

# Supporting Information

## Design, Synthesis, and Pharmacological Evaluation of Monocyclic Pyrimidinones as Novel Inhibitors of PDE5A

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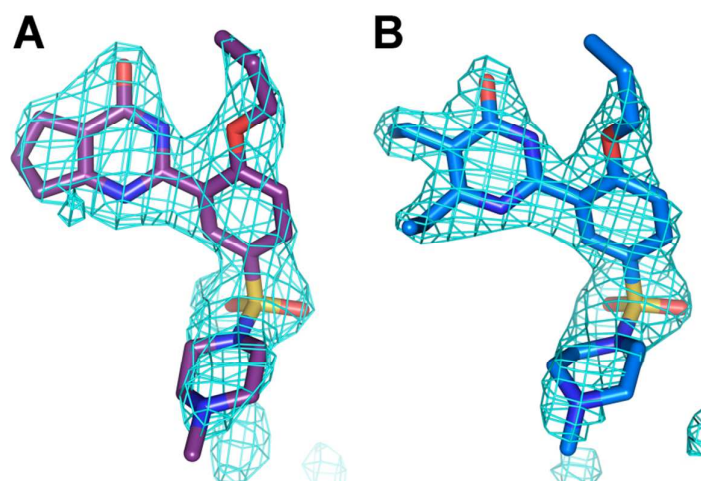
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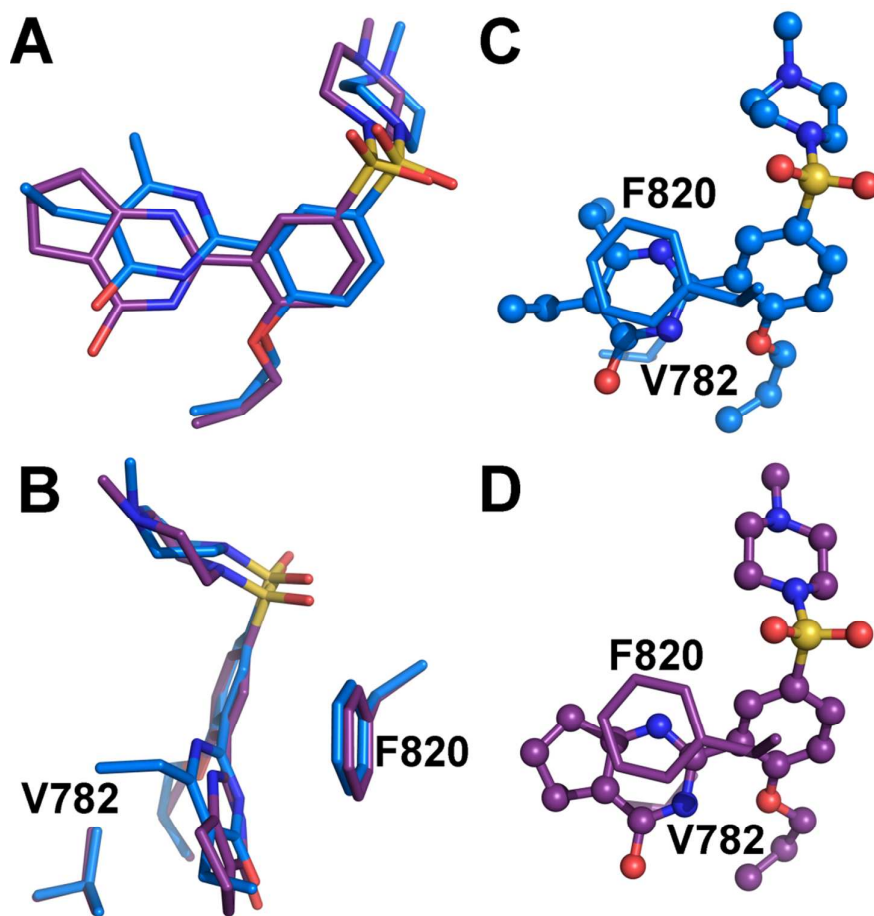
**Table S1** Data collection and refinement statistics

	<b>PDE5A/2</b>	<b>PDE5A/5</b>
Space group	P3 <sub>1</sub> 21	P3 <sub>1</sub> 21
Cell dimensions: a (Å)	90	90
b (Å)	90	90
c (Å)	120	120
Wavelength (Å)	0.9793	0.9793
*Reflections (unique)	32,512(2,427)	37,132(2,744)
Resolution range (Å)	2.40-46.38	2.28-46.06
Highest-resolution shell (Å)	2.40-2.46	2.28-2.34
*Redundancy	5.64(5.77)	3.83(3.82)
*I/σ(I)	10.56(4.21)	18.23(3.2)
*R <sub>merge</sub>	12.7(47.5)	6.2(52.6)
*Completeness (%)	99.9(100.0)	99.9(99.9)
R <sub>work</sub> /R <sub>free</sub> (%)	18.18/21.45	18.85/22.54
RMS values		
Bond length (Å)	0.007	0.008
Bond angle (°)	1.061	1.030
Number of non-hydrogen atoms		
Protein	2353	2290
Inhibitor	30	31
Water Oxygen	67	62
Others	1PEG,1MG,1ZN	1PEG,1MG,1ZN
Mean temperature factors (Å <sup>2</sup> )		
Protein	41.63	42.86
Inhibitor	47.53	40.93
Ramachandran plot		
Residues in most-favoured regions	281 (96.56%)	274(98.21%)
Residues in allowed regions	8(2.75%)	4(1.43%)
Residues in disallowed regions	2(0.69%)	1(0.36%)

\*Overall (highest resolution shell)



**Figures S1.**  $(F_o - F_c)$  difference electron-density maps contoured at  $3.0 \sigma$  for compounds **2** (A) and **5** (B) in their complex structures with PDE5 determined by X-ray diffraction.



**Figure S2.** The superimposition of the binding modes of the compounds **2** (purple) and **5** (blue) within PDE5. The complex structures of PDE5A/2 and PDE5A/5 was superimposed by fitting all the C $\alpha$  atoms of the enzyme. (A) The superimposition of compounds **2** and **5**. (B) The superimposition of compounds **2** and **5** as well as the two residues V782 and F820 in a perpendicular view to that shown in A. (C,D) The location of residues V782, F820, and the compounds **2** (C) and **5** (D) in the complex structures of PDE5A/2 and PDE5A/5, respectively. For the sake of clarity, the compounds in (C) and (D) were shown by balls and sticks.

### PDE Assays

Recombinant human PDE5A1, PDE6C, PDE7A1, PDE8A1, PDE9A2, PDE10A2, and PDE11A4 were purchased from BPS Bioscience. PDE1, PDE2, PDE3, and PDE4 were purified from rat brain, dog adrenal gland, rabbit blood platelet, and rat kidney, respectively. PDEs activity was analyzed using a tritium scintillation proximity assay (SPA) system, and the assay was performed according to the manufacturer's instructions (Amersham Biosciences). Assays were performed in the presence of 50 mM Tris–HCl (pH 7.5) containing 8.3 mM MgCl<sub>2</sub> and 1.7 mM EGTA. Each assay was performed in a 100  $\mu$ L reaction volume containing the above buffer, enzyme and around 0.05  $\mu$ Ci [3H]cGMP (for PDE5A, PDE6C, PDE9A2, PDE11A4) or 0.05  $\mu$ Ci [3H]cAMP (for PDE1A, PDE2A, PDE3A, PDE4A1, PDE7A1, PDE8A1, PDE10A2). The reaction was carried out at 30°C for 30 minutes and stopped by the addition of 50  $\mu$ L PDE SPA beads (1 mg) suspended in 18 mM zinc sulfate. The reaction mixture was left to be settled at a room temperature for 20 minutes before counting in MicroBeta TriLux (Perkin-Elmer Life Sciences, USA). For compound inhibition study on the PDEs, stock solutions of the compounds were prepared in 100% DMSO, diluted in deion water to the appropriate concentrations and added to the assay buffer to give a final concentration of < 1% DMSO. The amount of enzyme used in each reaction was such that the hydrolysis of substrates did not exceeded 15% so that the amount of product increased linearly with time. Duplicates were run in each assay.

PDE inhibitory activity was calculated from the equation below:

$$\% \text{PDEs inhibition} = \left[ 1 - \frac{(\text{CPM}_{\text{sample}} - \text{CPM}_{\text{blank}})}{(\text{CPM}_{\text{control}} - \text{CPM}_{\text{blank}})} \right] \times 100$$

In this equation, CPM<sub>sample</sub> represents radioactive value of sample obtained from the assay (with enzyme); CPM<sub>control</sub> represents radioactive value of solvent (water) which was used for diluting sample obtained from the assay (with enzyme); CPM<sub>blank</sub> represents radioactive value of the mixture of only buffer and substrate (without enzyme). IC<sub>50</sub> values were calculated from the concentration–inhibition curves by nonlinear regression analysis using GraphPad Prism.

### In vivo efficacy in the rat model

The test was carried out based on the methods reported. After fasted for 12 hours, 3 male SD rats were randomized into each group. After anesthetizing the rats with

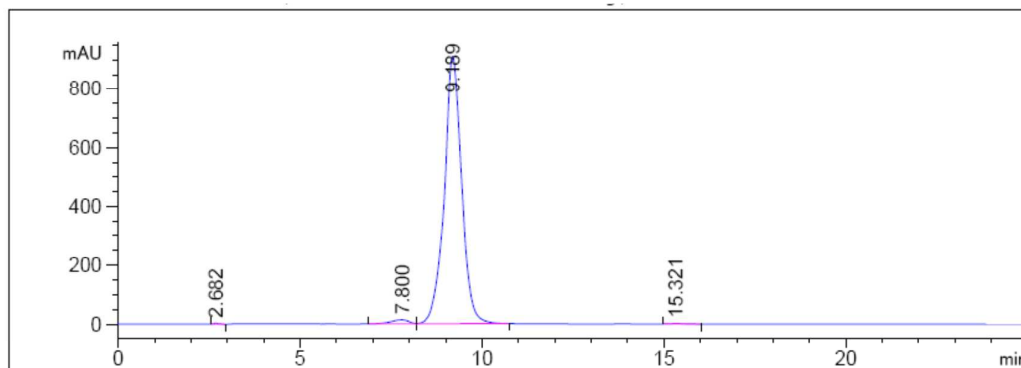
sodium pentobarbital (50 mg/kg, i.p.), the penile skin was incised and the prepuce was degloved to expose completely the corpora cavernosa (CC). A needle linked to an electrophysiology instrument was inserted into the CC on the right side in order to measure the intracavernous pressure (ICP). The right carotid artery was cannulated in a similar manner to the polyethylene tube in order to monitor the mean blood pressure (Bp) continuously. After exposing the lateral surface of the prostate via an incision in the midline inferior abdomen, a bipolar platinum microelectrode was placed on the cavernous nerve. Electric stimulation was performed at 2 Hz, for 60 s with a pulse duration of 5 ms and 3 V using a stimulator. The compounds were administered orally (10 mg/kg). The change of the ICP and Bp were monitored continuously before and after the administration. The effect of the compounds on the erection induced by electric stimulation was evaluated by the ratio of ICP to Bp.

### **Pharmacokinetics**

Male Sprague-Dawley rats, weighing 200-220g, were purchased from Sino-British SIPPR/BK lab. Animal Ltd. (Shanghai, China), and housed in a temperature ( $23 \pm 2$  °C) and moisture (RH:  $55 \pm 10\%$ ) controlled room, exposed to a controlled 12 h cycle of light and darkness, and allowed free access to food and water. Compound **5** was administered orally at a dose of 10 mg/kg and intravenously at a dose of 5 mg/kg after fasting for 12 h with free access to water. Blood samples were collected at 0, 0.25, 0.5, 1, 2, 4, 6, 8, and 10 h after oral administration, and at 0, 0.083, 0.25, 0.5, 1, 2, 4, 6, 8, and 10h after intravenous administration. Serum concentrations of **5** were analyzed using a LC/MS/MS method. Data used to generate the PK profile are the Mean  $\pm$  SD from three male rats (individual samples at all time points).

## HPLC chromatograms of novel compounds

### Compound 2



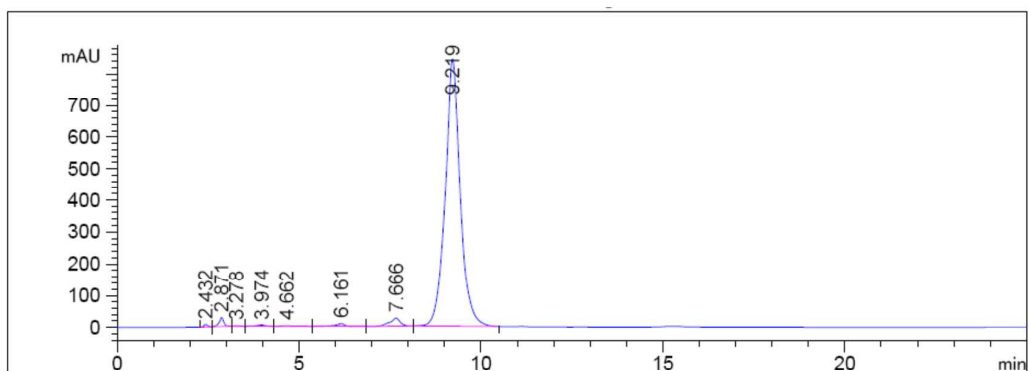
Signal 1: DAD1 A, Sig=220,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.682	BV	0.1279	29.89998	3.17534	0.0974
2	7.800	BV	0.5389	460.26630	13.32877	1.4990
3	9.189	VB	0.4951	3.01803e4	909.60791	98.2901
4	15.321	BB	0.4390	34.87043	1.17230	0.1136

Totals : 3.07053e4 927.28432

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# Compound 3



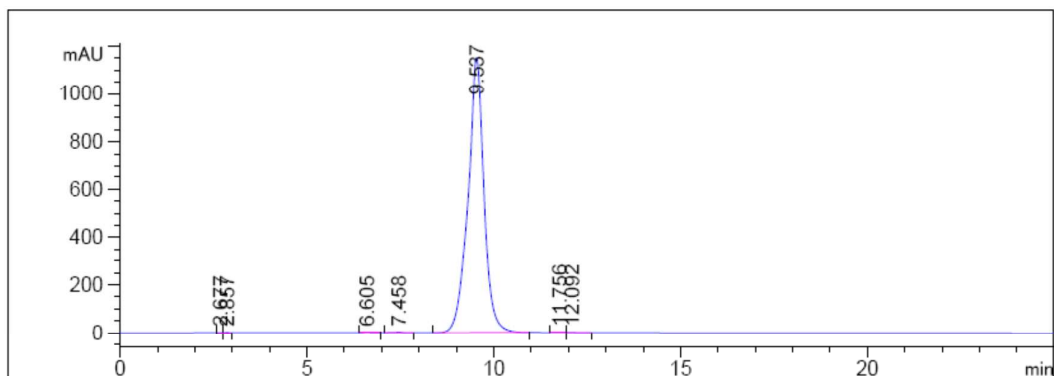
Signal 1: DAD1 A, Sig=220,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.432	BB	0.0977	55.24163	8.29760	0.2187
2	2.871	BB	0.1248	249.44574	28.31738	0.9877
3	3.278	BB	0.1208	15.70716	1.93372	0.0622
4	3.974	BB	0.2502	77.57486	4.47674	0.3072
5	4.662	BB	0.3751	63.94345	2.22641	0.2532
6	6.161	BB	0.2573	178.54768	9.58581	0.7070
7	7.666	BB	0.2787	508.37241	25.26694	2.0130
8	9.219	BB	0.4095	2.41056e4	843.23364	95.4510

Totals : 2.52544e4 923.33825

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Compound 5



Signal 1: DAD1 A, Sig=220,4 Ref=360,100

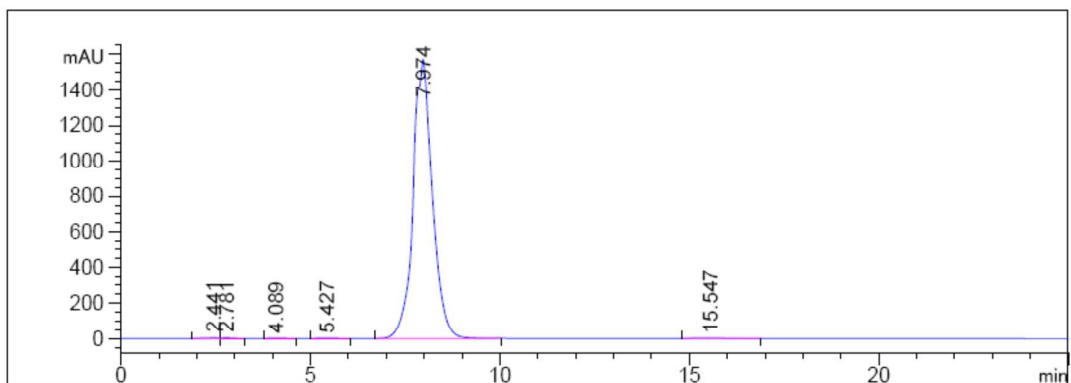
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.677	BV	0.0898	5.12911	8.32888e-1	0.0150
2	2.857	VV	0.1120	11.39016	1.54509	0.0333
3	6.605	BB	0.1852	6.86843	6.10749e-1	0.0201
4	7.458	BB	0.2348	35.36179	2.14025	0.1035
5	9.537	BB	0.4219	3.40809e4	1149.49573	99.7325
6	11.756	BV	0.2252	19.98406	1.30133	0.0585
7	12.092	VB	0.1720	12.68415	1.15572	0.0371

Totals : 3.41724e4 1157.08176

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Compound 9



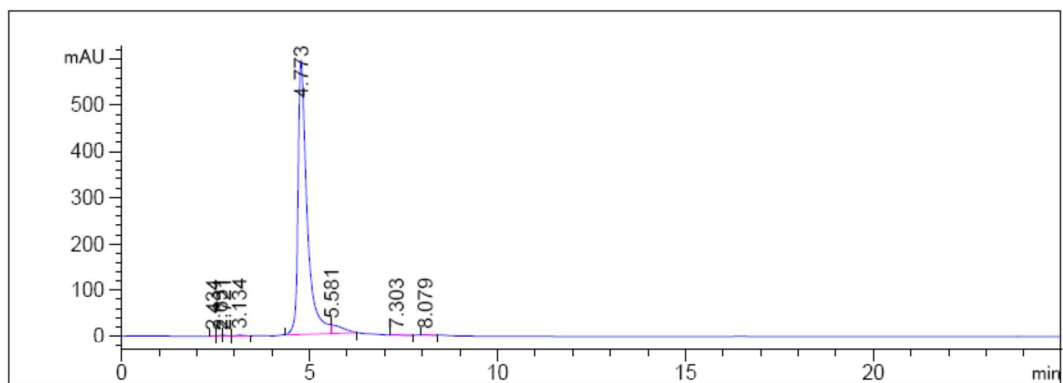
Signal 1: DAD1 A, Sig=220,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.441	BV	0.3298	97.13193	4.07885	0.1729
2	2.781	VB	0.3009	78.67293	3.94175	0.1401
3	4.089	BB	0.3020	19.98724	9.40411e-1	0.0356
4	5.427	BB	0.3742	46.79268	1.94864	0.0833
5	7.974	BB	0.4607	5.58238e4	1570.57800	99.3942
6	15.547	BB	0.7359	97.68318	1.71153	0.1739

Totals : 5.61641e4 1583.19920

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Compound 10



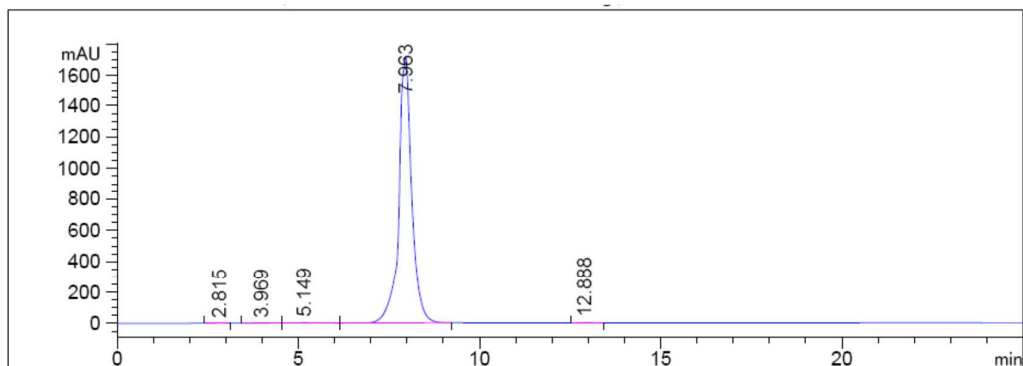
Signal 1: DAD1 A, Sig=220,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.434	BV	0.0960	3.56936	5.62654e-1	0.0342
2	2.631	VV	0.0913	12.81595	2.09683	0.1228
3	2.721	VV	0.1160	17.87897	2.12748	0.1713
4	3.134	VB	0.1545	30.72164	2.74576	0.2943
5	4.773	MF R	0.2460	9981.38867	594.19739	95.6162
6	5.581	FM R	0.3408	384.92148	18.82656	3.6873
7	7.303	BB	0.1391	6.22345	9.93581e-1	0.0596
8	8.079	BB	0.0831	1.49057	5.25029e-1	0.0143

Totals : 1.04390e4 622.07528

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## Compound 11

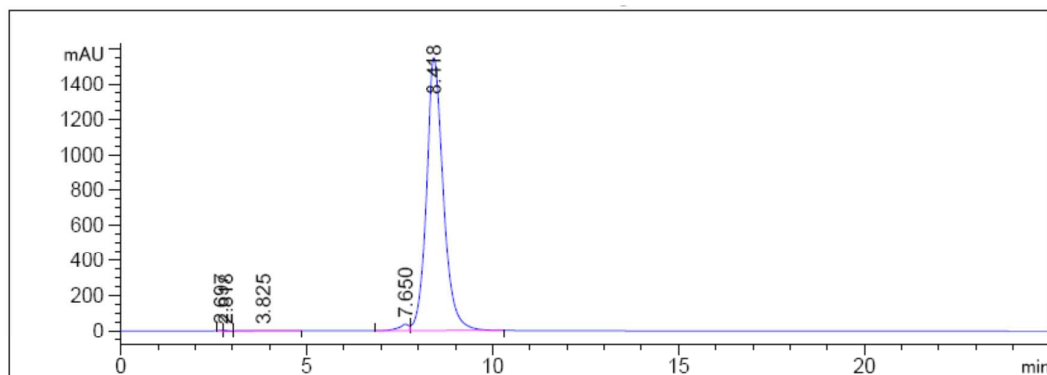


Signal 1: DAD1 A, Sig=220,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.815	BB	0.2961	33.82583	1.56550	0.0793
2	3.969	BB	0.3407	25.97938	1.03534	0.0609
3	5.149	BB	0.3484	60.32067	2.42350	0.1414
4	7.963	BB	0.3654	4.24806e4	1712.79590	99.5965
5	12.888	BB	0.3210	51.96140	2.45451	0.1218

Totals : 4.26527e4 1720.27475

## Compound 12

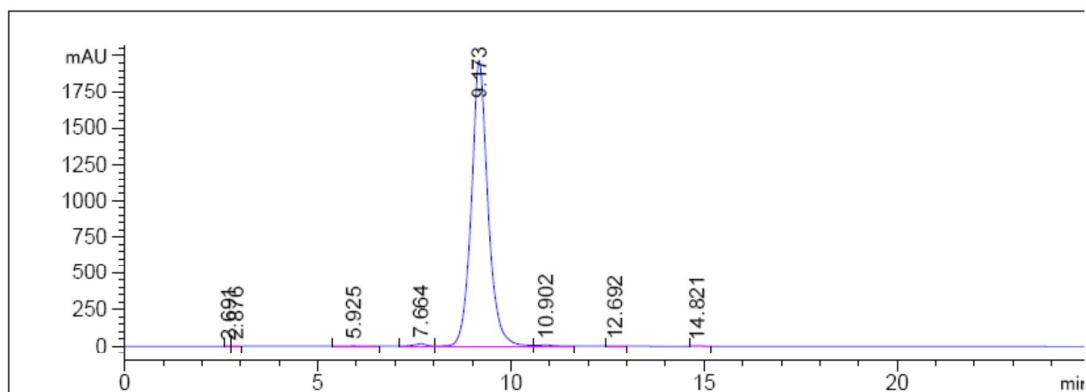


Signal 1: DAD1 A, Sig=220,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.697	BV	0.0842	11.91176	2.03715	0.0241
2	2.818	VV	0.1130	20.53636	2.52160	0.0416
3	3.825	VB	0.6210	41.43515	8.64850e-1	0.0839
4	7.650	BV	0.2622	691.16736	36.29197	1.3996
5	8.418	VB	0.4663	4.86182e4	1548.51147	98.4508

Totals : 4.93833e4 1590.22704

Compound 14



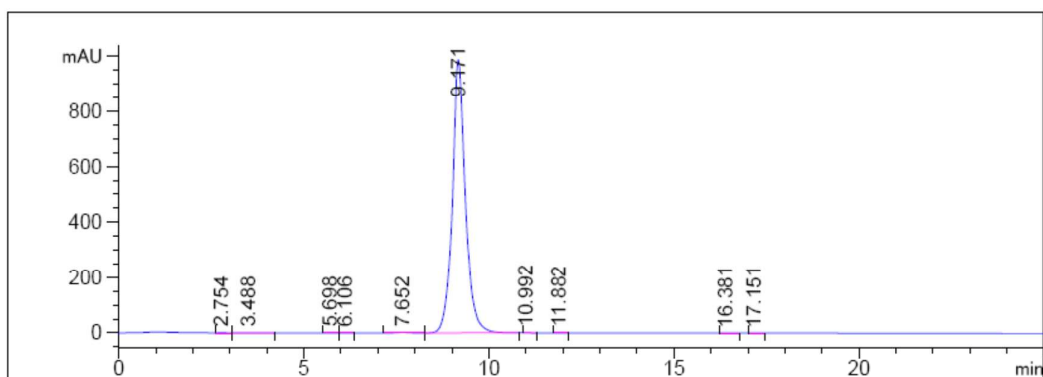
Signal 1: DAD1 A, Sig=220,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.691	BV	0.0869	5.67541	9.61655e-1	9.611e-3
2	2.876	VV	0.1098	16.32706	2.16836	0.0276
3	5.925	BB	0.3453	51.27264	1.98514	0.0868
4	7.664	BV	0.2750	325.03772	16.55895	0.5504
5	9.173	VB	0.4308	5.84300e4	1965.69922	98.9509
6	10.902	BB	0.3614	203.23392	7.51813	0.3442
7	12.692	BB	0.1764	11.60978	9.78447e-1	0.0197
8	14.821	BB	0.2058	6.34070	4.87254e-1	0.0107

Totals : 5.90495e4 1996.35716

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## Compound 15



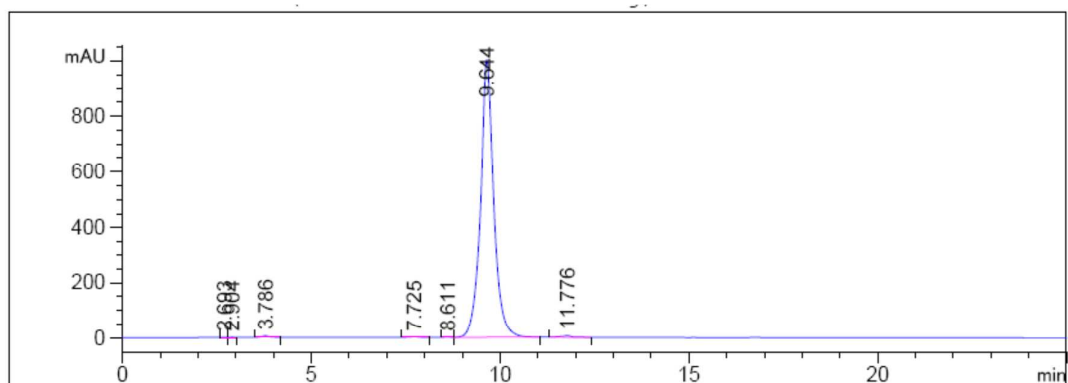
Signal 1: DAD1 A, Sig=220,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.754	VV	0.1840	18.80785	1.32173	0.0776
2	3.488	VB	0.4660	12.20166	3.20631e-1	0.0504
3	5.698	BV	0.1926	1.73406	1.18603e-1	7.156e-3
4	6.106	VV	0.1698	9.91336e-1	8.77506e-2	4.091e-3
5	7.652	BB	0.2785	42.70149	2.08855	0.1762
6	9.171	BB	0.3533	2.41492e4	987.44202	99.6636
7	10.992	BB	0.1233	8.56979e-1	1.20058e-1	3.537e-3
8	11.882	BB	0.1456	1.78848	1.93837e-1	7.381e-3
9	16.381	BB	0.2027	1.37399	9.85215e-2	5.670e-3
10	17.151	BB	0.1703	1.05779	8.32388e-2	4.365e-3

Totals : 2.42307e4 991.87493

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Compound 16



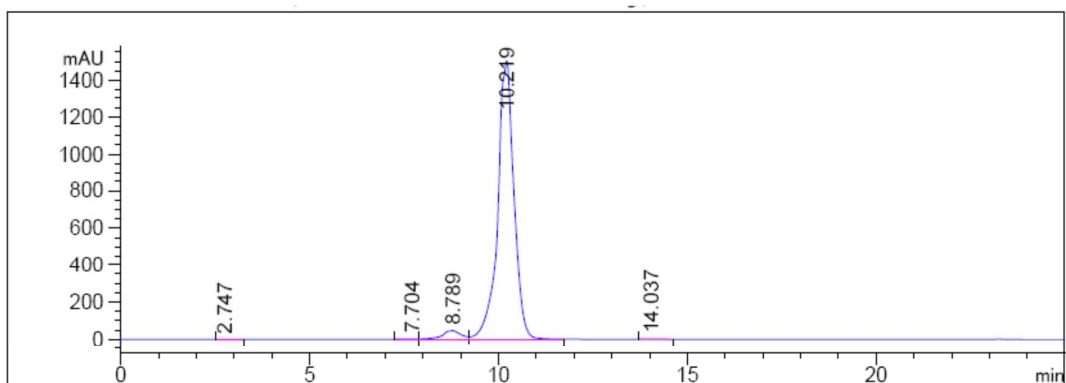
Signal 1: DAD1 A, Sig=220,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.693	BV	0.0940	5.38857	8.05687e-1	0.0218
2	2.904	VV	0.1010	7.31632	1.05347	0.0297
3	3.786	BB	0.1838	66.19927	5.08767	0.2684
4	7.725	BB	0.2231	36.24184	2.33490	0.1469
5	8.611	BV	0.1478	5.45448	5.69038e-1	0.0221
6	9.644	VB	0.3506	2.44462e4	1002.23566	99.1024
7	11.776	BB	0.2644	100.82639	5.19639	0.4087

Totals : 2.46676e4 1017.28281

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## Compound 17

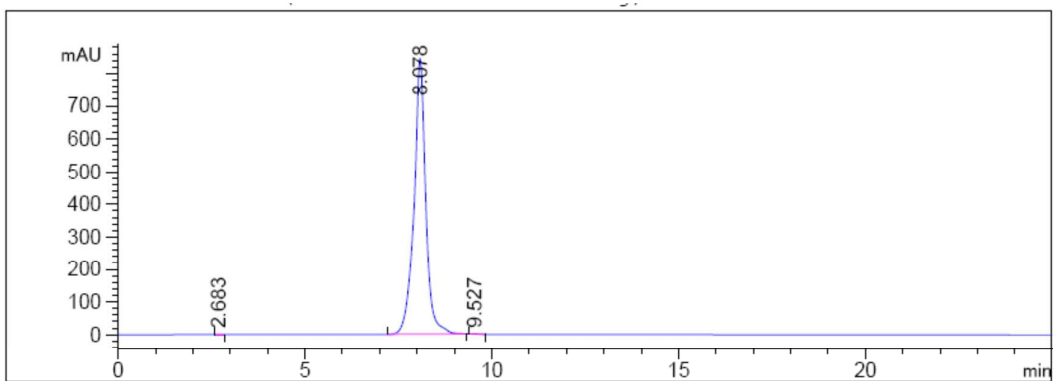


Signal 1: DAD1 A, Sig=220,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.747	BB	0.2160	9.62217	6.37750e-1	0.0207
2	7.704	BV	0.3721	54.74895	2.34778	0.1177
3	8.789	VV	0.4443	1573.00171	45.84112	3.3818
4	10.219	VB	0.3866	4.48347e4	1500.48645	96.3895
5	14.037	BB	0.3357	42.03625	1.85974	0.0904

Totals : 4.65141e4 1551.17284

## Compound 18

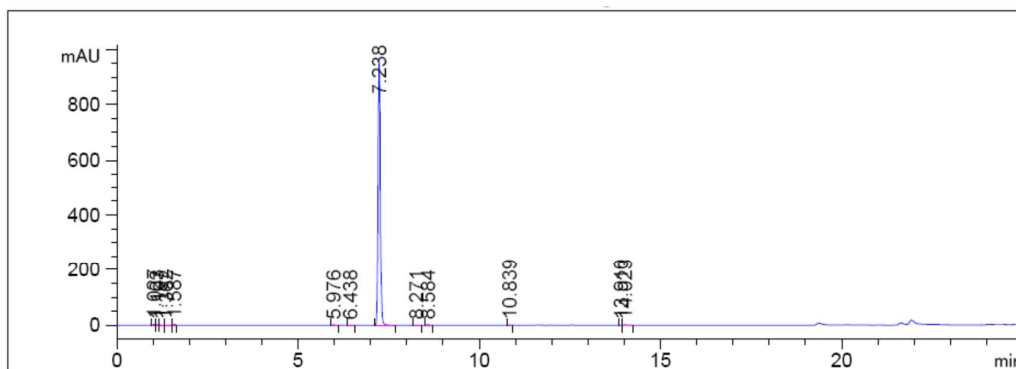


Signal 1: DAD1 A, Sig=220,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.683	BB	0.0928	3.53975	5.52285e-1	0.0192
2	8.078	BB	0.3125	1.84296e4	844.78271	99.9364
3	9.527	BB	0.1396	8.19396	9.60265e-1	0.0444

Totals : 1.84413e4 846.29526

# Compound 19



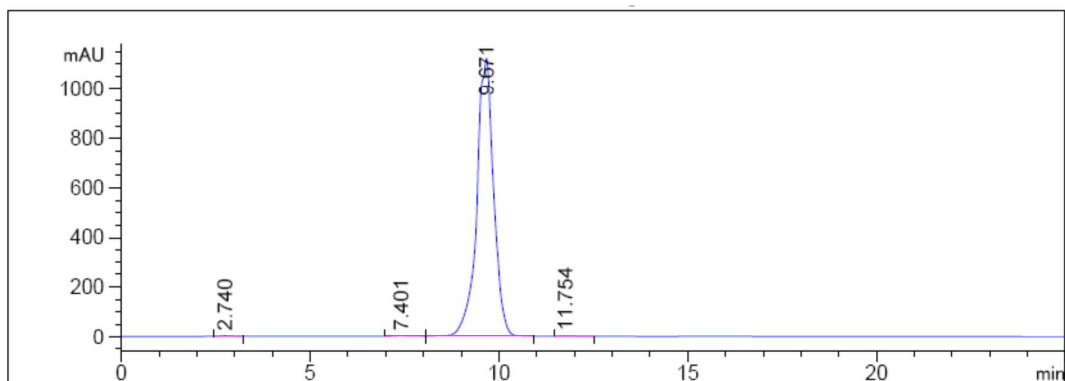
Signal 1: DAD1 A, Sig=220,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.027	BV	0.0592	12.32716	3.18151	0.2931
2	1.103	VV	0.0465	6.13435	1.86026	0.1458
3	1.197	VV	0.0769	6.48713	1.20390	0.1542
4	1.362	VV	0.1266	4.56747	4.81880e-1	0.1086
5	1.587	VV	0.0485	12.73649	4.07624	0.3028
6	5.976	BB	0.0654	9.08568	2.14389	0.2160
7	6.438	BB	0.0701	1.73642	3.88755e-1	0.0413
8	7.238	BB	0.0656	4124.84229	969.64282	98.0708
9	8.271	BB	0.1002	2.14039	2.96739e-1	0.0509
10	8.584	BB	0.0677	10.45311	2.36036	0.2485
11	10.839	BV	0.0627	2.37835	6.21186e-1	0.0565
12	13.910	VV	0.0629	1.69443	4.21071e-1	0.0403
13	14.023	VB	0.0818	11.40079	2.15125	0.2711

Totals : 4205.98405 988.82988

# Compound 24



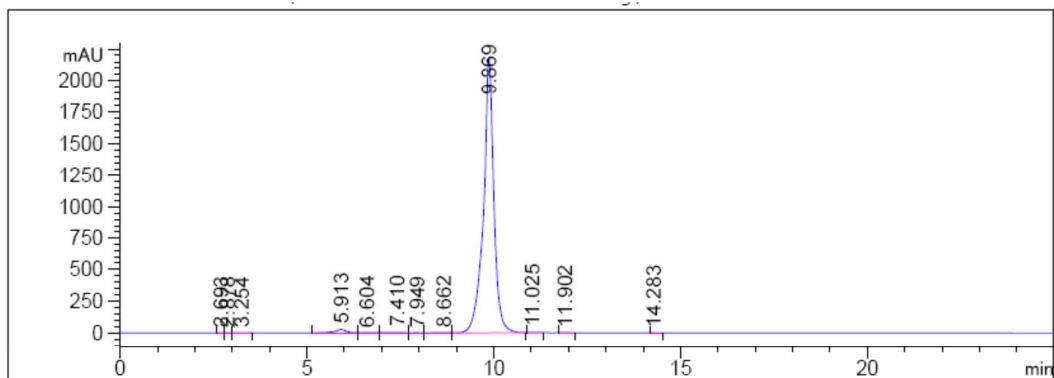


Signal 1: DAD1 A, Sig=220,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.740	BB	0.2887	40.67989	2.15032	0.1157
2	7.401	BV	0.4827	65.05402	1.86594	0.1851
3	9.671	VB	0.4042	3.50151e4	1121.52295	99.6048
4	11.754	BB	0.4061	33.17898	1.09320	0.0944

Totals : 3.51540e4 1126.63241

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Compound 25



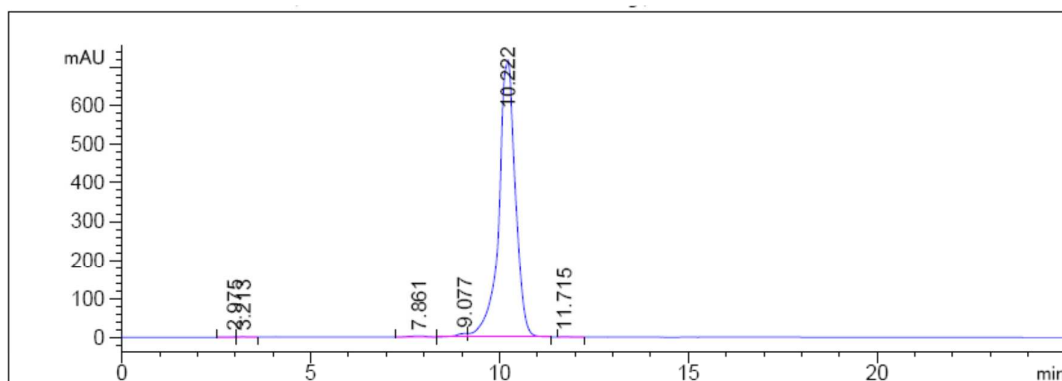
Signal 1: DAD1 A, Sig=220,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.693	BV	0.0909	10.55201	1.64442	0.0246
2	2.878	VV	0.1131	12.77536	1.60041	0.0297
3	3.254	VB	0.1926	13.50497	9.34767e-1	0.0314
4	5.913	BV	0.3145	603.12146	26.80430	1.4043
5	6.604	VV	0.3206	62.28036	2.64648	0.1450
6	7.410	VV	0.2997	65.57484	3.01521	0.1527
7	7.949	VV	0.1746	10.29826	9.06185e-1	0.0240
8	8.662	VV	0.2589	32.33676	1.80566	0.0753
9	9.869	VB	0.2713	4.20942e4	2180.13086	98.0091
10	11.025	BB	0.1613	14.82153	1.33723	0.0345
11	11.902	BB	0.1631	26.94684	2.51277	0.0627
12	14.283	BB	0.1233	2.84576	3.71926e-1	6.626e-3

Totals : 4.29493e4 2223.71024

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Compound 26



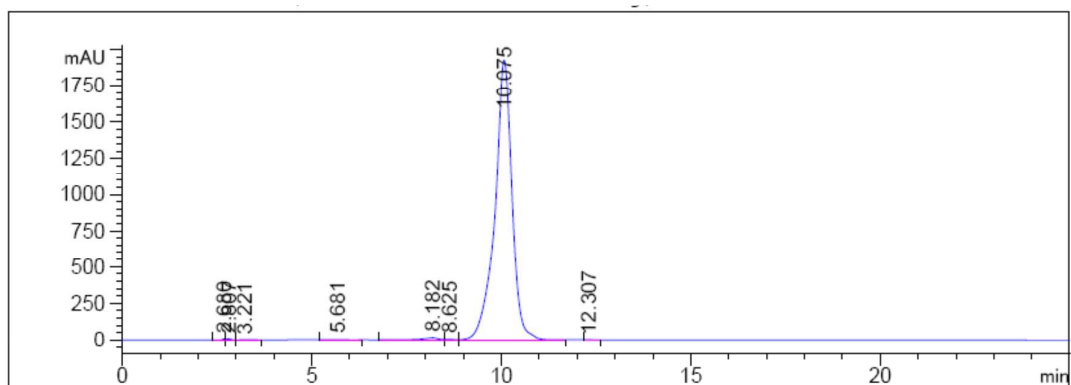
Signal 1: DAD1 A, Sig=220,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.975	BV	0.2594	14.43390	6.97526e-1	0.0654
2	3.213	VB	0.2838	19.68124	9.41816e-1	0.0892
3	7.861	BV	0.4354	79.37106	2.60526	0.3597
4	9.077	VV	0.3033	173.42979	8.67386	0.7859
5	10.222	VB	0.4003	2.17716e4	716.96167	98.6643
6	11.715	BB	0.2896	7.82345	4.31282e-1	0.0355

Totals : 2.20664e4 730.31142

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## Compound 27



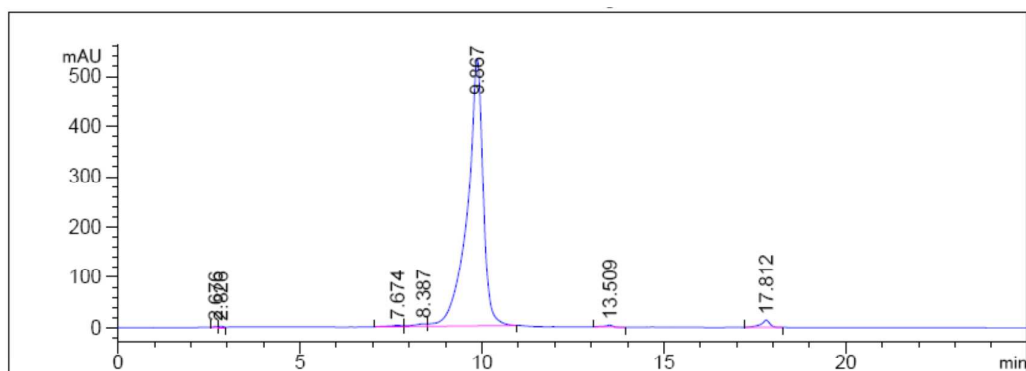
Signal 1: DAD1 A, Sig=220,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.680	BV	0.0861	39.09343	6.50727	0.0642
2	2.807	VV	0.1236	69.40466	8.65506	0.1139
3	3.221	VB	0.2672	28.91635	1.37565	0.0475
4	5.681	BB	0.3129	33.43967	1.75044	0.0549
5	8.182	BV	0.4389	439.61115	13.98020	0.7216
6	8.625	VV	0.2718	67.23055	3.73917	0.1104
7	10.075	VB	0.4549	6.02420e4	1925.88025	98.8796
8	12.307	BB	0.1484	4.89210	5.68472e-1	8.030e-3

Totals : 6.09246e4 1962.45651

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Compound 28



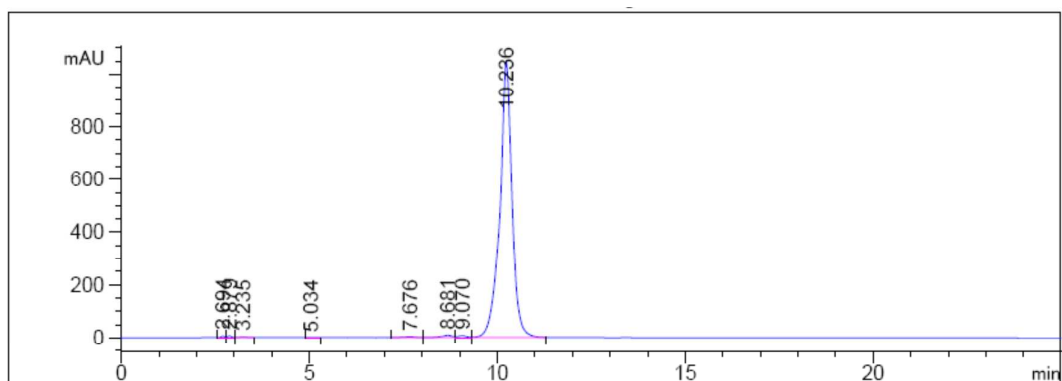
Signal 1: DAD1 A, Sig=220,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.676	BV	0.0841	11.99546	2.05481	0.0727
2	2.826	VV	0.1272	17.43382	2.13622	0.1057
3	7.674	BV	0.3411	61.33007	2.45821	0.3719
4	8.387	VV	0.3243	117.73526	5.00833	0.7139
5	9.867	VB	0.4168	1.59767e4	531.35901	96.8789
6	13.509	BB	0.2340	59.33834	3.64345	0.3598
7	17.812	BB	0.2393	246.88574	14.45211	1.4971

Totals : 1.64914e4 561.11214

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Compound 29



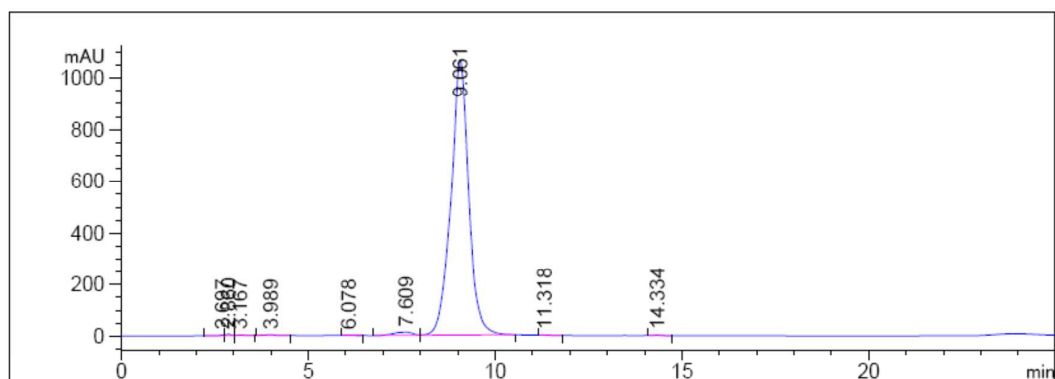
Signal 1: DAD1 A, Sig=220,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.694	BV	0.0967	37.91987	5.47892	0.1580
2	2.879	VV	0.1076	47.68562	6.35027	0.1987
3	3.235	VB	0.1874	28.03081	2.05175	0.1168
4	5.034	BB	0.1669	5.12682	4.64041e-1	0.0214
5	7.676	BV	0.3217	70.55417	3.16916	0.2941
6	8.681	VV	0.2709	164.24779	8.44403	0.6845
7	9.070	VV	0.2355	105.22010	6.47956	0.4385
8	10.236	VB	0.3197	2.35351e4	1049.04333	98.0879

Totals : 2.39939e4 1081.48107

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Compound 30



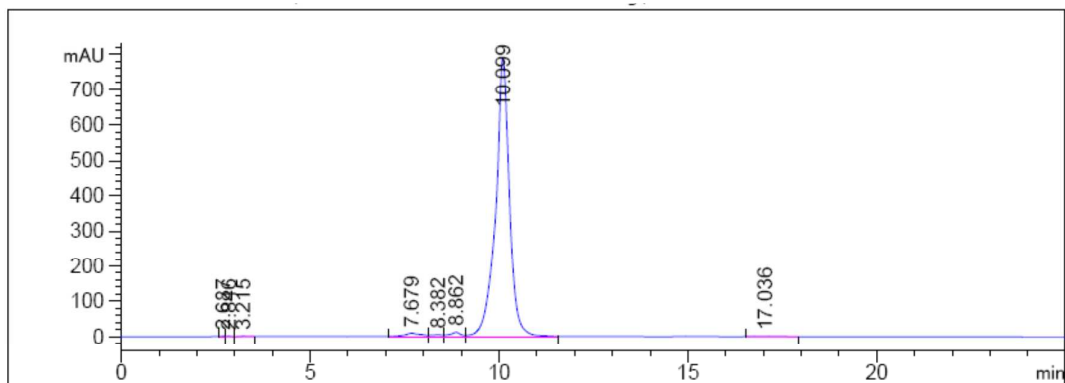
Signal 1: DAD1 A, Sig=220,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.697	BV	0.0996	14.55533	1.98273	0.0405
2	2.860	VV	0.1219	42.83889	5.32005	0.1193
3	3.167	VB	0.2215	15.46382	1.10365	0.0431
4	3.989	BB	0.2909	42.00998	2.23866	0.1170
5	6.078	BB	0.1728	8.41162	8.40007e-1	0.0234
6	7.609	BV	0.4724	438.46512	12.77718	1.2213
7	9.061	VB	0.4784	3.53079e4	1065.97620	98.3464
8	11.318	BB	0.2322	10.72654	7.81027e-1	0.0299
9	14.334	BB	0.2351	21.20993	1.39719	0.0591

Totals : 3.59016e4 1092.41668

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Compound 31



Signal 1: DAD1 A, Sig=220,4 Ref=360,100

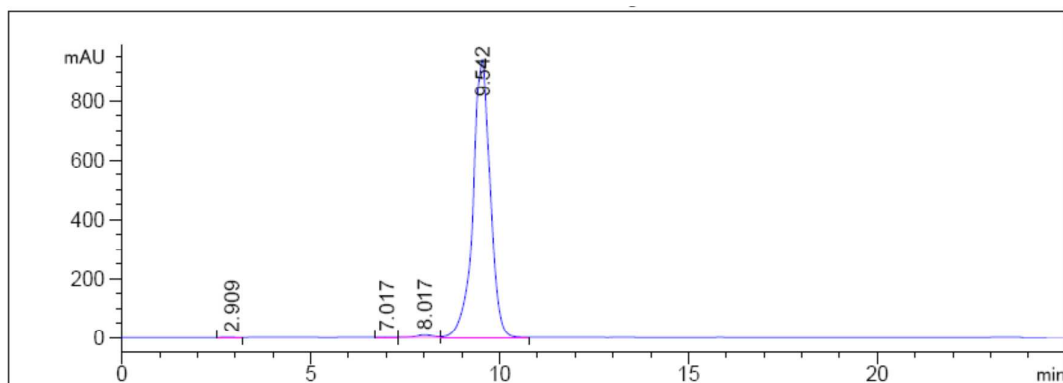
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.687	BV	0.0908	10.69815	1.66931	0.0517
2	2.846	VV	0.1396	12.59439	1.41891	0.0609
3	3.215	VB	0.2046	17.56045	1.27564	0.0849
4	7.679	BV	0.3778	258.92502	9.15943	1.2520
5	8.382	VV	0.2901	96.44301	4.49805	0.4663
6	8.862	VV	0.2633	218.34993	11.61788	1.0558
7	10.099	VB	0.3627	2.00246e4	787.40436	96.8231
8	17.036	BB	0.4991	42.45583	1.11272	0.2053

Totals : 2.06817e4 818.15630

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Compound 36



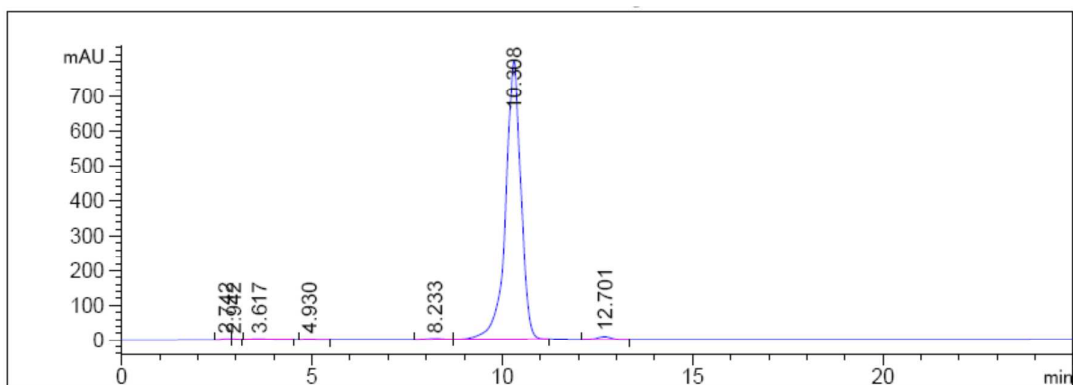
Signal 1: DAD1 A, Sig=220,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.909	BV	0.2610	15.24522	7.37976e-1	0.0506
2	7.017	BV	0.3301	15.15578	6.95889e-1	0.0504
3	8.017	VV	0.4794	246.55101	7.96022	0.8191
4	9.542	VB	0.4123	2.98227e4	939.58759	99.0799

Totals : 3.00997e4 948.98166

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Compound 37



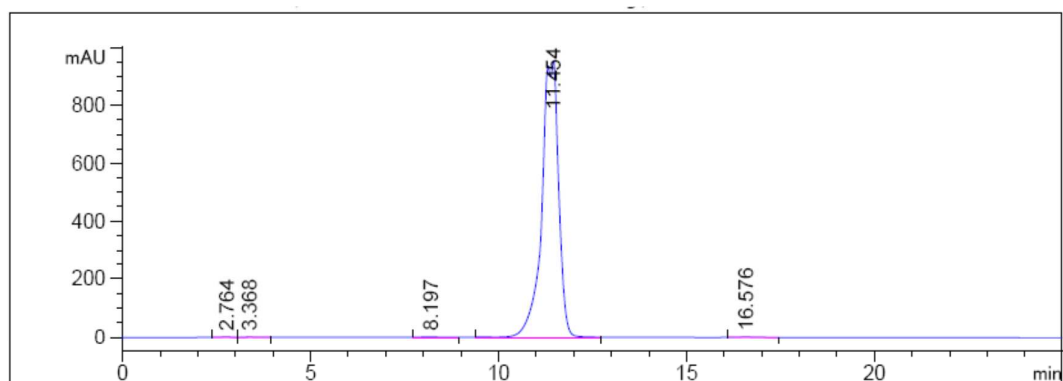
Signal 1: DAD1 A, Sig=220,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.742	BV	0.2055	29.16480	2.08151	0.1283
2	2.942	VB	0.1189	13.80542	1.56469	0.0607
3	3.617	BB	0.3375	42.45081	1.74678	0.1868
4	4.930	BB	0.3135	15.39694	6.86851e-1	0.0678
5	8.233	BV	0.3951	70.38641	2.60612	0.3097
6	10.308	VB	0.3674	2.23485e4	801.30280	98.3411
7	12.701	BB	0.3658	205.77980	8.51909	0.9055

Totals : 2.27255e4 818.50782

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Compound 38



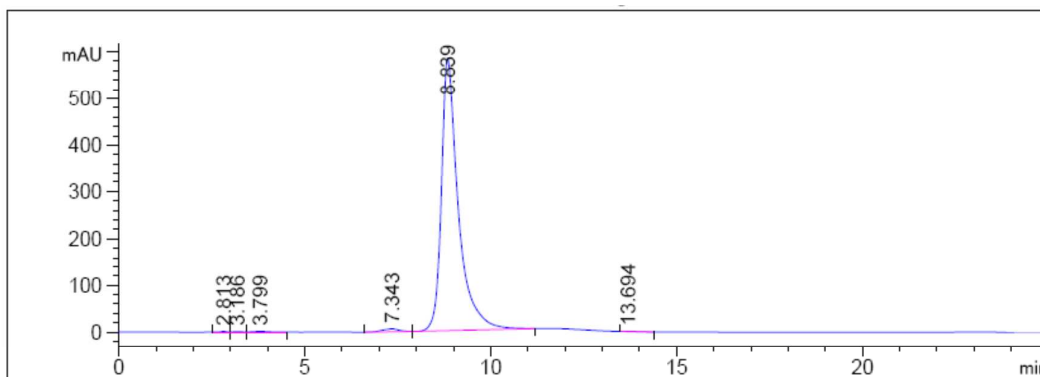
Signal 1: DAD1 A, Sig=220,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.764	BV	0.3245	27.36595	1.37307	0.0917
2	3.368	VB	0.4125	31.24514	1.10951	0.1047
3	8.197	BB	0.4785	30.22307	8.34498e-1	0.1013
4	11.454	BB	0.4038	2.97004e4	952.51892	99.5658
5	16.576	BB	0.5028	40.70169	1.28074	0.1364

Totals : 2.98299e4 957.11674

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Compound 39



Signal 1: DAD1 A, Sig=220,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.813	BV	0.1692	17.96299	1.57374	0.0963
2	3.186	VV	0.2000	17.28326	1.14586	0.0926
3	3.799	VB	0.3585	42.27412	1.61959	0.2265
4	7.343	BV	0.4036	184.72064	6.30796	0.9899
5	8.839	VB	0.4579	1.83857e4	583.01343	98.5232
6	13.694	BB	0.3379	13.35032	6.08581e-1	0.0715

Totals : 1.86613e4 594.26916

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