

Supporting Information.

C@PA: Computer-aided Pattern Analysis to Predict Multitarget ABC Transporter Inhibitors

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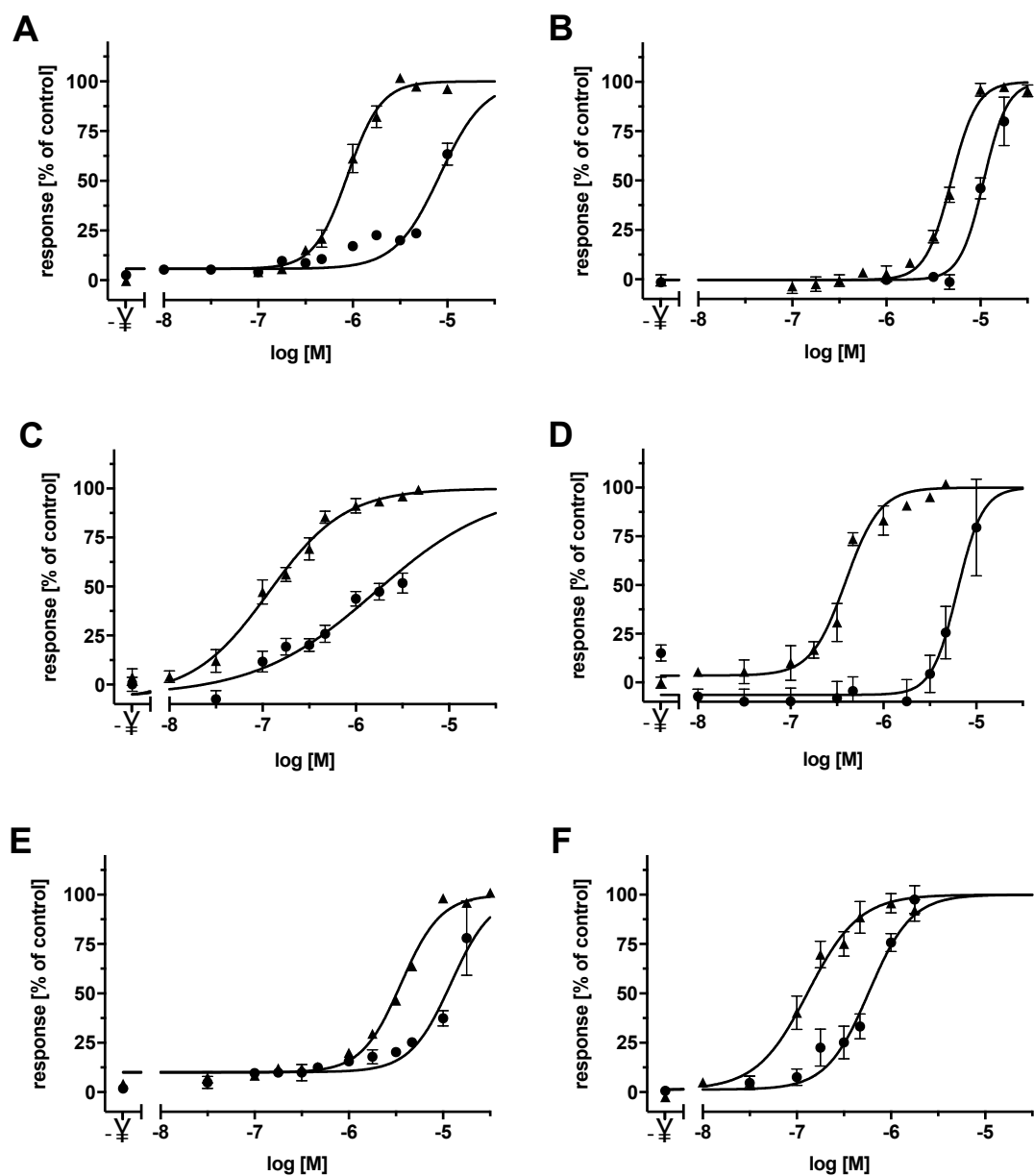
Supplementary Figure 1 A–F: Concentration-effect curves of compound **15** against ABCB1 (A and D), ABCC1 (B and E), and ABCG2 (C and F) as determined in calcein AM (A and B), pheophorbide A (C), Hoechst 33342 (D and F), and daunorubicin (E) assays.

Supplementary Figure 2 A–F: Concentration-effect curves of compound **18** against ABCB1 (A and D), ABCC1 (B and E), and ABCG2 (C and F) as determined in calcein AM (A and B), pheophorbide A (C), Hoechst 33342 (D and F), and daunorubicin (E) assays.

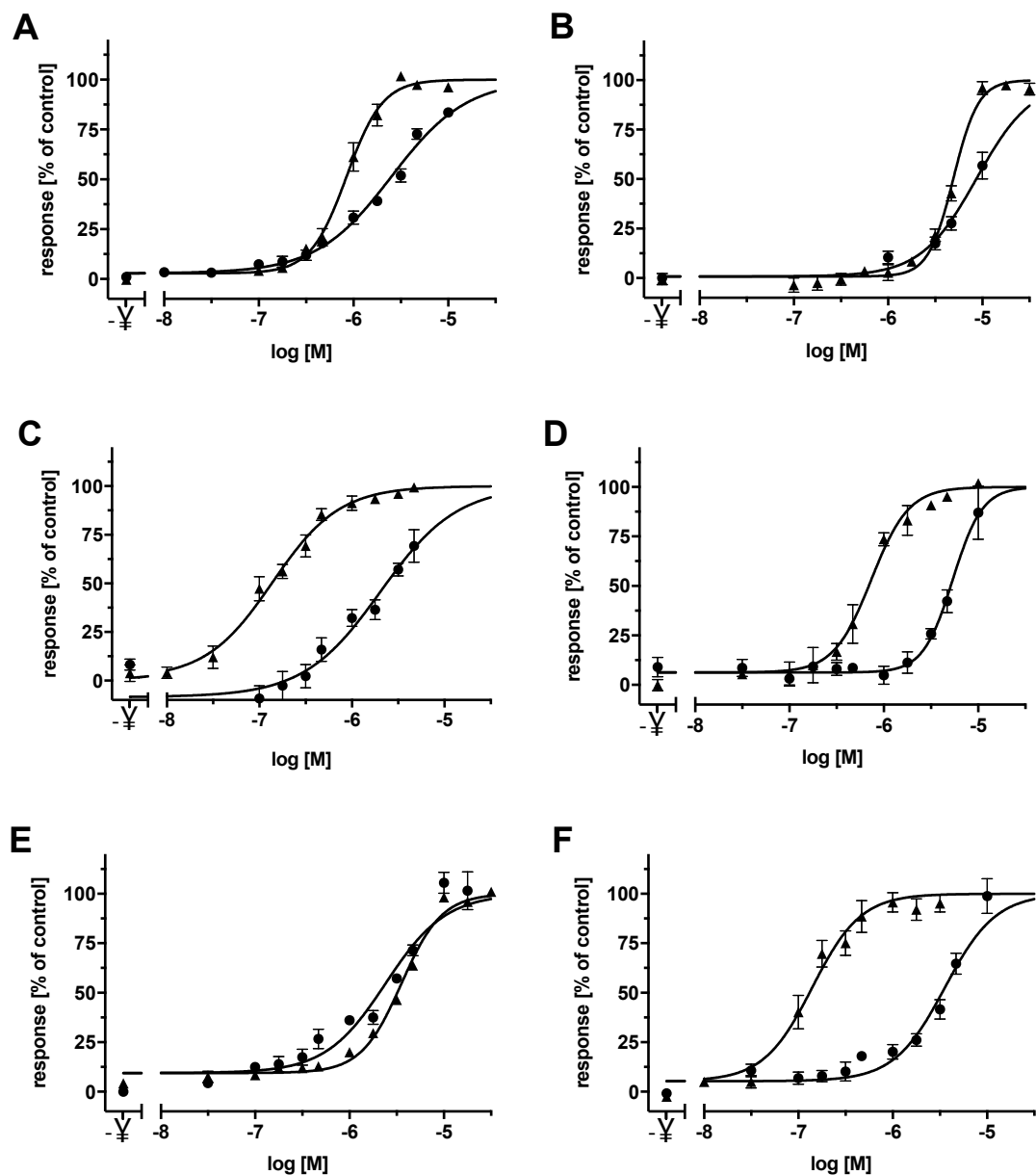
Supplementary Figure 3 A–F: Concentration-effect curves of compound **22** against ABCB1 (A and D), ABCC1 (B and E), and ABCG2 (C and F) as determined in calcein AM (A and B), pheophorbide A (C), Hoechst 33342 (D and F), and daunorubicin (E) assays.

Supplementary Figure 4 A–F: Concentration-effect curves of compound **26** against ABCB1 (A and D), ABCC1 (B and E), and ABCG2 (C and F) as determined in calcein AM (A and B), pheophorbide A (C), Hoechst 33342 (D and F), and daunorubicin (E) assays.

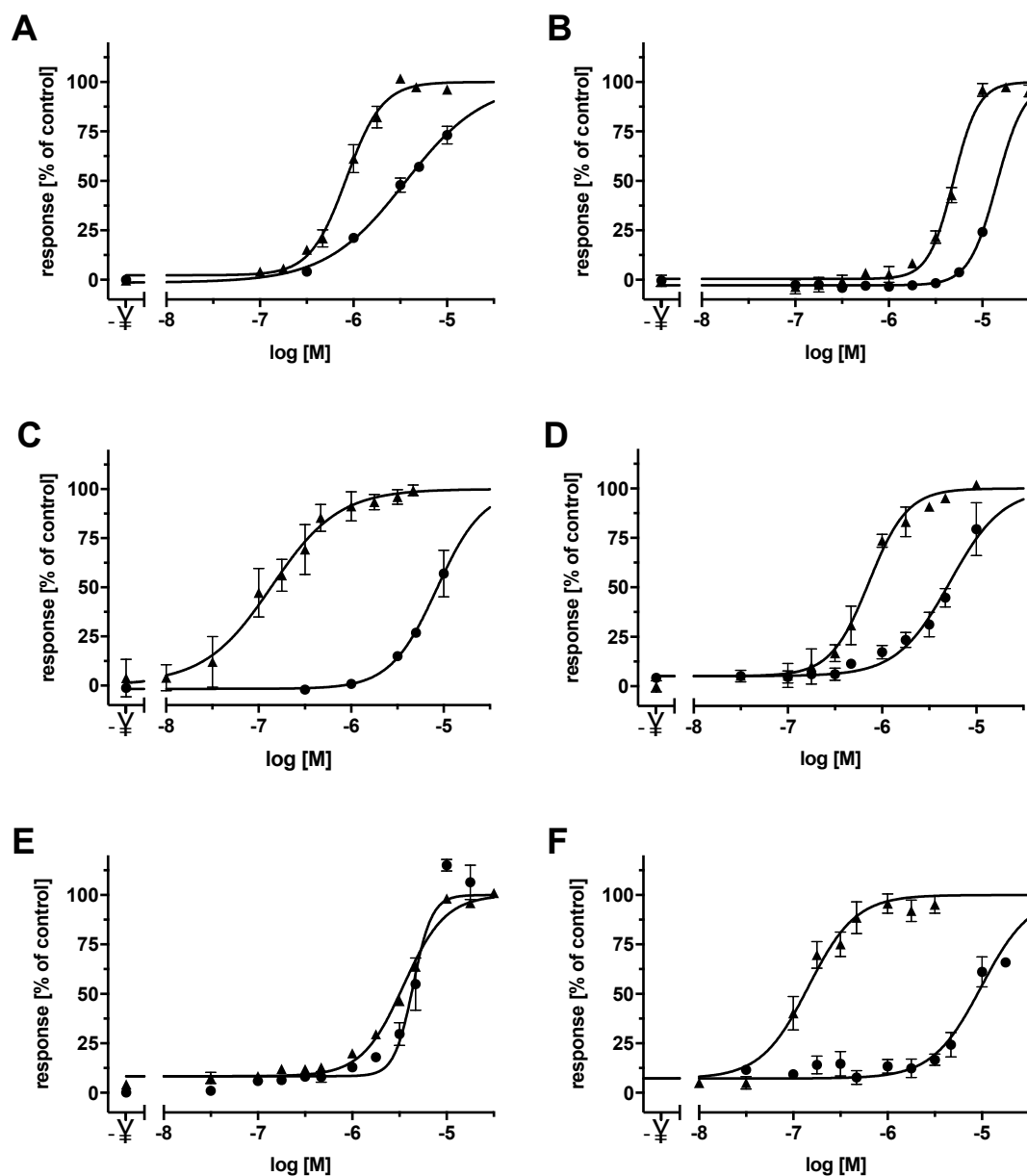
LC-MS data and NMR spectra of compounds 11–33.



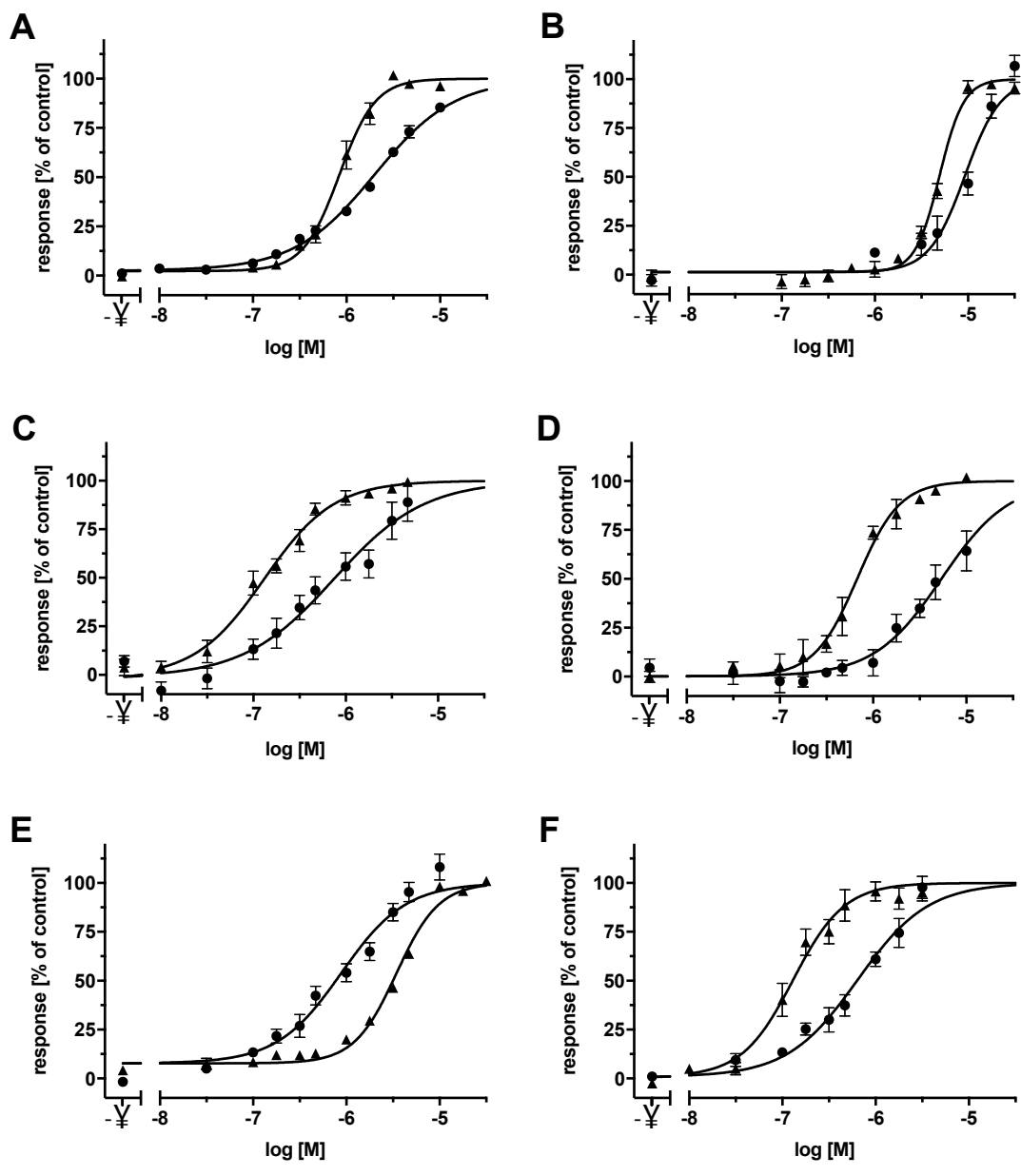
Supplementary Figure 1 A–F: Concentration-effect curves of compound **15** (●) as determined in calcein AM (A and B), pheophorbide A (C), Hoechst 33342 (D and F), and daunorubicin (E) assays using either ABCB1-overexpressing A2780/ADR cells (A and D), ABCC1-overexpressing H69AR cells (B and E), or ABCG2-overexpressing MDCK II BCRP cells (C and F). Data were normalized by defining the effect of 10 μ M cyclosporine A (▲; A, B, D, and E) and compound **34** (▲; C and F) as positive control (100%) and buffer medium was used as negative control (0%). Shown is mean \pm SEM of at least three independent experiments.



Supplementary Figure 2 A–F: Concentration-effect curves of compound **18** (●) as determined in calcein AM (A and B), pheophorbide A (C), Hoechst 33342 (D and F), and daunorubicin (E) assays using either ABCB1-overexpressing A2780/ADR cells (A and D), ABCC1-overexpressing H69AR cells (B and E), or ABCG2-overexpressing MDCK II BCRP cells (C and F). Data were normalized by defining the effect of 10 μ M cyclosporine A (▲; A, B, D, and E) and compound **34** (▲; C and F) as positive control (100%) and buffer medium was used as negative control (0%). Shown is mean \pm SEM of at least three independent experiments.



Supplementary Figure 3 A–F: Concentration-effect curves of compound **22** (●) as determined in calcein AM (A and B), pheophorbide A (C), Hoechst 33342 (D and F), and daunorubicin (E) assays using either ABCB1-overexpressing A2780/ADR cells (A and D), ABCC1-overexpressing H69AR cells (B and E), or ABCG2-overexpressing MDCK II BCRP cells (C and F). Data were normalized by defining the effect of 10 μ M cyclosporine A (▲; A, B, D, and E) and compound **34** (▲; C and F) as positive control (100%) and buffer medium was used as negative control (0%). Shown is mean \pm SEM of at least three independent experiments.



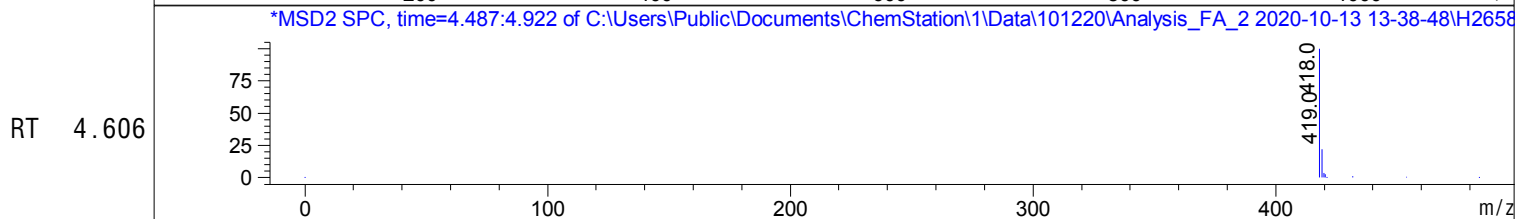
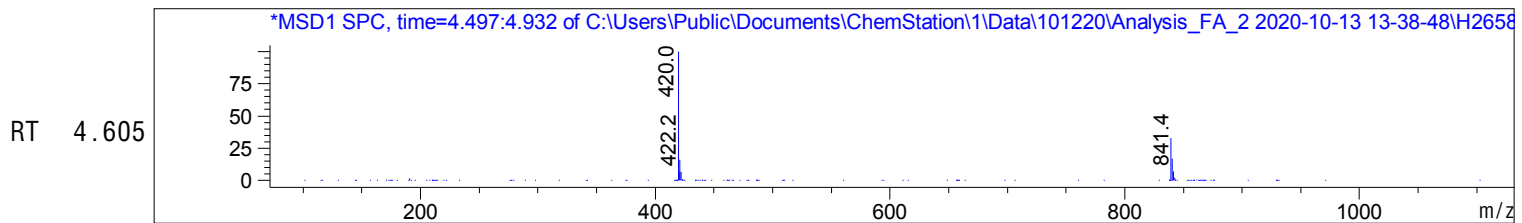
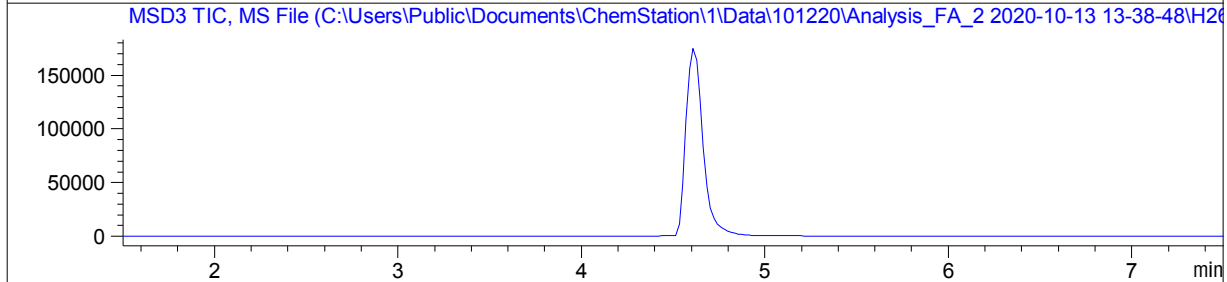
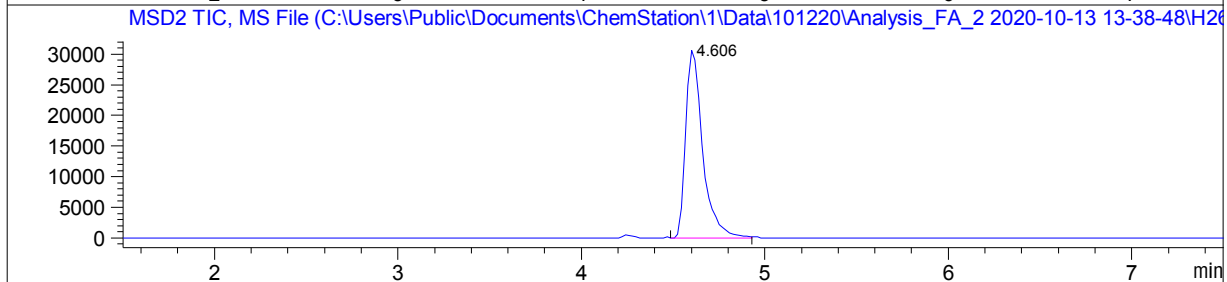
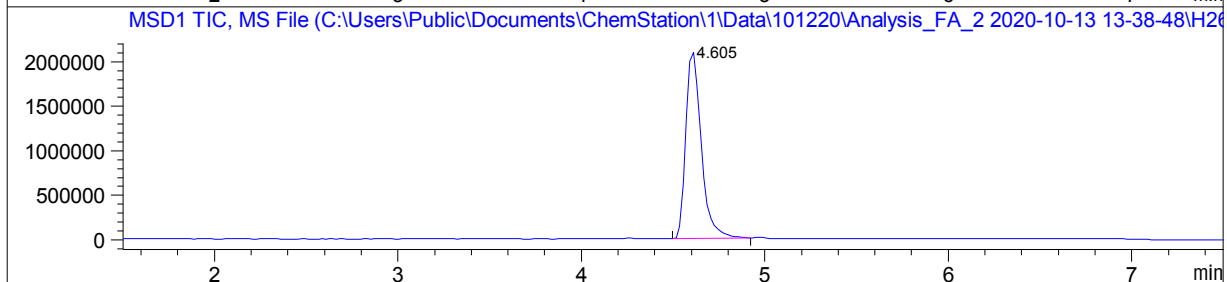
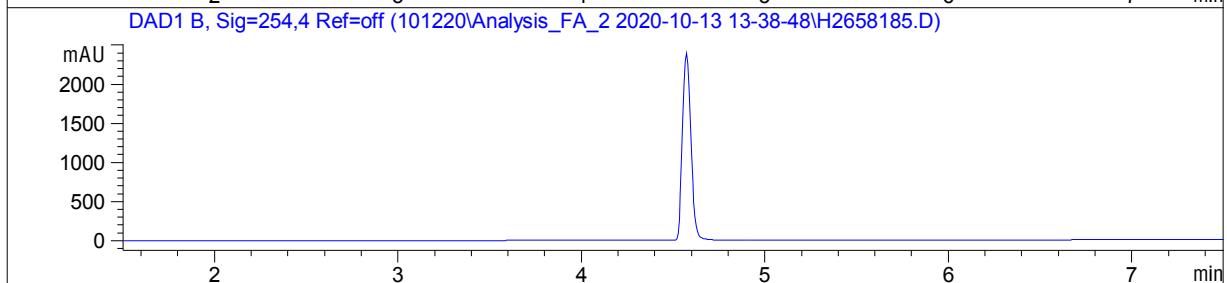
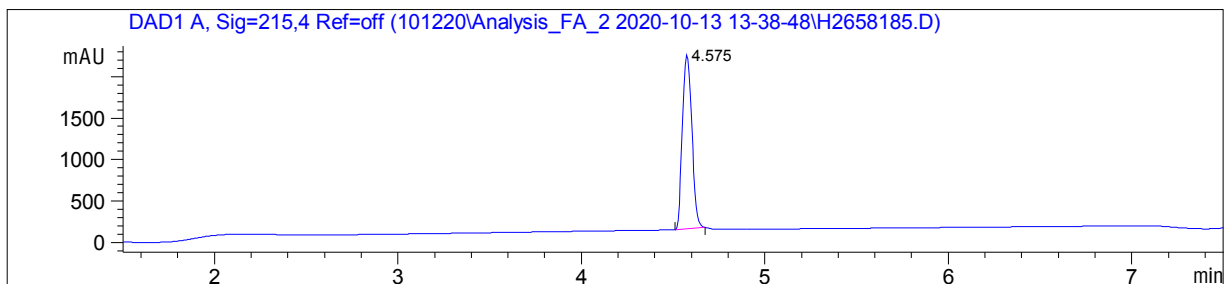
Supplementary Figure 4 A–F: Concentration-effect curves of compound **26** (●) as determined in calcein AM (A and B), pheophorbide A (C), Hoechst 33342 (D and F), and daunorubicin (E) assays using either ABCB1-overexpressing A2780/ADR cells (A and D), ABCC1-overexpressing H69AR cells (B and E), or ABCG2-overexpressing MDCK II BCRP cells (C and F). Data were normalized by defining the effect of 10 μ M cyclosporine A (▲; A, B, D, and E) and compound **34** (▲; C and F) as positive control (100%) and buffer medium was used as negative control (0%). Shown is mean \pm SEM of at least three independent experiments.

Compound 11

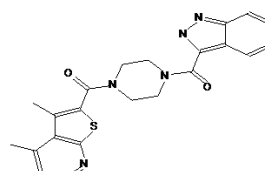
Sample H2658185

0.1%FA-ACN 5-95%ACN 6 min. Zorbax-Eclipse-Plus C18 4,6 x 100mm, 3.5 μ m.

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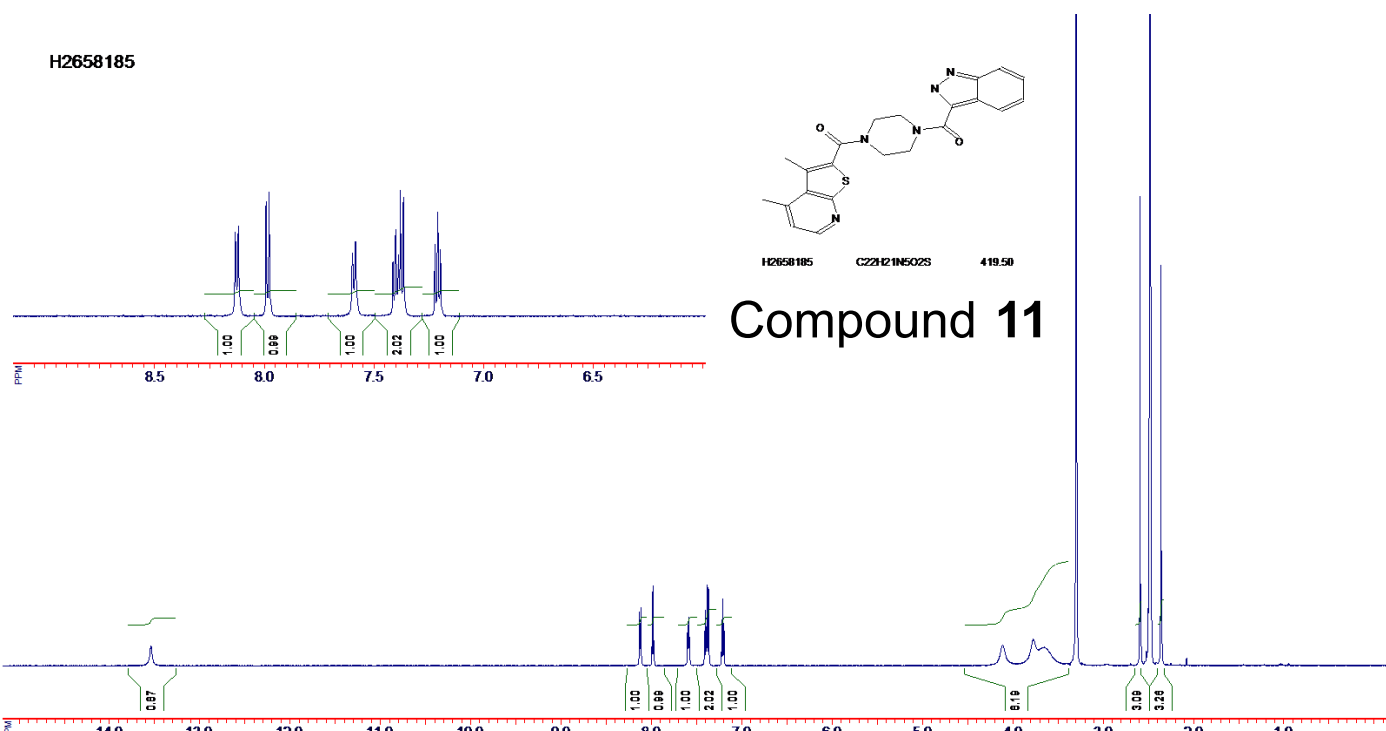


H2658185



H2658185 C22H21N5O2S 419.50

Compound 11



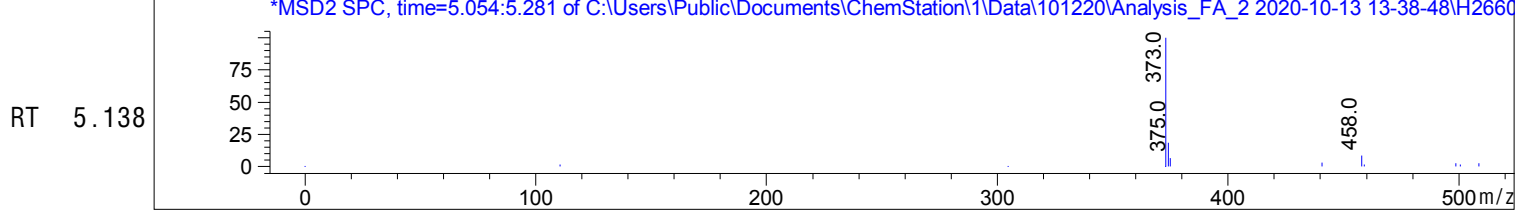
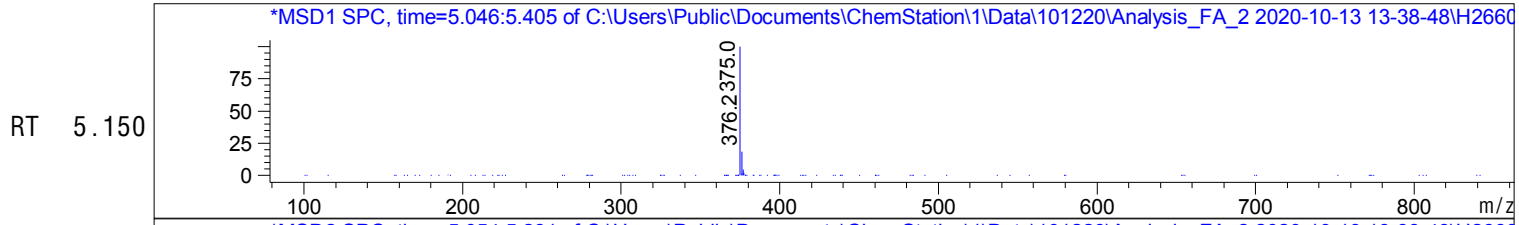
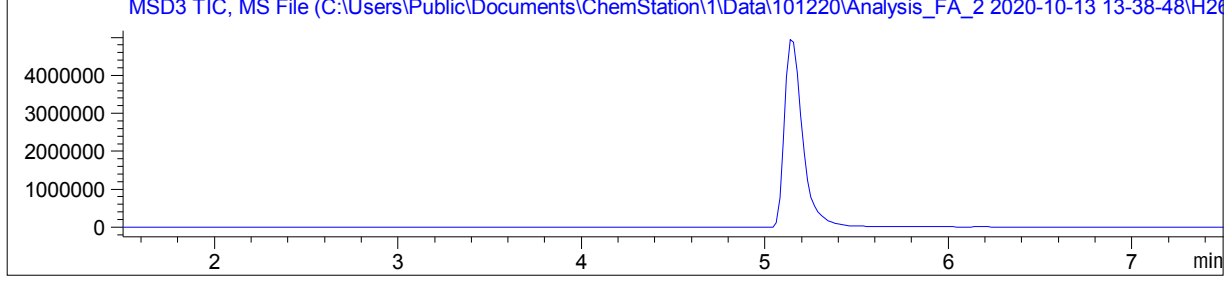
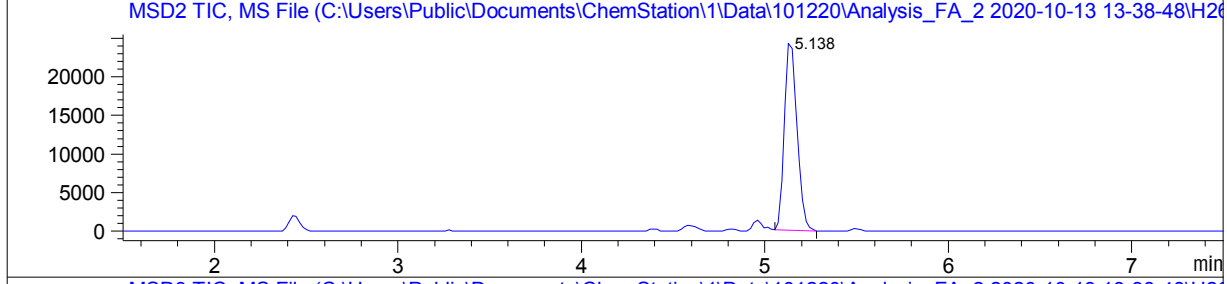
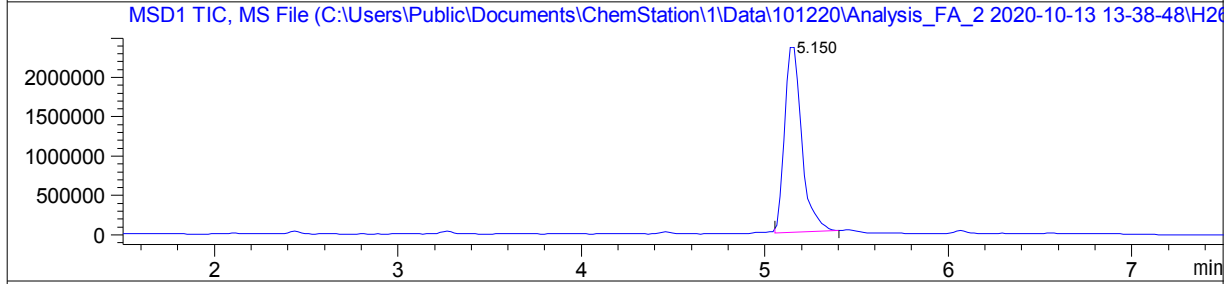
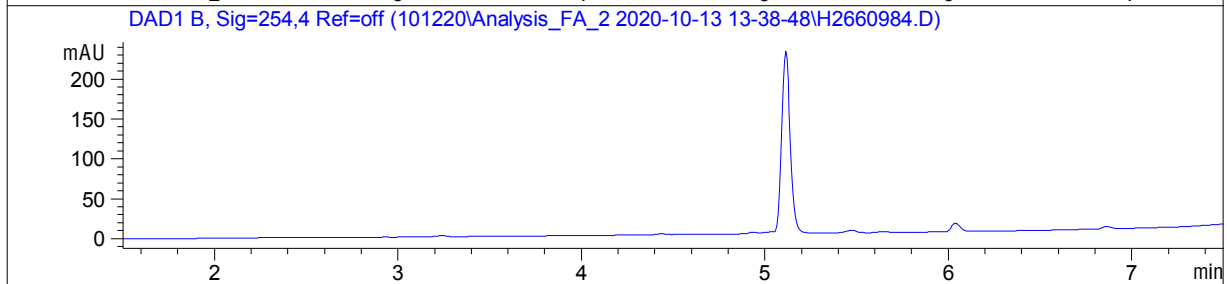
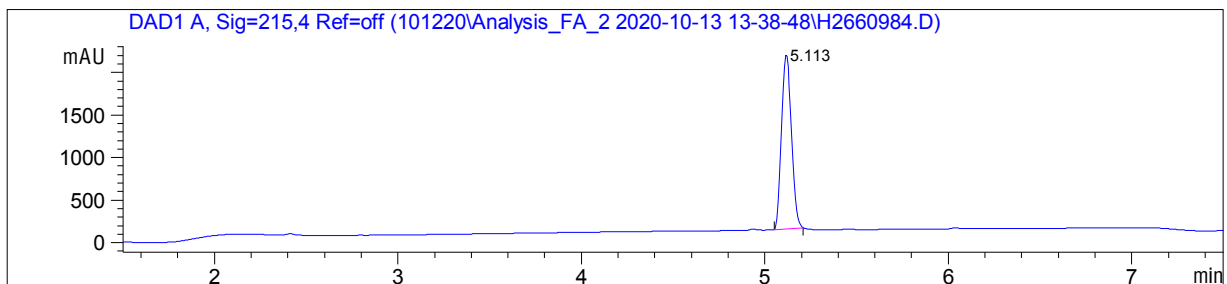
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Compound 12

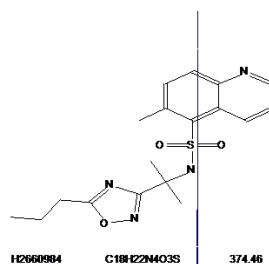
Sample H2660984

0.1%FA-ACN 5-95%ACN 6 min. Zorbax-Eclipse-Plus C18 4,6 x 100mm, 3.5 μ m.

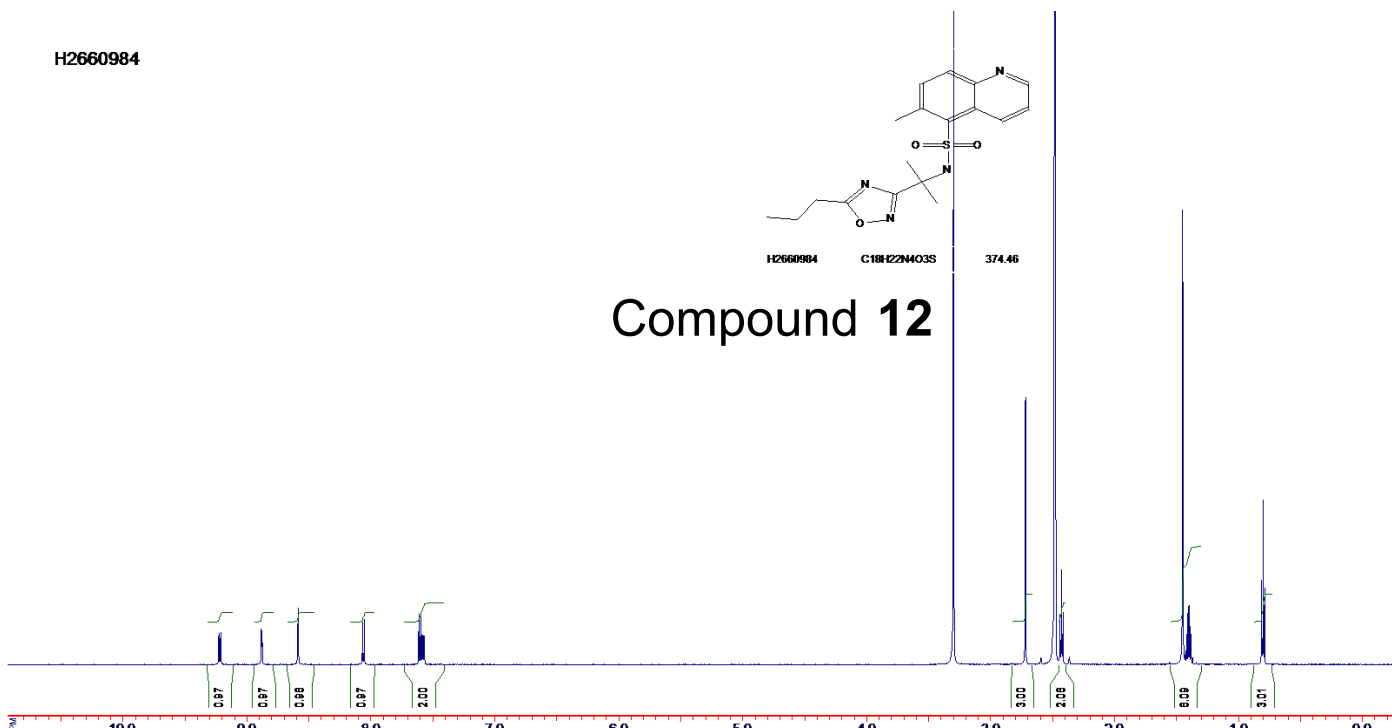
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H2660984



Compound 12

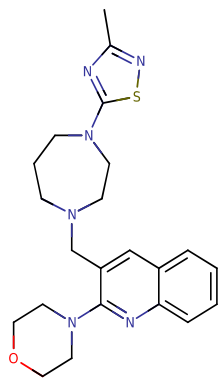
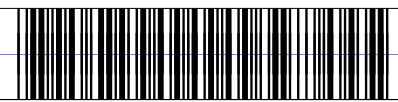


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Date: 26-Nov-2020	Solvent: dms0	SW: 11364 Hz	TE: 298 K	AQ: 2.82 sec, RD: 0.00 sec	H2660984

Compound 13

MaxPeak: 100.00%
Ret_Time: 0.981 min

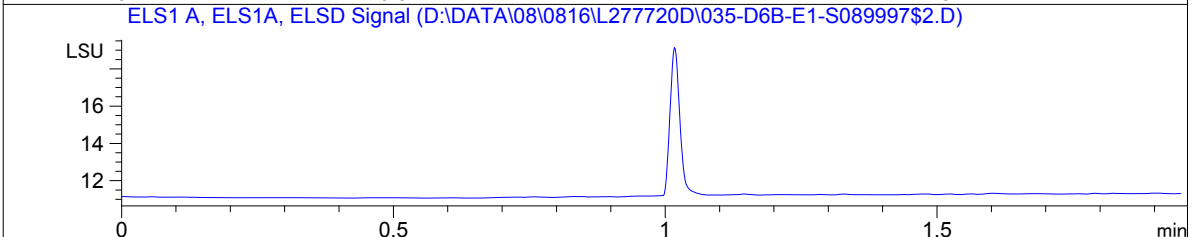
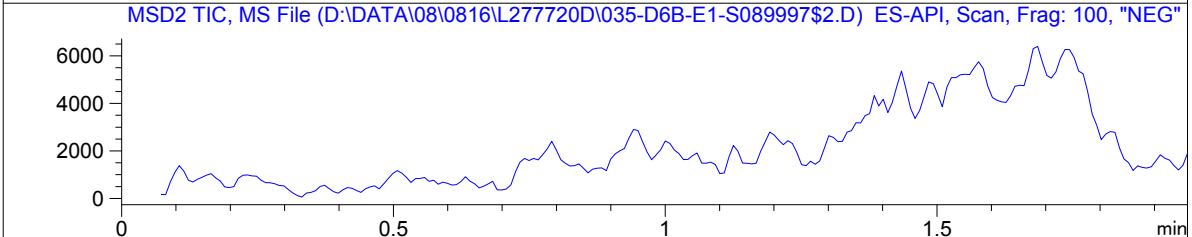
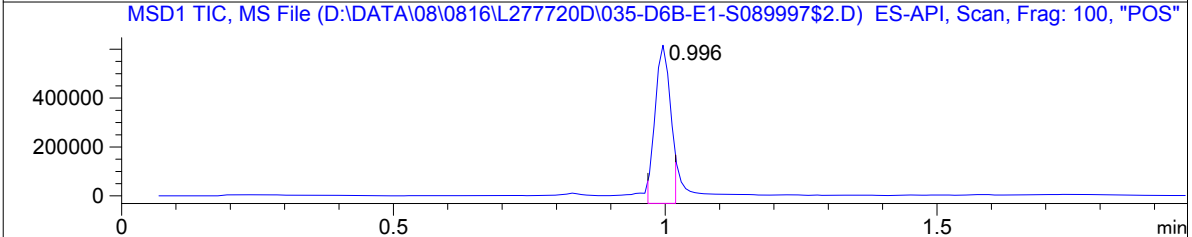
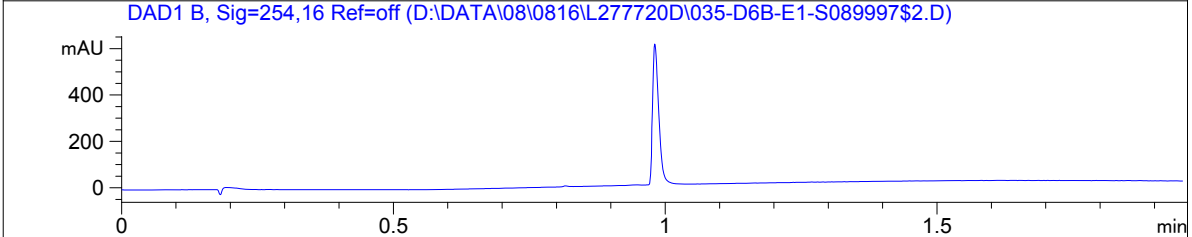
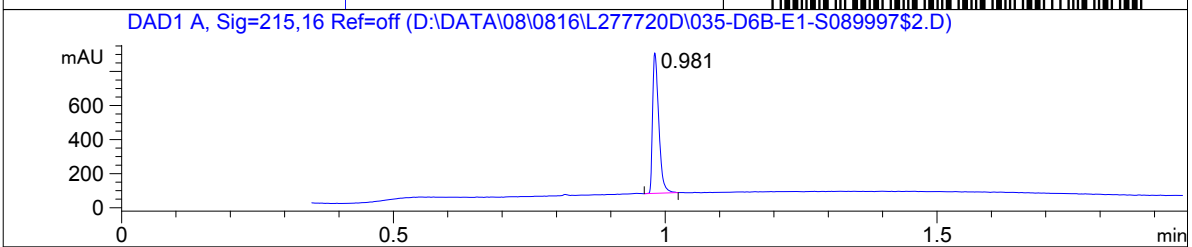
S089997\$2



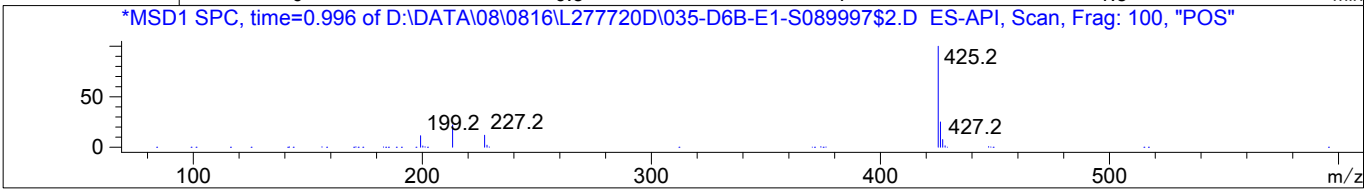
Mol Wt 424.56

Exact Mass 424.24

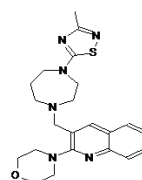
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RT 0.996

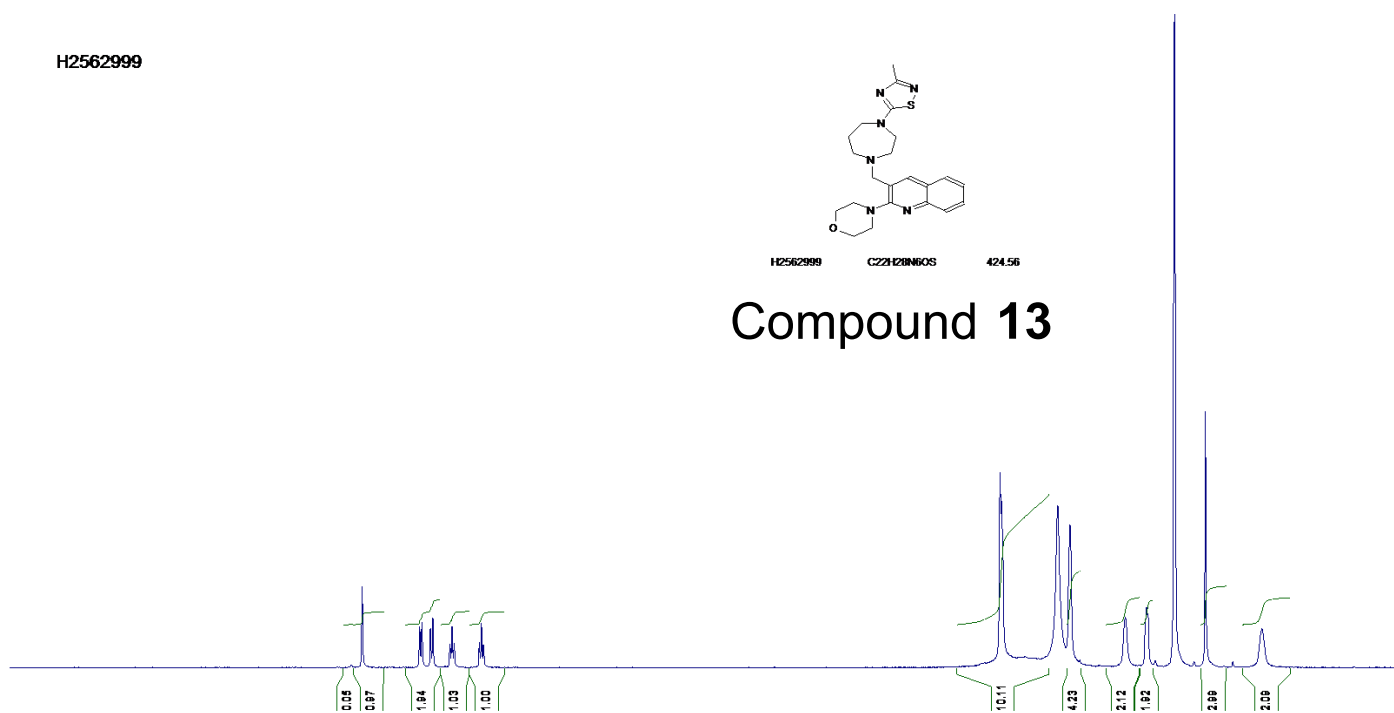


H2562999



H2562999 C21H28N6OS 424.56

Compound 13

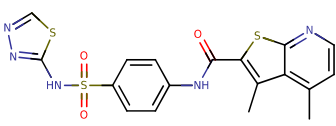


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Compound 14

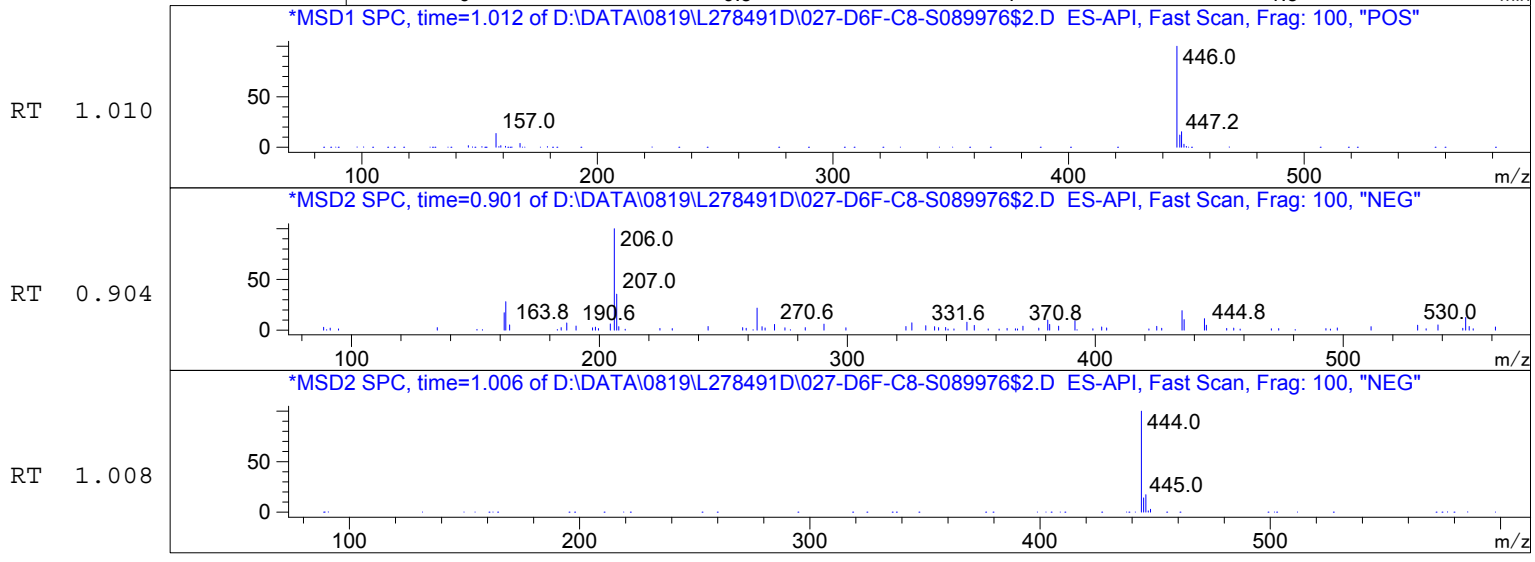
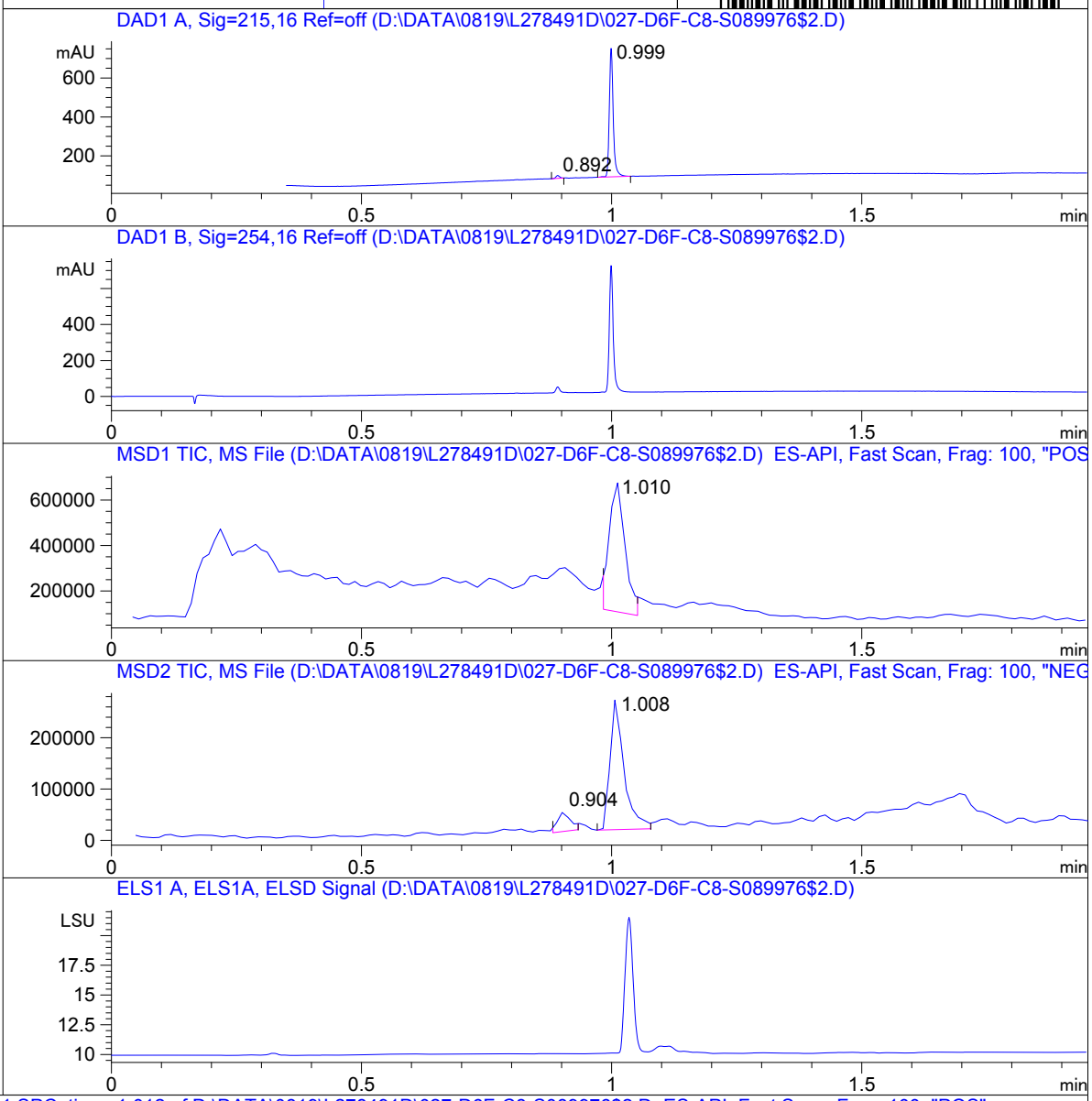
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Ret_Time: 0.999 min

S089976\$2

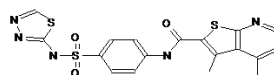


Mol Wt 445.54
Exact Mass 445.03

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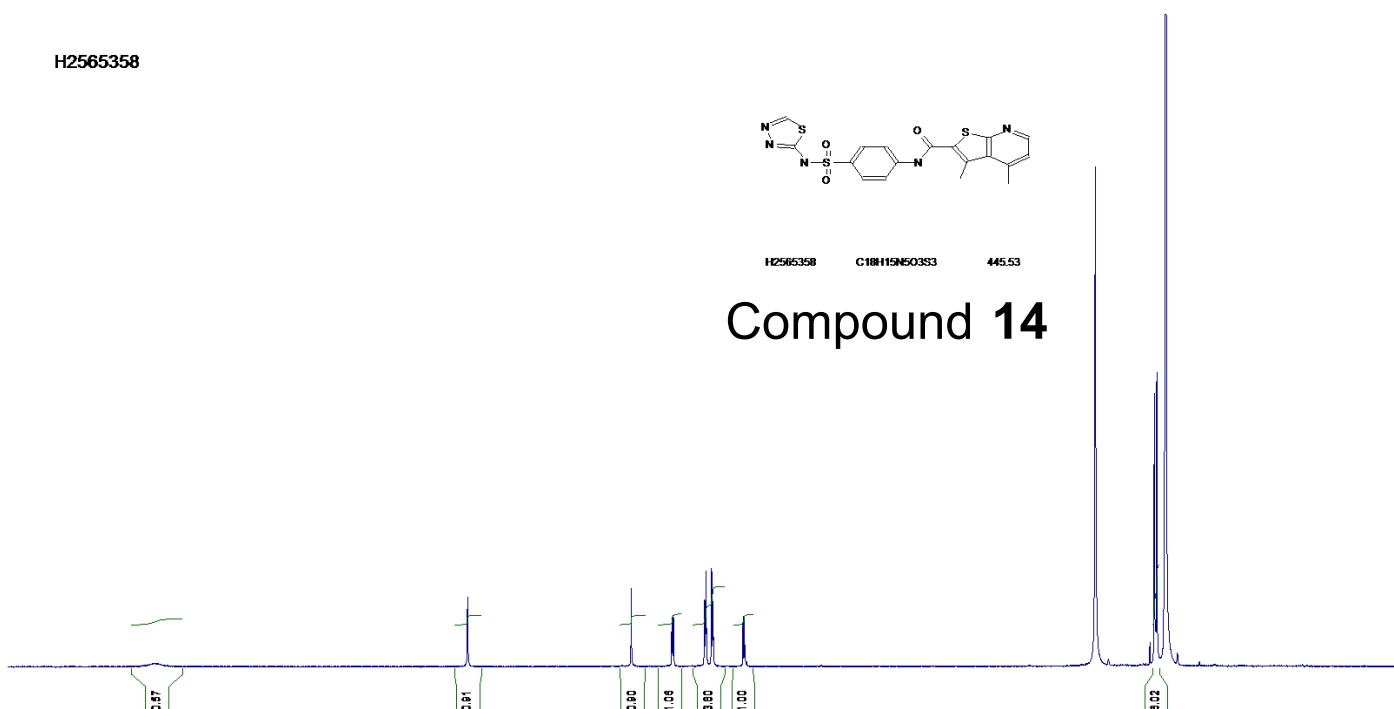


H2565358



H2565358 C18H15N5O3S3 445.53

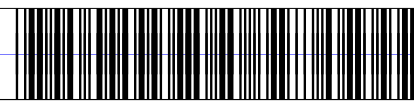
Compound 14



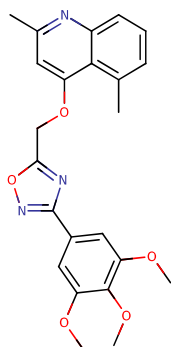
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Compound 15

S491337\$21

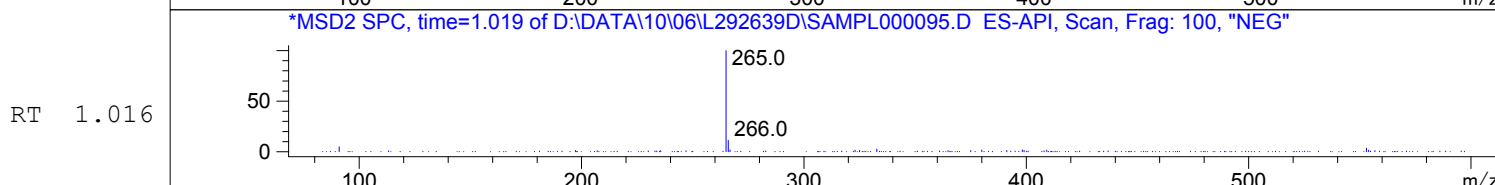
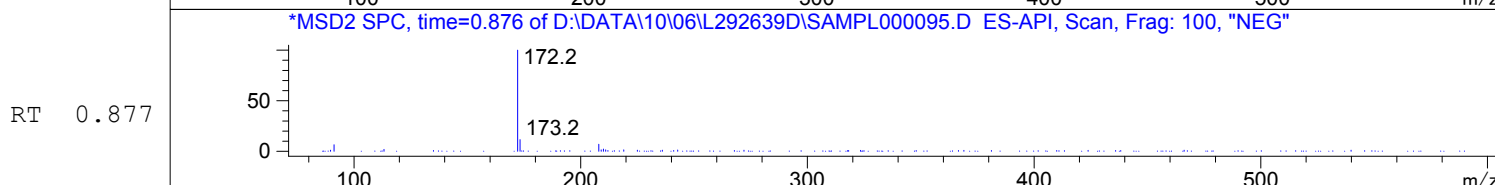
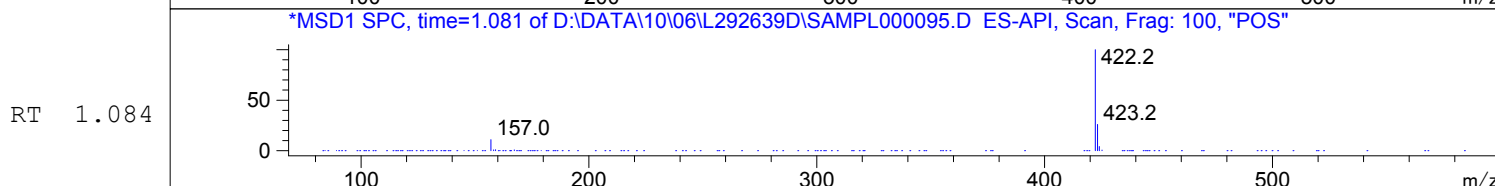
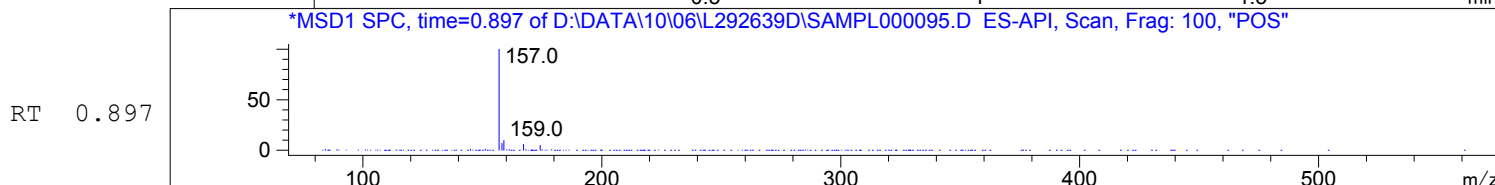
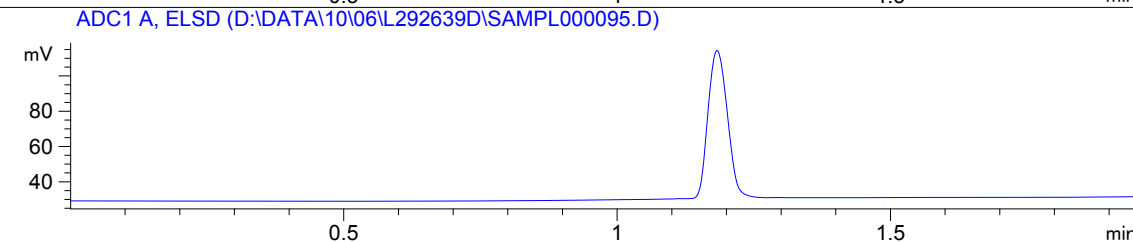
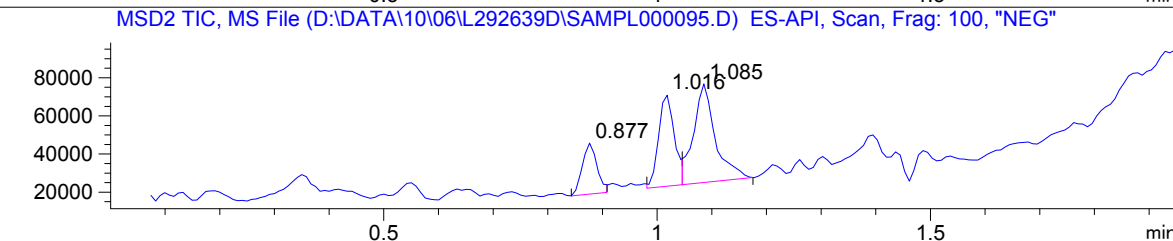
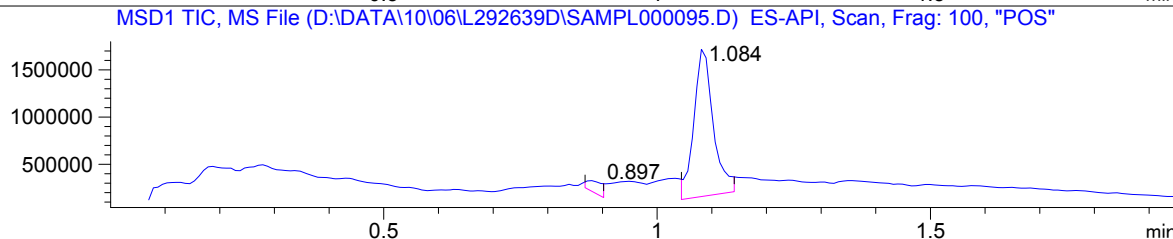
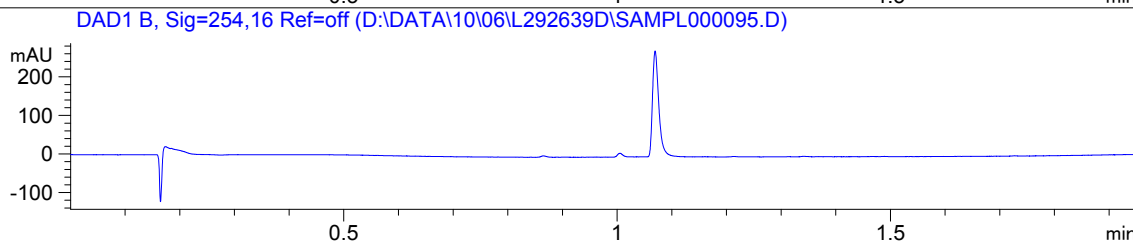
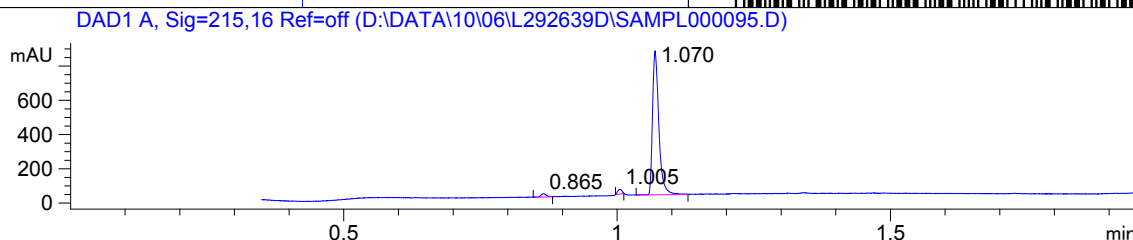


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Ret_Time: 1.070 min

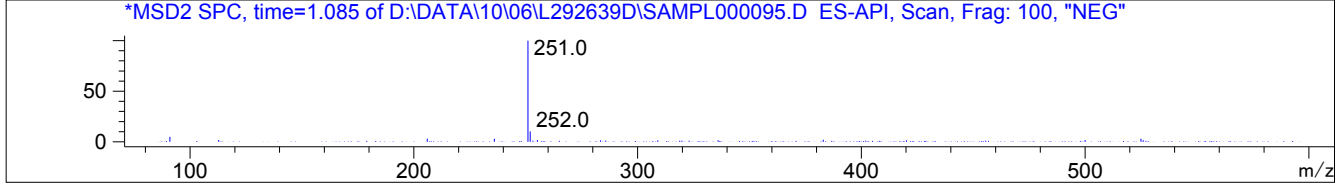


Mol Wt 421.45
Exact Mass 421.18

#	Time	Area%
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2	1.005	2.12
3	1.070	95.91



RT 1.085



SVK-25
SVK 25
1H

7.53
7.52
7.30
7.26
7.26
7.25
7.25
7.25
7.07

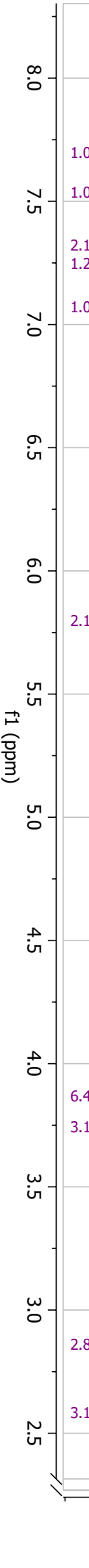
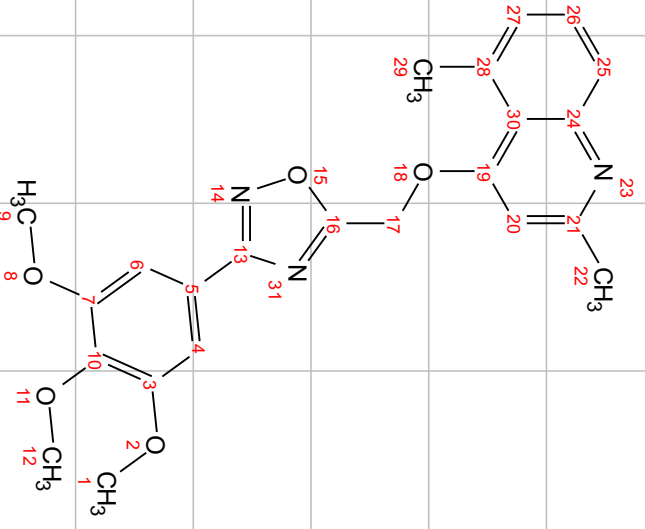
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B (dd) 7.53
C (s) 7.30
D (dt) 7.26
E (s) 7.07

F (s) 5.79

G (s) 3.86
H (s) 3.74

I (s) 2.86
J (s) 2.58

Compound 15

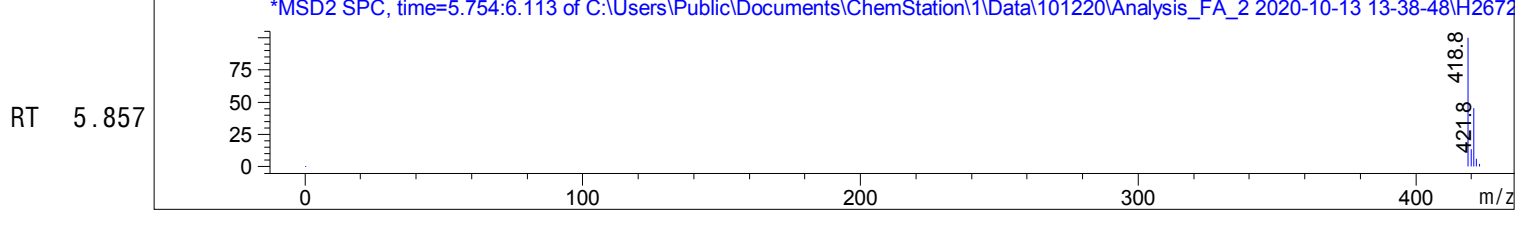
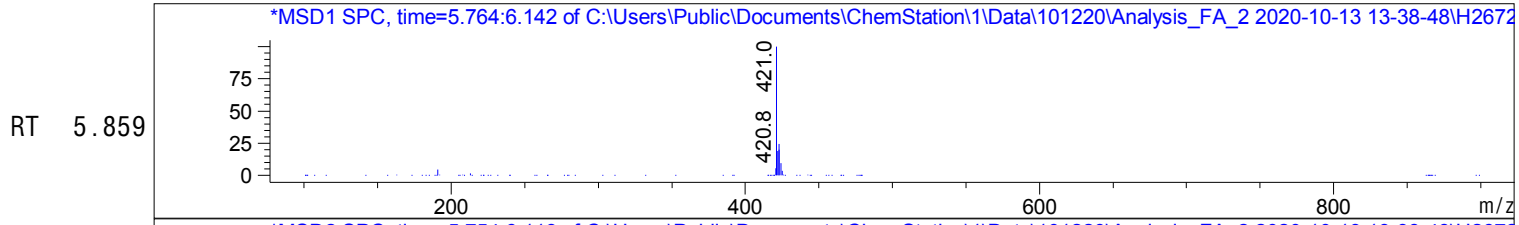
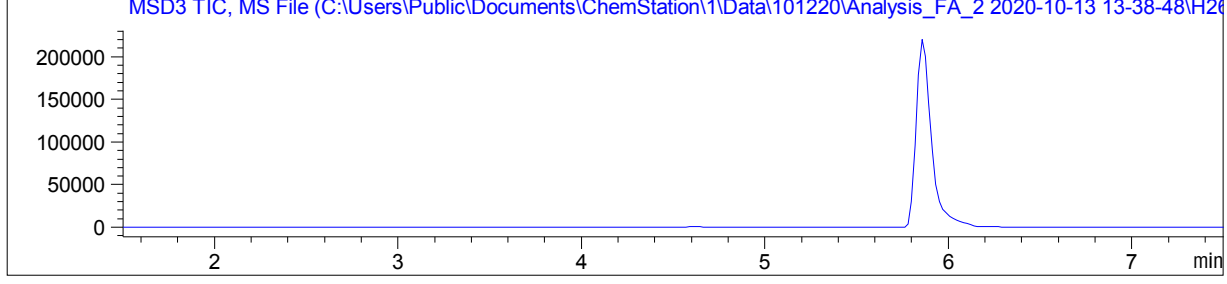
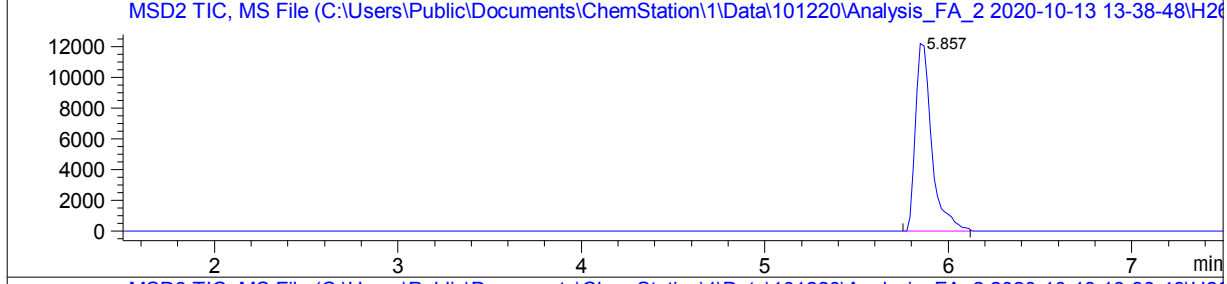
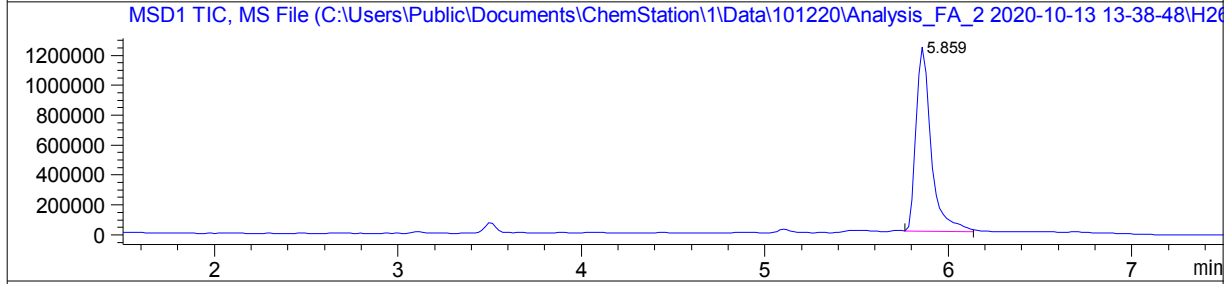
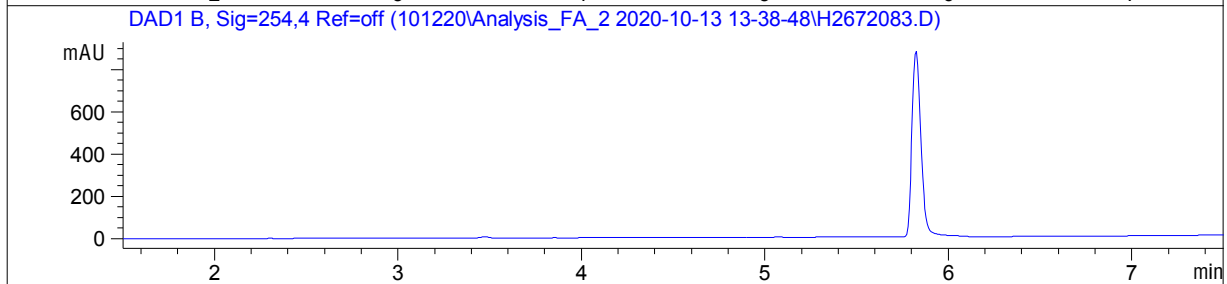
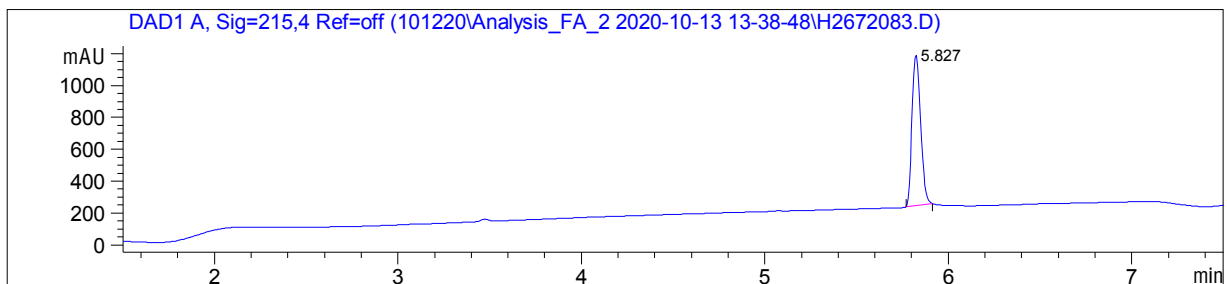


Compound 16

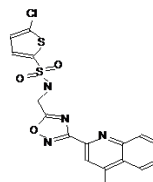
Sample H2672083

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#	Time	Area%
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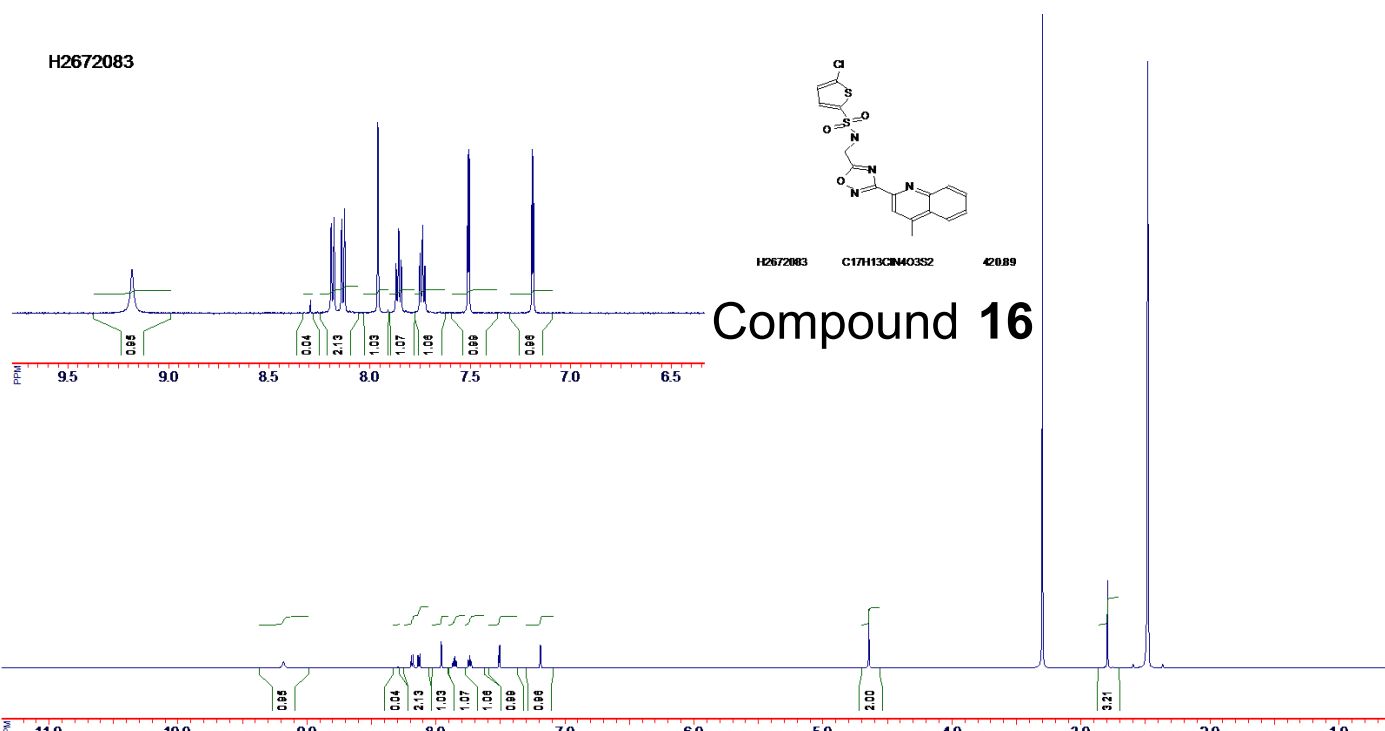


H2672083



H2672083 C17H13ClN4O3S2 428.99

Compound 16



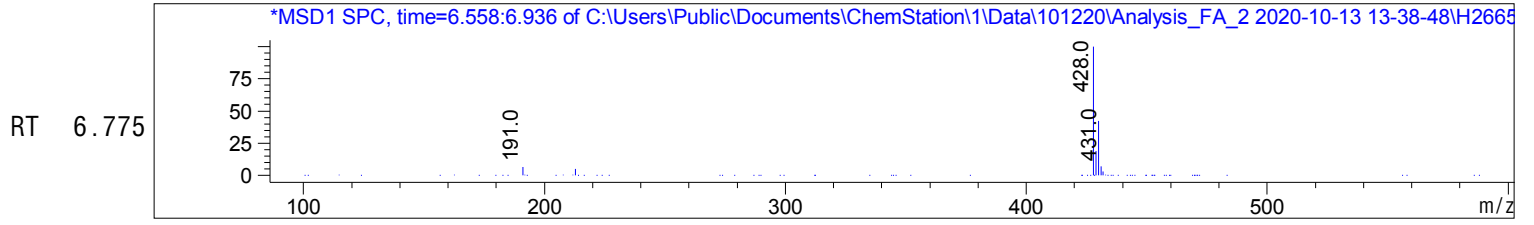
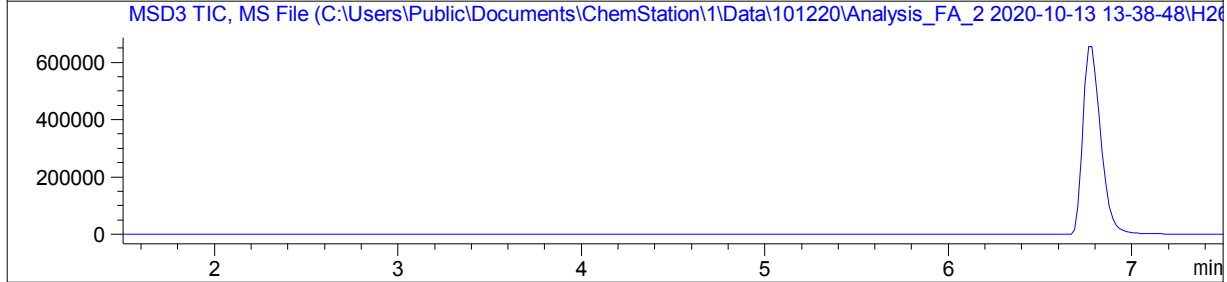
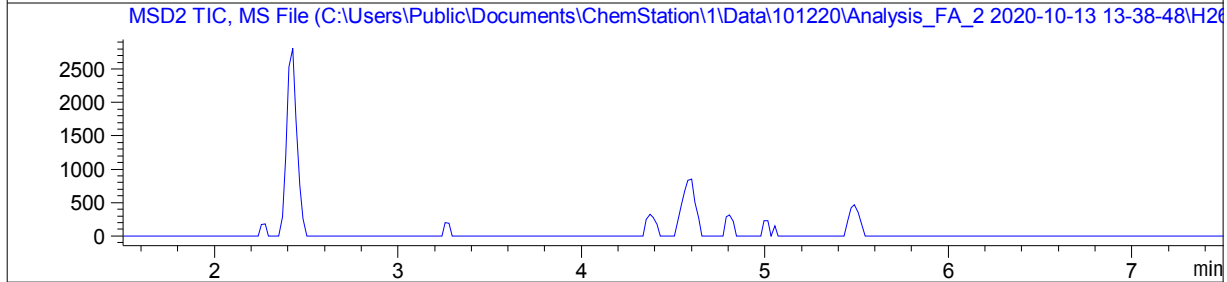
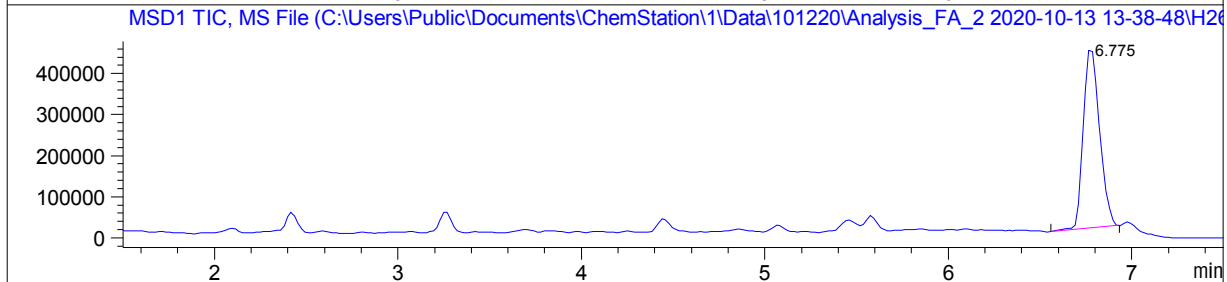
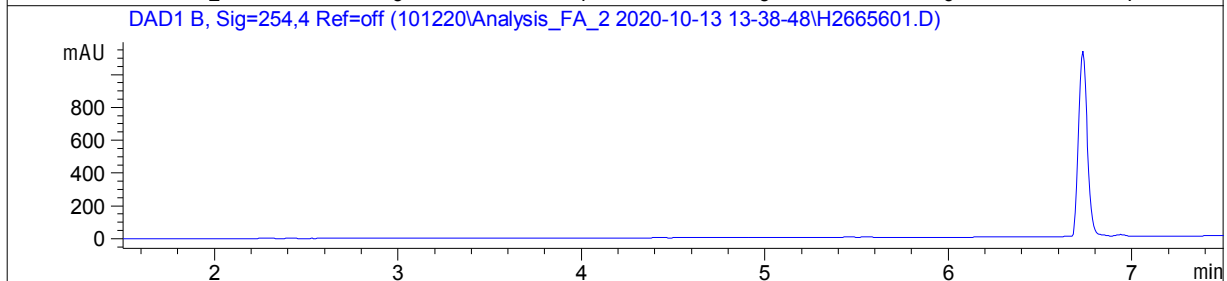
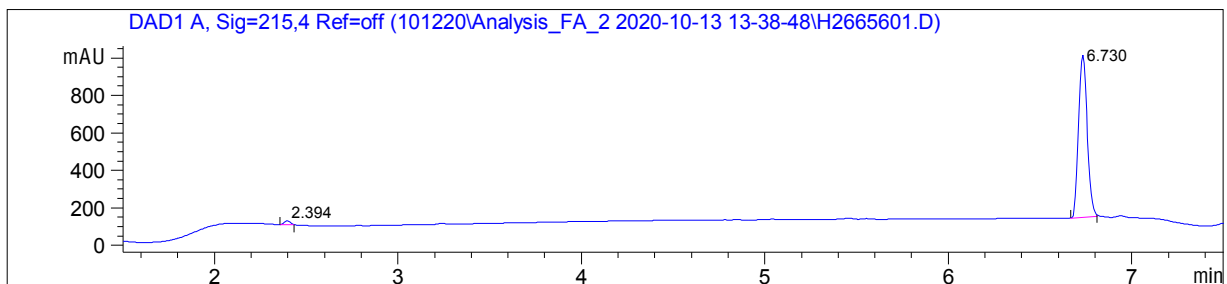
File name: H2672083	Host: H2672083	SF: 599.7811 MHz	NSC: 0	PW: 4.40 usec, RG: 44	SE 131072
Date: 26-Nov-2020	Solvent: dmsd	SW: 11364 Hz	TE: 298 K	AQ: 2.82 sec, RD: 0.00 sec	H2672083

Compound 17

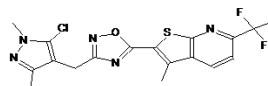
Sample
H2665601

0.1%FA-ACN 5-95%ACN 6 min. Zorbax-Eclipse-Plus C18 4,6 x
100mm, 3.5 mkm.

#	Time	Area%
1	2.394	1.75
2	6.730	98.25

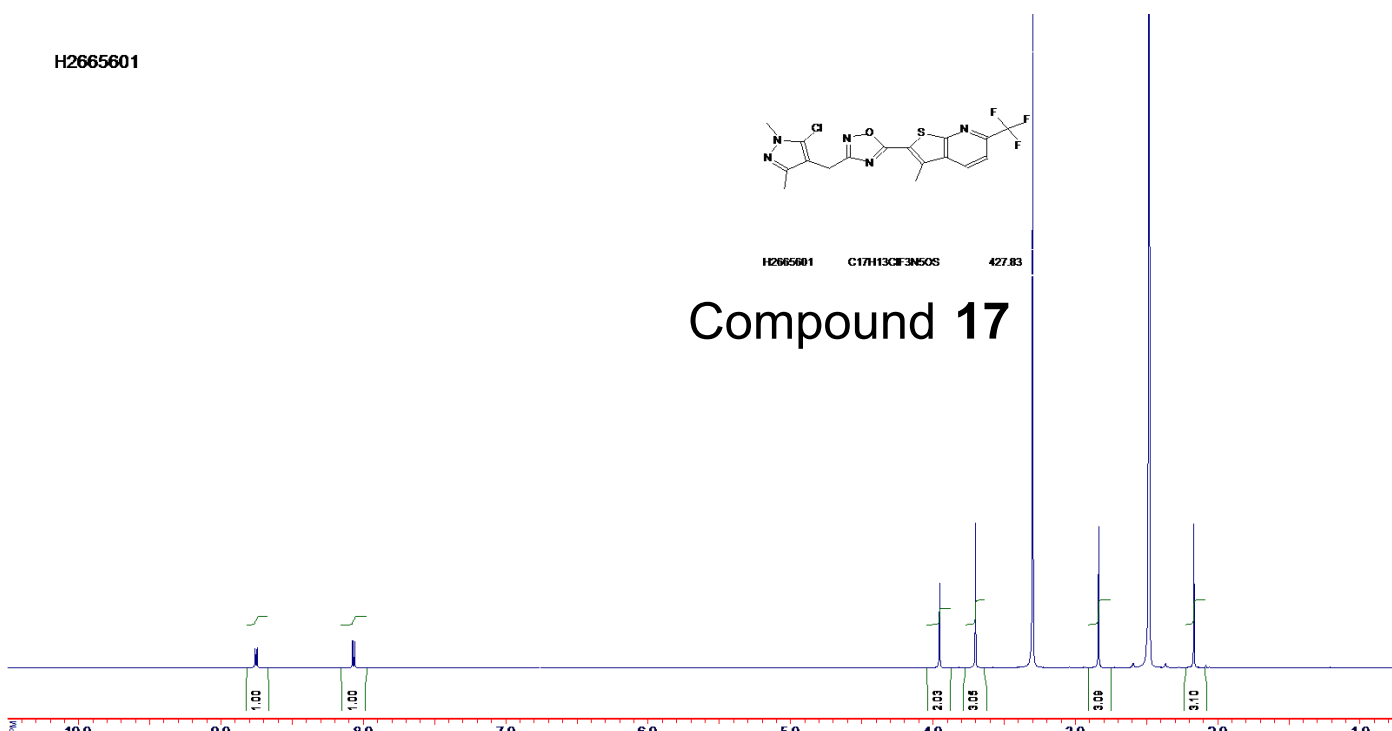


H2665601



H2665601 C17H13ClF3N5OS 427.83

Compound 17



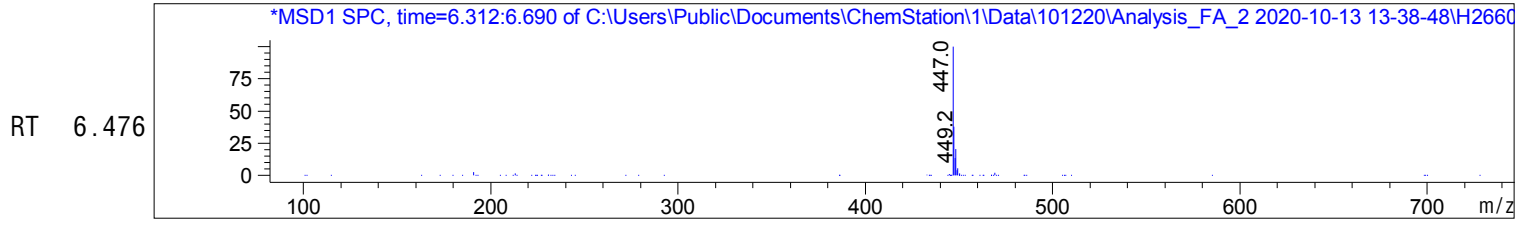
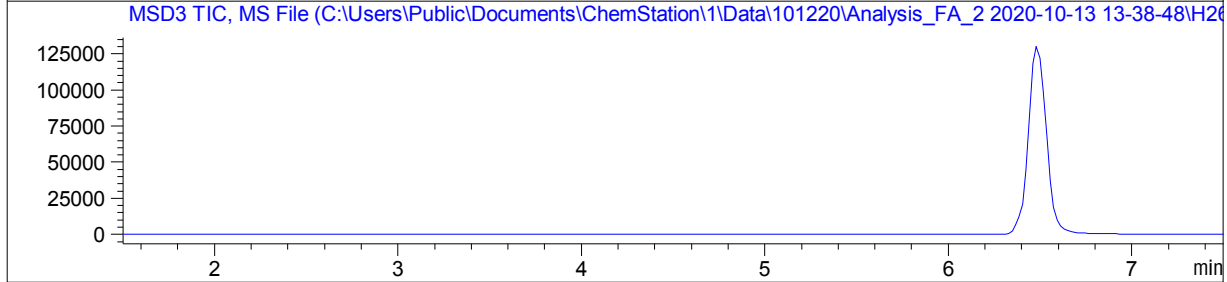
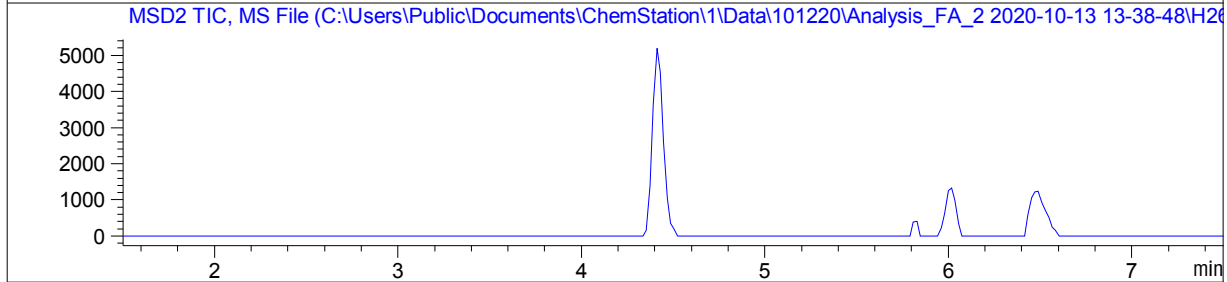
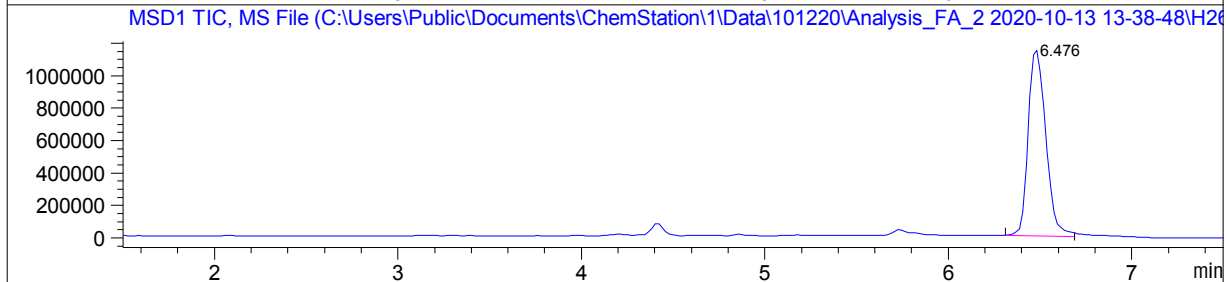
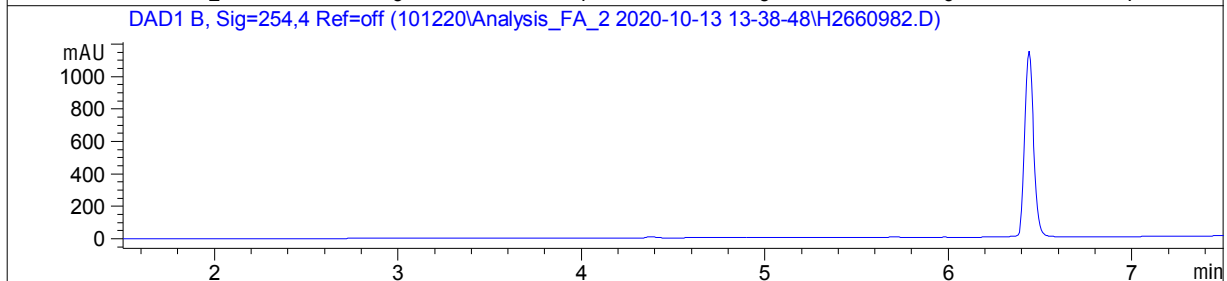
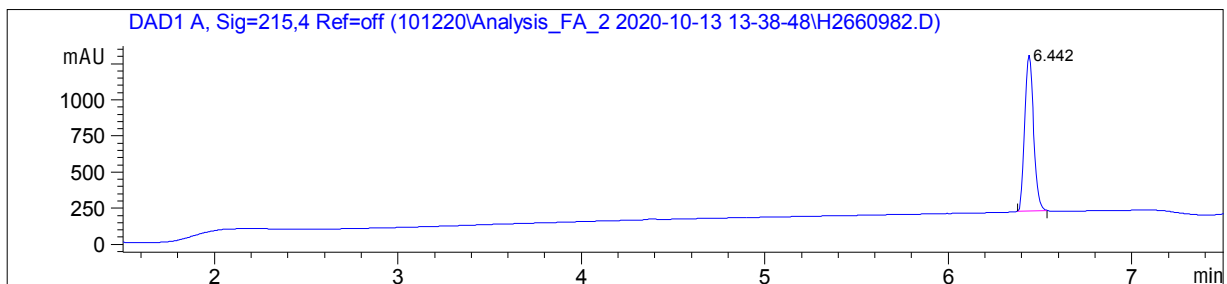
File name: H2665601	Host: char	SF: 599.7811 MHz	NSC: 0	PW: 4.40 usec, RG: 44	SE 131072
Date: 26-Nov-2020	Solvent: dmsd	SW: 11364 Hz	TE: 298 K	AQ: 2.82 sec, RD: 0.00 sec	H2665601

Compound 18

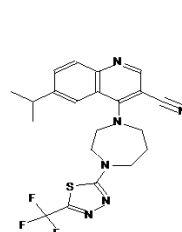
Sample H2660982

0.1%FA-ACN 5-95%ACN 6 min. Zorbax-Eclipse-Plus C18 4,6 x 100mm, 3.5 mkm.

#	Time	Area%
1	6.442	100.00

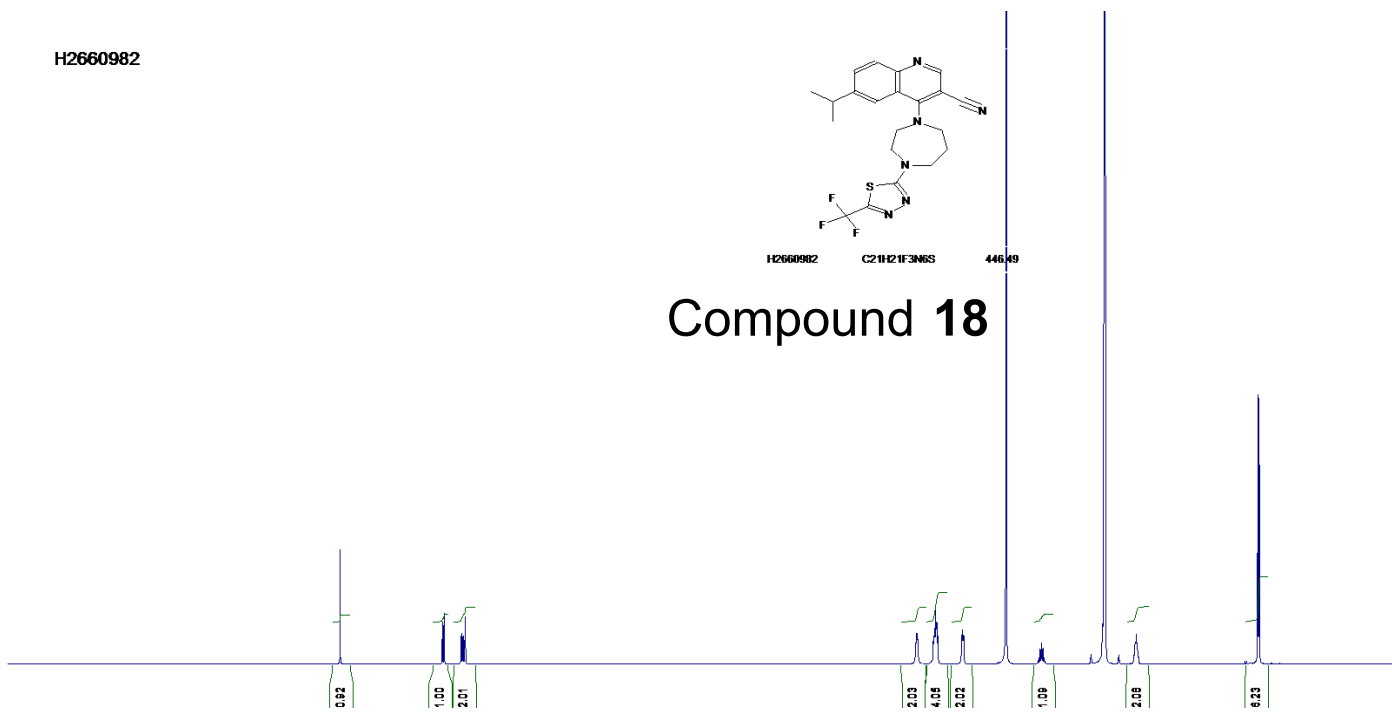


H2660982



H2660982 C21H21F3N6S 446.49

Compound 18



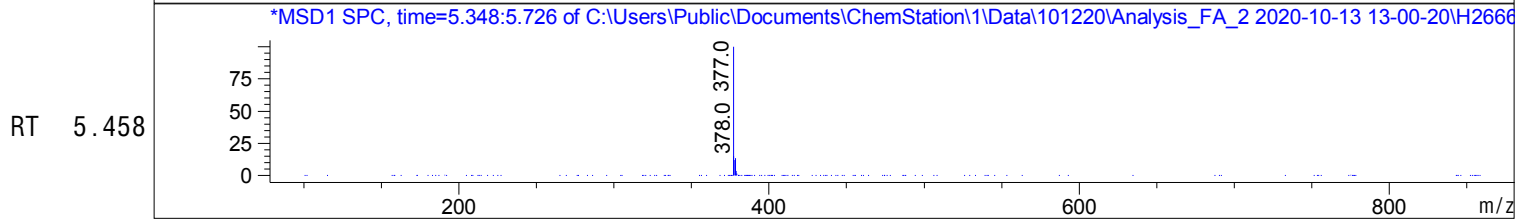
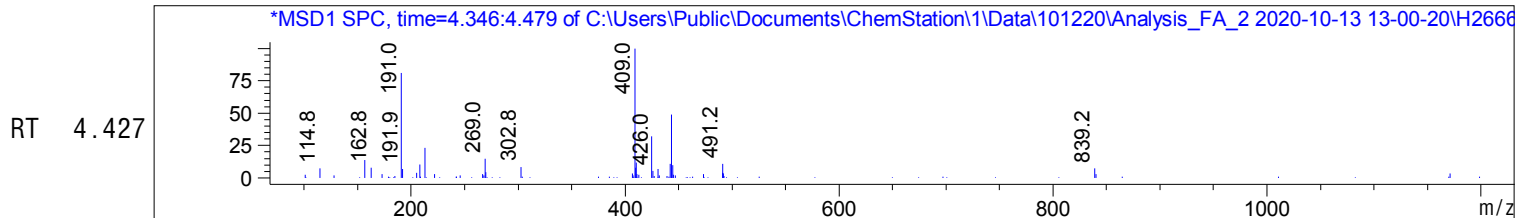
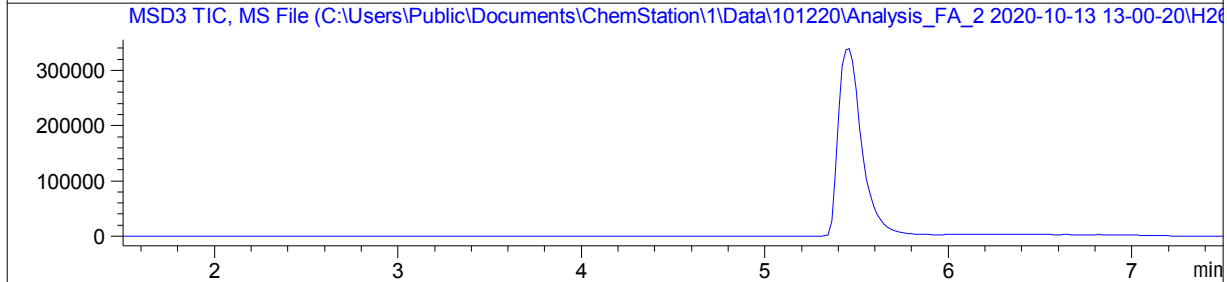
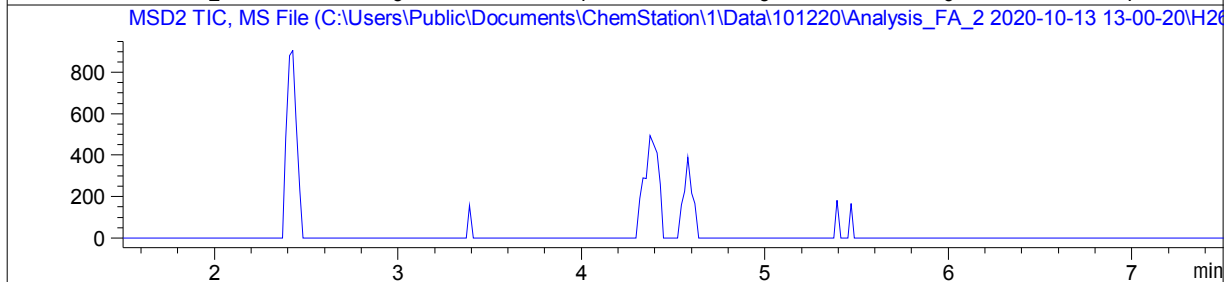
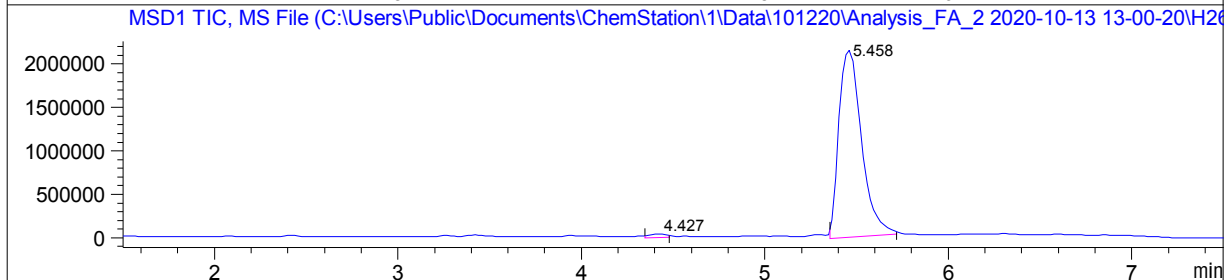
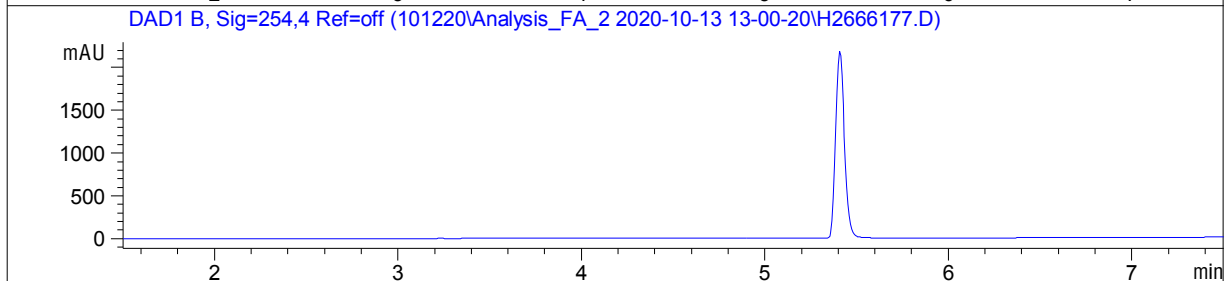
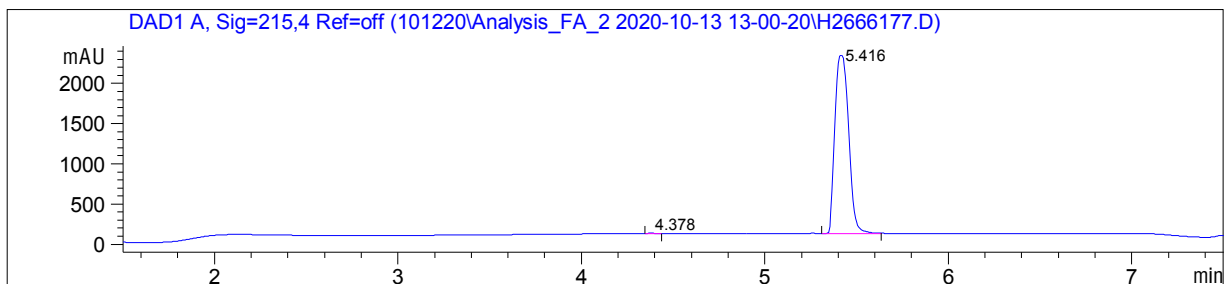
File name: H2660982	Host: H2660982	SF: 599.7811 MHz	NSC: 0	PW: 4.40 usec, RG: 44	SE 131072
Date: 26-Nov-2020	Solvent: dmsd	SW: 11364 Hz	TE: 298 K	AQ: 2.82 sec, RD: 0.00 sec	H2660982

Compound 19

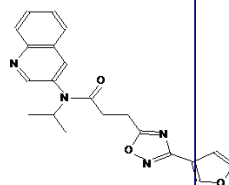
Sample H2666177

0.1%FA-ACN 5-95%ACN 6 min. Zorbax-Eclipse-Plus C18 4,6 x 100mm, 3.5 mkm.

#	Time	Area%
1	4.378	0.28
2	5.416	99.72

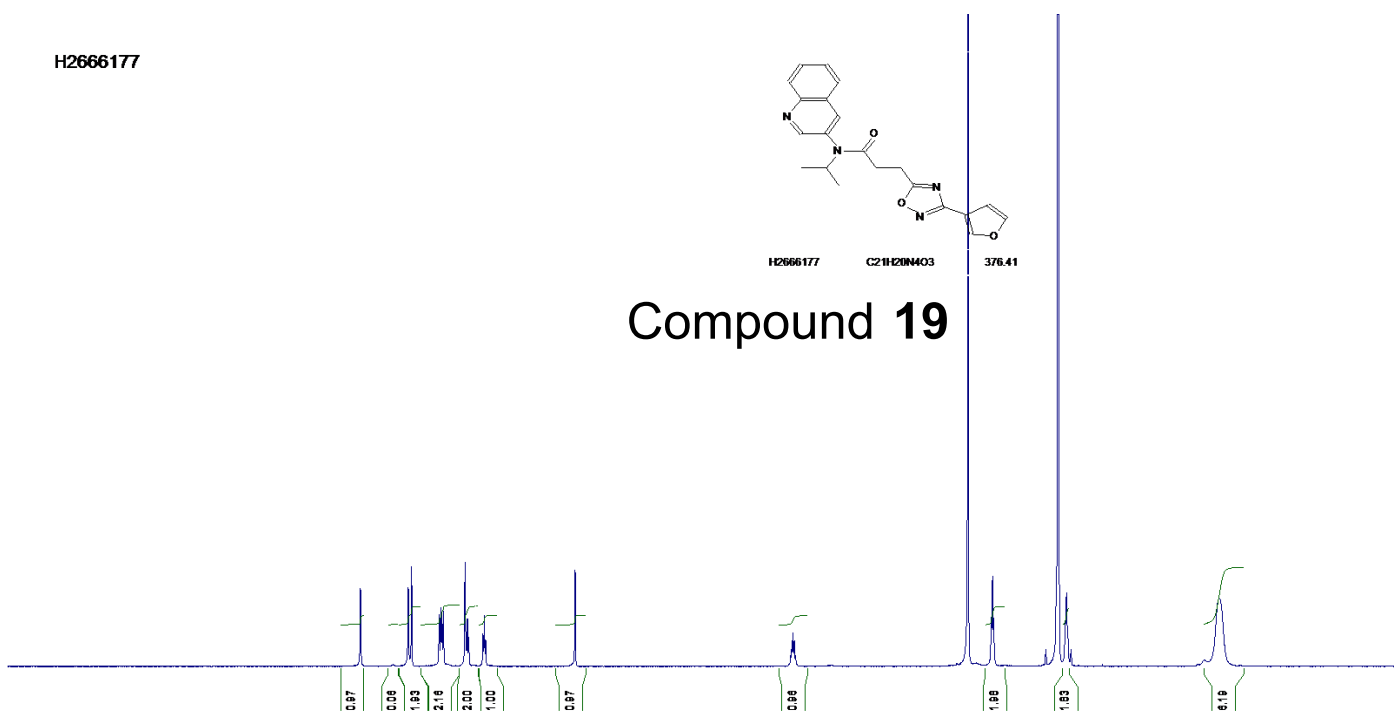


H2666177



H2666177 C21H20N4O3 376.41

Compound 19



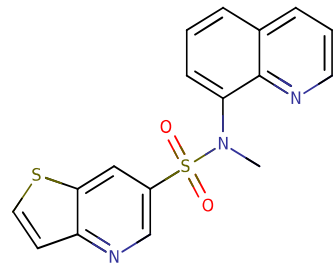
File name: H2666177	Host: H2666177	SF: 599.7811 MHz	NSC: 0	PW: 4.40 usec, RG: 44	SE 131072
Date: 26-Nov-2020	Solvent: dmsd	SW: 11364 Hz	TE: 298 K	AQ: 2.82 sec, RD: 0.00 sec	H2666177

Compound 20

S089986\$3

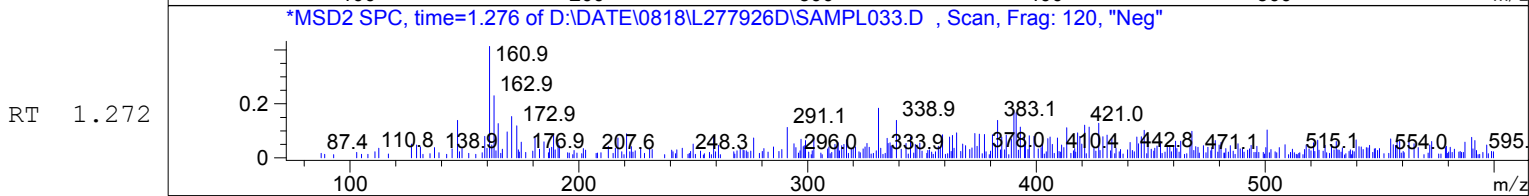
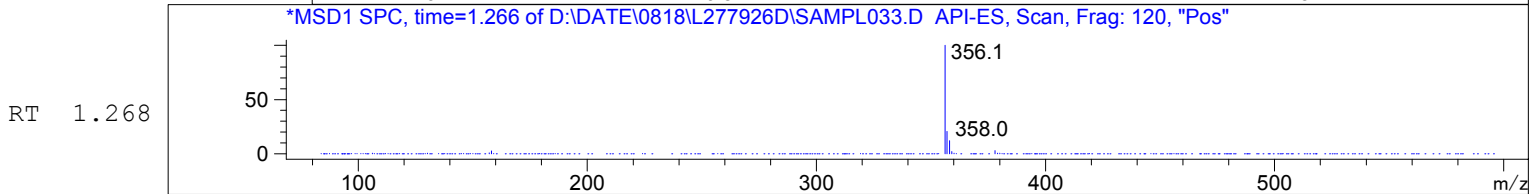
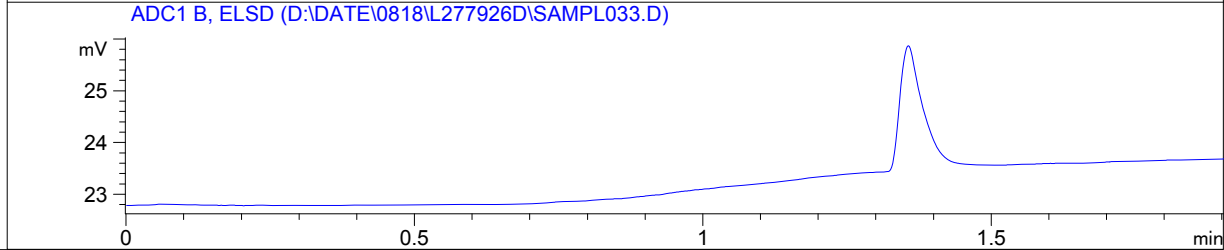
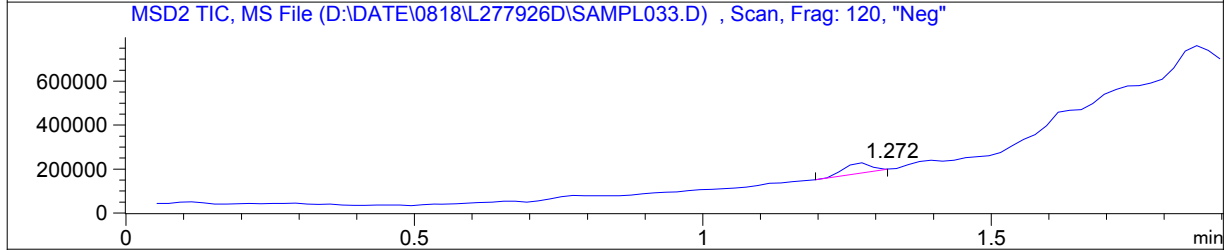
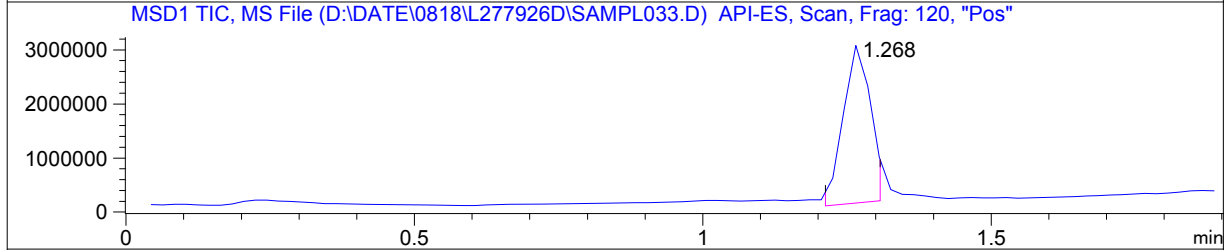
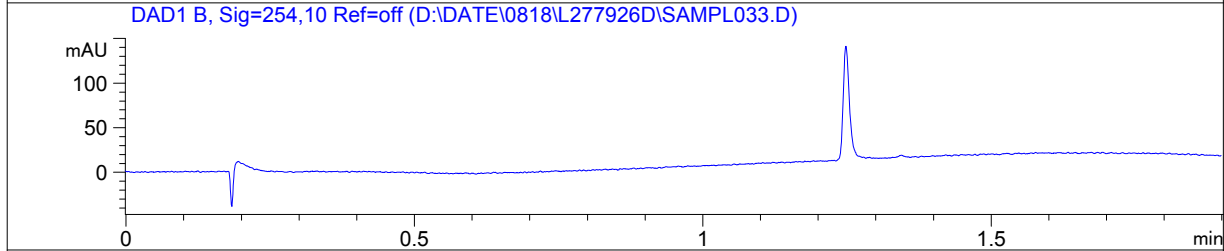
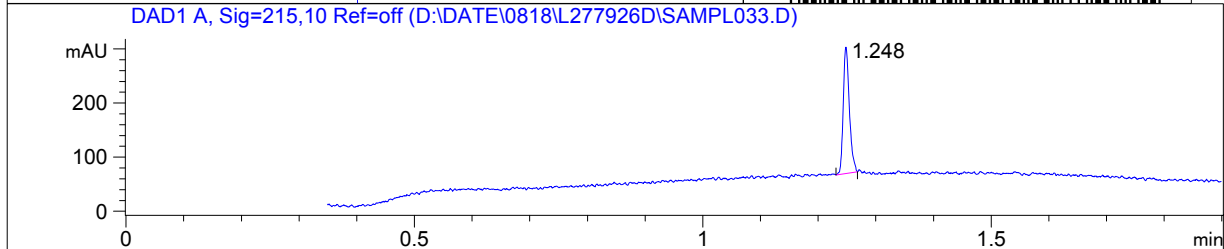


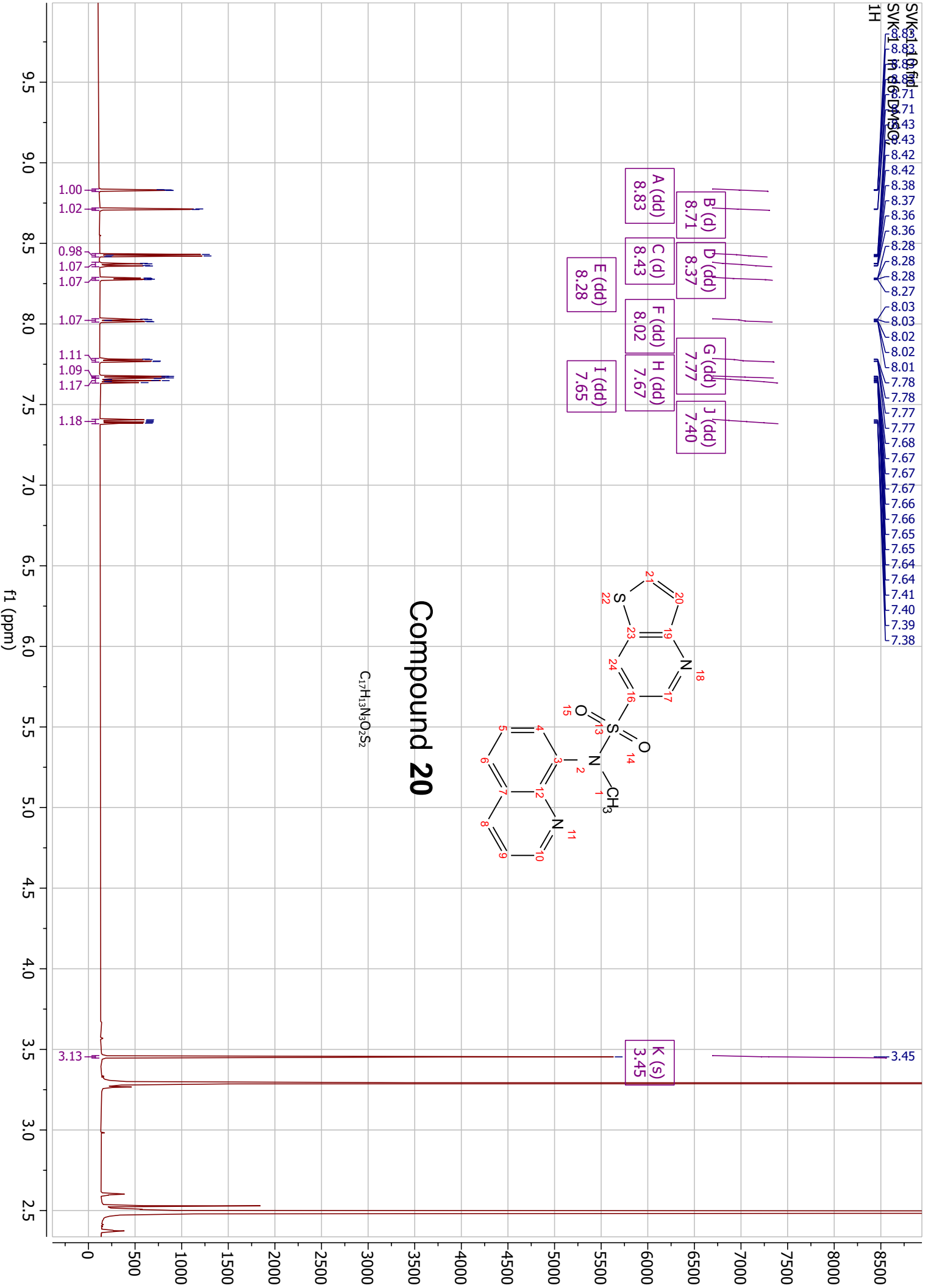
MaxPeak: 100.00%
Ret_Time: 1.248 min



Mol Wt 355.43
Exact Mass 355.05

#	Time	Area%
1	1.248	100.00

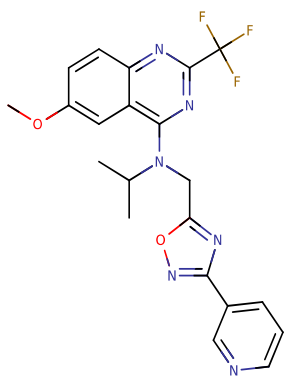




Compound 21

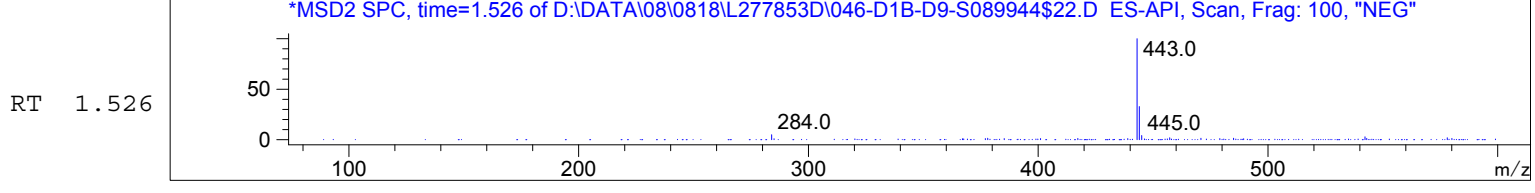
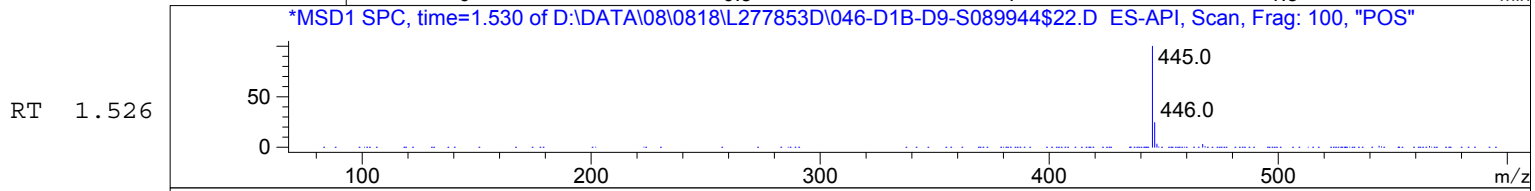
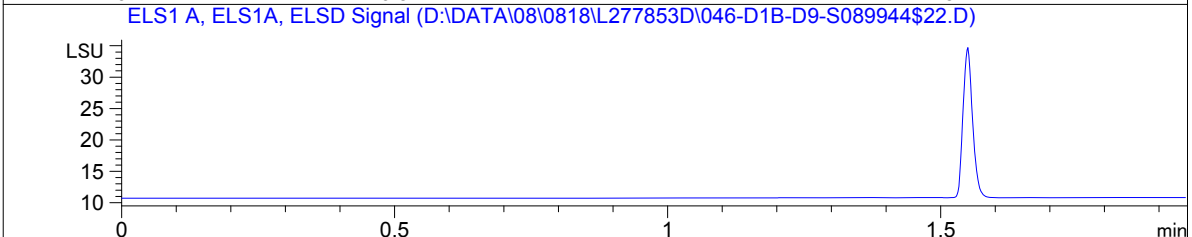
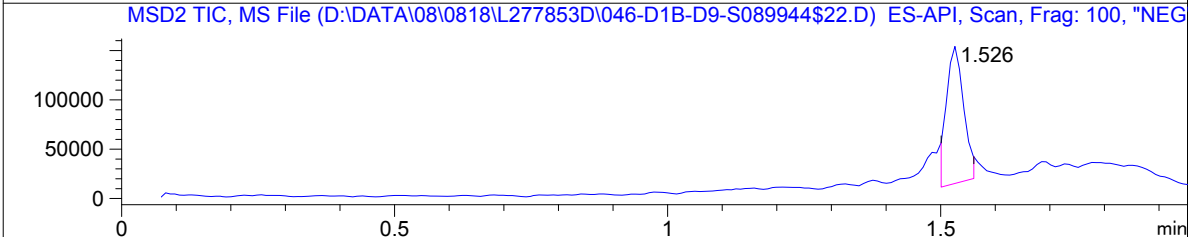
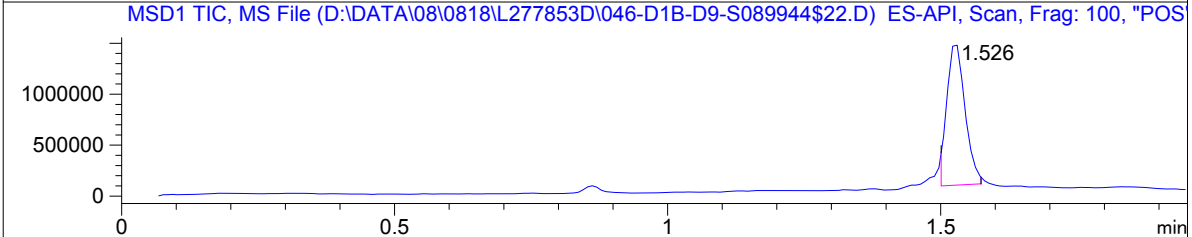
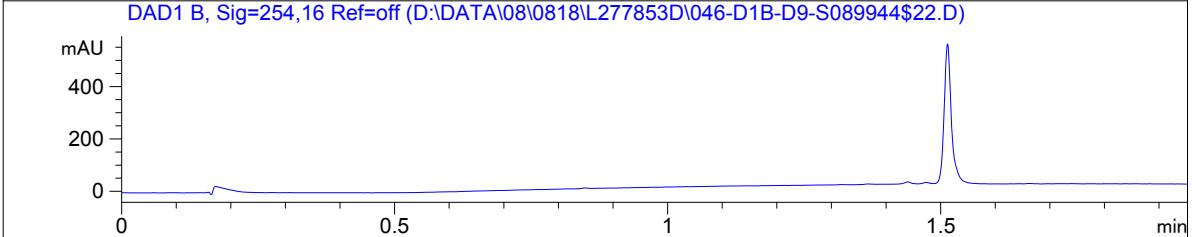
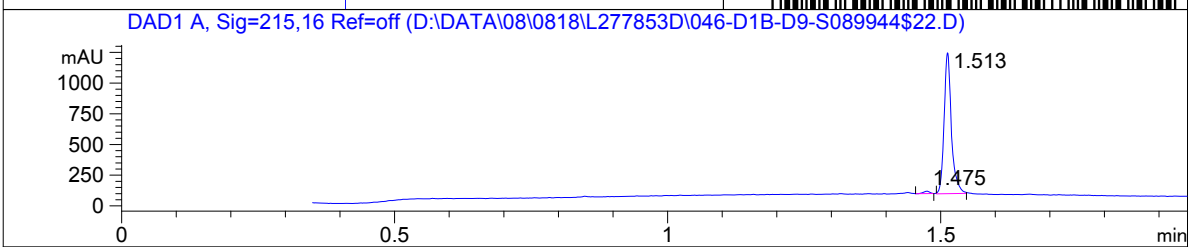
MaxPeak: 98.57%
Ret_Time: 1.513 min

S089944\$22

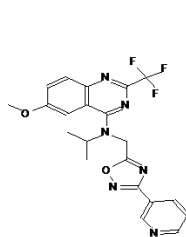


Mol Wt 444.41
Exact Mass 444.17

#	Time	Area%
1	1.475	1.43
2	1.513	98.57

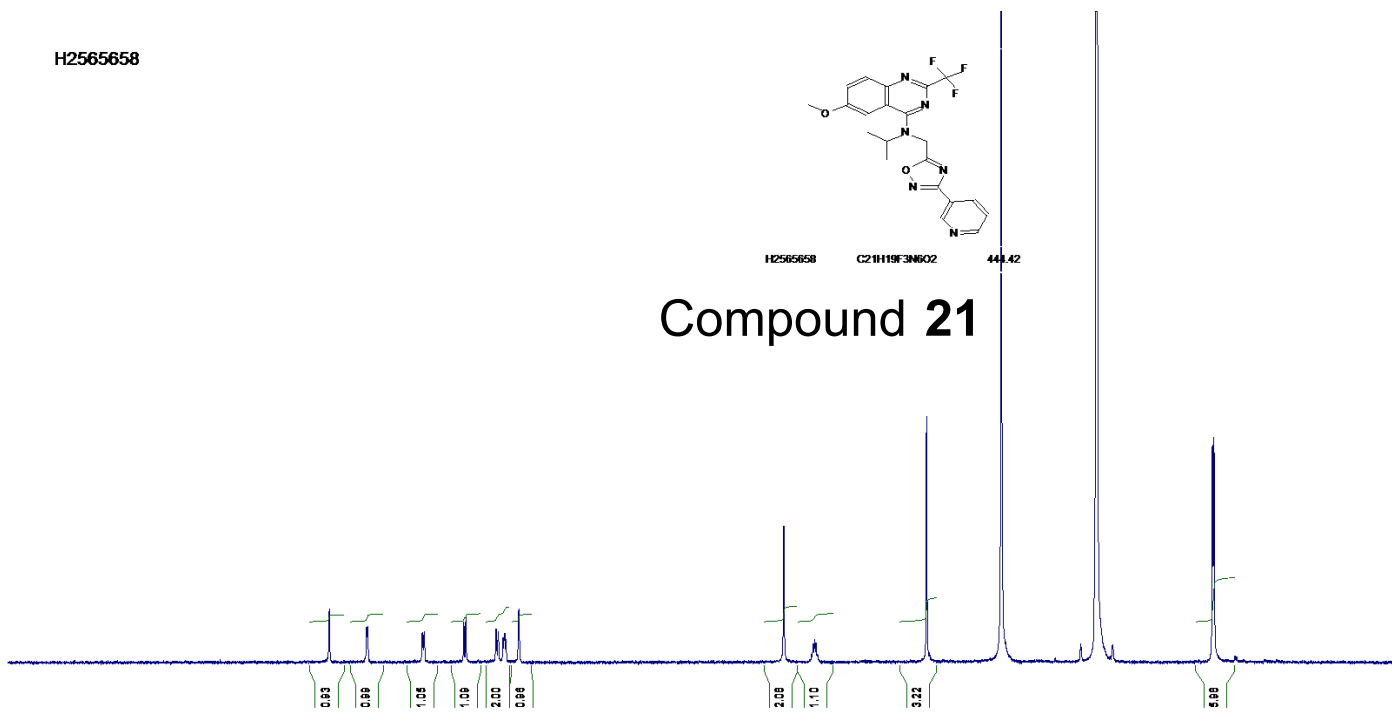


H2565658



H2565658 C21H19F3N6O2 444.42

Compound 21

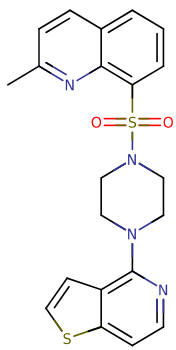


File name: H2565658	Host: H2565658	SF: 499.8207 MHz	NSC: 0	PW: 6.60 usec, RG: 40	SE: 131072
Date: 01-Dec-2020	Solvent: dms0	SW: 11364 Hz	TE: 298 K	AQ: 2.82 sec, RD: 0.00 sec	H2565658

Compound 22

MaxPeak: 100.00%
Ret_Time: 1.110 min

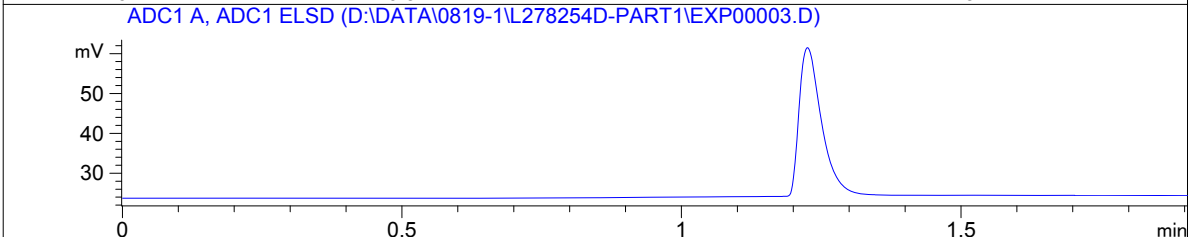
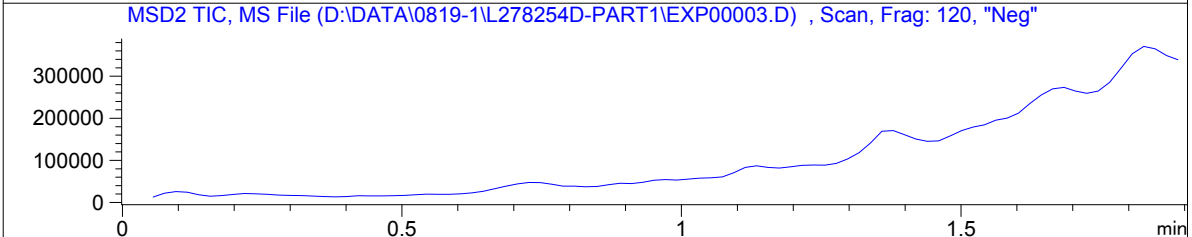
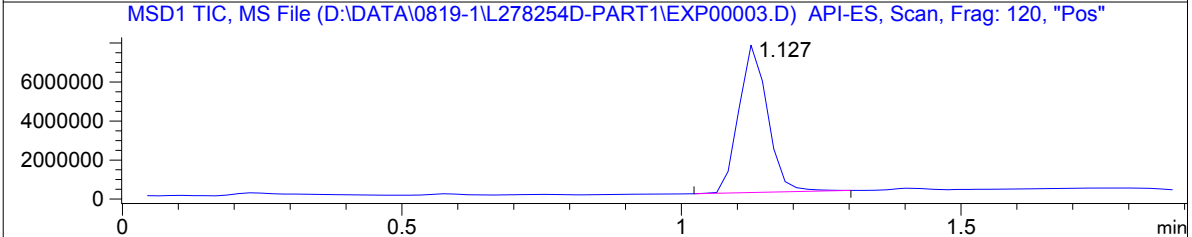
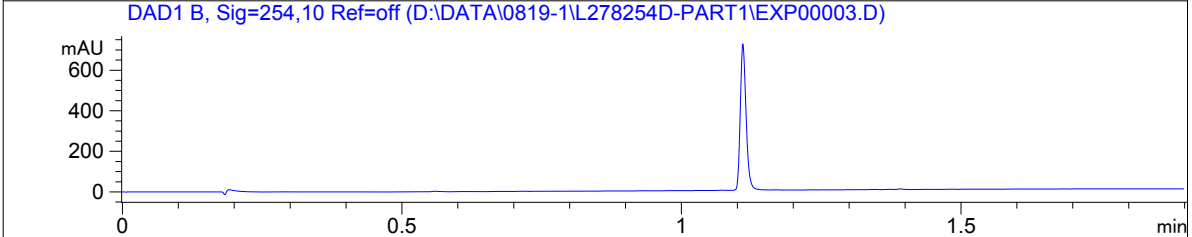
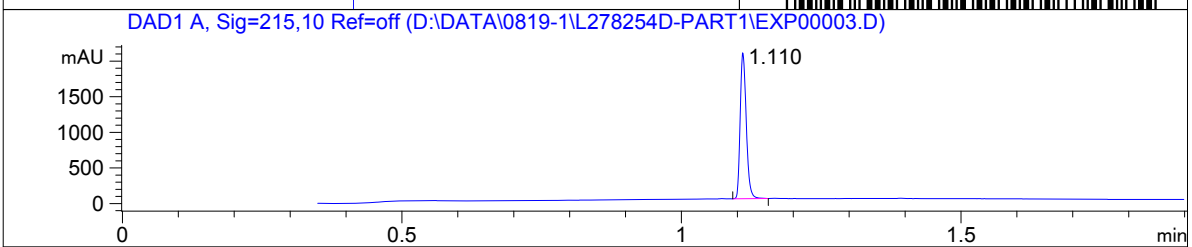
S089988\$5



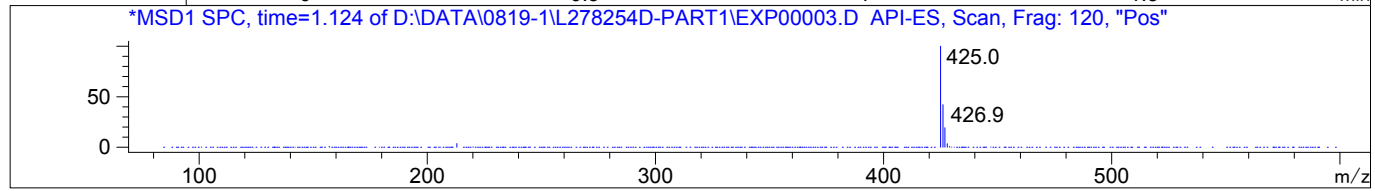
Mol Wt 424.54

Exact Mass 424.12

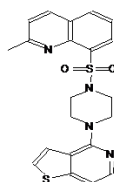
#	Time	Area%
1	1.110	100.00



RT 1.127



H2562997

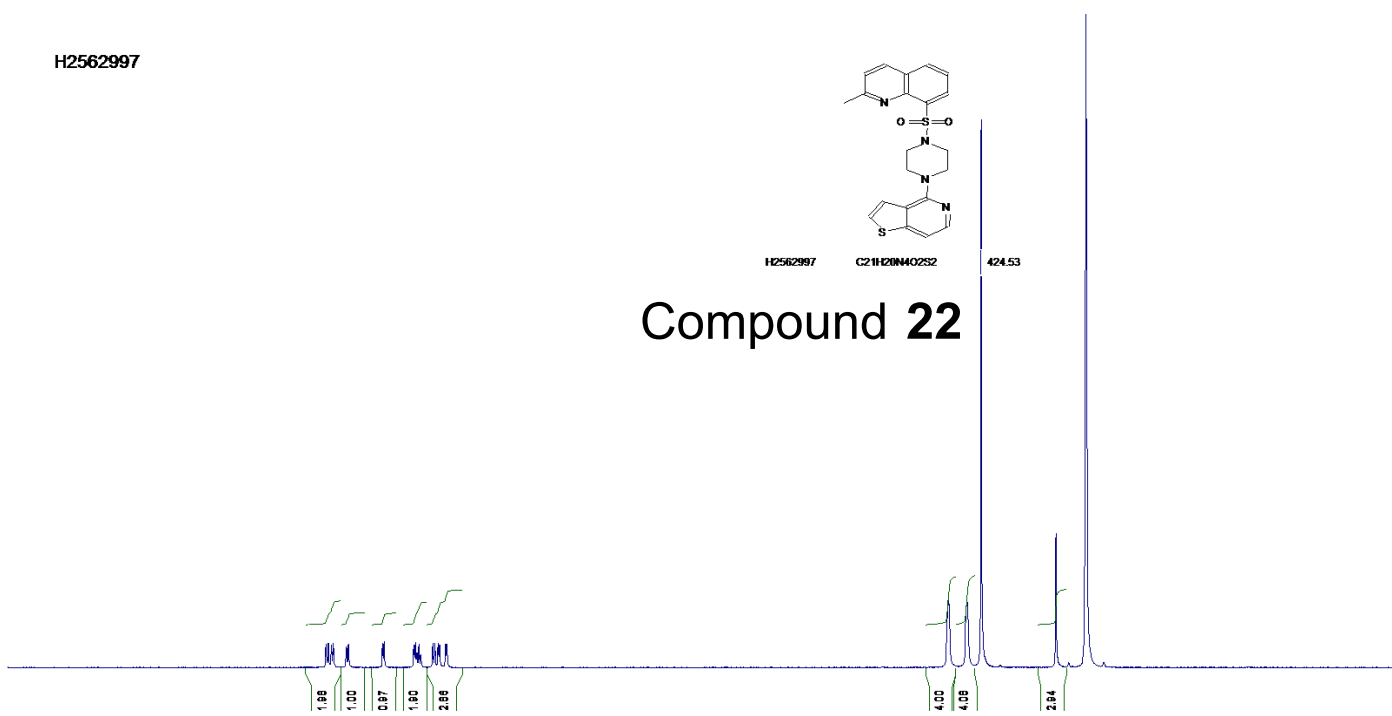


H2562997

C21H20N4O2S2

424.53

Compound 22

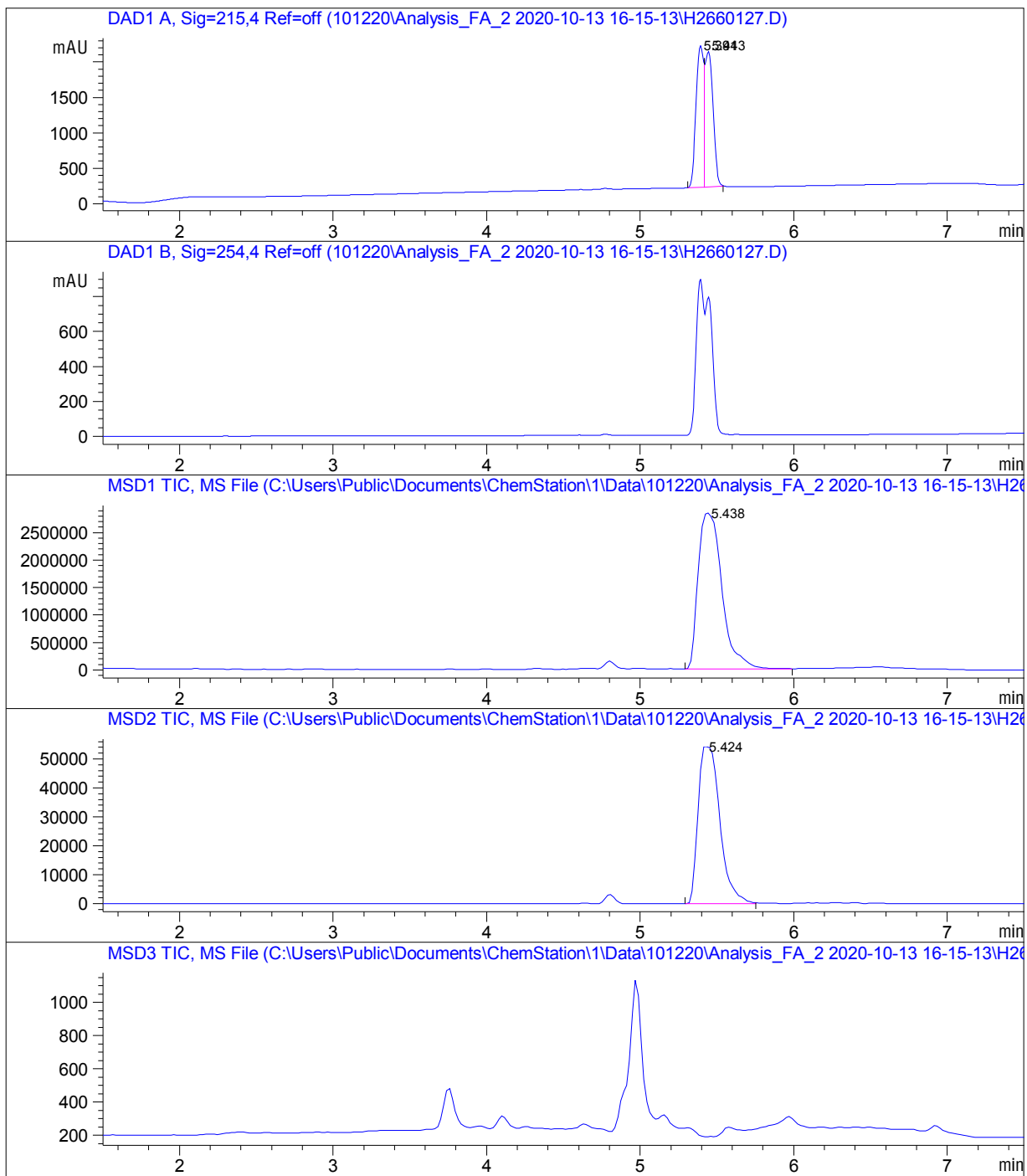


File name: H2562997	Host: char	SF: 499.8207 MHz	NSC: 0	PW: 6.60 usec, RG: 40	SE: 131072
Date: 01-Dec-2020	Solvent: dmso	SW: 11364 Hz	TE: 298 K	AQ: 2.82 sec, RD: 0.00 sec	H2562997

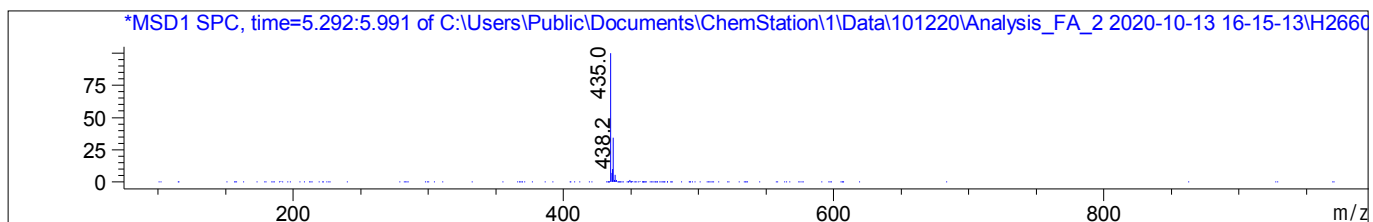
Compound 23

Sample 0.1%FA-ACN 5-95%ACN 6 min. Zorbax-Eclipse-Plus C18 4,6 x
H2660127 100mm, 3.5 mkm.

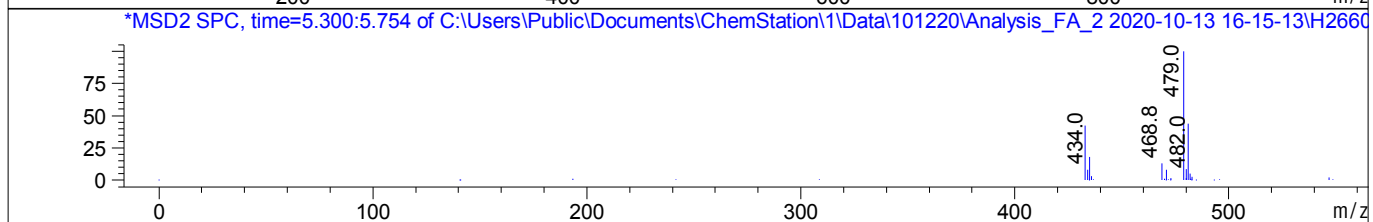
#	Time	Area%
1	5.391	53.36
2	5.443	46.64



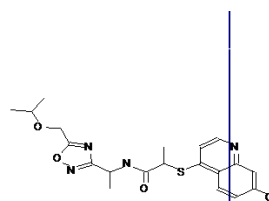
RT 5.438



RT 5.424

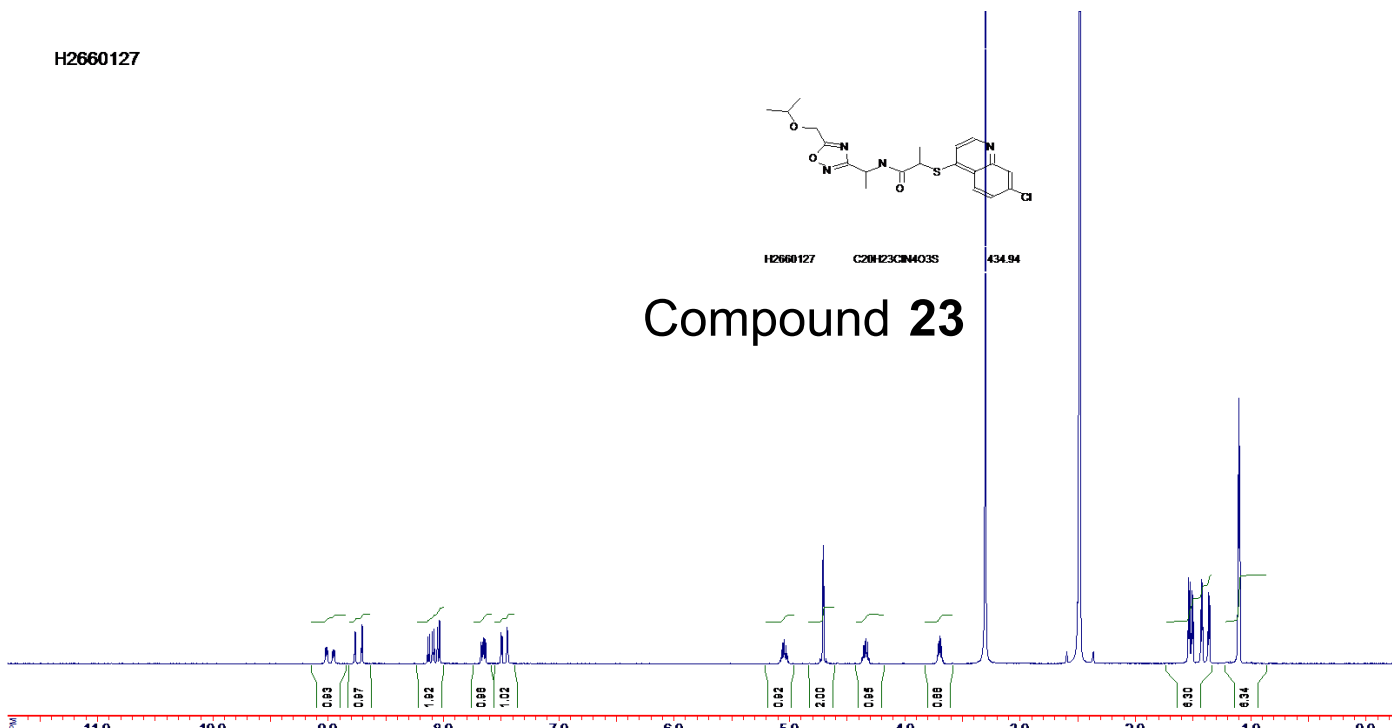


H2660127



H2660127 C20H23ClN4O3S 434.94

Compound 23



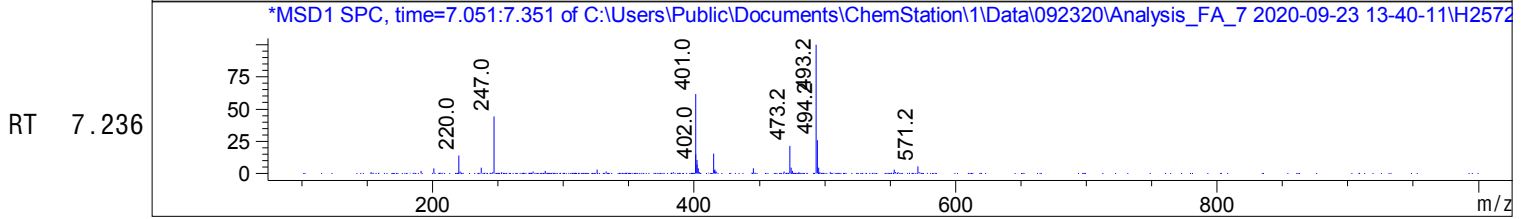
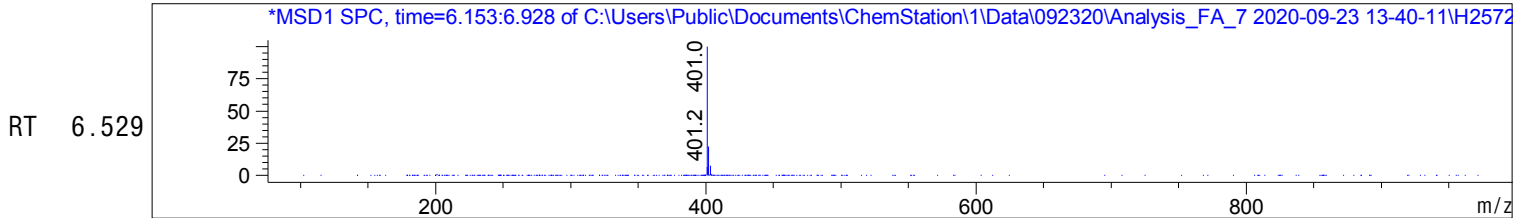
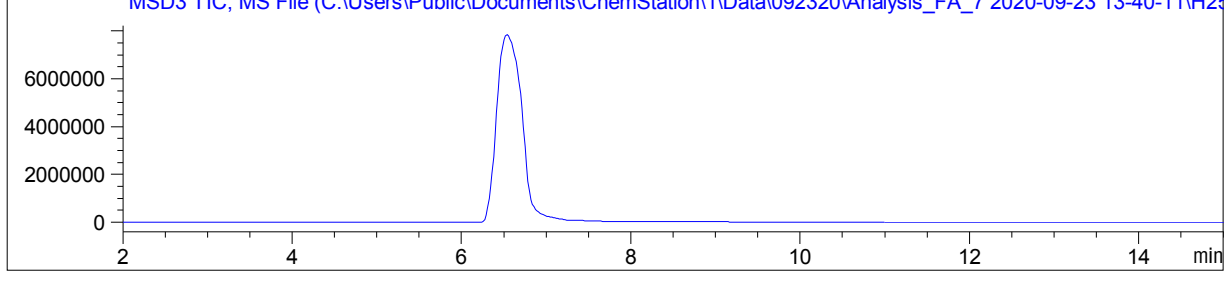
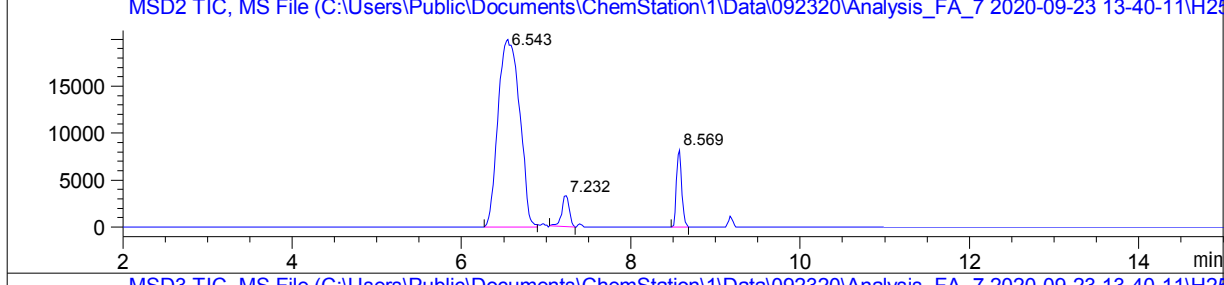
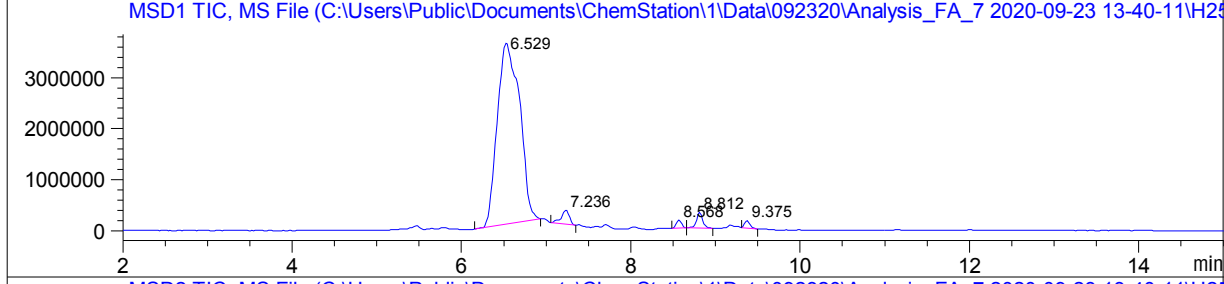
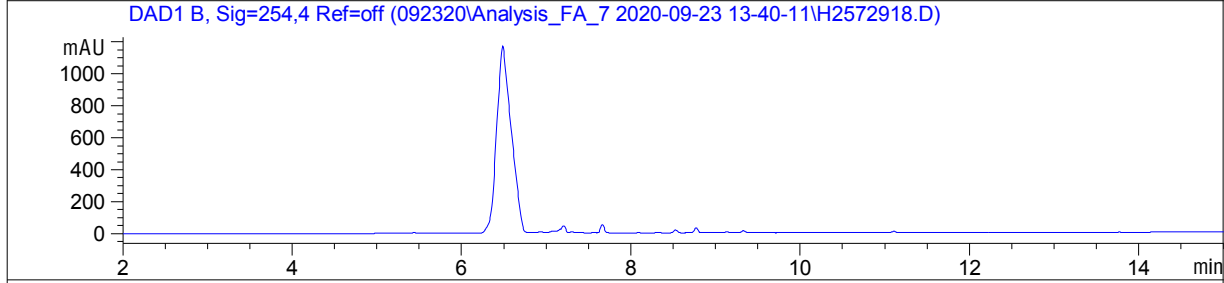
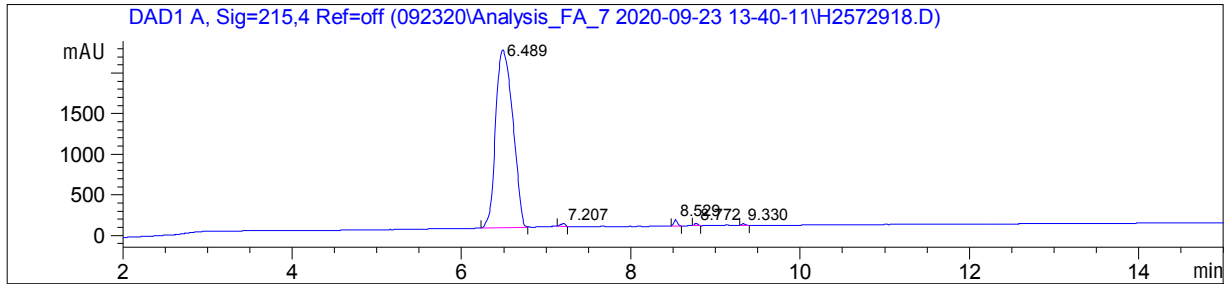
11.0	10.0	9.0	8.0	7.0	6.0	5.0	4.0	3.0	2.0	1.0	0.0
File name: H2660127		Hochbar		SF: 599.7811 MHz		NSC: 0		PW: 4.40 usec, RG: 44		SE 131072	
Date: 26-Nov-2020		Solvent: dmso		SW: 11364 Hz		TE: 298 K		AQ: 2.82 sec, RD: 0.00 sec		H2660127	

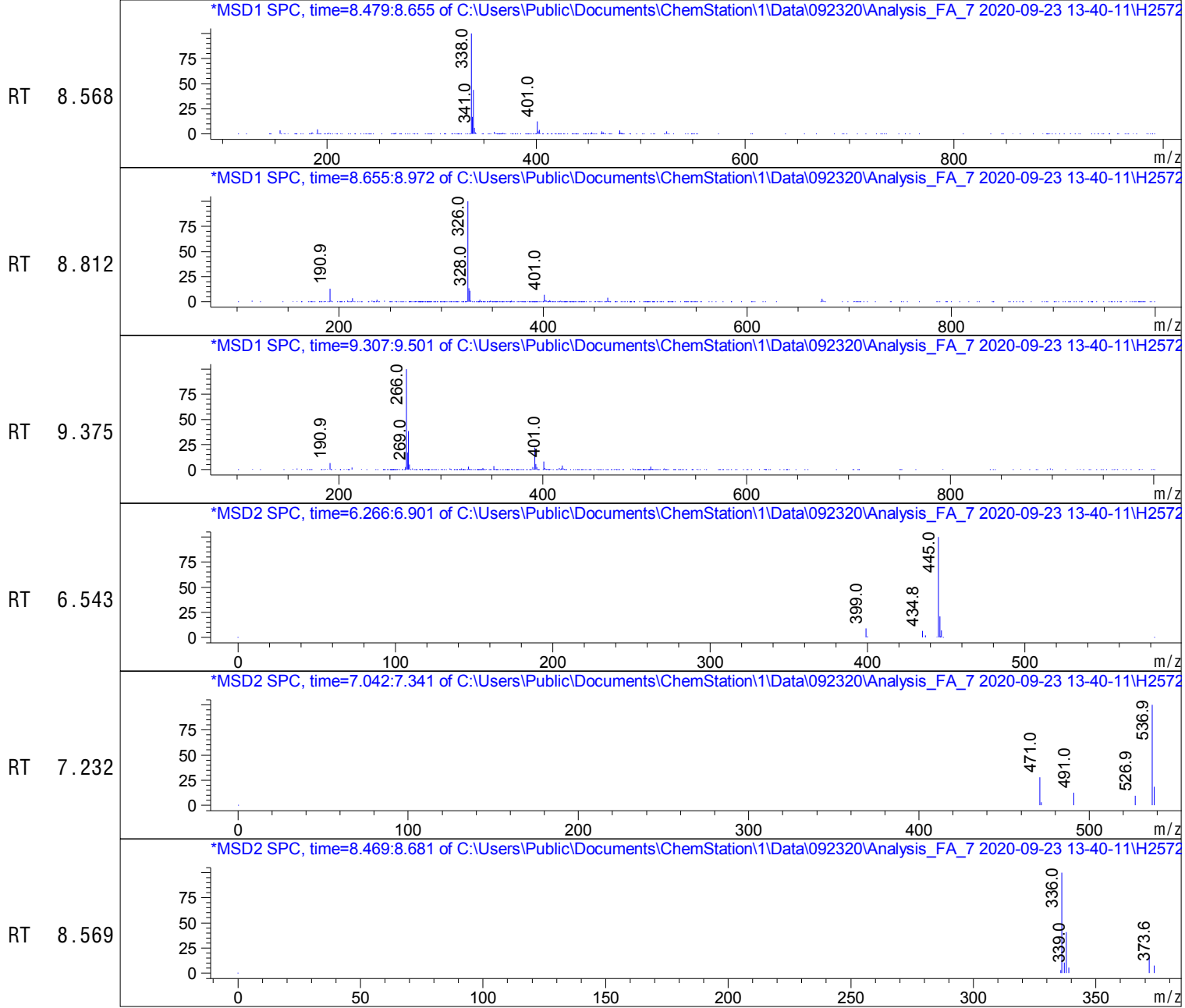
Compound 24

Sample H2572918

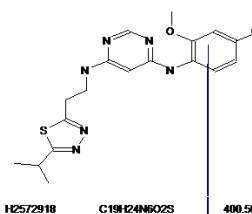
0.1%FA-ACN 5-95% ACN, 15 min. Kinetext C18 4,6 x 150mm, 2.6 u.

#	Time	Area%
1	6.489	98.38
2	7.207	0.45
3	8.529	0.70
4	8.772	0.27
5	9.330	0.20

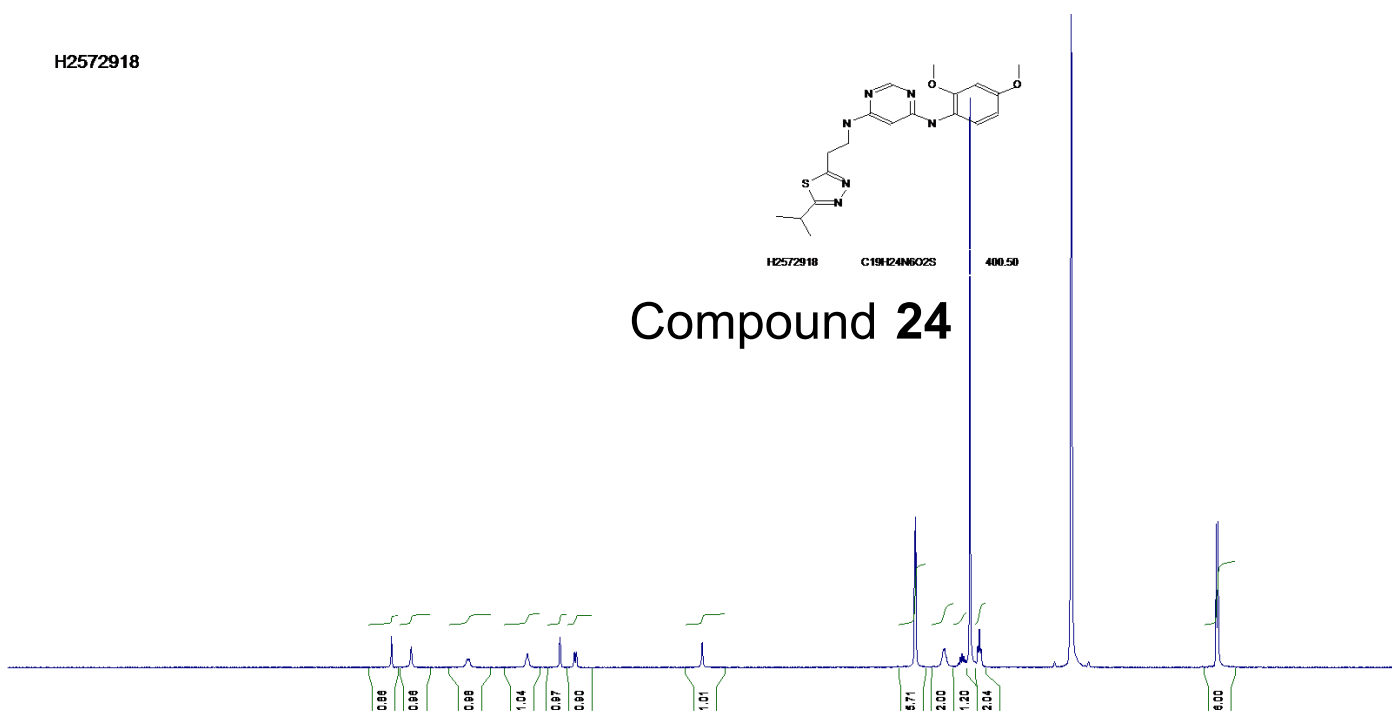




H2572918



Compound 24



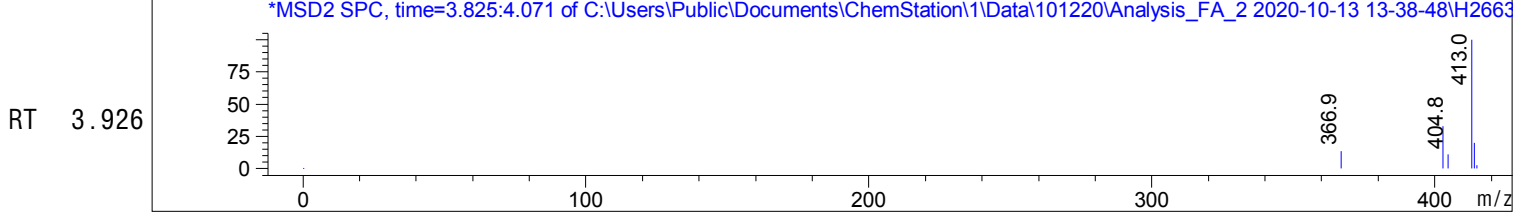
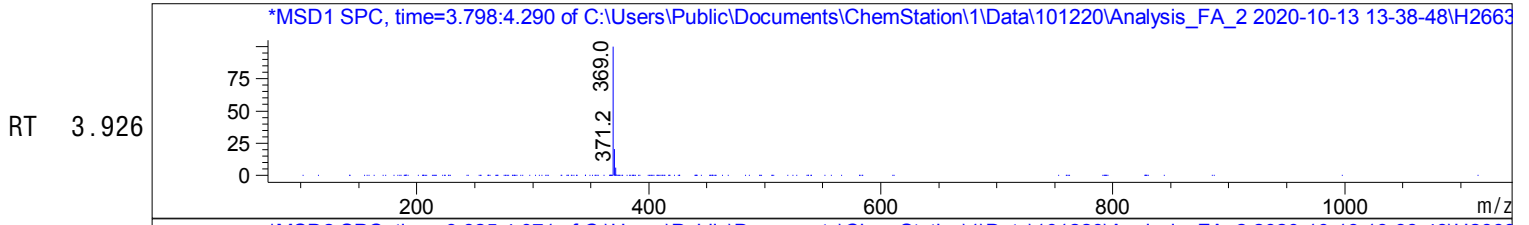
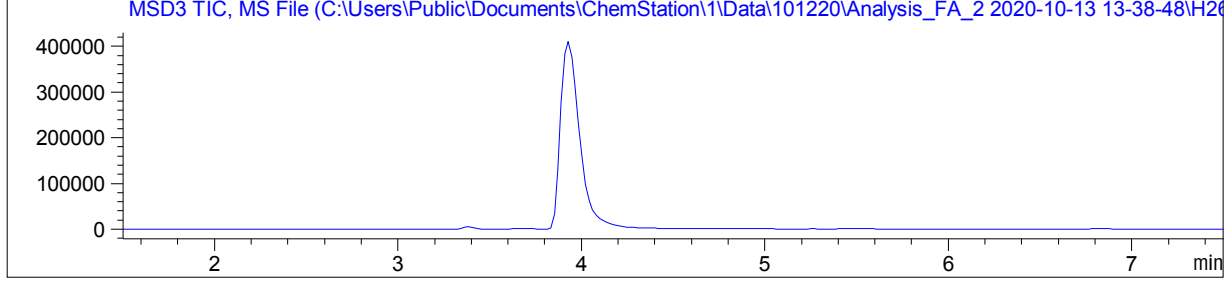
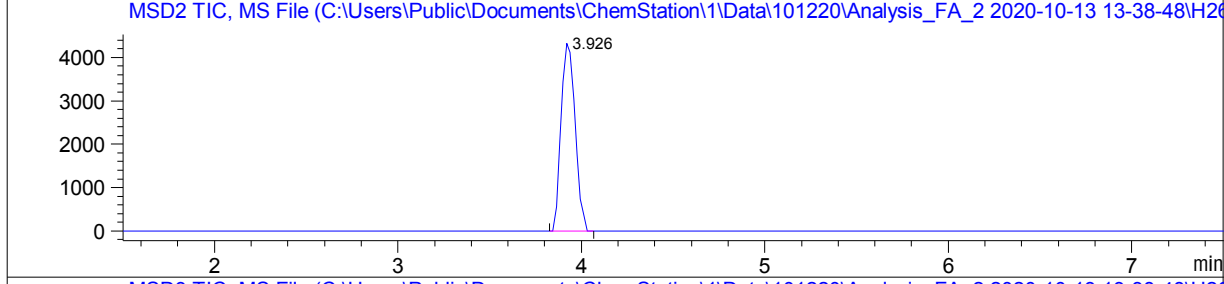
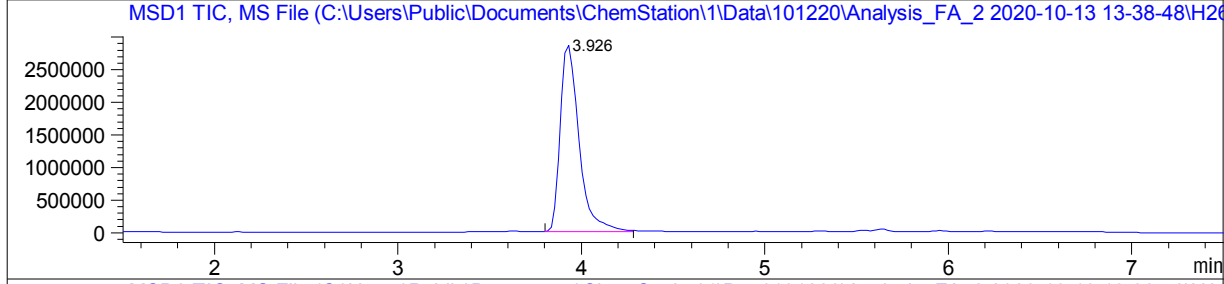
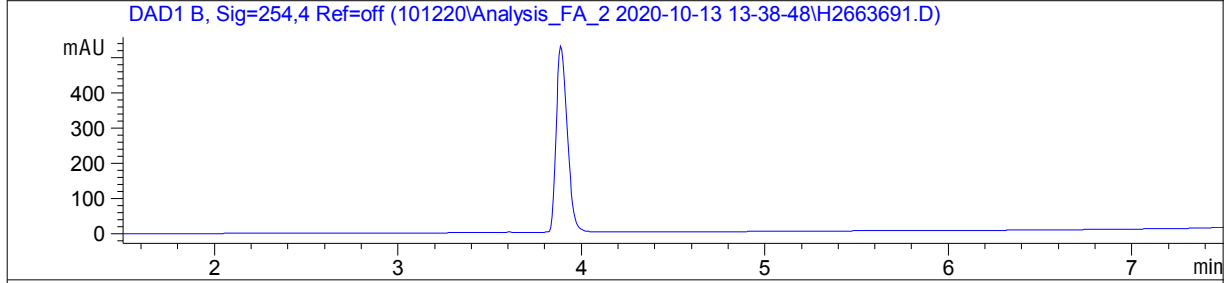
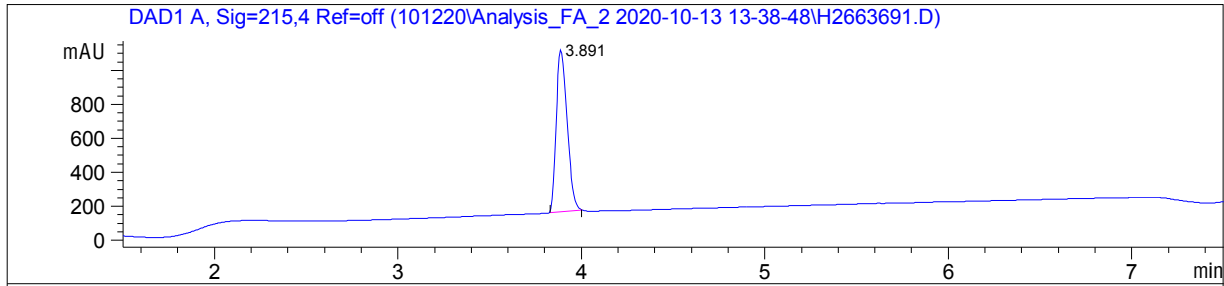
File name: H2572918	Host: Hsncbar	SF: 499.8207 MHz	NSC: 0	PW: 6.60 usec, RG: 40	SE: 131072
Date: 01-Dec-2020	Solvent: dmsd	SW: 11364 Hz	TE: 298 K	AQ: 2.82 sec, RD: 0.00 sec	H2572918

Compound 25

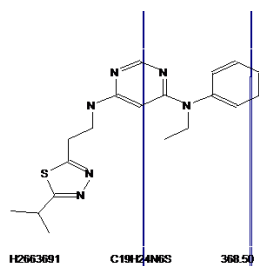
Sample H2663691

0.1%FA-ACN 5-95%ACN 6 min. Zorbax-Eclipse-Plus C18 4,6 x 100mm, 3.5 mkm.

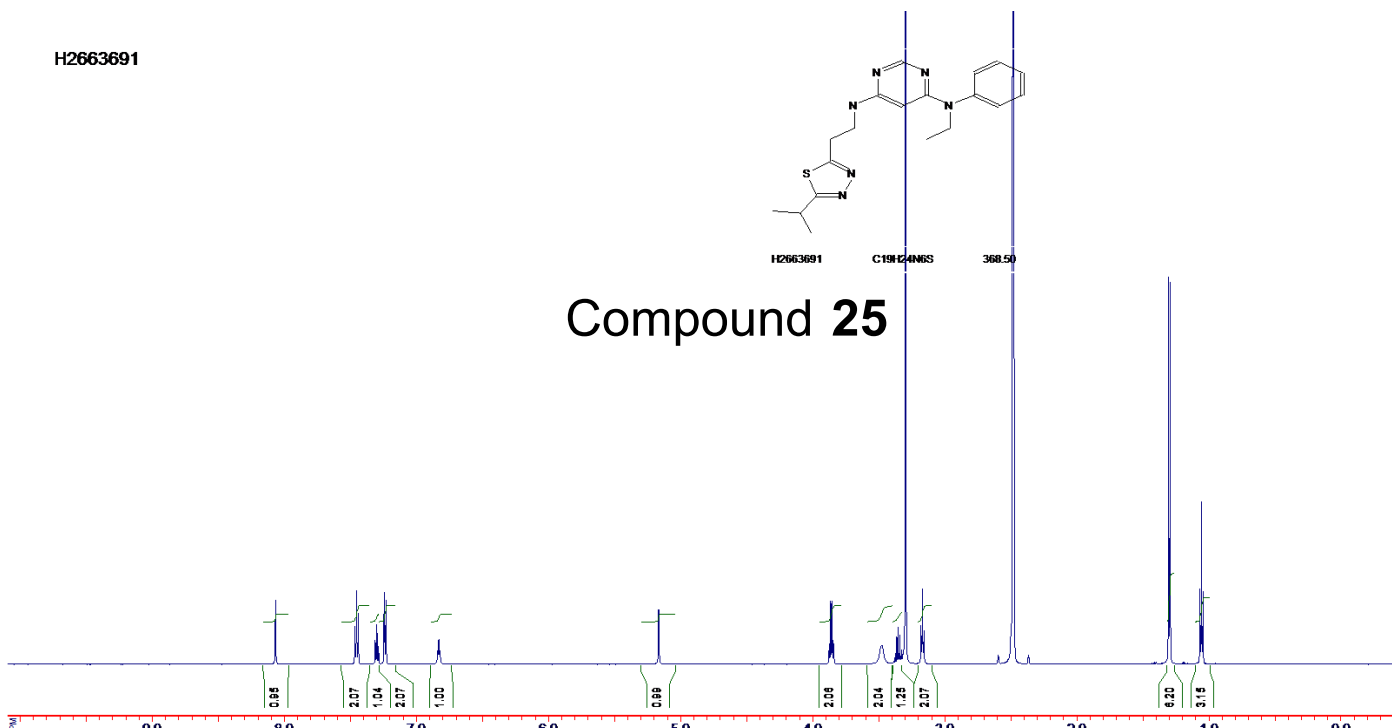
#	Time	Area%
1	3.891	100.00



H2663691



Compound 25



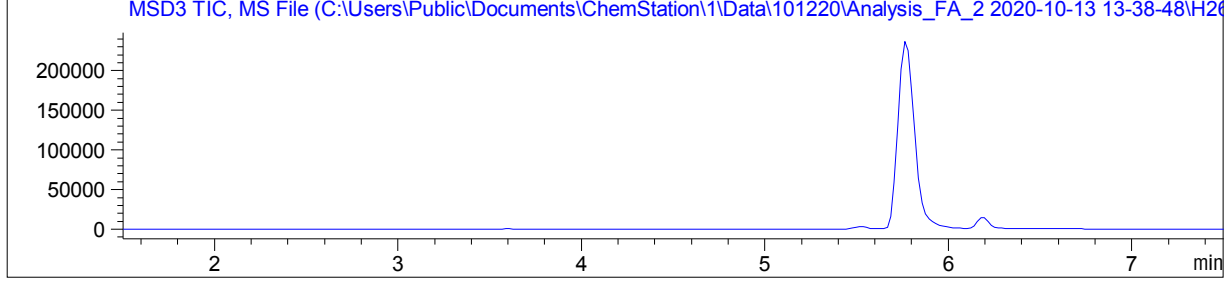
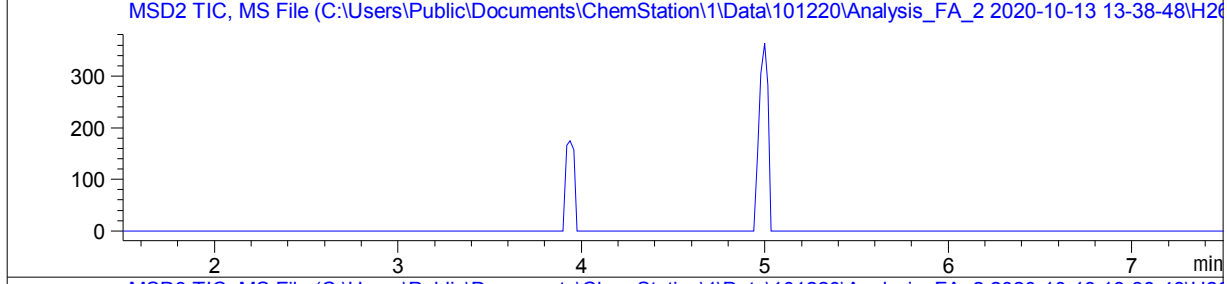
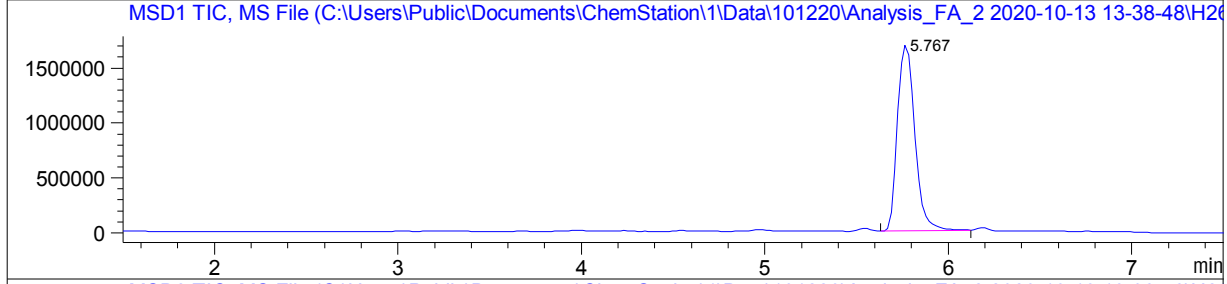
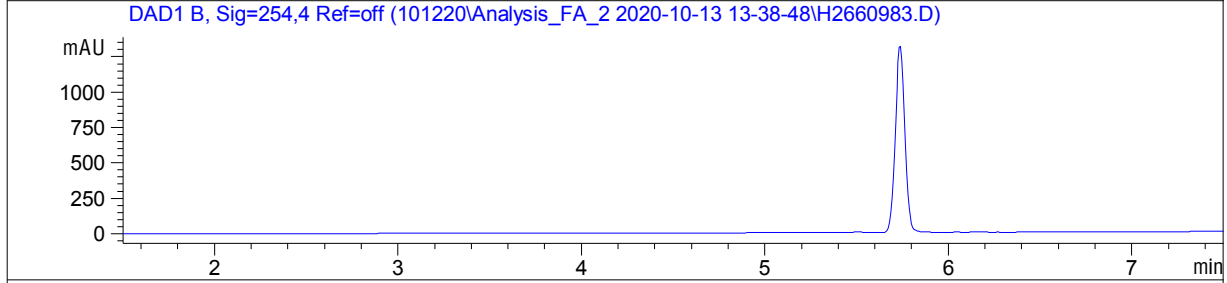
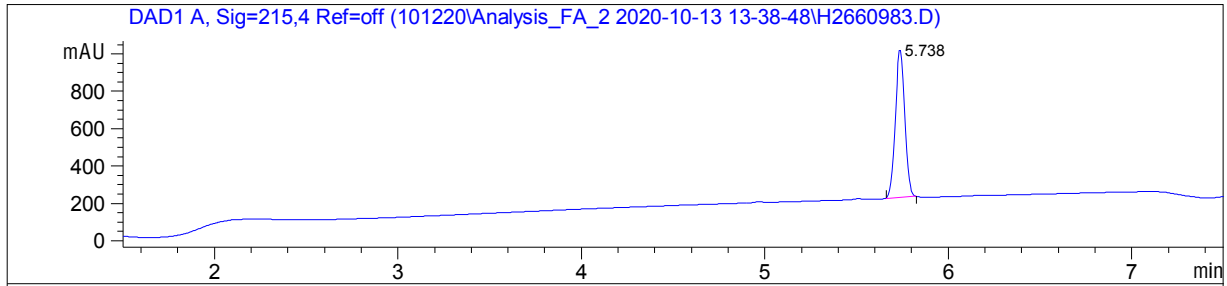
File name: H2663691	Hexachlor	SF: 599.7811 MHz	NSC: 0	PW: 4.40 usec, RG: 44	SE 131072
Date: 26-Nov-2020	Solvent: dms0	SW: 11364 Hz	TE: 298 K	AQ: 2.82 sec, RD: 0.00 sec	H2663691

Compound 26

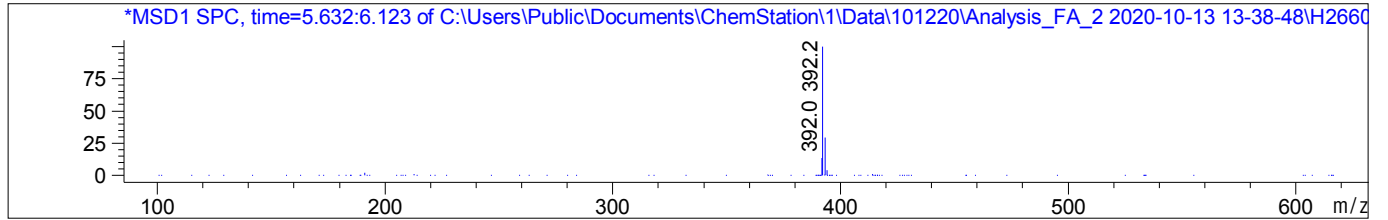
Sample H2660983

0.1%FA-ACN 5-95%ACN 6 min. Zorbax-Eclipse-Plus C18 4,6 x 100mm, 3.5 mkm.

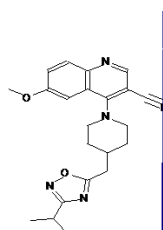
#	Time	Area%
1	5.738	100.00



RT 5.767



H2660983

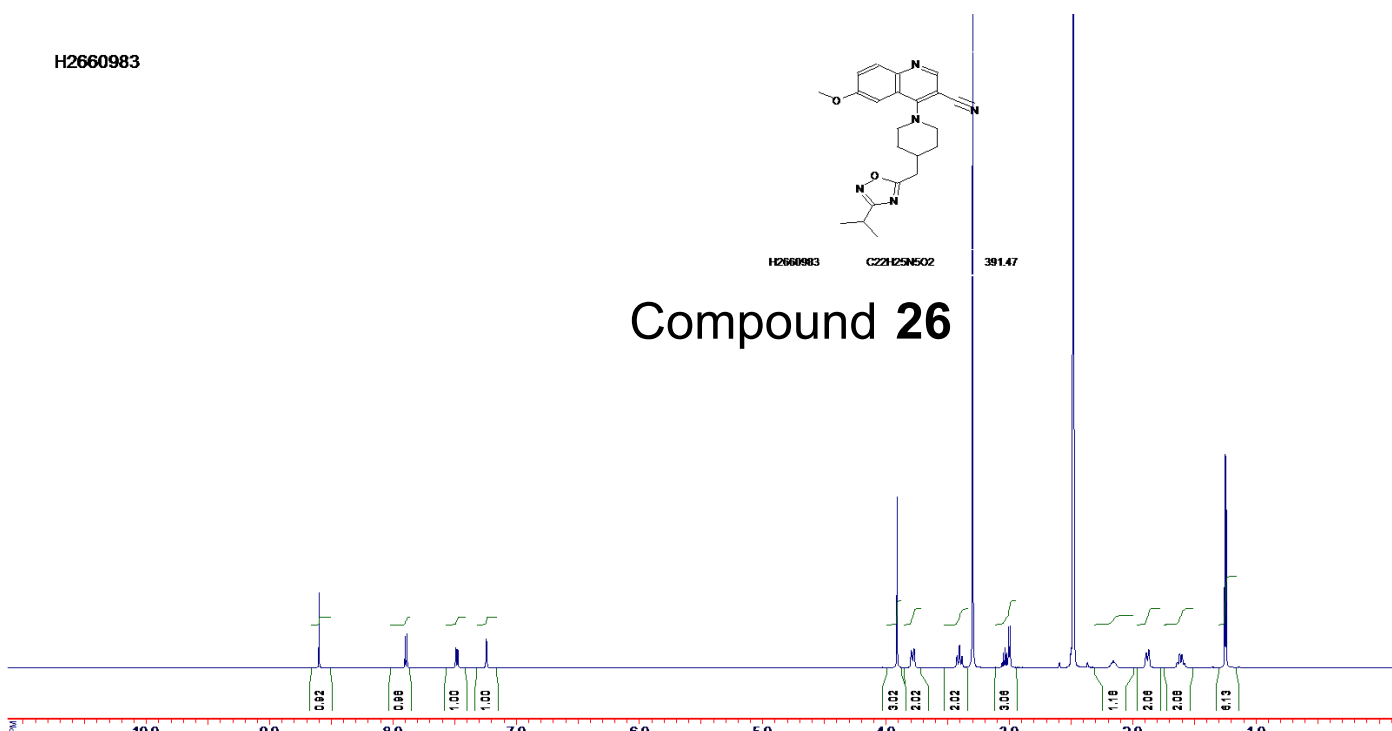


H2660983

C2H12N5O2

391.47

Compound 26



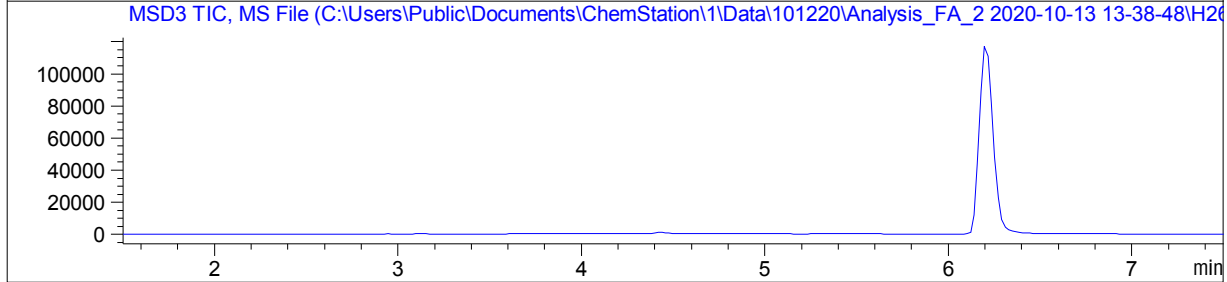
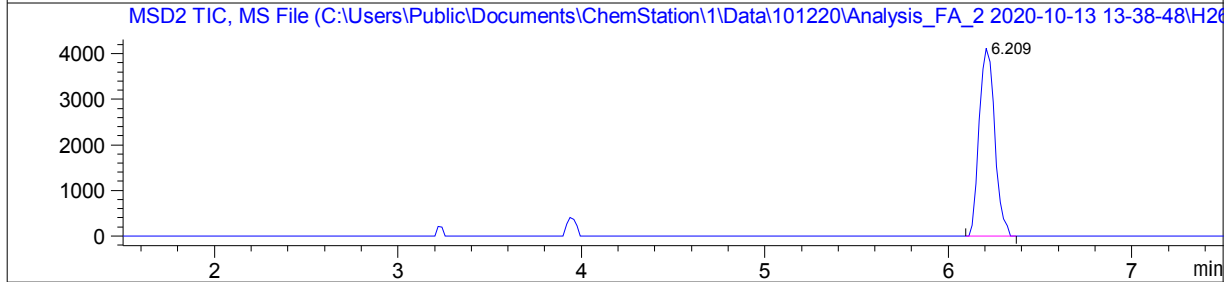
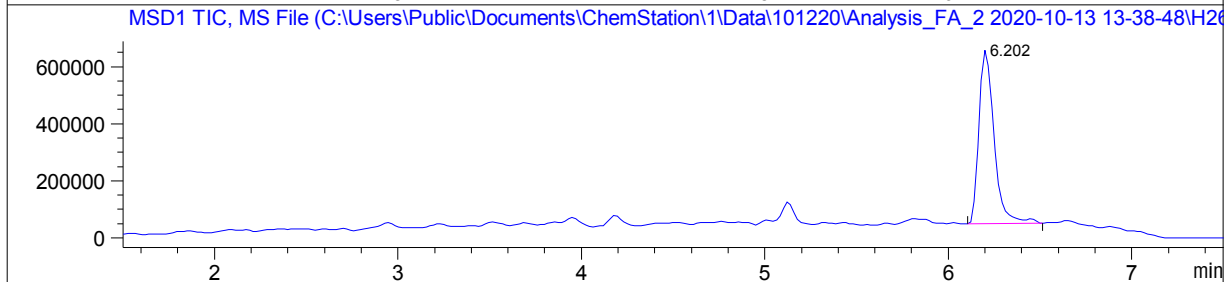
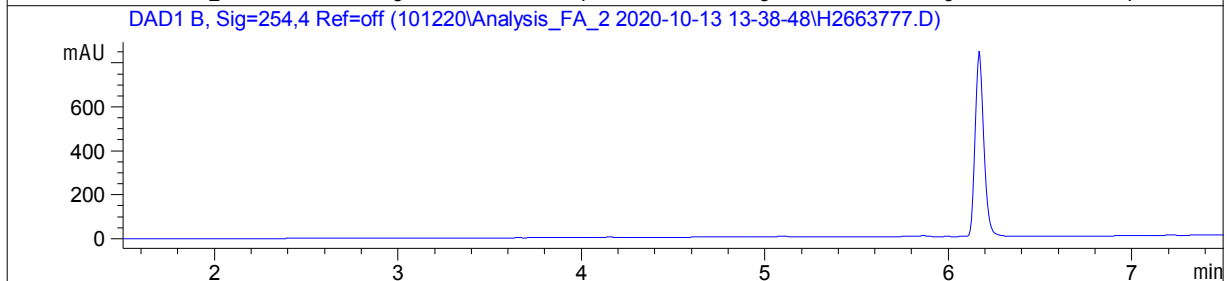
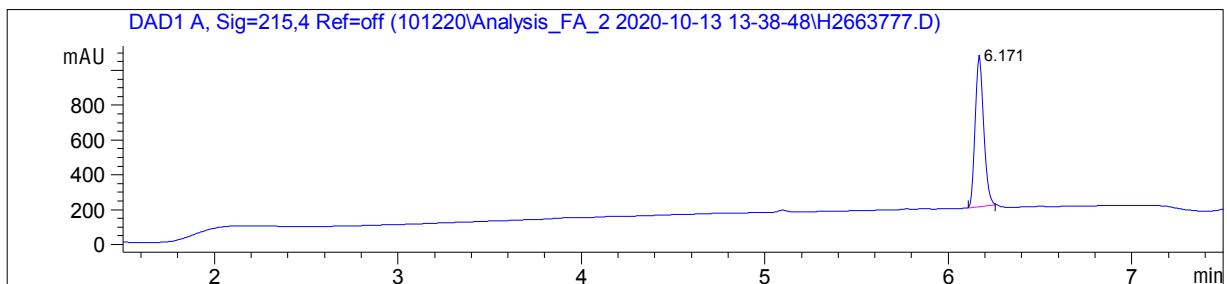
File name: H2660983	Host: Hachar	SF: 599.7811 MHz	NSC: 0	PW: 4.40 usec, RG: 44	SE 131072
Date: 26-Nov-2020	Solvent: dmsd	SW: 11364 Hz	TE: 298 K	AQ: 2.82 sec, RD: 0.00 sec	H2660983

Compound 27

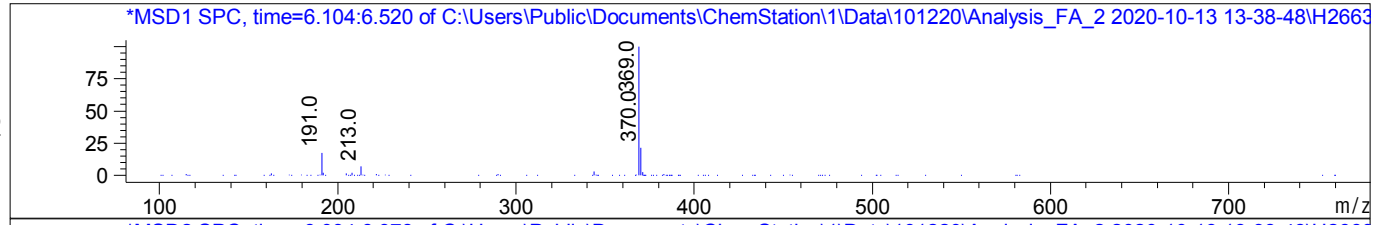
Sample H2663777

0.1%FA-ACN 5-95%ACN 6 min. Zorbax-Eclipse-Plus C18 4,6 x 100mm, 3.5 mk.

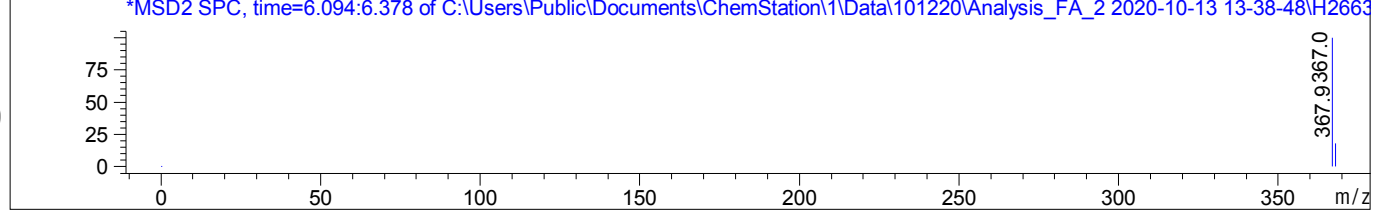
#	Time	Area%
1	6.171	100.00



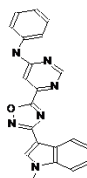
RT 6.202



RT 6.209



H2663777

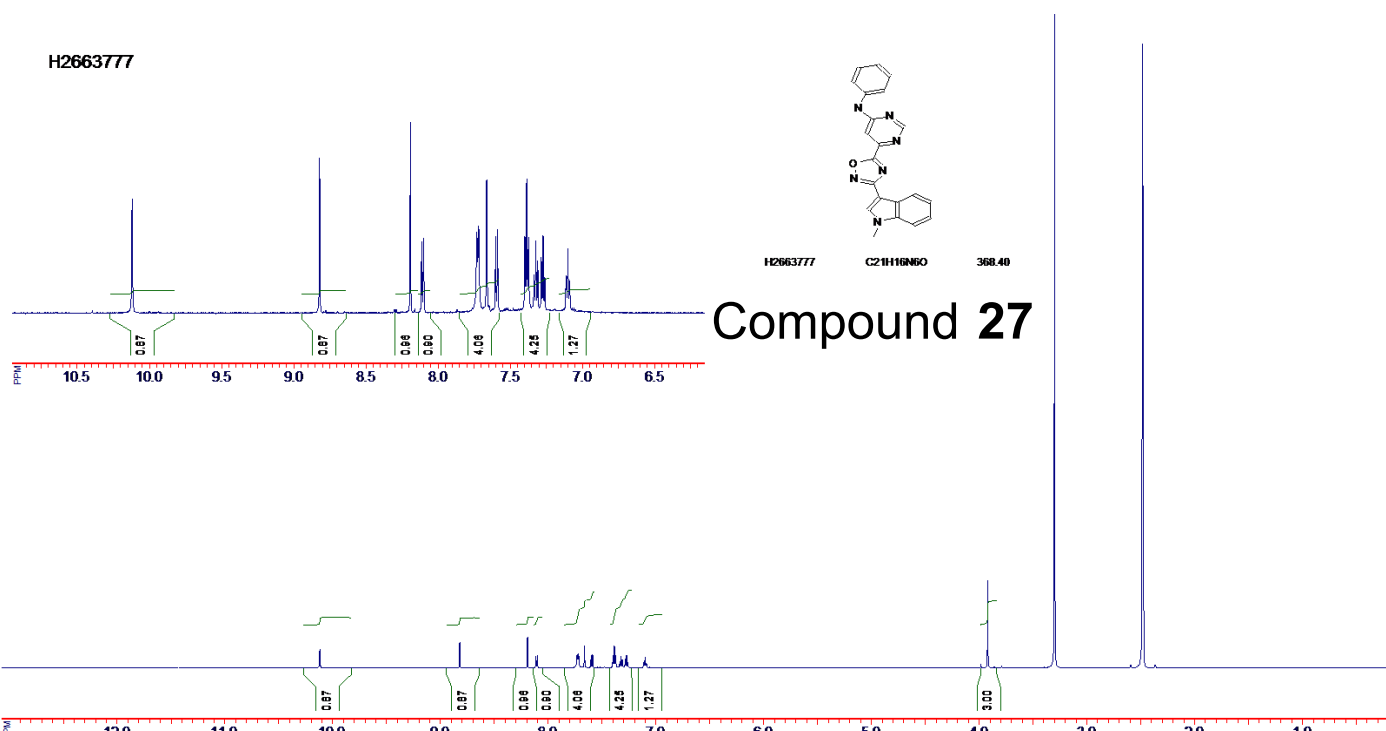


H2663777

C21H16N6O

368.40

Compound 27



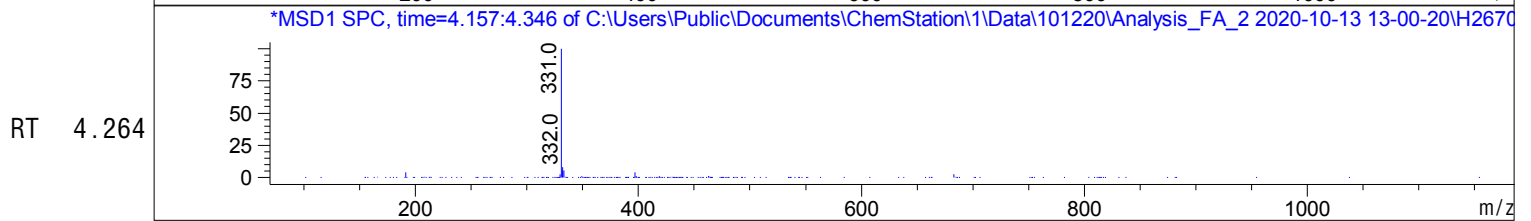
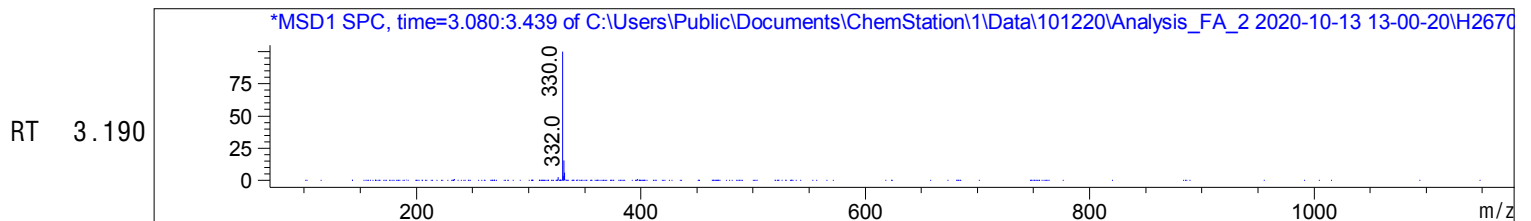
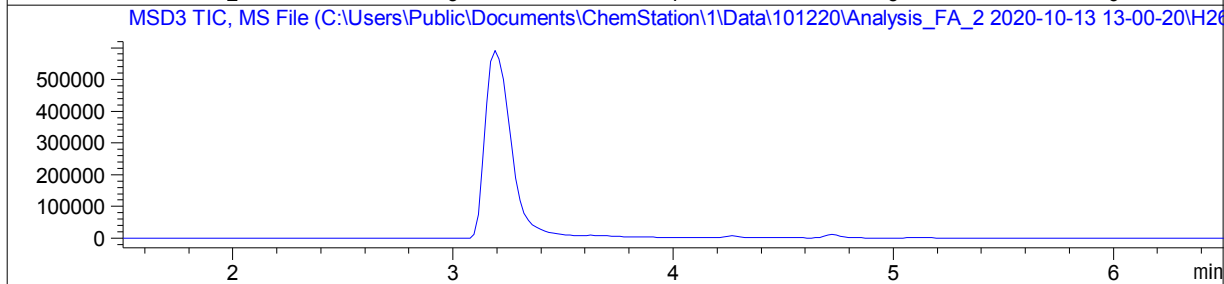
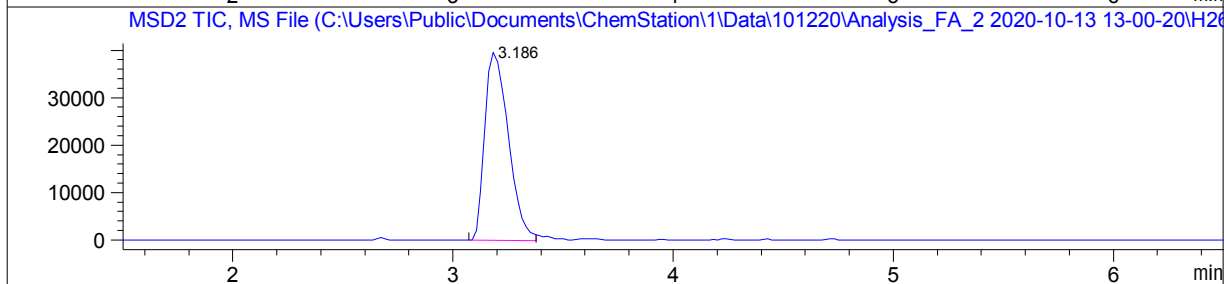
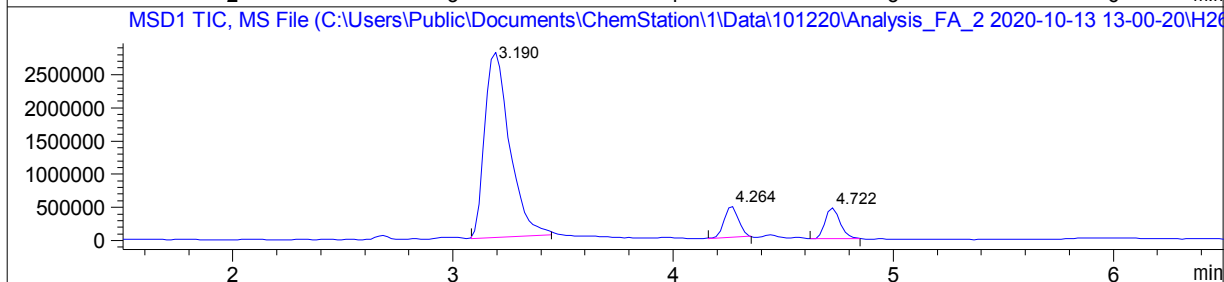
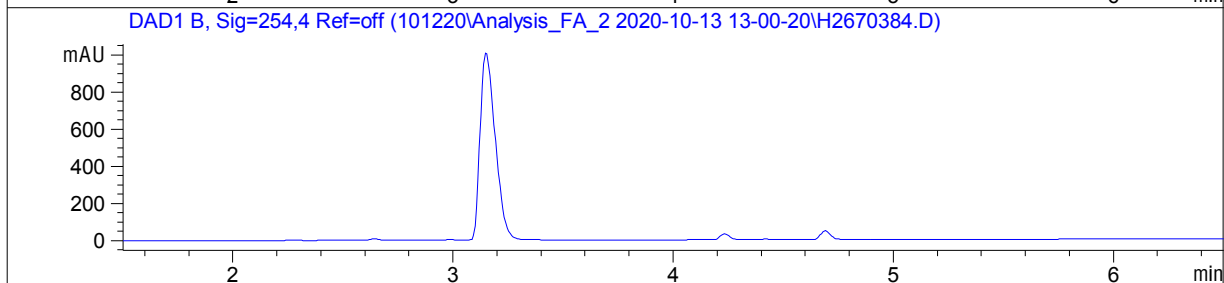
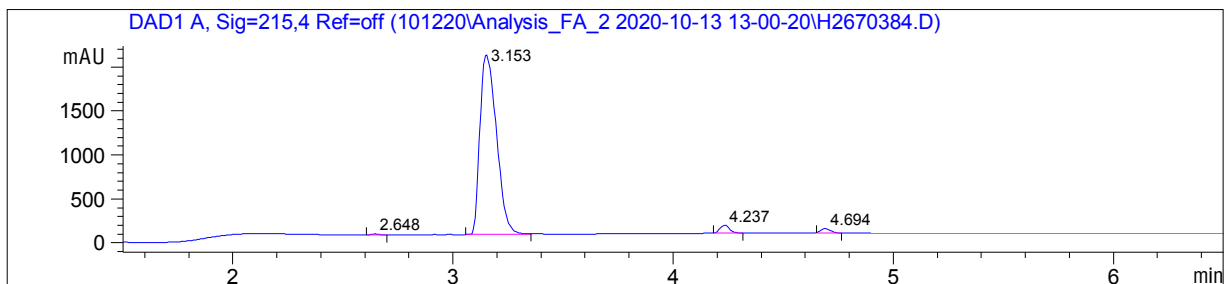
File name: H2663777	Host:char	SF: 599.7811 MHz	NSC: 0	PW: 4.40 usec, RG: 44	SE 131072
Date: 26-Nov-2020	Solvent: dms0	SW: 11364 Hz	TE: 298 K	AQ: 2.82 sec, RD: 0.00 sec	H2663777

Compound 28

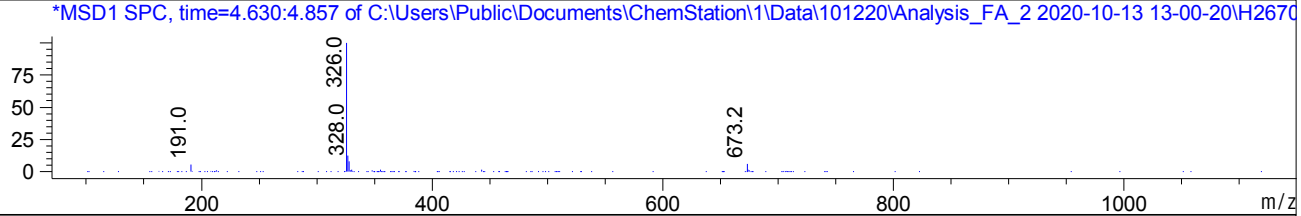
Sample H2670384

0.1%FA-ACN 5-95%ACN 6 min. Zorbax-Eclipse-Plus C18 4,6 x 100mm, 3.5 mkm.

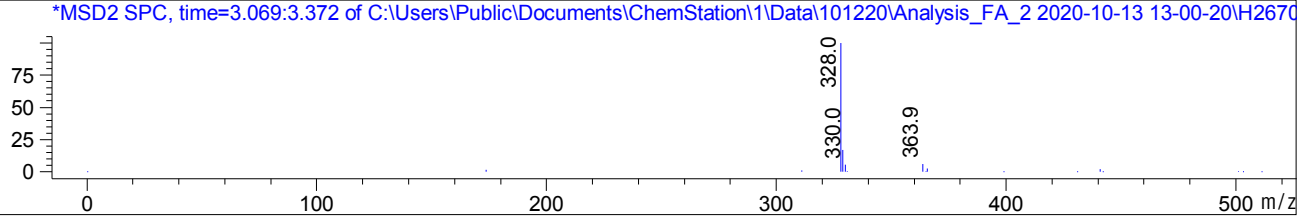
#	Time	Area%
1	2.648	0.35
2	3.153	95.66
3	4.237	2.50
4	4.694	1.49



RT 4.722

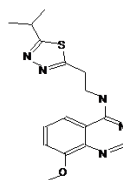


RT 3.186



H2670384

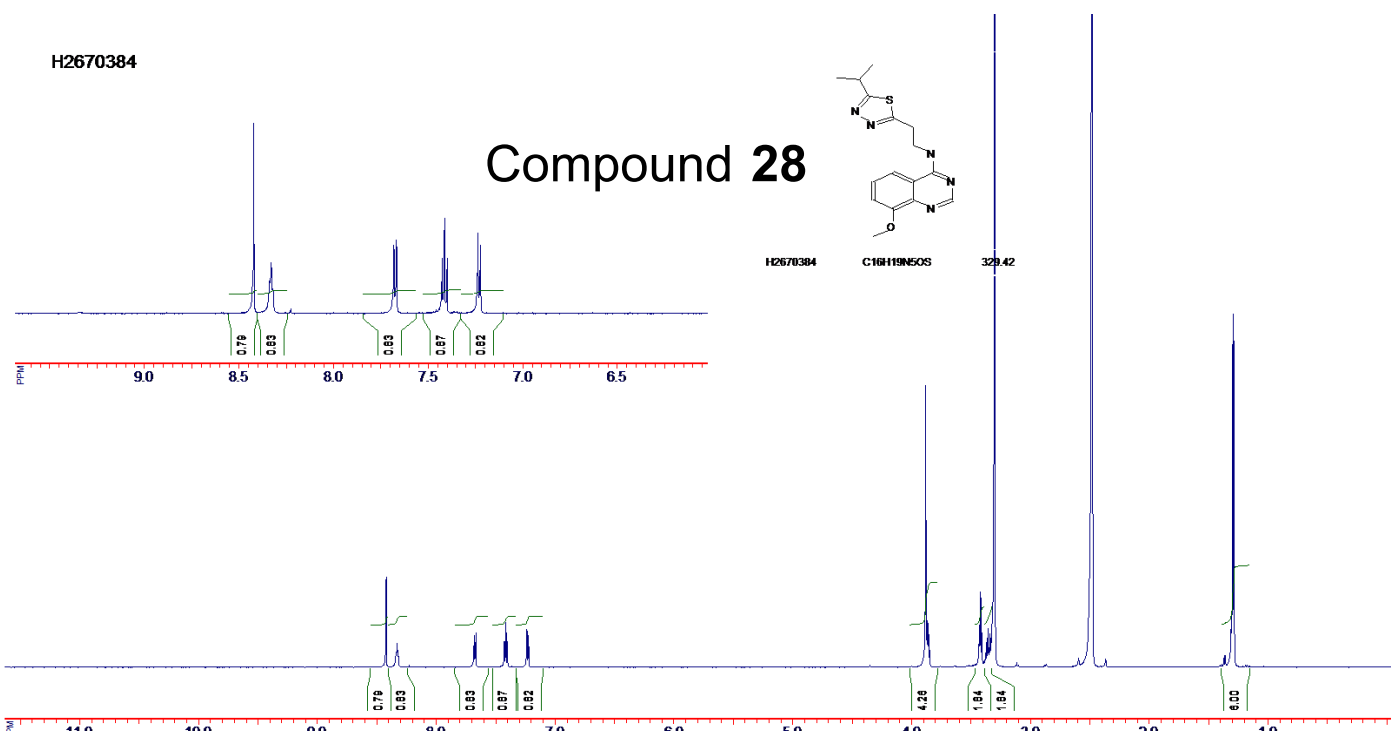
Compound 28



H2670384

C18H19N5OS

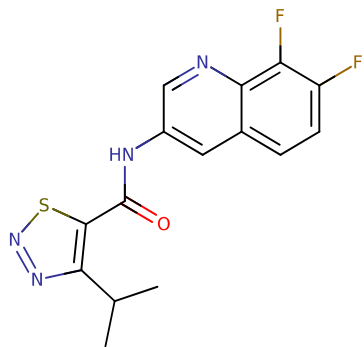
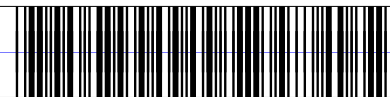
329.42



File name: H2670384	Host: H2670384	SF: 599.7811 MHz	NSC: 0	PW: 4.40 usec, RG: 44	SE 131072
Date: 26-Nov-2020	Solvent: dmsd	SW: 11364 Hz	TE: 298 K	AQ: 2.82 sec, RD: 0.00 sec	H2670384

MaxPeak: 100.00%
Ret_Time: 1.245 min

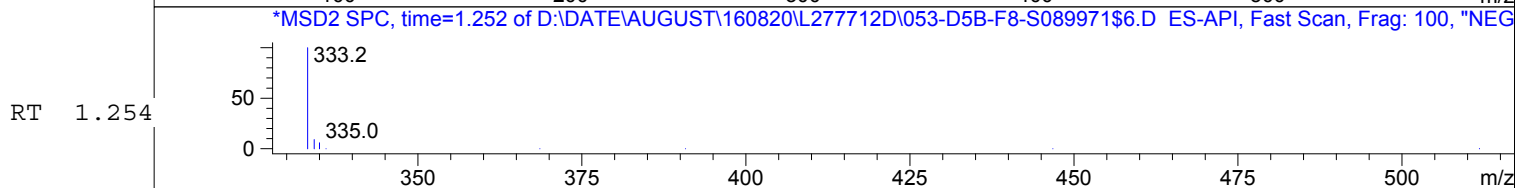
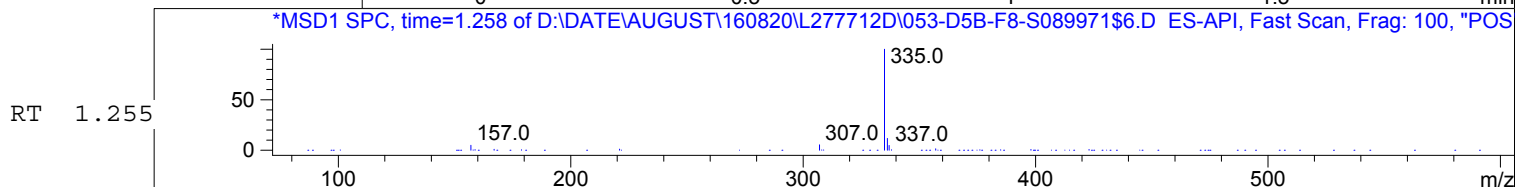
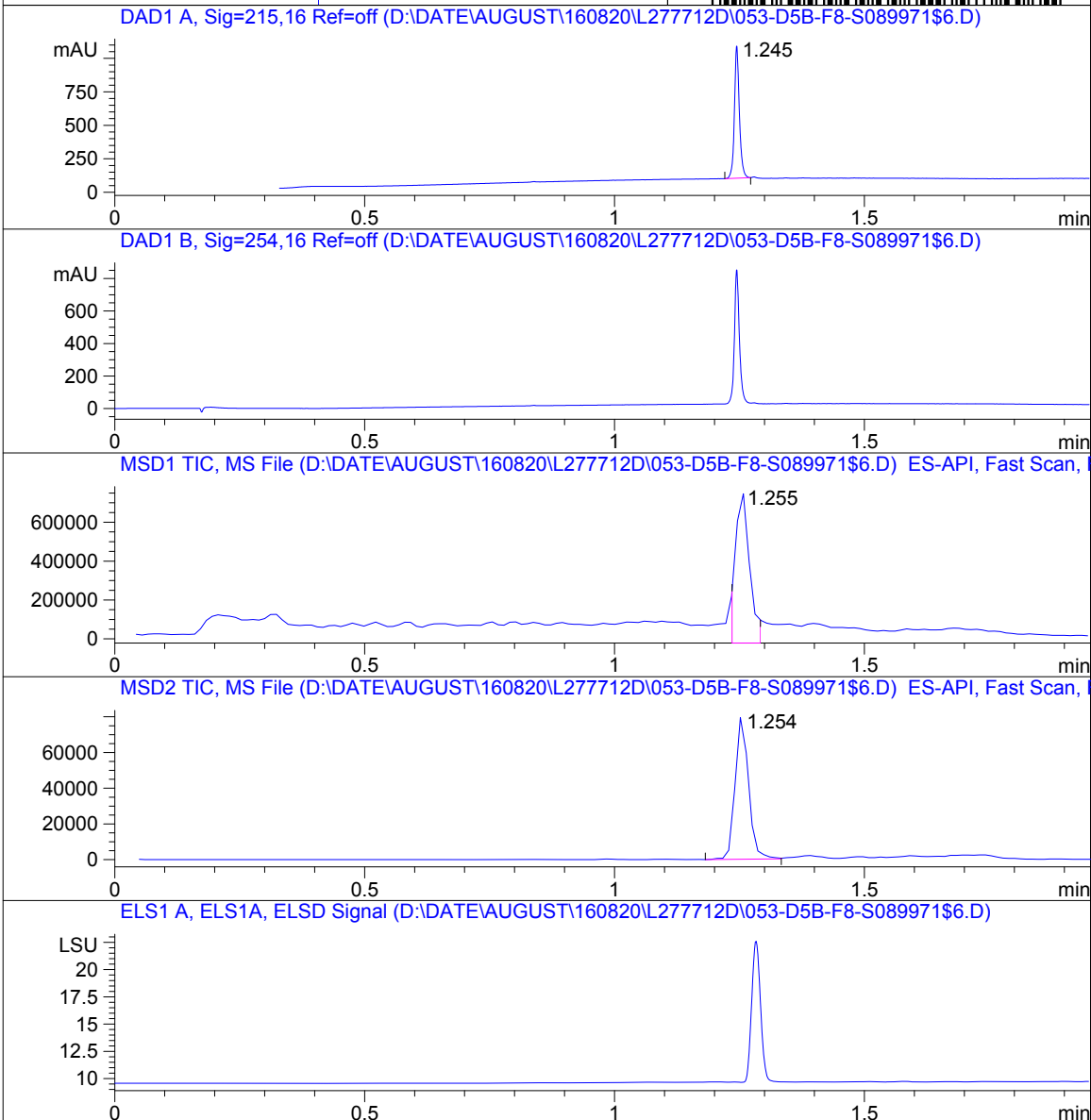
S089971\$6



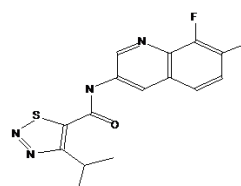
Mol Wt 334.34
Exact Mass 334.08

#	Time	Area%
1	1.245	100.00

Compound 29

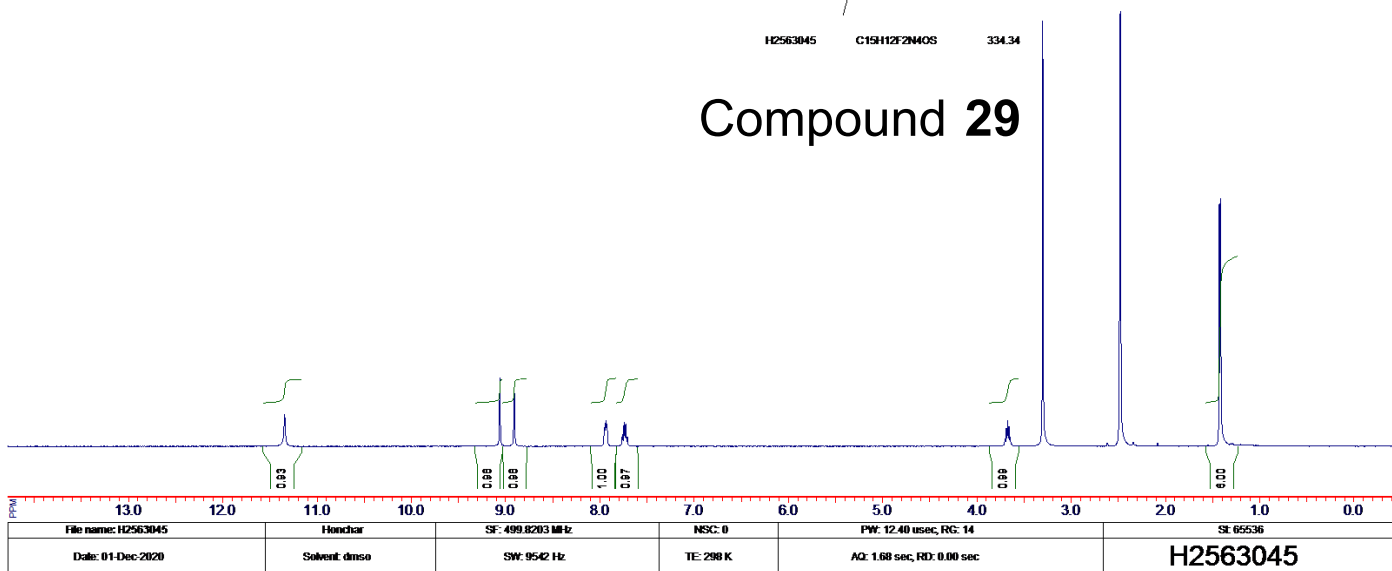


H2563045



H2563045 C15H12F2N4OS 334.34

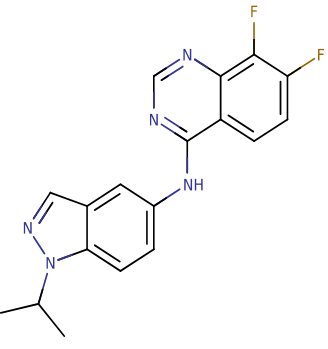
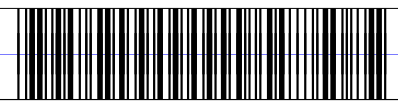
Compound 29



Compound 30

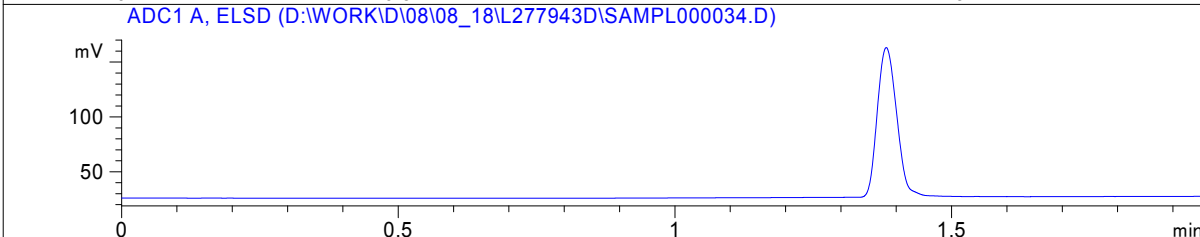
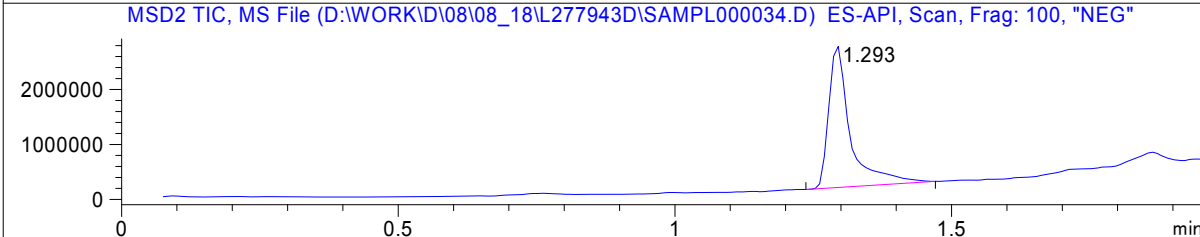
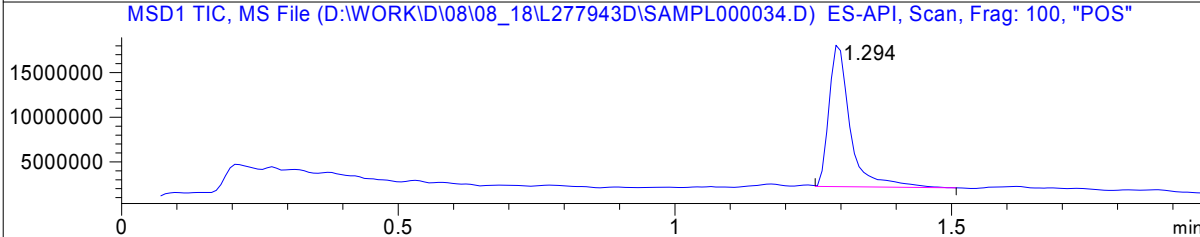
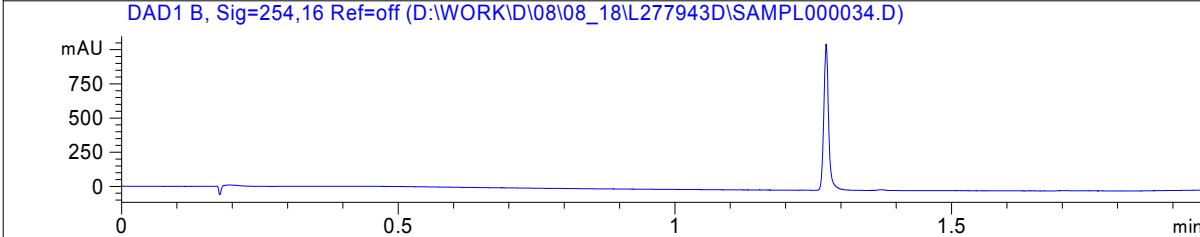
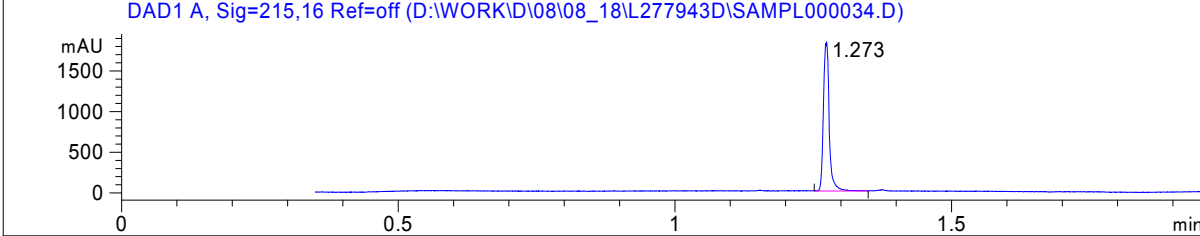
MaxPeak: 100.00%
Ret_Time: 1.273 min

S089954\$3

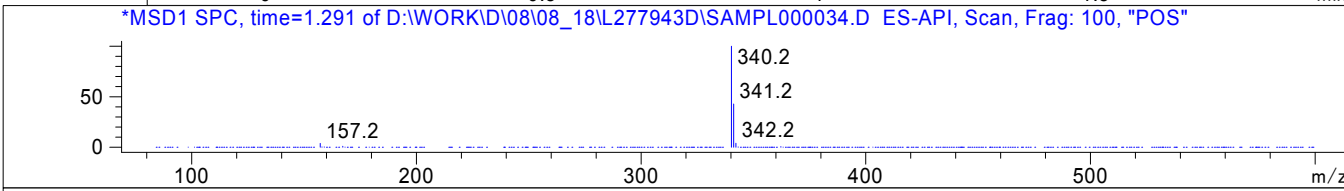


Mol Wt 339.34
Exact Mass 339.15

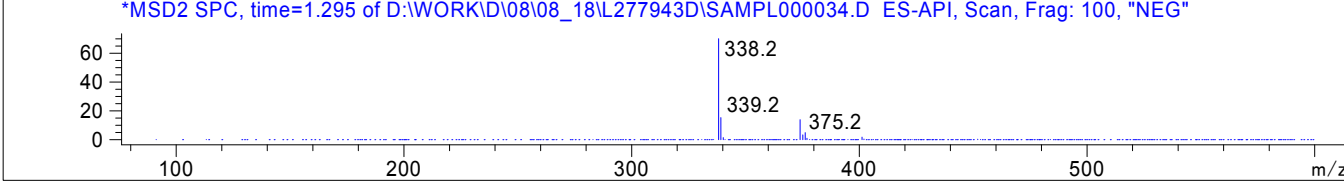
#	Time	Area%
1	1.273	100.00



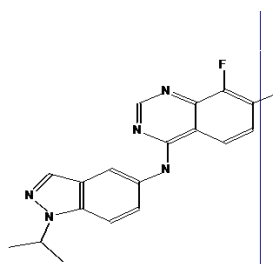
RT 1.294



RT 1.293



H2565633

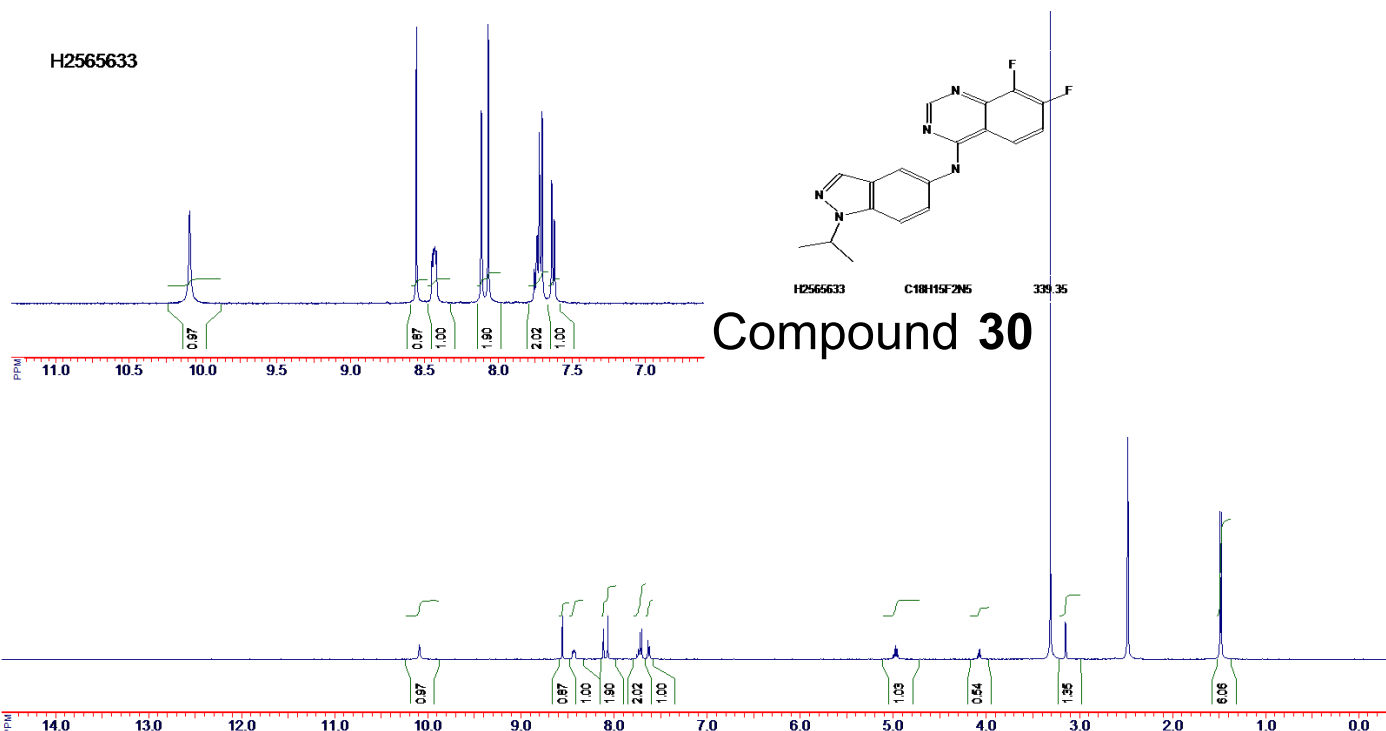


H2565633

C18H15F2N5

338.35

Compound 30



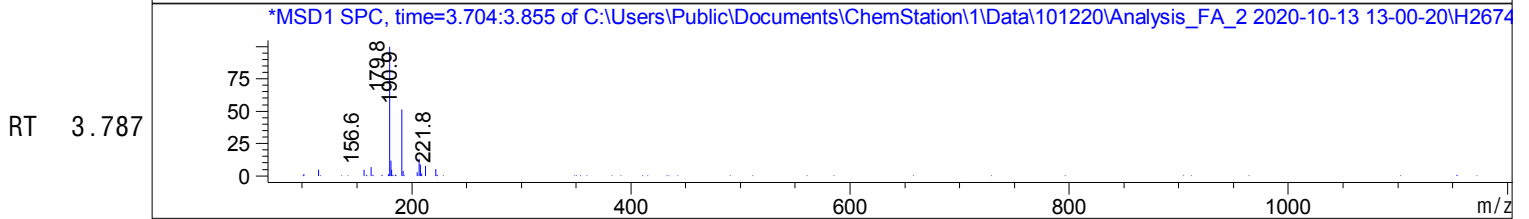
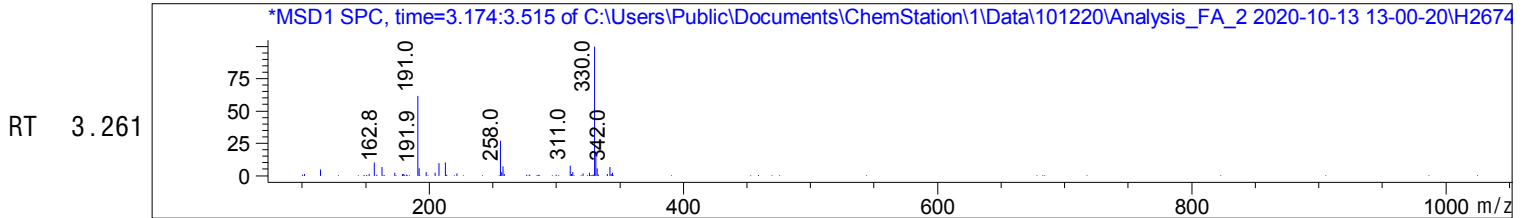
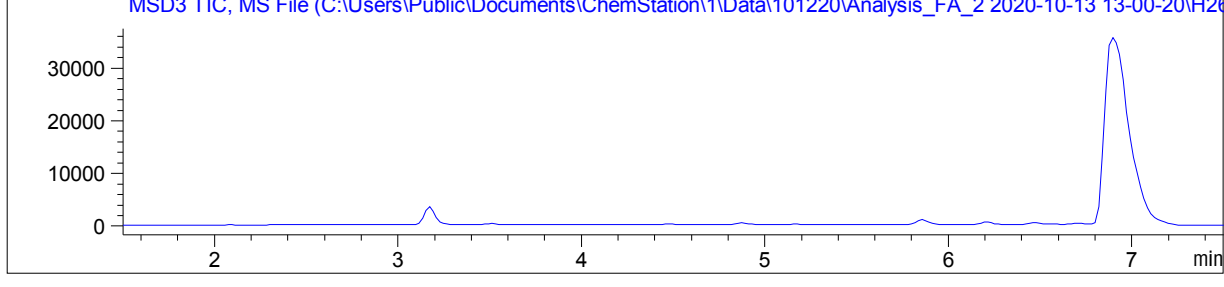
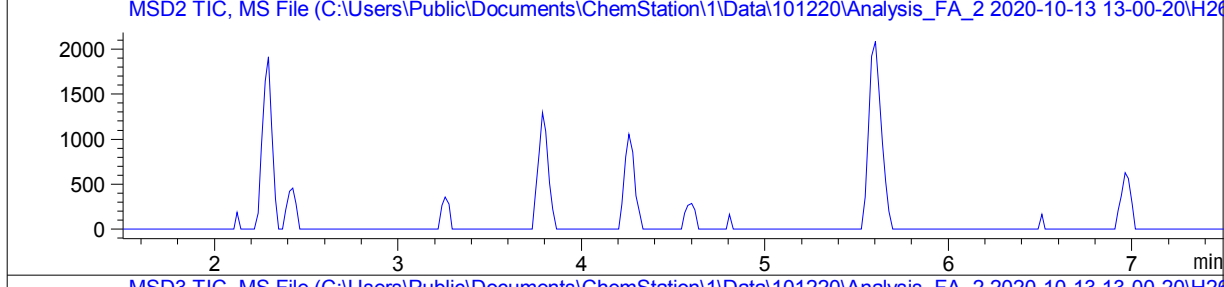
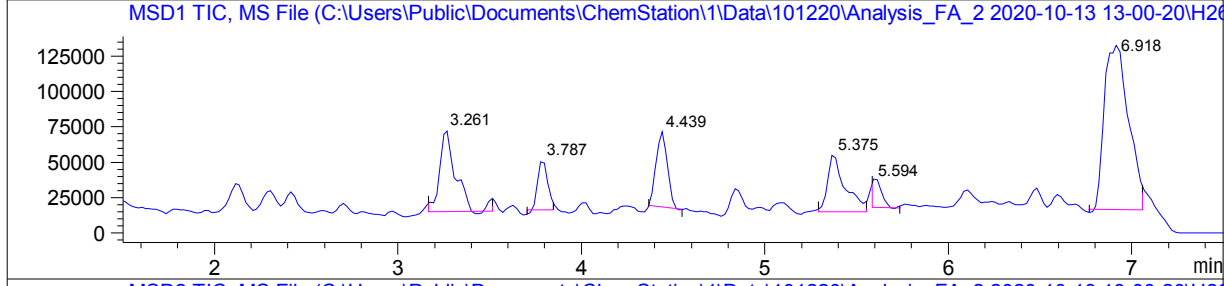
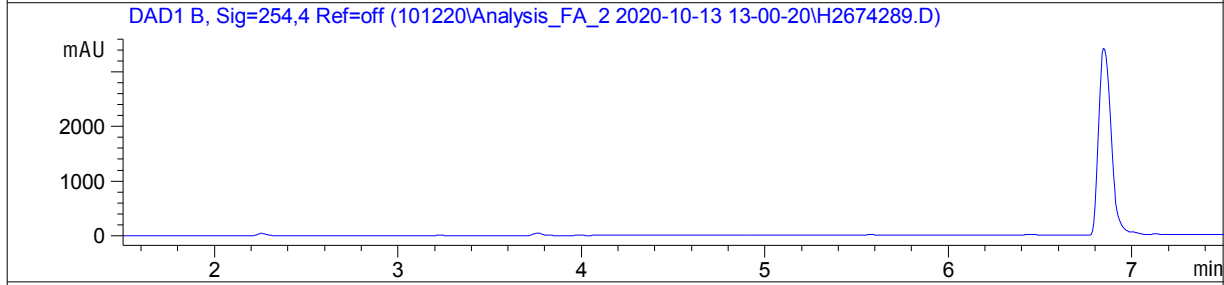
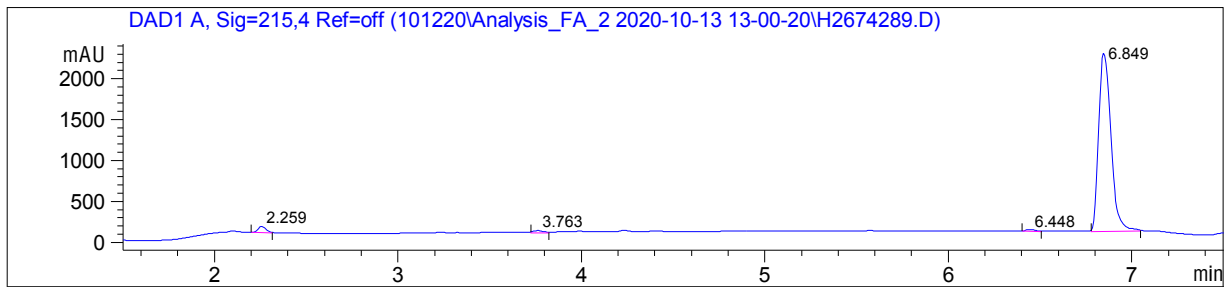
File name: H2565633	Operator: Victoria	SF: 499.0203 MHz	NSC: 0	PW: 12.40 usec, RG: 20	SI: 65536
Date: 01-Dec-2020	Solvent: dmsd	SW: 9542 Hz	TE: 298 K	AQ: 1.68 sec, RD: 0.00 sec	

Compound 31

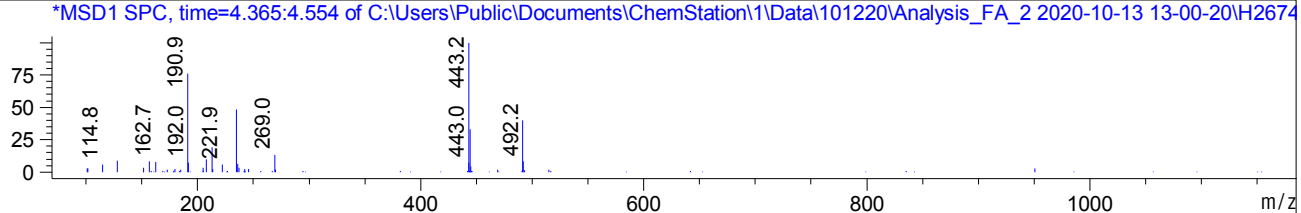
Sample
H2674289

0.1%FA-ACN 5-95%ACN 6 min. Zorbax-Eclipse-Plus C18 4,6 x
100mm, 3.5 mkm.

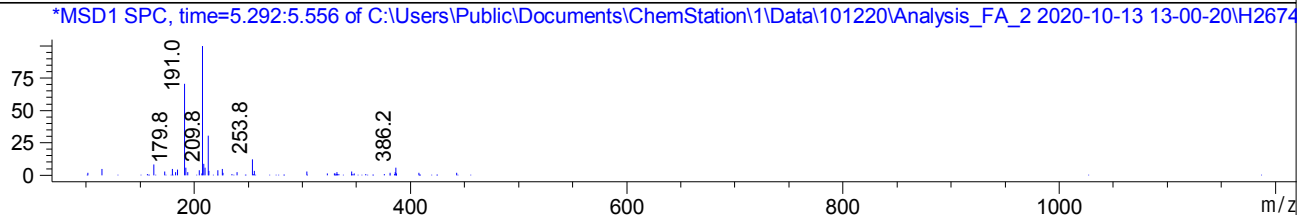
#	Time	Area%
1	2.259	2.14
2	3.763	0.89
3	6.448	0.80
4	6.849	96.18



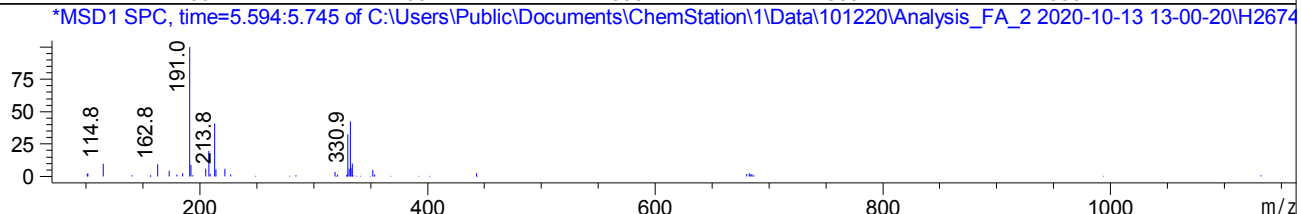
RT 4.439



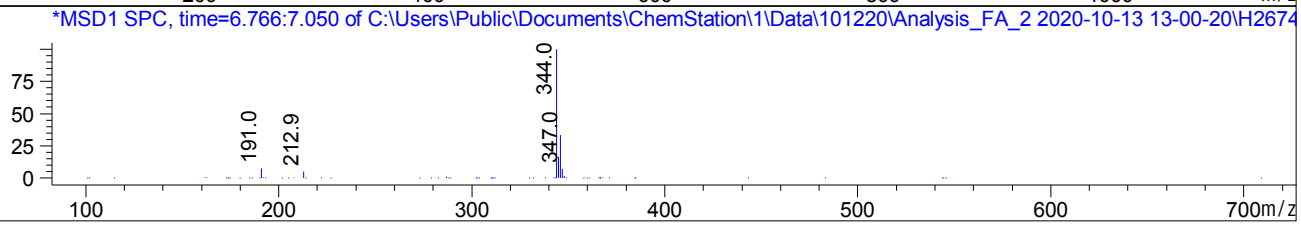
RT 5.375



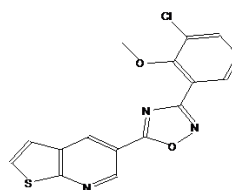
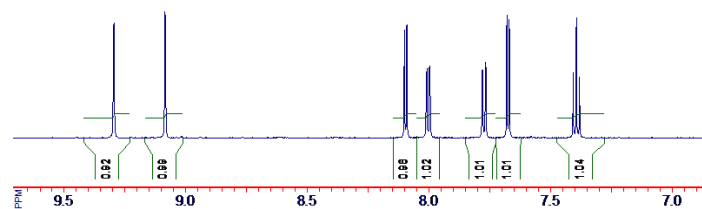
RT 5.594



RT 6.918

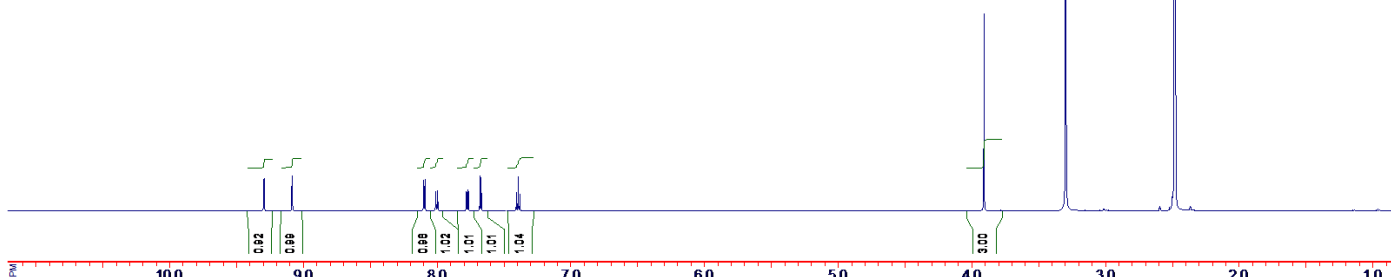


H2674289



H2674289 C16H10ClN3O2S 343.79

Compound 31

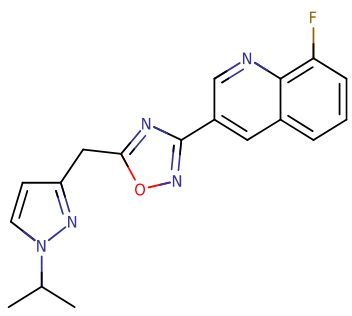
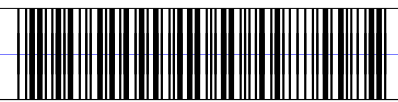


File name: H2674289	Host: Hachar	SF: 599.7811 MHz	NSC: 0	PW: 4.40 usec, RG: 44	SE 131072
Date: 26-Nov-2020	Solvent: dmso	SW: 11364 Hz	TE: 298 K	AQ: 2.82 sec, RD: 0.00 sec	H2674289

Compound 32

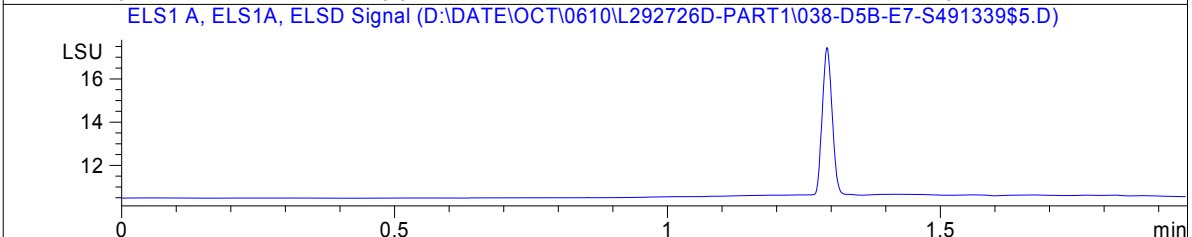
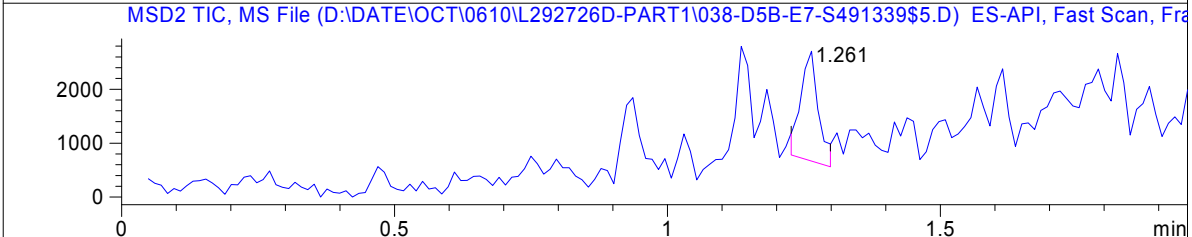
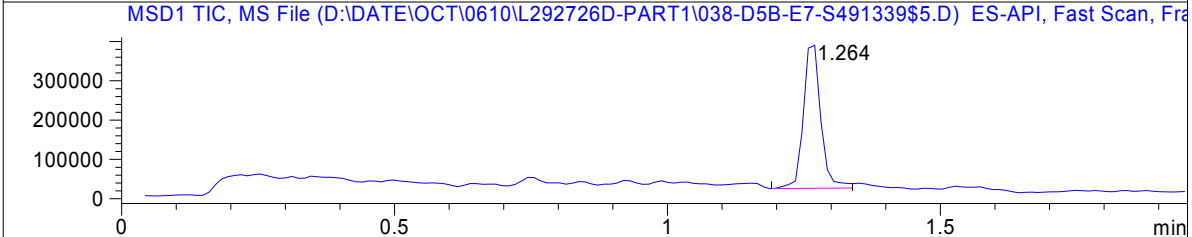
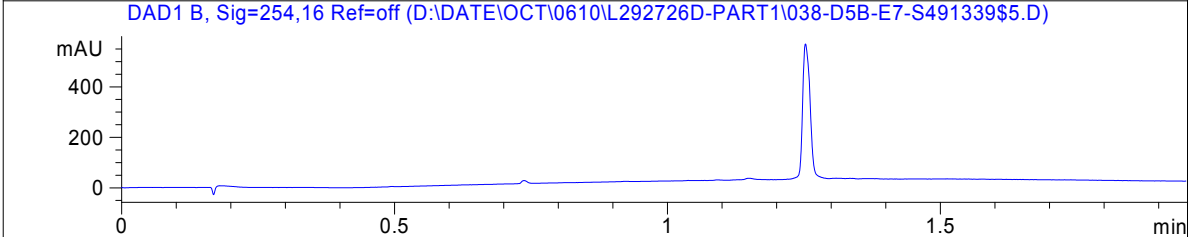
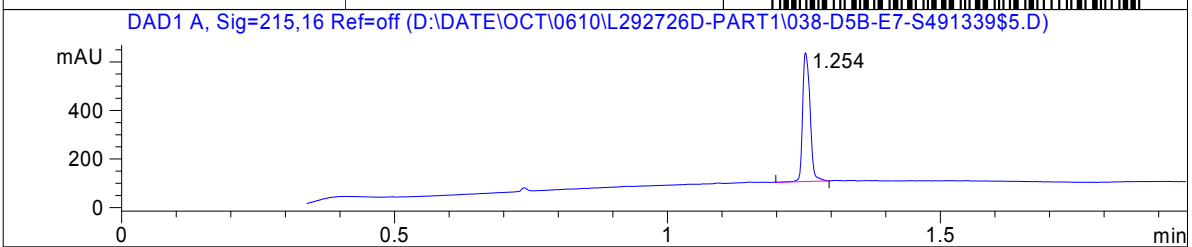
MaxPeak: 100.00%
Ret_Time: 1.254 min

S491339\$5

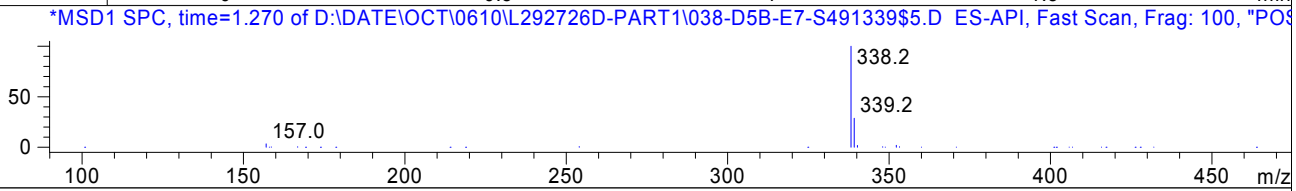


Mol Wt 337.35
Exact Mass 337.15

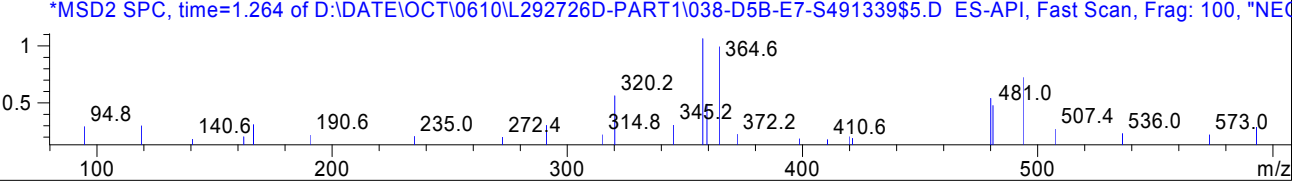
#	Time	Area%
1	1.254	100.00



RT 1.264

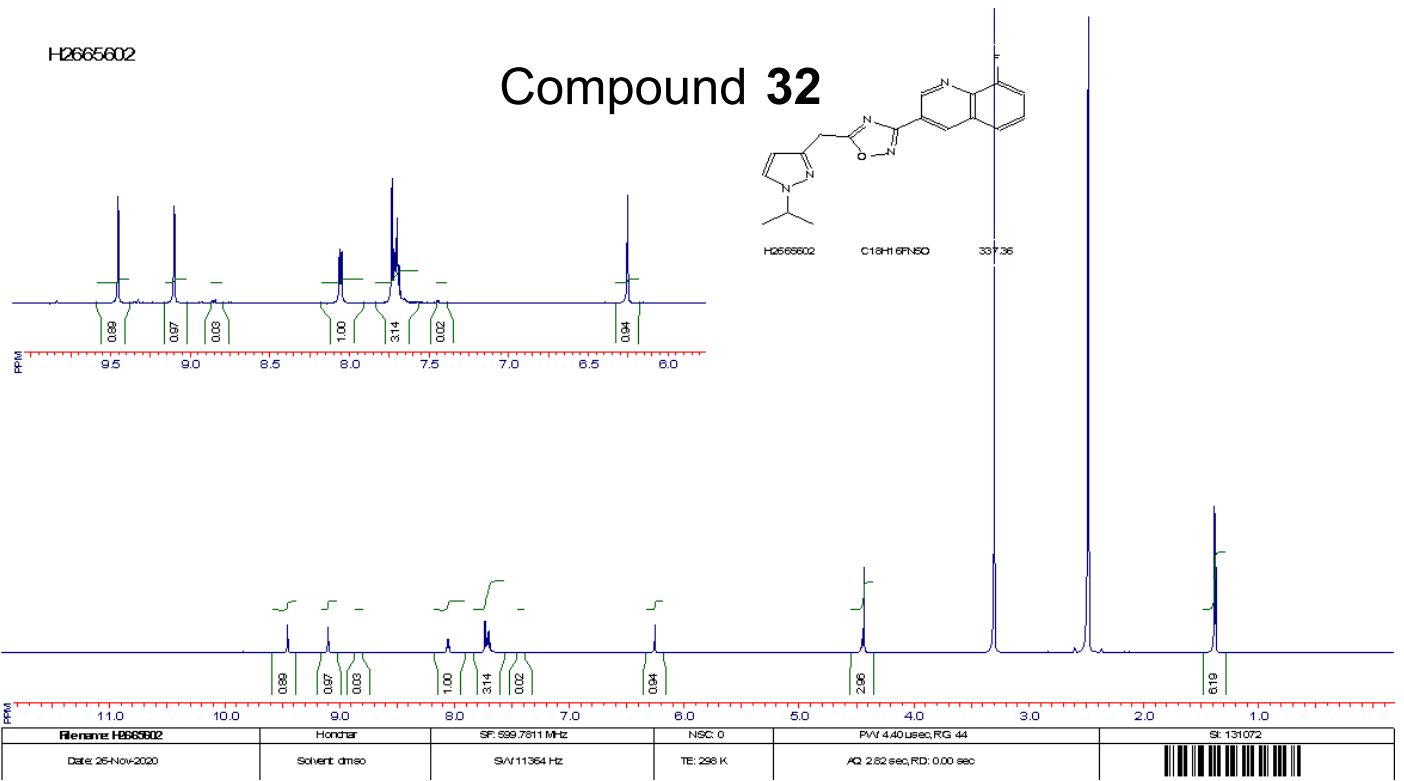
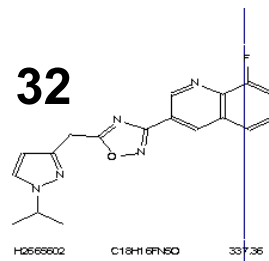



RT 1.261



H2665602

Compound 32

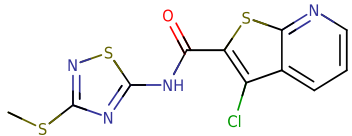
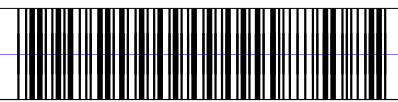


Filename: H2665602	Holder	SF: 599.7811 MHz	NSC: 0	PW: 4.40 usec, RG: 44	SI: 131072
Date: 25-Nov-2020	Solvent: dms0	SN: 11364 Hz	TE: 296 K	AQ: 2.82 sec, RD: 0.00 sec	

Compound 33

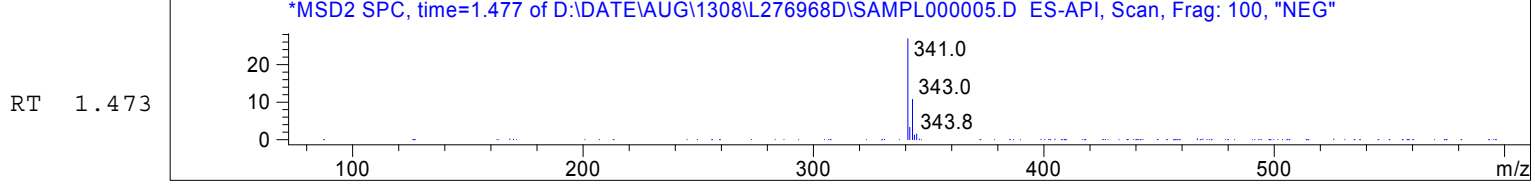
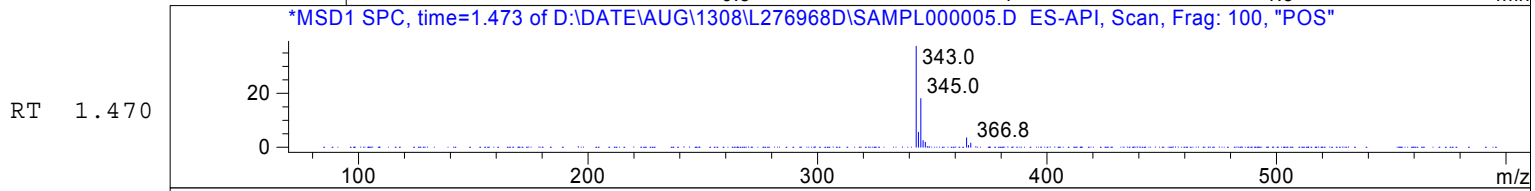
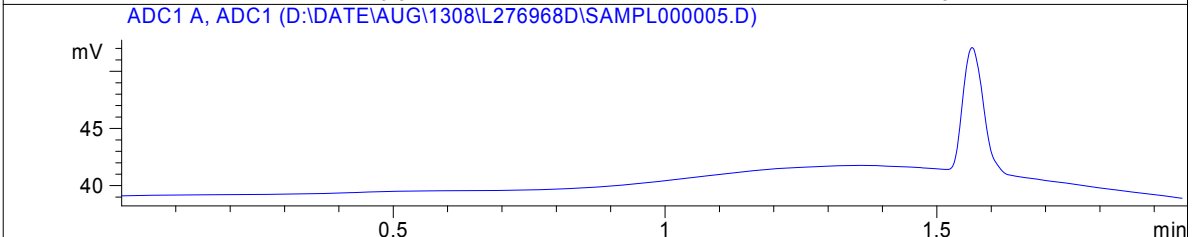
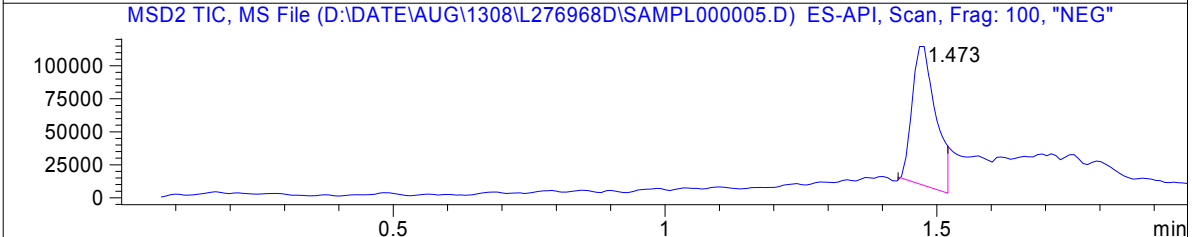
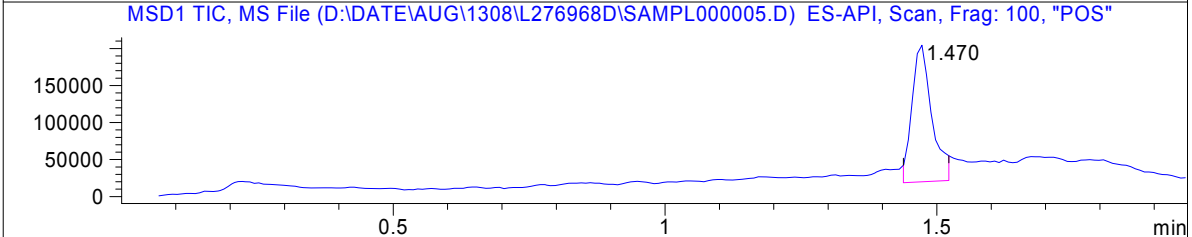
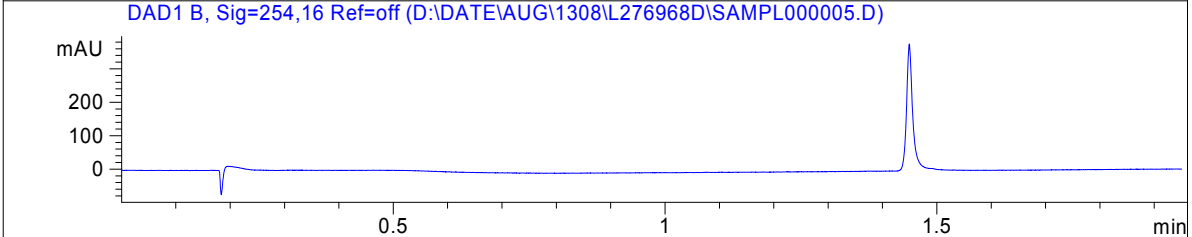
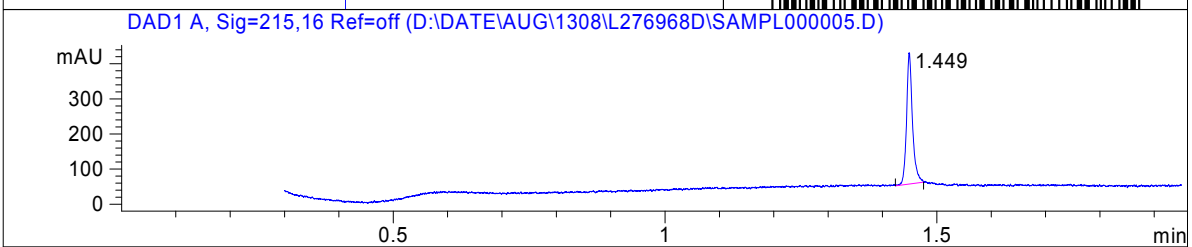
MaxPeak: 100.00%
Ret_Time: 1.449 min

S089995\$3

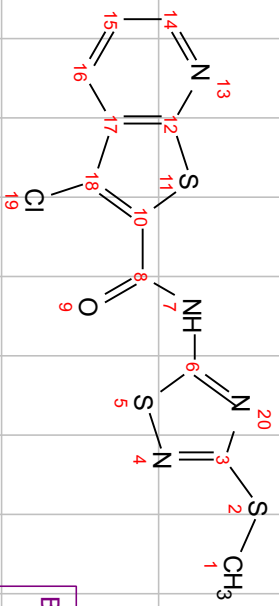


Mol Wt 342.85
Exact Mass 341.94

#	Time	Area%
1	1.449	100.00

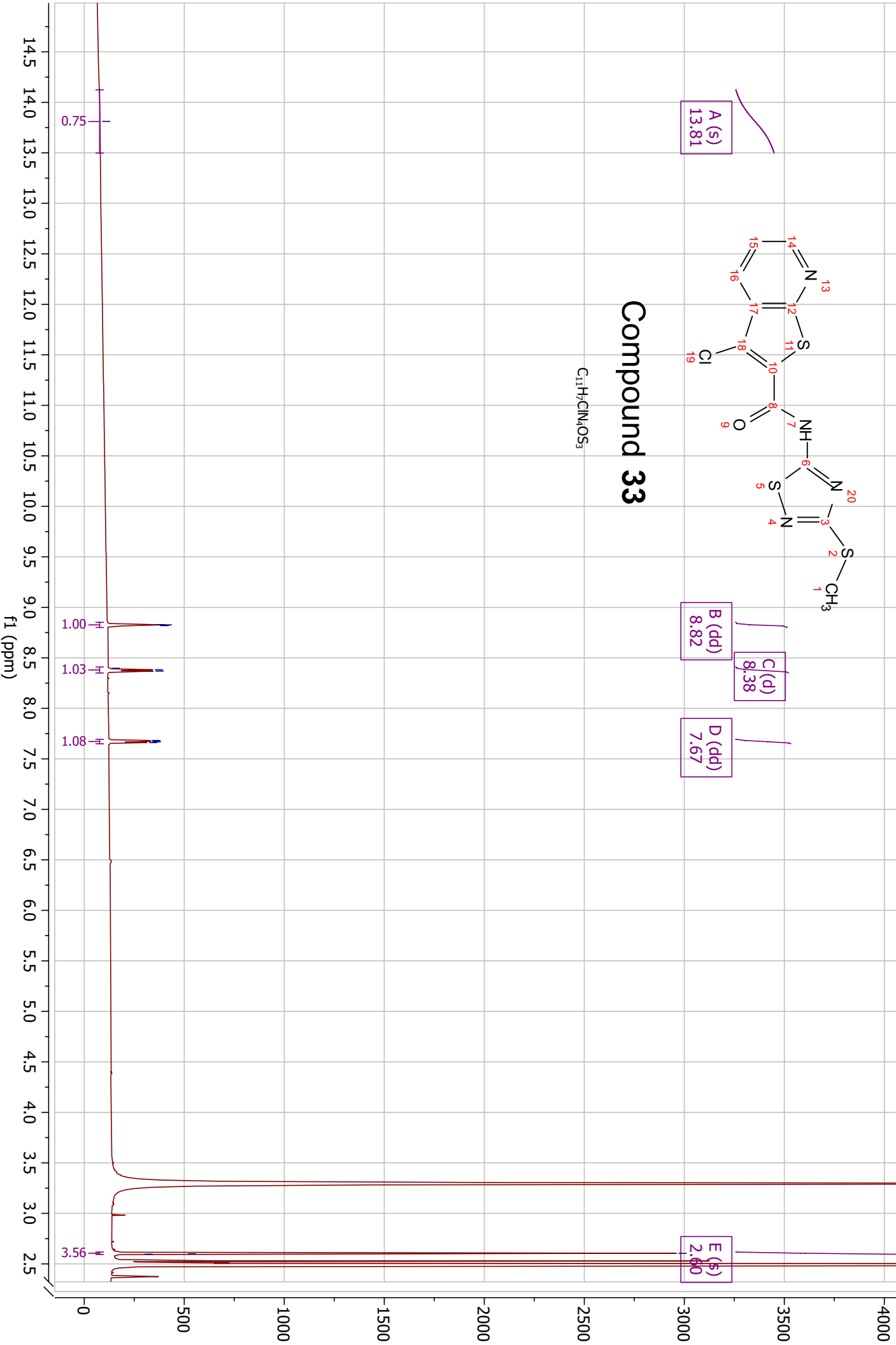


SVK-6.10.fid
SVK 6 in d6-DMSO;
1H



Compound 33

$C_{11}H_{12}ClN_4OS_3$



8.83
8.83
8.82
8.82
8.40
8.38
8.37
7.68
7.67
7.67
7.66

2.60
2.60
2.60