

Supporting Information

# Discovery of Arylsulfonamides as Dual Orexin Receptor Agonists

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Compound purity by HPLC

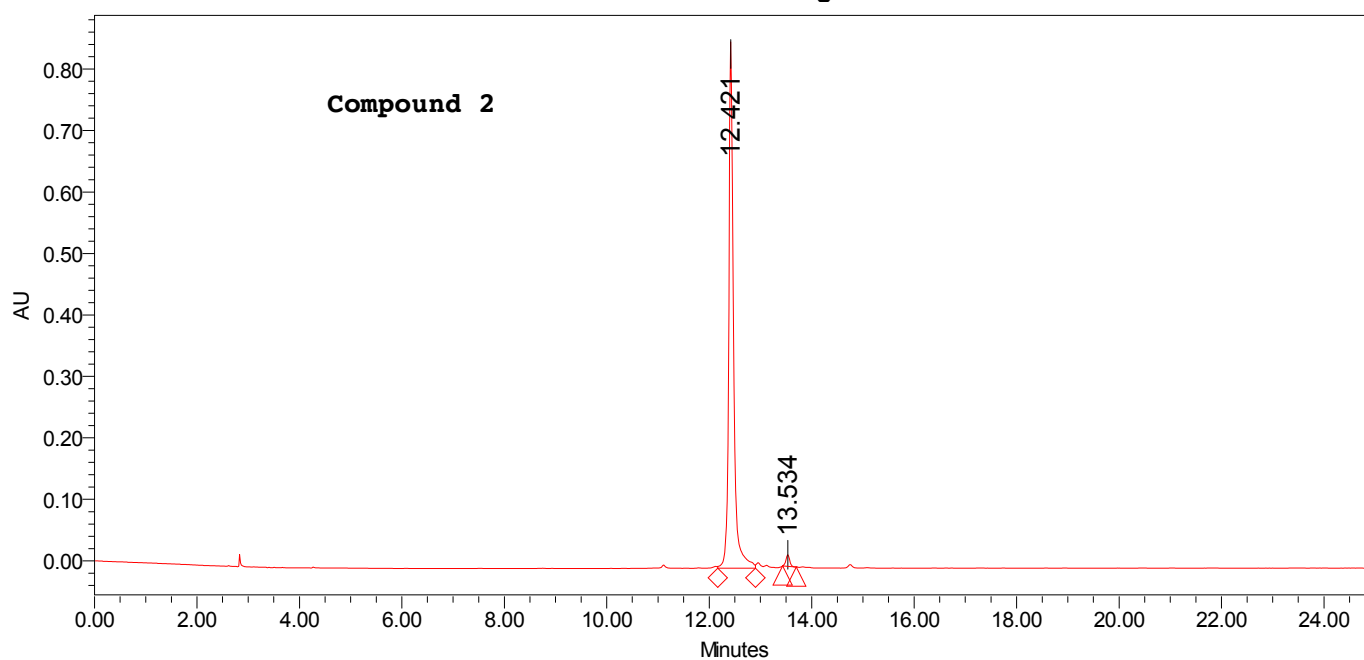
Compound	Retention time (min)	Purity (%)
2	12.421	98.3
6	13.372	98.4
7	13.576	>99
8	12.923	>99
9	13.105	99.0
10	11.049	96.8
11	11.084	95.0
12	15.528	99.0
13	11.274	95.1
14	12.154	96.9
15	15.874	>99
16	14.823	95.1
17	13.976	98.1
18	11.910	95.2
19	13.367	95.0
20	12.836	95.6
21	14.411	96.2
22	12.928	>99
23	14.793	>99
24	12.713	98.3
25	12.302	98.9
26	12.720	>99
27	13.467	>99
28	13.683	98.7
29	13.635	98.7
30	14.107	98.9
31	13.028	95.3
32	16.023	96.2
33	12.592	95.6
34	12.506	98.4
35	13.091	96.1

<b>36</b>	15.585	>99
<b>37</b>	12.767	98.6
<b>38</b>	12.642	>99
<b>39</b>	12.517	98.2
<b>40</b>	12.497	>99
<b>41</b>	12.653	98.1
<b>42</b>	12.395	97.8
<b>43</b>	13.951	98.5
<b>44</b>	12.455	>99

## SAMPLE INFORMATION

Sample Name:	13937-054	Acquired By:	walkup
Sample Type:	Unknown	Sample Set Name:	DehuiDavidHPLC
Vial:	1	Acq. Method Set:	MethodSetAB5T95B15Min
Injection #:	1	Processing Method:	220W280W15MIN
Injection Volume:	20.00 ul	Channel Name:	W2996 280.0nm-4.0
Run Time:	30.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA 280.0 nm at 4.0
Date Acquired:	1/27/2021 7:35:50 PM EST		
Date Processed:	4/2/2021 3:27:05 PM EST		

## Auto-Scaled Chromatogram



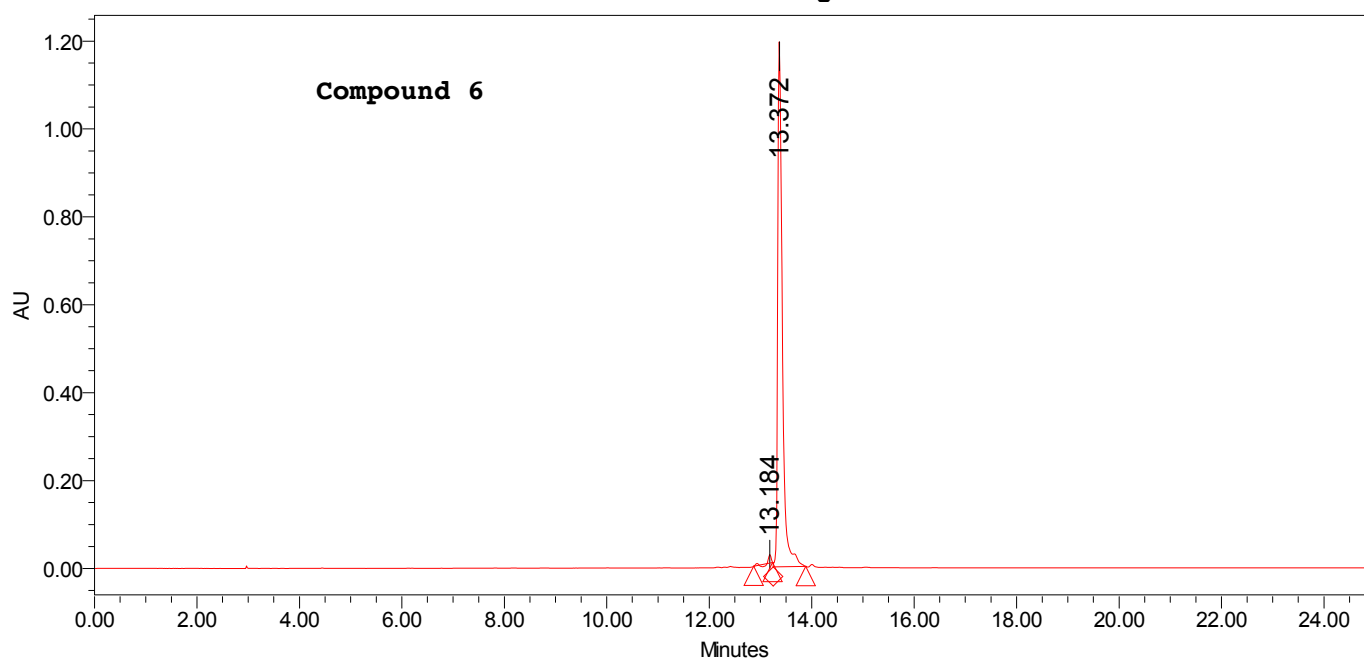
## Peak Results

	RT	Area	% Area	Height
1	12.421	5498165	98.29	851114
2	13.534	95466	1.71	18474

## SAMPLE INFORMATION

Sample Name:	13937-081	Acquired By:	walkup
Sample Type:	Unknown	Sample Set Name:	DehuiDavidHPLC
Vial:	5	Acq. Method Set:	MethodSetAB5T95B15Min
Injection #:	1	Processing Method:	220W280W15MIN
Injection Volume:	20.00 ul	Channel Name:	W2996 280.0nm-4.0
Run Time:	30.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA 280.0 nm at 4.0
Date Acquired:	1/27/2021 9:39:58 PM EST		
Date Processed:	4/2/2021 3:59:12 PM EST		

## Auto-Scaled Chromatogram



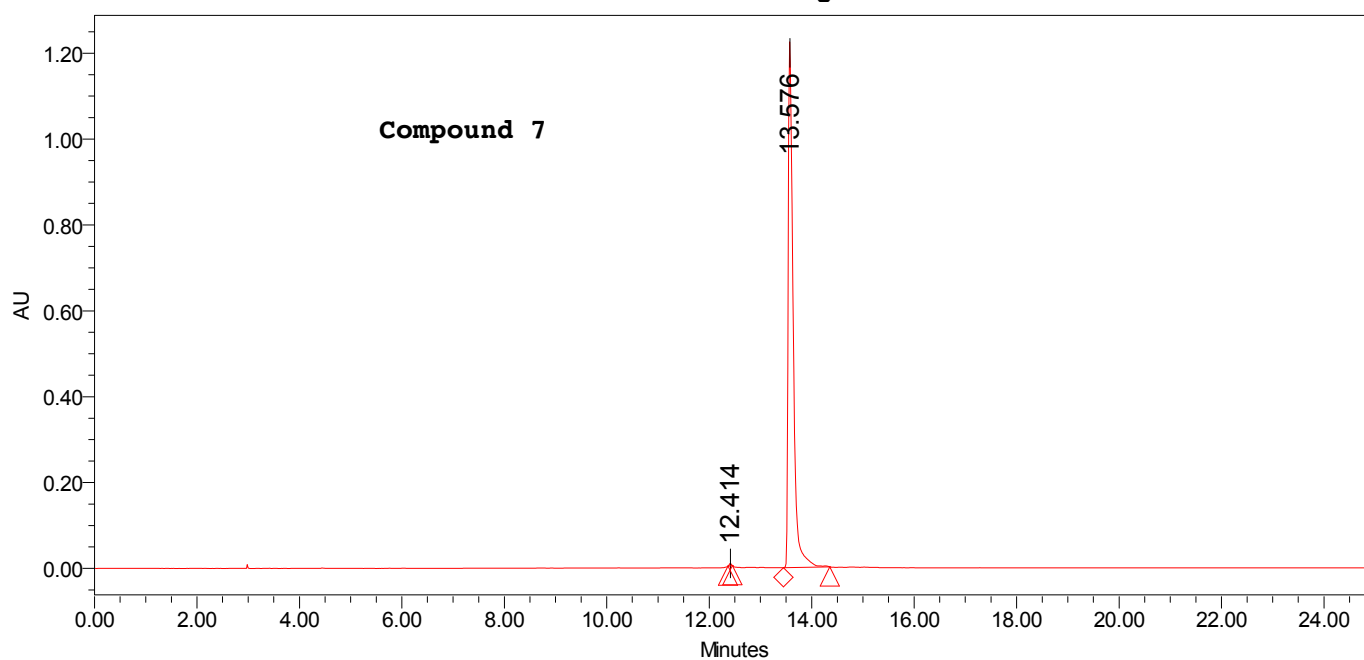
## Peak Results

	RT	Area	% Area	Height
1	13.184	118486	1.58	18186
2	13.372	7396048	98.42	1204050

## SAMPLE INFORMATION

Sample Name:	13937-074	Acquired By:	walkup
Sample Type:	Unknown	Sample Set Name:	DehuiDavidHPLC
Vial:	2	Acq. Method Set:	MethodSetAB5T95B15Min
Injection #:	1	Processing Method:	220W280W15MIN
Injection Volume:	20.00 ul	Channel Name:	W2996 280.0nm-4.0
Run Time:	30.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA 280.0 nm at 4.0
Date Acquired:	1/27/2021 8:06:52 PM EST		
Date Processed:	4/2/2021 4:00:39 PM EST		

## Auto-Scaled Chromatogram



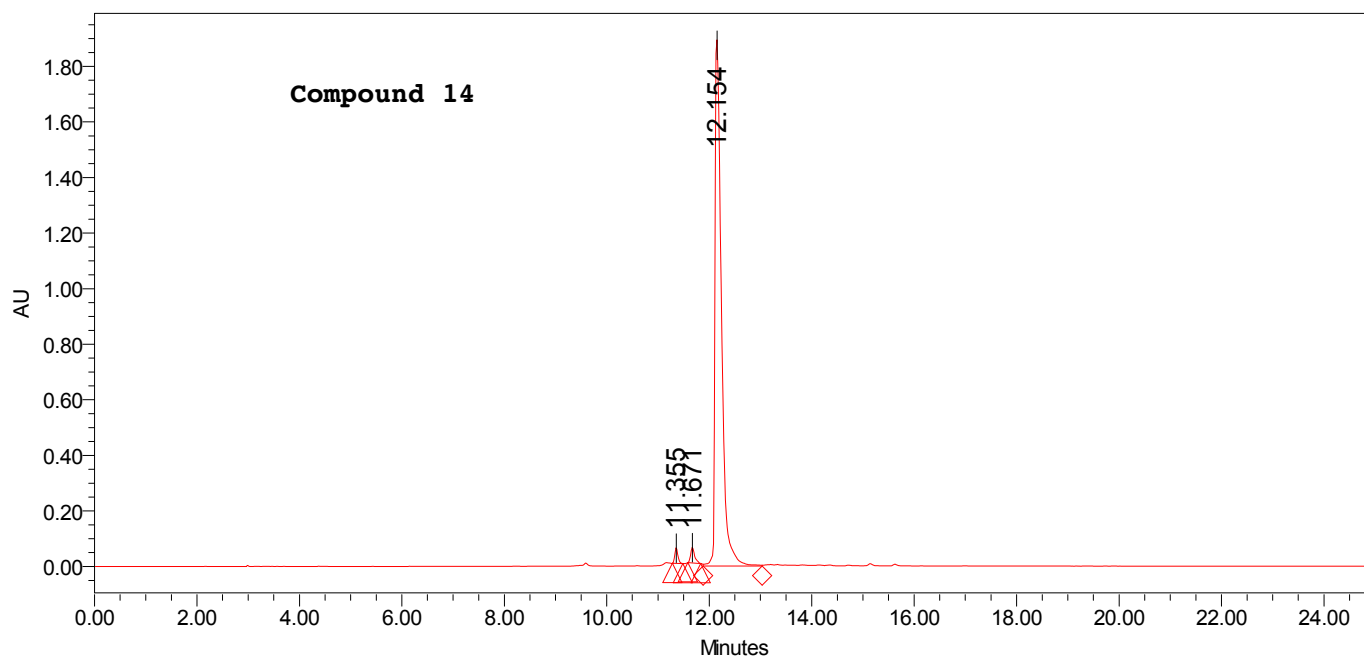
## Peak Results

	RT	Area	% Area	Height
1	12.414	15531	0.19	5298
2	13.576	8317200	99.81	1256770

## SAMPLE INFORMATION

Sample Name:	14045-085	Acquired By:	walkup
Sample Type:	Unknown	Sample Set Name:	DehuiDavidHPLC
Vial:	12	Acq. Method Set:	MethodSetAB5T95B15Min
Injection #:	1	Processing Method:	220W280W15MIN
Injection Volume:	20.00 ul	Channel Name:	W2996 280.0nm-4.0
Run Time:	30.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA 280.0 nm at 4.0
Date Acquired:	1/28/2021 1:17:08 AM EST		
Date Processed:	4/2/2021 4:03:30 PM EST		

## Auto-Scaled Chromatogram



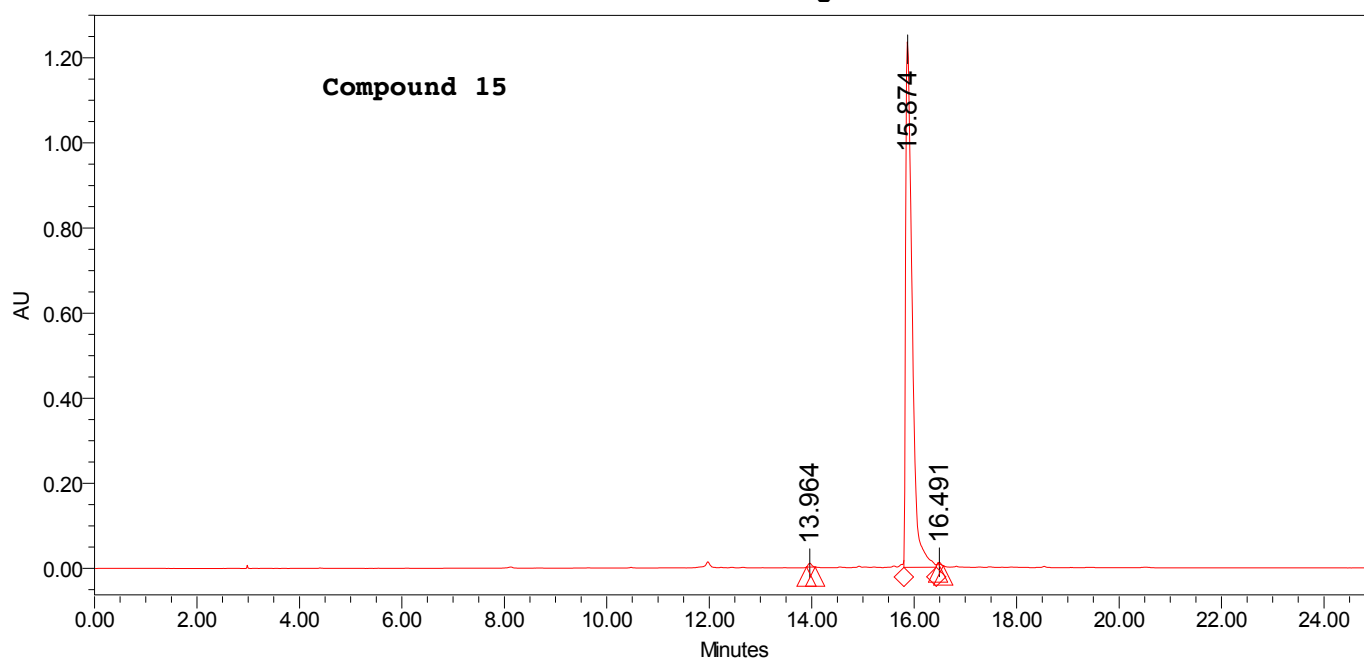
## Peak Results

	RT	Area	% Area	Height
1	11.355	233116	1.35	54519
2	11.671	300555	1.74	54890
3	12.154	16725811	96.91	1914526

## SAMPLE INFORMATION

Sample Name:	14045-093	Acquired By:	walkup
Sample Type:	Unknown	Sample Set Name:	DehuiDavidHPLC
Vial:	13	Acq. Method Set:	MethodSetAB5T95B15Min
Injection #:	1	Processing Method:	220W280W15MIN
Injection Volume:	20.00 ul	Channel Name:	W2996 280.0nm-4.0
Run Time:	30.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA 280.0 nm at 4.0
Date Acquired:	1/28/2021 1:48:11 AM EST		
Date Processed:	4/2/2021 4:07:03 PM EST		

## Auto-Scaled Chromatogram



## Peak Results

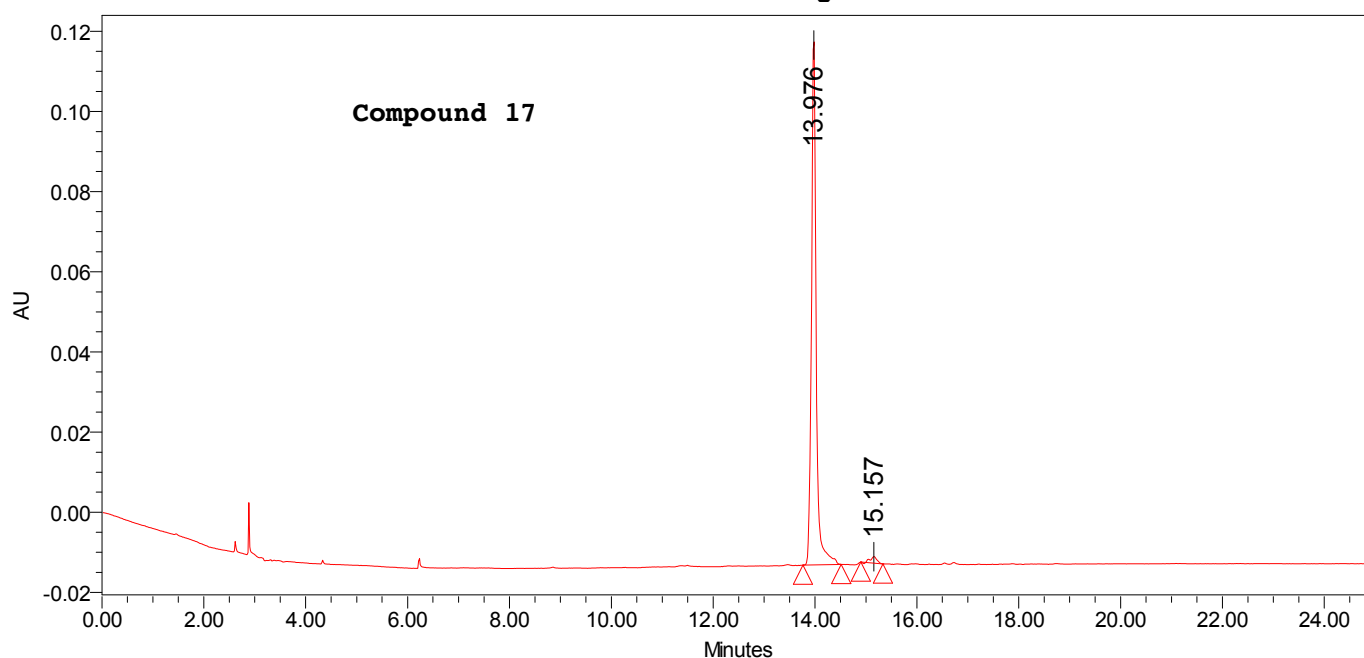
	RT	Area	% Area	Height
1	13.964	42013	0.39	8978
2	15.874	10856650	99.51	1266499
3	16.491	11883	0.11	3511



## SAMPLE INFORMATION

Sample Name:	DZ14227-23	Acquired By:	walkup
Sample Type:	Unknown	Sample Set Name:	DZ142272325
Vial:	25	Acq. Method Set:	MethodSetAB5T95B15Min
Injection #:	1	Processing Method:	220W280W15MIN
Injection Volume:	20.00 ul	Channel Name:	W2996 280.0nm-4.0
Run Time:	30.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA 280.0 nm at 4.0
Date Acquired:	9/1/2020 7:35:26 PM EDT		
Date Processed:	4/2/2021 4:27:47 PM EST		

## Auto-Scaled Chromatogram



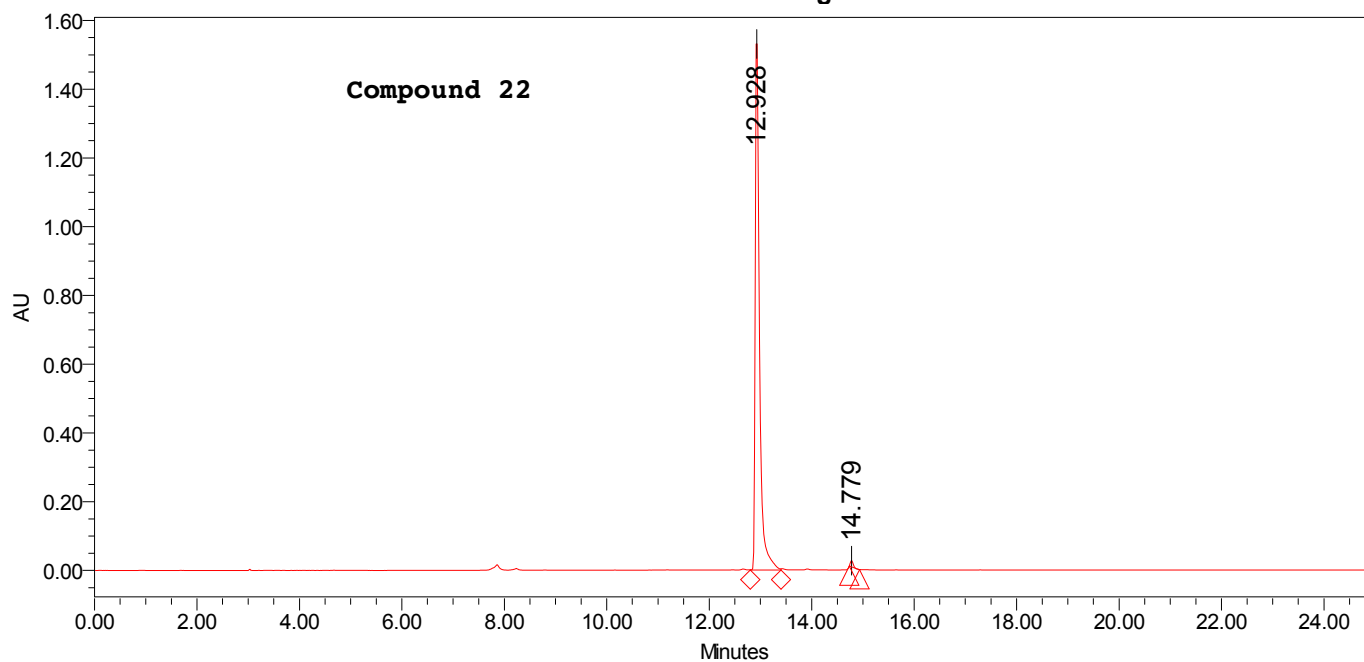
## Peak Results

	RT	Area	% Area	Height
1	13.976	841421	98.10	130310
2	15.157	16278	1.90	1659

## SAMPLE INFORMATION

Sample Name:	14045-181	Acquired By:	walkup
Sample Type:	Unknown	Sample Set Name:	DehuiDavidHPLC
Vial:	17	Acq. Method Set:	MethodSetAB5T95B15Min
Injection #:	1	Processing Method:	220W280W15MIN
Injection Volume:	20.00 ul	Channel Name:	W2996 280.0nm-4.0
Run Time:	30.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA 280.0 nm at 4.0
Date Acquired:	1/28/2021 3:52:18 AM EST		
Date Processed:	4/2/2021 4:13:14 PM EST		

## Auto-Scaled Chromatogram



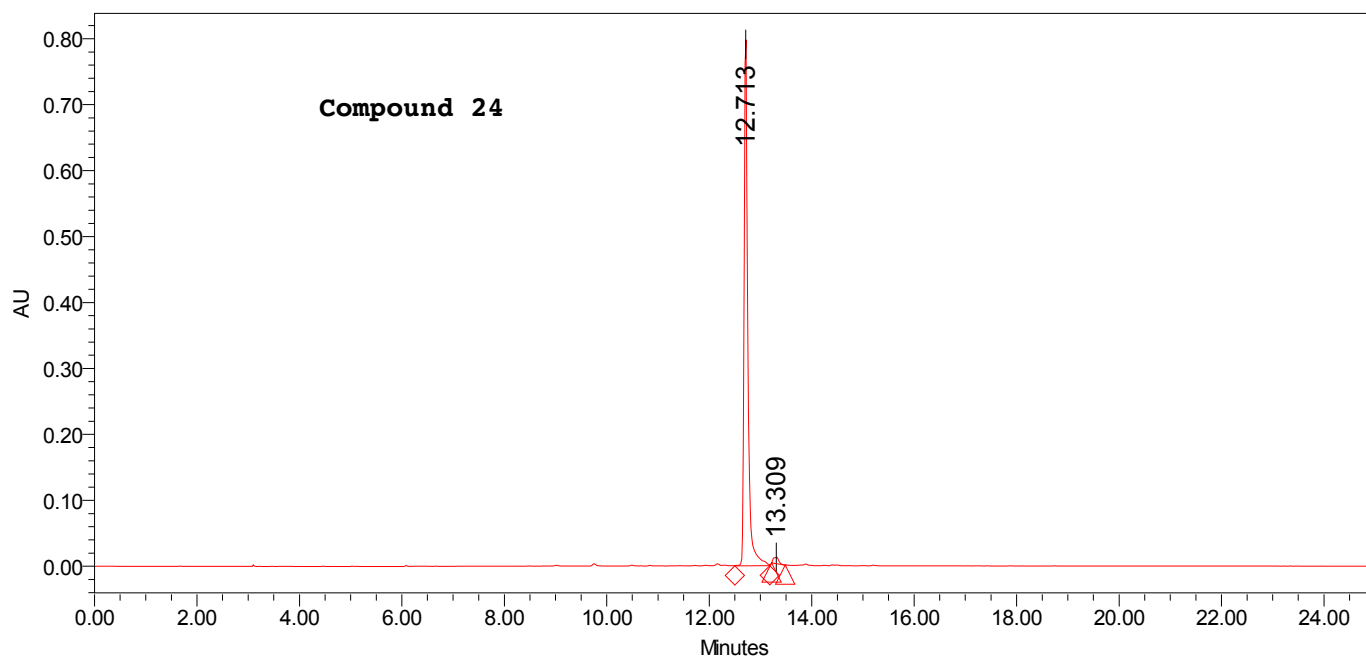
## Peak Results

	RT	Area	% Area	Height
1	12.928	9081791	99.21	1563802
2	14.779	72481	0.79	18104

## SAMPLE INFORMATION

Sample Name:	14171-57	Acquired By:	walkup
Sample Type:	Unknown	Sample Set Name:	DZOXAgonist paper
Vial:	98	Acq. Method Set:	MethodSetAB5T95B15Min
Injection #:	1	Processing Method:	220W280W15MIN
Injection Volume:	10.00 ul	Channel Name:	W2996 280.0nm-4.0
Run Time:	30.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA 280.0 nm at 4.0
Date Acquired:	9/4/2020 7:42:29 PM EDT		
Date Processed:	4/2/2021 4:29:40 PM EST		

## Auto-Scaled Chromatogram



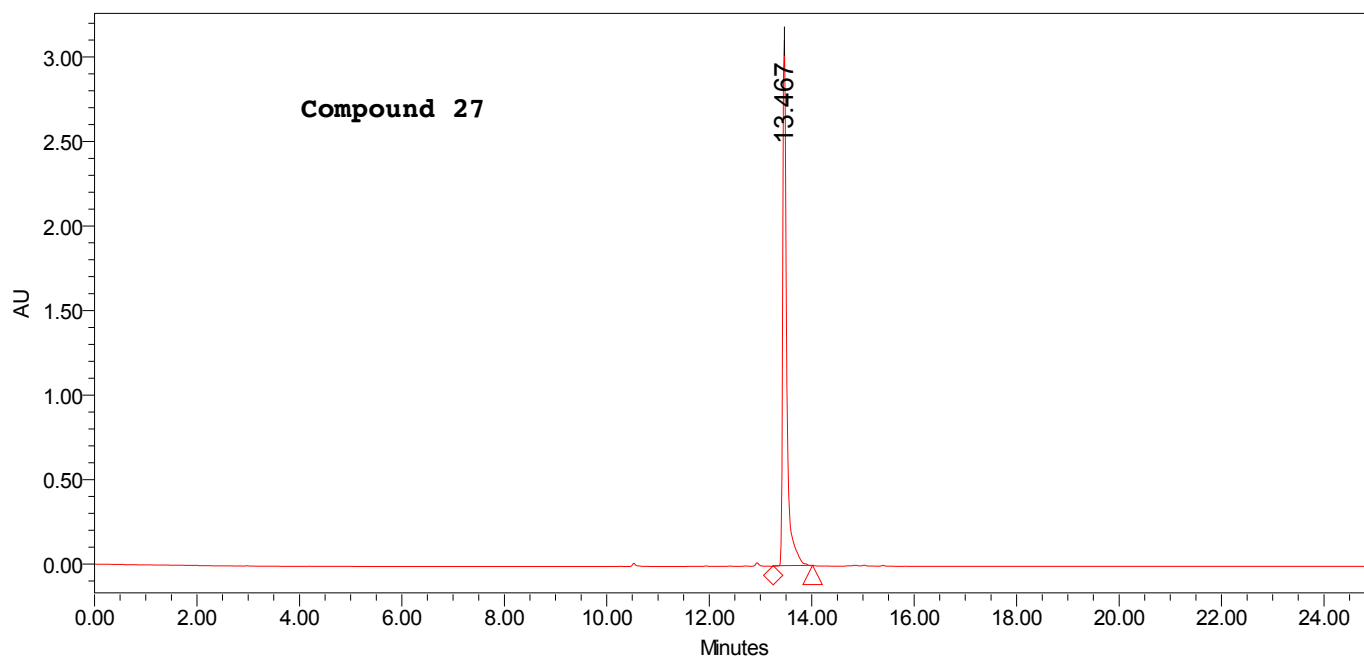
## Peak Results

	RT	Area	% Area	Height
1	12.713	4034950	98.29	785179
2	13.309	70221	1.71	9906

## SAMPLE INFORMATION

Sample Name:	14171-62	Acquired By:	walkup
Sample Type:	Unknown	Sample Set Name:	DZ1417162OXpaper
Vial:	1	Acq. Method Set:	MethodSetAB5T95B15Min
Injection #:	1	Processing Method:	220W280W15MIN
Injection Volume:	10.00 ul	Channel Name:	W2996 280.0nm-4.0
Run Time:	30.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA 280.0 nm at 4.0
Date Acquired:	9/5/2020 3:47:42 PM EDT		
Date Processed:	4/2/2021 4:31:33 PM EST		

## Auto-Scaled Chromatogram



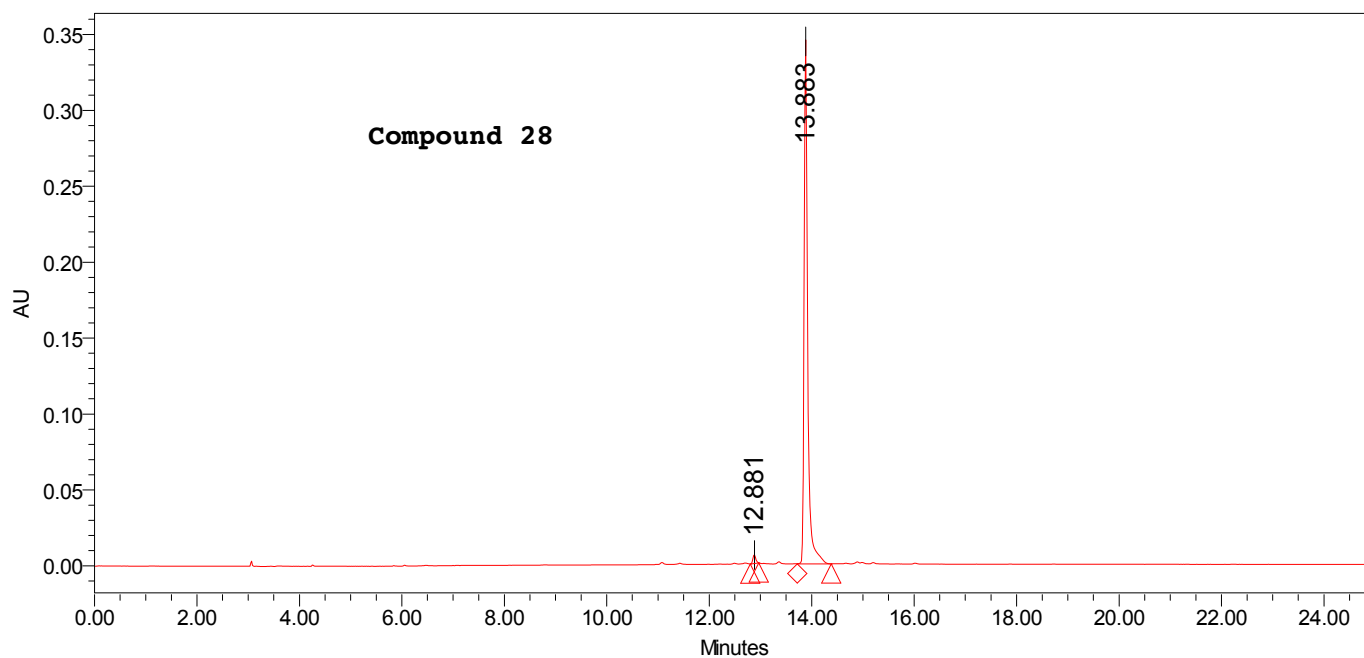
## Peak Results

	RT	Area	% Area	Height
1	13.467	16853280	100.00	3135157

## SAMPLE INFORMATION

Sample Name:	14171-65	Acquired By:	walkup
Sample Type:	Unknown	Sample Set Name:	DZOXAgonist paper
Vial:	100	Acq. Method Set:	MethodSetAB5T95B15Min
Injection #:	1	Processing Method:	220W280W15MIN
Injection Volume:	10.00 ul	Channel Name:	W2996 280.0nm-4.0
Run Time:	30.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA 280.0 nm at 4.0
Date Acquired:	9/4/2020 8:44:24 PM EDT		
Date Processed:	4/2/2021 4:32:39 PM EST		

## Auto-Scaled Chromatogram



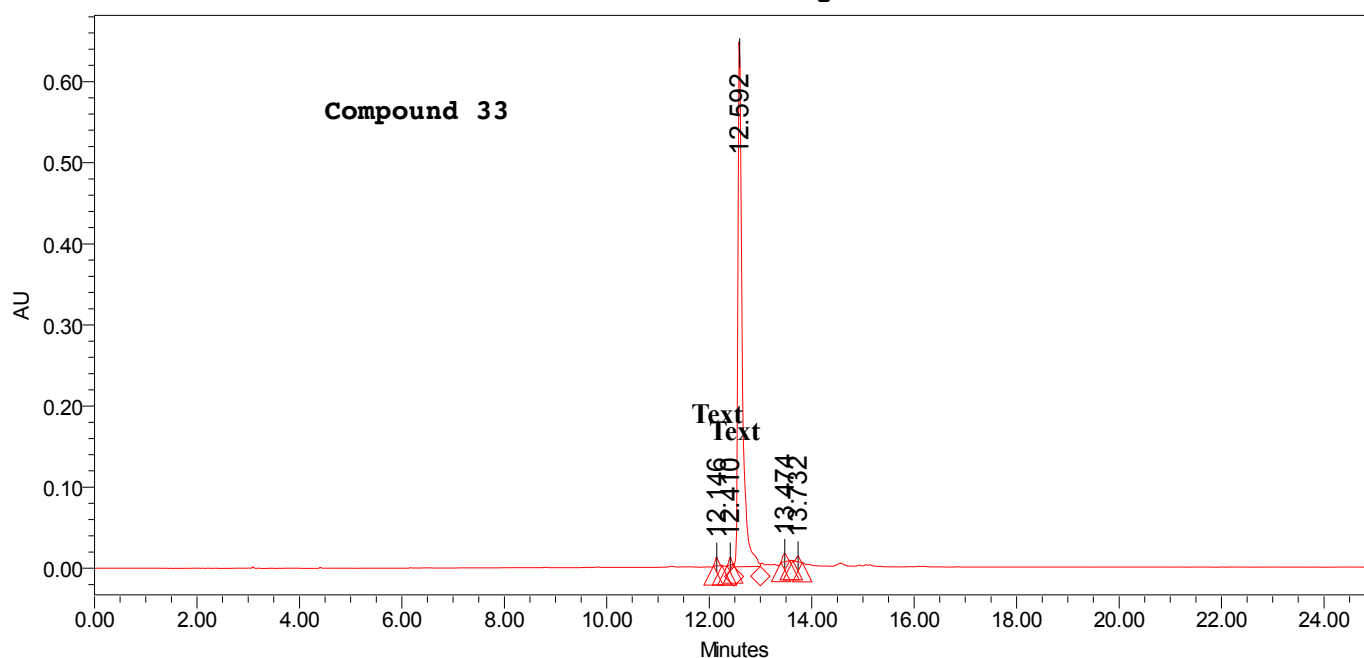
## Peak Results

	RT	Area	% Area	Height
1	12.881	22097	1.30	5511
2	13.883	1680846	98.70	335519

## SAMPLE INFORMATION

Sample Name:	14171-113	Acquired By:	walkup
Sample Type:	Unknown	Sample Set Name:	DZOXAgonist paper
Vial:	106	Acq. Method Set:	MethodSetAB5T95B15Min
Injection #:	1	Processing Method:	220W280W15MIN
Injection Volume:	10.00 ul	Channel Name:	W2996 280.0nm-4.0
Run Time:	30.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA 280.0 nm at 4.0
Date Acquired:	9/4/2020 11:50:09 PM EDT		
Date Processed:	4/2/2021 4:36:56 PM EST		

## Auto-Scaled Chromatogram



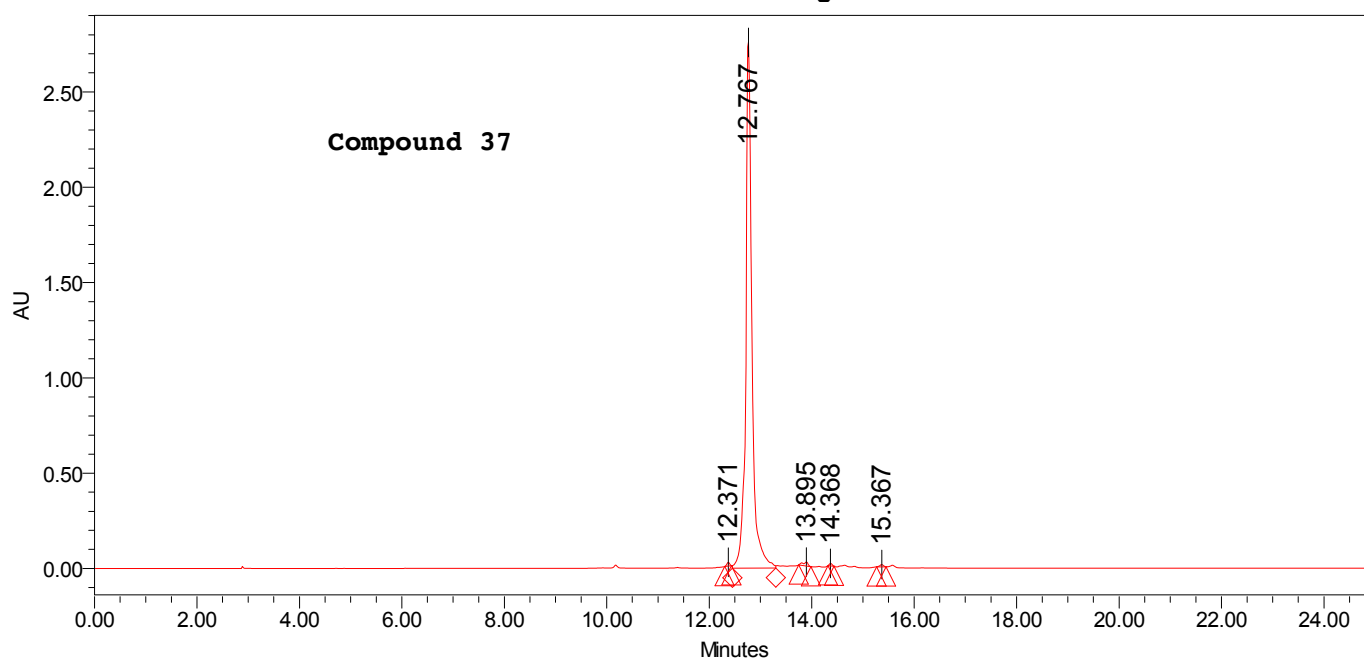
## Peak Results

	RT	Area	% Area	Height
1	12.146	47544	1.20	10379
2	12.410	34343	0.87	9099
3	12.592	3792449	95.63	646464
4	13.474	58210	1.47	10043
5	13.732	33009	0.83	6942

## SAMPLE INFORMATION

Sample Name:	14171-116	Acquired By:	walkup
Sample Type:	Unknown	Sample Set Name:	DZOXAgonist paper
Vial:	109	Acq. Method Set:	MethodSetAB5T95B15Min
Injection #:	1	Processing Method:	220W280W15MIN
Injection Volume:	30.00 ul	Channel Name:	W2996 280.0nm-4.0
Run Time:	30.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA 280.0 nm at 4.0
Date Acquired:	9/5/2020 1:23:09 AM EDT		
Date Processed:	4/2/2021 4:38:39 PM EST		

## Auto-Scaled Chromatogram



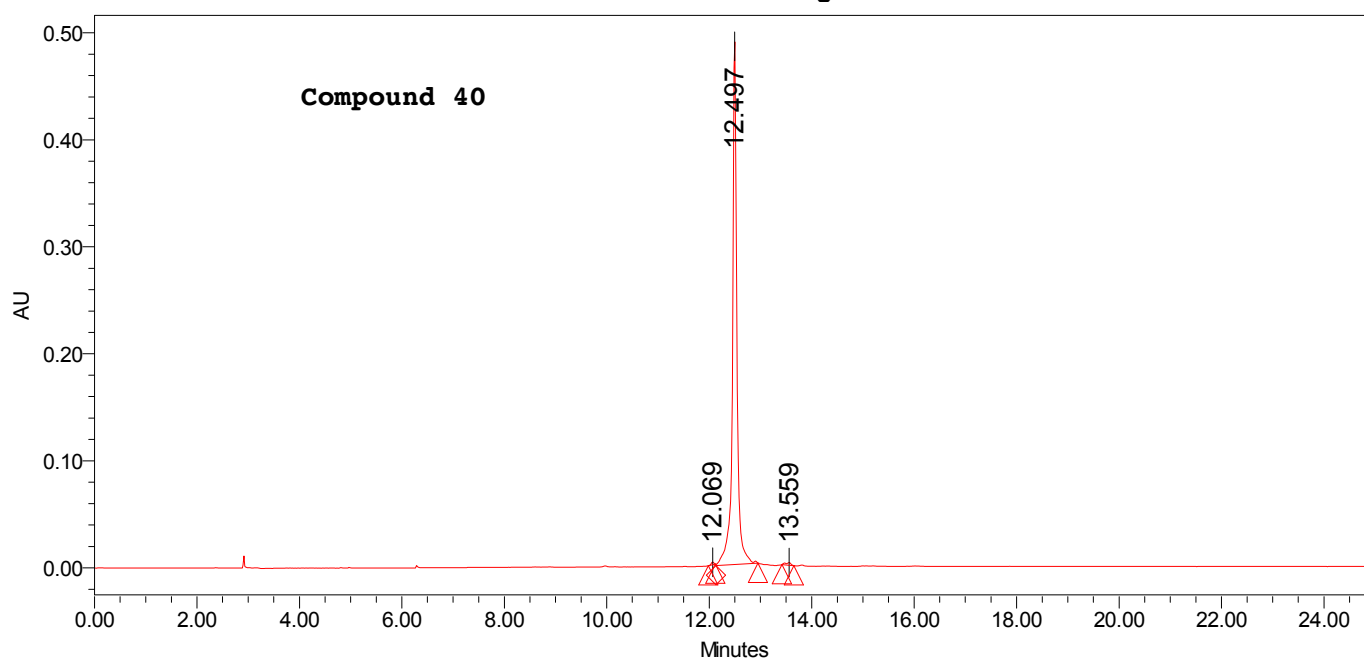
## Peak Results

	RT	Area	% Area	Height
1	12.371	75931	0.32	19529
2	12.767	23094517	98.59	2789966
3	13.895	145299	0.62	21135
4	14.368	52928	0.23	13121
5	15.367	56836	0.24	11613

## SAMPLE INFORMATION

Sample Name:	14171-143	Acquired By:	walkup
Sample Type:	Unknown	Sample Set Name:	DZOXAgonist paper
Vial:	114	Acq. Method Set:	MethodSetAB5T95B15Min
Injection #:	1	Processing Method:	220W280W15MIN
Injection Volume:	30.00 ul	Channel Name:	W2996 280.0nm-4.0
Run Time:	30.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA 280.0 nm at 4.0
Date Acquired:	9/5/2020 3:58:14 AM EDT		
Date Processed:	4/2/2021 4:40:01 PM EST		

## Auto-Scaled Chromatogram



## Peak Results

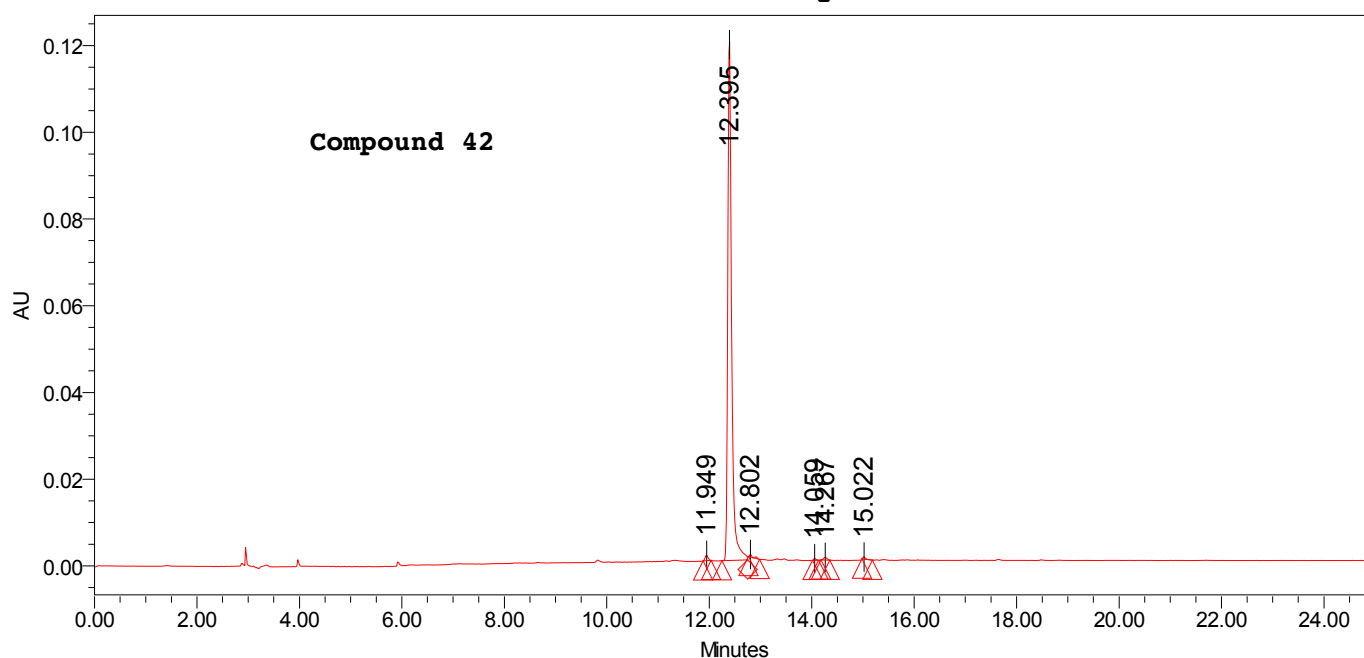
	RT	Area	% Area	Height
1	12.069	9075	0.30	2385
2	12.497	3007715	99.09	482507
3	13.559	18681	0.62	2539



## SAMPLE INFORMATION

Sample Name:	DZ14171-171	Acquired By:	walkup
Sample Type:	Unknown	Sample Set Name:	14171170195
Vial:	27	Acq. Method Set:	MethodSetAB5T95B15Min
Injection #:	1	Processing Method:	220W280W15MIN
Injection Volume:	10.00 ul	Channel Name:	W2996 280.0nm-4.0
Run Time:	30.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA 280.0 nm at 4.0
Date Acquired:	8/31/2020 8:13:45 PM EDT		
Date Processed:	4/2/2021 4:46:38 PM EST		

## Auto-Scaled Chromatogram



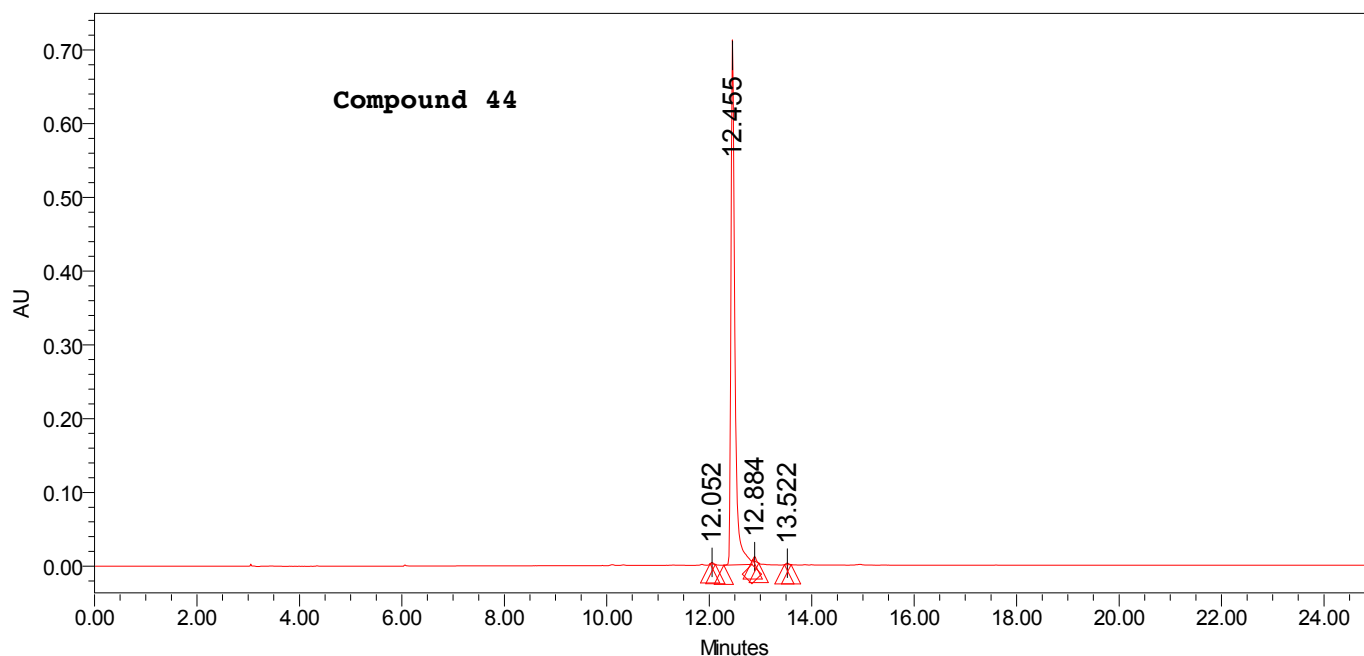
## Peak Results

	RT	Area	% Area	Height
1	11.949	5247	0.82	1249
2	12.395	625949	97.82	118736
3	12.802	2897	0.45	561
4	14.059	1235	0.19	356
5	14.267	2749	0.43	596
6	15.022	1850	0.29	500

## SAMPLE INFORMATION

Sample Name:	DZ14171-195	Acquired By:	walkup
Sample Type:	Unknown	Sample Set Name:	14171170195
Vial:	28	Acq. Method Set:	MethodSetAB5T95B15Min
Injection #:	1	Processing Method:	220W280W15MIN
Injection Volume:	10.00 ul	Channel Name:	W2996 280.0nm-4.0
Run Time:	30.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA 280.0 nm at 4.0
Date Acquired:	8/31/2020 8:44:46 PM EDT		
Date Processed:	4/2/2021 4:49:27 PM EST		

## Auto-Scaled Chromatogram

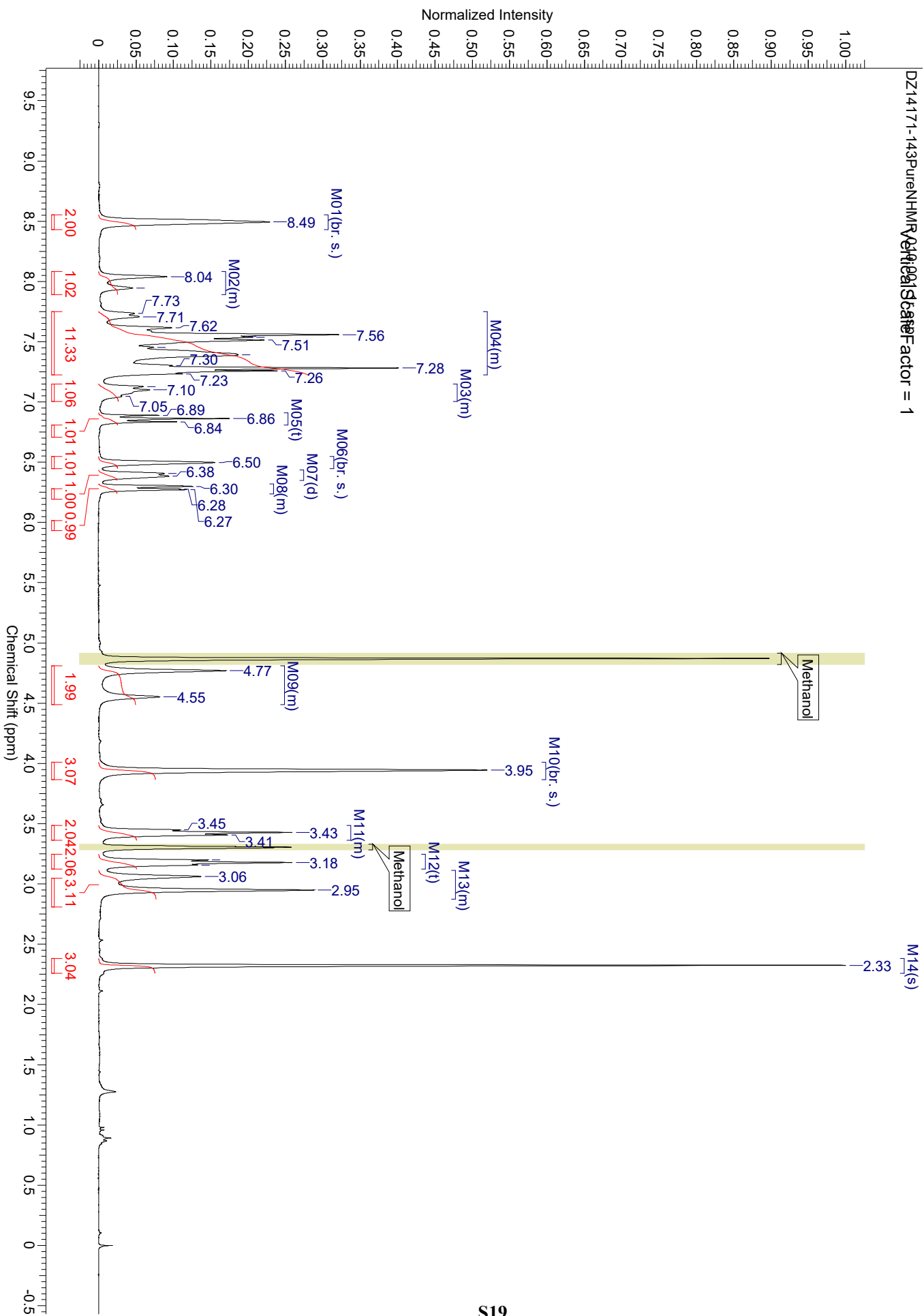


## Peak Results

	RT	Area	% Area	Height
1	12.052	7038	0.18	2102
2	12.455	3786738	99.07	700017
3	12.884	19634	0.51	5712
4	13.522	8852	0.23	2185

# Compound 40

DZ14171-143PureNHMR 01/19/2015 Gain Factor = 1



# Compound 40

