
Dilution            :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: MSD1 TIC, MS File

Signal 2: MSD2 TIC, MS File

Signal 3: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.991	BB	0.0480	1606.82959	515.60278	20.4509
2	7.193	BB	0.0488	3599.23340	1176.28821	45.8091
3	8.018	BV	0.0501	1194.73254	376.76279	15.2059
4	8.764	BV	0.0473	1456.22791	477.04208	18.5341

Totals :   7857.02344 2545.69586

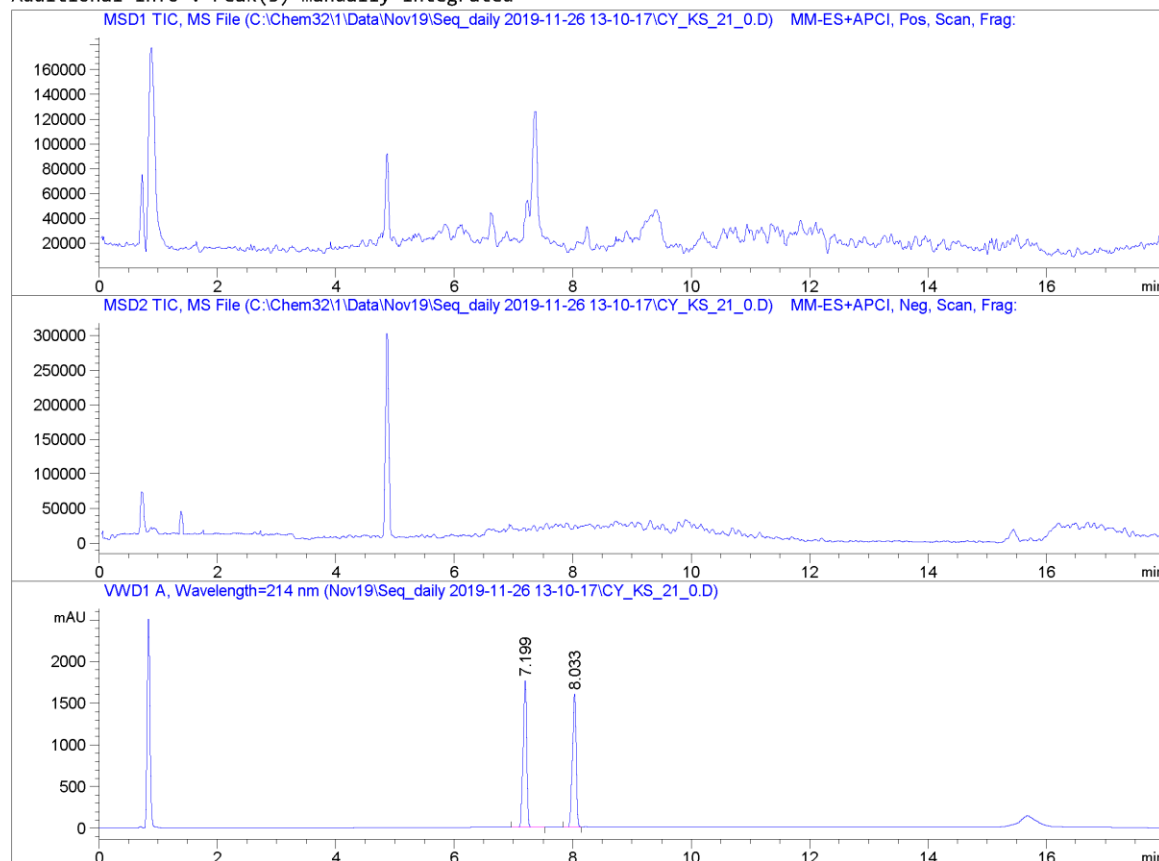
===
*** End of Report ***

Scheme 8 – Borylation Reaction with Non-preheated Catalyst Solution

Data File C:\Chem32\1\Data\Nov19\Seq_daily 2019-11-26 13-10-17\CY_KS_21_0.D
Sample Name: CY_KS_21_0

```
==================================================================
Acq. Operator   : SYSTEM                      Seq. Line :   8
Acq. Instrument : 6130B LCMS                   Location :   51
Injection Date  : 26-Nov-19 3:29:58 PM             Inj :   1
                                            Inj Volume : 10.000 µl
Method          : C:\Chem32\1\Data\Nov19\Seq_daily 2019-11-26 13-10-17\PORO_AMMACE_214_70.M (
                  Sequence Method)
Last changed    : 26-Nov-19 2:13:51 PM by SYSTEM
Method Info     : method for Poroshell 120 4.6 x75 x2.7um
```

Additional Info : Peak(s) manually integrated


```
==================================================================
                    Area Percent Report
==================================================================

Sorted By           :     Signal
Multiplier          :     1.0000
Dilution            :     1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: MSD1 TIC, MS File

Signal 2: MSD2 TIC, MS File

Signal 3: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.199	VB	0.0618	7343.55420	1760.91309	51.1996
2	8.033	BV	0.0657	6999.43408	1595.62891	48.8004

Totals :   1.43430e4 3356.54199

```
======================================================================
```
*** End of Report ***

Data File C:\Chem32\1\Data\Nov19\Seq_daily 2019-11-26 13-10-17\CY_KS_21_1.D
Sample Name: CY_KS_21_1

```
==================================================================
Acq. Operator   : SYSTEM                      Seq. Line :   9
Acq. Instrument : 6130B LCMS                   Location :   52
Injection Date  : 26-Nov-19 3:49:32 PM             Inj :   1
                                            Inj Volume : 10.000 µl
Method          : C:\Chem32\1\Data\Nov19\Seq_daily 2019-11-26 13-10-17\PORO_AMMACE_214_70.M (
                  Sequence Method)
Last changed    : 26-Nov-19 2:13:51 PM by SYSTEM
Method Info     : method for Poroshell 120 4.6 x75 x2.7um
```

Additional Info : Peak(s) manually integrated


```
==================================================================
                     Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: MSD1 TIC, MS File

Signal 2: MSD2 TIC, MS File

Signal 3: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.983	BB	0.0596	496.07339	124.55663	4.2278
2	7.200	VB	0.0609	5901.26367	1441.25977	50.2936
3	8.034	BV	0.0649	4124.48828	956.32281	35.1510
4	8.787	VV	0.0624	1211.79822	286.57910	10.3276

Totals :   1.17336e4   2808.71832

==
*** End of Report ***

Data File C:\Chem32\1\Data\Nov19\Seq_daily 2019-11-26 13-10-17\CY_KS_21_2.D
Sample Name: CY_KS_21_2

```
==================================================================
Acq. Operator   : SYSTEM                      Seq. Line :  10
Acq. Instrument : 6130B LCMS                  Location :   53
Injection Date  : 26-Nov-19 4:09:08 PM              Inj :   1
                                        Inj Volume : 10.000 µl
Method          : C:\Chem32\1\Data\Nov19\Seq_daily 2019-11-26 13-10-17\PORO_AMMACE_214_70.M (
                  Sequence Method)
Last changed    : 26-Nov-19 2:13:51 PM by SYSTEM
Method Info     : method for Poroshell 120 4.6 x75 x2.7um
```

Additional Info : Peak(s) manually integrated


```
==================================================================
                    Area Percent Report
==================================================================

Sorted By            :     Signal
Multiplier           :     1.0000
Dilution             :     1.0000
Use Multiplier & Dilution Factor with ISTDs
```
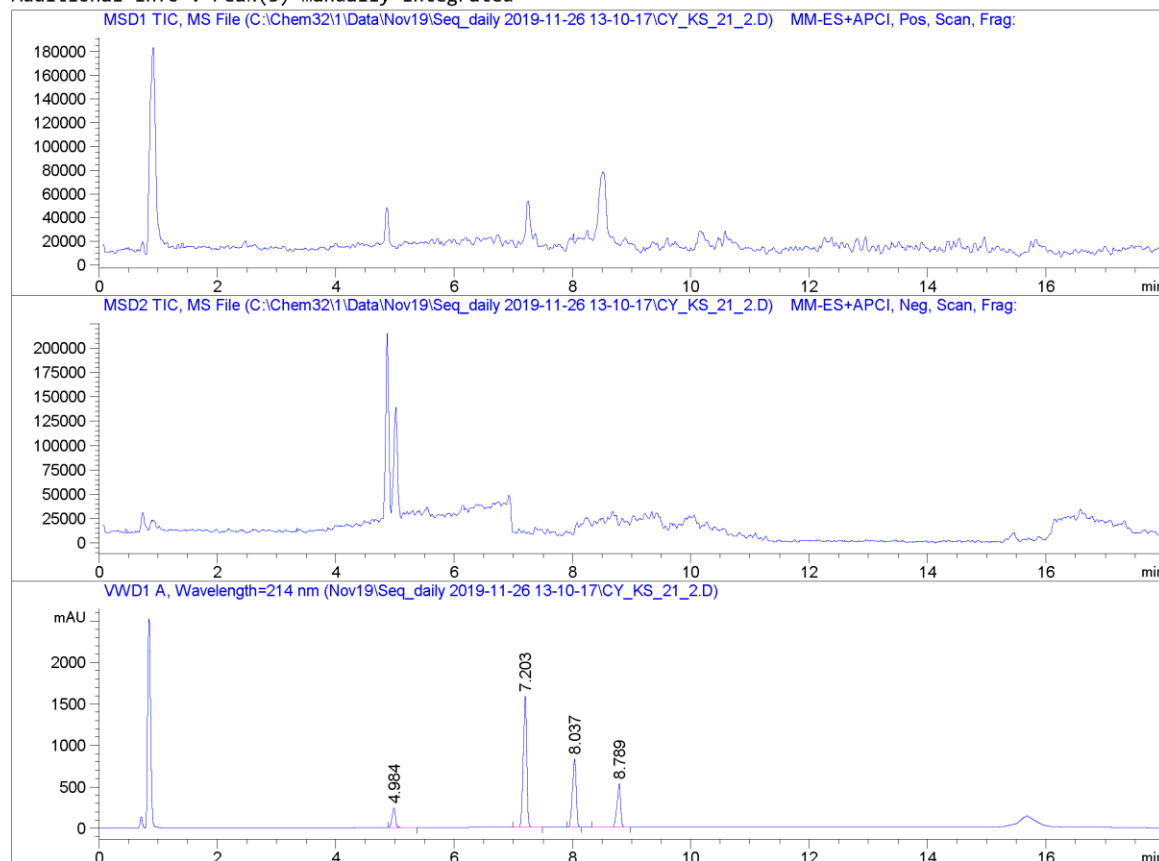
Data File C:\Chem32\1\Data\Nov19\Seq_daily 2019-11-26 13-10-17\CY_KS_21_2.D
Sample Name: CY_KS_21_2

Signal 1: MSD1 TIC, MS File

Signal 2: MSD2 TIC, MS File

Signal 3: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.984	VV	0.0616	998.71948	240.24475	7.4890
2	7.203	VB	0.0613	6523.60986	1579.24976	48.9180
3	8.037	BV	0.0637	3583.00903	826.92700	26.8676
4	8.789	BV	0.0614	2230.45972	523.48090	16.7254

Totals :   1.33358e4   3169.90240
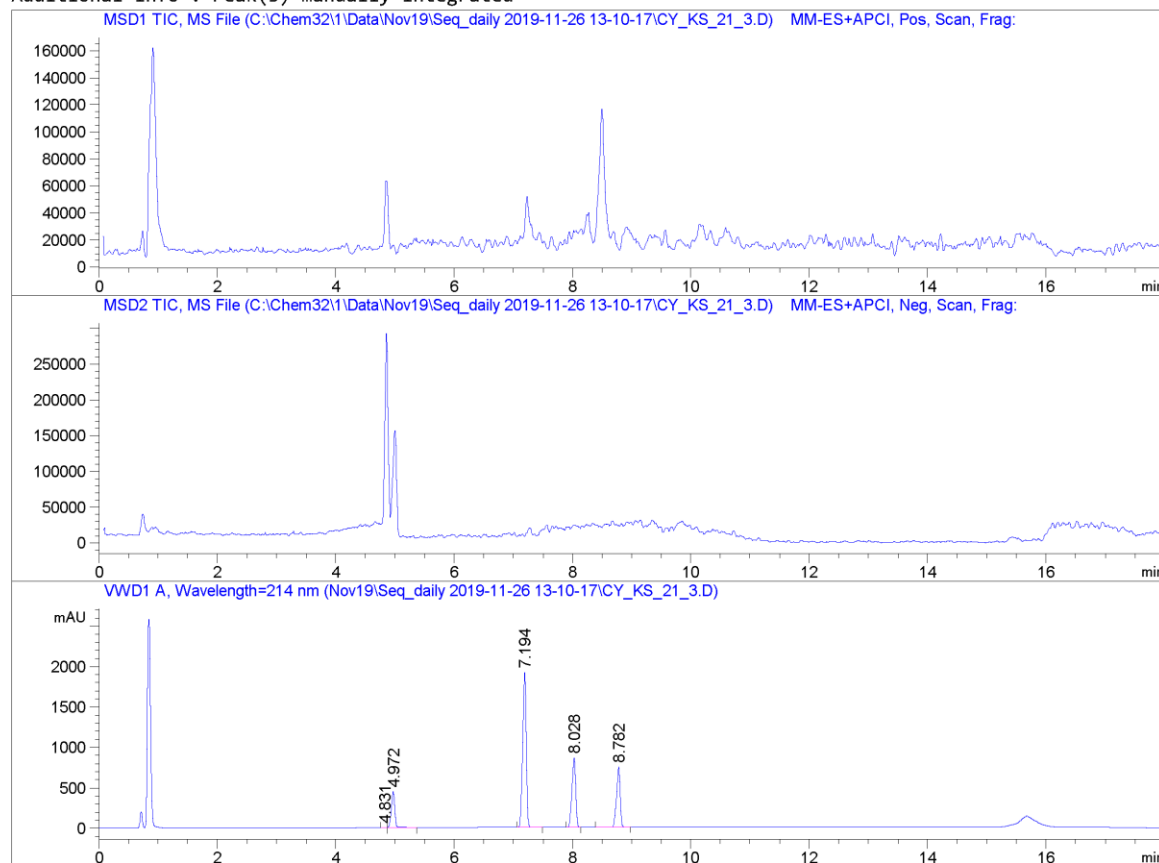
===
*** End of Report ***

Data File C:\Chem32\1\Data\Nov19\Seq_daily 2019-11-26 13-10-17\CY_KS_21_3.D
Sample Name: CY_KS_21_3

```
=================================================================
Acq. Operator   : SYSTEM                     Seq. Line :  11
Acq. Instrument : 6130B LCMS                 Location :   54
Injection Date  : 26-Nov-19 4:28:44 PM            Inj :   1
                                          Inj Volume : 10.000 µl
Method          : C:\Chem32\1\Data\Nov19\Seq_daily 2019-11-26 13-10-17\PORO_AMMACE_214_70.M (
                  Sequence Method)
Last changed    : 26-Nov-19 2:13:51 PM by SYSTEM
Method Info     : method for Poroshell 120 4.6 x75 x2.7um
```

Additional Info : Peak(s) manually integrated


```
=================================================================
                    Area Percent Report
=================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: MSD1 TIC, MS File

Signal 2: MSD2 TIC, MS File

Signal 3: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.831	BV	0.0526	5.90045	1.74397	0.0353
2	4.972	VV	0.0627	1842.22656	446.28290	11.0092
3	7.194	BB	0.0619	8001.80029	1913.68896	47.8189
4	8.028	BV	0.0654	3743.63257	859.81769	22.3720
5	8.782	BV	0.0625	3140.00464	741.88239	18.7647

Totals :   1.67336e4   3963.41591

==
*** End of Report ***

Data File C:\Chem32\1\Data\Nov19\Seq_daily 2019-11-26 13-10-17\CY_KS_21_4.D
Sample Name: CY_KS_21_4

```
==================================================================
Acq. Operator   : SYSTEM                      Seq. Line :  14
Acq. Instrument : 6130B LCMS                   Location :   55
Injection Date  : 26-Nov-19 5:27:54 PM              Inj :   1
                                             Inj Volume : 10.000 µl
Method          : C:\Chem32\1\Data\Nov19\Seq_daily 2019-11-26 13-10-17\PORO_AMMACE_214_70.M (
                  Sequence Method)
Last changed    : 26-Nov-19 2:13:51 PM by SYSTEM
Method Info     : method for Poroshell 120 4.6 x75 x2.7um
```

Additional Info : Peak(s) manually integrated


```
==================================================================
                    Area Percent Report
==================================================================

Sorted By          :      Signal
Multiplier         :      1.0000
Dilution           :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```
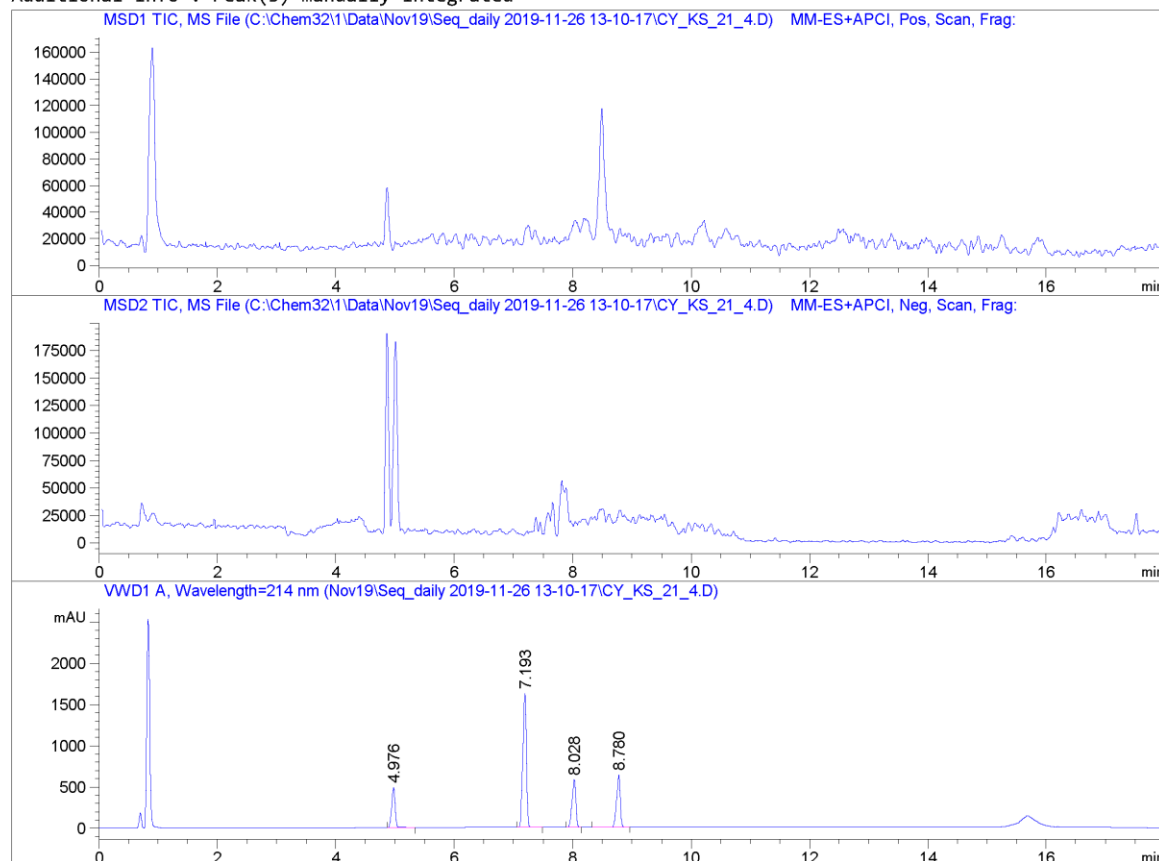
Signal 1: MSD1 TIC, MS File

Signal 2: MSD2 TIC, MS File

Signal 3: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.976	VV	0.0629	2030.24597	490.44662	14.4207
2	7.193	BB	0.0632	6763.53760	1621.19019	48.0410
3	8.028	BV	0.0657	2523.23267	575.54480	17.9224
4	8.780	VV	0.0626	2761.67383	631.83099	19.6160

Totals :   1.40787e4   3319.01260

==
*** End of Report ***

Data File C:\Chem32\1\Data\Nov19\Seq_daily 2019-11-26 13-10-17\CY_KS_21_5.D
Sample Name: CY_KS_21_5

```
==================================================================
Acq. Operator   : SYSTEM                       Seq. Line :  15
Acq. Instrument : 6130B LCMS                    Location :   56
Injection Date  : 26-Nov-19 5:47:32 PM               Inj :   1
                                            Inj Volume : 10.000 µl
Method          : C:\Chem32\1\Data\Nov19\Seq_daily 2019-11-26 13-10-17\PORO_AMMACE_214_70.M (
                  Sequence Method)
Last changed    : 26-Nov-19 2:13:51 PM by SYSTEM
Method Info     : method for Poroshell 120 4.6 x75 x2.7um
```

Additional Info : Peak(s) manually integrated


```
==================================================================
                    Area Percent Report
==================================================================

Sorted By           :      Signal
Multiplier          :      1.0000
Dilution            :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```
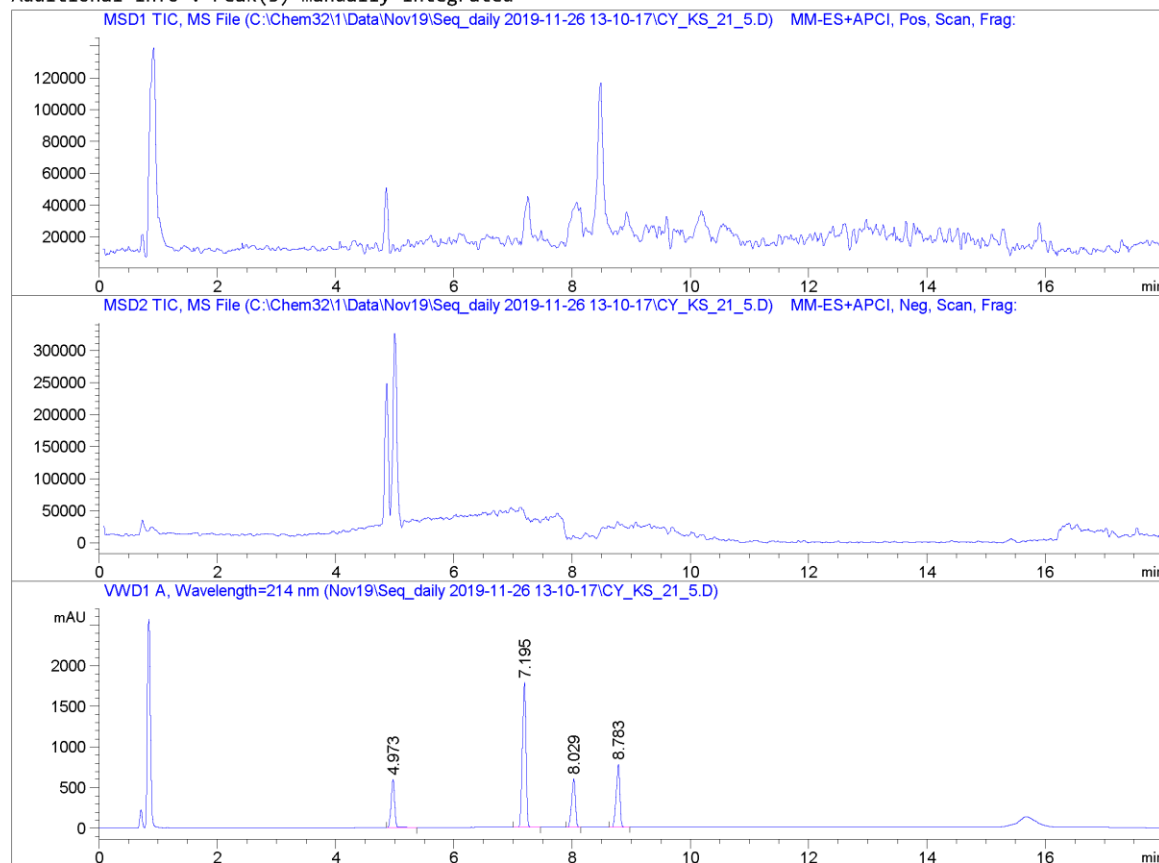
Signal 1: MSD1 TIC, MS File

Signal 2: MSD2 TIC, MS File

Signal 3: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.973	VV	0.0630	2454.64478	591.52423	15.5047
2	7.195	BV	0.0621	7472.76025	1781.17200	47.2015
3	8.029	BV	0.0657	2598.99829	593.48499	16.4165
4	8.783	BV	0.0630	3305.21948	773.07556	20.8773

Totals :   1.58316e4   3739.25677

===
                          *** End of Report ***

Data File C:\Chem32\1\Data\Nov19\Seq_daily 2019-11-26 13-10-17\CY_KS_21_6.D
Sample Name: CY_KS_21_6

```
==================================================================
Acq. Operator   : SYSTEM                      Seq. Line :  17
Acq. Instrument : 6130B LCMS                   Location :   57
Injection Date  : 26-Nov-19 6:27:22 PM             Inj :   1
                                           Inj Volume : 10.000 µl
Method          : C:\Chem32\1\Data\Nov19\Seq_daily 2019-11-26 13-10-17\PORO_AMMACE_214_70.M (
                  Sequence Method)
Last changed    : 26-Nov-19 2:13:51 PM by SYSTEM
Method Info     : method for Poroshell 120 4.6 x75 x2.7um
```

Additional Info : Peak(s) manually integrated


```
==================================================================
                      Area Percent Report
==================================================================

Sorted By          :       Signal
Multiplier         :       1.0000
Dilution           :       1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: MSD1 TIC, MS File

Signal 2: MSD2 TIC, MS File

Signal 3: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.969	VV	0.0614	2786.43335	673.43005	19.6341
2	7.192	BV	0.0623	6795.67432	1613.15320	47.8846
3	8.026	BV	0.0646	2032.14758	460.48703	14.3192
4	8.779	VB	0.0618	2577.52051	599.82239	18.1621

Totals :   1.41918e4   3346.89267

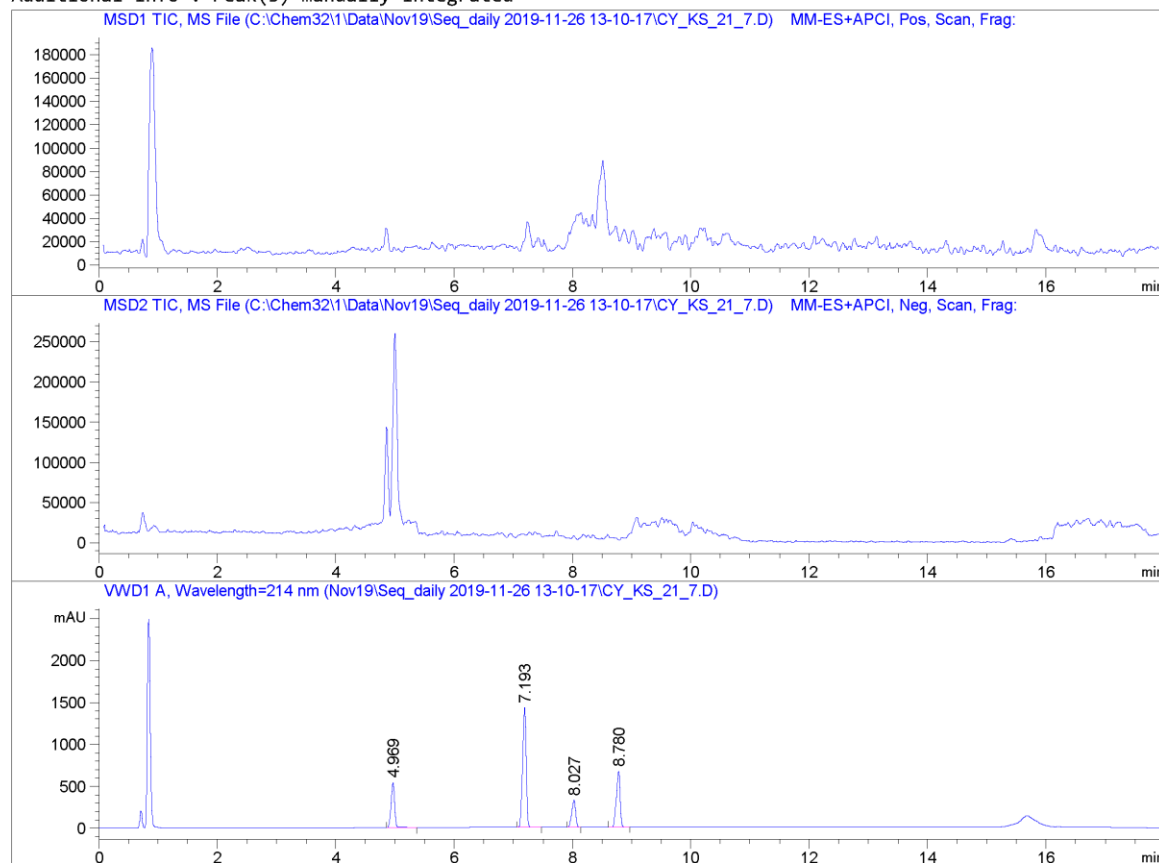===
                         *** End of Report ***

Data File C:\Chem32\1\Data\Nov19\Seq_daily 2019-11-26 13-10-17\CY_KS_21_7.D
Sample Name: CY_KS_21_7

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :  18
Acq. Instrument : 6130B LCMS                     Location :   58
Injection Date  : 26-Nov-19 6:46:57 PM               Inj :   1
                                             Inj Volume : 10.000 µl
Method          : C:\Chem32\1\Data\Nov19\Seq_daily 2019-11-26 13-10-17\PORO_AMMACE_214_70.M (
                  Sequence Method)
Last changed    : 26-Nov-19 2:13:51 PM by SYSTEM
Method Info     : method for Poroshell 120 4.6 x75 x2.7um
```

Additional Info : Peak(s) manually integrated


```
==================================================================
                    Area Percent Report
==================================================================

Sorted By          :      Signal
Multiplier         :      1.0000
Dilution           :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: MSD1 TIC, MS File

Signal 2: MSD2 TIC, MS File

Signal 3: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.969	BV	0.0635	2273.87061	542.35571	17.9416
2	7.193	BB	0.0624	6046.22070	1429.55090	47.7068
3	8.027	BV	0.0665	1444.36121	324.48328	11.3965
4	8.780	BV	0.0625	2909.26050	667.66852	22.9551

Totals :   1.26737e4 2964.05841

===
*** End of Report ***

Data File C:\Chem32\1\Data\Nov19\Seq_daily 2019-11-26 13-10-17\CY_KS_21_8.D
Sample Name: CY_KS_21_8

```
==================================================================
Acq. Operator   : SYSTEM                      Seq. Line :  19
Acq. Instrument : 6130B LCMS                  Location :   59
Injection Date  : 26-Nov-19 7:06:31 PM            Inj :   1
                                          Inj Volume : 10.000 µl
Method          : C:\Chem32\1\Data\Nov19\Seq_daily 2019-11-26 13-10-17\PORO_AMMACE_214_70.M (
                  Sequence Method)
Last changed    : 26-Nov-19 2:13:51 PM by SYSTEM
Method Info     : method for Poroshell 120 4.6 x75 x2.7um
```

Additional Info : Peak(s) manually integrated


```
==================================================================
                    Area Percent Report
==================================================================

Sorted By           :      Signal
Multiplier          :      1.0000
Dilution            :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```
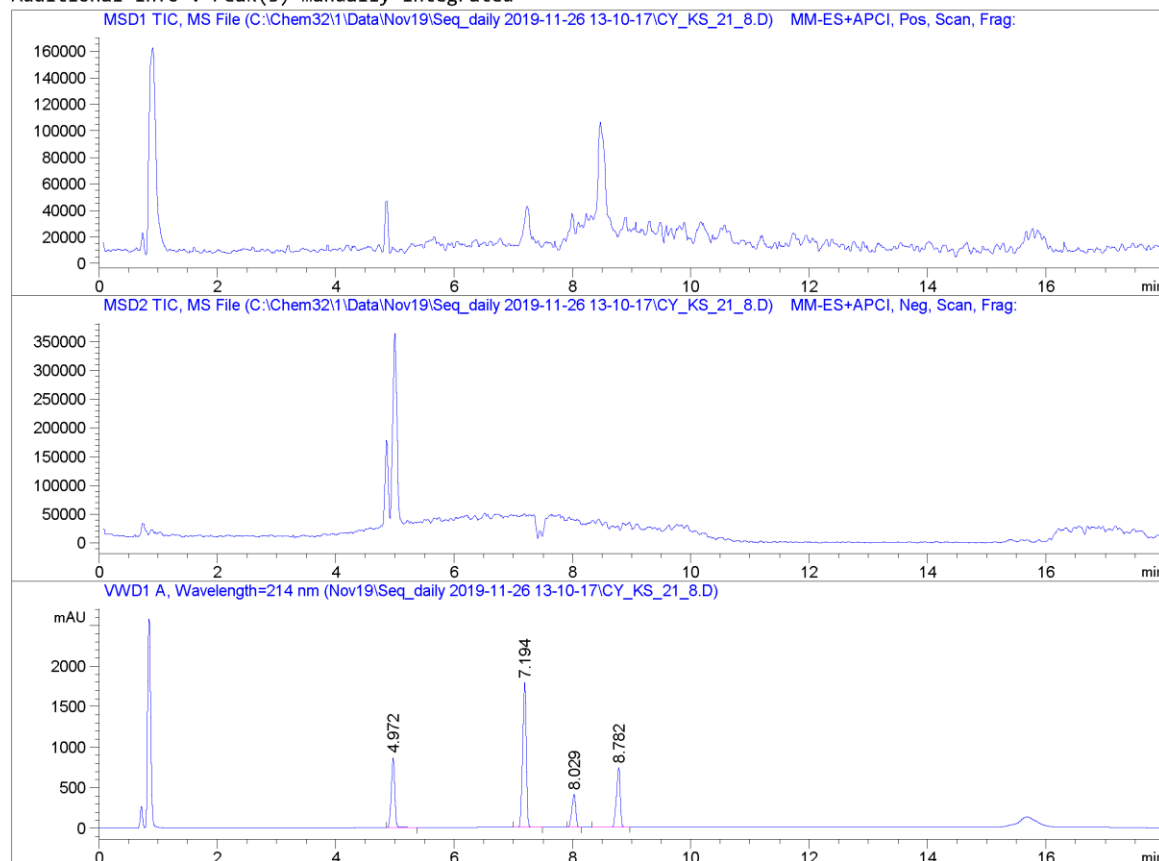
Data File C:\Chem32\1\Data\Nov19\Seq_daily 2019-11-26 13-10-17\CY_KS_21_8.D
Sample Name: CY_KS_21_8

Signal 1: MSD1 TIC, MS File

Signal 2: MSD2 TIC, MS File

Signal 3: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.972	VV	0.0630	3595.41870	866.59143	22.0969
2	7.194	BB	0.0643	7607.51514	1784.80261	46.7547
3	8.029	BV	0.0666	1820.84729	408.46149	11.1907
4	8.782	BV	0.0645	3247.34546	736.75909	19.9577

Totals :   1.62711e4 3796.61462

===
*** End of Report ***

Data File C:\Chem32\1\Data\Nov19\Seq_daily 2019-11-26 13-10-17\CY_KS_21_9.D
Sample Name: CY_KS_21_9

```
===================================================================
Acq. Operator   : SYSTEM                    Seq. Line :  20
Acq. Instrument : 6130B LCMS                 Location :   60
Injection Date  : 26-Nov-19 7:26:08 PM           Inj :   1
                                          Inj Volume : 10.000 µl
Method          : C:\Chem32\1\Data\Nov19\Seq_daily 2019-11-26 13-10-17\PORO_AMMACE_214_70.M (
                  Sequence Method)
Last changed    : 26-Nov-19 2:13:51 PM by SYSTEM
Method Info     : method for Poroshell 120 4.6 x75 x2.7um
```

Additional Info : Peak(s) manually integrated


```
===================================================================
                    Area Percent Report
===================================================================

Sorted By           :     Signal
Multiplier          :     1.0000
Dilution            :     1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: MSD1 TIC, MS File

Signal 2: MSD2 TIC, MS File

Signal 3: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.970	VV	0.0633	2214.12158	530.49738	17.9647
2	7.191	VB	0.0627	5872.97852	1382.46716	47.6515
3	8.026	BV	0.0654	1320.62268	294.62619	10.7151
4	8.780	BV	0.0634	2917.13647	657.61914	23.6687

Totals :   1.23249e4   2865.20987

===
                      *** End of Report ***

Data File C:\Chem32\1\Data\Nov19\Seq_daily 2019-11-26 13-10-17\CY_KS_21_10.D
Sample Name: CY_KS_21_10

```
==================================================================
Acq. Operator   : SYSTEM                     Seq. Line :  24
Acq. Instrument : 6130B LCMS                 Location :   69
Injection Date  : 26-Nov-19 8:44:52 PM            Inj :   1
                                           Inj Volume : 10.000 µl
Method          : C:\Chem32\1\Data\Nov19\Seq_daily 2019-11-26 13-10-17\PORO_AMMACE_214_70.M (
                  Sequence Method)
Last changed    : 26-Nov-19 2:13:51 PM by SYSTEM
Method Info     : method for Poroshell 120 4.6 x75 x2.7um
```

Additional Info : Peak(s) manually integrated


```
==================================================================
                    Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```
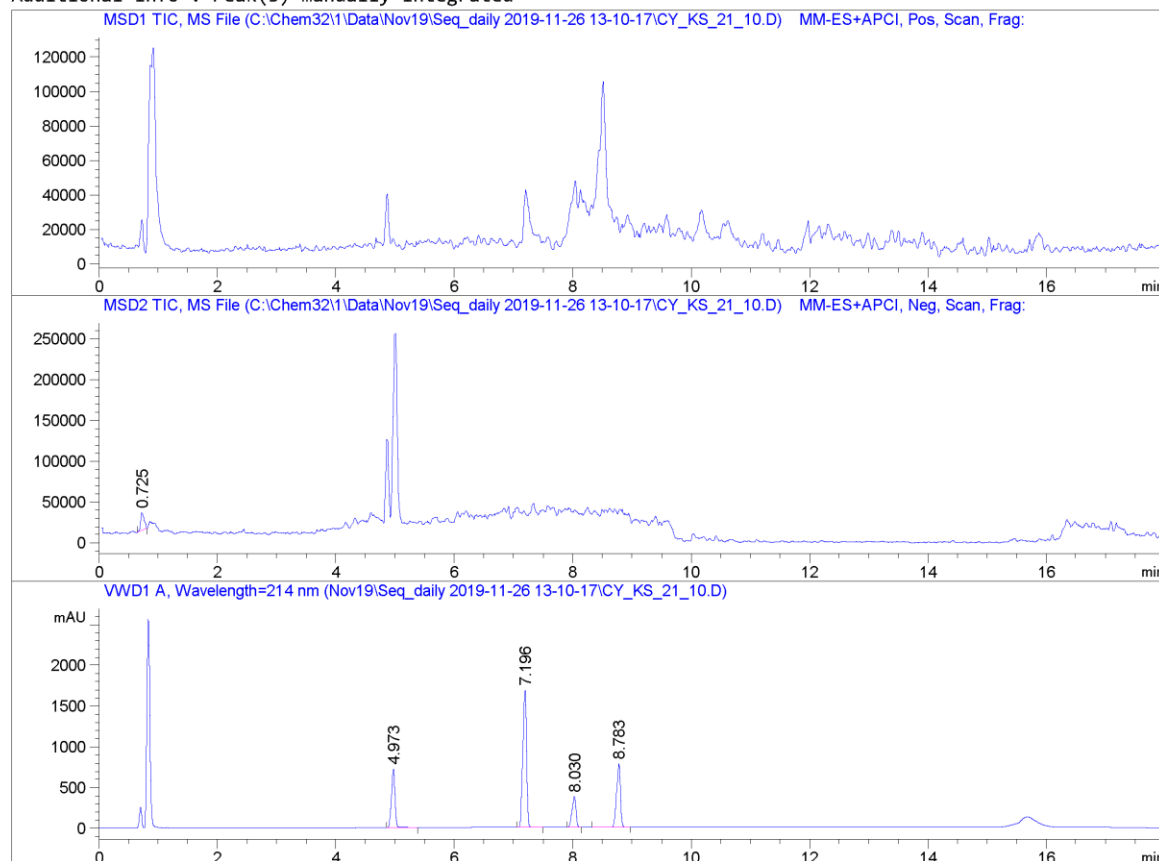
Signal 1: MSD1 TIC, MS File

Signal 2: MSD2 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	0.725	BB	0.0630	8.93777e4	2.21501e4	100.0000

Totals :   8.93777e4 2.21501e4

Signal 3: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.973	VV	0.0640	3066.78076	723.77808	19.5501
2	7.196	BB	0.0640	7358.13770	1686.30530	46.9067
3	8.030	BV	0.0680	1714.08752	373.96356	10.9270
4	8.783	BV	0.0660	3547.74805	781.92694	22.6162

Totals :   1.56868e4 3565.97388

===
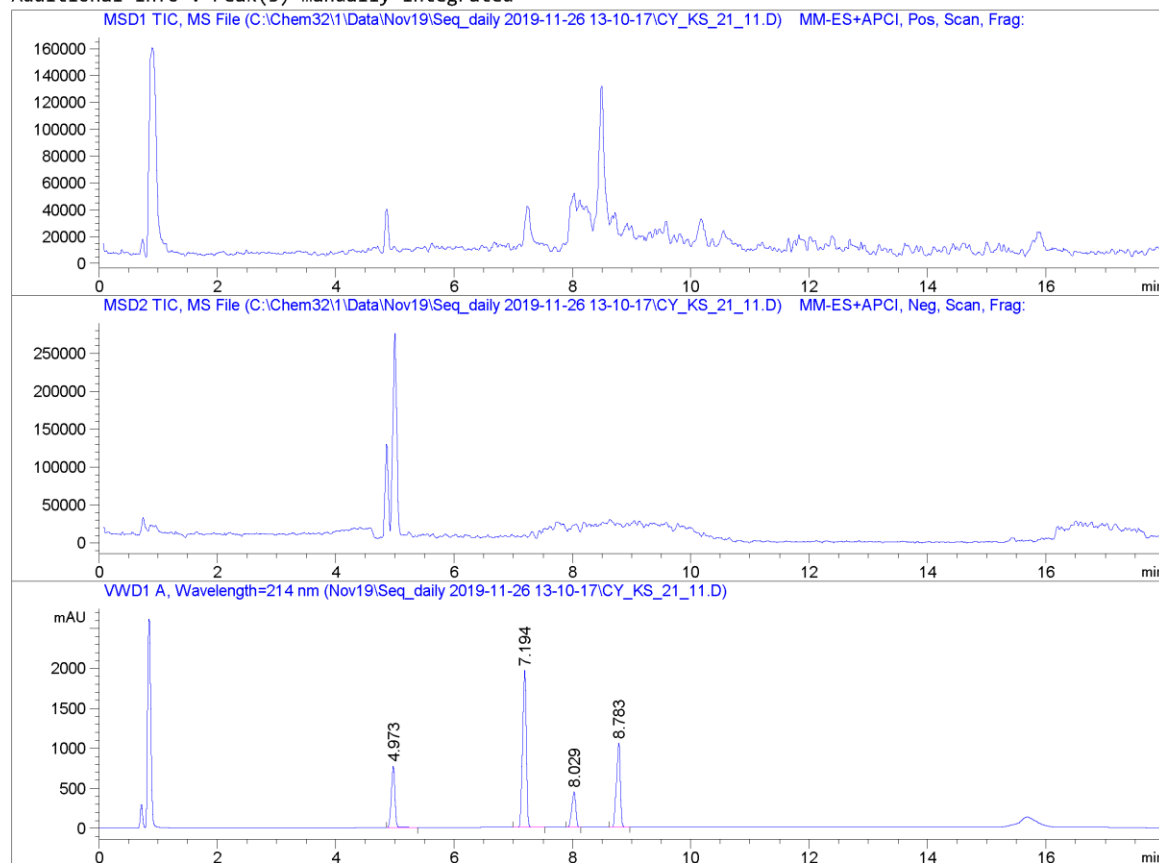*** End of Report ***

Data File C:\Chem32\1\Data\Nov19\Seq_daily 2019-11-26 13-10-17\CY_KS_21_11.D
Sample Name: CY_KS_21_11

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :  25
Acq. Instrument : 6130B LCMS                     Location :   70
Injection Date  : 26-Nov-19 9:04:32 PM               Inj :   1
                                           Inj Volume : 10.000 µl
Method          : C:\Chem32\1\Data\Nov19\Seq_daily 2019-11-26 13-10-17\PORO_AMMACE_214_70.M (
                  Sequence Method)
Last changed    : 26-Nov-19 2:13:51 PM by SYSTEM
Method Info     : method for Poroshell 120 4.6 x75 x2.7um
```

Additional Info : Peak(s) manually integrated


```
==================================================================
                  Area Percent Report
==================================================================
```

```
Sorted By          :      Signal
Multiplier         :      1.0000
Dilution           :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: MSD1 TIC, MS File

Signal 2: MSD2 TIC, MS File

Signal 3: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.973	VV	0.0645	3308.16919	772.48804	17.6441
2	7.194	VB	0.0660	8666.34668	1964.11804	46.2220
3	8.029	BV	0.0683	2036.13196	442.26819	10.8597
4	8.783	BV	0.0658	4738.74072	1048.40881	25.2741

Totals :   1.87494e4   4227.28308

===
*** End of Report ***