

Supporting Information

Optimization of Novel 1-Methyl-1*H*-Pyrazole-5-carboxamides Leads to High Potency Larval Development Inhibitors of the Barber's Pole Worm

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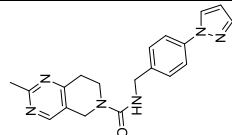
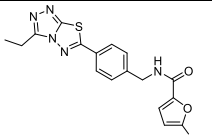
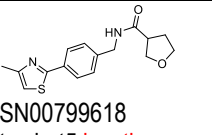
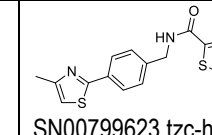
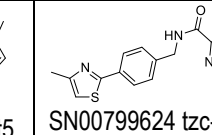
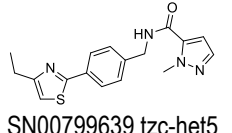
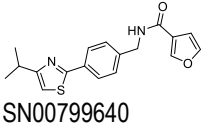
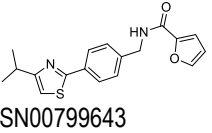
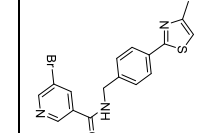
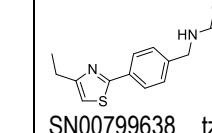
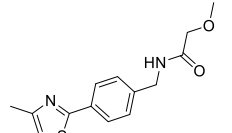
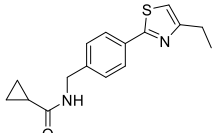
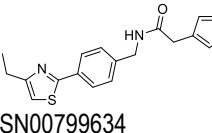
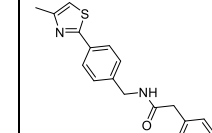
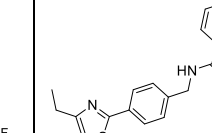
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SAR SUPPLEMENTARY INFORMATION

Table 1 Initial SAR of broadly related analogues to initial hit **SN00799639**

 SN00772011 py_misc inactive	 SN00794046 ttzc inactive	 SN00799618 tzc-het5 inactive	 SN00799623 tzc-het5 inactive	 SN00799624 tzc-het5 emol id: 32964923 inactive
 SN00799639 tzc-het5 emol id:33060302 original	 SN00799640 tzc-het5 inactive	 SN00799643 tzc-het5 inactive	 SN00799629 tzc_het6 inactive	 SN00799638 tzc_het6 inactive
 SN00799627 tzc_misc inactive	 SN00799636 tzc_misc inactive	 SN00799634 tzc_misc_bn inactive	 SN00799621 tzc_misc_bn inactive	 SN00799635 tzc_ph inactive

Sample Name: TGL-639-37

Compound 37

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Acq. Operator :
Acq. Instrument : 1260ANALYTICAL Location : P1-D-07
Injection Date : 16/10/2018 8:54:27 AM Inj Volume : 0.200 µl

Method : C:\CHEM32\1\METHODS\ROUTINE_PEAK PURITY GRAD METHOD#1.M
Last changed : 16/10/2018 8:53:51 AM
(modified after loading)

Method Info : Standard Peak Purity Gradient Method for Monash Agilent Analytical

Sample Info : Easy-Access Method: 'PP Gradient'

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Instrument Conditions	:	At Start	At Stop
Column Temp. (left)	:	35.0	35.0 °C
Column Temp. (right)	:	35.0	35.0 °C
Pressure	:	224.8	94.3 bar
Flow	:	1.000	1.000 ml/min

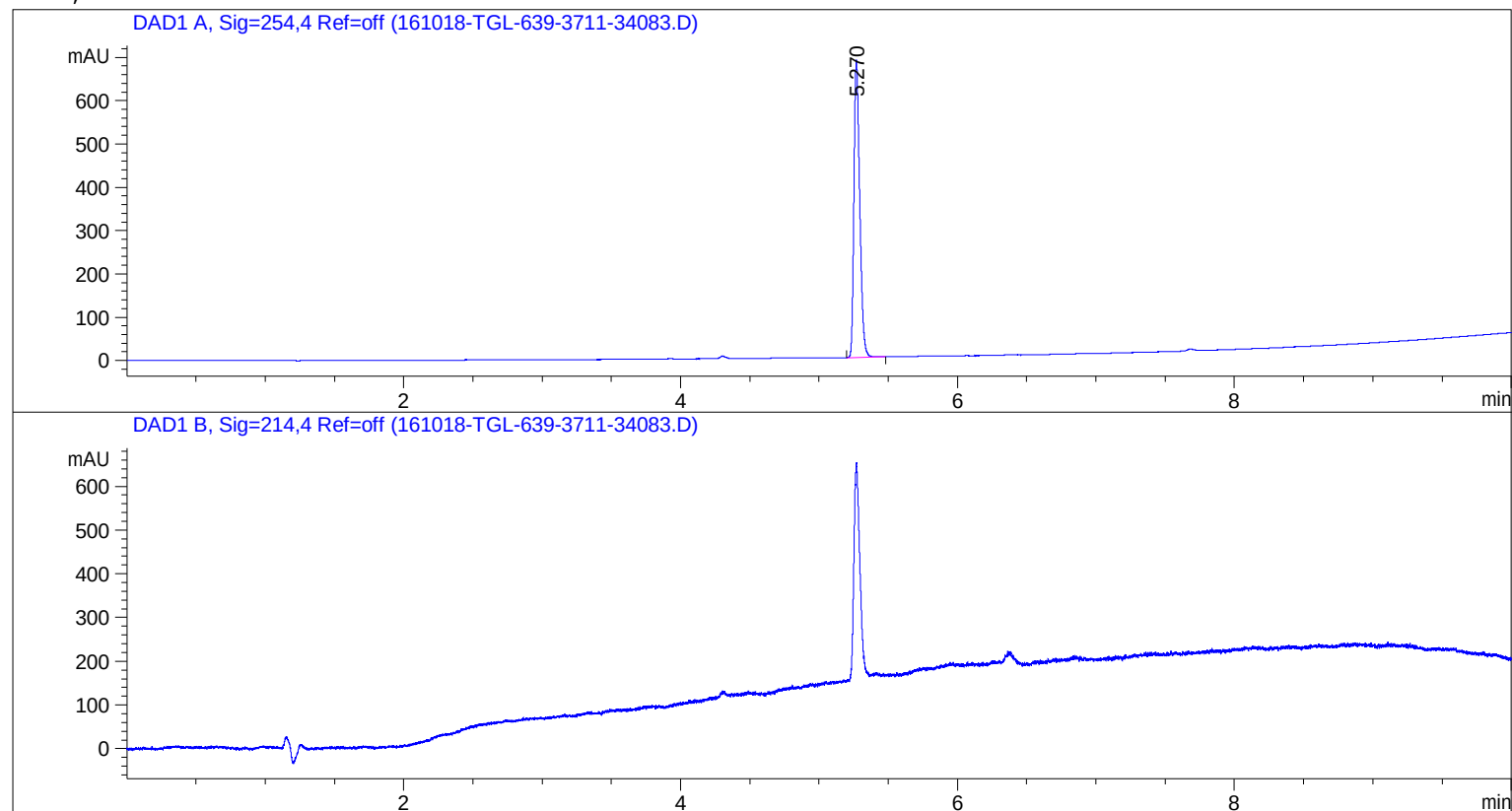
Detector Lamp Burn Times: Current On-Time Accumulated On-Time

DAD 1, UV Lamp	:	21.18	1490.1 h
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Solvent Description :

PMP1, Solvent A : Water 0.1% TFA

PMP1, Solvent B : ACN 0.1% TFA



Sample Name: TGL-639-37

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

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.270	BB	0.0433	1985.25818	685.61157	100.0000

Totals : 1985.25818 685.61157

Signal 2: DAD1 B, Sig=214,4 Ref=off

=====
Summed Peaks Report
=====

Signal 1: DAD1 A, Sig=254,4 Ref=off

Signal 2: DAD1 B, Sig=214,4 Ref=off

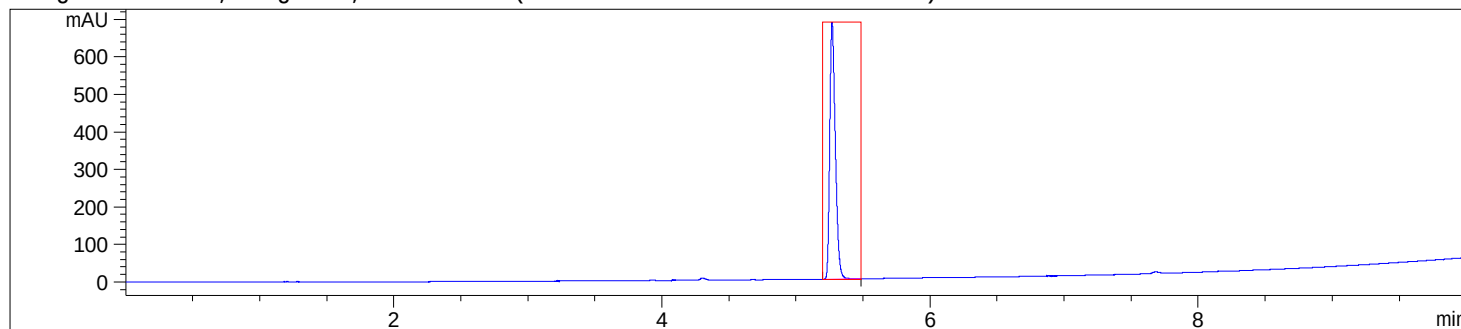
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Final Summed Peaks Report
=====

Signal 1: DAD1 A, Sig=254,4 Ref=off

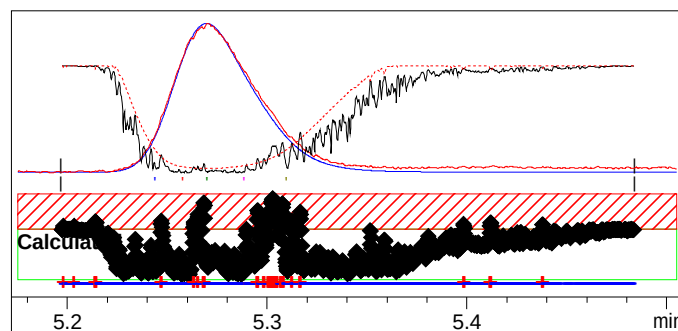
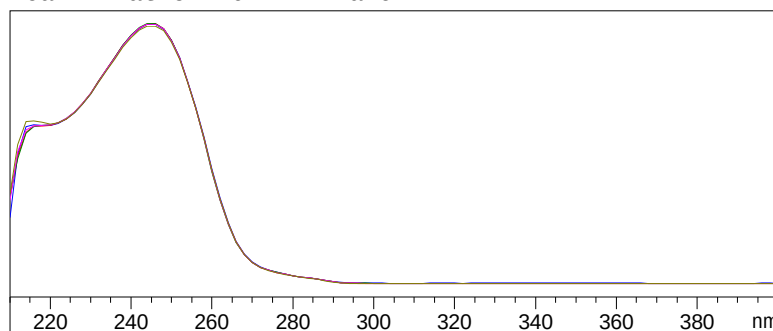
Signal 2: DAD1 B, Sig=214,4 Ref=off

Sample Name: TGL-639-37

Signal DAD1 A, Sig=254,4 Ref=off (161018-TGL-639-3711-34083.D)



Peak :1 at 5.270 min Name : ?



-> The purity factor exceeds the calculated threshold limit. <-

Purity factor : 755.129 (96 of 1333 spectra exceed the calculated threshold limit.)

Threshold : 776.345 (Calculated with 96 of 1333 spectra)

Reference : Peak start and end spectra (integrated) (5.197 / 5.484)

Spectra : 5 (Selection automatic, 5)

Noise Threshold: 3.212 (12 spectra, St.Dev 1.0403 + 3 * 0.724)

*** End of Report ***

Sample Name: TGL-639-38

Compound 38

=====

Acq. Operator :
Acq. Instrument : 1260ANALYTICAL Location : P2-A-08
Injection Date : 15/10/2018 5:48:45 PM Inj Volume : 2.000 µl

Method : C:\CHEM32\1\METHODS\ROUTINE_PEAK PURITY GRAD METHOD#1.M
Last changed : 15/10/2018 5:48:07 PM
(modified after loading)

Method Info : Standard Peak Purity Gradient Method for Monash Agilent Analytical

Sample Info : Easy-Access Method: 'PP Gradient'

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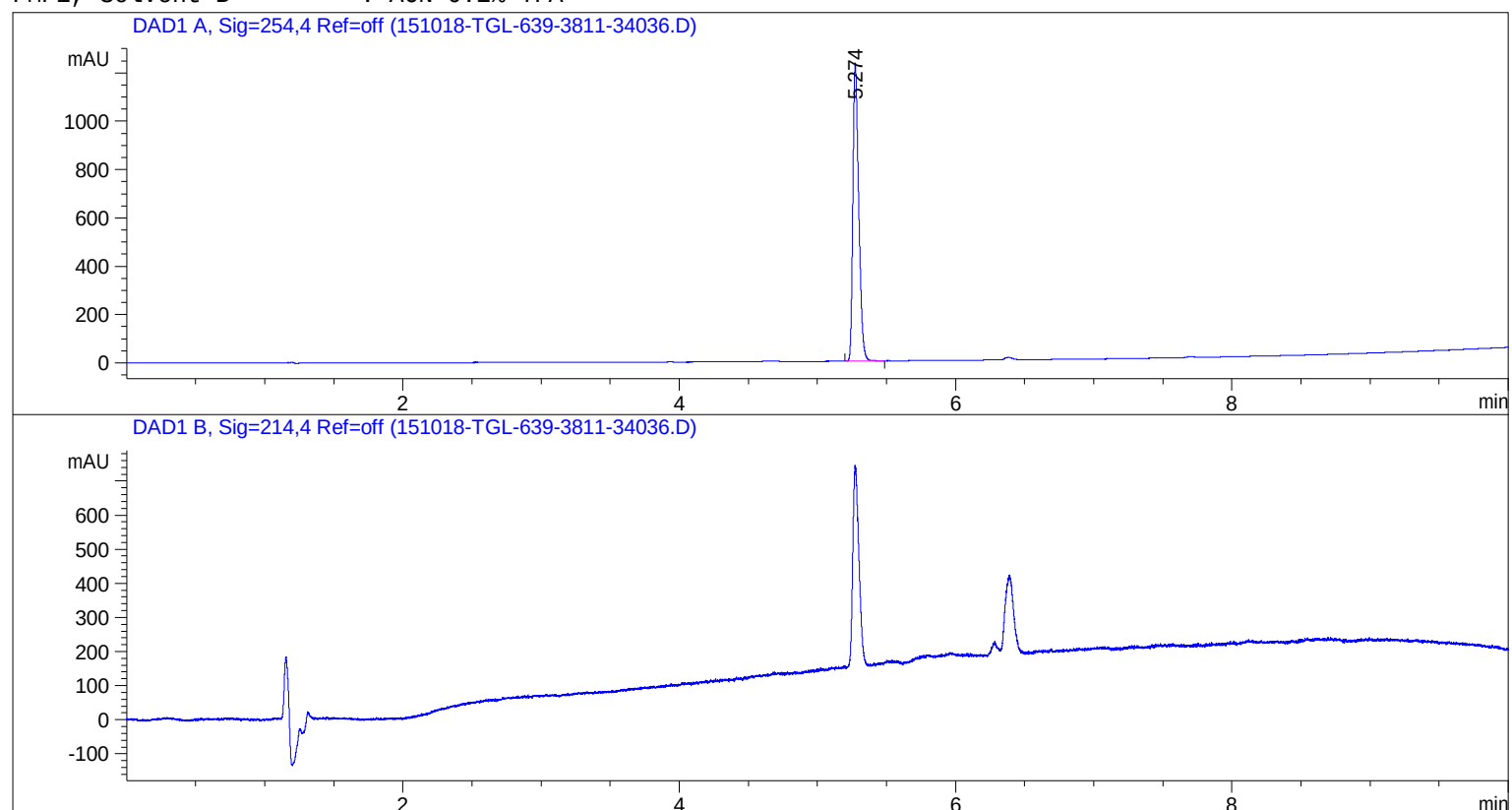
Instrument Conditions : At Start At Stop

Column Temp. (left)	: 35.0	35.0 °C
Column Temp. (right)	: 35.0	35.0 °C
Pressure	: 228.1	95.4 bar
Flow	: 1.000	1.000 ml/min

Detector Lamp Burn Times: Current On-Time Accumulated On-Time

DAD 1, UV Lamp	: 6.08	1475.0 h
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Solvent Description :
PMP1, Solvent A : Water 0.1% TFA
PMP1, Solvent B : ACN 0.1% TFA



Sample Name: TGL-639-38

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Area Percent Report
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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.274	BV	0.0444	3630.90063	1232.40955	100.0000

Totals : 3630.90063 1232.40955

Signal 2: DAD1 B, Sig=214,4 Ref=off

=====
Summed Peaks Report
=====

Signal 1: DAD1 A, Sig=254,4 Ref=off

Signal 2: DAD1 B, Sig=214,4 Ref=off

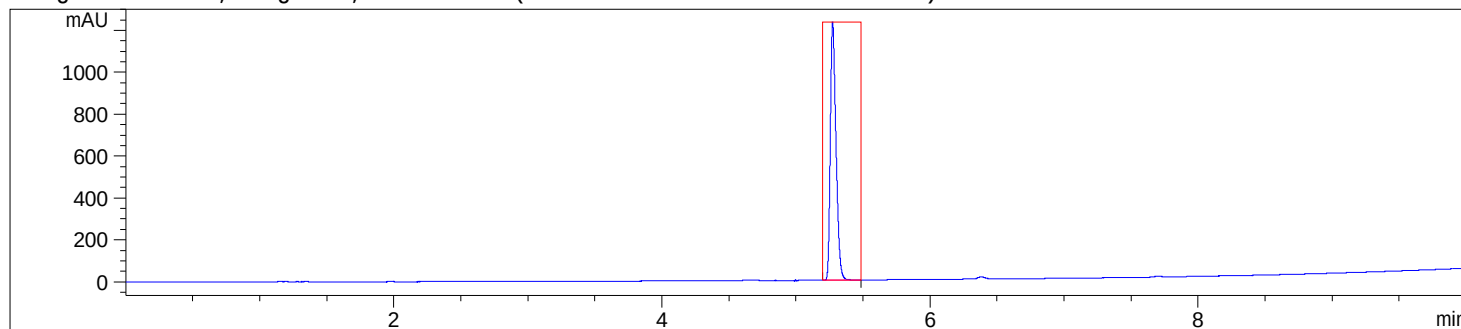
=====
Final Summed Peaks Report
=====

Signal 1: DAD1 A, Sig=254,4 Ref=off

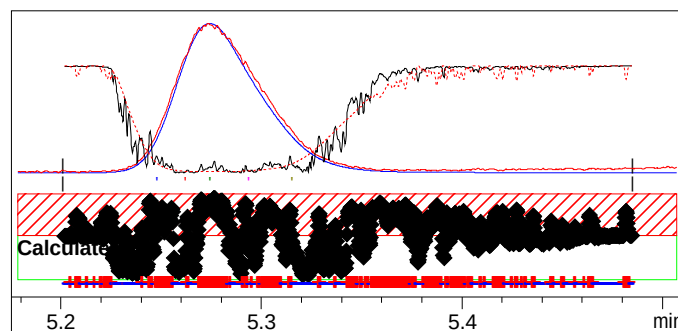
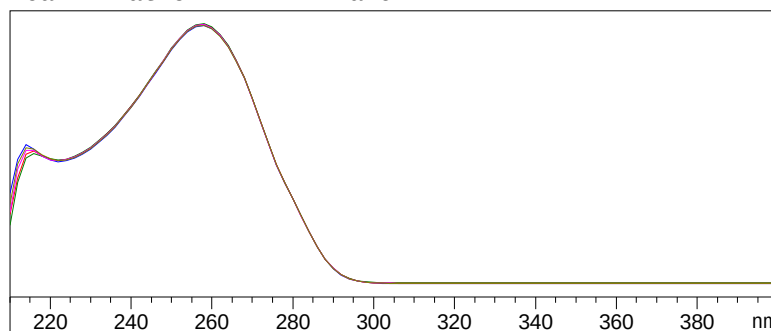
Signal 2: DAD1 B, Sig=214,4 Ref=off

Sample Name: TGL-639-38

Signal DAD1 A, Sig=254,4 Ref=off (151018-TGL-639-3811-34036.D)



Peak :1 at 5.274 min Name : ?



-> The purity factor exceeds the calculated threshold limit. <-

Purity factor : 514.476 (652 of 1337 spectra exceed the calculated threshold limit.)

Threshold : 685.643 (Calculated with 652 of 1337 spectra)

Reference : Peak start and end spectra (integrated) (5.201 / 5.485)

Spectra : 5 (Selection automatic, 5)

Noise Threshold: 2.203 (12 spectra, St.Dev 0.911 + 3 * 0.4306)

Warning : Spectral absorbances > 1000 mAU (see help for more information)

*** End of Report ***

Sample Name: TGL-639-54

Compound 54

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Acq. Operator :
Acq. Instrument : 1260ANALYTICAL Location : P1-D-05
Injection Date : 16/10/2018 9:26:10 AM Inj Volume : 0.200 µl

Method : C:\CHEM32\1\METHODS\ROUTINE_PEAK PURITY GRAD METHOD#1.M
Last changed : 16/10/2018 9:25:34 AM
(modified after loading)

Method Info : Standard Peak Purity Gradient Method for Monash Agilent Analytical

Sample Info : Easy-Access Method: 'PP Gradient'

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Instrument Conditions	At Start	At Stop
Column Temp. (left)	35.0	35.0 °C
Column Temp. (right)	35.0	35.0 °C
Pressure	224.1	93.9 bar
Flow	1.000	1.000 ml/min

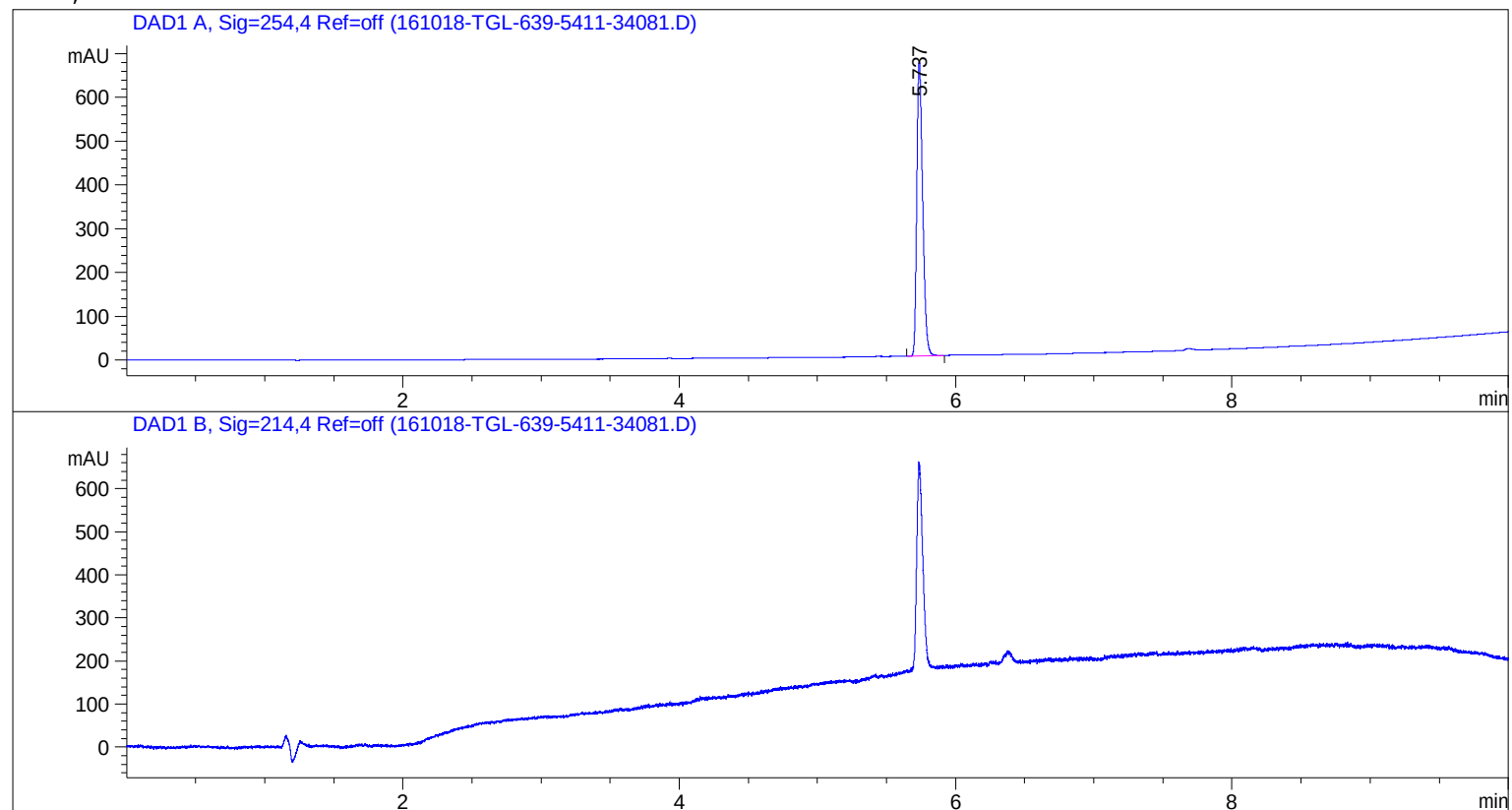
Detector Lamp Burn Times: Current On-Time Accumulated On-Time

DAD 1, UV Lamp	21.71	1490.6 h
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Solvent Description :

PMP1, Solvent A : Water 0.1% TFA

PMP1, Solvent B : ACN 0.1% TFA



Sample Name: TGL-639-54

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Area Percent Report
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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.737	BV	0.0443	1985.63513	675.32037	100.0000

Totals : 1985.63513 675.32037

Signal 2: DAD1 B, Sig=214,4 Ref=off

=====
Summed Peaks Report
=====

Signal 1: DAD1 A, Sig=254,4 Ref=off

Signal 2: DAD1 B, Sig=214,4 Ref=off

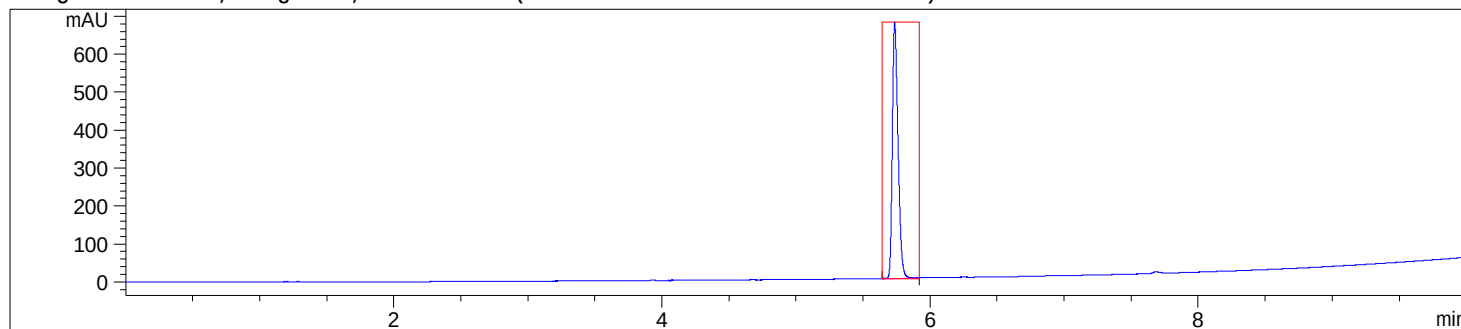
=====
Final Summed Peaks Report
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Signal 1: DAD1 A, Sig=254,4 Ref=off

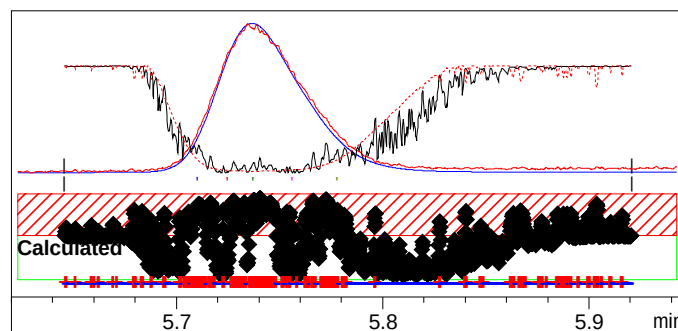
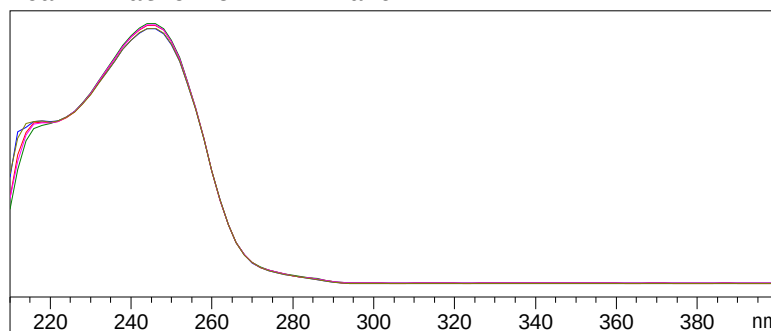
Signal 2: DAD1 B, Sig=214,4 Ref=off

Sample Name: TGL-639-54

Signal DAD1 A, Sig=254,4 Ref=off (161018-TGL-639-5411-34081.D)



Peak :1 at 5.737 min Name : ?



-> The purity factor exceeds the calculated threshold limit. <-

Purity factor : 633.423 (468 of 1216 spectra exceed the calculated threshold limit.)

Threshold : 739.268 (Calculated with 468 of 1216 spectra)

Reference : Peak start and end spectra (integrated) (5.645 / 5.921)

Spectra : 5 (Selection automatic, 5)

Noise Threshold: 1.854 (12 spectra, St.Dev 0.7872 + 3 * 0.3555)

*** End of Report ***

Sample Name: TGL-639-55

Compound 55

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Acq. Operator :
Acq. Instrument : 1260ANALYTICAL Location : P2-B-04
Injection Date : 15/10/2018 7:08:16 PM Inj Volume : 2.000 µl

Method : C:\CHEM32\1\METHODS\ROUTINE_PEAK PURITY GRAD METHOD#1.M
Last changed : 15/10/2018 7:07:37 PM
(modified after loading)

Method Info : Standard Peak Purity Gradient Method for Monash Agilent Analytical

Sample Info : Easy-Access Method: 'PP Gradient'

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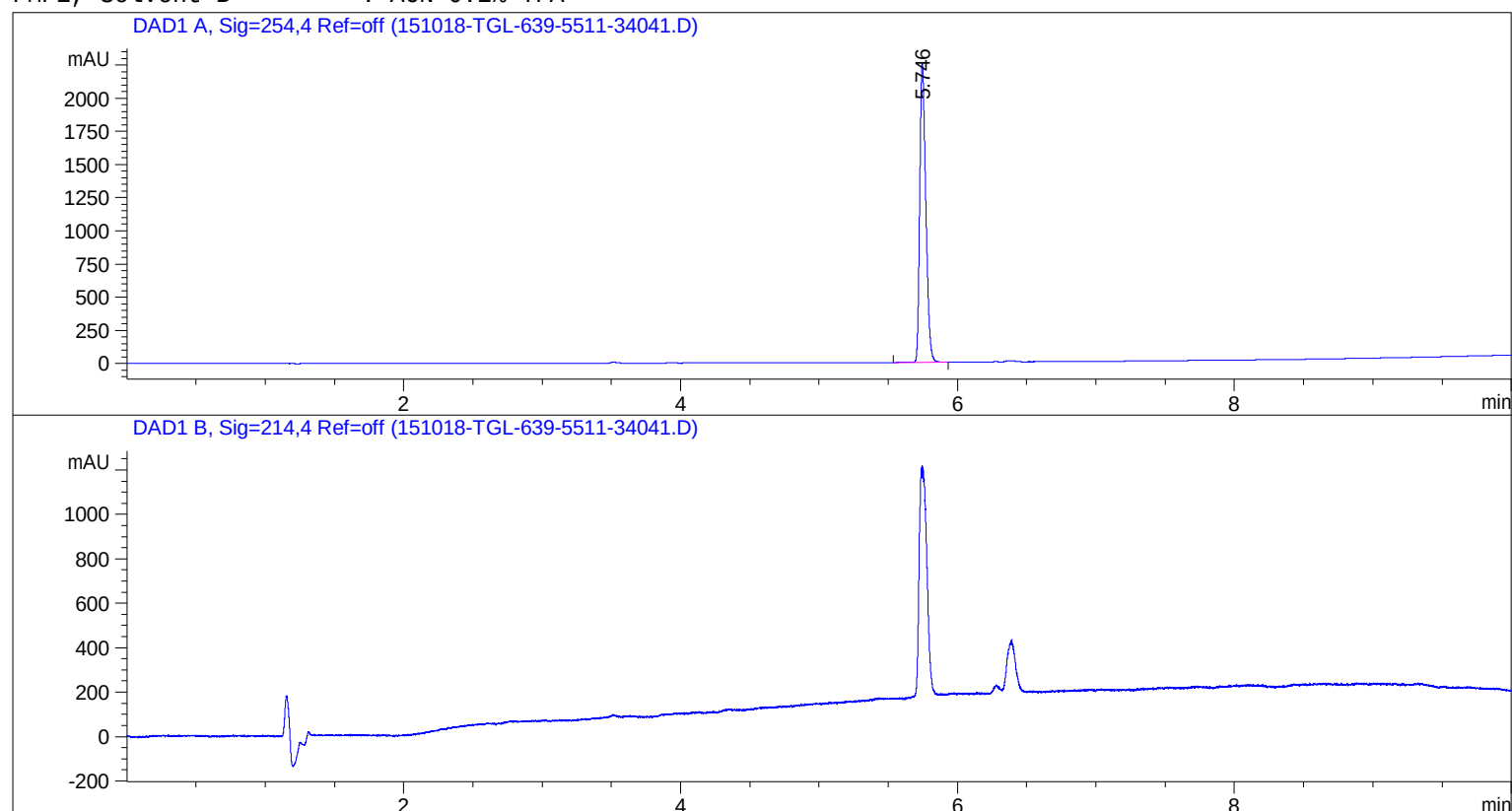
Instrument Conditions : At Start At Stop

Column Temp. (left)	: 35.0	35.0 °C
Column Temp. (right)	: 35.0	35.0 °C
Pressure	: 225.8	95.4 bar
Flow	: 1.000	1.000 ml/min

Detector Lamp Burn Times: Current On-Time Accumulated On-Time

DAD 1, UV Lamp	: 7.41	1476.3 h
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Solvent Description :
PMP1, Solvent A : Water 0.1% TFA
PMP1, Solvent B : ACN 0.1% TFA



Sample Name: TGL-639-55

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Area Percent Report
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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.746	BV	0.0460	6859.01660	2251.33667	100.0000

Totals : 6859.01660 2251.33667

Signal 2: DAD1 B, Sig=214,4 Ref=off

=====
Summed Peaks Report
=====

Signal 1: DAD1 A, Sig=254,4 Ref=off

Signal 2: DAD1 B, Sig=214,4 Ref=off

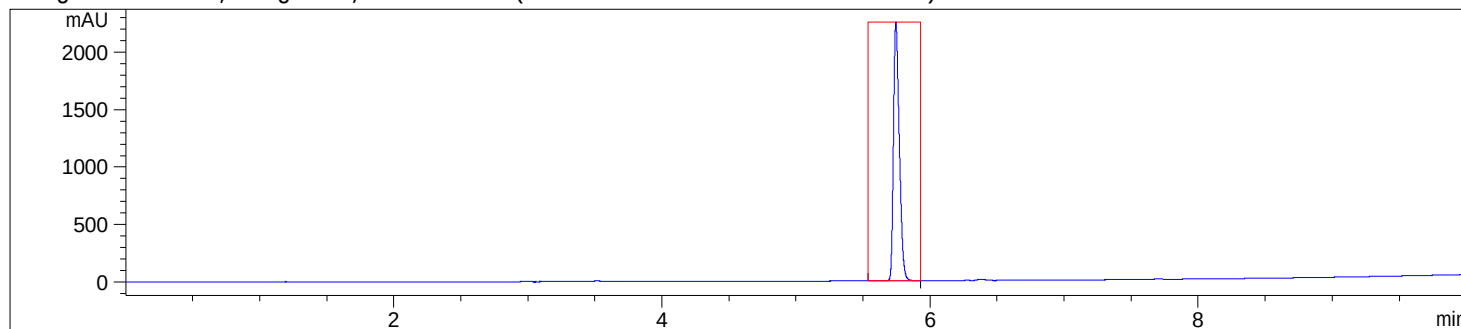
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Final Summed Peaks Report
=====

Signal 1: DAD1 A, Sig=254,4 Ref=off

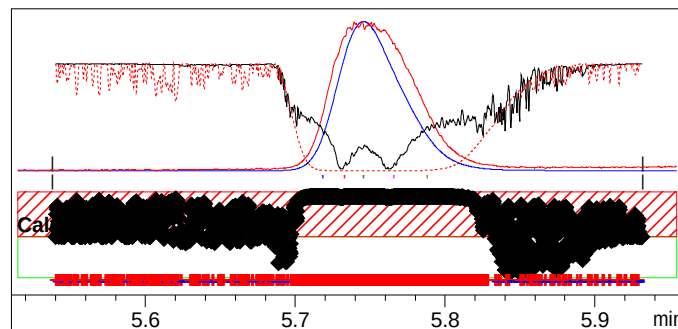
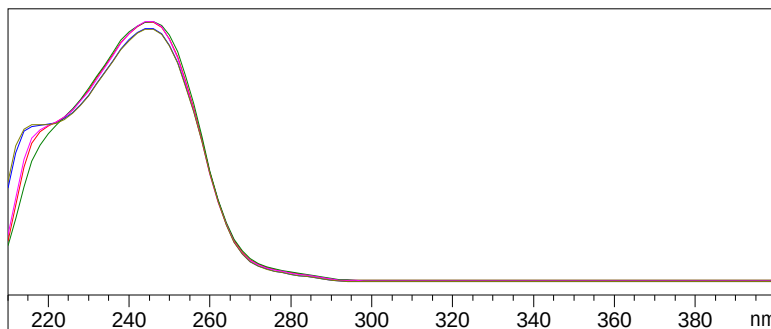
Signal 2: DAD1 B, Sig=214,4 Ref=off

Sample Name: TGL-639-55

Signal DAD1 A, Sig=254,4 Ref=off (151018-TGL-639-5511-34041.D)



Peak :1 at 5.746 min Name : ?



-> The purity factor exceeds the calculated threshold limit. <-

Purity factor : 526.894 (1388 of 1732 spectra exceed the calculated threshold limit.)

Threshold : 757.203 (Calculated with 1388 of 1732 spectra)

Reference : Peak start and end spectra (integrated) (5.538 / 5.932)

Spectra : 5 (Selection automatic, 5)

Noise Threshold: 1.017 (12 spectra, St.Dev 0.4493 + 3 * 0.1892)

Warning : Spectral absorbances > 1000 mAU (see help for more information)

*** End of Report ***

Sample Name: TGL-639-56

Compound 56

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Acq. Operator :
Acq. Instrument : 1260ANALYTICAL Location : P2-B-05
Injection Date : 15/10/2018 7:24:09 PM Inj Volume : 2.000 µl

Method : C:\CHEM32\1\METHODS\ROUTINE_PEAK PURITY GRAD METHOD#1.M
Last changed : 15/10/2018 7:23:31 PM
(modified after loading)

Method Info : Standard Peak Purity Gradient Method for Monash Agilent Analytical

Sample Info : Easy-Access Method: 'PP Gradient'

=====

Instrument Conditions	At Start	At Stop
Column Temp. (left)	35.0	35.0 °C
Column Temp. (right)	35.0	35.0 °C
Pressure	225.8	95.0 bar
Flow	1.000	1.000 ml/min

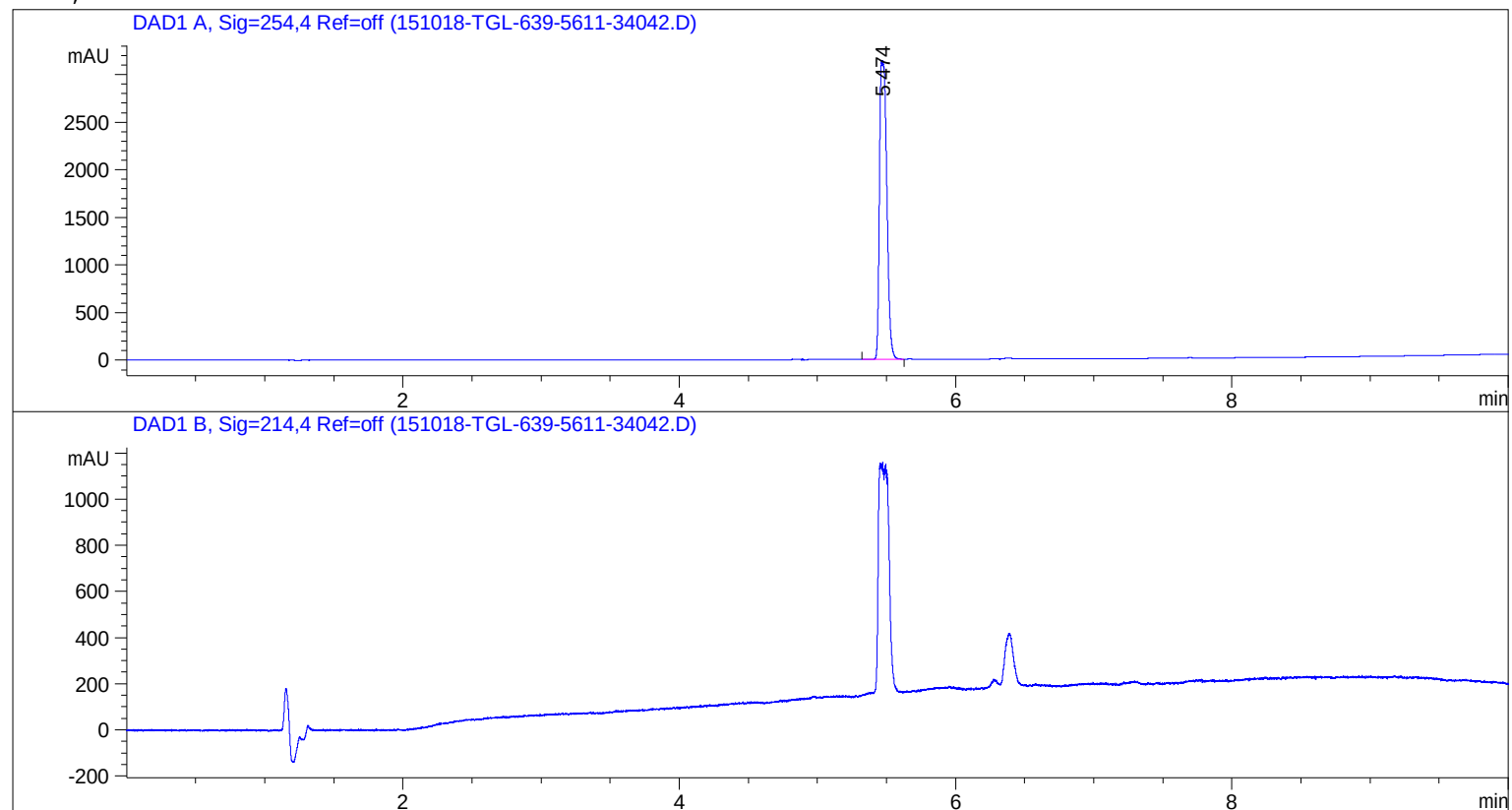
Detector Lamp Burn Times: Current On-Time Accumulated On-Time

DAD 1, UV Lamp	7.67	1476.5 h
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Solvent Description :

PMP1, Solvent A : Water 0.1% TFA

PMP1, Solvent B : ACN 0.1% TFA



Sample Name: TGL-639-56

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Area Percent Report
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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.474	VV	0.0449	1.15159e4	3133.66968	100.0000

Totals : 1.15159e4 3133.66968

Signal 2: DAD1 B, Sig=214,4 Ref=off

=====
Summed Peaks Report
=====

Signal 1: DAD1 A, Sig=254,4 Ref=off

Signal 2: DAD1 B, Sig=214,4 Ref=off

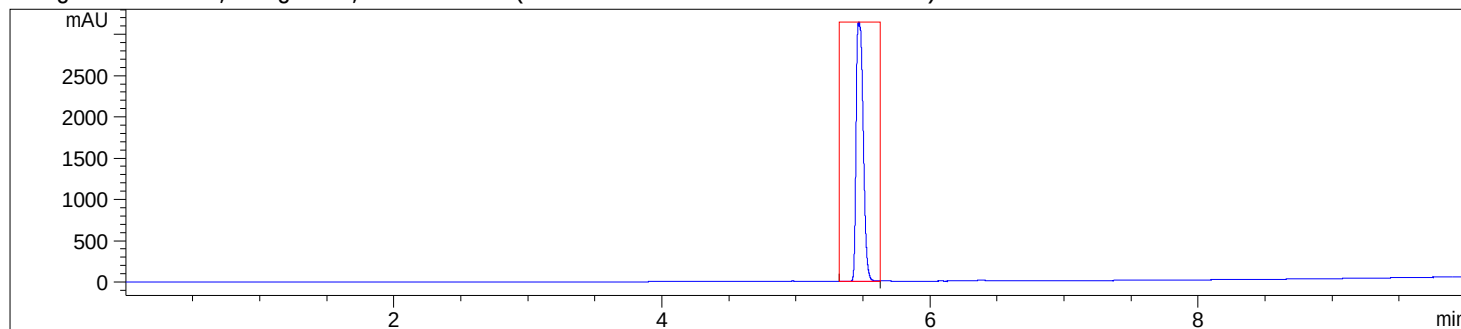
=====
Final Summed Peaks Report
=====

Signal 1: DAD1 A, Sig=254,4 Ref=off

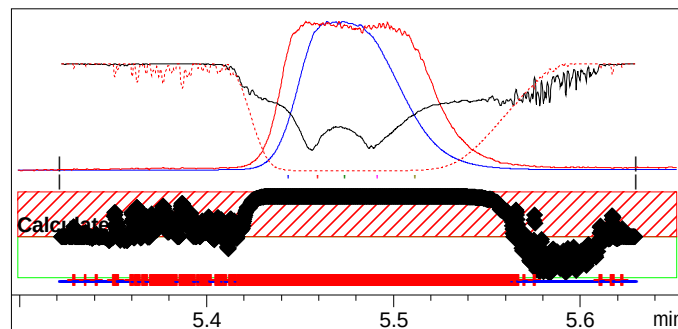
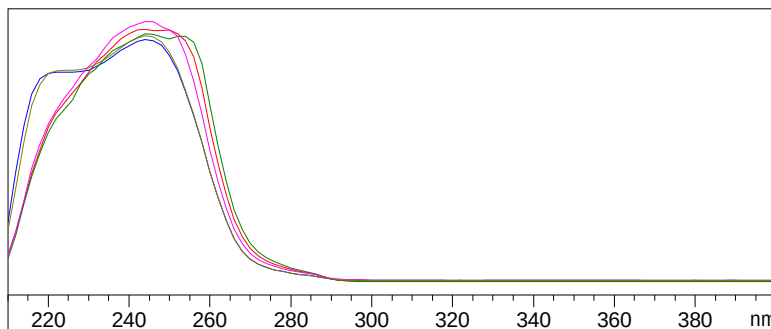
Signal 2: DAD1 B, Sig=214,4 Ref=off

Sample Name: TGL-639-56

Signal DAD1 A, Sig=254,4 Ref=off (151018-TGL-639-5611-34042.D)



Peak :1 at 5.474 min Name : ?



-> The purity factor exceeds the calculated threshold limit. <-

Purity factor : 701.367 (997 of 1433 spectra exceed the calculated threshold limit.)

Threshold : 818.124 (Calculated with 997 of 1433 spectra)

Reference : Peak start and end spectra (integrated) (5.321 / 5.630)

Spectra : 5 (Selection automatic, 5)

Noise Threshold: 2.405 (12 spectra, St.Dev 0.6937 + 3 * 0.5705)

Warning : Spectral absorbances > 1000 mAU (see help for more information)

*** End of Report ***

Sample Name: TGL-639-57

Compound 57

=====

Acq. Operator :
Acq. Instrument : 1260ANALYTICAL Location : P1-D-06
Injection Date : 16/10/2018 9:10:19 AM Inj Volume : 0.200 µl

Method : C:\CHEM32\1\METHODS\ROUTINE_PEAK PURITY GRAD METHOD#1.M
Last changed : 16/10/2018 9:09:42 AM
(modified after loading)

Method Info : Standard Peak Purity Gradient Method for Monash Agilent Analytical

Sample Info : Easy-Access Method: 'PP Gradient'

=====

Instrument Conditions	At Start	At Stop
Column Temp. (left)	35.0	35.0 °C
Column Temp. (right)	35.0	35.0 °C
Pressure	224.2	93.9 bar
Flow	1.000	1.000 ml/min

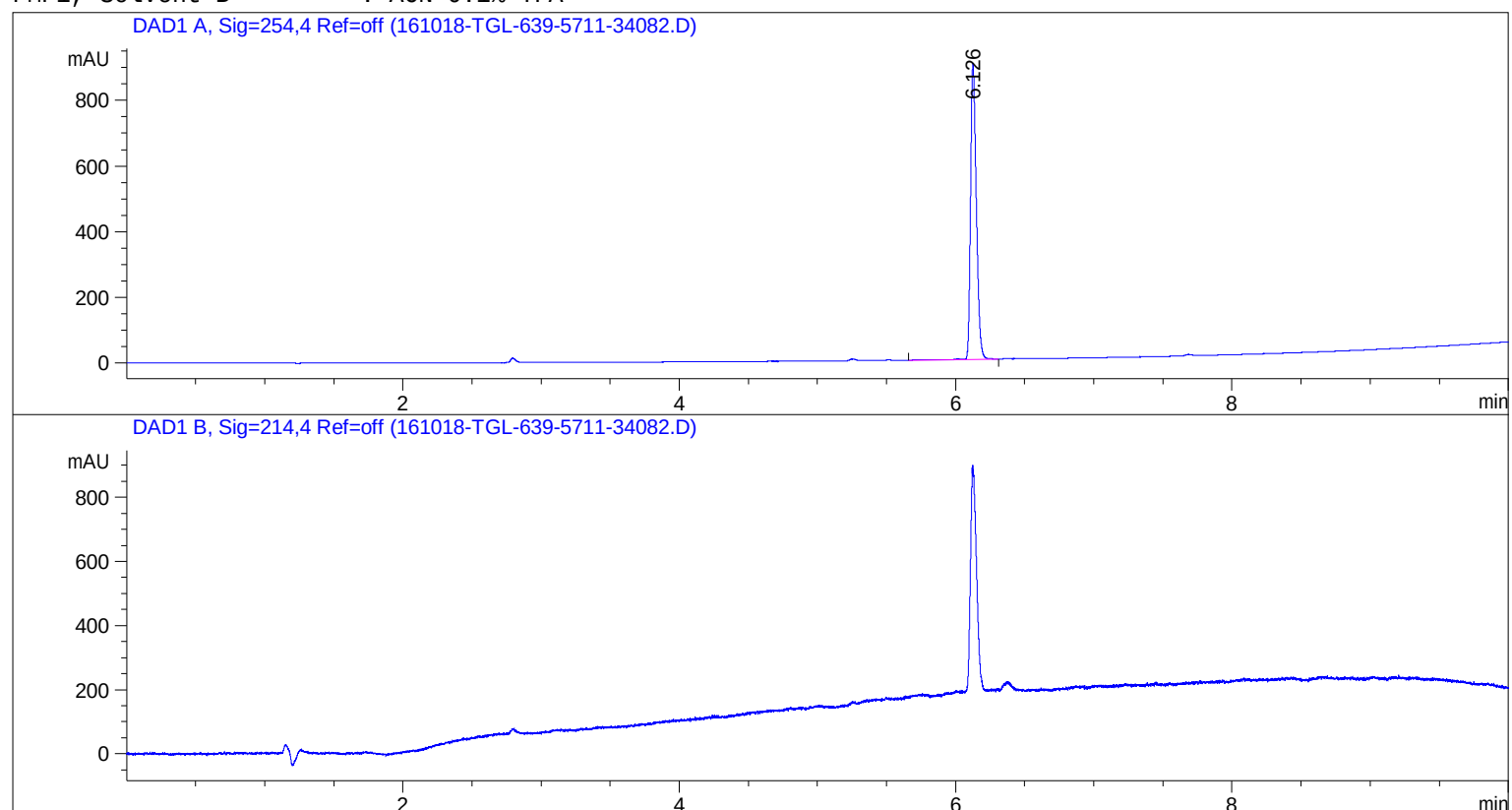
Detector Lamp Burn Times: Current On-Time Accumulated On-Time

DAD 1, UV Lamp	21.44	1490.3 h
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Solvent Description :

PMP1, Solvent A : Water 0.1% TFA

PMP1, Solvent B : ACN 0.1% TFA



Sample Name: TGL-639-57

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

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.126	BV	0.0438	2615.44897	901.48932	100.0000

Totals : 2615.44897 901.48932

Signal 2: DAD1 B, Sig=214,4 Ref=off

=====
Summed Peaks Report
=====

Signal 1: DAD1 A, Sig=254,4 Ref=off

Signal 2: DAD1 B, Sig=214,4 Ref=off

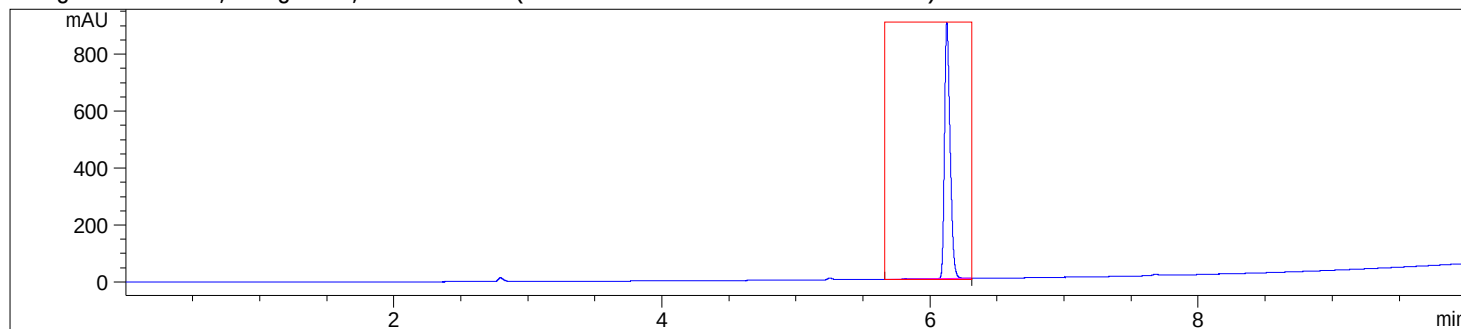
=====
Final Summed Peaks Report
=====

Signal 1: DAD1 A, Sig=254,4 Ref=off

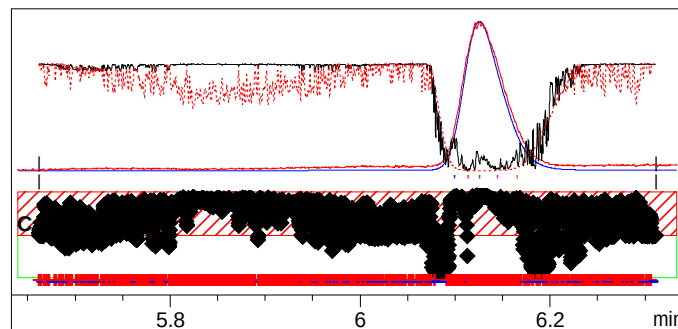
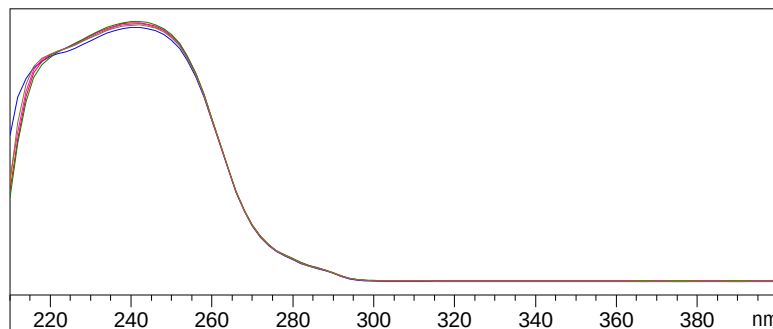
Signal 2: DAD1 B, Sig=214,4 Ref=off

Sample Name: TGL-639-57

Signal DAD1 A, Sig=254,4 Ref=off (161018-TGL-639-5711-34082.D)



Peak :1 at 6.126 min Name : ?



-> The purity factor exceeds the calculated threshold limit. <-

Purity factor : 250.786 (2421 of 2938 spectra exceed the calculated threshold limit.)

Threshold : 724.381 (Calculated with 2421 of 2938 spectra)

Reference : Peak start and end spectra (integrated) (5.662 / 6.312)

Spectra : 5 (Selection automatic, 5)

Noise Threshold: 1.136 (12 spectra, St.Dev 0.5253 + 3 * 0.2035)

Warning : Spectral absorbances > 1000 mAU (see help for more information)

*** End of Report ***

Sample Name: TGL-639-60

Compound 60

=====

Acq. Operator :
Acq. Instrument : 1260ANALYTICAL Location : P2-B-09
Injection Date : 15/10/2018 8:27:41 PM Inj Volume : 2.000 µl

Acq. Method : C:\CHEM32\1\METHODS\ROUTINE_PEAK PURITY GRAD METHOD#1.M
Last changed : 15/10/2018 8:27:03 PM
(modified after loading)

Analysis Method : C:\CHEM32\1\METHODS\ROUTINE_PEAK PURITY GRAD METHOD#1.M
Last changed : 23/06/2014 10:41:01 AM

Method Info : Standard Peak Purity Gradient Method for Monash Agilent Analytical

Sample Info : Easy-Access Method: 'PP Gradient'

Additional Info : Peak(s) manually integrated

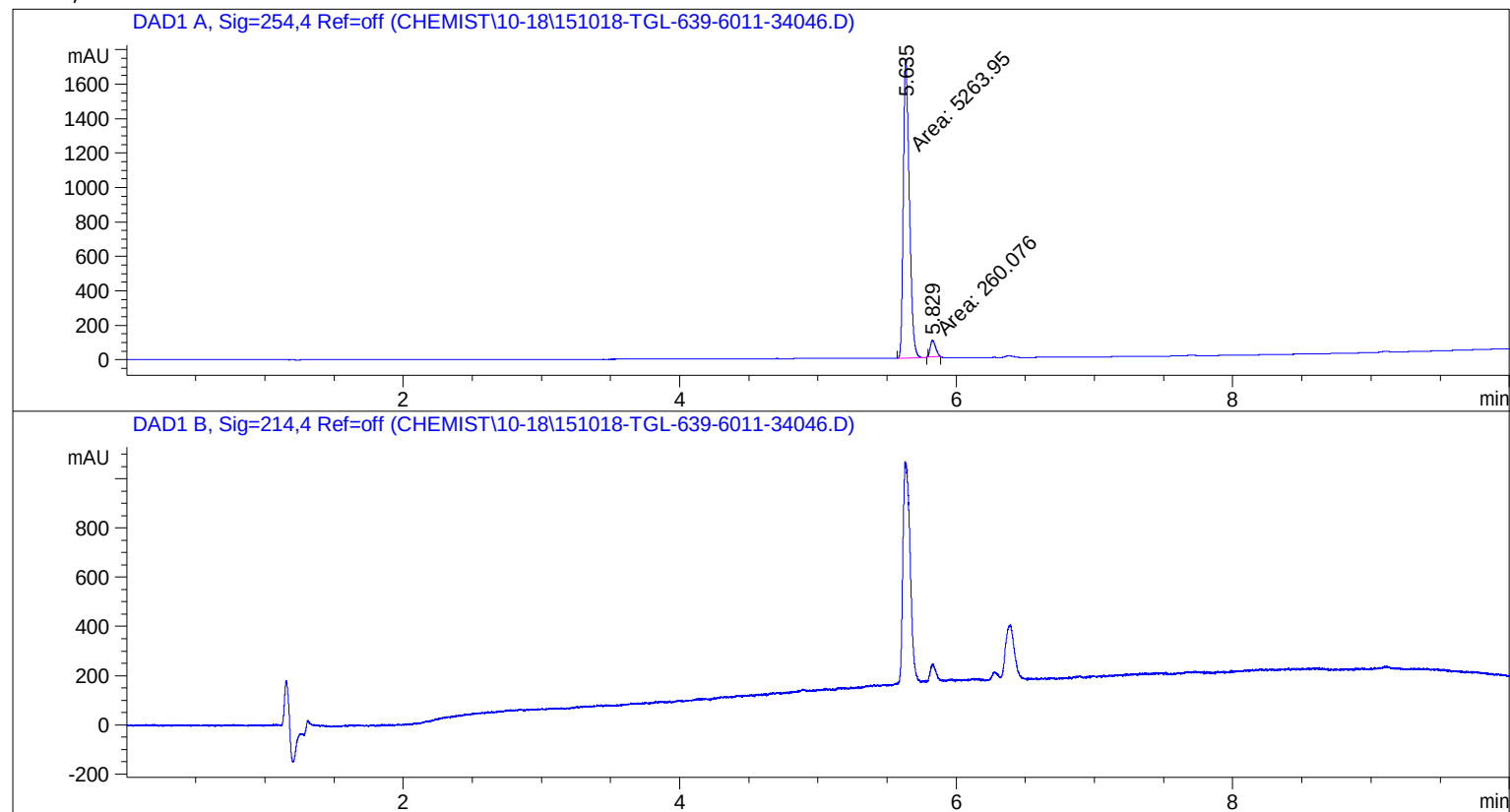
=====

Instrument Conditions	At Start	At Stop
Column Temp. (left)	35.0	35.0 °C
Column Temp. (right)	35.0	35.0 °C
Pressure	226.1	95.2 bar
Flow	1.000	1.000 ml/min

Detector Lamp Burn Times: Current On-Time Accumulated On-Time

DAD 1, UV Lamp	8.73	1477.6 h
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Solvent Description :
PMP1, Solvent A : Water 0.1% TFA
PMP1, Solvent B : ACN 0.1% TFA



Sample Name: TGL-639-60

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

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.635	MM	0.0506	5263.94971	1733.16821	95.2919
2	5.829	MM	0.0452	260.07559	95.81357	4.7081

Totals : 5524.02530 1828.98178

Signal 2: DAD1 B, Sig=214,4 Ref=off

=====
Summed Peaks Report
=====

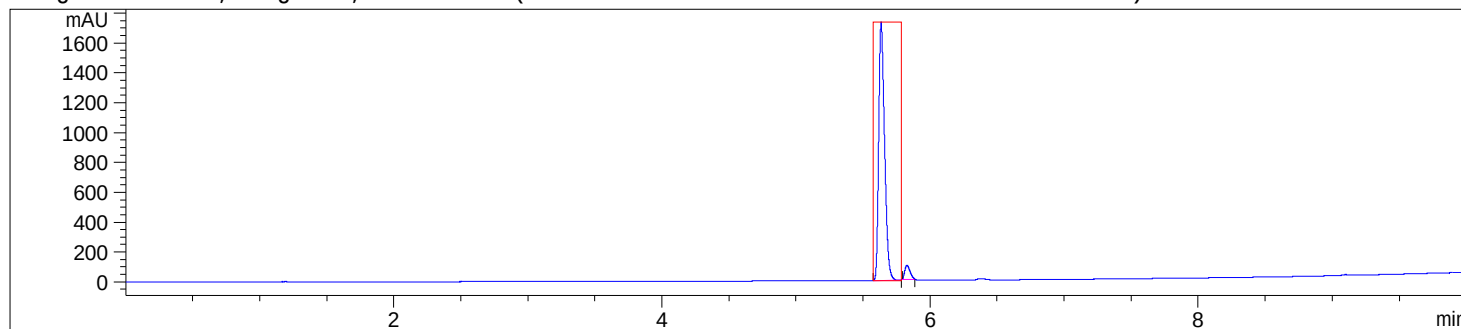
Signal 1: DAD1 A, Sig=254,4 Ref=off
Signal 2: DAD1 B, Sig=214,4 Ref=off

=====
Final Summed Peaks Report
=====

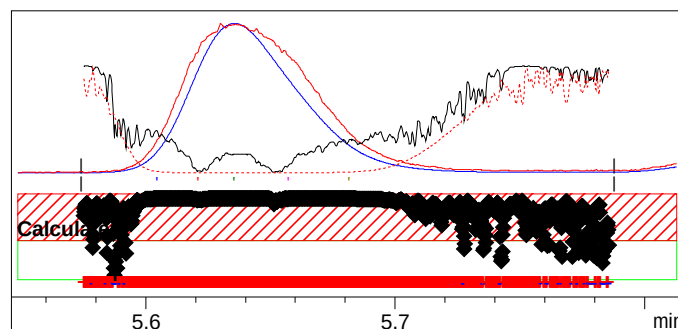
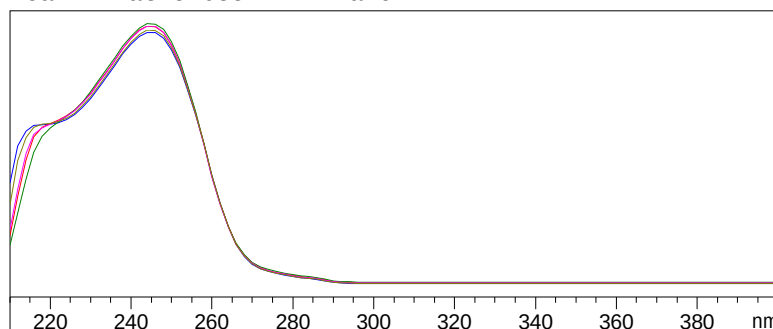
Signal 1: DAD1 A, Sig=254,4 Ref=off
Signal 2: DAD1 B, Sig=214,4 Ref=off

Sample Name: TGL-639-60

Signal DAD1 A, Sig=254,4 Ref=off (CHEMIST\10-18\151018-TGL-639-6011-34046.D)



Peak :1 at 5.635 min Name : ?



-> The purity factor exceeds the calculated threshold limit. <-

Purity factor : 791.139 (938 of 991 spectra exceed the calculated threshold limit.)

Threshold : 934.496 (Calculated with 938 of 991 spectra)

Reference : Peak start and end spectra (integrated) (5.574 / 5.788)

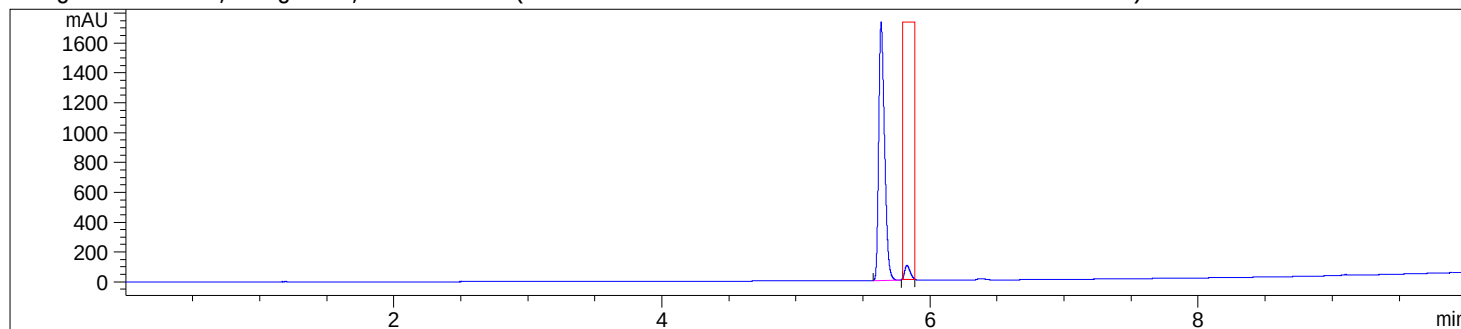
Spectra : 5 (Selection automatic, 5)

Noise Threshold: 0.721 (12 spectra, St.Dev 0.297 + 3 * 0.1415)

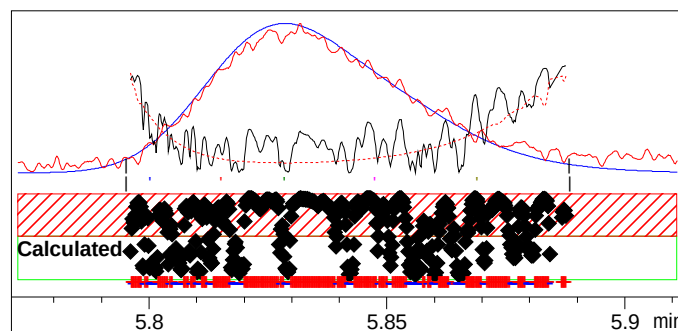
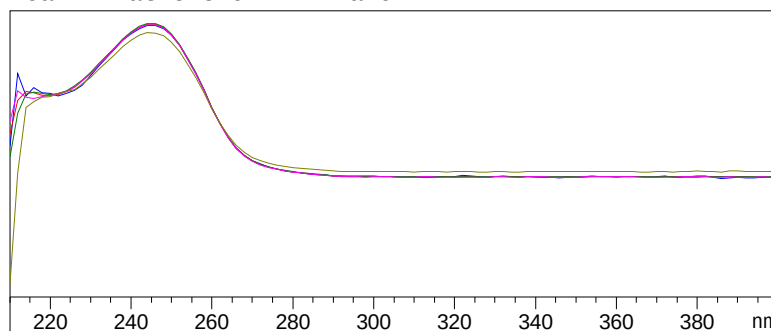
Warning : Spectral absorbances > 1000 mAU (see help for more information)

Sample Name: TGL-639-60

Signal DAD1 A, Sig=254,4 Ref=off (CHEMIST\10-18\151018-TGL-639-6011-34046.D)



Peak :2 at 5.829 min Name : ?



-> The purity factor exceeds the calculated threshold limit. <-

Purity factor : 917.496 (283 of 429 spectra exceed the calculated threshold limit.)

Threshold : 975.473 (Calculated with 283 of 429 spectra)

Reference : Peak start and end spectra (integrated) (5.795 / 5.888)

Spectra : 5 (Selection automatic, 5)

Noise Threshold: 0.721 (12 spectra, St.Dev 0.297 + 3 * 0.1415)

*** End of Report ***

Sample Name: TGL-639-63

Compound 63

=====

Acq. Operator :
Acq. Instrument : 1260ANALYTICAL Location : P2-C-02
Injection Date : 15/10/2018 8:59:29 PM Inj Volume : 2.000 µl

Method : C:\CHEM32\1\METHODS\ROUTINE_PEAK PURITY GRAD METHOD#1.M
Last changed : 15/10/2018 8:58:51 PM
(modified after loading)

Method Info : Standard Peak Purity Gradient Method for Monash Agilent Analytical

Sample Info : Easy-Access Method: 'PP Gradient'

=====

Instrument Conditions : At Start At Stop

Column Temp. (left)	: 35.0	35.0 °C
Column Temp. (right)	: 35.0	35.0 °C
Pressure	: 225.6	95.0 bar
Flow	: 1.000	1.000 ml/min

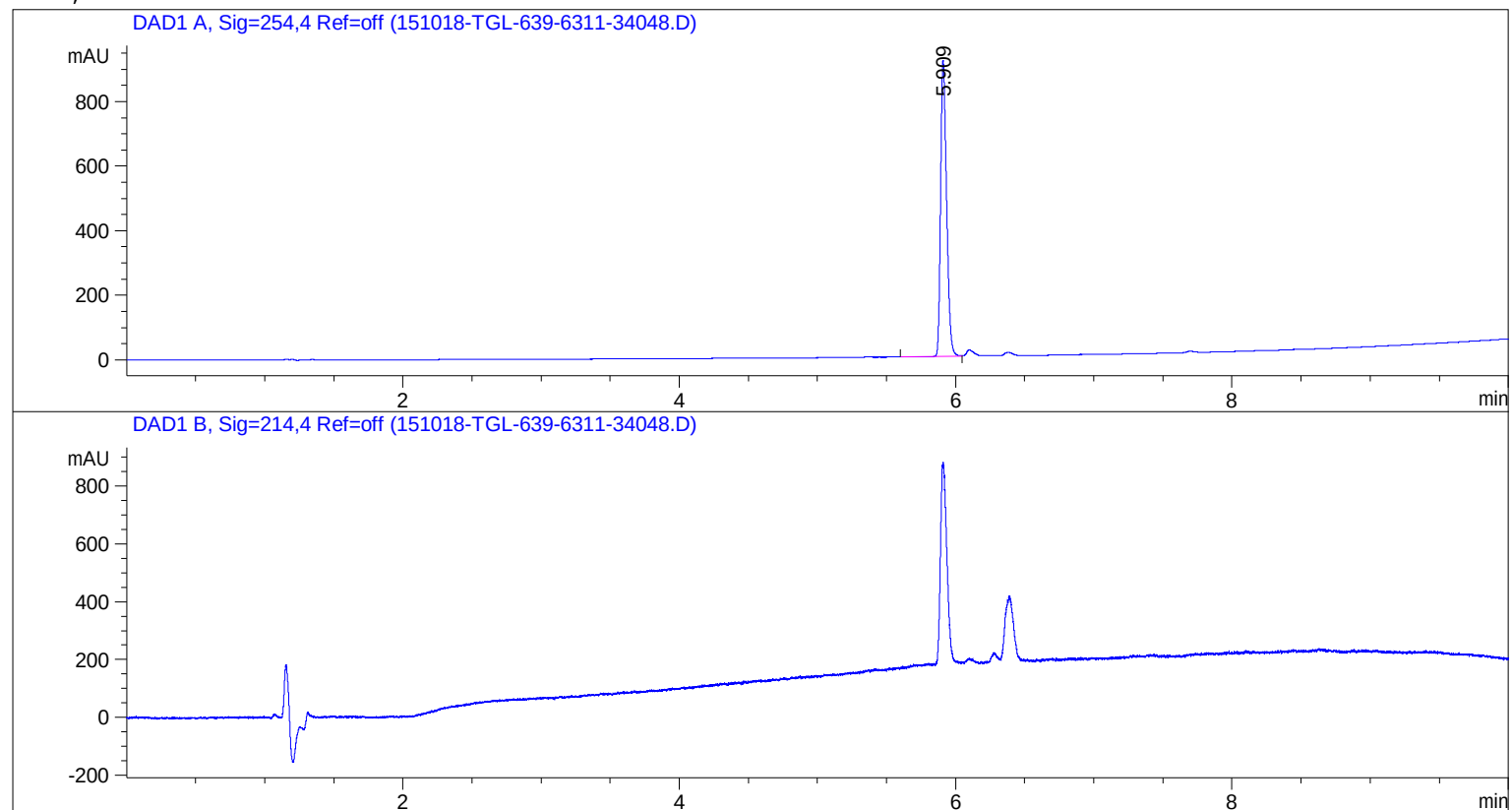
Detector Lamp Burn Times: Current On-Time Accumulated On-Time

DAD 1, UV Lamp	: 9.26	1478.1 h
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Solvent Description :

PMP1, Solvent A : Water 0.1% TFA

PMP1, Solvent B : ACN 0.1% TFA



Sample Name: TGL-639-63

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

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.909	BV	0.0456	2760.50684	917.19354	100.0000

Totals : 2760.50684 917.19354

Signal 2: DAD1 B, Sig=214,4 Ref=off

=====
Summed Peaks Report
=====

Signal 1: DAD1 A, Sig=254,4 Ref=off

Signal 2: DAD1 B, Sig=214,4 Ref=off

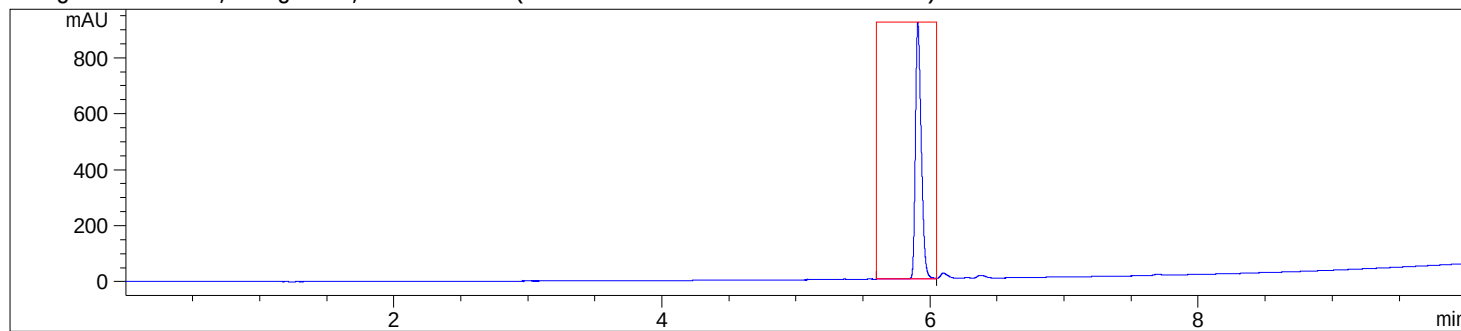
=====
Final Summed Peaks Report
=====

Signal 1: DAD1 A, Sig=254,4 Ref=off

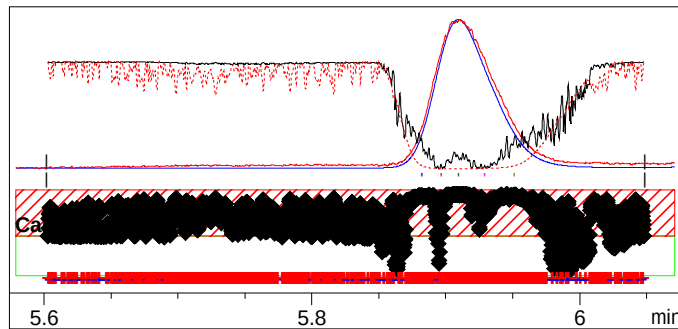
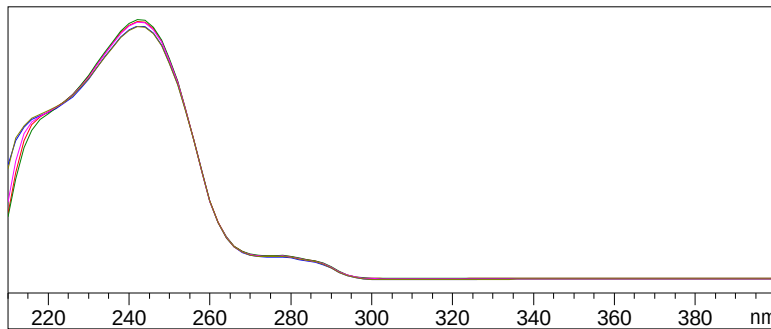
Signal 2: DAD1 B, Sig=214,4 Ref=off

Sample Name: TGL-639-63

Signal DAD1 A, Sig=254,4 Ref=off (151018-TGL-639-6311-34048.D)



Peak :1 at 5.909 min Name : ?



-> The purity factor exceeds the calculated threshold limit. <-

Purity factor : 375.234 (1758 of 2054 spectra exceed the calculated threshold limit.)

Threshold : 668.947 (Calculated with 1758 of 2054 spectra)

Reference : Peak start and end spectra (integrated) (5.602 / 6.048)

Spectra : 5 (Selection automatic, 5)

Noise Threshold: 1.179 (12 spectra, St.Dev 0.4087 + 3 * 0.2567)

Warning : Spectral absorbances > 1000 mAU (see help for more information)

*** End of Report ***