

Supporting Information

Design, Synthesis, and Biological Evaluation of *N*-Carboxyphenylpyrrole Derivatives as Potent HIV Fusion Inhibitors Targeting gp41

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Elemental Analysis Data

Compounds #	Formula	Calculation			Found		
		C	H	N	C	H	N
A ₁	C ₁₁ H ₈ ClNO ₂	59.61	3.64	6.32	60.10	3.65	5.92
A ₂	C ₁₁ H ₉ NO ₃	65.02	4.46	6.89	65.18	4.12	6.34
A ₃	C ₁₁ H ₉ NO ₂	70.58	4.85	7.48	70.59	4.82	7.36
A ₄	C ₁₁ H ₉ N ₅	62.55	4.29	33.16	62.17	4.22	33.97
A ₅	C ₁₂ H ₁₁ NO ₃ ·1/8 H ₂ O	65.72	5.17	6.39	65.64	5.05	6.12
A ₆	C ₁₁ H ₉ NO ₂	70.58	4.85	7.48	70.30	4.66	7.16
A ₇	C ₁₂ H ₁₁ NO ₂ ·1/8 H ₂ O	70.84	5.57	6.88	70.68	5.44	6.80
A ₈	C ₁₁ H ₉ NO ₃	65.02	4.46	6.89	65.64	4.49	6.51
A ₉	C ₁₂ H ₁₁ NO ₂	71.63	5.51	6.96	71.38	5.49	6.82
A ₁₀	C ₁₃ H ₁₃ NO ₂ ·1/8 H ₂ O	71.79	6.09	6.44	71.79	6.05	6.33
A ₁₁	C ₁₃ H ₁₂ ClNO ₂	62.53	4.84	5.61	62.37	4.82	5.49
A ₁₂	C ₁₃ H ₁₃ NO ₃ ·1/8 H ₂ O	66.92	5.68	6.00	67.30	5.85	5.64
A ₁₃	C ₁₃ H ₁₃ NO ₂	72.54	6.09	6.51	72.52	6.13	6.31
A ₁₄	C ₁₃ H ₁₃ N ₅	65.25	5.48	29.27	65.43	5.71	28.95
A ₁₆	C ₁₃ H ₁₃ NO ₂	72.54	6.09	6.51	72.62	6.16	6.39
A ₁₇	C ₁₄ H ₁₅ NO ₂	73.34	6.59	6.11	73.83	6.90	5.87
A ₁₈	C ₁₃ H ₁₂ ClNO ₂ ·1/8 H ₂ O	61.97	4.87	5.56	61.95	4.69	5.24
A ₁₉	C ₁₄ H ₁₅ NO ₂	73.34	6.59	6.11	73.44	6.73	5.82
A ₂₀	C ₁₂ H ₁₄ N ₂ O ₂ S	57.58	5.64	11.19	57.51	5.62	10.83
B ₁	C ₁₁ H ₉ BrN ₂ O ₃	44.47	3.05	9.43	44.75	2.82	9.25
B ₂	C ₁₁ H ₉ ClN ₂ O ₃ ·1/2 H ₂ O	50.48	3.47	10.71	50.72	3.34	10.58
B ₁₄	C ₁₂ H ₉ NO ₅	58.30	3.67	5.67	58.11	3.53	5.45
B ₁₆	C ₁₀ H ₆ F ₃ NOS ₂	43.32	2.18	5.05	43.01	2.01	4.73
B ₁₇	C ₁₀ H ₉ NO ₂ S ₂	50.19	3.79	5.85	50.13	3.66	5.60

HPLC Conditions:

HPLC analysis were performed on ZORBAX Eclipse XDB-C8, 5 μ m, 4.6 \times 150 mm column; sample injection volume 5 μ L, at 254 nm wavelength.

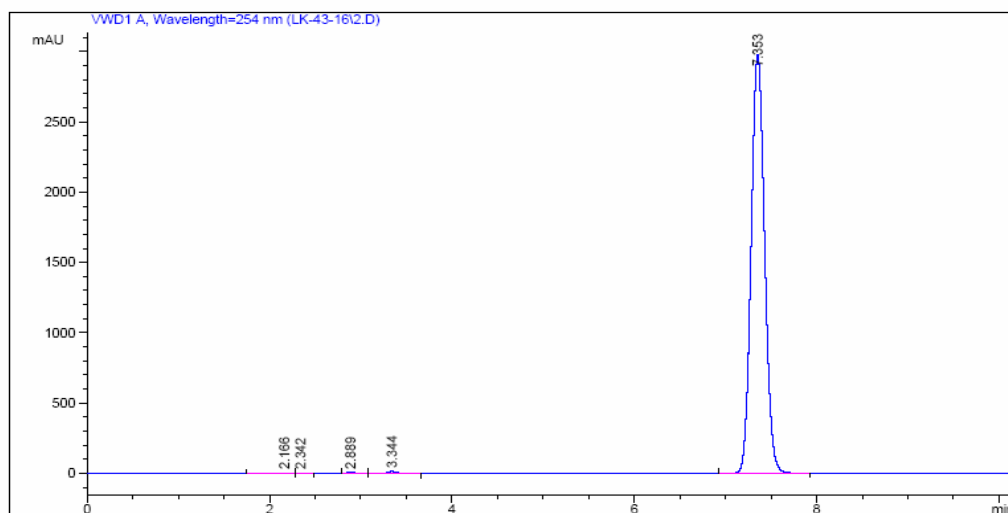
Mobile phase 1: water/CH₃CN 30:70; flow rate 0.8 mL/min.

Mobile phase 2: water/CH₃OH 20:80; flow rate 0.6 mL/min.

Summary of HPLC purity data for final compounds

Code#	HPLC-1		HPLC-2	
	Retention time (min)	Purity %	Retention time (min)	Purity %
A₁₅	7.35	98.6	7.77	95.9
B₃	2.96	98.7	2.57	96.7
B₄	2.18	97.1	2.71	98.6
B₅	1.94	99.6	1.40	100
B₆	1.47	99.2	2.65	98.4
B₇	1.55	96.2	3.25	97.2
B₈	1.49	99.8	2.63	95.9
B₉	2.91	97.1	5.70	97.4
B₁₀	1.54	97.1	2.95	97.9
B₁₁	2.28	96.9	2.75	98.3
B₁₂	1.91	98.9	2.06	97.5
B₁₃	1.44	98.5	2.58	99.5
B₁₅	2.01	97.5	1.85	98.5
B₁₈	2.07	99.6	2.65	98.5
B₁₉	2.05	99.8	2.05	98.9
B₂₀	2.05	99.8	2.05	99.7
B₂₁	2.15	99.5	2.14	99.2
B₂₂	2.13	99.7	2.90	98.2

A15: HPLC-1 (H₂O/CH₃CN 30:70, flow rate 0.8 mL/min)



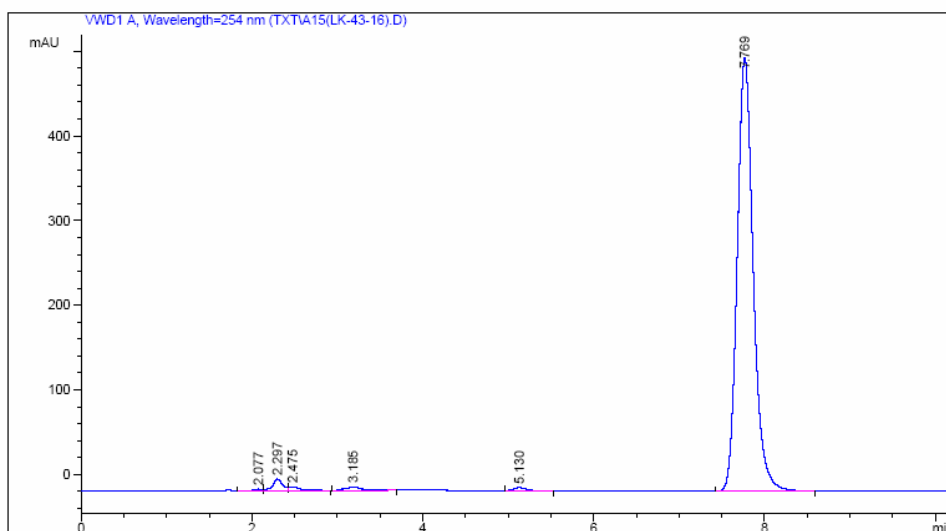
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Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

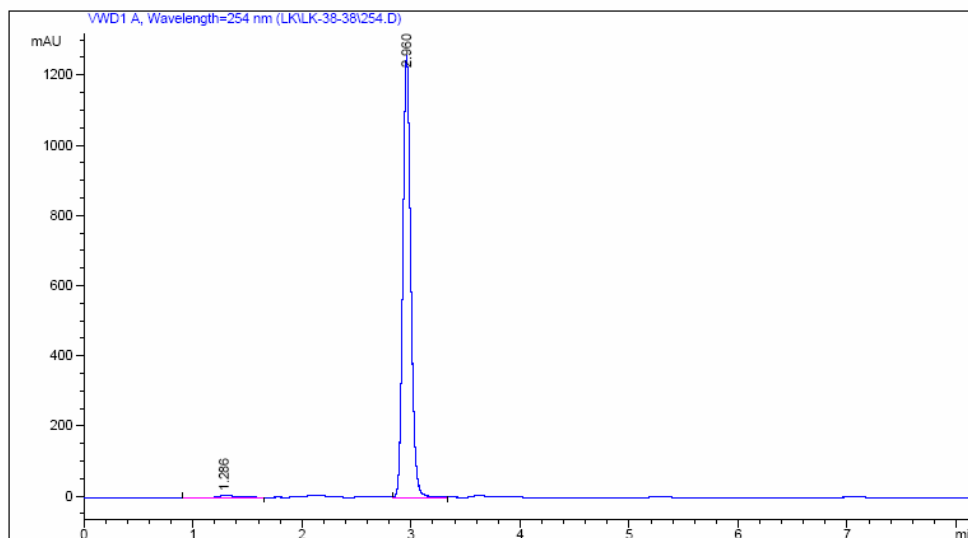
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	2.166	VV	0.3385	155.15916	6.02190	0.5000
2	2.342	VV	0.1382	47.27467	4.68332	0.1524
3	2.889	VV	0.1209	79.37608	9.21665	0.2558
4	3.344	VB	0.1363	145.79961	14.85626	0.4699
5	7.353	BV	0.1592	3.06014e4	2979.09424	98.6219

A15: HPLC-2 (H₂O/CH₃OH 20:80, flow rate 0.6 mL/min)



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
3	2.475	VB	0.1414	52.86165	5.03558	0.7599
4	3.185	BB	0.1927	60.57285	4.31952	0.8707
5	5.130	BB	0.1559	39.19286	3.82646	0.5634
6	7.769	BB	0.1983	6668.06201	512.71582	95.8550

B3: HPLC-1 (H₂O/CH₃CN 30:70, flow rate 0.8 mL/min)



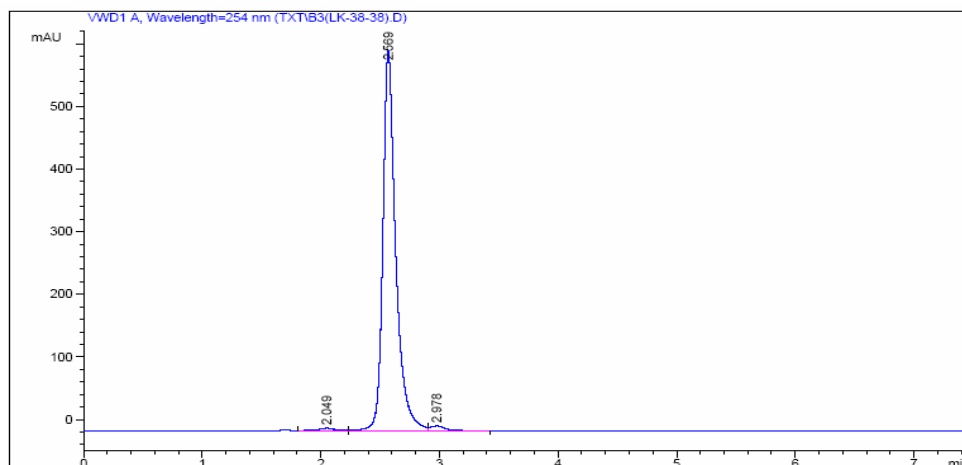
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Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	1.286	BV	0.1513	82.24670	7.09297	1.2728
2	2.960	VV	0.0780	6379.42529	1259.15625	98.7272

B3: HPLC-2 (H₂O/CH₃OH 20:80, flow rate 0.6 mL/min)



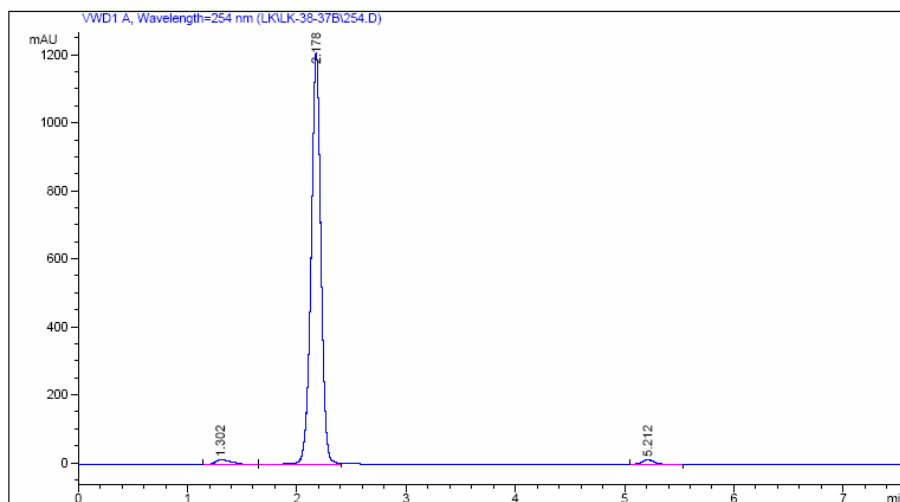
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Multiplier : 1.0000
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Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	2.049	VV	0.1725	63.84985	4.94400	1.3382
2	2.569	VV	0.1103	4615.87158	608.51855	96.7426

B4: HPLC-1 (H₂O/CH₃CN 30:70, flow rate 0.8 mL/min)



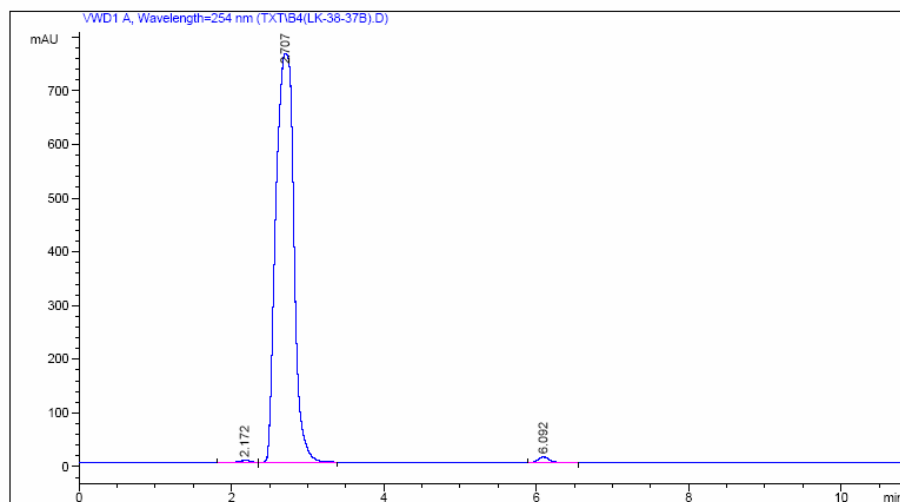
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Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
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Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	1.302	BV	0.1381	130.55939	12.93653	1.6852
2	2.178	VV	0.0943	7521.70703	1210.77722	97.0886

B4: HPLC-2 (H₂O/CH₃OH 20:80, flow rate 0.6 mL/min)



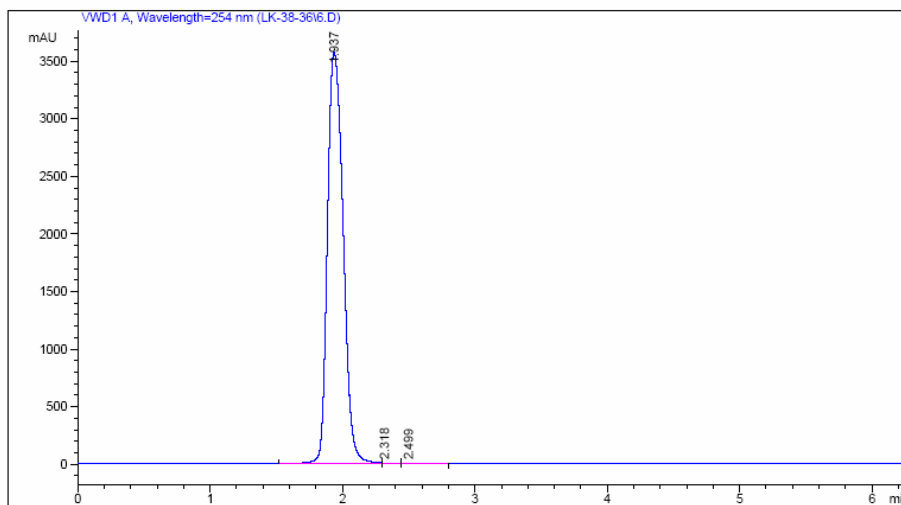
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Use Multiplier & Dilution Factor with ISTDs
  
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Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	2.172	BV	0.1752	55.14525	4.19585	0.4342
2	2.707	VV	0.2702	1.25288e4	762.92651	98.6496

B5: HPLC-1 (H₂O/CH₃CN 30:70, flow rate 0.8 mL/min)



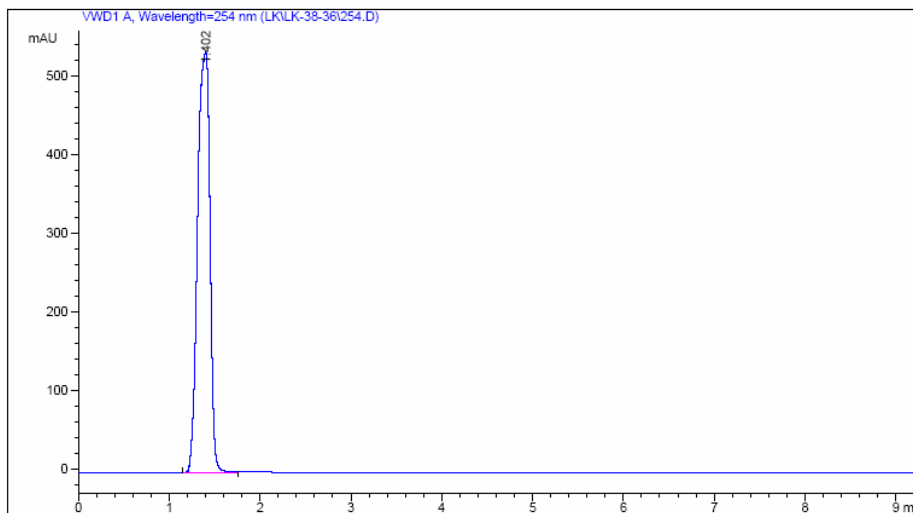
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Signal 1: VWD1 A, Wavelength=254 nm

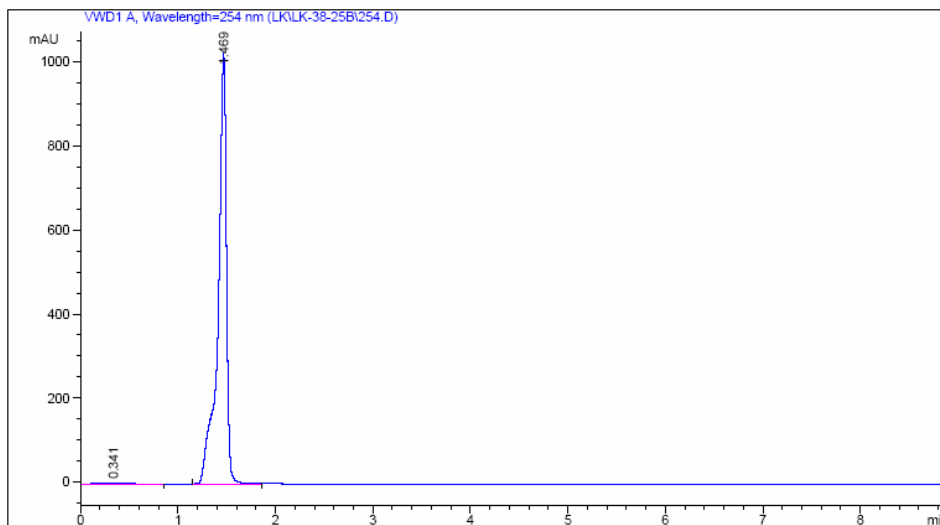
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	1.937	VV	0.1346	2.96692e4	3579.32153	99.5673

B5: HPLC-2 (H₂O/CH₃OH 20:80, flow rate 0.6 mL/min)



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	1.402	BB	0.1539	5060.80371	535.58734	100.0000

B6: HPLC-1 (H₂O/CH₃CN 30:70, flow rate 0.8 mL/min)



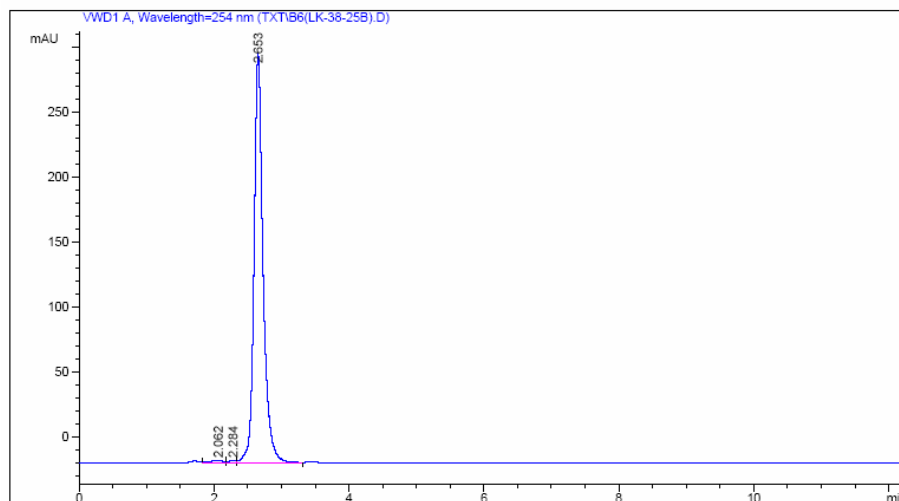
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 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	0.341	BB	0.2972	48.96991	2.52936	0.7833
2	1.469	BV	0.0880	6202.45459	1026.25085	99.2167

B6: HPLC-2 (H₂O/CH₃OH 20:80, flow rate 0.6 mL/min)



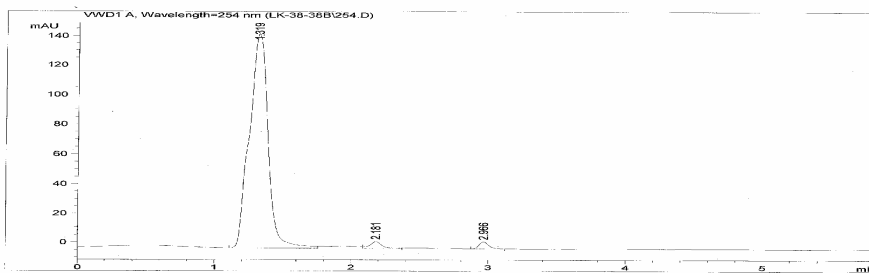
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 Sample Name: CLS1

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
3	2.653	VV	0.1370	2961.17188	315.90558	98.4139

B7: HPLC-1 (H₂O/CH₃CN 30:70, flow rate 0.8 mL/min)

Data File: C:\Chem32\1\DATA\LK-38-38B\254.D

Sample Name: LK-38-38B
 Acq. Operator : LK
 Acq. Instrument : Instrument 1
 Injection Date : 2008-3-20 16:01:43 Location : Vial 1
 Method : C:\Chem32\1\METHODS\DEF.LC.M
 Last Changed : 2008-3-20 13:25:25 By LK
 Sample Info : (modified after loading)



Area Percent Report

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

Signal 1: VWD1 A, Wavelength=254 nm

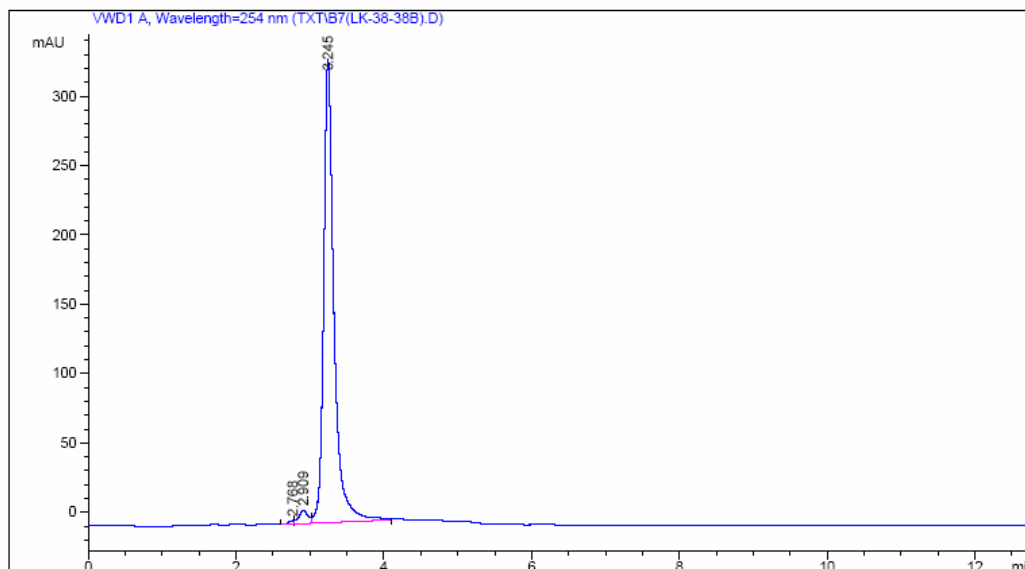
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	1.319	VB	0.1414	1380.96692	145.44109	96.2776
2	2.151	VB	0.0327	29.42029	4.56044	2.0511
3	2.966	BV	0.0753	23.37164	4.71405	1.6712
Totals :				1434.35885	154.71557	

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Instrument 1 2008-3-20 16:08:25 LK

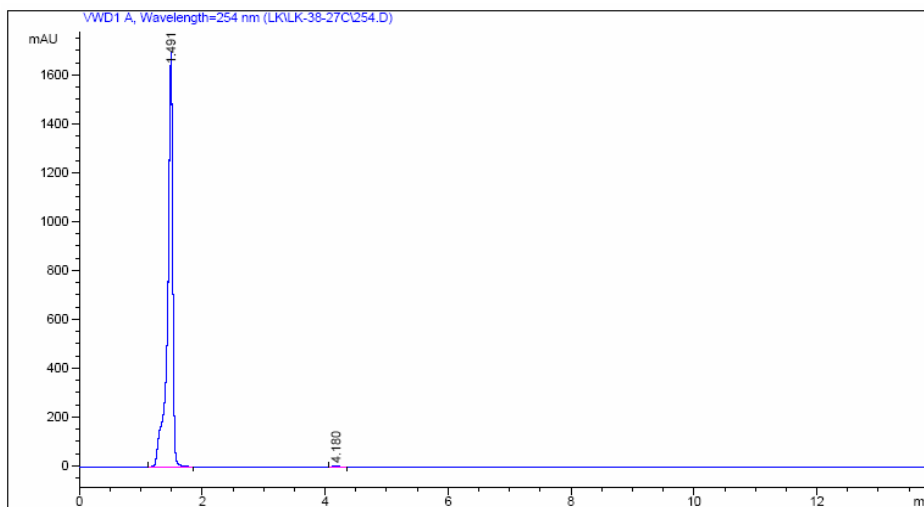
Page 1 of 1

B7: HPLC-2 (H₂O/CH₃OH 20:80, flow rate 0.6 mL/min)



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
3	3.245	VB	0.1412	3257.99023	334.88025	97.2077

B8: HPLC-1 (H₂O/CH₃CN 30:70, flow rate 0.8 mL/min)



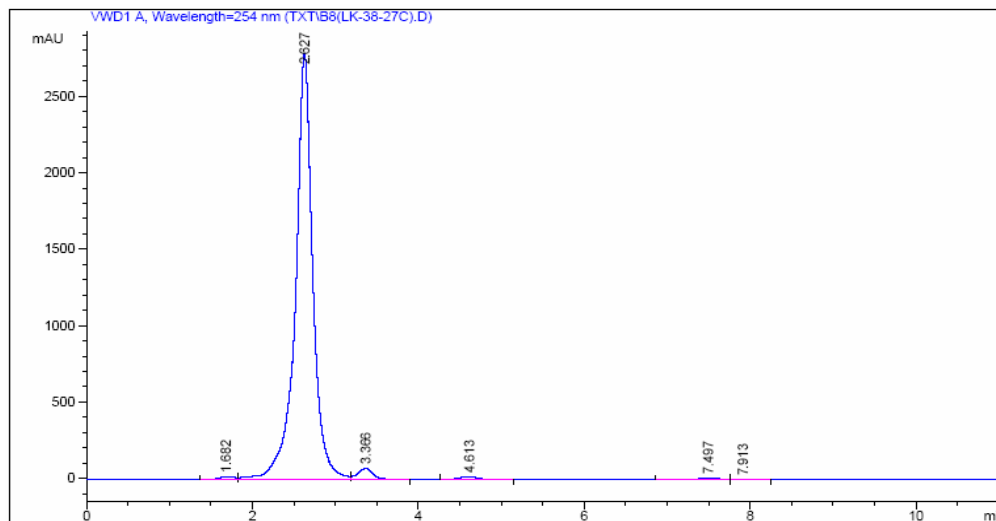
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Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	1.491	BV	0.0816	9747.08008	1696.78491	99.7949

B8: HPLC-2 (H₂O/CH₃OH 20:80, flow rate 0.6 mL/min)



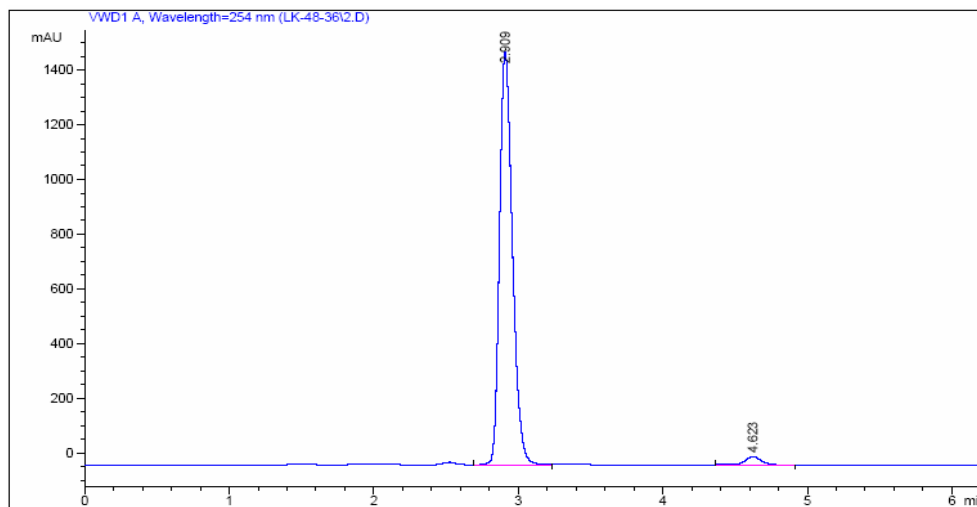
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Sorted By : Signal
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 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	1.682	BV	0.1906	265.06256	21.05449	0.6228
2	2.627	VV	0.2084	4.08059e4	2791.78735	95.8767

B9: HPLC-1 (H₂O/CH₃CN 30:70, flow rate 0.8 mL/min)



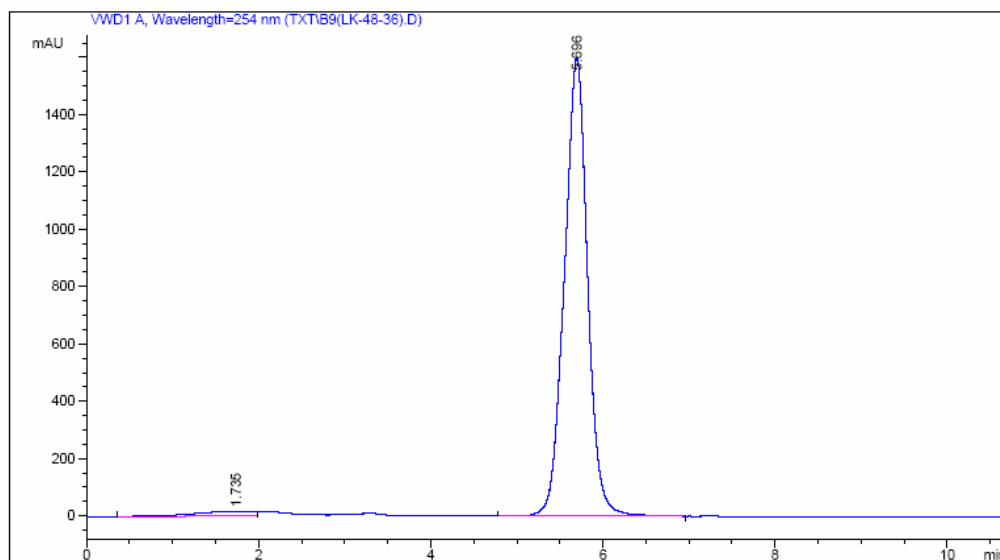
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Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
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Signal 1: VWD1 A, Wavelength=254 nm

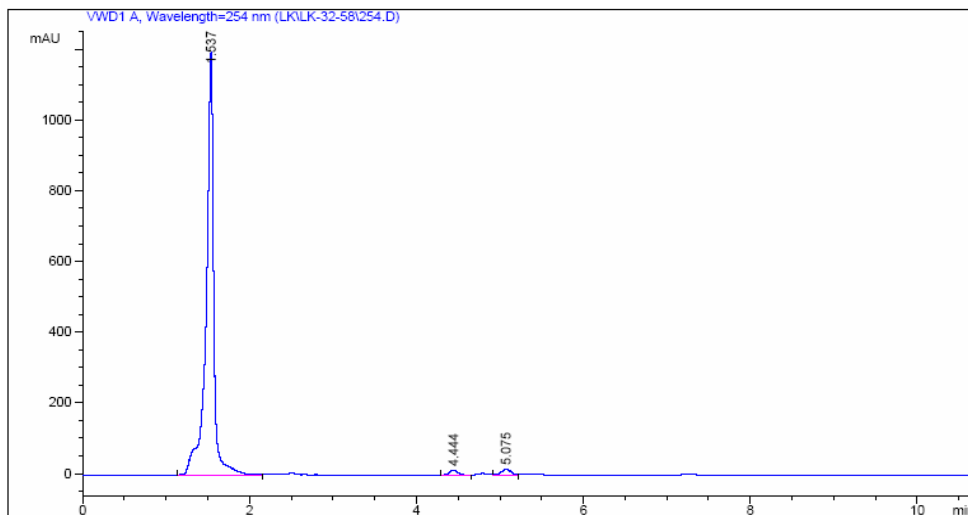
Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area %	Height [mAU]	Area %
1	2.909	VV	0.0960	9430.32813	97.1153	1513.35547	97.1153

B9: HPLC-2 (H₂O/CH₃OH 20:80, flow rate 0.6 mL/min)



Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area %	Height [mAU]	Area %
1	1.735	BV	0.6871	809.01007	2.6338	17.06408	2.6338
2	5.696	BB	0.2750	2.99073e4	97.3662	1599.10913	97.3662

B10: HPLC-1 (H₂O/CH₃CN 30:70, flow rate 0.8 mL/min)



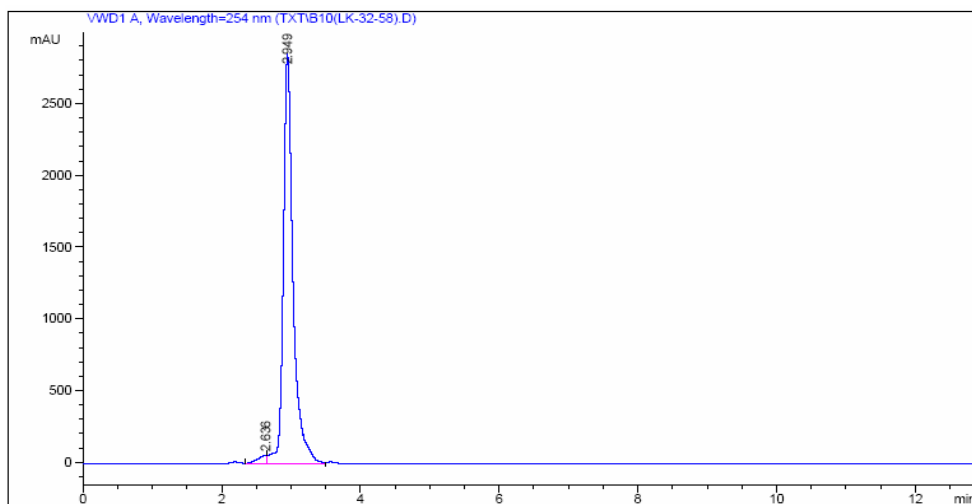
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                          Area Percent Report
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Sorted By      :      Signal
Multiplier    :      1.0000
Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
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Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area %	Height [mAU]
1	1.537	BV	0.0871	7586.87061	97.0817	1196.93848

B10: HPLC-2 (H₂O/CH₃OH 20:80, flow rate 0.6 mL/min)



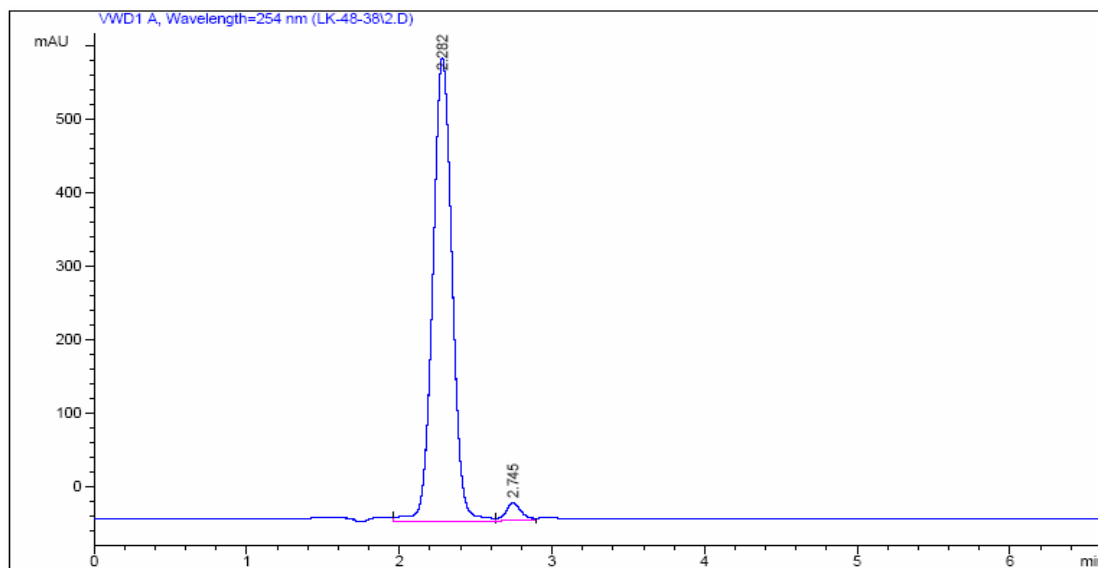
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Multiplier    :      1.0000
Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
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Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area %	Height [mAU]
1	2.636	VV	0.1429	609.58398	2.1212	61.73075
2	2.949	VV	0.1438	2.81281e4	97.8788	2860.39429

B11: HPLC-1 (H₂O/CH₃CN 30:70, flow rate 0.8 mL/min)



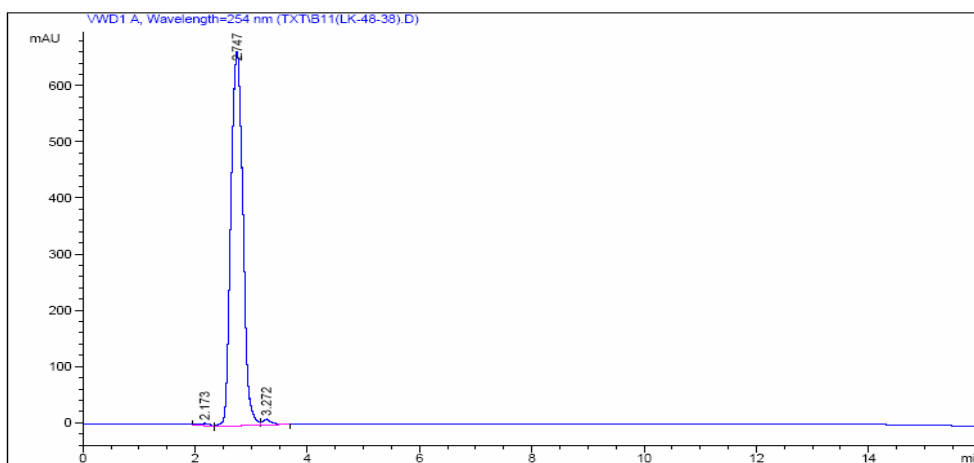
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Sorted By : Signal
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 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	2.282	VV	0.1361	5550.82520	630.96332	96.9352

B11: HPLC-2 (H₂O/CH₃OH 20:80, flow rate 0.6 mL/min)



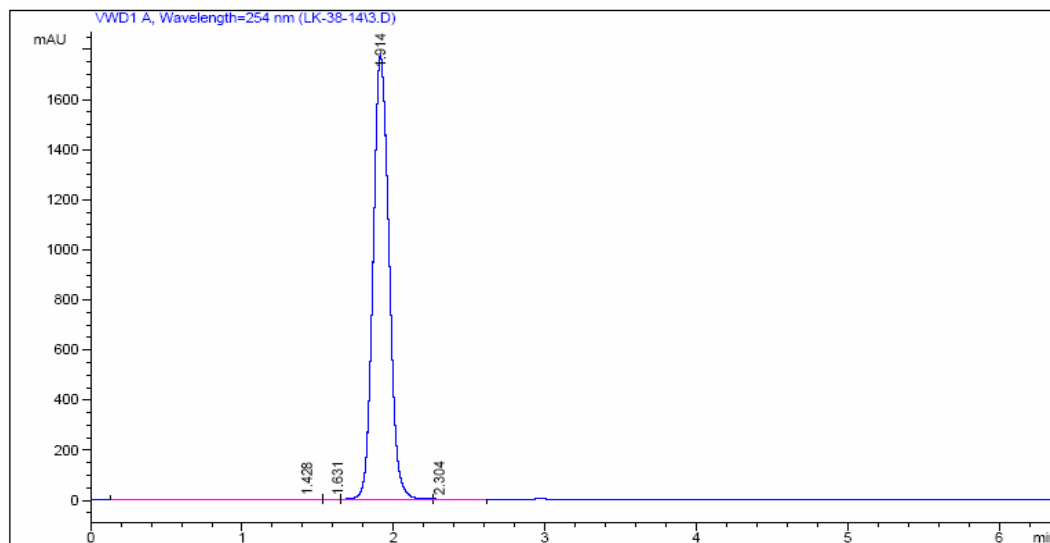
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Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	2.173	BV	0.2340	54.90606	3.97336	0.5455
2	2.747	VV	0.2300	9896.56250	666.54462	98.3260

B12: HPLC-1 (H₂O/CH₃CN 30:70, flow rate 0.8 mL/min)



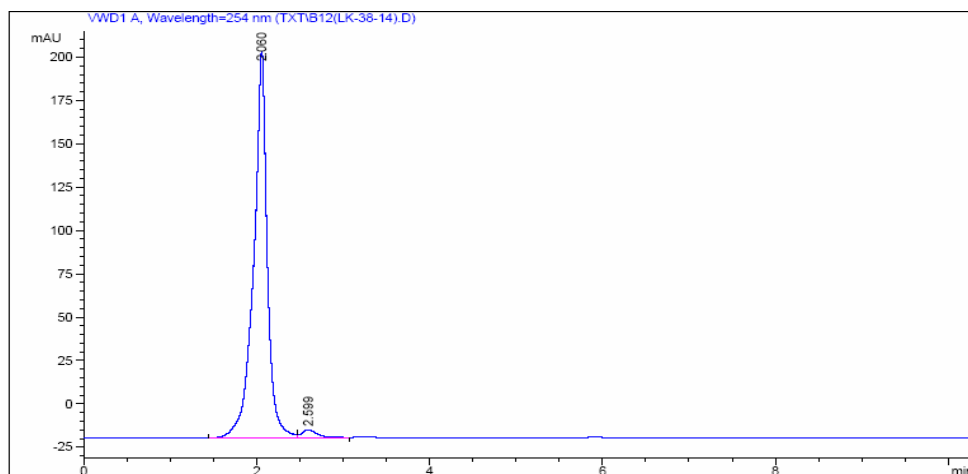
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Sorted By : Signal
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 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	1.428	BV	0.4312	85.71160	2.41682	0.6511
2	1.631	VV	0.0848	15.65988	2.60160	0.1190
3	1.914	VV	0.1146	1.30213e4	1776.35046	98.9080

B12: HPLC-2 (H₂O/CH₃OH 20:80, flow rate 0.6 mL/min)



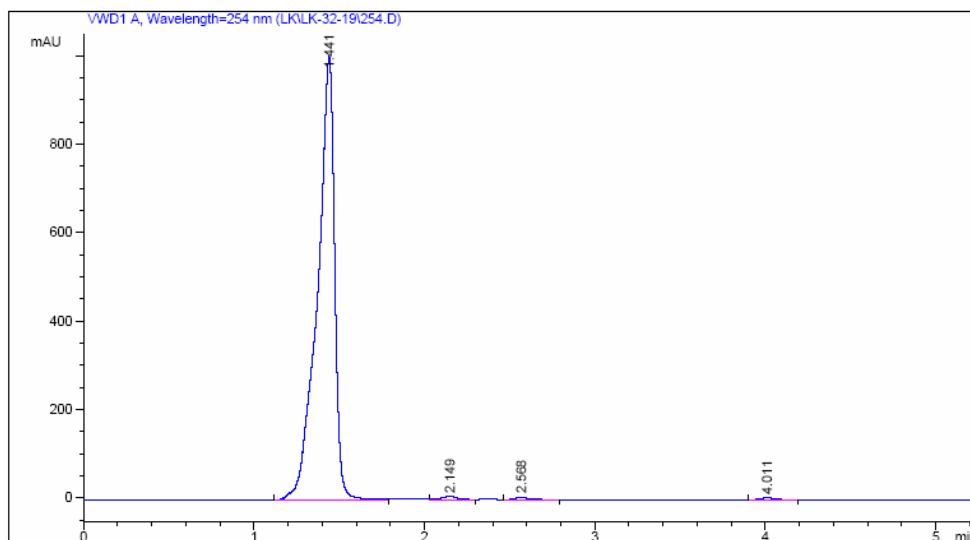
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 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	2.060	BV	0.1497	2446.26587	223.29013	97.4603

B13: HPLC-1 (H₂O/CH₃CN 30:70, flow rate 0.8 mL/min)



```

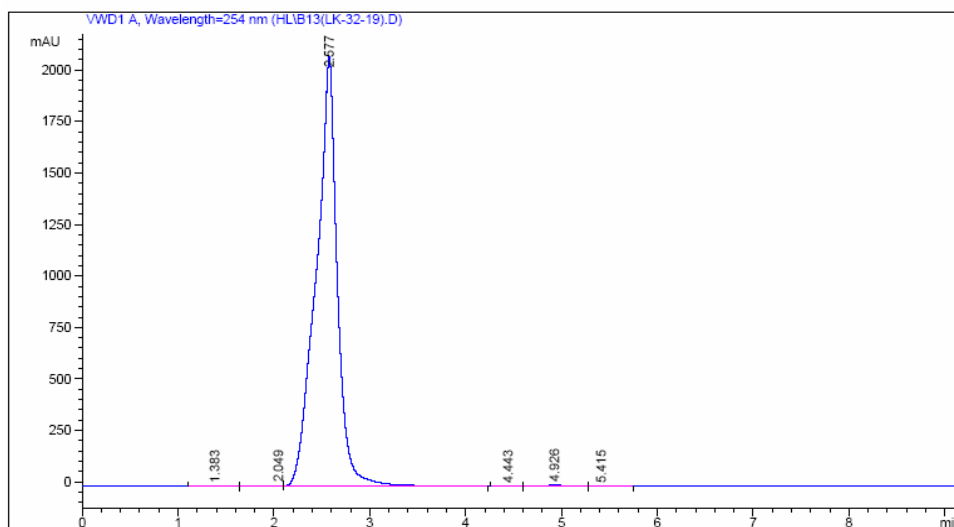
=====
                        Area Percent Report
=====

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

Signal 1: VWD1 A, Wavelength=254 nm

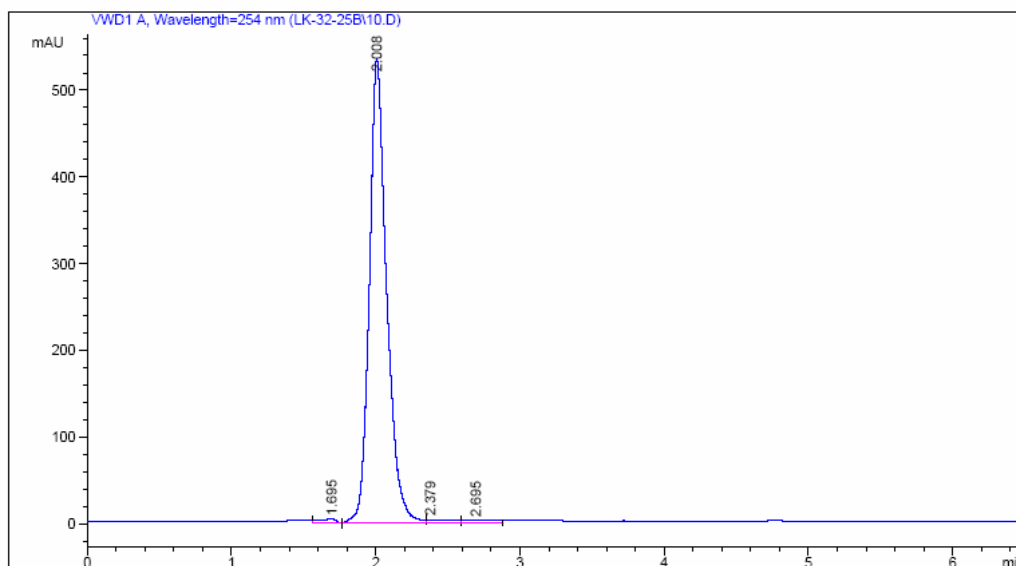
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	1.441	BV	0.1005	7015.16748	1002.95532	98.5273

B13: HPLC-2 (H₂O/CH₃OH 20:80, flow rate 0.6 mL/min)



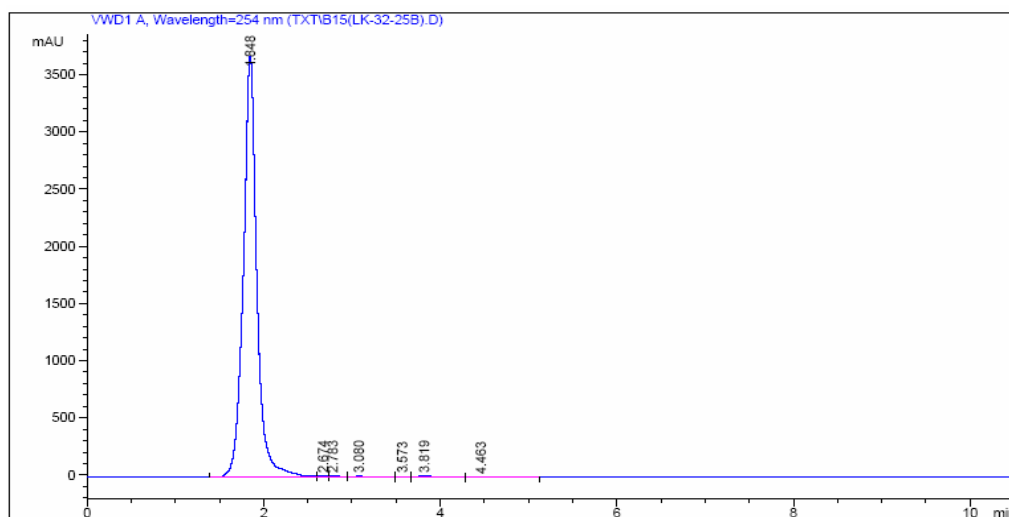
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
3	2.577	VB	0.2039	3.20494e4	2087.45288	99.5493
4	4.443	BV	0.2333	18.03419	1.07675	0.0560
5	4.926	VV	0.1905	89.57513	6.84766	0.2782
6	5.415	VB	0.2623	8.32586	4.38531e-1	0.0259

B15: HPLC-1 (H₂O/CH₃CN 30:70, flow rate 0.8 mL/min)



Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	1.695	VV	0.1083	36.68132	4.71187	0.8019
2	2.008	VV	0.1191	4461.09326	535.11725	97.5286
3	2.379	VV	0.1494	38.69138	3.34806	0.8459
4	2.695	VV	0.1947	37.67315	2.50111	0.8236

B15: HPLC-2 (H₂O/CH₃OH 20:80, flow rate 0.6 mL/min)



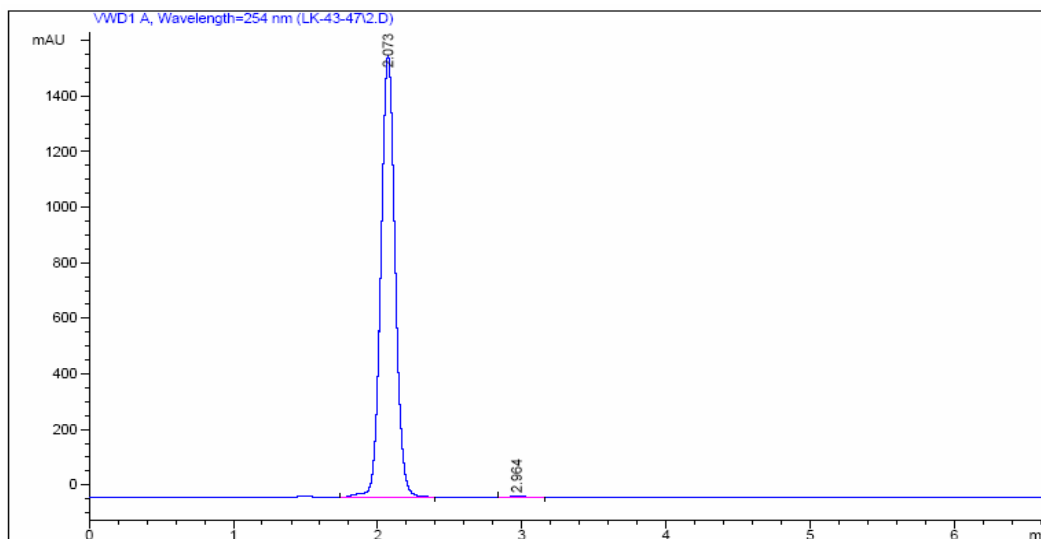
=====
Area Percent Report
=====

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

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	1.848	BV	0.1525	3.94418e4	3685.48682	98.4877

B18: HPLC-1 (H₂O/CH₃CN 30:70, flow rate 0.8 mL/min)



```

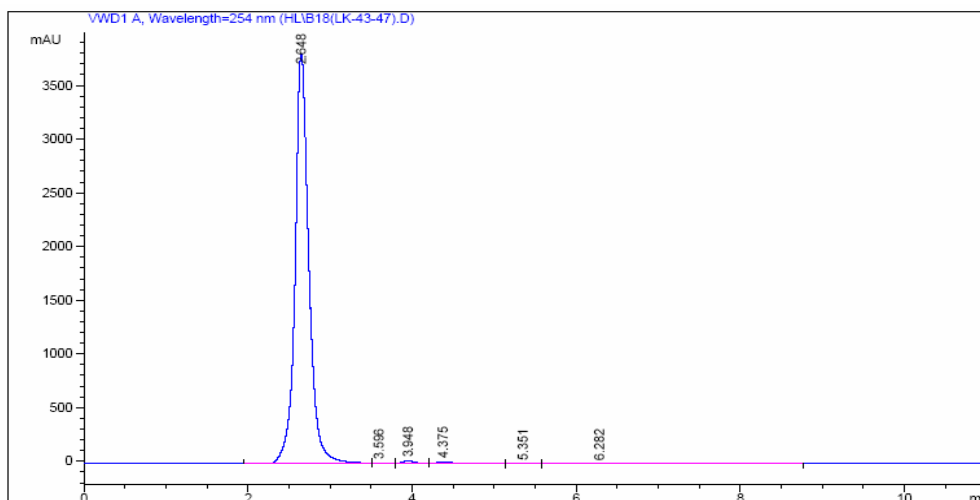
=====
                          Area Percent Report
=====

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

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	2.073	VV	0.1072	1.10542e4	1593.14136	99.5603

B18: HPLC-2 (H₂O/CH₃OH 20:80, flow rate 0.6 mL/min)



```

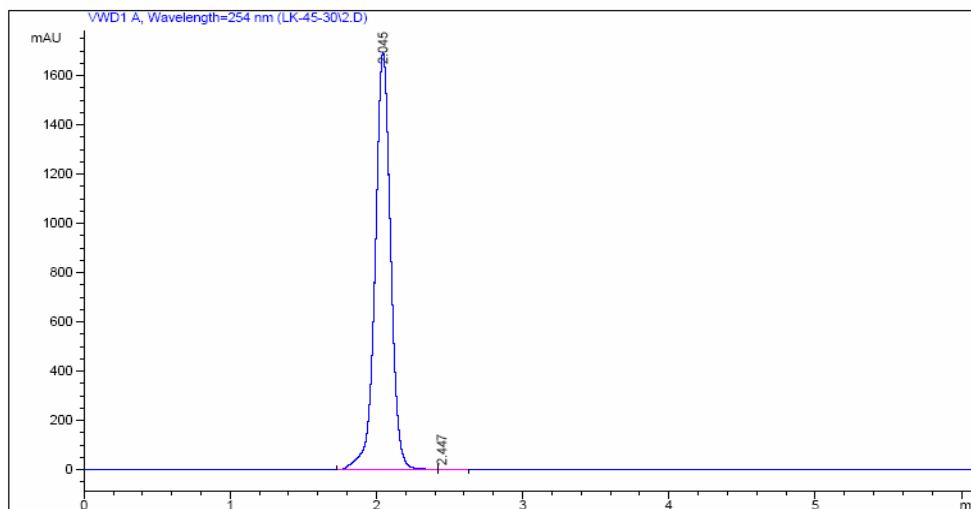
=====
                          Area Percent Report
=====

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

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	2.648	BV	0.1696	4.45519e4	3817.99048	98.4591

B19: HPLC-1 (H₂O/CH₃CN 30:70, flow rate 0.8 mL/min)



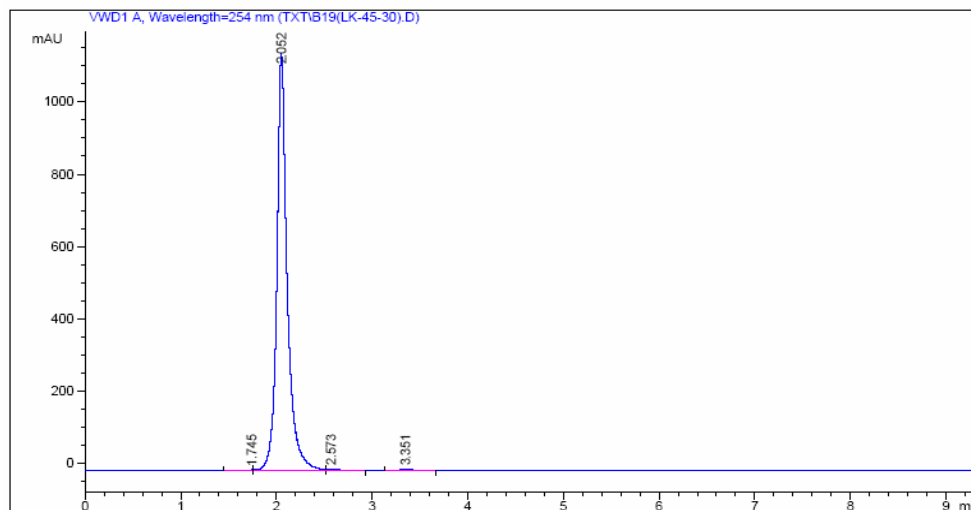
=====
 Area Percent Report
 =====

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

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	2.045	VV	0.1126	1.25565e4		1696.57605	99.7842

B19: HPLC-2 (H₂O/CH₃OH 20:80, flow rate 0.6 mL/min)



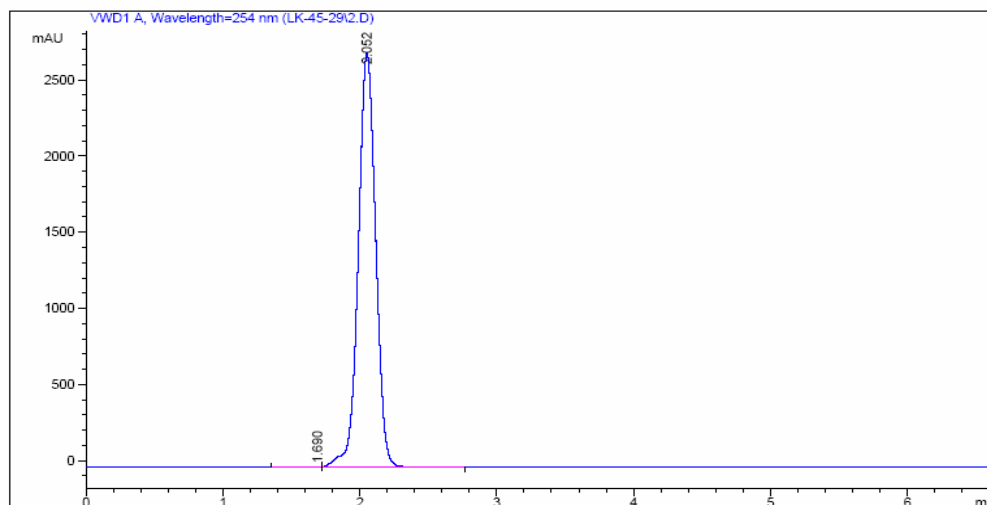
=====
 Area Percent Report
 =====

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

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	1.745	BV	0.0922	14.74195		2.34809	0.1668
2	2.052	VV	0.1073	8744.52930		1154.88965	98.9323

B20: HPLC-1 (H₂O/CH₃CN 30:70, flow rate 0.8 mL/min)



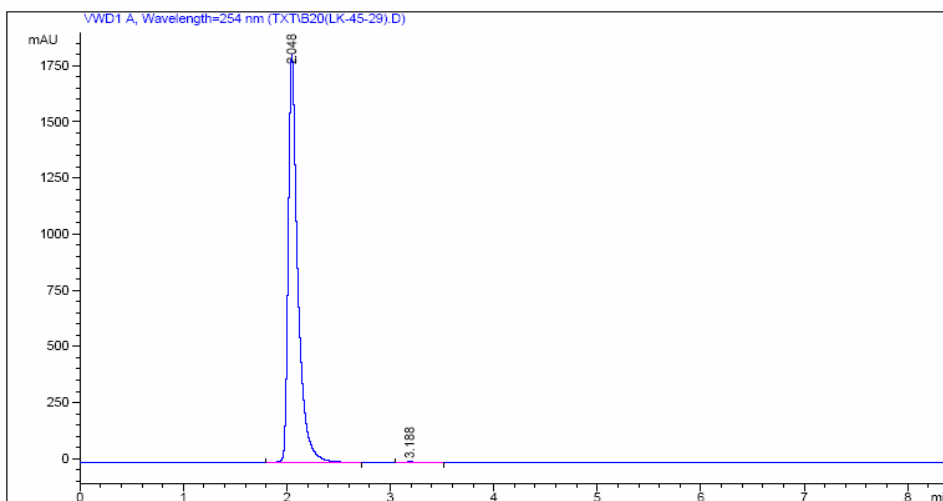
```

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

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width   Area      Height   Area
# [min]          [min] mAU     *s      [mAU]    %
-----|-----|-----|-----|-----|-----|
  1  1.690 BV     0.1275  58.08959  6.15739  0.2398
  2  2.052 VV     0.1370  2.41636e4 2723.82471 99.7602
    
```

B20: HPLC-2 (H₂O/CH₃OH 20:80, flow rate 0.6 mL/min)



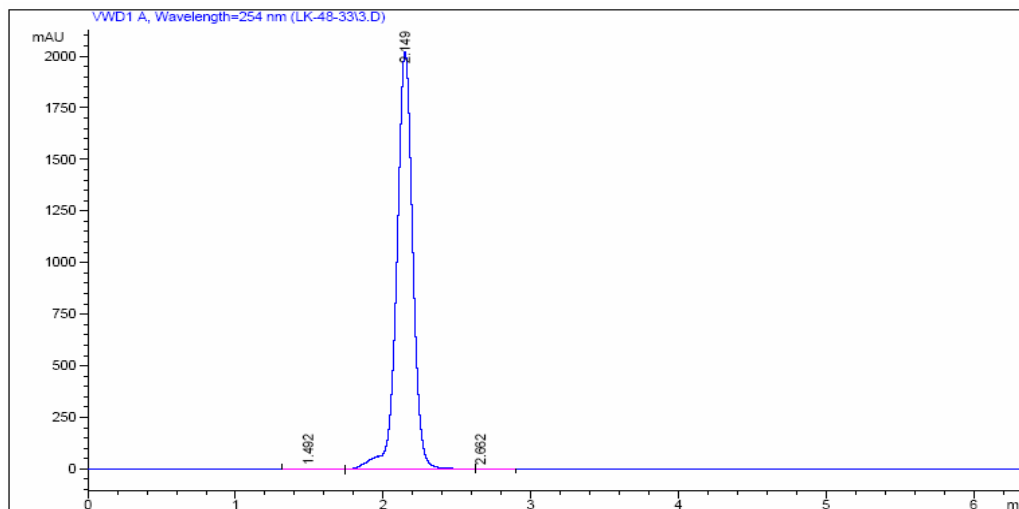
```

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

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width   Area      Height   Area
# [min]          [min] mAU     *s      [mAU]    %
-----|-----|-----|-----|-----|
  1  2.048 VV     0.0924  1.16889e4 1821.20483 99.6620
    
```

B21: HPLC-1 (H₂O/CH₃CN 30:70, flow rate 0.8 mL/min)



```

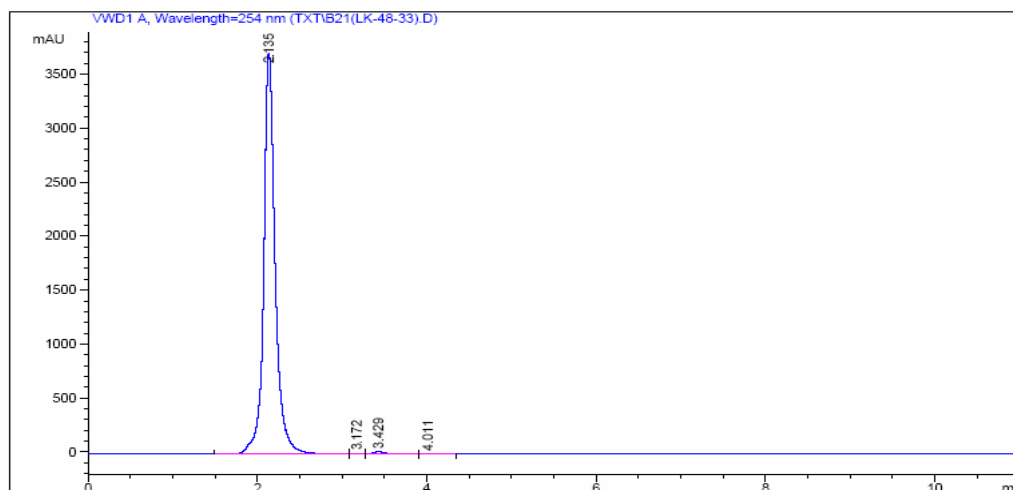
=====
                          Area Percent Report
=====

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

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	1.492	BV	0.2458	47.97275	2.67226	2.67226	0.3102
2	2.149	VV	0.1148	1.53851e4	2025.02637	2025.02637	99.4692

B21: HPLC-2 (H₂O/CH₃OH 20:80, flow rate 0.6 mL/min)



```

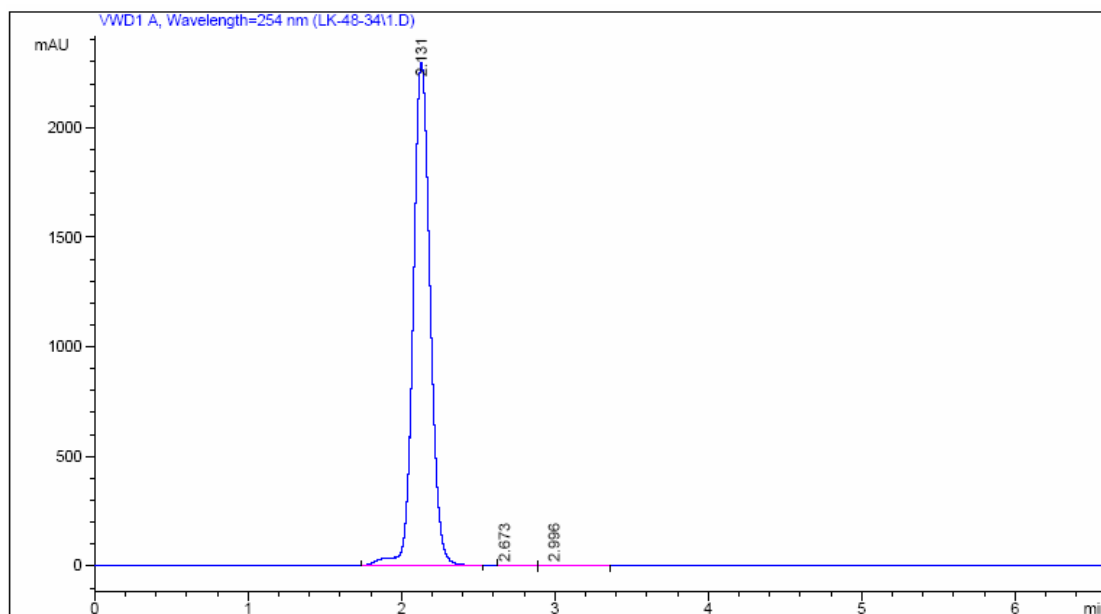
=====
                          Area Percent Report
=====

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

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	2.135	BV	0.1375	3.49668e4	3715.42896	3715.42896	99.1581

B22: HPLC-1 (H₂O/CH₃CN 30:70, flow rate 0.8 mL/min)



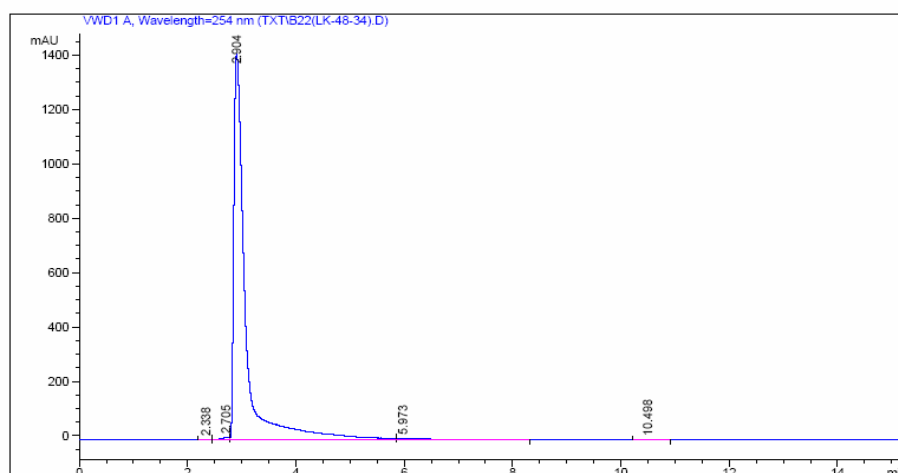
=====
 Area Percent Report
 =====

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

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	2.131	VV	0.1194	1.77742e4	2297.73096	99.7049

B22: HPLC-2 (H₂O/CH₃OH 20:80, flow rate 0.6 mL/min)



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
3	2.904	VV	0.2196	2.12571e4	1421.26331	98.1732
4	5.973	VB	0.5376	249.75653	5.86450	1.1535
5	10.498	BB	0.2431	32.86382	2.09083	0.1518