

## SUPPORTING INFORMATION

# **Systematic Structure Modifications of Multi-target Prostate Cancer Clinical Candidate Galeterone to Produce Novel Androgen Receptor Down-regulating Agents as an Approach to Treatment of Advanced Prostate Cancer**

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<sup>#</sup>These authors contributed equally to the work performed in this manuscript.

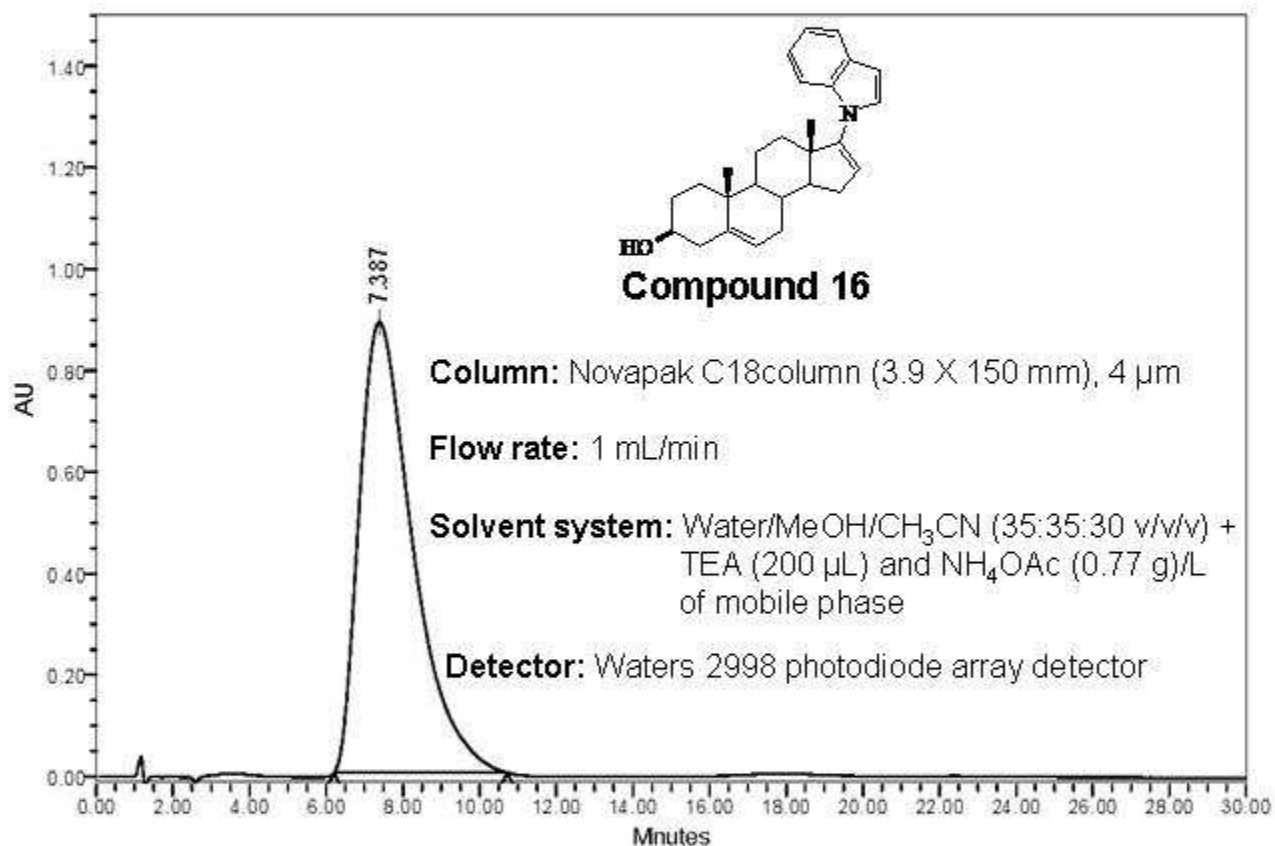
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**Contents:** HPLC chromatograms and high resolution mass spectral data for compounds **16 – 22, 25, 28, 31** and **33 – 49**. This material is available free of charge via the internet at <http://pubs.acs.org>

**SAMPLE INFORMATION**

Sample Name: VNPT144  
 Sample Type: Unknown  
 Vial: 23  
 Injection #: 1  
 Injection Volume: 20.00 ul  
 Run Time: 30.0 Minutes  
 Sample Set Name: Puru Sample Set 2

Acquired By: System  
 Date Acquired: 4/13/2012 12:08:12 AM  
 Acq. Method Set: VN124  
 Date Processed: 4/13/2012 10:49:19 AM  
 Processing Method: VN124venky  
 Channel Name: WIn Ch1  
 Proc. Chnl. Descr.: FDA 242.7 nm



**PDA Result Table**

	Name	RT	Area	Purity (#1) Angle	Purity (#1) Threshold	Purity Flag	Match (#1) Spect. Name	Match (#1) Angle	Match (#1) Threshold	PDA Match Flag
1		7.387	85848846			No				No

Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (µV*sec)	% Area	Height (µV)	Int Type	Amount
1	7.387							85848846	100.00	887465	bb	

# Mass Spectrum List Report

## Analysis Info

Analysis Name VNPT144\_pos\_000001.d

Method XMASS\_Method

Sample Name: VNPT144\_pos  
VNPT144\_pos: in 1:1 THF:MeOH w/ NaCl.

Acquisition Date 12/13/2010 3:22:31 PM

Operator FTMS\_USER

Instrument apex-Qe

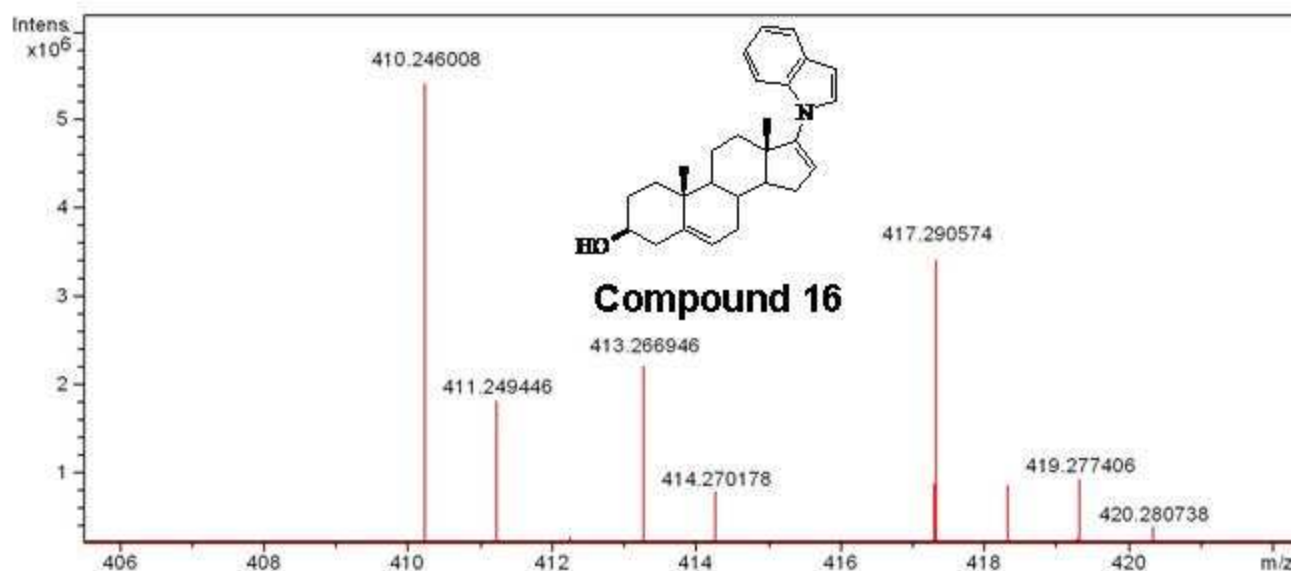
## Acquisition Parameter

Sample Name: VNPT144

Exact Mass of (C<sub>27</sub>H<sub>33</sub>NO)Na<sup>+</sup>: 410.245436u

Observed Mass: 410.246008u

Difference: 1.4 ppm

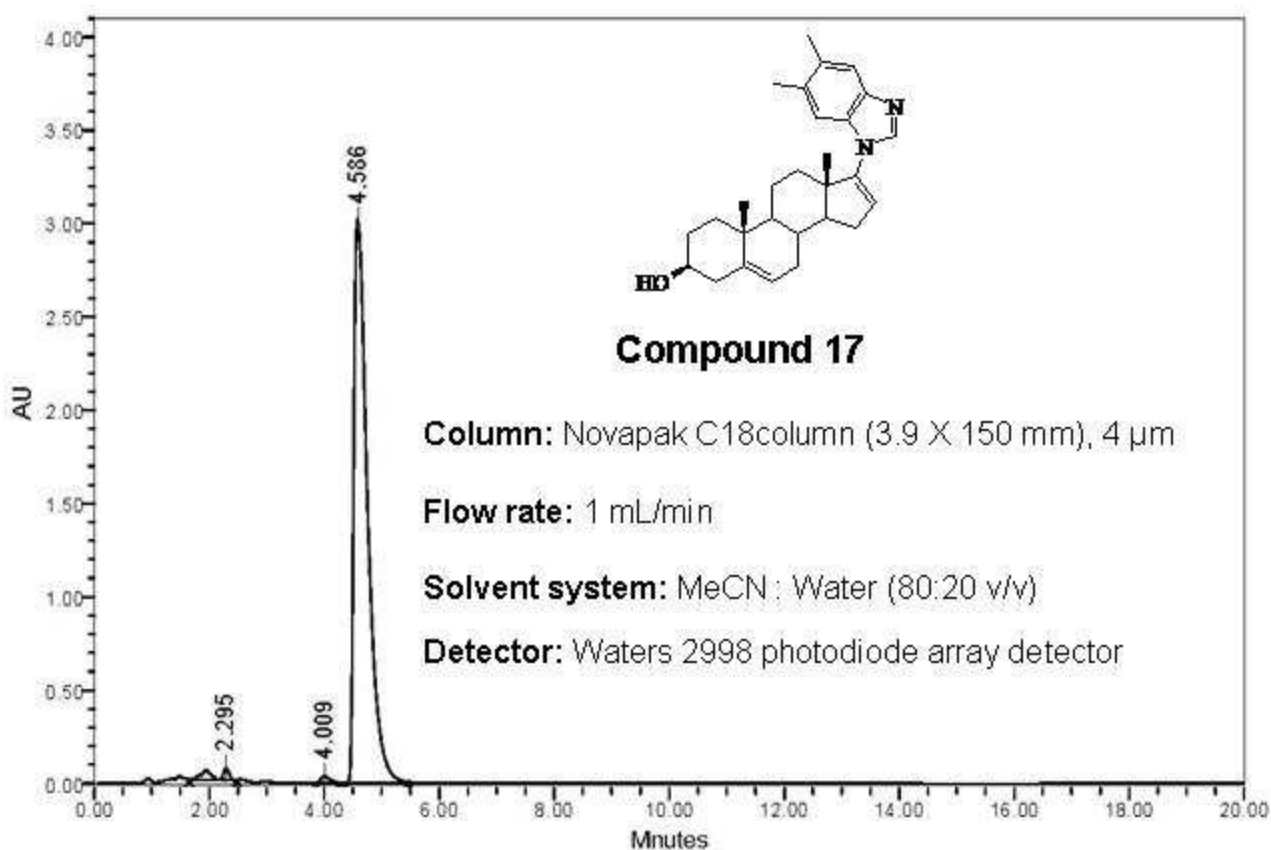


#	m/z	I
1	134.556119	403440
2	136.518053	429200
3	137.090914	1156049
4	137.291678	400945
5	146.927649	602594
6	160.827351	458290
7	171.361692	392829
8	184.232201	400095
9	184.451713	462658
10	210.584345	566629
11	228.484673	592840
12	228.484951	837320
13	233.292188	459175
14	319.930282	415031
15	342.717320	1126513
16	342.726527	727665
17	368.109441	577251
18	368.117713	982627
19	368.120246	1038051
20	368.124977	1222243
21	368.127888	1354723
22	368.131810	1103587
23	368.135190	3157987

**SAMPLE INFORMATION**

Sample Name: VNPT140  
 Sample Type: Unknown  
 Vial: 22  
 Injection #: 2  
 Injection Volume: 10.00 ul  
 Run Time: 20.0 Minutes  
 Sample Set Name:

Acquired By: System  
 Date Acquired: 4/16/2012 4:51:57 PM  
 Acq. Method Set: VN124  
 Date Processed: 4/16/2012 5:46:42 PM  
 Processing Method: VN124venky  
 Channel Name: WWin Ch1  
 Proc. Chnl. Descr.: FDA 242.7 nm



**Compound 17**

**Column:** Novapak C18column (3.9 X 150 mm), 4 µm

**Flow rate:** 1 mL/min

**Solvent system:** MeCN : Water (80:20 v/v)

**Detector:** Waters 2998 photodiode array detector

**PDA Result Table**

Name	RT	Area	Purity (#1) Angle	Purity (#1) Threshold	Purity Flag	Match (#1) Spect. Name	Match (#1) Angle	Match (#1) Threshold	PDA Match Flag
1	2.295	1082619			No				No
2	4.009	365305			No				No

Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (µV*sec)	% Area	Height (µV)	Int Type	Amount
1	2.295							1082619	2.11	63749	bb	
2	4.009							365305	0.71	35251	bb	
3	4.586							49772396	97.17	3024747	bb	

## Mass Spectrum List Report

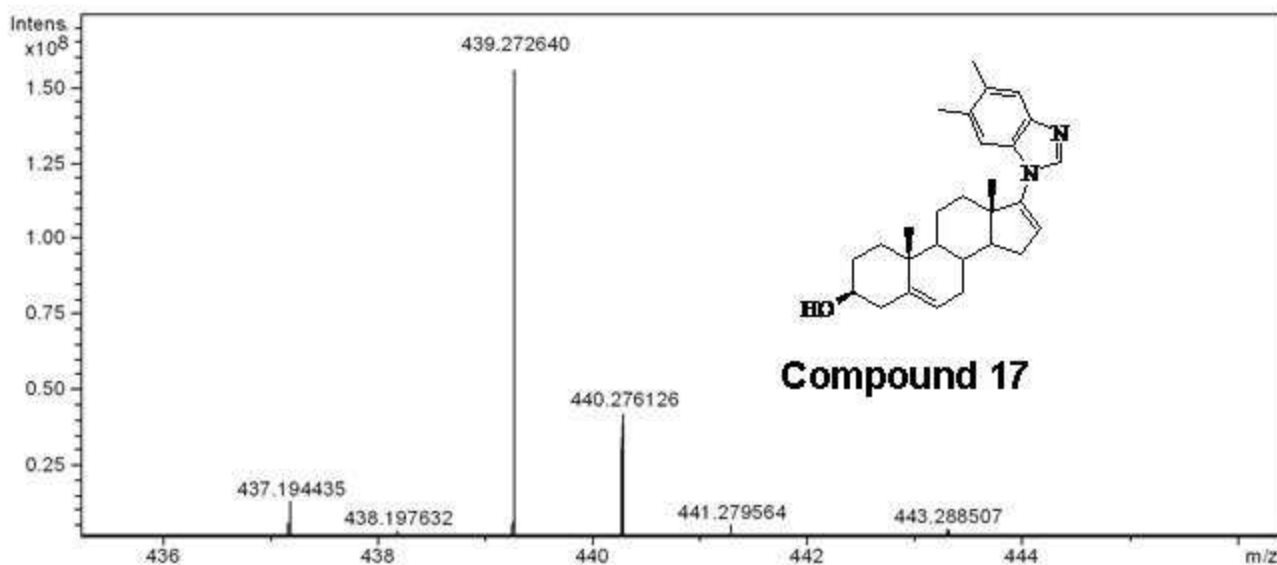
### Analysis Info

Analysis Name VNPT140\_pos\_000001.d  
Method XMASS\_Method  
Sample Name: VNPT140\_pos  
VNPT140\_pos: in 1:1 THF:MeOH w/ NaCl.

Acquisition Date 12/13/2010 3:19:04 PM  
Operator FTMS\_USER  
Instrument apex-Qe

### Acquisition Parameter

Sample Name: VNPT140  
Exact Mass of (C<sub>28</sub>H<sub>36</sub>N<sub>2</sub>O)Na<sup>+</sup>: 439.271985u  
Observed Mass: 439.272640u  
Difference: 1.5 ppm

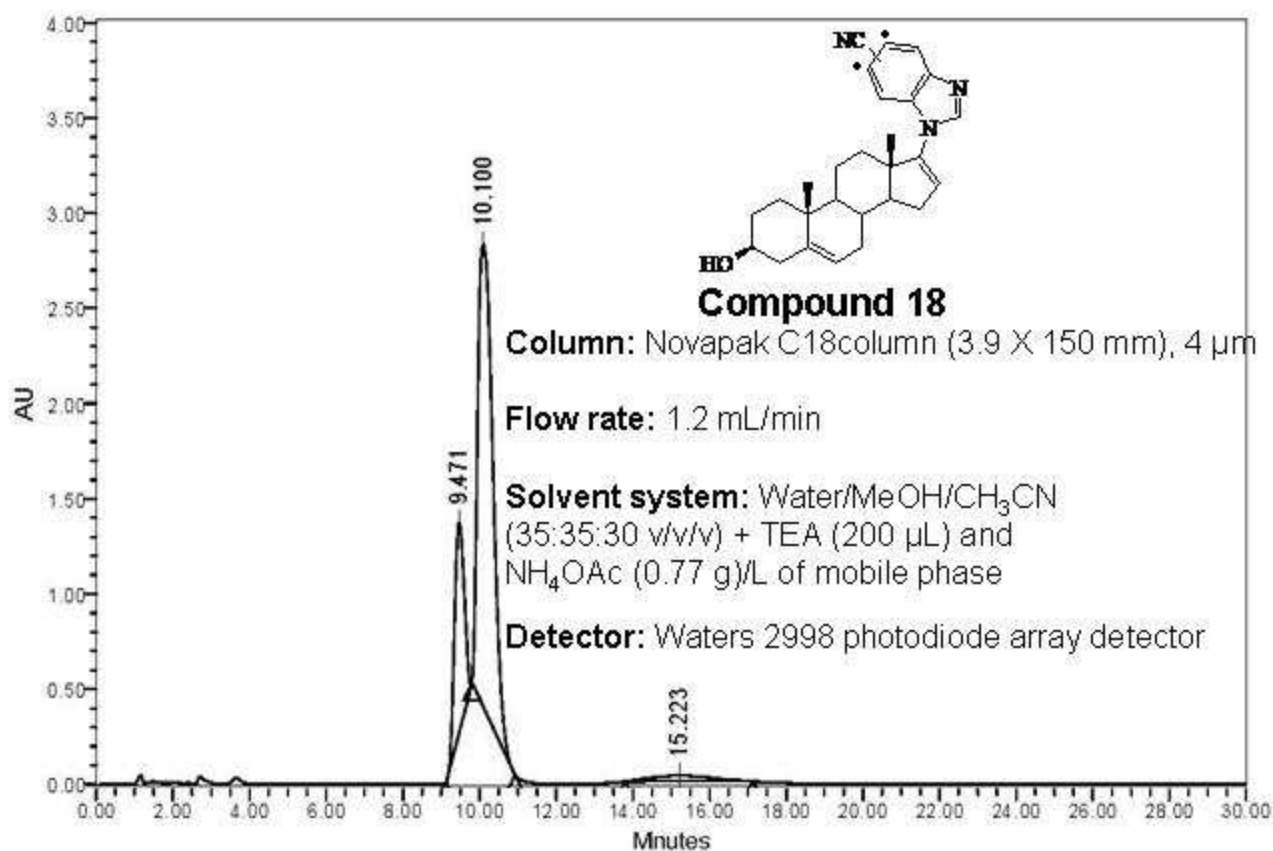


#	m/z	I
1	417.286515	48179623
2	417.288766	56356263
3	417.290328	336768423
4	418.290242	30903724
5	418.293937	87600556
6	418.295491	9670060
7	419.293856	6751666
8	419.297519	9850290
9	437.190212	5807665
10	437.194435	12582449
11	439.268445	43593283
12	439.270729	17509955
13	439.272640	159493699
14	440.271999	23744076
15	440.274570	7175756
16	440.276126	42069580
17	441.279564	5295701
18	463.304164	6043451
19	467.263083	11276138
20	467.267955	26709866
21	468.271269	8023926
22	507.330461	11391325
23	510.310388	5251458

**SAMPLE INFORMATION**

Sample Name: VNPT191  
 Sample Type: Unknown  
 Vial: 28  
 Injection #: 1  
 Injection Volume: 20.00 ul  
 Run Time: 30.0 Minutes  
 Sample Set Name: Puru Sample Set 2

Acquired By: System  
 Date Acquired: 4/13/2012 2:44:27 AM  
 Acq. Method Set: VN124  
 Date Processed: 4/13/2012 11:35:55 AM  
 Processing Method: VN124venky  
 Channel Name: WIn Ch1  
 Proc. Chnl. Descr.: FDA 242.7 nm



**PDA Result Table**

	Name	RT	Area	Purity (#1) Angle	Purity (#1) Threshold	Purity Flag	Match (#1) Spect. Name	Match (#1) Angle	Match (#1) Threshold	PDA Match Flag
1		9.471	19310379			No				No
2		10.100	66248525			No				No

Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (µV*sec)	% Area	Height (µV)	Int Type	Amount
1	9.471							19310379	21.71	1104336	bb	
2	10.100							66248525	74.46	2427980	bb	
3	15.223							3407799	3.83	30204	bb	

# Mass Spectrum List Report

## Analysis Info

Analysis Name VNPT191\_pos\_000001.d  
Method XMASS\_Method  
Sample Name: VNPT191\_pos  
VNPT191\_pos: in ACN w/ 0.1% FA.

Acquisition Date 3/20/2012 1:25:02 PM  
Operator FTMS\_USER  
Instrument apex-Qe

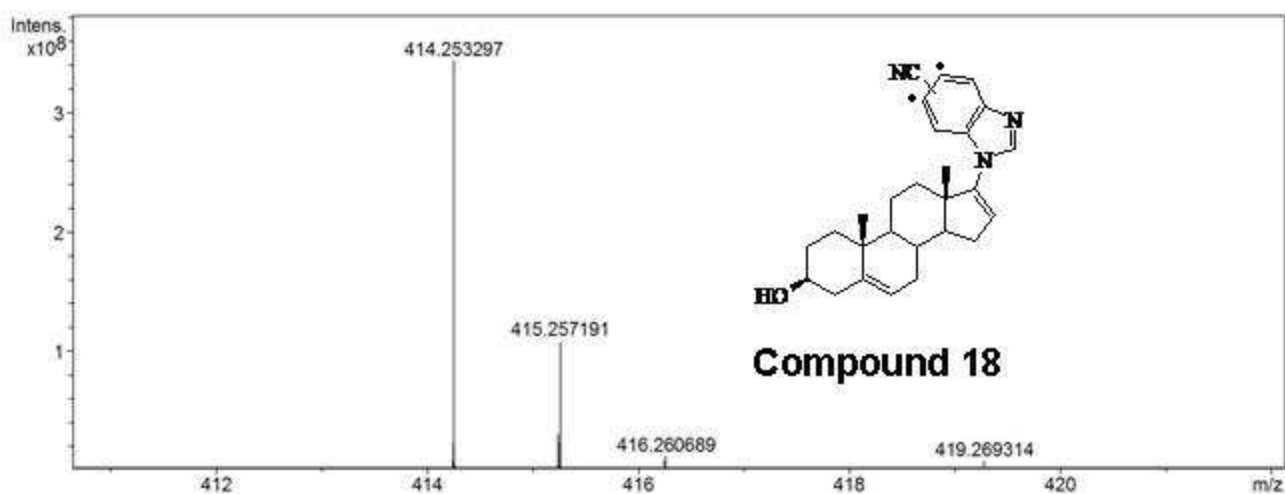
## Acquisition Parameter

Sample: VNPT191

Exact Mass of (C<sub>27</sub>H<sub>31</sub>N<sub>3</sub>O)H<sup>+</sup> = 414.253989u

Observed Mass = 414.253297u

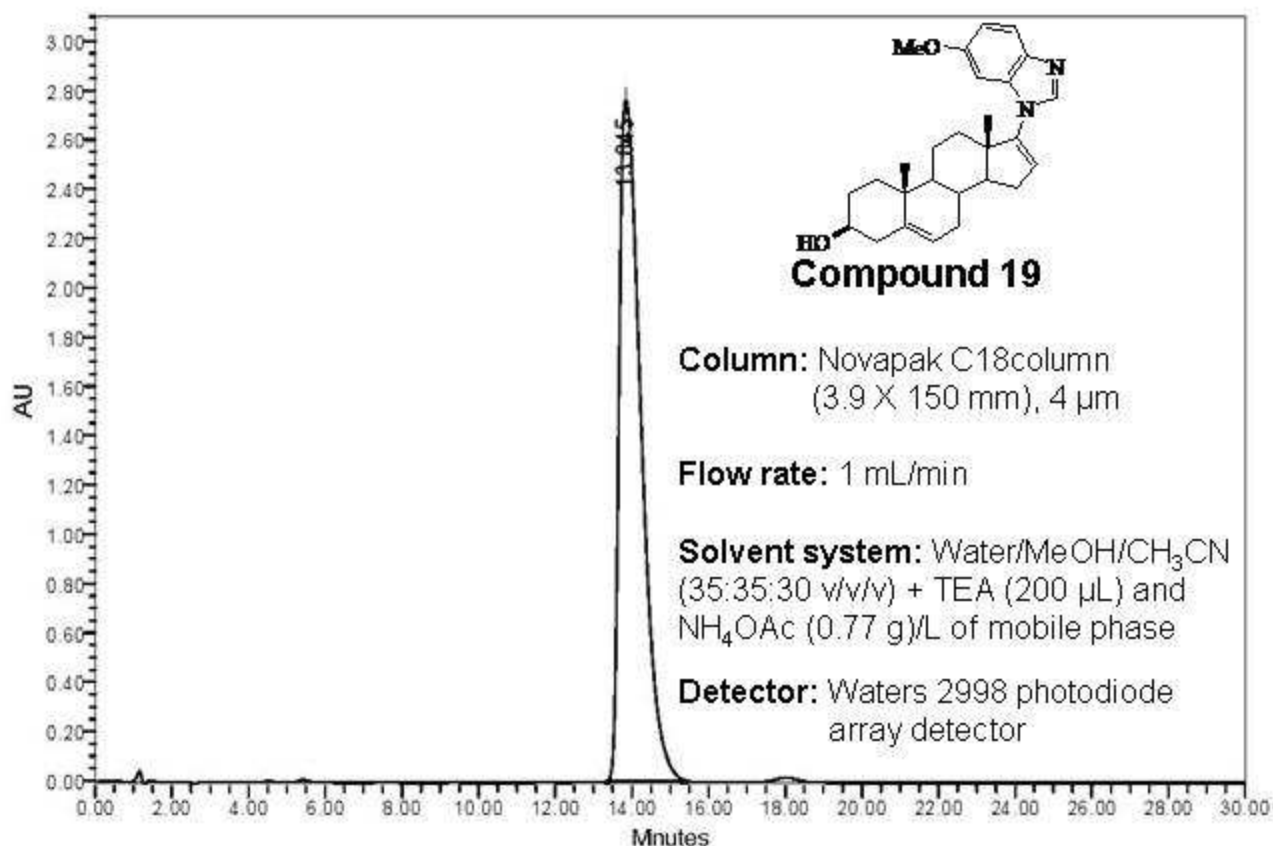
Difference = -1.7 ppm



m/z	I
207.126701	4337469
207.128455	2215349
207.129525	1581085
215.089036	8511228
231.062976	7850492
277.011287	2583461
277.013816	1696005
277.020245	1632293
285.130902	4250548
301.104836	6320597
397.191074	1913074
405.253657	5370636
413.222364	2013990
414.242579	1509161
414.244566	8293673
414.247990	1461545
414.249367	4661033
414.251438	110091049
414.253297	343300905
414.254584	13818665
414.255045	8760105

### SAMPLE INFORMATION

Sample Name:	VNPT187A	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	4/13/2012 2:13:13 AM
Vial:	27	Acq. Method Set:	VN124
Injection #:	1	Date Processed:	4/13/2012 11:28:42 AM
Injection Volume:	20.00 ul	Processing Method:	VN124venky
Run Time:	30.0 Minutes	Channel Name:	WIn Ch1
Sample Set Name:	Puru Sample Set 2	Proc. Chnl. Descr.:	FDA 242.7 nm



**PDA Result Table**

Name	RT	Area	Purity (#1) Angle	Purity (#1) Threshold	Purity Flag	Match (#1) Spect. Name	Match (#1) Angle	Match (#1) Threshold	PDA Match Flag
1	13.845	109561301			No				No

Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (μV*sec)	% Area	Height (μV)	Int Type	Amount
1	13.845							109561301	100.00	2761138	bb	



# Mass Spectrum List Report

## Analysis Info

Analysis Name VNPT187A\_pos\_000001.d  
Method XMASS\_Method  
Sample Name: VNPT187A\_pos  
VNPT187A\_pos: in 1:1 THF:MeOH w/ NaCl

Acquisition Date 3/20/2012 11:59:30 AM  
Operator FTMS\_USER  
Instrument apex-Qe

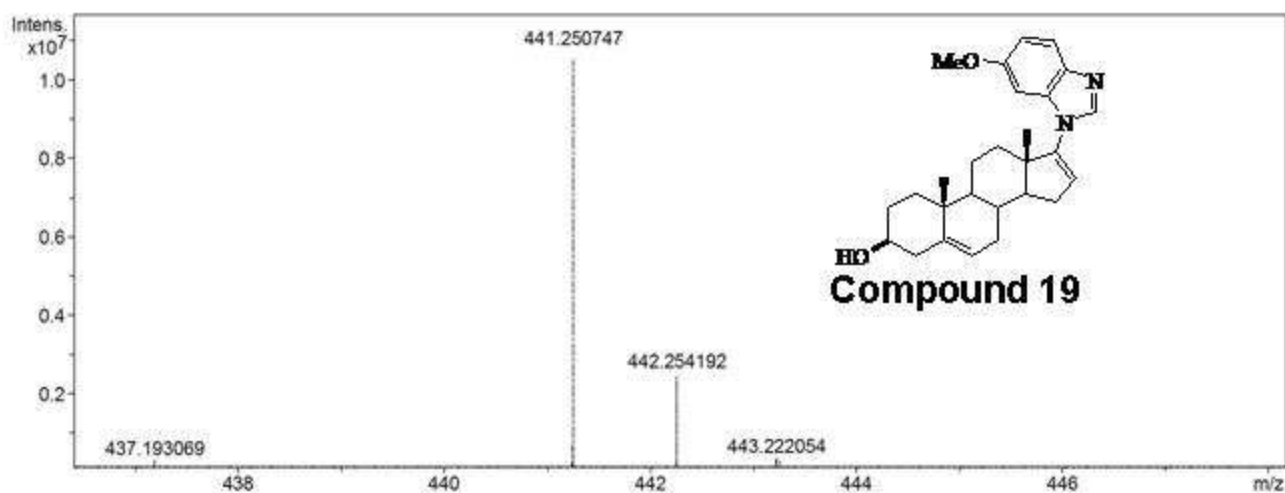
## Acquisition Parameter

Sample: VNPT187A

Exact Mass of (C<sub>27</sub>H<sub>34</sub>N<sub>2</sub>O<sub>2</sub>)Na<sup>+</sup> = 441.251249u

Observed Mass = 441.250747u

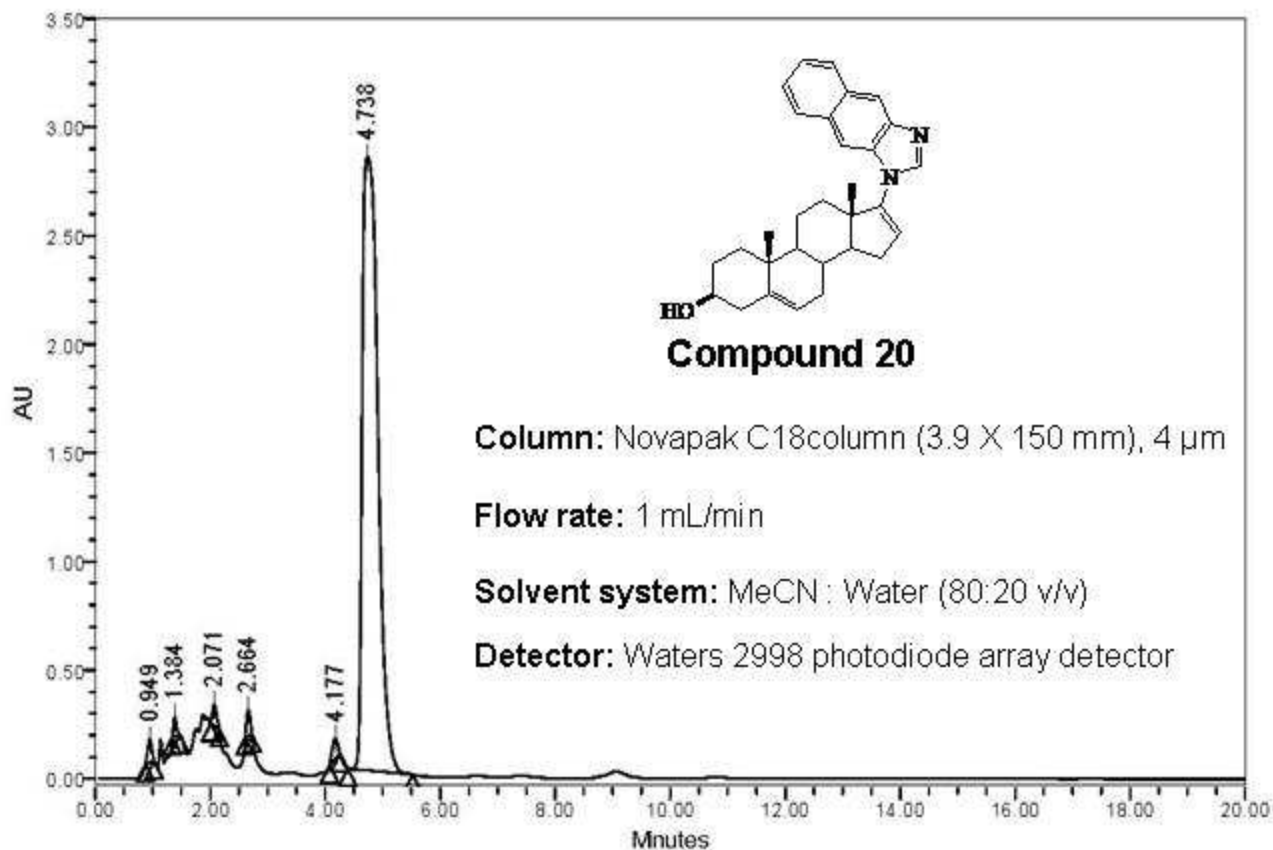
Difference = -1.1 ppm



m/z	I
209.637209	1277661
215.088640	5082059
215.088862	39289163
215.089088	3149387
215.089208	1519403
216.092282	2614315
231.062858	1213227
270.519635	3796859
288.289493	16748969
289.292912	2627244
310.271487	1429486
316.320766	8756739
317.324173	1284359
413.211522	2652484
413.265839	3925828
419.258192	1587540
419.264983	1192788
419.265443	1809748
419.266760	8172372
419.267792	17296212
419.268571	229661524

**SAMPLE INFORMATION**

Sample Name:	VNLT103	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	4/17/2012 11:46:21 AM
Vial:	30	Acq. Method Set:	VN124
Injection #:	1	Date Processed:	4/17/2012 12:12:35 PM
Injection Volume:	10.00 ul	Processing Method:	VN124venky
Run Time:	20.0 Minutes	Channel Name:	WWin Ch1
Sample Set Name:		Proc. Chnl. Descr.:	FDA 253.4 nm



**PDA Result Table**

Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (μV*sec)	% Area	Height (μV)	Int Type	Amount
1	0.949							531560	0.95	107993	bb	
2	1.384							328823	0.59	89008	bb	
3	2.071							486019	0.87	97144	bb	
4	2.664							511337	0.92	119703	bb	
5	4.177							608542	1.09	92684	bb	
6	4.738							53212442	95.57	2821779	bb	
6	4.738	53212442			No				No			

## Mass Spectrum List Report

### Analysis Info

Analysis Name VNLT-103\_pos\_000001.d

Method XMASS\_Method

Sample Name: VNLT-103\_pos

VNLT-103\_pos: in 1:1 THF:MeOH w/ NaCl.

Acquisition Date 12/13/2010 3:05:09 PM

Operator FTMS\_USER

Instrument apex-Qe

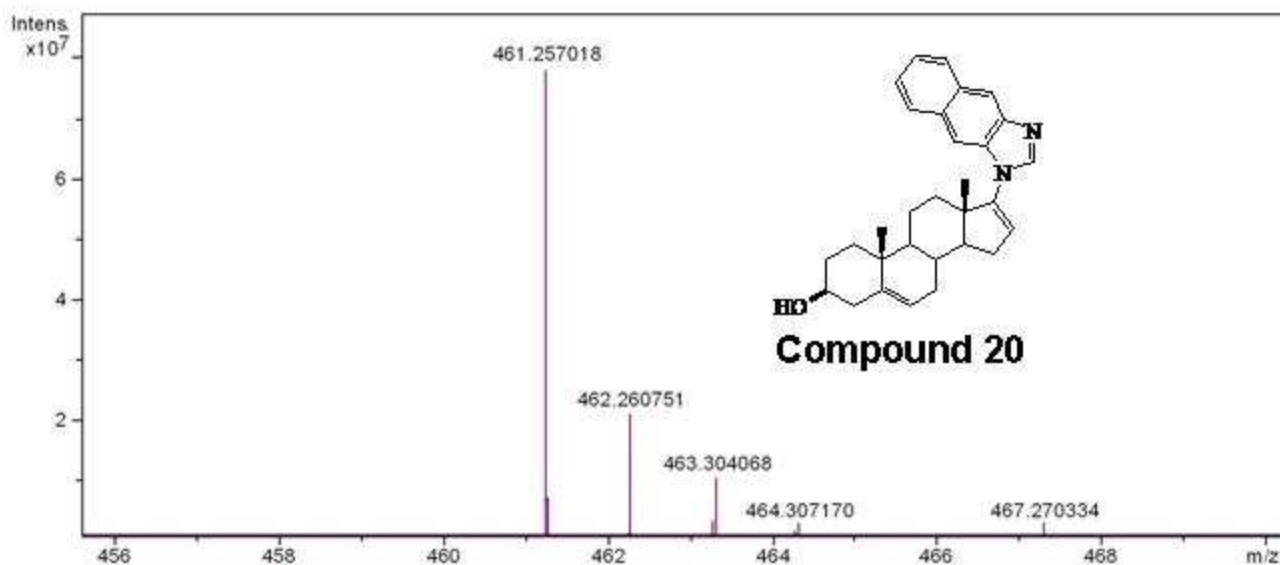
### Acquisition Parameter

Sample Name: VNLT-103

Exact Mass of (C<sub>30</sub>H<sub>34</sub>N<sub>2</sub>O)Na<sup>+</sup>: 461.256350u

Observed Mass: 461.257018u

Difference: 1.5 ppm

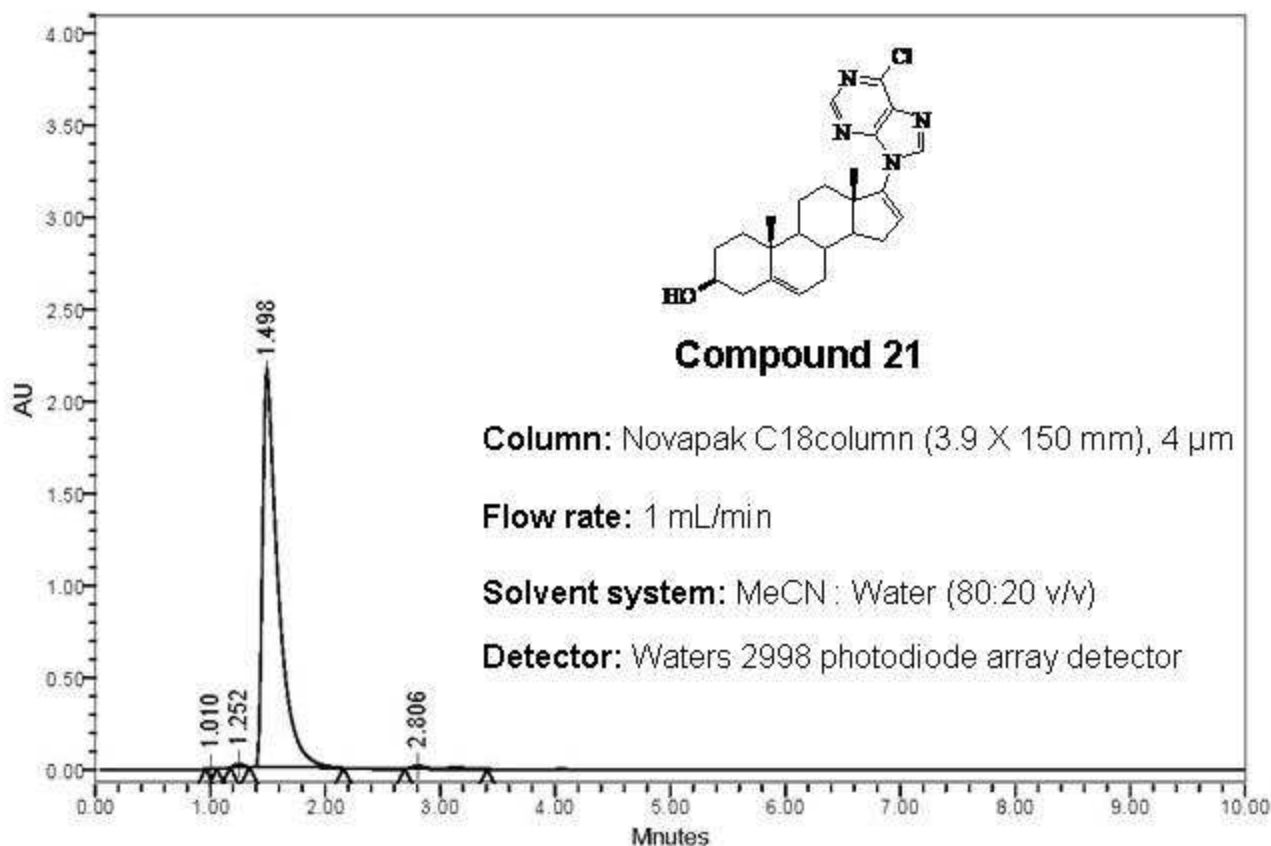


#	m/z	I
1	437.194422	10919097
2	439.271531	36199628
3	439.275009	197373133
4	439.277670	9440461
5	439.278693	5455053
6	440.275437	18947286
7	440.278470	64466134
8	441.281875	10353888
9	461.254853	20049346
10	461.257018	78360002
11	461.258911	7368130
12	462.257447	6120911
13	462.260751	21302735
14	463.304068	10739164
15	489.252458	18485058
16	490.255652	5525328
17	505.247336	5511212
18	507.330416	21573706
19	508.333743	6129753
20	529.280941	10645891
21	529.283634	39874947
22	530.286910	14201233
23	540.302036	14971412

**SAMPLE INFORMATION**

Sample Name: VNFP39  
 Sample Type: Unknown  
 Vial: 20  
 Injection #: 1  
 Injection Volume: 10.00 ul  
 Run Time: 10.0 Mnutes  
 Sample Set Name:

Acquired By: System  
 Date Acquired: 4/17/2012 5:44:59 PM  
 Acq. Method Set: VN124  
 Date Processed: 4/17/2012 5:59:38 PM  
 Processing Method: VN124venky  
 Channel Name: WWin Ch1  
 Proc. Chnl. Descr.: FDA 242.7 nm



**PDA Result Table**

Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (μV*sec)	% Area	Height (μV)	Int Type	Amount
1	1.010							18739	0.09	5560	bb	
2	1.252							96373	0.47	18627	bb	
3	1.498							20236004	98.21	2182717	bb	
4	2.806							254360	1.23	15767	bb	
4	2.806	254360			No				No			

# Mass Spectrum List Report

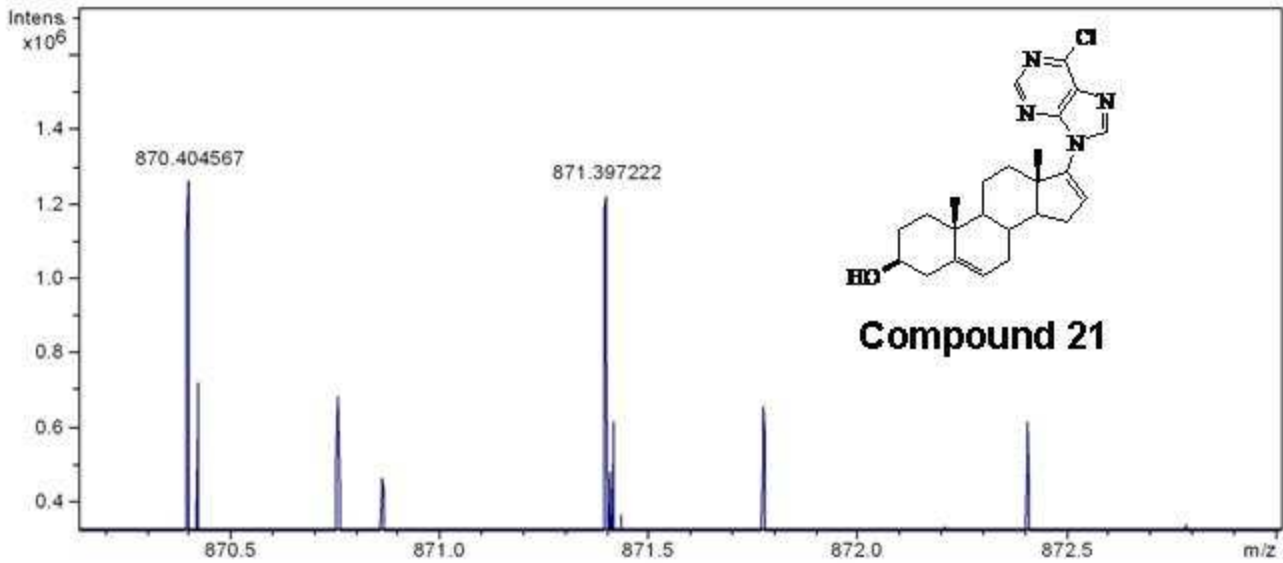
## Analysis Info

Analysis Name VNPP39\_pos\_000002.d  
Method XMASS\_Method  
Sample Name: VNPP39\_pos  
VNPP39\_pos: in 1:1 THF:MeOH w/ NaCl.

Acquisition Date 12/13/2010 9:30:30 AM  
Operator FTMS\_USER  
Instrument apex-Qe

## Acquisition Parameter

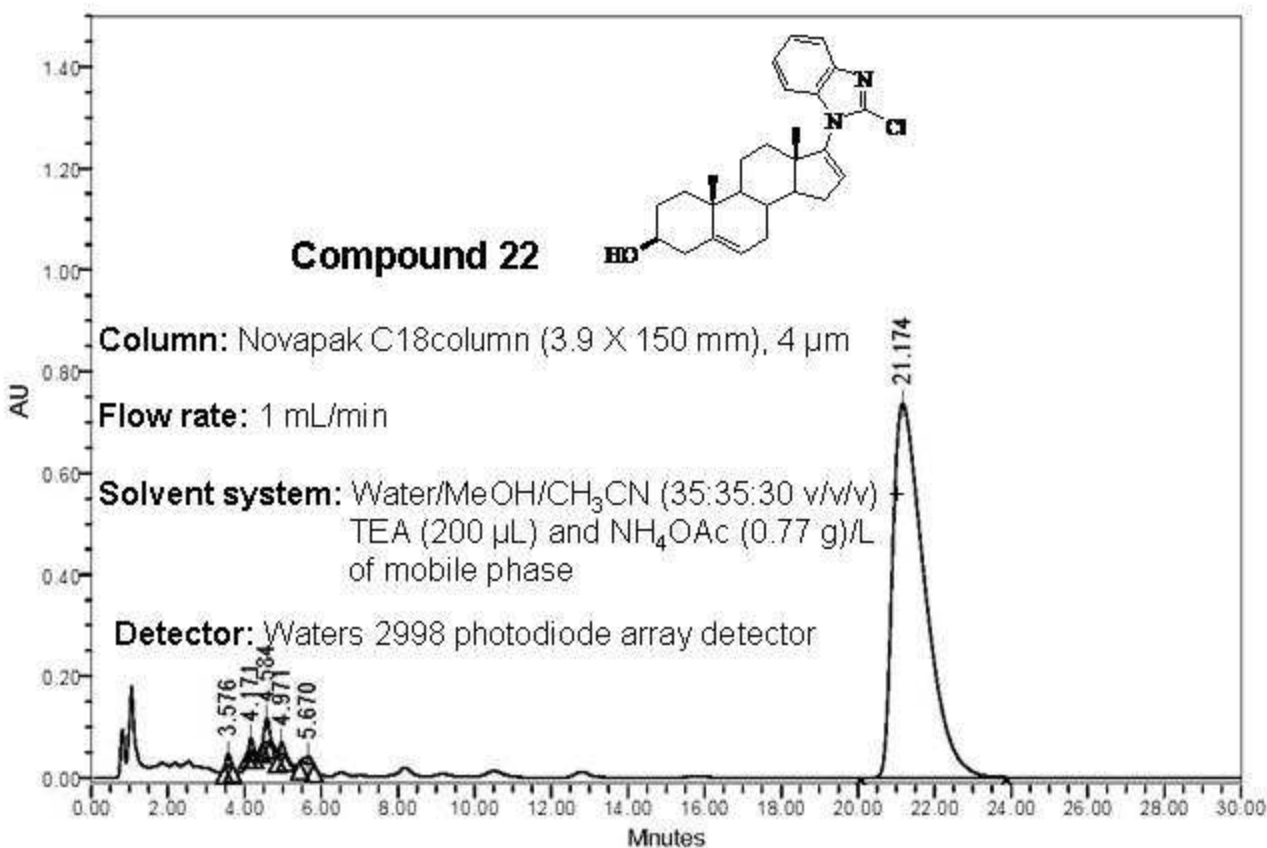
Sample Name: VNPP39  
Exact Mass of (C<sub>24</sub>H<sub>29</sub>ClN<sub>4</sub>O)<sub>2</sub>Na<sup>+</sup>: 871.395200u  
Observed Mass: 871.397222u  
Difference: 2.3 ppm



#	m/z	I
1	99.184985	3542938
2	99.185669	3037728
3	99.185994	5406510
4	99.186475	2818354
5	99.453074	2867801
6	99.453612	44023753
7	99.453821	16366319
8	99.454003	6816989
9	99.454145	12029385
10	99.454293	8032589
11	99.454580	4681961
12	107.305349	2956982
13	107.305676	34732250
14	107.305868	17211162
15	107.306174	35874138
16	107.556313	2485458
17	129.448204	6045547
18	129.448776	8152491
19	129.449287	2872347
20	136.518144	2742312
21	143.074745	22627634
22	143.076532	47352114
23	143.076995	7450674

### SAMPLE INFORMATION

Sample Name: VNFP59	Acquired By: System
Sample Type: Unknown	Date Acquired: 4/16/2012 1:37:35 PM
Vial: 19	Acq. Method Set: VN124
Injection #: 1	Date Processed: 4/16/2012 2:17:34 PM
Injection Volume: 20.00 ul	Processing Method: VN124venky
Run Time: 30.0 Minutes	Channel Name: WIn Ch1
Sample Set Name:	Proc. Chnl. Descr.: FDA 280.5 nm



**PDA Result Table**

Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (μV*sec)	% Area	Height (μV)	Int Type	Amount
1	3.576							175488	0.40	23050	bb	
2	4.171							160111	0.37	25692	bb	
3	4.584							398089	0.91	47115	bb	
4	4.971							185460	0.42	23414	bb	
5	5.670							190574	0.44	13719	bb	
6	21.174							42572398	97.46	736593	bb	
6	21.174	42572398			No					No		

## Mass Spectrum List Report

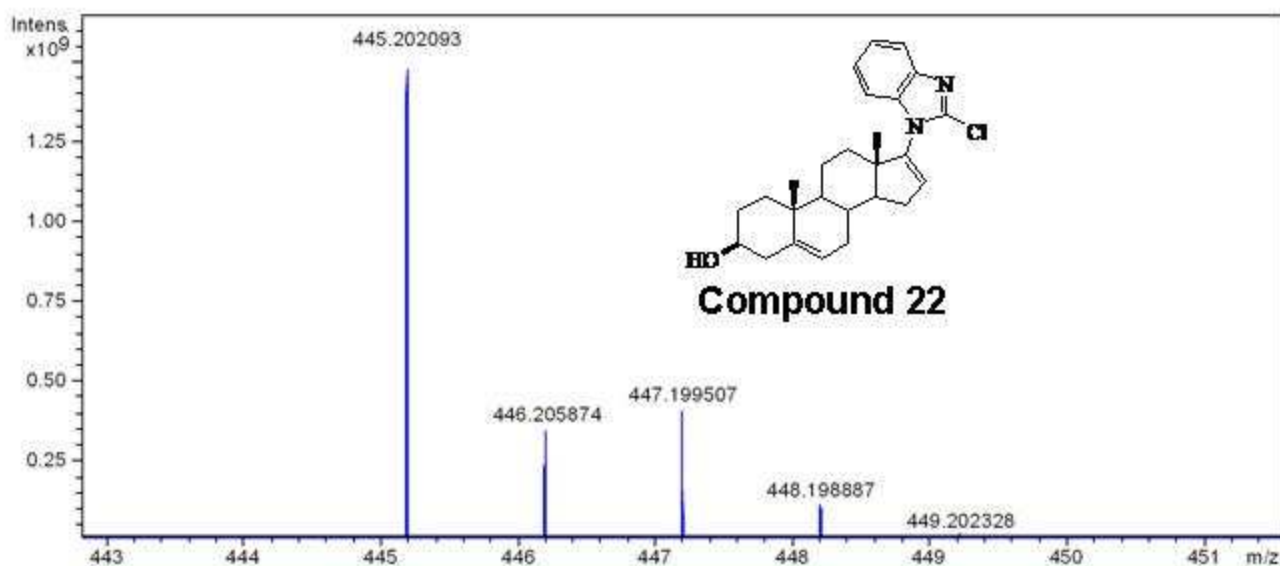
### Analysis Info

Analysis Name VNPP59\_pos\_000002.d  
Method XMASS\_Method  
Sample Name: VNPP59\_pos  
VNPP59\_pos: in 1:1 THF:MeOH w/ NaCl.

Acquisition Date 12/13/2010 9:43:14 AM  
Operator FTMS\_USER  
Instrument apex-Qe

### Acquisition Parameter

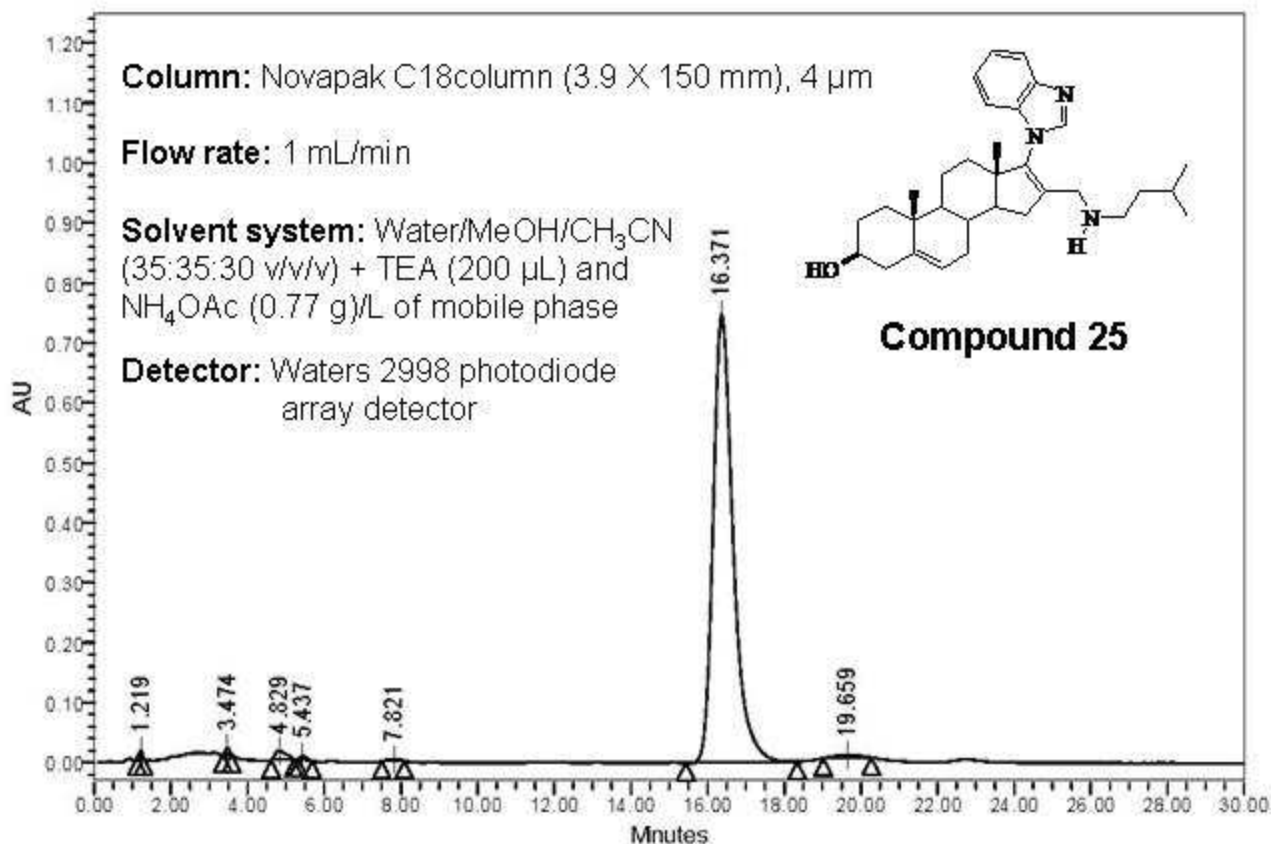
Sample Name: VNPP59  
Exact Mass of (C<sub>26</sub>H<sub>31</sub>ClN<sub>2</sub>O)<sup>+</sup>: 445.201712u  
Observed Mass: 445.202093u  
Difference: < 1.0 ppm



#	m/z	I
1	413.263186	302941245
2	413.266736	610632765
3	414.266758	119604306
4	414.270408	147817554
5	423.216757	166266149
6	423.220701	325027109
7	424.220302	61932863
8	424.224006	90080575
9	425.213951	71566682
10	425.217651	112166234
11	445.196902	480085969
12	445.198174	490178513
13	445.200271	509970385
14	445.202093	1522632657
15	445.203601	191989713
16	445.204694	91424721
17	445.205767	56133585
18	446.201800	245401589
19	446.205874	352815093
20	447.195579	284723225
21	447.199507	412715033
22	447.201211	54593561
23	447.205035	47532057

**SAMPLE INFORMATION**

Sample Name:	VNPT71	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	4/19/2012 12:55:10 PM
Vial:	8	Acq. Method Set:	VN124
Injection #:	1	Date Processed:	4/19/2012 1:30:52 PM
Injection Volume:	10.00 ul	Processing Method:	VN124venky
Run Time:	30.0 Mnutes	Channel Name:	WVln Ch1
Sample Set Name:		Proc. Chnl. Descr.:	FDA 242.7 nm



**PDA Result Table**

Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (µV*sec)	% Area	Height (µV)	Int Type	Amount
1	1.219							60206	0.22	11525	bb	
2	3.474							82996	0.30	10745	bb	
3	4.829							295707	1.06	15150	bb	
4	5.437							64475	0.23	5858	bb	
5	7.821							65687	0.24	3017	bb	
6	16.371							27032179	97.14	746417	bb	
7	19.659							227051	0.82	4775	bb	
6	16.371	27032179				No					No	



# Mass Spectrum List Report

## Analysis Info

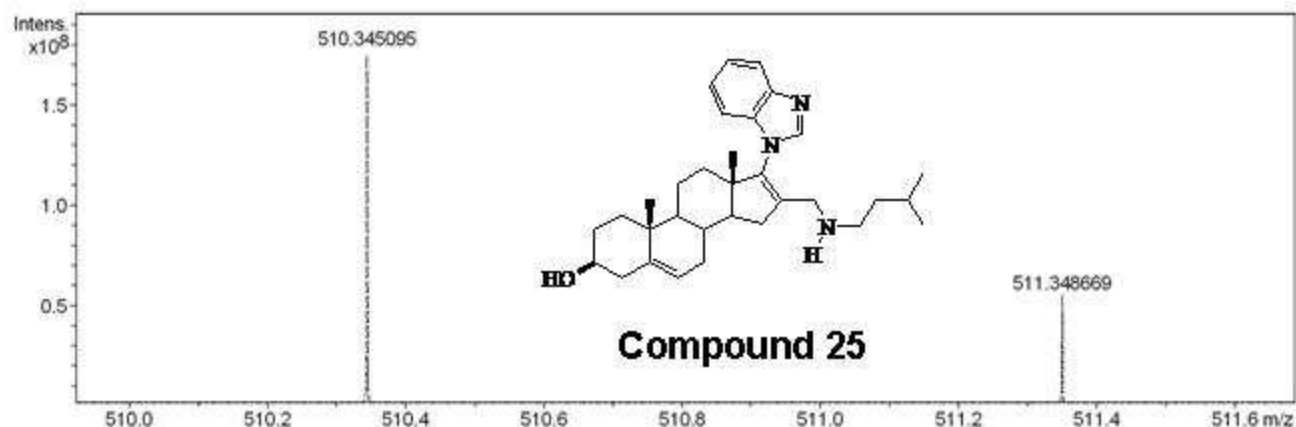
Analysis Name	VNPT71_pos_000001.d	Acquisition Date	3/1/2010 10:54:23 AM
Method	XMASS_Method	Operator	FTMS_USER
Sample Name:	VNPT71_pos	Instrument	apex-Qe
VNPT71_pos: in 1:1 THF:MeOH w/ NaCl			

Sample Name: VNPT71

Exact Mass of (C<sub>32</sub>H<sub>45</sub>N<sub>3</sub>O)Na<sup>+</sup> = 510.345484u

Observed Mass = 510.345095u

Difference = < -1.0 ppm



#	m/z	I
1	211.797033	6437307
2	212.363528	20741435
3	215.088084	10641562
4	215.088707	43305274
5	469.378734	8267224
6	488.363169	574656097
7	488.364171	53333601
8	488.364845	22531681
9	488.365489	12303969
10	488.366118	8089185
11	489.364160	9109096
12	489.364665	7872104
13	489.366524	186617448
14	490.370124	24776303
15	500.362103	13508277
16	500.363300	65736373
17	501.366849	21163708
18	508.389666	17800941
19	510.342453	6648570
20	510.345095	176688890
21	510.346908	8974074
22	511.348669	55381761

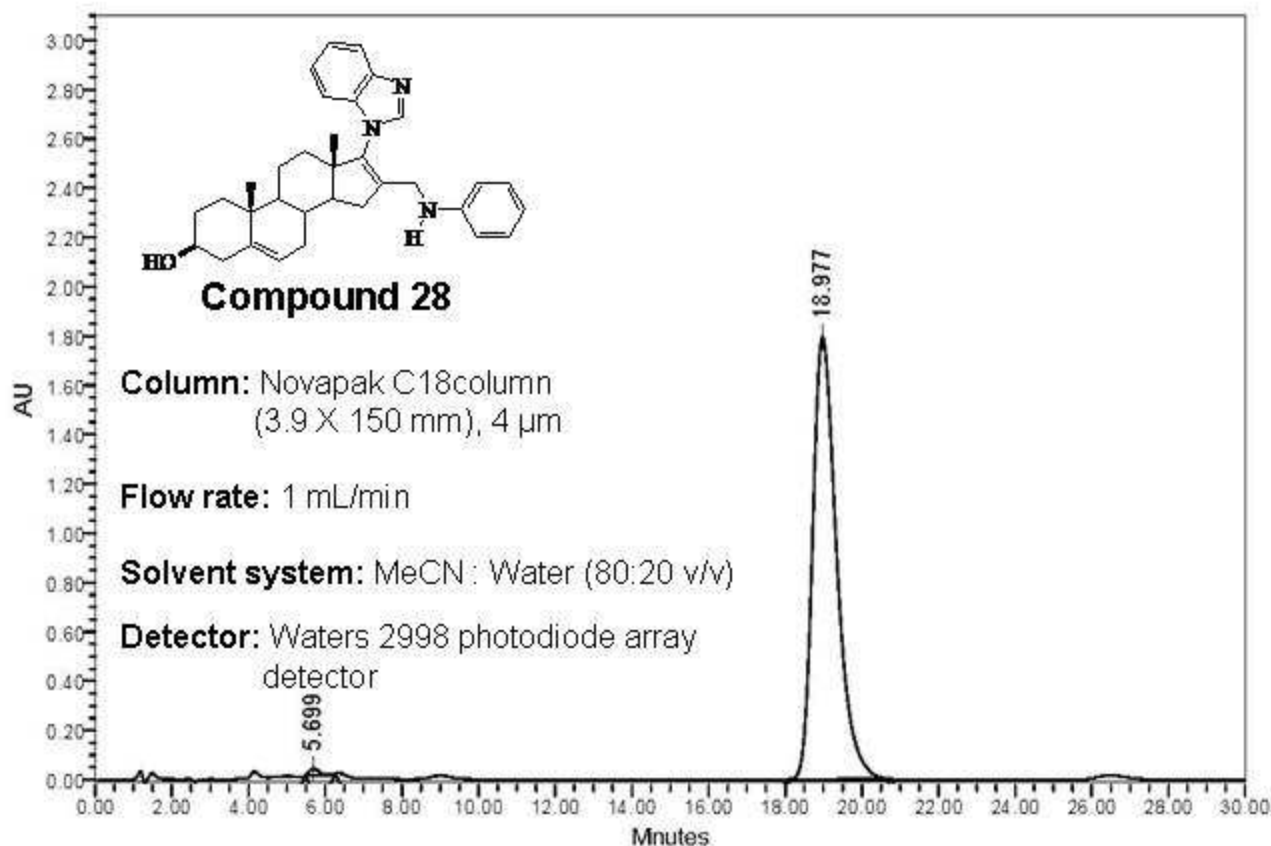
Reported by User: System

Project Name: FDA\_Default

**SAMPLE INFORMATION**

Sample Name: VNPT72  
 Sample Type: Unknown  
 Vial: 9  
 Injection #: 1  
 Injection Volume: 20.00 ul  
 Run Time: 30.0 Mnutes  
 Sample Set Name: Furu Sample Set 2

Acquired By: System  
 Date Acquired: 4/12/2012 4:50:33 PM  
 Acq. Method Set: VN124  
 Date Processed: 4/12/2012 5:43:12 PM  
 Processing Method: VN124venky  
 Channel Name: WIn Ch1  
 Proc. Chnl. Descr.: FDA 242.7 nm



**PDA Result Table**

Name	RT	Area	Purity (#1) Angle	Purity (#1) Threshold	Purity Flag	Match (#1) Spect. Name	Match (#1) Angle	Match (#1) Threshold	PDA Match Flag
1	5.699	497110			No				No
2	18.977	77612908			No				No

Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (μV*sec)	% Area	Height (μV)	Int Type	Amount
1	5.699							497110	0.64	25559	bb	
2	18.977							77612908	99.36	1794102	bb	

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## Analysis Info

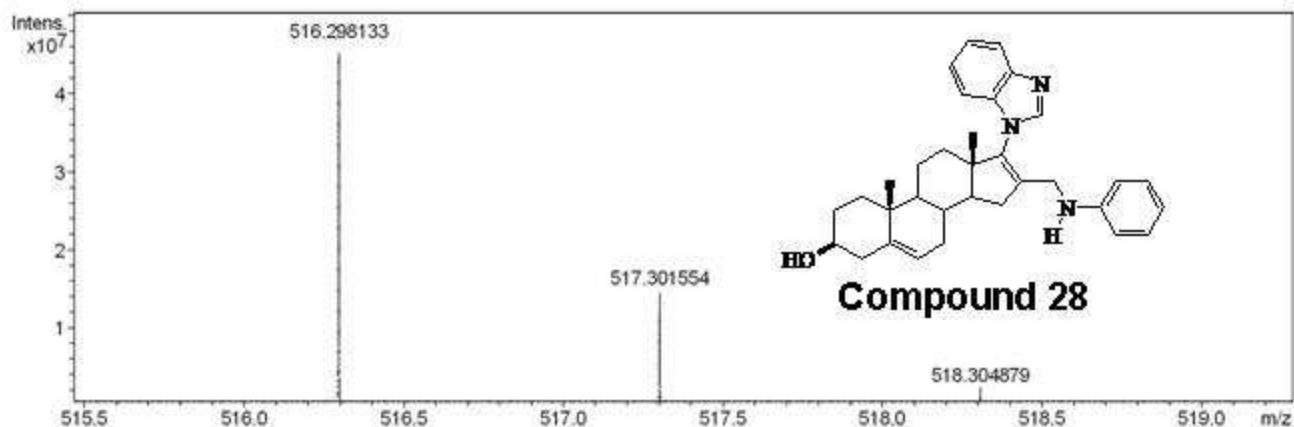
Analysis Name VNPT72\_pos\_000001.d Acquisition Date 3/1/2010 11:00:00 AM  
Method XMASS\_Method Operator FTMS\_USER  
Sample Name: VNPT72\_pos Instrument apex-Qe  
VNPT72\_pos: in 1:1 THF:MeOH w/ NaCl

Sample Name: VNPT72

Exact Mass of (C<sub>33</sub>H<sub>39</sub>N<sub>3</sub>O)Na<sup>+</sup> = 516.298534u

Observed Mass = 516.298133u

Difference = < -1.0 ppm

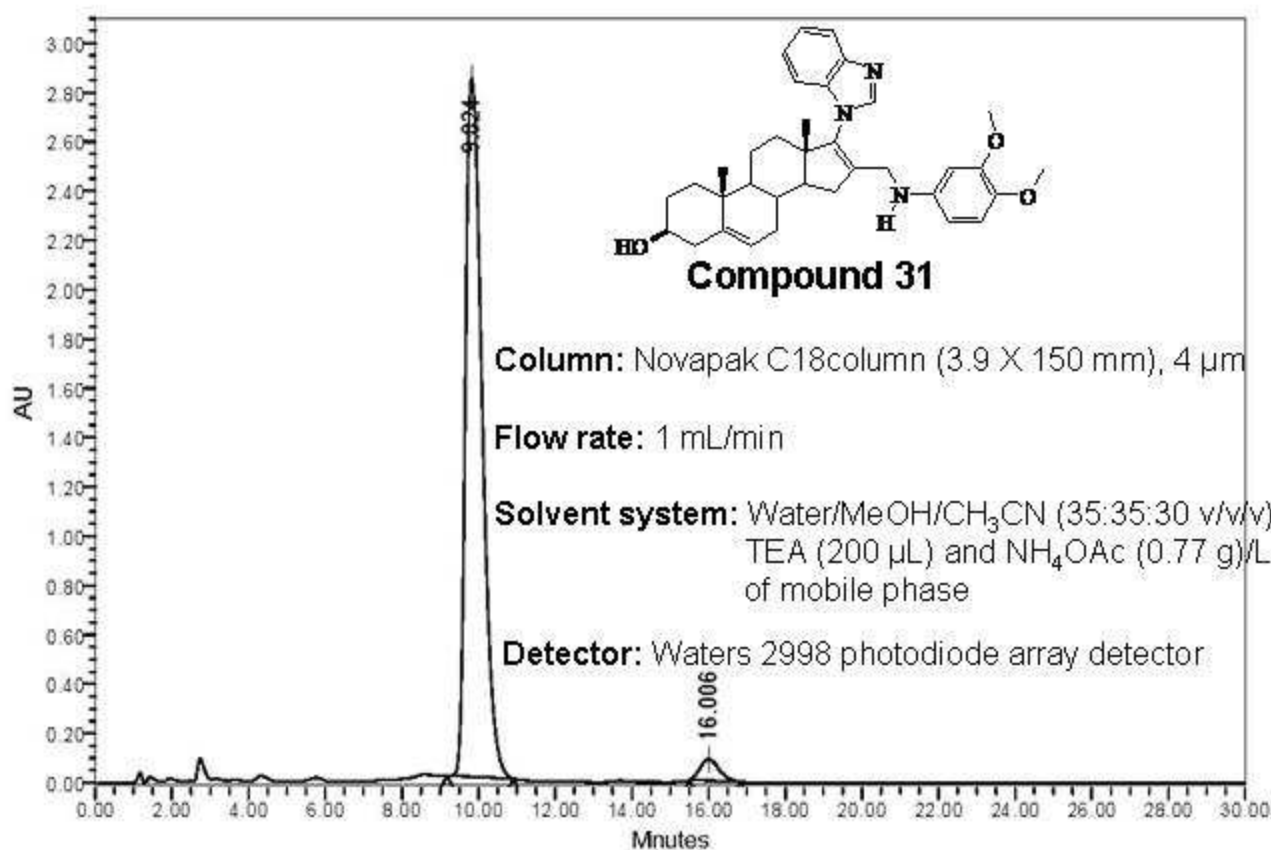


#	m/z	I
1	208.542848	5053828
2	209.078912	21073955
3	213.073022	3912097
4	215.088125	20083487
5	215.088638	72098079
6	216.092021	5912607
7	231.083607	3138334
8	231.119985	3176286
9	245.098553	4383474
10	245.099293	8099890
11	494.310209	2711484
12	494.310857	3752380
13	494.311509	4743612
14	494.314377	38997436
15	494.315937	561417660
16	494.316981	63049148
17	494.317641	25628092
18	494.318283	13630908
19	494.318940	8752572
20	494.319569	5909948
21	494.320228	4488636
22	494.320854	3342780

**SAMPLE INFORMATION**

Sample Name: VNPT85  
 Sample Type: Unknown  
 Vial: 10  
 Injection #: 1  
 Injection Volume: 20.00 ul  
 Run Time: 30.0 Minutes  
 Sample Set Name: Furu Sample Set 2

Acquired By: System  
 Date Acquired: 4/12/2012 5:21:50 PM  
 Acq. Method Set: VN124  
 Date Processed: 4/12/2012 6:09:21 PM  
 Processing Method: VN124venky  
 Channel Name: WWin Ch1  
 Proc. Chnl. Descr.: FDA 242.7 nm



**PDA Result Table**

Name	RT	Area	Purity (#1) Angle	Purity (#1) Threshold	Purity Flag	Match (#1) Spect. Name	Match (#1) Angle	Match (#1) Threshold	PDA Match Flag
1	9.824	85109342			No				No
2	16.006	2948948			No				No

Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (μV*sec)	% Area	Height (μV)	Int Type	Amount
1	9.824							85109342	96.65	2831130	bb	
2	16.006							2948948	3.35	86580	bb	

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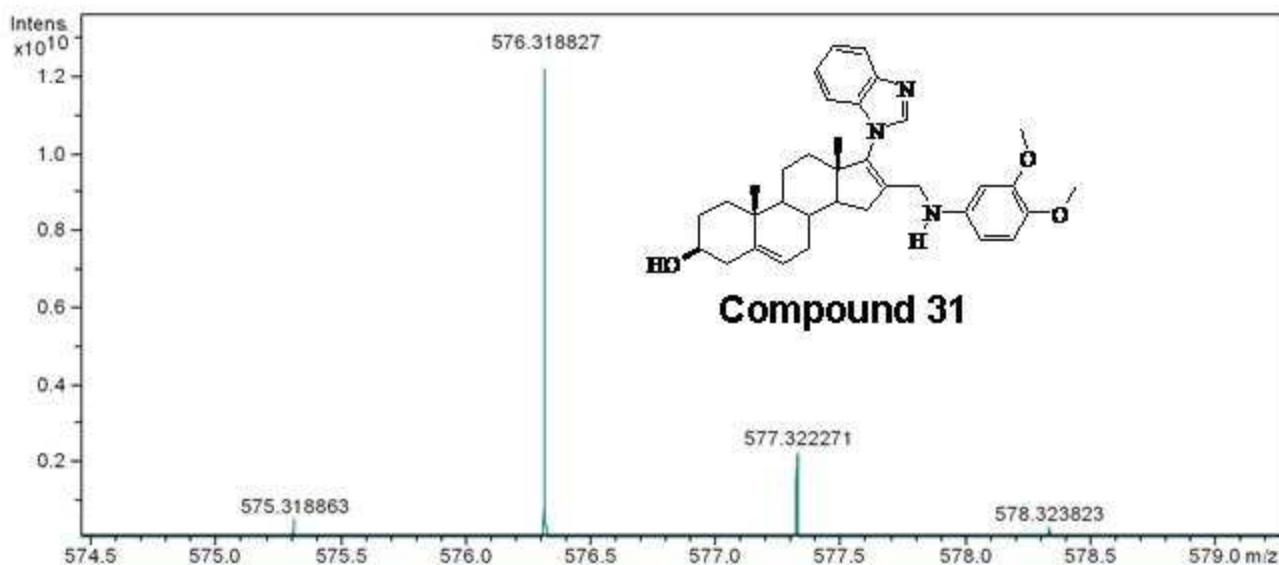
### Analysis Info

Analysis Name VNPT85\_pos\_000001.d  
Method XMASS\_Method  
Sample Name: VNPT85\_pos  
VNPT85\_pos: in 1:1 THF:MeOH w/ NaCl.

Acquisition Date 12/13/2010 9:58:53 AM  
Operator FTMS\_USER  
Instrument apex-Qe

### Acquisition Parameter

Sample Name: VNPT85  
Exact Mass of (C<sub>35</sub>H<sub>43</sub>N<sub>3</sub>O<sub>3</sub>)Na<sup>+</sup>: 576.319663u  
Observed Mass: 576.318827u  
Difference: -1.5 ppm



#	m/z	I
1	104.559218	33793815
2	115.265512	208863415
3	115.305605	136110263
4	115.345740	42790071
5	144.082437	58001569
6	189.603830	54713133
7	189.712316	34044719
8	191.888100	42187618
9	191.999087	163289957
10	191.999533	45611877
11	192.221687	436902762
12	192.332870	101170029
13	192.333198	148314989
14	288.164855	109355579
15	553.410476	43231973
16	554.332671	121481968
17	554.335691	302820080
18	554.338815	117811952
19	555.263893	38873850
20	555.335906	44018427
21	555.338877	93498107
22	555.343306	44083963
23	574.321872	53701486

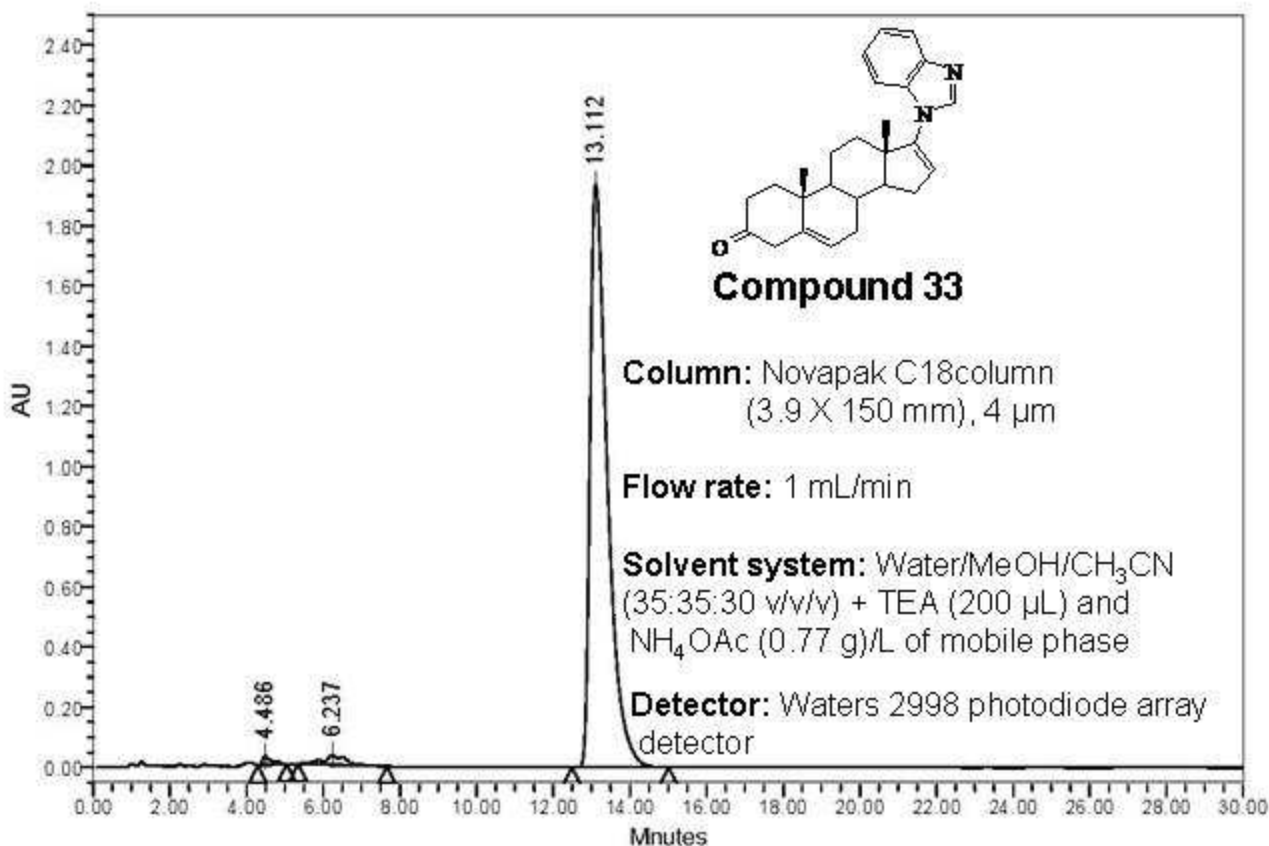
Reported by User: System

Project Name: FDA\_Default

**SAMPLE INFORMATION**

Sample Name: VNPT92  
 Sample Type: Unknown  
 Vial: 15  
 Injection #: 2  
 Injection Volume: 10.00 ul  
 Run Time: 30.0 Minutes  
 Sample Set Name:

Acquired By: System  
 Date Acquired: 4/19/2012 12:21:43 PM  
 Acq. Method Set: VN124  
 Date Processed: 4/19/2012 1:11:33 PM  
 Processing Method: VN124venky  
 Channel Name: W/in Ch1  
 Proc. Chnl. Descr.: FDA 242.7 nm



**PDA Result Table**

Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (μV*sec)	% Area	Height (μV)	Int Type	Amount
1	4.486							487872	0.78	29481	bb	
2	6.237							1308902	2.09	32125	bb	
3	13.112							60874384	97.13	1938660	bb	
3	13.112	60874384				No				No		

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### Analysis Info

Analysis Name: VNPT92\_pos\_000001.d

Method: XMASS\_Method

Sample Name: VNPT92\_pos

VNPT92\_pos: in 1:1 THF:MeOH w/ NaCl.

Acquisition Date: 12/13/2010 2:56:24 PM

Operator: FTMS\_USER

Instrument: apex-Qe

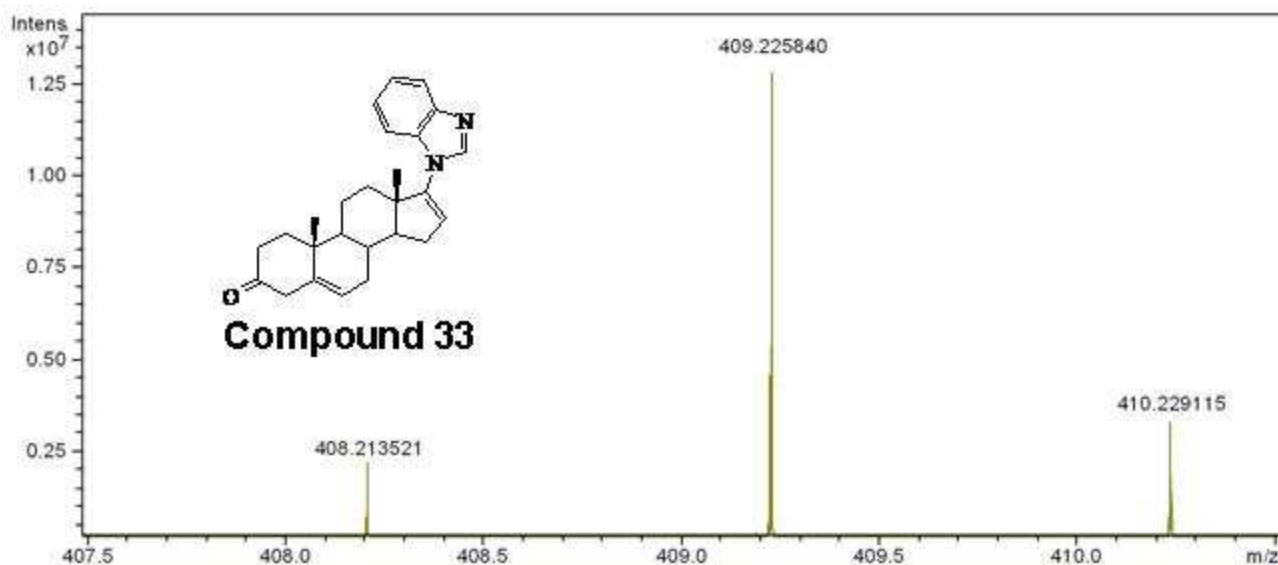
### Acquisition Parameter

Sample Name: VNPT92

Exact Mass of (C<sub>26</sub>H<sub>30</sub>N<sub>2</sub>O)Na<sup>+</sup>: 409.225035u

Observed Mass: 409.22584u

Difference: 2.0 ppm

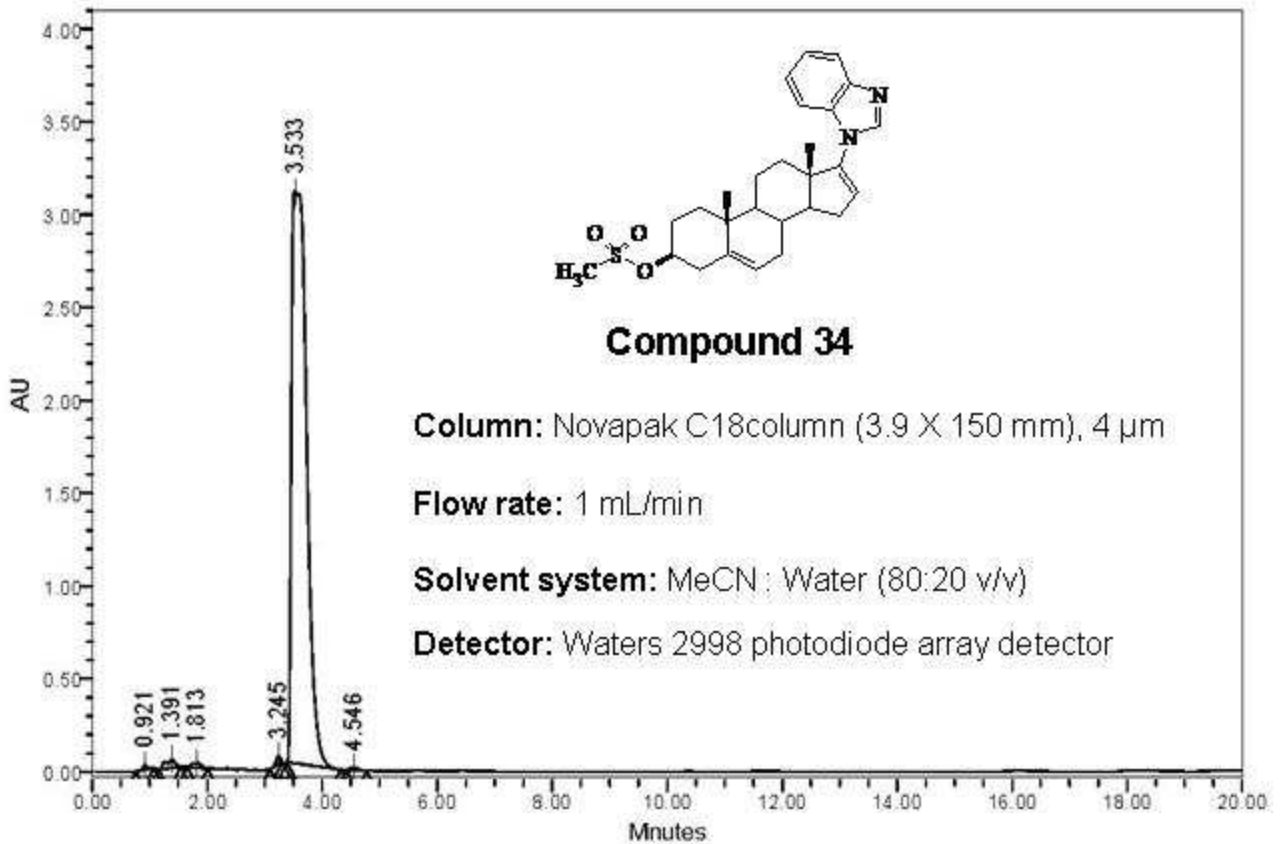


#	m/z	I
1	137.090933	2302848
2	342.717283	2674180
3	368.135593	2290701
4	385.228031	2892305
5	387.241298	4228626
6	387.243645	9944594
7	388.247091	3527187
8	401.219969	2389537
9	401.222860	18296353
10	402.226480	7476771
11	403.238687	5930532
12	407.207573	3683884
13	407.210005	10640940
14	409.223325	4535857
15	409.225840	13131313
16	410.229115	3411507
17	413.267057	2642491
18	423.202097	2519645
19	423.204968	13635185
20	424.208468	3366497
21	425.220782	5736038
22	437.191570	3405472
23	437.194387	13807264

**SAMPLE INFORMATION**

Sample Name: VNPT88  
 Sample Type: Unknown  
 Vial: 12  
 Injection #: 1  
 Injection Volume: 5.00 ul  
 Run Time: 20.0 Minutes  
 Sample Set Name:

Acquired By: System  
 Date Acquired: 4/17/2012 4:18:02 PM  
 Acq. Method Set: VN124  
 Date Processed: 4/17/2012 4:44:33 PM  
 Processing Method: VN124venky  
 Channel Name: WIn Ch1  
 Proc. Chnl. Descr.: FDA 242.7 nm



**PDA Result Table**

Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (µV*sec)	% Area	Height (µV)	Int Type	Amount
1	0.921							111335	0.19	22065	bb	
2	1.391							530162	0.92	46499	bb	
3	1.813							287257	0.50	26807	bb	
4	3.245							238659	0.41	42892	bb	
5	3.533							56331766	97.75	3097112	bb	
6	4.546							127688	0.22	14225	bb	
6	4.546		127688		No				No			



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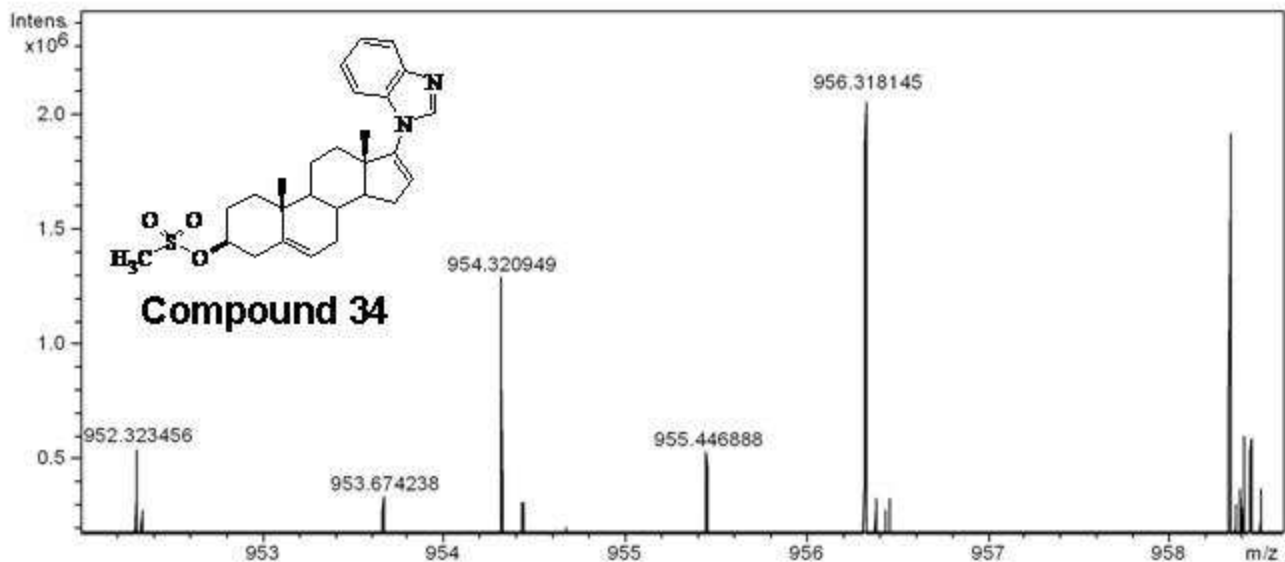
## Analysis Info

Analysis Name VNPT88\_pos\_000001.d  
Method XMASS\_Method  
Sample Name: VNPT88\_pos  
VNPT88\_pos: in 1:1 THF:MeOH w/ NaCl.

Acquisition Date 12/13/2010 10:10:21 AM  
Operator FTMS\_USER  
Instrument apex-Qe

## Acquisition Parameter

Sample Name: VNPT88  
Exact Mass of (C<sub>27</sub>H<sub>34</sub>N<sub>2</sub>O<sub>4</sub>S)<sub>2</sub>Na<sup>+</sup>: 955.447248u  
Observed Mass: 955.446888u  
Difference: < -1.0 ppm

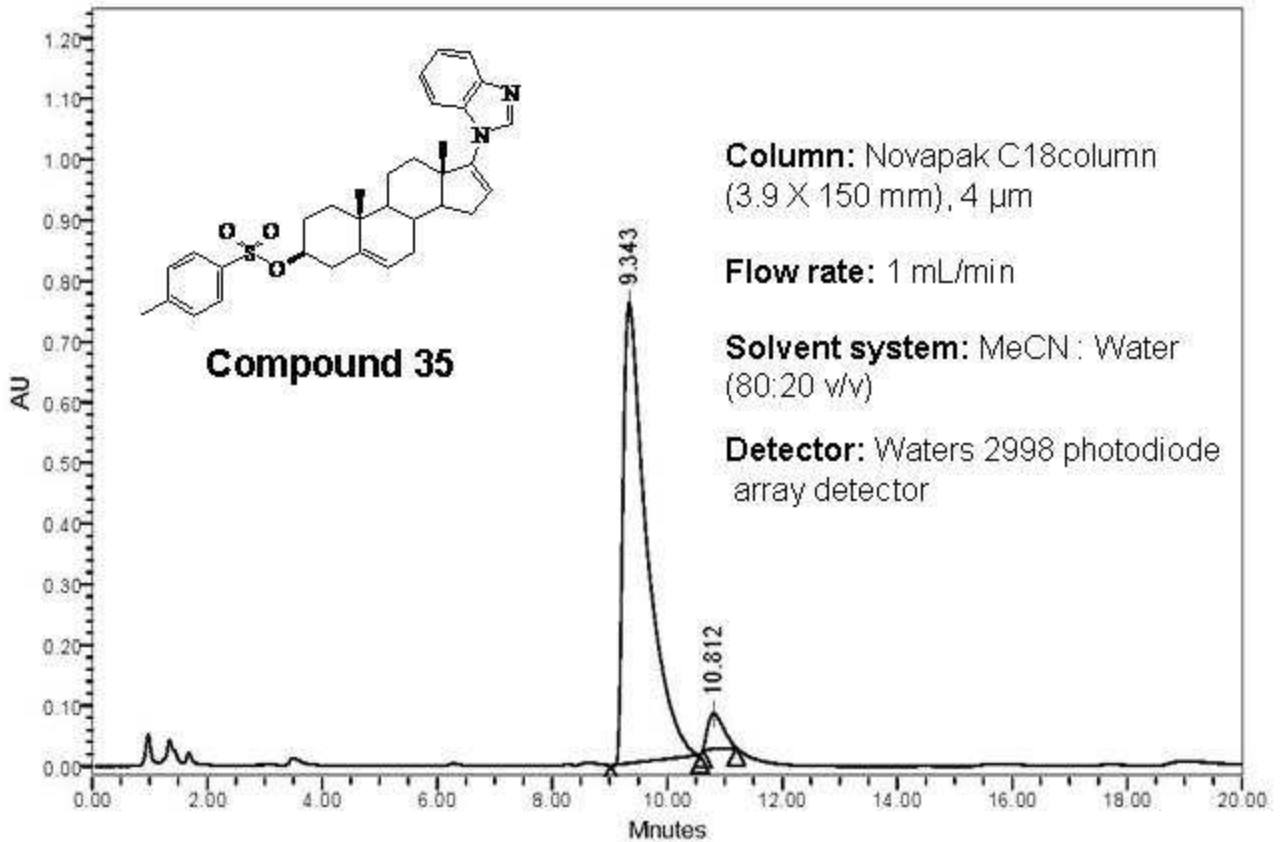


#	m/z	I
1	92.810928	762789
2	93.447502	1444669
3	121.423903	1207111
4	123.748557	549667
5	136.518139	437753
6	167.502441	830149
7	185.622592	1579337
8	185.623909	2056905
9	186.124356	625745
10	210.584300	1979814
11	233.617105	6074250
12	233.621378	752650
13	234.118752	1538965
14	342.717353	603861
15	371.237072	1004863
16	371.238050	1050175
17	371.238945	539967
18	371.240253	3637823
19	371.243932	11222591
20	371.245617	169455167
21	371.248499	91926079
22	371.251769	3413567
23	372.241528	617530

**SAMPLE INFORMATION**

Sample Name: VNPT96  
 Sample Type: Unknown  
 Vial: 16  
 Injection #: 1  
 Injection Volume: 5.00 ul  
 Run Time: 20.0 Mnutes  
 Sample Set Name:

Acquired By: System  
 Date Acquired: 4/17/2012 2:57:03 PM  
 Acq. Method Set: VN124  
 Date Processed: 4/17/2012 3:27:47 PM  
 Processing Method: VN124venky  
 Channel Name: WIn Ch1  
 Proc. Chnl. Descr.: FDA 238.5 nm



**PDA Result Table**

Name	RT	Area	Purity (#1) Angle	Purity (#1) Threshold	Purity Flag	Match (#1) Spect. Name	Match (#1) Angle	Match (#1) Threshold	PDA Match Flag
1	9.343	21631487			No				No
2	10.812	1105449			No				No

Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (µV*sec)	% Area	Height (µV)	Int Type	Amount
1	9.343							21631487	95.14	759568	bb	
2	10.812							1105449	4.86	58691	bb	

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## Analysis Info

Analysis Name VNPT96\_pos\_000001.d

Method XMASS\_Method

Sample Name: VNPT96\_pos

VNPT96\_pos: in 1:1 THF:MeOH w/ NaCl.

Acquisition Date 12/13/2010 3:00:37 PM

Operator FTMS\_USER

Instrument apex-Qe

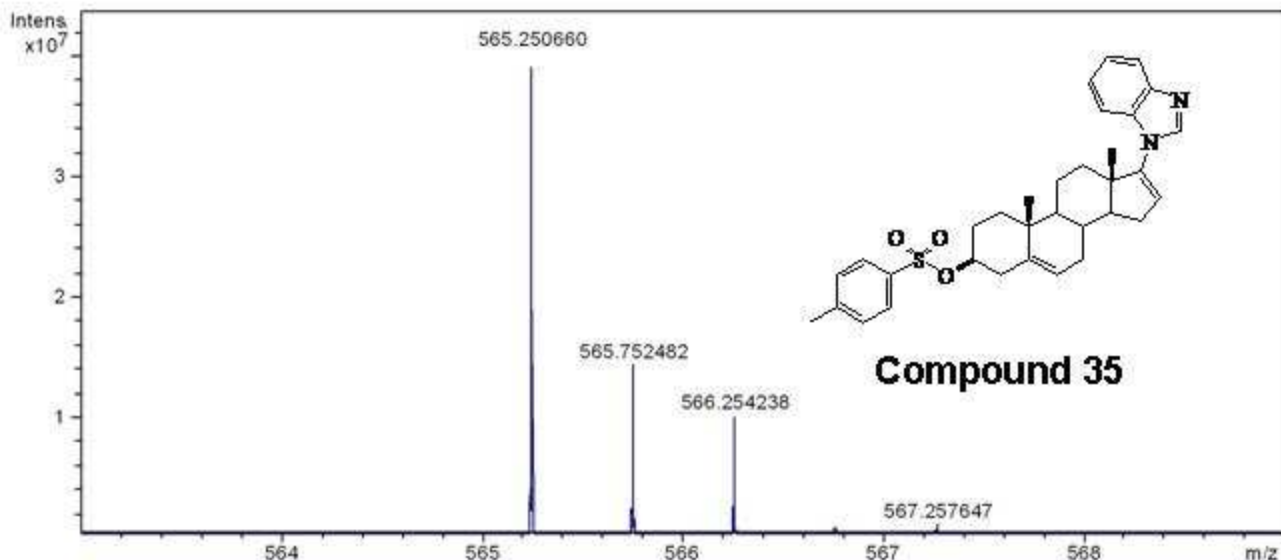
## Acquisition Parameter

Sample Name: VNPT96

Exact Mass of (C<sub>33</sub>H<sub>38</sub>N<sub>2</sub>O<sub>3</sub>S)Na<sup>+</sup>: 565.249535u

Observed Mass: 565.250660u

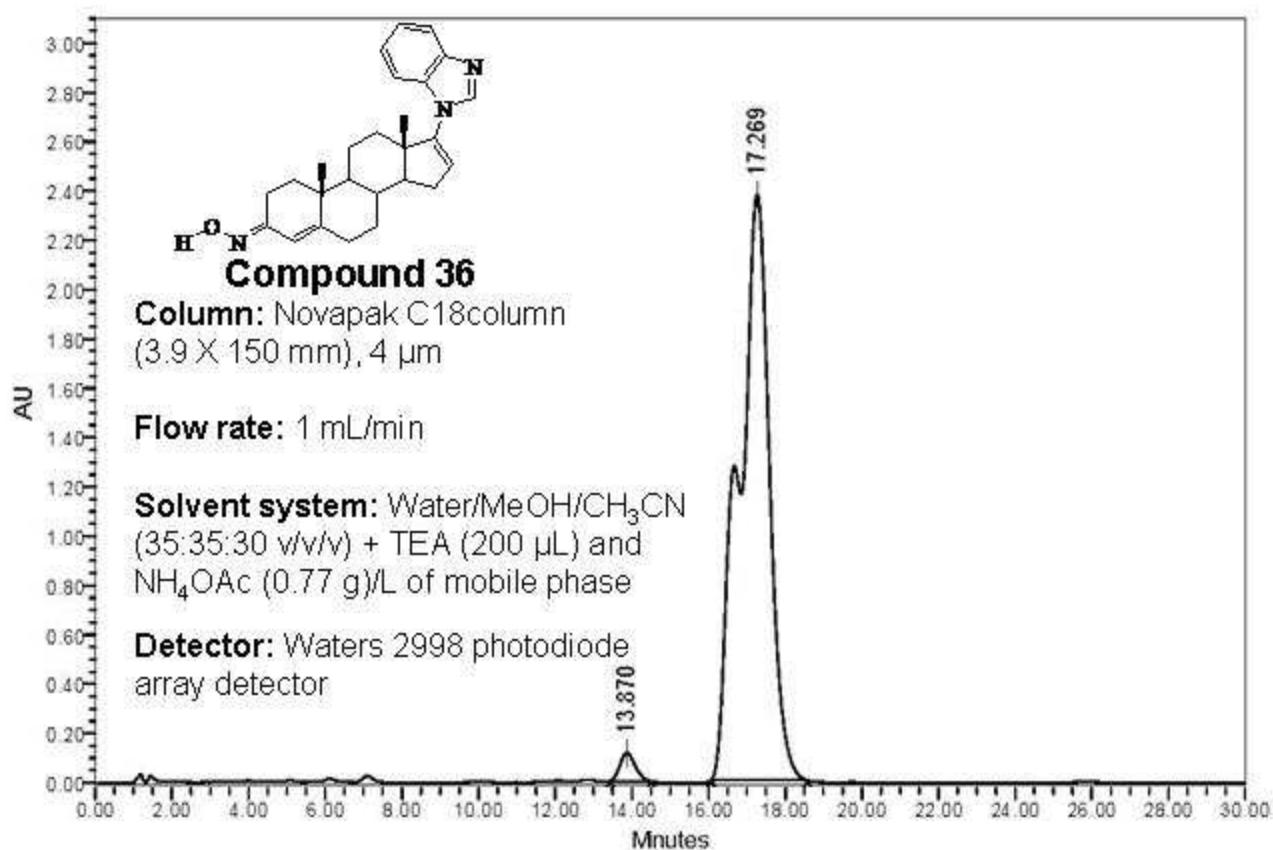
Difference: 2.0 ppm



#	m/z	I
1	371.245638	39013499
2	371.248473	92384379
3	372.249059	20368505
4	372.250628	5581945
5	372.251966	21924985
6	373.252490	4173943
7	393.228538	3966041
8	393.230669	11574361
9	403.272364	5889112
10	403.275085	12258392
11	417.288318	3827823
12	417.290650	11332719
13	507.330448	3972863
14	543.262606	27447376
15	543.268069	532983888
16	544.267334	17625177
17	544.269248	16248921
18	544.271785	159232089
19	544.275636	7544921
20	545.264304	15765602
21	545.275212	23621730
22	546.267946	5662826
23	551.356667	4714646

**SAMPLE INFORMATION**

Sample Name:	VNPT56EZ	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	4/12/2012 2:11:35 PM
Vial:	4	Acq. Method Set:	VN124
Injection #:	1	Date Processed:	4/12/2012 4:51:36 PM
Injection Volume:	20.00 ul	Processing Method:	VN124venky
Run Time:	30.0 Minutes	Channel Name:	WIn Ch1
Sample Set Name:		Proc. Chnl. Descr.:	FDA 242.7 nm



**PDA Result Table**

Name	RT	Area	Purity (#1) Angle	Purity (#1) Threshold	Purity Flag	Match (#1) Spect. Name	Match (#1) Angle	Match (#1) Threshold	PDA Match Flag
1	13.870	3135516			No				No
2	17.269	131270485			No				No

Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (μV*sec)	% Area	Height (μV)	Int Type	Amount
1	13.870							3274849	2.41	117424	bb	
2	17.269							132434535	97.59	2383008	bb	

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## Analysis Info

Analysis Name VNPT56\_pos\_000001.d

Method XMASS\_Method

Sample Name: VNPT56\_pos  
VNPT56\_pos: in 1:1 THF:MeOH w/ NaCl.

Acquisition Date 12/13/2010 2:26:55 PM

Operator FTMS\_USER

Instrument apex-Qe

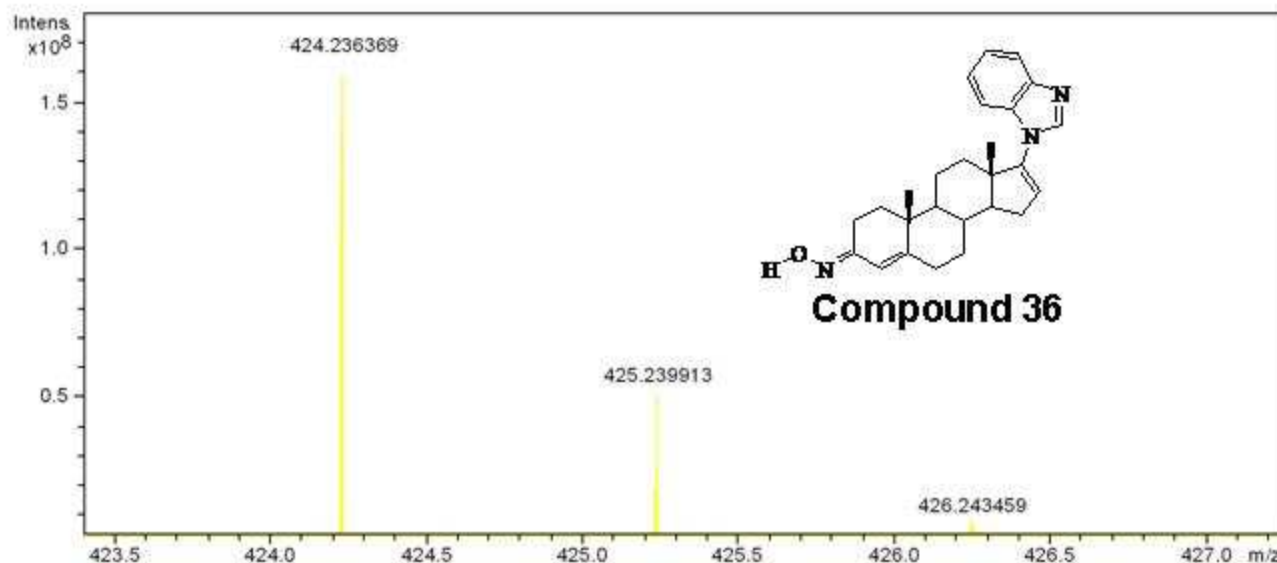
## Acquisition Parameter

Sample Name: VNPT56

Exact Mass of (C<sub>26</sub>H<sub>31</sub>N<sub>3</sub>O)<sup>Na+</sup>: 424.235934u

Observed Mass: 424.236369u

Difference: < 1.0 ppm



#	m/z	I
1	368.128009	3737047
2	368.135383	6376919
3	368.139193	4440535
4	402.252054	20780227
5	402.254405	99906755
6	403.255310	6900927
7	403.257980	28226751
8	404.261260	4080827
9	424.233761	55407799
10	424.236369	164099255
11	424.237833	19223735
12	424.238837	8901815
13	424.239795	5143735
14	424.240772	3601591
15	425.237028	19016890
16	425.239913	52950202
17	426.243459	8574142
18	437.190333	4228346
19	437.194291	11052282
20	463.304059	6389252
21	482.195620	5676821
22	483.276248	8722215
23	488.656117	3899262

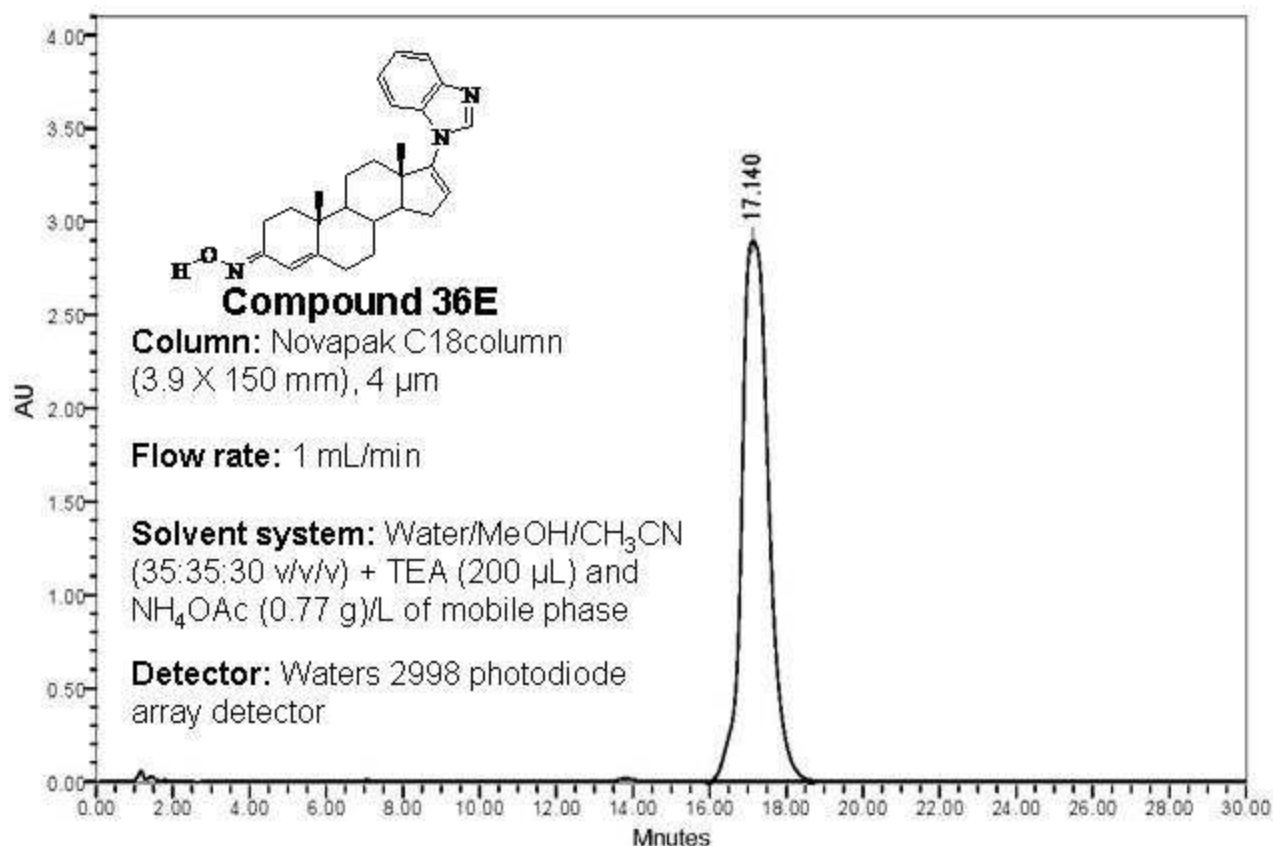
Reported by User: System

Project Name: FDA\_Default

**SAMPLE INFORMATION**

Sample Name: VNPT56E  
 Sample Type: Unknown  
 Vial: 6  
 Injection #: 1  
 Injection Volume: 20.00 ul  
 Run Time: 30.0 Minutes  
 Sample Set Name: Puru Sample Set 1

Acquired By: System  
 Date Acquired: 4/12/2012 3:15:39 PM  
 Acq. Method Set: VN124  
 Date Processed: 4/12/2012 5:05:48 PM  
 Processing Method: VN124venky  
 Channel Name: WIn Ch1  
 Proc. Chnl. Descr.: FDA 242.7 nm



**PDA Result Table**

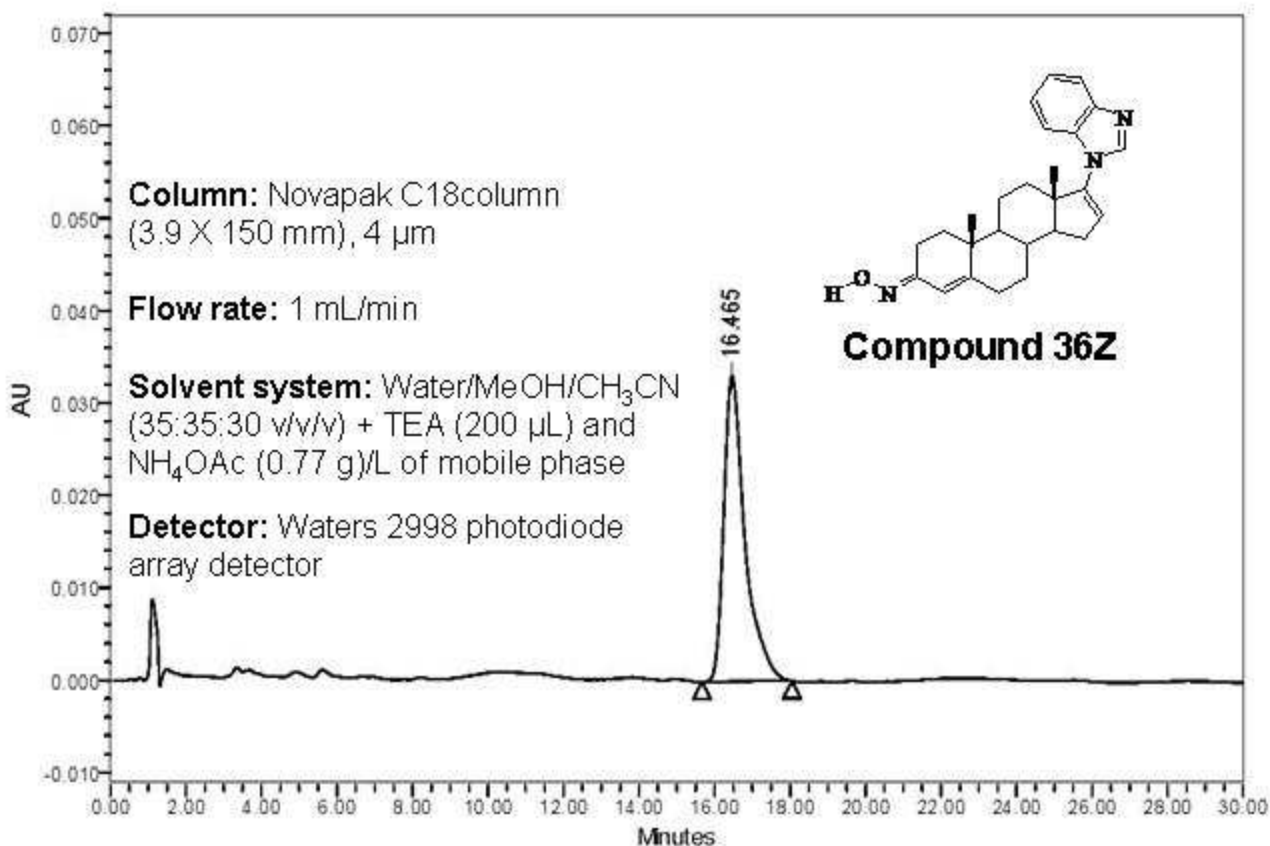
Name	RT	Area	Purity (#1) Angle	Purity (#1) Threshold	Purity Flag	Match (#1) Spect. Name	Match (#1) Angle	Match (#1) Threshold	PDA Match Flag
1	17.140	140318033			No				No

Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (µV*sec)	% Area	Height (µV)	Int Type	Amount
1	17.140							140318033	100.00	2894291	bb	

### SAMPLE INFORMATION

Sample Name: VNPT56Z  
 Sample Type: Unknown  
 Vial: 7  
 Injection #: 1  
 Injection Volume: 20.00 ul  
 Run Time: 30.0 Minutes  
 Sample Set Name: Furu Sample Set 1

Acquired By: System  
 Date Acquired: 4/12/2012 3:46:56 PM  
 Acq. Method Set: VNI24  
 Date Processed: 4/16/2012 12:41:23 PM  
 Processing Method: VNI24venky  
 Channel Name: WIn Ch1  
 Proc. Chnl. Descr.: FDA 308.4 nm



PDA Result Table

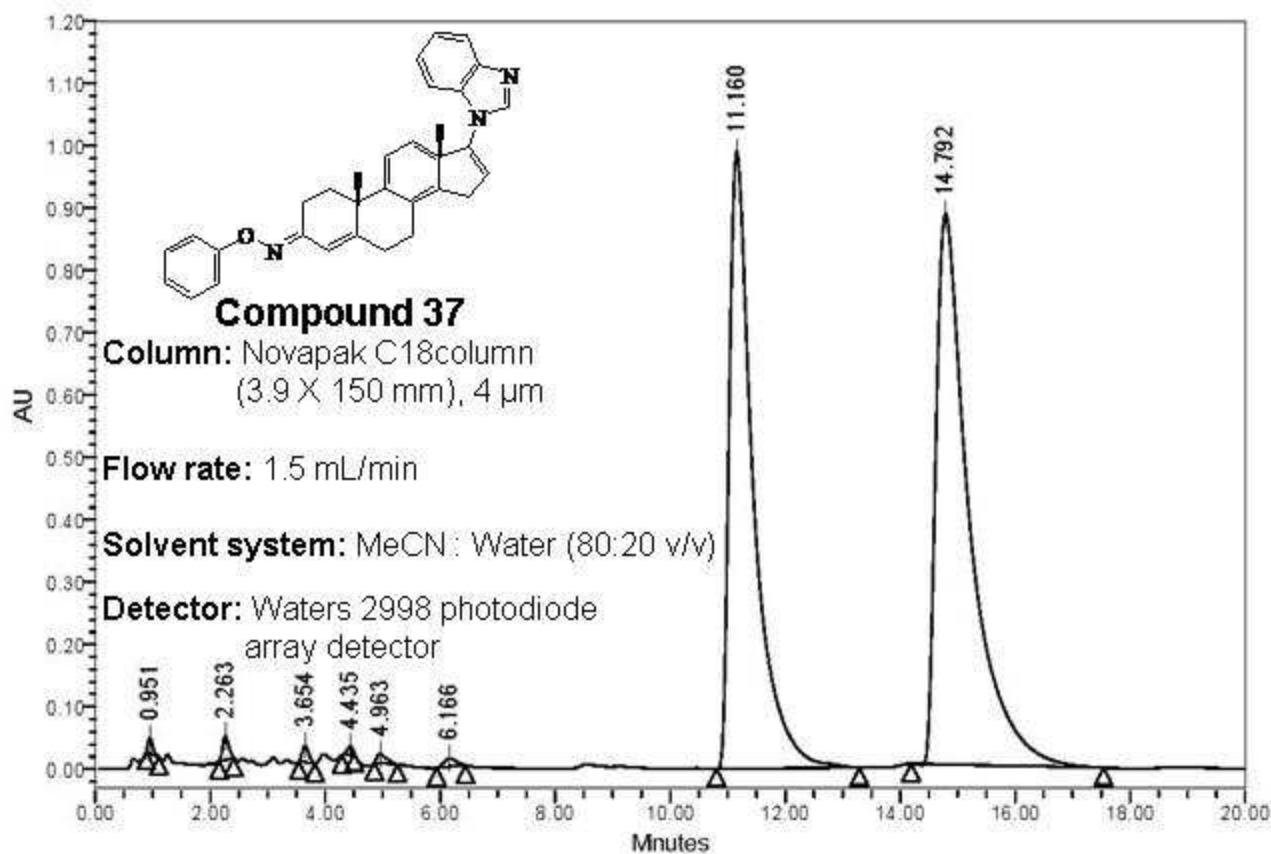
Name	RT	Area	Purity (#1) Angle	Purity (#1) Threshold	Purity Flag	Match (#1) Spect. Name	Match (#1) Angle	Match (#1) Threshold	PDA Match Flag
1	16.465	1289423			No				No

Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (μV*sec)	% Area	Height (μV)	Int Type	Amount
1	16.465							1289423	100.00	33076	bb	

**SAMPLE INFORMATION**

Sample Name: VNPT86EZ  
 Sample Type: Unknown  
 Vial: 33  
 Injection #: 1  
 Injection Volume: 10.00 ul  
 Run Time: 20.0 Mnutes  
 Sample Set Name:

Acquired By: System  
 Date Acquired: 4/17/2012 2:31:15 PM  
 Acq. Method Set: VN124  
 Date Processed: 4/17/2012 2:58:37 PM  
 Processing Method: VN124venky  
 Channel Name: WWin Ch1  
 Proc. Chnl. Descr.: FDA 242.7 nm



**PDA Result Table**

Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (µV*sec)	% Area	Height (µV)	Int Type	Amount
1	0.951							147967	0.22	24144	bb	
2	2.263							279566	0.42	38471	bb	
3	3.654							210600	0.32	26908	bb	
4	4.435							77454	0.12	11811	bb	
5	4.963							170556	0.26	14388	bb	
6	6.166							199059	0.30	13315	bb	
7	11.160							29047288	44.15	990268	bb	
8	14.792							35665664	54.20	882686	bb	



# Mass Spectrum List Report

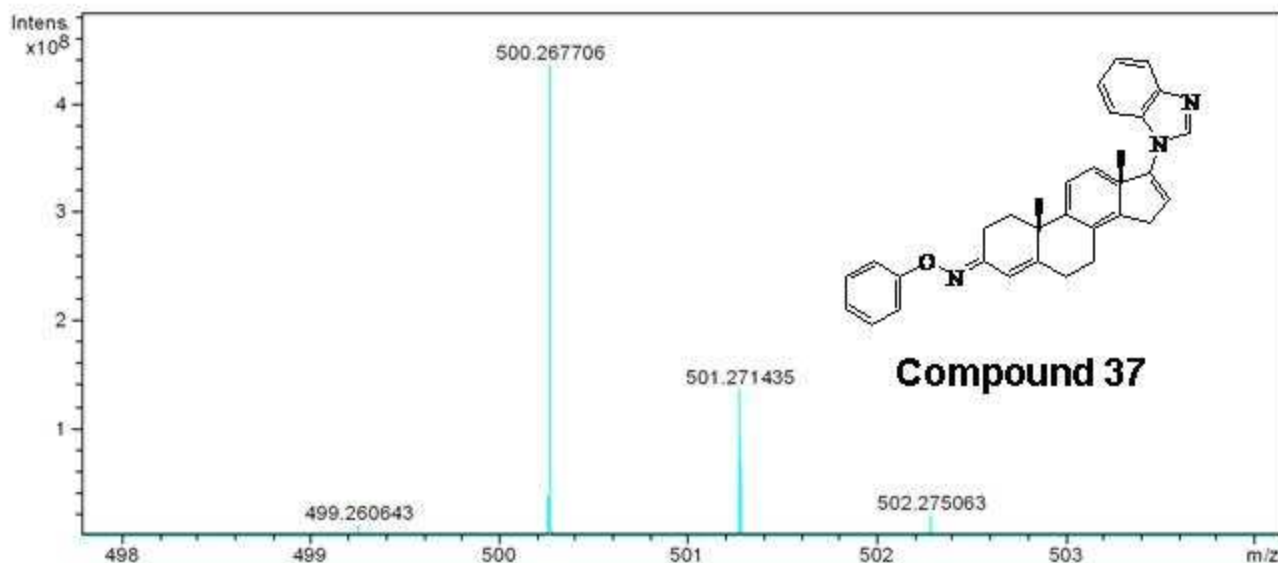
## Analysis Info

Analysis Name VNPT86\_pos\_000002.d  
Method XMASS\_Method  
Sample Name: VNPT86\_pos  
VNPT86\_pos: in 1:1 THF:MeOH w/ NaCl.

Acquisition Date 12/13/2010 2:43:43 PM  
Operator FTMS\_USER  
Instrument apex-Qe

## Acquisition Parameter

Sample Name: VNPT86  
Exact Mass of (C<sub>32</sub>H<sub>35</sub>N<sub>3</sub>O)Na<sup>+</sup>: 500.267234u  
Observed Mass: 500.267706u  
Difference: < 1.0 ppm

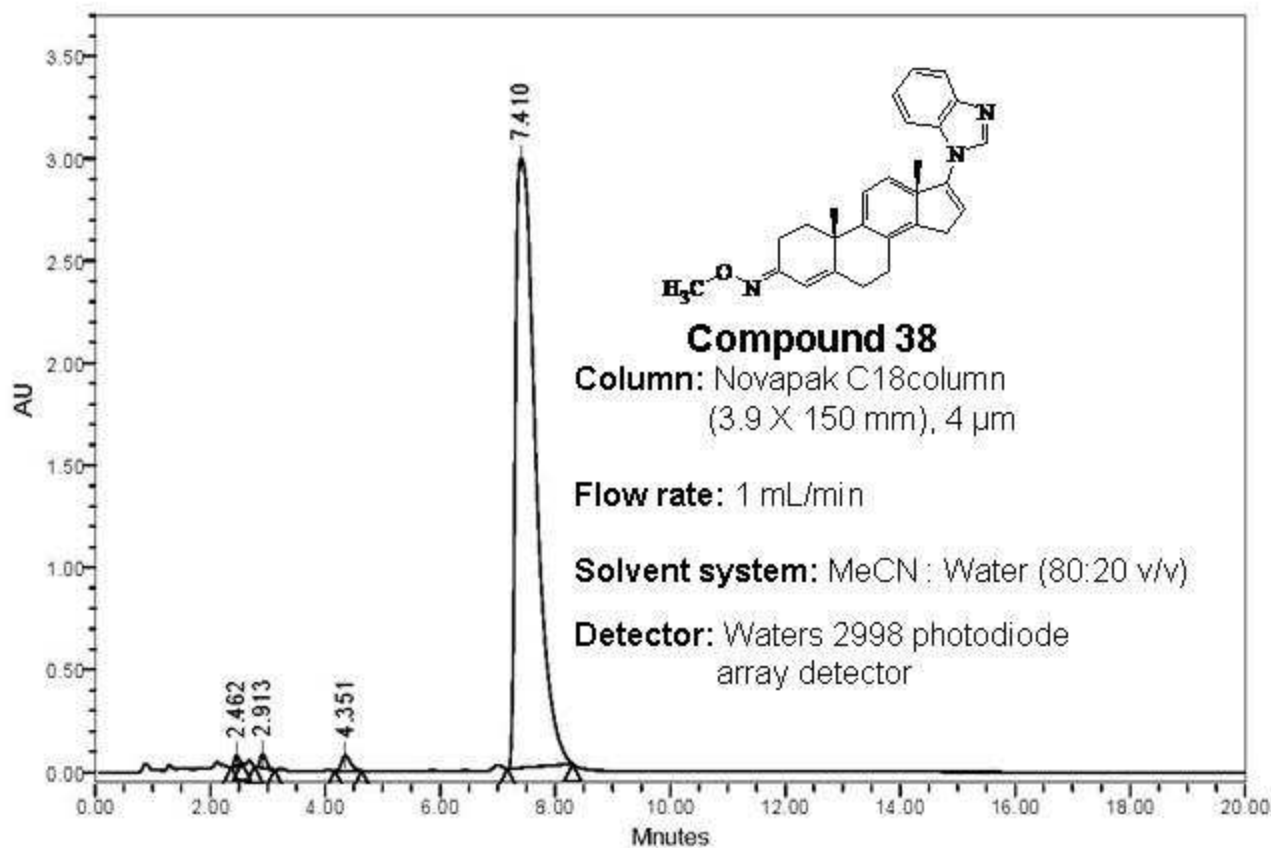


#	m/z	I
1	250.132714	6161166
2	437.194380	8789105
3	463.304092	5616992
4	478.281369	4172295
5	478.283427	10476039
6	478.286387	40480264
7	479.289697	13168147
8	499.260643	10297096
9	500.257456	5318420
10	500.261569	38760212
11	500.265386	46083860
12	500.267706	433630996
13	500.271389	16985876
14	500.272725	10055444
15	500.274065	6876948
16	500.275372	4841236
17	501.265880	18083617
18	501.269136	26095393
19	501.271435	134197025
20	501.275116	6324001
21	502.269589	4384557
22	502.272551	5713709
23	502.275063	19107629

**SAMPLE INFORMATION**

Sample Name: VNPT90EZ  
 Sample Type: Unknown  
 Vial: 13  
 Injection #: 2  
 Injection Volume: 5.00 ul  
 Run Time: 20.0 Mnutes  
 Sample Set Name:

Acquired By: System  
 Date Acquired: 4/16/2012 6:40:40 PM  
 Acq. Method Set: VN124  
 Date Processed: 4/16/2012 7:02:11 PM  
 Processing Method: VN124venky  
 Channel Name: WIn Ch1  
 Proc. Chnl. Descr.: FDA 242.7 nm



**PDA Result Table**

Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (µV*sec)	% Area	Height (µV)	Int Type	Amount
1	2.462							276523	0.37	49900	bb	
2	2.913							510130	0.69	66982	bb	
3	4.351							821480	1.11	77988	bb	
4	7.410							72353889	97.83	2982634	bb	
4	7.410	72353889			No				No			

## Mass Spectrum List Report

### Analysis Info

Analysis Name VNPT90\_pos\_000001.d

Method XMASS\_Method

Sample Name: VNPT90\_pos  
VNPT90\_pos: in 1:1 THF:MeOH w/ NaCl.

Acquisition Date 12/13/2010 2:48:12 PM

Operator FTMS\_USER

Instrument apex-Qe

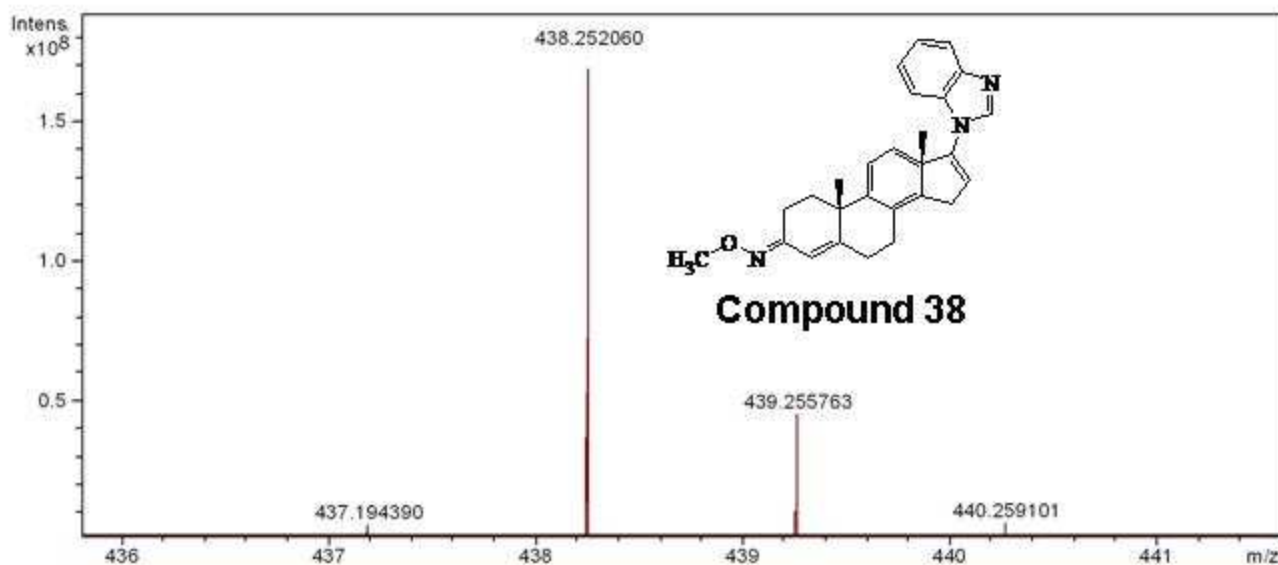
### Acquisition Parameter

Sample Name: VNPT90

Exact Mass of (C<sub>27</sub>H<sub>33</sub>N<sub>3</sub>O)Na<sup>+</sup>: 438.251584u

Observed Mass: 438.252060u

Difference: 1.1 ppm

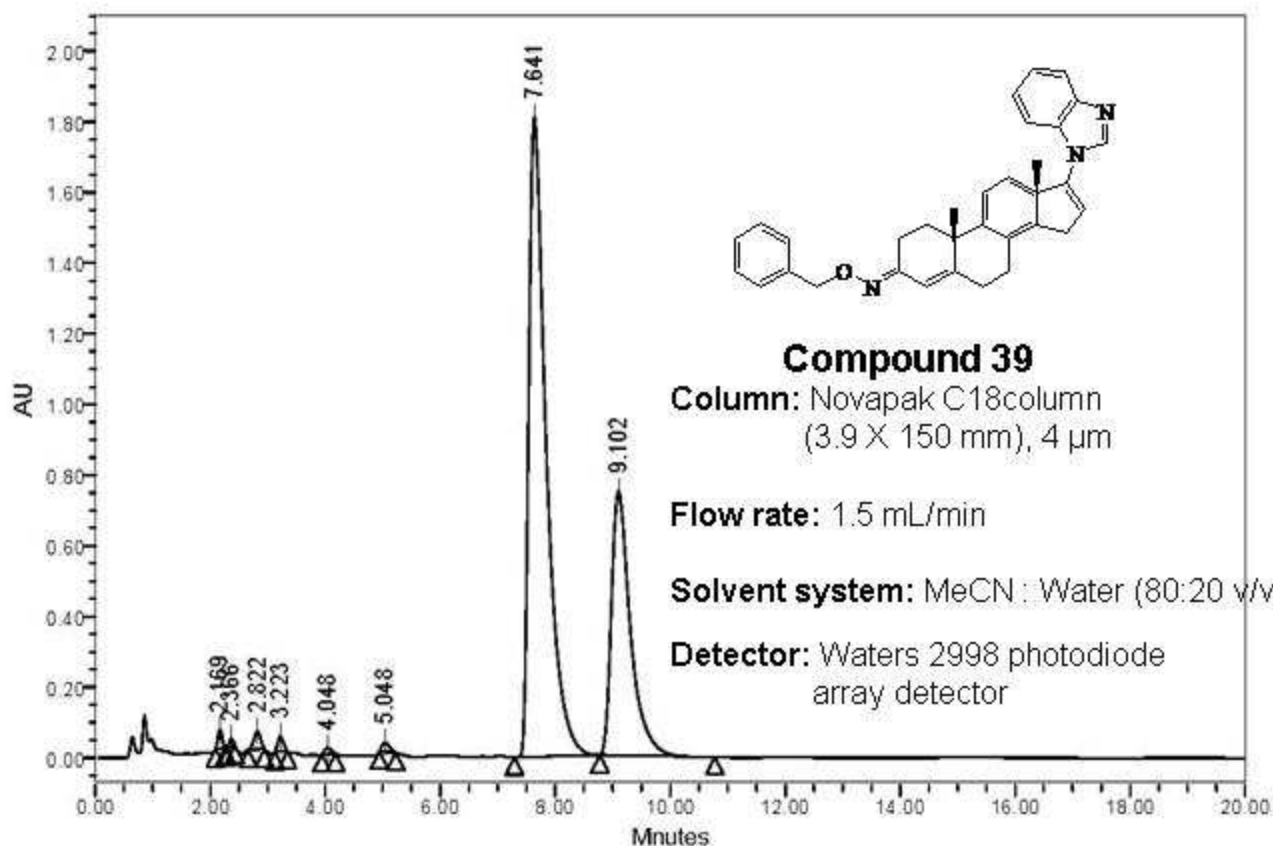


#	m/z	I
1	219.124631	2574927
2	413.266960	8050259
3	416.267615	17567324
4	416.270108	71315036
5	417.270928	7669343
6	417.273591	24768095
7	418.276985	4046435
8	437.194390	5367501
9	438.248374	20856533
10	438.250131	38055637
11	438.252060	174108373
12	438.256591	3182293
13	439.251788	7808733
14	439.253076	10653405
15	439.255763	45002461
16	440.259101	5836517
17	443.292697	5840638
18	461.291776	2971562
19	463.247635	3695551
20	463.303667	2658240
21	463.305263	2664896
22	463.307719	16158656
23	464.310818	5484491

**SAMPLE INFORMATION**

Sample Name: VNPT91EZ  
 Sample Type: Unknown  
 Vial: 14  
 Injection #: 1  
 Injection Volume: 10.00 ul  
 Run Time: 20.0 Mnutes  
 Sample Set Name:

Acquired By: System  
 Date Acquired: 4/18/2012 12:06:02 PM  
 Acq. Method Set: VN124  
 Date Processed: 4/18/2012 12:36:11 PM  
 Processing Method: VN124venky  
 Channel Name: WIn Ch1  
 Proc. Chnl. Descr.: FDA 242.7 nm



**PDA Result Table**

Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (μV*sec)	% Area	Height (μV)	Int Type	Amount
1	2.169							281170	0.50	52418	bb	
2	2.366							108346	0.19	23308	bb	
3	2.822							405503	0.72	51482	bb	
4	3.223							294087	0.52	42465	bb	
5	4.048							131555	0.23	17038	bb	
6	5.048							242246	0.43	26854	bb	
7	7.641							37898416	67.06	1810460	bb	
8	9.102							17155637	30.35	748129	bb	

# Mass Spectrum List Report

## Analysis Info

Analysis Name VNPT91\_pos\_000001.d

Method XMASS\_Method

Sample Name: VNPT91\_pos

VNPT91\_pos: in 1:1 THF:MeOH w/ NaCl.

Acquisition Date 12/13/2010 2:51:51 PM

Operator FTMS\_USER

Instrument apex-Qe

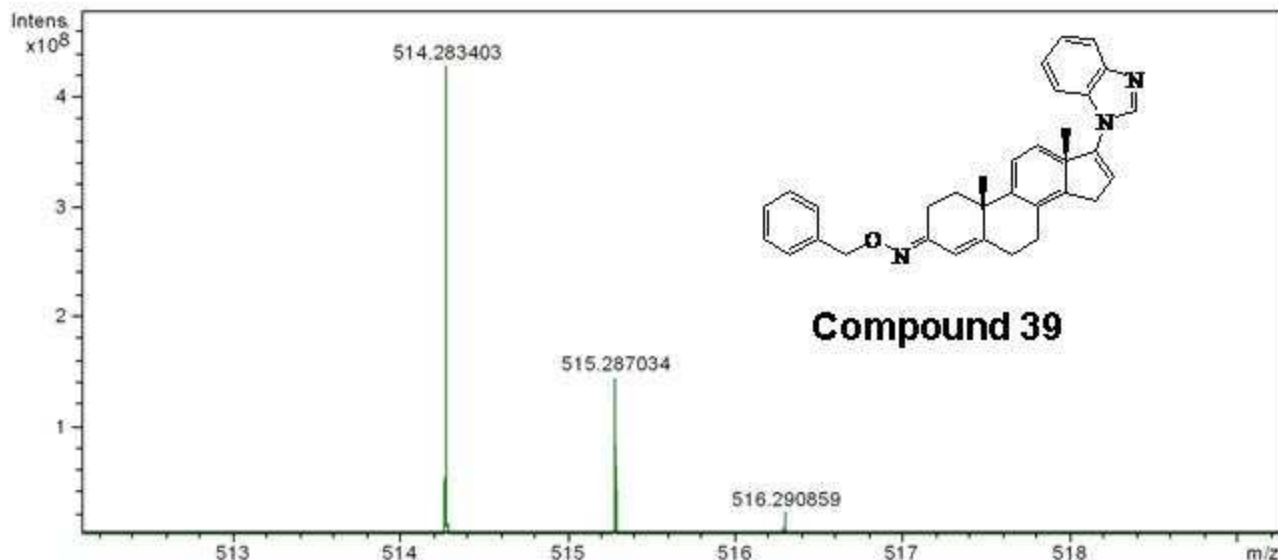
## Acquisition Parameter

Sample Name: VNPT91

Exact Mass of (C<sub>33</sub>H<sub>37</sub>N<sub>3</sub>O)<sup>Na+</sup>: 514.282884u

Observed Mass: 514.283403u

Difference: 1.0 ppm

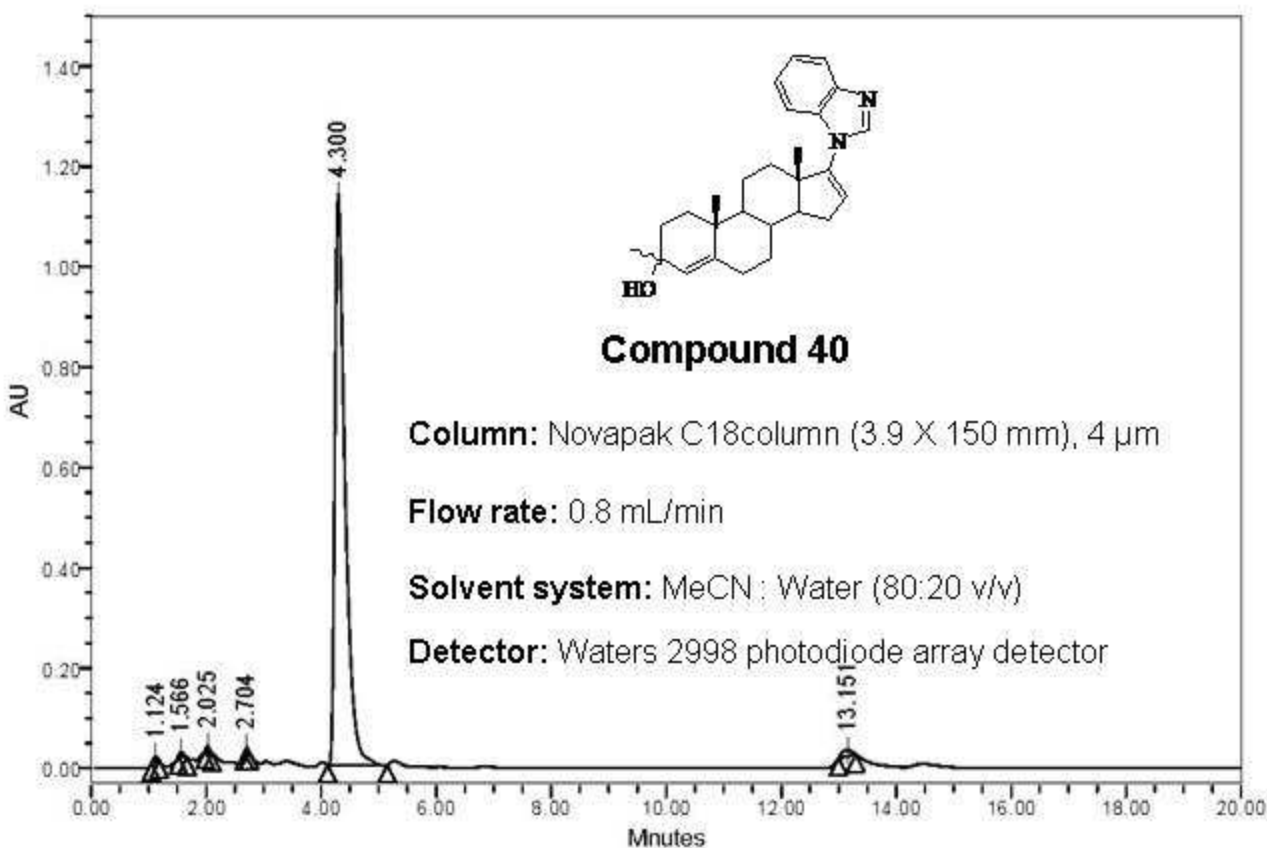


#	m/z	I
1	257.140458	7961506
2	413.267041	9796655
3	437.194474	6372640
4	492.296638	45985994
5	492.301584	187543755
6	493.300248	25276638
7	493.303108	9834718
8	493.305230	59355358
9	494.303758	6232305
10	494.308746	9810162
11	507.330529	6953455
12	514.278070	64991861
13	514.283403	427602549
14	514.287283	18092661
15	514.288720	11080309
16	514.290105	7660149
17	515.281541	34255496
18	515.282982	27841160
19	515.287034	144355976
20	516.285144	6963867
21	516.290859	21934747
22	528.263300	6980474
23	530.272963	7154590

### SAMPLE INFORMATION

Sample Name: VNPT135  
 Sample Type: Unknown  
 Vial: 21  
 Injection #: 2  
 Injection Volume: 10.00 ul  
 Run Time: 20.0 Mnutes  
 Sample Set Name:

Acquired By: System  
 Date Acquired: 4/18/2012 12:51:36 PM  
 Acq. Method Set: VN124  
 Date Processed: 4/18/2012 1:26:05 PM  
 Processing Method: VN124venky  
 Channel Name: WIn Ch1  
 Proc. Chnl. Descr.: FDA 261.6 nm



PDA Result Table

Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (μV*sec)	% Area	Height (μV)	Int Type	Amount
1	1.124							51733	0.36	10202	bb	
2	1.566							47653	0.33	9677	bb	
3	2.025							43769	0.30	11467	bb	
4	2.704							28431	0.20	9262	bb	
5	4.300							14097027	97.79	1139189	bb	
6	13.151							146781	1.02	12631	bb	
6	13.151	146781			No				No			

## Mass Spectrum List Report

### Analysis Info

Analysis Name VNPT135\_pos\_000001.d

Method XMASS\_Method

Sample Name: VNPT135\_pos

VNPT135\_pos: in 1:1 THF:MeOH w/ NaCl.

Acquisition Date 12/13/2010 3:15:24 PM

Operator FTMS\_USER

Instrument apex-Qe

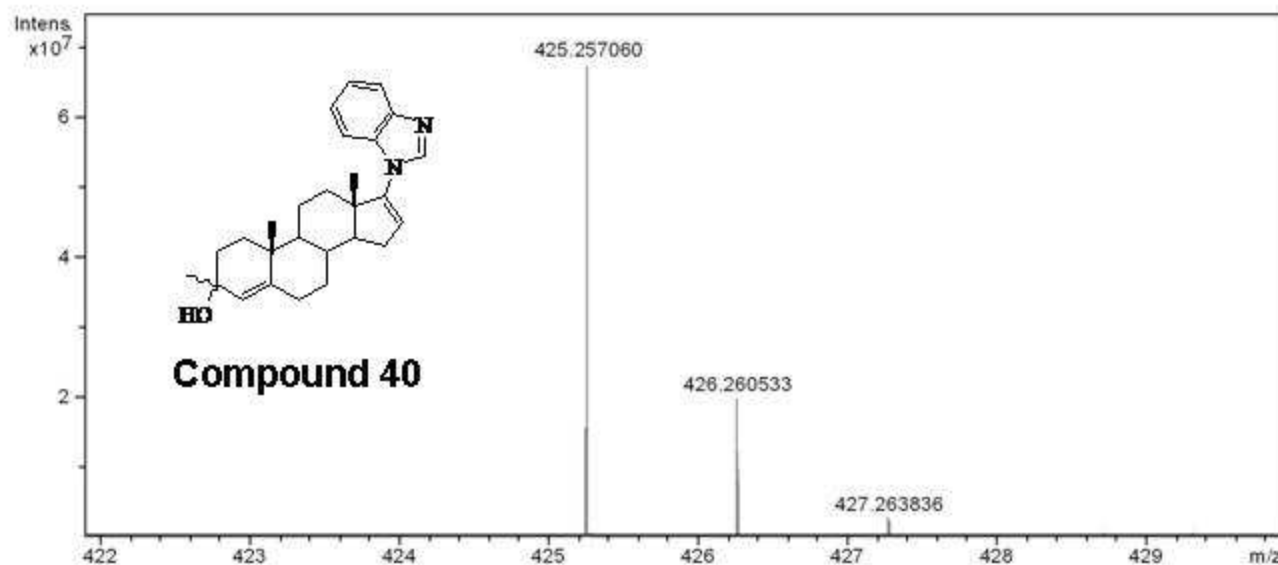
### Acquisition Parameter

Sample Name: VNPT135

Exact Mass of (C<sub>27</sub>H<sub>34</sub>N<sub>2</sub>O)Na<sup>+</sup>: 425.256335u

Observed Mass: 425.257060u

Difference: 1.7 ppm



#	m/z	I
1	403.271288	36826730
2	403.273131	33826410
3	403.274930	122072682
4	403.277216	6772330
5	403.278083	4212330
6	404.274853	23309931
7	404.276519	11656811
8	404.278251	49163883
9	405.278221	4771436
10	405.281837	6237804
11	425.253455	16060075
12	425.254614	14722731
13	425.257060	67481259
14	426.257035	6530736
15	426.260533	19984048
16	426.266079	8052400
17	437.194395	9666291
18	441.249109	6147856
19	441.251922	30699281
20	442.255364	9125656
21	443.288145	8040224
22	443.289864	9060128
23	443.292625	44625696

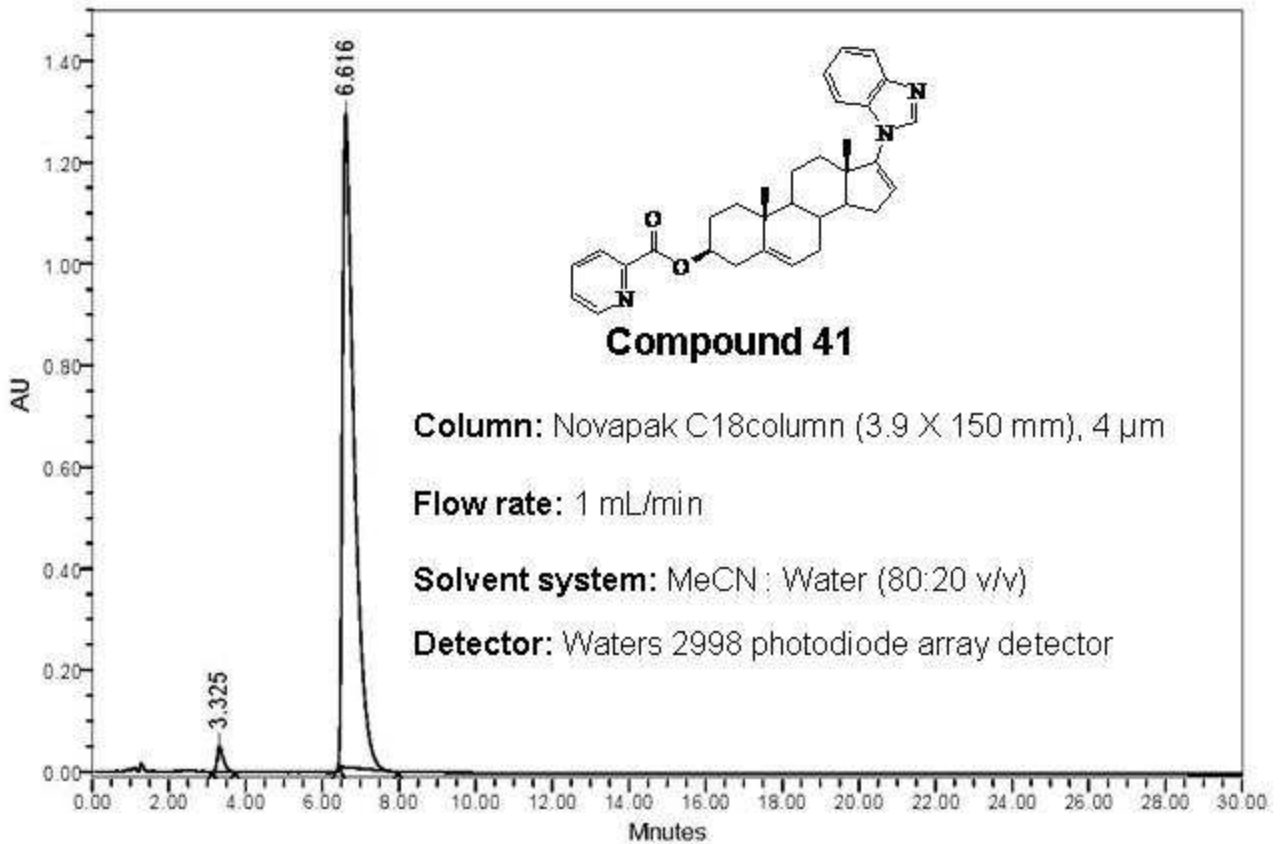
Reported by User: System

Project Name: FDA\_Default

**SAMPLE INFORMATION**

Sample Name: VNPT179  
 Sample Type: Unknown  
 Vial: 26  
 Injection #: 1  
 Injection Volume: 20.00 ul  
 Run Time: 30.0 Minutes  
 Sample Set Name:

Acquired By: System  
 Date Acquired: 4/16/2012 3:50:31 PM  
 Acq. Method Set: VN124  
 Date Processed: 4/16/2012 5:15:43 PM  
 Processing Method: VN124venky  
 Channel Name: WIn Ch1  
 Proc. Chnl. Descr.: FDA 242.7 nm



**PDA Result Table**

Name	RT	Area	Purity (#1) Angle	Purity (#1) Threshold	Purity Flag	Match (#1) Spect. Name	Match (#1) Angle	Match (#1) Threshold	PDA Match Flag
1	3.325	551467			No				No
2	6.616	27187061			No				No

Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (µV*sec)	% Area	Height (µV)	Int Type	Amount
1	3.325							551467	1.99	49837	bb	
2	6.616							27187061	98.01	1290219	bb	



# Mass Spectrum List Report

## Analysis Info

Analysis Name VNPT179\_pos\_000001.d  
Method XMASS\_Method  
Sample Name: VNPT179\_pos  
VNPT179\_pos: in 1:1 THF:MeOH w/ NaCl.

Acquisition Date 3/20/2012 11:47:08 AM  
Operator FTMS\_USER  
Instrument apex-Qe

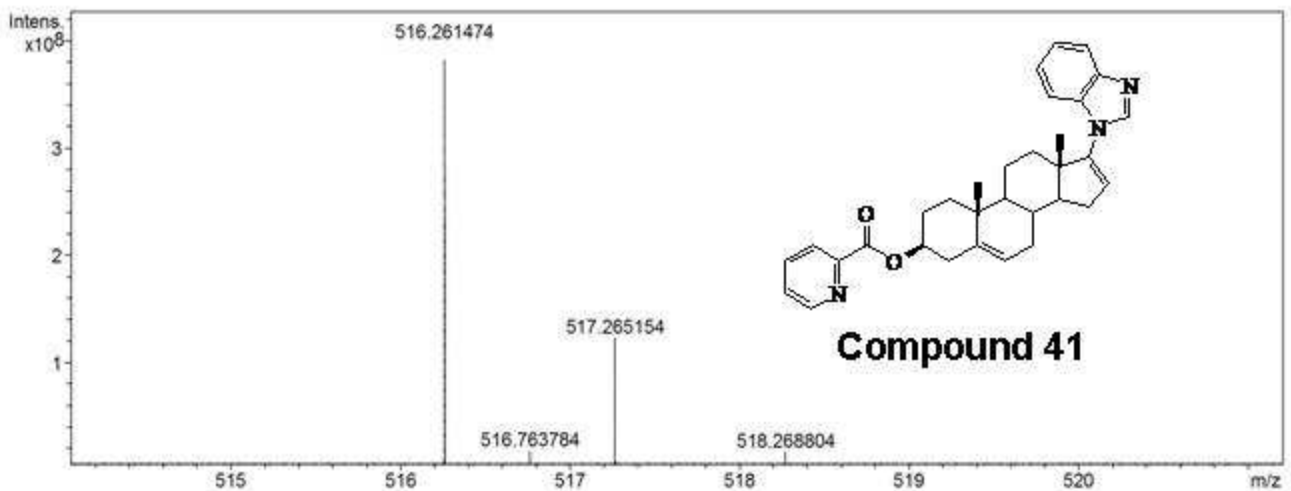
## Acquisition Parameter

Sample: VNPT179

Exact Mass of (C<sub>32</sub>H<sub>35</sub>N<sub>3</sub>O<sub>2</sub>)Na<sup>+</sup> = 516.262148u

Observed Mass = 516.261474u

Difference = -1.3 ppm

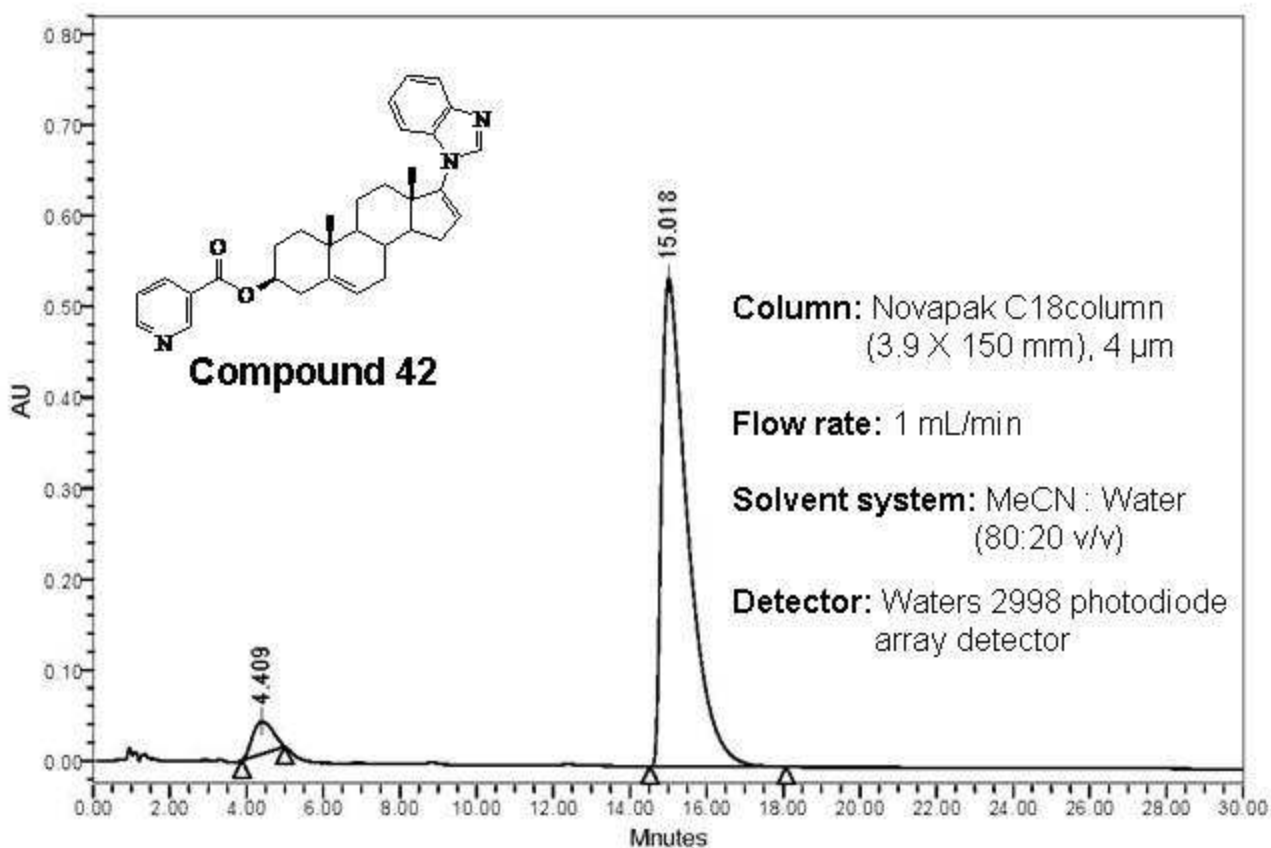


m/z	I
197.934590	1822853
198.377329	5411965
215.088630	1580010
215.088993	34418026
215.089216	2782186
288.289811	2729377
413.265369	3316464
413.266167	25123568
414.269713	3206388
494.278329	3346440
494.279957	67017736
495.283499	20823052
516.245880	3133532
516.258064	8555612
516.258869	6937692
516.261474	396909660
516.763784	17362014
517.259856	2213472
517.261533	2603104
517.262460	2534496
517.263060	2675808

**SAMPLE INFORMATION**

Sample Name: VNPT177B  
 Sample Type: Unknown  
 Vial: 34  
 Injection #: 1  
 Injection Volume: 20.00 ul  
 Run Time: 30.0 Minutes  
 Sample Set Name:

Acquired By: System  
 Date Acquired: 4/16/2012 3:19:08 PM  
 Acq. Method Set: VNI24  
 Date Processed: 4/16/2012 3:50:49 PM  
 Processing Method: VNI24venky  
 Channel Name: WIn Ch1  
 Proc. Chnl. Descr.: FDA 260.5 nm



**PDA Result Table**

Name	RT	Area	Purity (#1) Angle	Purity (#1) Threshold	Purity Flag	Match (#1) Spect. Name	Match (#1) Angle	Match (#1) Threshold	PDA Match Flag
1	4.409	1300457			No				No
2	15.018	25447192			No				No

# Mass Spectrum List Report

## Analysis Info

Analysis Name VNPT177B\_pos\_000001.d  
Method XMASS\_Method  
Sample Name: VNPT177B\_pos  
VNPT177B\_pos: in 1:1 THF:MeOH w/ NaCl

Acquisition Date 3/20/2012 11:43:04 AM  
Operator FTMS\_USER  
Instrument apex-Qe

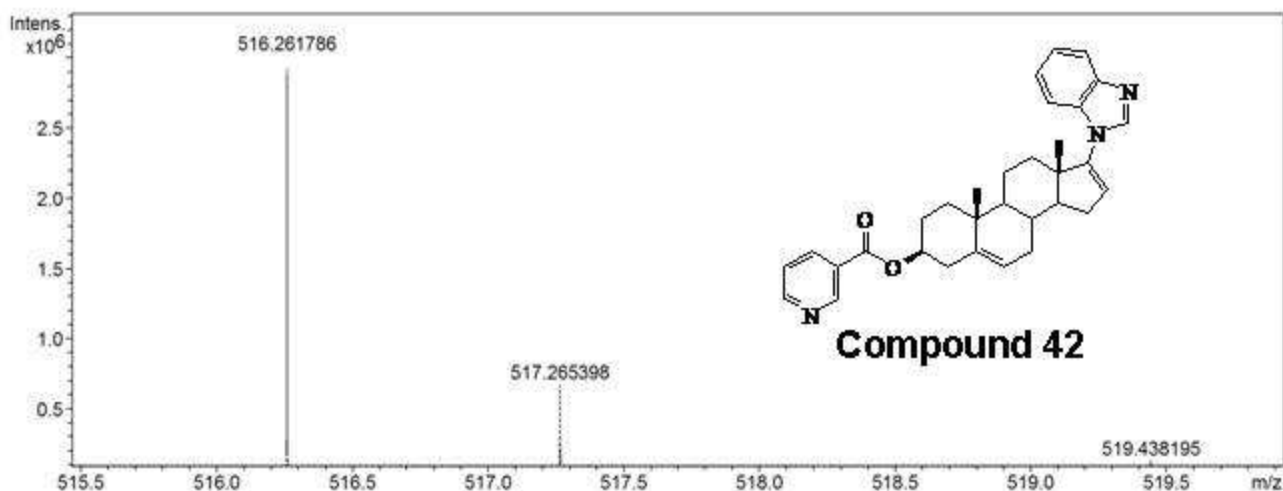
## Acquisition Parameter

Sample: VNPT177B

Exact Mass of (C<sub>32</sub>H<sub>35</sub>N<sub>3</sub>O<sub>2</sub>)Na<sup>+</sup> = 516.262148u

Observed Mass = 516.261786u

Difference = < -1.0 ppm

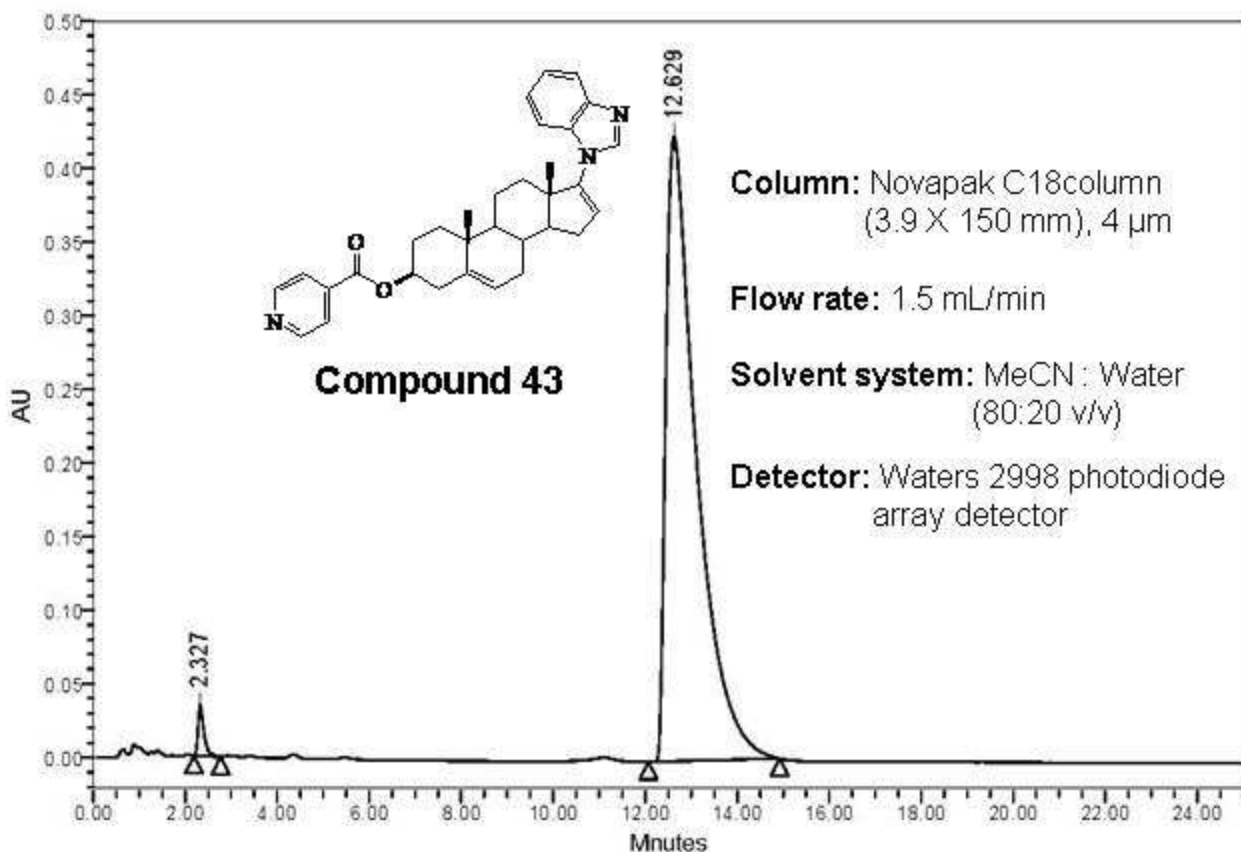


m/z	I
185.062451	1490630
209.097058	1390642
209.499908	904522
215.086193	1017311
215.088455	1842847
215.088911	49435935
215.089145	3093279
215.089265	1611839
215.089387	947647
215.089509	687919
216.092342	2405503
231.062890	2400542
245.099516	853453
247.140256	660689
247.143846	705169
273.047555	1148229
288.288980	986446
288.289607	14552526
289.293048	1163668
301.140993	1604117
310.271618	586250

**SAMPLE INFORMATION**

Sample Name: VNPT178  
 Sample Type: Unknown  
 Vial: 25  
 Injection #: 1  
 Injection Volume: 10.00 ul  
 Run Time: 25.0 Mnutes  
 Sample Set Name:

Acquired By: System  
 Date Acquired: 4/17/2012 1:20:21 PM  
 Acq. Method Set: VN124  
 Date Processed: 4/17/2012 5:50:01 PM  
 Processing Method: VN124venky  
 Channel Name: WIn Ch1  
 Proc. Chnl. Descr.: FDA 254.8 nm



**PDA Result Table**

Name	RT	Area	Purity (#1) Angle	Purity (#1) Threshold	Purity Flag	Match (#1) Spect. Name	Match (#1) Angle	Match (#1) Threshold	PDA Match Flag
1	2.327	306176			No				No
2	12.629	19652190			No				No

Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (µV*sec)	% Area	Height (µV)	Int Type	Amount
1	2.327							306176	1.53	34529	bb	
2	12.629							19652190	98.47	424202	bb	

# Mass Spectrum List Report

## Analysis Info

Analysis Name: VNPT178\_pos\_000001.d  
Method: XMASS\_Method  
Sample Name: VNPT178\_pos  
VNPT178\_pos: in 1:1 THF:MeOH w/ NaCl.

Acquisition Date: 3/20/2012 11:38:43 AM  
Operator: FTMS\_USER  
Instrument: apex-Qe

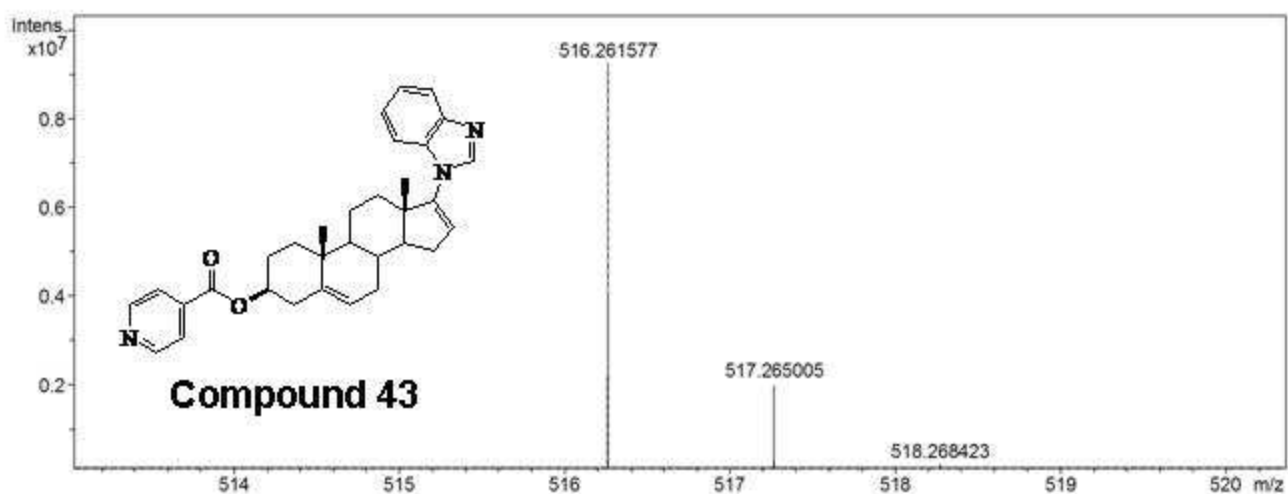
## Acquisition Parameter

Sample: VNPT178

Exact Mass of (C<sub>32</sub>H<sub>35</sub>N<sub>3</sub>O<sub>2</sub>)Na<sup>+</sup> = 516.262148u

Observed Mass = 516.261577u

Difference = -1.1 ppm

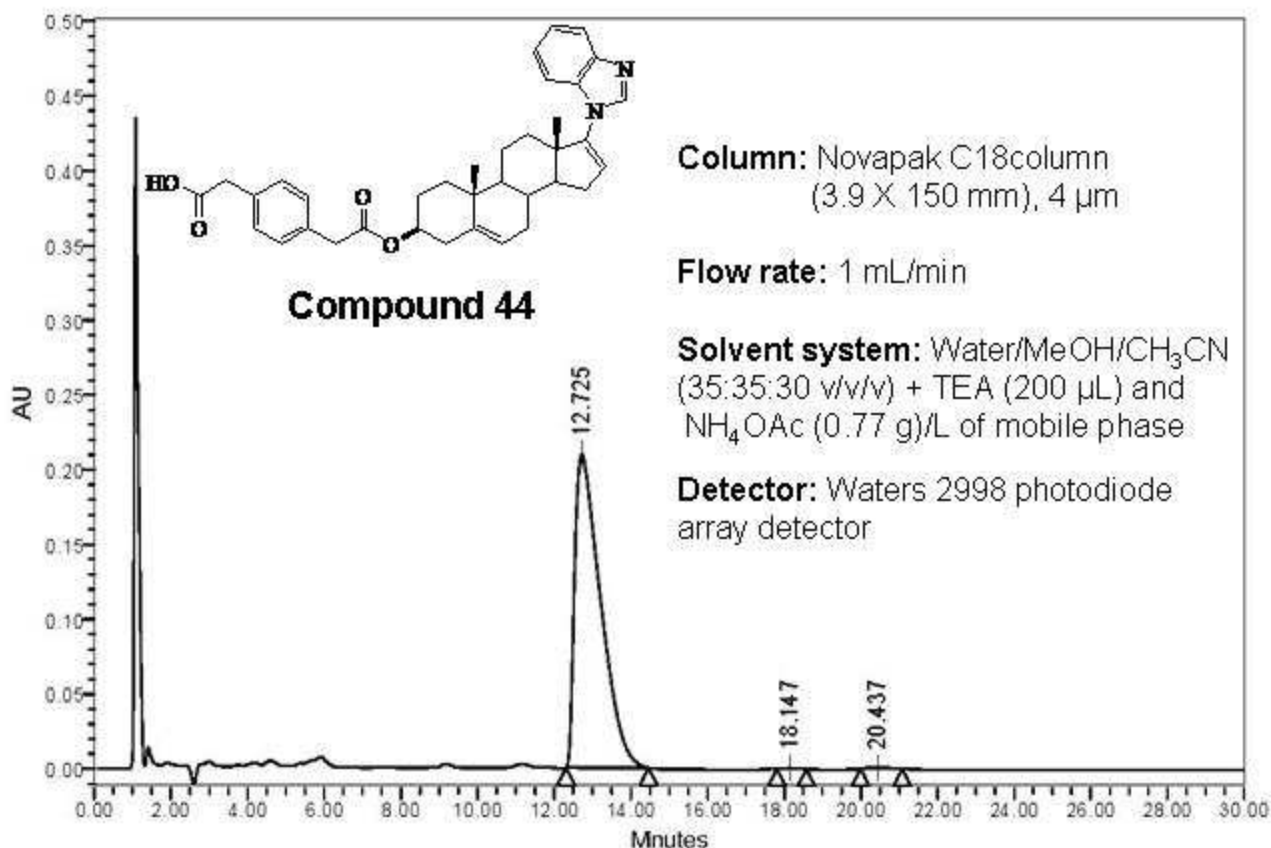


m/z	I
185.062477	1065821
209.097140	2554732
215.088622	3864074
215.088876	36556586
216.092292	1936729
231.062860	1750153
273.047517	1827067
288.289553	7934390
301.140957	1170096
316.320830	4056634
360.323466	1730833
389.258530	1145729
413.265859	16268233
414.269355	2832844
429.239902	3820018
494.265021	2184844
494.275782	1652364
494.276404	2849932
494.276992	4674700
494.277485	3841164
494.279453	160095372

**SAMPLE INFORMATION**

Sample Name: VNFP307C  
 Sample Type: Unknown  
 Vial: 32  
 Injection #: 1  
 Injection Volume: 20.00 ul  
 Run Time: 30.0 Minutes  
 Sample Set Name: Puru Sample Set 2

Acquired By: System  
 Date Acquired: 4/13/2012 4:49:26 AM  
 Acq. Method Set: VN124  
 Date Processed: 4/13/2012 12:05:26 PM  
 Processing Method: VN124venky  
 Channel Name: WWin Ch1  
 Proc. Chnl. Descr.: PDA 242.7 nm



**PDA Result Table**

Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (µV*sec)	% Area	Height (µV)	Int Type	Amount
1	12.725							9835773	99.54	209607	bb	
2	18.147							14037	0.14	544	bb	
3	20.437							31755	0.32	870	bb	
	20.437	31755			No				No			

# Mass Spectrum List Report

## Analysis Info

Analysis Name VNPT307C\_pos\_000001.d  
Method XMASS\_Method  
Sample Name: VNPT307C\_pos  
VNPT307C\_pos: in 1:1 THF:MeOH w/ NaCl.

Acquisition Date 3/20/2012 11:30:04 AM  
Operator FTMS\_USER  
Instrument apex-Qe

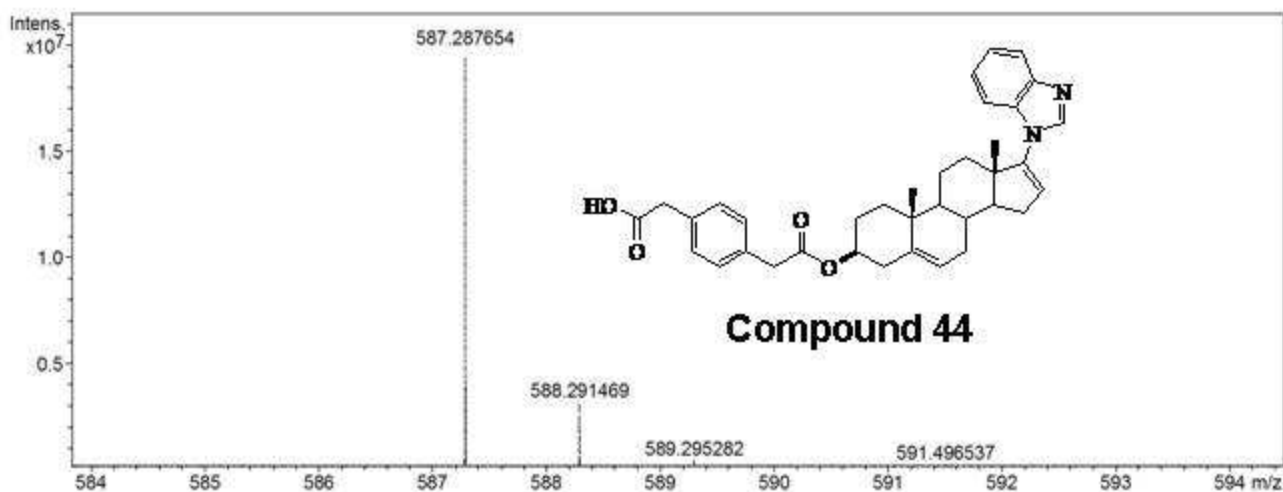
## Acquisition Parameter

Sample: VNPT307C

Exact Mass of (C<sub>36</sub>H<sub>40</sub>N<sub>2</sub>O<sub>4</sub>)Na<sup>+</sup> = 587.288029u

Observed Mass = 587.287654u

Difference = < -1.0 ppm

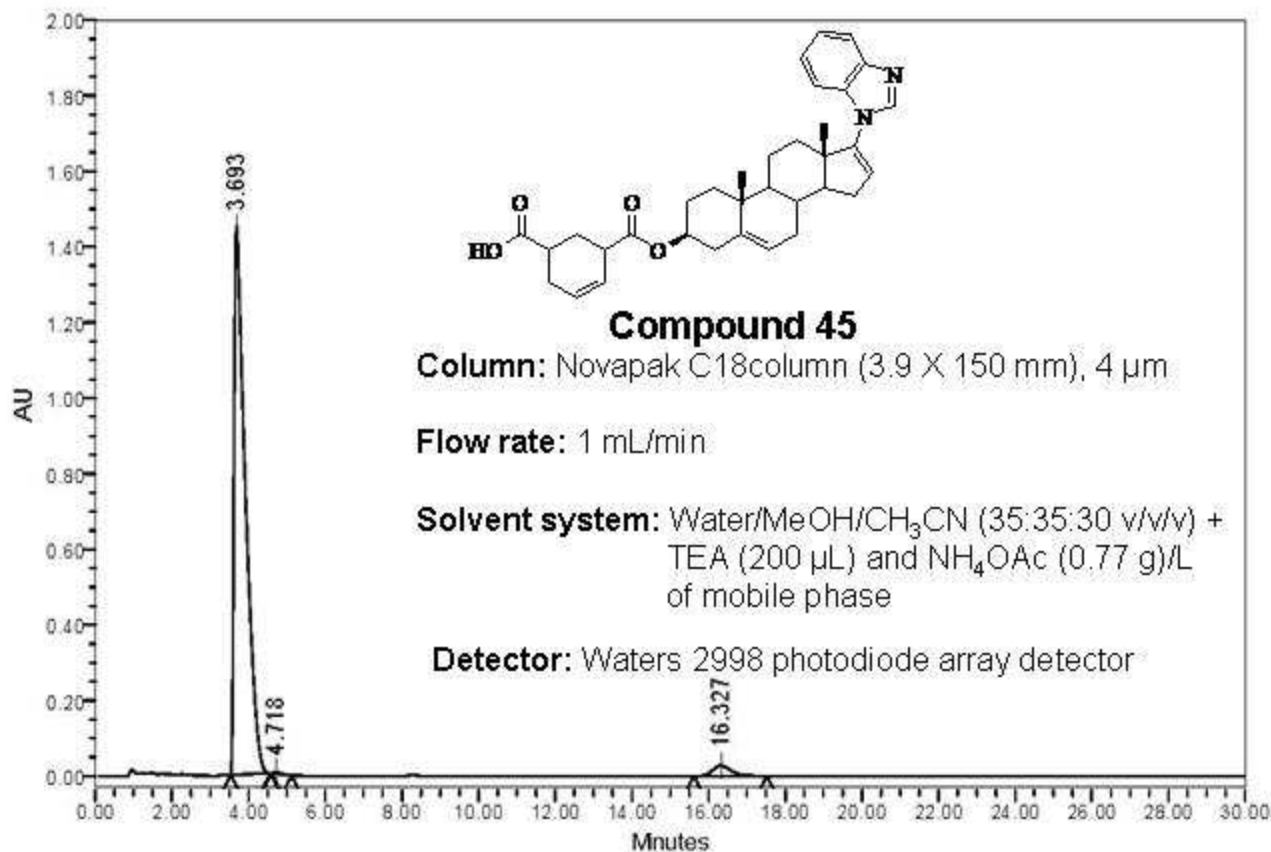


m/z	I
184.723590	1413539
185.062424	3832089
215.088615	2539430
215.088961	35047206
231.062920	3051173
288.289724	1830199
413.265200	2912084
413.266025	30145364
413.266860	2572116
414.269513	4845397
429.240036	16276324
429.240877	1447268
430.243262	1568869
522.595663	2752675
522.596907	25943203
522.598278	2046115
523.600455	7666858
550.610122	2990436
550.621650	1256804
550.622477	2005348
550.624122	6589797

**SAMPLE INFORMATION**

Sample Name: VNFP305  
 Sample Type: Unknown  
 Vial: 29  
 Injection #: 1  
 Injection Volume: 20.00 ul  
 Run Time: 30.0 Mnutes  
 Sample Set Name:

Acquired By: System  
 Date Acquired: 4/19/2012 1:28:31 PM  
 Acq. Method Set: VN124  
 Date Processed: 4/19/2012 2:25:22 PM  
 Processing Method: VN124venky  
 Channel Name: WIn Ch1  
 Proc. Chnl. Descr.: FDA 242.7 nm



**PDA Result Table**

Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (μV*sec)	% Area	Height (μV)	Int Type	Amount
1	3.693							29609358	96.73	1453562	bb	
2	4.718							52987	0.17	3831	bb	
3	16.327							948867	3.10	27735	bb	



# Mass Spectrum List Report

## Analysis Info

Analysis Name VNPT305\_pos\_000001.d  
Method XMASS\_Method  
Sample Name: VNPT305\_pos  
VNPT305\_pos: in 1:1 THF:MeOH w/ NaCl.

Acquisition Date 3/20/2012 11:21:17 AM  
Operator FTMS\_USER  
Instrument apex-Qe

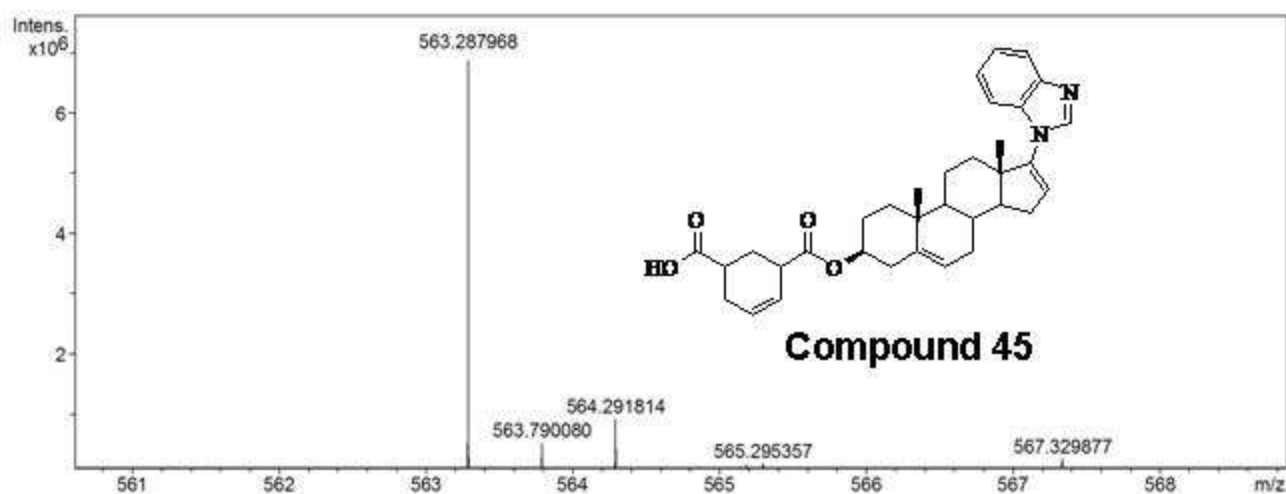
## Acquisition Parameter

Sample: VNPT305

Exact Mass of (C<sub>34</sub>H<sub>40</sub>N<sub>2</sub>O<sub>4</sub>)Na<sup>+</sup> = 563.288029u

Observed Mass = 563.287968u

Difference = < -1.0 ppm

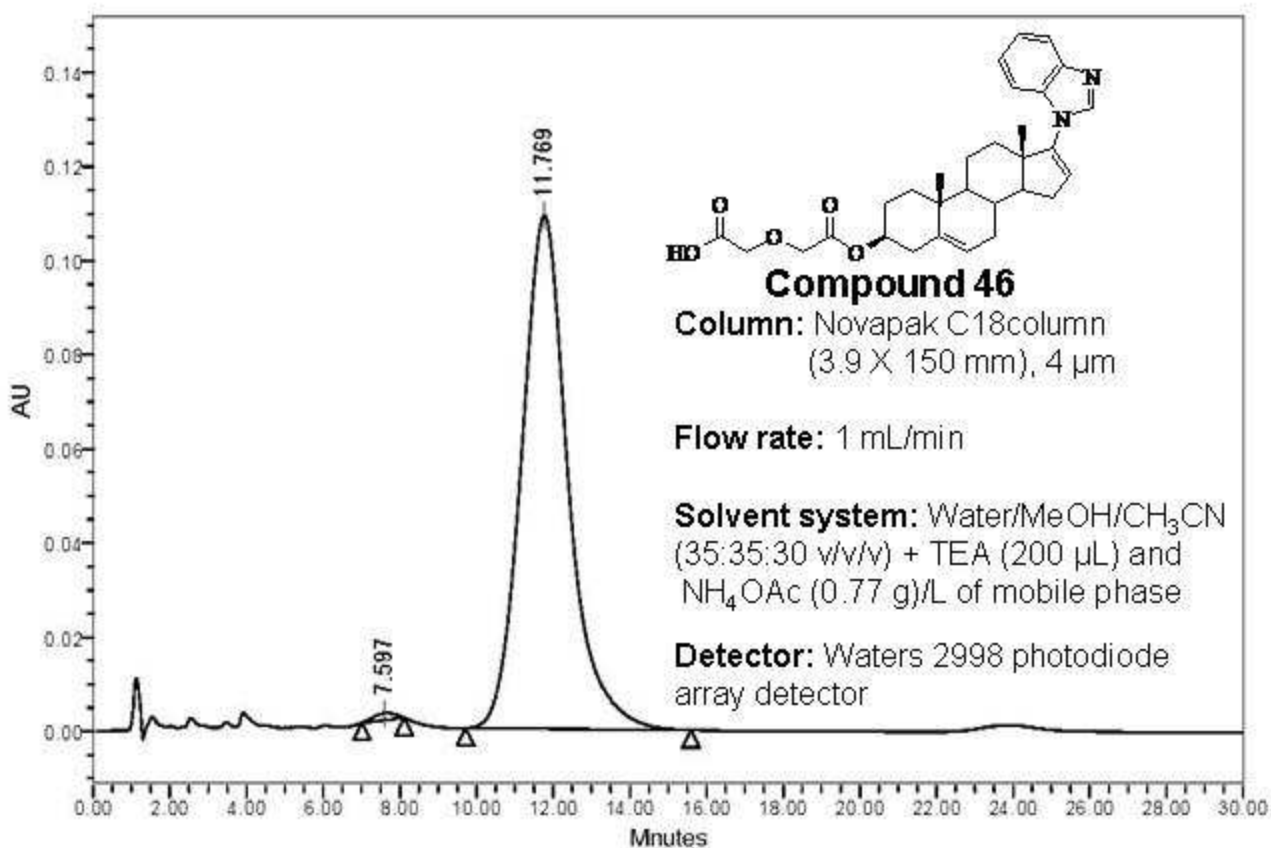


m/z	I
184.723534	788919
185.062355	2047755
209.499911	826085
215.088626	1621843
215.088971	16155155
231.062933	3294610
275.314670	741804
283.094117	7861642
299.068021	10771920
300.071368	842837
413.266271	5815272
414.269588	750188
429.239295	807968
429.240195	8858656
430.243867	649763
475.193433	752823
475.194206	696759
522.597101	12162398
523.600407	1687906
541.305990	10032548
542.309702	1342632

### SAMPLE INFORMATION

Sample Name: VNFP306  
 Sample Type: Unknown  
 Vial: 31  
 Injection #: 1  
 Injection Volume: 20.00 ul  
 Run Time: 30.0 Minutes  
 Sample Set Name: Furu Sample Set 2

Acquired By: System  
 Date Acquired: 4/13/2012 4:18:11 AM  
 Acq. Method Set: VN124  
 Date Processed: 4/16/2012 1:07:01 PM  
 Processing Method: VN124venky  
 Channel Name: WIn Ch1  
 Proc. Chnl. Descr.: FDA 309.3 nm



PDA Result Table

Name	RT	Area	Purity (#1) Angle	Purity (#1) Threshold	Purity Flag	Match (#1) Spect. Name	Match (#1) Angle	Match (#1) Threshold	PDA Match Flag
1	7.597	58941			No				No
2	11.769	9196748			No				No

Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (µV*sec)	% Area	Height (µV)	Int Type	Amount
1	7.597							58941	0.64	1464	bb	
2	11.769							9196748	99.36	109087	bb	

# Mass Spectrum List Report

## Analysis Info

Analysis Name VNPT306\_pos\_000001.d  
Method XMASS\_Method  
Sample Name: VNPT306\_pos  
VNPT306\_pos: in 1:1 THF:MeOH w/ NaCl.

Acquisition Date 3/20/2012 11:25:50 AM  
Operator FTMS\_USER  
Instrument apex-Qe

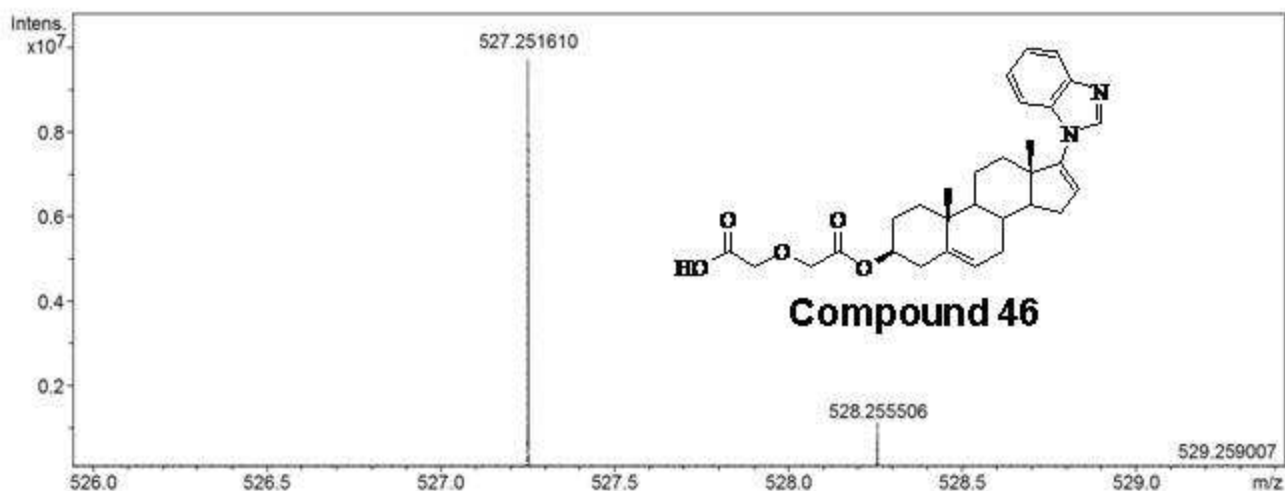
## Acquisition Parameter

Sample: VNPT306

Exact Mass of (C<sub>30</sub>H<sub>36</sub>N<sub>2</sub>O<sub>5</sub>)Na<sup>+</sup> = 527.251643u

Observed Mass = 527.251610u

Difference = < -1.0 ppm

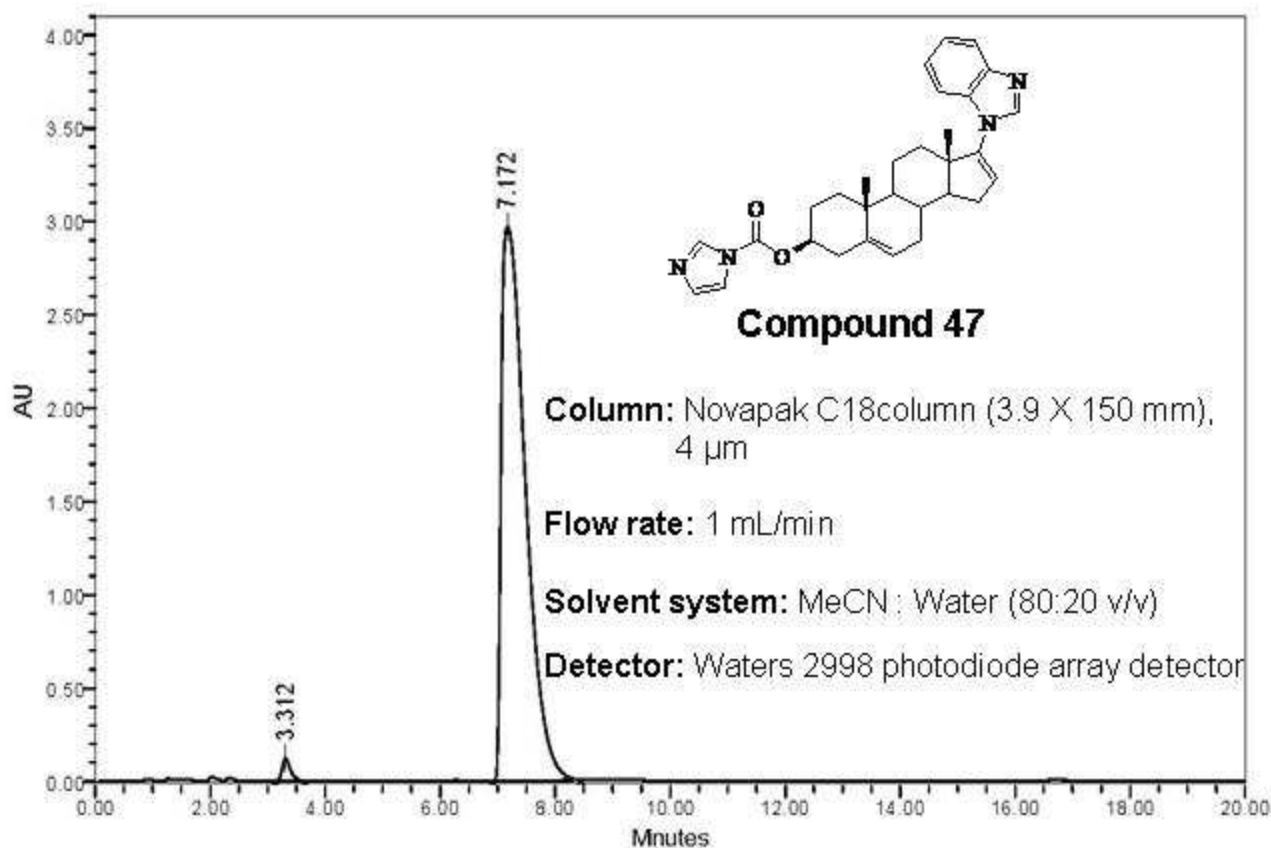


m/z	I
184.723567	1354535
185.062420	4080649
209.499907	859991
215.088620	1381261
215.088997	17456685
215.089199	1567213
231.062948	2398701
275.314597	985332
275.319017	841972
413.266188	19946348
414.269687	1766383
429.238362	942233
429.240104	21519257
430.243703	1700380
505.270133	1121166
522.597030	27270358
522.598186	2472150
523.600619	7920858
527.250311	1060074
527.251610	9858282
528.255506	1114862

**SAMPLE INFORMATION**

Sample Name: VNPT55  
 Sample Type: Unknown  
 Vial: 3  
 Injection #: 1  
 Injection Volume: 10.00 ul  
 Run Time: 20.0 Minutes  
 Sample Set Name:

Acquired By: System  
 Date Acquired: 4/16/2012 5:14:35 PM  
 Acq. Method Set: VN124  
 Date Processed: 4/16/2012 5:37:09 PM  
 Processing Method: VN124venky  
 Channel Name: WIn Ch1  
 Proc. Chnl. Descr.: FDA 242.7 nm



**PDA Result Table**

Name	RT	Area	Purity (#1) Angle	Purity (#1) Threshold	Purity Flag	Match (#1) Spect. Name	Match (#1) Angle	Match (#1) Threshold	PDA Match Flag
1	3.312	1208766			No				No
2	7.172	86587610			No				No

Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (μV*sec)	% Area	Height (μV)	Int Type	Amount
1	3.312							1208766	1.38	121508	bb	
2	7.172							86587610	98.62	2971456	bb	

# Mass Spectrum List Report

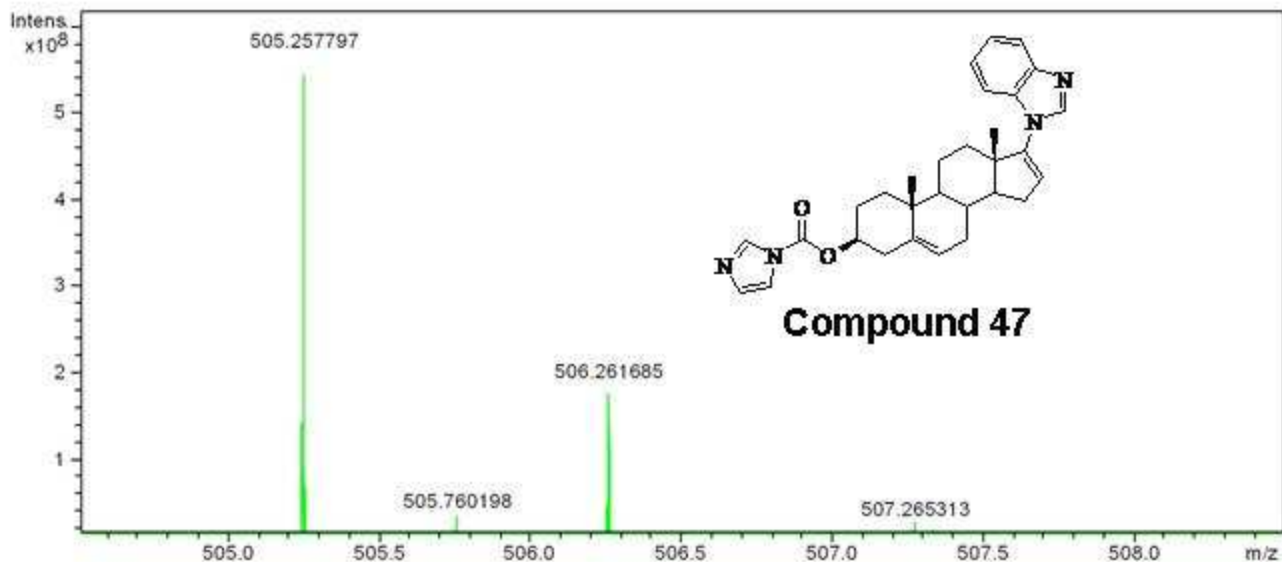
## Analysis Info

Analysis Name VNPT55\_pos\_000003.d  
Method XMASS\_Method  
Sample Name: VNPT55\_pos  
VNPT55\_pos: in 1:1 THF:MeOH w/ NaCl.

Acquisition Date 12/13/2010 2:21:55 PM  
Operator FTMS\_USER  
Instrument apex-Qe

## Acquisition Parameter

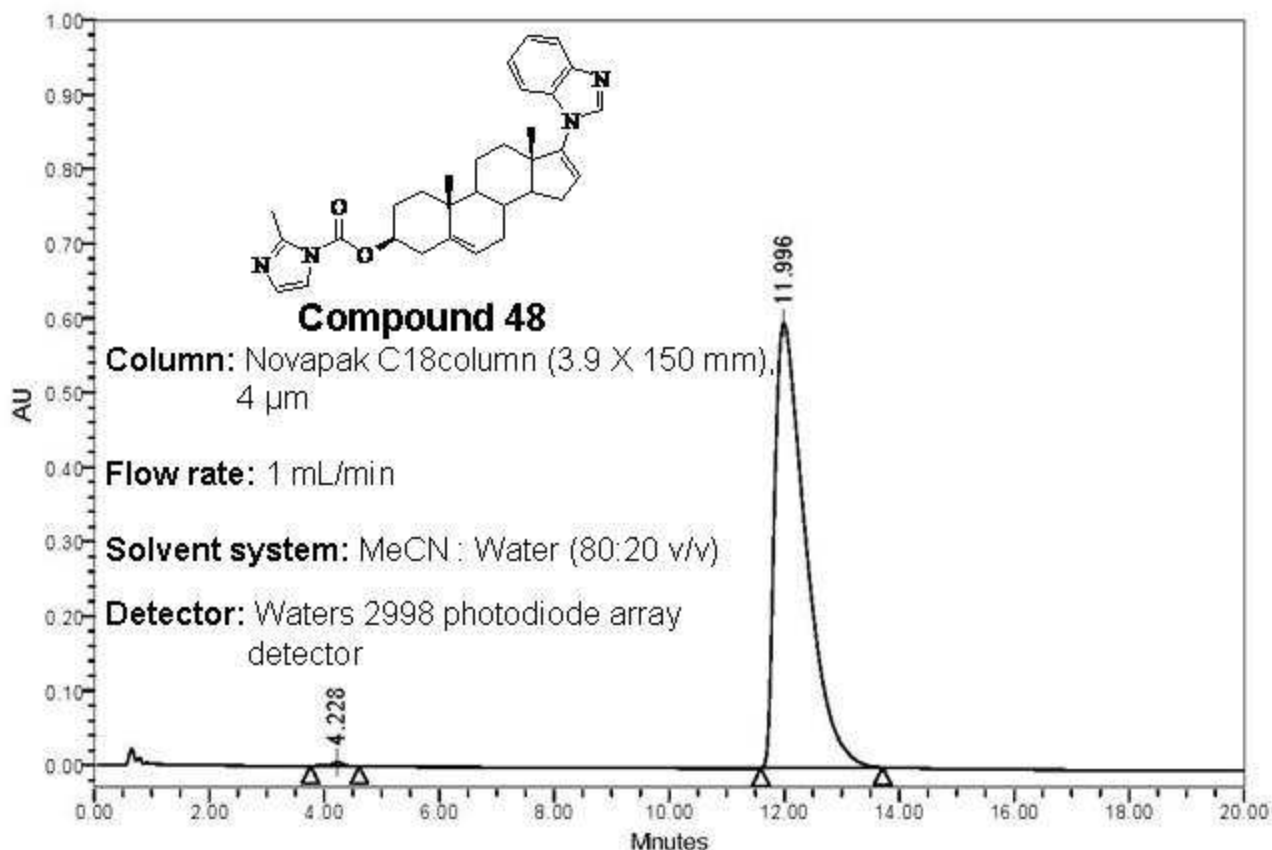
Sample Name: VNPT55  
Exact Mass of (C<sub>30</sub>H<sub>34</sub>N<sub>4</sub>O<sub>2</sub>)Na<sup>+</sup>: 505.257397u  
Observed Mass: 505.257797u  
Difference: < 1.0 ppm



#	m/z	I
1	371.248676	11977620
2	437.194304	19395642
3	447.265010	19674327
4	461.268391	14628311
5	463.304127	10950144
6	483.270994	36534184
7	483.272990	19404712
8	483.274223	40040360
9	483.276045	286324848
10	483.278097	29095848
11	483.279379	13154216
12	484.274508	16029630
13	484.277525	12203966
14	484.279676	85981118
15	485.283277	11655124
16	500.268386	11671843
17	505.252033	141310353
18	505.255574	63699345
19	505.257797	564984209
20	505.262526	18012561
21	505.263850	12339601
22	505.265141	8595857
23	505.754534	17463708

**SAMPLE INFORMATION**

Sample Name:	VNPT124	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	4/18/2012 3:46:28 PM
Vial:	17	Acq. Method Set:	VN124
Injection #:	1	Date Processed:	4/18/2012 4:12:16 PM
Injection Volume:	15.00 ul	Processing Method:	VN124venky
Run Time:	20.0 Minutes	Channel Name:	WIn Ch1
Sample Set Name:		Proc. Chnl. Descr.:	FDA 242.7 nm



**PDA Result Table**

Name	RT	Area	Purity (#1) Angle	Purity (#1) Threshold	Purity Flag	Match (#1) Spect. Name	Match (#1) Angle	Match (#1) Threshold	PDA Match Flag
1	4.228	85756			No				No
2	11.996	22321100			No				No

# Mass Spectrum List Report

## Analysis Info

Analysis Name VNPT124\_pos\_000001.d

Method XMASS\_Method

Sample Name: VNPT124\_pos

VNPT124\_pos; in 1:1 THF:MeOH w/ NaCl.

Acquisition Date 12/13/2010 3:09:48 PM

Operator FTMS\_USER

Instrument apex-Qe

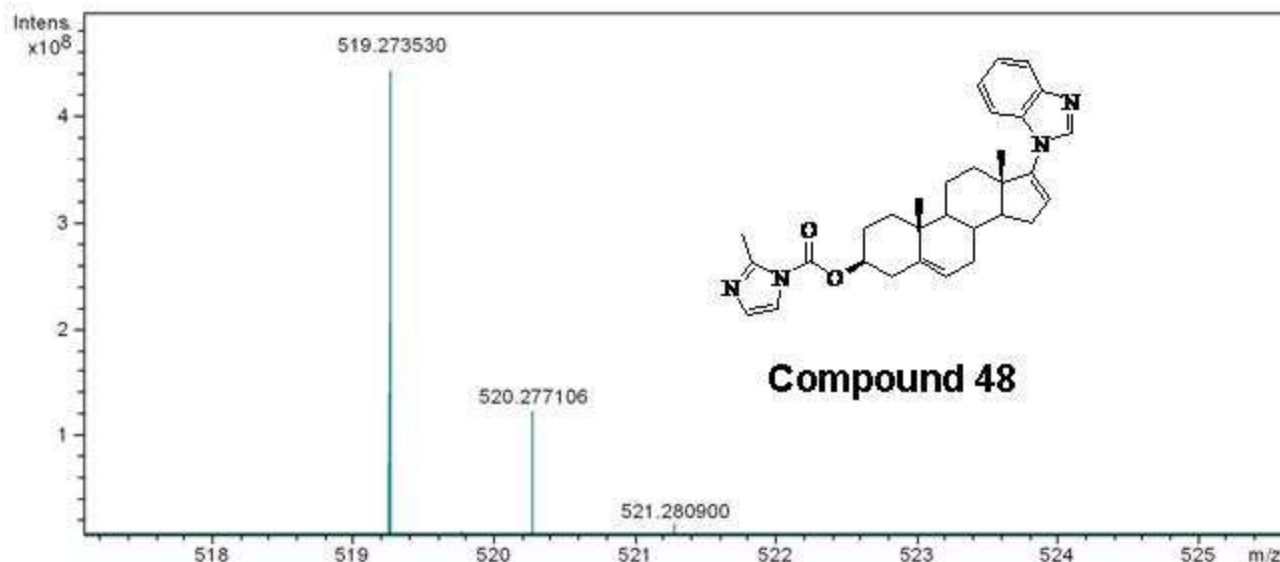
## Acquisition Parameter

Sample Name: VNPT124

Exact Mass of (C<sub>31</sub>H<sub>36</sub>N<sub>4</sub>O<sub>2</sub>)Na<sup>+</sup>: 519.273048u

Observed Mass: 519.273048u

Difference: < 1.0 ppm



#	m/z	I
1	259.635577	8467253
2	437.194366	14273672
3	453.302128	9473279
4	463.304118	6124888
5	475.284244	14331345
6	476.287497	4847068
7	497.288537	5080782
8	497.289576	8302286
9	497.292015	50081486
10	498.295472	17133275
11	507.330366	15601484
12	519.263745	5126119
13	519.273530	452767720
14	519.275741	46772200
15	519.277296	19607528
16	519.278741	11366376
17	519.280143	7053288
18	519.281571	5115880
19	519.775808	10325998
20	520.270138	4567029
21	520.273080	11505653
22	520.277106	123056117
23	520.281089	5930997

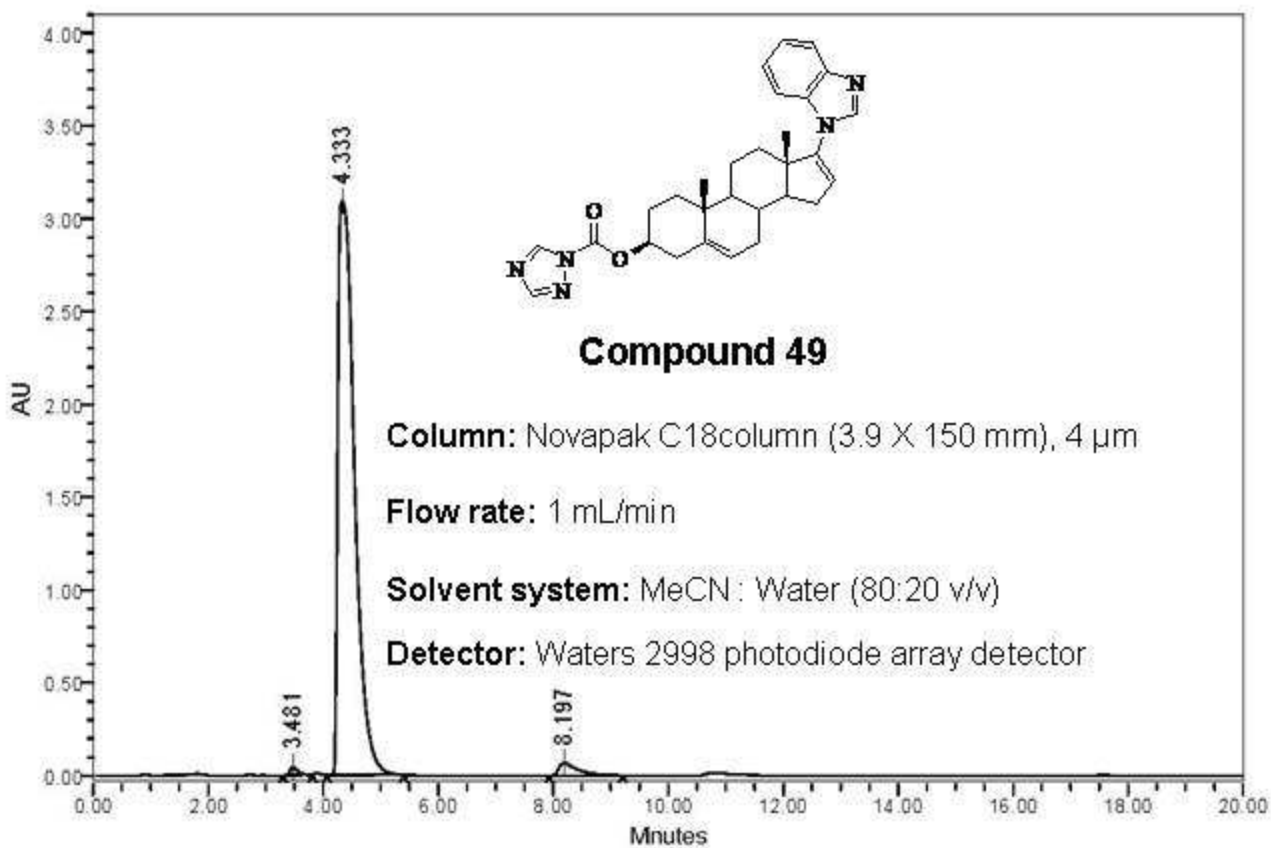
Reported by User: System

Project Name: FDA\_Default

**SAMPLE INFORMATION**

Sample Name: VNPT153B  
 Sample Type: Unknown  
 Vial: 24  
 Injection #: 1  
 Injection Volume: 5.00 ul  
 Run Time: 20.0 Minutes  
 Sample Set Name:

Acquired By: System  
 Date Acquired: 4/17/2012 4:39:33 PM  
 Acq. Method Set: VN124  
 Date Processed: 4/17/2012 5:02:57 PM  
 Processing Method: VN124venky  
 Channel Name: WWin Ch1  
 Proc. Chnl. Descr.: FDA 242.7 nm



**PDA Result Table**

Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (μV*sec)	% Area	Height (μV)	Int Type	Amount
1	3.481							430247	0.67	45813	bb	
2	4.333							62017322	96.79	3091354	bb	
3	8.197							1625863	2.54	68672	bb	



# Mass Spectrum List Report

## Analysis Info

Analysis Name VNPT153B\_pos\_000001.d  
Method XMASS\_Method  
Sample Name: VNPT153B\_pos  
VNPT153B\_pos: in 1:1 THF:MeOH w/ NaCl

Acquisition Date 3/20/2012 11:34:29 AM  
Operator FTMS\_USER  
Instrument apex-Qe

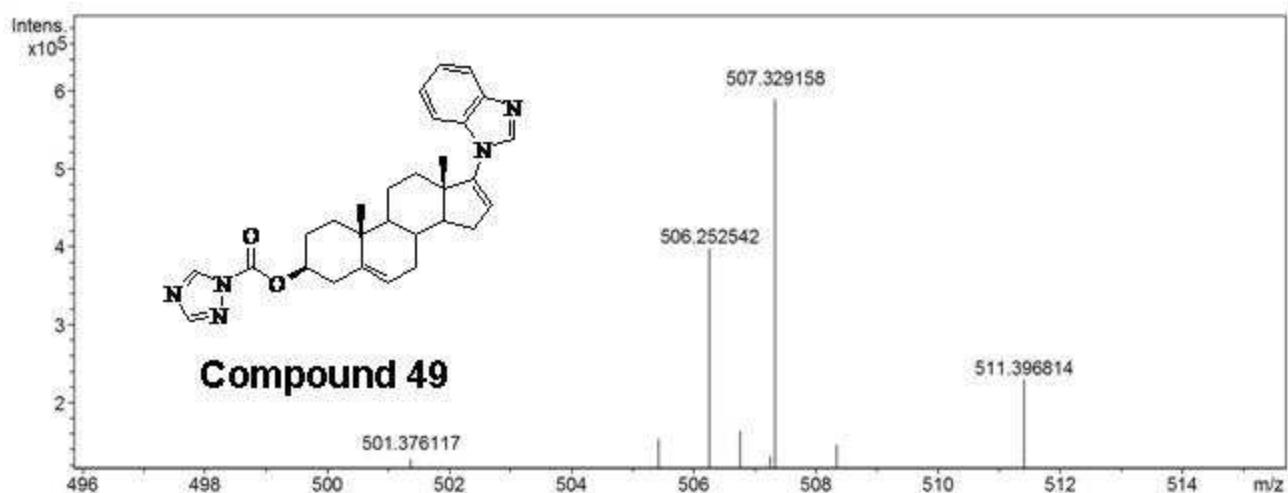
## Acquisition Parameter

Sample: VNPT153B

Exact Mass of (C<sub>29</sub>H<sub>33</sub>N<sub>5</sub>O<sub>2</sub>)Na<sup>+</sup> = 506.252646u

Observed Mass = 506.252542u

Difference = < -1.0 ppm



m/z	I
184.315475	139658
184.723645	874819
184.949376	116849
185.062462	2233145
193.872434	121730
193.996706	121389
195.643278	209406
204.161043	125813
209.499908	874755
213.073307	237163
214.140641	425445
214.729692	1642449
215.083463	149318
215.086190	1015528
215.088571	3477104
215.088905	54268720
216.089478	115767
216.091969	499152
216.092332	2510608
216.825607	113252
217.093155	223540