SUPPORTING INFORMATION

Systematic design of adenosine analogs as inhibitors of a *Clostridioides difficile*-specific DNA adenine methyltransferase required for normal sporulation and persistence

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Table S1. Elemental Analyses for Final Compounds **10-12**, **14-21**, and **31-42**.

Lab code	Compd	Formula	Calculated, %			Found, %		
			C	H	N	C	H	N
MC4742	**10**	$C_{24}H_{25}N_5O_4$	64.42	5.63	15.65	64.52	5.63	15.60
MC4736	**11**	$C_{22}H_{23}N_5O_4$	62.70	5.50	16.62	62.82	5.50	16.55
MC4737	**12**	$C_{22}H_{23}N_5O_4$	62.70	5.50	16.62	62.81	5.51	16.56
MC4741	**14**	$C_{19}H_{23}N_5O_4$	59.21	6.02	18.17	59.30	6.04	18.10
MC4800	**15**	$C_{19}H_{24}N_6O_4$	56.99	6.04	20.99	57.11	6.05	20.92
MC4761	**16**	$C_{19}H_{23}N_5O_5$	56.85	5.78	17.45	56.97	5.78	17.39
MC4760	**17**	$C_{20}H_{25}N_5O_5$	57.82	6.07	16.86	57.92	6.08	16.81
MC4756	**18**	$C_{20}H_{25}N_5O_4$	60.14	6.31	17.53	60.25	6.32	17.47
MC4757	**19**	$C_{21}H_{27}N_5O_4$	61.00	6.58	16.94	61.12	6.58	16.87
MC4795	**20**	$C_{15}H_{23}N_5O_5$	50.98	6.56	19.82	51.11	6.58	19.76
MC4758	**21**	$C_{22}H_{29}N_5O_4$	61.81	6.84	16.38	61.91	6.85	16.32
MC4764	**31**	$C_{22}H_{28}N_6O_4$	59.99	6.41	19.08	60.09	6.42	19.01
MC4770	**32**	$C_{21}H_{23}N_7O_4$	57.66	5.30	22.41	57.78	5.30	22.34
MC4771	**33**	$C_{17}H_{24}N_6O_4$	54.24	6.43	22.33	54.36	6.44	22.26
MC4776	**34**	$C_{18}H_{28}N_6O_4$	55.09	7.19	21.41	55.20	7.19	21.35
MC4769	**35**	$C_{17}H_{26}N_6O_5$	51.77	6.64	21.31	51.90	6.65	21.25
MC4778	**36**	$C_{18}H_{29}N_7O_4$	53.06	7.17	24.06	53.18	7.18	23.99
MC4830	**37**	$C_{21}H_{32}N_6O_6$	54.30	6.94	18.09	54.44	6.95	18.02
MC4777	**38**	$C_{22}H_{34}N_6O_6$	55.22	7.16	17.56	55.34	7.18	17.50
MC4799	**39**	$C_{23}H_{36}N_6O_6$	56.08	7.37	17.06	56.20	7.38	17.00
MC4831	**40**	$C_{22}H_{34}N_6O_6$	55.22	7.16	17.56	55.35	7.17	17.49
MC4832	**41**	$C_{23}H_{34}N_6O_6$	56.31	6.99	17.13	56.43	7.00	17.07
MC4919	**42**	$C_{18}H_{28}N_6O_4$	55.09	7.19	21.41	55.22	7.19	21.34

Table S2. Summary of X-ray data collection at wavelength=1Å of beamline APS 222-ID and refinement statistics (*) of space group $P2_12_12_1$ ($\alpha=\beta=\gamma=90°$)

Date Collected	03/2021	06/2021	06/2021	06/2021	06/2021	06/2021	07/2021
compound	214 (MTA)	**2** (161; MC4679)	**3** (162; MC4680)	**8** (163; MC4681)	**4** (164; MC4682)	**6** (165; MC4683)	**9** (168: APNEA)
PDB Code	8CXS	8CXU	8CXV	8CXY	8CXW	8CXX	8CY2
Cell dimensions (Å)	81.97, 161.16, 230.80	81.45, 161.24, 229.52	81.46, 161.34, 229.79	81.36, 161.36, 229.75	81.33, 161.63, 229.60	81.76, 161.47, 230.27	81.53, 161.81, 230.34
Resolution (Å)	41.87-2.49 (2.89-2.49)	44.86-2.28 (2.37-2.28)	44.88-2.26 (2.37-2.26)	48.71-2.19 (2.27-2.19)	46.80-2.78 (2.89-2.78)	44.29-2.34 (2.43-2.34)	45.17-2.81 (2.89 -2.81)
[a] R_{merge}	0.292 (2.295)	0.233 (1.70)	0.244 (2.09)	0.166 (1.93)	0.224 (1.51)	0.165 (1.46)	0.465 (3.28)
R_{pim}	0.074 (0.700)	0.072 (0.733)	0.070 (0.788)	0.040 (0.575)	0.110 (0.789)	0.048 (0.499)	0.141 (1.081)
$CC_{1/2}$, CC*	(0.469, 0.799)	(0.410, 0.762	(0.344, 0.715)	(0.762, 0.930)	(0.394, 0.752)	(0.503, 0.818)	(0.402, 0.758)
[b] <I/σI>	11.4 (1.3)	10.0 (0.9)	10.9 (1.0)	14.9 (1.4)	7.4 (1.1)	14.4 (1.2)	8.0 (1.1)
Completeness (%)	99.6 (94.9)	93.5 (74.8)	95.0 (90.5)	95.0 (83.4)	99.6 (99.6)	96.5 (76.0)	99.9 (99.9)
Redundancy	14.9 (10.1)	8.9 (4.8)	12.4 (6.8)	14.4 (9.1)	5.1 (4.5)	12.1 (8.1)	11.6 (9.9)
Observed reflections	1,578,071	1,147,875	1,650,078	2,167,132	390,186	1,497,945	861,139
Unique reflections	106,240	129,038	133,608	147,745	76,354	123,740	74,091
Refinement							
Resolution (Å)	2.49	2.28	2.26	2.19	2.78	2.34	2.81
No. reflections	106,072	128,797	133,381	147,569	76,256	123,583	73,994
[c] R_{work} / [d] R_{free}	0.179 / 0.213	0.186 / 0.222	0.177 / 0.205	0.174 / 0.203	0.184 / 0.230	0.179 / 0.206	0.171 / 0.222
No. Atoms							
Protein	13,408	13,407	13,421	13,401	13,372	13,464	13,280
DNA	1704	1704	1704	1704	1704	1704	1704
Inhibitor	60	81	81	81	87	84	84
Solvent	440	629	736	759	406	582	348
B Factors (Å^2)							
Protein	51.1	46.2	48.0	48.7	51.7	52.8	56.0
DNA	56.1	50.2	54.8	54.9	59.7	59.6	64.5
Inhibitor	53.1	55.4	54.5	48.9	64.9	70.3	65.3
Solvent	41.2	41.9	43.8	45.3	38.4	46.8	44.5
R.m.s. deviations							
Bond lengths (Å)	0.003	0.003	0.004	0.004	0.003	0.003	0.004
Bond angles (°)	0.6	0.6	0.6	0.6	0.5	0.6	0.6

* Values in parenthesis correspond to highest resolution shell;
[a] $R_{merge} = \Sigma\ |\ I - \langle I \rangle\ | / \Sigma\ I$, where I is the observed intensity and <I> is the averaged intensity from multiple observations;
[b] <I/σI> = averaged ratio of the intensity (I) to the error of the intensity (σI);
[c] $R_{work} = \Sigma\ |\ Fobs - Fcal\ | / \Sigma\ |\ Fobs\ |$, where Fobs and Fcal are the observed and calculated structure factors, respectively;
[d] R_{free} was calculated using a randomly chosen subset (5%) of the reflections not used in refinement.

Table S2 (Continues) Summary of X-ray data collection at wavelength=1Å of beamline APS 22-ID and refinement statistics (*) of space group $P2_12_12_1$ ($\alpha=\beta=\gamma=90°$)

Date Collected	09/2021	11/2021	11/2021	11/2021	03/2022	03/2022	03/2021
Inhibitor	**14** (174; MC4741)	**18** (178; MC4756)	**19** (179; MC5757)	**16** (181; MC4761)	**15** (197; MC4800)	**39** (199; MC4799)	**1** (101; MC4624)
PDB Code	8CXZ	8CY0	8CY1	8CY4	8CY3	8CY5	8CXT
Cell dimensions (Å)	81.44, 161.43, 229.71	81.37, 160.86, 230.38	81.25, 161.57, 229.93	81.31, 161.76, 229.95	81.24, 161.24, 229.58	81.55, 161.23, 230.29	82.21, 161.67, 230.80
Resolution (Å)	45.89-2.35 (2.43-2.35)	47.01-2.65 (2.74-2.65)	44.89-2.38 (2.48-2.38)	44.10-2.34 (2.43-2.34)	46.9-2.65 (2.74-2.65)	47.03-2.50 (2.58-2.50)	44.23-2.61 (2.74-2.61)
[a] R_{merge}	0.210 (1.36)	0.281 (1.89)	0.282 (1.80)	0.251 (1.73)	0.279 (1.64)	0.244 (1.35)	0.337 (2.535)
R_{pim}	0.071 (0.519)	0.116 (0.926)	0.100 (0.728)	0.076 (0.661)	0.083 (0.646)	0.057 (0.642)	0.063 (0.678)
$CC_{1/2}$, CC*	(0.356, 0.724)	(0.363, 0.730)	(0.374, 0.738)	(0.472 ,0.801)	(0.387, 0.747)	(0.431, 0.776)	(0.468, 0.799)
[b] $\langle I/\sigma I \rangle$	12.4 (1.2)	8.1 (1.1)	8.0 (0.81)	10.2 (0.95)	8.6 (0.8)	12.7 (1.0)	11.3 (1.2)
Completeness (%)	99.5 (97.4)	99.8 (99.6)	96.2 (77.7)	96.6 (86.9)	97.3 (85.5)	99.3 (93.4)	100.0 (99.8)
Redundancy	12.7 (6.6)	6.6 (4.5)	8.6 (4.9)	10.9 (6.3)	11.3 (6.0)	12.6 (4.4)	23.8 (9.7)
Observed reflections	1,588,738	582,034	1,012,216	1,339,925	966,027	1,329,225	2,164,493
Unique reflections	125,490	88,696	117,552	122,653	85,741	105,385	91,039
Refinement							
Resolution (Å)	2.35	2.65	2.38	2.34	2.65	2.50	2.61
No. reflections	125,292	88,571	117,266	121,299	85,314	105,232	90,810
[c] R_{work} / [d] R_{free}	0.174 / 0.204	0.173 / 0.221	0.182 / 0.227	0.173 / 0.207	0.190 / 0.226	0.177 / 0.210	0.189 / 0.224
No. Atoms							
Protein	13,424	13,368	13,386	13,402	13,368	13,397	13,241
DNA	1704	1704	1704	1704	1704	1704	1704
Inhibitor	84	87	90	87	87	105	78
Solvent	849	498	747	818	305	609	136
B Factors (Å^2)							
Protein	53.2	58.3	58.1	51.1	74.9	65.0	68.9
DNA	61,2	68.0	68.1	58,0	85.9	73.0	73.5
Inhibitor	53.4	62.8	63.2	55.1	78.4	66.9	79.8
Solvent	48.0	47.7	51.0	45.8	60.4	55.2	56.2
R.m.s. deviations							
Bond lengths (Å)	0.003	0.003	0.003	0.003	0.003	0.002	0.003
Bond angles (°)	0.6	0.5	0.6	0.6	0.5	0.5	0.6

* Values in parenthesis correspond to highest resolution shell;

[a] $R_{merge} = \Sigma\ |\ I - \langle I \rangle\ | / \Sigma\ I$, where I is the observed intensity and $\langle I \rangle$ is the averaged intensity from multiple observations;

[b] $\langle I/\sigma I \rangle$ = averaged ratio of the intensity (I) to the error of the intensity (σI);

[c] $R_{work} = \Sigma\ |\ Fobs - Fcal\ | / \Sigma\ |\ Fobs\ |$, where Fobs and Fcal are the observed and calculated structure factors, respectively;

[d] R_{free} was calculated using a randomly chosen subset (5%) of the reflections not used in refinement.

Table S3. The predicted cell permeability of compounds **16**, **38**, and **39**

Compound		Caco2 permeability (P_{app})		Human intestinal absorption		References
		pkCSM ($\times 10^{-6}$ cm/s)	PreADMET ($\times 10^{-6}$ cm/s)	pkCSM (%)	PreADMET (%)	
16	-	1.77	1.68	63.9	74.4	-
38	-	1.85	1.93	60.6	73.5	-
39	-	1.78	1.57	61.5	76.2	-
7	Nitrobenzylthioinosine	0.79	0.33	73.9	64.9	In cells [1]
9	APNEA	1.81	1.45	62.1	74.0	In cells/tissues [2,3] *In vivo* [4,5]
13	A2AR-agonist-1	1.81	0.54	70.0	75.7	*In vivo* [6]

We have performed *in silico* cell permeability prediction using two different tools: pkCSM (https://biosig.lab.uq.edu.au/)[7] and PreADMET (https://preadmet.webservice.bmdrc.org/). Both tools enable the prediction of Caco-2 cell permeability and human intestinal absorption.

A

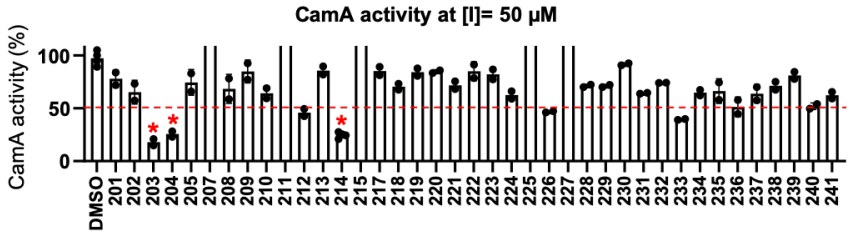

Figure S1

B

Compound	name	Reference/note	Compound	name	Reference/note
201 (dcSAM)	Decarboxyliertes SAM	a gift from Dr. Bernard Blessington, Bradford University, Bradford, UK	221	TL106 *N*6-benzylthioethyl-2'-deoxyadenosine	Qian et al. *Chem. Commun. 54*, 13945-13948, 2018
202 (da-SAM)	Deaminiertes SAM (epimeric mixture)	iBorchardt el al. *J. Med. Chem.* **19**, 1104-1110, 1976	222	TL104 *N*6-hydroxyethyl-2'-deoxyadenosine	Brock et al. *Chem. Res. Toxicol.* **17**, 1047-1056, 2004
203 (DMTA)	5'-dimethylthioadenosine	Borchardt, R.T. *J. Am. Chem. Soc.* **101**, 458-463, 1979	223	TL100-2 *N*6-(*S*-(homocysteinyl)-ethyl)-2'-deoxyadenosine	N/A
204	sinefungin	a gift from Dr. M. Niedenthal, Lilly Research Laboratories, Indianapolis, IN, USA	224 (AEA)	5'-aminoethyladenosine	N/A
205	Aza-SAM	a gift from Dr. Mike Blackburn, The University of Sheffield, Sheffield, U.K.)	225 (CMTA)	5'-carboxymethylthioadenosine	Gillet et al. *Experientia* **35**, 1007-1009, 1979
206	L-SAH (not used in the assay – reaction product)	Sigma-Aldrich	226	5'-deoxy-5'-chloroadenosine	Kikugawa et al. *J. Med. Chem.* **15**, 387-390, 1972
207	D-SAH	Sigma-Aldrich	227	5'-phthalimidoadenosine	M. Pignot, Dissertation, TU Dortmund, Germany, 1999
208 (dc-SAH)	Decarboxyliertes SAH	Pignot et al. *Eur. J. Org. Chem.* **3**, 549–555, 2000	228	5'-deoxy-5'-acetylthioadenosine	Pignot et al. *Eur. J. Org. Chem.* **3**, 549–555, 2000
209	5-'-adenosyl-L-cysteine	Sigma-Aldrich	229	(*South*)-SAH	a gift from Dr. Victor Marquez, National Cancer Institute, Frederick, MD, USA
210 (CPTA)	5'-carboxypropyl-thioadenosine (deaminiated SAH, daSAH)	Pignot et al. *Eur. J. Org. Chem.* **3**, 549–555, 2000	230	(*North*)-SAH	a gift from Dr. Victor Marquez, National Cancer Institute, Frederick, MD, USA
211	CPTA methylester	Pignot et al. *Eur. J. Org. Chem.* **3**, 549–555, 2000	231	5'-ethylthioadenosine	Kikugawa et al. *J. Med. Chem.* **15**, 387-390, 1972
212 (AETA)	5'-aminoethylthioadenosine	Goedecke et al. *Nat. Struct. Biol.* **8**, 121-125, 2001	232	5'-propythioadenosine	Kikugawa et al. *J. Med. Chem.* **15**, 387-390, 1972
213 (CETA)	5'-carboxyethylthioadenosine	Srivastava et al. *Med. Chem. Lett.* **17**, 6239-6244, 2007	233	5'-butylthioadenosine	Kikugawa et al. *J. Med. Chem.* **15**, 387-390, 1972
214 (MTA)	5'-methylthioadenosine	Sigma-Aldrich	234	5'-methylbutylthioadenosine [as epimeric mixture from 5'-butylthioadenosine (**233**)]	Gillet et al. *Experientia 35*, 1007-1009, 1979
215	5'-thioadenosine	Pignot et al. *Eur. J. Org. Chem.* **3**, 549–555, 2000	235	5'-methylpropylthioadenosine [as epimeric mixture from 5'-propylthioadenosine (**232**)]	Gnegy and Lotspeich, *J. Med. Chem.* **19**, 1191-1195, 1976
216	Adenosine (not used)	Sigma-Aldrich	236	5'-methylethylthioadenosine [as epimeric mixture from 5'-ethylthioadenosine (**231**)]	Gnegy and Lotspeich, *J. Med. Chem.* **19**, 1191-1195, 1976, 1976
217	L-methionine	Sigma-Aldrich	237 (AEAA)	5'-aminoethylamino-5'-deoxyadenosine	M. Kolb et al. *J. Med. Chem.* **25**, 550-556, 1982
218	5'-aminoadenosine	M. Pignot, Dissertation, TU Dortmund, Germany, 1999	238 (phETA)	5'-phenylethythio-5'-deoxyadenosine	Kai *et al.* Chem. Commun. **50**, 8586-8589, 2014
219	*N*6-methyl-2'-deoxyadenosine	MBI Fermentas, Vilnius, Lithuania	239 (ML43)	Bisubstrate inhibitor	New synthesis (see next page)
220	TL107-2 *N*6-(*S*-(homocysteinyl)-methyl)-2'-deoxyadenosine	Wahnon et al. *J. Am. Chem. Soc.* **123**, 976-977, 2001	240	5'-iodo-5'-deoxyadenosine	TCI Europe, Zwijndrecht, Belgium
			241	5'-tosyladenosine	Sigma-Aldrich

Figure S1. (A) Screen of CamA inhibition against SAM analogs at [I]=50 μM, in the presence of 40 μM co-substrate SAM. Three compounds, **203** (dMTA), **204** (sinefungin) and **214** (MTA), have inhibitions at >50% CamA activity. Compounds **207**, **211**, **215**, **225** and **227** might interfere with the Promega MTase-Glo™ luminescent assay used in the study (see Figure S3). (**B**) Compound information (see HPLC traces of compounds 201-241).

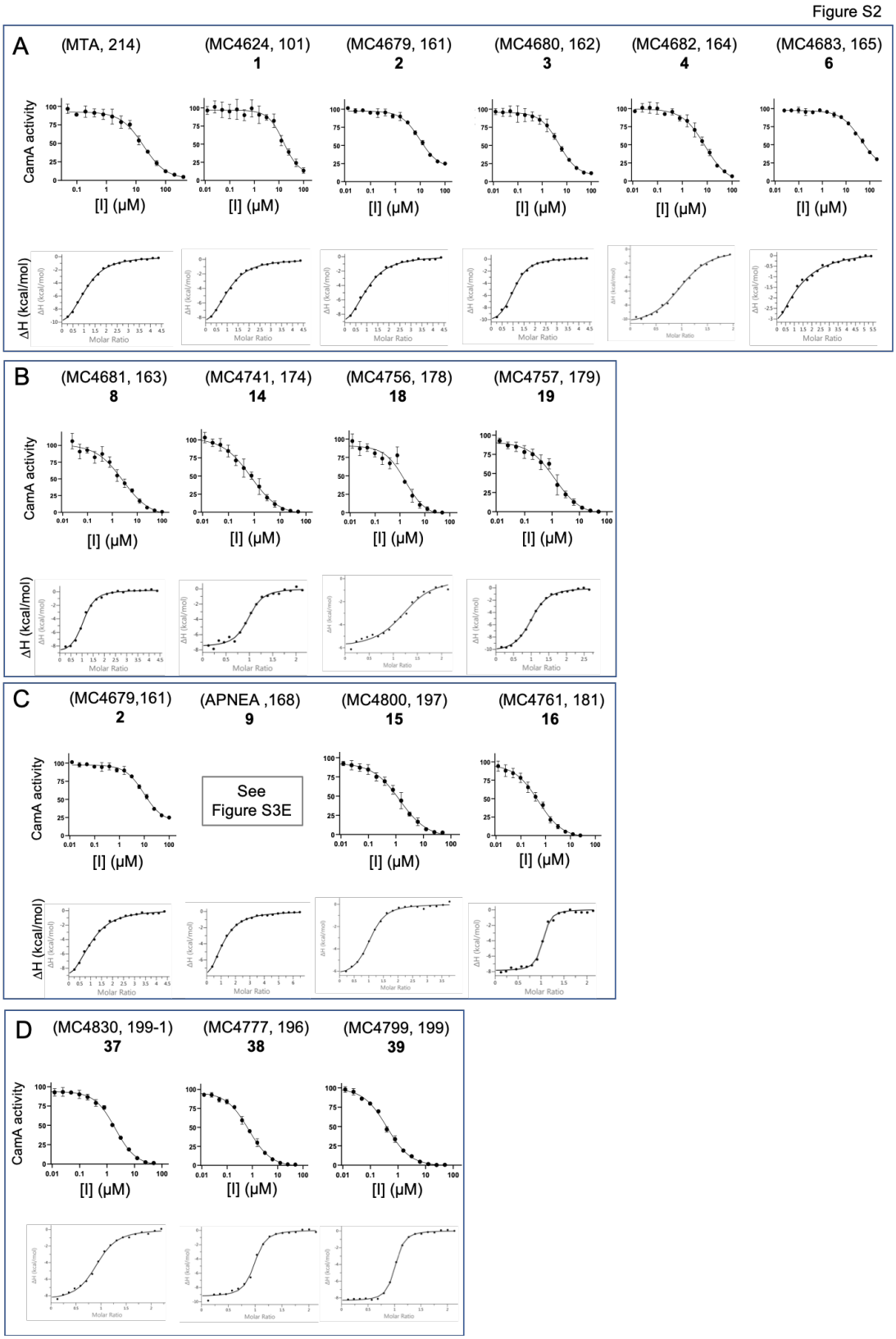

Figure S2. Raw data of MTase-GloTM inhibition assay (top panels) and ITC measurements (bottom panels). (**A**) Related to Figure 3. (**B**) Related to Figure 4. (**C**) Related to Figure 5. (**D**) Related to Figure 6.

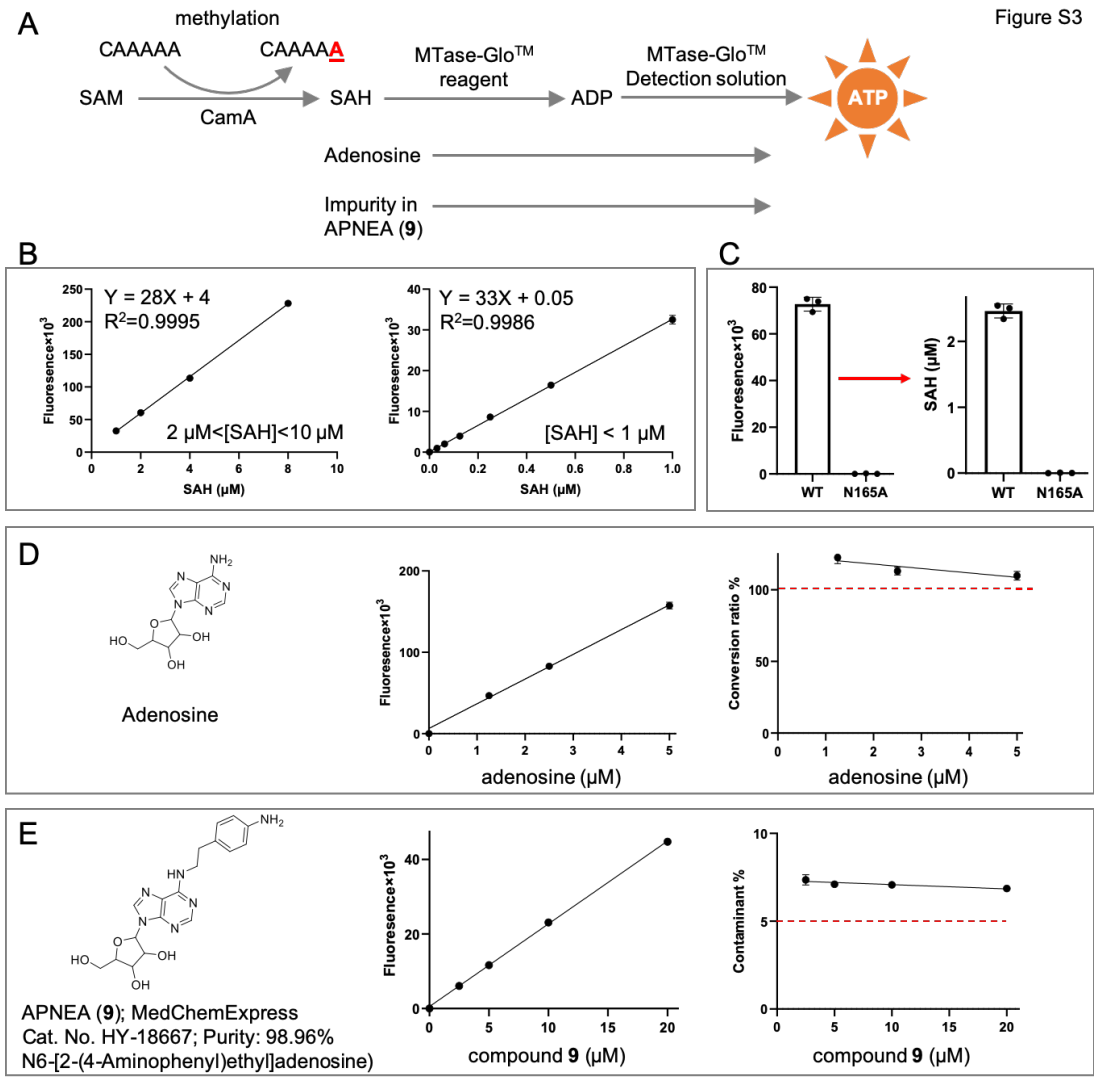

Figure S3

Figure S3. APNEA (compound 9) contains an impurity that interferes with MTase-Glo™ assay. (**A**) Schematic steps of CamA-mediated methylation. After the methylation reaction is complete, the MTase-Glo™ Reagent and Detection Solution (provided by Promega) convert SAH to ATP and measure the light from the luciferase reaction. (**B**) Standard curves for the Promega bioluminescence assay as a function of SAH concentrations in the range of above or below 1 μM (left and right panels) ($N = 2$). (**C**) Enzymatic activity of CamA wild-type (WT) and catalytic mutant (N165A) (left: the raw reading of luminescence signal; right: converted SAH concentration). There is no component in the methylation reaction that interference with the luminescent assay. (**D**) Adenosine acts like SAH in the MTase-Glo™ assay which converts nearly 100% of adenosine to ATP. (**E**) APNEA (compound **9**) contains a >5% impurity which interferes with MTase-Glo™ assay.

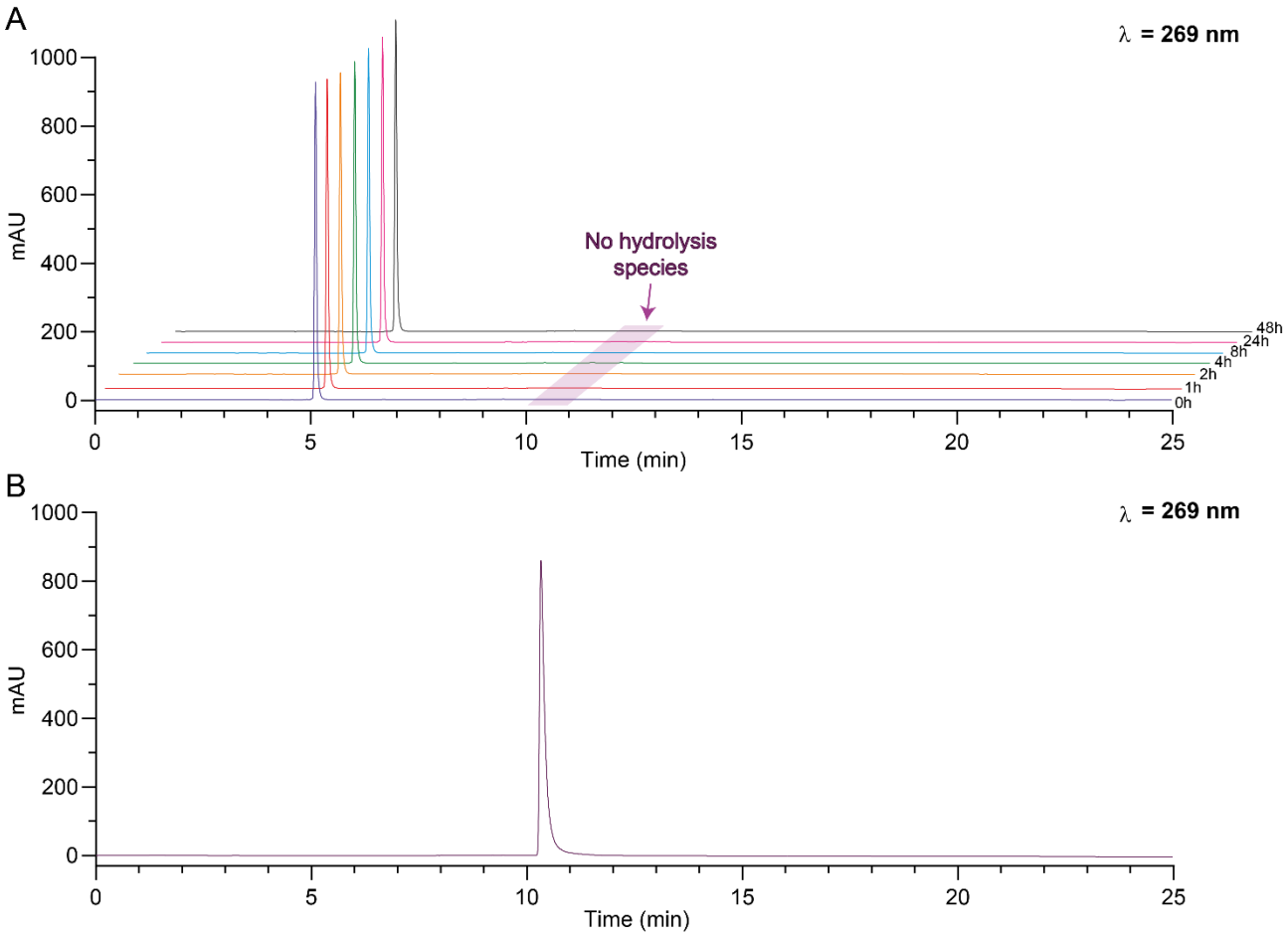

Figure S4. Evaluation of compound **39** stability in assay buffer. We assessed the stability of compound **39** in a water solution containing 50 mM Tris-HCl pH 7.5 and 100 mM NaCl, similar to the enzymatic inhibition assay buffer. Specifically, we dissolved the compound in the buffer (c = 0.5 mg/mL), incubated the solution at 37 °C and then performed analytical HPLC under the same conditions described in the Experimental section. HPLC runs were performed at time 0 and after 1, 2, 4, 8, 24, and 48 h of incubation (**A**). As a comparison, the hydrolysis/deprotection product of **39**, i.e. compound **42**, was also dissolved in the same buffer and analyzed via HPLC (**B**). There is no significant difference between the HPLC profiles of compound **39** at different incubation times and no hydrolysis product formation was observed at any time point, thereby compound **39** is chemically stable under the tested conditions. This observation agrees with that *tert*-butyl carbamate moiety is resistant to hydrolysis under physiological pH conditions[8]. Indeed, given the presence of the additional oxygen, three possible resonance structures can be found which contribute to the increased stability of carbamates compared to amides[9]. Moreover, carbamates are being increasingly chosen as peptide mimetic groups because of their metabolic stability and many examples of carbamate-containing drugs, such as the anthelminthic drugs albendazole and mebendazole, the chemotherapeutic mitomycin C, and the antiasthma agent zafirlukast[10].

References

(1) Griffiths, M. et al. Cloning of a human nucleoside transporter implicated in the cellular uptake of adenosine and chemotherapeutic drugs. Nat Med. 3(1): 89-93 (1997)

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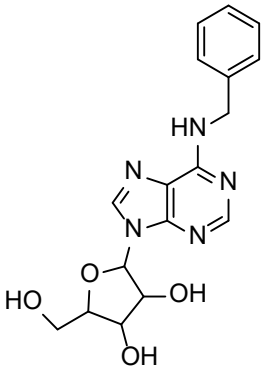
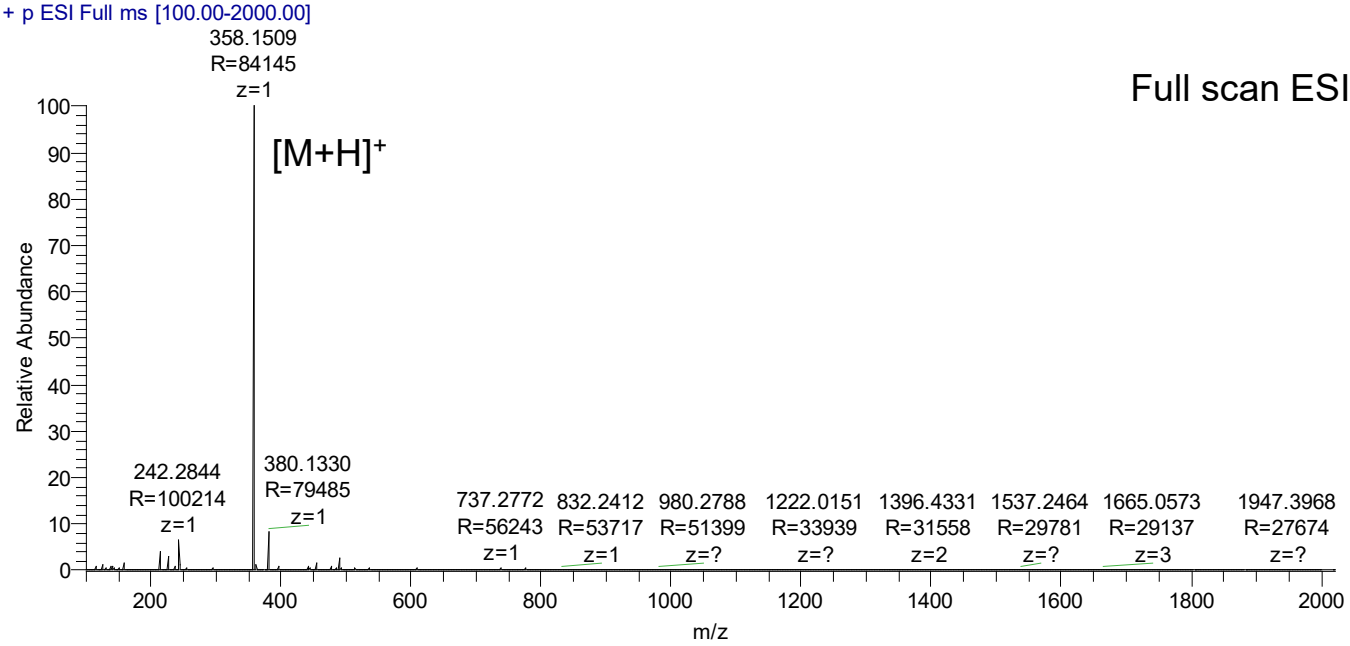
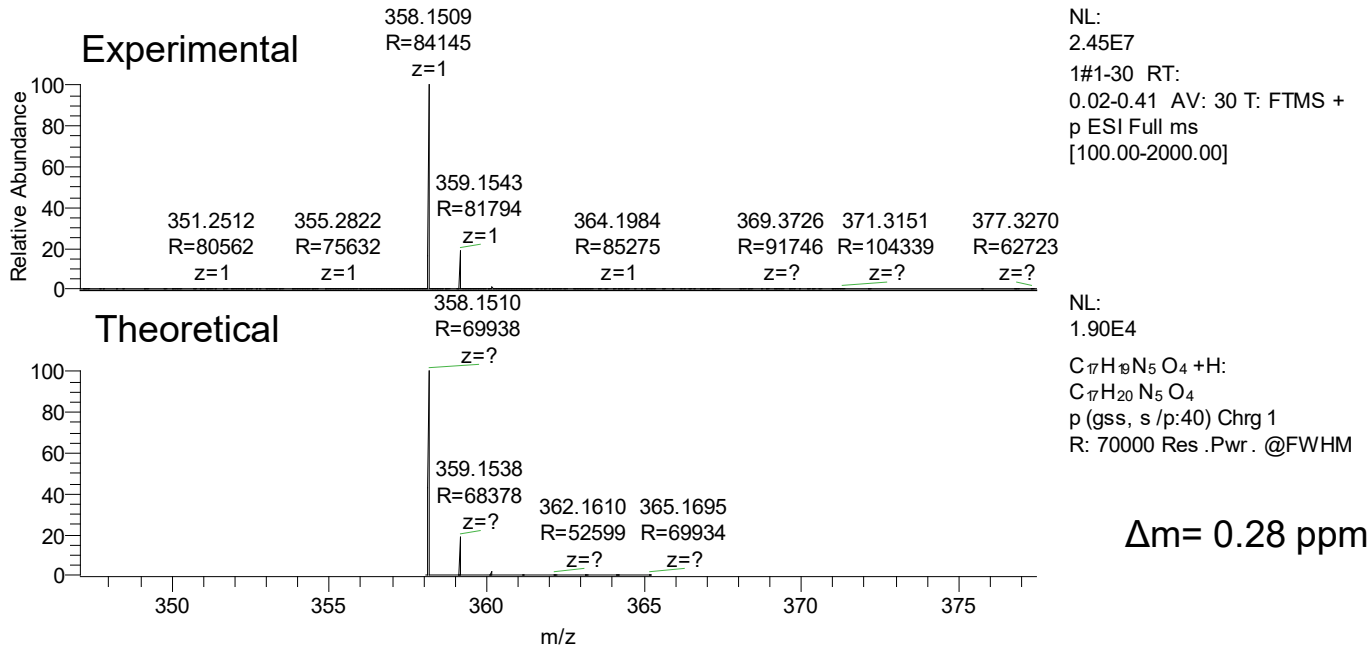
1



1 #1-30 RT: 0.02-0.41 AV: 30 NL: 2.45E7 T: FTMS
+ p ESI Full ms [100.00-2000.00]



Full scan ESI(+)



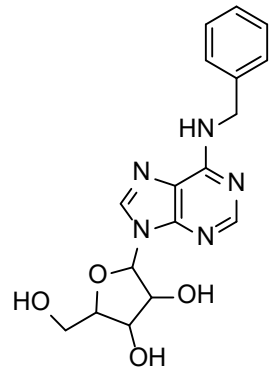
NL:
2.45E7
1#1-30 RT:
0.02-0.41 AV: 30 T: FTMS +
p ESI Full ms
[100.00-2000.00]

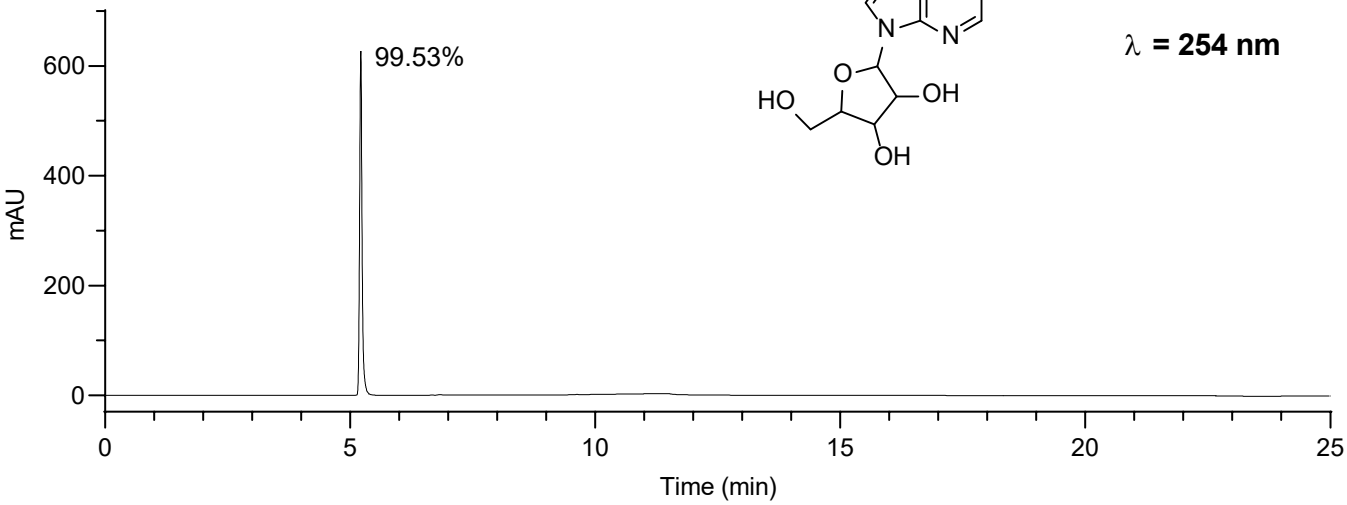
NL:
1.90E4

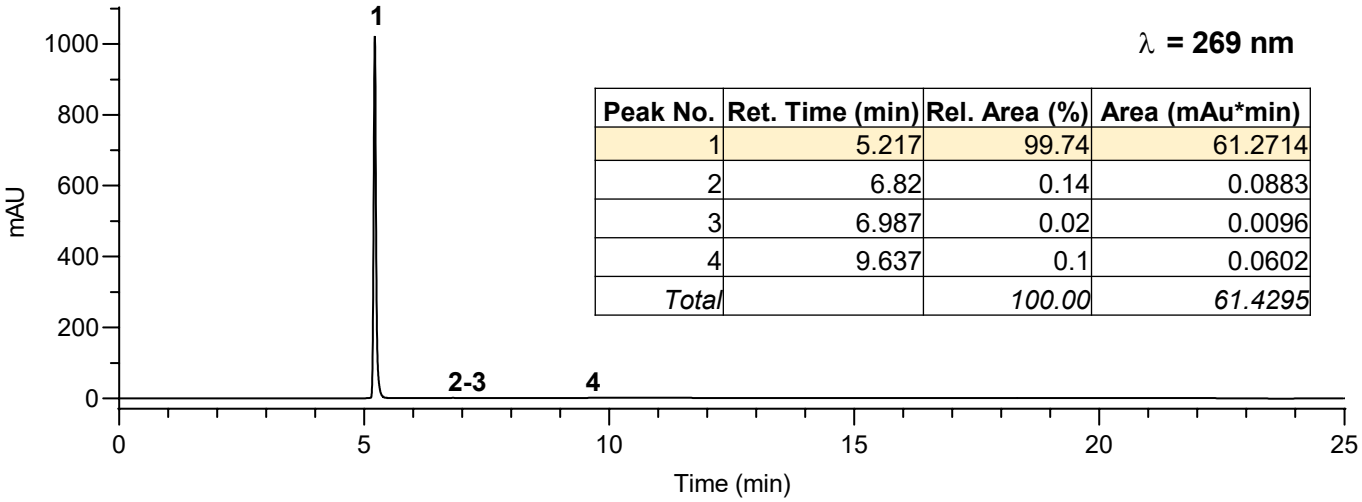
$C_{17}H_{19}N_5O_4$ +H:
$C_{17}H_{20}N_5O_4$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr. @FWHM

Δm= 0.28 ppm

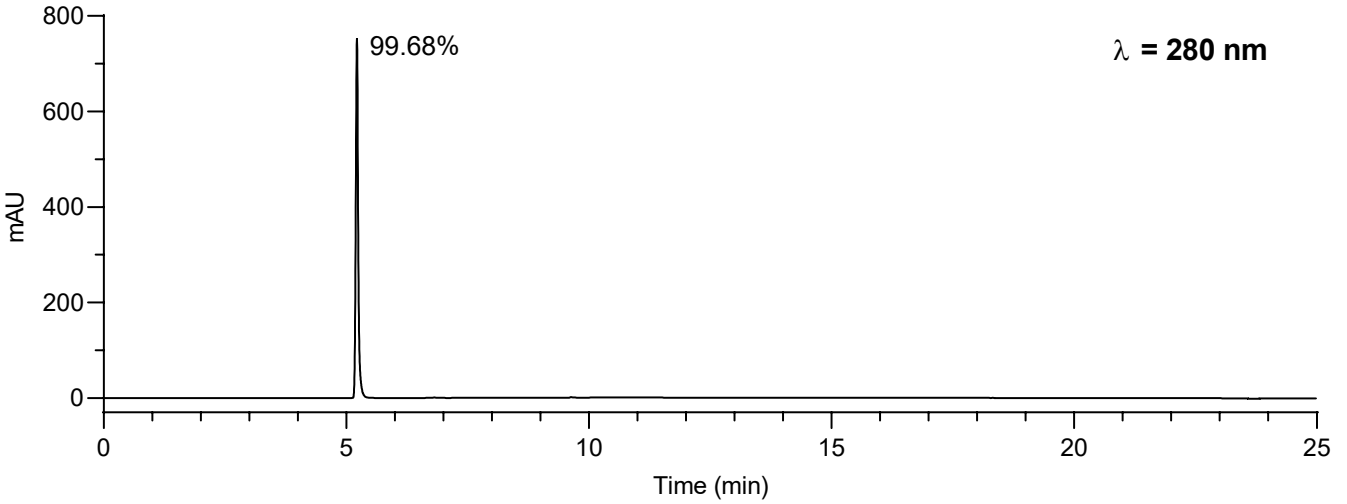
1







Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	5.217	99.74	61.2714
2	6.82	0.14	0.0883
3	6.987	0.02	0.0096
4	9.637	0.1	0.0602
Total		*100.00*	*61.4295*



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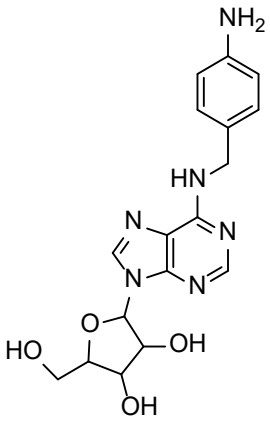
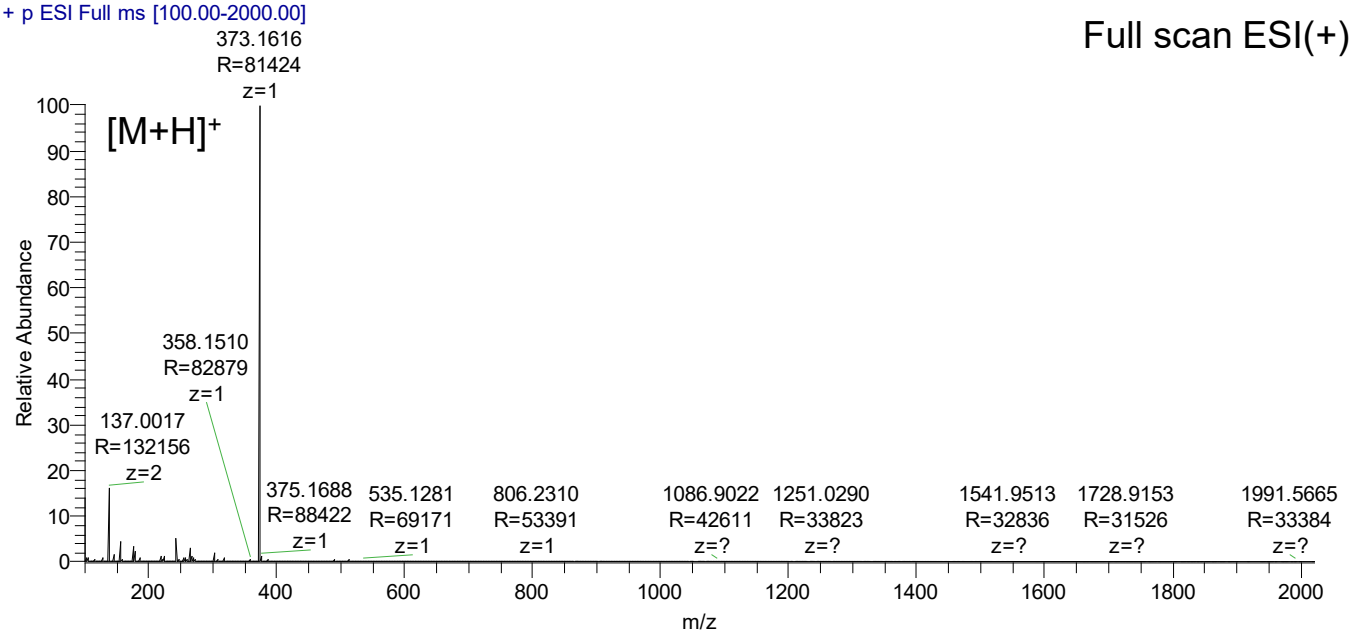
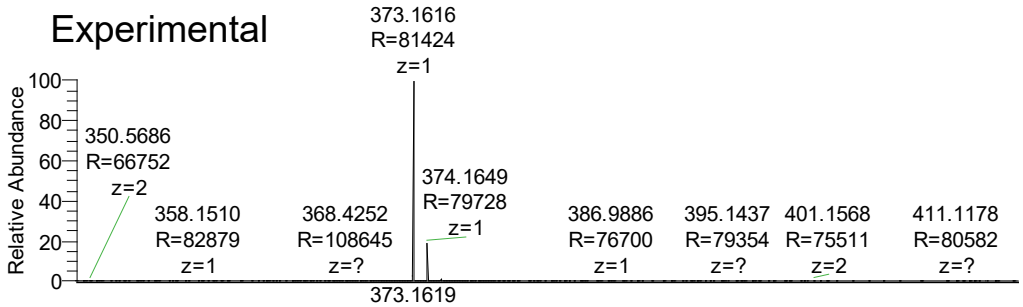


2 #1-17 RT: 0.02-0.23 AV: 17 NL: 5.55E7 T: FTMS
+ p ESI Full ms [100.00-2000.00]

Full scan ESI(+)

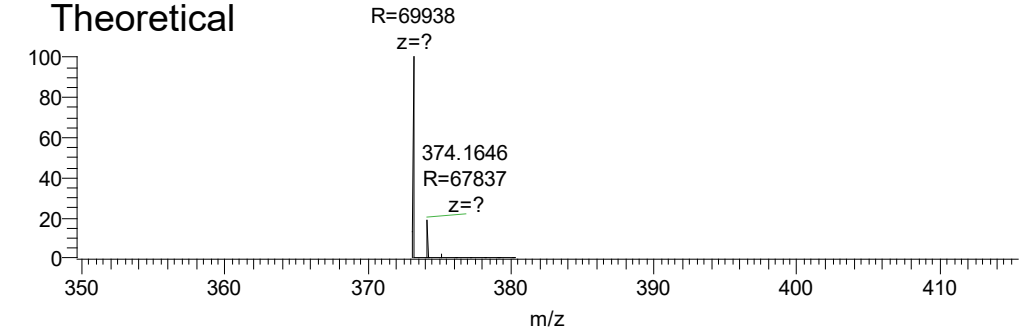


Experimental



NL:
5.55E7
2#1-17 RT:
0.02-0.23 AV: 17 T: FTMS +
p ESI Full ms
[100.00-2000.00]

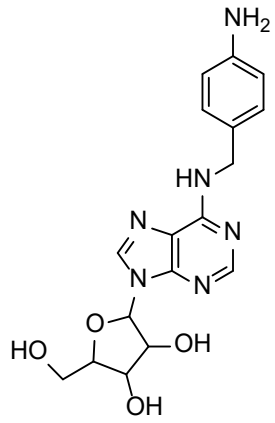
Theoretical

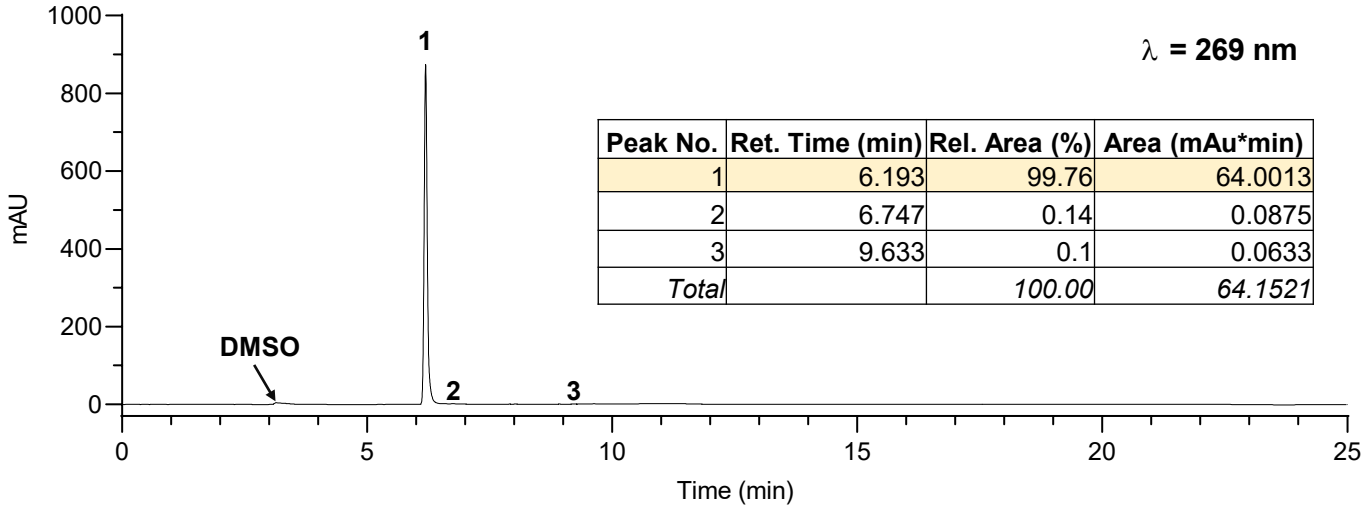


NL:
1.89E4
$C_{17}H_{20}N_6O_4$ +H:
$C_{17}H_{21}N_6O_4$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM

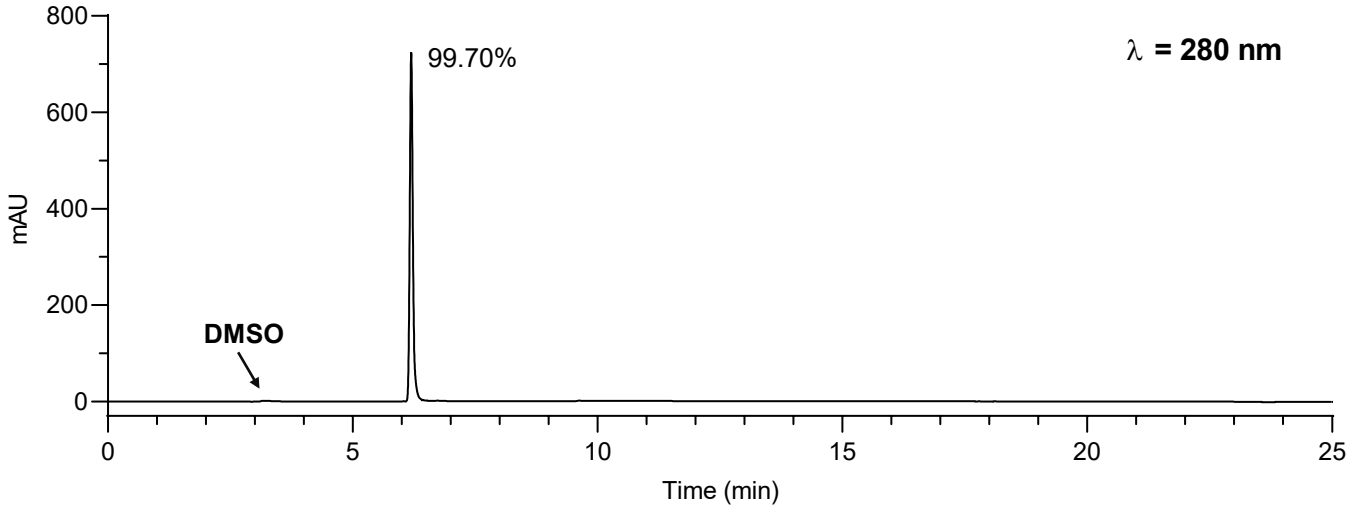
Δm= 0.80ppm

2





Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	6.193	99.76	64.0013
2	6.747	0.14	0.0875
3	9.633	0.1	0.0633
Total		*100.00*	*64.1521*



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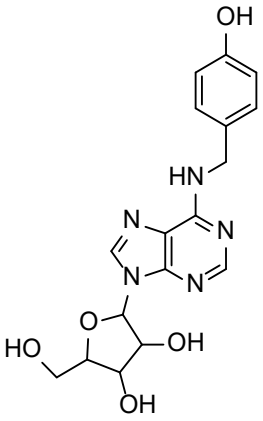
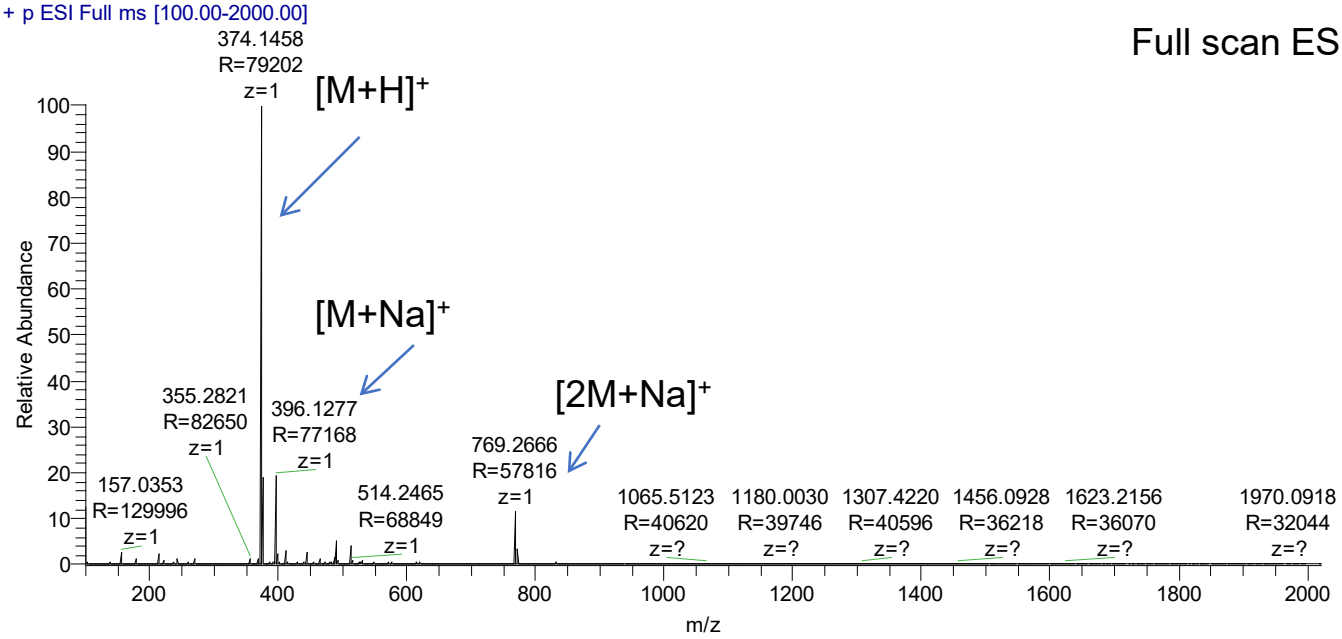
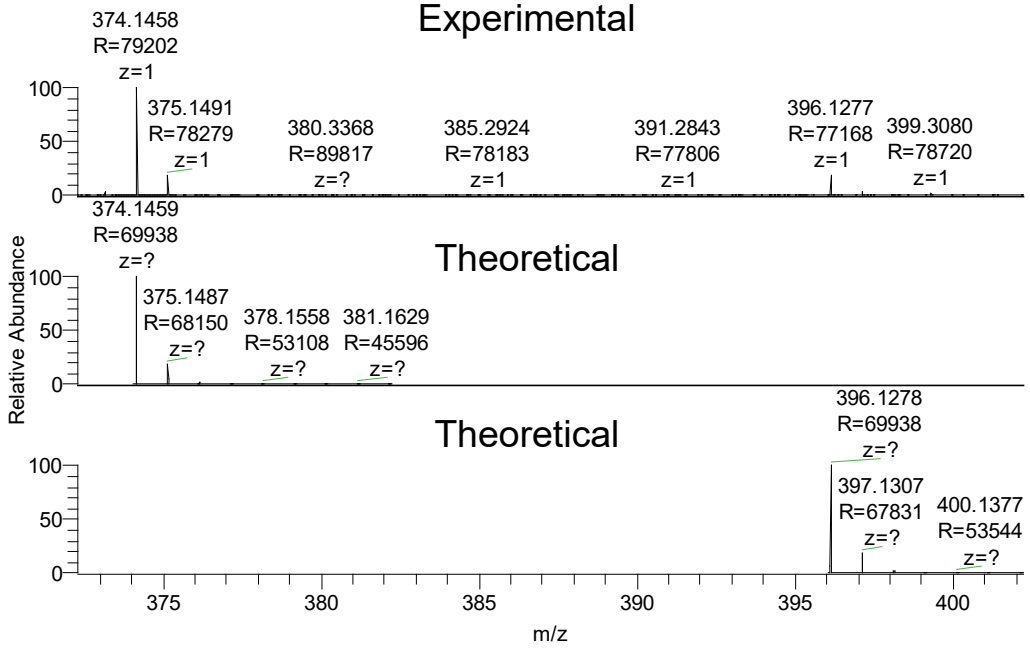


3 #2-30 RT: 0.03-0.42 AV: 29 NL: 1.36E7 T: FTMS
+ p ESI Full ms [100.00-2000.00]

Full scan ESI(+)





NL:
1.36E7
3#2-30 RT:
0.03-0.42 AV: 29 T: FTMS +
p ESI Full ms
[100.00-2000.00]

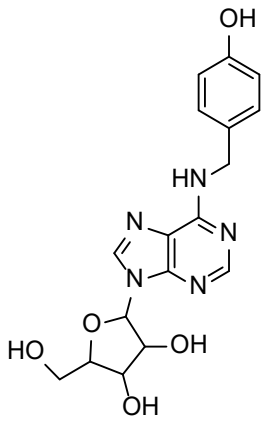
NL:
1.89E4
Δm= 0.27ppm

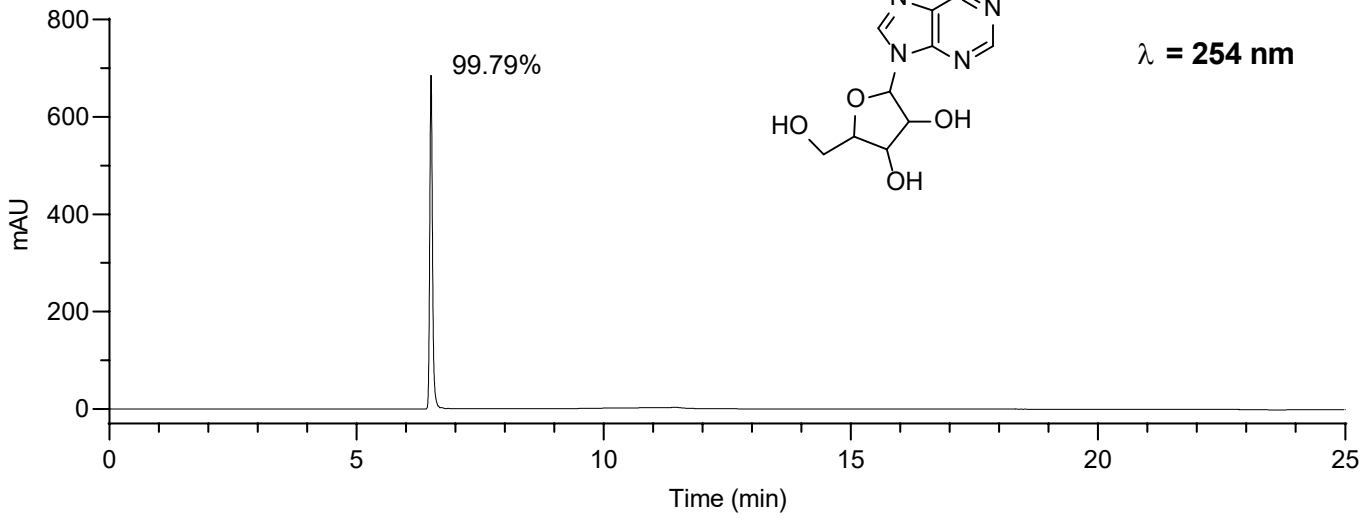
$C_{17}H_{19}N_5O_5$ +H:
$C_{17}H_{20}N_5O_5$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM

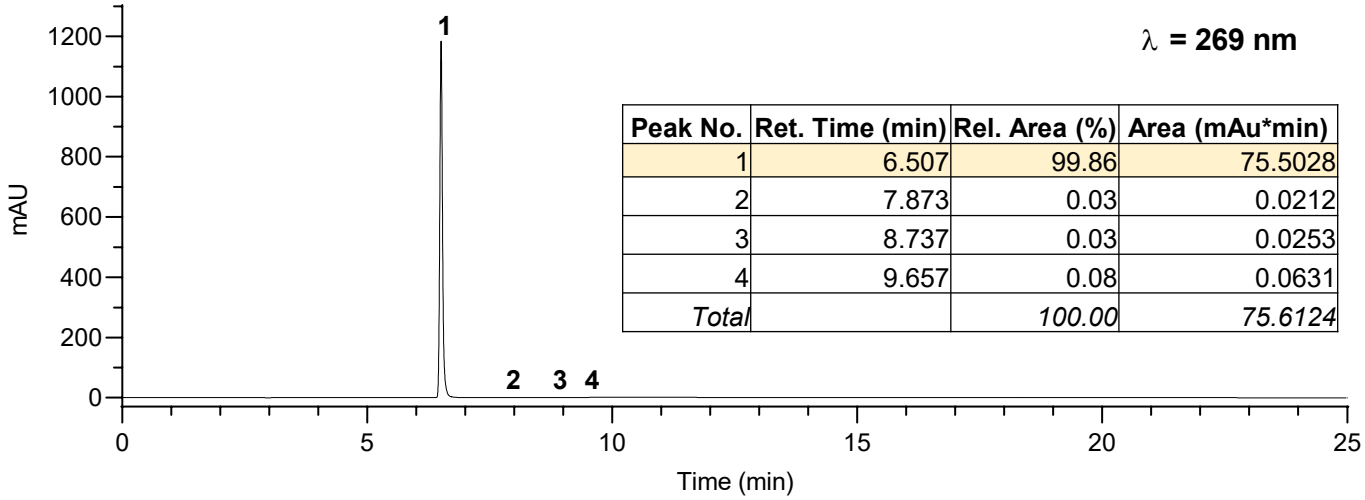
NL:
1.89E4
Δm= 0.25ppm

$C_{17}H_{19}N_5O_5$ +Na:
$C_{17}H_{19}N_5O_5Na_1$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM

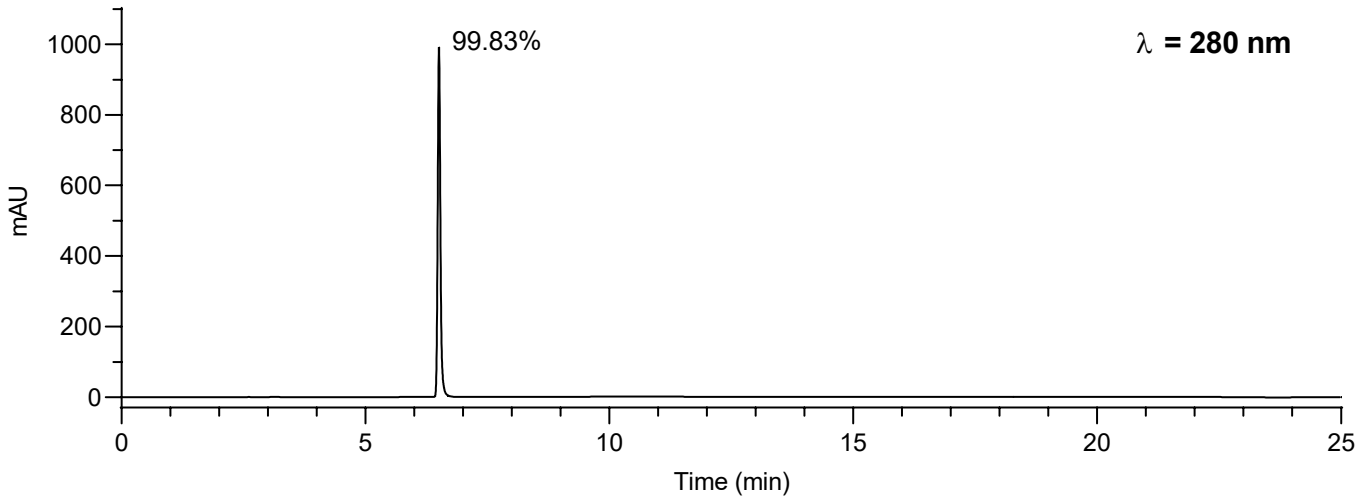
3







Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	6.507	99.86	75.5028
2	7.873	0.03	0.0212
3	8.737	0.03	0.0253
4	9.657	0.08	0.0631
Total		*100.00*	*75.6124*



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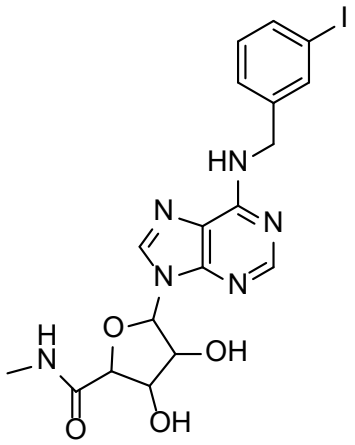
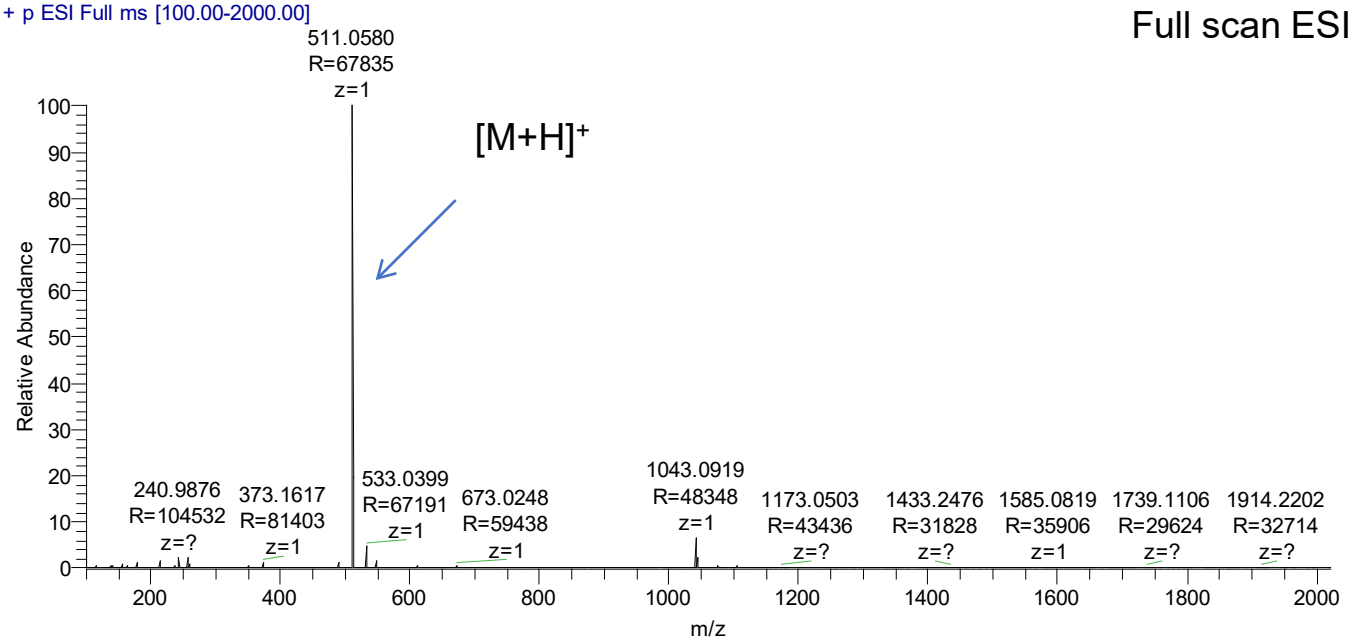
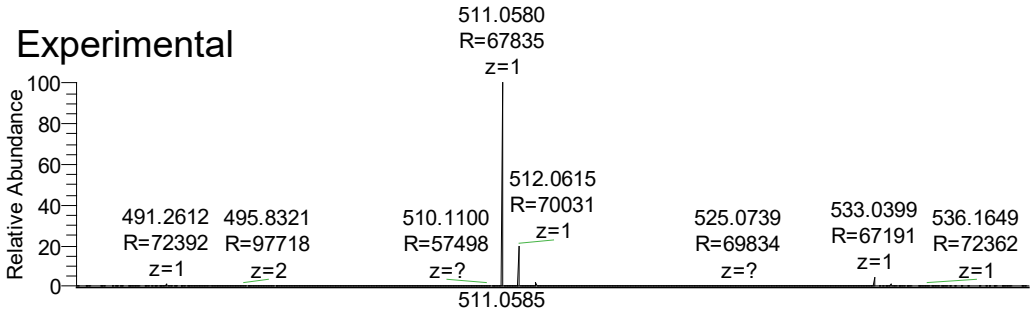


4 #1-10 RT: 0.02-0.14 AV: 10 NL: 6.90E7 T: FTMS
+ p ESI Full ms [100.00-2000.00]

Full scan ESI(+)

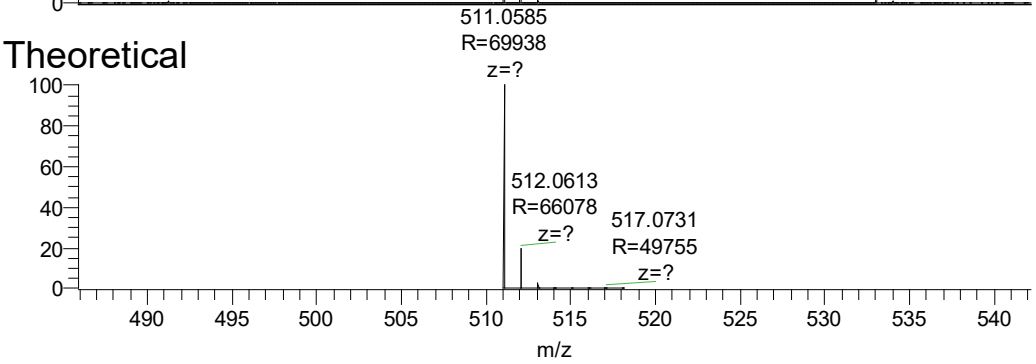


Experimental



NL:
6.90E7
4#1-10 RT:
0.02-0.14 AV: 10 T: FTMS +
p ESI Full ms
[100.00-2000.00]

Theoretical

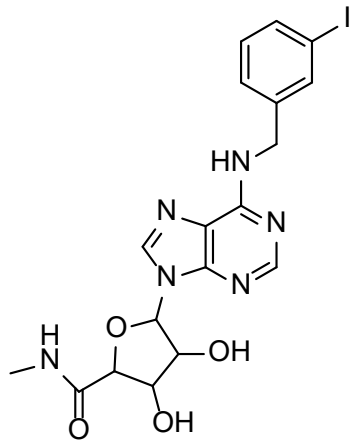


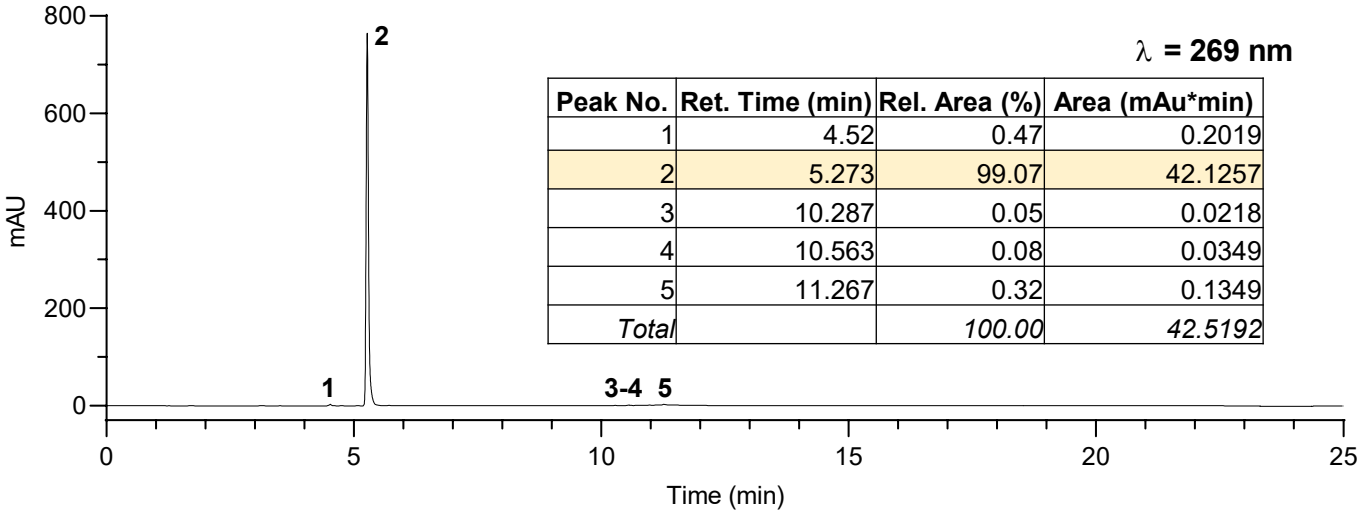
NL:
1.87E4

$C_{18}H_{19}IN_6O_4$ +H:
$C_{18}H_{20}I_1N_6O_4$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr. @FWHM

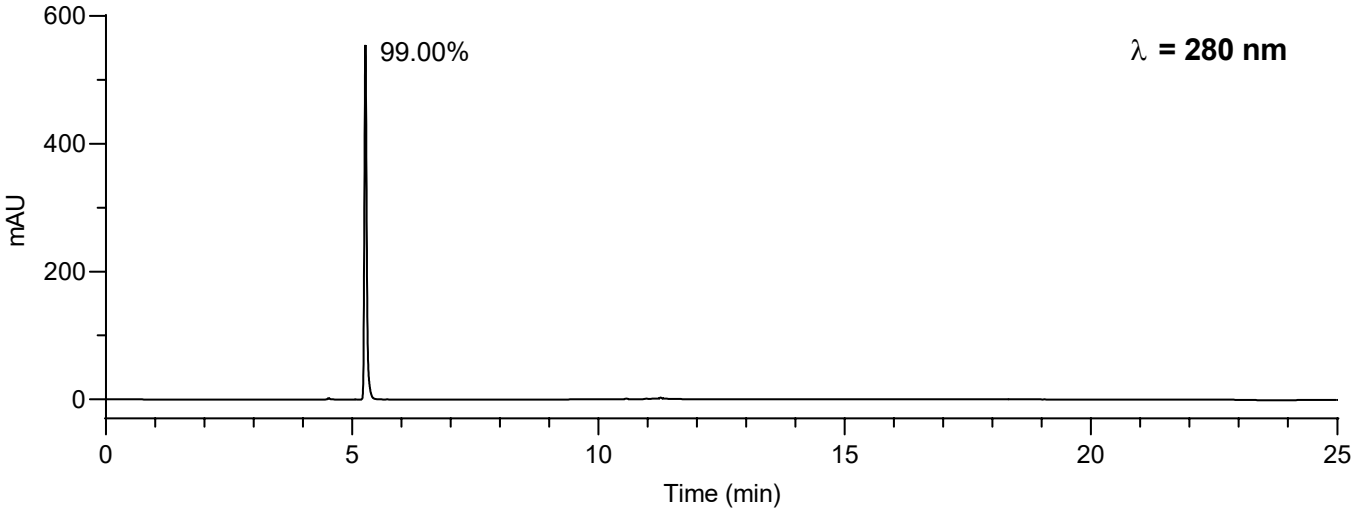
Δm= 0.98ppm

4

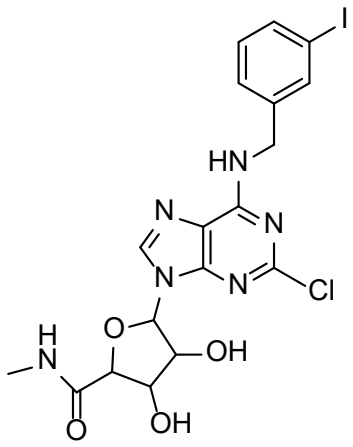




Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	4.52	0.47	0.2019
2	5.273	99.07	42.1257
3	10.287	0.05	0.0218
4	10.563	0.08	0.0349
5	11.267	0.32	0.1349
Total		*100.00*	*42.5192*

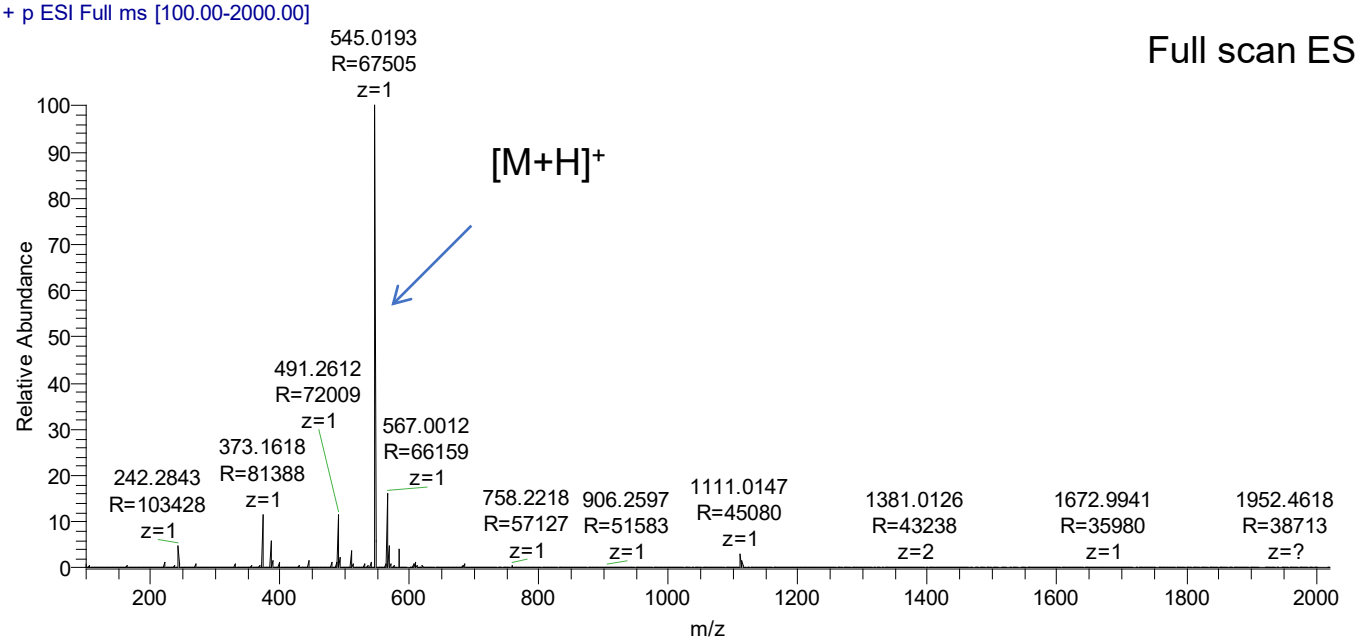


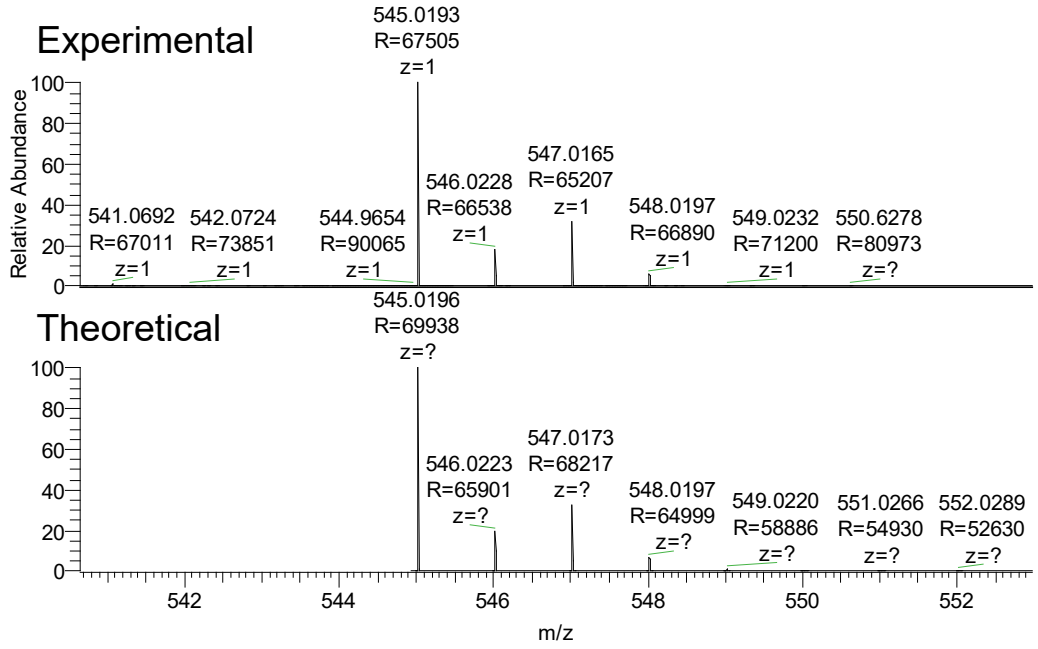
5



5 #1-30 RT: 0.02-0.41 AV: 30 NL: 1.49E7 T: FTMS
+ p ESI Full ms [100.00-2000.00]

Full scan ESI(+)



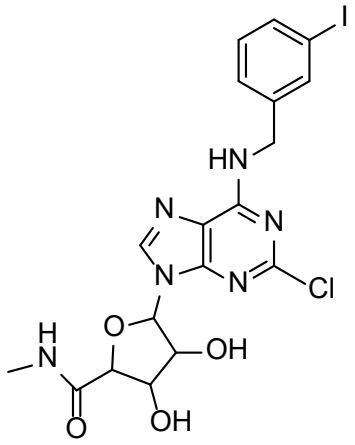


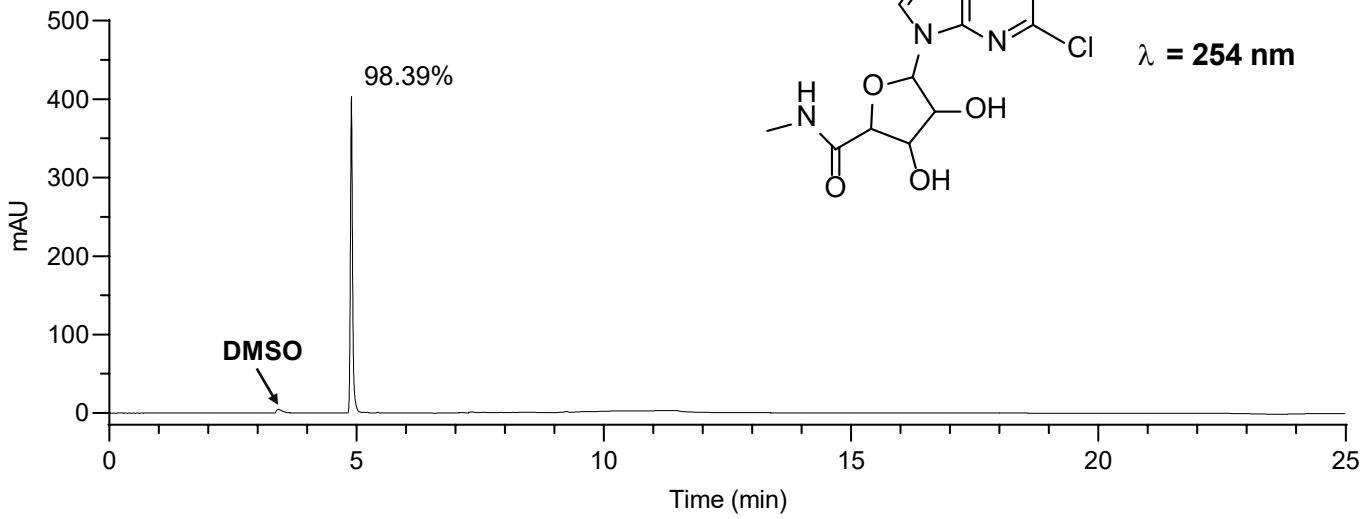
NL:
1.49E7
5#1-30 RT:
0.02-0.41 AV: 30 T: FTMS +
p ESI Full ms
[100.00-2000.00]

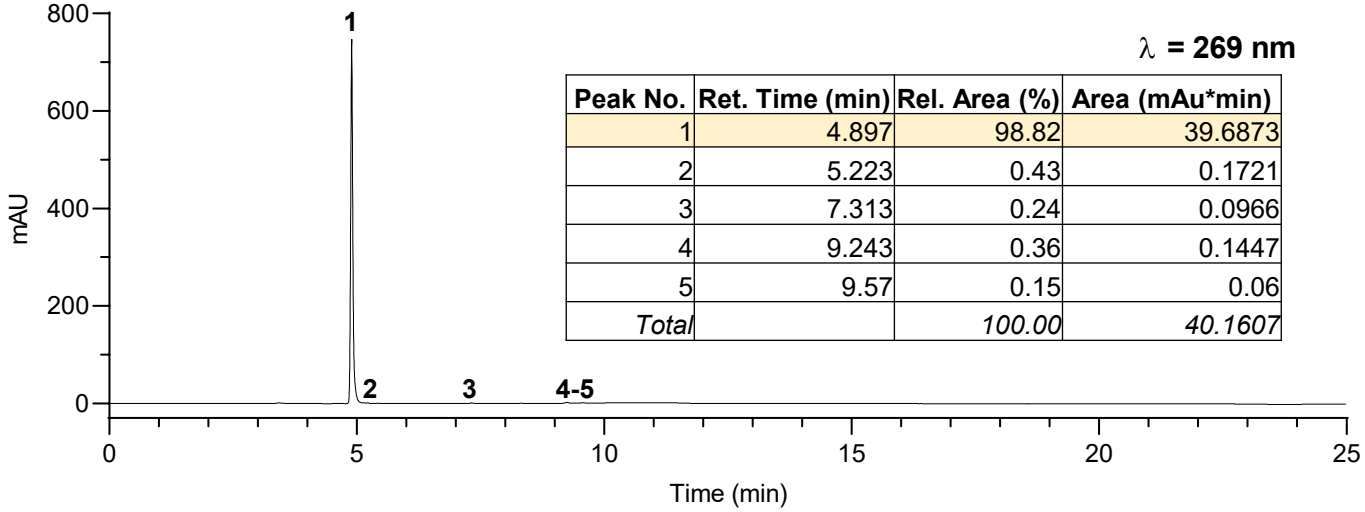
NL:
1.42E4
$C_{18}H_{18}ClIN_6O_4$ +H:
$C_{18}H_{19}Cl_1I_1N_6O_4$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr. @FWHM

Δm= 0.55ppm

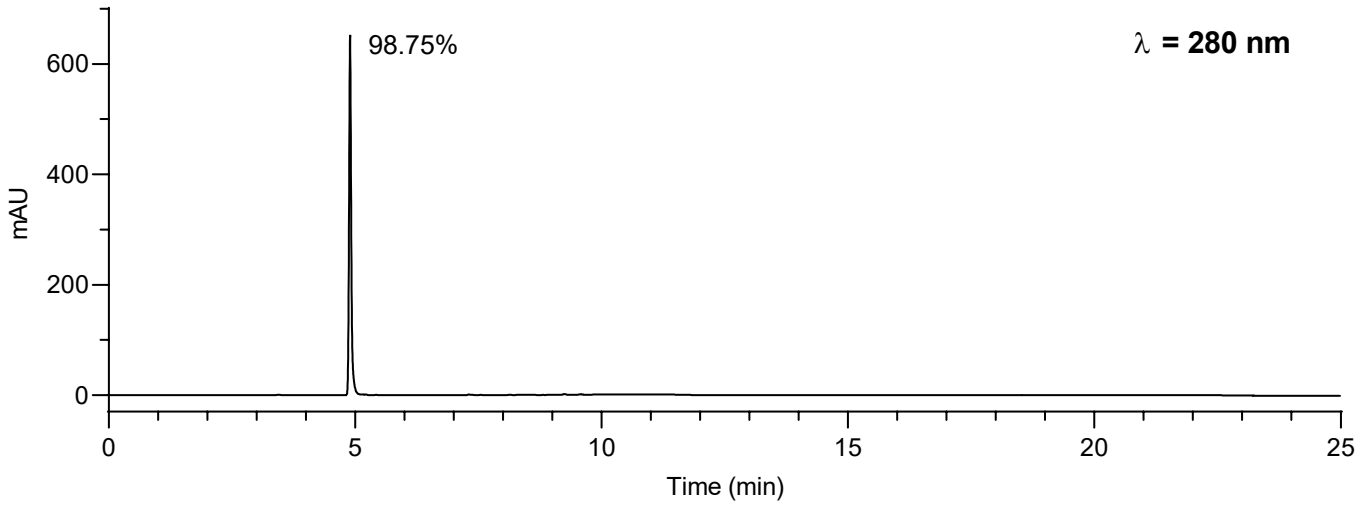
5



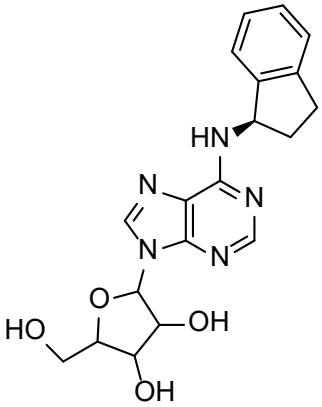




Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	4.897	98.82	39.6873
2	5.223	0.43	0.1721
3	7.313	0.24	0.0966
4	9.243	0.36	0.1447
5	9.57	0.15	0.06
Total		*100.00*	*40.1607*

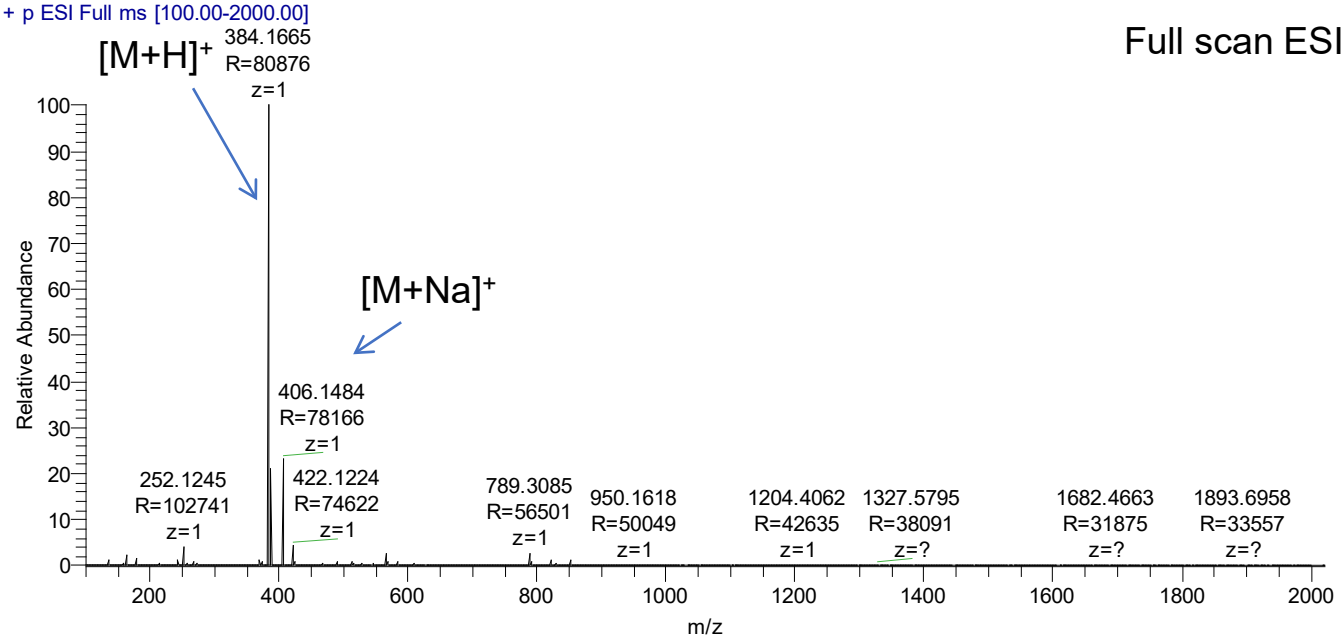


6

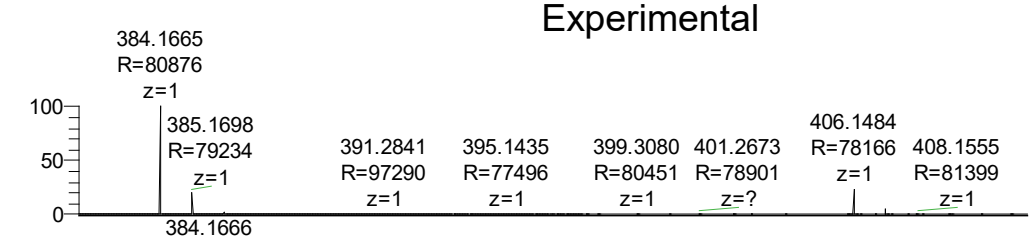


6 #1-30 RT: 0.02-0.41 AV: 30 NL: 3.52E7 T: FTMS
+ p ESI Full ms [100.00-2000.00]

Full scan ESI(+)

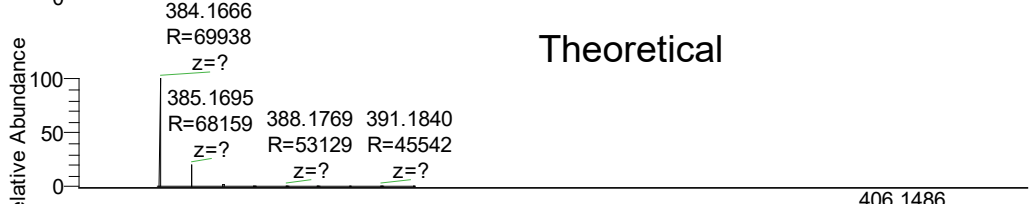


Experimental



NL:
3.52E7
6#1-30 RT:
0.02-0.41 AV: 30 T: FTMS +
p ESI Full ms
[100.00-2000.00]

Theoretical

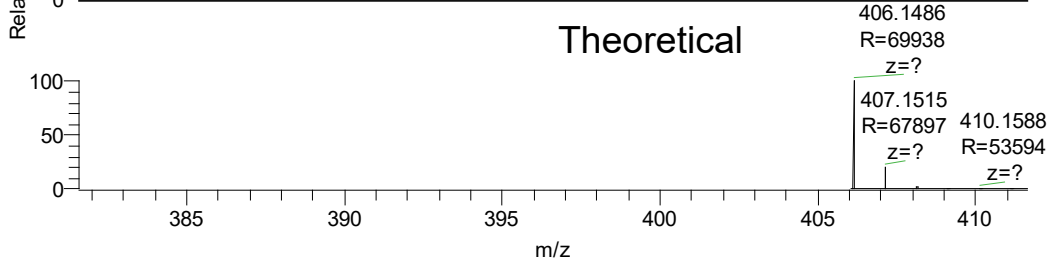


NL:
1.85E4

Δm= 0.26 ppm

$C_{19}H_{21}N_5O_4$ +H:
$C_{19}H_{22}N_5O_4$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM

Theoretical

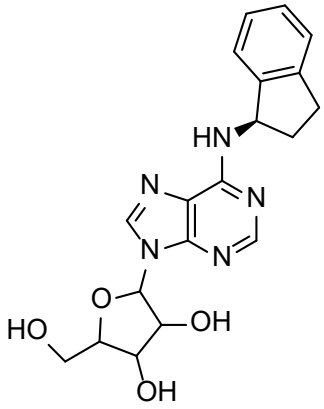


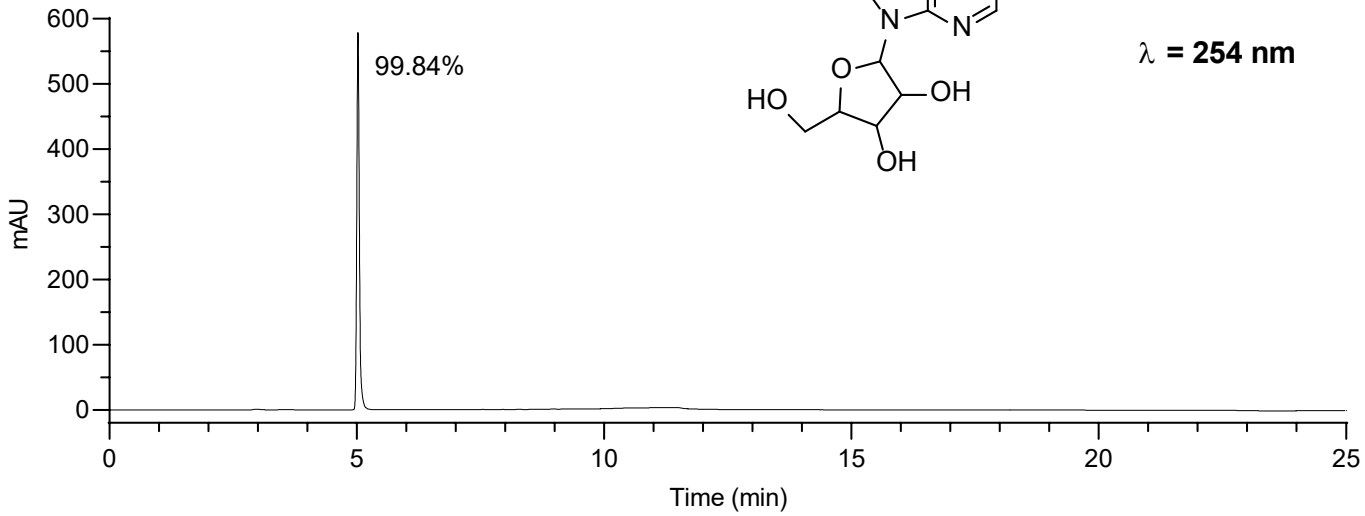
NL:
1.86E4

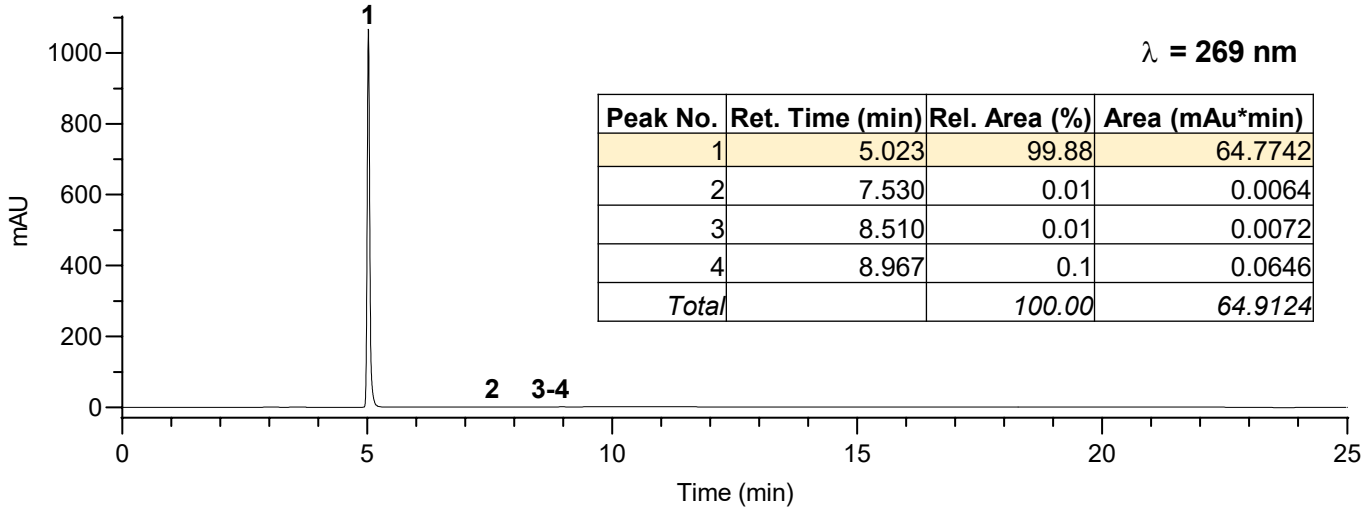
Δm= 0.49 ppm

$C_{19}H_{21}N_5O_4$ +Na:
$C_{19}H_{21}N_5O_4Na_1$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM

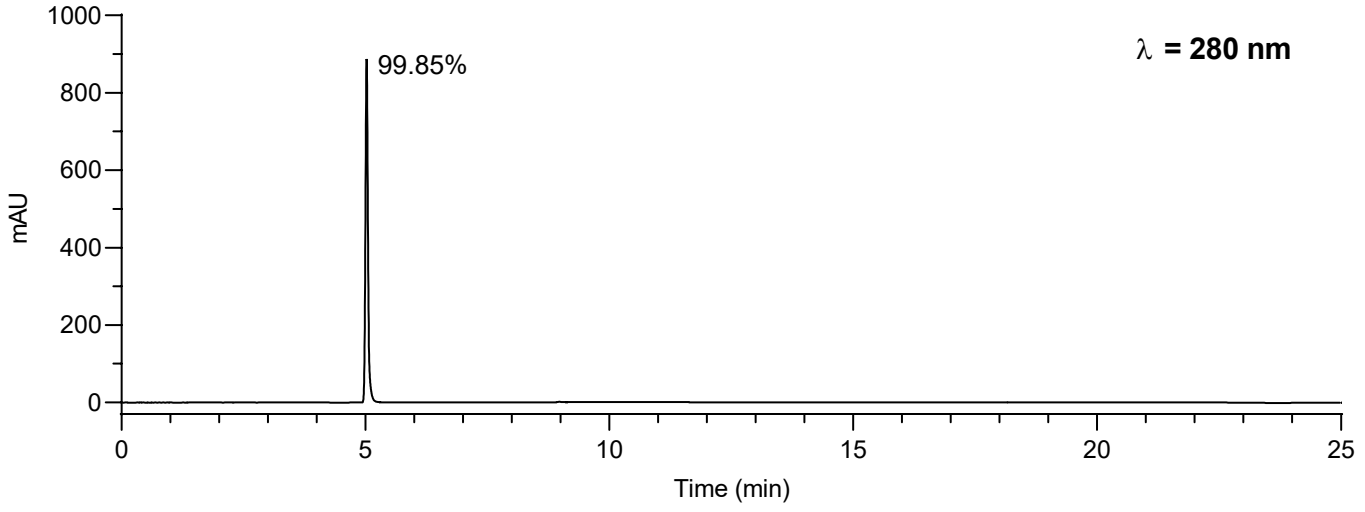
6



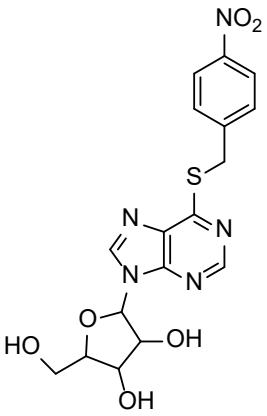




Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	5.023	99.88	64.7742
2	7.530	0.01	0.0064
3	8.510	0.01	0.0072
4	8.967	0.1	0.0646
Total		*100.00*	*64.9124*

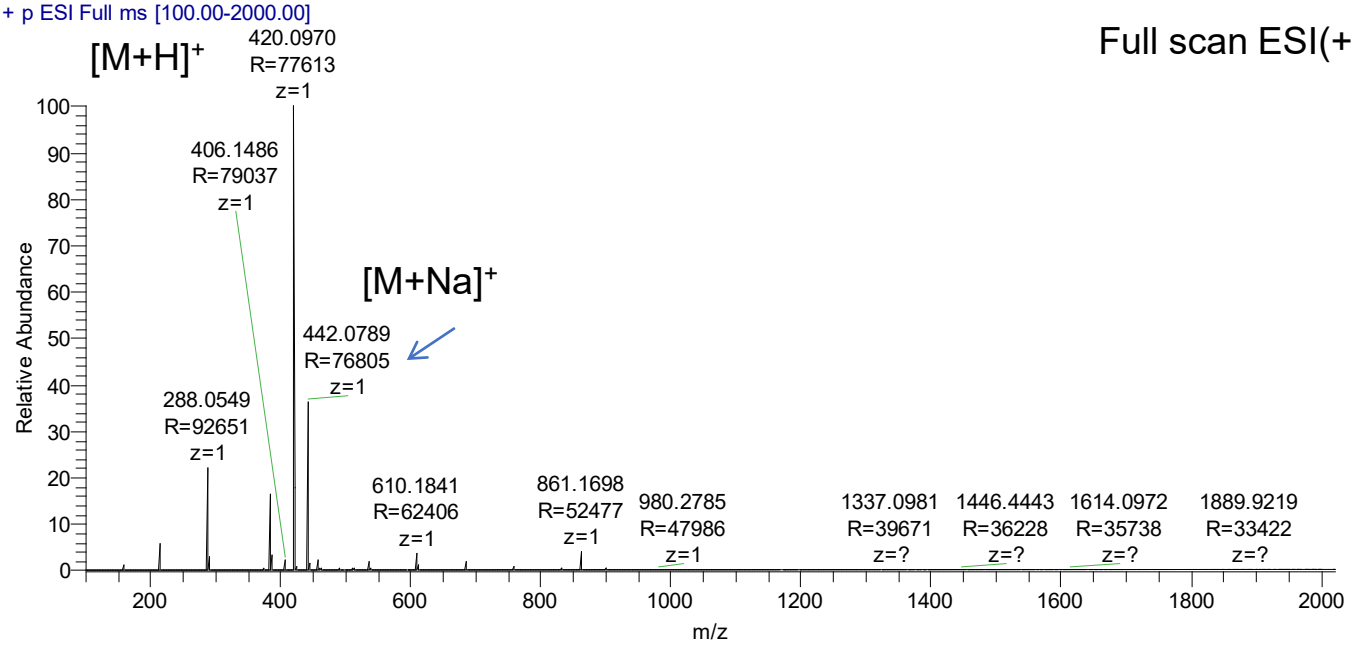


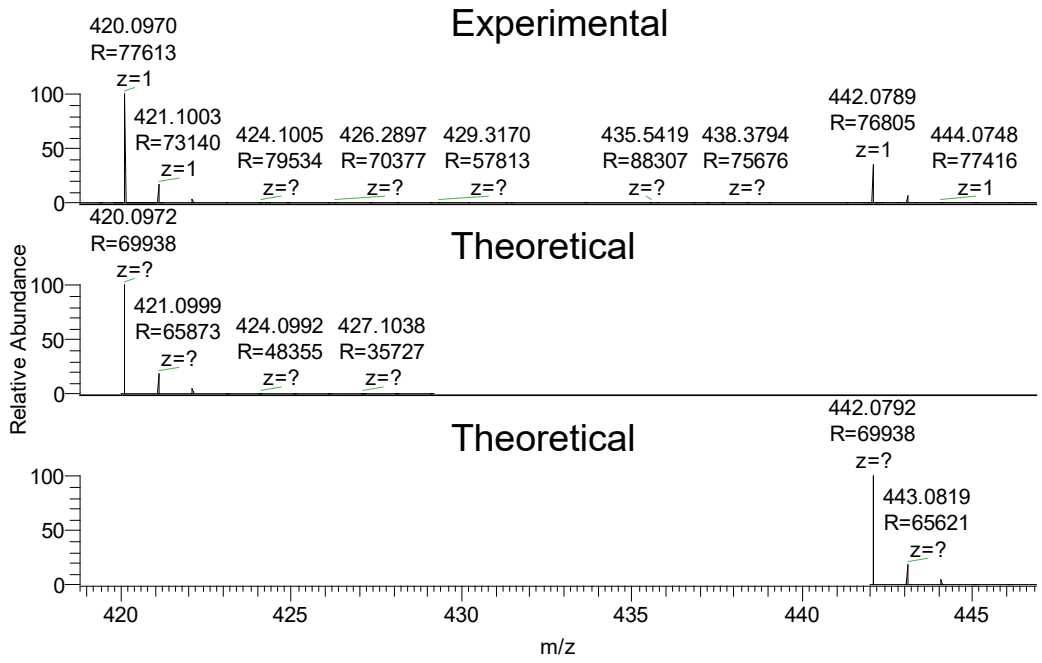
7



7 #1-29 RT: 0.02-0.40 AV: 29 NL: 2.02E7 T: FTMS
+ p ESI Full ms [100.00-2000.00]

Full scan ESI(+)





NL:
2.02E7
7#1-29 RT:
0.02-0.40 AV: 29 T: FTMS +
p ESI Full ms
[100.00-2000.00]

NL:
1.79E4

Δm= 0.48 ppm

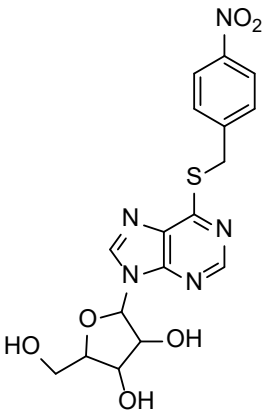
$C_{17}H_{17}N_5O_6S$ +H:
$C_{17}H_{18}N_5O_6S_1$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM

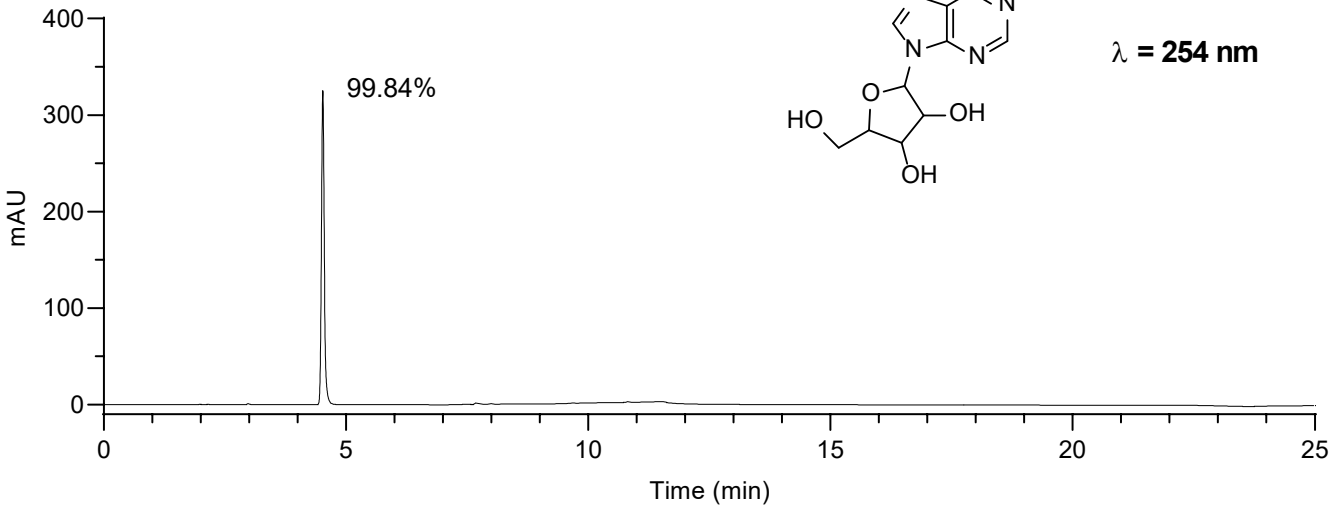
NL:
1.79E4

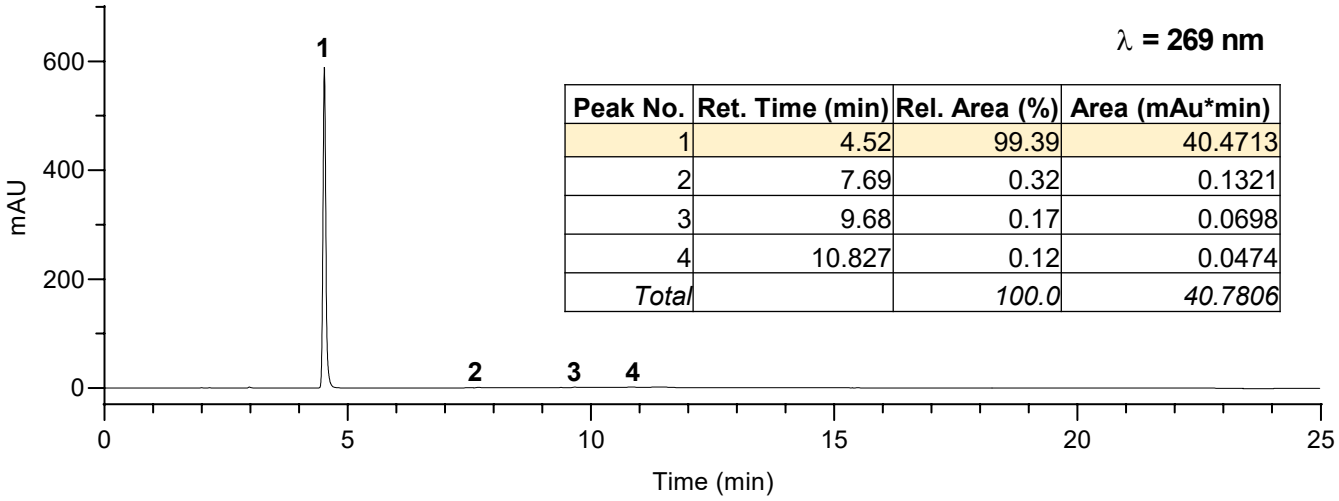
Δm= 0.68 ppm

$C_{17}H_{17}N_5O_6S$ +Na:
$C_{17}H_{17}N_5O_6S_1Na_1$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM

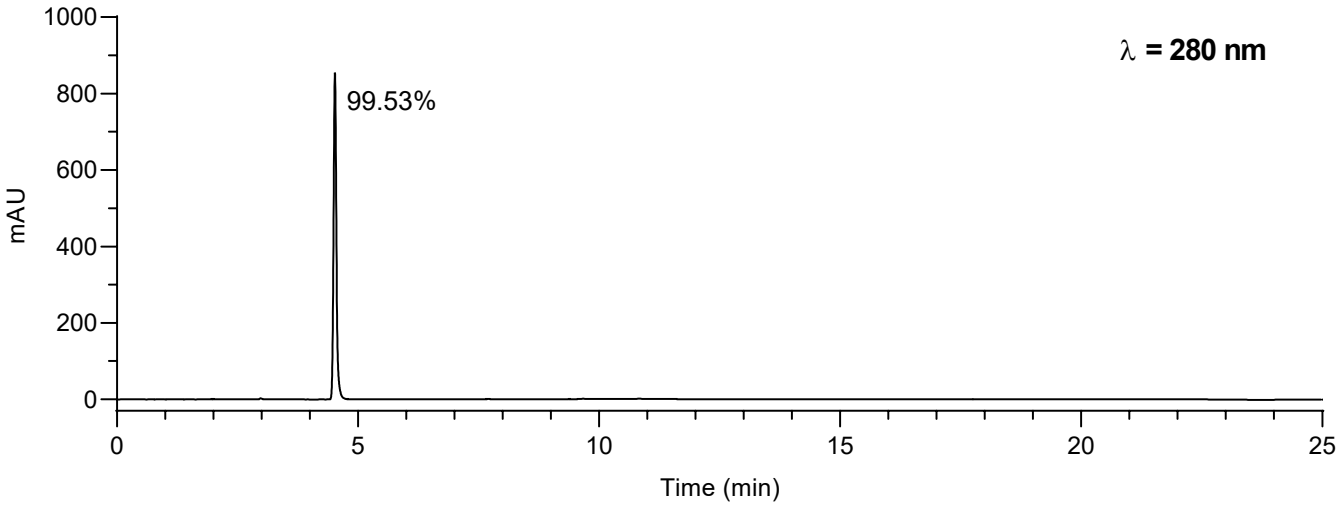
7



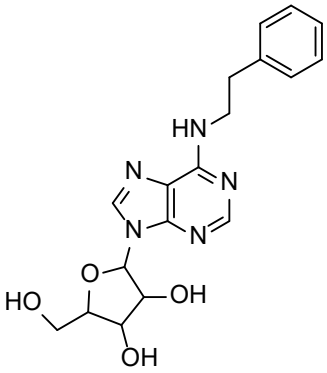




Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	4.52	99.39	40.4713
2	7.69	0.32	0.1321
3	9.68	0.17	0.0698
4	10.827	0.12	0.0474
Total		*100.0*	*40.7806*

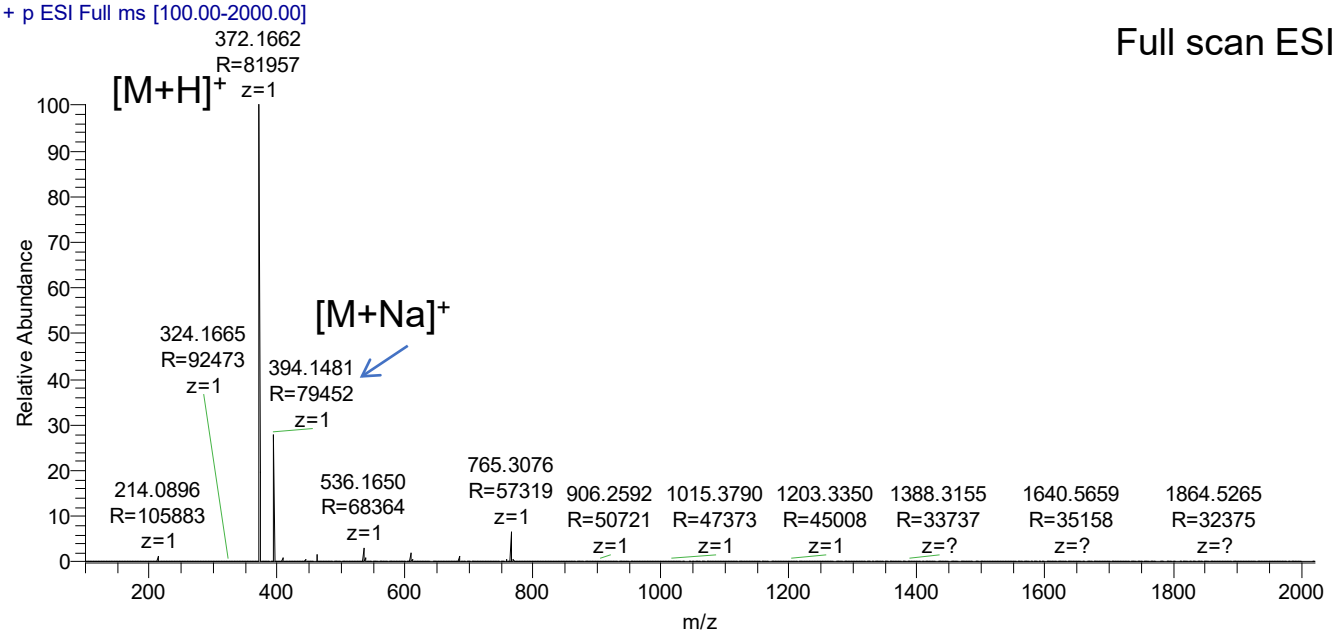


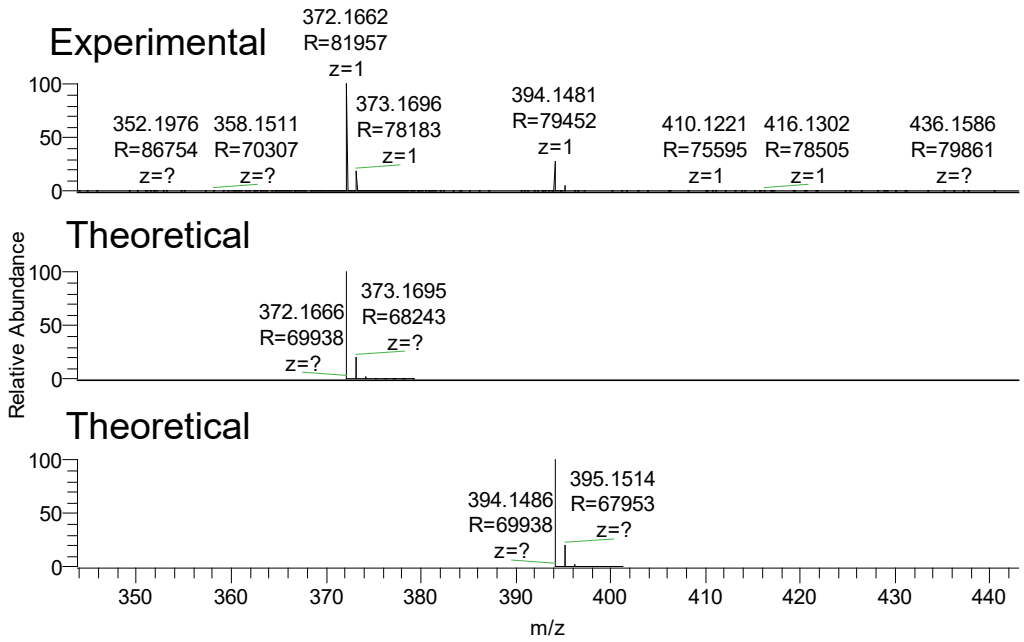
8



8 #2-30 RT: 0.03-0.41 AV: 29 NL: 1.30E8 T: FTMS
+ p ESI Full ms [100.00-2000.00]

Full scan ESI(+)



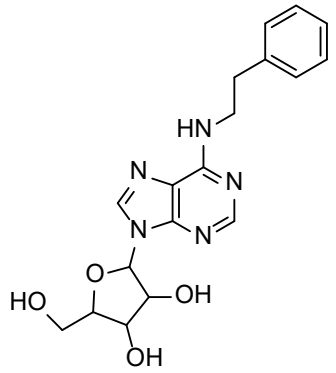


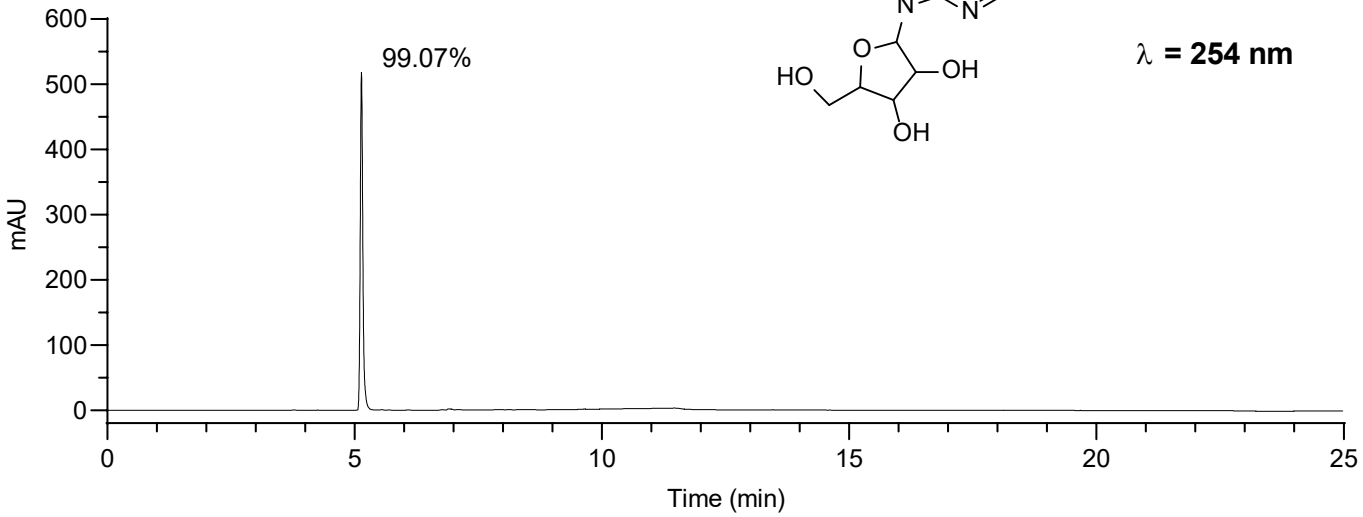
NL:
1.30E8
8#2-30 RT:
0.03-0.41 AV: 29 T: FTMS +
p ESI Full ms
[100.00-2000.00]

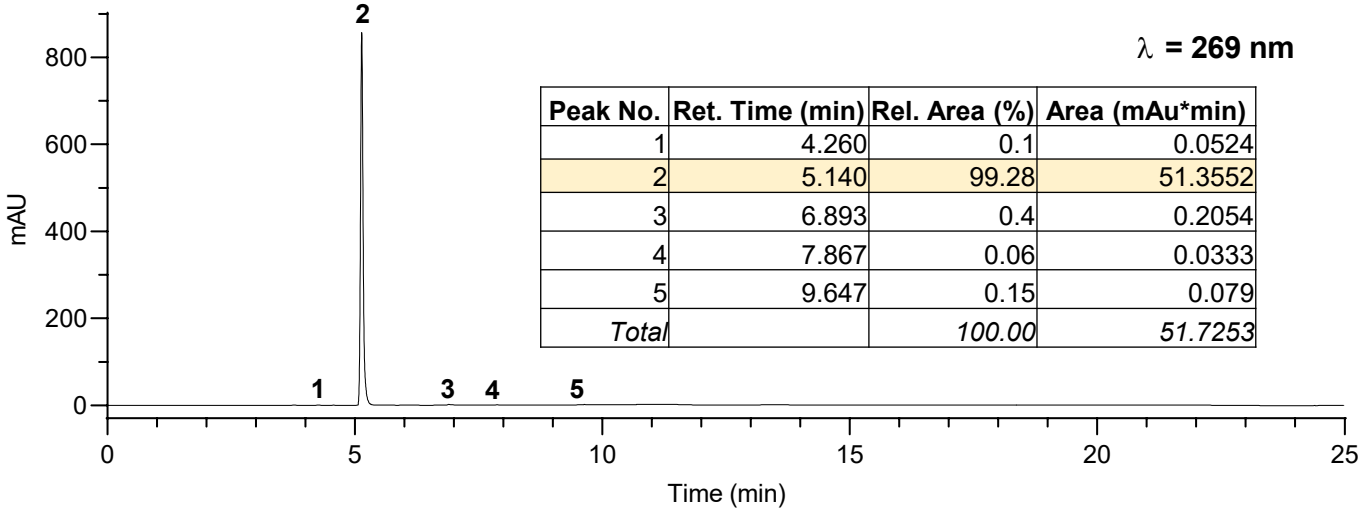
NL:
1.87E4 Δm= 0.85ppm
$C_{18}H_{21}N_5O_4$ +H:
$C_{18}H_{22}N_5O_4$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM

NL:
1.88E4 Δm= 1.27 ppm
$C_{18}H_{21}N_5O_4$ +Na:
$C_{18}H_{21}N_5O_4Na_1$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM

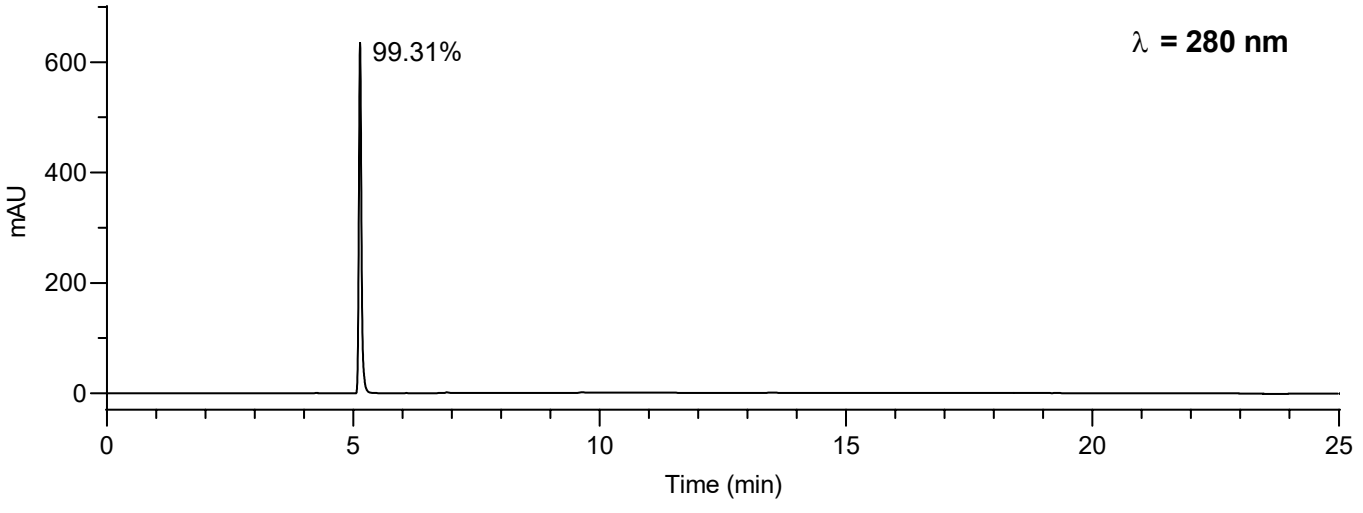
8



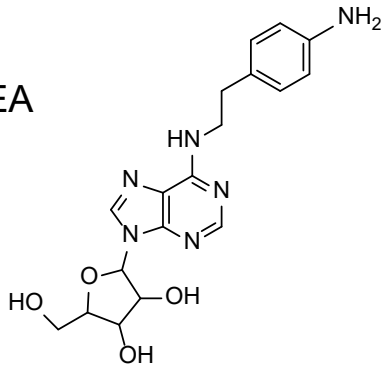




Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	4.260	0.1	0.0524
2	5.140	99.28	51.3552
3	6.893	0.4	0.2054
4	7.867	0.06	0.0333
5	9.647	0.15	0.079
Total		*100.00*	*51.7253*

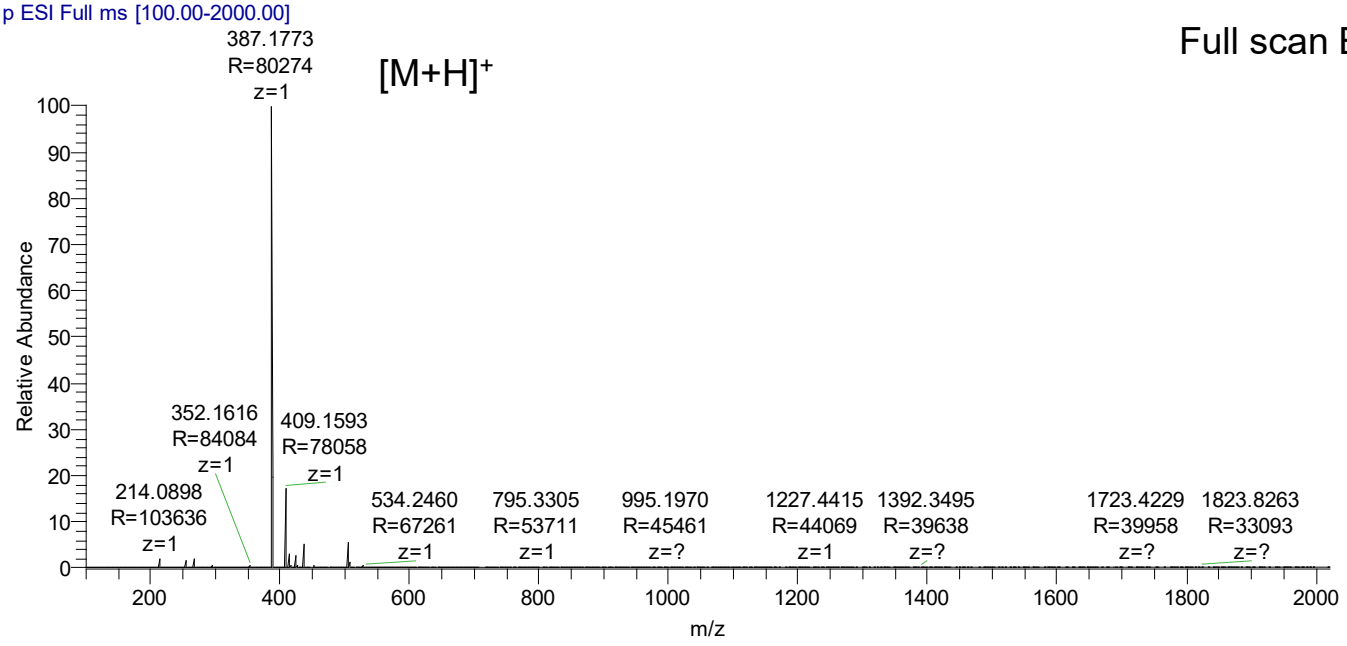


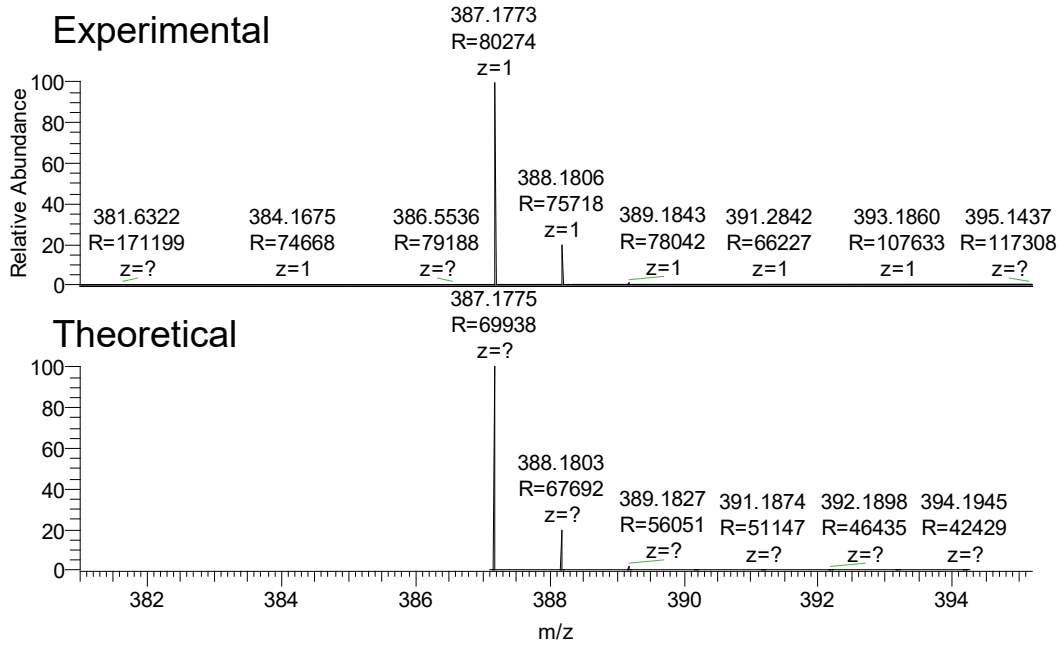
9 - APNEA



9_APNEA #1-30 RT: 0.02-0.41 AV: 30 NL: 5.42E7 T: FTMS +
p ESI Full ms [100.00-2000.00]

Full scan ESI(+)



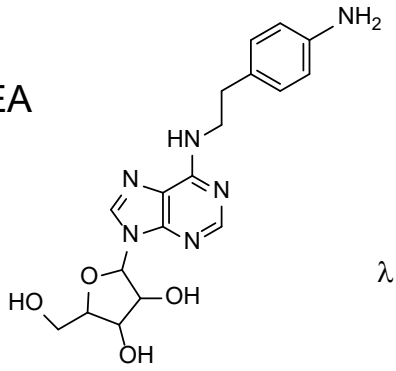


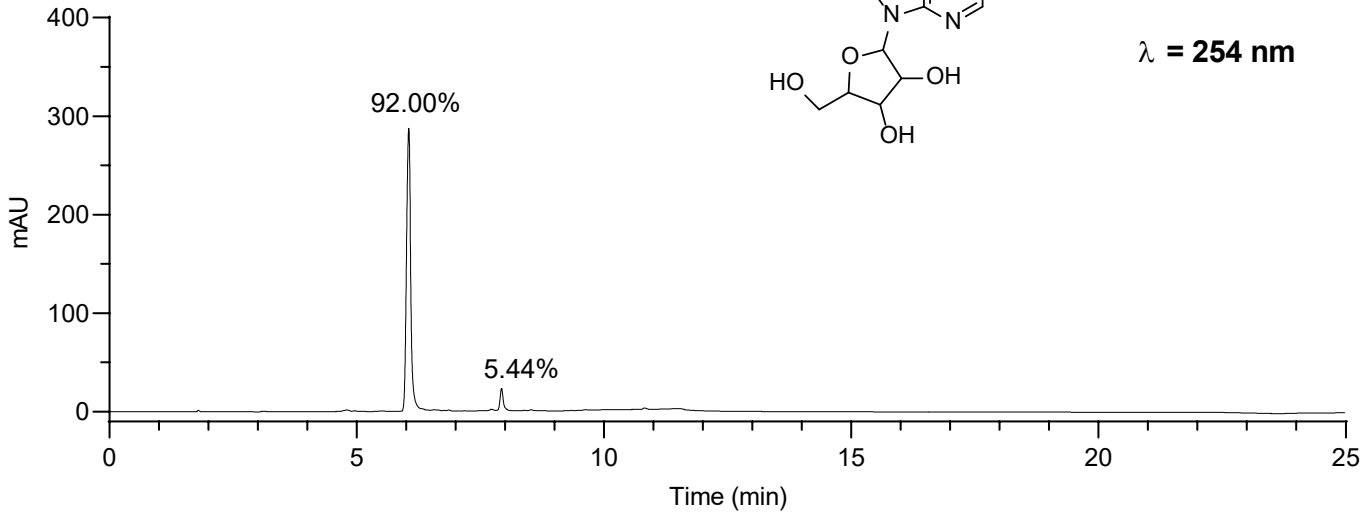
NL:
5.42E7
9_APNEA#1-30 RT:
0.02-0.41 AV: 30 T: FTMS +
p ESI Full ms
[100.00-2000.00]

NL:
1.87E4
$C_{18}H_{22}N_6O_4$ +H:
$C_{18}H_{23}N_6O_4$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr. @FWHM

Δm= 0.52 ppm

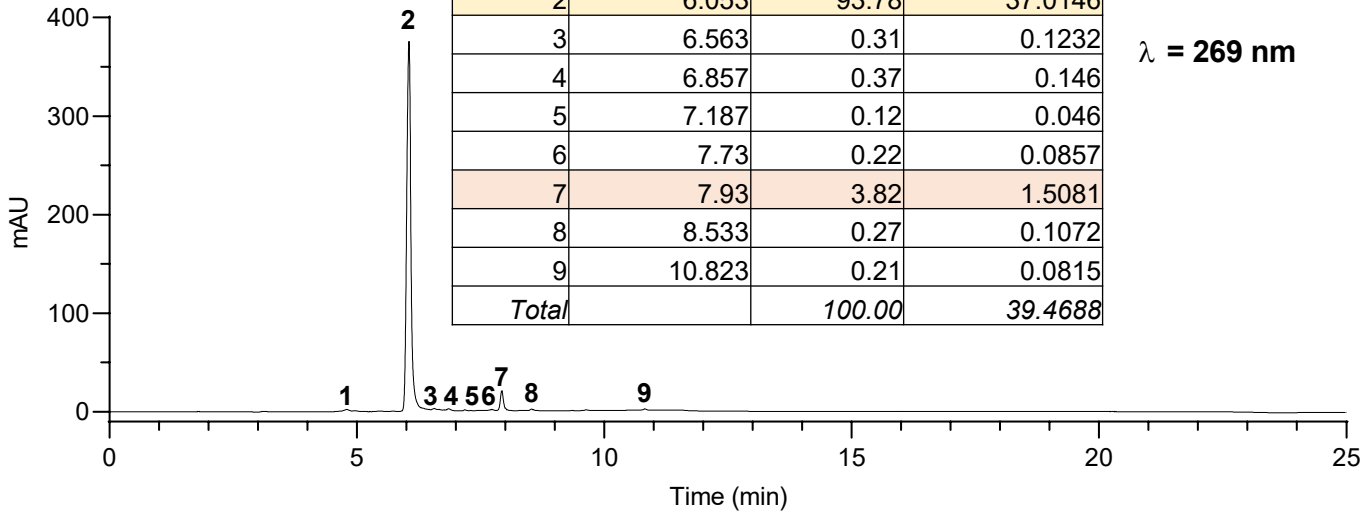
9 - APNEA



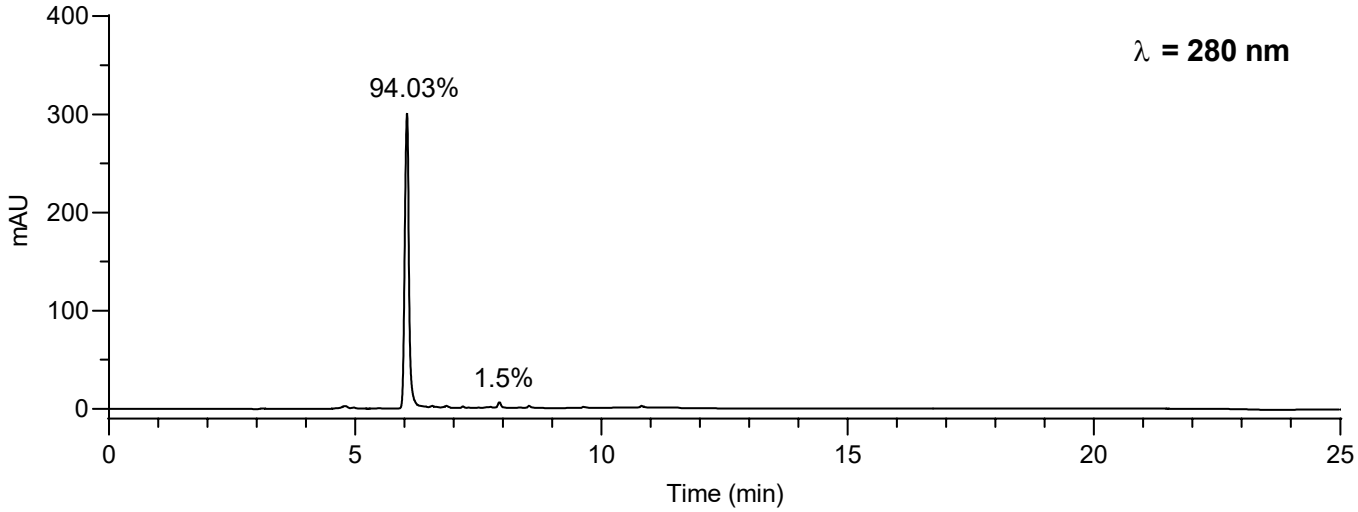


λ = 254 nm

Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	4.8	0.9	0.3565
2	6.053	93.78	37.0146
3	6.563	0.31	0.1232
4	6.857	0.37	0.146
5	7.187	0.12	0.046
6	7.73	0.22	0.0857
7	7.93	3.82	1.5081
8	8.533	0.27	0.1072
9	10.823	0.21	0.0815
Total		*100.00*	*39.4688*

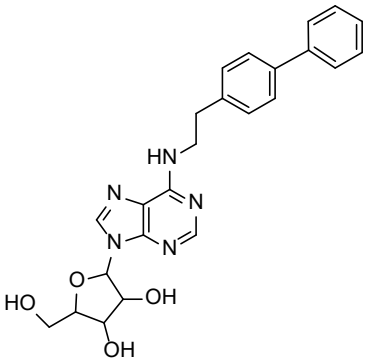


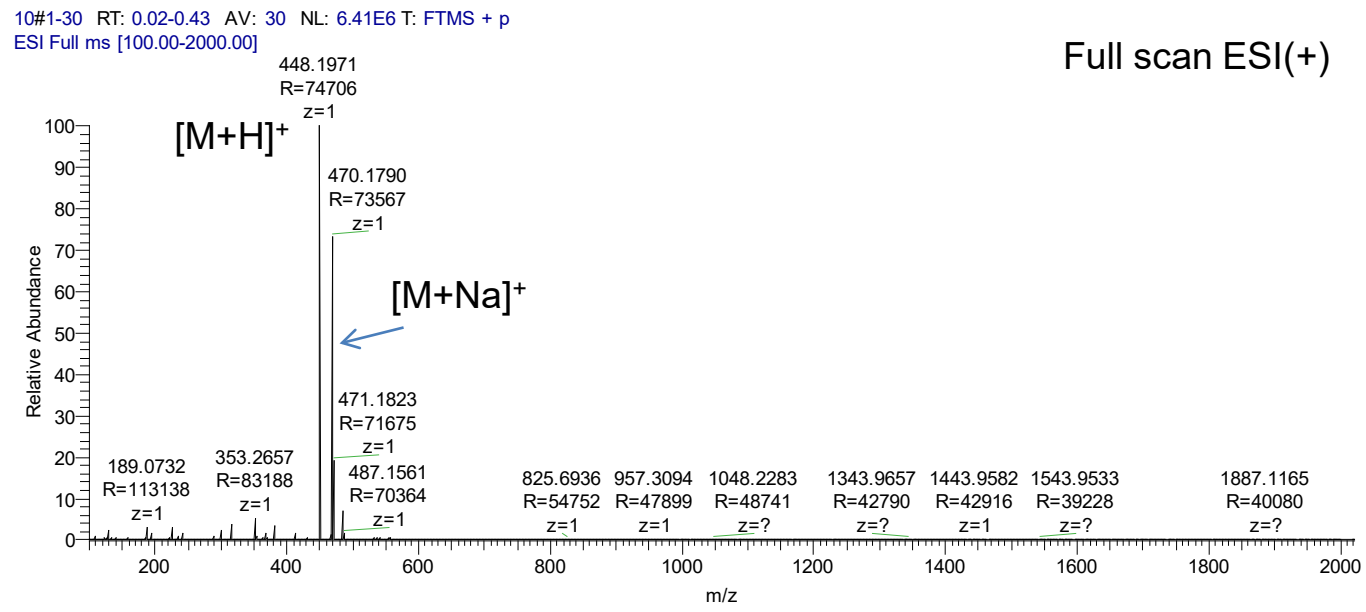
λ = 269 nm

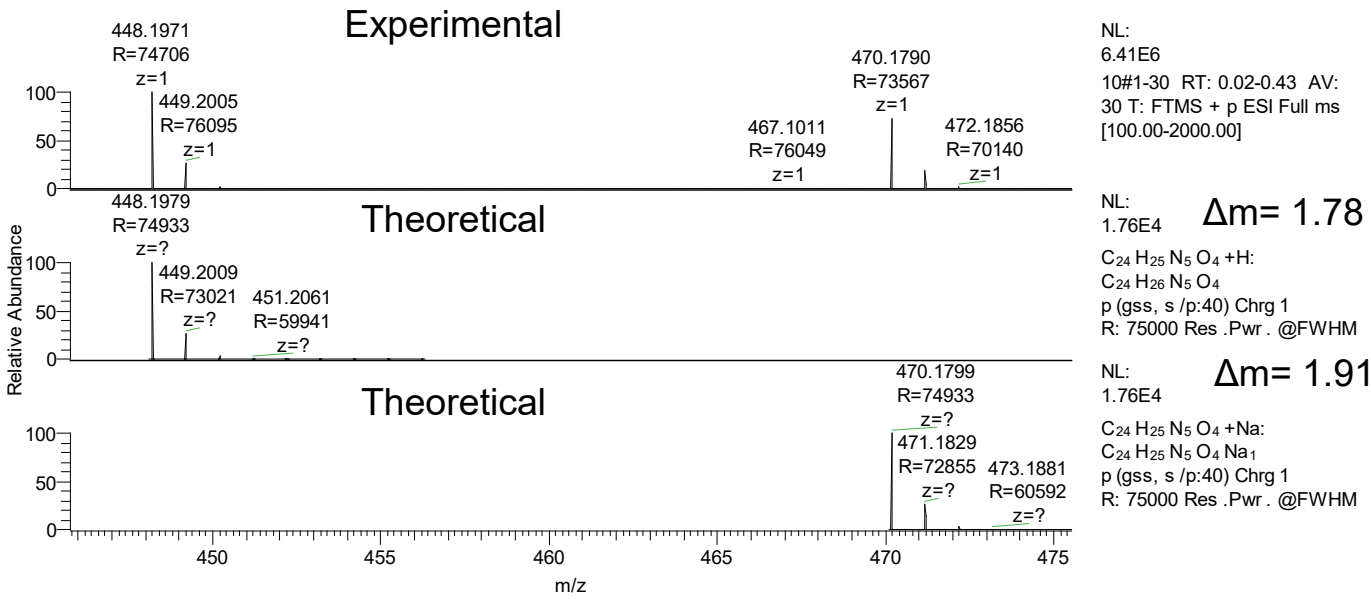


λ = 280 nm

10







NL:
6.41E6
10#1-30 RT: 0.02-0.43 AV: 30 T: FTMS + p ESI Full ms [100.00-2000.00]

NL:
1.76E4

Δm= 1.78 ppm

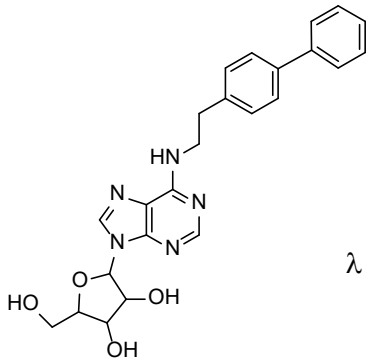
$C_{24}H_{25}N_5O_4$ +H:
$C_{24}H_{26}N_5O_4$
p (gss, s /p:40) Chrg 1
R: 75000 Res .Pwr . @FWHM

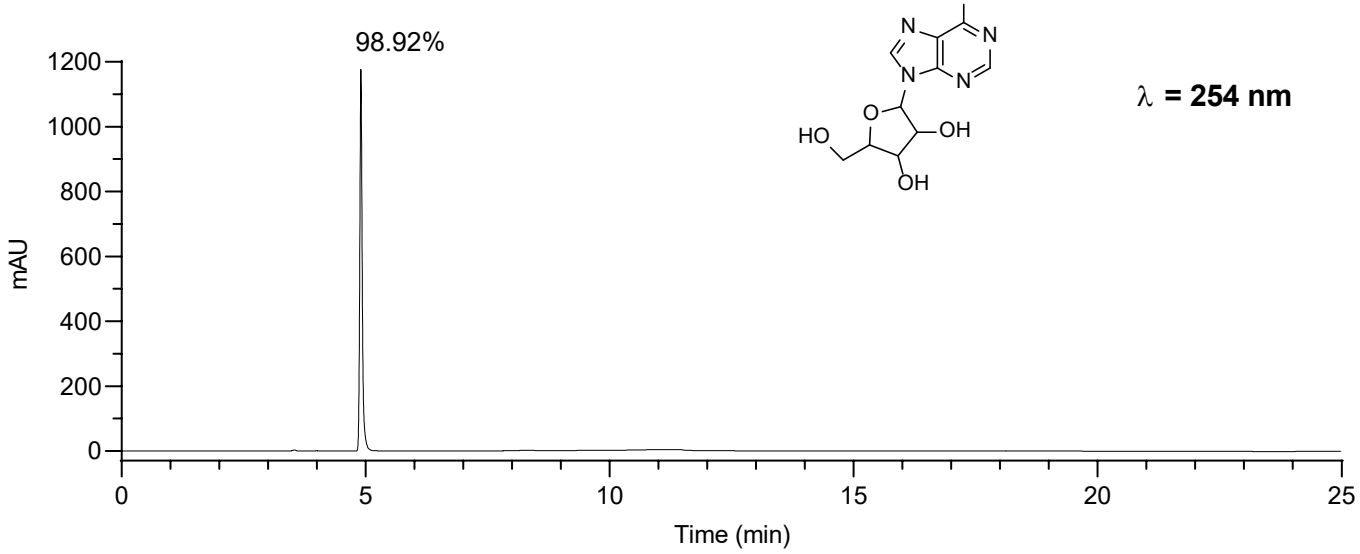
NL:
1.76E4

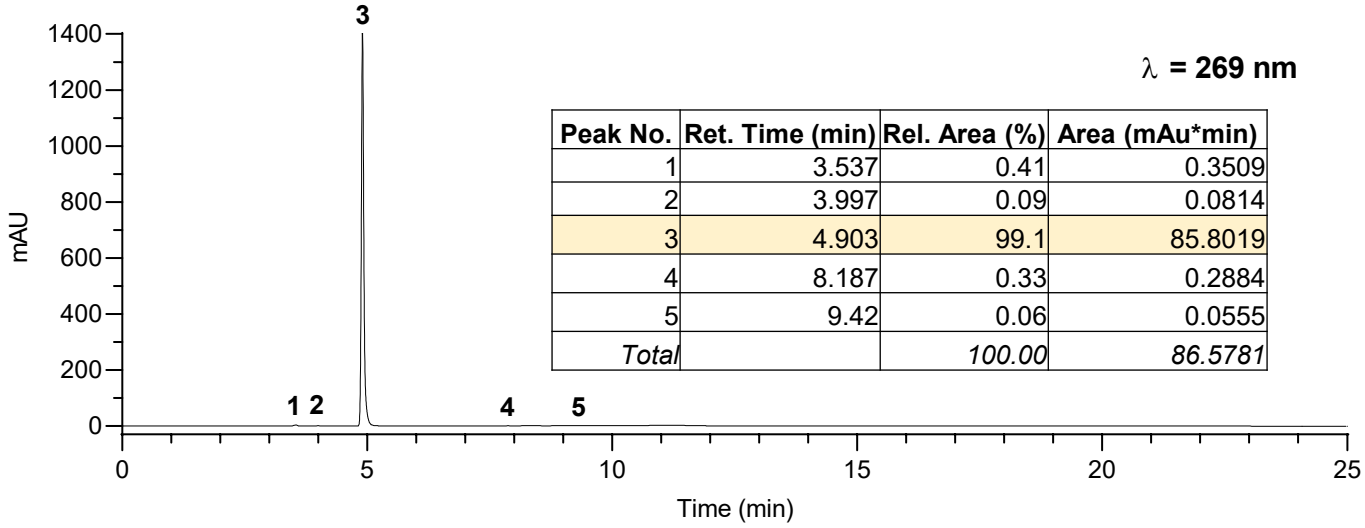
Δm= 1.91ppm

$C_{24}H_{25}N_5O_4$ +Na:
$C_{24}H_{25}N_5O_4Na_1$
p (gss, s /p:40) Chrg 1
R: 75000 Res .Pwr . @FWHM

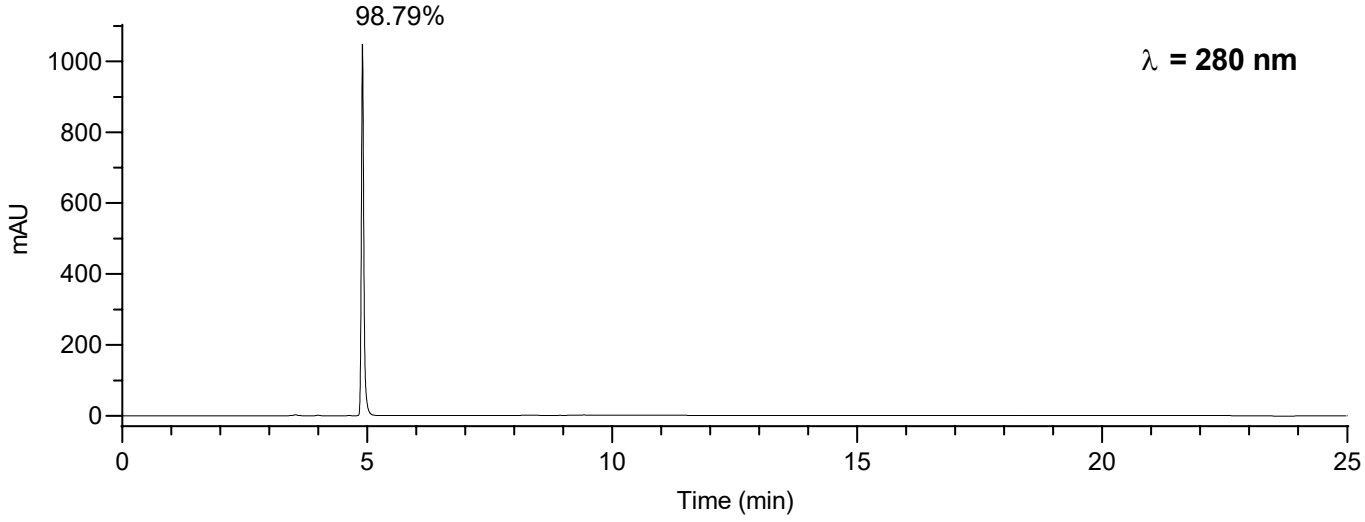
10



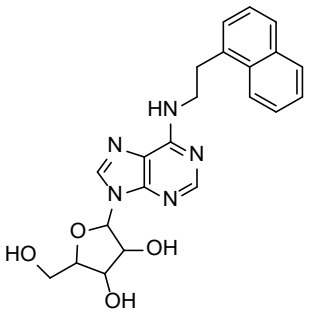


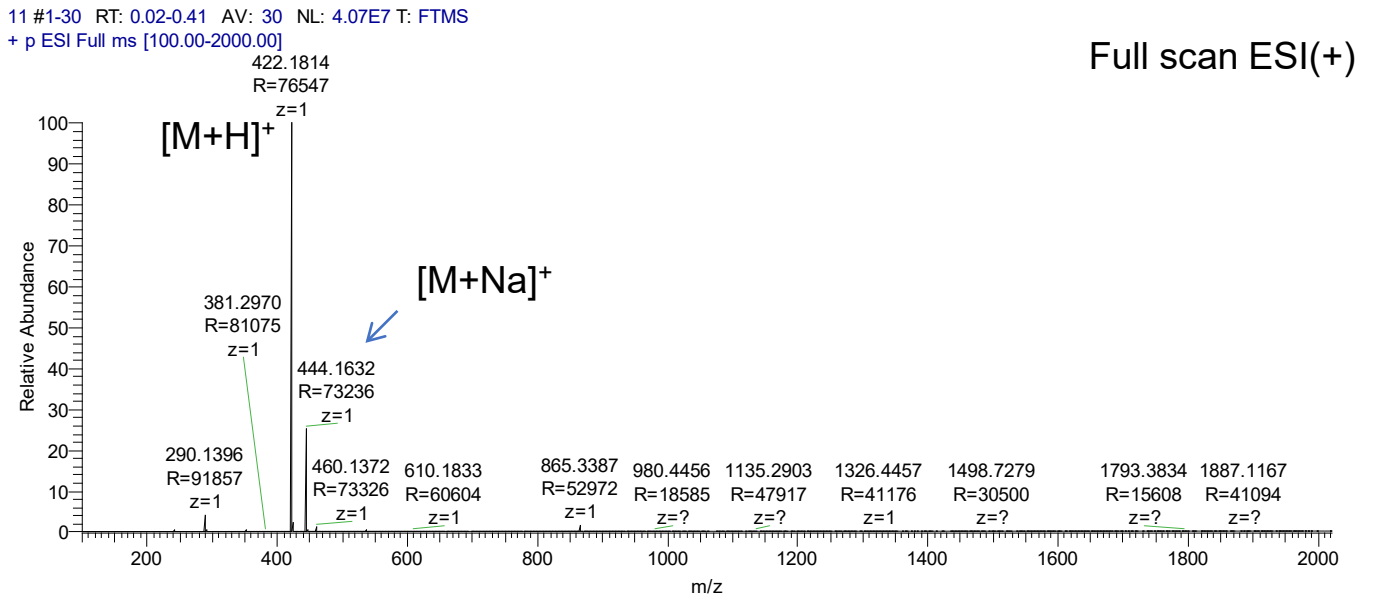


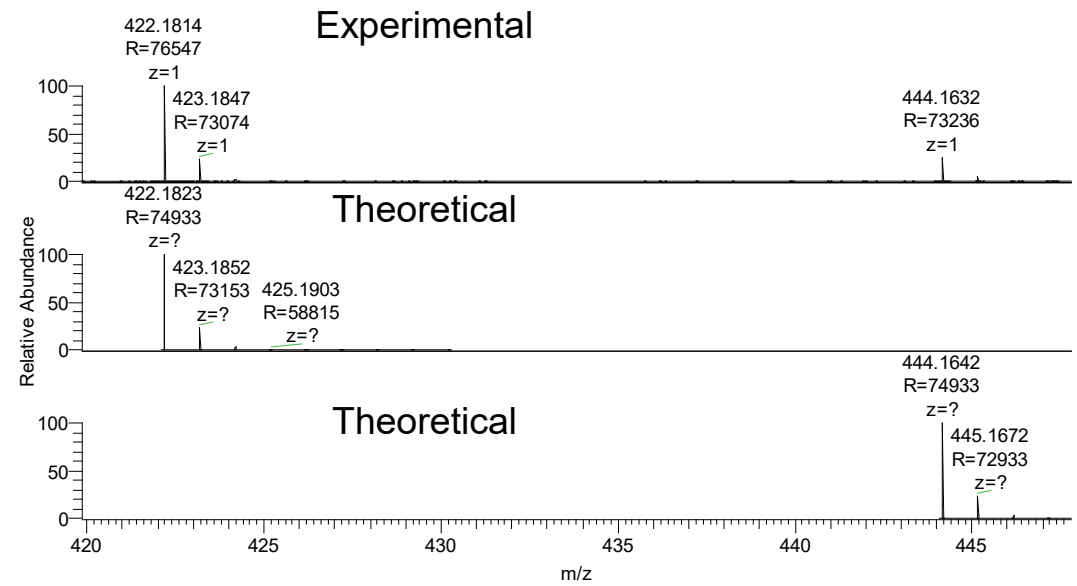
Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	3.537	0.41	0.3509
2	3.997	0.09	0.0814
3	4.903	99.1	85.8019
4	8.187	0.33	0.2884
5	9.42	0.06	0.0555
Total		*100.00*	*86.5781*



11







NL:
4.07E7
11#1-30 RT: 0.02-0.41 AV: 30 T: FTMS + p ESI Full ms [100.00-2000.00]

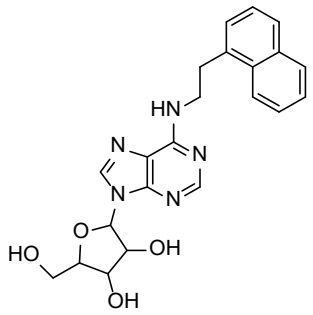
NL:
1.80E4
$C_{22}H_{23}N_5O_4$ +H:
$C_{22}H_{24}N_5O_4$
p (gss, s /p:40) Chrg 1
R: 75000 Res .Pwr . @FWHM

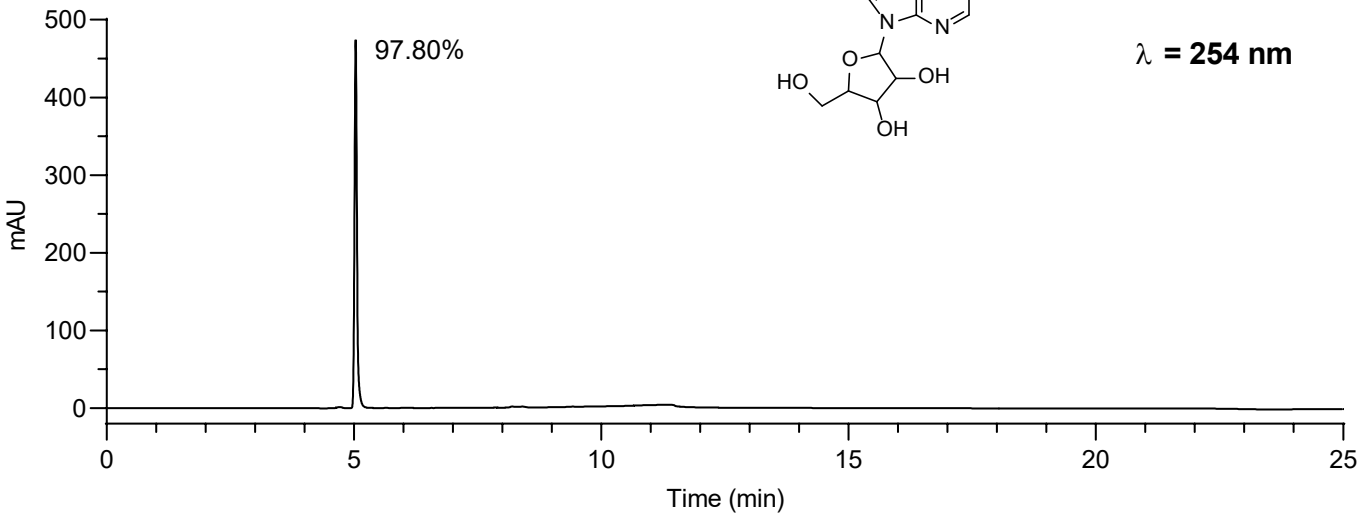
Δm= 2.13ppm

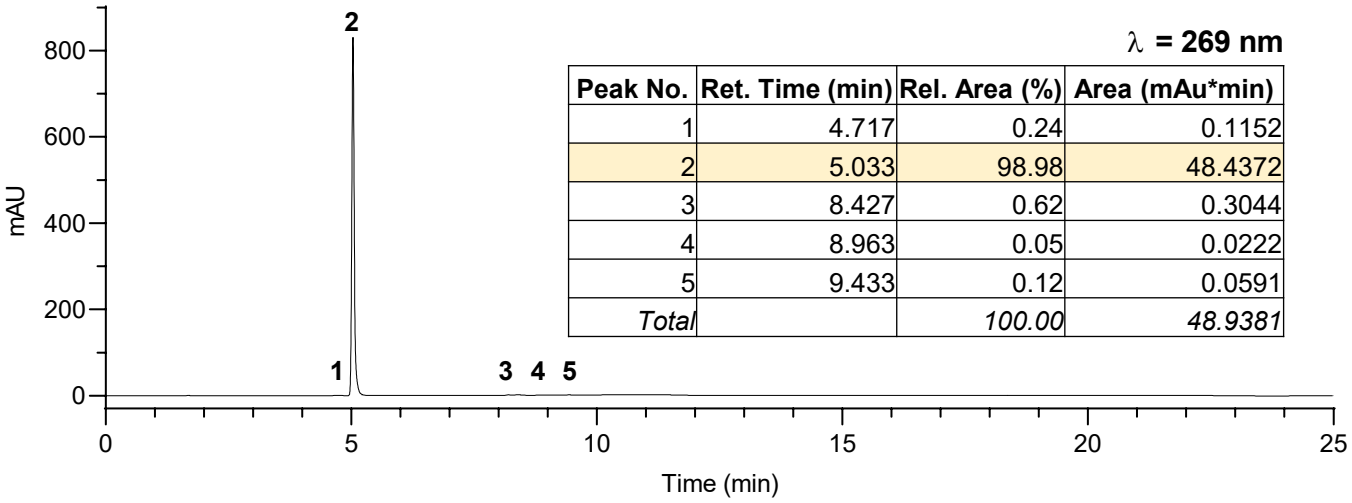
NL:
1.80E4
$C_{22}H_{23}N_5O_4$ +Na:
$C_{22}H_{23}N_5O_4Na_1$
p (gss, s /p:40) Chrg 1
R: 75000 Res .Pwr . @FWHM

Δm= 2.25ppm

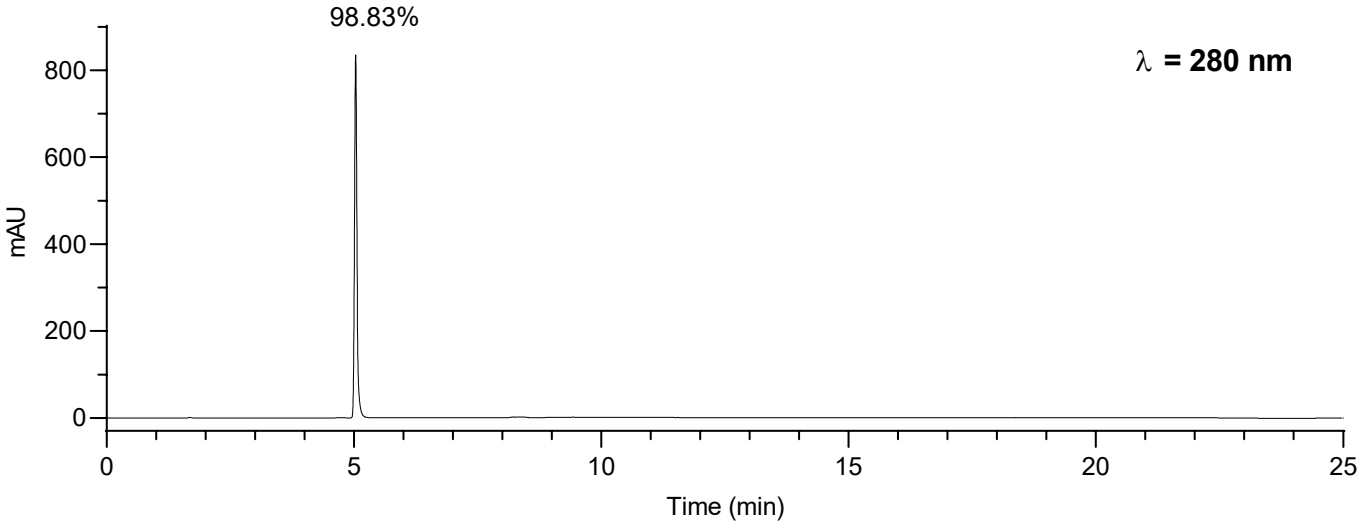
11



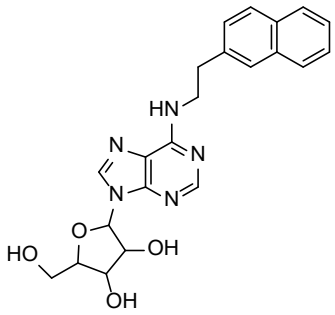




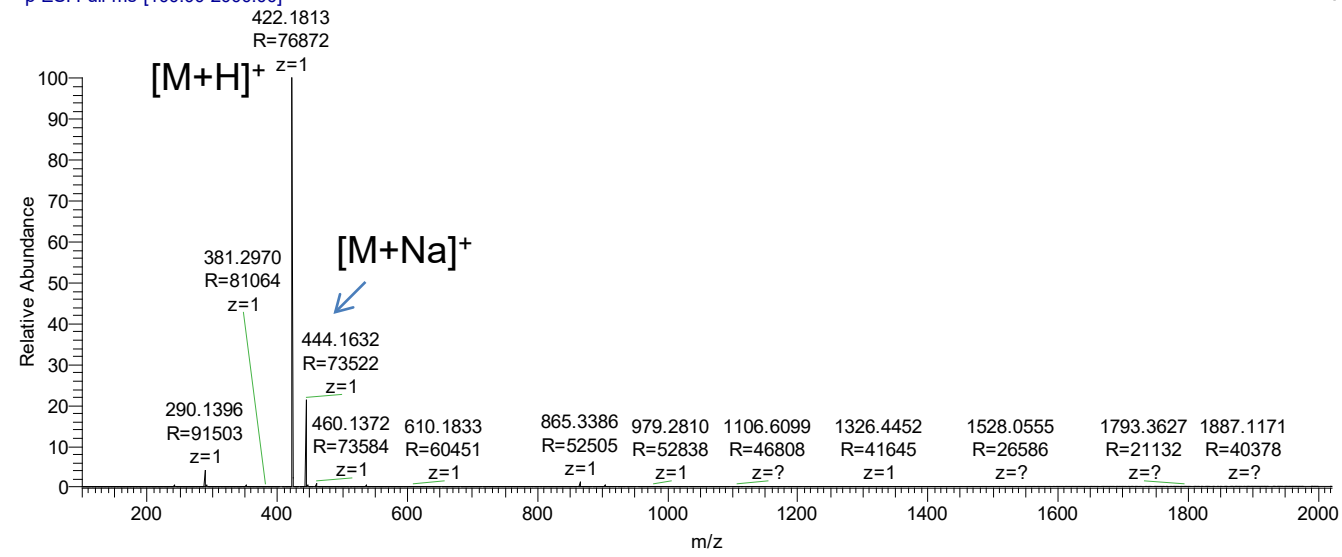
Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	4.717	0.24	0.1152
2	5.033	98.98	48.4372
3	8.427	0.62	0.3044
4	8.963	0.05	0.0222
5	9.433	0.12	0.0591
Total		*100.00*	*48.9381*

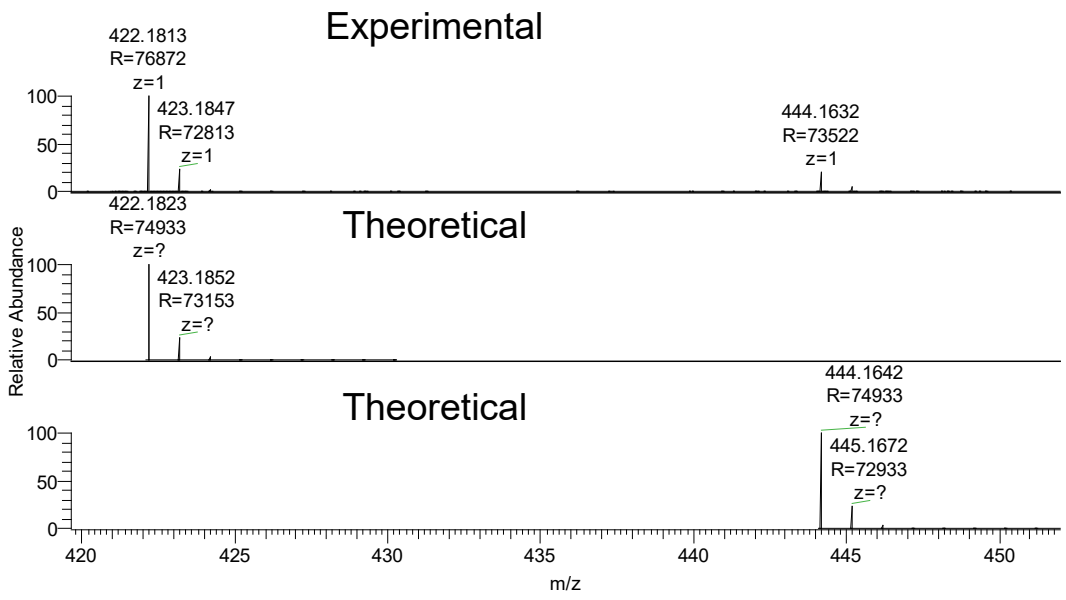


12



Full scan ESI(+)





NL:
4.08E7
12#1-30 RT: 0.02-0.41 AV: 30 T: FTMS + p ESI Full ms [100.00-2000.00]

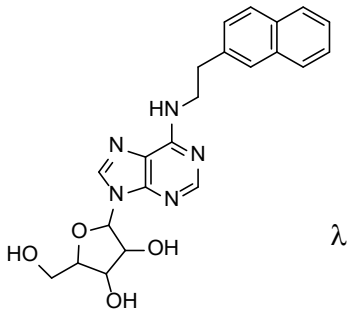
NL:
1.80E4
$C_{22}H_{23}N_5O_4$ +H:
$C_{22}H_{24}N_5O_4$
p (gss, s /p:40) Chrg 1
R: 75000 Res .Pwr . @FWHM

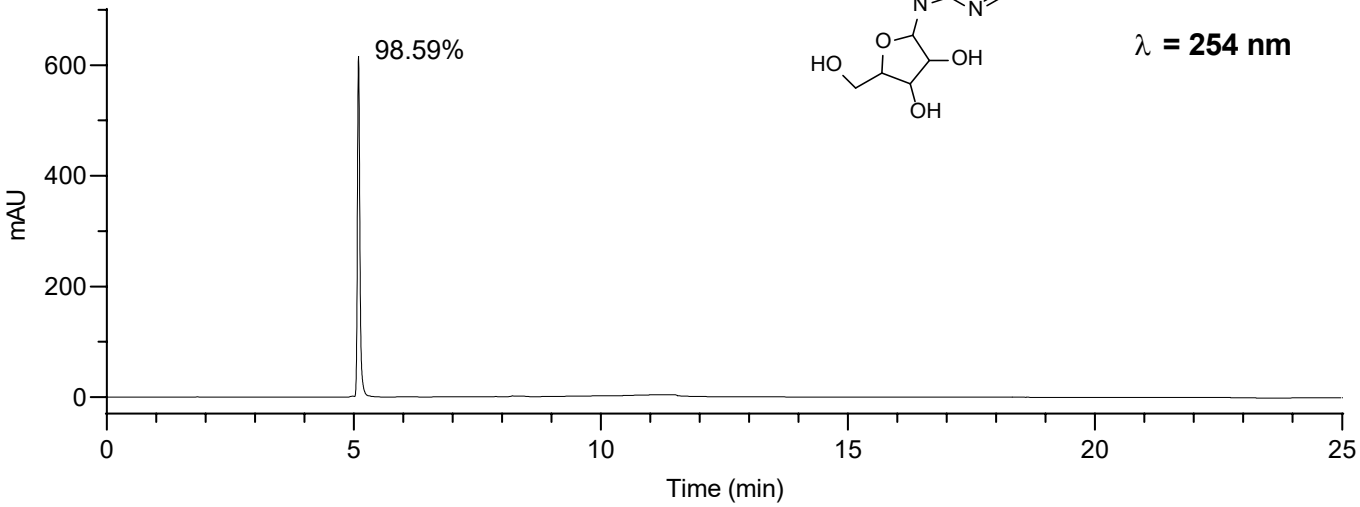
Δm= 2.36ppm

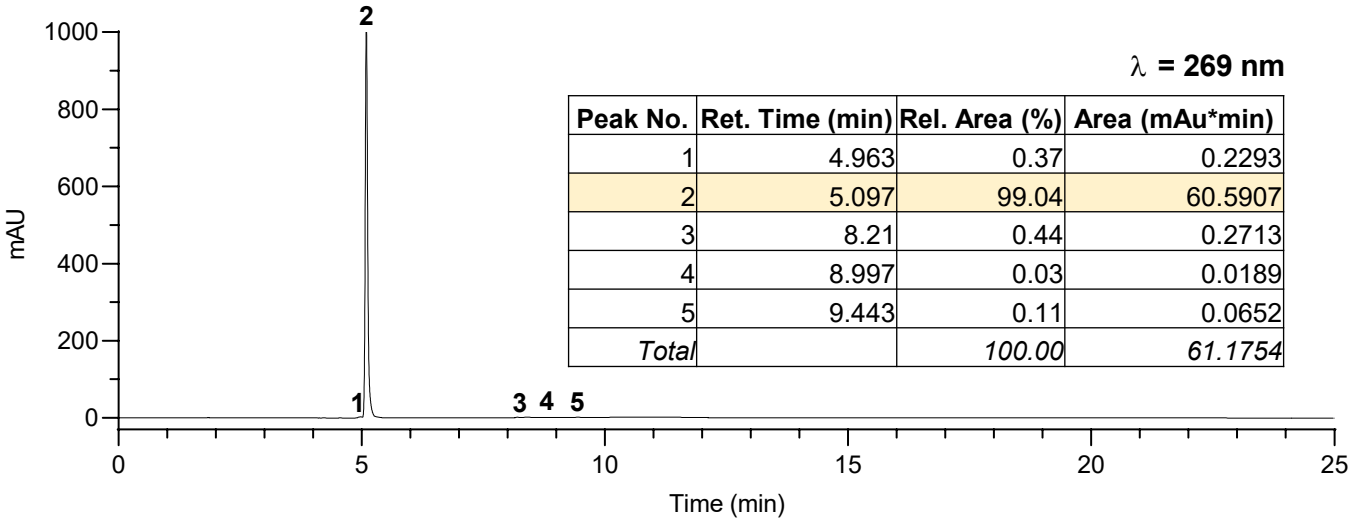
NL:
1.80E4
$C_{22}H_{23}N_5O_4$ +Na:
$C_{22}H_{23}N_5O_4Na_1$
p (gss, s /p:40) Chrg 1
R: 75000 Res .Pwr . @FWHM

Δm= 2.25ppm

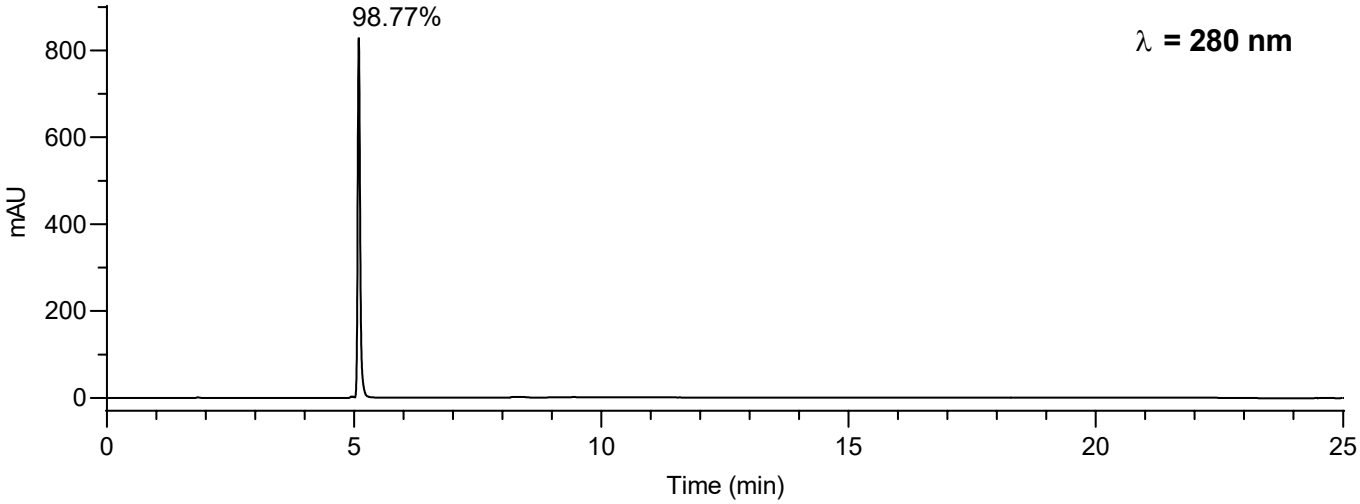
12



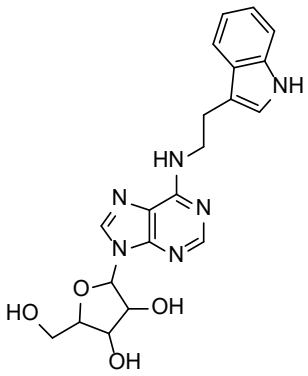




Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	4.963	0.37	0.2293
2	5.097	99.04	60.5907
3	8.21	0.44	0.2713
4	8.997	0.03	0.0189
5	9.443	0.11	0.0652
Total		*100.00*	*61.1754*

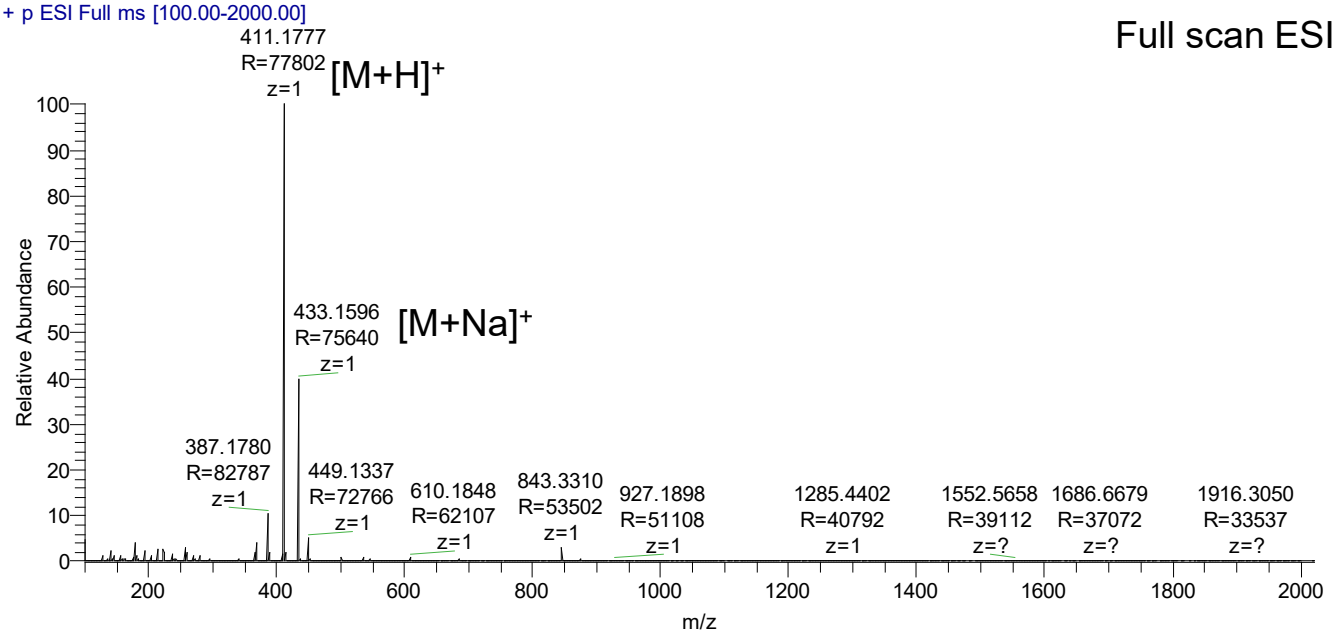


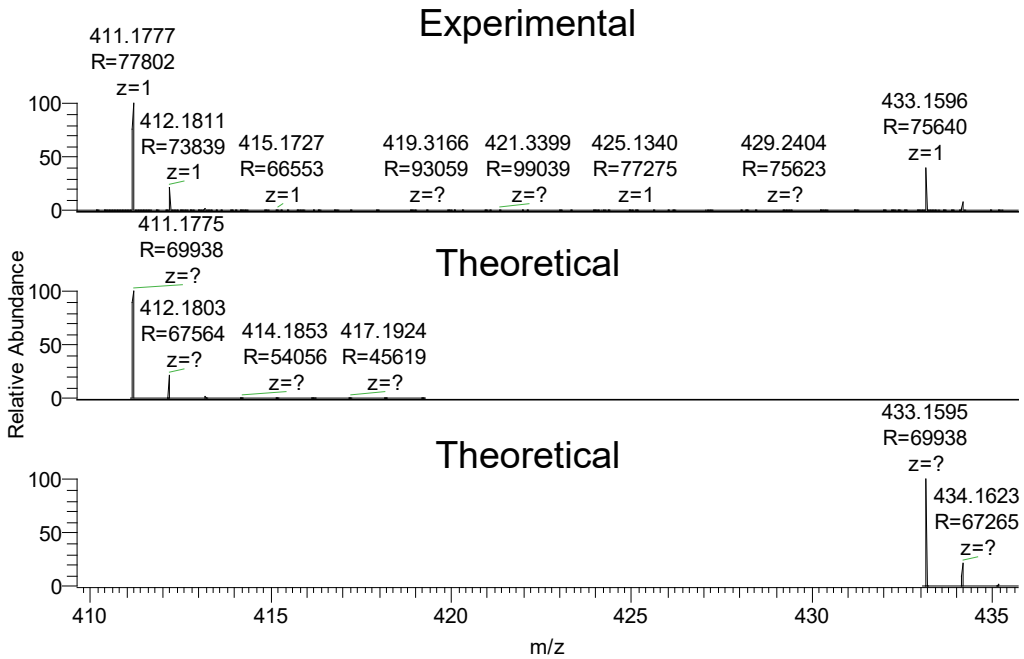
13



13 #2-30 RT: 0.03-0.42 AV: 29 NL: 1.11E7 T: FTMS
+ p ESI Full ms [100.00-2000.00]

Full scan ESI(+)



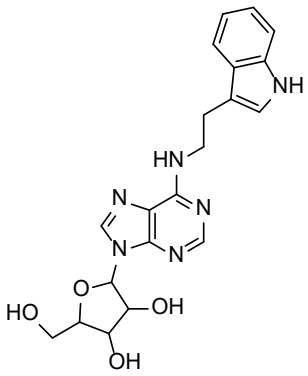


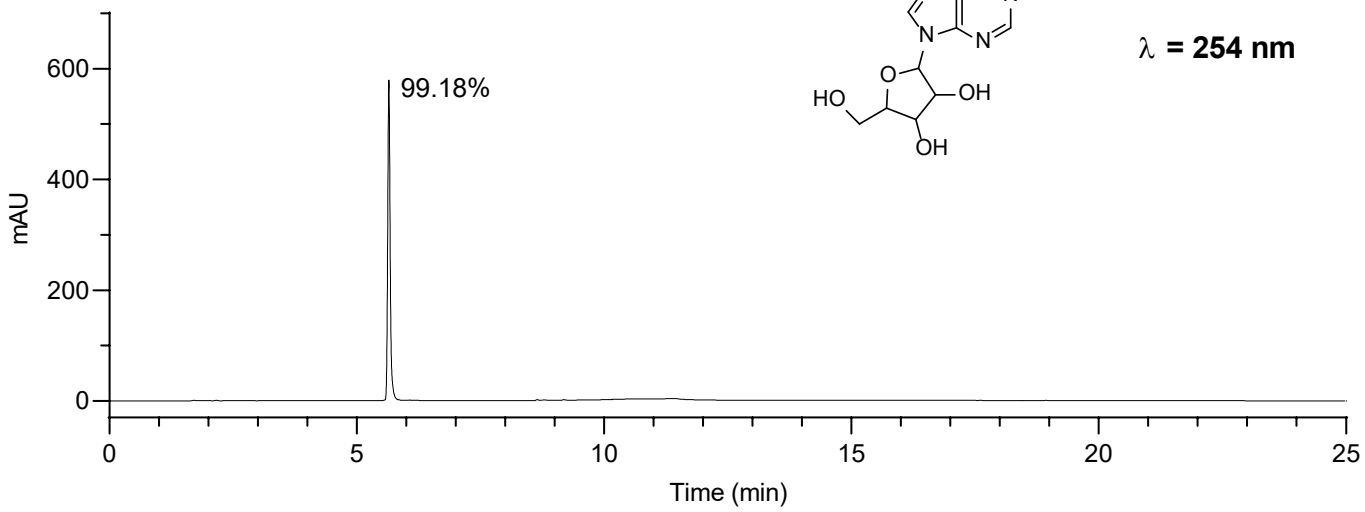
NL:
1.11E7
13#2-30 RT: 0.03-0.42 AV: 29 T: FTMS + p ESI Full ms [100.00-2000.00]

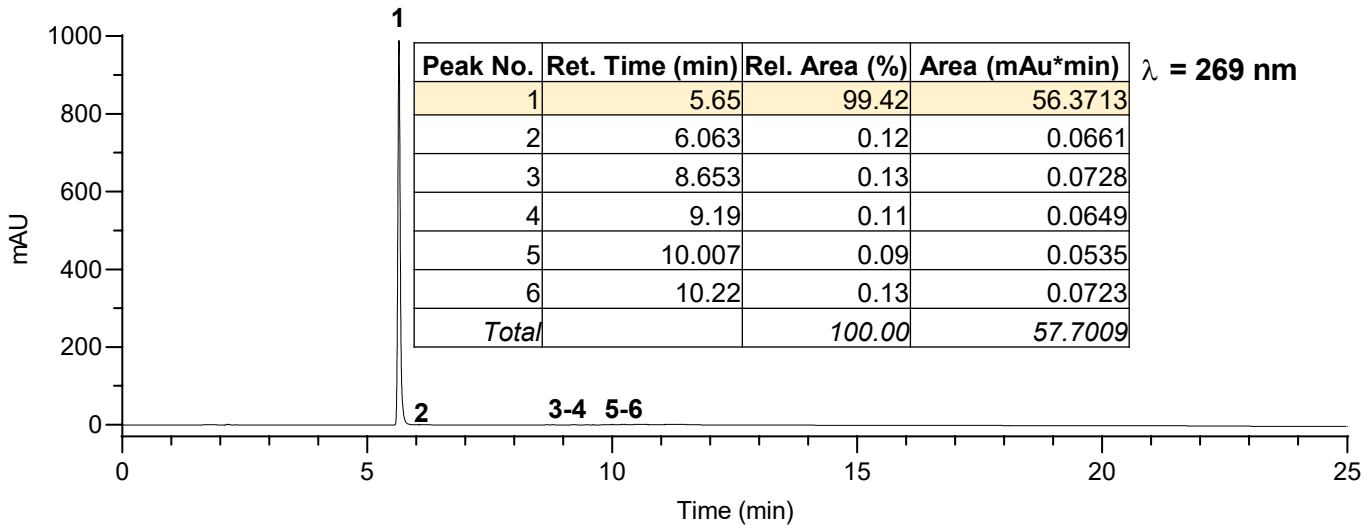
NL: Δm= 0.49ppm
1.83E4
$C_{20}H_{22}N_6O_4$ +H:
$C_{20}H_{23}N_6O_4$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM

NL: Δm= 0.23ppm
1.83E4
$C_{20}H_{22}N_6O_4$ +Na:
$C_{20}H_{22}N_6O_4Na_1$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM

13

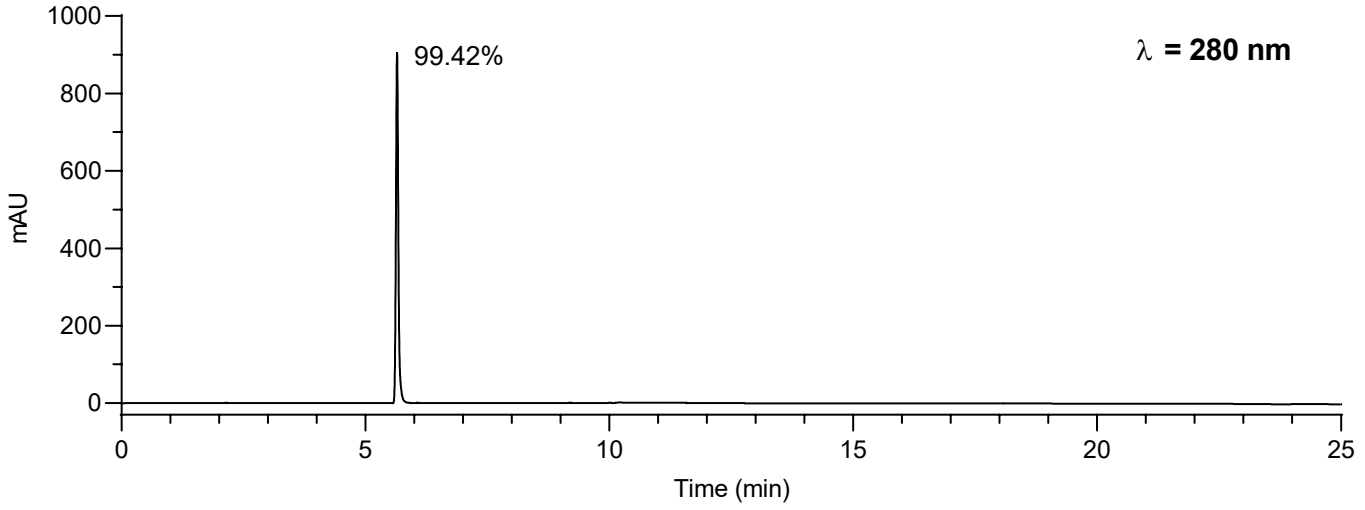




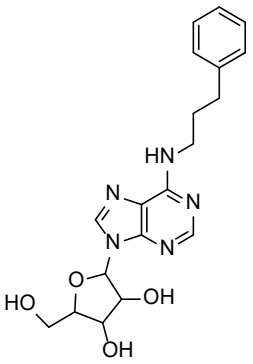


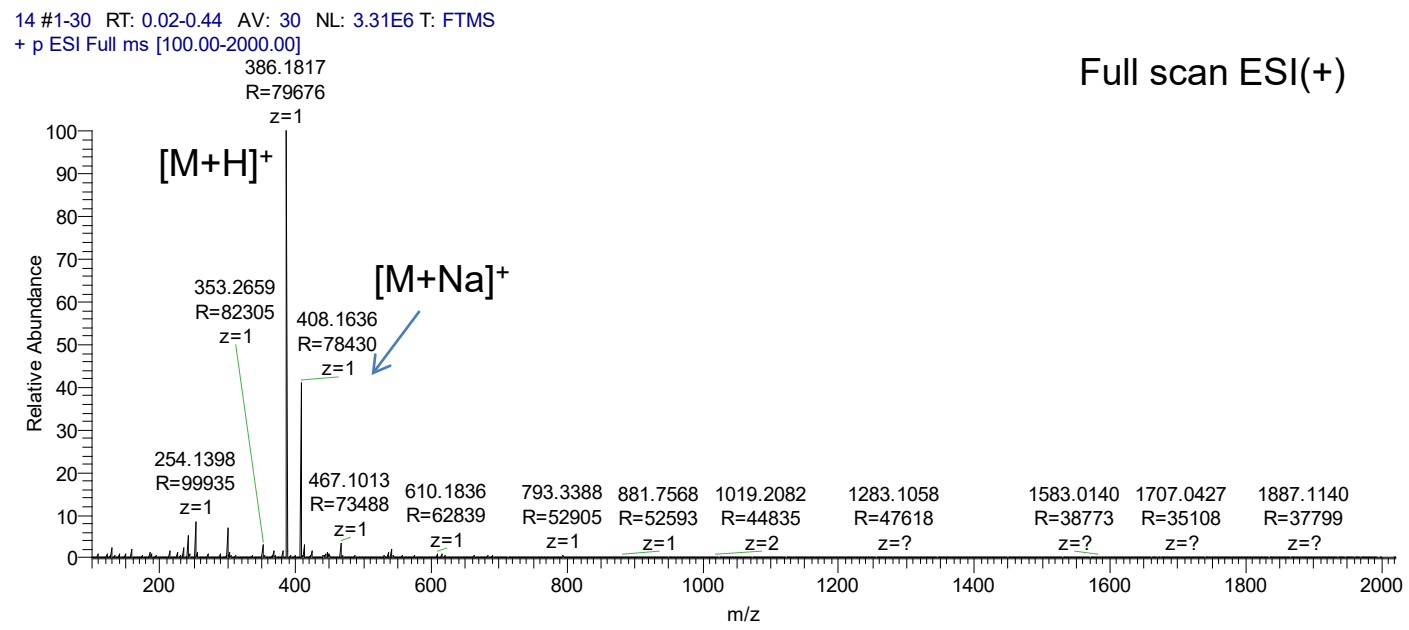
Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	5.65	99.42	56.3713
2	6.063	0.12	0.0661
3	8.653	0.13	0.0728
4	9.19	0.11	0.0649
5	10.007	0.09	0.0535
6	10.22	0.13	0.0723
Total		*100.00*	*57.7009*

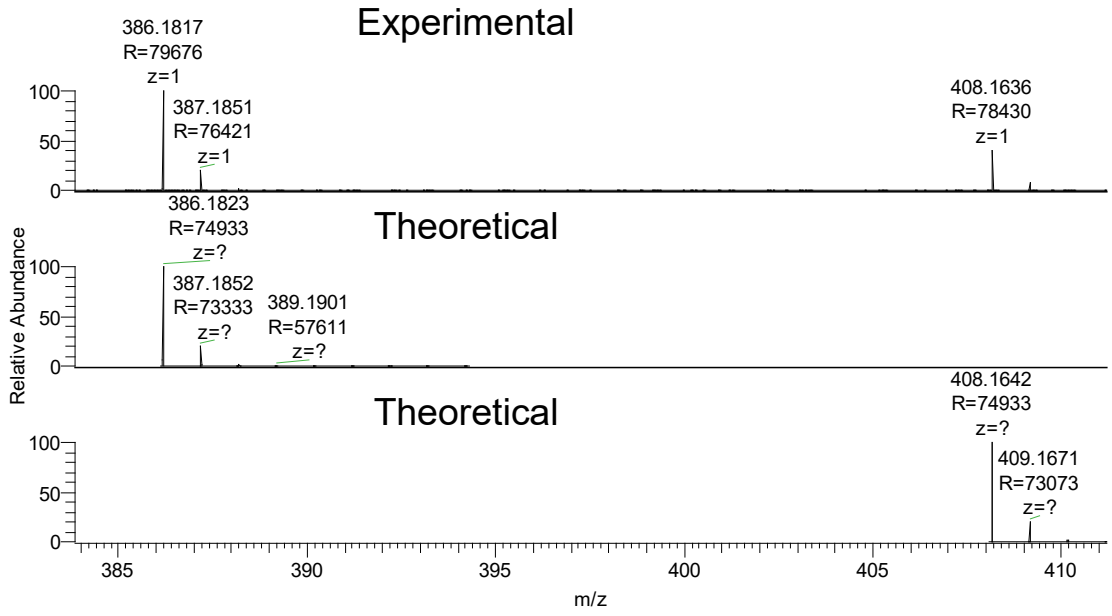
λ = 269 nm



14







NL:
3.31E6
14#1-30 RT: 0.02-0.44 AV: 30 T: FTMS + p ESI Full ms [100.00-2000.00]

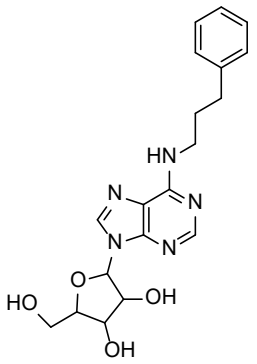
NL:
1.85E4
Δm= 1.55ppm

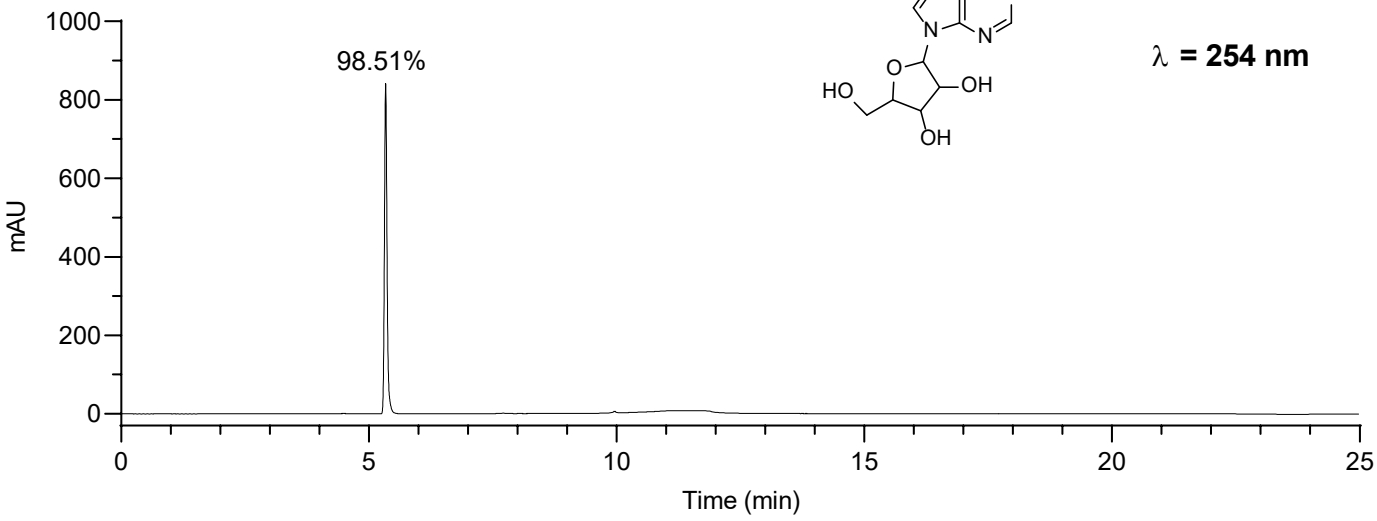
$C_{19}H_{23}N_5O_4$ +H:
$C_{19}H_{24}N_5O_4$
p (gss, s /p:40) Chrg 1
R: 75000 Res .Pwr . @FWHM

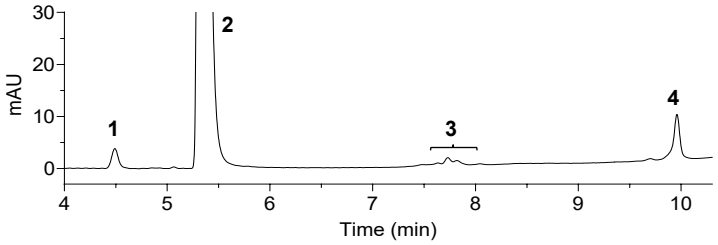
NL:
1.85E4
Δm= 1.47ppm

$C_{19}H_{23}N_5O_4$ +Na:
$C_{19}H_{23}N_5O_4Na_1$
p (gss, s /p:40) Chrg 1
R: 75000 Res .Pwr . @FWHM

14

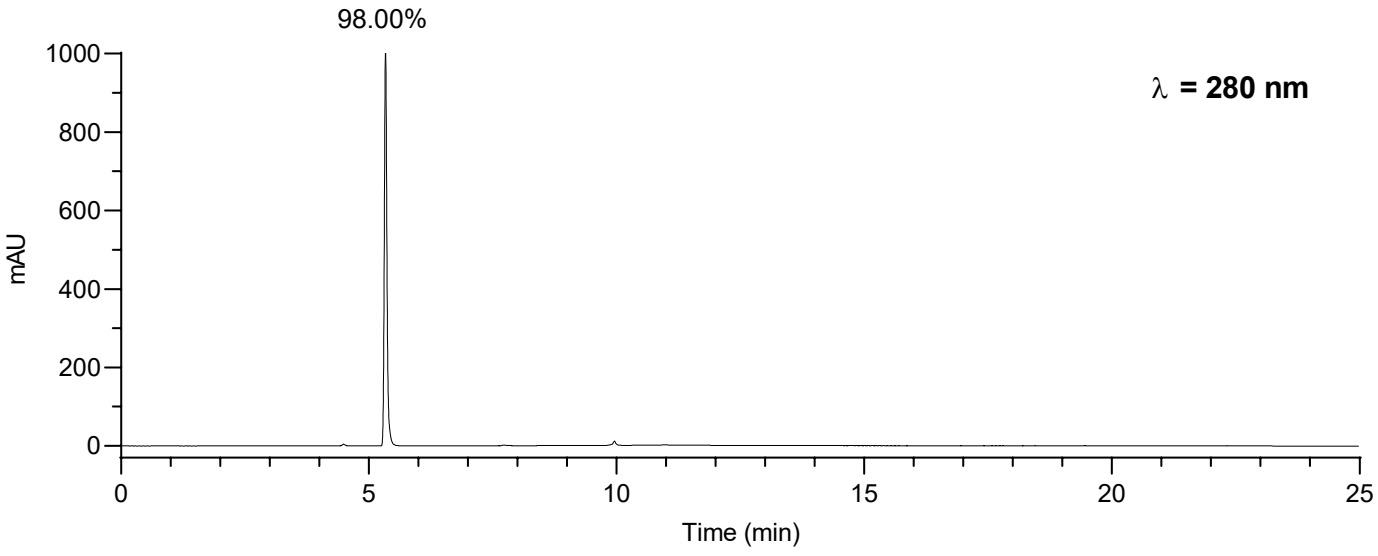




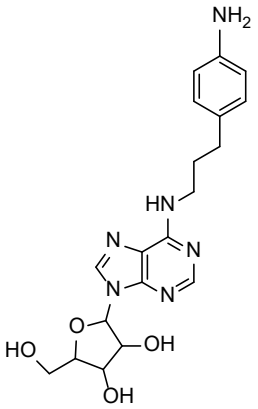


λ = 269 nm

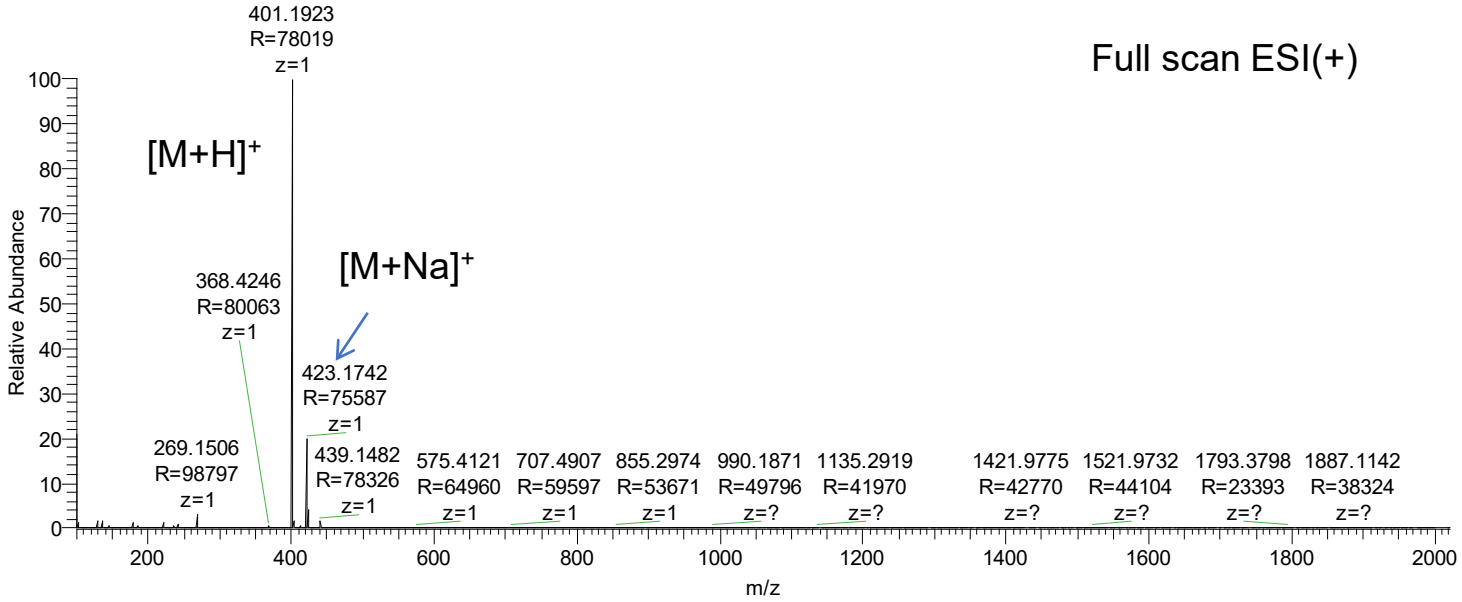
Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	4.49	0.33	0.274
2	5.337	98.56	81.5944
3	7.73	0.4	0.3321
4	9.96	0.71	0.5908
Total		*100.00*	*82.7913*

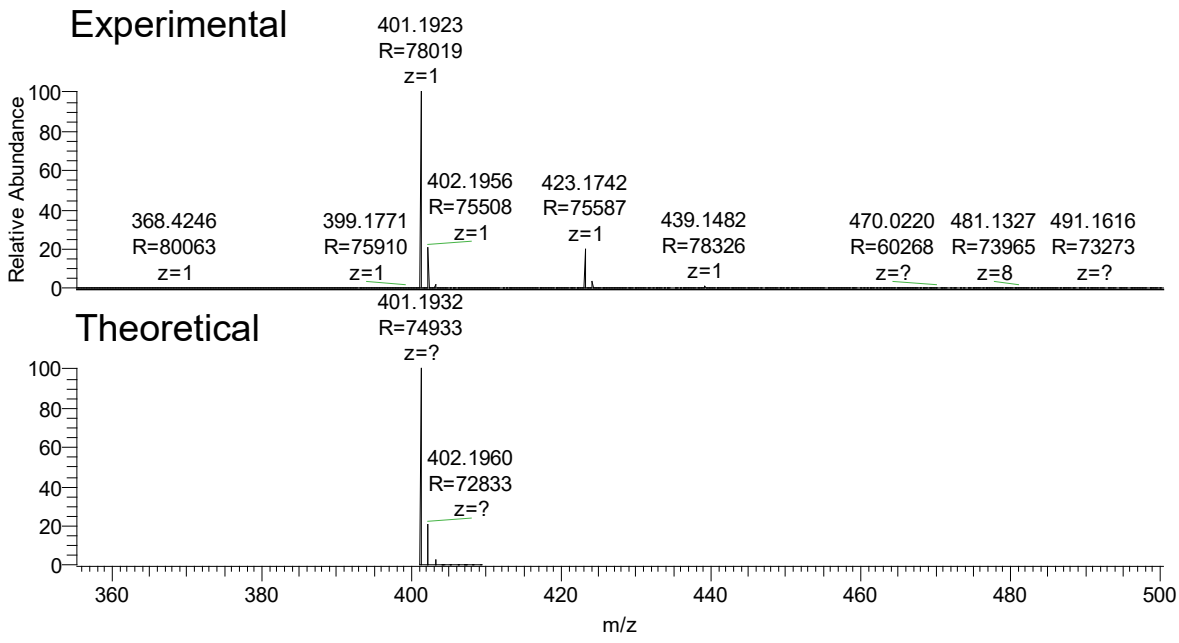


15



15 #1-30 RT: 0.02-0.42 AV: 30 NL: 1.59E7 T: FTMS
+ p ESI Full ms [100.00-2000.00]



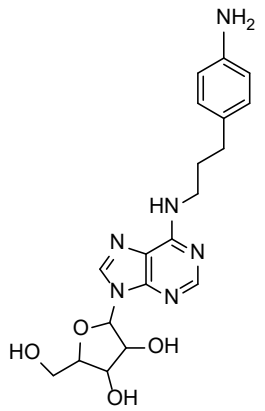


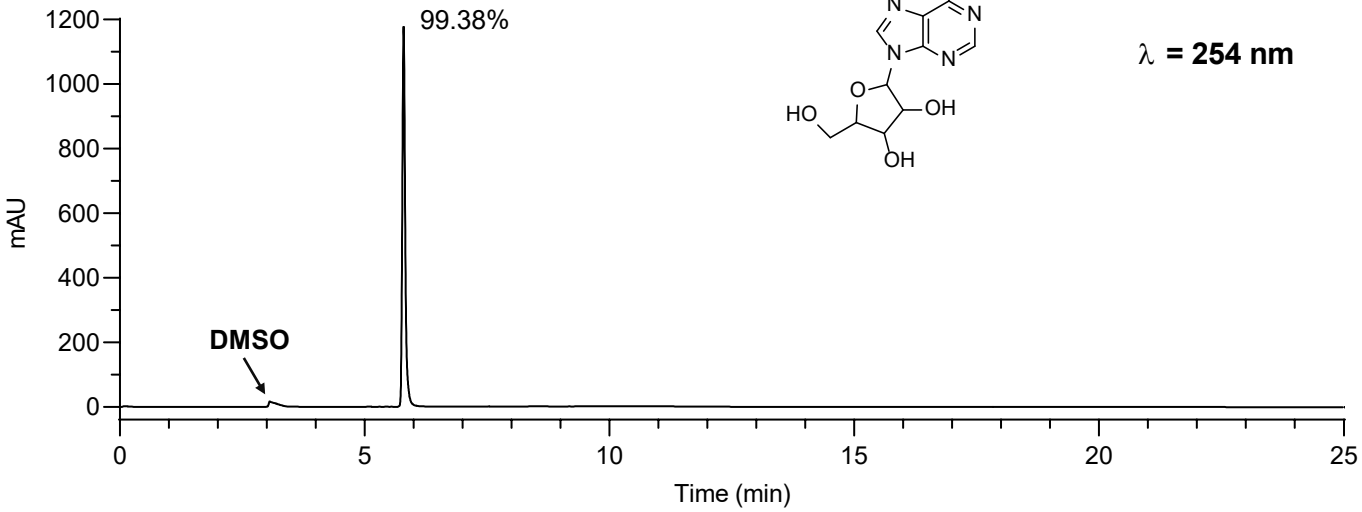
NL:
1.59E7
15#1-30 RT:
0.02-0.42 AV: 30 T: FTMS +
p ESI Full ms
[100.00-2000.00]

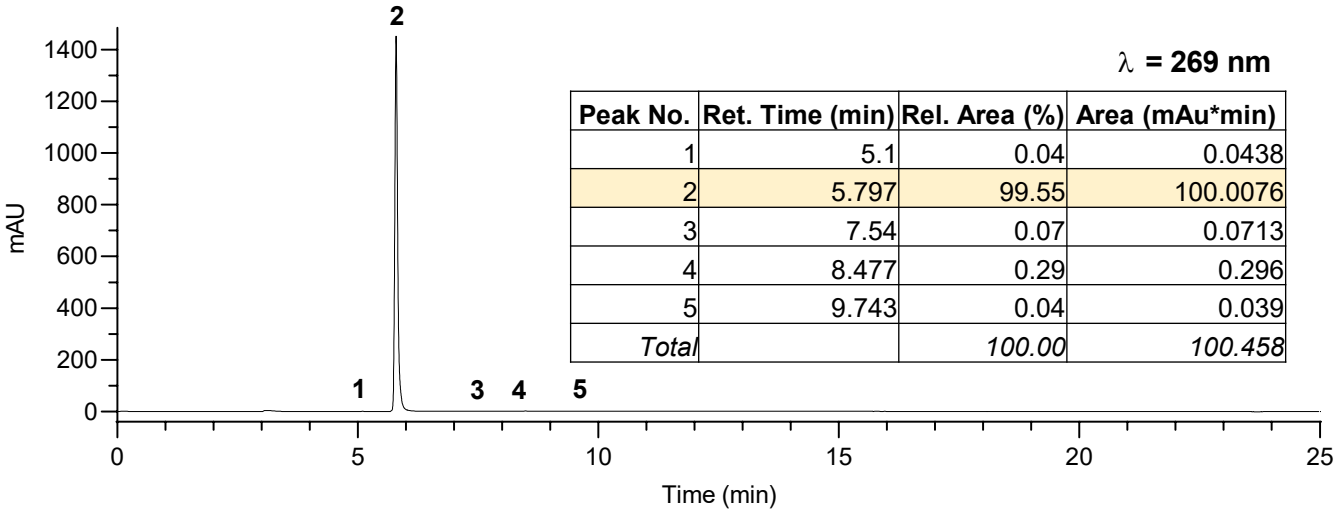
NL:
1.85E4
$C_{19}H_{24}N_6O_4$ +H:
$C_{19}H_{25}N_6O_4$
p (gss, s /p:40) Chrg 1
R: 75000 Res .Pwr . @FWHM

Δm= 2.24ppm

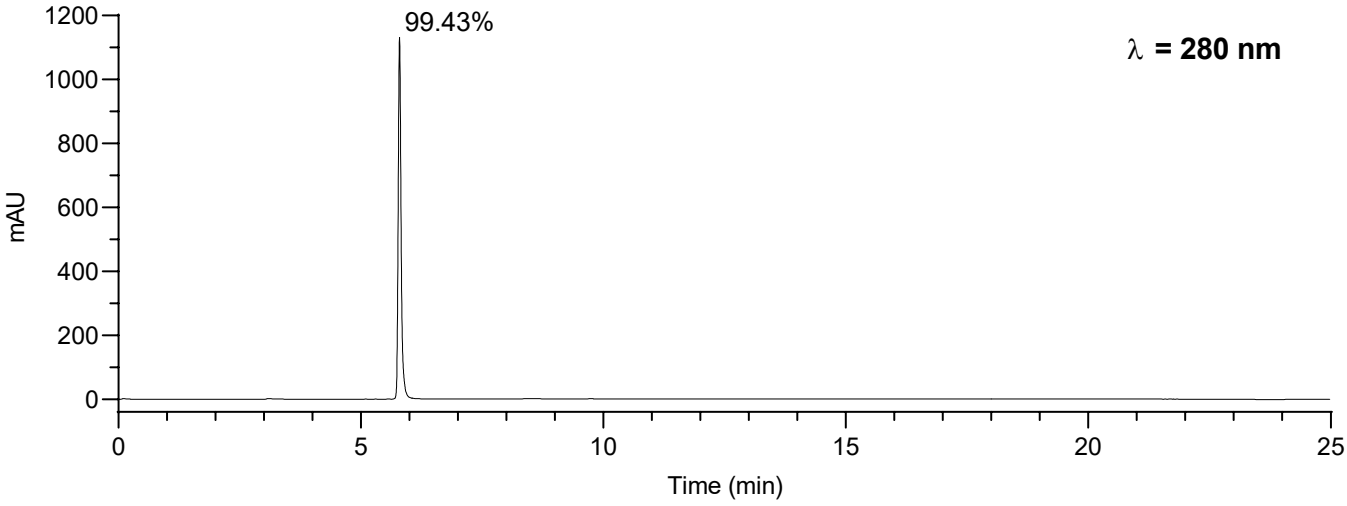
15



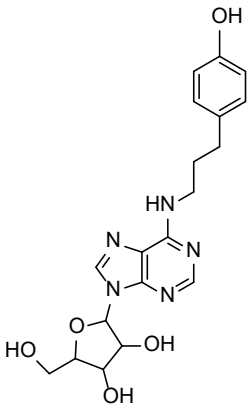




Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	5.1	0.04	0.0438
2	5.797	99.55	100.0076
3	7.54	0.07	0.0713
4	8.477	0.29	0.296
5	9.743	0.04	0.039
Total		*100.00*	*100.458*

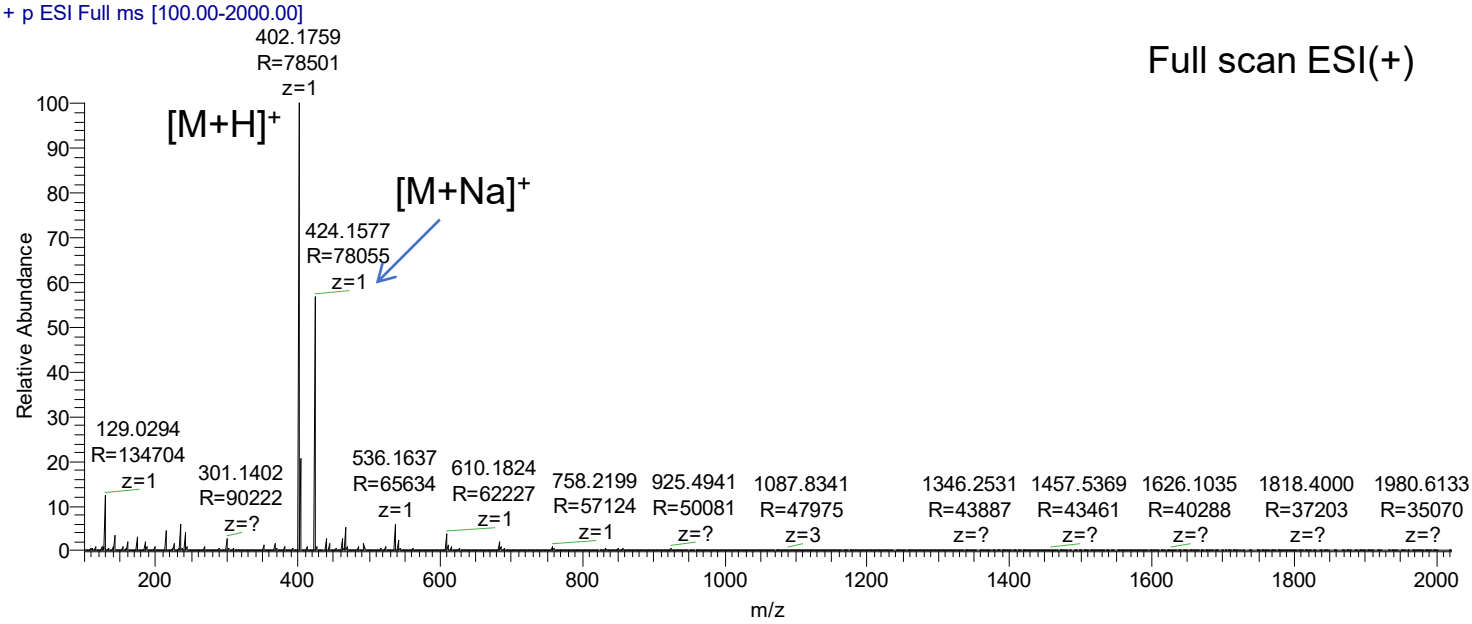


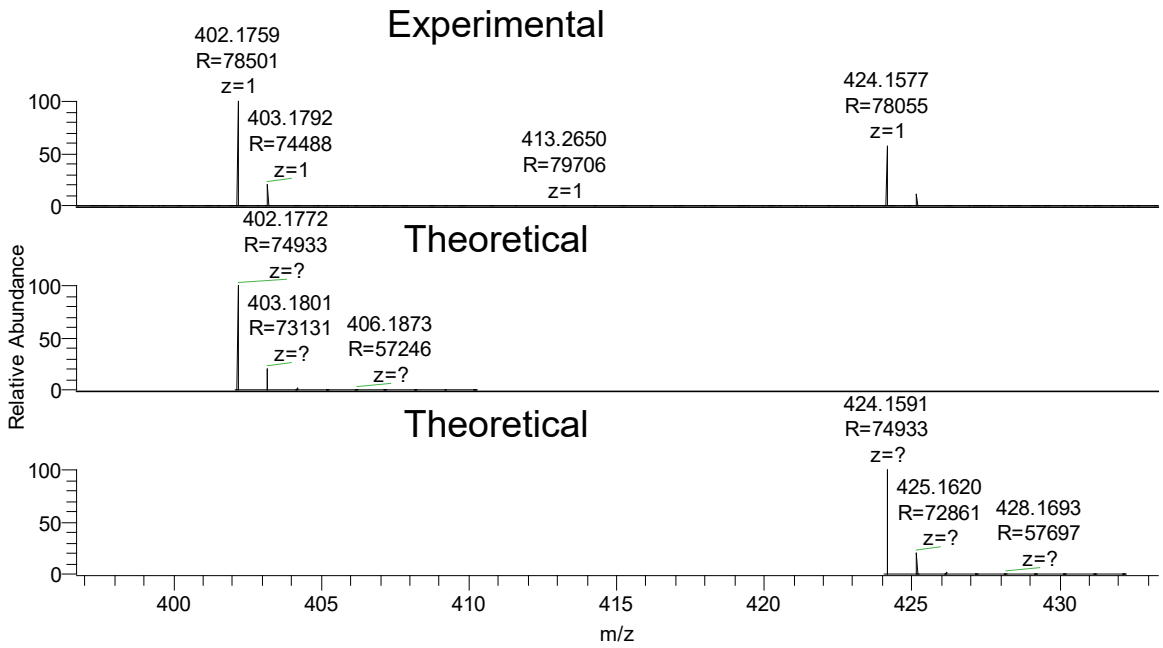
16



16 #1-30 RT: 0.02-0.46 AV: 30 NL: 1.34E6 T: FTMS
+ p ESI Full ms [100.00-2000.00]

Full scan ESI(+)





NL:
1.34E6
16#1-30 RT: 0.02-0.46 AV: 30 T: FTMS + p ESI Full ms [100.00-2000.00]

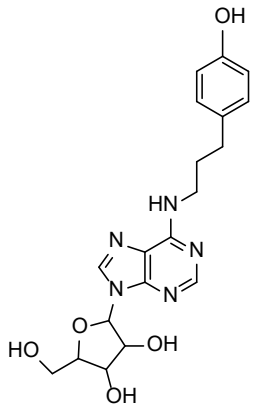
NL:
1.85E4
Δm= 3.24ppm

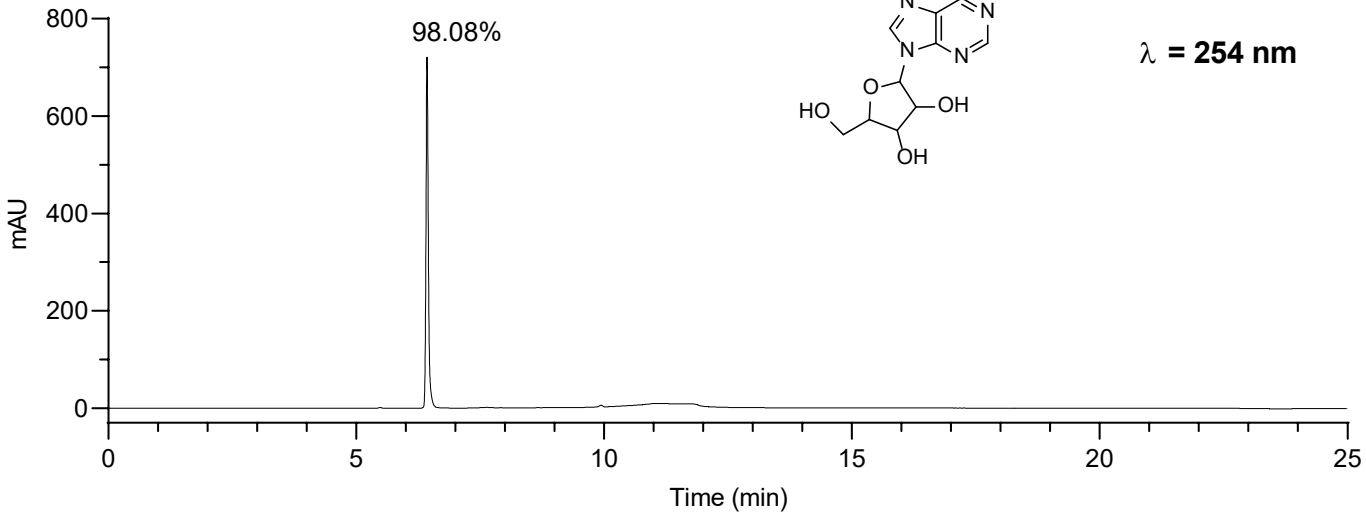
$C_{19}H_{23}N_5O_5$ +H:
$C_{19}H_{24}N_5O_5$
p (gss, s /p:40) Chrg 1
R: 75000 Res .Pwr . @FWHM

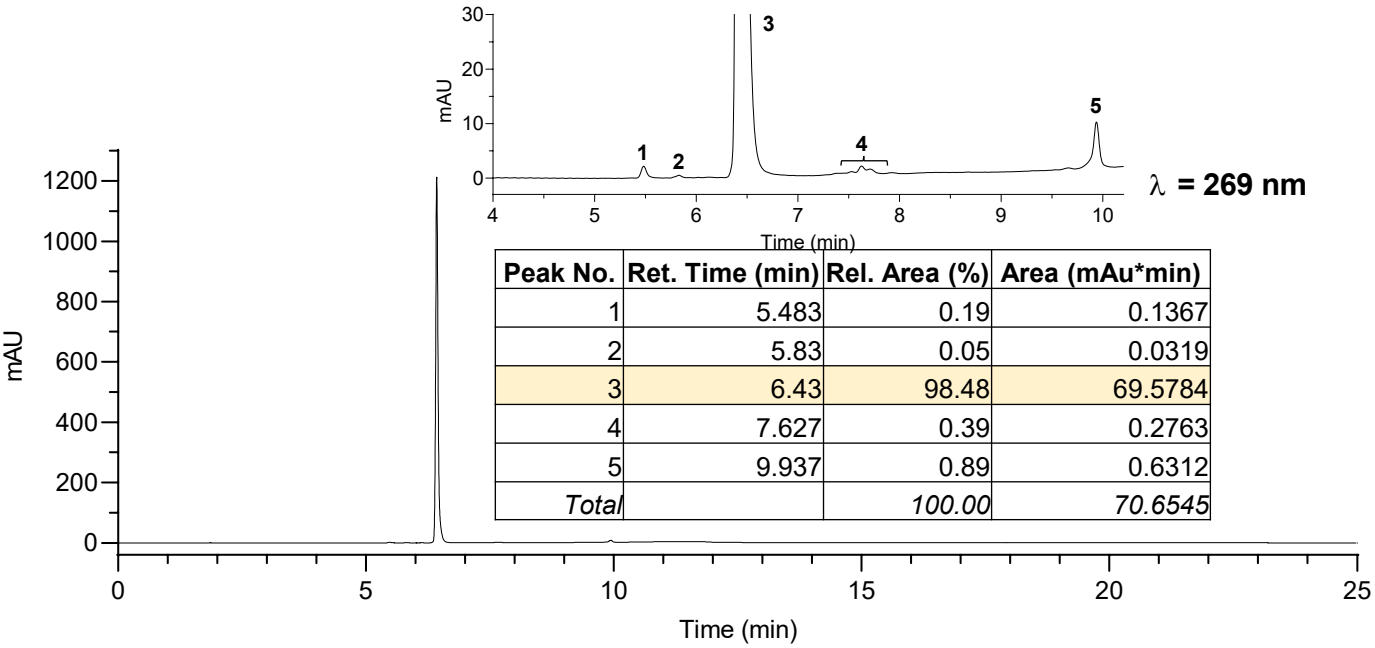
NL:
1.85E4
Δm= 3.30ppm

$C_{19}H_{23}N_5O_5$ +Na:
$C_{19}H_{23}N_5O_5Na_1$
p (gss, s /p:40) Chrg 1
R: 75000 Res .Pwr . @FWHM

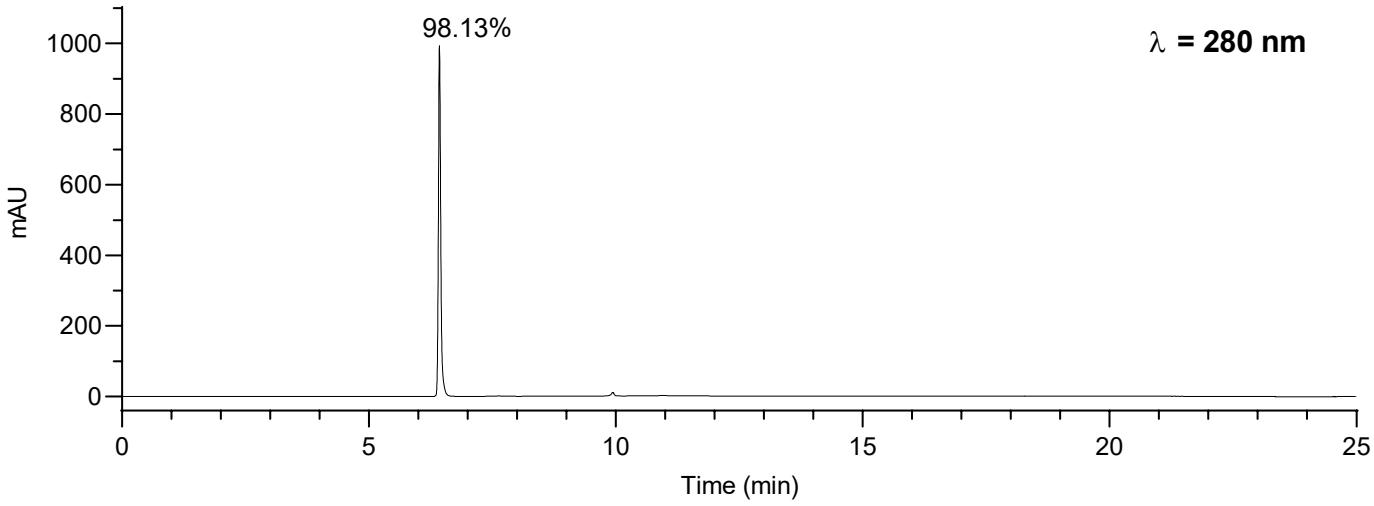
16



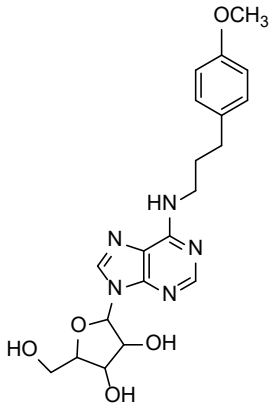


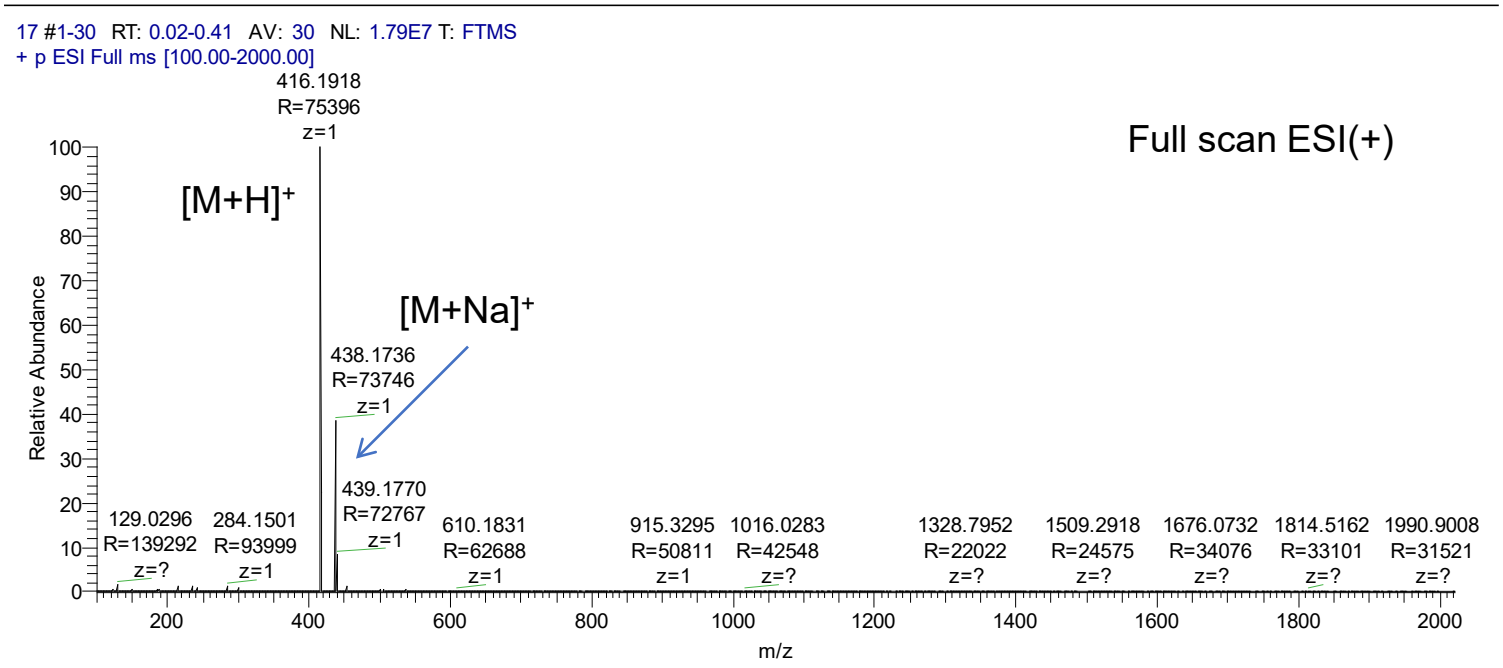


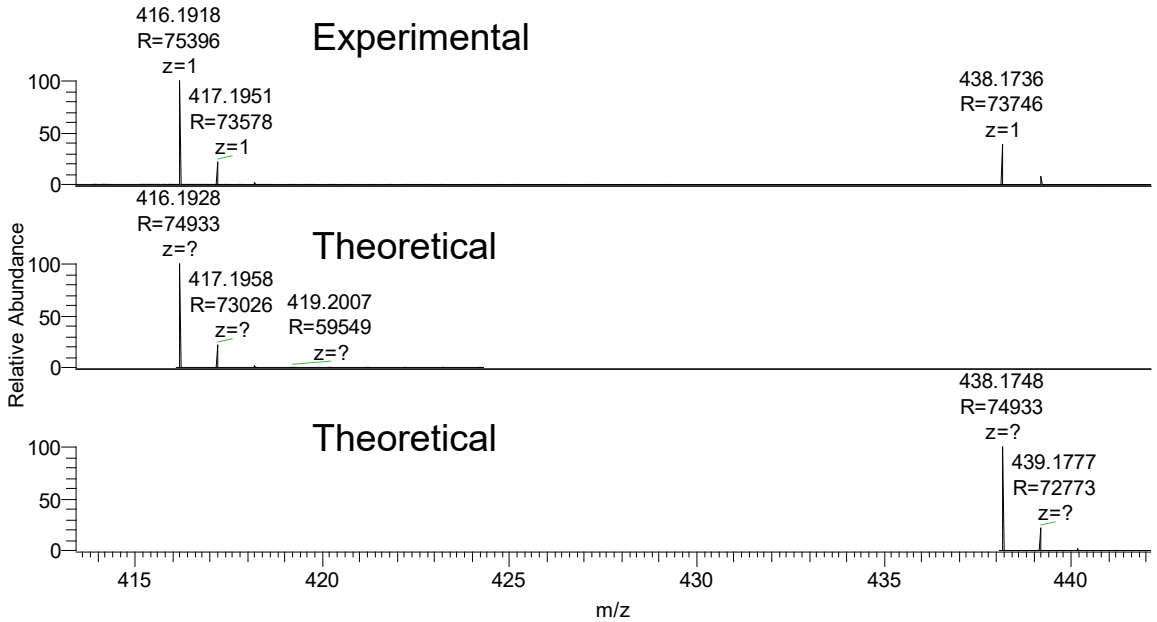
Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	5.483	0.19	0.1367
2	5.83	0.05	0.0319
3	6.43	98.48	69.5784
4	7.627	0.39	0.2763
5	9.937	0.89	0.6312
Total		*100.00*	*70.6545*



17





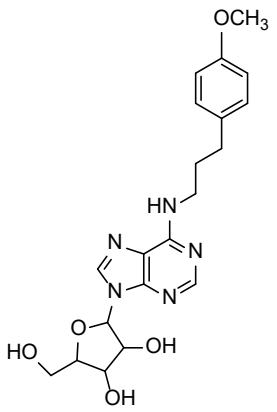


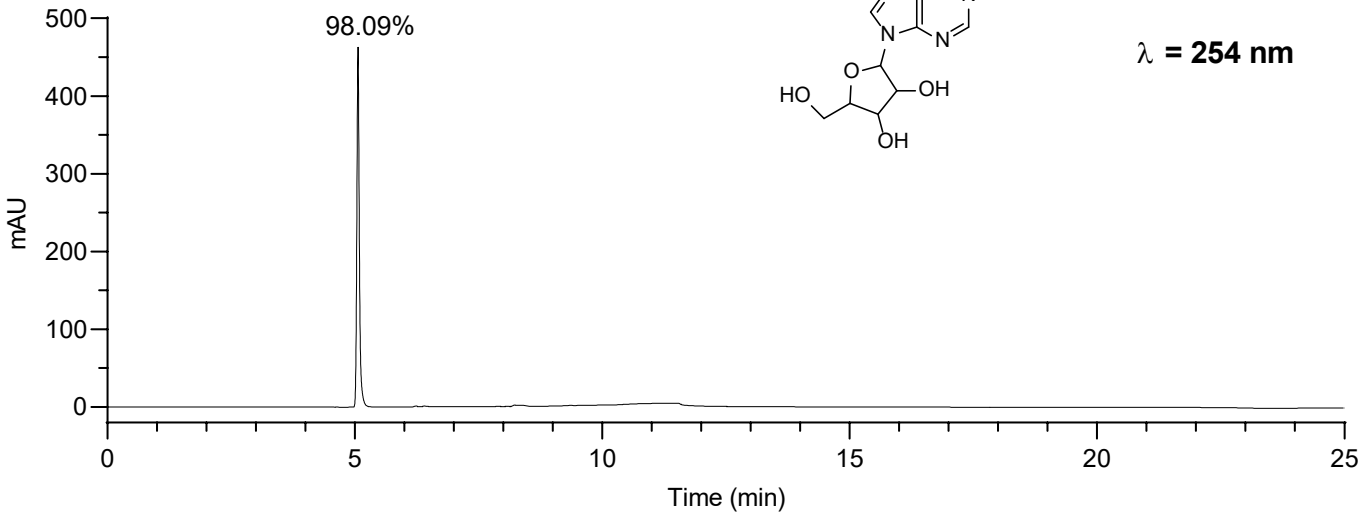
NL:
1.79E7
17#1-30 RT: 0.02-0.41 AV: 30 T: FTMS + p ESI Full ms [100.00-2000.00]

NL: Δm=2.40 ppm
1.83E4
$C_{20}H_{25}N_5O_5$ +H:
$C_{20}H_{26}N_5O_5$
p (gss, s /p:40) Chrg 1
R: 75000 Res .Pwr . @FWHM

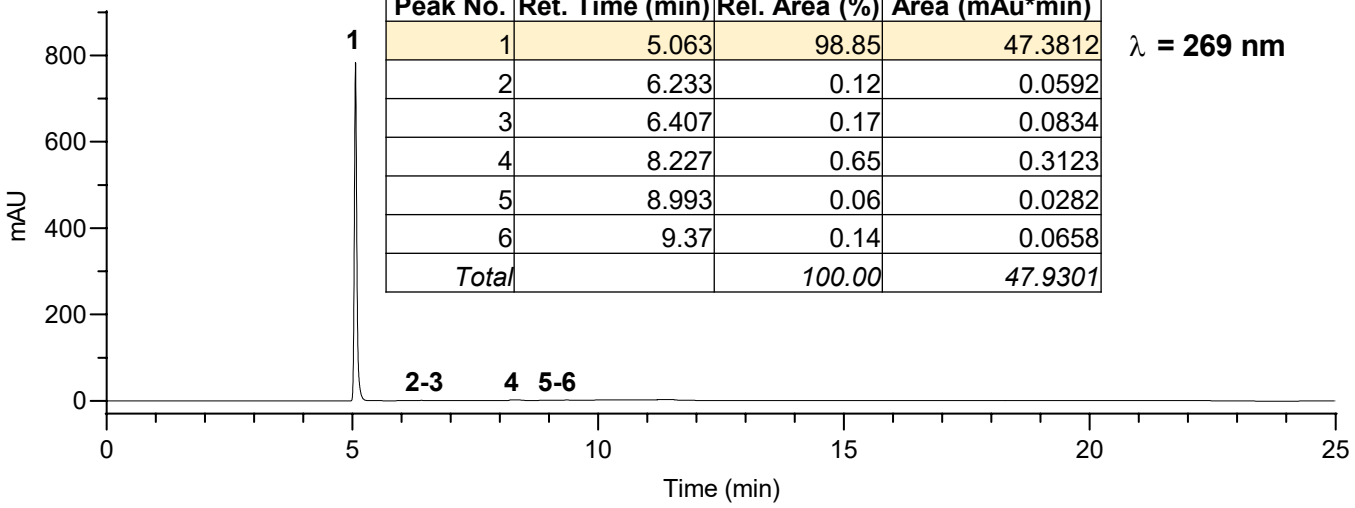
NL: Δm= 2.74ppm
1.83E4
$C_{20}H_{25}N_5O_5$ +Na:
$C_{20}H_{25}N_5O_5Na_1$
p (gss, s /p:40) Chrg 1
R: 75000 Res .Pwr . @FWHM

17



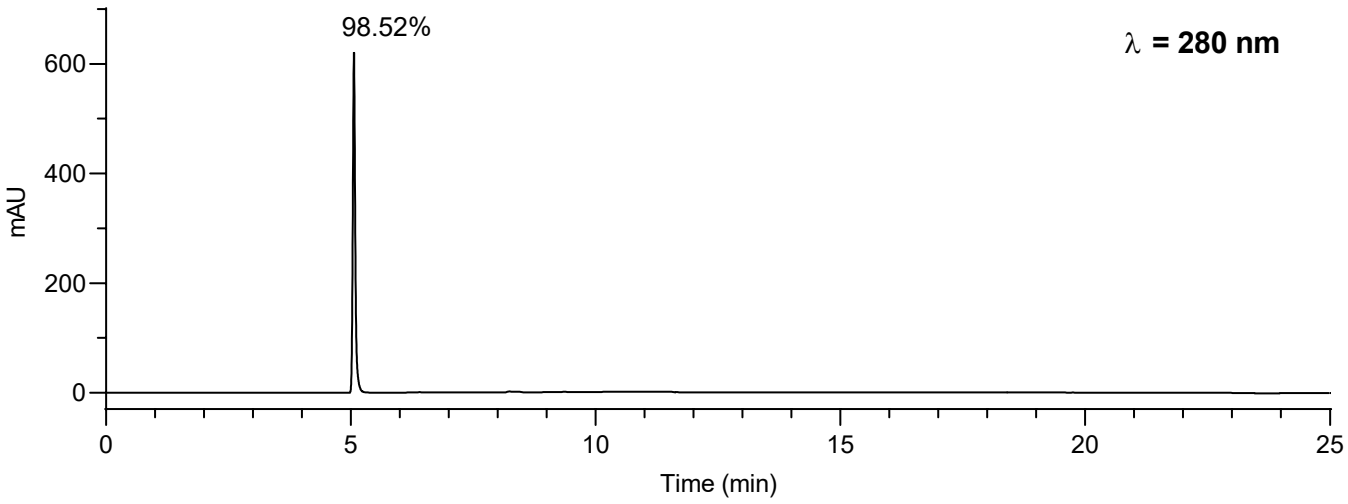


λ = 254 nm



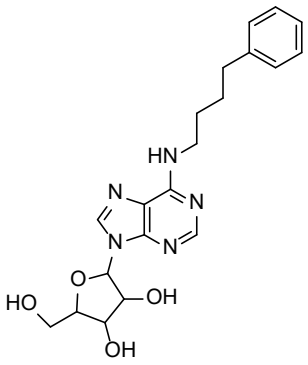
Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	5.063	98.85	47.3812
2	6.233	0.12	0.0592
3	6.407	0.17	0.0834
4	8.227	0.65	0.3123
5	8.993	0.06	0.0282
6	9.37	0.14	0.0658
Total		*100.00*	*47.9301*

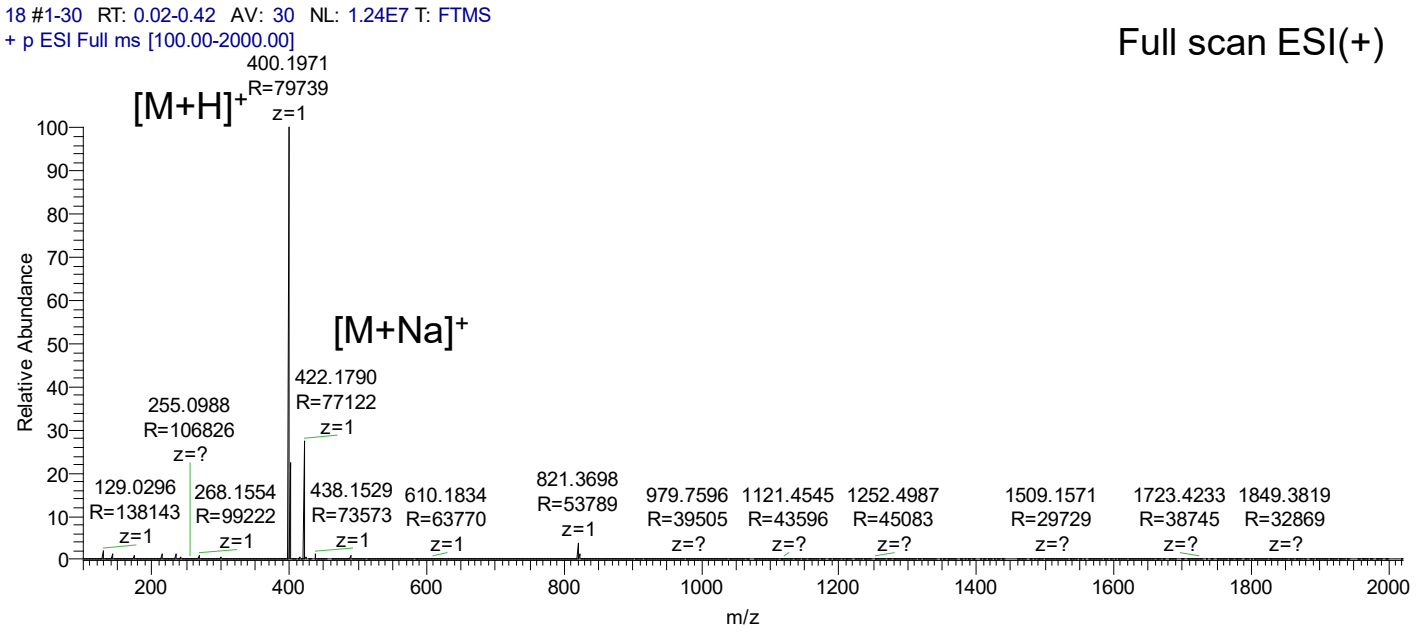
λ = 269 nm

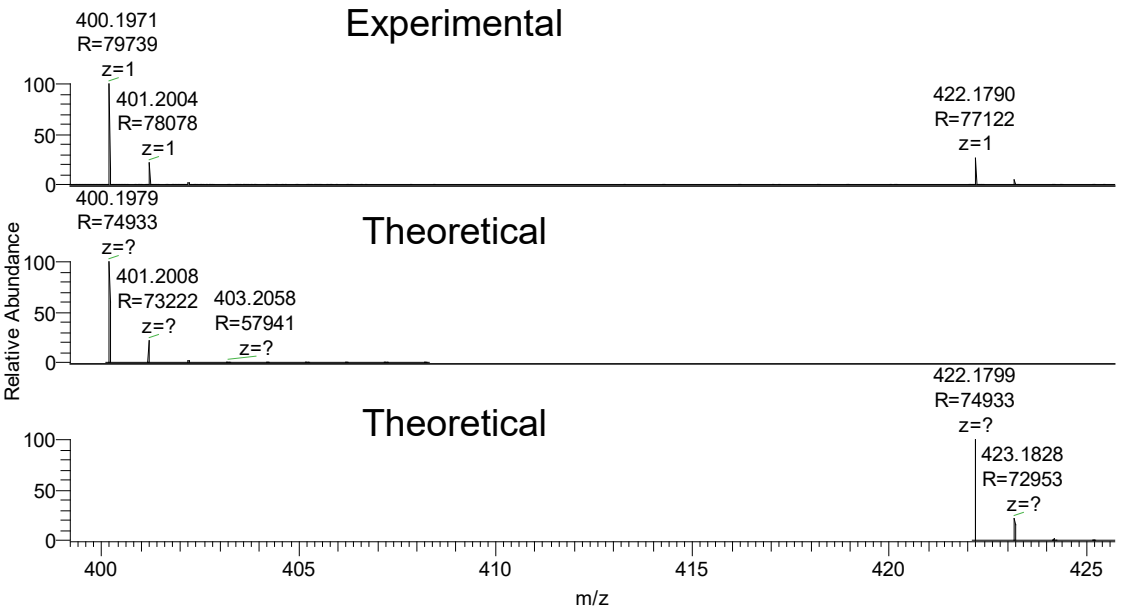


λ = 280 nm

18





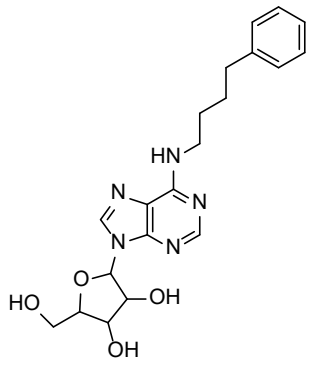


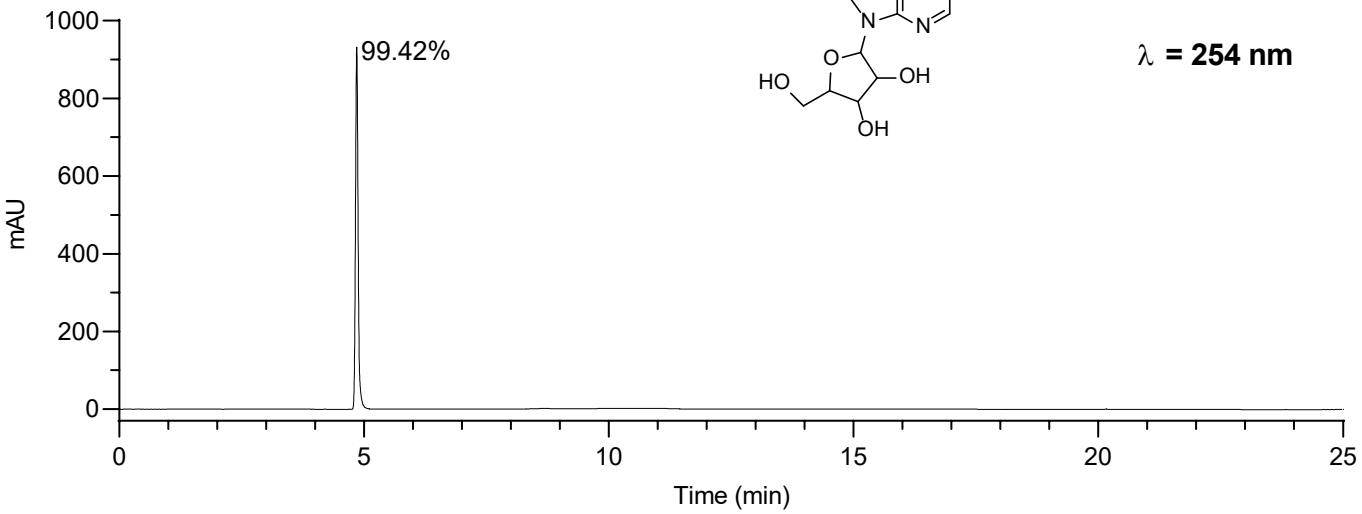
NL:
1.24E7
18#1-30 RT: 0.02-0.42 AV: 30 T: FTMS + p ESI Full ms [100.00-2000.00]

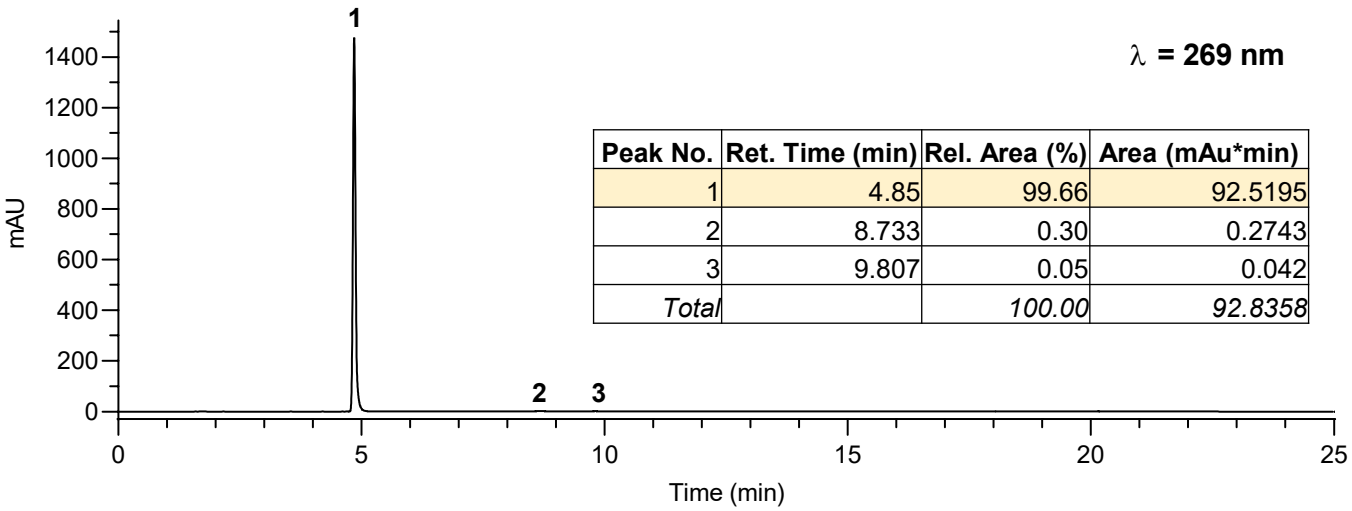
NL:
1.83E4
Δm=2.00 ppm
$C_{20}H_{25}N_5O_4$ +H:
$C_{20}H_{26}N_5O_4$
p (gss, s /p:40) Chrg 1
R: 75000 Res .Pwr . @FWHM

NL:
1.83E4
Δm= 2.13ppm
$C_{20}H_{25}N_5O_4$ +Na:
$C_{20}H_{25}N_5O_4Na_1$
p (gss, s /p:40) Chrg 1
R: 75000 Res .Pwr . @FWHM

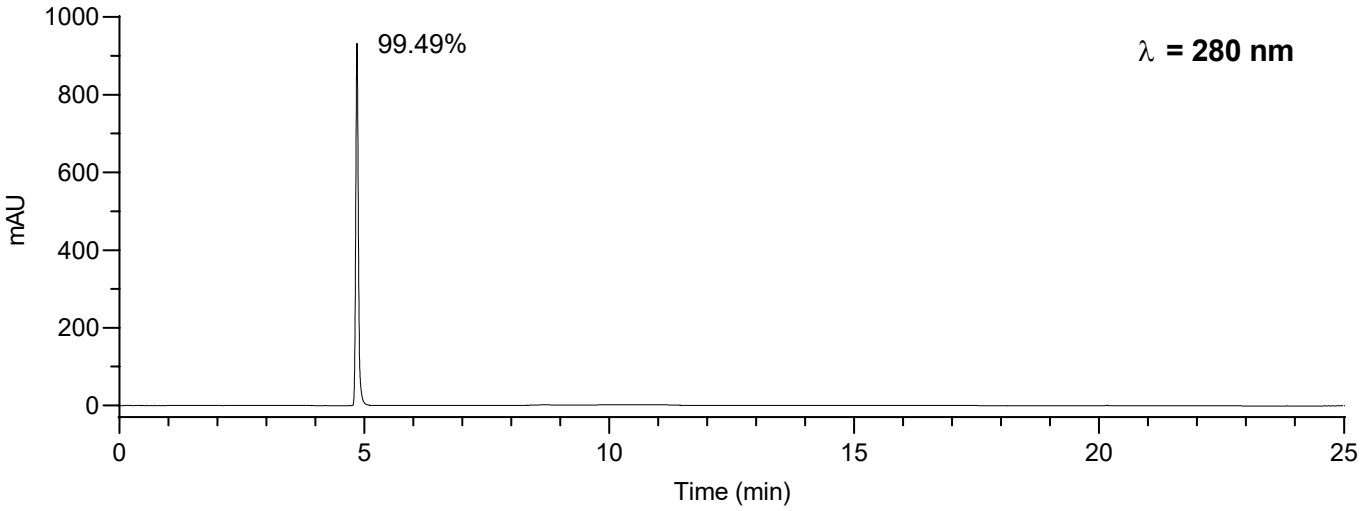
18



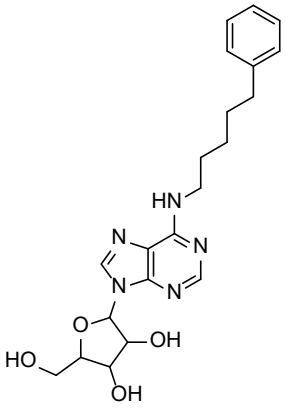




Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	4.85	99.66	92.5195
2	8.733	0.30	0.2743
3	9.807	0.05	0.042
Total		*100.00*	*92.8358*

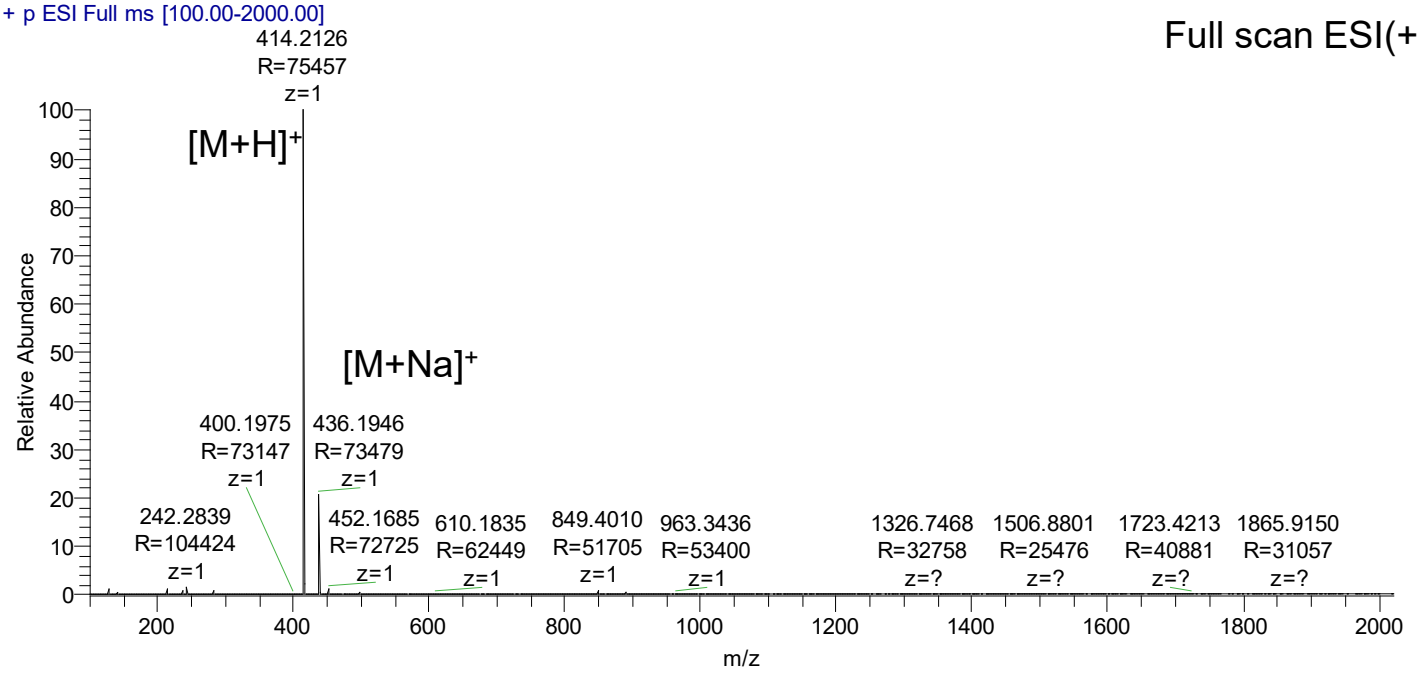


19

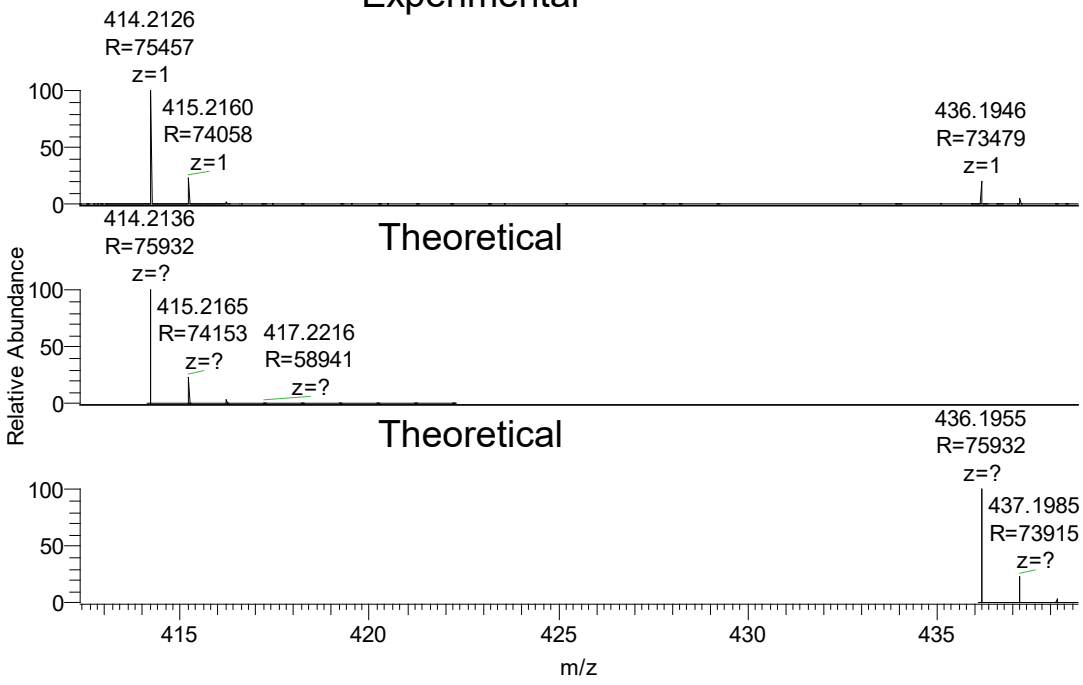


19 #1-30 RT: 0.02-0.41 AV: 30 NL: 2.54E7 T: FTMS
+ p ESI Full ms [100.00-2000.00]

Full scan ESI(+)



Experimental

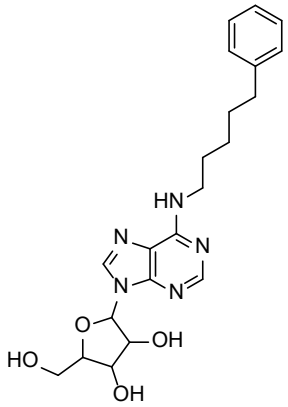


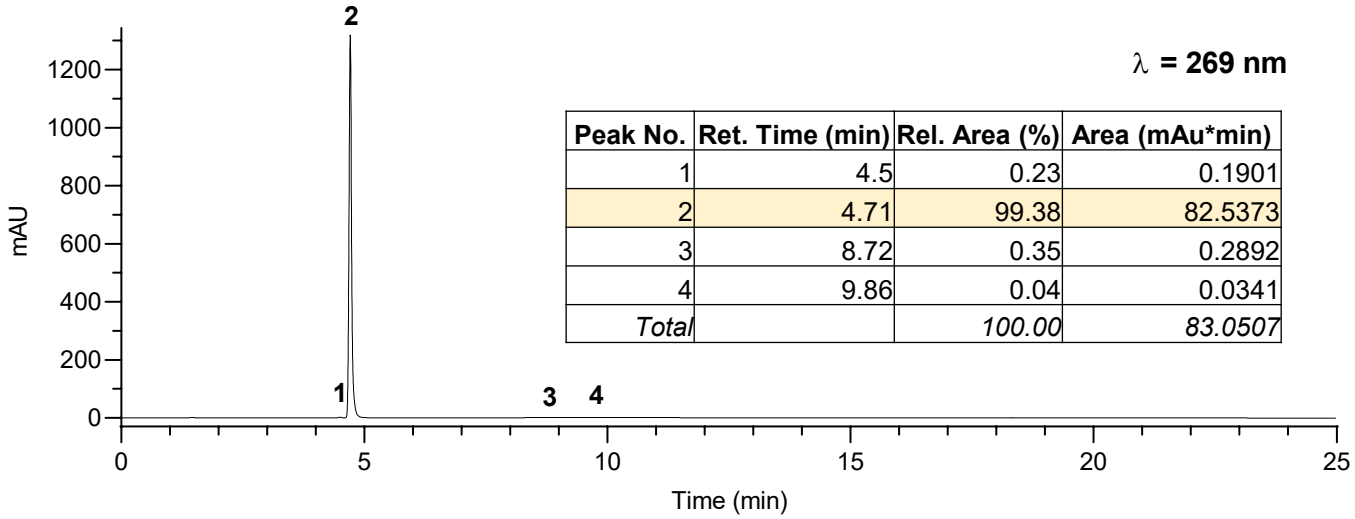
NL:
2.54E7
19#1-30 RT: 0.02-0.41 AV: 30 T: FTMS + p ESI Full ms [100.00-2000.00]

NL: Δm=2.41ppm
1.81E4
$C_{21}H_{27}N_5O_4$ +H:
$C_{21}H_{28}N_5O_4$
p (gss, s /p:40) Chrg 1
R: 76000 Res .Pwr . @FWHM

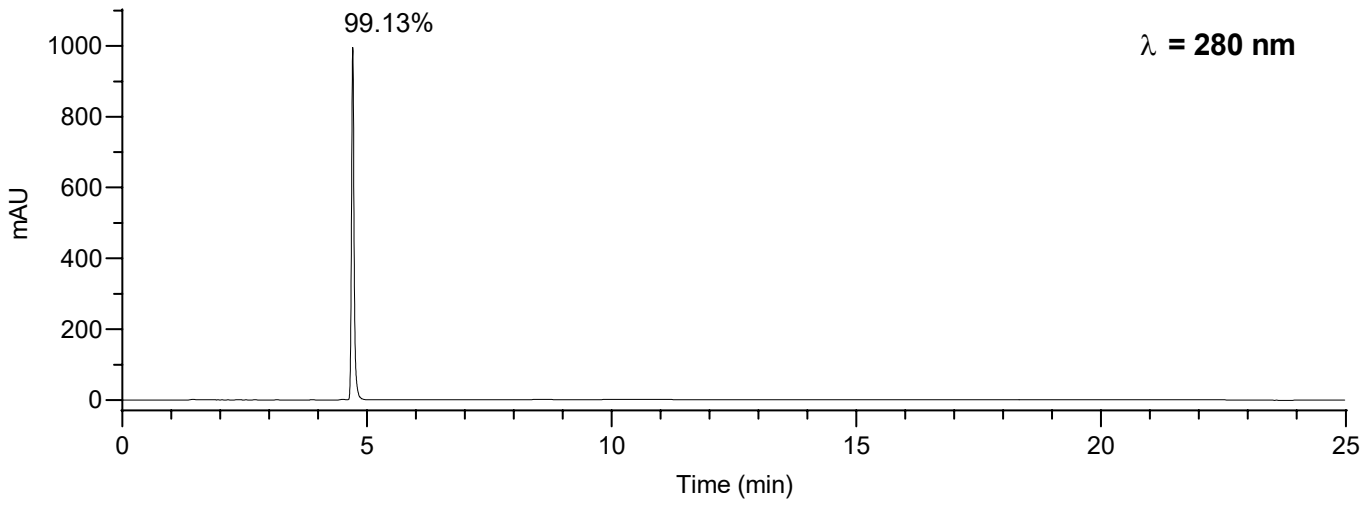
NL: Δm= 2.06 ppm
1.81E4
$C_{21}H_{27}N_5O_4$ +Na:
$C_{21}H_{27}N_5O_4Na_1$
p (gss, s /p:40) Chrg 1
R: 76000 Res .Pwr . @FWHM

19

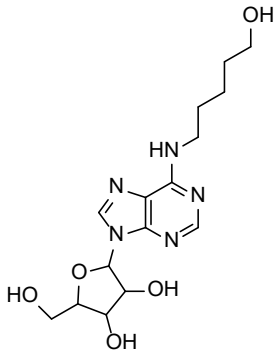




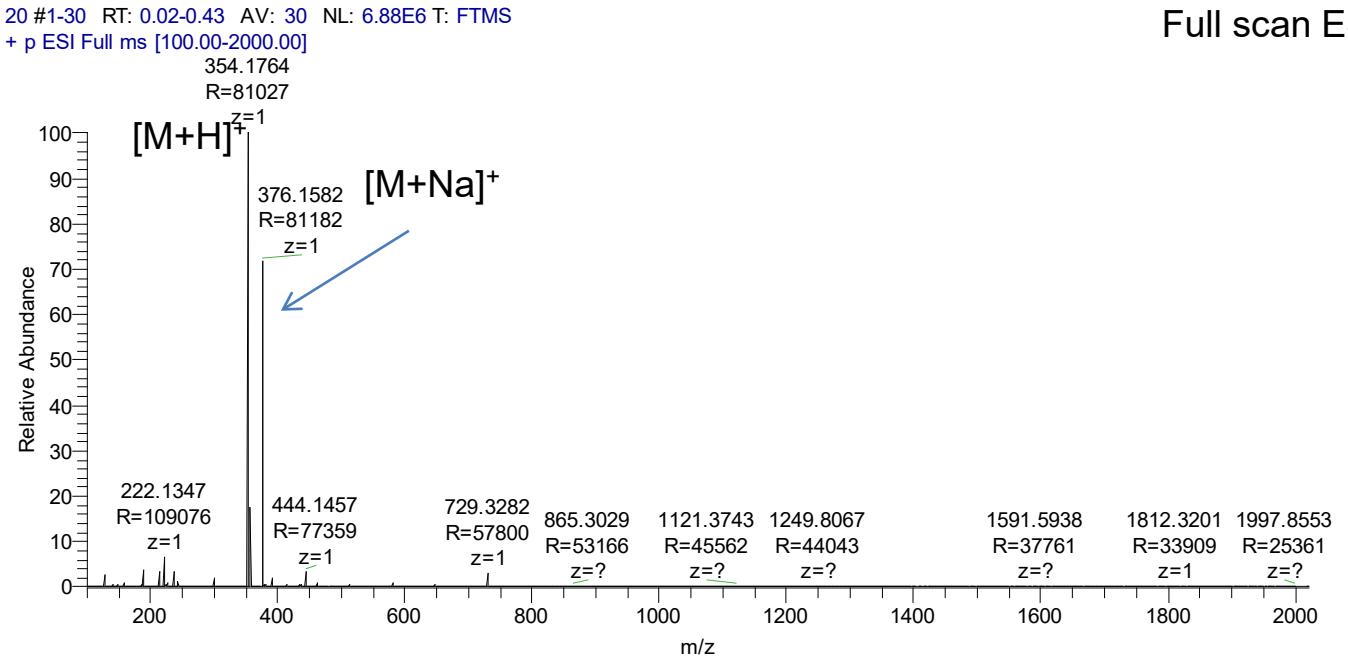
Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	4.5	0.23	0.1901
2	4.71	99.38	82.5373
3	8.72	0.35	0.2892
4	9.86	0.04	0.0341
Total		*100.00*	*83.0507*

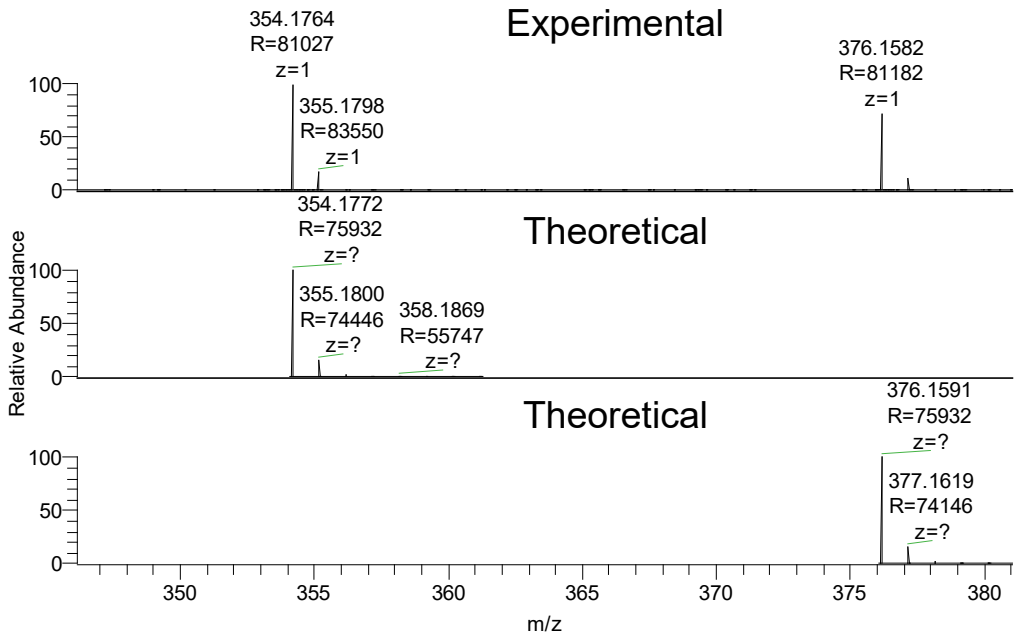


20



Full scan ESI(+)





NL:
6.88E6
20#1-30 RT: 0.02-0.43 AV:
30 T: FTMS + p ESI Full ms
[100.00-2000.00]

Δm=2.26ppm

NL:
1.93E4

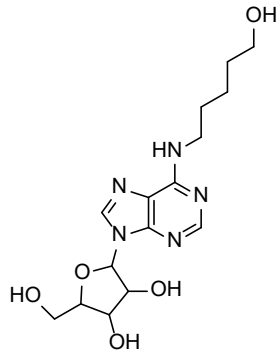
$C_{15}H_{23}N_5O_5$ +H:
$C_{15}H_{24}N_5O_5$
p (gss, s /p:40) Chrg 1
R: 76000 Res .Pwr . @FWHM

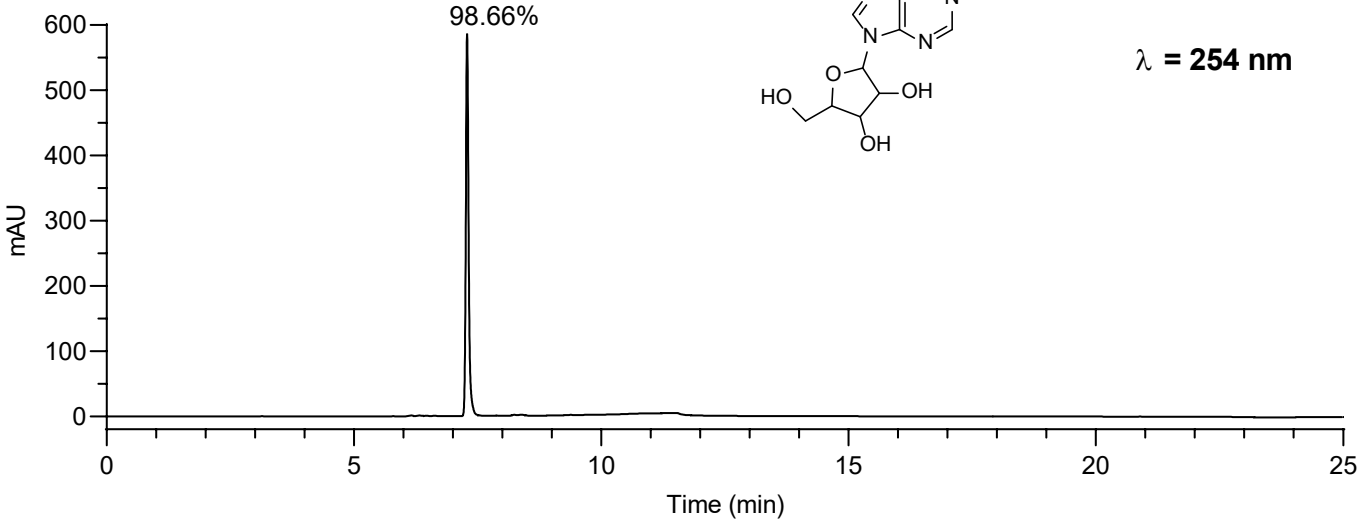
Δm= 2.39ppm

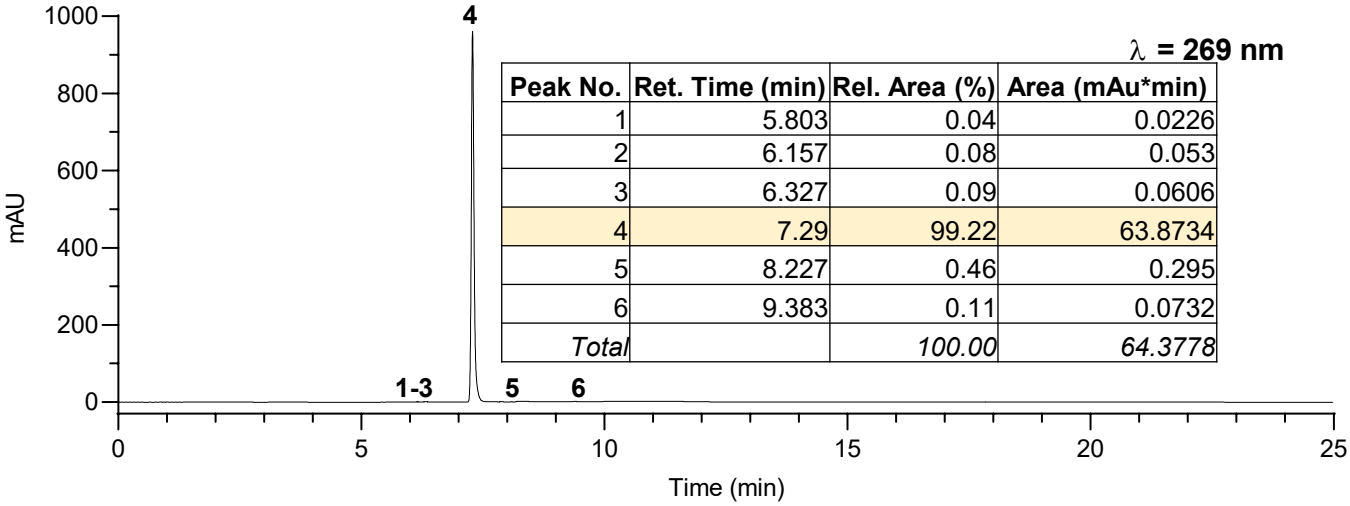
NL:
1.93E4

$C_{15}H_{23}N_5O_5$ +Na:
$C_{15}H_{23}N_5O_5Na_1$
p (gss, s /p:40) Chrg 1
R: 76000 Res .Pwr . @FWHM

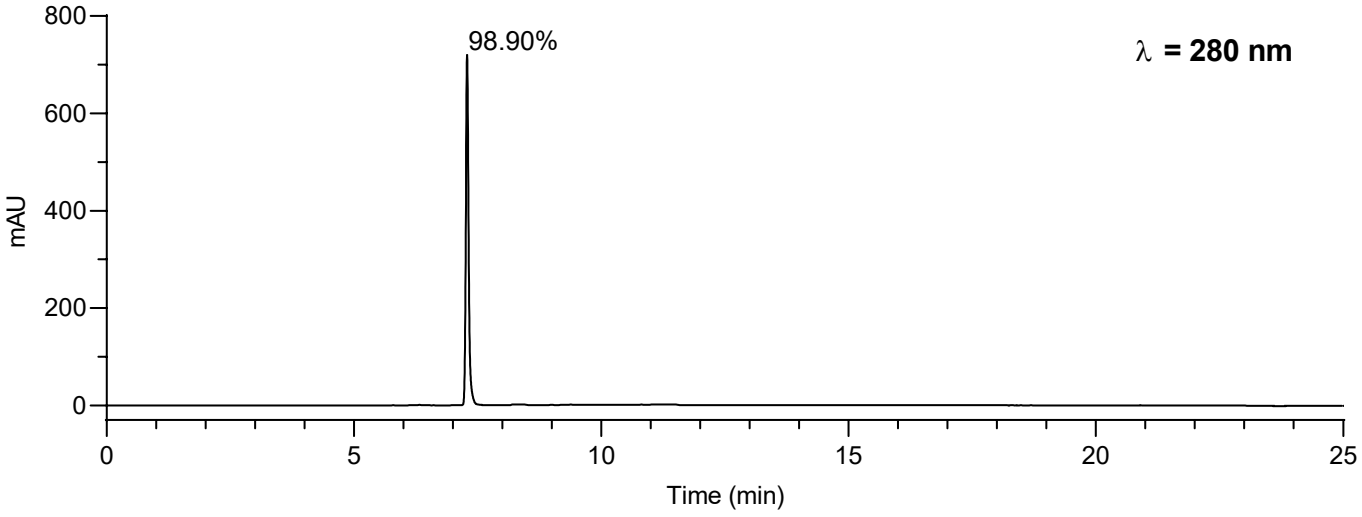
20



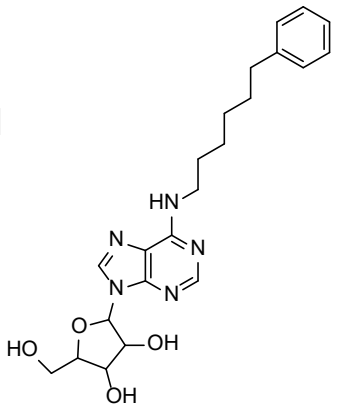




Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	5.803	0.04	0.0226
2	6.157	0.08	0.053
3	6.327	0.09	0.0606
4	7.29	99.22	63.8734
5	8.227	0.46	0.295
6	9.383	0.11	0.0732
Total		*100.00*	*64.3778*

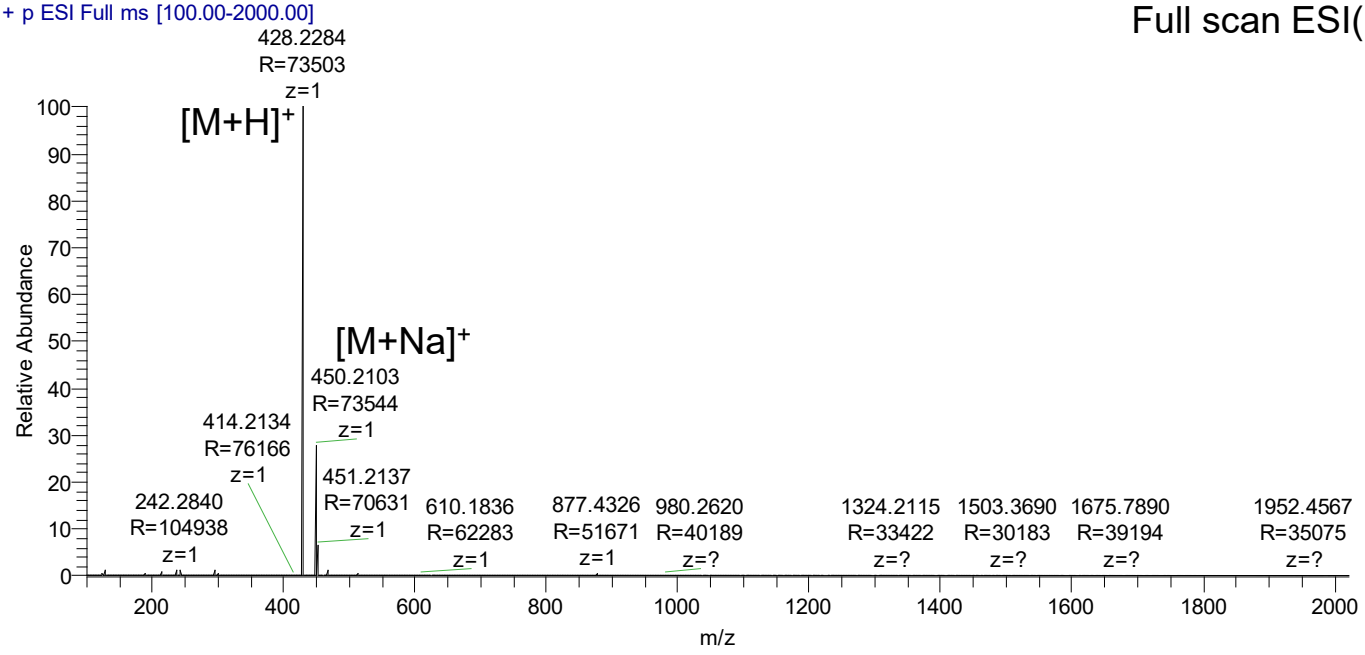


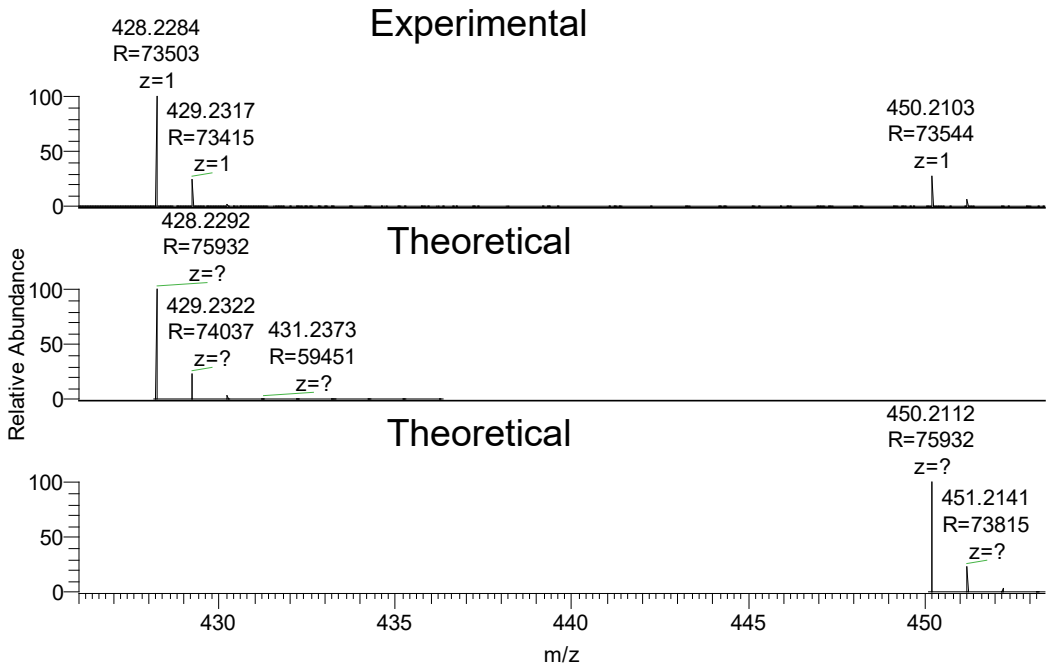
21



21 #1-29 RT: 0.02-0.40 AV: 29 NL: 2.48E7 T: FTMS
+ p ESI Full ms [100.00-2000.00]

Full scan ESI(+)





NL:
2.48E7
21#1-29 RT: 0.02-0.40 AV: 29 T: FTMS + p ESI Full ms [100.00-2000.00]

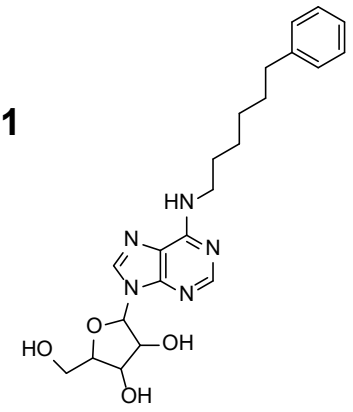
NL: Δm=1.87 ppm
1.79E4

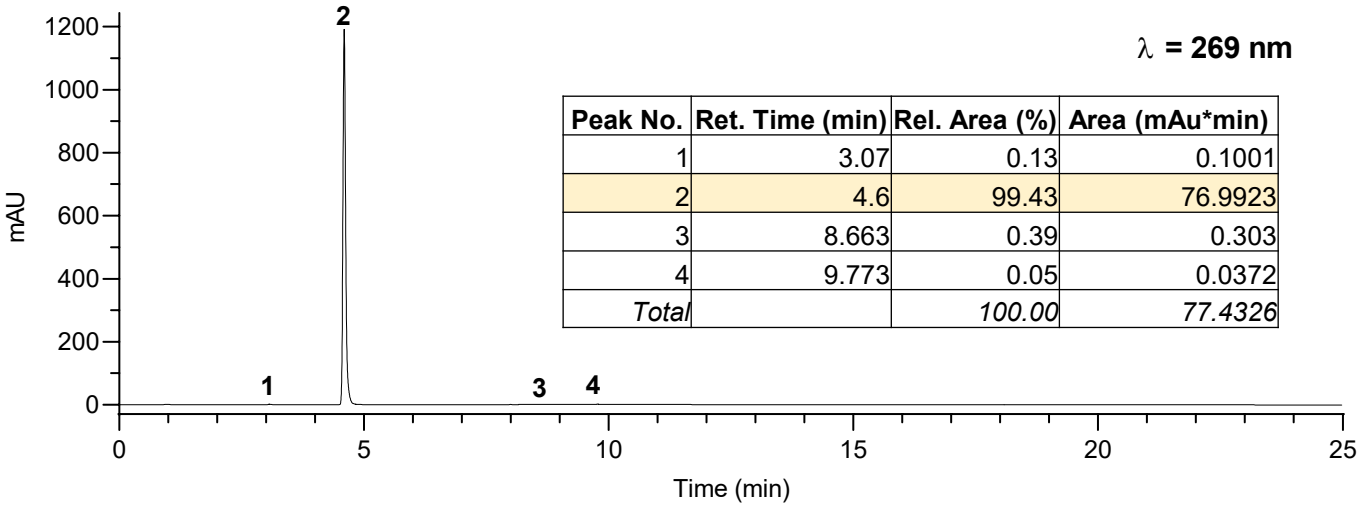
$C_{22}H_{29}N_5O_4$ +H:
$C_{22}H_{30}N_5O_4$
p (gss, s /p:40) Chrg 1
R: 76000 Res .Pwr . @FWHM

NL: Δm= 2.00 ppm
1.79E4

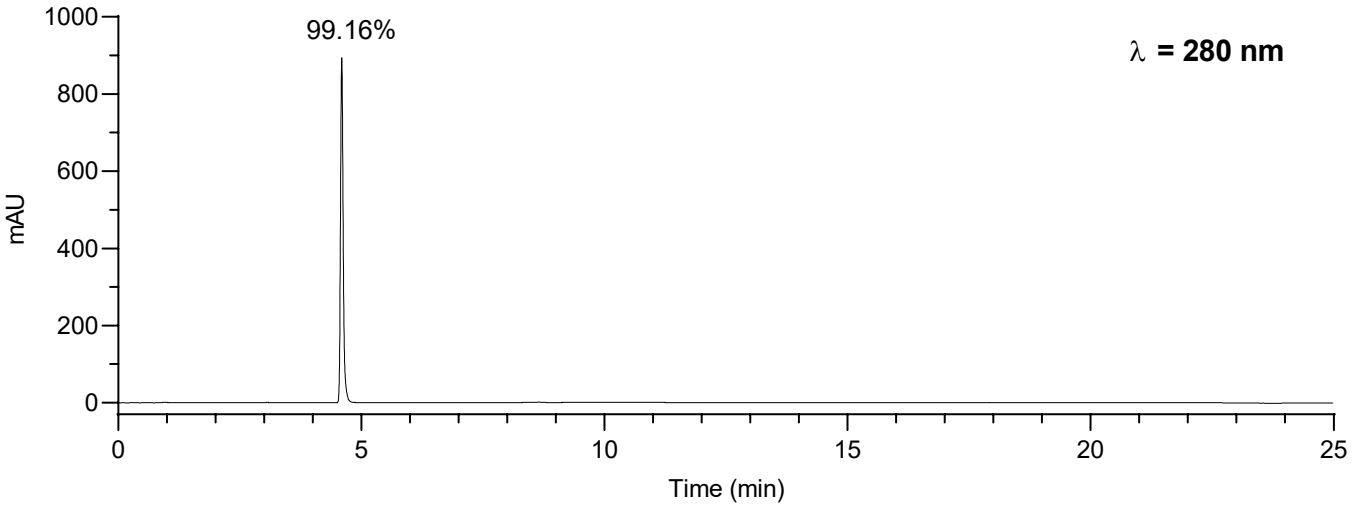
$C_{22}H_{29}N_5O_4$ +Na:
$C_{22}H_{29}N_5O_4Na_1$
p (gss, s /p:40) Chrg 1
R: 76000 Res .Pwr . @FWHM

21

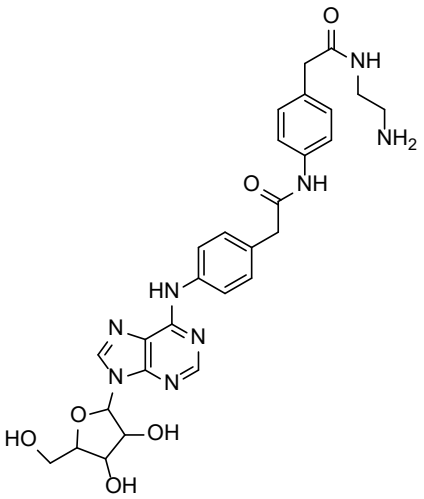




Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	3.07	0.13	0.1001
2	4.6	99.43	76.9923
3	8.663	0.39	0.303
4	9.773	0.05	0.0372
Total		*100.00*	*77.4326*

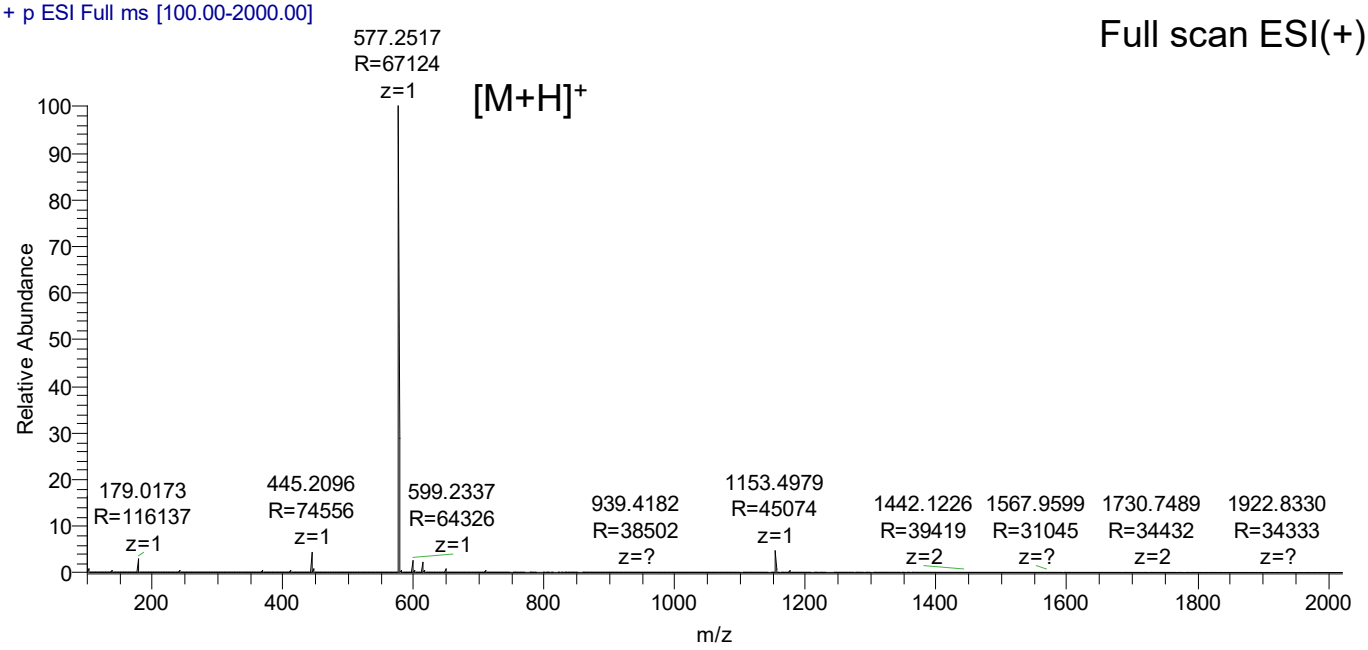


22

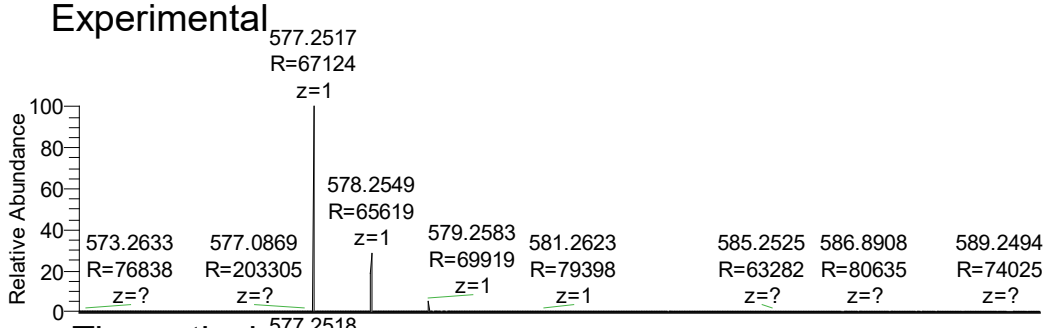


22 #1-30 RT: 0.02-0.41 AV: 30 NL: 9.48E7 T: FTMS
+ p ESI Full ms [100.00-2000.00]

Full scan ESI(+)

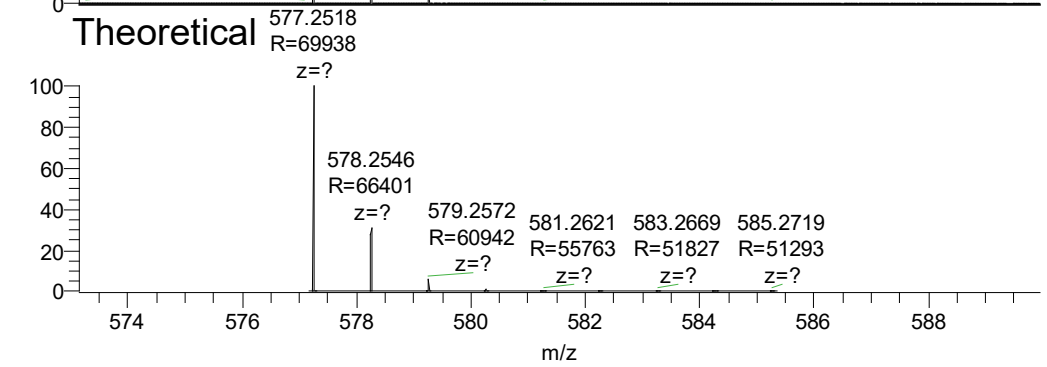


Experimental



NL:
9.48E7
22#1-30 RT:
0.02-0.41 AV: 30 T: FTMS +
p ESI Full ms
[100.00-2000.00]

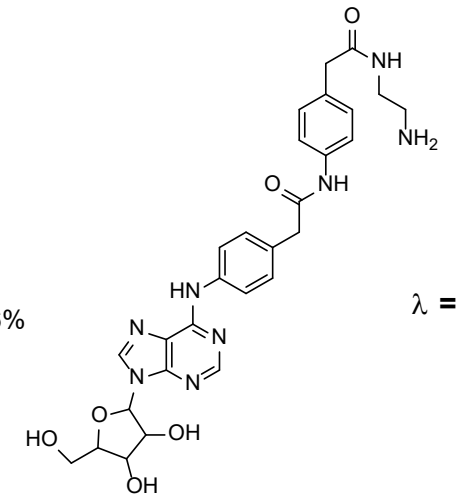
Theoretical

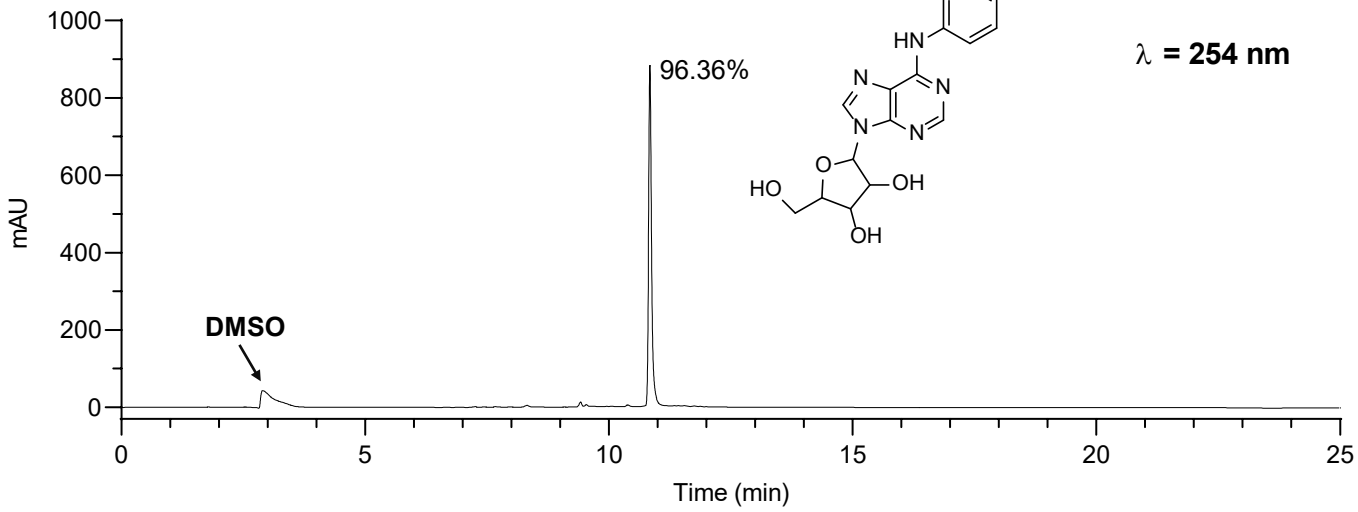


NL:
1.66E4
$C_{28}H_{32}N_8O_6$ +H:
$C_{28}H_{33}N_8O_6$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM

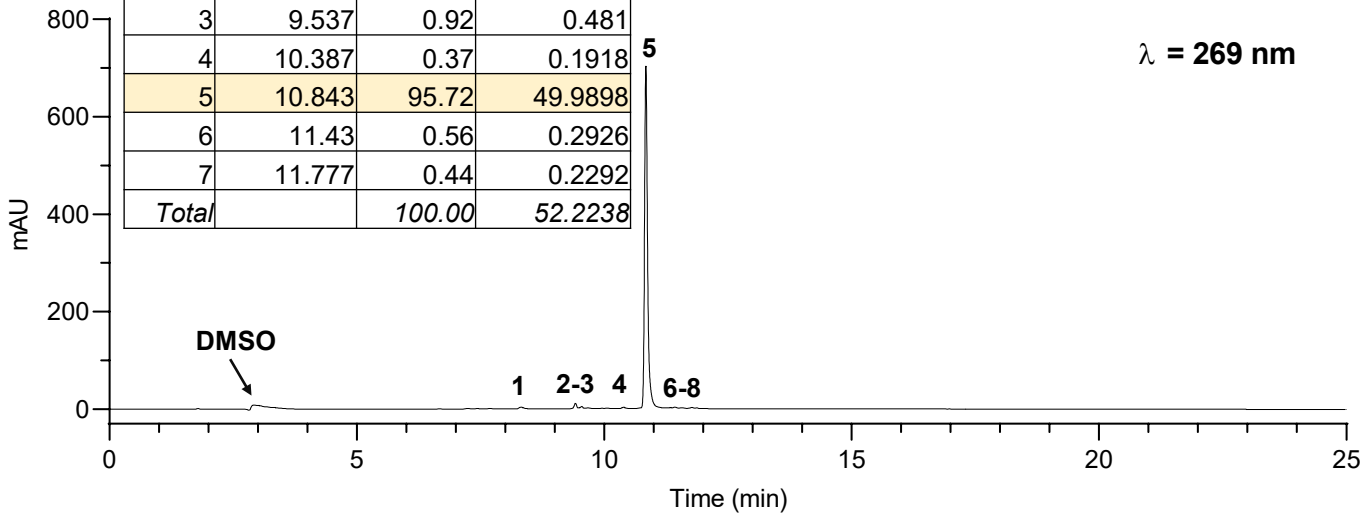
Δm= 0.17ppm

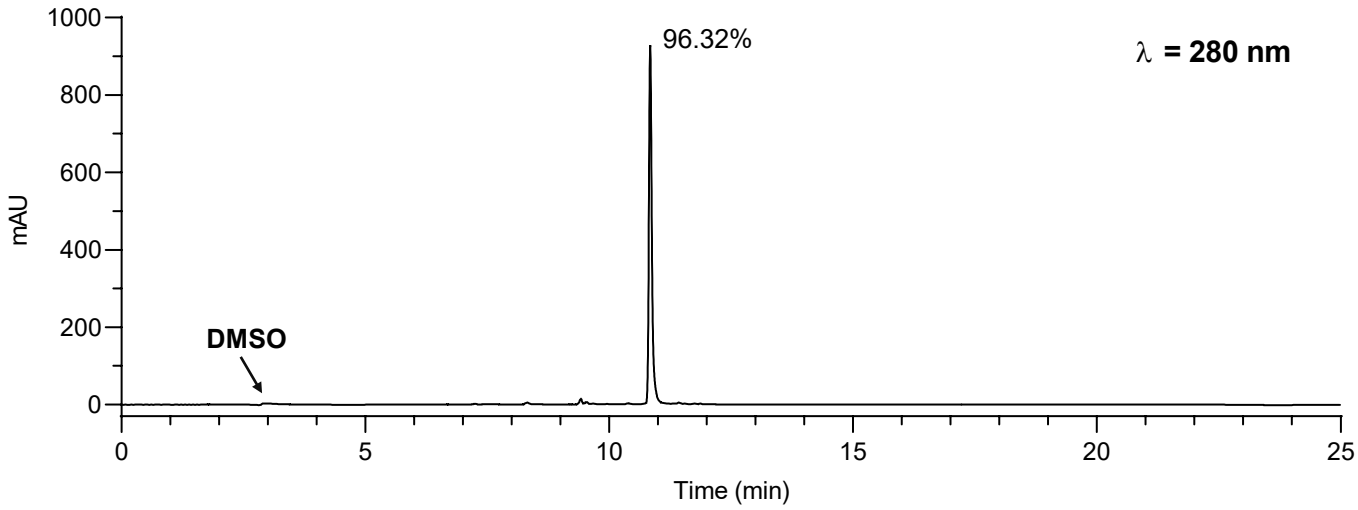
22



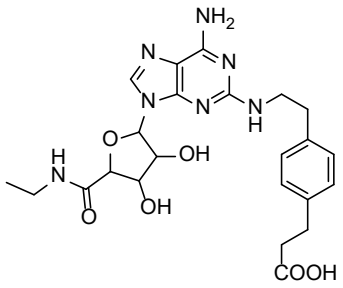


Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	8.317	0.71	0.3723
2	9.417	1.28	0.6671
3	9.537	0.92	0.481
4	10.387	0.37	0.1918
5	10.843	95.72	49.9898
6	11.43	0.56	0.2926
7	11.777	0.44	0.2292
Total		*100.00*	*52.2238*



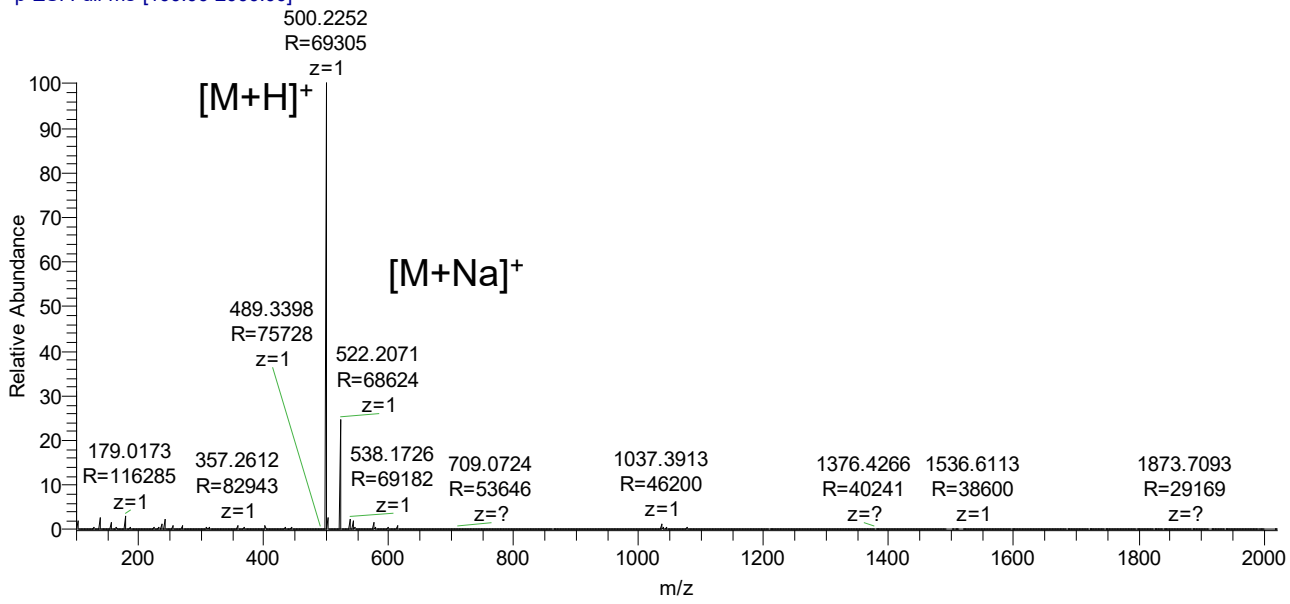


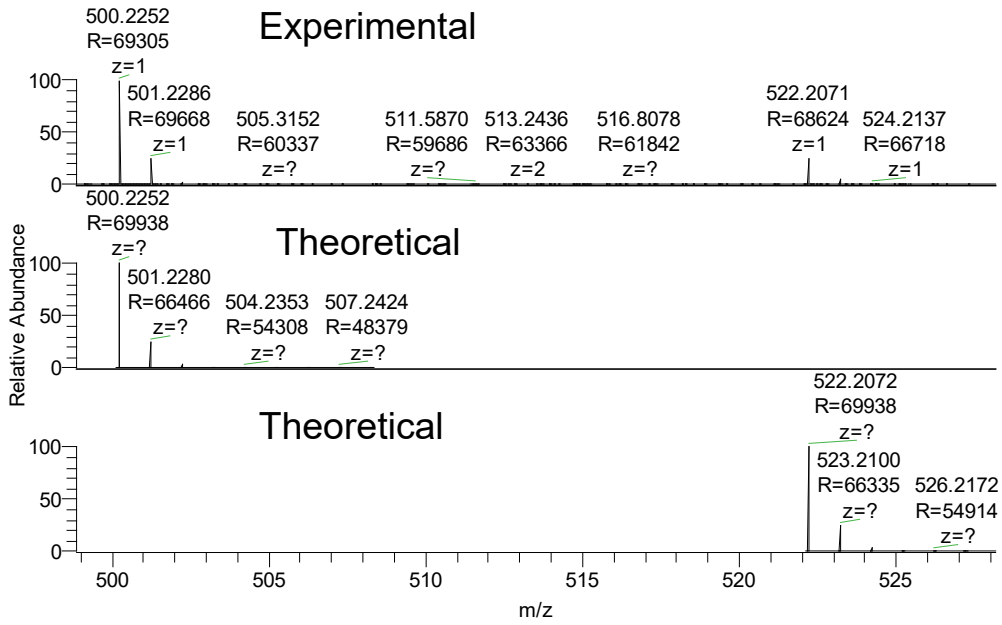
23



23 #1-30 RT: 0.02-0.41 AV: 30 NL: 2.96E7 T: FTMS + p ESI Full ms [100.00-2000.00]

Full scan ESI(+)





NL:
2.96E7
23#1-30 RT: 0.02-0.41 AV: 30 T: FTMS + p ESI Full ms [100.00-2000.00]

NL:
1.75E4

Δm= 0.00ppm

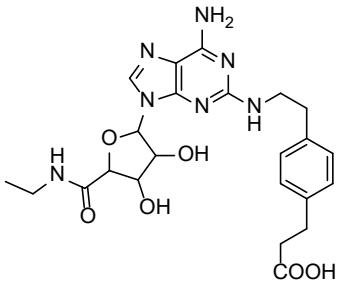
$C_{23}H_{29}N_7O_6$ +H:
$C_{23}H_{30}N_7O_6$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM

NL:
1.75E4

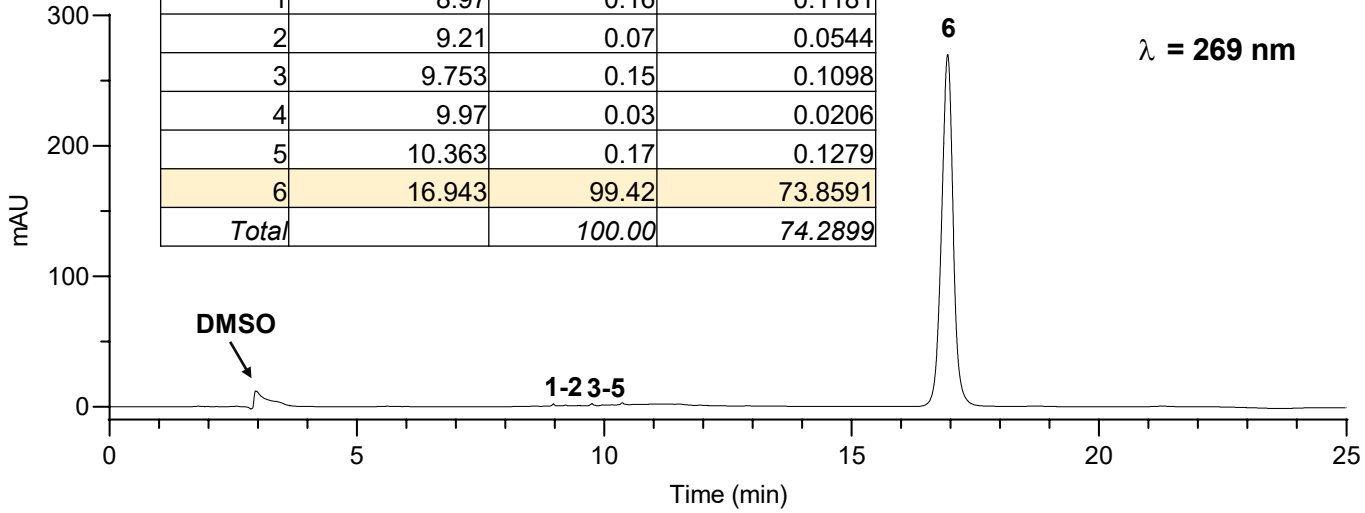
Δm= 0.19ppm

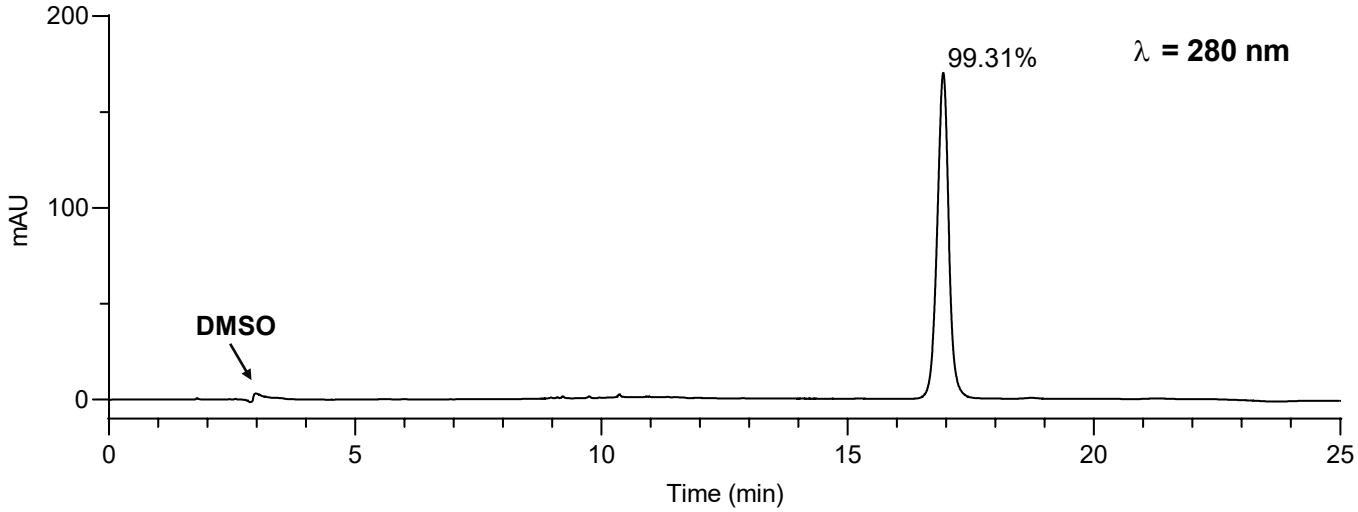
$C_{23}H_{29}N_7O_6$ +Na:
$C_{23}H_{29}N_7O_6Na_1$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM

23

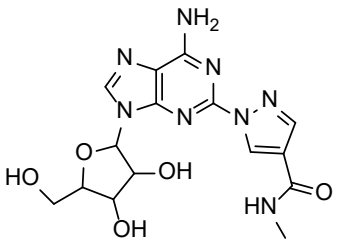


Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	8.97	0.16	0.1181
2	9.21	0.07	0.0544
3	9.753	0.15	0.1098
4	9.97	0.03	0.0206
5	10.363	0.17	0.1279
6	16.943	99.42	73.8591
Total		*100.00*	*74.2899*



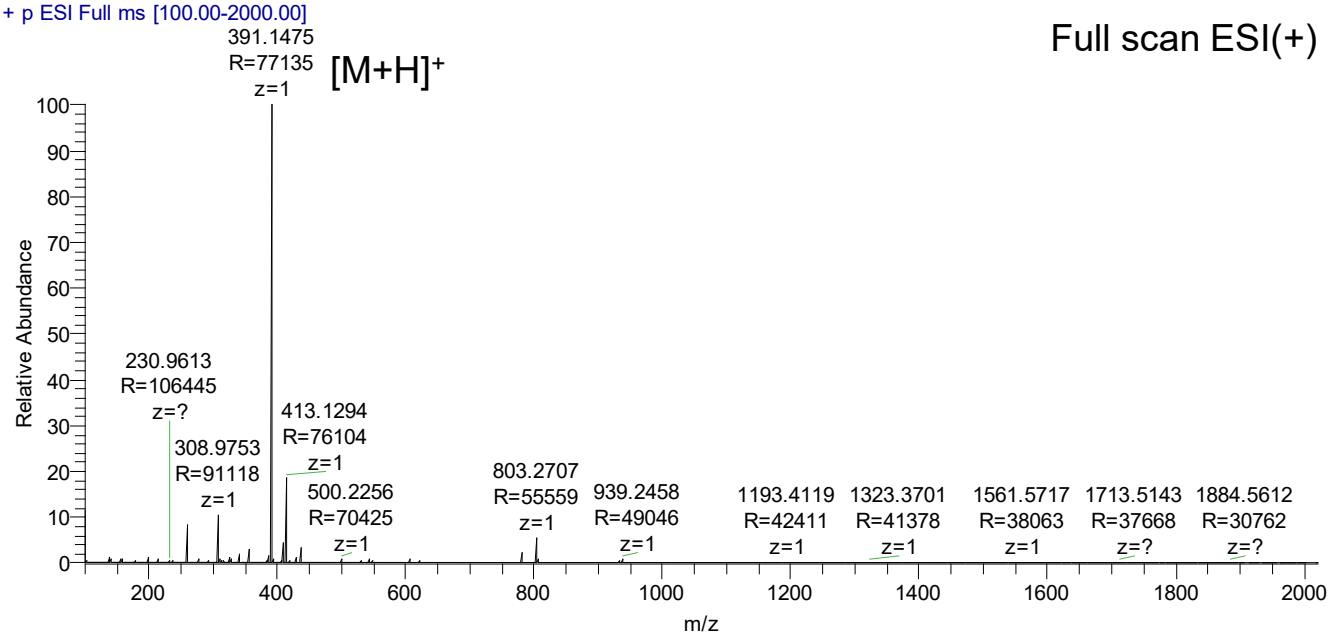


24

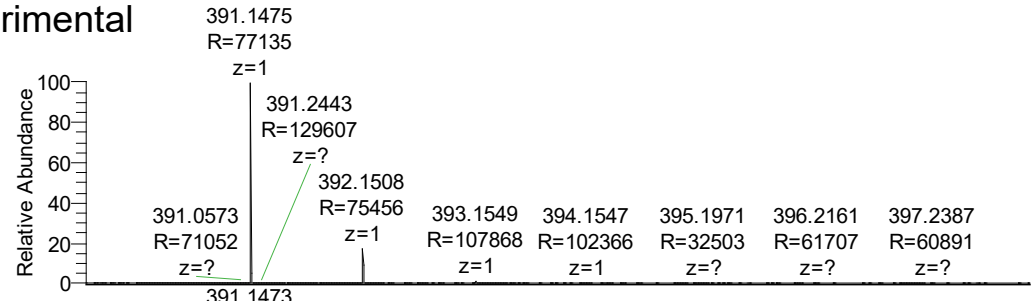


24 #1-30 RT: 0.02-0.42 AV: 30 NL: 1.17E7 T: FTMS
+ p ESI Full ms [100.00-2000.00]

Full scan ESI(+)

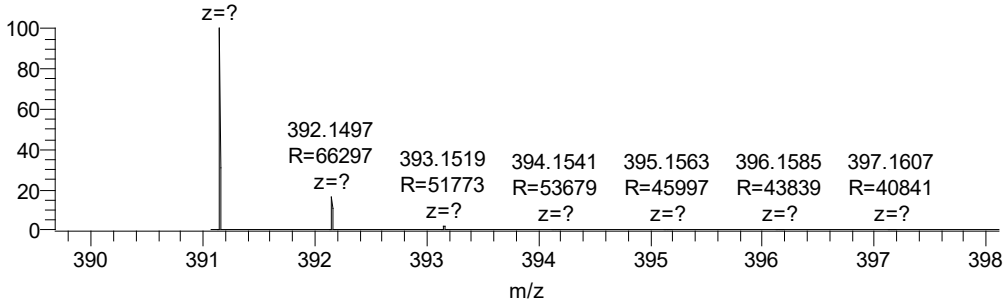


Experimental



NL:
1.17E7
24#1-30 RT:
0.02-0.42 AV: 30 T: FTMS +
p ESI Full ms
[100.00-2000.00]

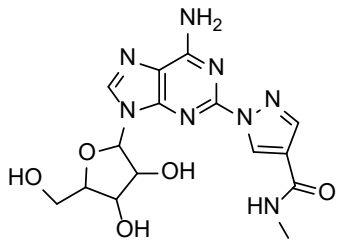
Theoretical

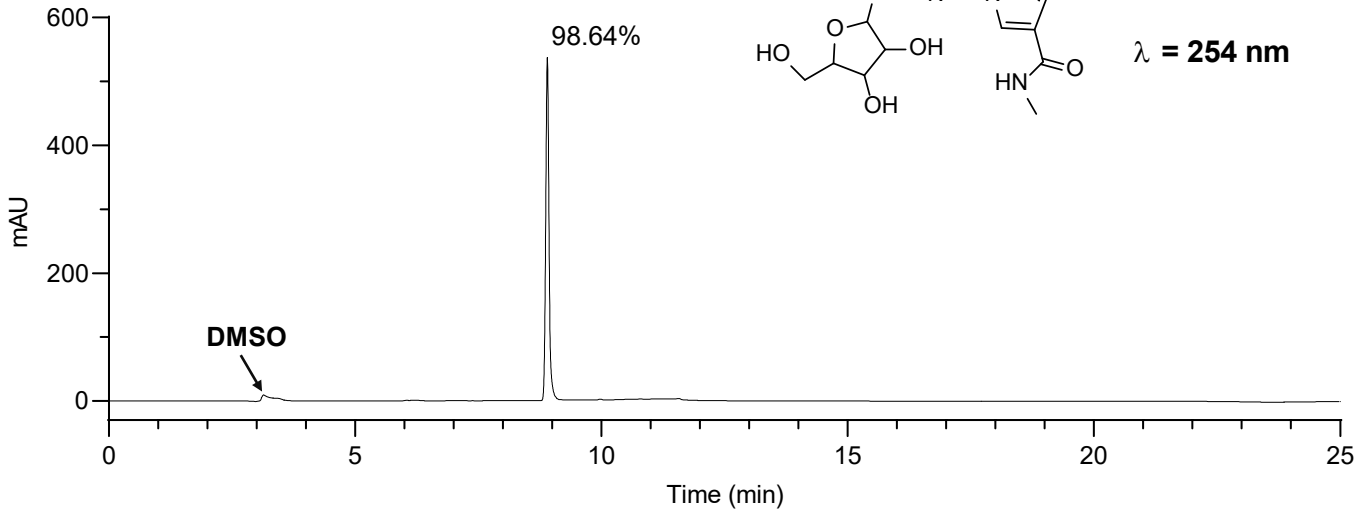


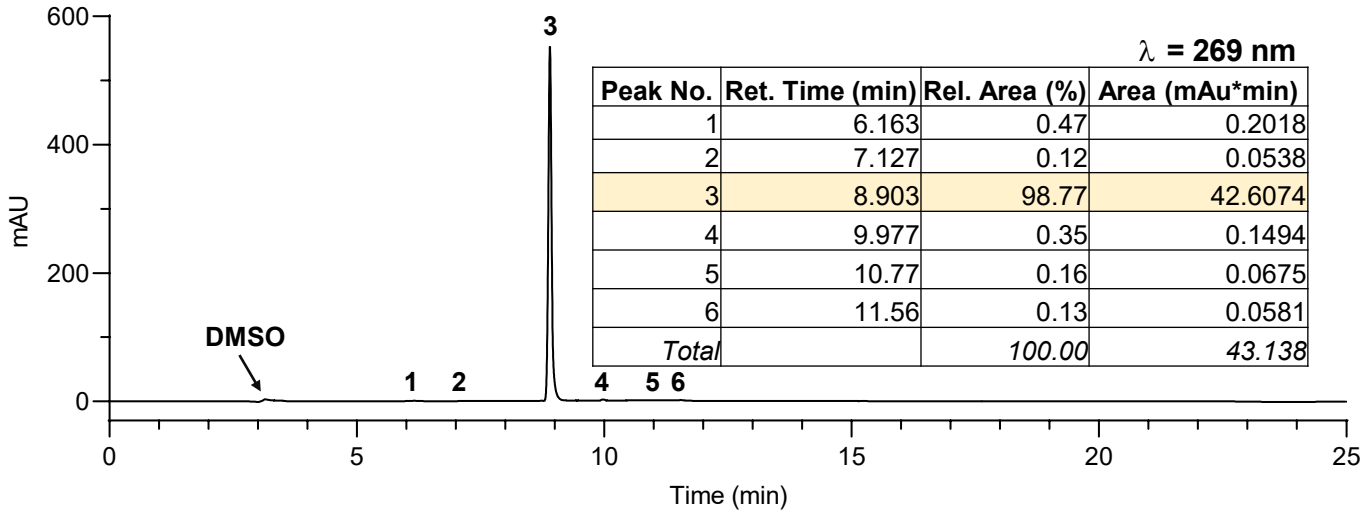
NL:
1.91E4
$C_{15}H_{18}N_8O_5$ +H:
$C_{15}H_{19}N_8O_5$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr. @FWHM

Δm= 0.51ppm

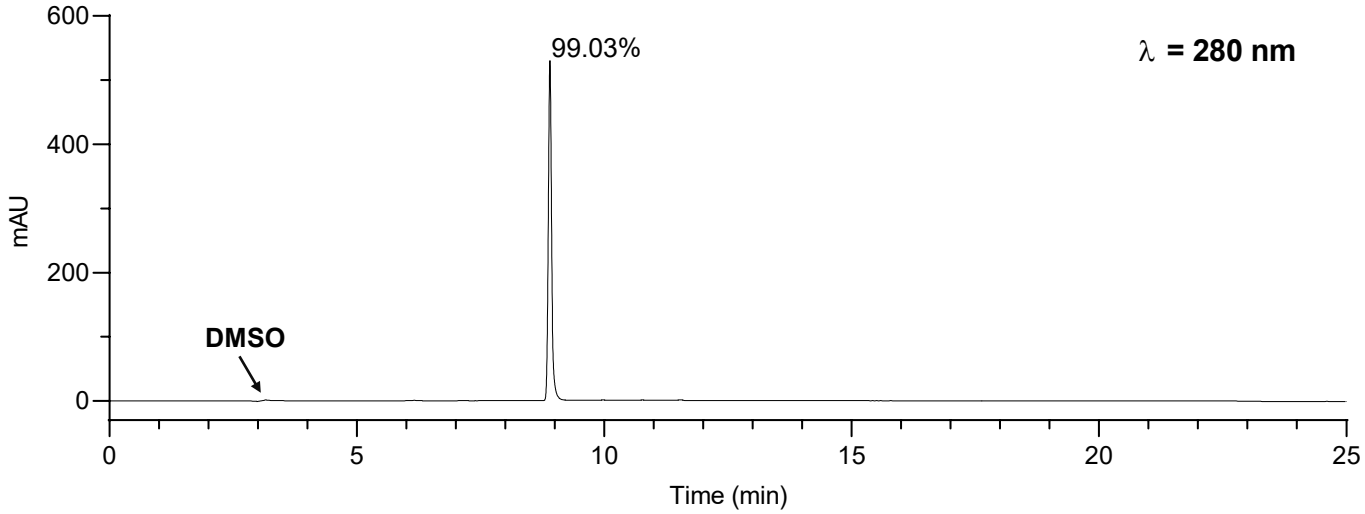
24



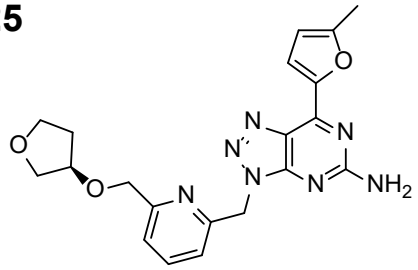




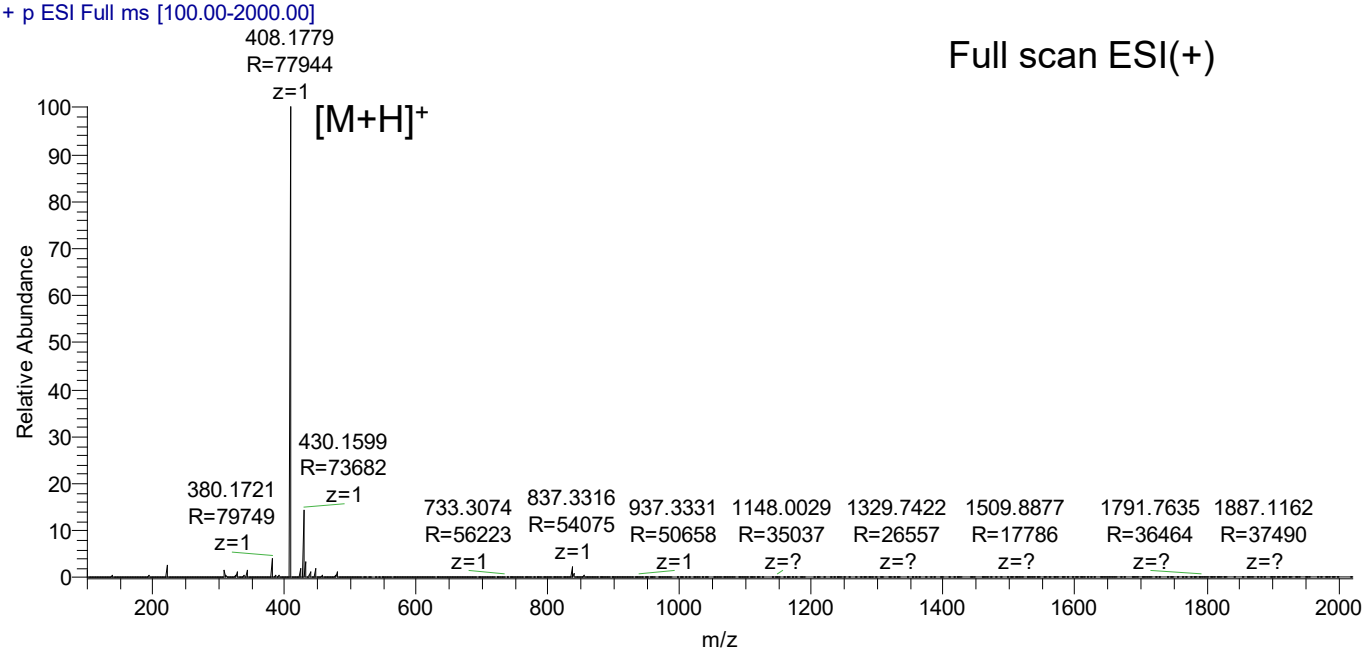
Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	6.163	0.47	0.2018
2	7.127	0.12	0.0538
3	8.903	98.77	42.6074
4	9.977	0.35	0.1494
5	10.77	0.16	0.0675
6	11.56	0.13	0.0581
Total		*100.00*	*43.138*

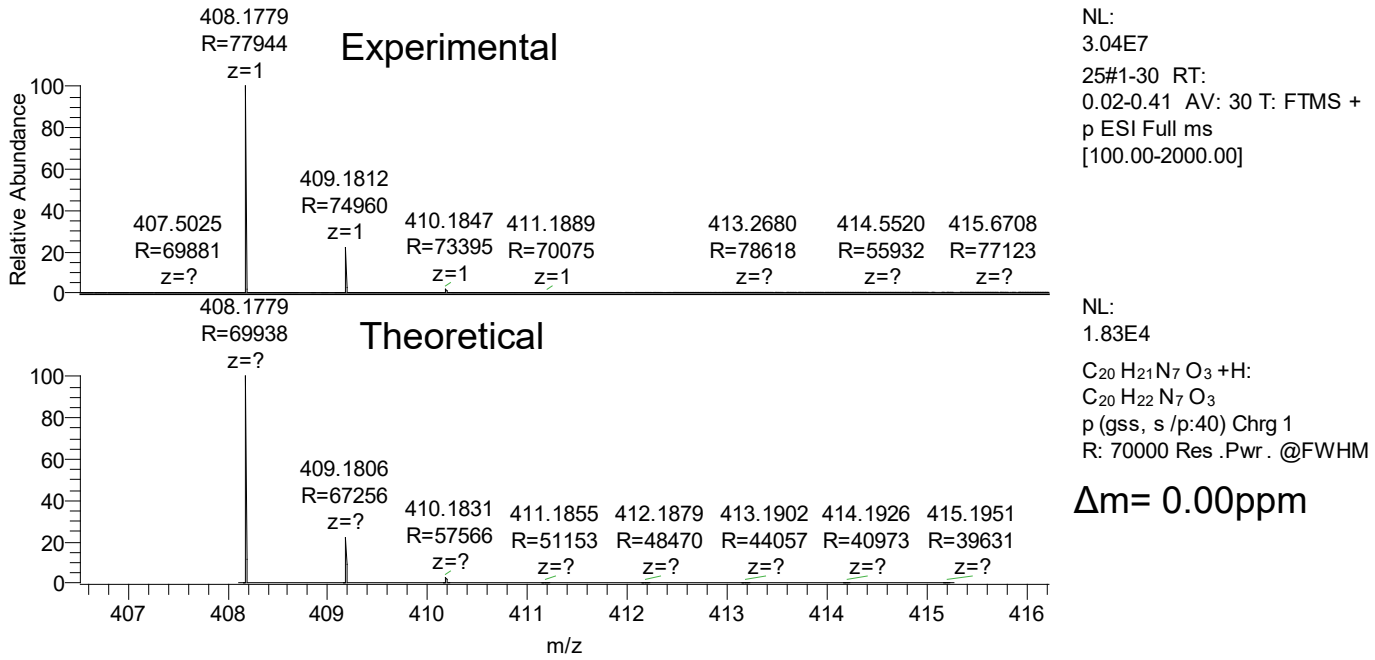


25

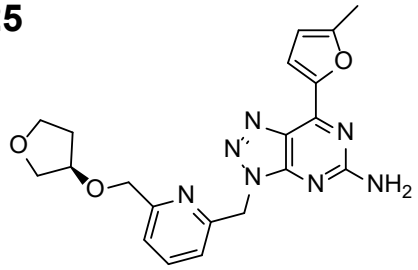


25 #1-30 RT: 0.02-0.41 AV: 30 NL: 3.04E7 T: FTMS
+ p ESI Full ms [100.00-2000.00]

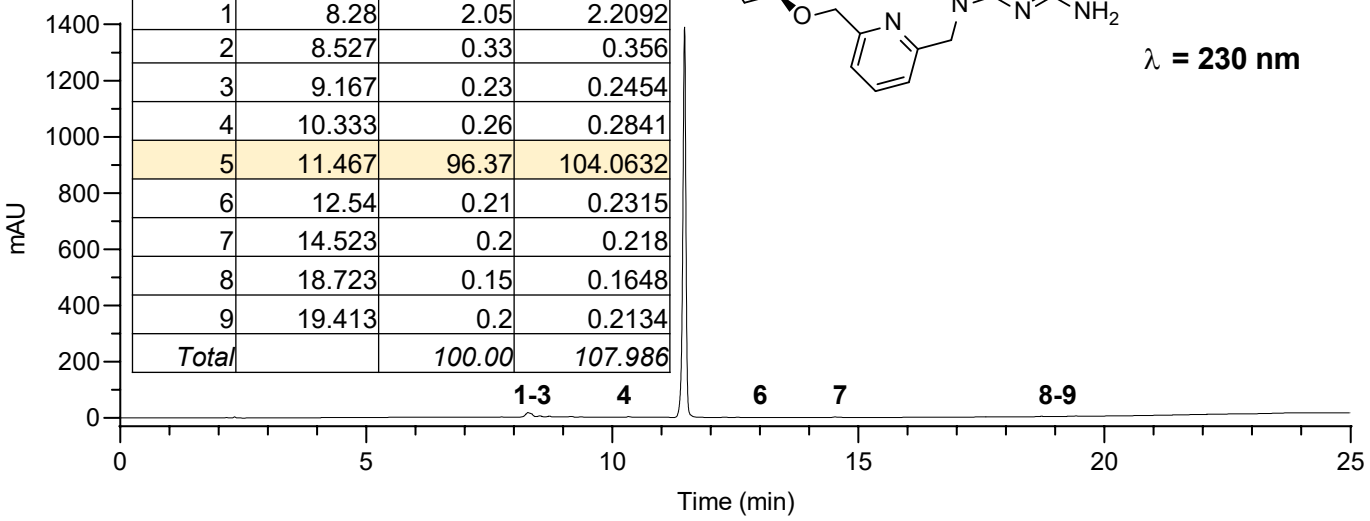


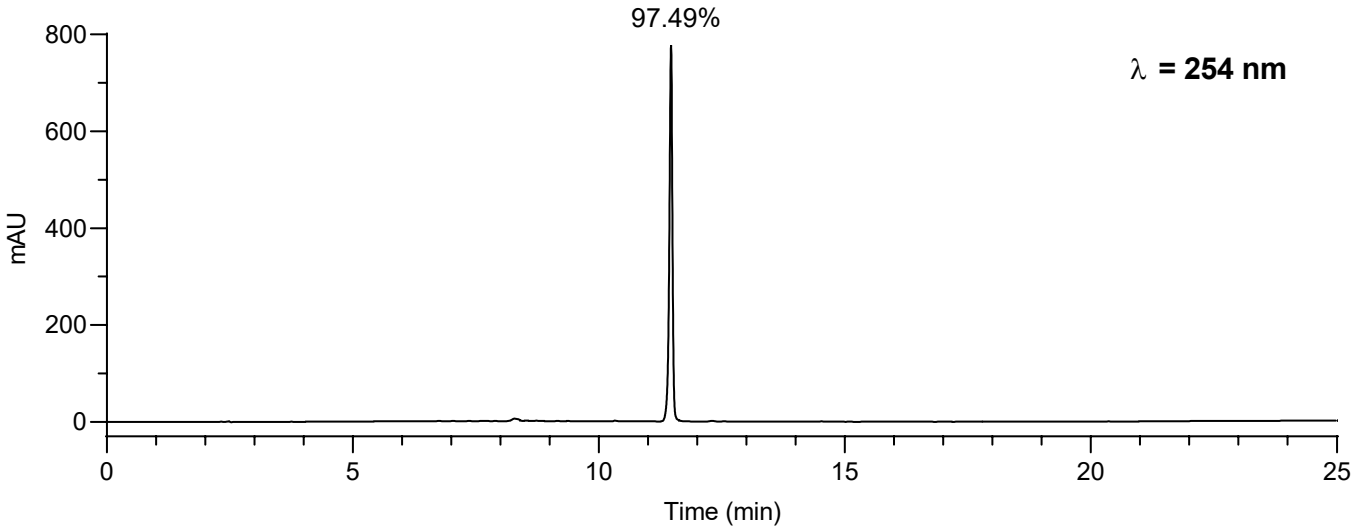


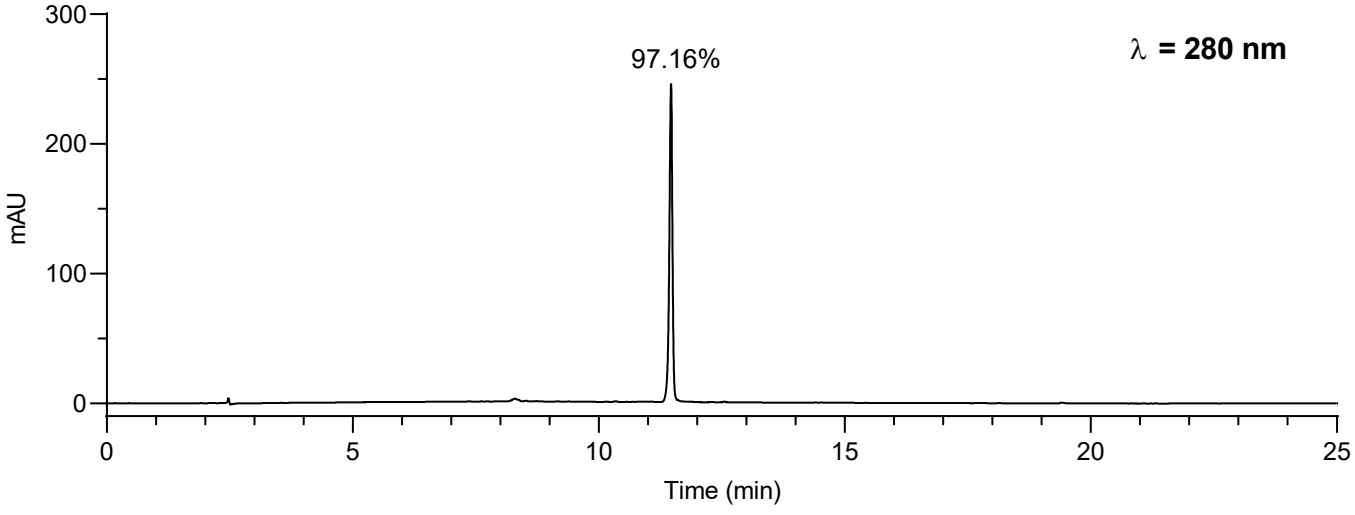
25



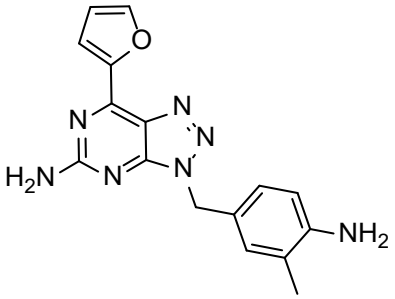
Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	8.28	2.05	2.2092
2	8.527	0.33	0.356
3	9.167	0.23	0.2454
4	10.333	0.26	0.2841
5	11.467	96.37	104.0632
6	12.54	0.21	0.2315
7	14.523	0.2	0.218
8	18.723	0.15	0.1648
9	19.413	0.2	0.2134
Total		*100.00*	*107.986*



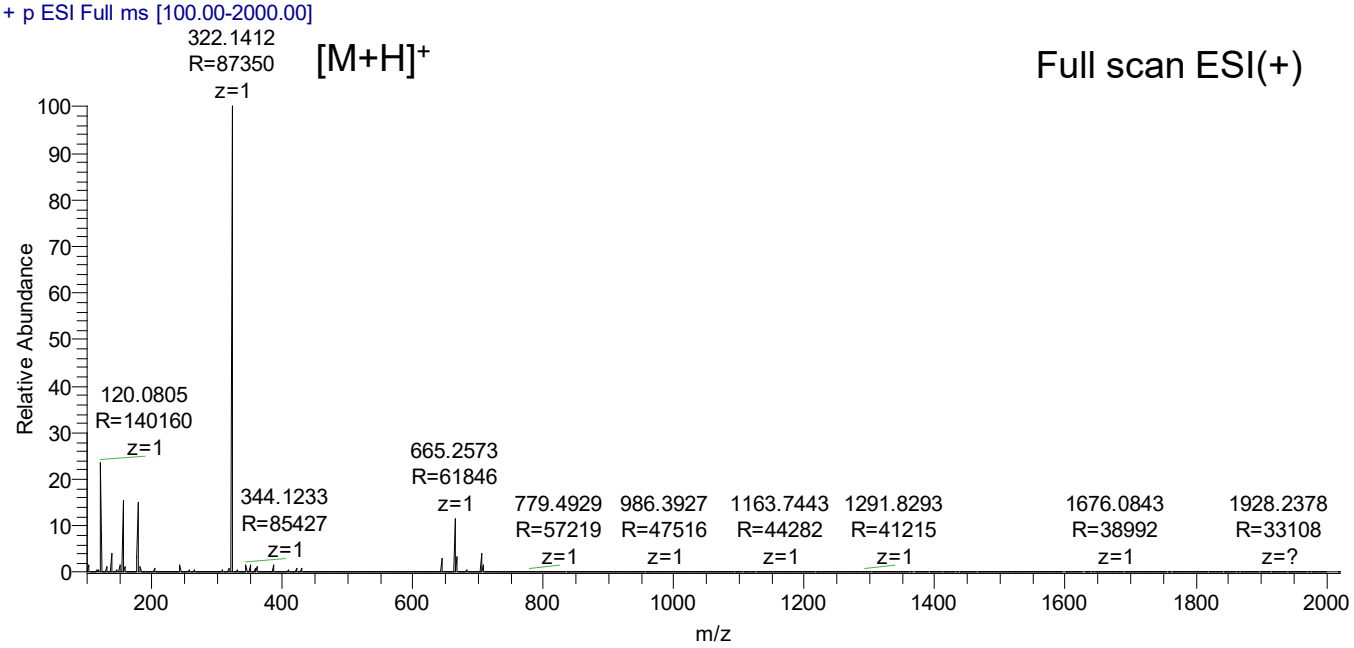


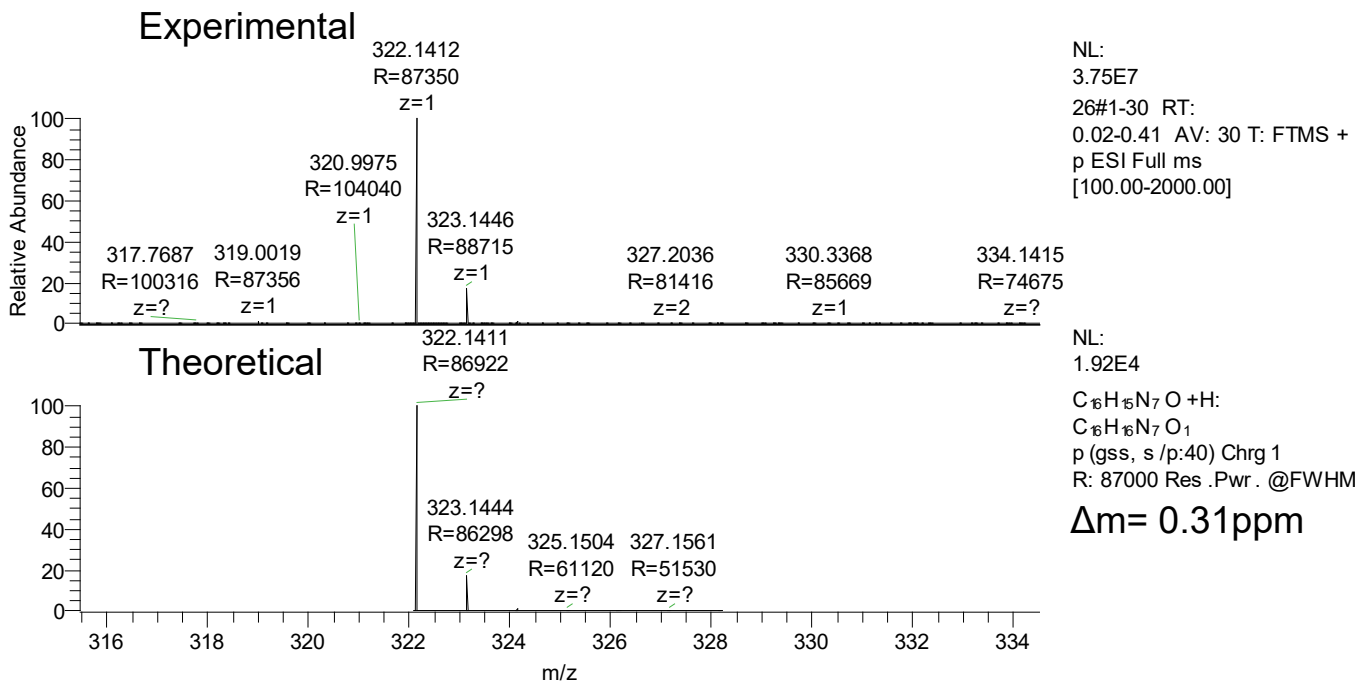


26

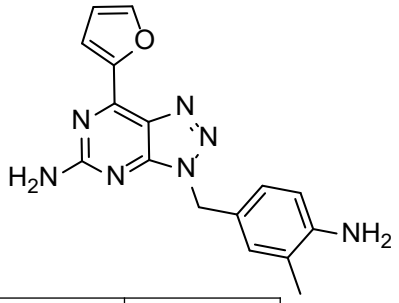


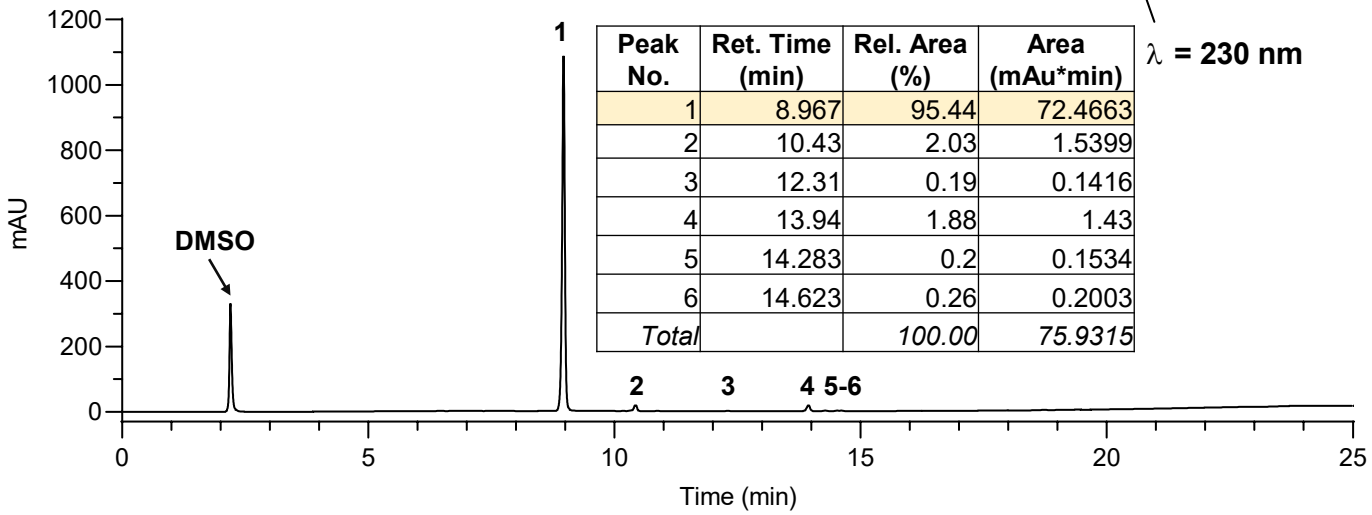
26 #1-30 RT: 0.02-0.41 AV: 30 NL: 3.75E7 T: FTMS
+ p ESI Full ms [100.00-2000.00]





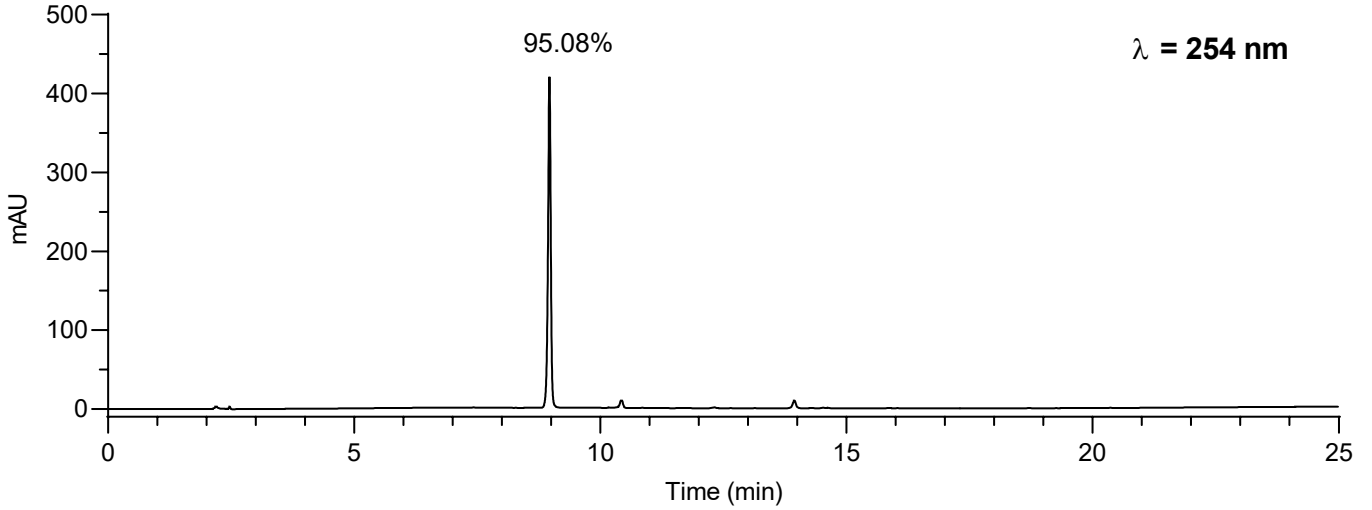
26



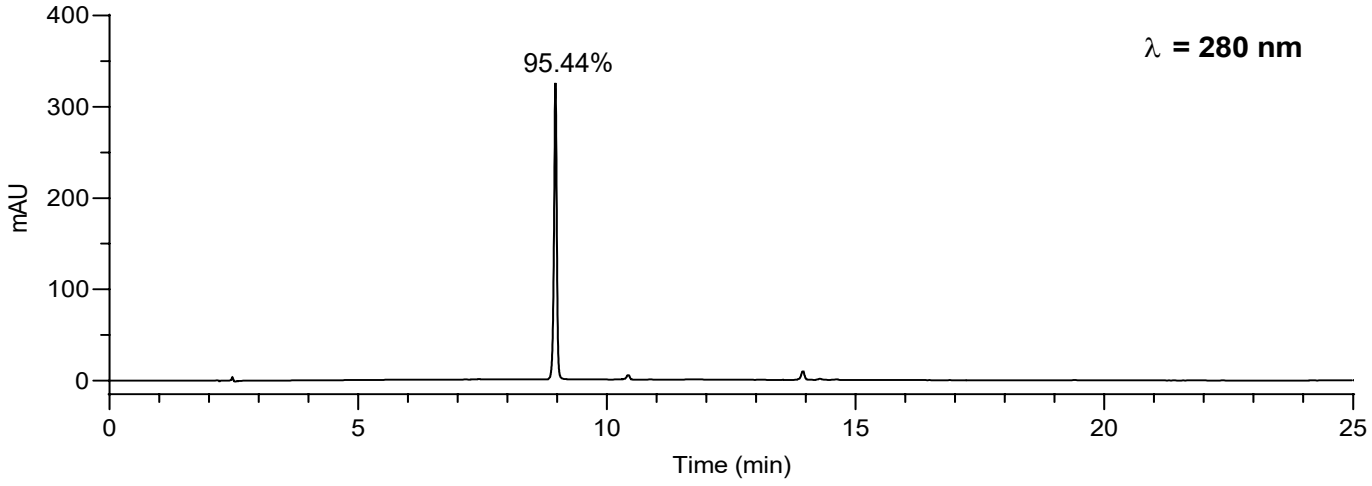


Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	8.967	95.44	72.4663
2	10.43	2.03	1.5399
3	12.31	0.19	0.1416
4	13.94	1.88	1.43
5	14.283	0.2	0.1534
6	14.623	0.26	0.2003
Total		*100.00*	*75.9315*

λ = 230 nm

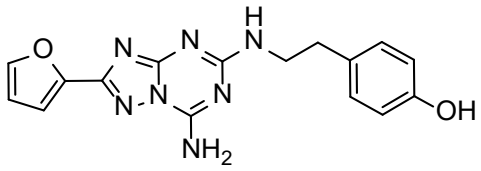


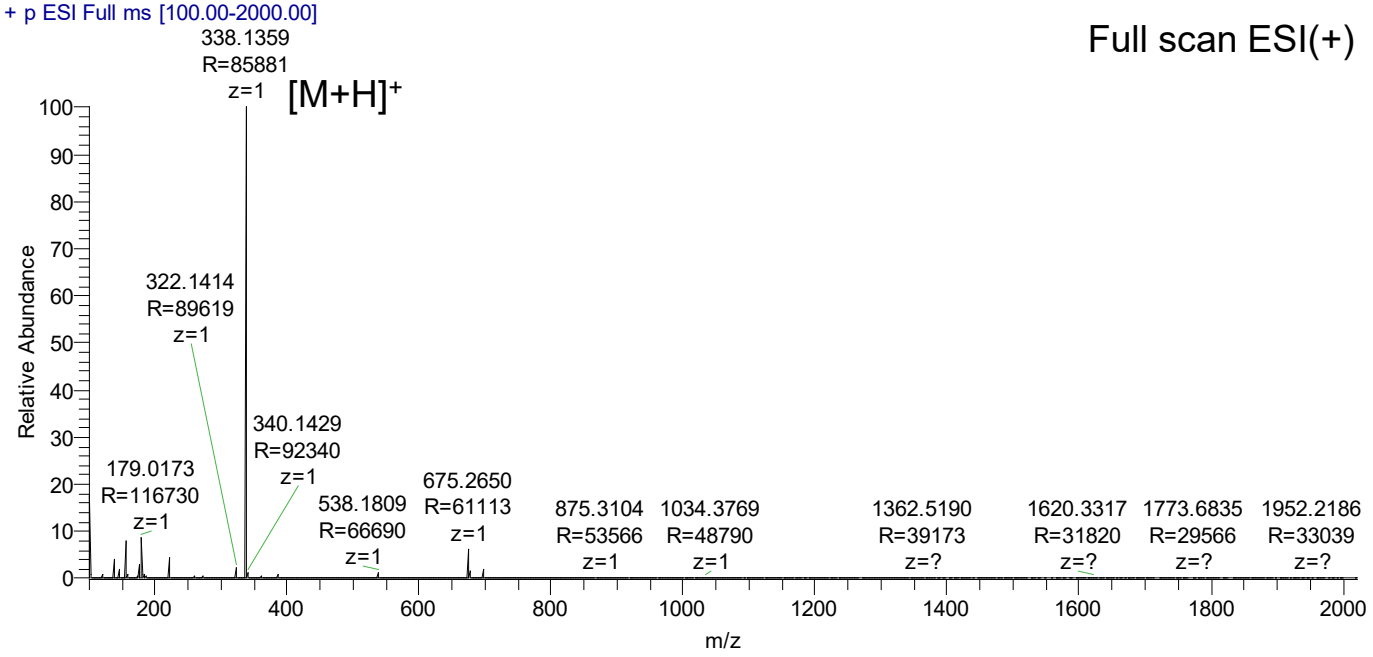
λ = 254 nm

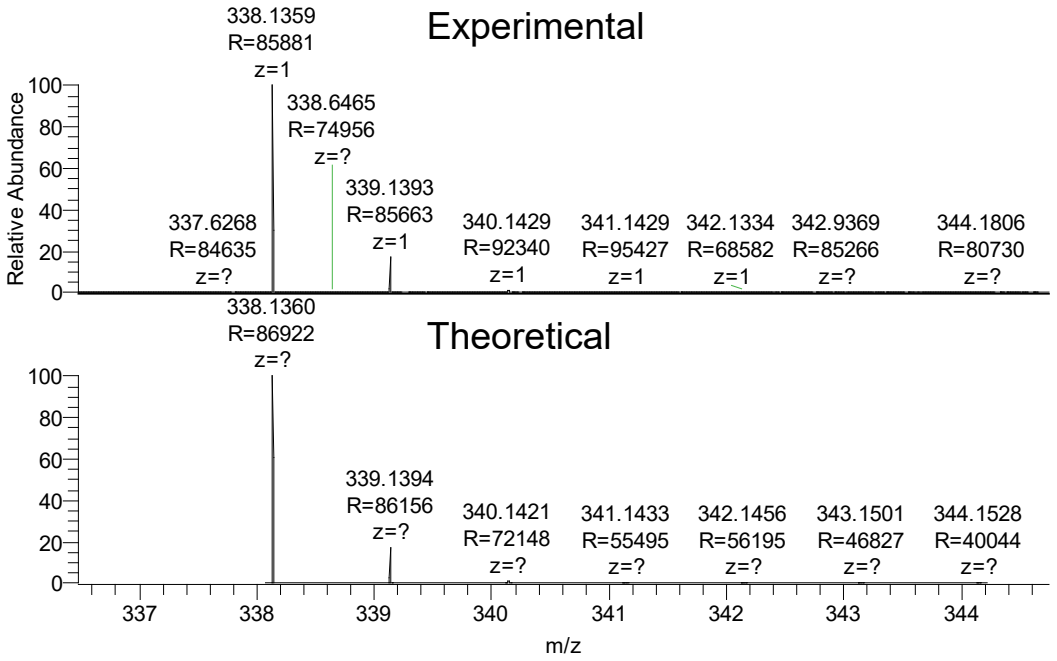


λ = 280 nm

27





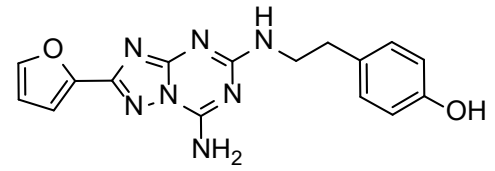


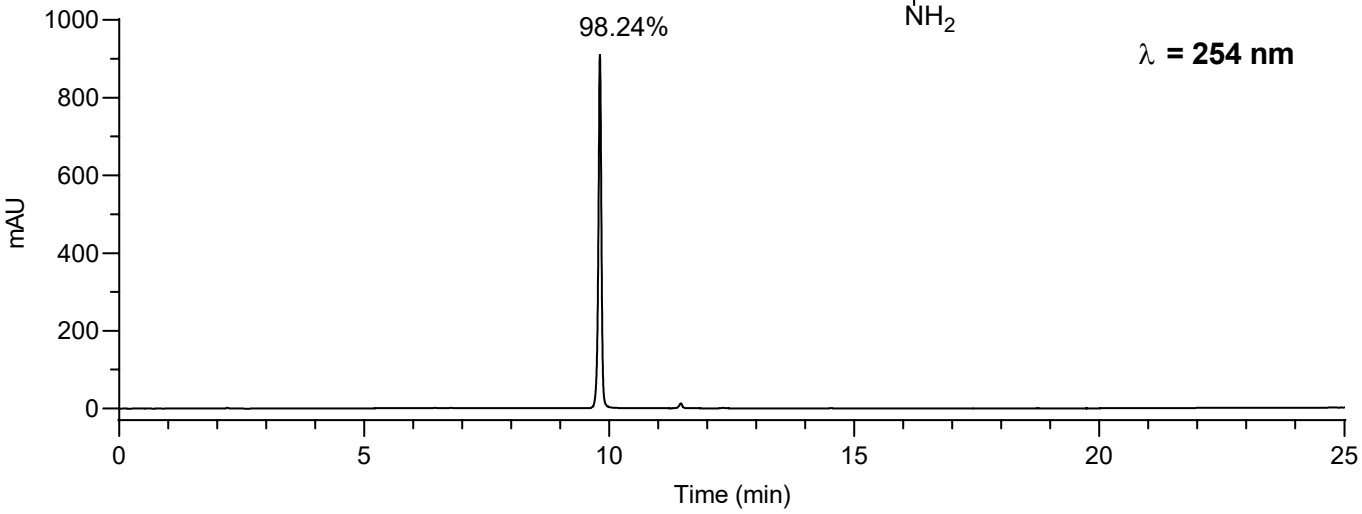
NL:
1.74E7
27#2-29 RT:
0.03-0.40 AV: 28 T: FTMS +
p ESI Full ms
[100.00-2000.00]

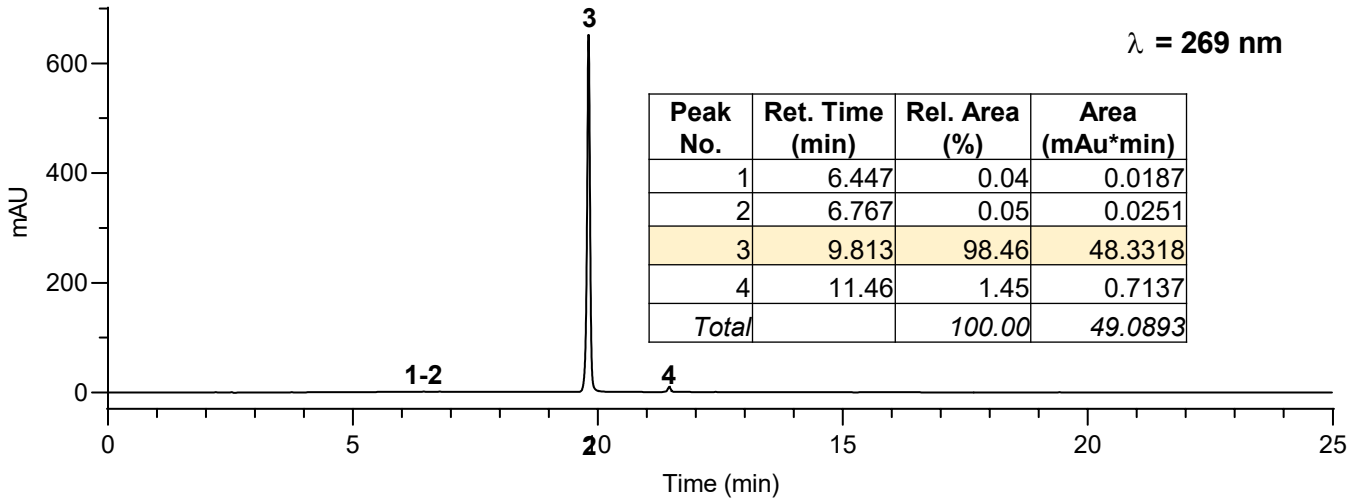
NL:
1.91E4
$C_{16}H_{15}N_7O_2$ +H:
$C_{16}H_{16}N_7O_2$
p (gss, s /p:40) Chrg 1
R: 87000 Res .Pwr. @FWHM

Δm= 0.30ppm

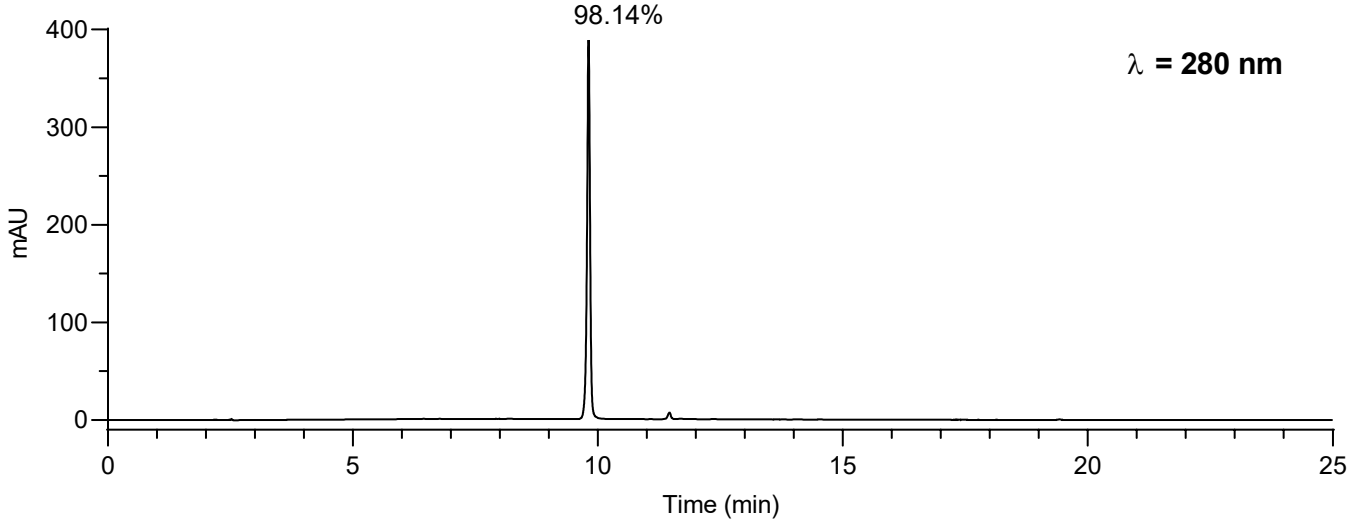
27



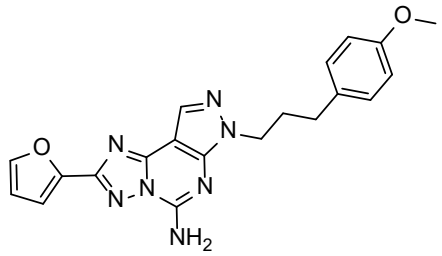




Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	6.447	0.04	0.0187
2	6.767	0.05	0.0251
3	9.813	98.46	48.3318
4	11.46	1.45	0.7137
Total		*100.00*	*49.0893*

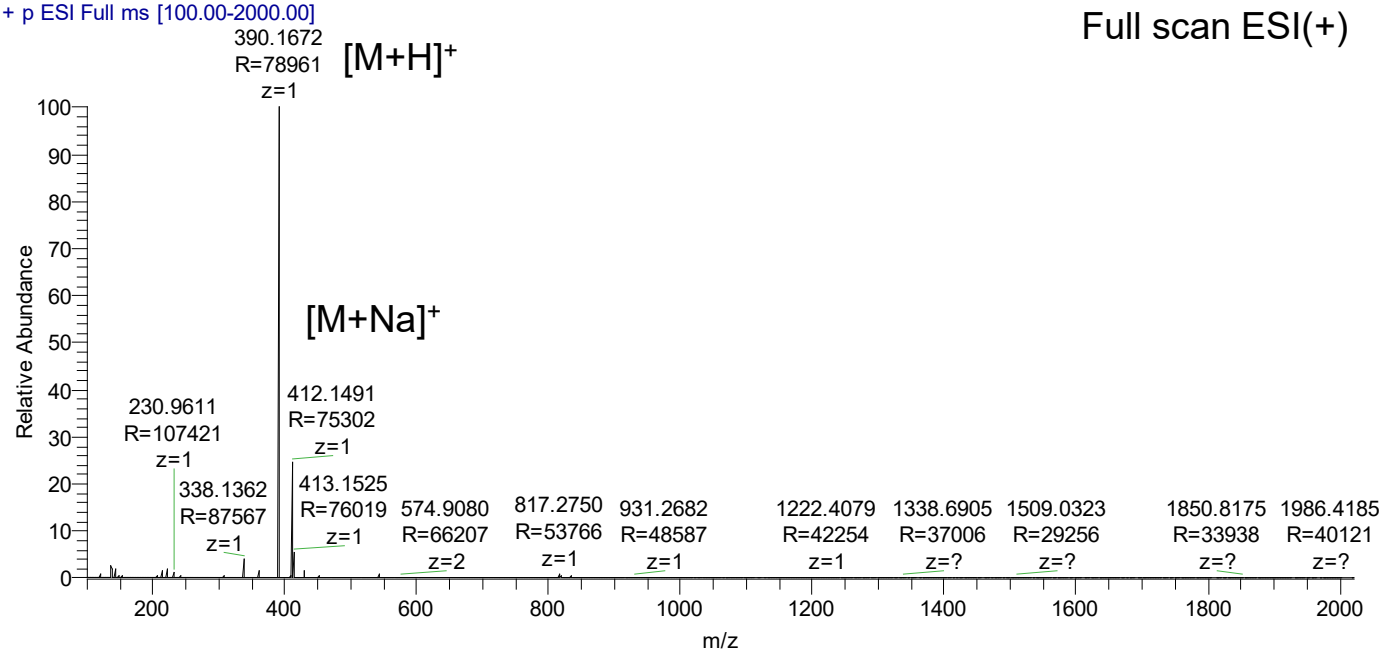


28

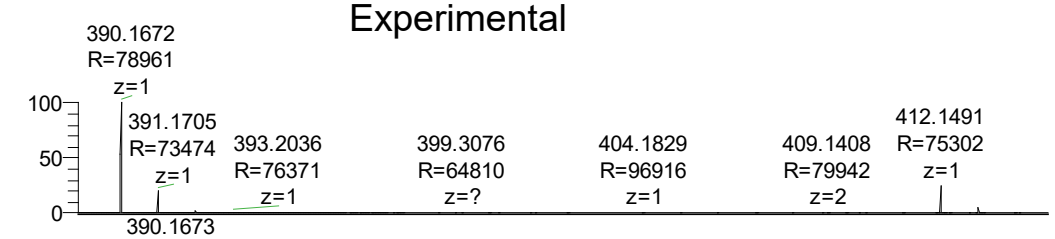


28 #1-30 RT: 0.02-0.41 AV: 30 NL: 2.35E7 T: FTMS
+ p ESI Full ms [100.00-2000.00]

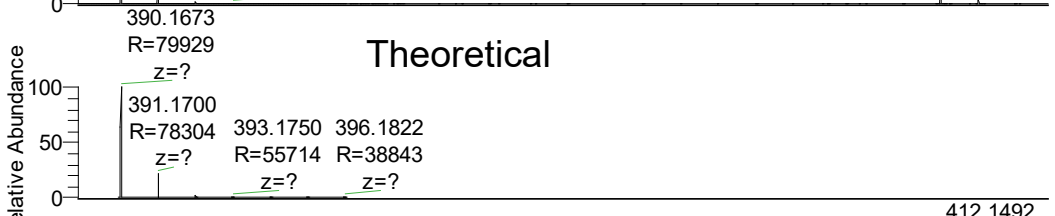
Full scan ESI(+)



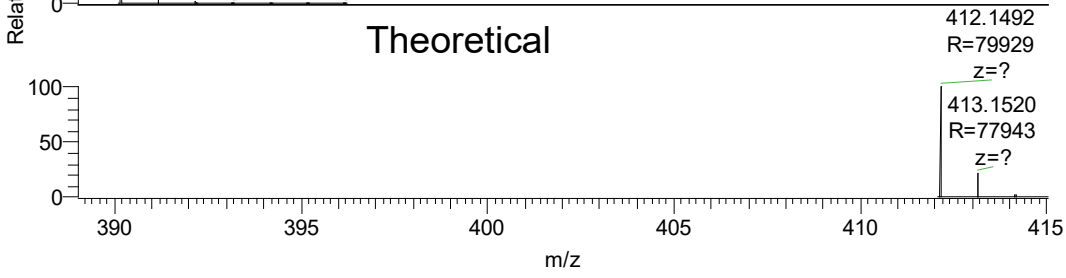
Experimental



Theoretical



Theoretical

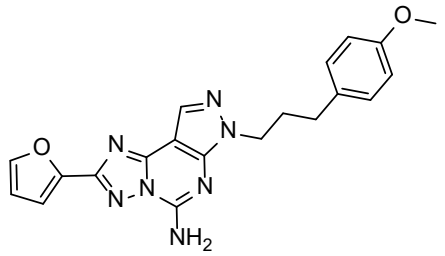


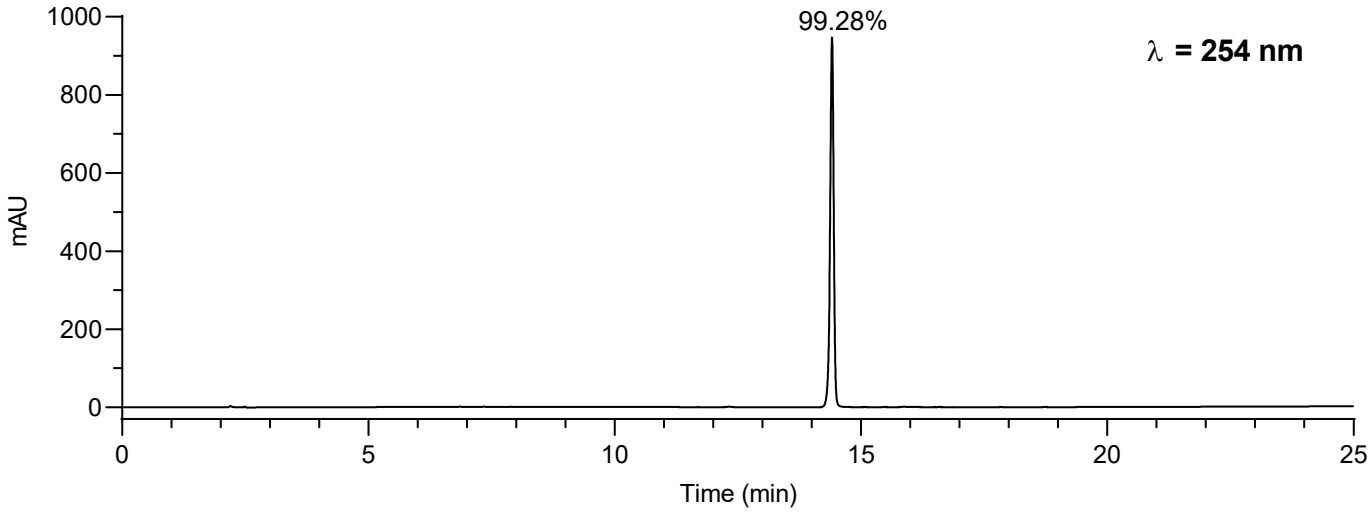
NL:
2.35E7
28#1-30 RT: 0.02-0.41 AV: 30 T: FTMS + p ESI Full ms [100.00-2000.00]

NL: Δm= 0.26ppm
1.83E4
$C_{20}H_{19}N_7O_2$ +H:
$C_{20}H_{20}N_7O_2$
p (gss, s /p:40) Chrg 1
R: 80000 Res .Pwr . @FWHM

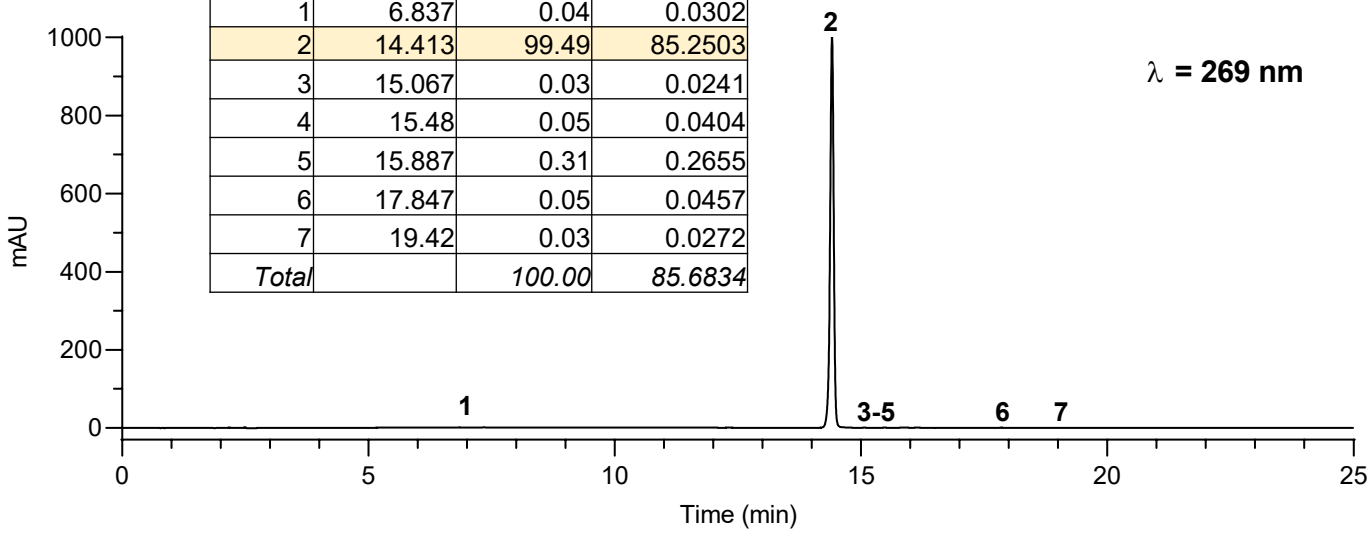
NL: Δm= 0.24ppm
1.83E4
$C_{20}H_{19}N_7O_2$ +Na:
$C_{20}H_{19}N_7O_2Na_1$
p (gss, s /p:40) Chrg 1
R: 80000 Res .Pwr . @FWHM

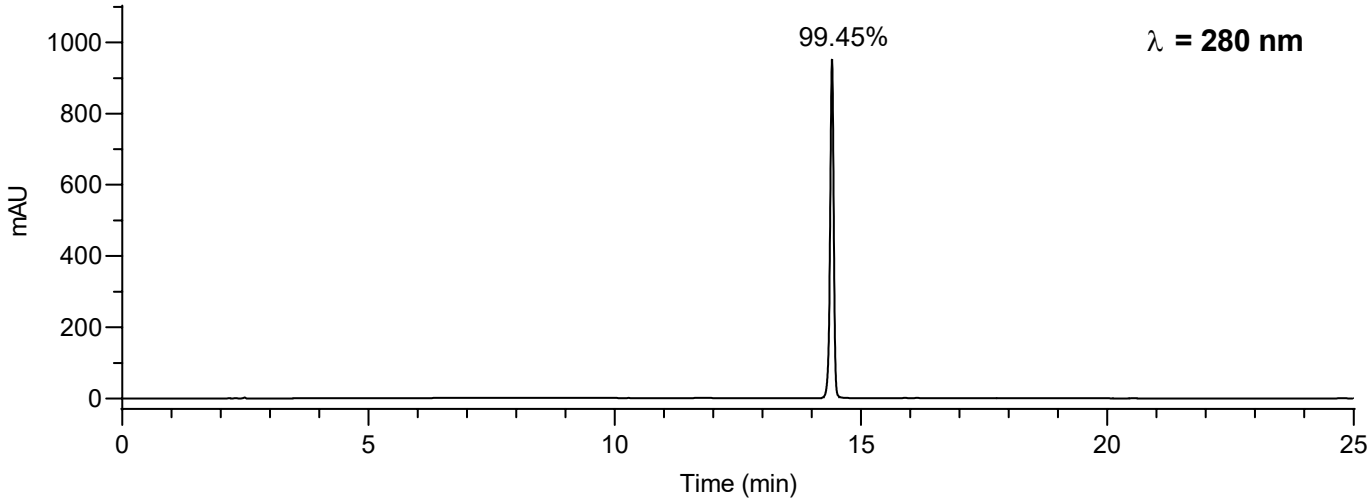
28



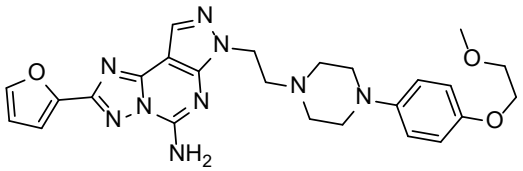


Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	6.837	0.04	0.0302
2	14.413	99.49	85.2503
3	15.067	0.03	0.0241
4	15.48	0.05	0.0404
5	15.887	0.31	0.2655
6	17.847	0.05	0.0457
7	19.42	0.03	0.0272
Total		*100.00*	*85.6834*

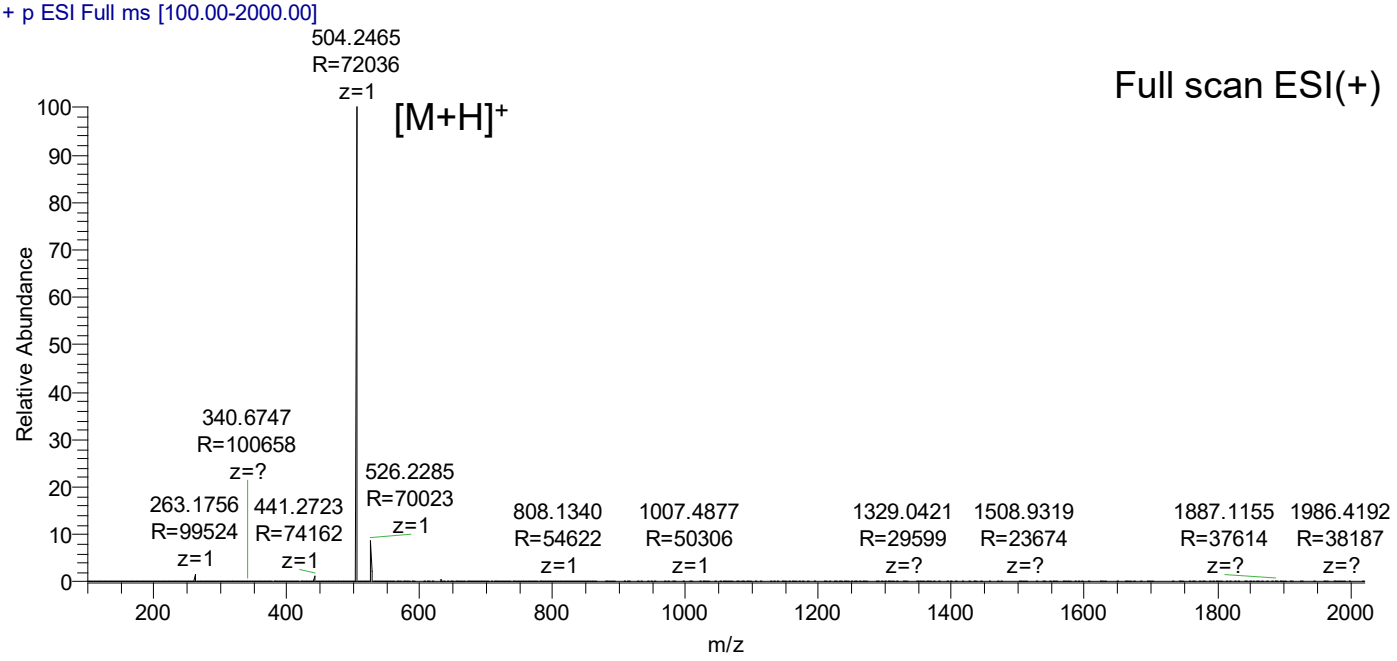


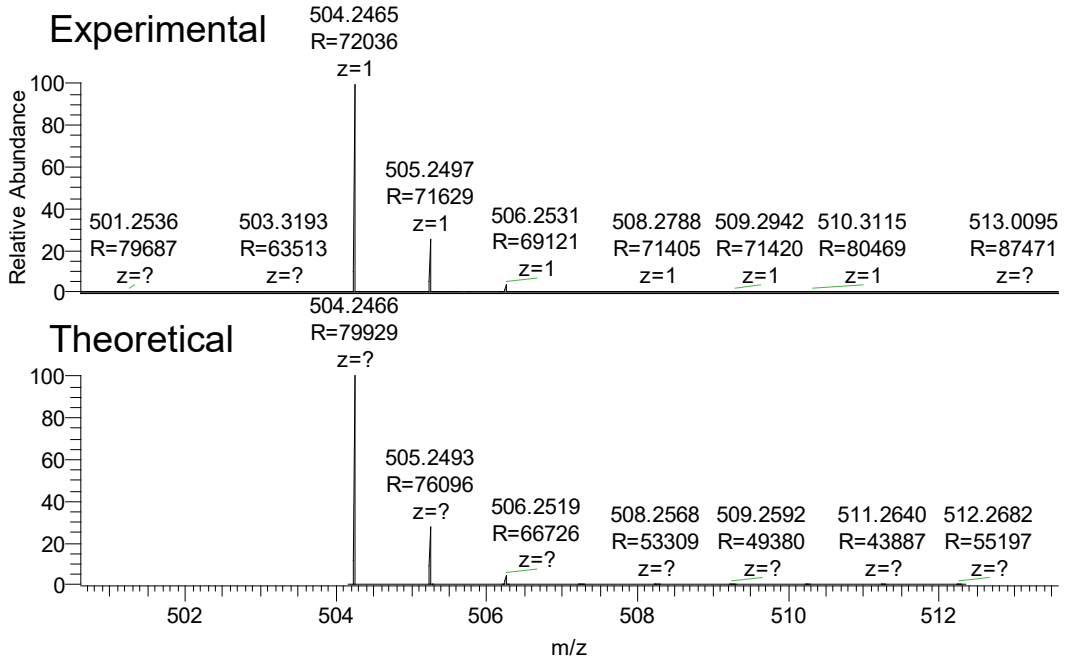


29



29 #1-30 RT: 0.02-0.41 AV: 30 NL: 1.18E8 T: FTMS
+ p ESI Full ms [100.00-2000.00]



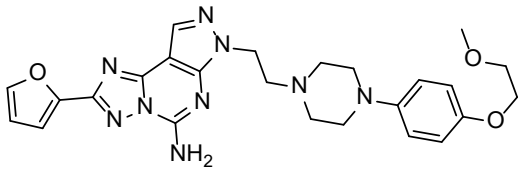


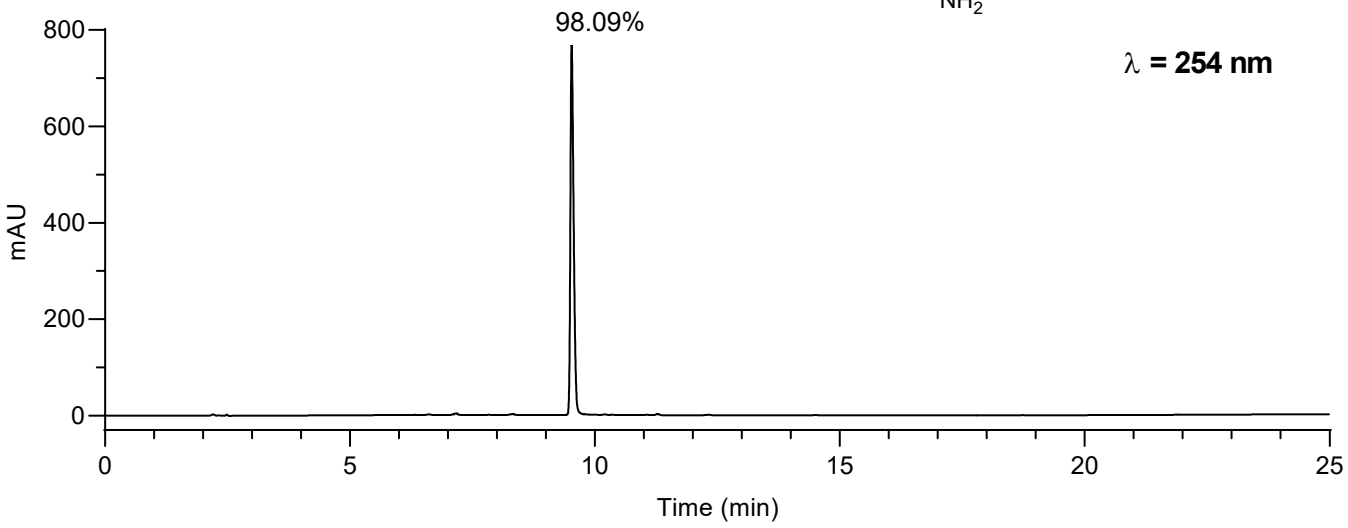
NL:
1.18E8
29#1-30 RT:
0.02-0.41 AV: 30 T: FTMS +
p ESI Full ms
[100.00-2000.00]

NL:
1.72E4
$C_{25}H_{29}N_9O_3$ +H:
$C_{25}H_{30}N_9O_3$
p (gss, s /p:40) Chrg 1
R: 80000 Res .Pwr. @FWHM

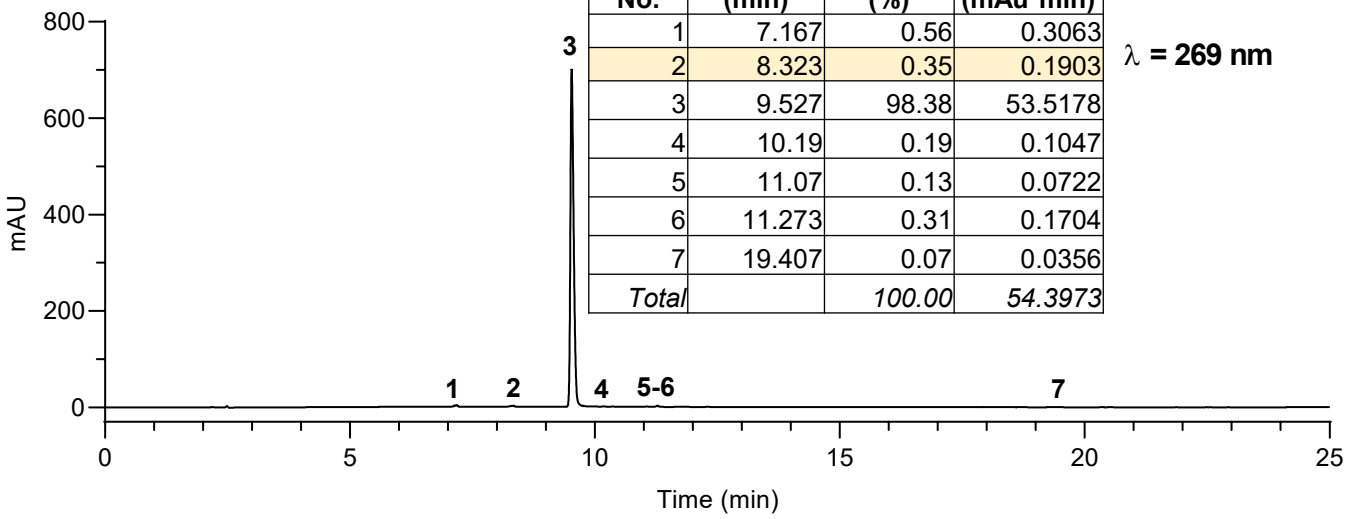
Δm=0.20 ppm

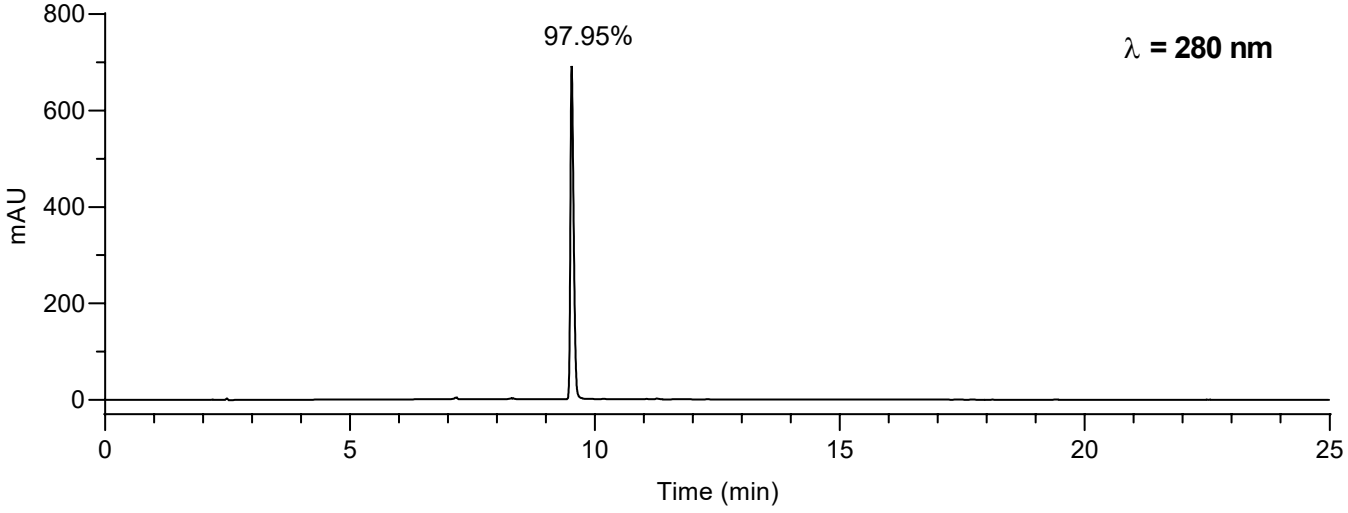
29



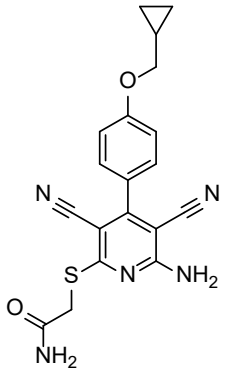


Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	7.167	0.56	0.3063
2	8.323	0.35	0.1903
3	9.527	98.38	53.5178
4	10.19	0.19	0.1047
5	11.07	0.13	0.0722
6	11.273	0.31	0.1704
7	19.407	0.07	0.0356
Total		*100.00*	*54.3973*



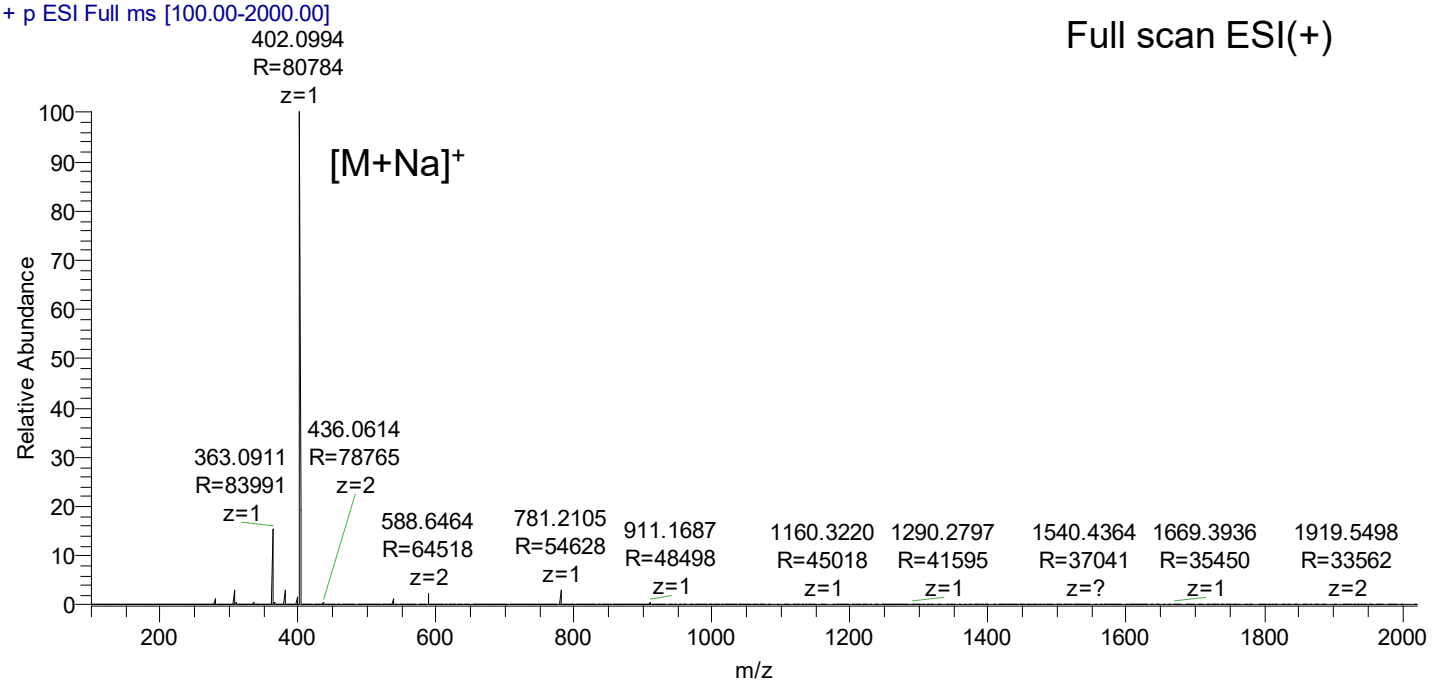


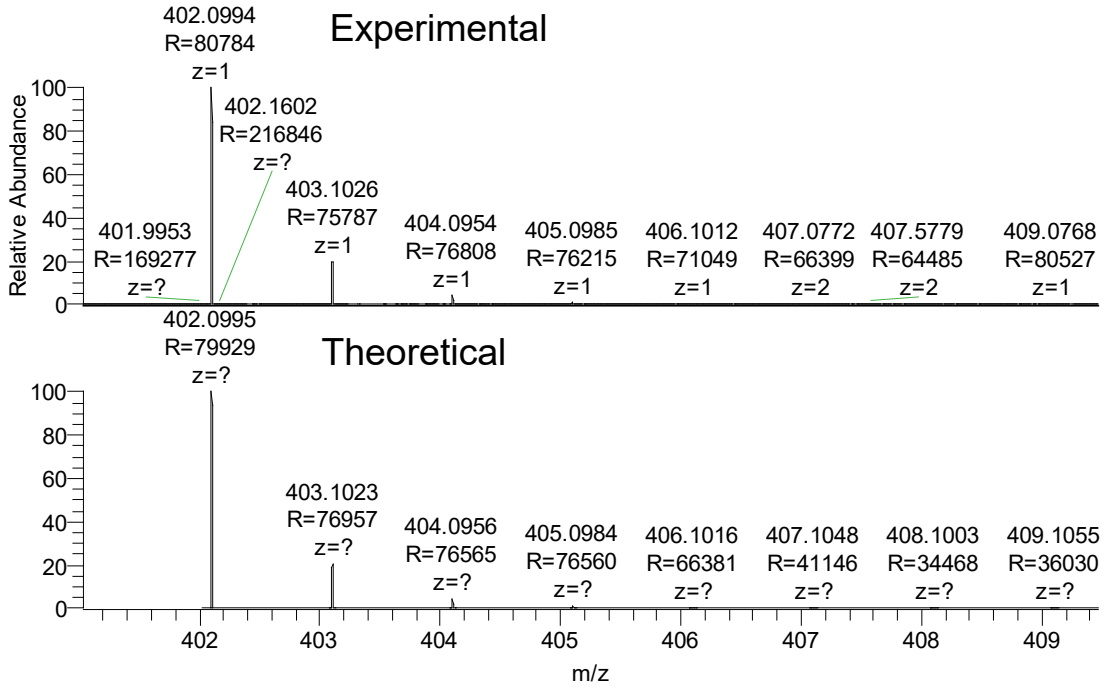
30



30 #2-28 RT: 0.03-0.39 AV: 27 NL: 3.03E7 T: FTMS
+ p ESI Full ms [100.00-2000.00]

Full scan ESI(+)



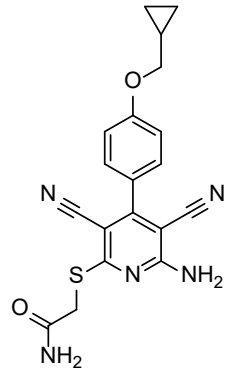


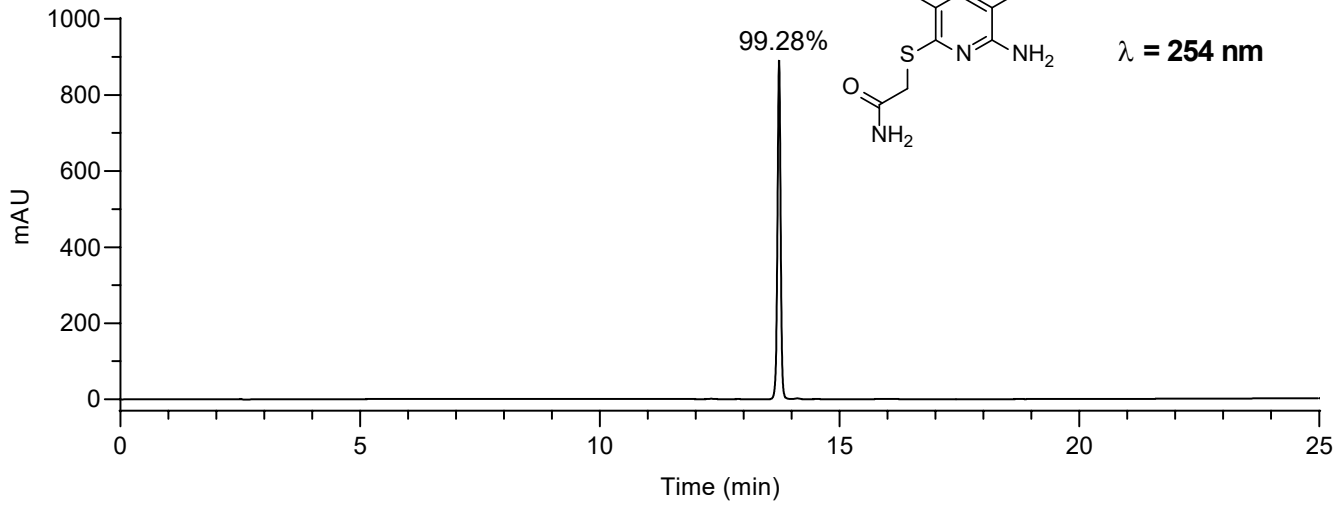
NL:
3.03E7
30#2-28 RT:
0.03-0.39 AV: 27 T: FTMS +
p ESI Full ms
[100.00-2000.00]

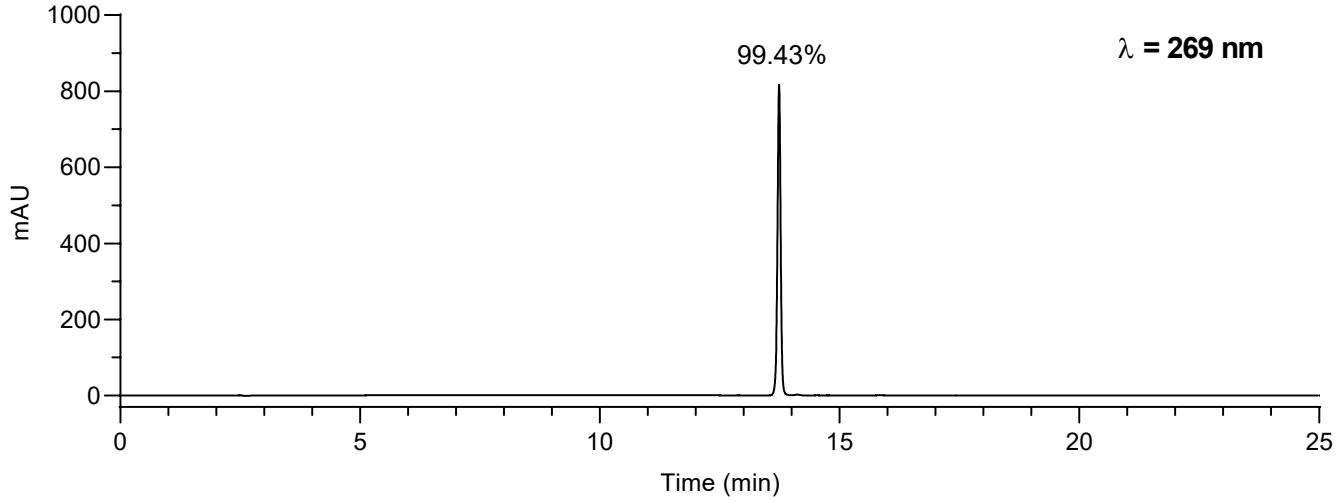
NL:
1.77E4
$C_{19}H_{17}N_5O_2S$ +Na:
$C_{19}H_{17}N_5O_2S_1Na_1$
p (gss, s /p:40) Chrg 1
R: 80000 Res .Pwr. @FWHM

Δm= 0.25 ppm

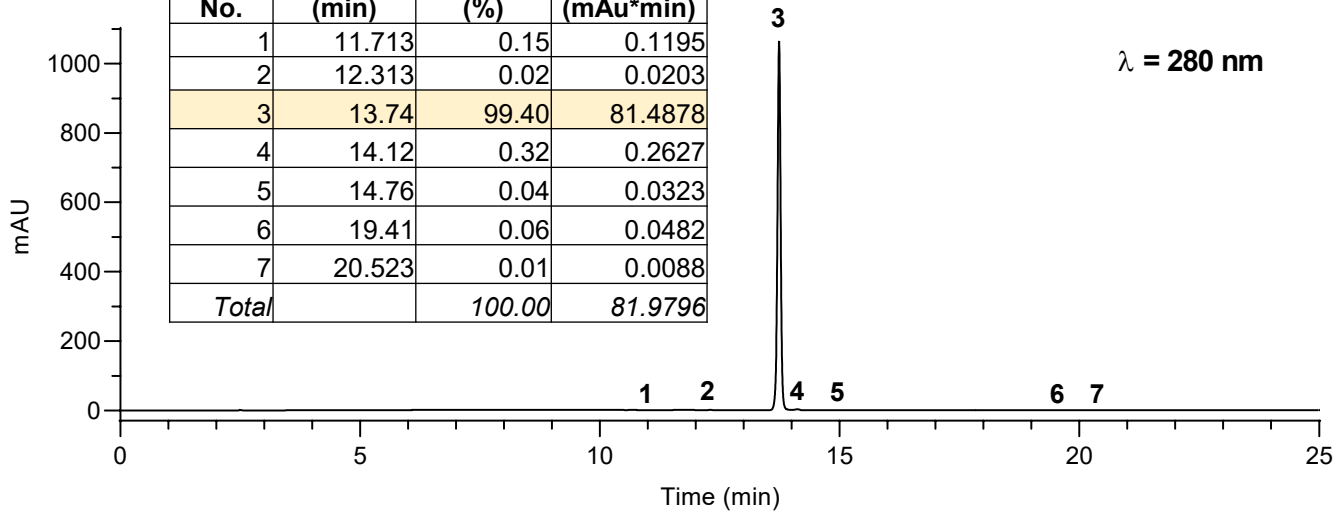
30



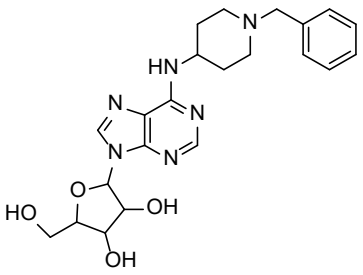




Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	11.713	0.15	0.1195
2	12.313	0.02	0.0203
3	13.74	99.40	81.4878
4	14.12	0.32	0.2627
5	14.76	0.04	0.0323
6	19.41	0.06	0.0482
7	20.523	0.01	0.0088
Total		*100.00*	*81.9796*

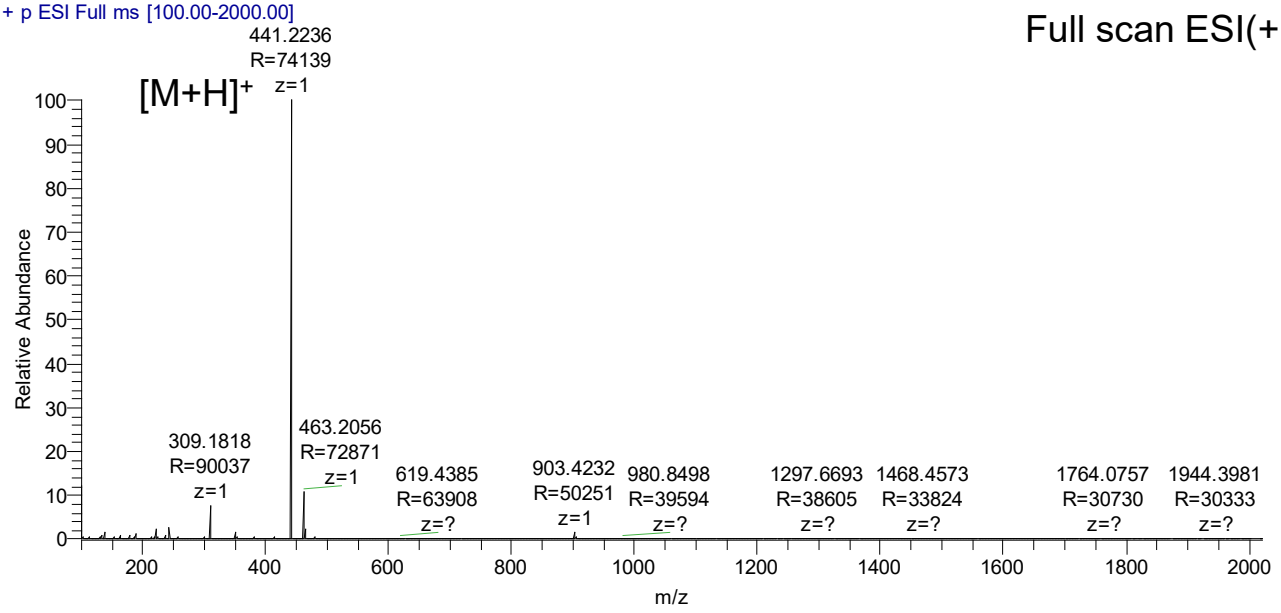


31

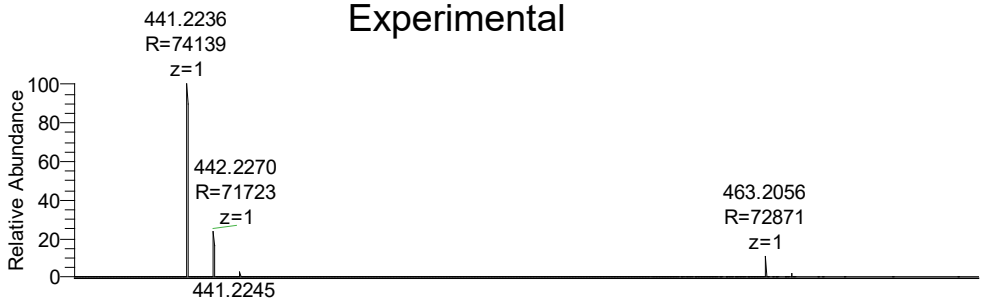


31 #1-30 RT: 0.02-0.42 AV: 30 NL: 1.46E7 T: FTMS
+ p ESI Full ms [100.00-2000.00]

Full scan ESI(+)

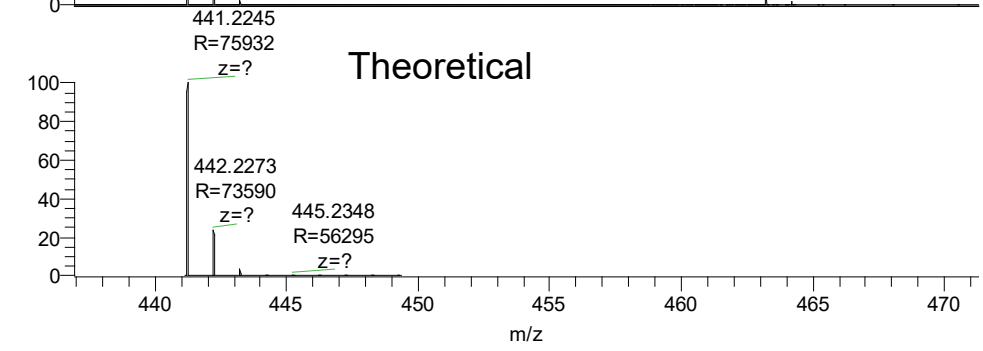


Experimental



NL:
1.46E7
31#1-30 RT:
0.02-0.42 AV: 30 T: FTMS +
p ESI Full ms
[100.00-2000.00]

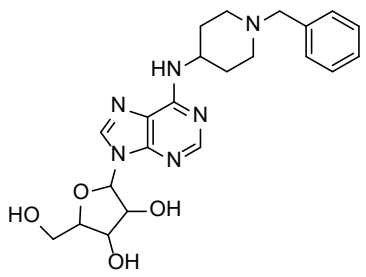
Theoretical

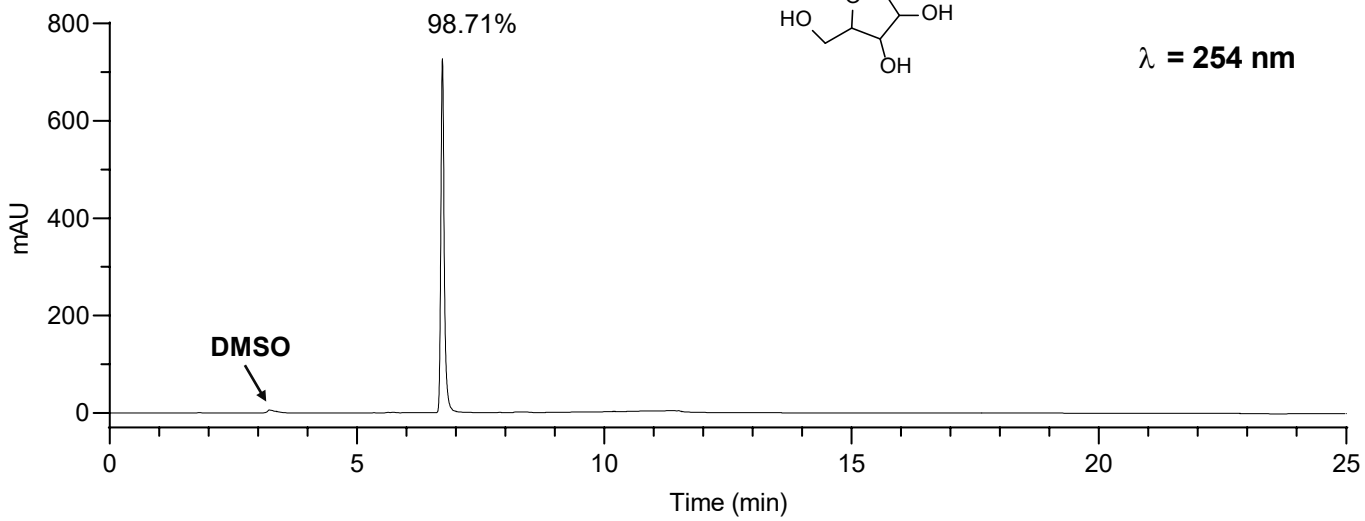


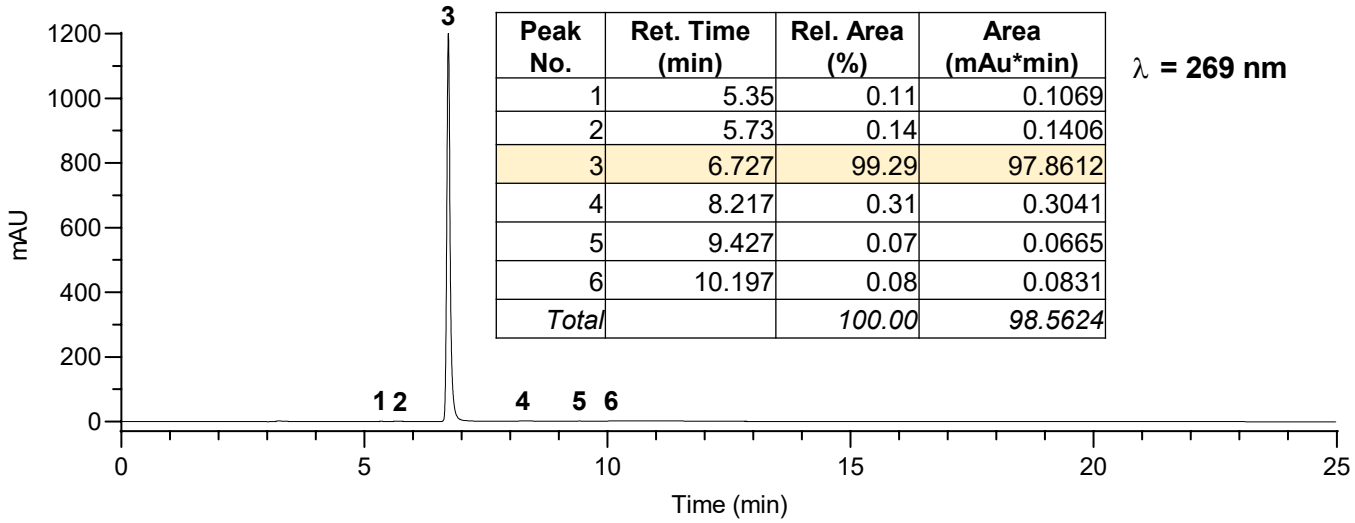
NL:
1.79E4
$C_{22}H_{28}N_6O_4$ +H:
$C_{22}H_{29}N_6O_4$
p (gss, s /p:40) Chrg 1
R: 76000 Res .Pwr. @FWHM

Δm= 2.04 ppm

31

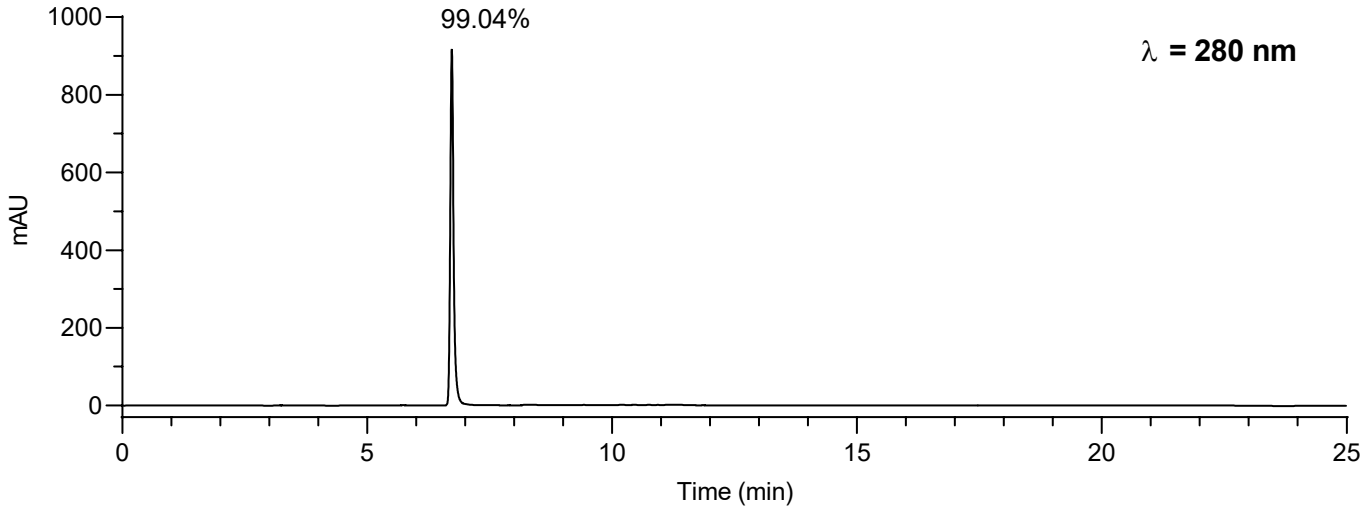




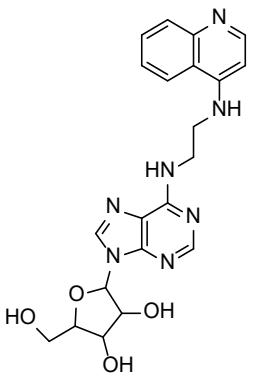


Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	5.35	0.11	0.1069
2	5.73	0.14	0.1406
3	6.727	99.29	97.8612
4	8.217	0.31	0.3041
5	9.427	0.07	0.0665
6	10.197	0.08	0.0831
Total		*100.00*	*98.5624*

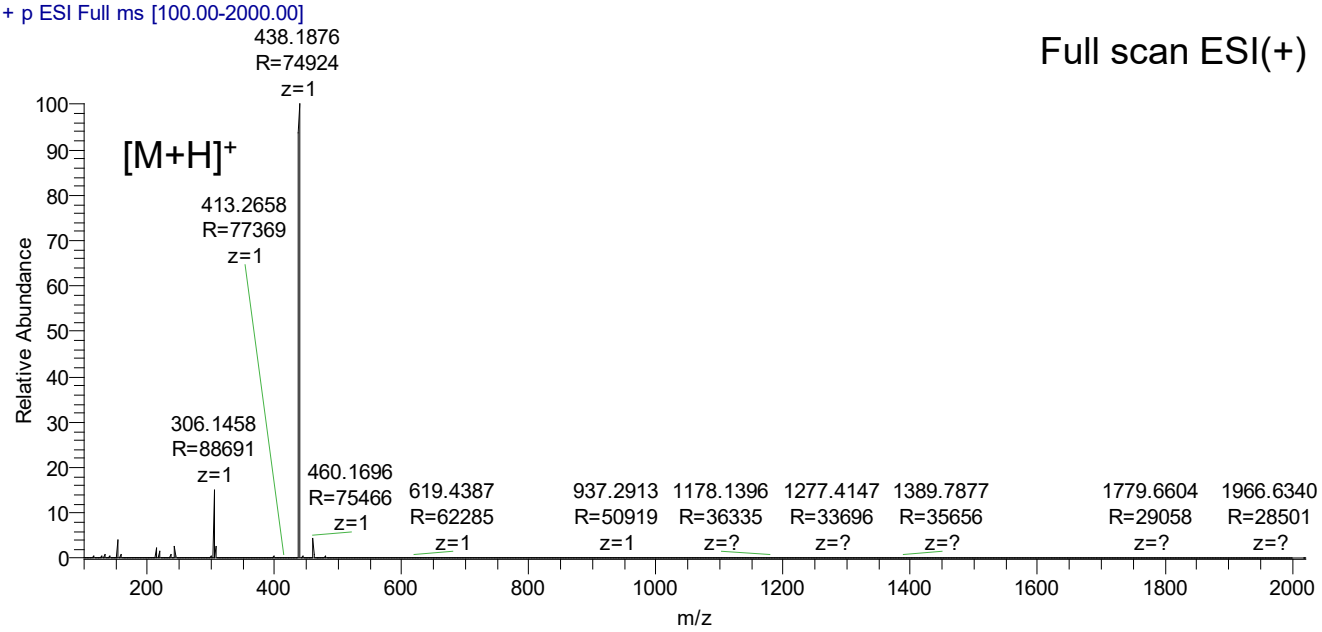
λ = 269 nm

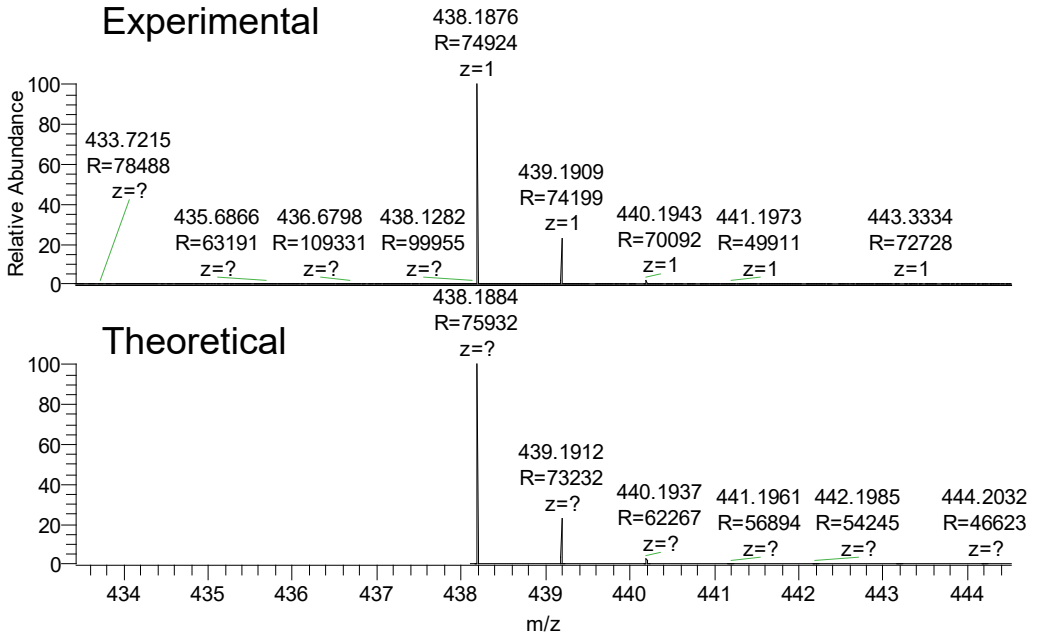


32



32 #1-30 RT: 0.02-0.42 AV: 30 NL: 1.49E7 T: FTMS
+ p ESI Full ms [100.00-2000.00]



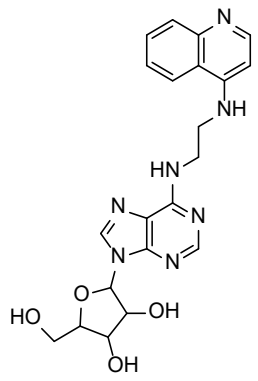


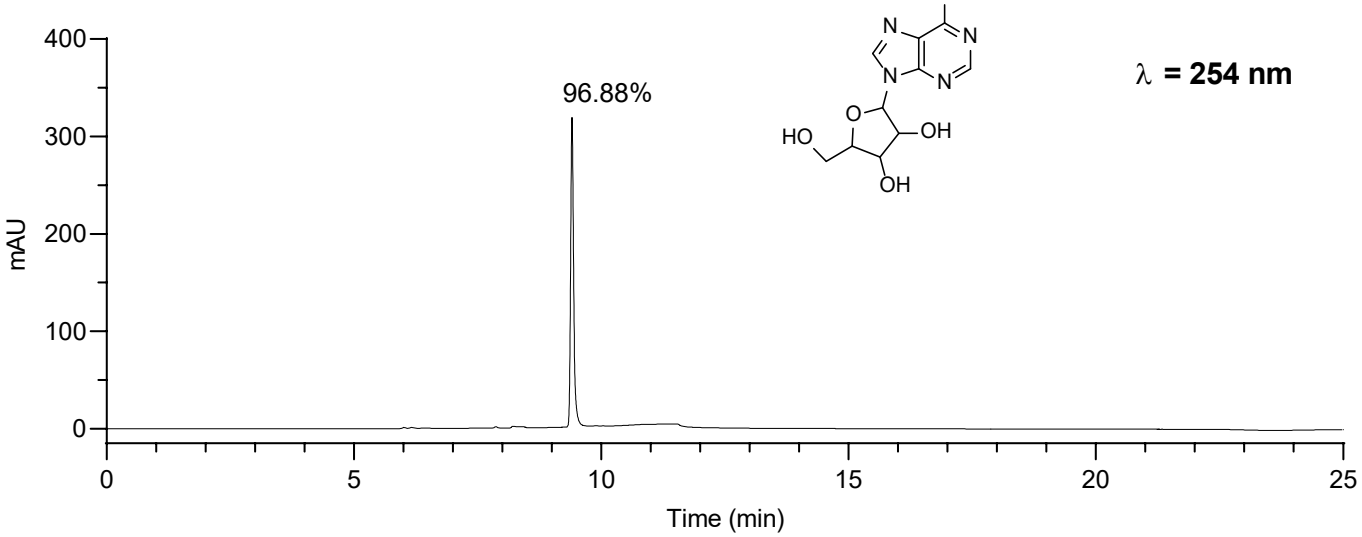
NL:
1.49E7
32#1-30 RT:
0.02-0.42 AV: 30 T: FTMS +
p ESI Full ms
[100.00-2000.00]

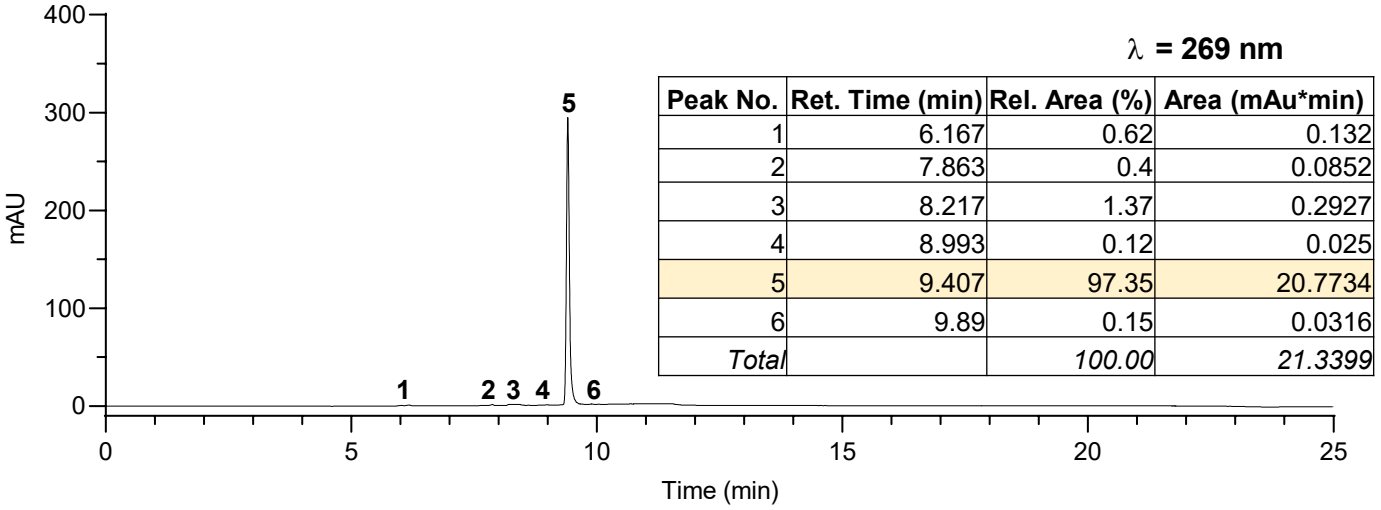
NL:
1.80E4
$C_{21}H_{23}N_7O_4$ +H:
$C_{21}H_{24}N_7O_4$
p (gss, s /p:40) Chrg 1
R: 76000 Res .Pwr . @FWHM

Δm= 1.83 ppm

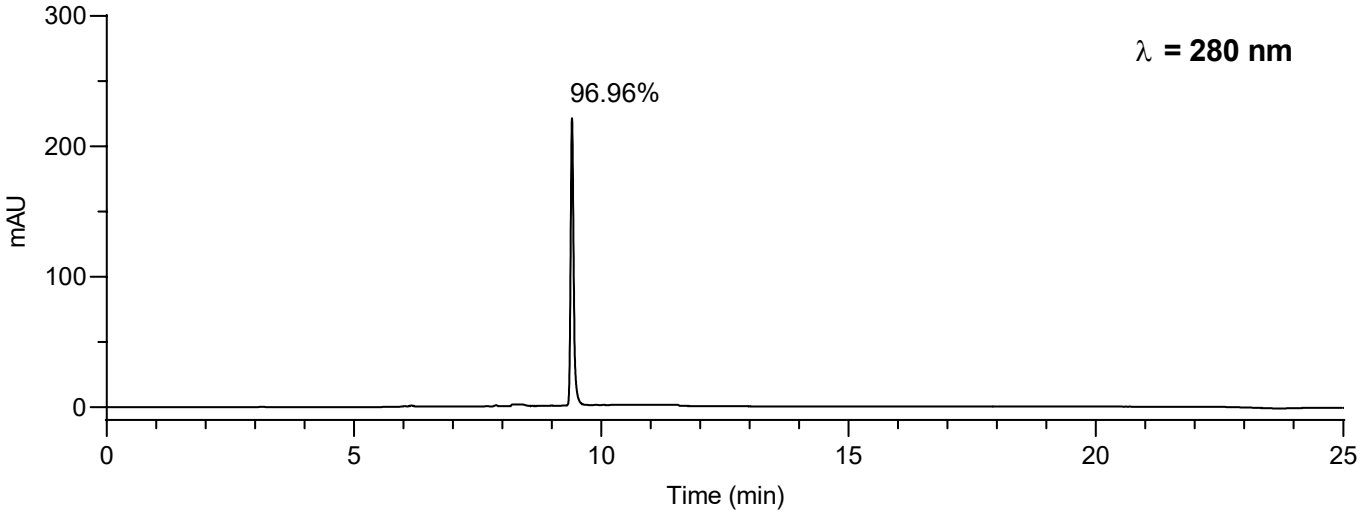
32



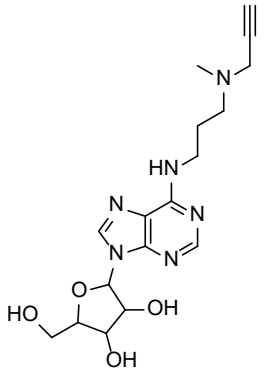


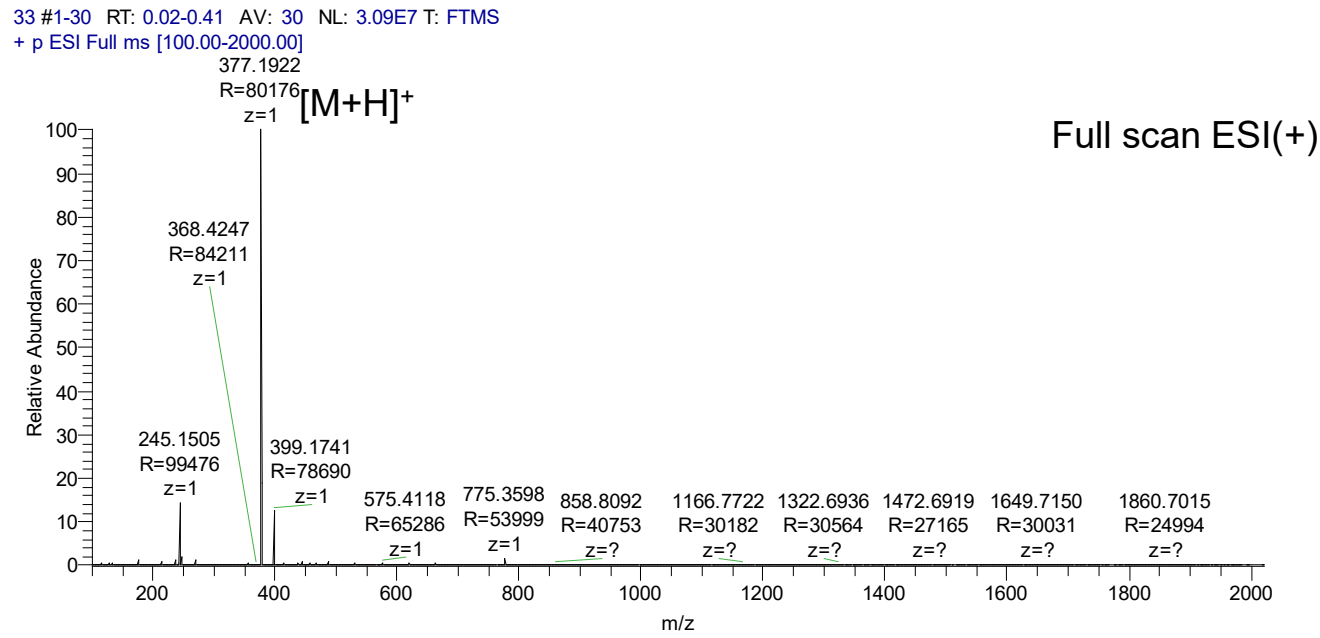


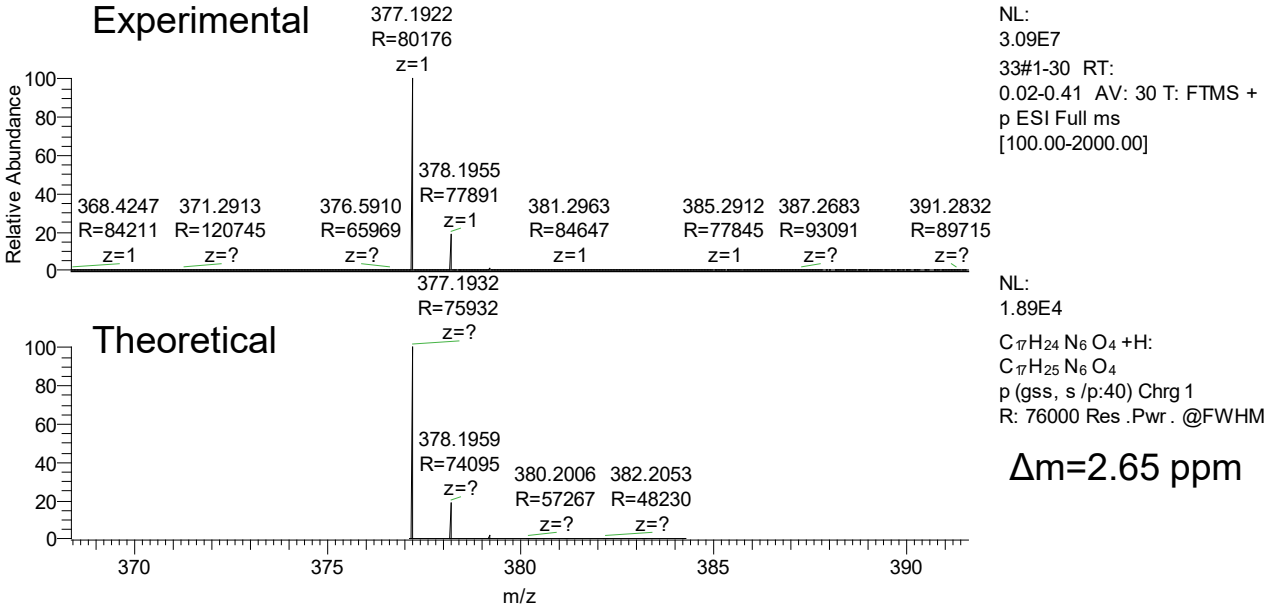
Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	6.167	0.62	0.132
2	7.863	0.4	0.0852
3	8.217	1.37	0.2927
4	8.993	0.12	0.025
5	9.407	97.35	20.7734
6	9.89	0.15	0.0316
Total		*100.00*	*21.3399*



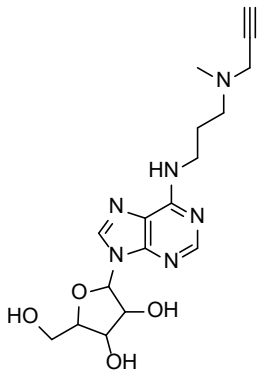
33

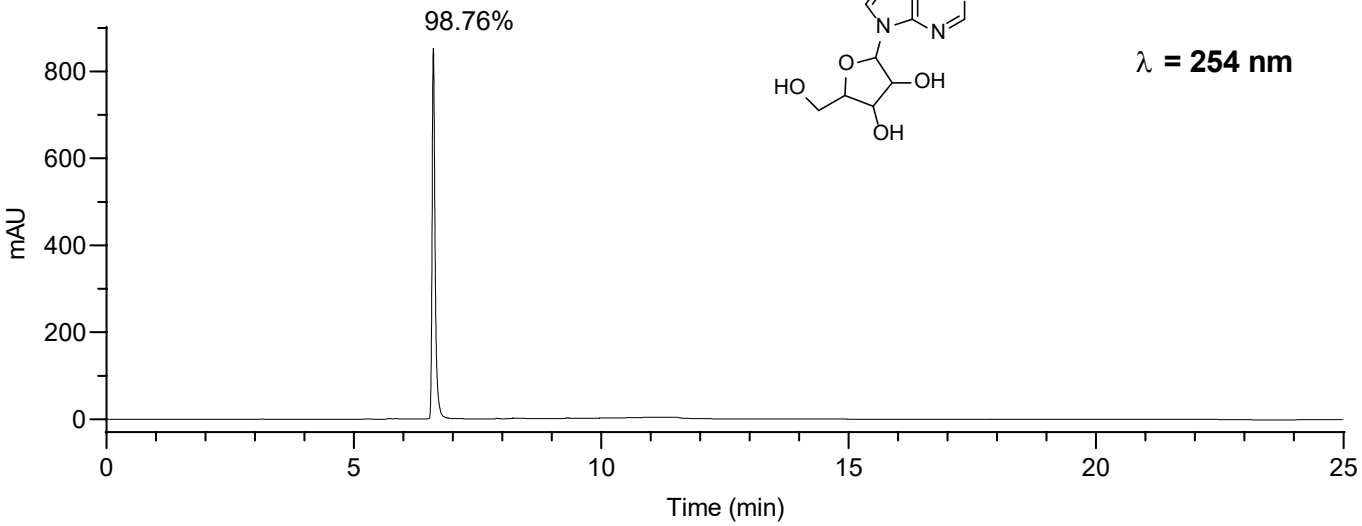

N
HN
N
N
N
N
O
HO
OH
OH


33 #1-30 RT: 0.02-0.41 AV: 30 NL: 3.09E7 T: FTMS
+ p ESI Full ms [100.00-2000.00]
377.1922
R=80176
z=1
[M+H]+
Full scan ESI(+)
368.4247
R=84211
z=1
245.1505
R=99476
z=1
399.1741
R=78690
z=1
575.4118
R=65286
z=1
775.3598
R=53999
z=1
858.8092
R=40753
z=?
1166.7722
R=30182
z=?
1322.6936
R=30564
z=?
1472.6919
R=27165
z=?
1649.7150
R=30031
z=?
1860.7015
R=24994
z=?
Relative Abundance
m/z

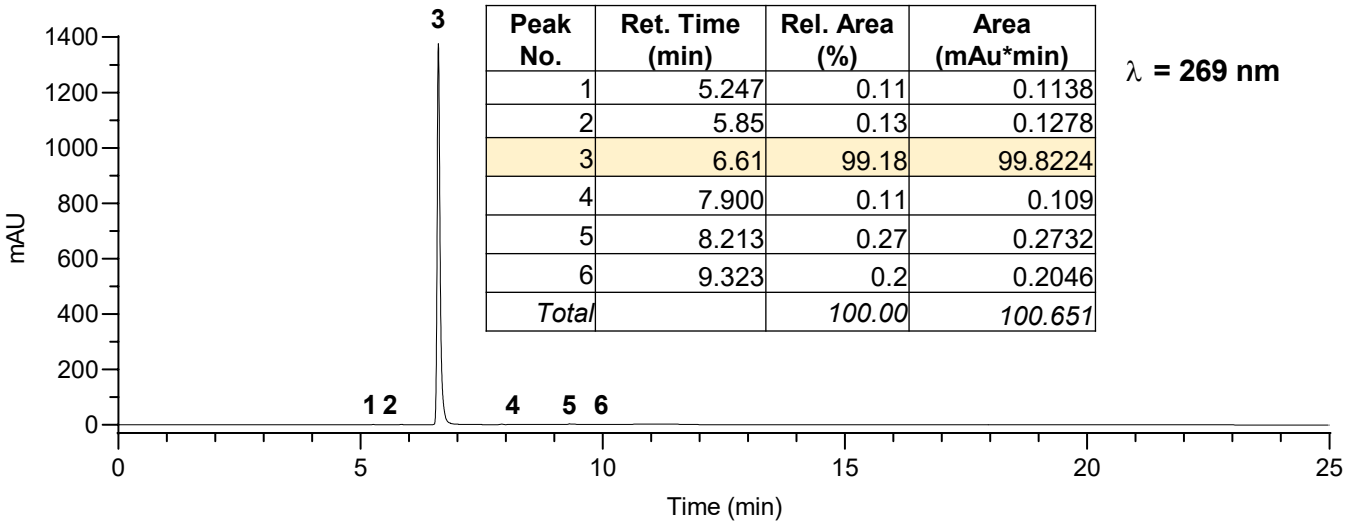

Experimental
377.1922
R=80176
z=1
368.4247
R=84211
z=1
371.2913
R=120745
z=?
376.5910
R=65969
z=?
378.1955
R=77891
z=1
381.2963
R=84647
z=1
385.2912
R=77845
z=1
387.2683
R=93091
z=?
391.2832
R=89715
z=?
Relative Abundance
NL:
3.09E7
33#1-30 RT:
0.02-0.41 AV: 30 T: FTMS +
p ESI Full ms
[100.00-2000.00]
Theoretical
377.1932
R=75932
z=?
378.1959
R=74095
z=?
380.2006
R=57267
z=?
382.2053
R=48230
z=?
NL:
1.89E4
C17H24N6O4 +H:
C17H25N6O4
p (gss, s /p:40) Chrg 1
R: 76000 Res .Pwr . @FWHM
Δm=2.65 ppm
m/z

33



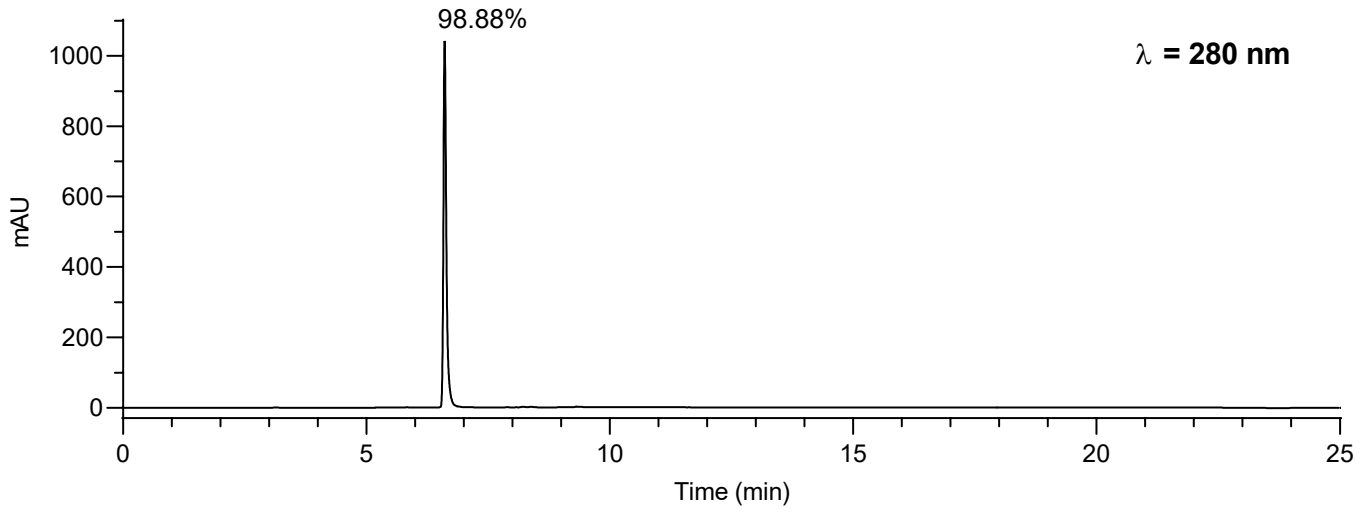


λ = 254 nm



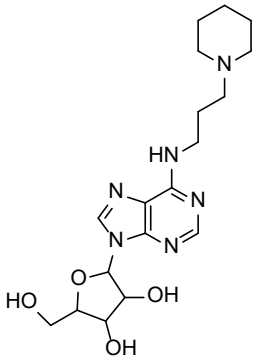
Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	5.247	0.11	0.1138
2	5.85	0.13	0.1278
3	6.61	99.18	99.8224
4	7.900	0.11	0.109
5	8.213	0.27	0.2732
6	9.323	0.2	0.2046
Total		*100.00*	*100.651*

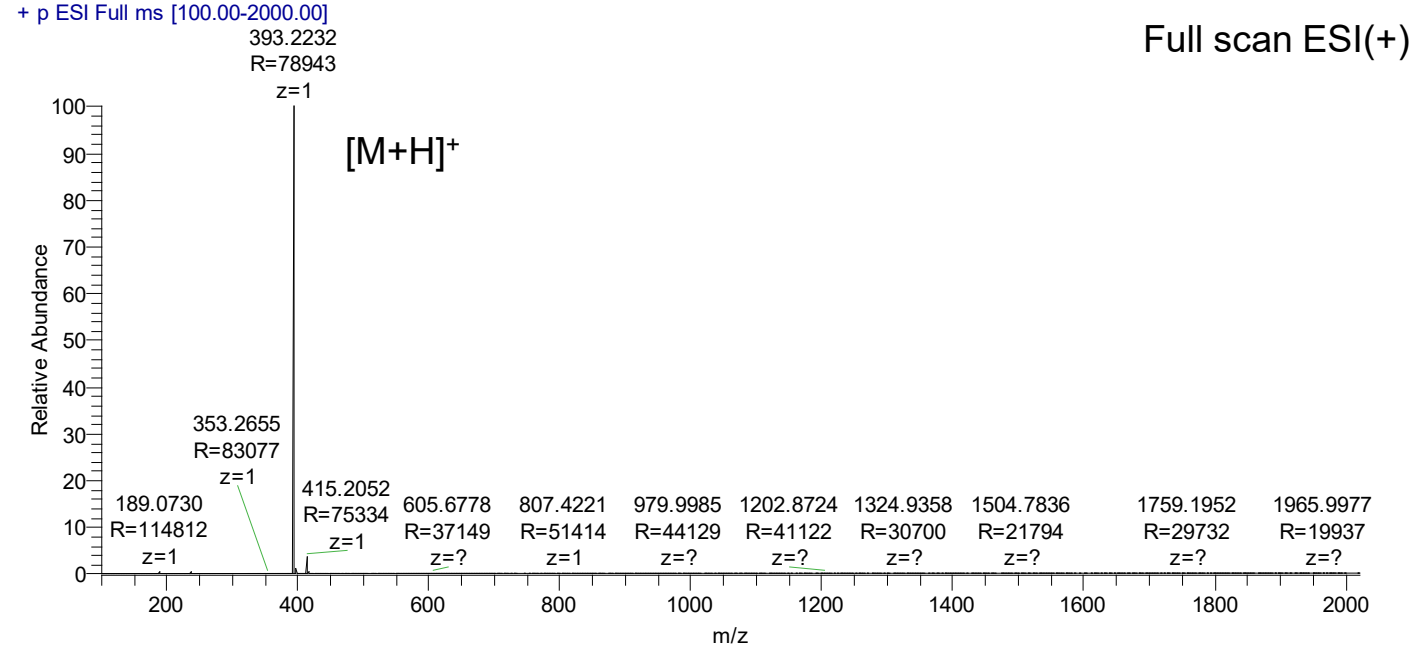
λ = 269 nm

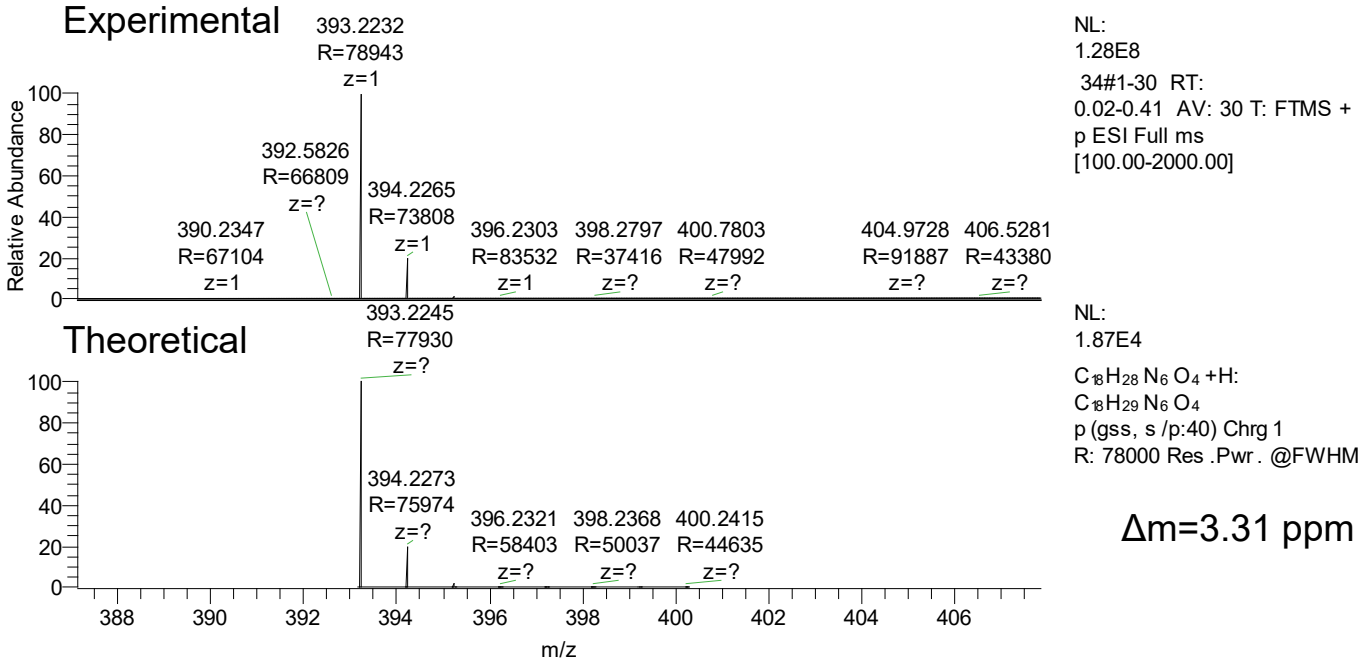


λ = 280 nm

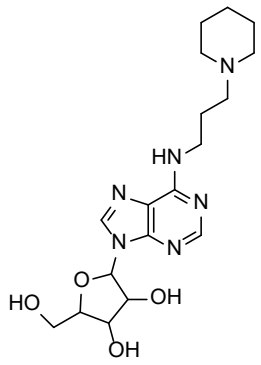
34

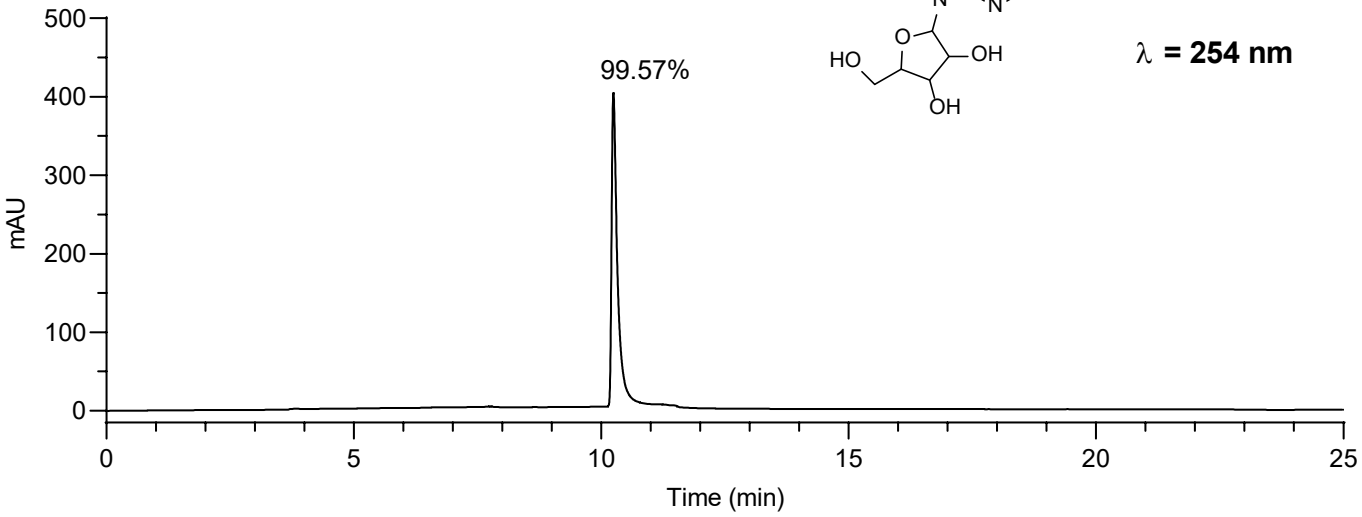

N
HN
N
N
N
N
O
HO
OH
OH

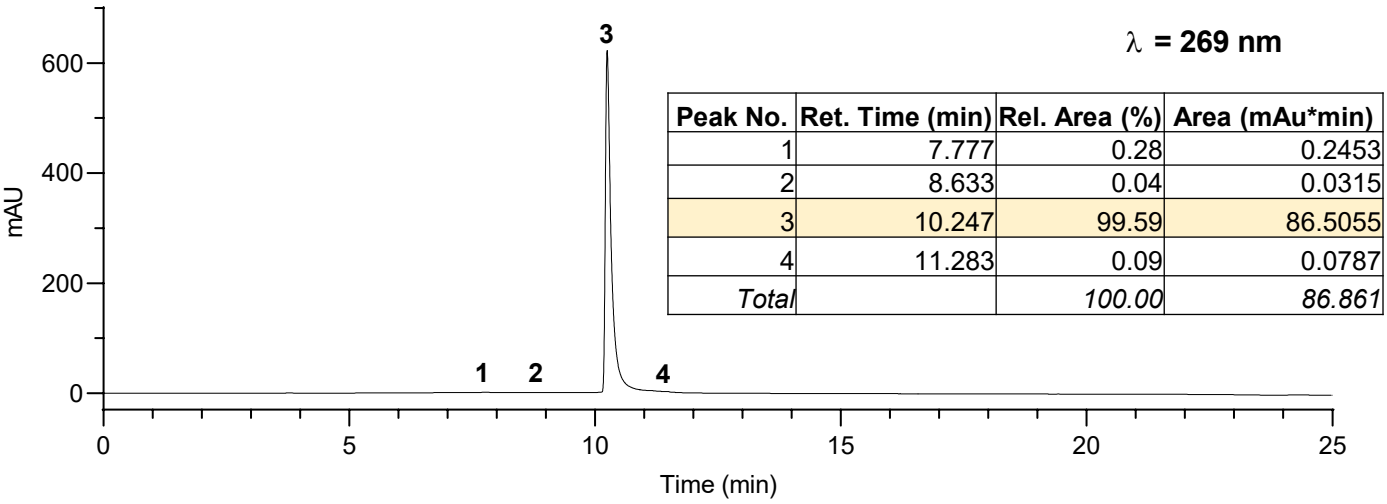

34 #1-30 RT: 0.02-0.41 AV: 30 NL: 1.28E8 T: FTMS
+ p ESI Full ms [100.00-2000.00]
Full scan ESI(+)
393.2232
R=78943
z=1
[M+H]+
Relative Abundance
353.2655
R=83077
z=1
189.0730
R=114812
z=1
415.2052
R=75334
z=1
605.6778
R=37149
z=?
807.4221
R=51414
z=1
979.9985
R=44129
z=?
1202.8724
R=41122
z=?
1324.9358
R=30700
z=?
1504.7836
R=21794
z=?
1759.1952
R=29732
z=?
1965.9977
R=19937
z=?
m/z


Experimental
393.2232
R=78943
z=1
Relative Abundance
392.5826
R=66809
z=?
394.2265
R=73808
z=1
390.2347
R=67104
z=1
396.2303
R=83532
z=1
398.2797
R=37416
z=?
400.7803
R=47992
z=?
404.9728
R=91887
z=?
406.5281
R=43380
z=?
NL:
1.28E8
34#1-30 RT:
0.02-0.41 AV: 30 T: FTMS +
p ESI Full ms
[100.00-2000.00]
Theoretical
393.2245
R=77930
z=?
394.2273
R=75974
z=?
396.2321
R=58403
z=?
398.2368
R=50037
z=?
400.2415
R=44635
z=?
NL:
1.87E4
C18H28N6O4+H:
C18H29N6O4
p (gss, s /p:40) Chrg 1
R: 78000 Res .Pwr. @FWHM
Δm=3.31 ppm
m/z

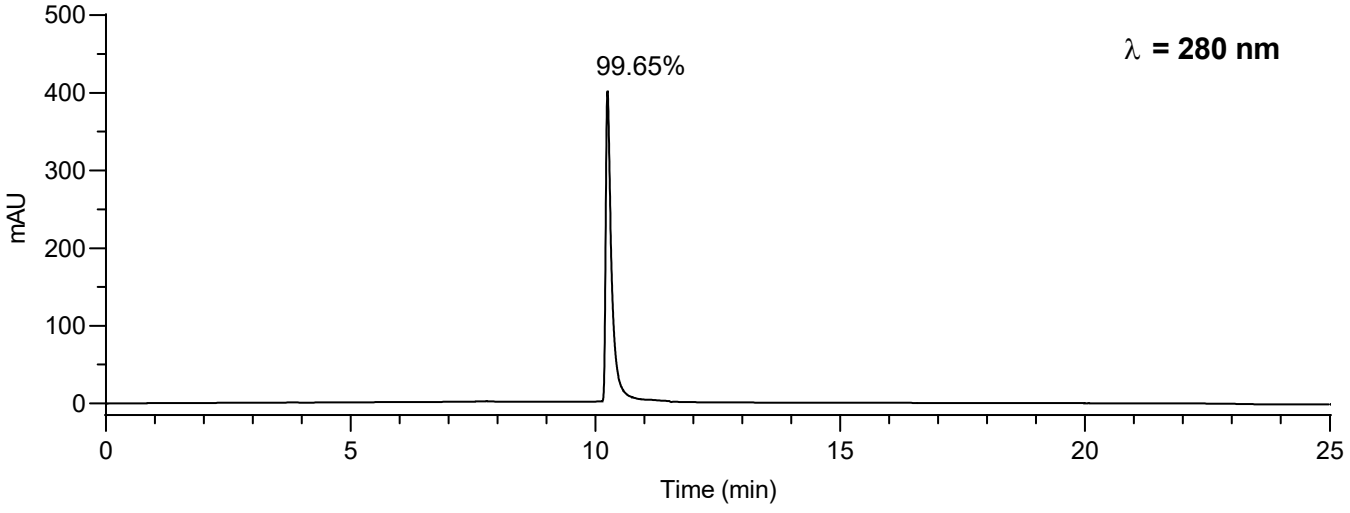
34



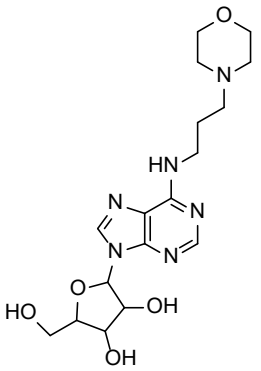




Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	7.777	0.28	0.2453
2	8.633	0.04	0.0315
3	10.247	99.59	86.5055
4	11.283	0.09	0.0787
Total		*100.00*	*86.861*

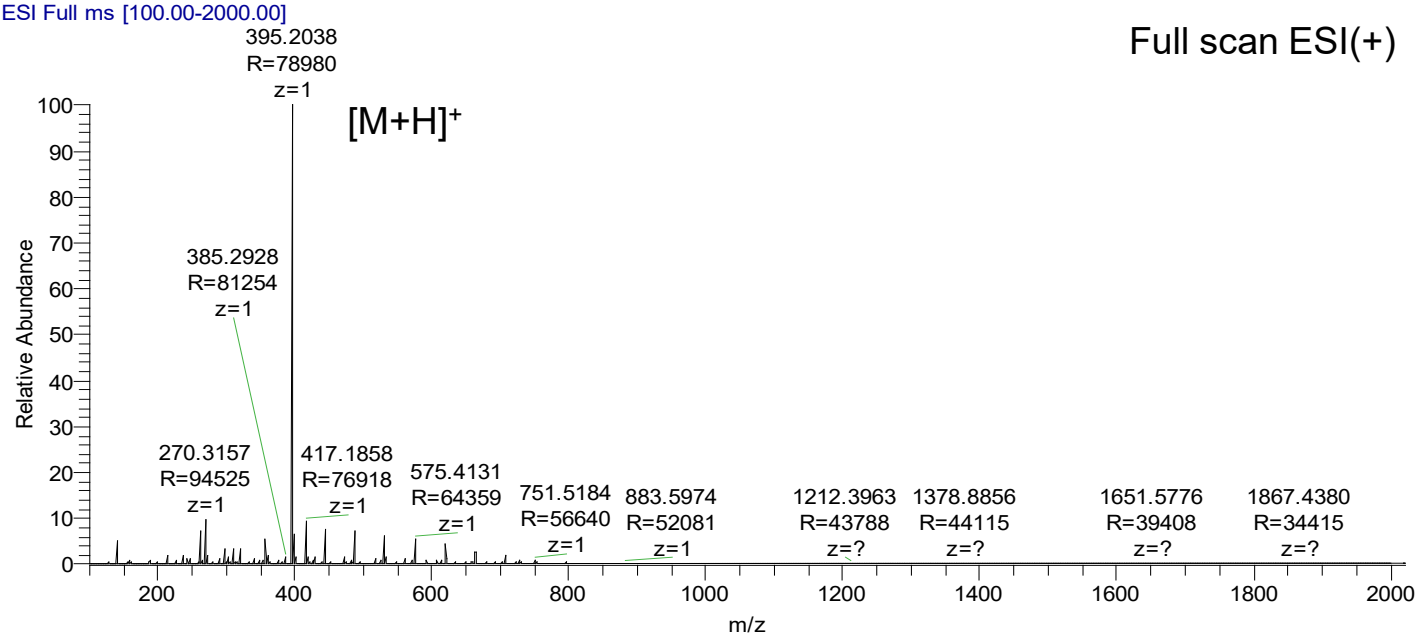


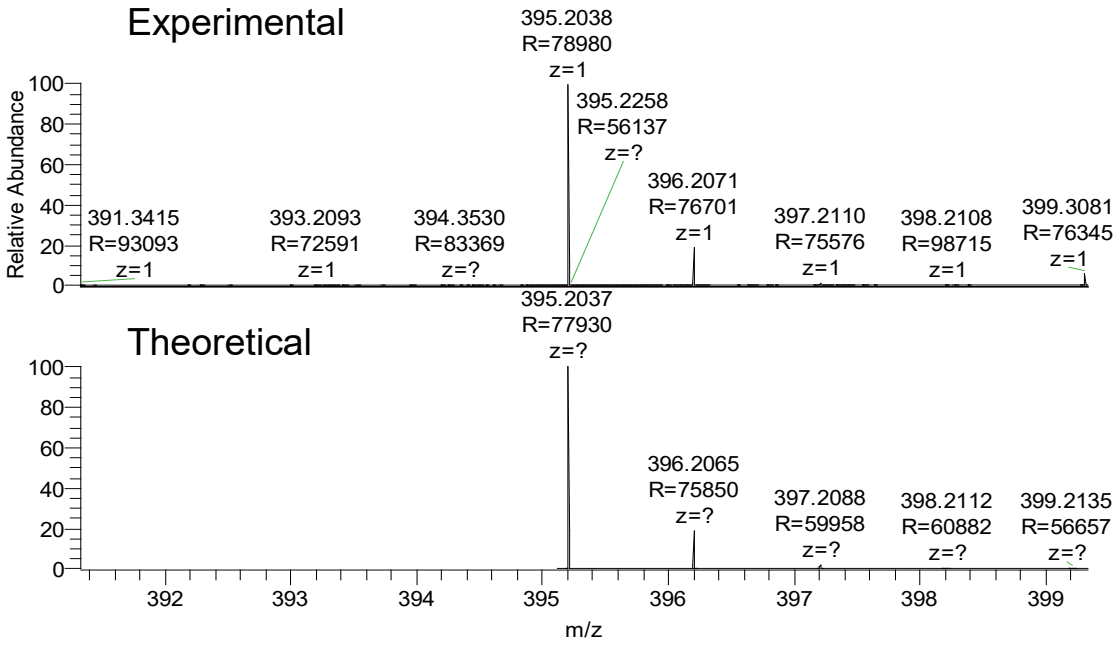
35



35 #1-30 RT: 0.02-0.41 AV: 30 NL: 1.24E7 T: FTMS + p
ESI Full ms [100.00-2000.00]

Full scan ESI(+)



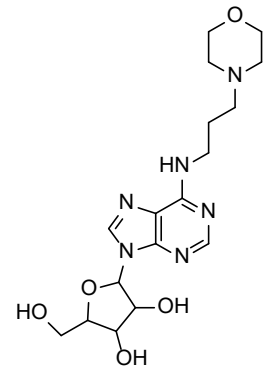


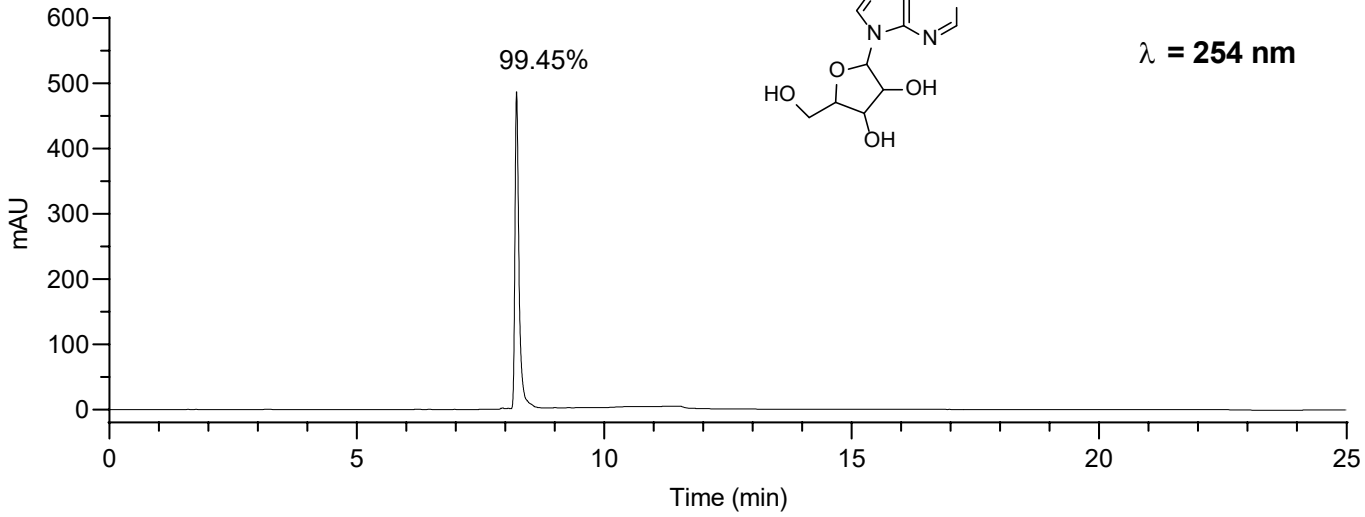
NL:
1.24E7
35#1-30 RT: 0.02-0.41 AV: 30 T: FTMS + p ESI Full ms [100.00-2000.00]

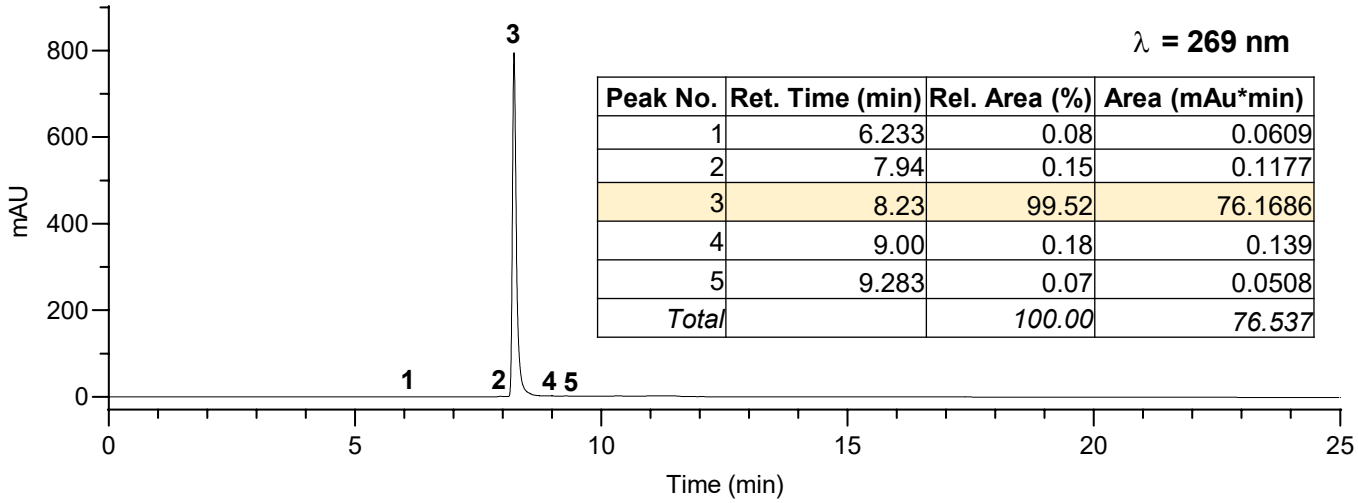
NL:
1.88E4
$C_{17}H_{26}N_6O_5$ +H:
$C_{17}H_{27}N_6O_5$
p (gss, s /p:40) Chrg 1
R: 78000 Res .Pwr . @FWHM

Δm= 0.25 ppm

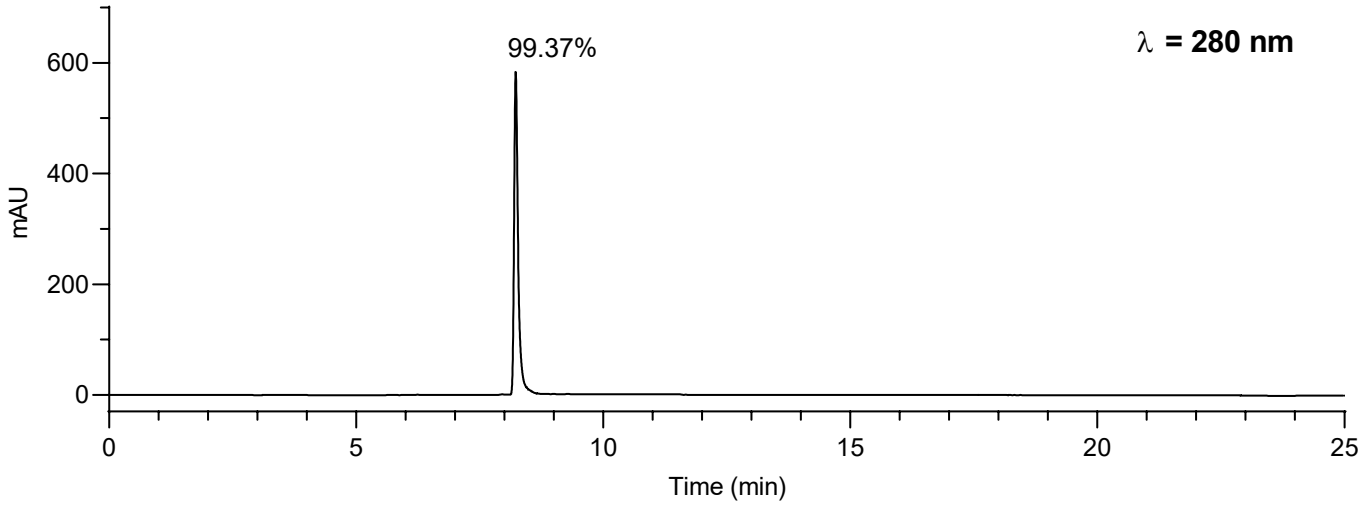
35



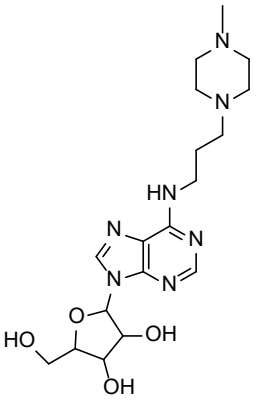




Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	6.233	0.08	0.0609
2	7.94	0.15	0.1177
3	8.23	99.52	76.1686
4	9.00	0.18	0.139
5	9.283	0.07	0.0508
Total		*100.00*	*76.537*

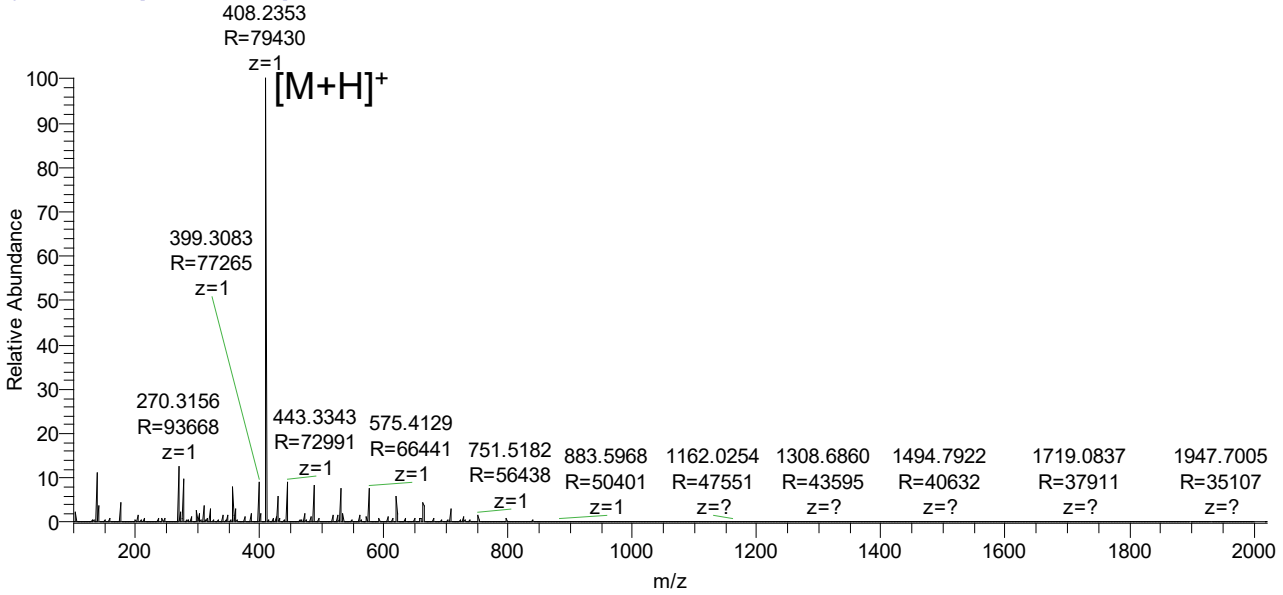


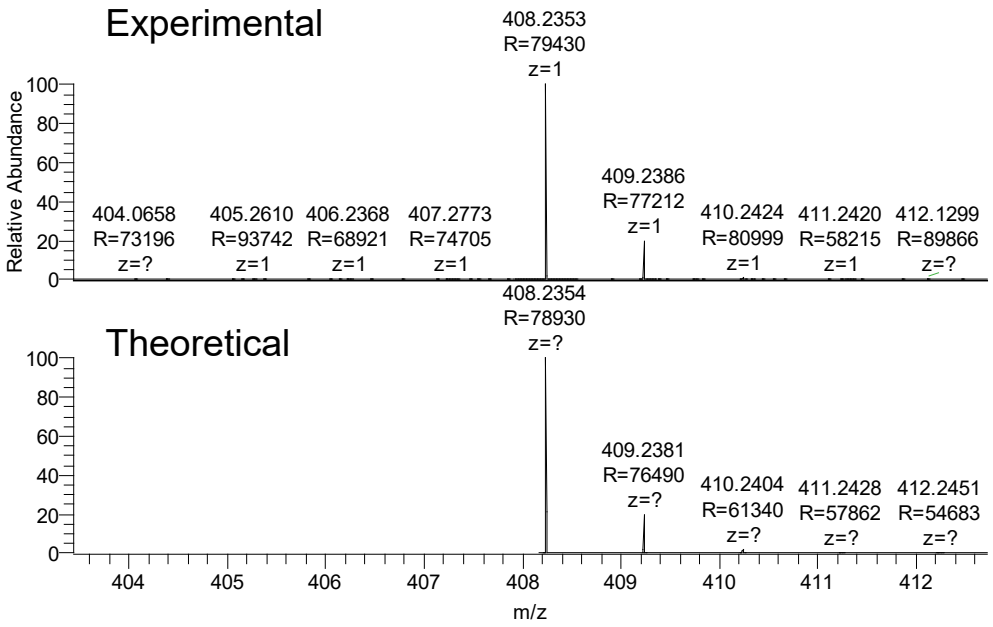
36



36 #2-26 RT: 0.03-0.36 AV: 25 NL: 5.60E6 T: FTMS + p ESI Full ms [100.00-2000.00]

Full scan ESI(+)



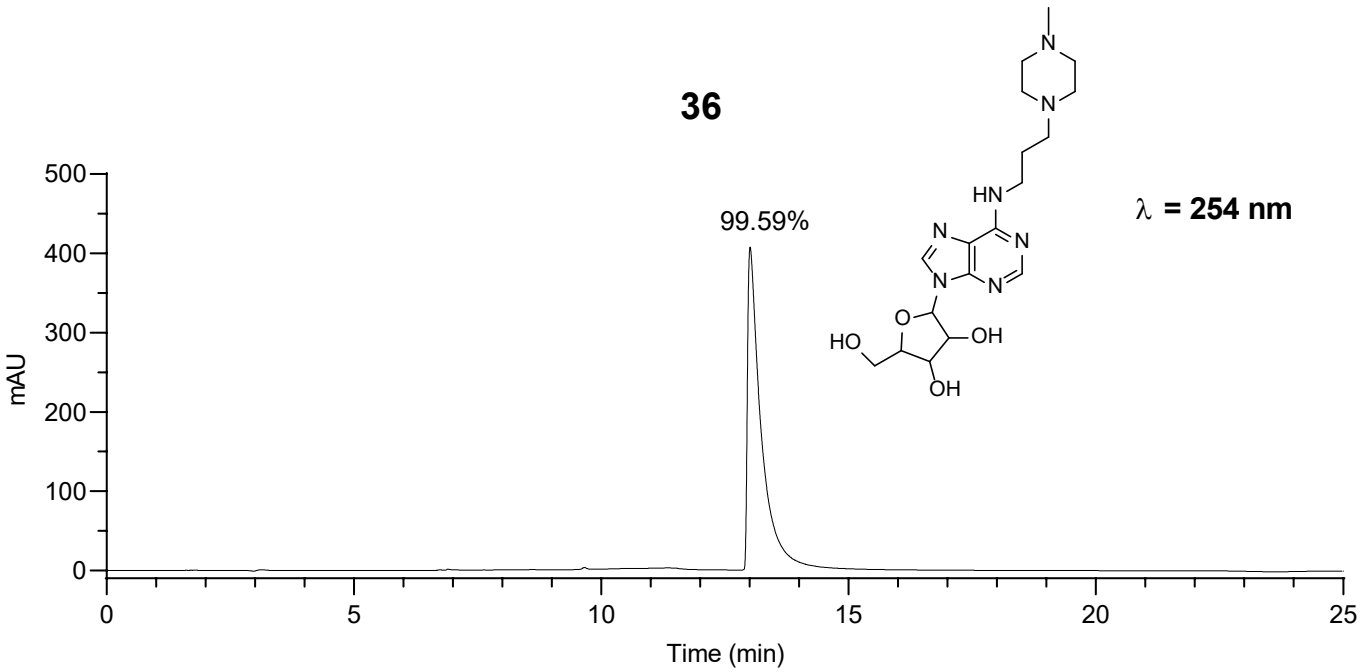


NL:
5.60E6
36#2-26 RT:
0.03-0.36 AV: 25 T: FTMS +
p ESI Full ms
[100.00-2000.00]

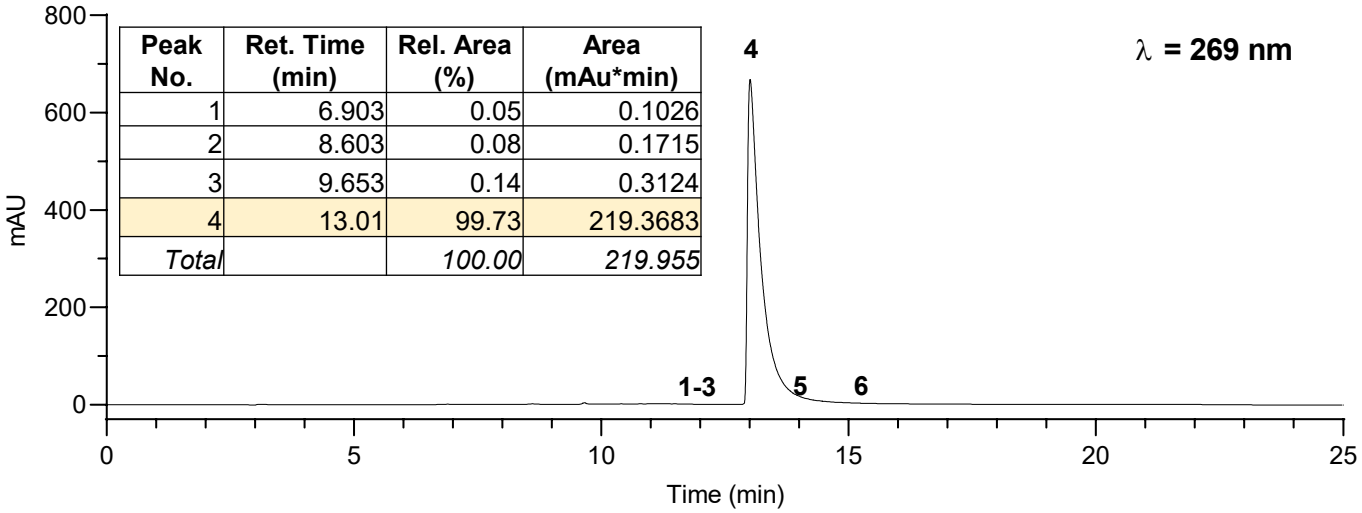
NL:
1.86E4
$C_{18}H_{29}N_7O_4$ +H:
$C_{18}H_{30}N_7O_4$
p (gss, s /p:40) Chrg 1
R: 79000 Res .Pwr . @FWHM

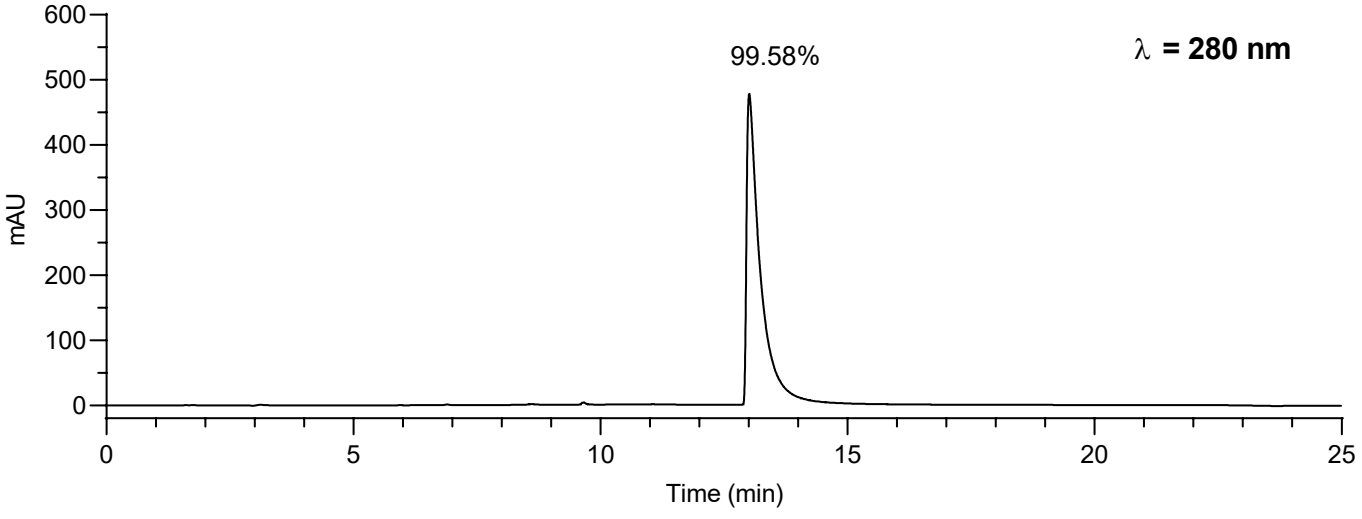
Δm= 0.24ppm

36

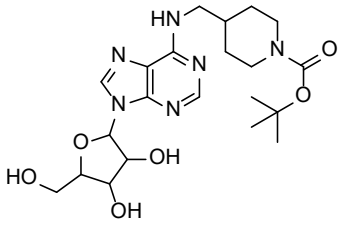


Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	6.903	0.05	0.1026
2	8.603	0.08	0.1715
3	9.653	0.14	0.3124
4	13.01	99.73	219.3683
Total		*100.00*	*219.955*

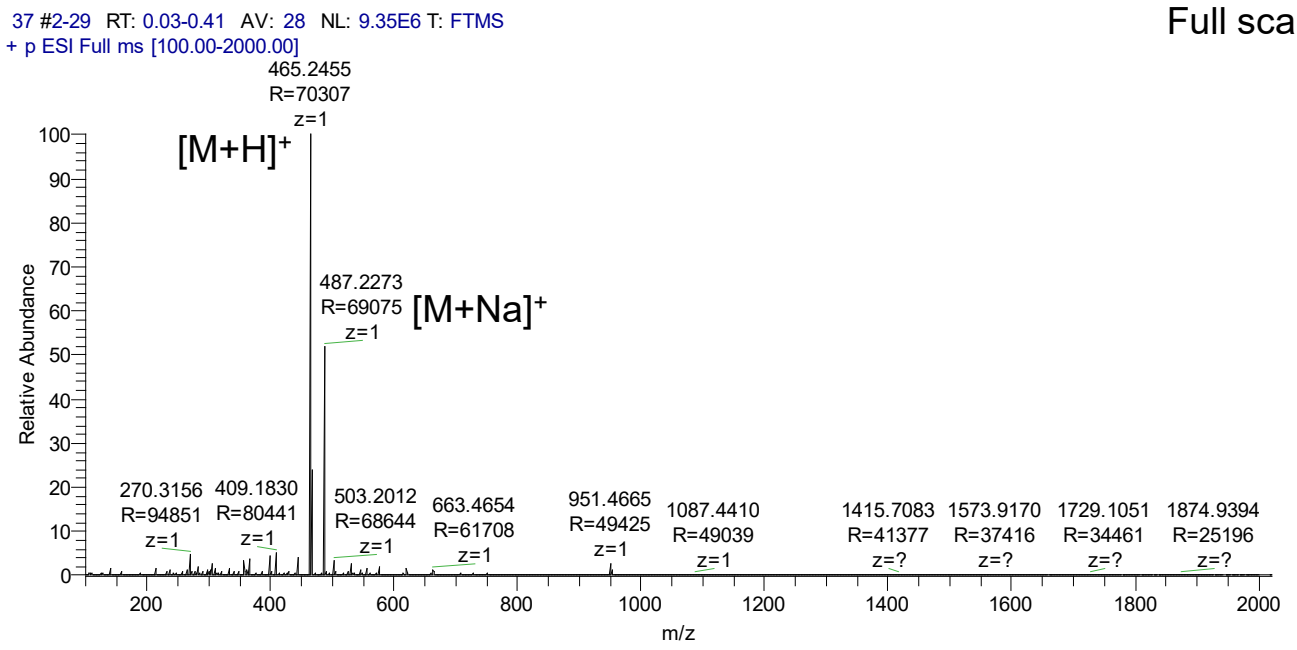


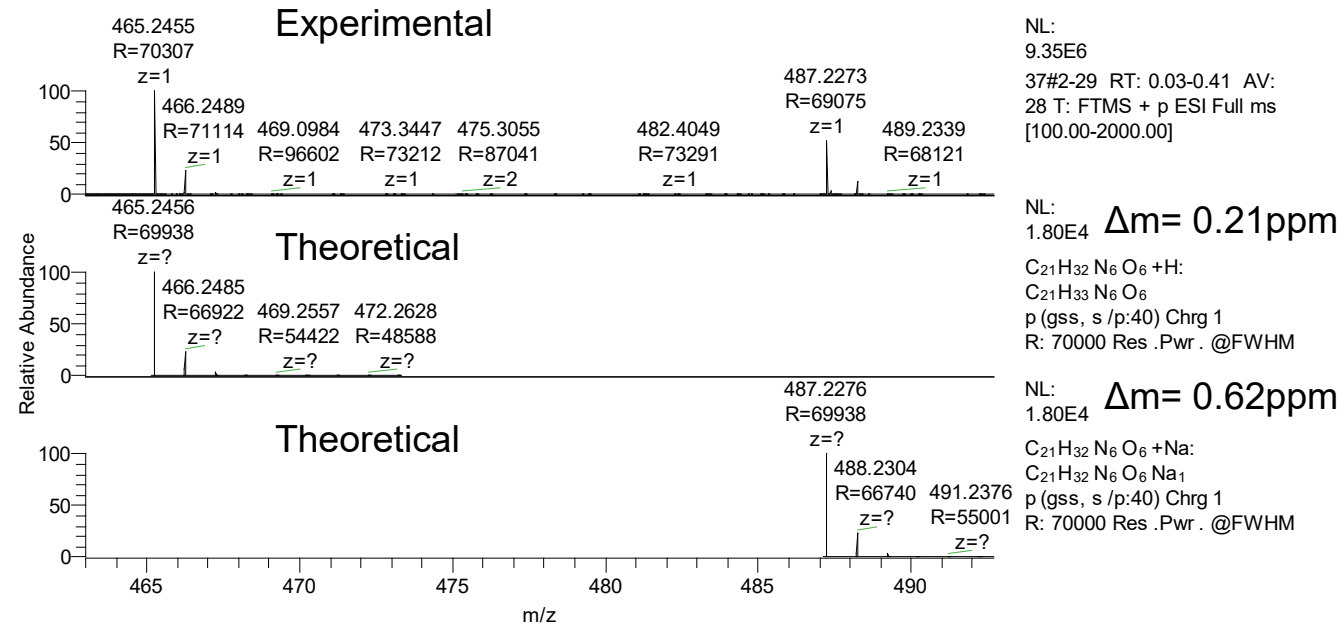


37



Full scan ESI(+)





NL:
9.35E6
37#2-29 RT: 0.03-0.41 AV: 28 T: FTMS + p ESI Full ms [100.00-2000.00]

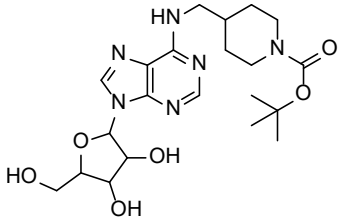
NL:
1.80E4 **Δm= 0.21ppm**

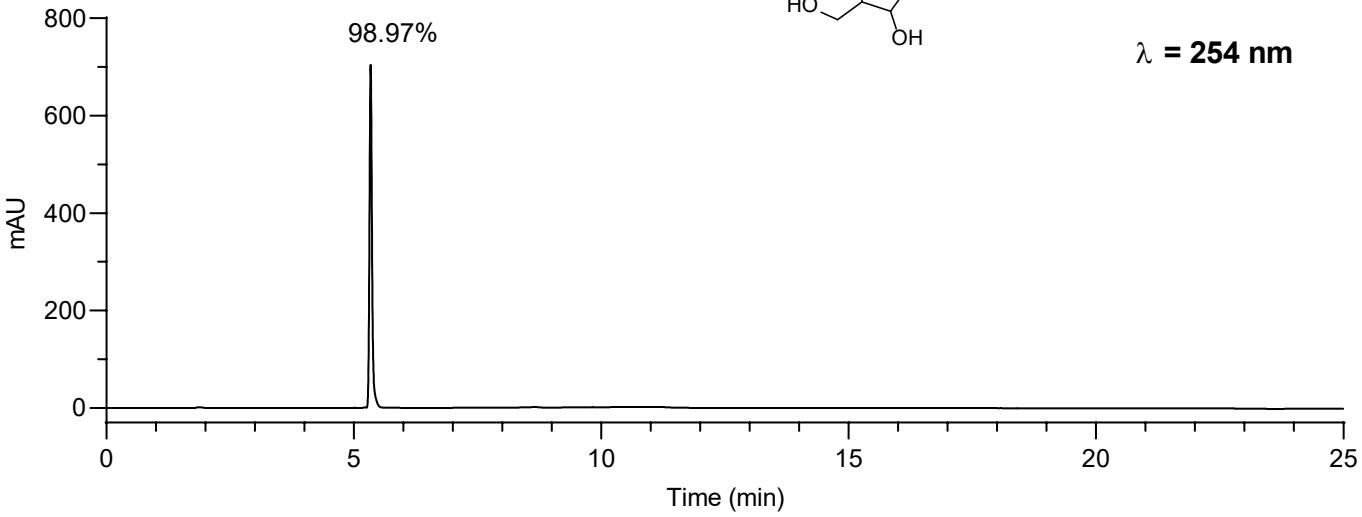
$C_{21}H_{32}N_6O_6$ +H:
$C_{21}H_{33}N_6O_6$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM

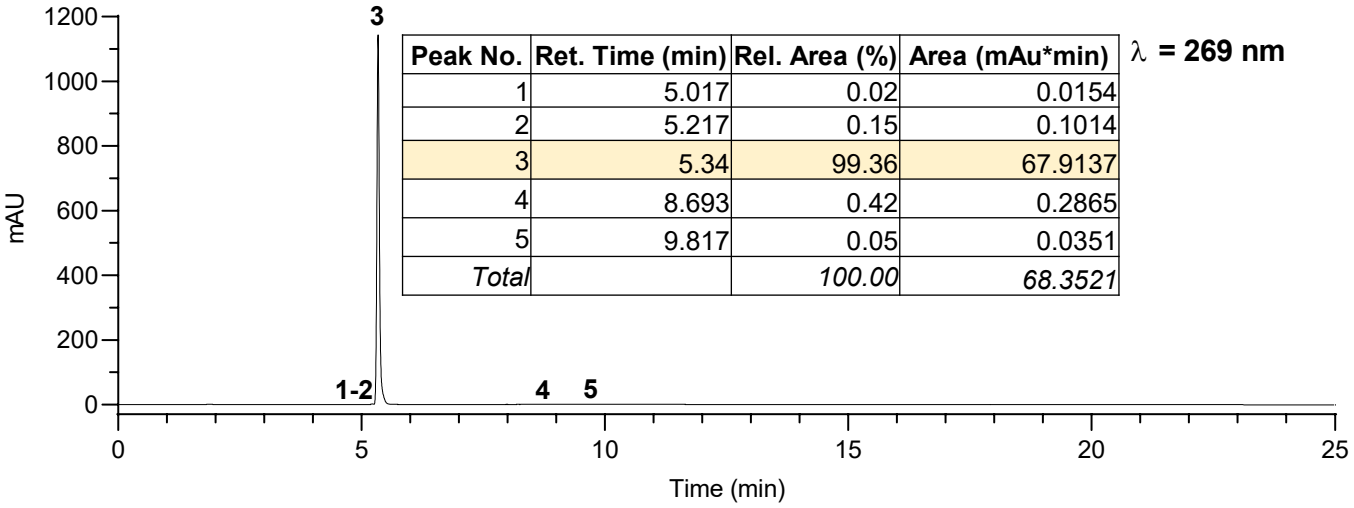
NL:
1.80E4 **Δm= 0.62ppm**

$C_{21}H_{32}N_6O_6$ +Na:
$C_{21}H_{32}N_6O_6Na_1$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM

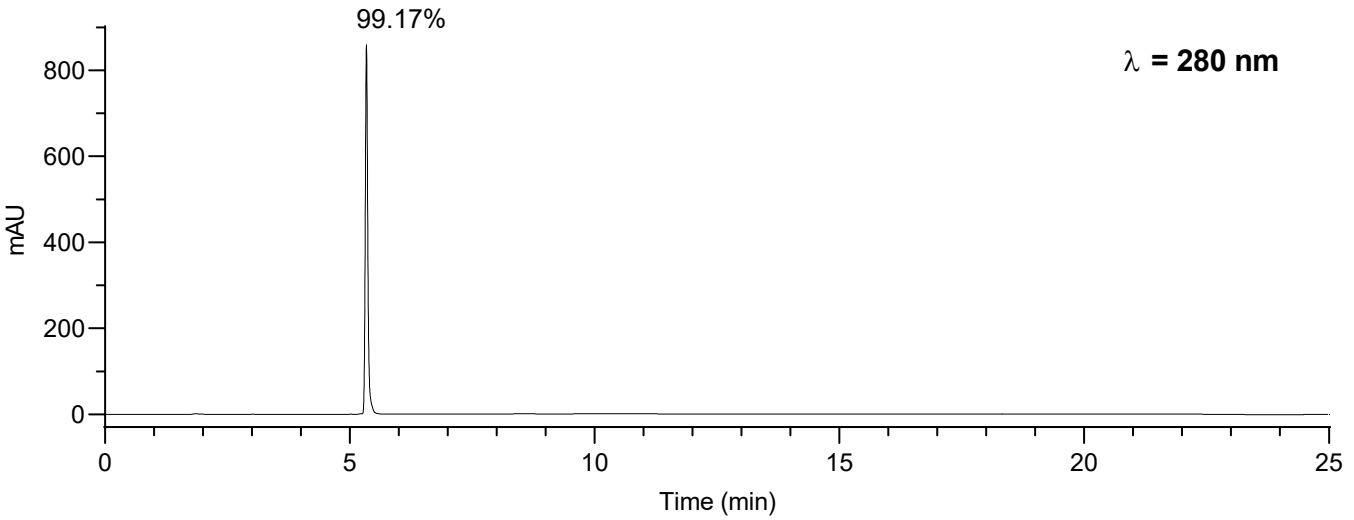
37



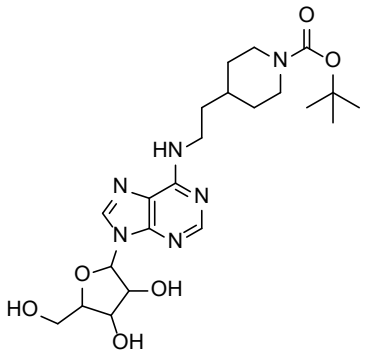




Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	5.017	0.02	0.0154
2	5.217	0.15	0.1014
3	5.34	99.36	67.9137
4	8.693	0.42	0.2865
5	9.817	0.05	0.0351
Total		*100.00*	*68.3521*

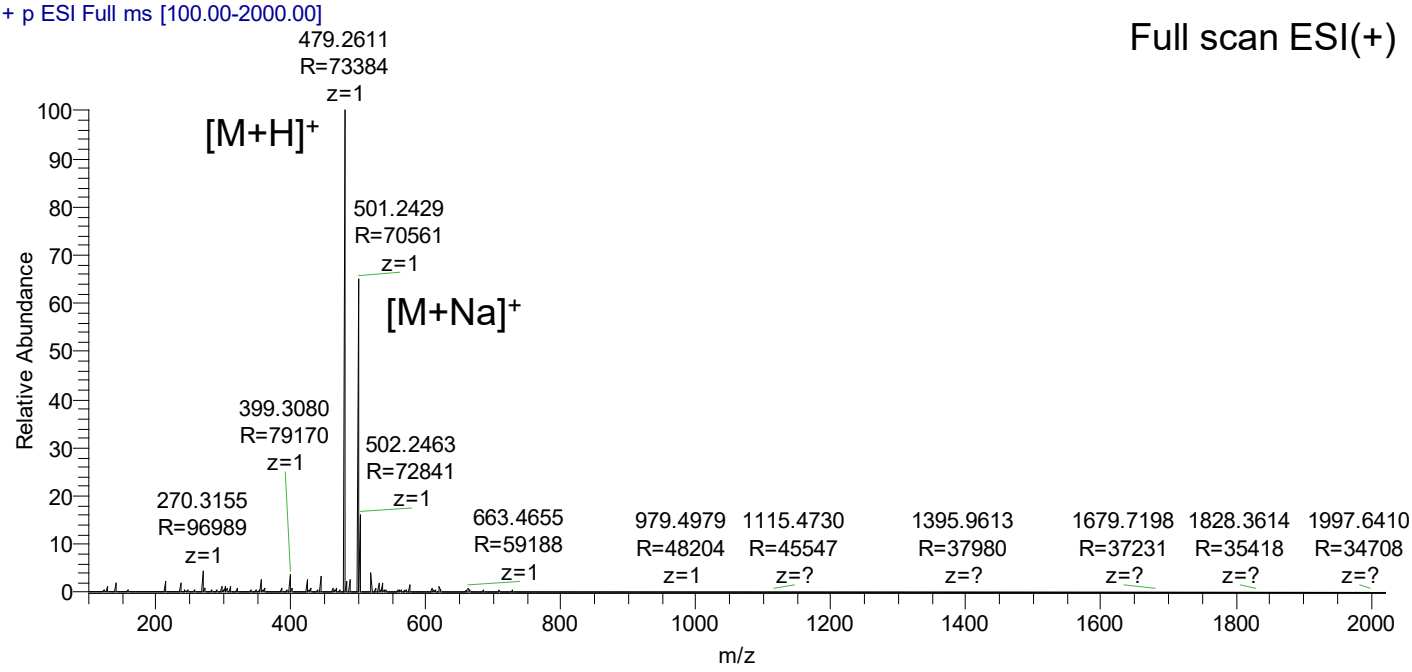


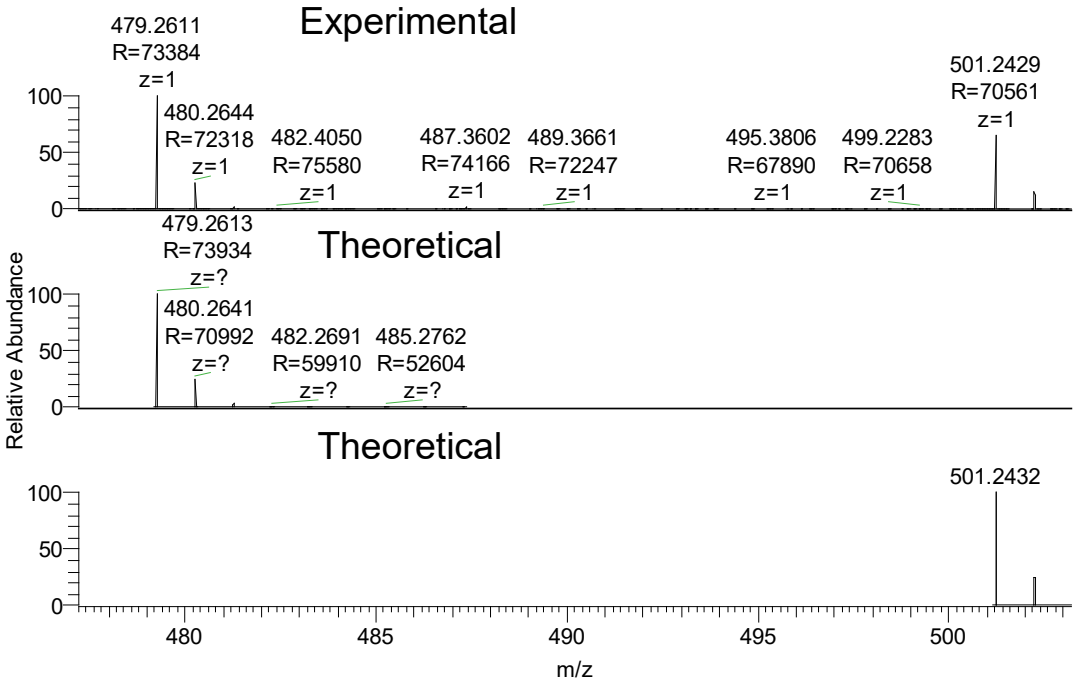
38



38 #1-30 RT: 0.02-0.42 AV: 30 NL: 1.51E7 T: FTMS
+ p ESI Full ms [100.00-2000.00]

Full scan ESI(+)





NL:
1.51E7
38#1-30 RT: 0.02-0.42 AV: 30 T: FTMS + p ESI Full ms [100.00-2000.00]

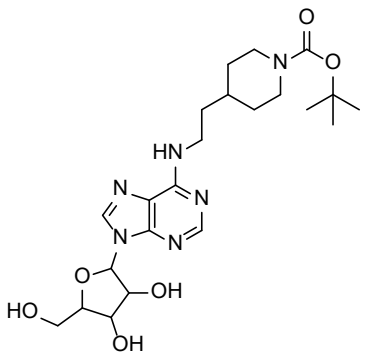
NL:
1.78E4 Δm= 0.42 ppm

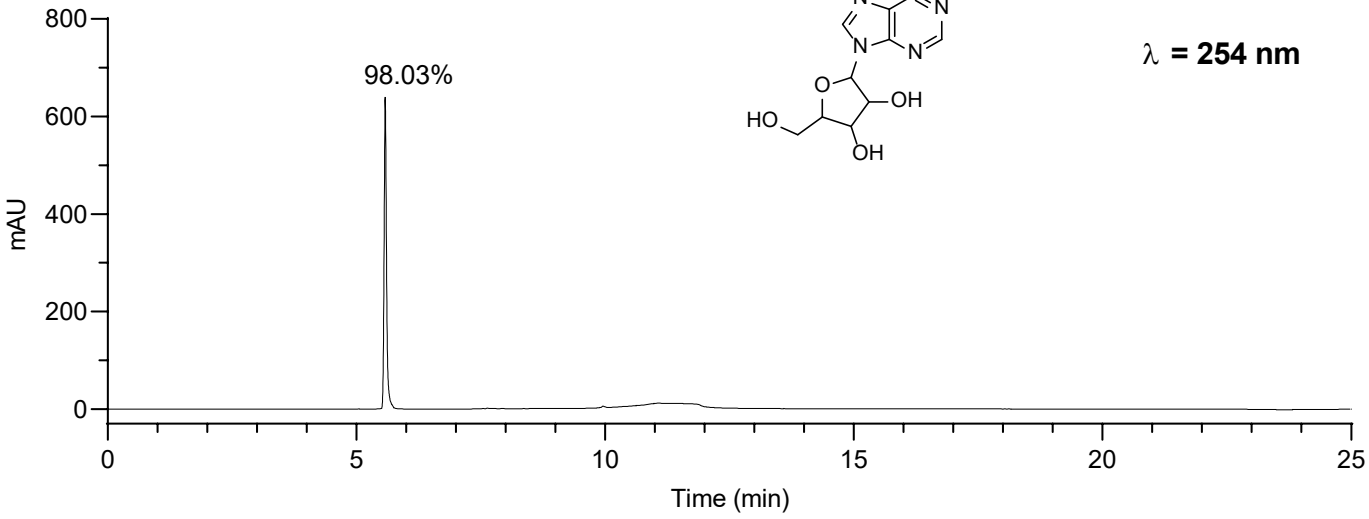
$C_{22}H_{34}N_6O_6$ +H:
$C_{22}H_{35}N_6O_6$
p (gss, s /p:40) Chrg 1
R: 74000 Res .Pwr . @FWHM

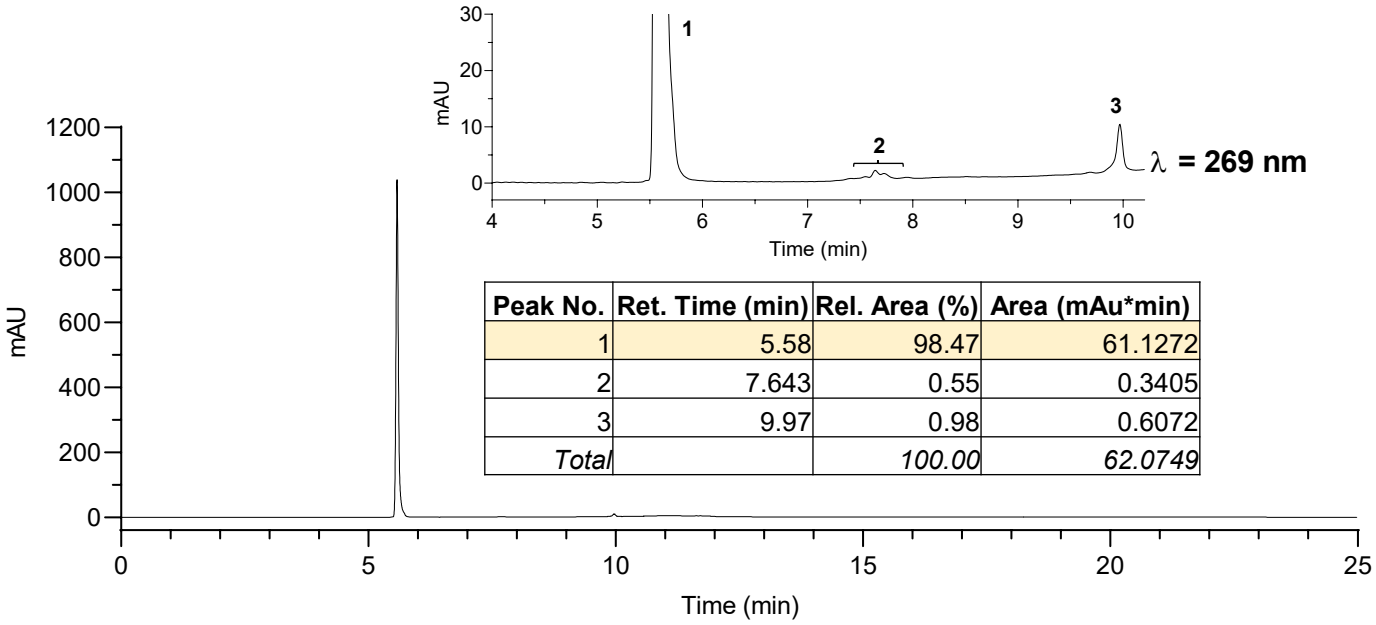
NL:
1.78E4 Δm= 0.60ppm

$C_{22}H_{34}N_6O_6$ +Na:
$C_{22}H_{34}N_6O_6Na_1$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM

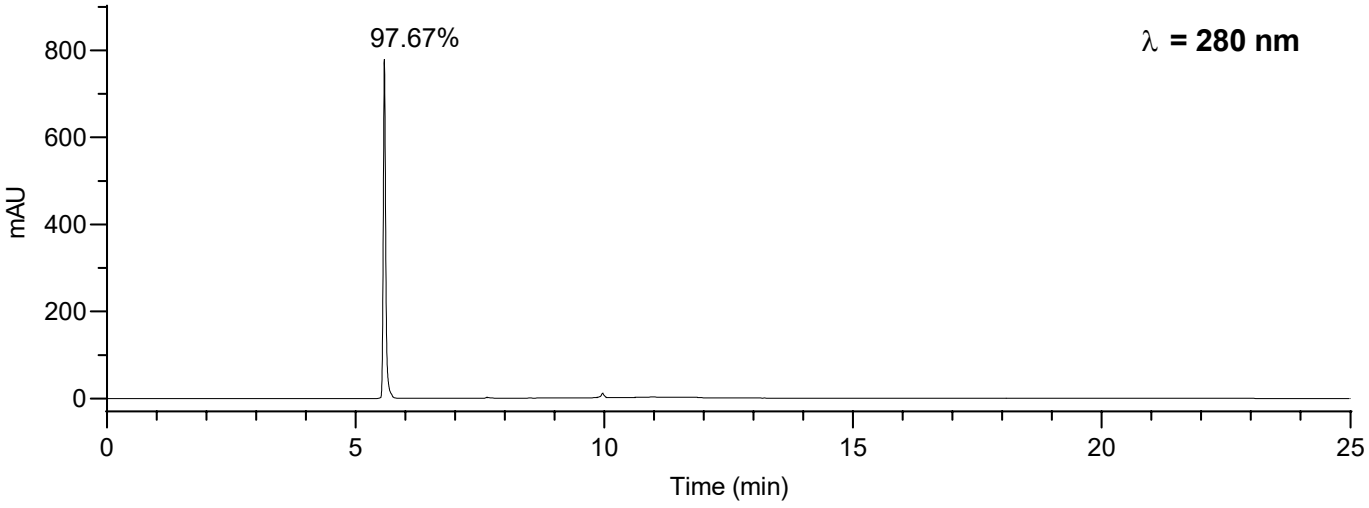
38



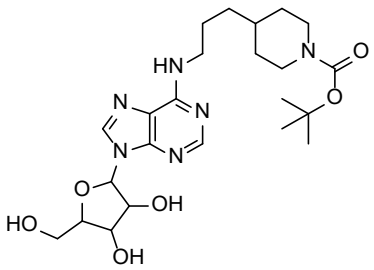




Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	5.58	98.47	61.1272
2	7.643	0.55	0.3405
3	9.97	0.98	0.6072
Total		*100.00*	*62.0749*

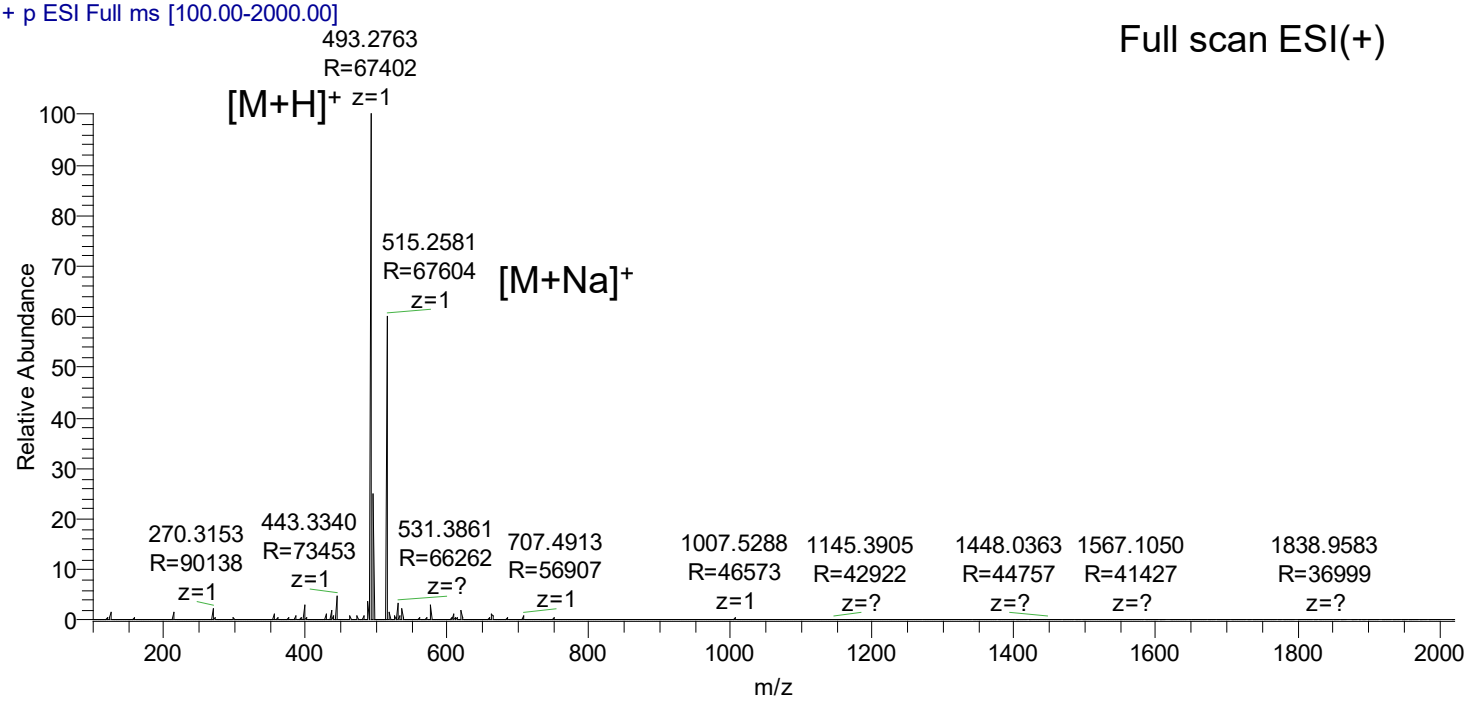


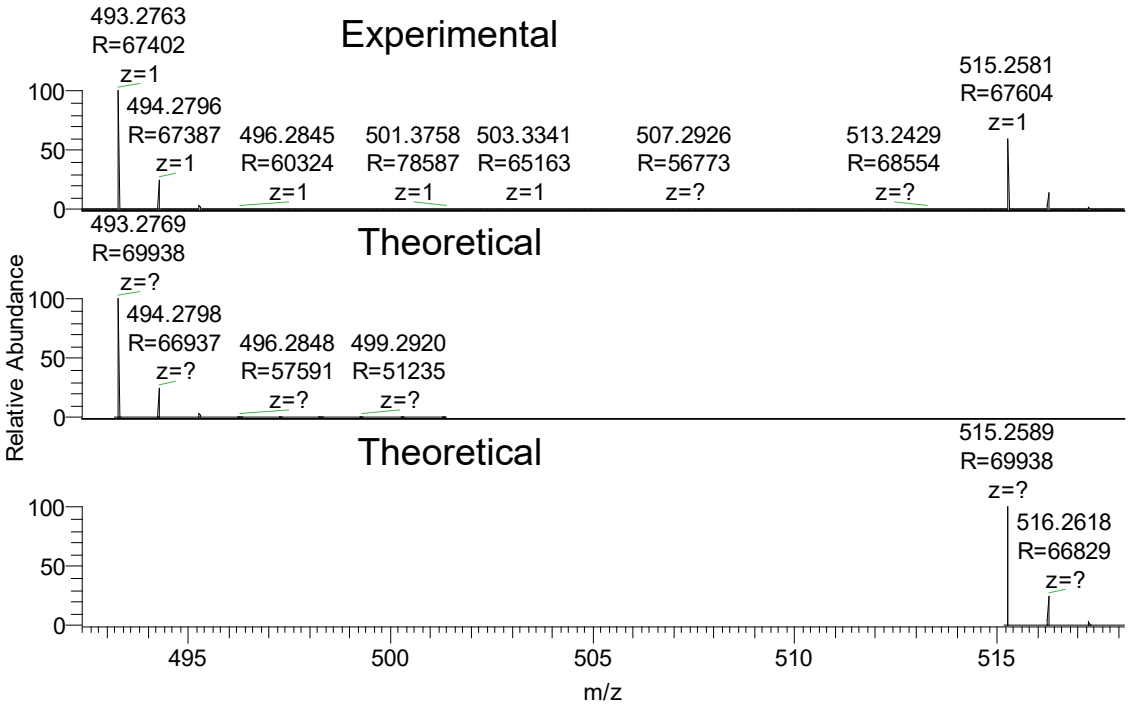
39



39 #1-29 RT: 0.02-0.40 AV: 29 NL: 2.97E7 T: FTMS + p ESI Full ms [100.00-2000.00]

Full scan ESI(+)





NL:
2.97E7
39#1-29 RT: 0.02-0.40 AV: 29 T: FTMS + p ESI Full ms [100.00-2000.00]

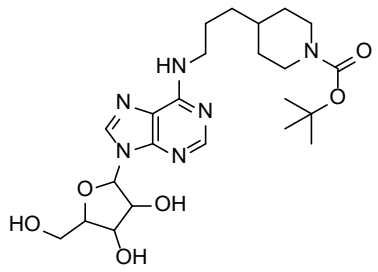
NL: Δm= 1.22ppm
1.76E4

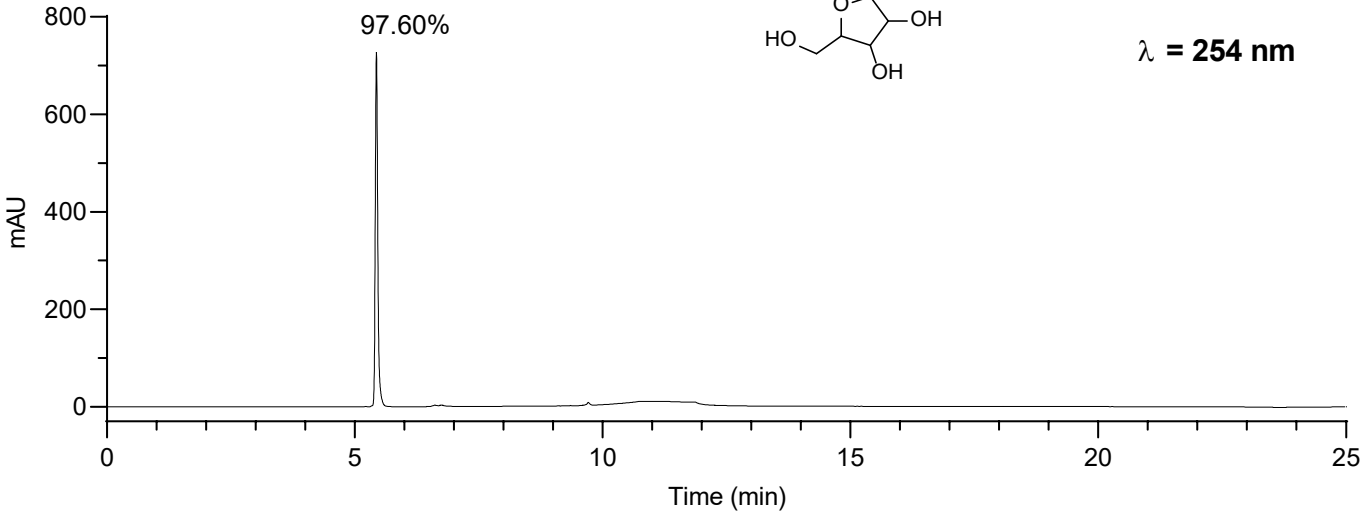
$C_{23}H_{36}N_6O_6$ +H:
$C_{23}H_{37}N_6O_6$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM

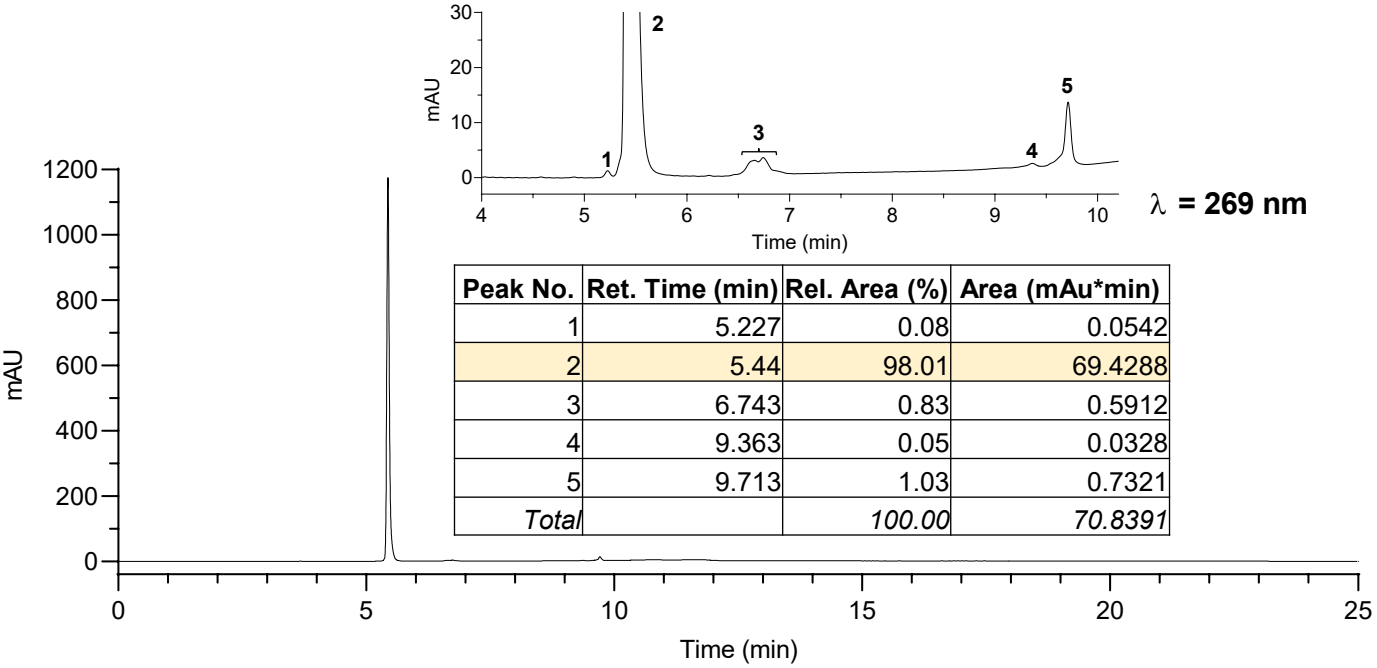
NL: Δm=1.55 ppm
1.76E4

$C_{23}H_{36}N_6O_6$ +Na:
$C_{23}H_{36}N_6O_6Na_1$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM

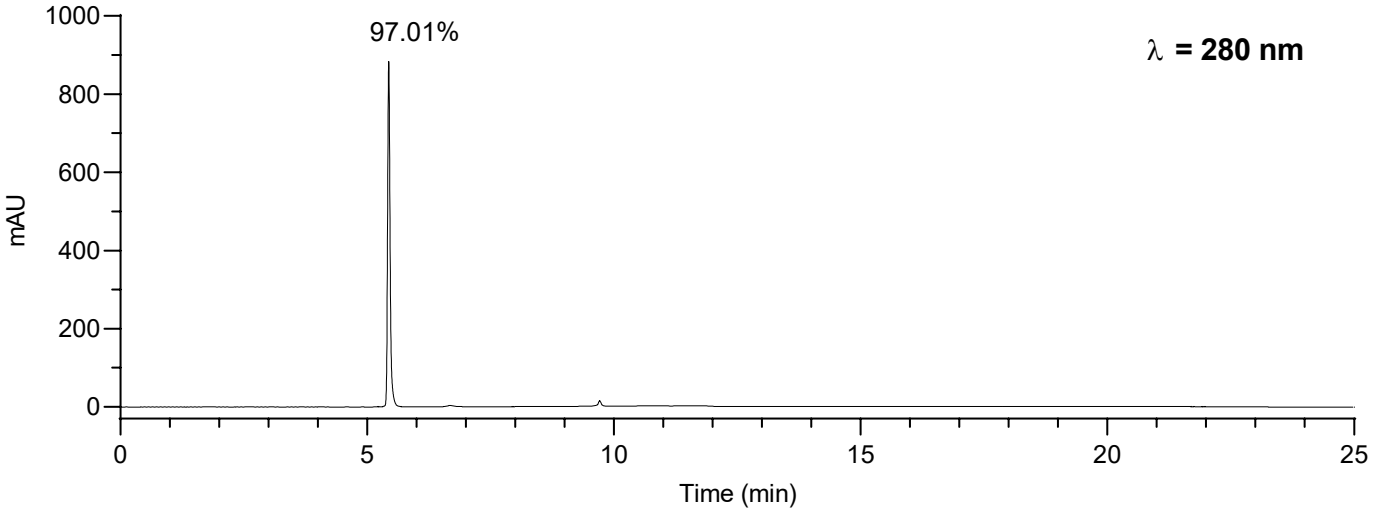
39



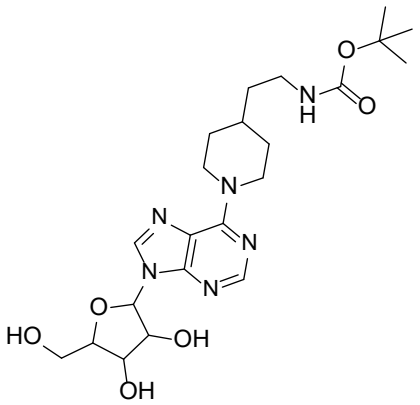




Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	5.227	0.08	0.0542
2	5.44	98.01	69.4288
3	6.743	0.83	0.5912
4	9.363	0.05	0.0328
5	9.713	1.03	0.7321
Total		*100.00*	*70.8391*

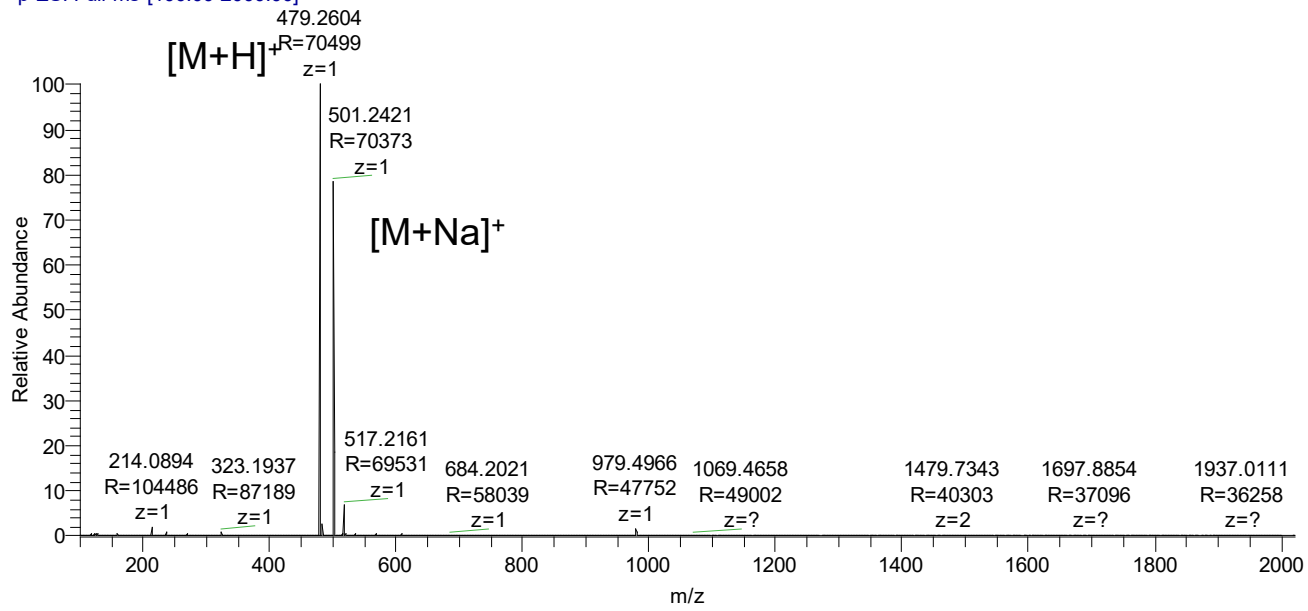


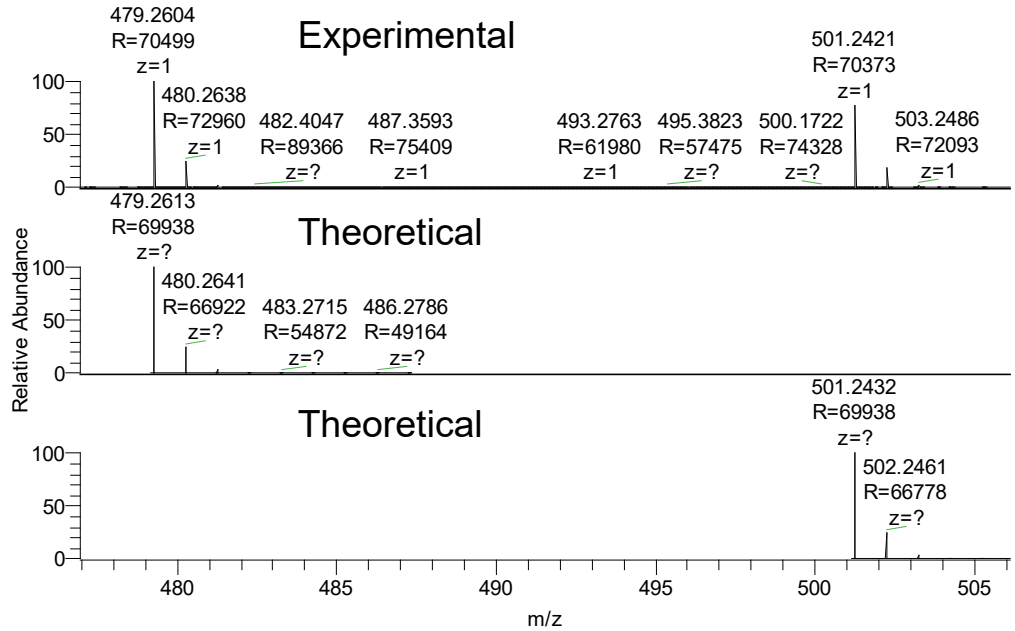
40



40 #1-30 RT: 0.02-0.45 AV: 30 NL: 2.94E6 T: FTMS
+ p ESI Full ms [100.00-2000.00]

Full scan ESI(+)





NL:
2.94E6
40#1-30 RT: 0.02-0.45 AV: 30 T: FTMS + p ESI Full ms [100.00-2000.00]

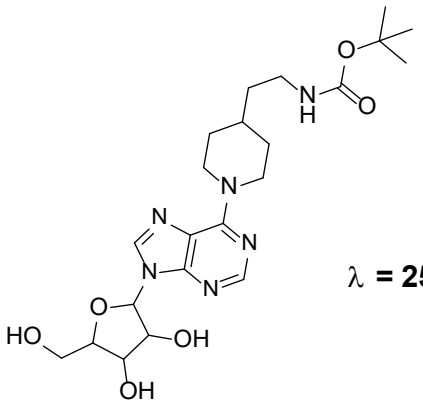
NL: Δm= 1.90 ppm
1.78E4

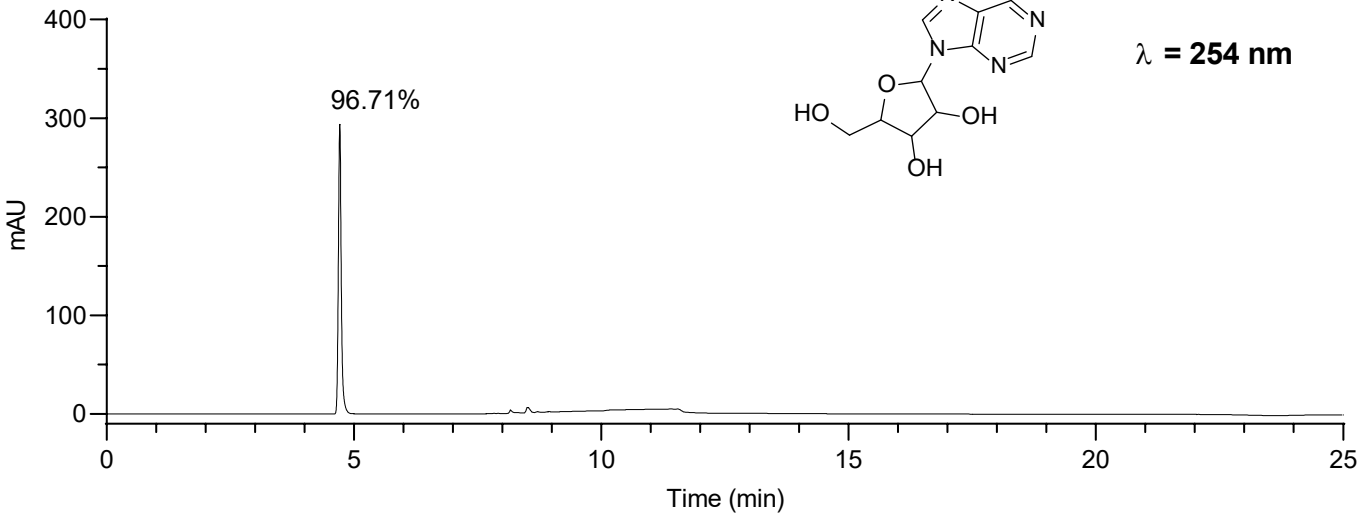
$C_{22}H_{34}N_6O_6$ +H:
$C_{22}H_{35}N_6O_6$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM

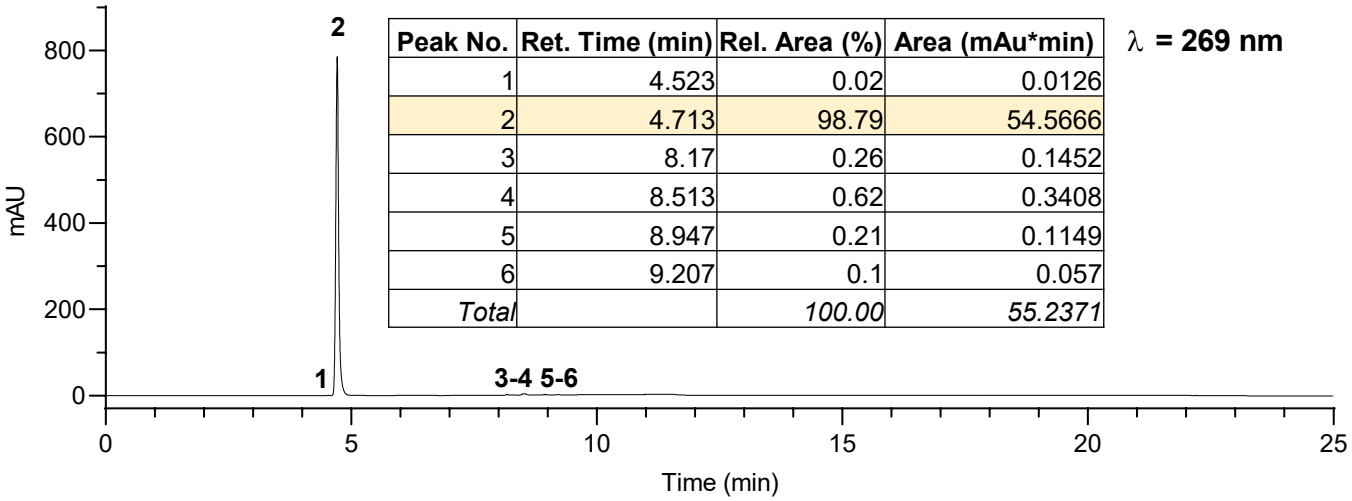
NL: Δm=2.19 ppm
1.78E4

$C_{22}H_{34}N_6O_6$ +Na:
$C_{22}H_{34}N_6O_6Na_1$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM

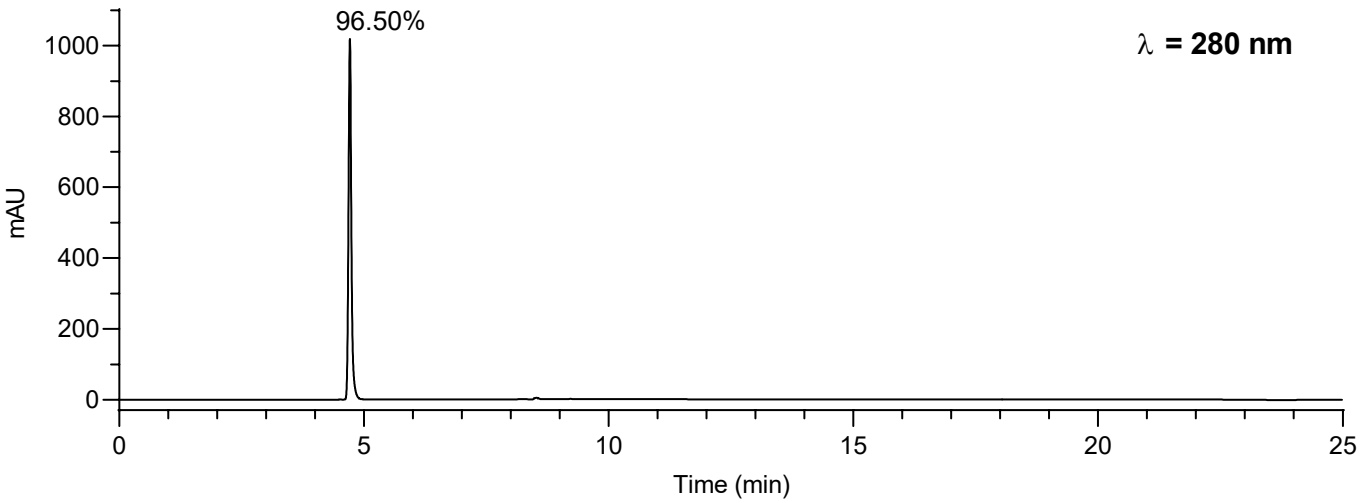
40



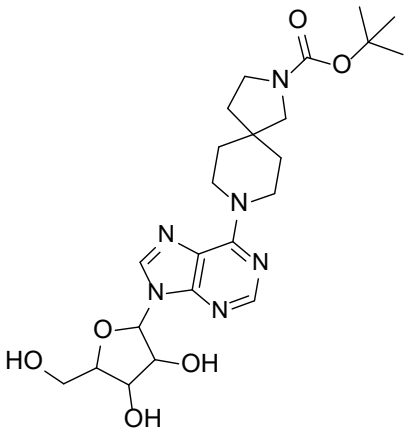




Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	4.523	0.02	0.0126
2	4.713	98.79	54.5666
3	8.17	0.26	0.1452
4	8.513	0.62	0.3408
5	8.947	0.21	0.1149
6	9.207	0.1	0.057
Total		*100.00*	*55.2371*

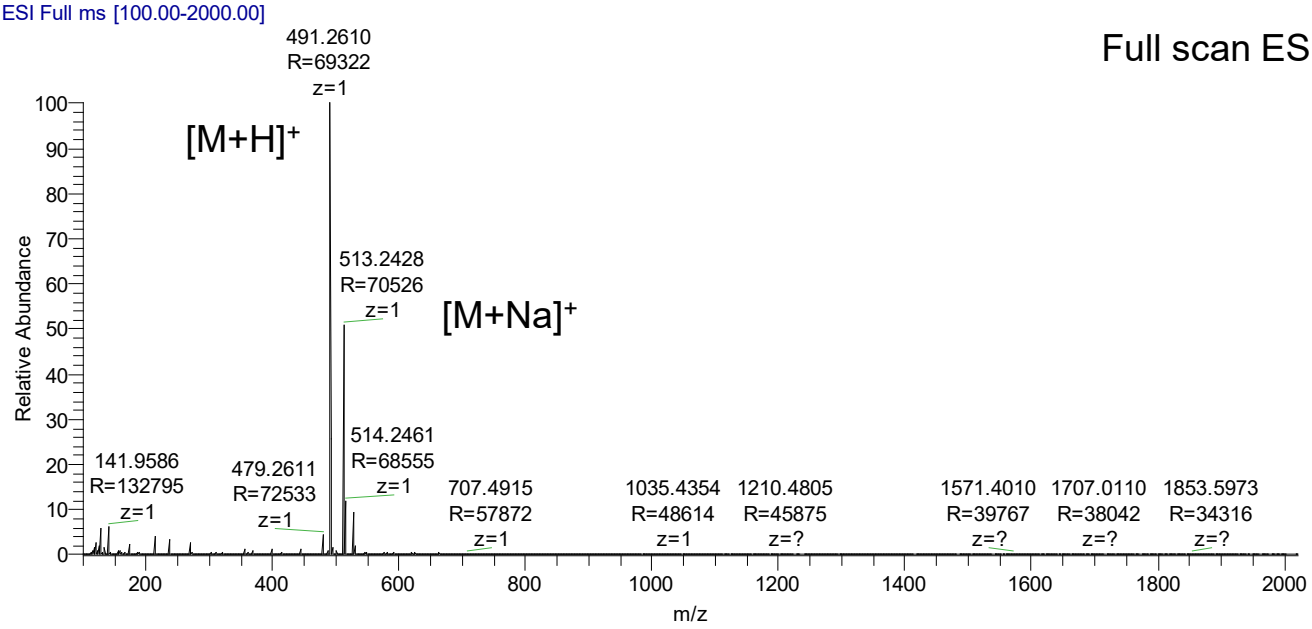


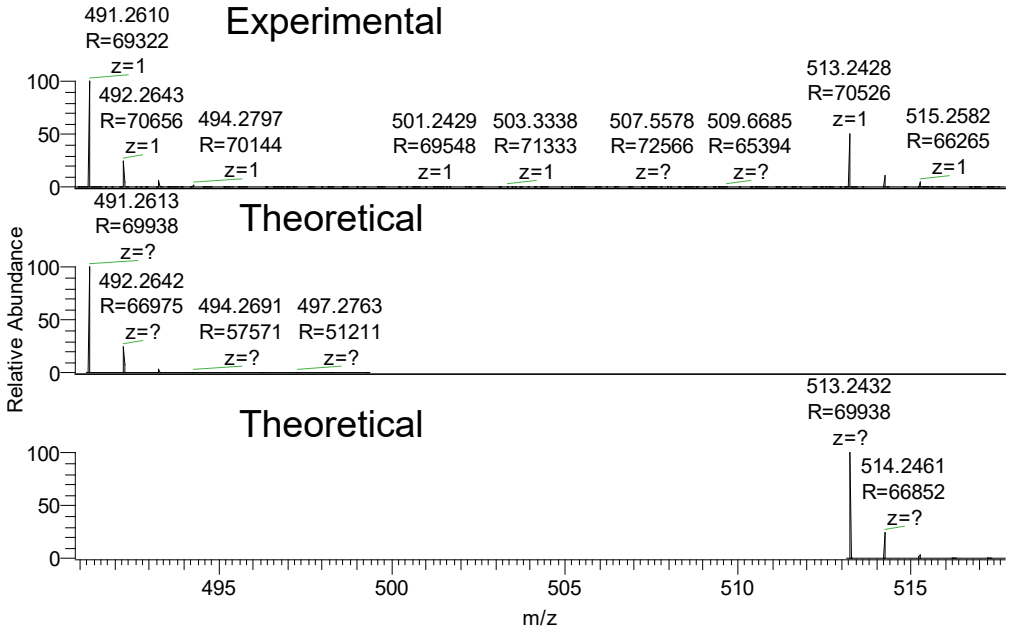
41



41#1-29 RT: 0.02-0.44 AV: 29 NL: 8.40E5 T: FTMS + p ESI Full ms [100.00-2000.00]

Full scan ESI(+)





NL:
8.40E5
41#1-29 RT: 0.02-0.44 AV: 29 T: FTMS + p ESI Full ms [100.00-2000.00]

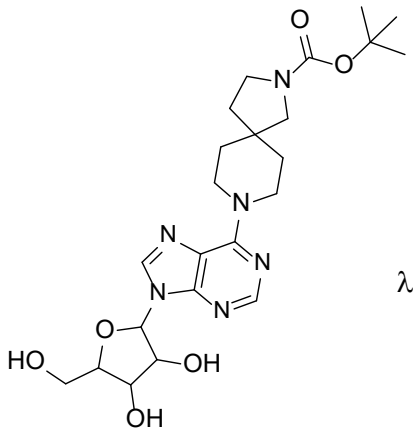
NL:
1.76E4 Δm= 0.61 ppm

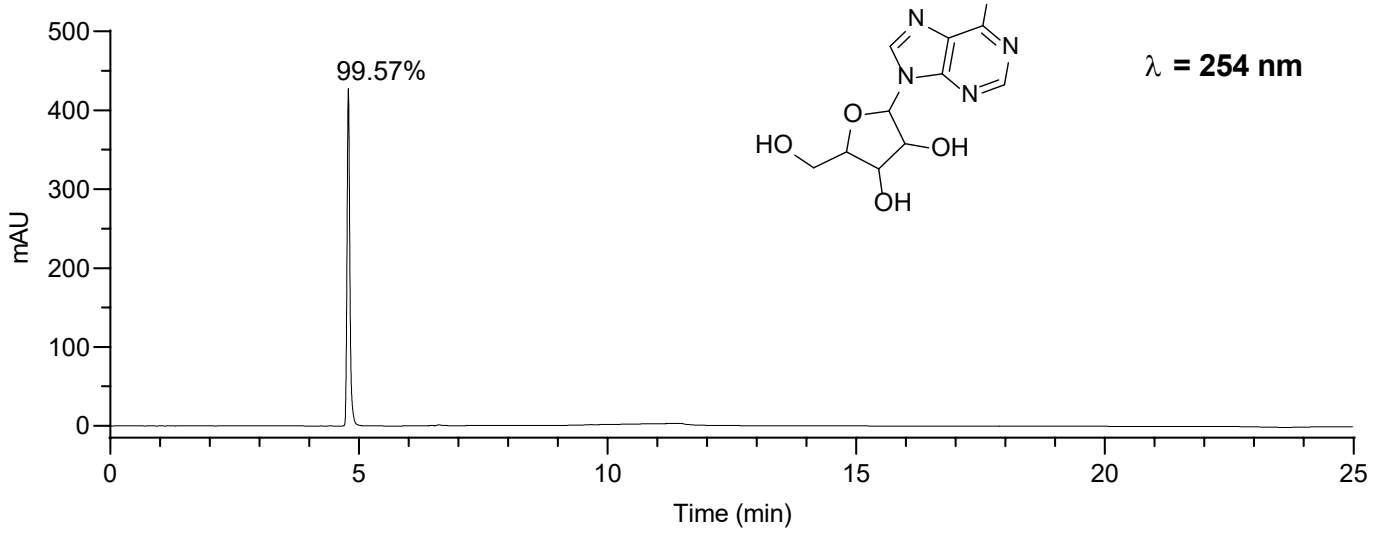
$C_{23}H_{34}N_6O_6$ +H:
$C_{23}H_{35}N_6O_6$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM

NL:
1.76E4 Δm= 0.78 ppm

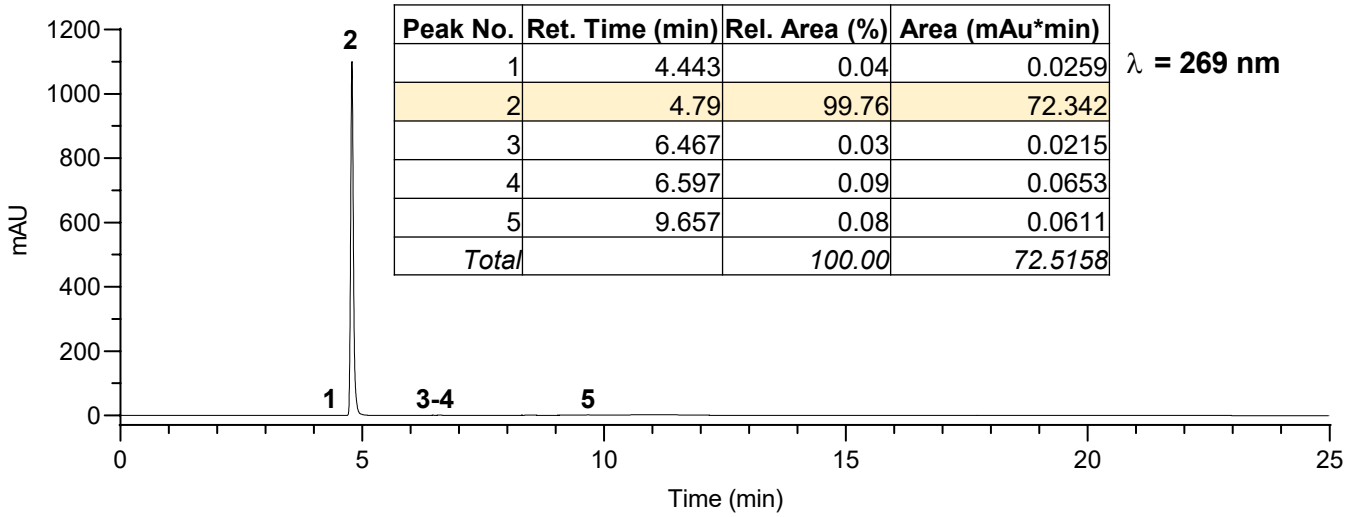
$C_{23}H_{34}N_6O_6$ +Na:
$C_{23}H_{34}N_6O_6Na_1$
p (gss, s /p:40) Chrg 1
R: 70000 Res .Pwr . @FWHM

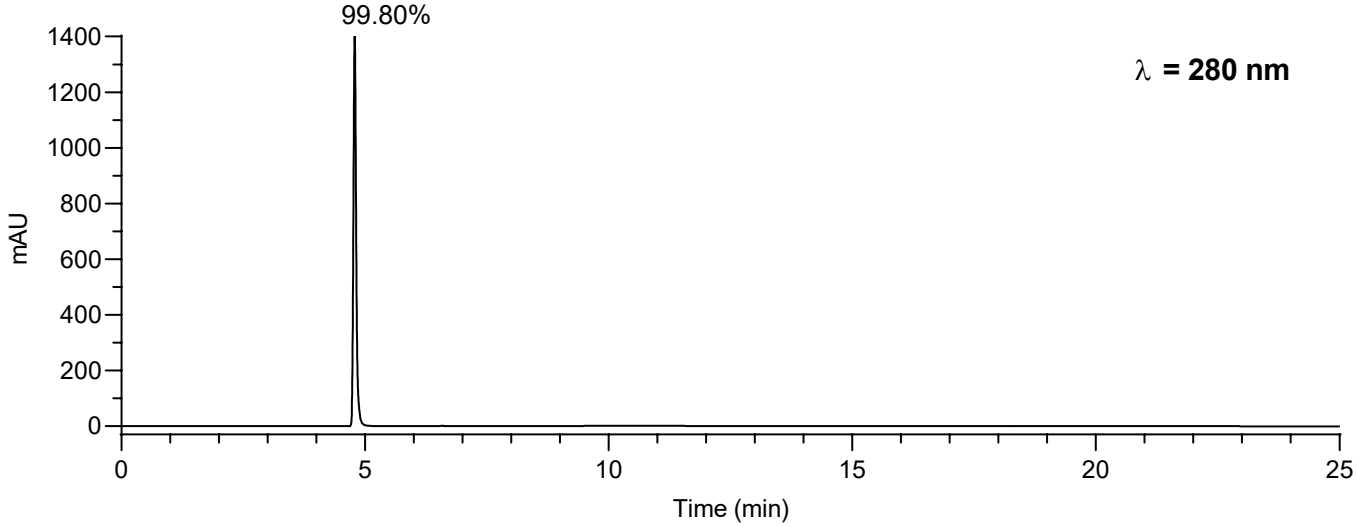
41



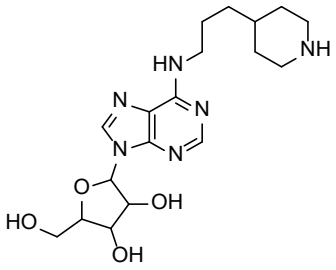


Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	4.443	0.04	0.0259
2	4.79	99.76	72.342
3	6.467	0.03	0.0215
4	6.597	0.09	0.0653
5	9.657	0.08	0.0611
Total		*100.00*	*72.5158*

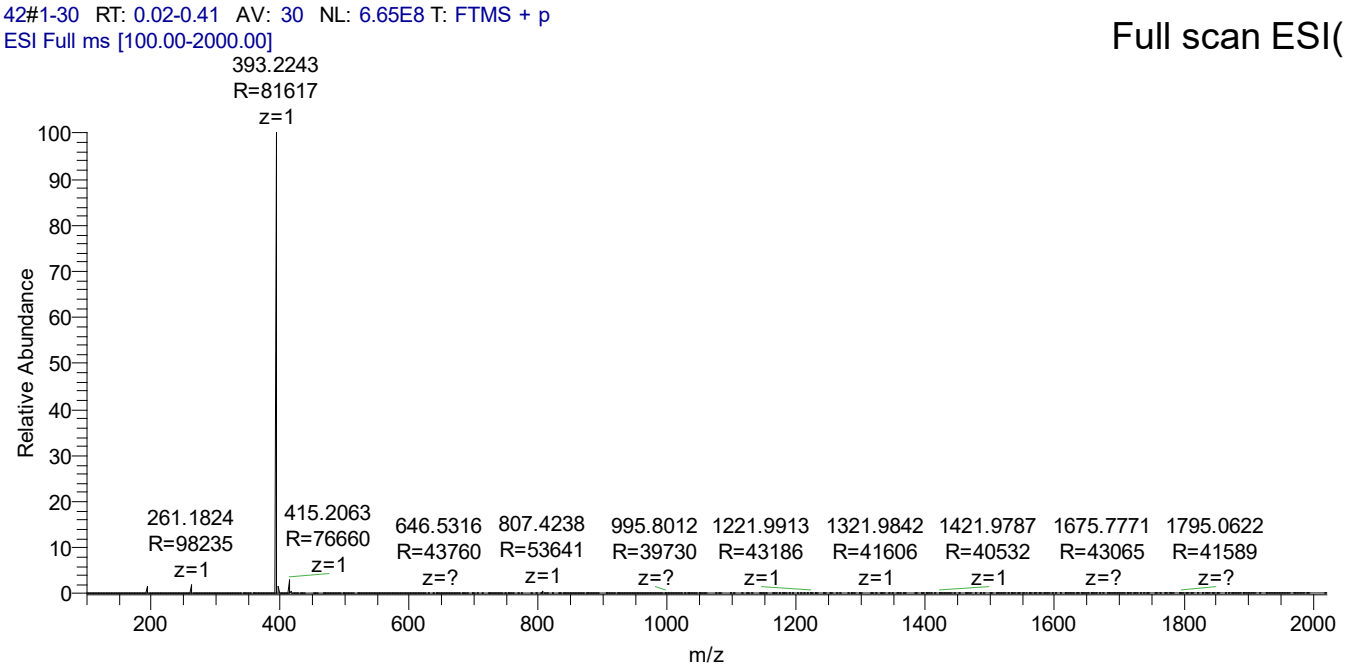


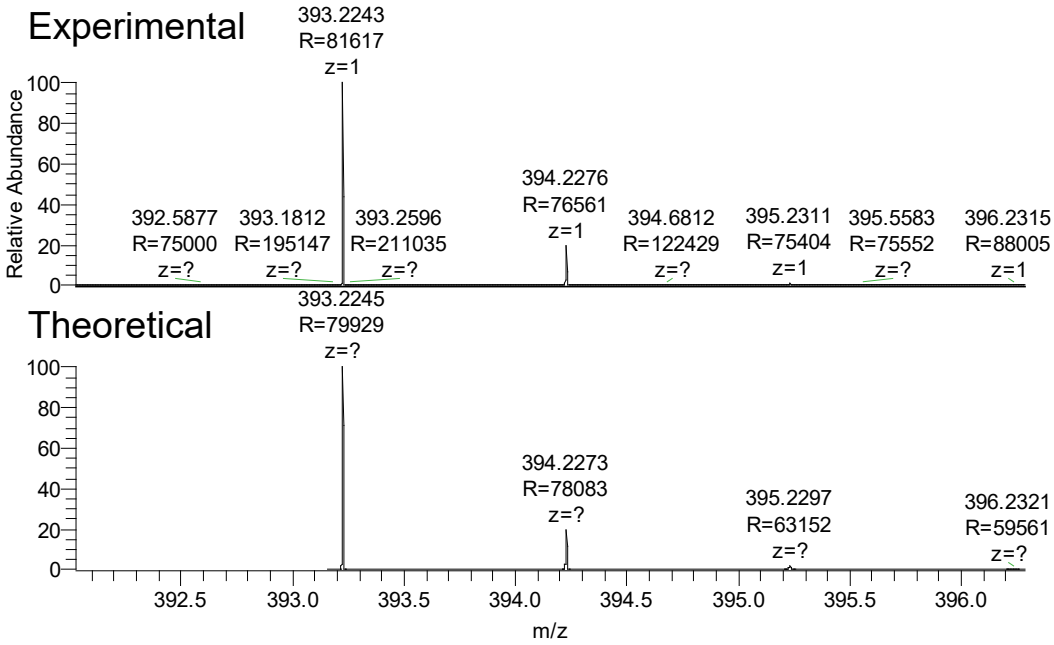


42



Full scan ESI(+)



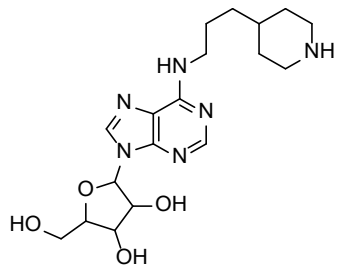


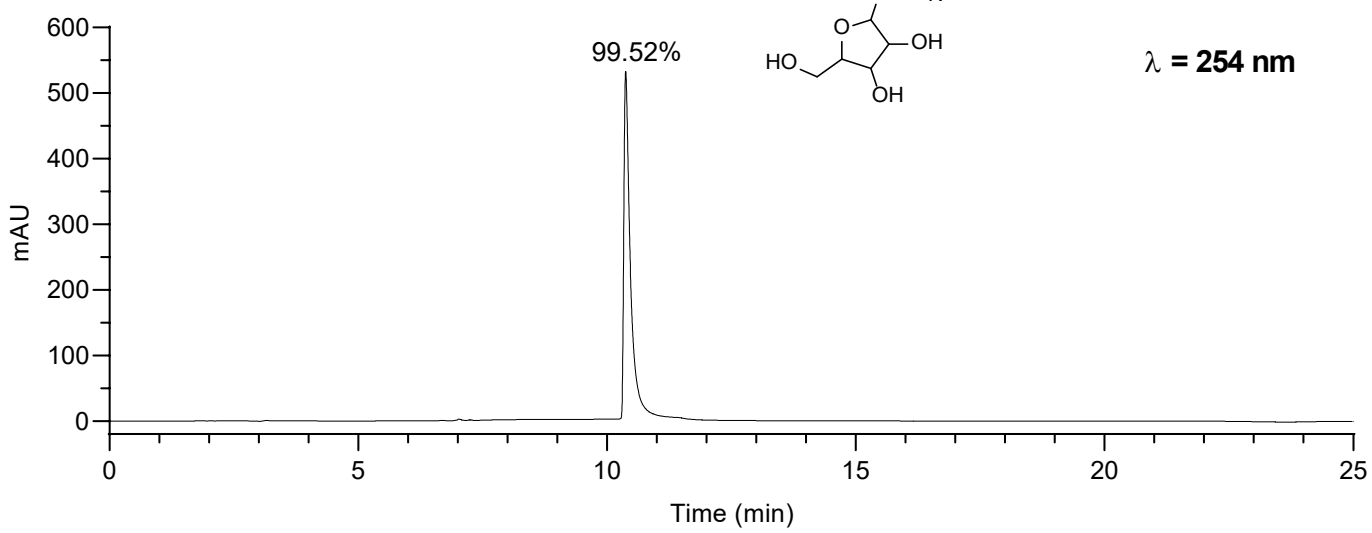
NL:
6.65E8
421-30 RT: 0.02-0.41 AV: 30
T: FTMS + p ESI Full ms
[100.00-2000.00]

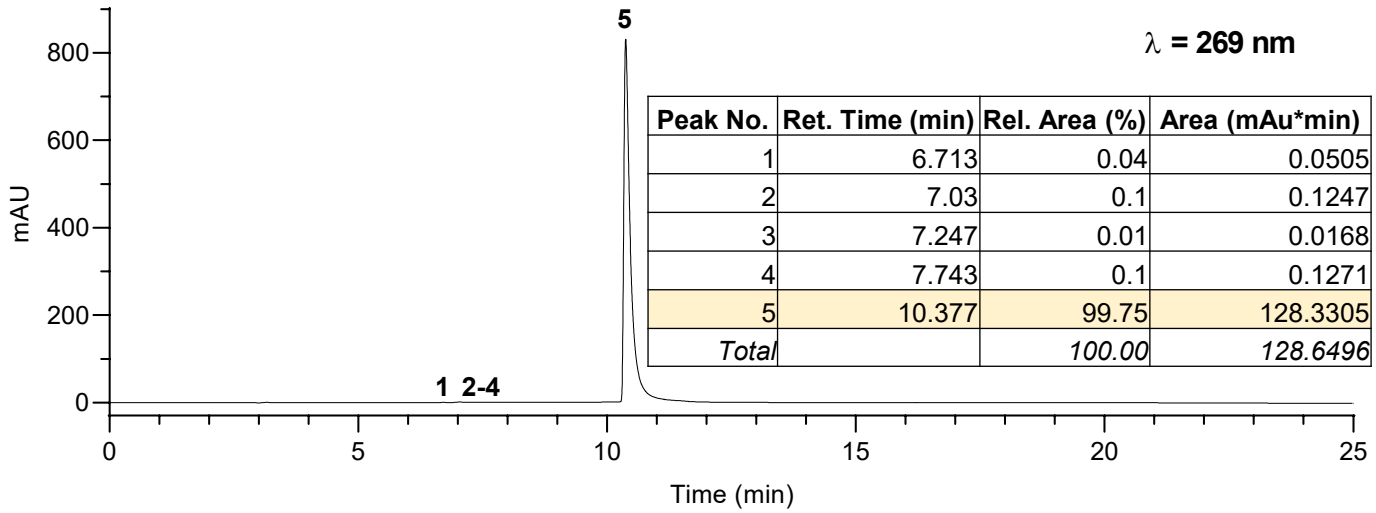
NL:
1.87E4
$C_{18}H_{28}N_6O_4$ +H:
$C_{18}H_{29}N_6O_4$
p (gss, s /p:40) Chrg 1
R: 80000 Res .Pwr . @FWHM

Δm= 0.51 ppm

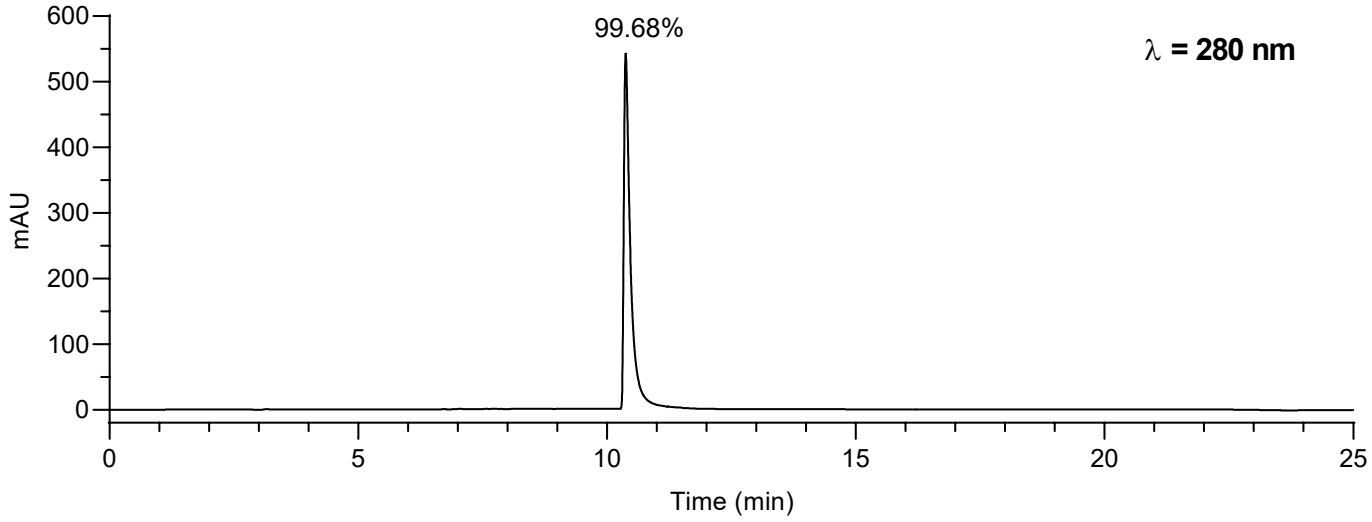
42





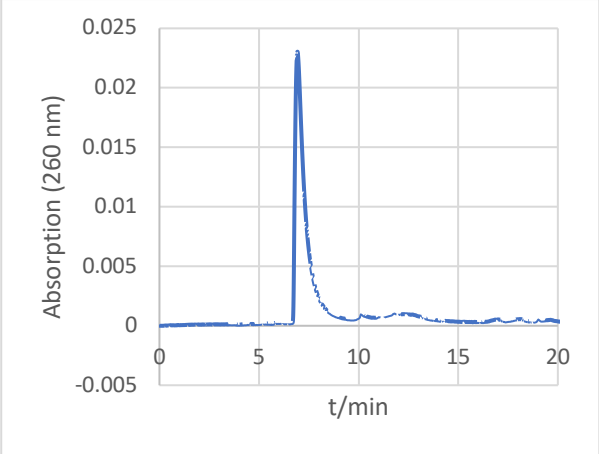


Peak No.	Ret. Time (min)	Rel. Area (%)	Area (mAu*min)
1	6.713	0.04	0.0505
2	7.03	0.1	0.1247
3	7.247	0.01	0.0168
4	7.743	0.1	0.1271
5	10.377	99.75	128.3305
Total		*100.00*	*128.6496*

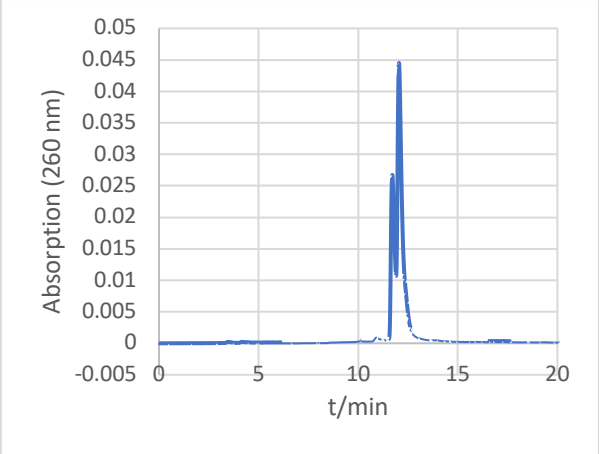


Reversed phase HPLC analysis of compounds from Figure S1. Compounds were analyzed by reversed phase HPLC (MZ-Aqua Perfect C-18 column, 250 x 4.6 mm, 5 µm, 120 Å, equipped with a C-18 pre-column, 8.0 mm x 4.0 mm, 5 µm, 120 Å) using acetonitrile gradient A (0% – 7% in 15 min and 7% – 70% in 5 min) or gradient B (4.9% – 52.5% in 30 min and 52.5 – 70% in 1 min) in aqueous TFA solution (0.01 % TFA) with a flow of 1 mL/min and detection at 260 nm.

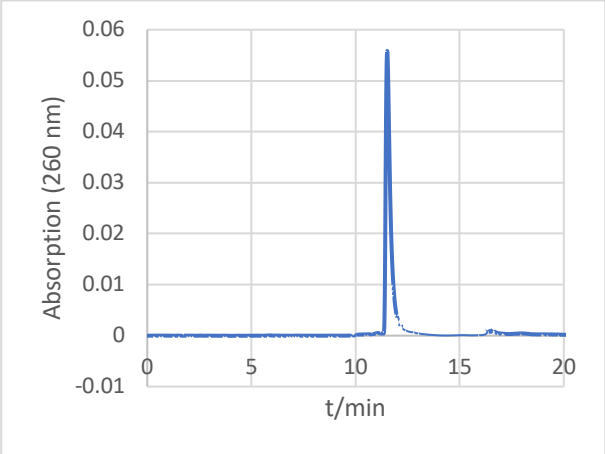
201 (dcSAM), gradient A



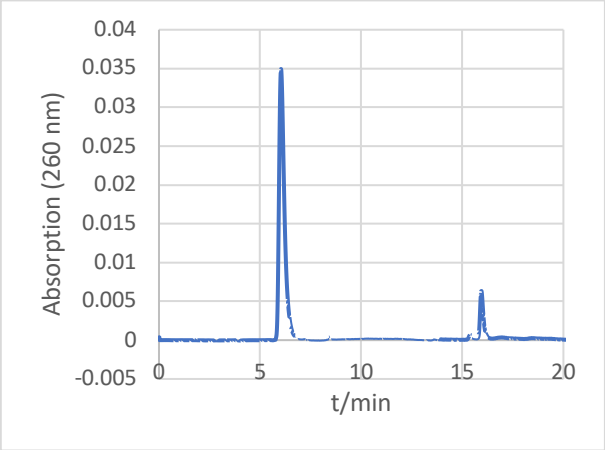
202 (daSAM), gradient A



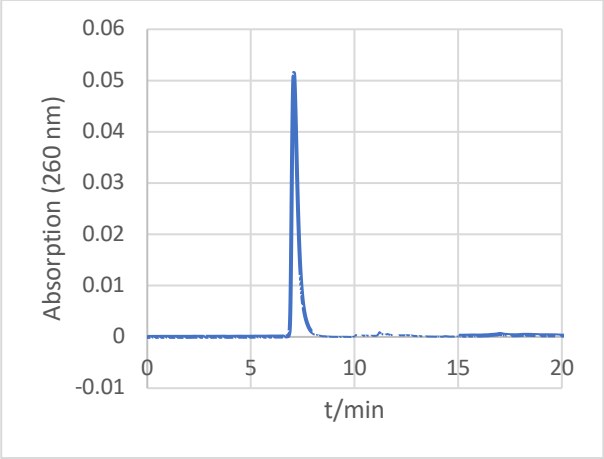
203 (DMTA), gradient A



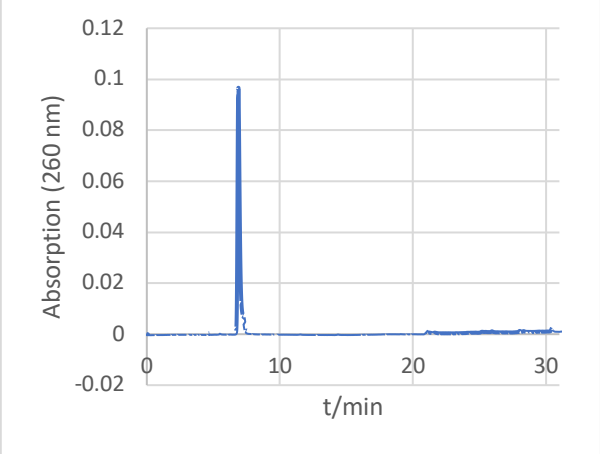
204 (sinefungin), gradient A



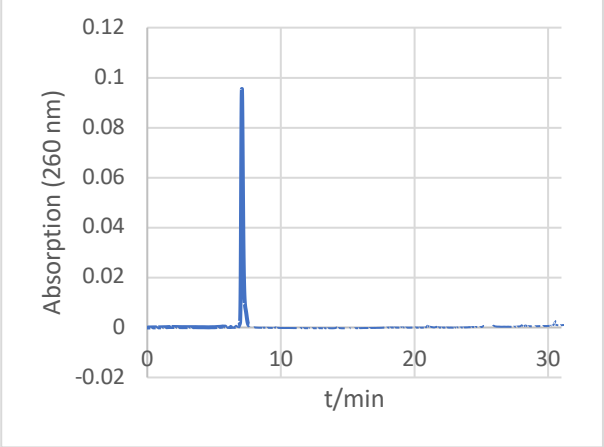
205 (Aza-SAM), gradient A



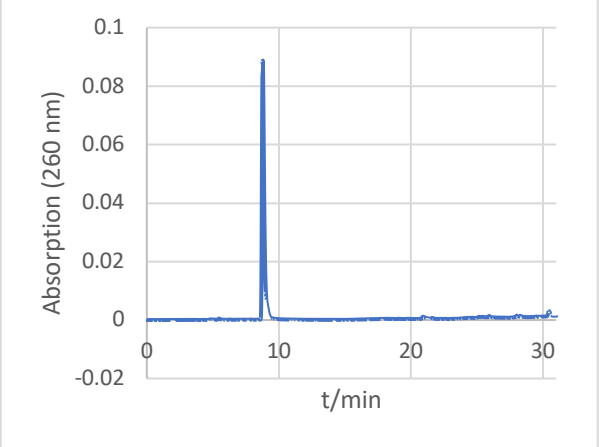
206 (L-SAH), gradient B



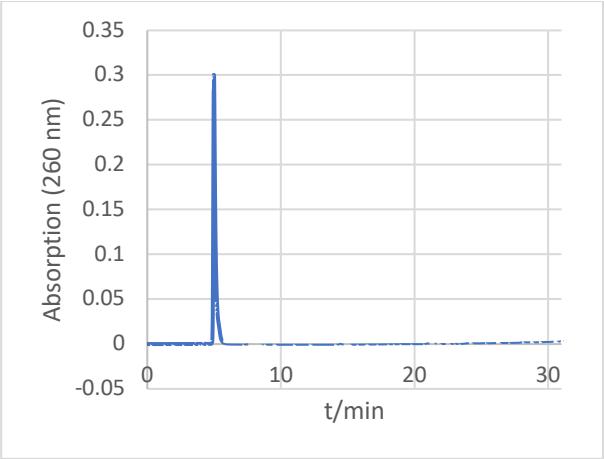
207 (D-SAH), gradient B



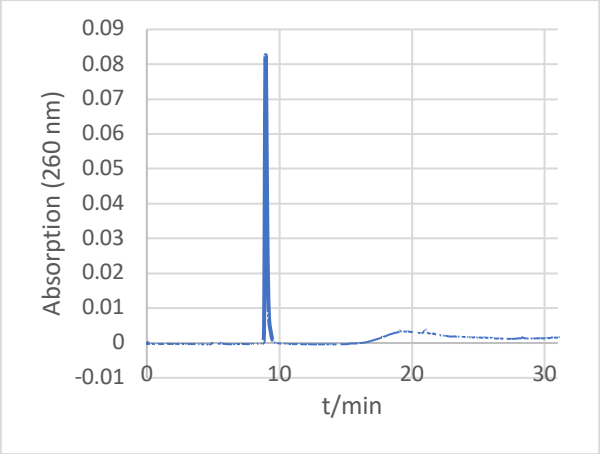
208 (dc-SAH), gradient B



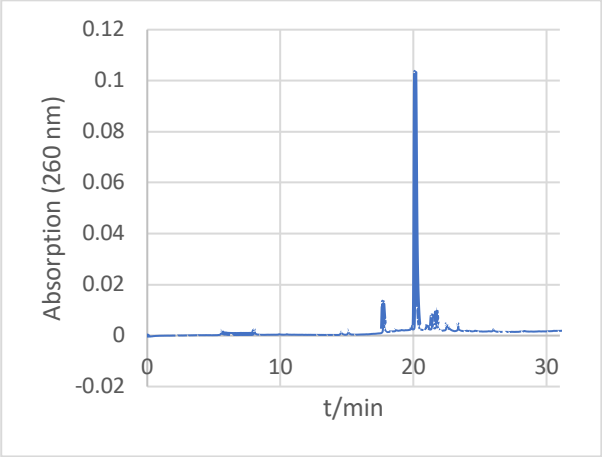
209 (5'-adenosyl-L-cysteine), gradient B



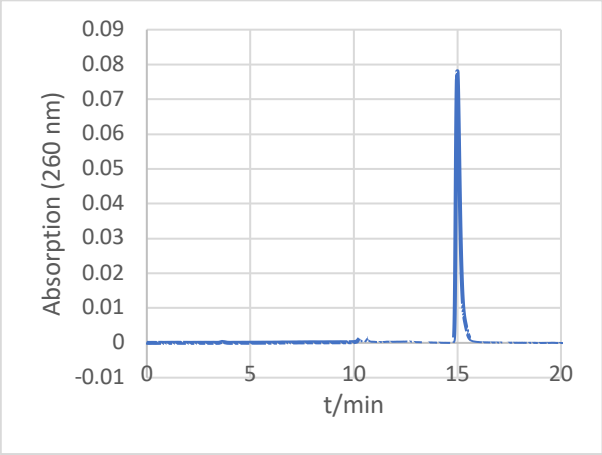
210 (CPTA), gradient B



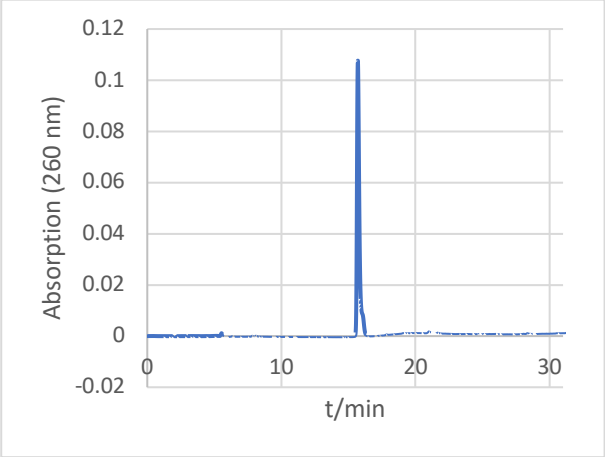
211 (CPTA methylester), gradient B



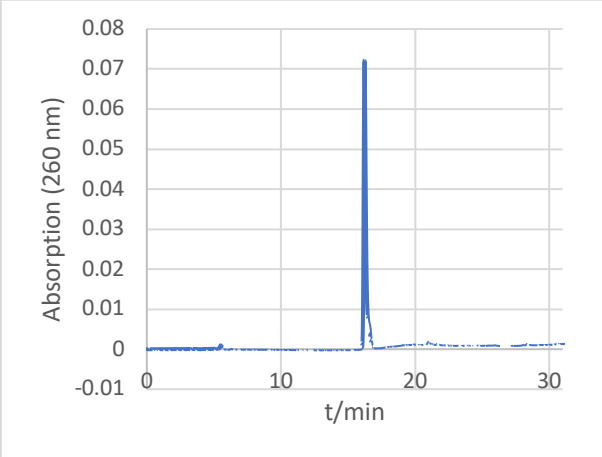
212 (AETA), gradient A



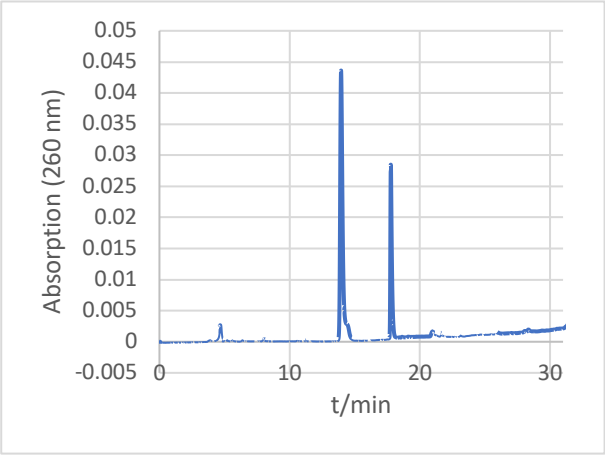
213 (CETA), gradient B



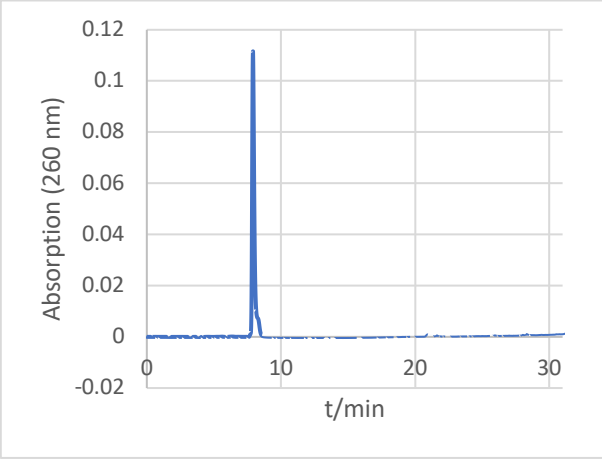
214 (MTA), gradient B



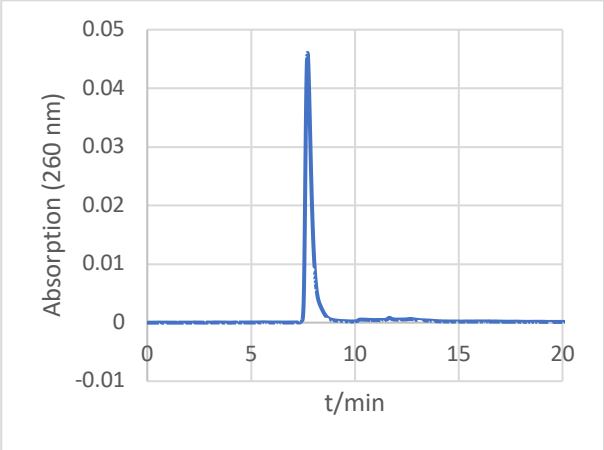
215 (5'-thioadenosine), gradient B



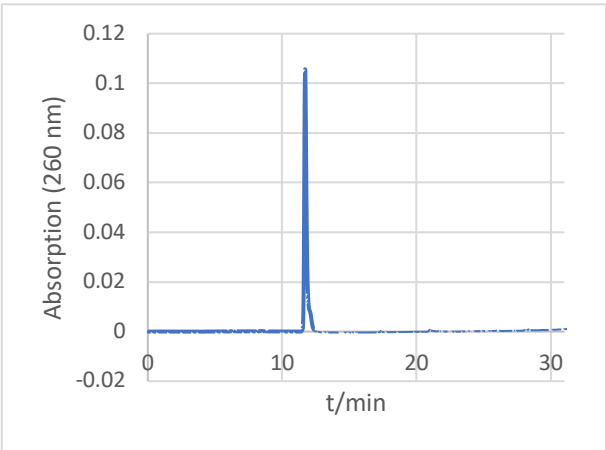
216 (adenosine), gradient B



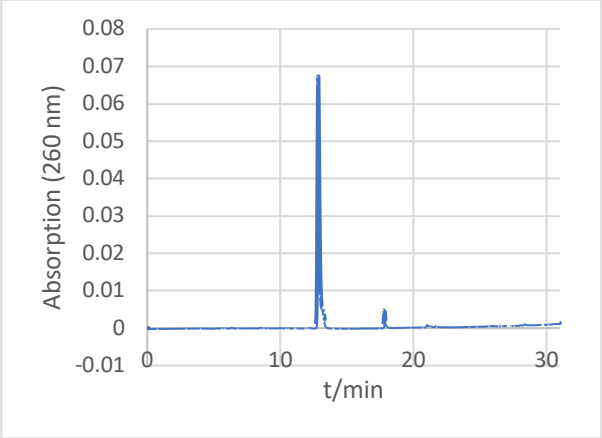
218 (5'-aminoadenosine), gradient A



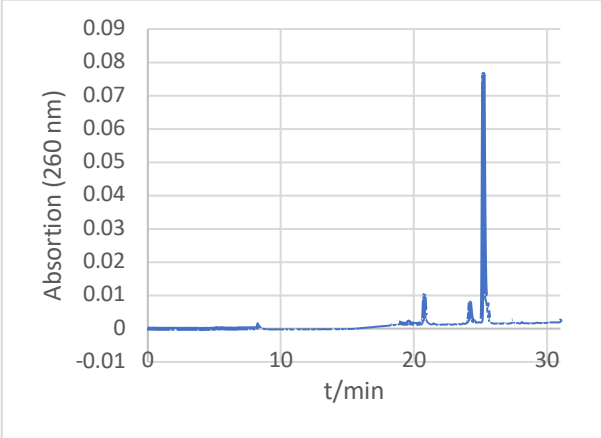
219 (*N*6-methyl-2'-deoxyadenosine), gradient B



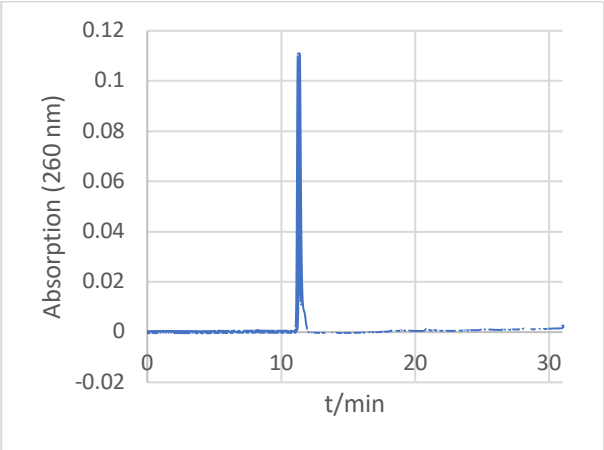
220 (TL-107-2), gradient B



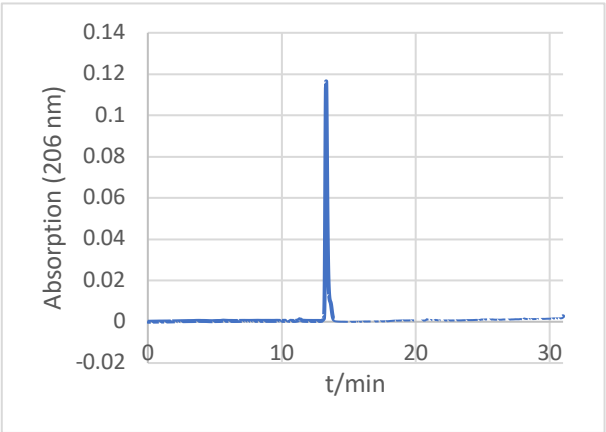
221 (TL-106), gradient B



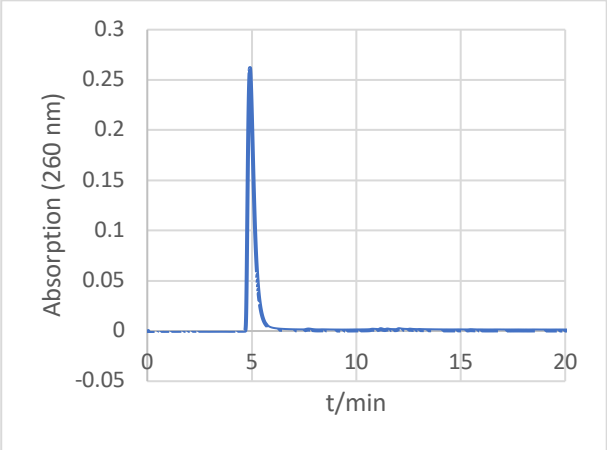
222 (TL-104), gradient B



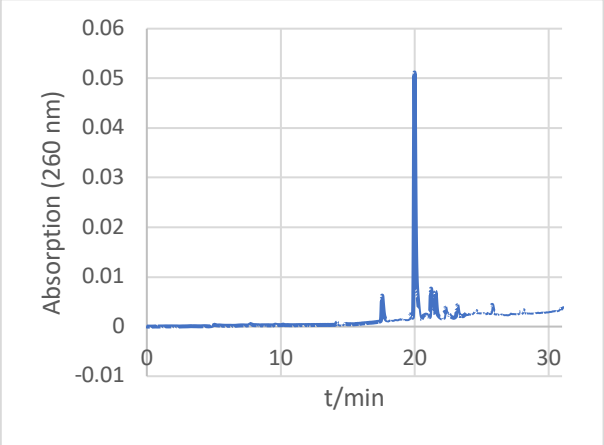
223 (TL-100-2), gradient B



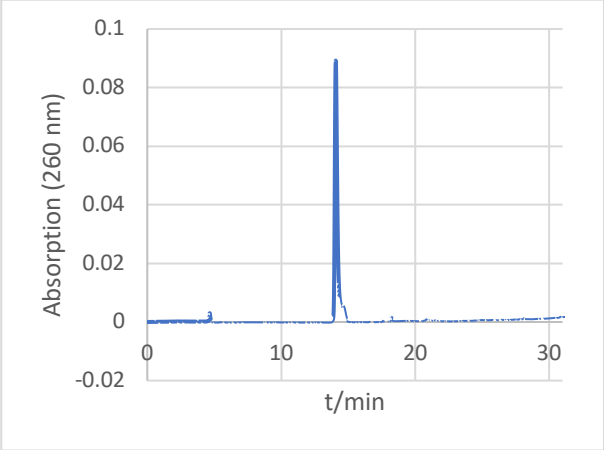
224 (AEA), gradient A



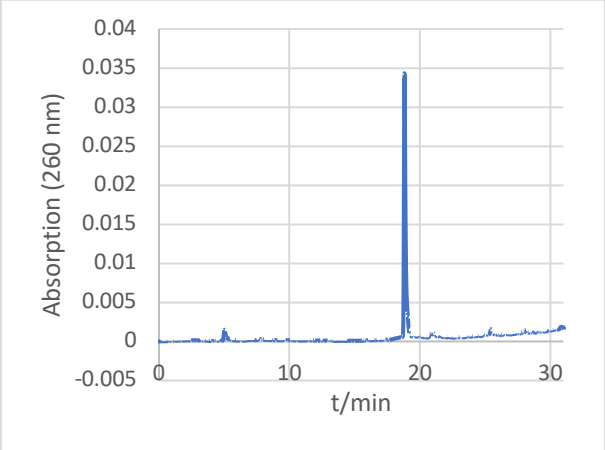
225 (CMTA), gradient B



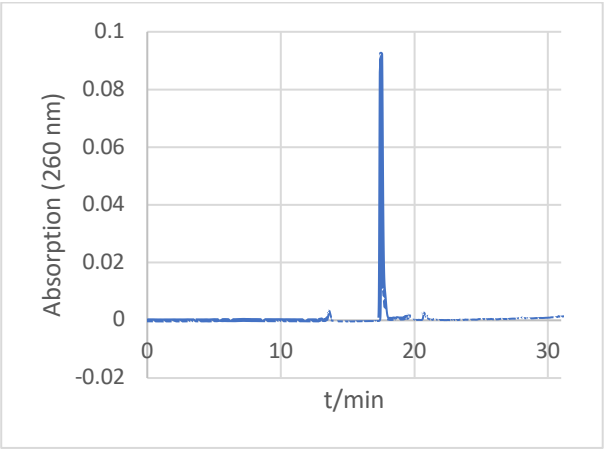
226 (5'-deoxy-5'-chloroadenosine), gradient B



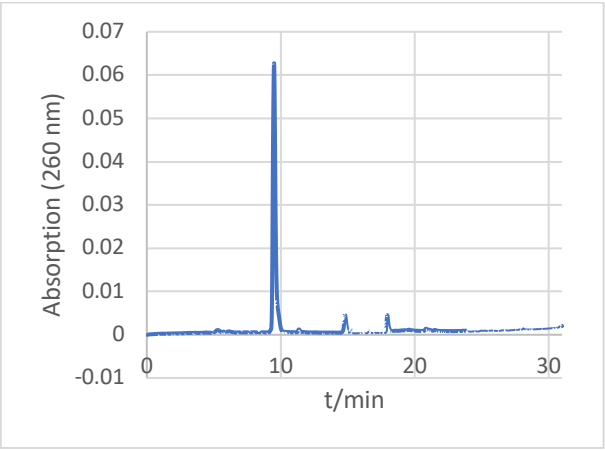
227 (5'-phthalimidoadenosine), gradient B



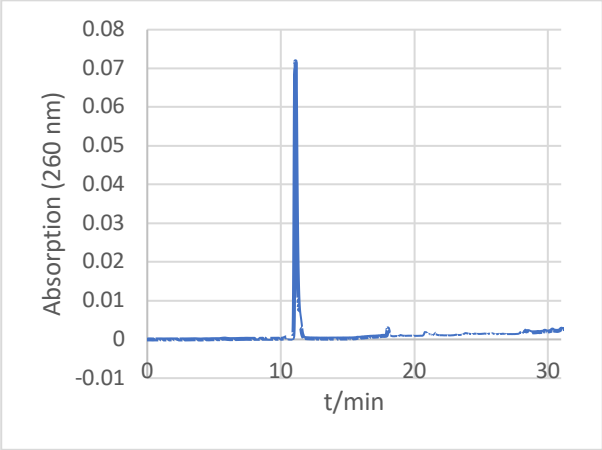
228 (5'-deoxy-5'-acetyladenosine), gradient B



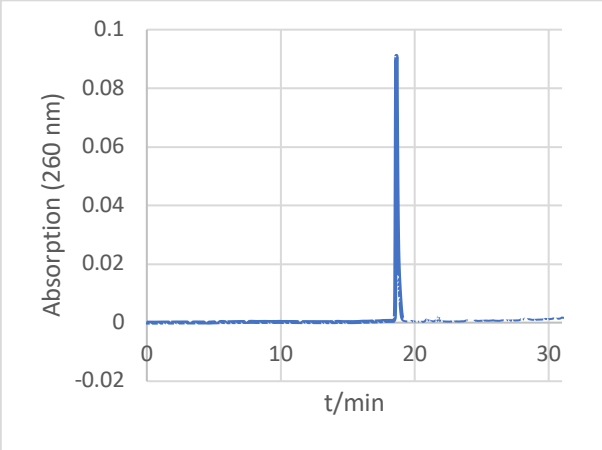
229 (*South*-SAH), gradient B



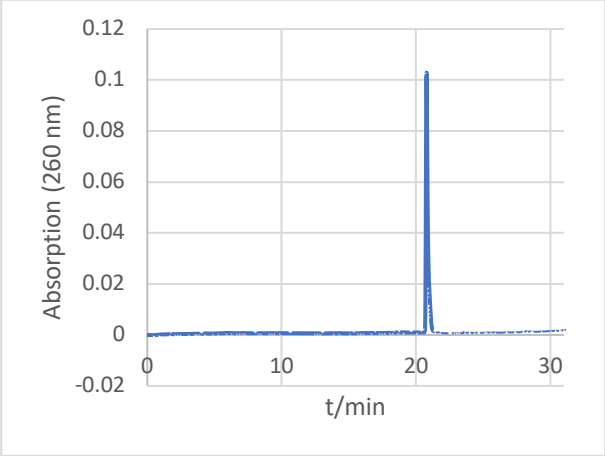
230 (*North*-SAH), gradient B



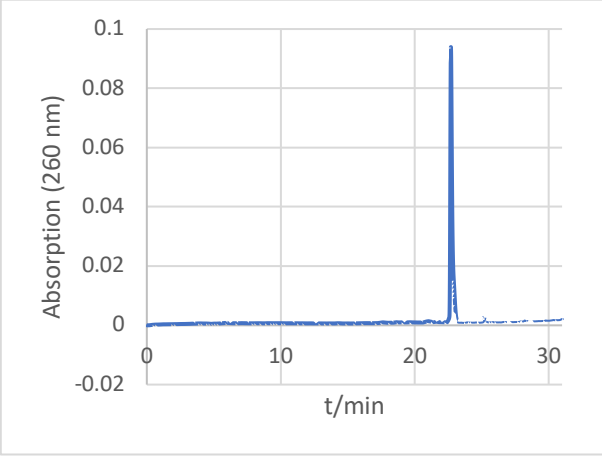
231 (5'-ethylthioadenosine), gradient B



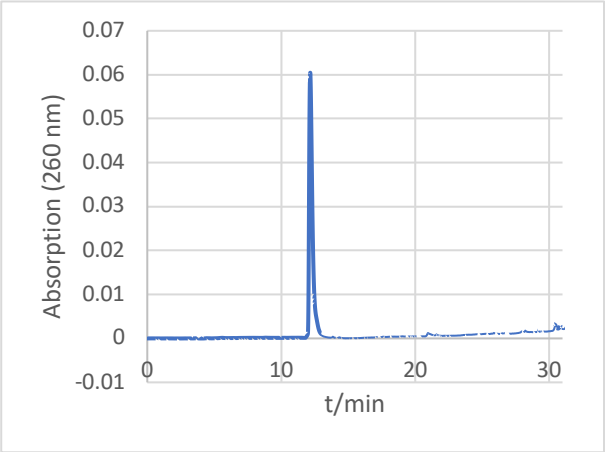
232 (5'-propylthioadenosine), gradient B



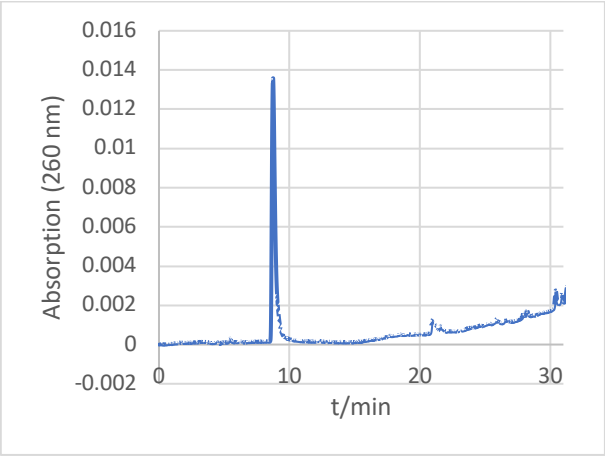
233 (5'-butylthioadenosine), gradient B



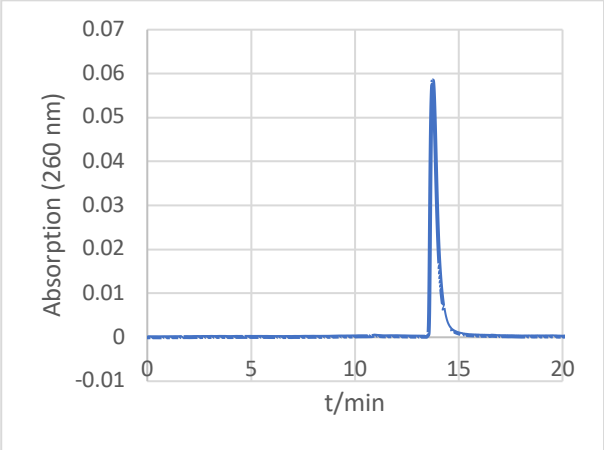
234 (5'-methylbutylthioadenosine), gradient B



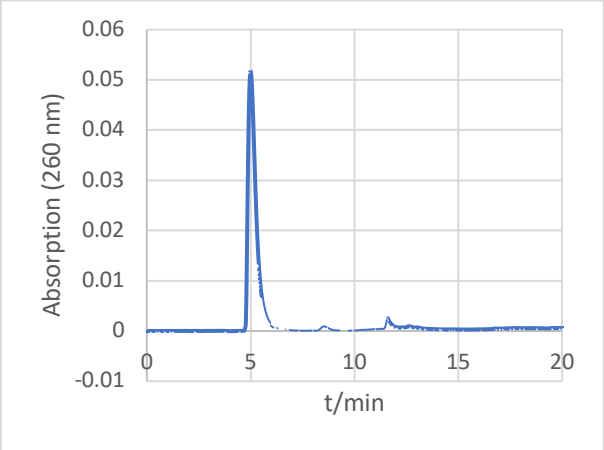
235 (5'-methylpropylthioadenosine), gradient B



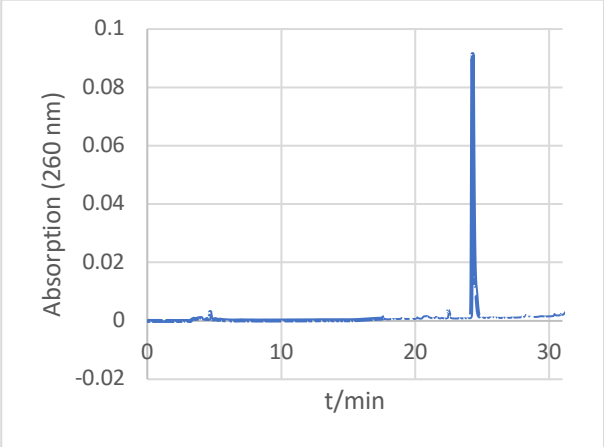
236 (5'-methylethylthioadenosine), gradient A



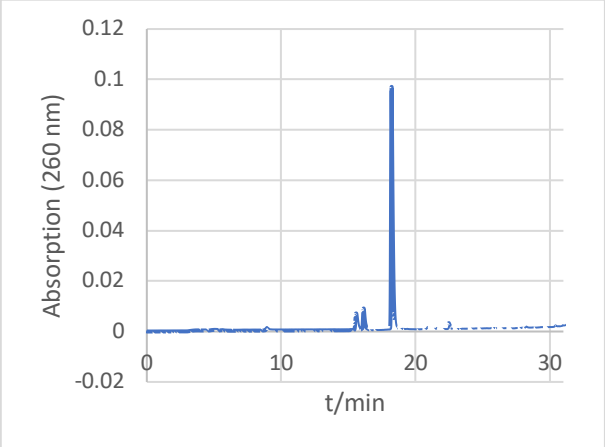
237 (AEAA), gradient A



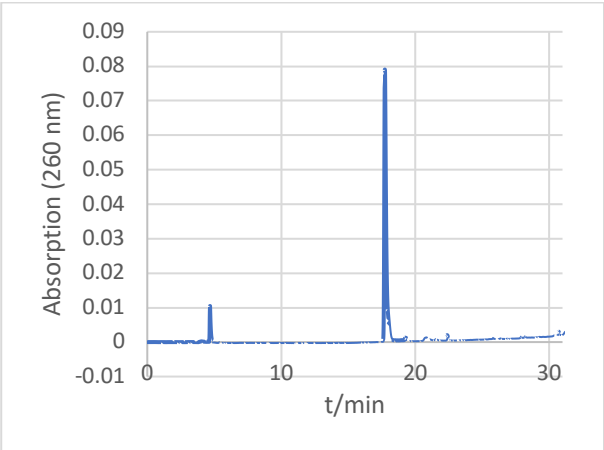
238 (phETA), gradient B



239 (Bisubstrate inhibitor), gradient B



240 (5'-iodo-5'-deoxyadenosine), gradient B



241 (5'-tosyladenosine), gradient B