

# Supplementary Materials for

## Large library docking for novel SARS-CoV-2 main protease non-covalent and covalent inhibitors

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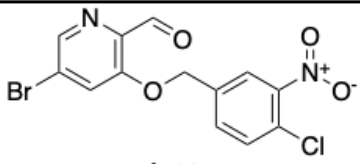
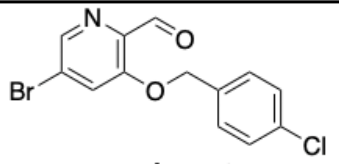
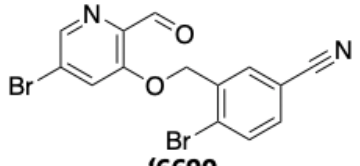
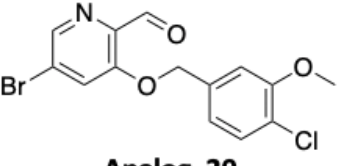
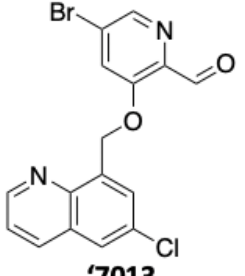
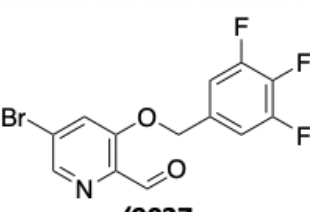
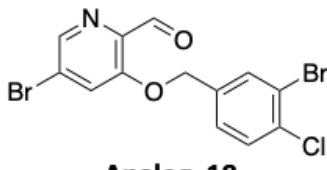
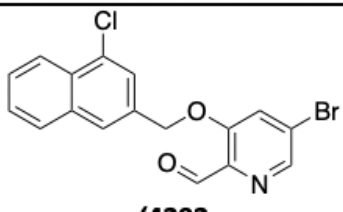
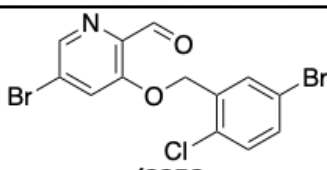
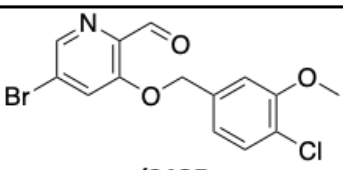
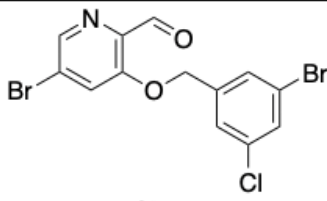
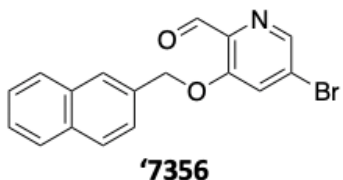
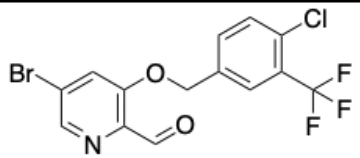
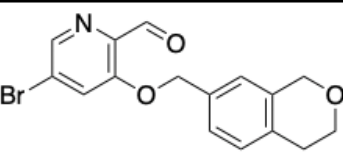
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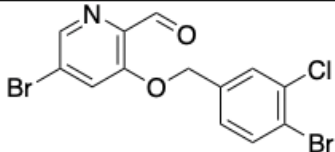
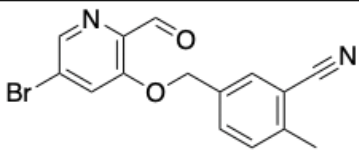
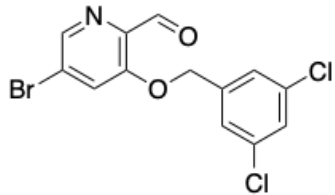
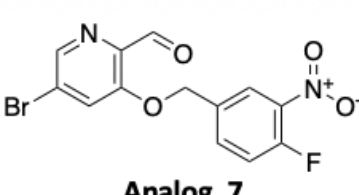
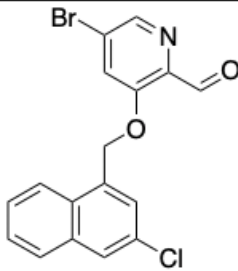
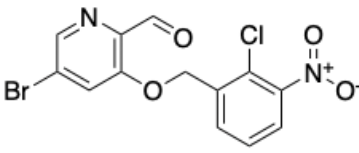
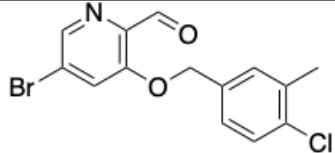
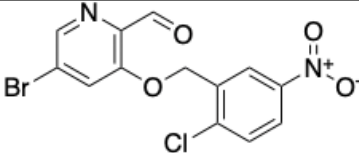
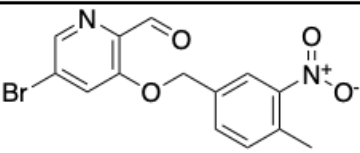
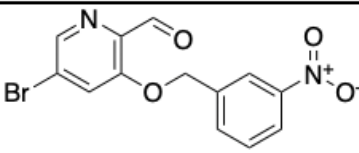
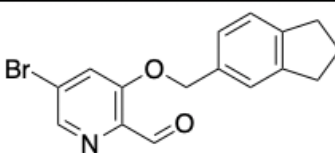
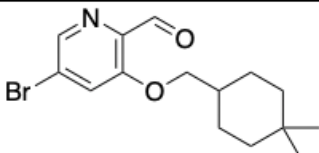
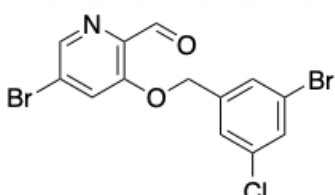
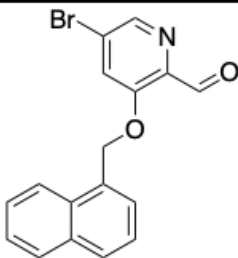
Tables S2 to S5  
Figures S1 to S12

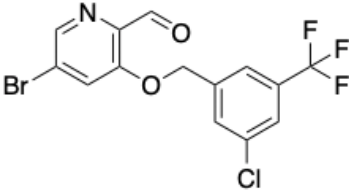
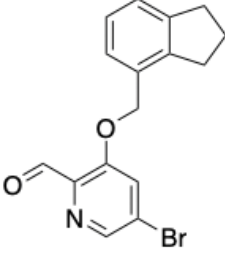
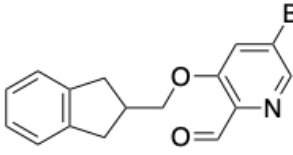
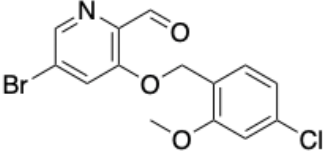
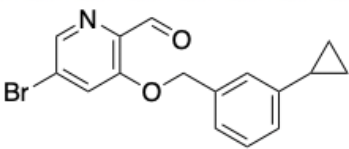
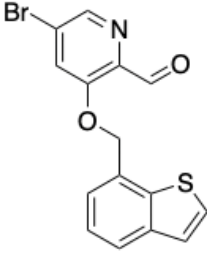
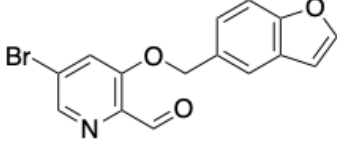
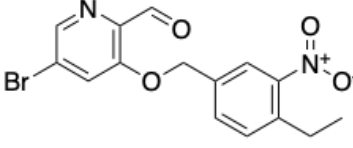
### **Other Supplementary Material for this manuscript includes the following:**

Table S1 (.xlsx)

**Supplementary Table 2. Analogs of covalent docking hit '3620 with improved potencies.**

Compound	IC50 [ $\mu$ M]	Compound	IC50 [ $\mu$ M]
 <p><b>'7021</b></p>	1	 <p><b>Analog_12</b></p>	22
 <p><b>'6690</b></p>	2	 <p><b>Analog_20</b></p>	22
 <p><b>'7013</b></p>	5	 <p><b>'9037</b></p>	23
 <p><b>Analog_18</b></p>	6	 <p><b>'4202</b></p>	24
 <p><b>'8252</b></p>	6	 <p><b>'9125</b></p>	25
 <p><b>'6117</b></p>	7	 <p><b>'7356</b></p>	26
 <p><b>Analog_19</b></p>	9	 <p><b>'8474</b></p>	27

 <p><b>'4217</b></p>	9	 <p><b>'0481</b></p>	27
 <p><b>'9033</b></p>	9	 <p><b>Analog_7</b></p>	28
 <p><b>'9122</b></p>	9	 <p><b>Analog_8</b></p>	33
 <p><b>Analog_17</b></p>	11	 <p><b>Analog_10</b></p>	34
 <p><b>Analog_6</b></p>	12	 <p><b>Analog_11</b></p>	35
 <p><b>Analog_49</b></p>	13	 <p><b>'9009</b></p>	38
 <p><b>'0156</b></p>	14	 <p><b>'3251</b></p>	40

 <p><b>'9028</b></p>	14	 <p><b>'3250</b></p>	40
 <p><b>'4221</b></p>	19	 <p><b>Analog_21</b></p>	43
 <p><b>'3264</b></p>	20	 <p><b>'3252</b></p>	45
 <p><b>'4212</b></p>	20	 <p><b>'3564</b></p>	48

**Supplementary Table 3. Antiviral activities.**

Compound	Antiviral IC <sub>50</sub> <sup>a</sup> [μM]	Antiviral IC <sub>90</sub> <sup>a</sup> [μM]	CC <sub>10</sub> <sup>b</sup> [μM]
<b>'7021</b>	6.2	7.3	8.03
<b>'7356</b>	19.53	19.9	6.93

<sup>a</sup> Efficacy in RT-qPCR viral infectivity assay in X cells.

<sup>b</sup> Reduction in cell viability (cytotoxicity).

**Supplementary Table 4. Pan-viral enzymatic activities of '7021.**

Viral M <sup>Pro</sup>	IC50 [ $\mu$ M]
MERS	50
SARS-CoV-1	8
SARS-CoV-2	1

**Supplementary Table 5. Crystallographic statistics.**

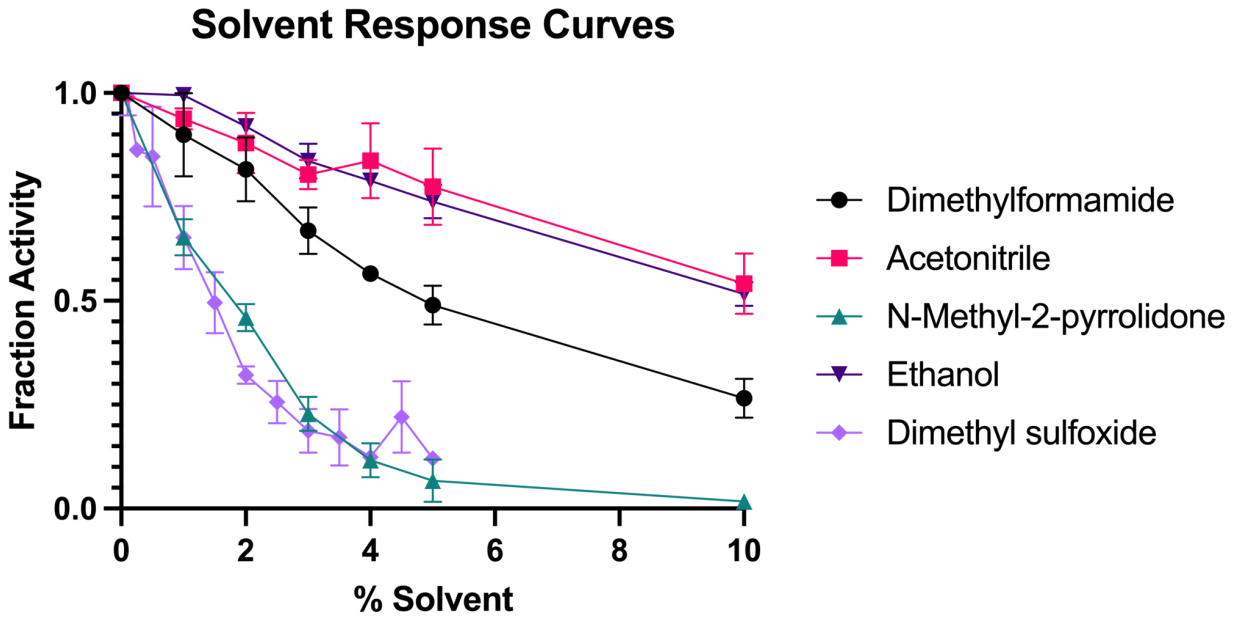
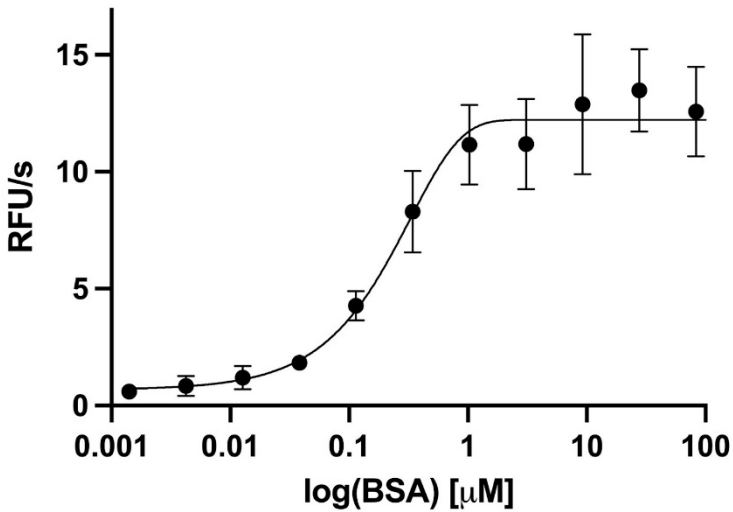
Ligand	'5548	'7356	'6111	SG-0001	'9121	'7021	'8252	'9218
PDB ID	8DIG	8DIF	8DIH	8DII	8DIC	8DIB	8DID	8DIE
Resolution range (Å)	72.62 - 2.45 (2.538 - 2.45)	48.44 - 1.98 (2.051 - 1.98)	44.39 - 2.12 (2.196 - 2.12)	48.6 - 2.59 (2.683 - 2.59)	38.13 - 2.09 (2.165 - 2.09)	38.73 - 2.17 (2.248 - 2.17)	38.22 - 1.95 (2.02 - 1.95)	38.64 - 1.9 (1.968 - 1.9)
Space group	P 21 21 21	P 1 21 1	C 1 2 1	I 1 2 1	P 1 21 1	P 1 21 1	P 1 21 1	P 1 21 1
a, b, c (Å)	67.779, 102.704, 102.704	44.897, 53.624, 115.04	114.102, 53.917, 45.258	45.041, 53.835, 115.11	44.346, 53.814, 115.824	44.911, 53.72, 115.527	44.238, 53.666, 115.632	44.923, 53.751, 115.119
a, b, c (°)	90, 90, 90	90, 101.151, 90	90, 101.253, 90	90, 101.13, 90	90, 100.459, 90	90, 100.833, 90	90, 100.938, 90	90, 101.062, 90
Total reflections	52786 (4222)	74588 (6993)	29895 (2343)	17080 (1724)	63019 (6332)	56799 (5689)	76834 (7688)	83998 (8382)
Unique reflections	26433 (2151)	37368 (3516)	14998 (1188)	8552 (864)	31556 (3170)	28435 (2848)	38463 (3848)	42036 (4194)
Multiplicity	2.0 (2.0)	2.0 (2.0)	2.0 (2.0)	2.0 (2.0)	2.0 (2.0)	2.0 (2.0)	2.0 (2.0)	2.0 (2.0)
Completeness (%)	97.69 (80.05)	99.03 (92.87)	96.99 (77.24)	99.74 (99.77)	98.17 (98.84)	98.18 (98.41)	98.14 (98.54)	94.67 (79.45)
Mean I/sigma(I)	10.82 (1.33)	13.42 (1.00)	19.51 (1.83)	8.81 (0.84)	8.94 (0.98)	8.68 (0.89)	7.58 (0.98)	4.57 (0.59)
Wilson B-factor	44.04	36.71	48.65	56.27	39.01	40.42	30.04	33.18
R-merge	0.05895 (0.6349)	0.0362 (0.8374)	0.01881 (0.4432)	0.06999 (0.9217)	0.05198 (0.7831)	0.05847 (0.8779)	0.05816 (0.7736)	0.1022 (1.824)
R-meas	0.08337 (0.8979)	0.0512 (1.184)	0.0266 (0.6267)	0.09899 (1.304)	0.07351 (1.107)	0.08269 (1.242)	0.08226 (1.094)	0.1446 (2.579)
R-pim	0.05895 (0.6349)	0.0362 (0.8374)	0.01881 (0.4432)	0.06999 (0.9217)	0.05198 (0.7831)	0.05847 (0.8779)	0.05816 (0.7736)	0.1022 (1.824)
CC1/2	0.997 (0.513)	1 (0.41)	1 (0.625)	0.995 (0.333)	0.999 (0.474)	0.998 (0.397)	0.998 (0.513)	0.993 (0.201)
CC*	0.999 (0.823)	1 (0.763)	1 (0.877)	0.999 (0.707)	1 (0.802)	1 (0.754)	1 (0.823)	0.998 (0.579)
<b>Refinement</b>								
Reflections used in refinement	26397 (2118)	37312 (3502)	14996 (1188)	8548 (862)	31513 (3163)	28394 (2844)	38390 (3844)	40479 (3371)
Reflections used for R-free	1317 (116)	1835 (176)	723 (54)	419 (45)	1615 (173)	1341 (143)	1894 (224)	2128 (174)
R-work	0.2138 (0.3321)	0.2432 (0.3608)	0.2114 (0.3256)	0.2164 (0.3640)	0.2275 (0.3419)	0.2267 (0.3265)	0.2574 (0.3563)	0.2534 (0.3559)
R-free	0.2717 (0.3771)	0.2955 (0.3532)	0.2760 (0.3358)	0.2672 (0.3837)	0.2764 (0.3772)	0.2814 (0.3331)	0.2915 (0.4119)	0.3032 (0.3935)
CC(work)	0.954 (0.748)	0.957 (0.639)	0.964 (0.698)	0.957 (0.515)	0.959 (0.639)	0.962 (0.651)	0.954 (0.698)	0.953 (0.502)
CC(free)	0.922 (0.479)	0.953 (0.613)	0.963 (0.738)	0.947 (0.420)	0.932 (0.465)	0.955 (0.574)	0.948 (0.514)	0.916 (0.400)
Number of non-hydrogen atoms	4589	4365	2317	2347	4502	4579	4531	4604
macromolecules	4540	4269	2267	2310	4433	4506	4413	4509
ligands	25	42	25	25	38	42	38	42
solvent	24	54	25	12	31	31	80	53
Protein residues	601	585	303	303	599	599	591	605
RMS(bonds)	0.008	0.01	0.008	0.002	0.009	0.004	0.015	0.009
RMS(angles)	0.94	0.99	1.01	0.57	0.98	0.7	1.14	0.92
Ramachandran favored (%)	94.76	97.68	96.62	96.66	97.23	98.11	97.33	97.45
Ramachandran allowed (%)	5.24	2.32	3.38	3.34	2.6	1.72	2.49	2.38
Ramachandran outliers (%)	0	0	0	0	0.17	0.17	0.18	0.17
Rotamer outliers (%)	0	0.23	0	0	0.43	0	0.21	0
Clashscore	7.5	3.99	4.71	5.48	6.71	3.84	8.22	5.1



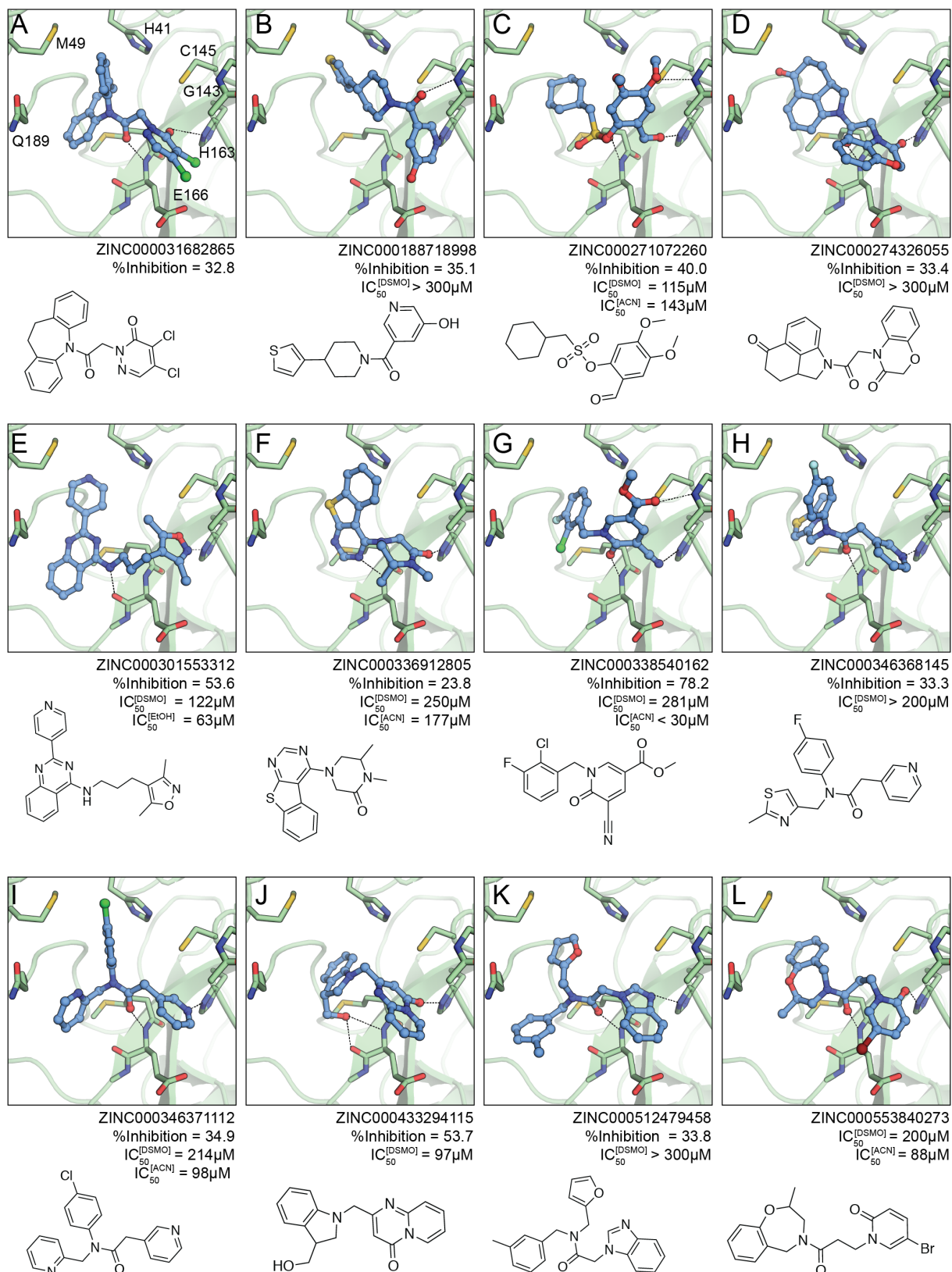
Average B-factor	49.4	40.26	56.53	63.66	44.1	48.58	33.91	37.93
macromolecules	49.35	40.11	56.35	63.09	43.98	48.12	33.78	37.84
ligands	60.21	54.15	73.4	122.98	61.63	99.97	55.66	50.55
solvent	48.32	41.14	55.62	49.68	39.64	46.39	30.93	35.8

(One crystal for each structure)

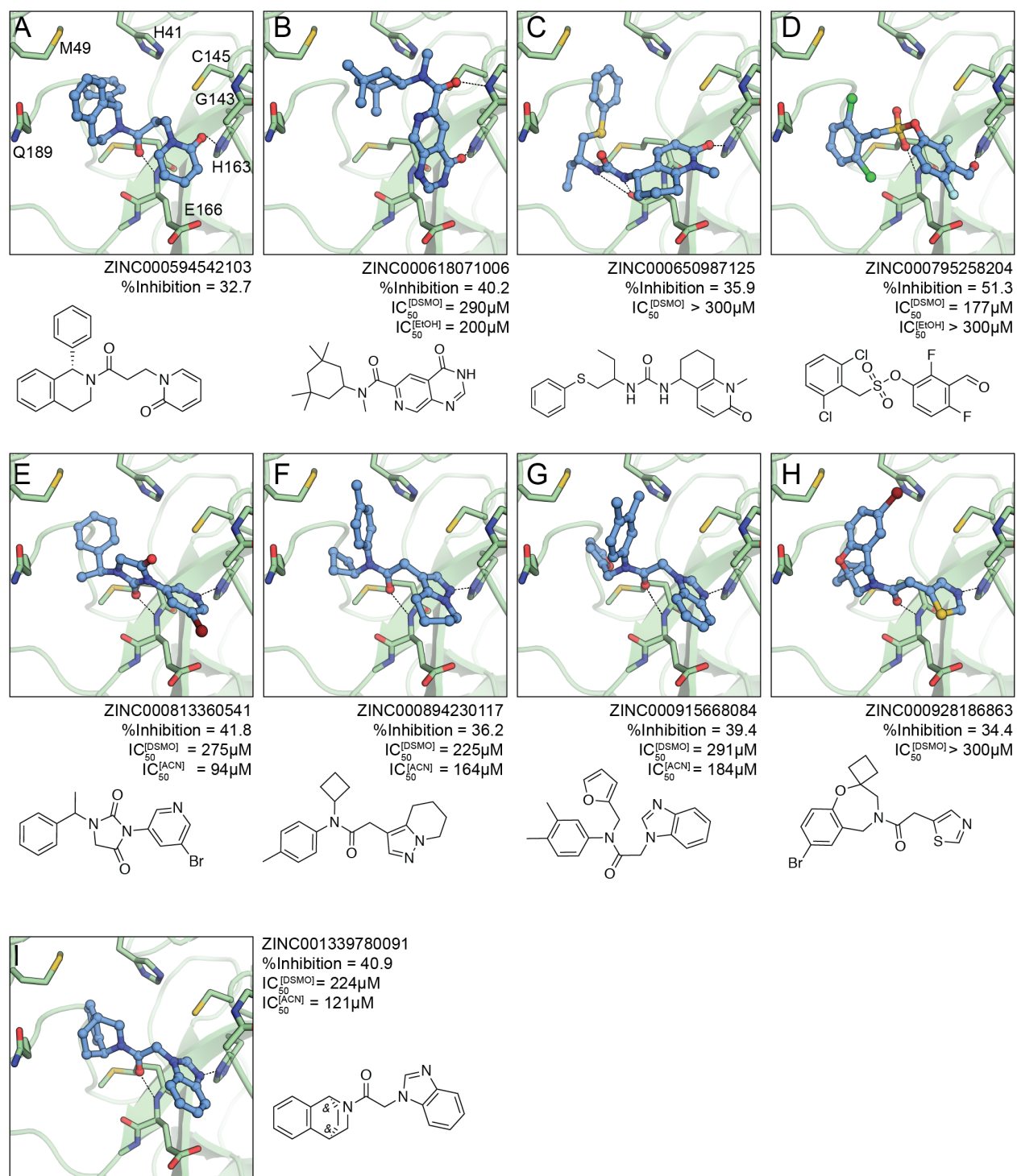
\* Values in parentheses are for the highest-resolution shell.

**A****B**

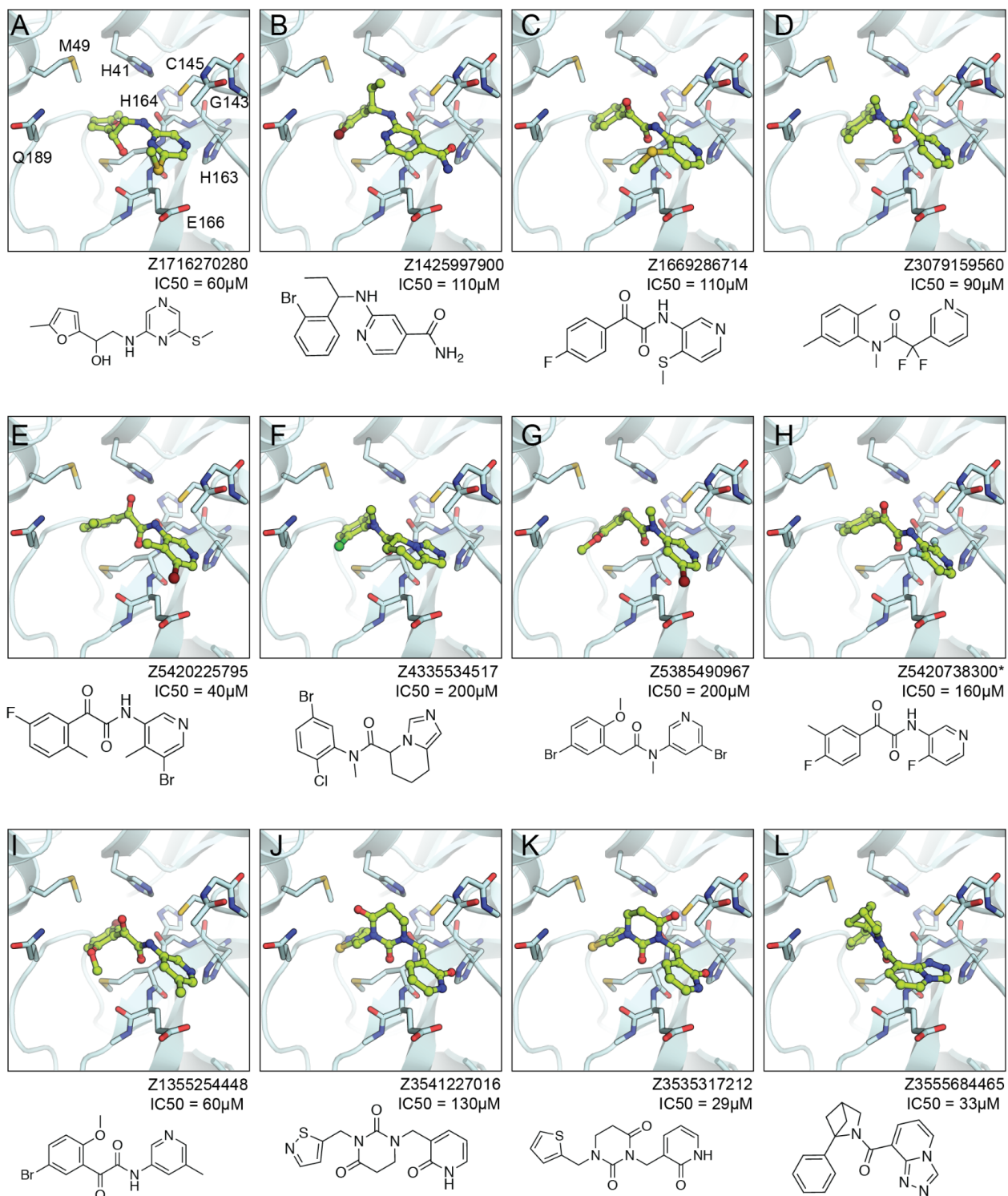
**Supplementary Figure 1. Assay optimization for solvent and detergent. (A)** The effect of solvents on enzymatic activity of M<sup>Pro</sup>. **(B)** Activity loss from removal of detergent rescued with addition of BSA.



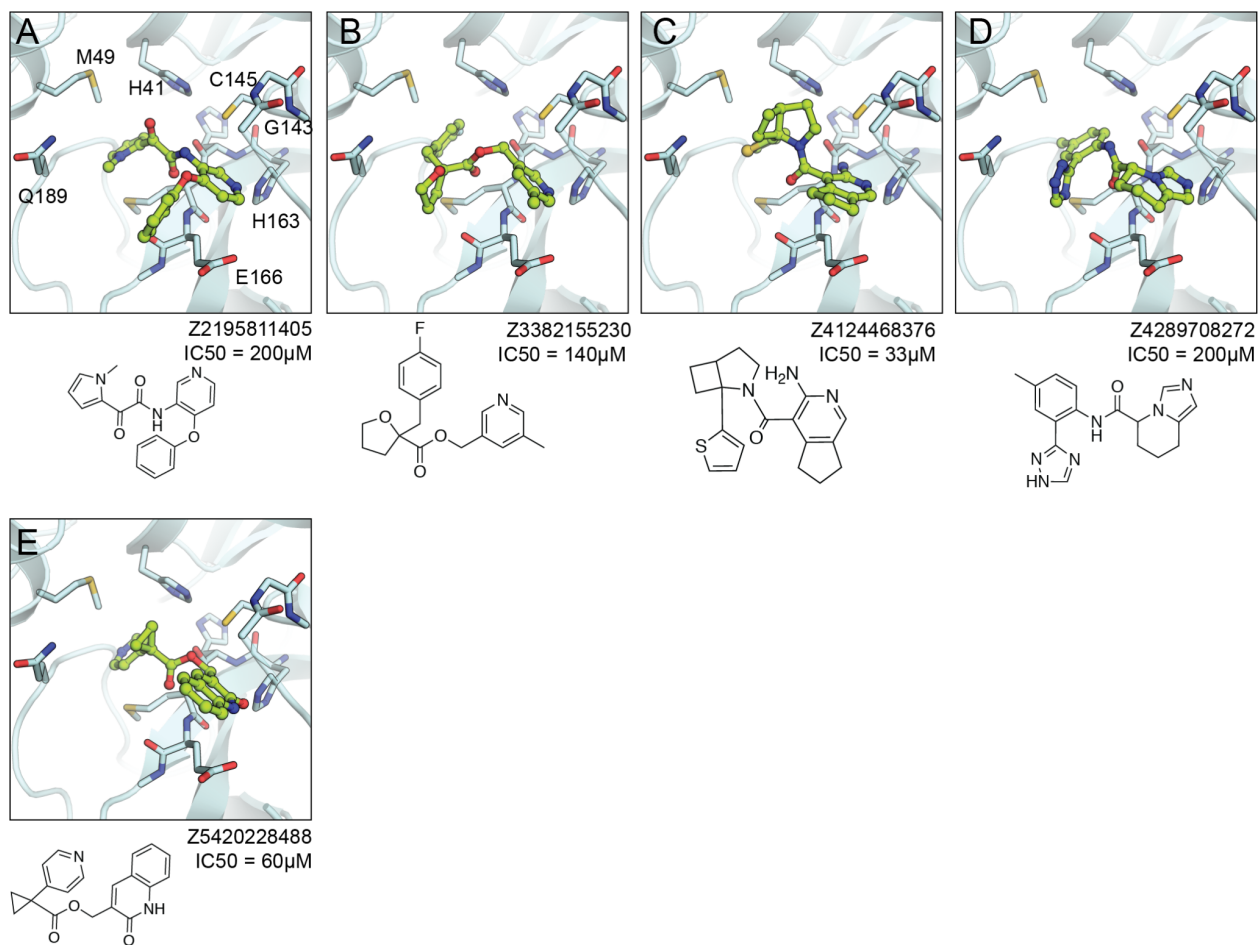
**Supplementary Figure 2.1 Non-covalent docking hits or compounds with >30% inhibition from first virtual screen.**



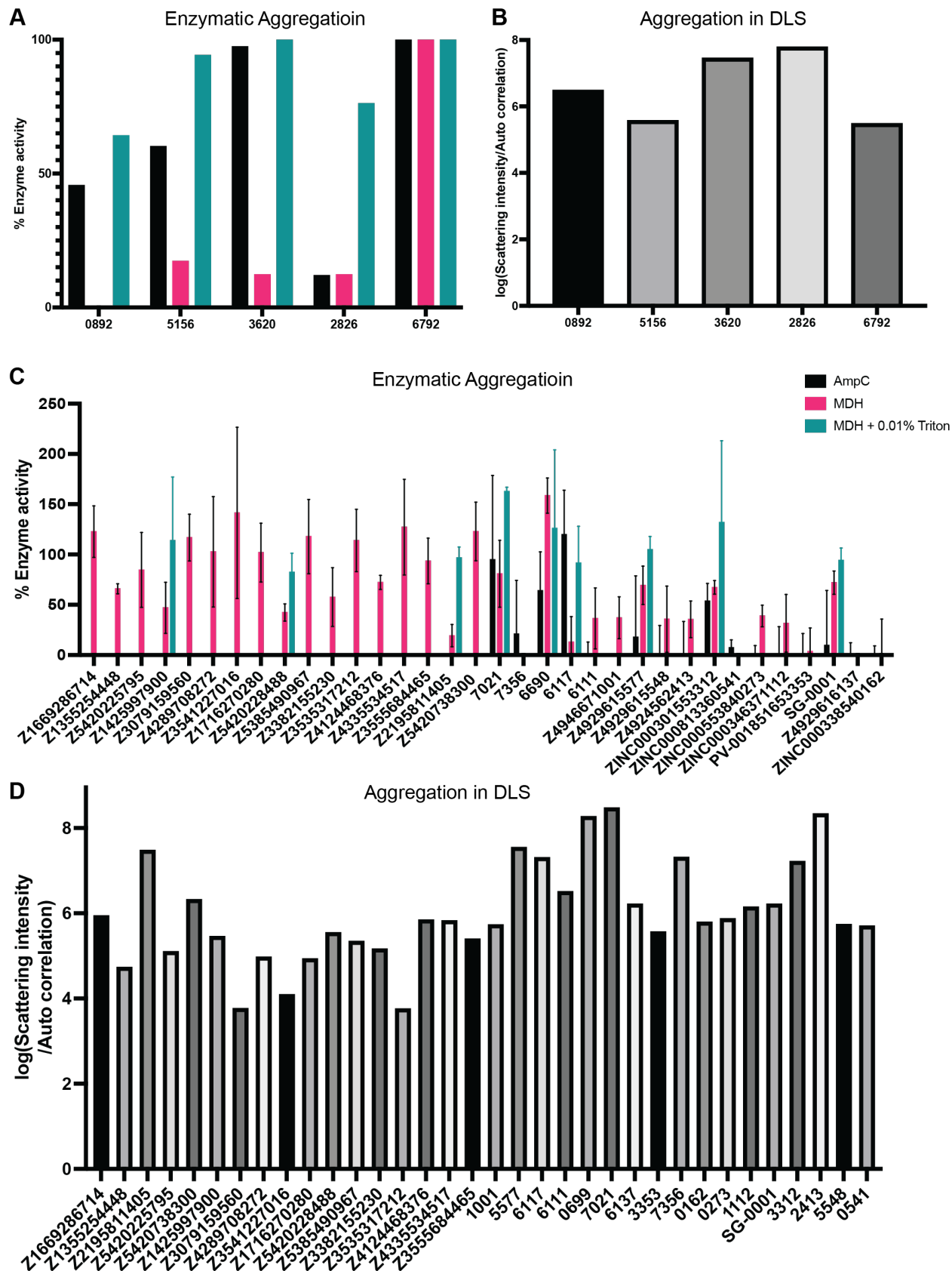
**Supplementary Figure 2.2 Non-covalent docking hits or compounds with >30% inhibition from first virtual screen.**



**Supplementary Figure 2.3 Non-covalent docking hits from second virtual screen.**

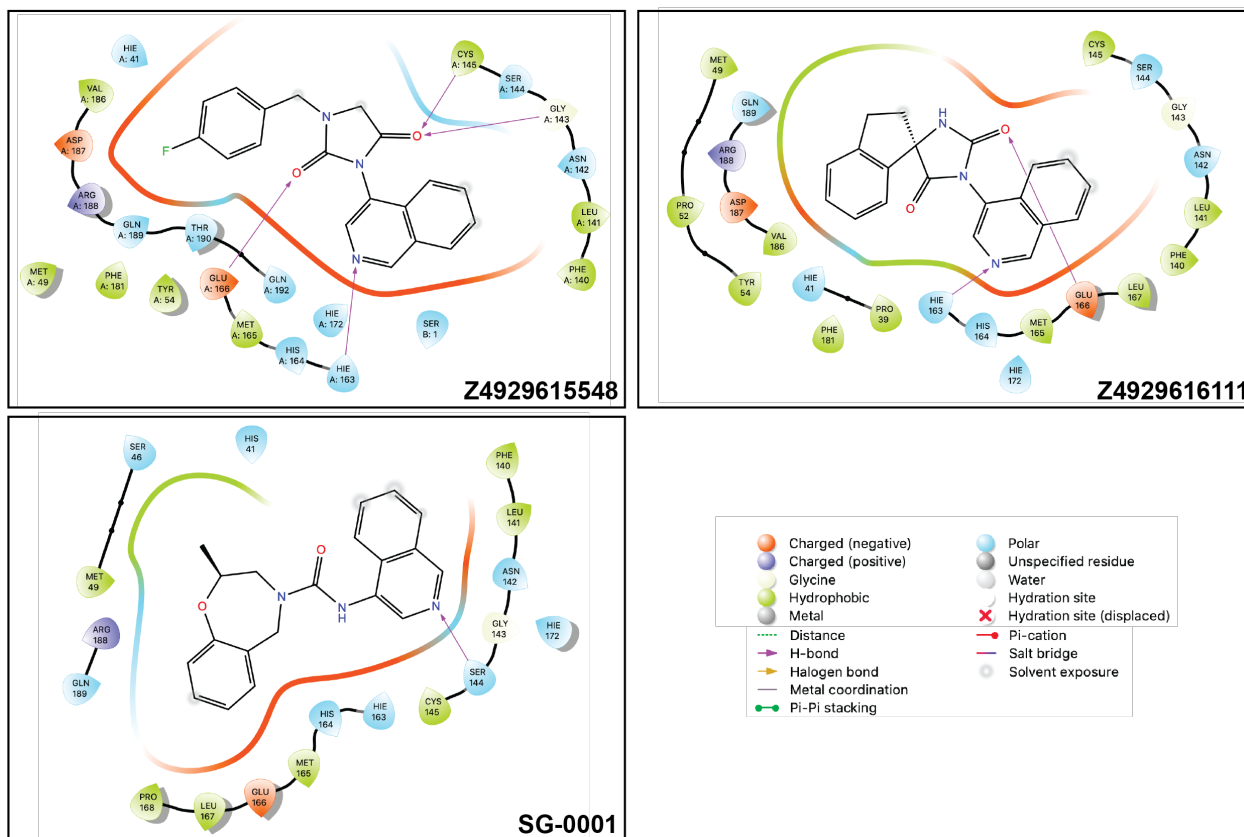


**Supplementary Figure 2.4 Non-covalent docking hits from second virtual screen.**

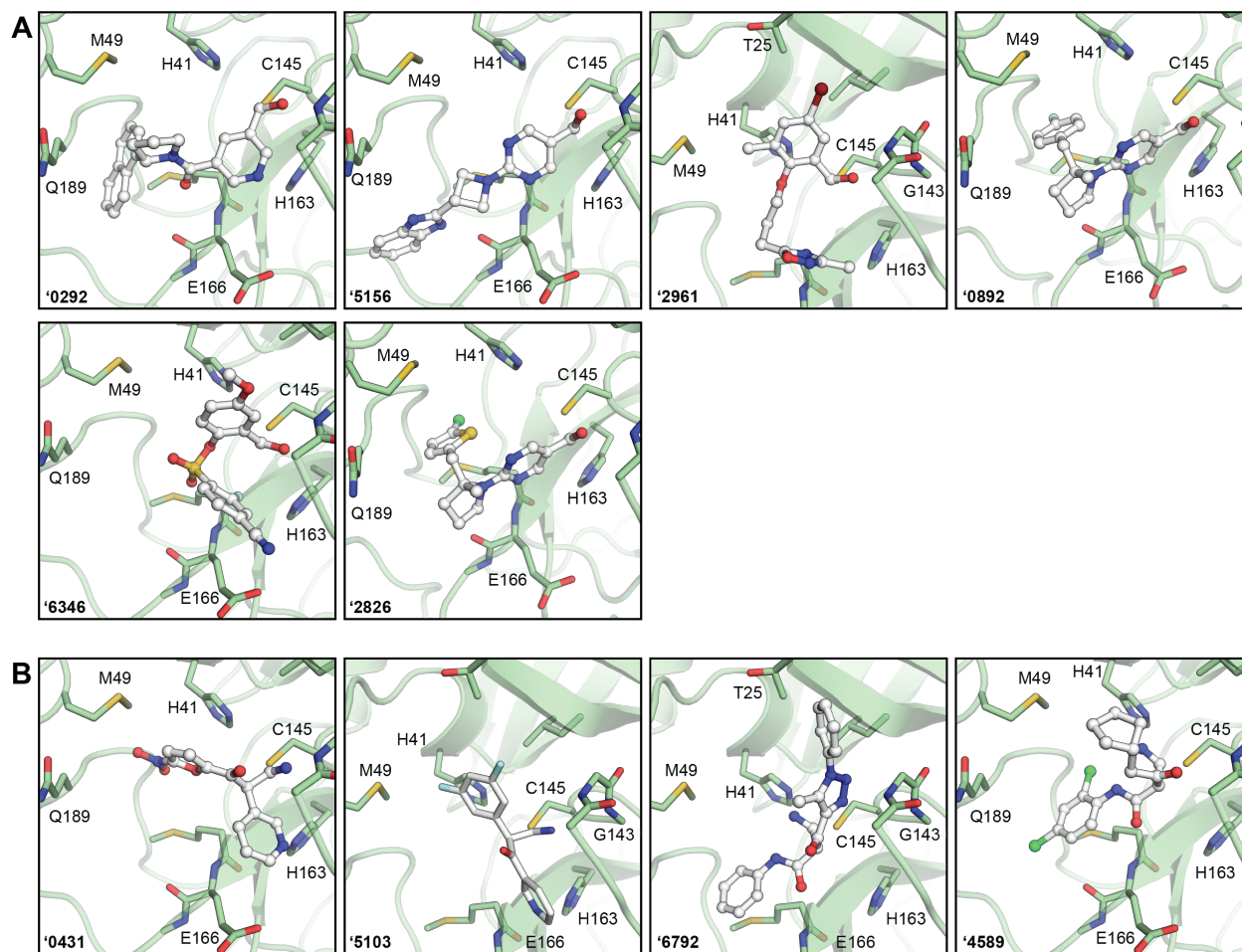


**Supplementary Figure 3. Evaluating aggregation potential of initial docking hits and potent analogs.** (A,C) Enzymatic inhibition by aggregation tested against AmpC and MDH (with or without 0.01% Triton X-100 detergent). (B,D) Compounds observed in DLS for forming colloidal-like particles where values above  $10^6$  have the potential for aggregating.

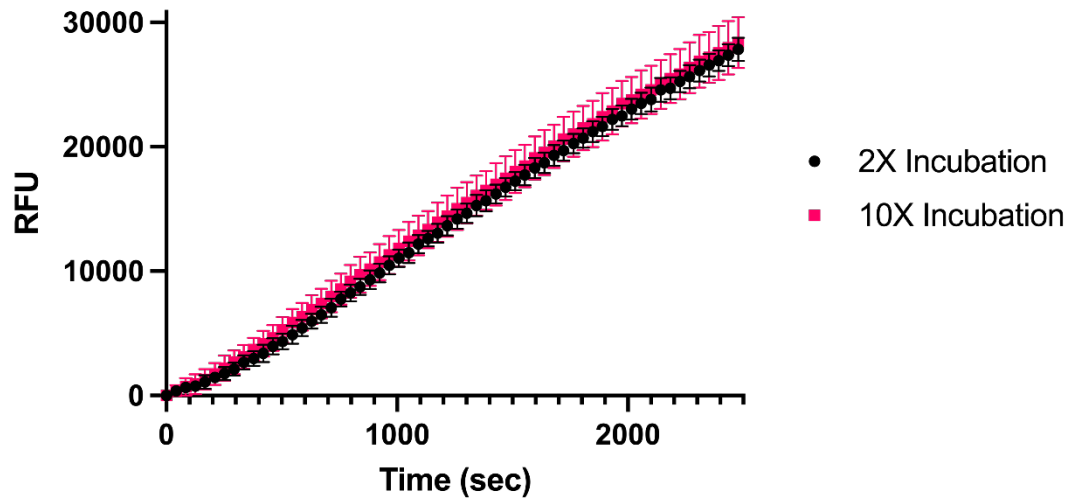




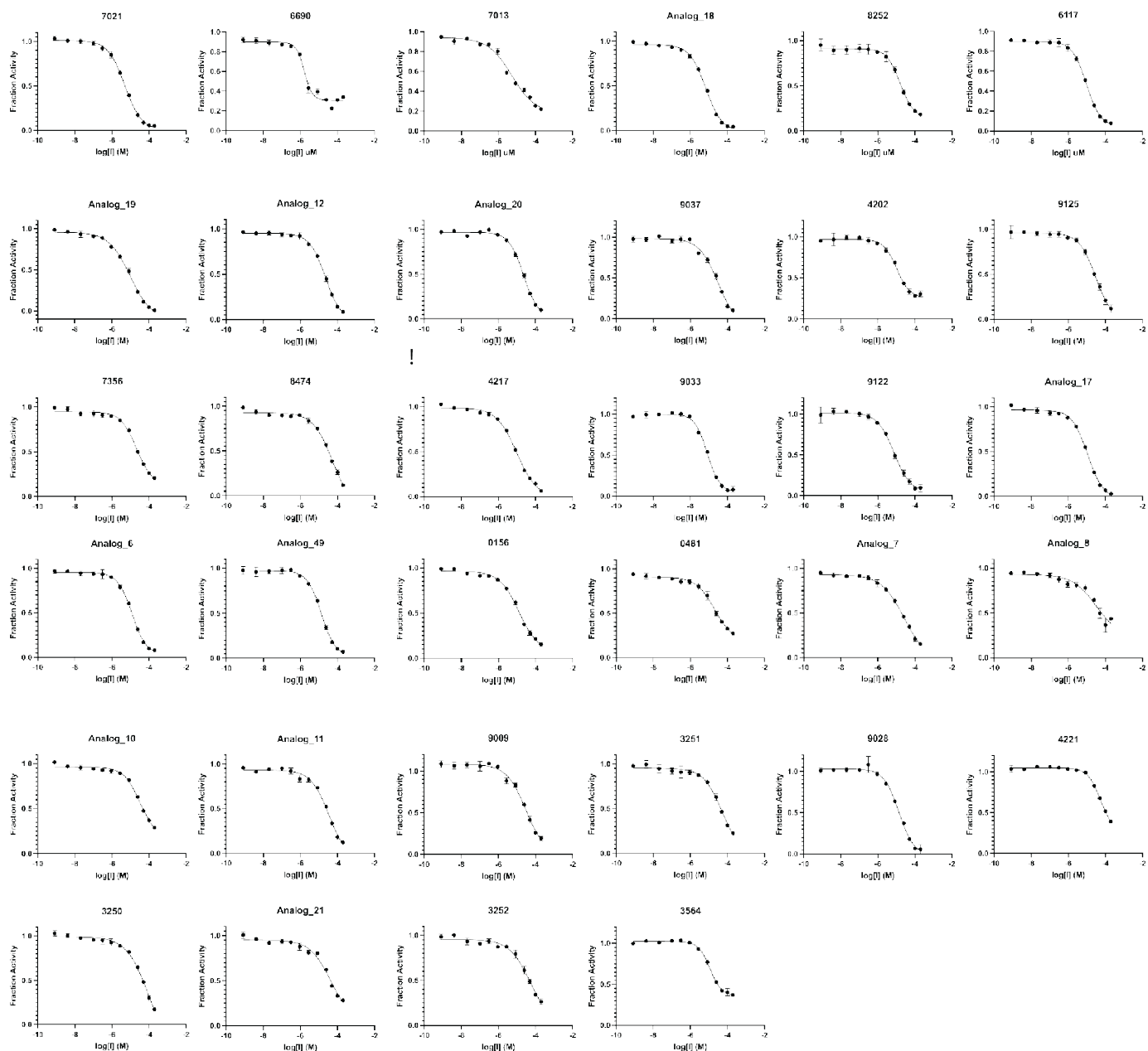
Supplementary Figure 4. LigPlot visualization of M<sup>Pro</sup>-noncovalent inhibitor interactions in newly solved structures.



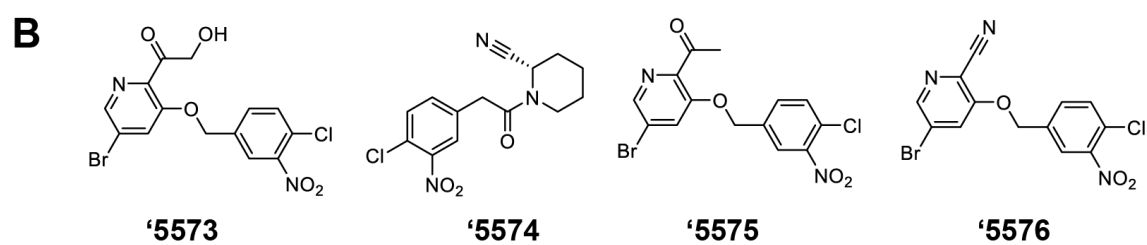
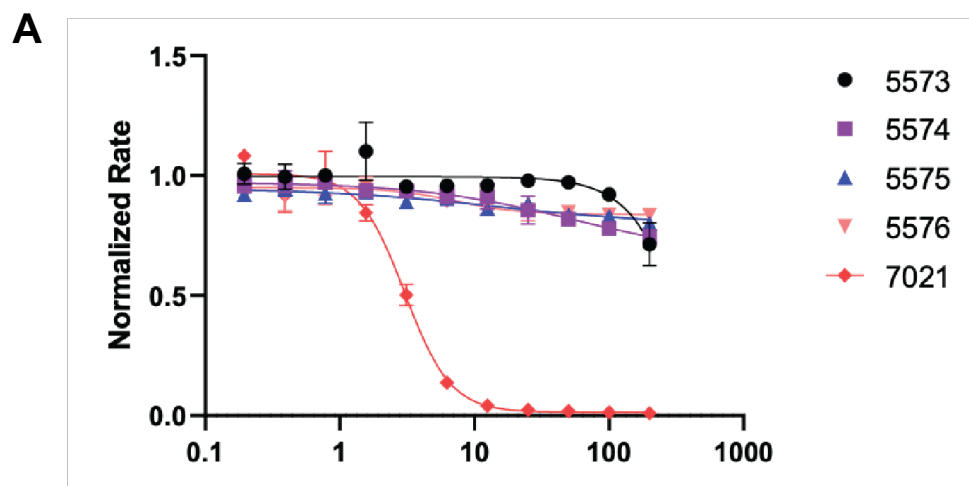
**Supplementary Figure 5. Docked poses of covalent hits. (A) Aldehydes. (B) Nitriles.** Covalent bonds between the warhead and Cys145 and not explicitly modeled in docking.



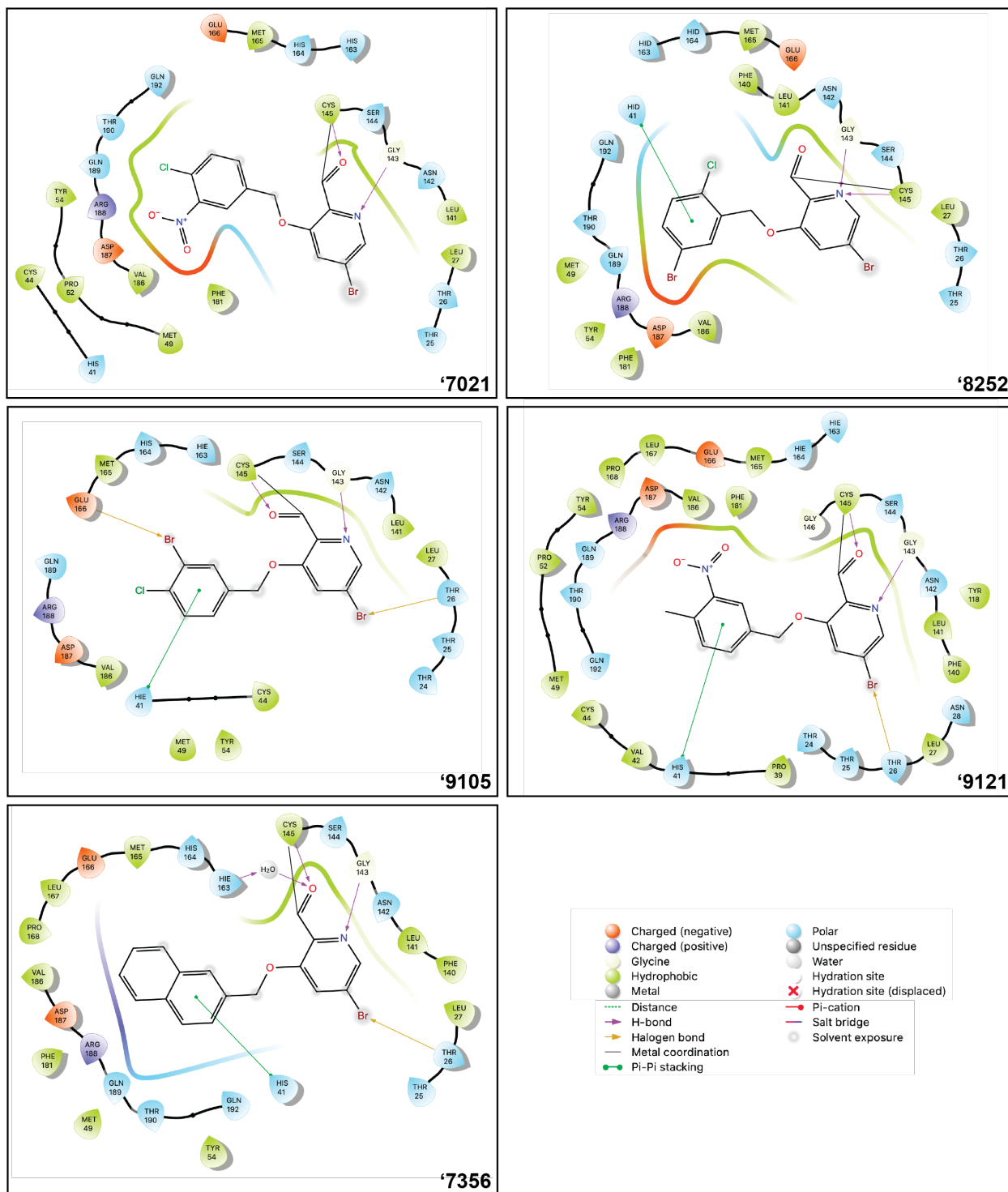
**Supplementary Figure 6. Reversibility of compound '7021.** Both 2X and 10X concentrations of enzyme and '7021 inhibitor were co-incubated for 1-hour. By Le Chatelier's principle, the 10X incubation should lead to more inhibited enzyme product. Both 2X and 10X incubations were diluted to 1X concentrations with final substrate concentration of 1X NSP7. Both co-incubations yielded the same velocity, evincing concentration dependent diffusion of the enzyme-inhibitor complex, thus evincing the reversibility of the '7021 compound.



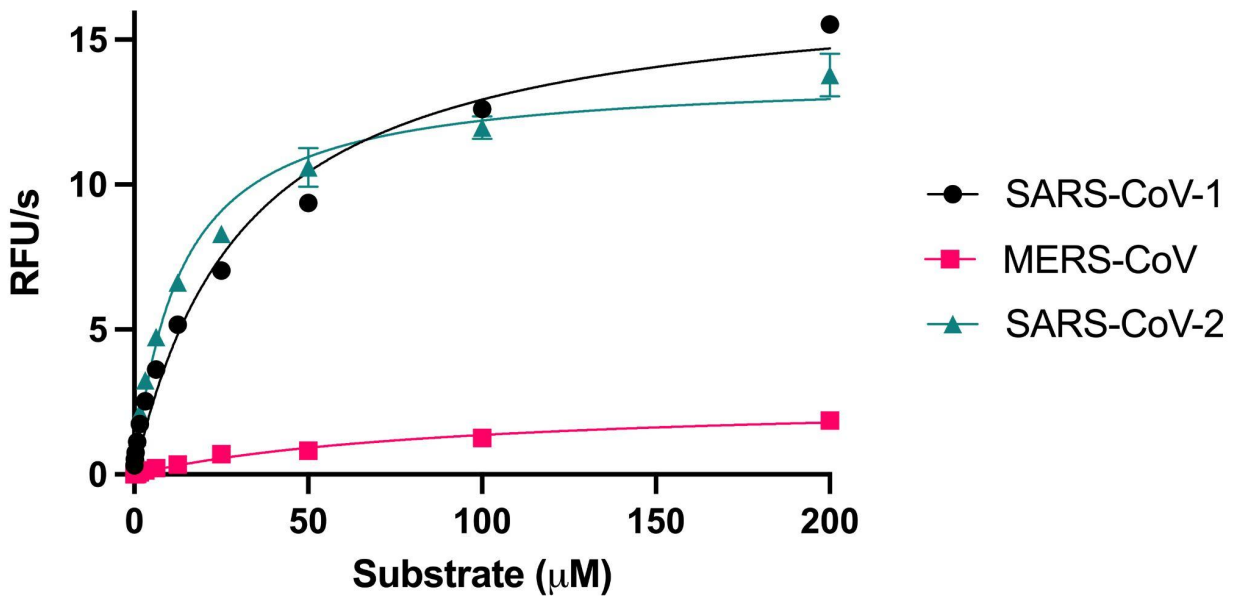
**Supplementary Figure 7. '3620 analogs with improved potencies. IC<sub>50</sub> values in Table S2.**



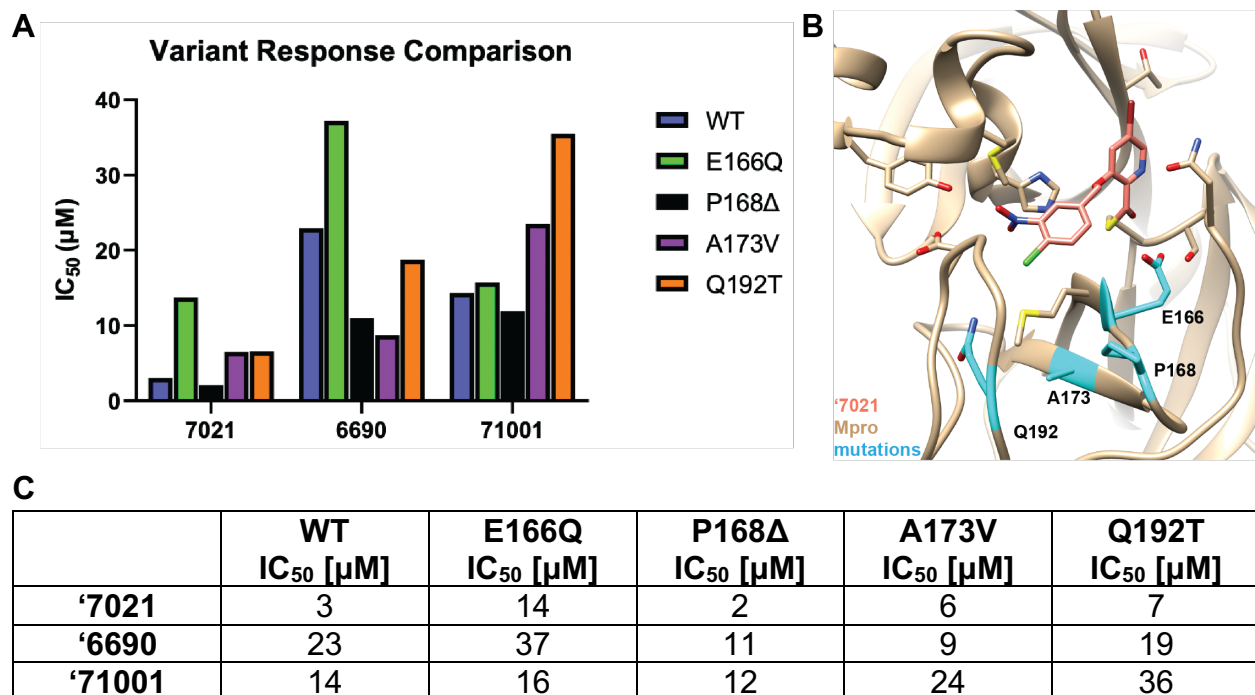
**Supplementary Figure 8. '7021 analogs with different electrophiles did not inhibit  $M^{Pro}$ .**



**Supplementary Figure 9. LigPlot visualization of M<sup>Pro</sup>-covalent inhibitor interactions in newly solved structures.**



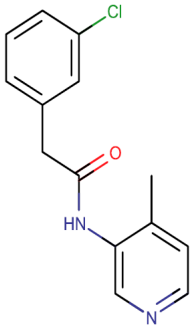
**Supplementary Figure 10. Pan-viral enzymatic activities.** Michaelis-Menten kinetics were ran side-by-side with the optimized NSP7 substrate for SARS-CoV-2 (green), SARS-CoV-1 (black), and MERS (red) major proteases.  $K_M$  values were found to be  $12\mu\text{M}$ ,  $30\mu\text{M}$ , and  $90\mu\text{M}$  for SARS-CoV-2, SARS-CoV-1, and MERS, respectively. All proceeding inhibitory assays were ran with  $K_M$  concentrations of substrate.



**Supplementary Figure 11. Compound activities against mutant SARS-CoV-2 M<sup>Pro</sup>.** (A, C) IC<sub>50</sub> values for '7021, '6690, and '71001 against a panel of M<sup>Pro</sup> mutants. (B) Mutations (blue carbons) shown on the '7021 SARS-CoV-2 M<sup>Pro</sup> crystal structure. WT, wildtype. All measurements were done in triplicate.



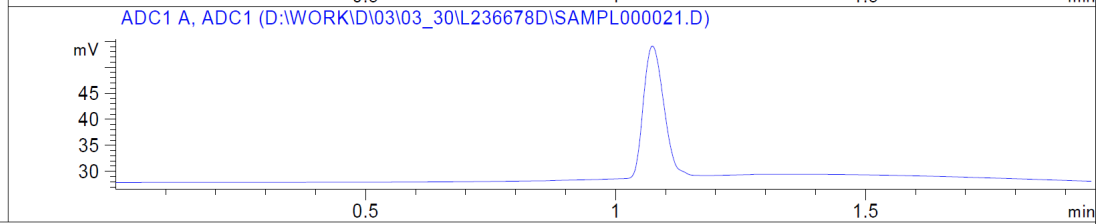
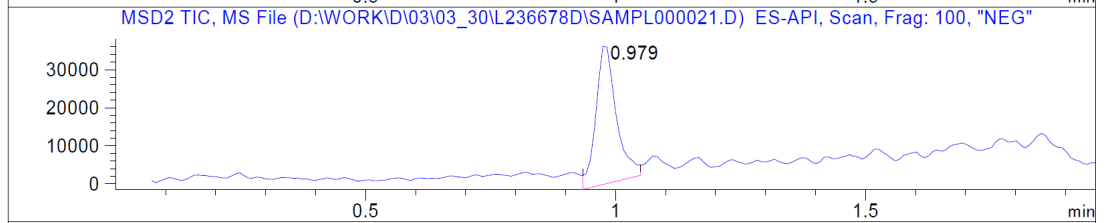
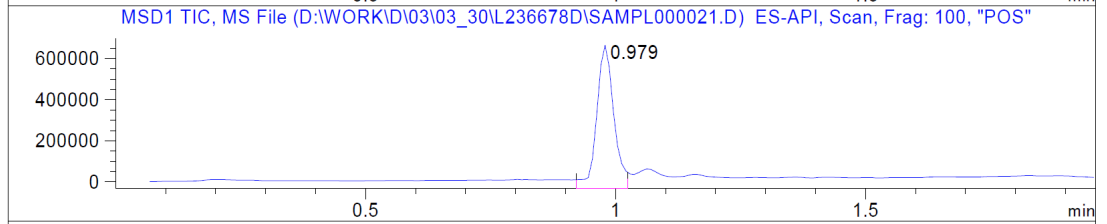
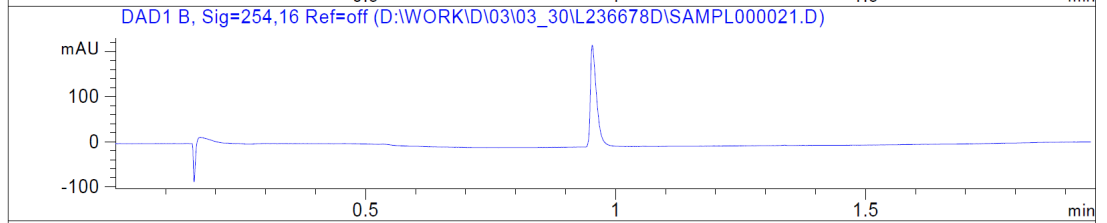
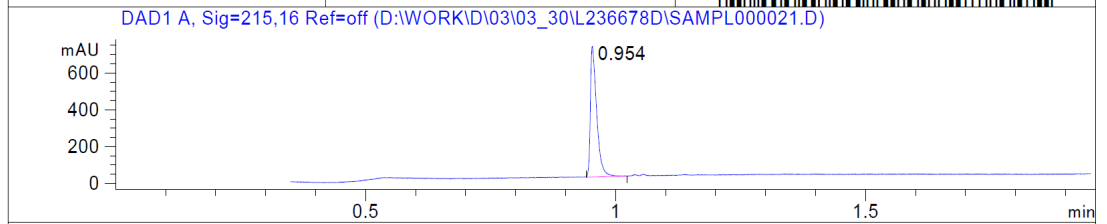
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Ret\_Time: 0.954 min



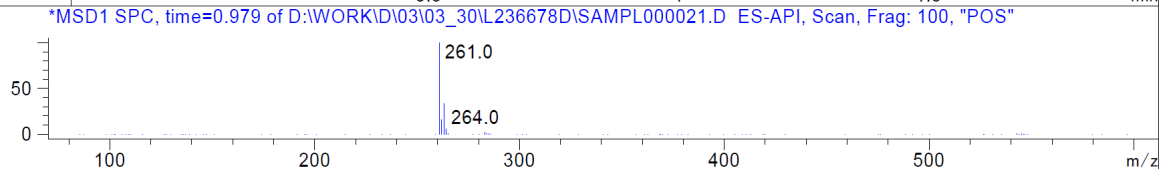
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**Exact Mass** 260.09

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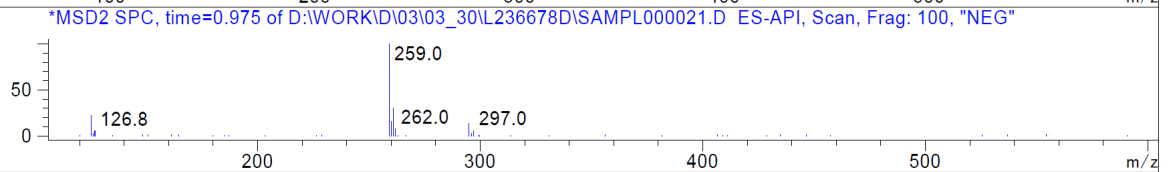
Q216097\$2



RT 0.979

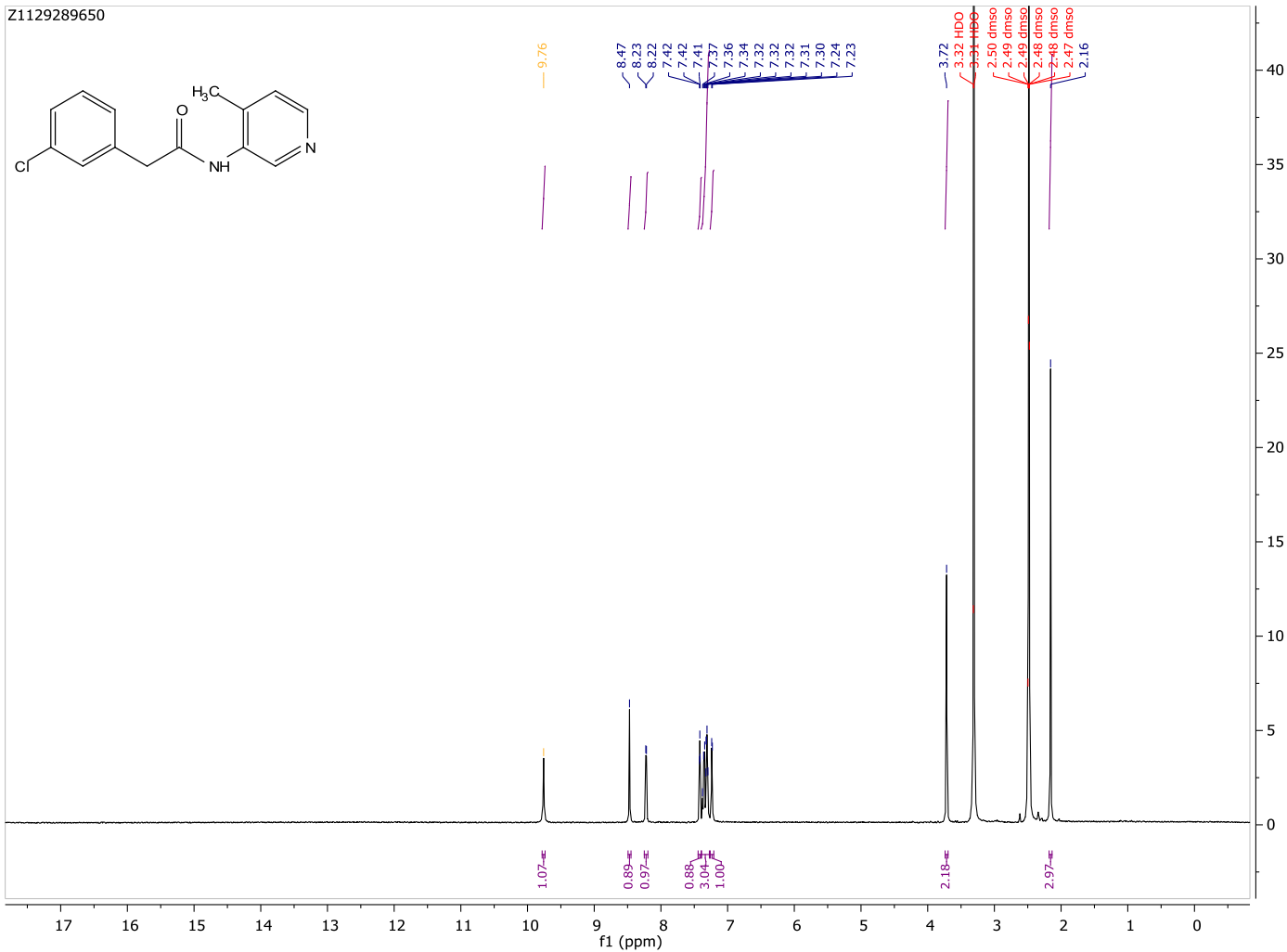
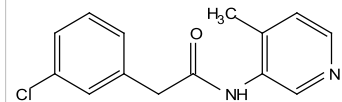


RT 0.979



Z1129289650

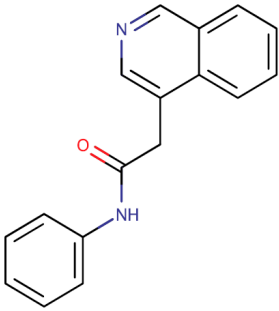
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Q272221\$1

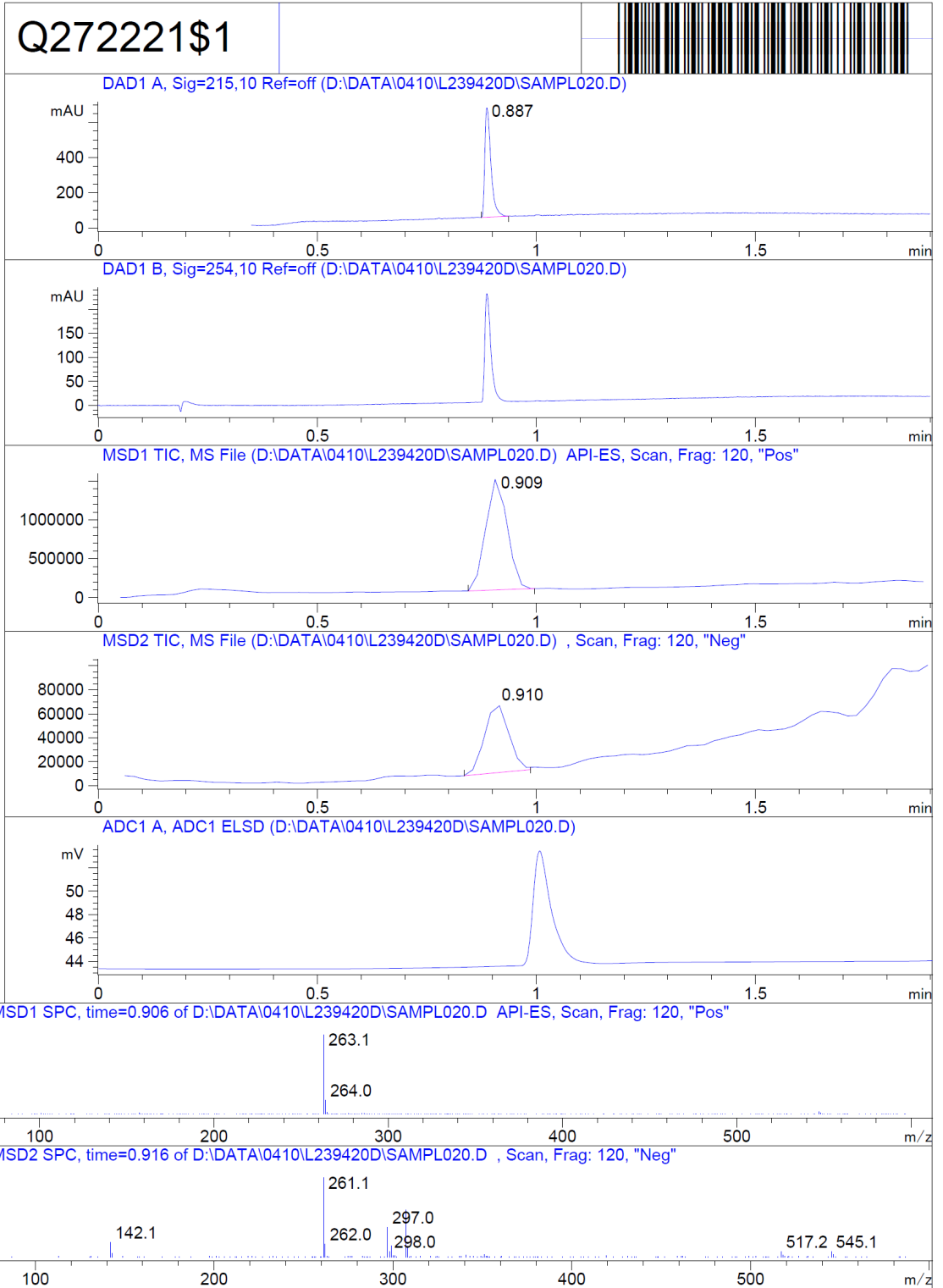


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Ret\_Time: 0.887 min



Mol Wt 262.31  
Exact Mass 262.13

#	Time	Area%
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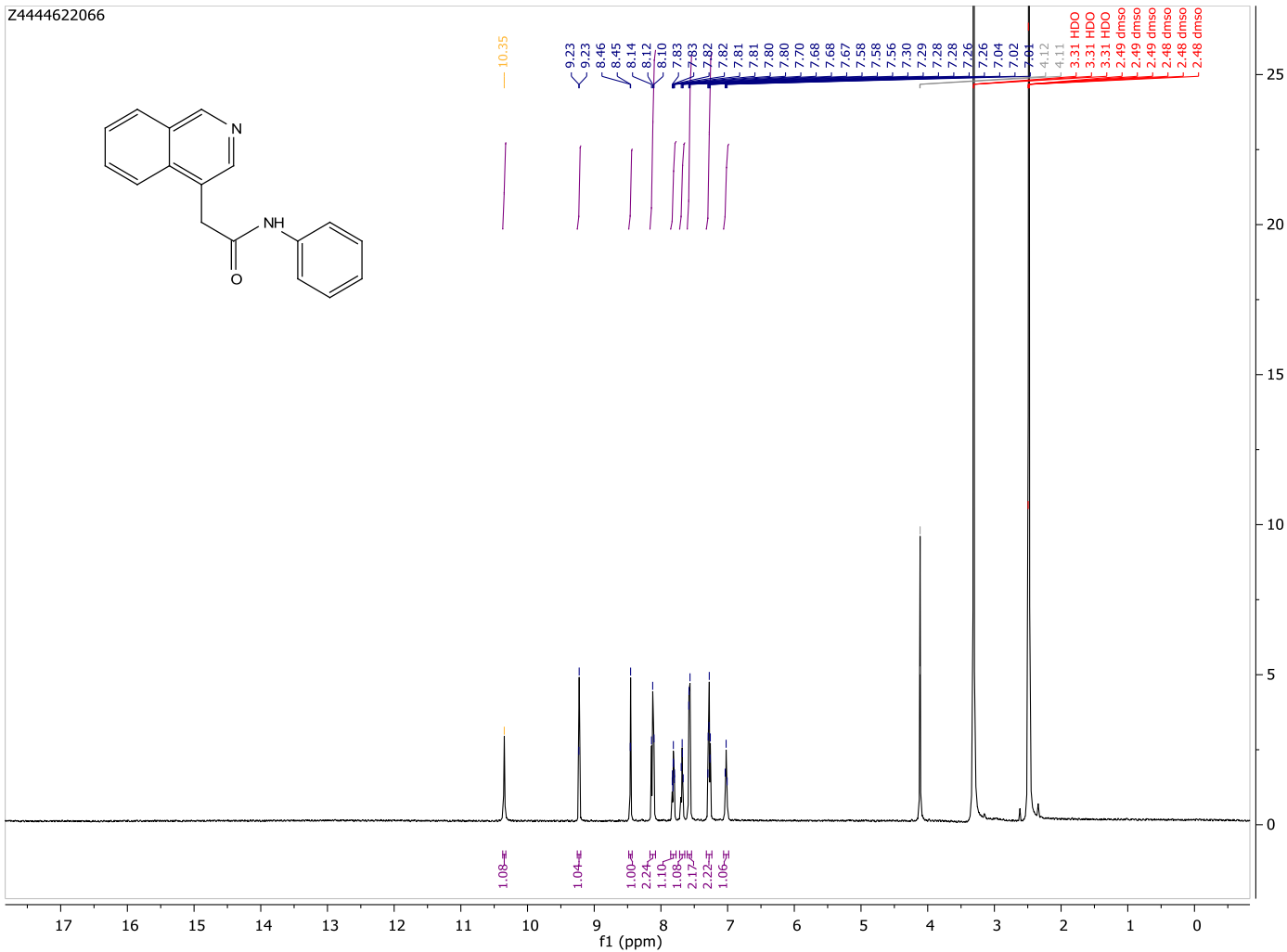
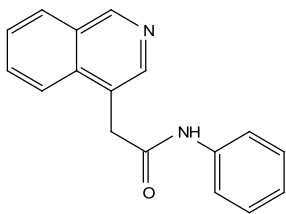


RT 0.909

RT 0.910

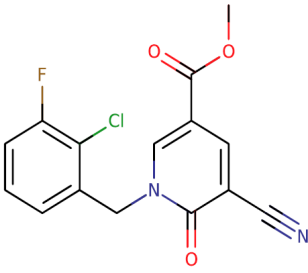
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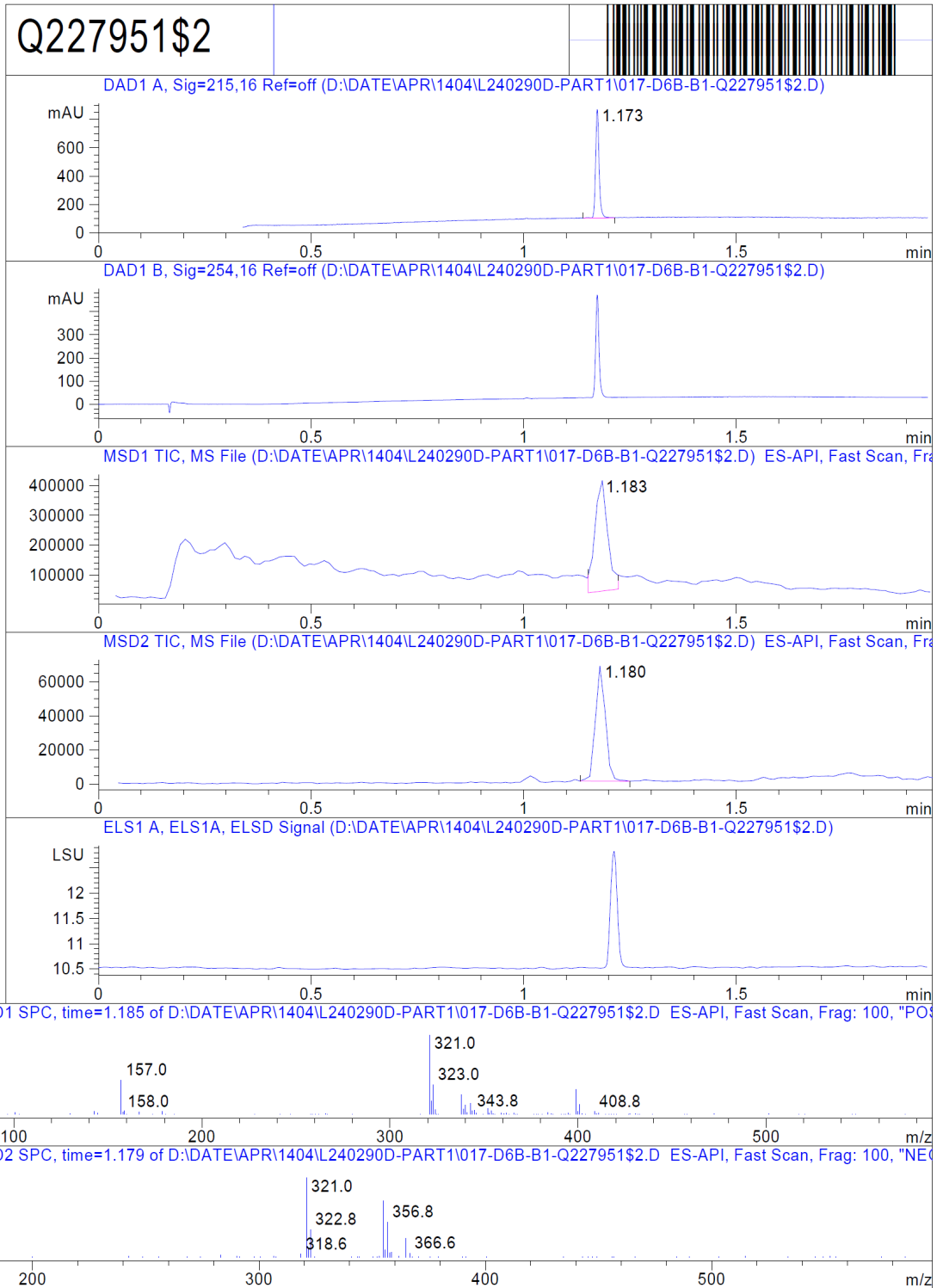
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Q227951\$2



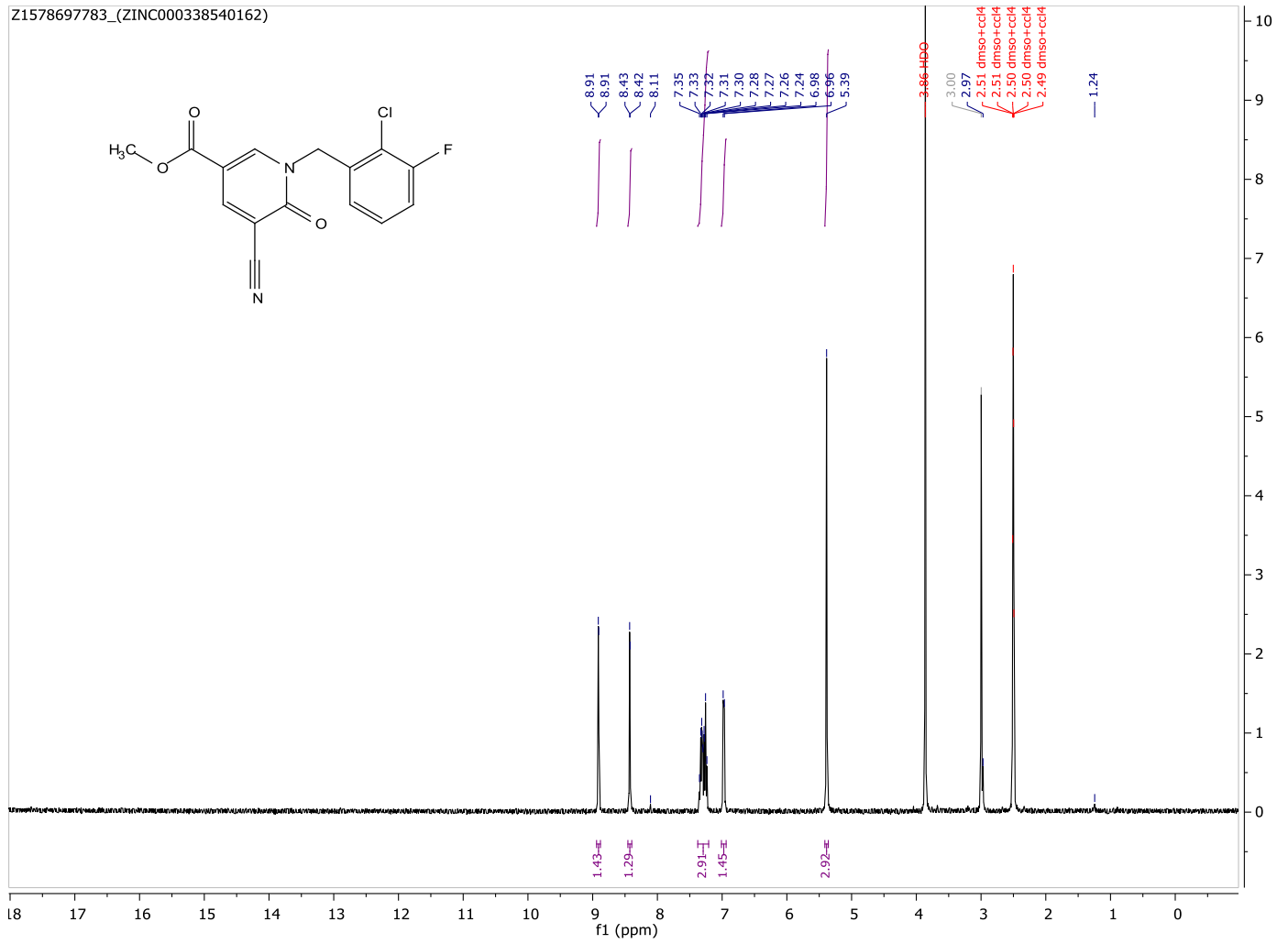
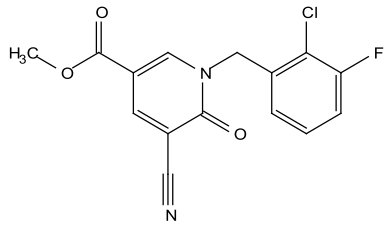
Mol Wt 320.7  
Exact Mass 320.04

#	Time	Area%
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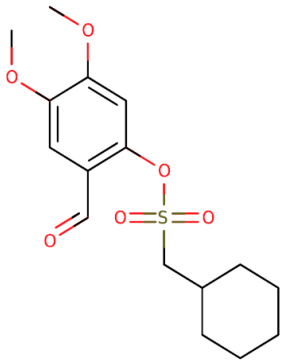


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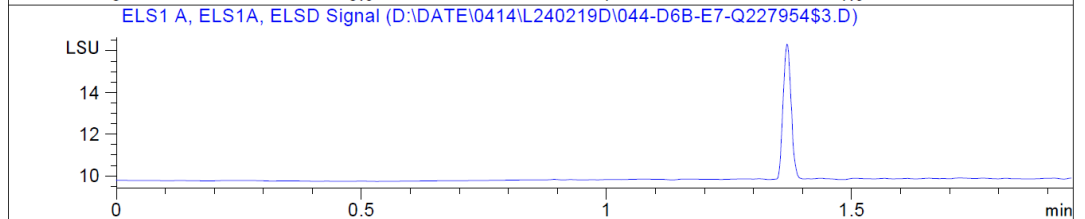
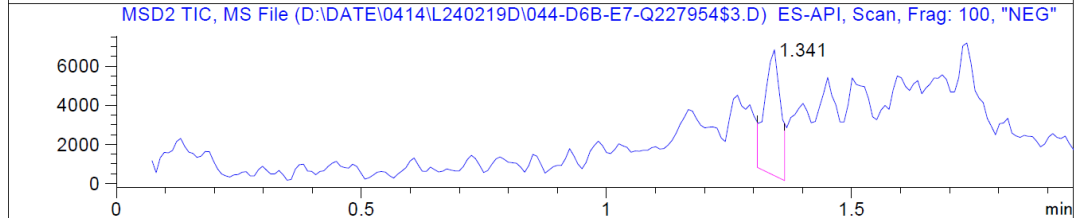
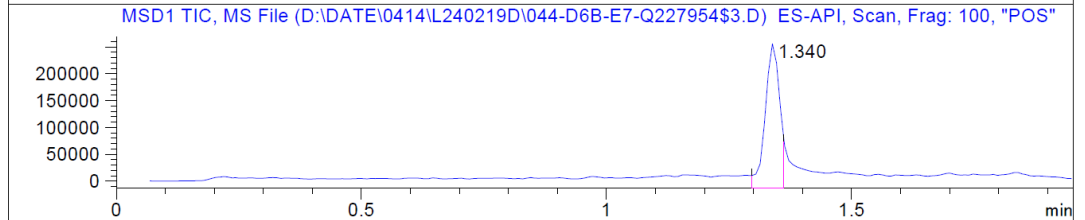
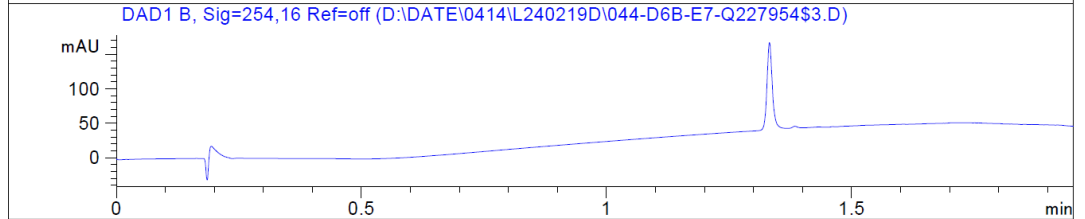
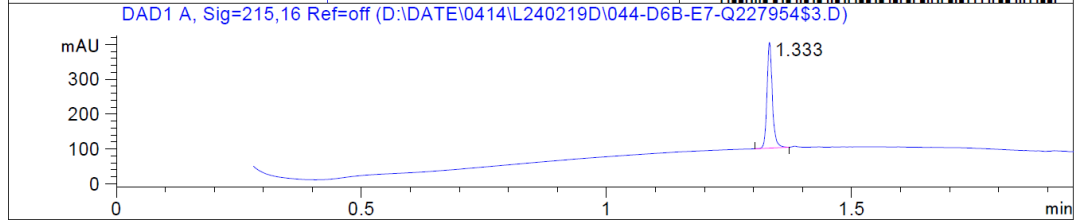
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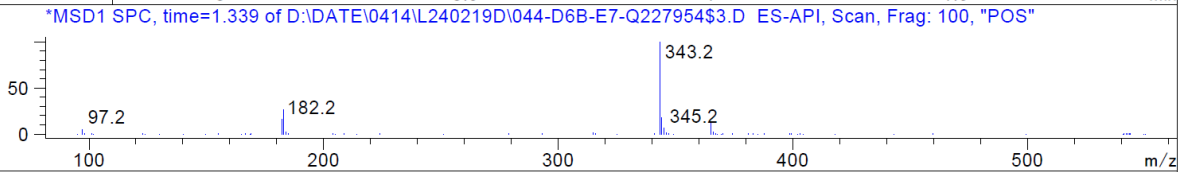
Mol Wt 342.41  
Exact Mass 342.13

#	Time	Area%
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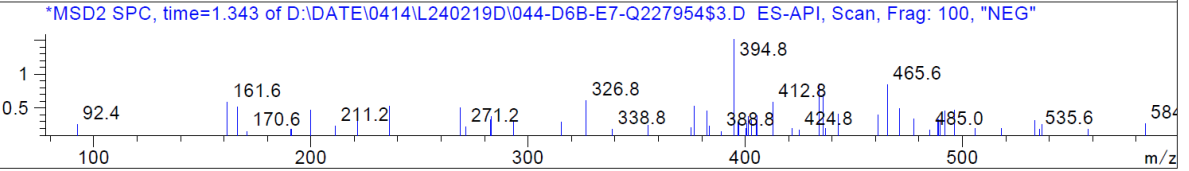
Q227954\$3



RT 1.340

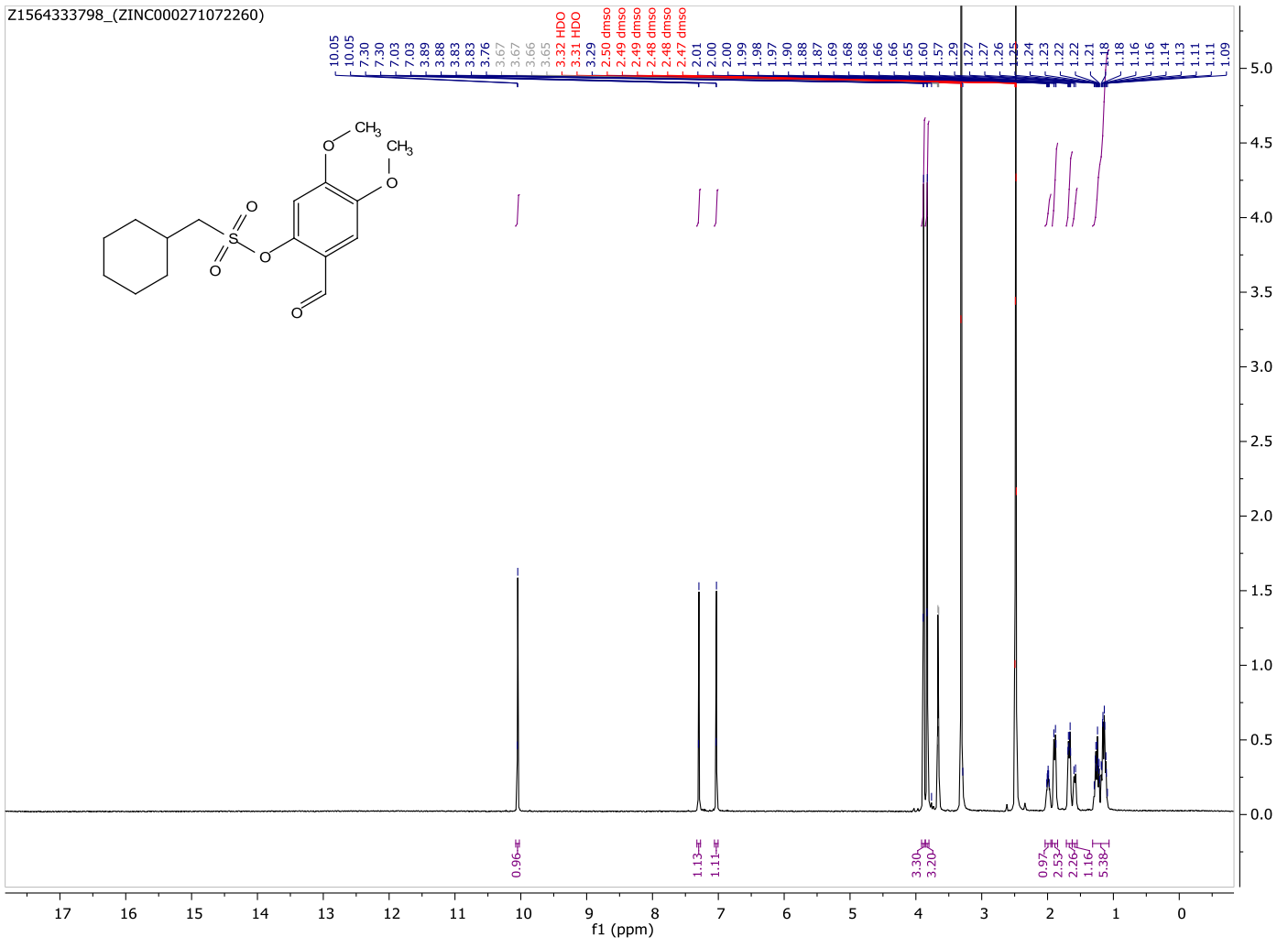


RT 1.341



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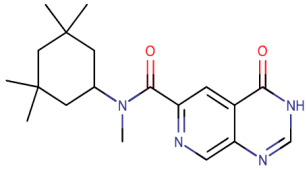
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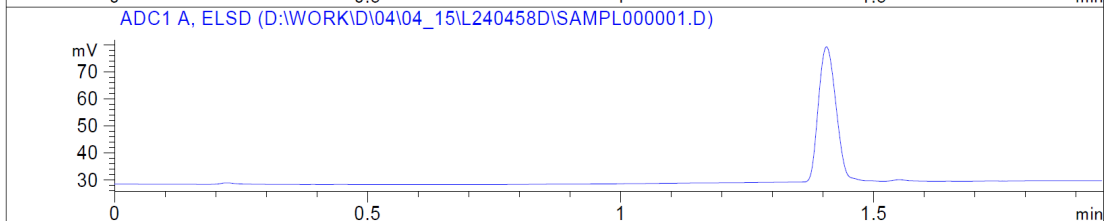
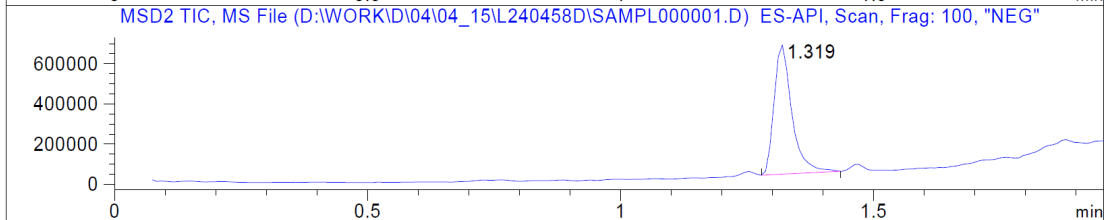
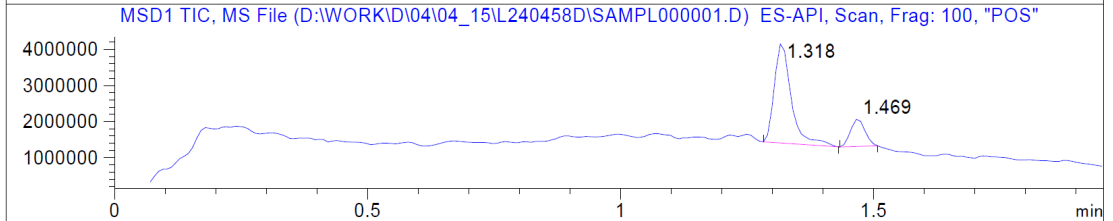
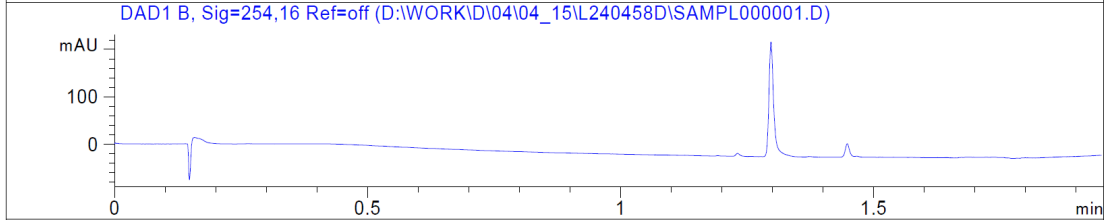
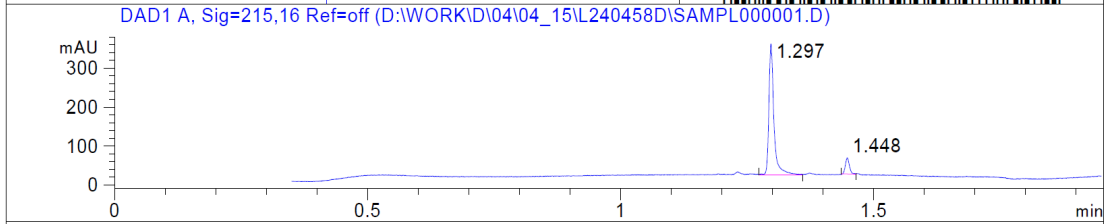
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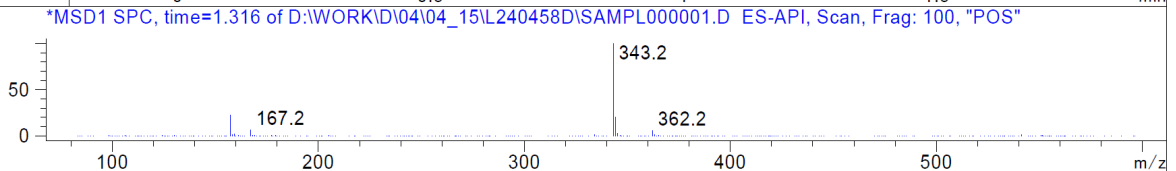


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Exact Mass 342.24

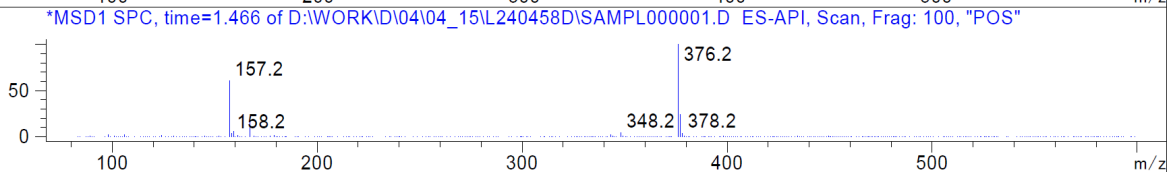
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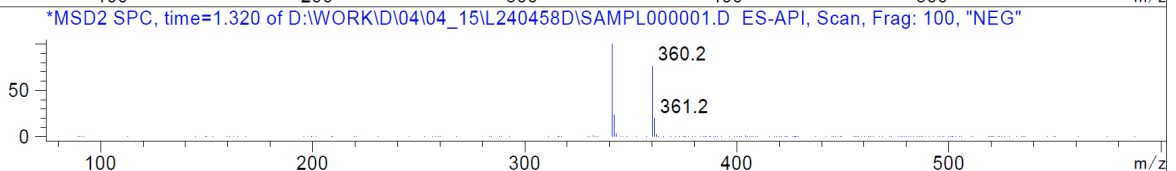
RT 1.318



RT 1.469

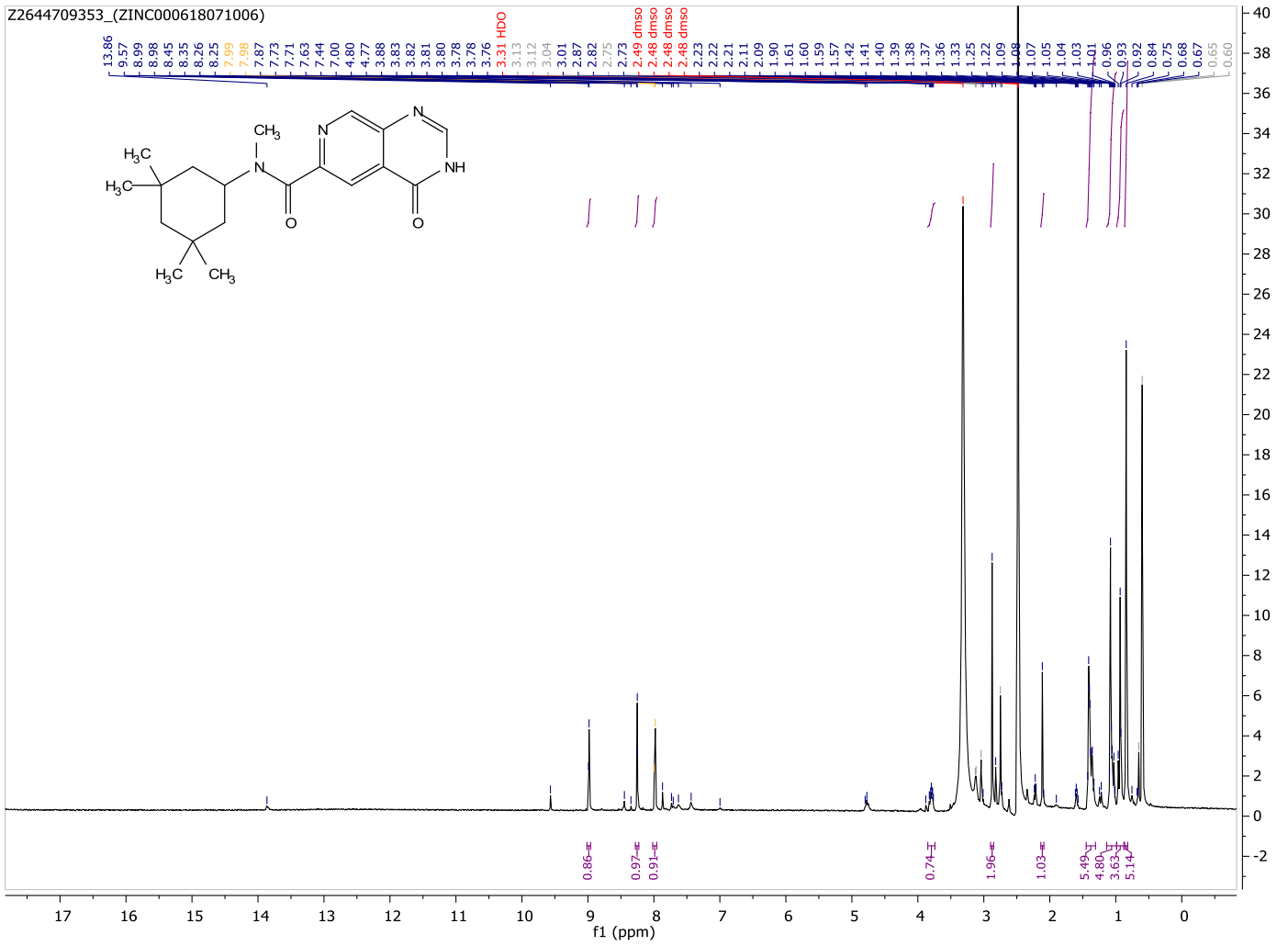
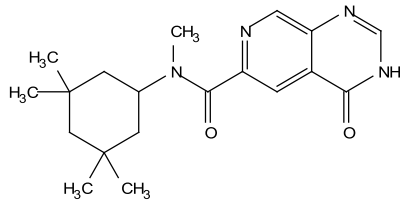


RT 1.319



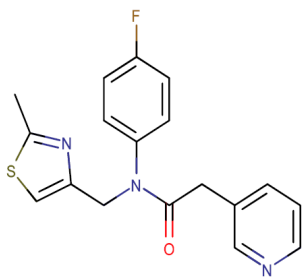
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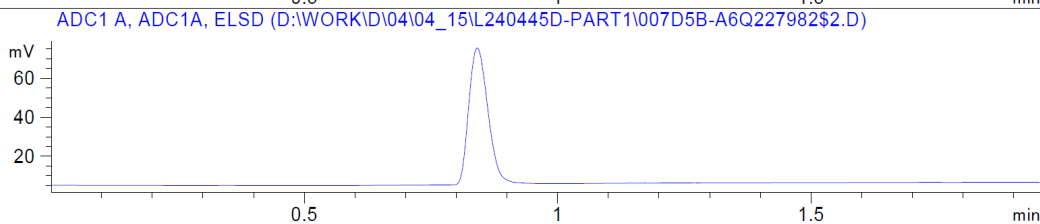
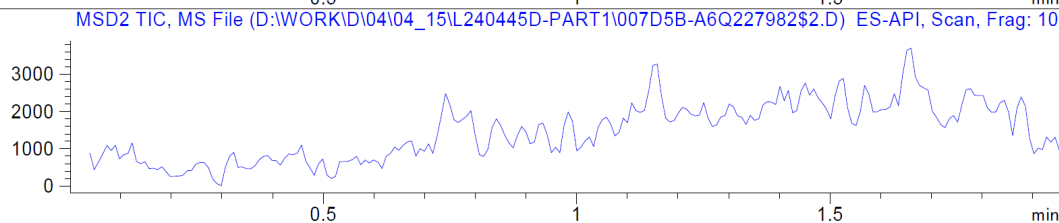
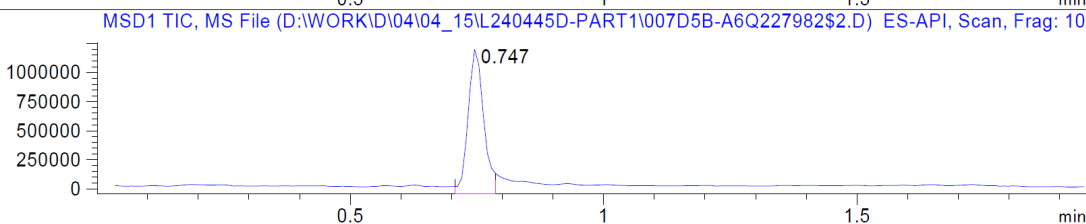
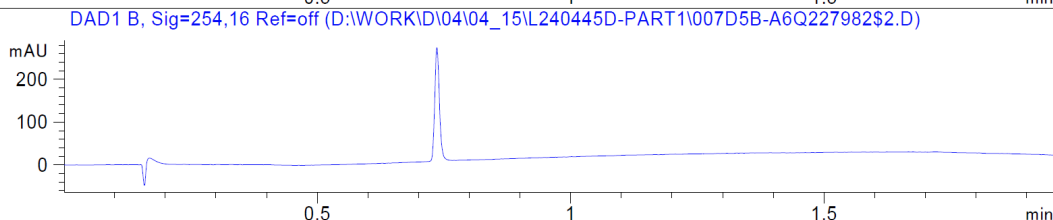
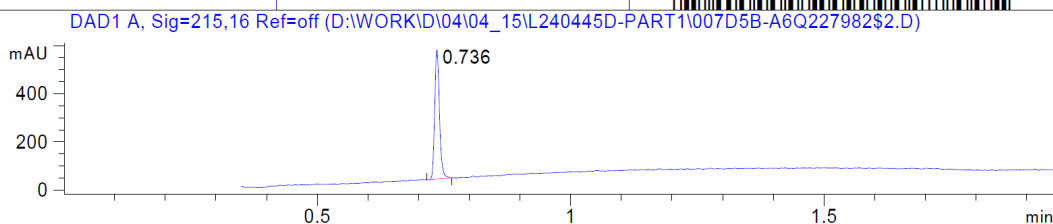
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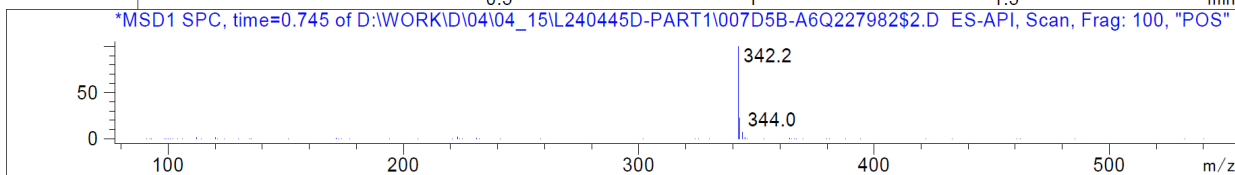


Mol Wt 341.4  
Exact Mass 341.12

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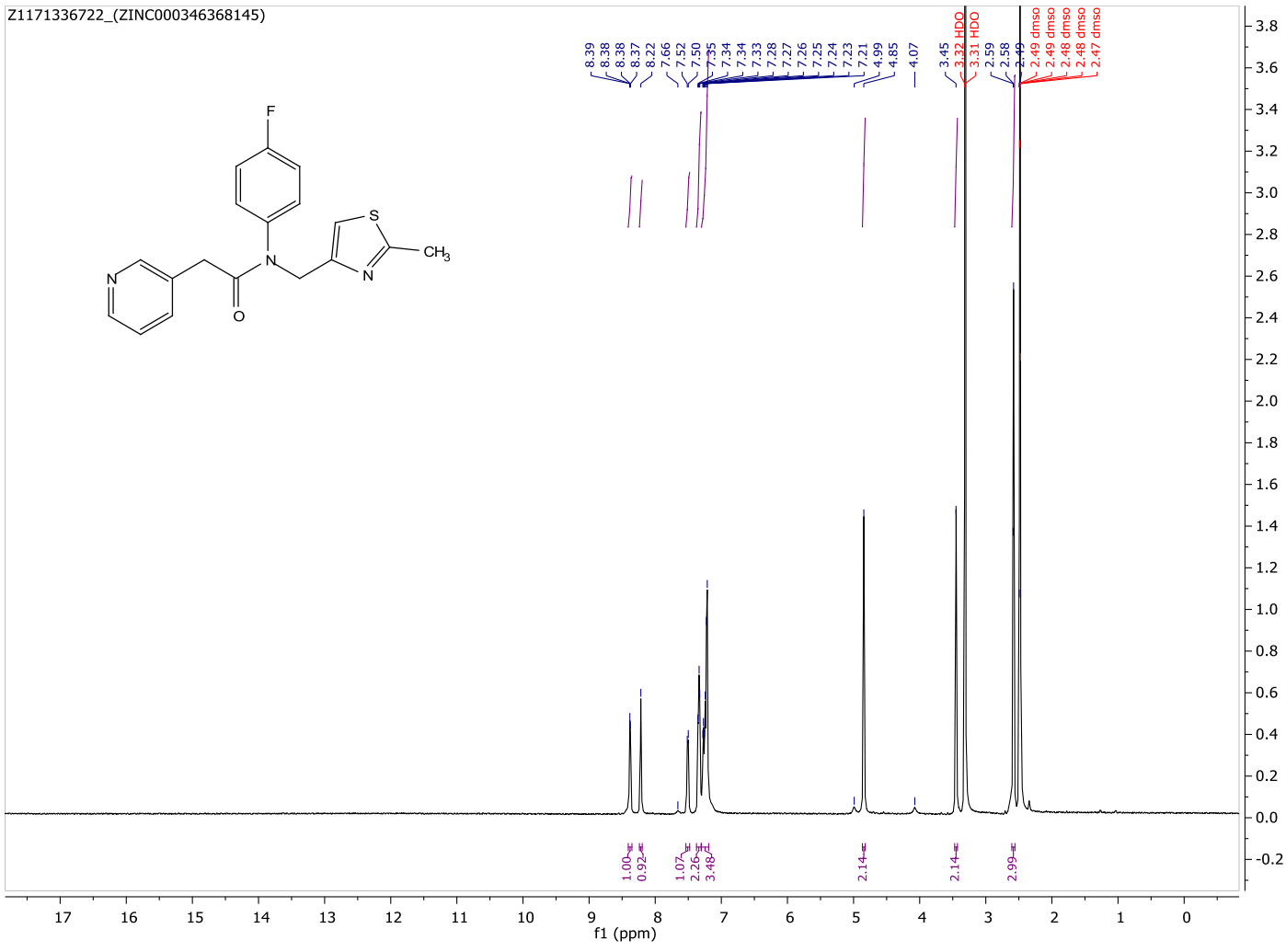
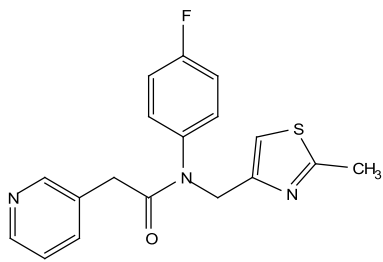


RT 0.747



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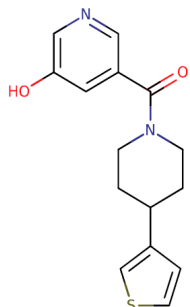
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# Q227994\$1

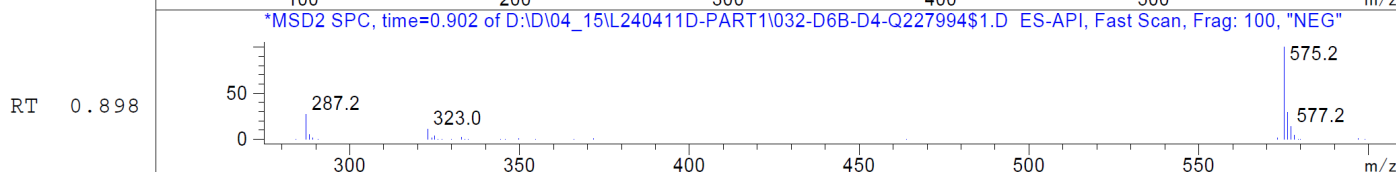
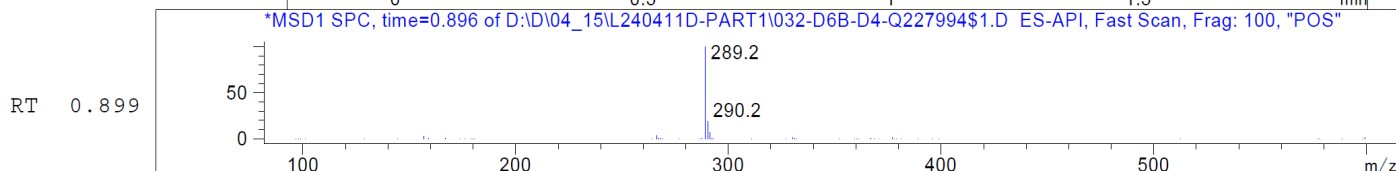
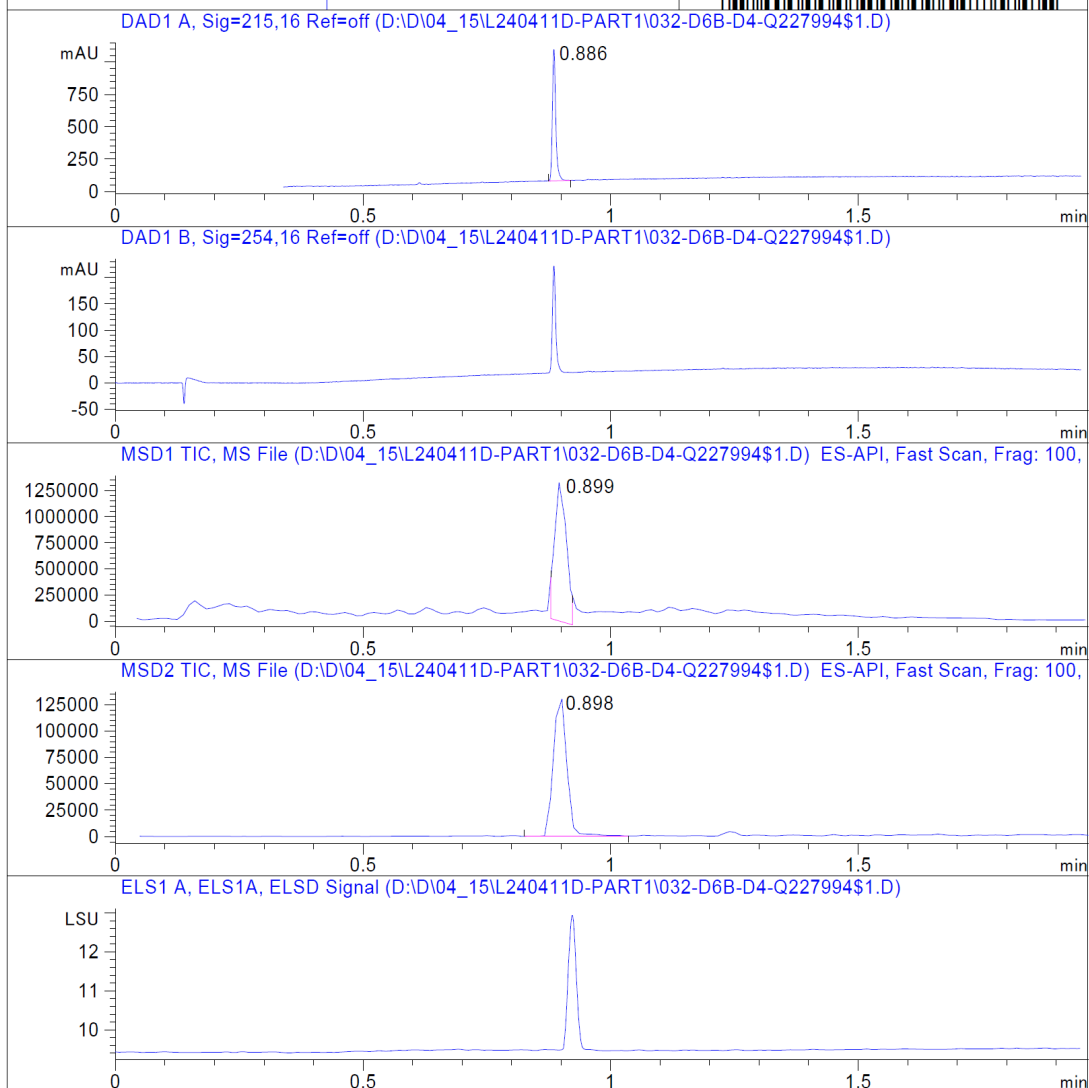


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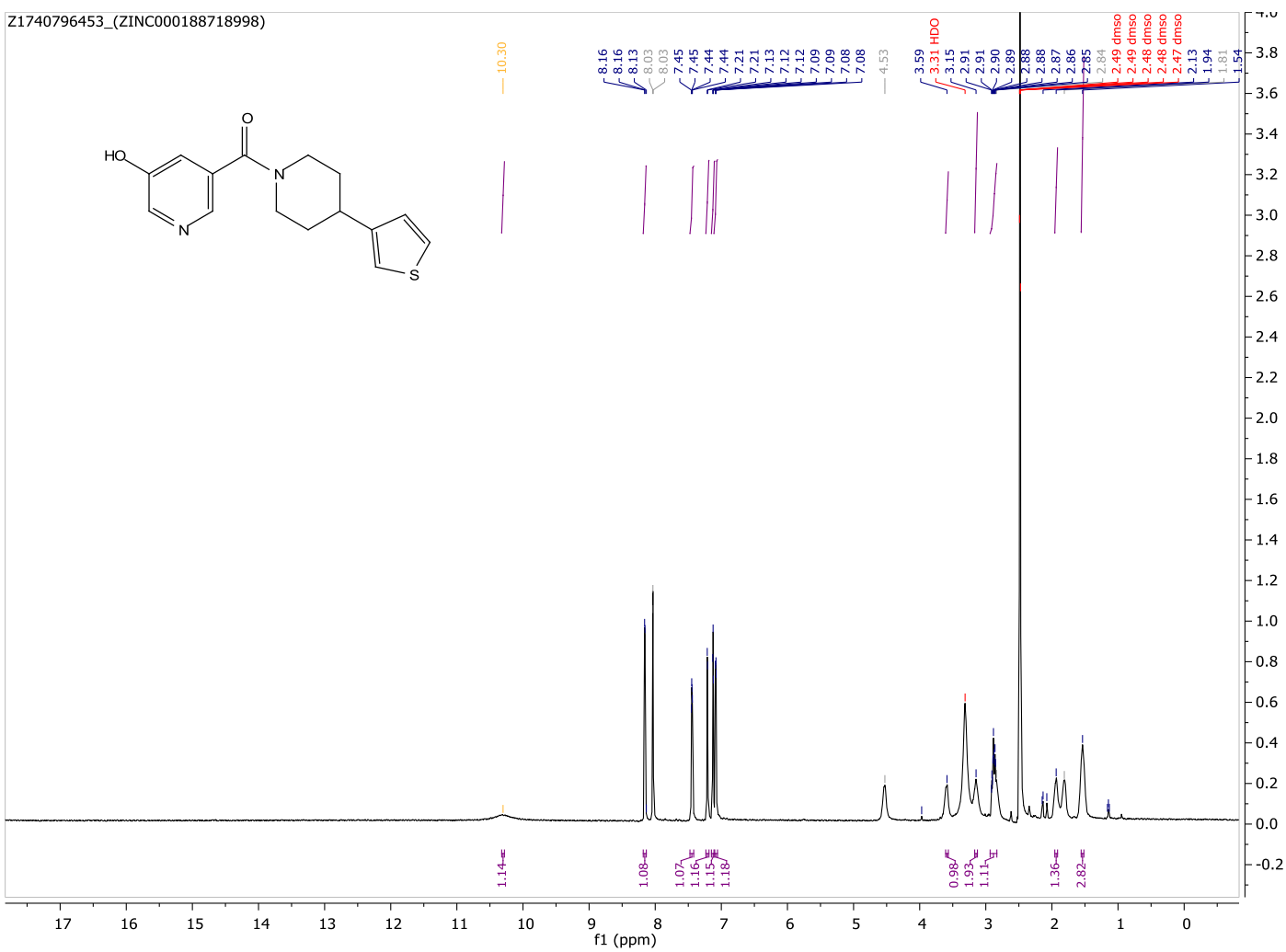
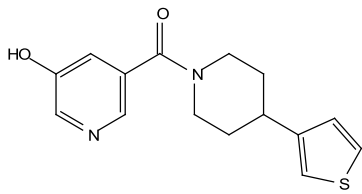
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**Exact Mass** 288.11

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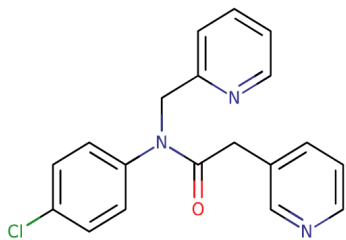
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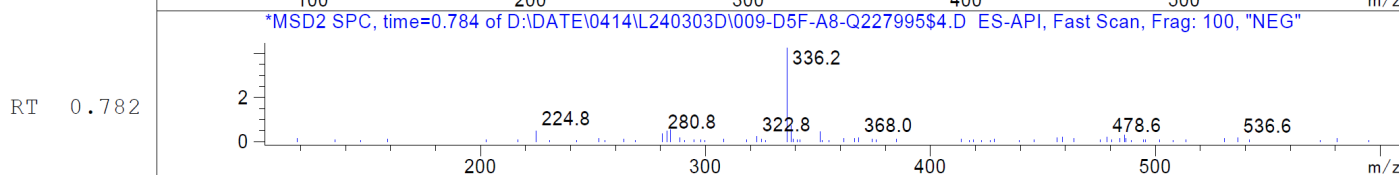
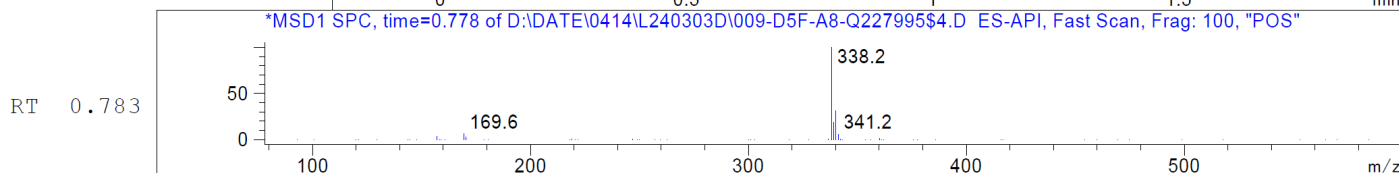
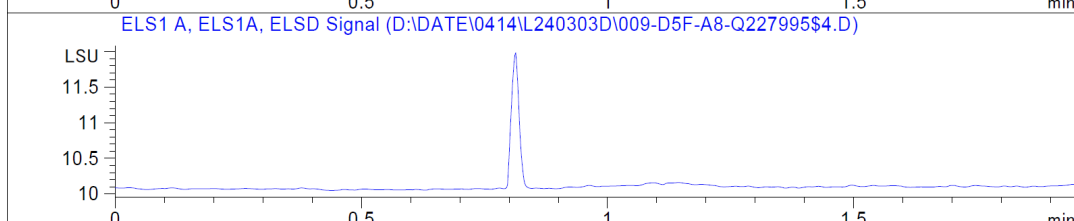
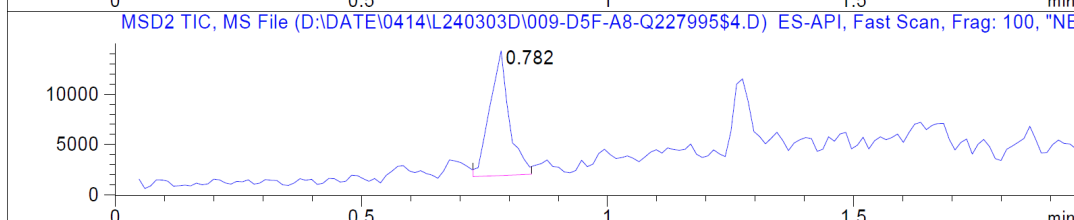
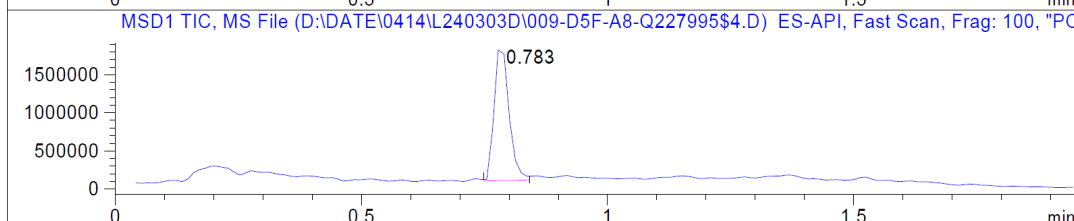
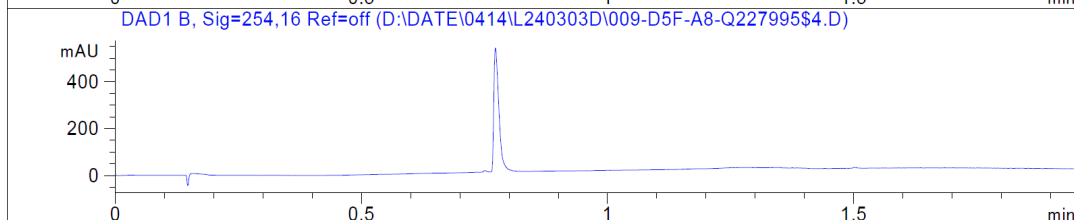
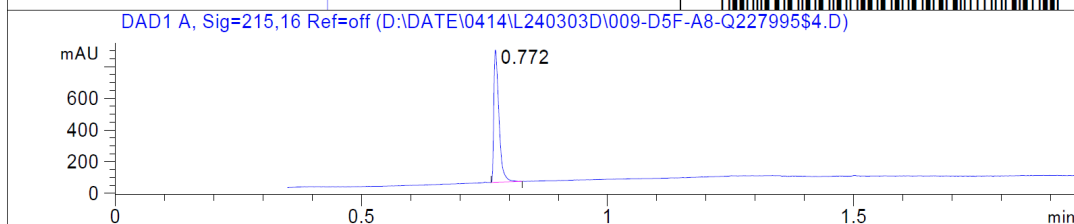
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Q227995\$4



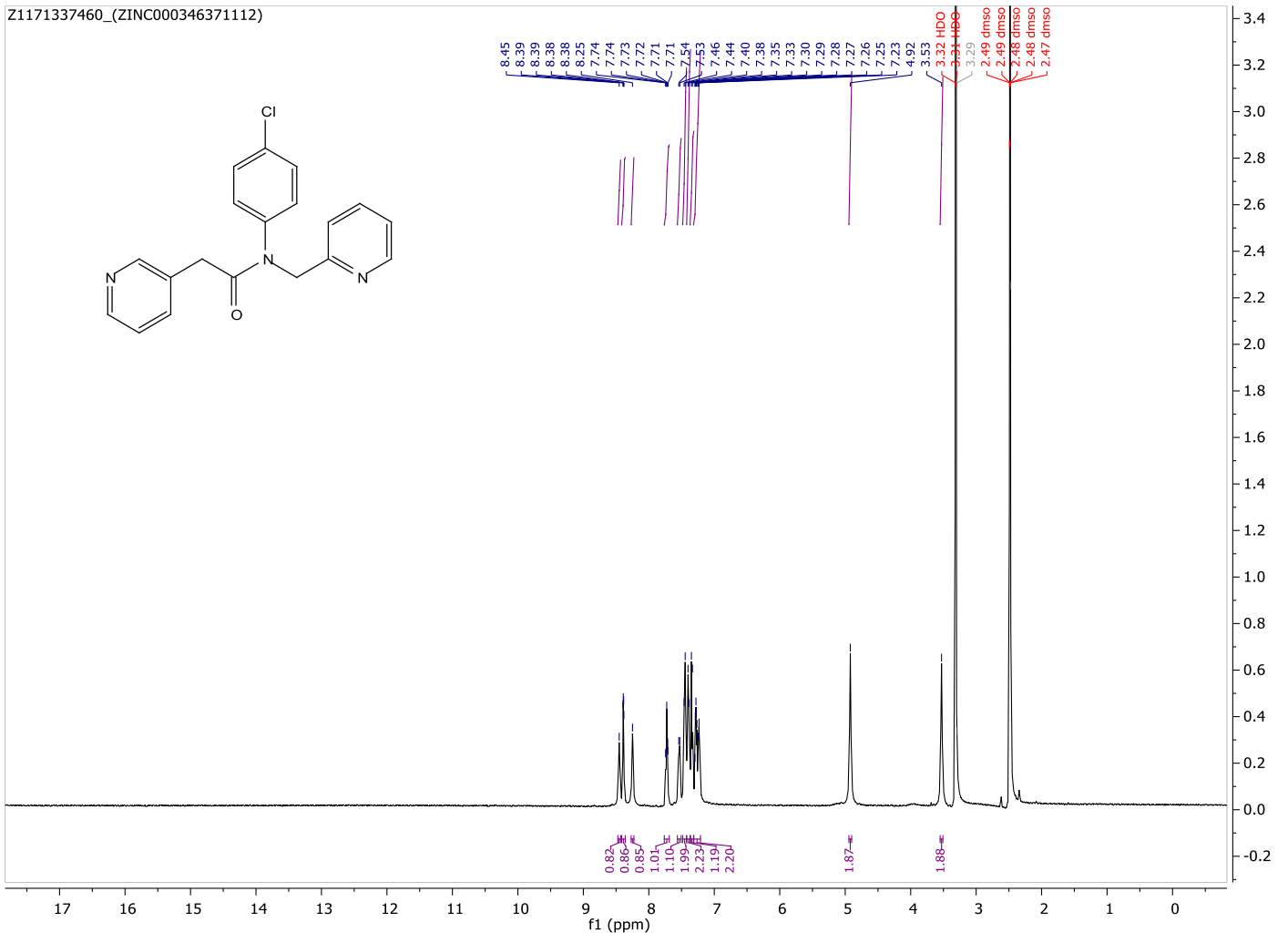
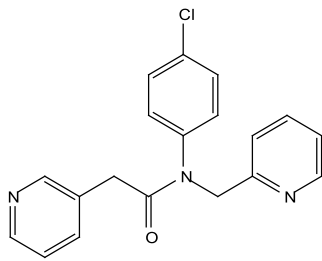
Mol Wt 337.8  
Exact Mass 337.12

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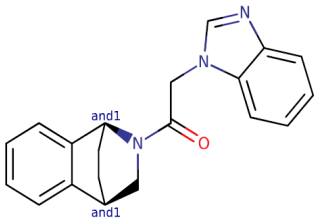
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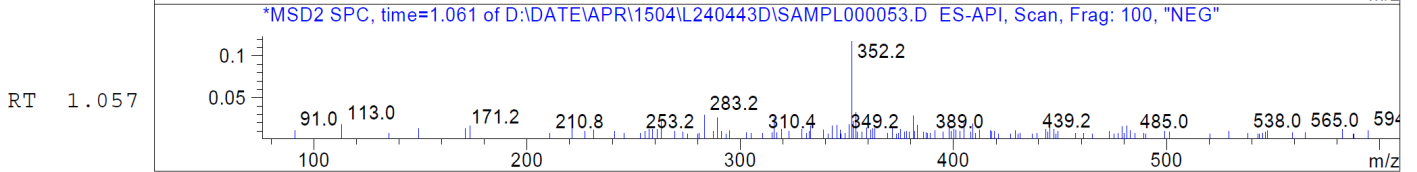
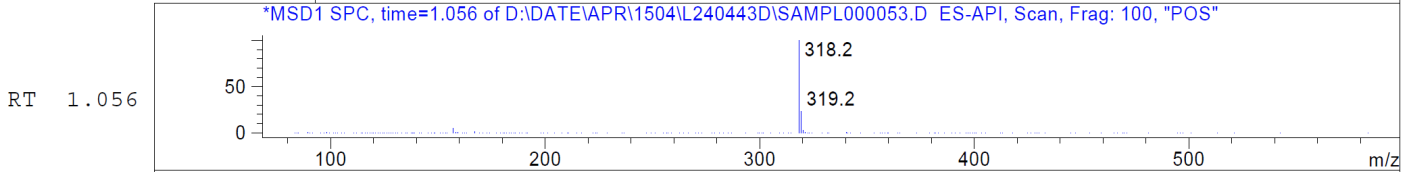
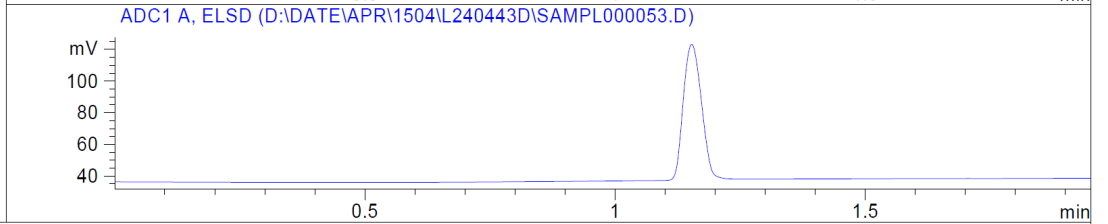
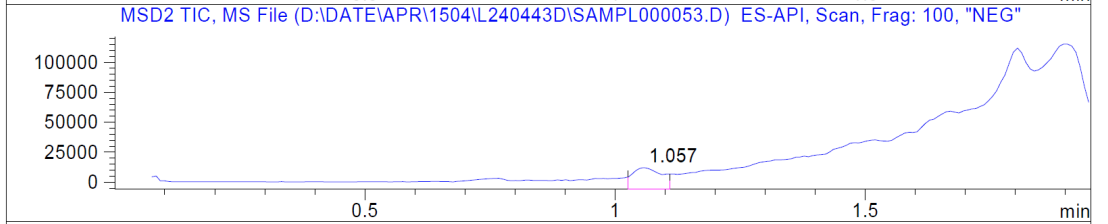
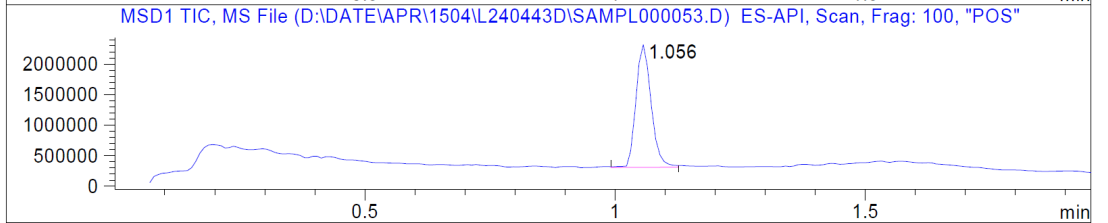
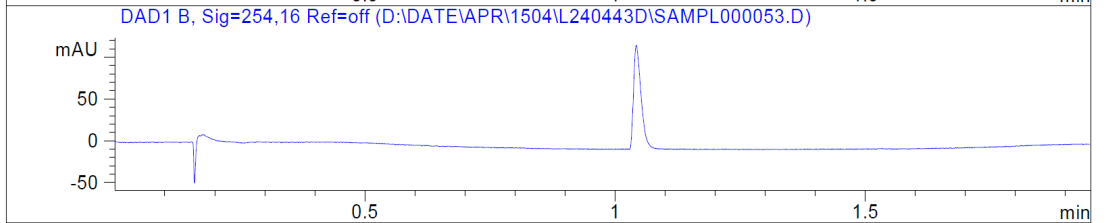
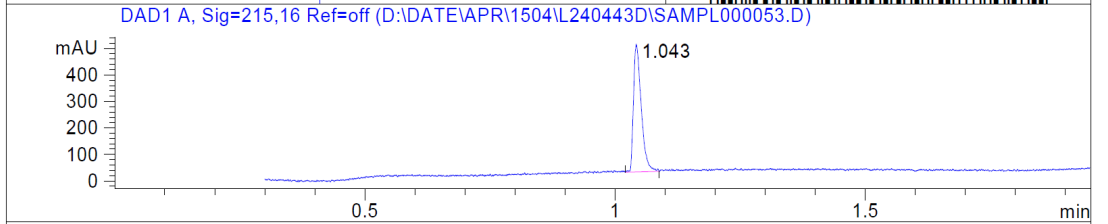
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Q227980\$2



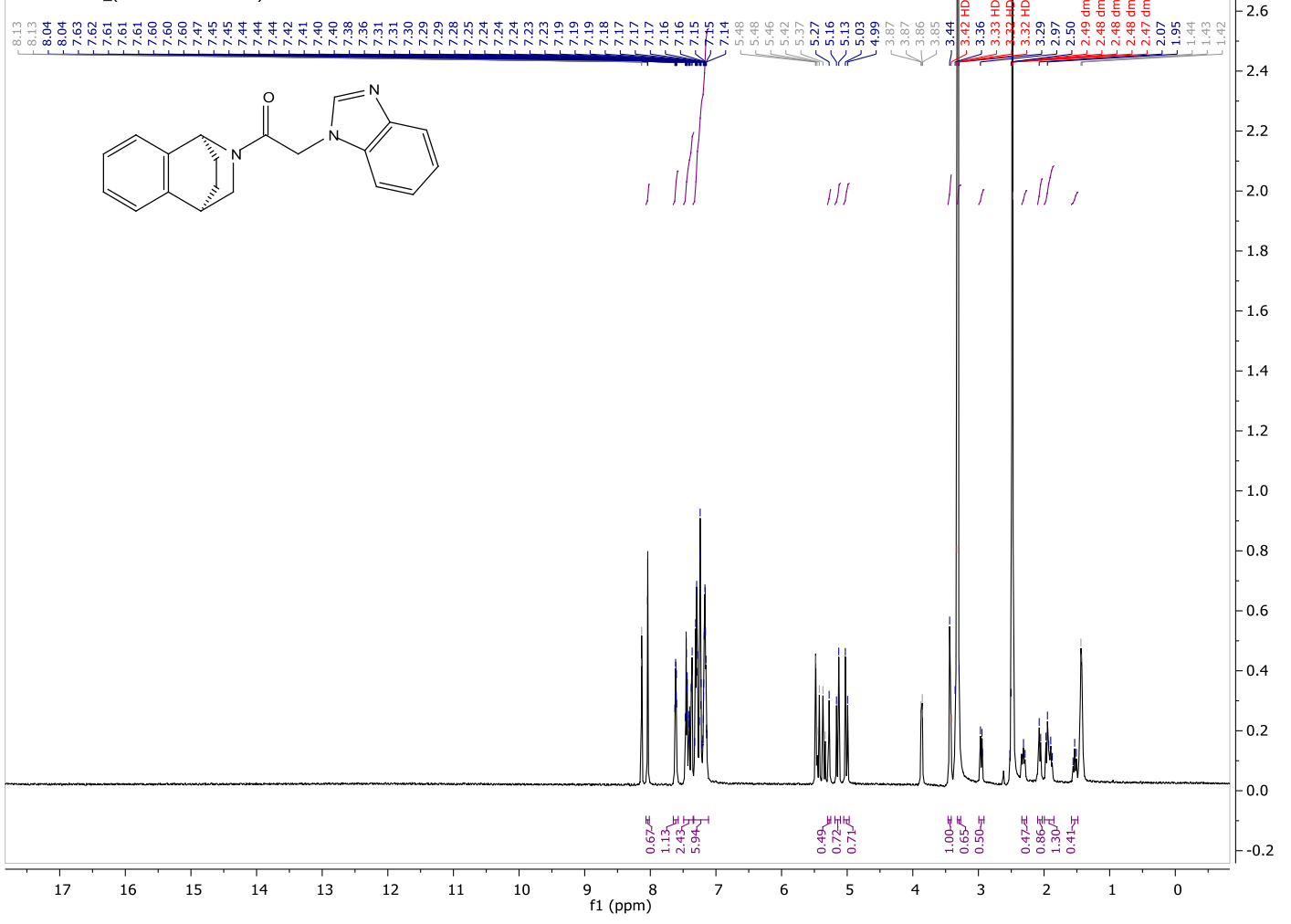
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Exact Mass 317.18

#	Time	Area%
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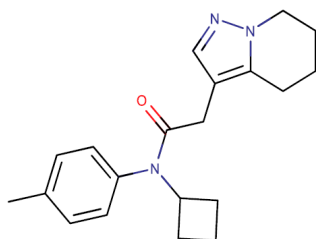
Z2876049675\_(ZINC001339780091)

Z2876049675\_(ZINC001339780091)



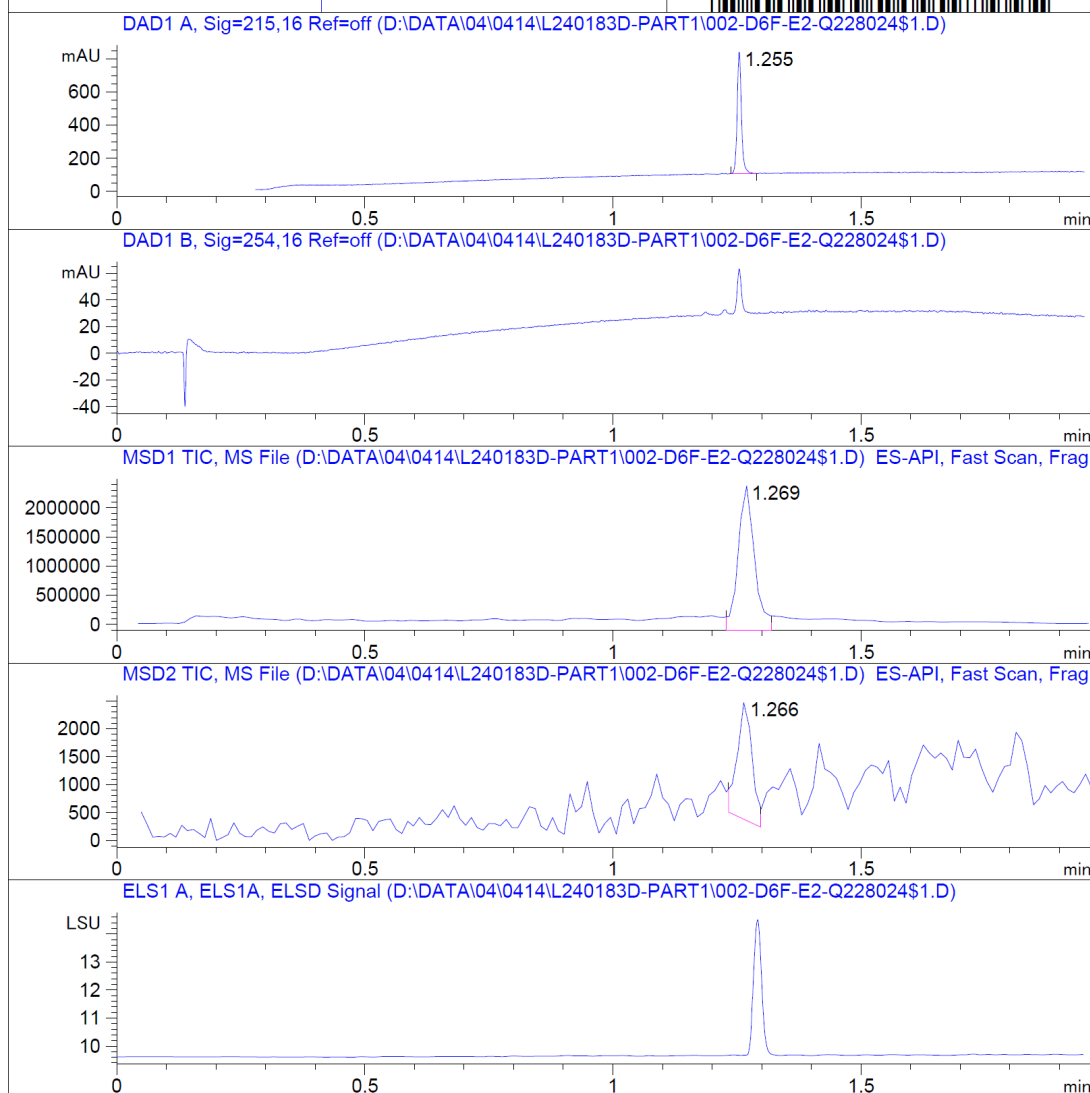
MaxPeak: 100.00%  
Ret\_Time: 1.255 min

# Q228024\$1

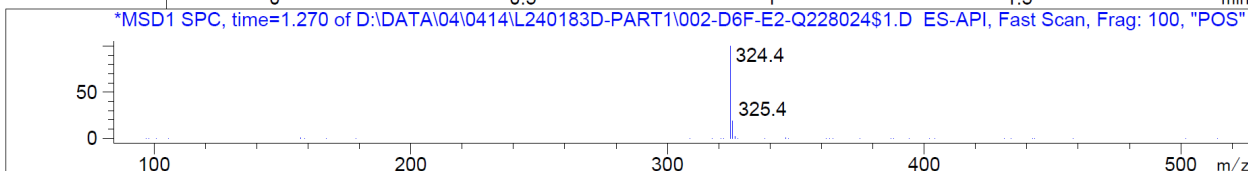


**Mol Wt** 323.43  
**Exact Mass** 323.24

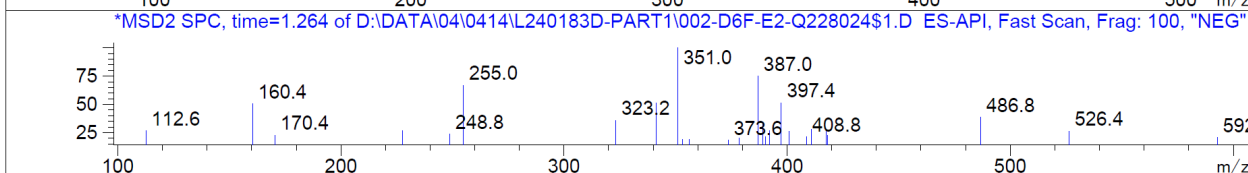
#	Time	Area%
1	1.255	100.00



RT 1.269

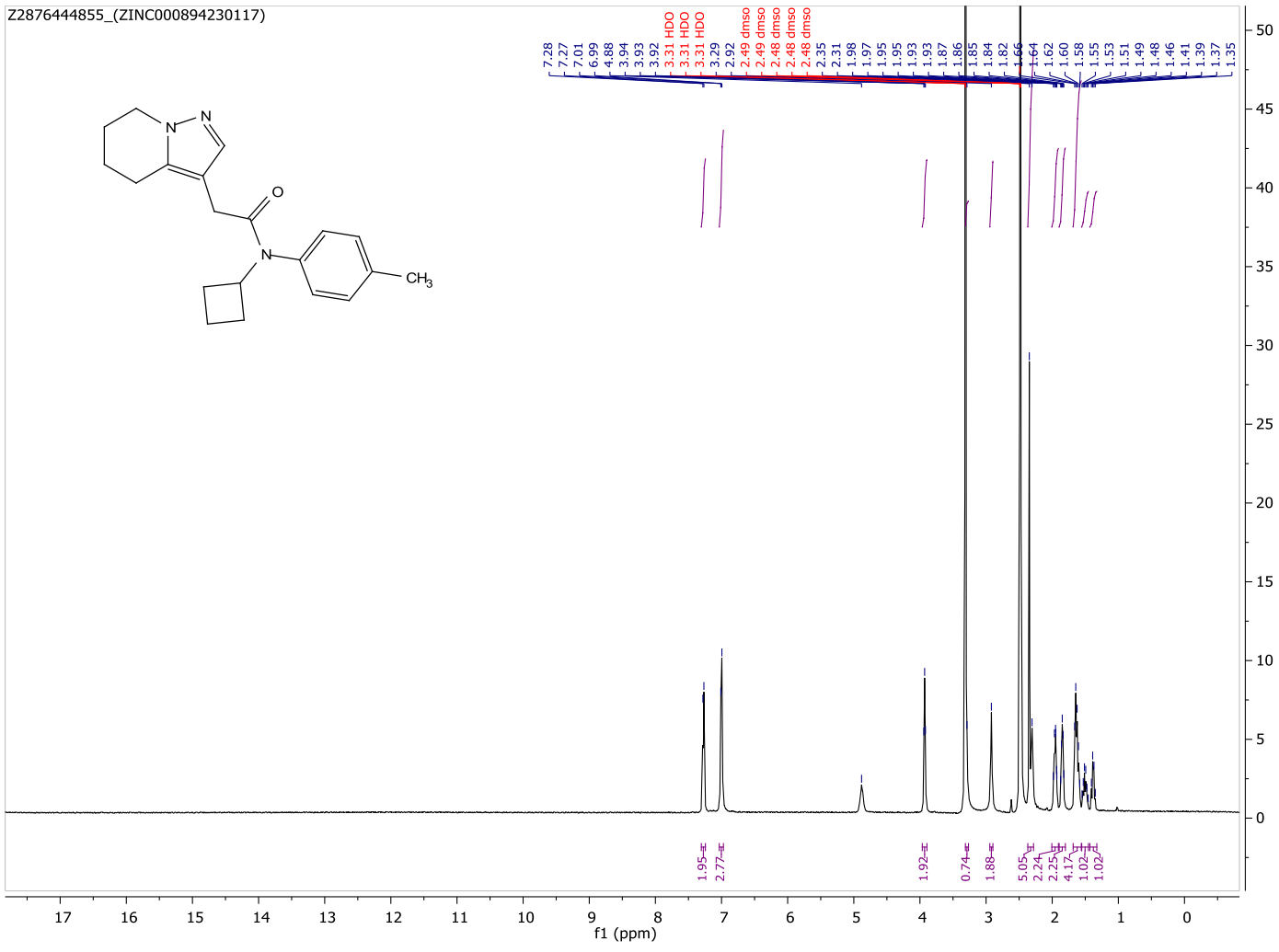
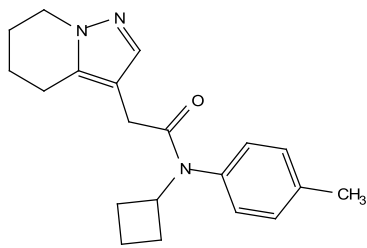


RT 1.266

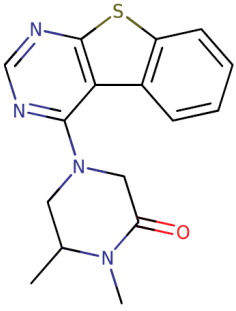


Z2876444855\_(ZINC000894230117)

Z2876444855\_(ZINC000894230117)



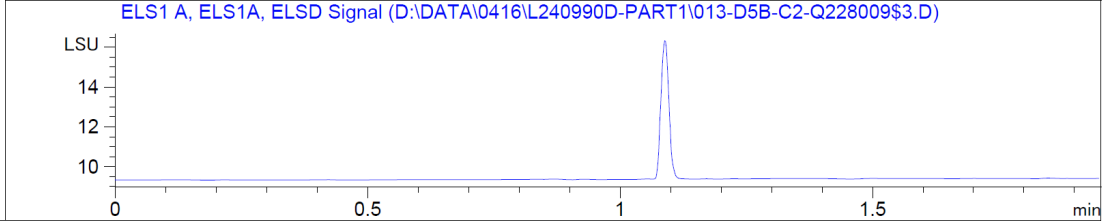
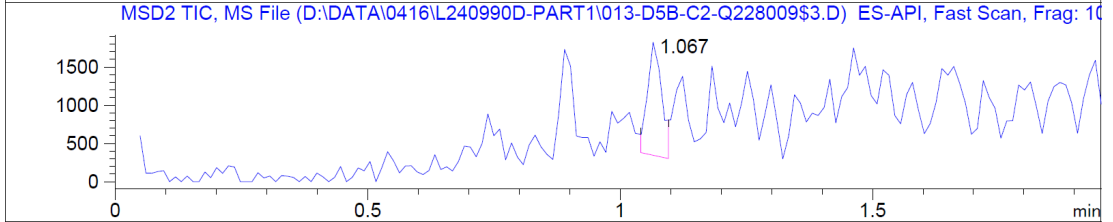
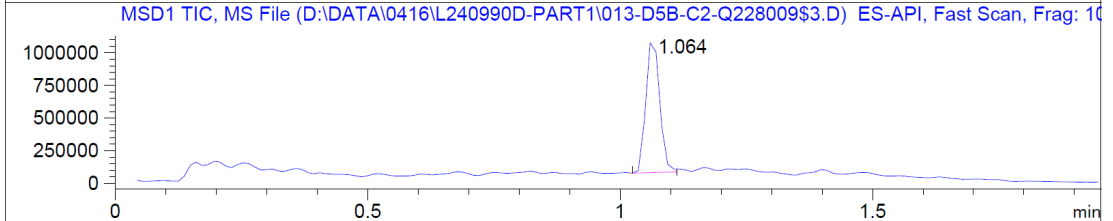
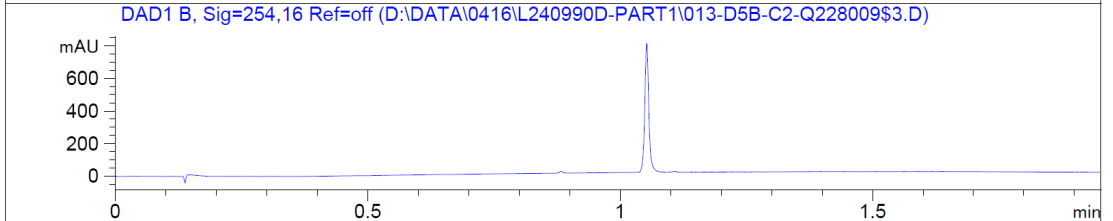
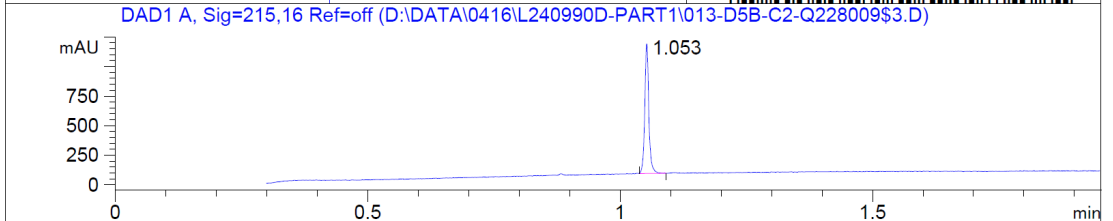
MaxPeak: 100.00%  
Ret\_Time: 1.053 min



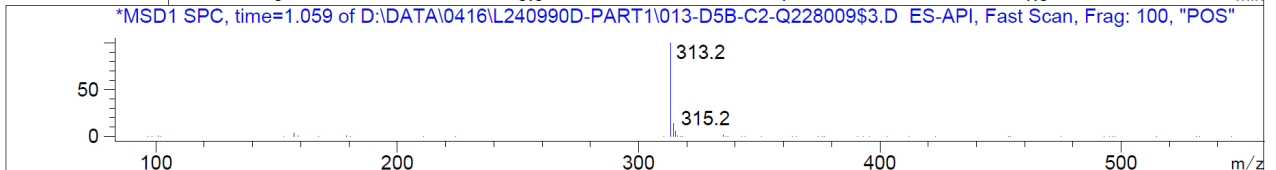
Mol Wt 312.39  
Exact Mass 312.12

#	Time	Area%
1	1.053	100.00

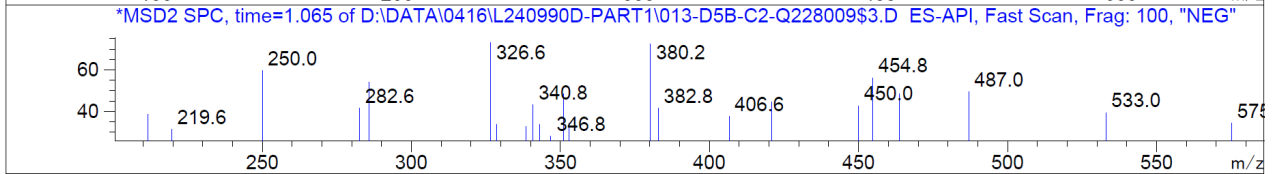
# Q228009\$3



RT 1.064

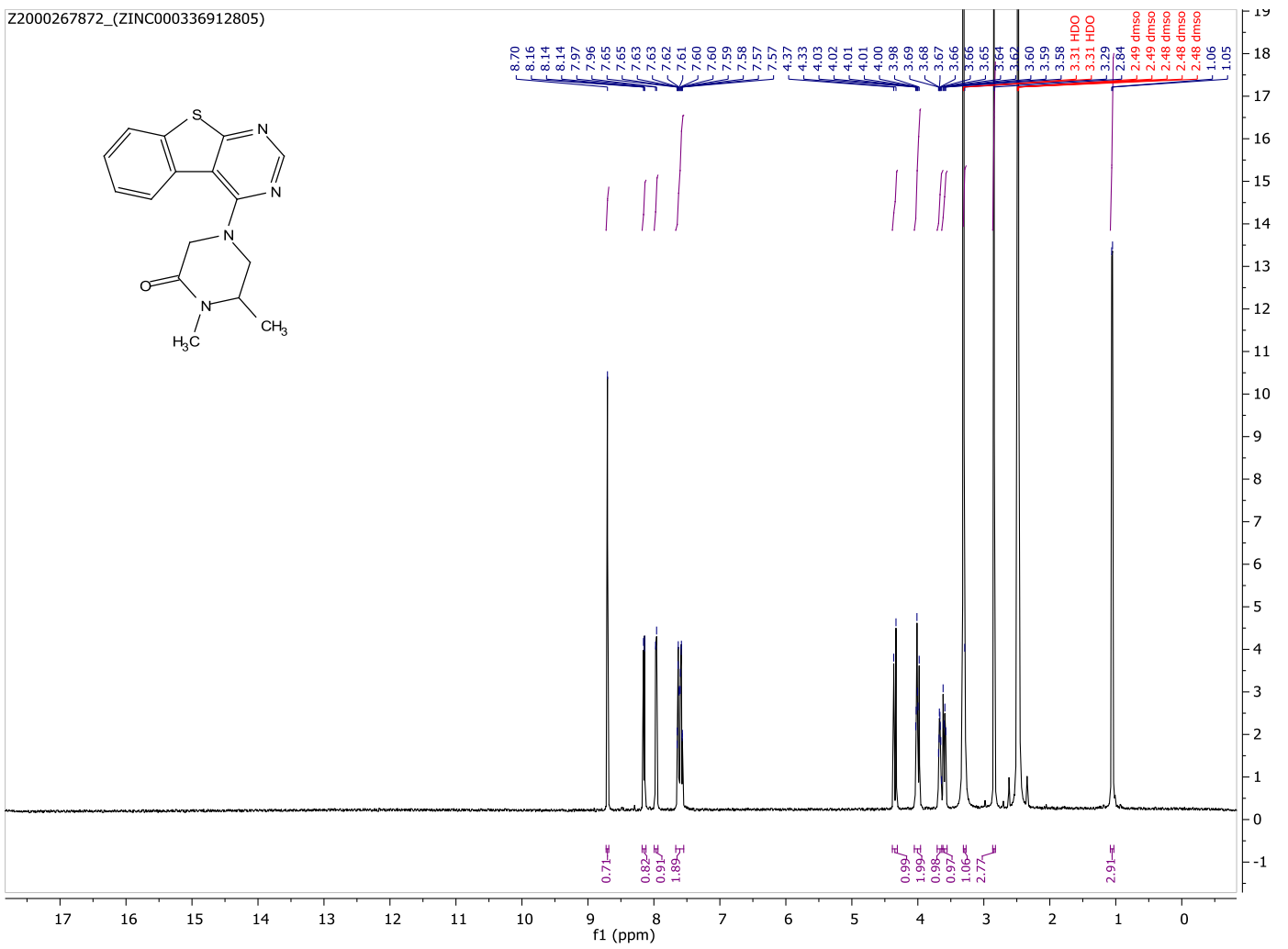
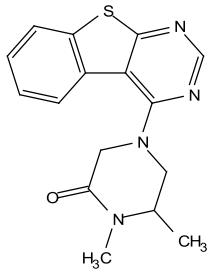


RT 1.067

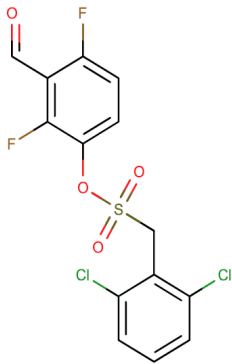


Z2000267872\_(ZINC000336912805)

Z2000267872\_(ZINC000336912805)



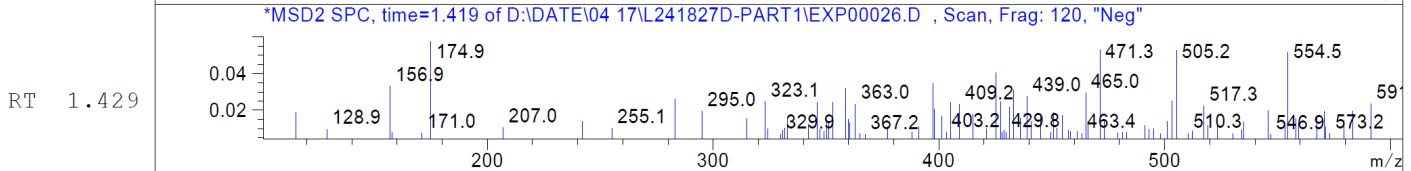
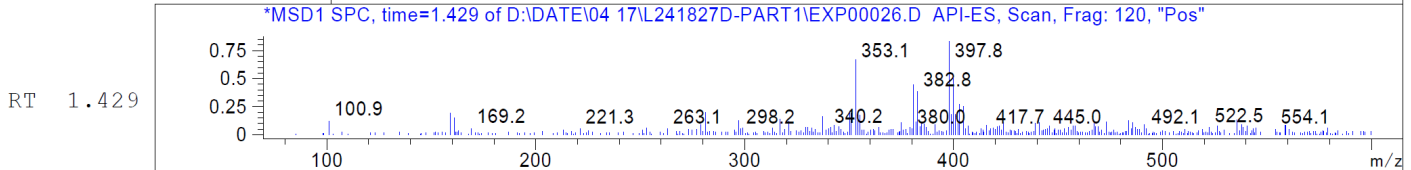
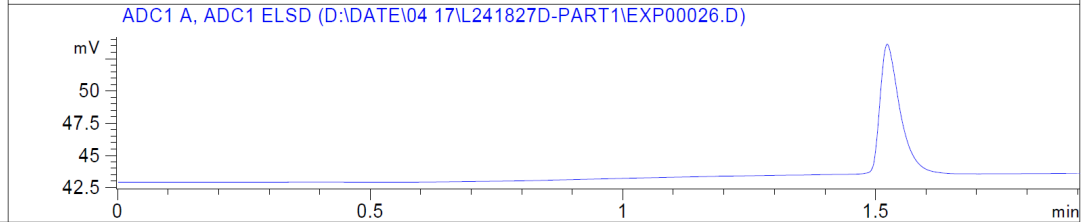
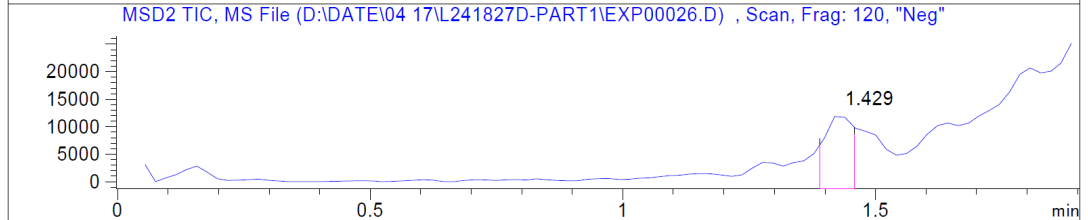
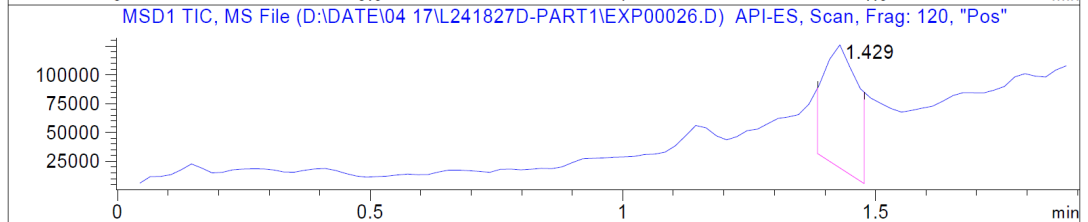
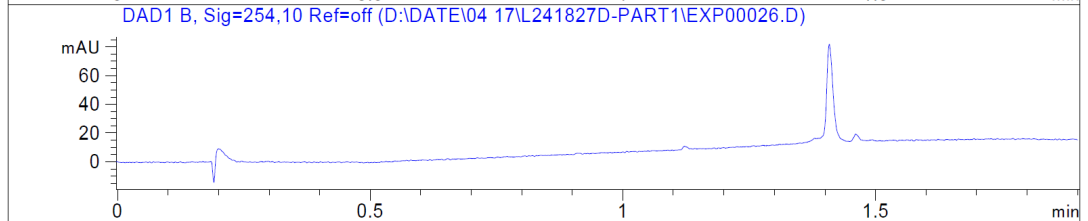
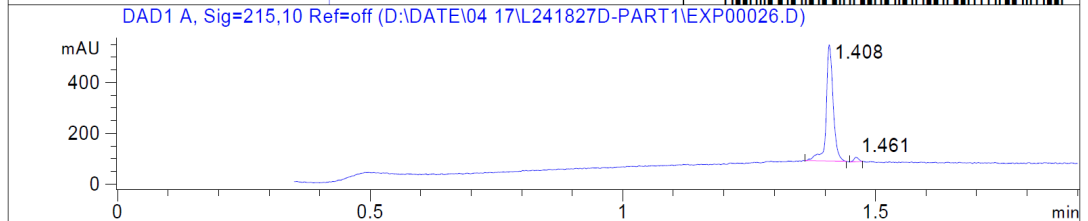
MaxPeak: 97.45%  
Ret\_Time: 1.408 min



Mol Wt 381.18  
Exact Mass 379.95

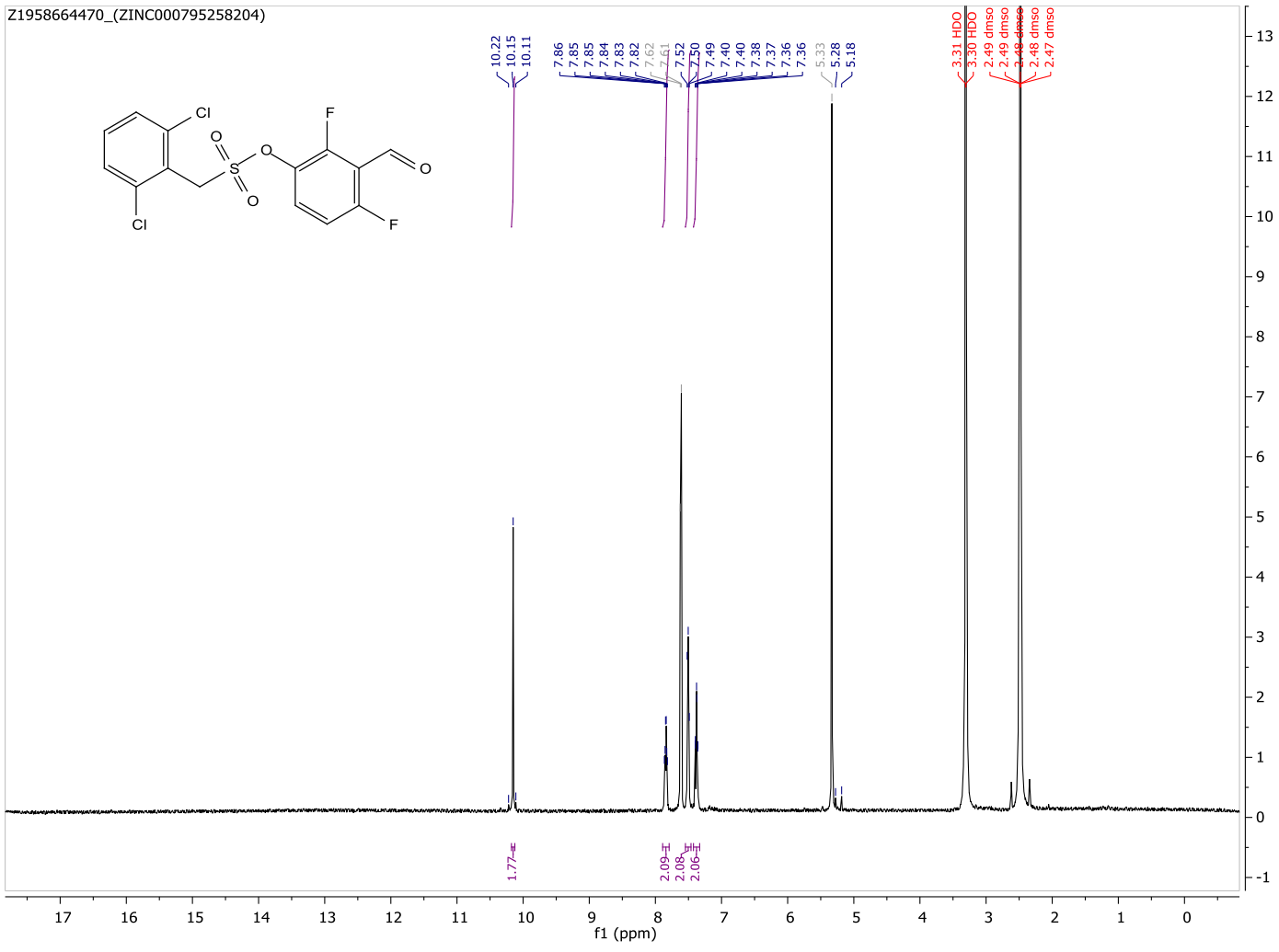
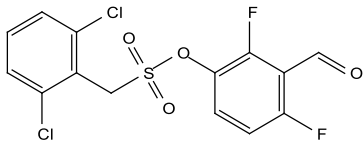
#	Time	Area%
1	1.408	97.45
2	1.461	2.55

Q260270\$3



Z1958664470\_(ZINC000795258204)

Z1958664470\_(ZINC000795258204)

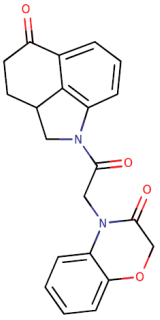




# Q260236\$1

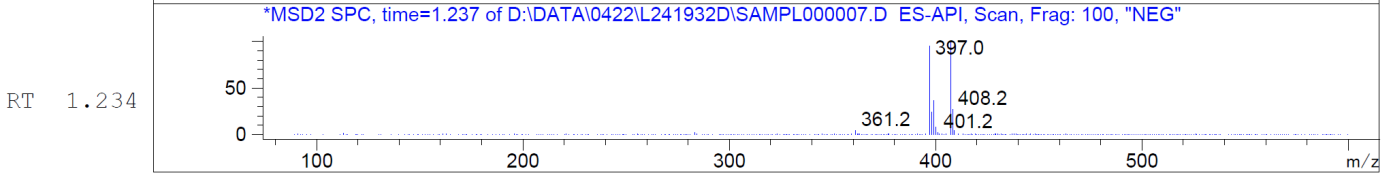
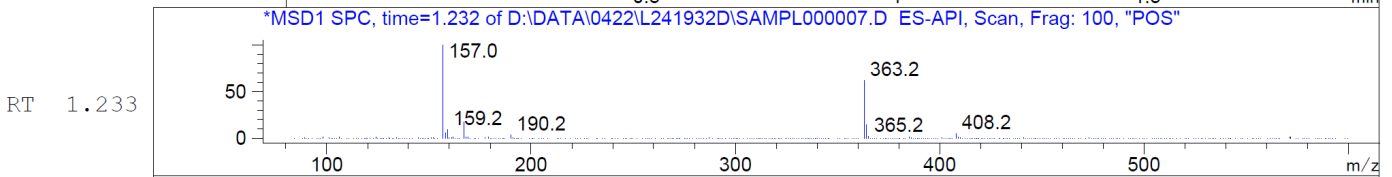
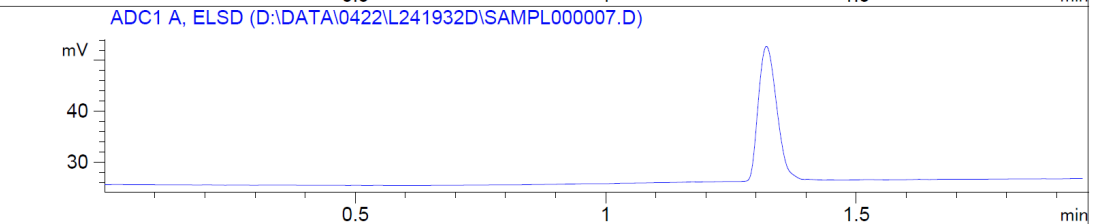
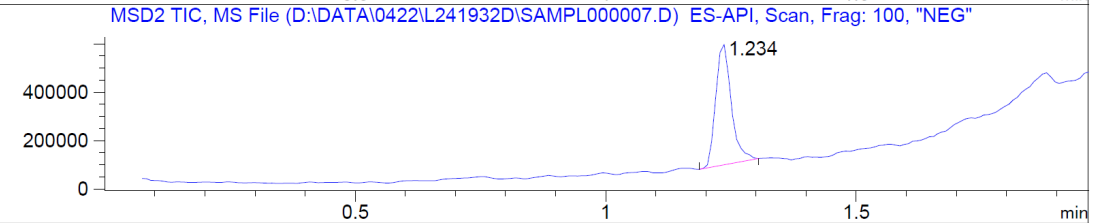
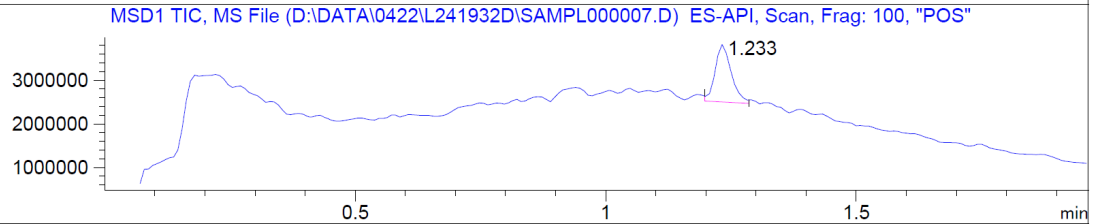
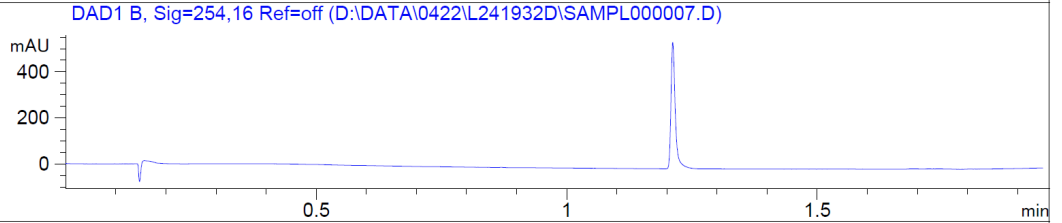
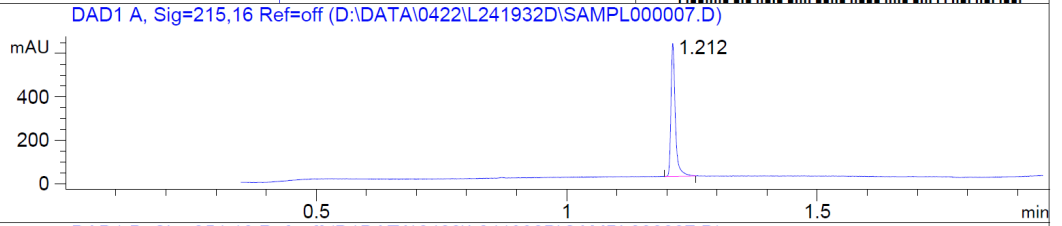


MaxPeak: 100.00%  
Ret\_Time: 1.212 min



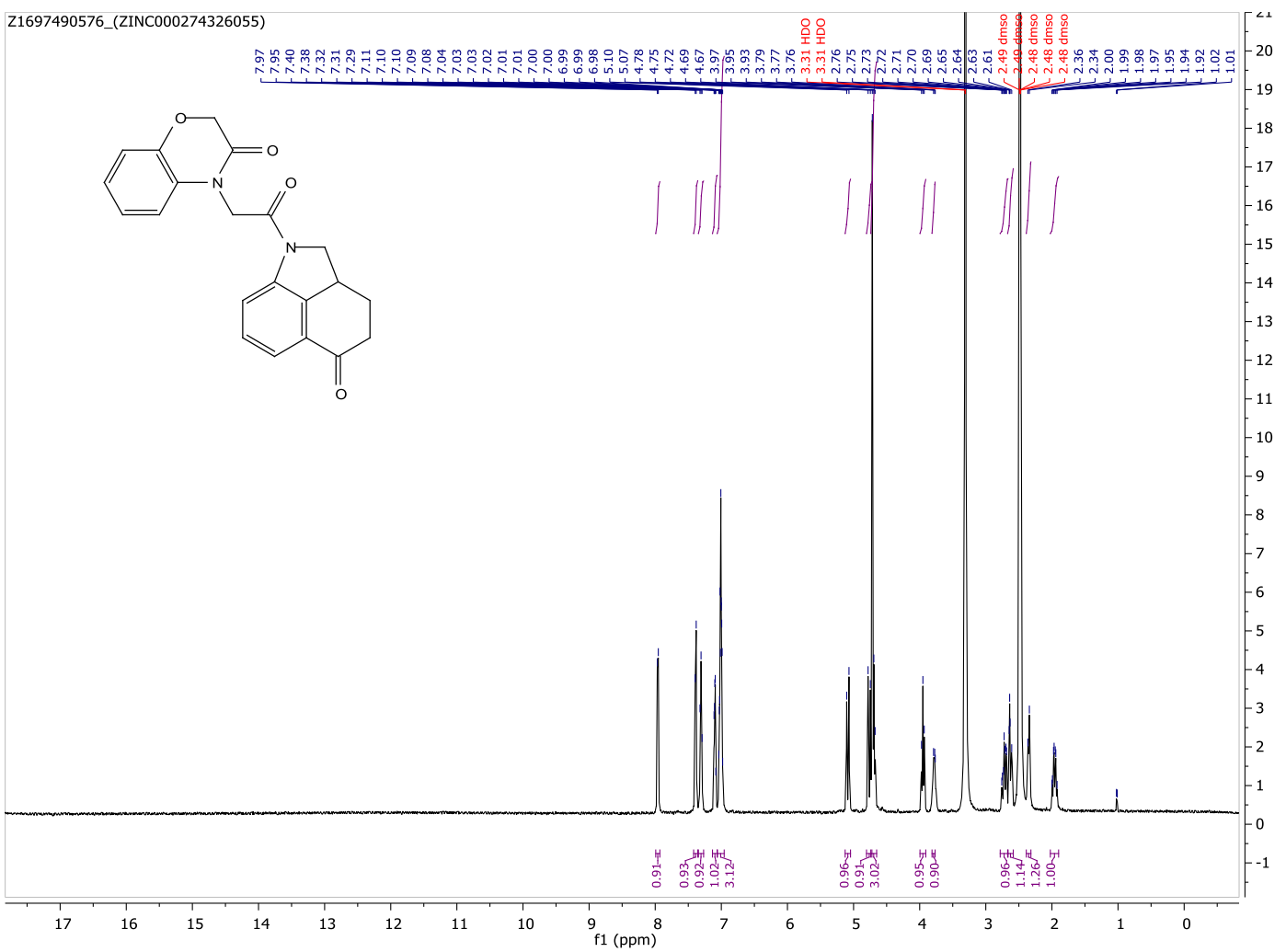
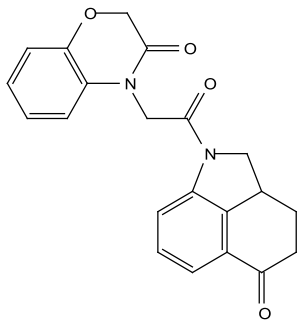
Mol Wt 362.38  
Exact Mass 362.14

#	Time	Area%
1	1.212	100.00



Z1697490576\_(ZINC000274326055)

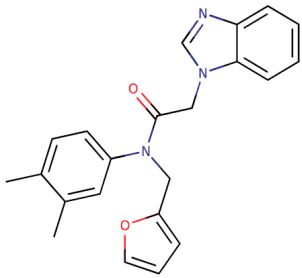
Z1697490576\_(ZINC000274326055)



# Q260188\$1

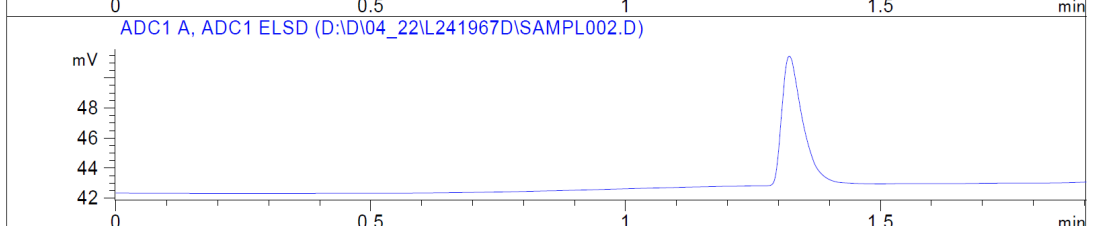
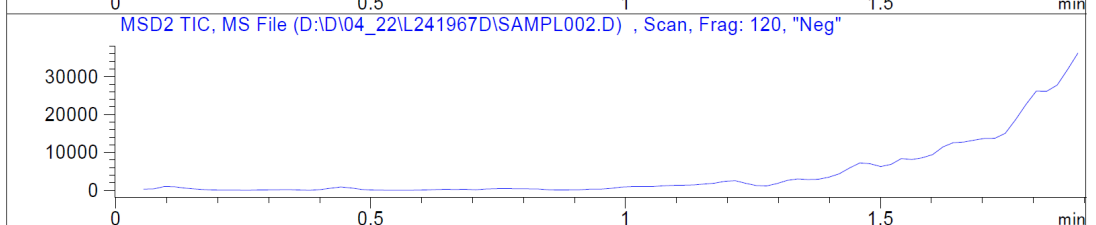
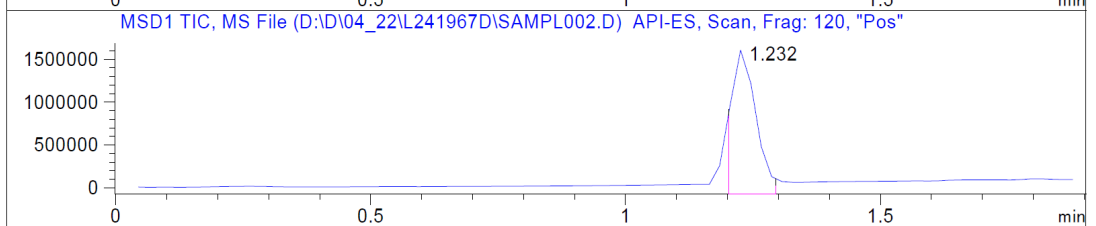
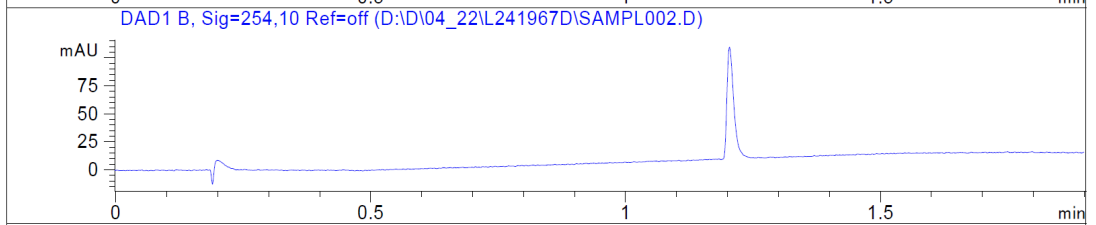
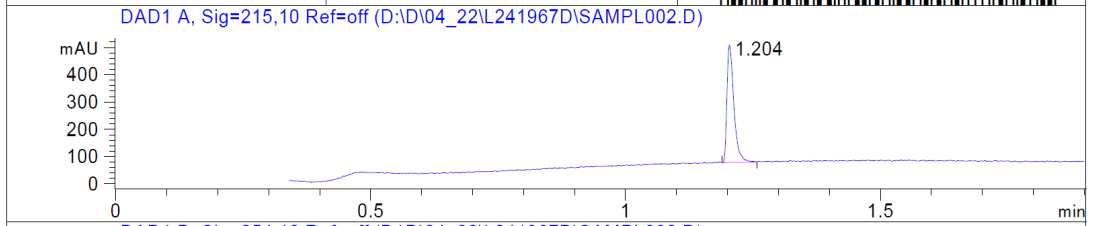


MaxPeak: 100.00%  
Ret\_Time: 1.204 min

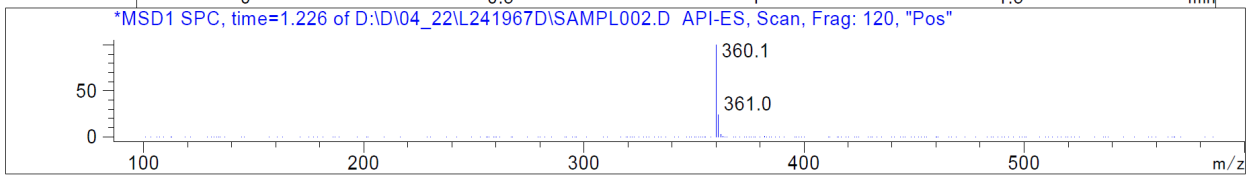


**Mol Wt** 359.42  
**Exact Mass** 359.19

#	Time	Area%
1	1.204	100.00

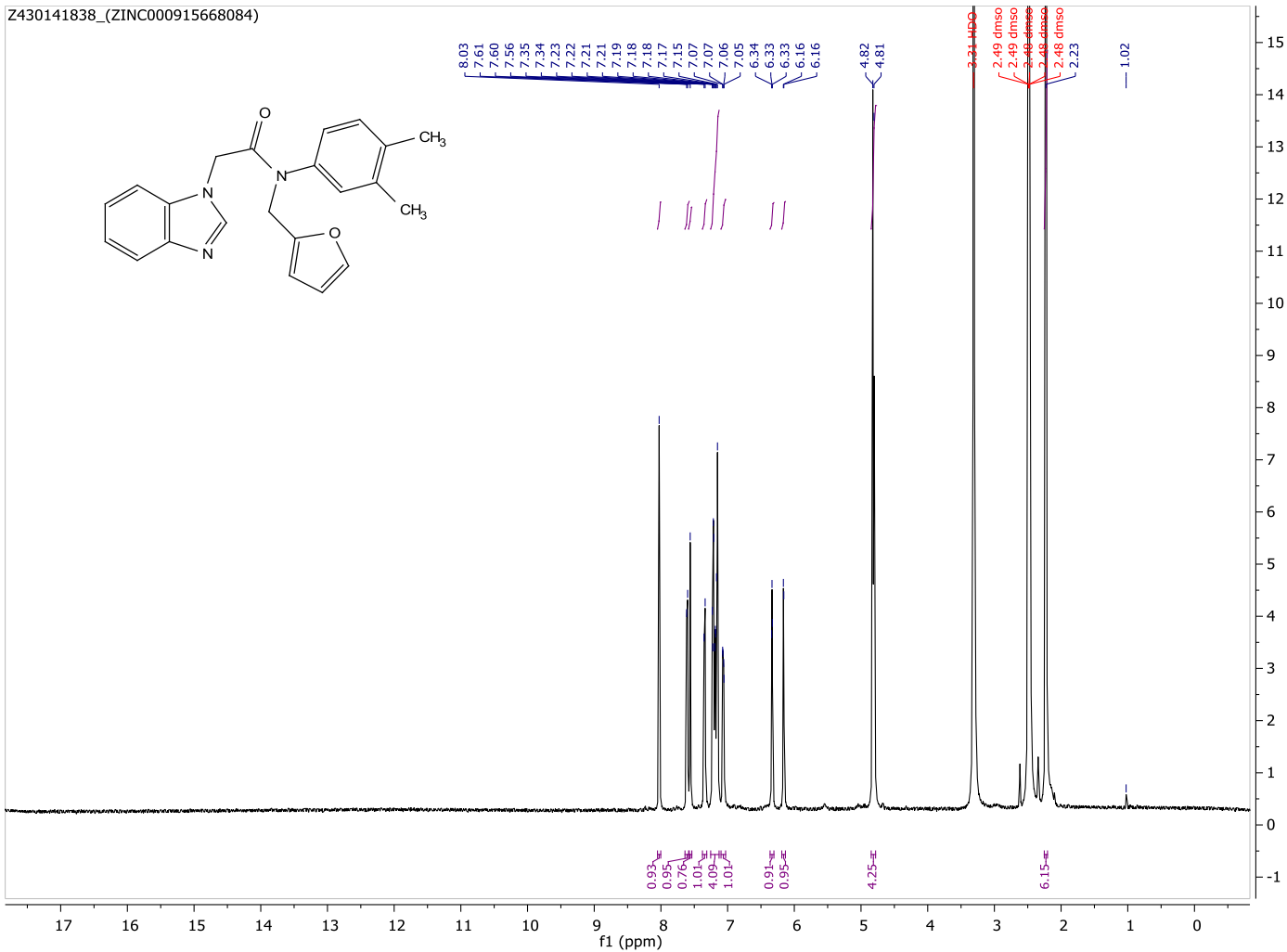
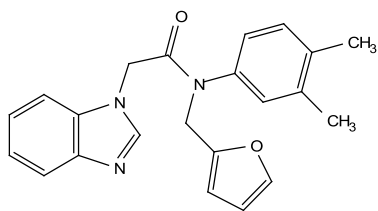


RT 1.232

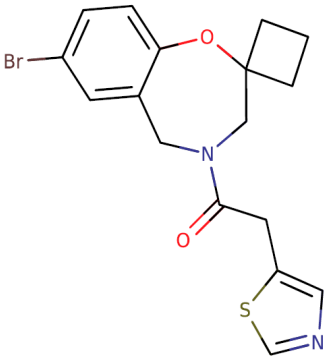


Z430141838\_(ZINC000915668084)

Z430141838\_(ZINC000915668084)



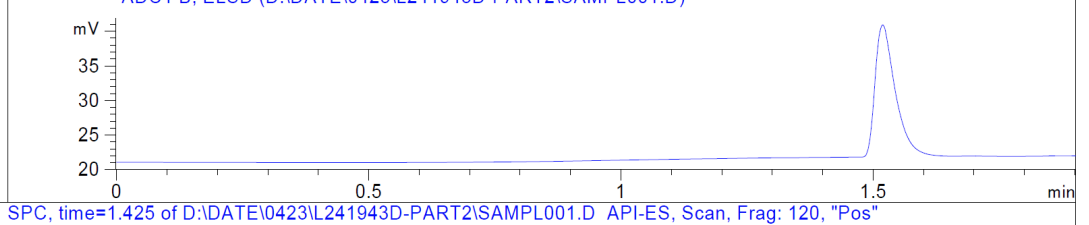
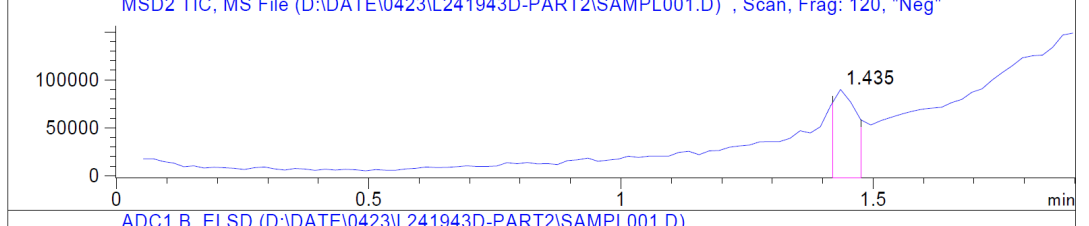
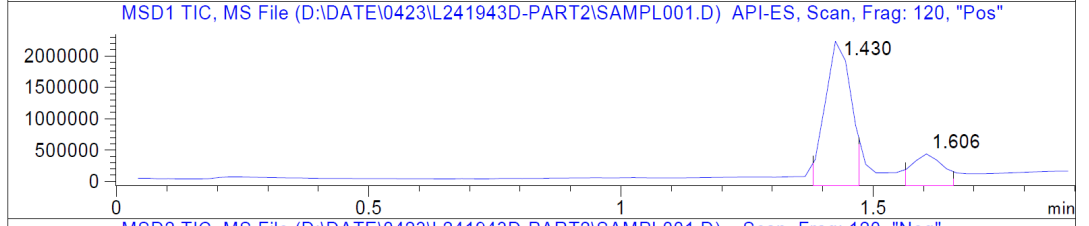
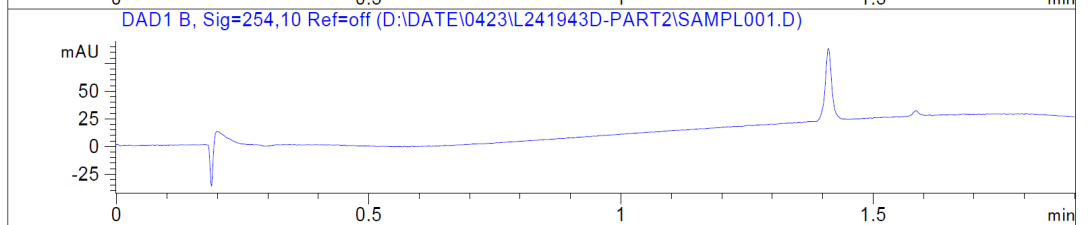
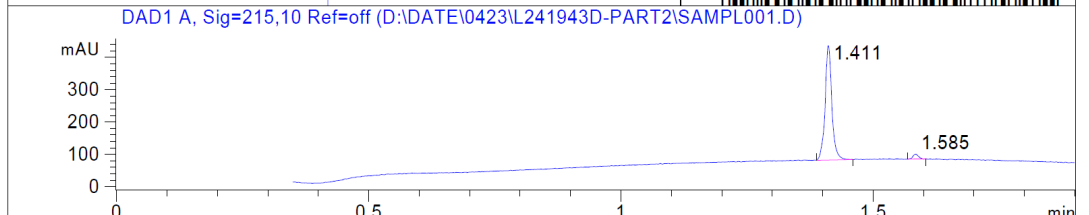
MaxPeak: 96.66%  
Ret\_Time: 1.411 min



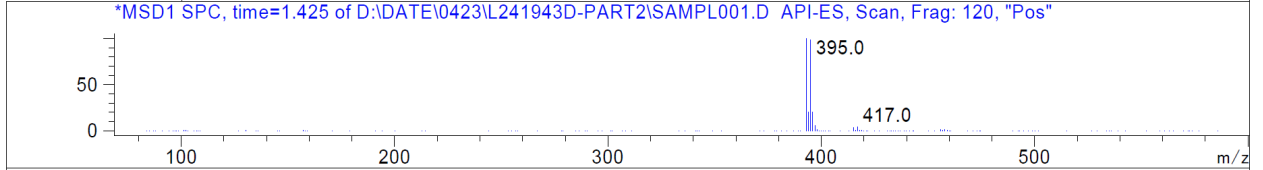
Mol Wt 393.3  
Exact Mass 394.04

#	Time	Area%
1	1.411	96.66
2	1.585	3.34

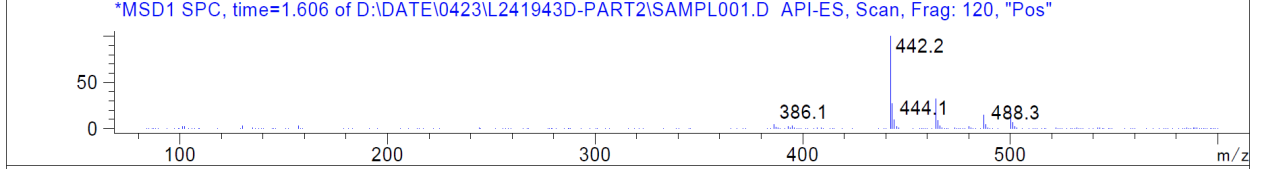
Q260276\$1



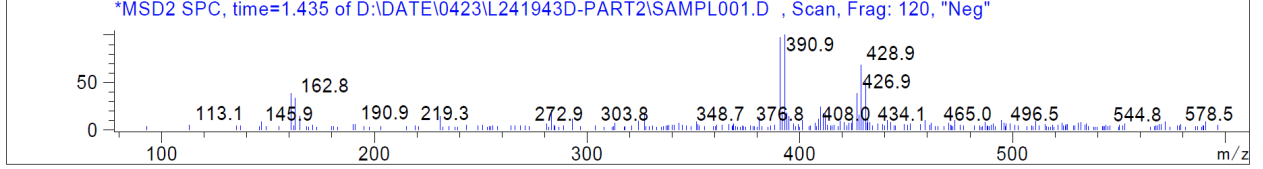
RT 1.430



RT 1.606

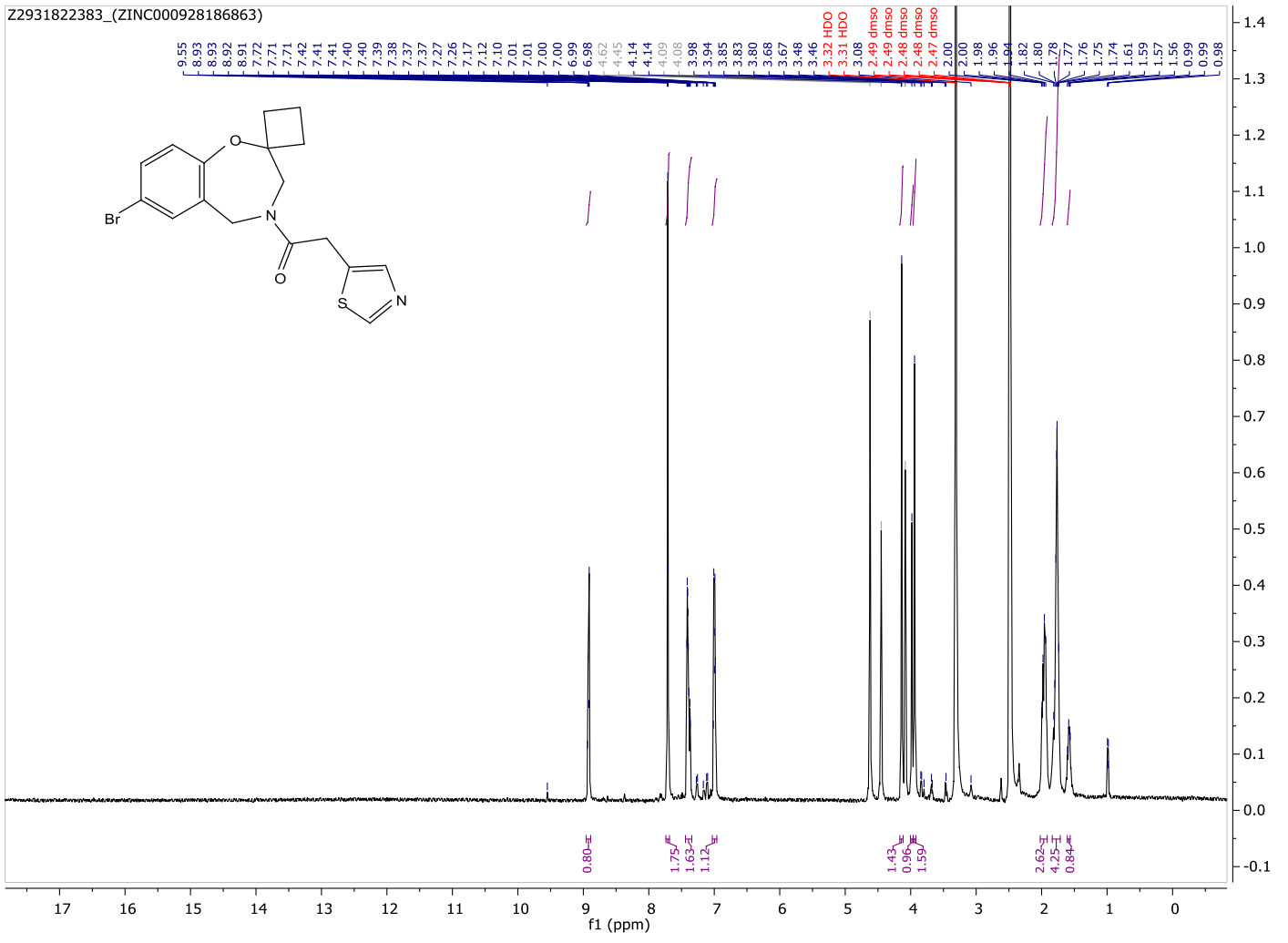
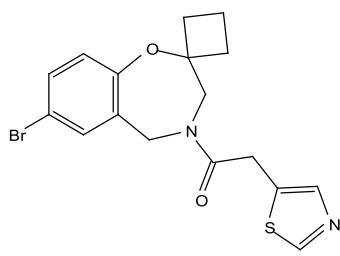


RT 1.435

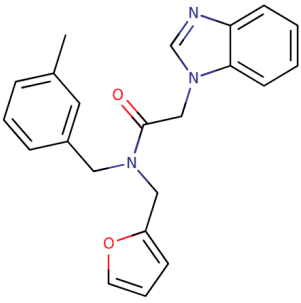


Z2931822383\_(ZINC000928186863)

Z2931822383\_(ZINC000928186863)



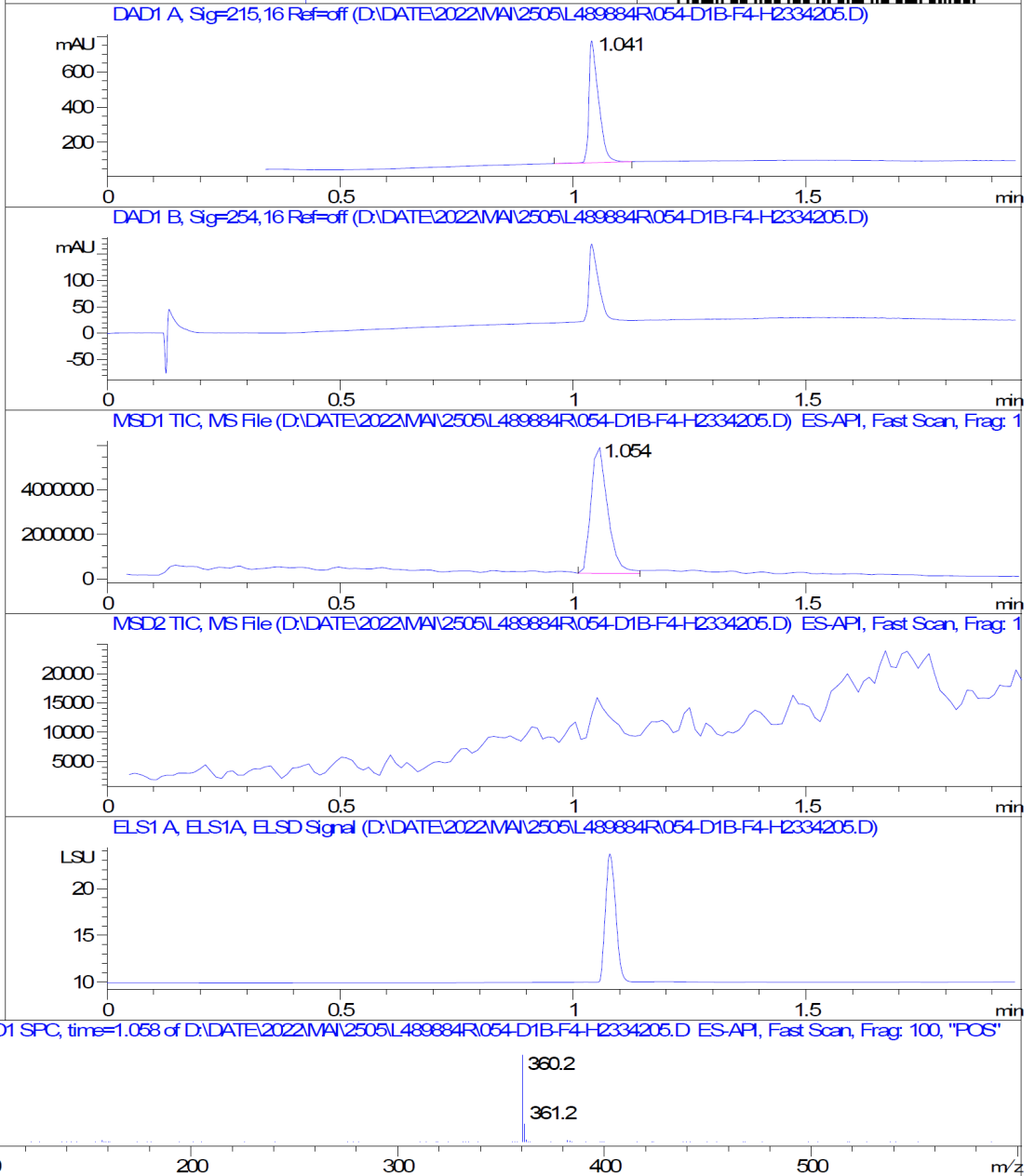
MaxPeak: 100.00%  
Ret\_Time: 1.041 min



Mol Wt 359.42  
Exact Mass 359.19

#	Time	Area%
1	1.041	100.00

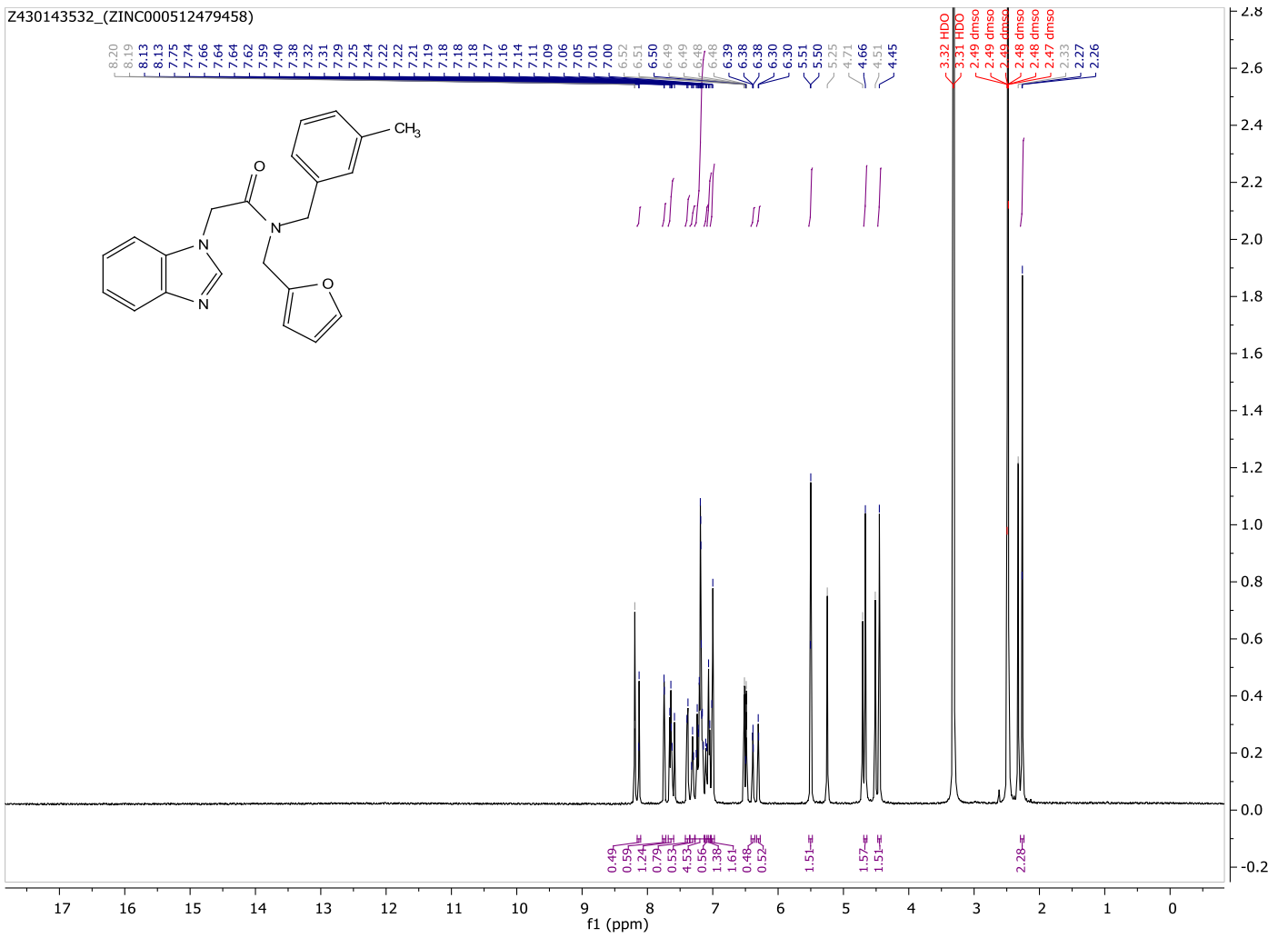
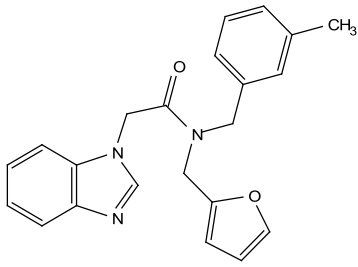
# H2334205



RT 1.054

Z430143532\_(ZINC000512479458)

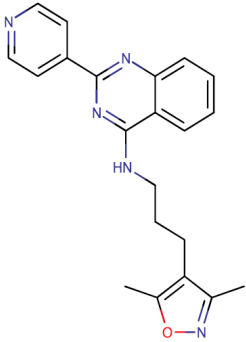
Z430143532\_(ZINC000512479458)





MaxPeak: 100.00%  
Ret\_Time: 1.099 min

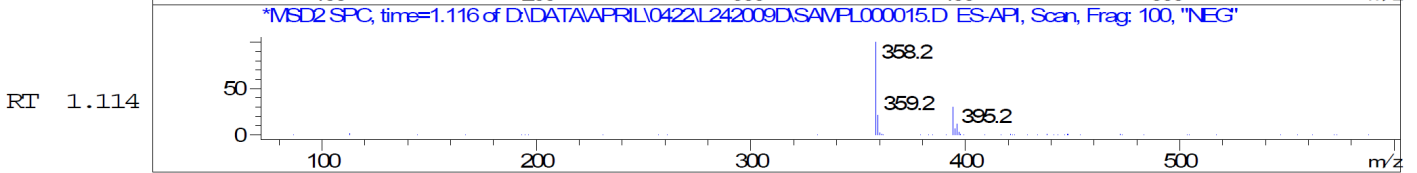
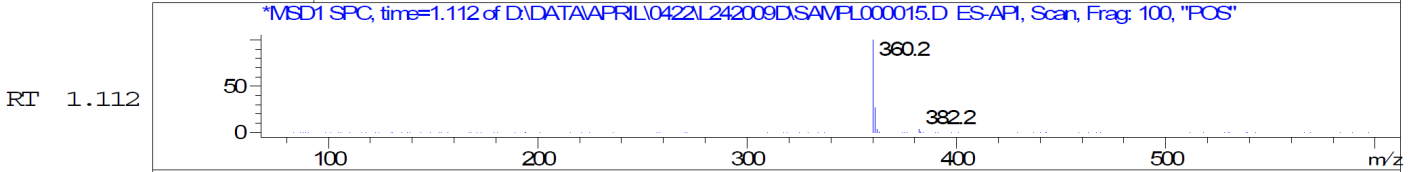
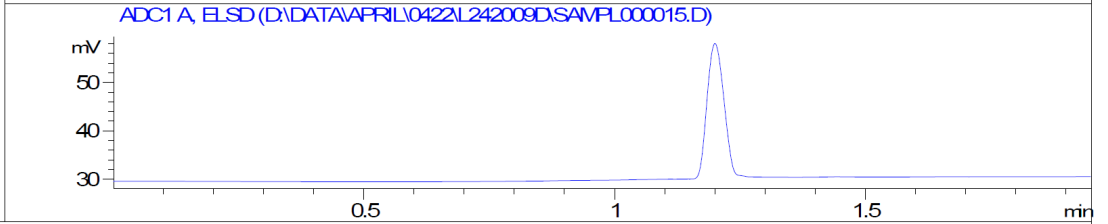
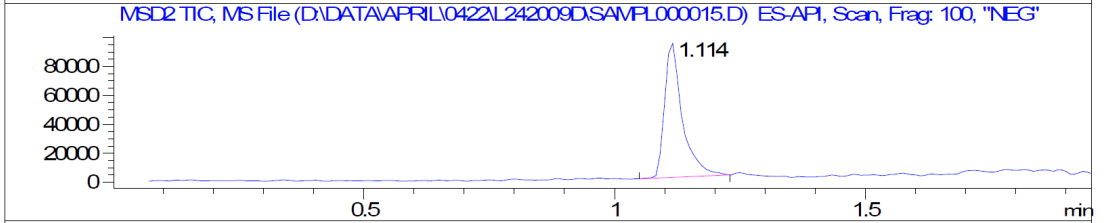
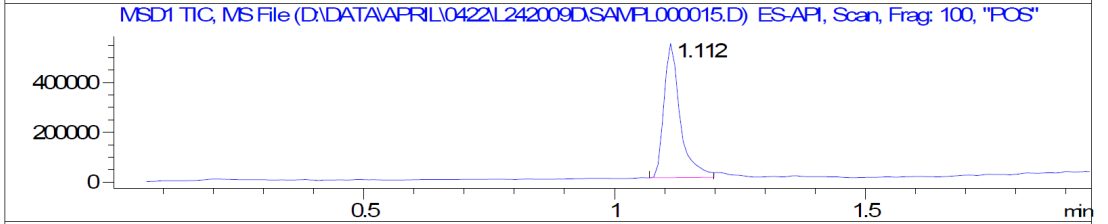
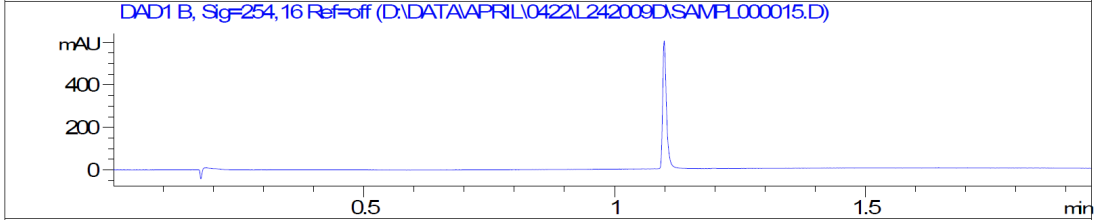
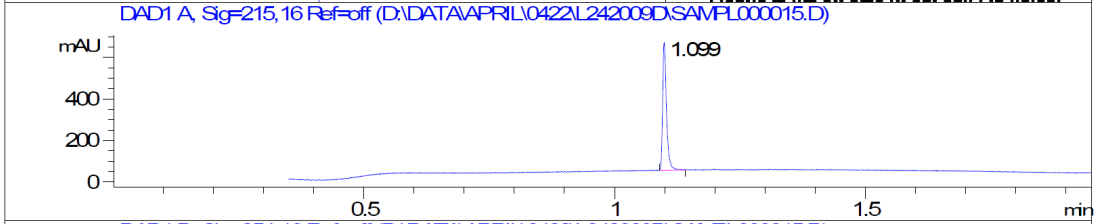
Q260300\$2



Mol Wt 359.42

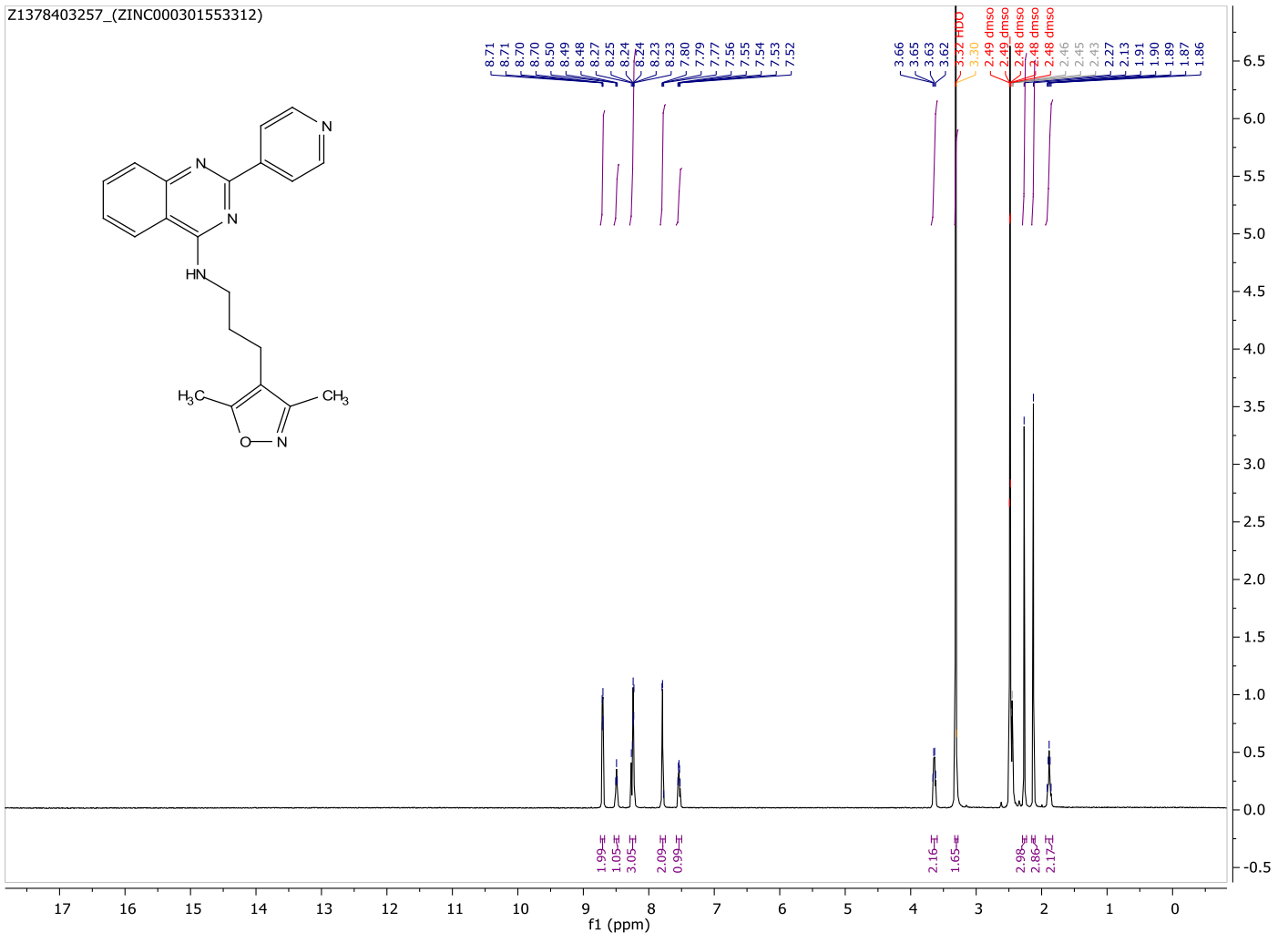
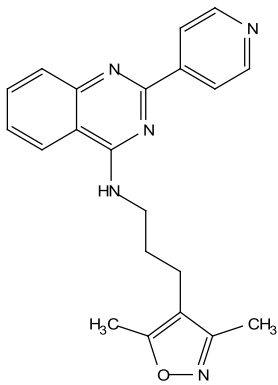
Exact Mass 359.2

#	Time	Area%
1	1.099	100.00



Z1378403257\_(ZINC000301553312)

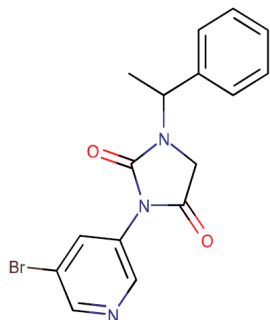
Z1378403257\_(ZINC000301553312)



# Q260256\$3

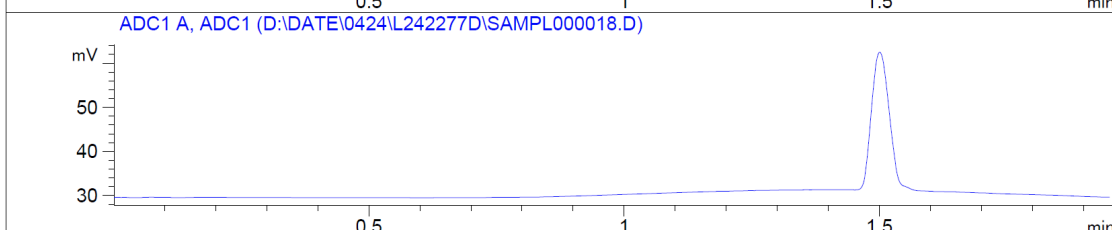
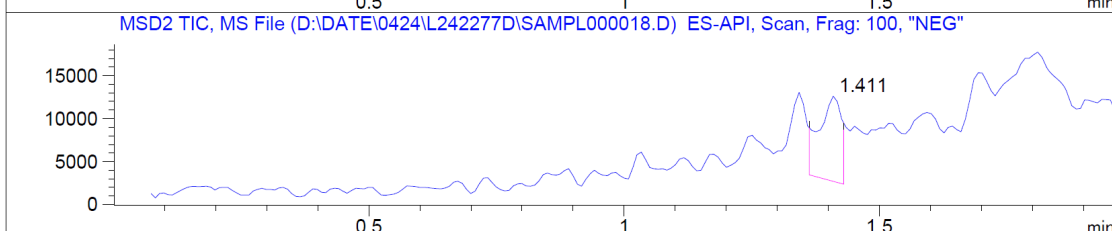
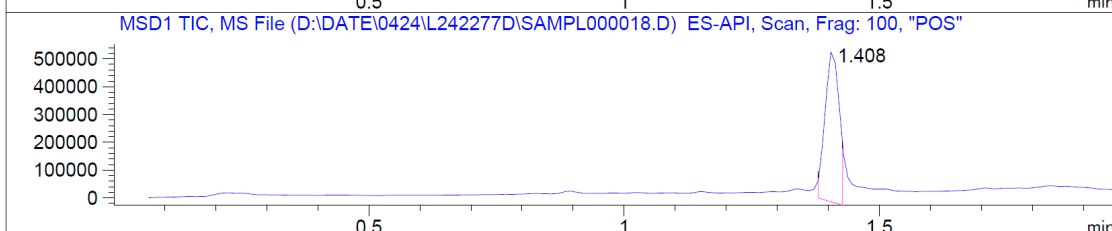
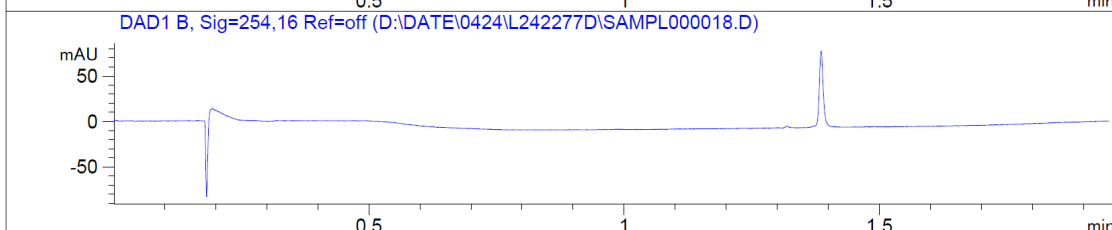
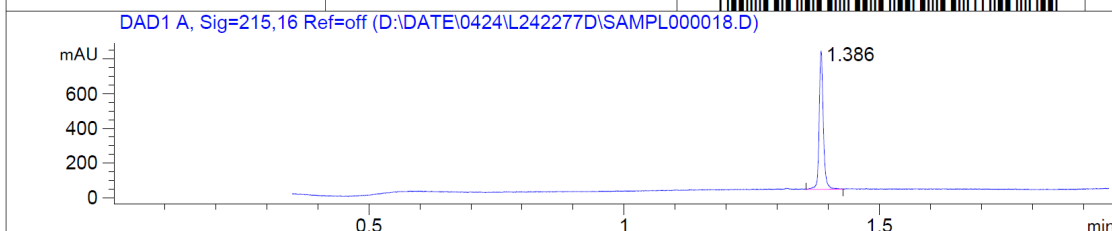


MaxPeak: 100.00%  
Ret\_Time: 1.386 min

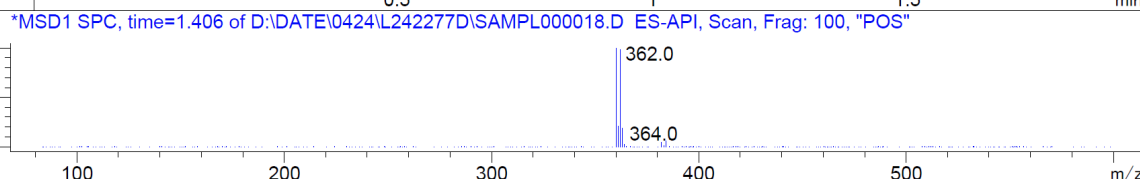


Mol Wt 360.2  
Exact Mass 359.04

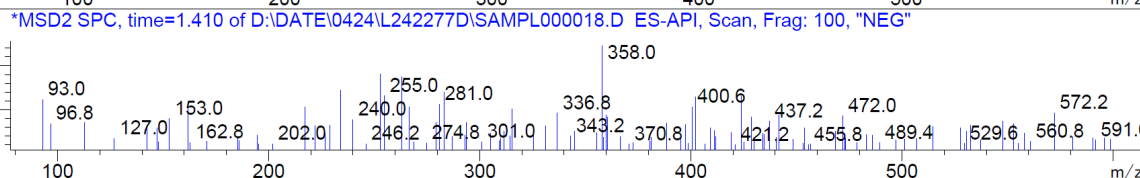
#	Time	Area%
1	1.386	100.00



RT 1.408

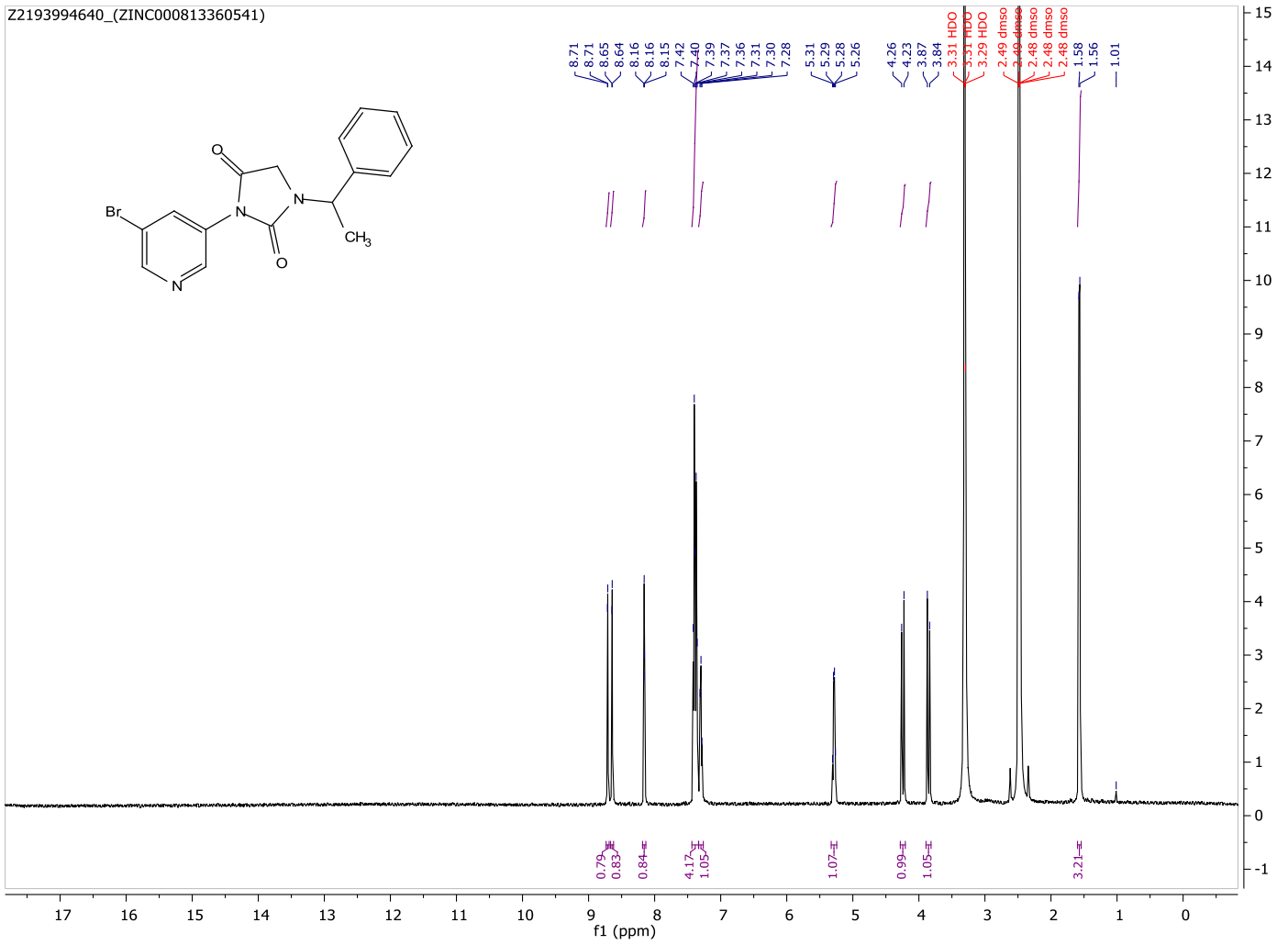
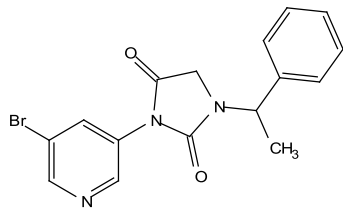


RT 1.411

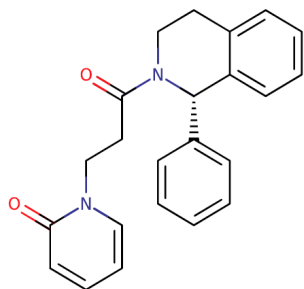


Z2193994640\_(ZINC000813360541)

Z2193994640\_(ZINC000813360541)



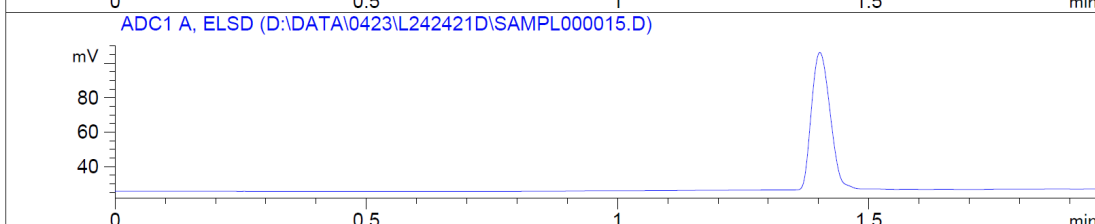
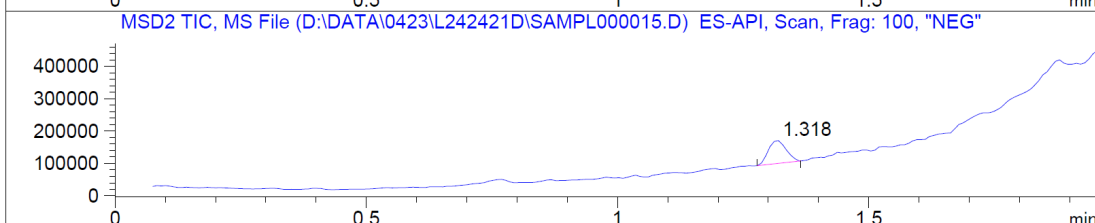
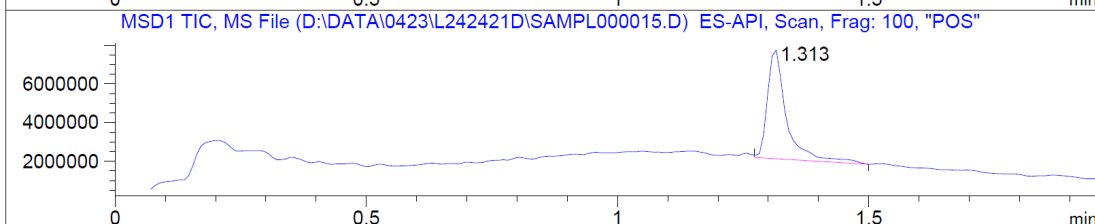
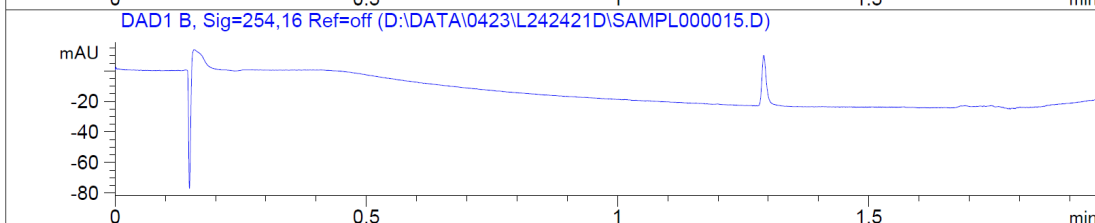
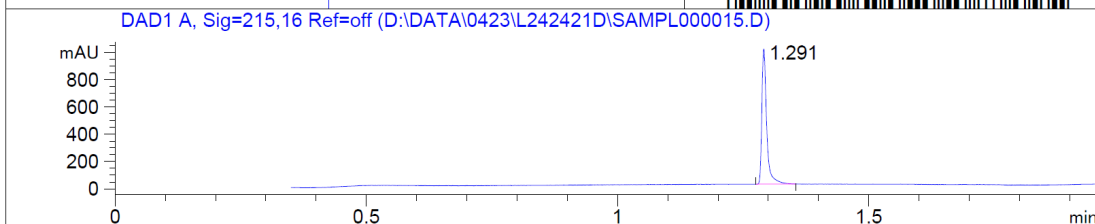
MaxPeak: 100.00%  
 Ret\_Time: 1.291 min



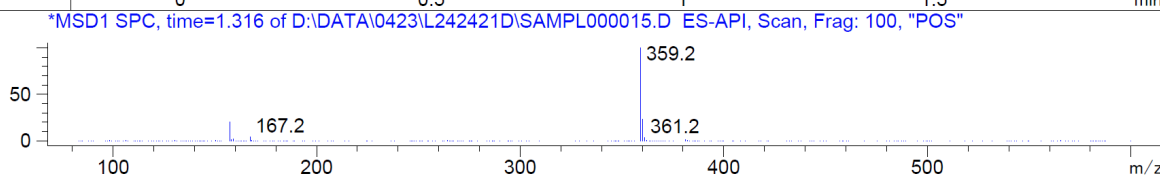
**Mol Wt** 358.43  
**Exact Mass** 358.2

#	Time	Area%
1	1.291	100.00

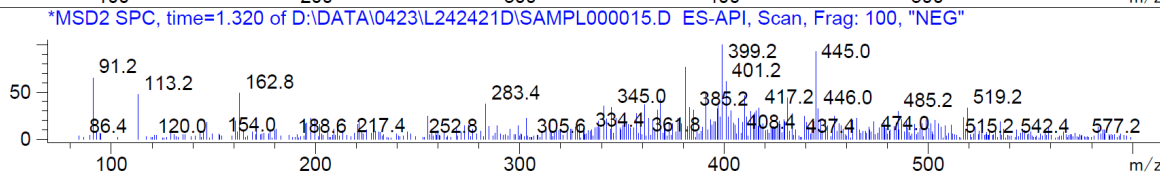
Q260233\$2



RT 1.313

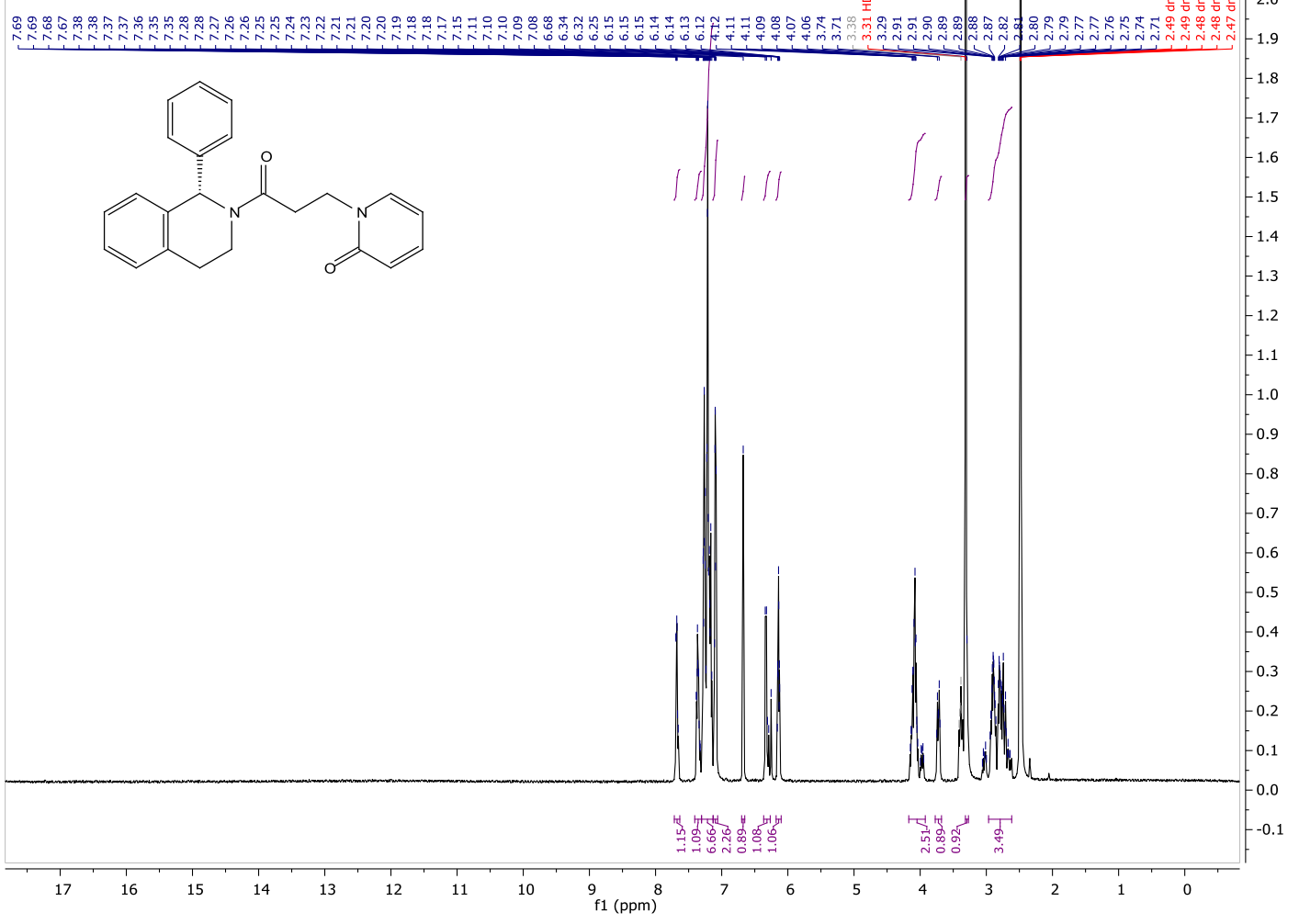


RT 1.318



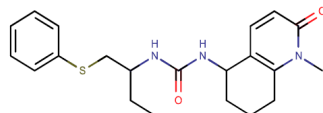
Z2232119003\_(ZINC000594542103)

Z2232119003\_(ZINC000594542103)



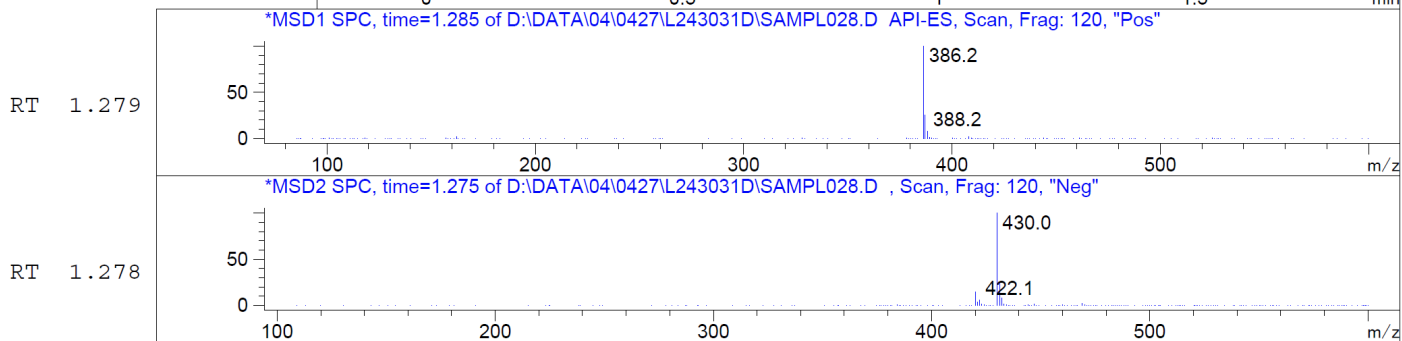
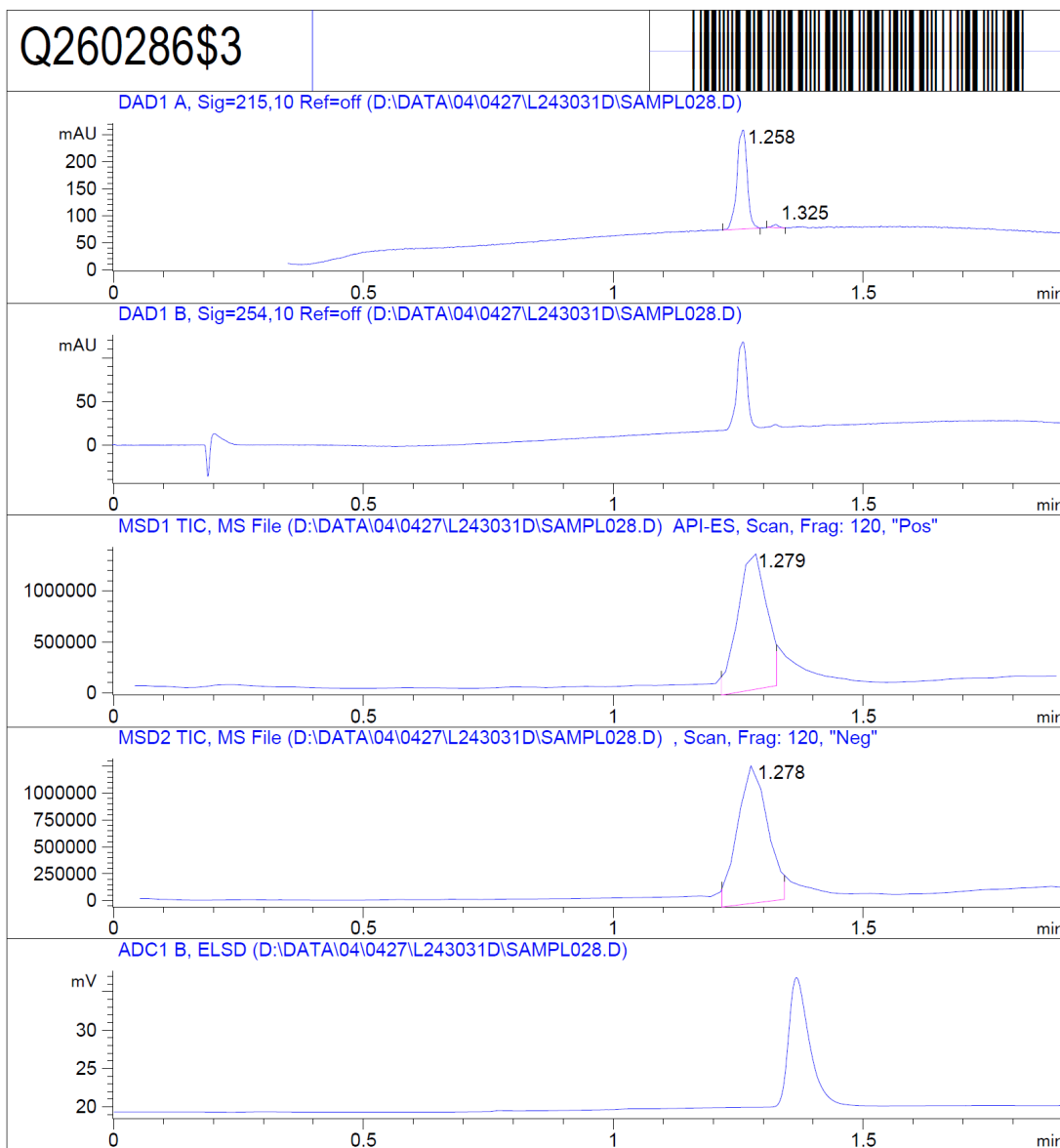
MaxPeak: 98.15%  
Ret\_Time: 1.258 min

Q260286\$3



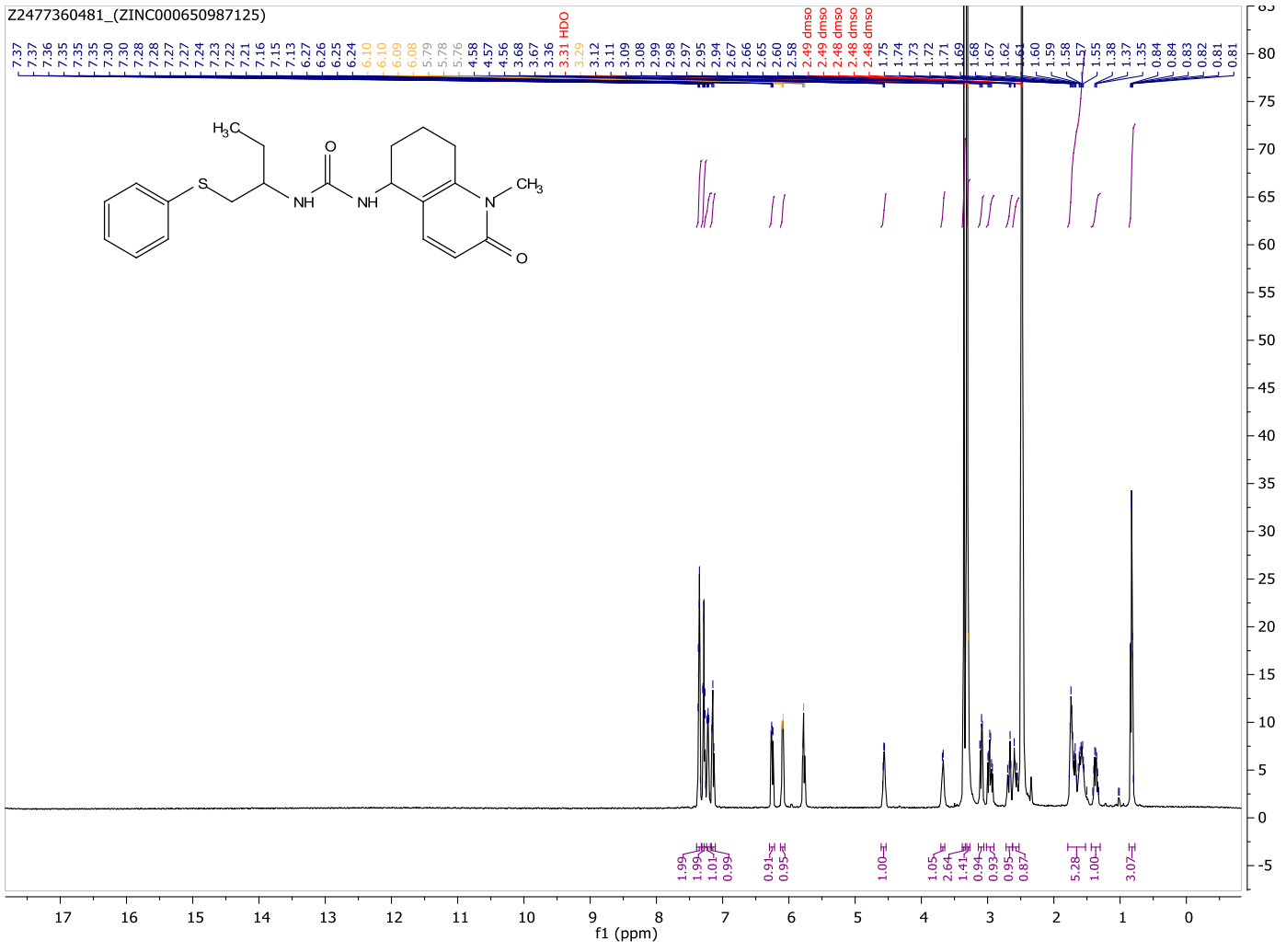
Mol Wt 385.52  
Exact Mass 385.22

#	Time	Area%
1	1.258	98.15
2	1.325	1.85



Z2477360481\_(ZINC000650987125)

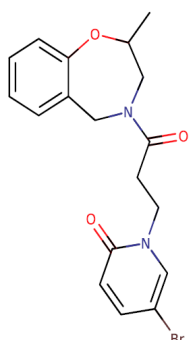
Z2477360481\_(ZINC000650987125)





MaxPeak: 100.00%  
Ret\_Time: 1.300 min

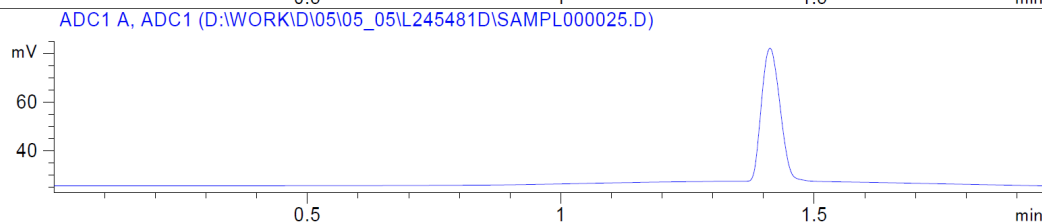
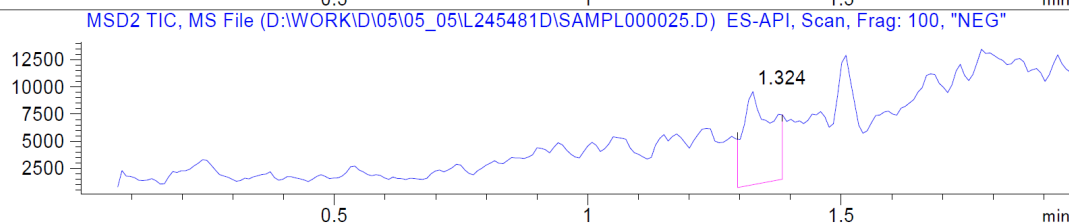
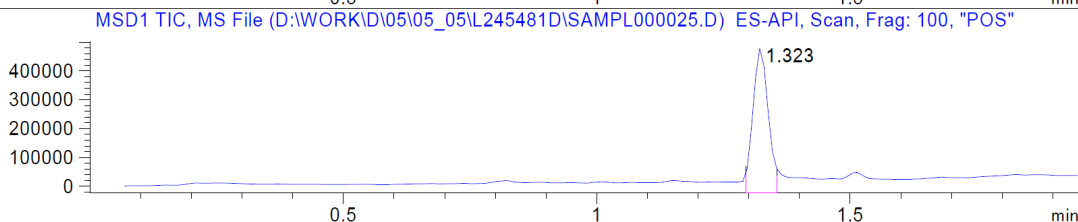
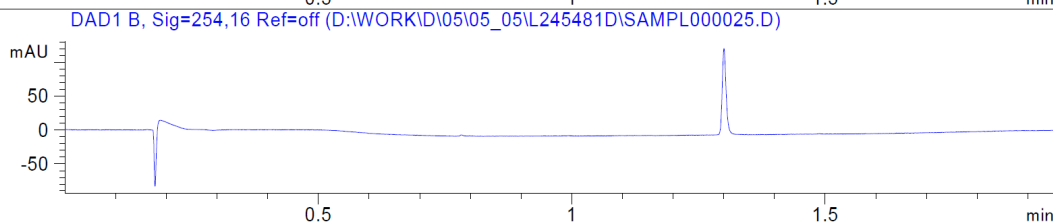
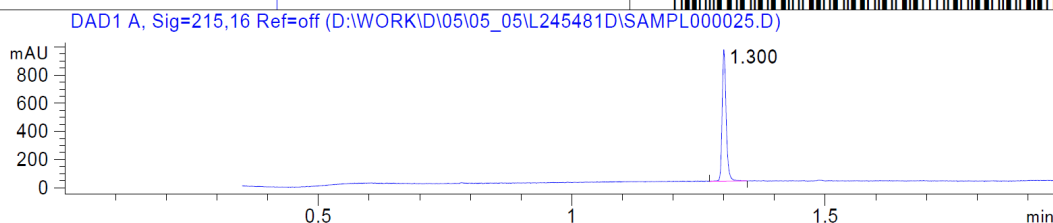
Q260214\$114



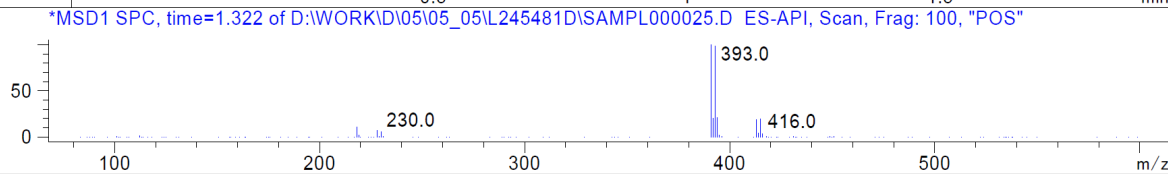
Mol Wt 391.26

Exact Mass 390.08

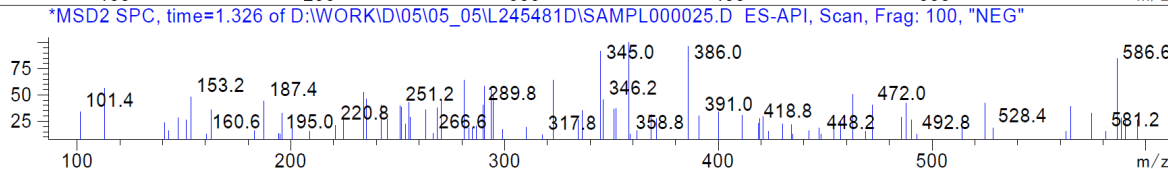
#	Time	Area%
1	1.300	100.00



RT 1.323

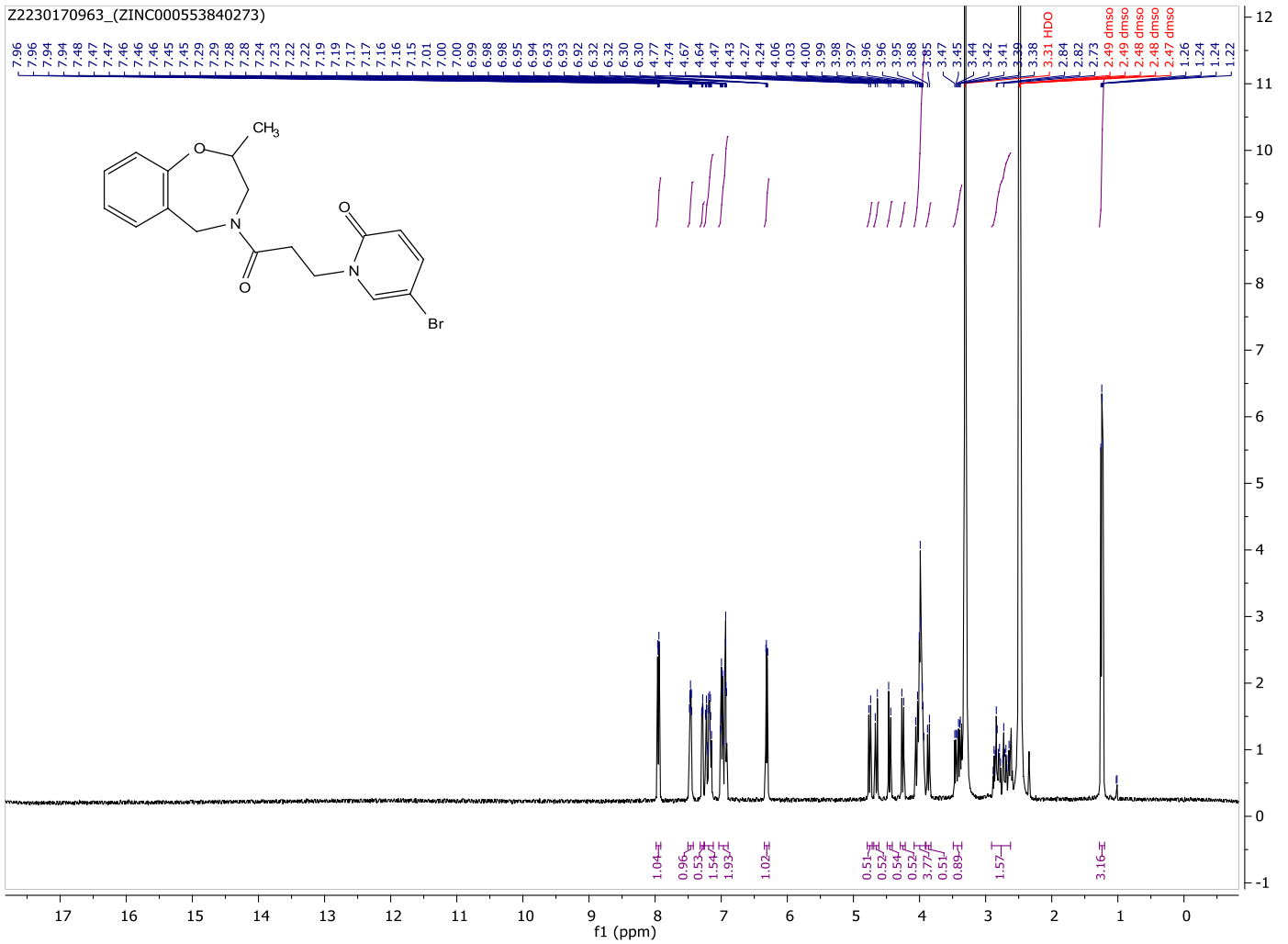
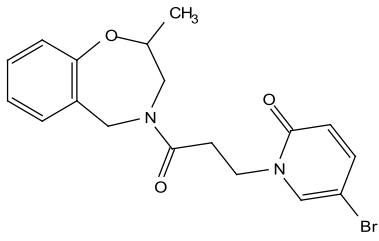


RT 1.324

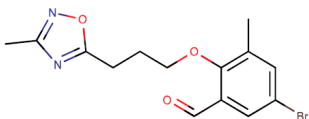


Z2230170963\_(ZINC000553840273)

Z2230170963\_(ZINC000553840273)



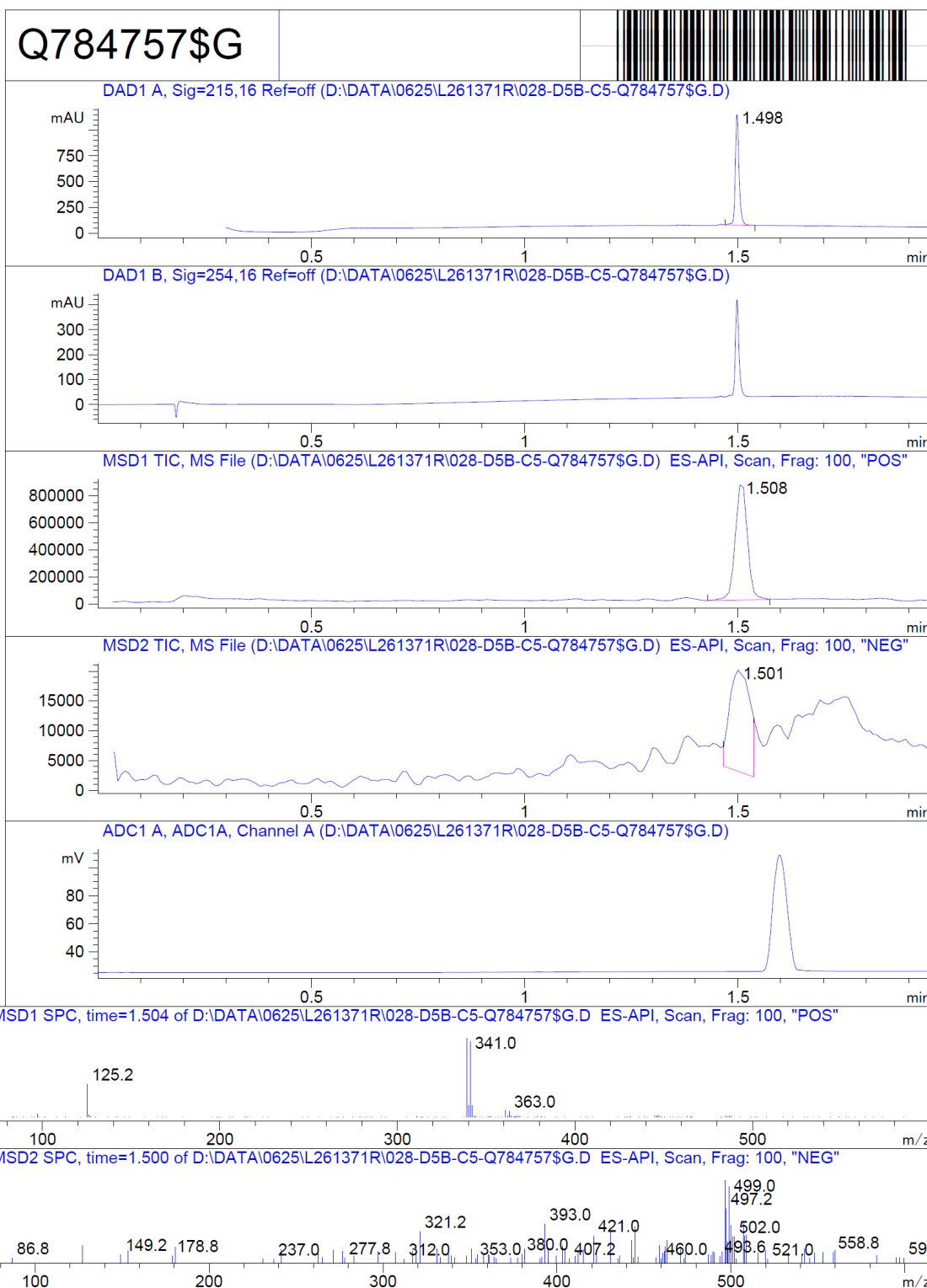
MaxPeak: 100.00%  
Ret\_Time: 1.498 min



Mol Wt 339.18  
Exact Mass 338.04

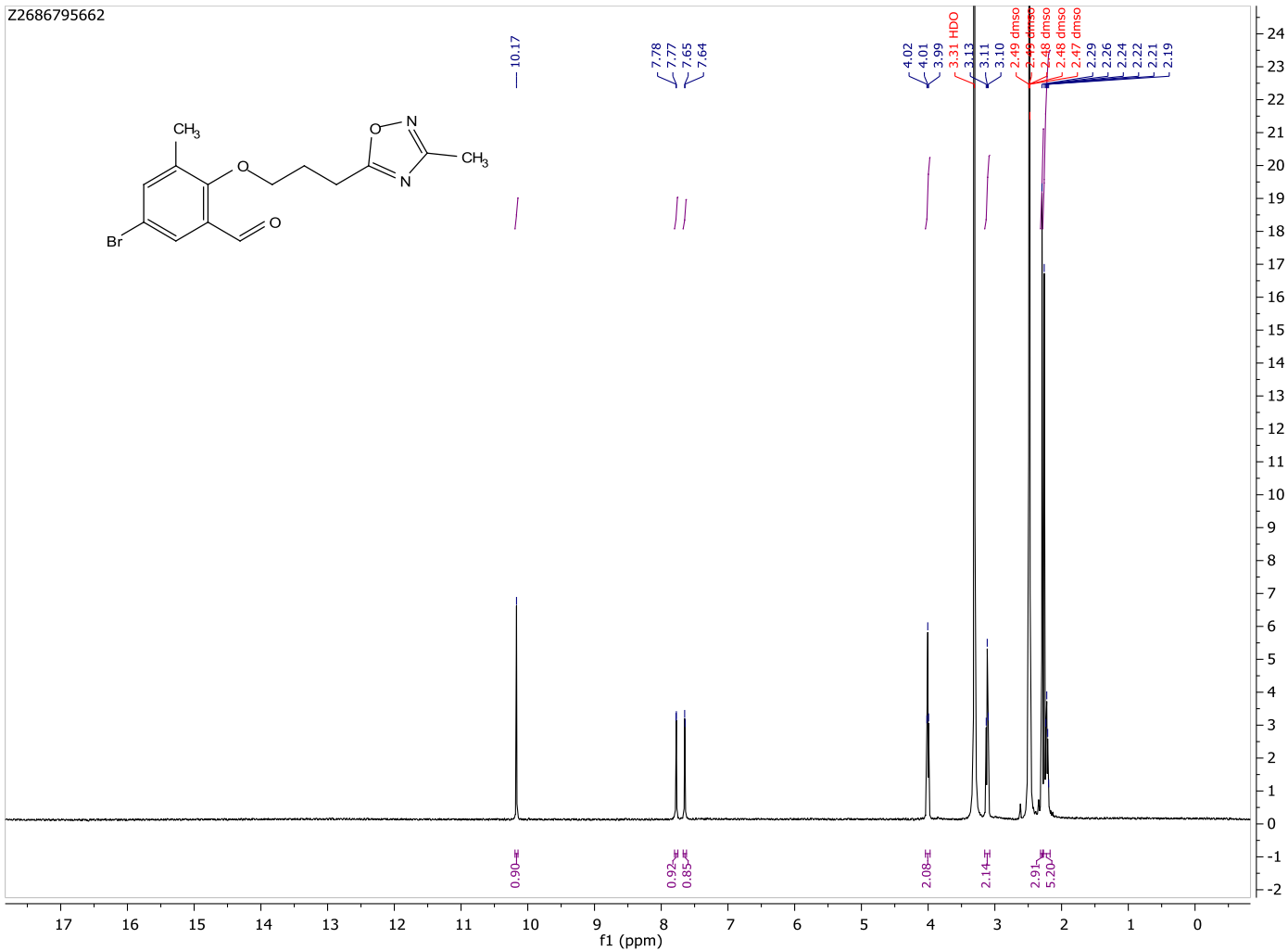
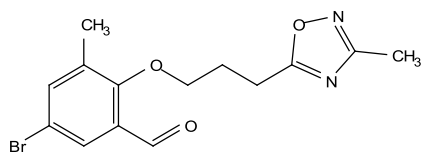
#	Time	Area%
1	1.498	100.00

# Q784757\$G



Z2686795662

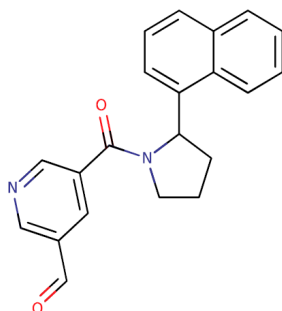
Z2686795662



# Q763572\$3



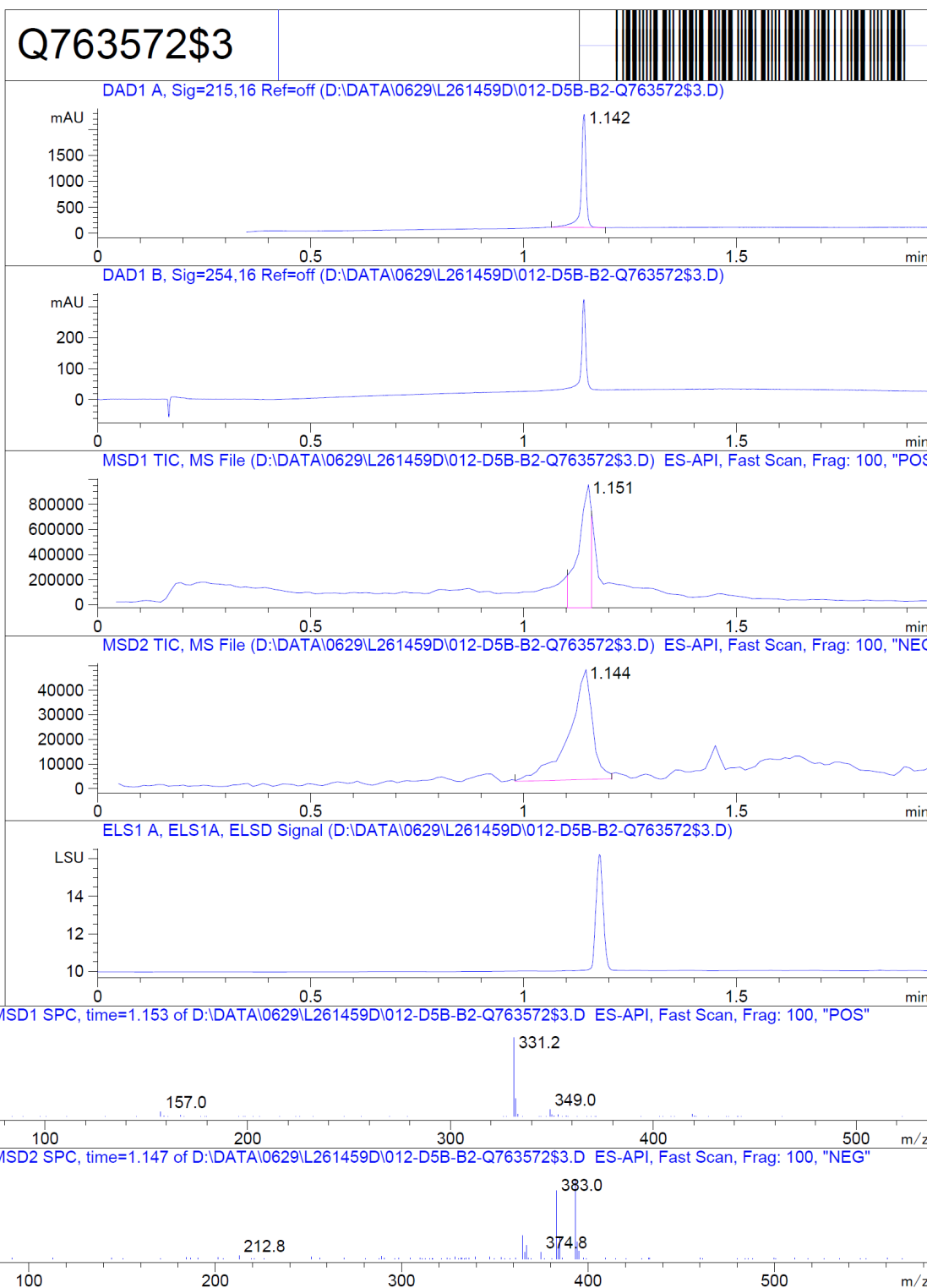
MaxPeak: 100.00%  
Ret\_Time: 1.142 min



Mol Wt 330.38

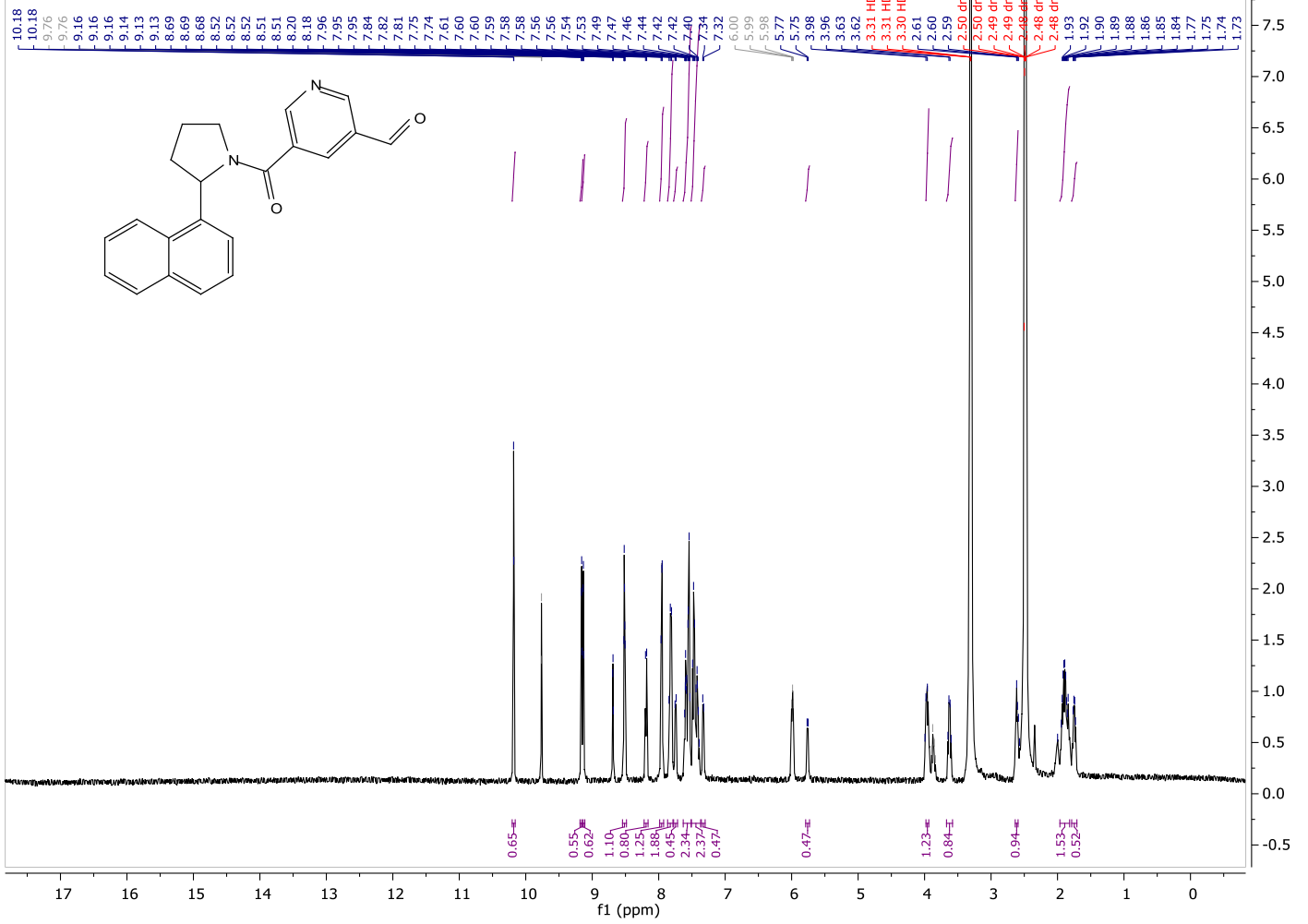
Exact Mass 330.16

#	Time	Area%
1	1.142	100.00



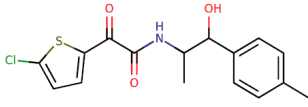
Z4497434908

Z4497434908



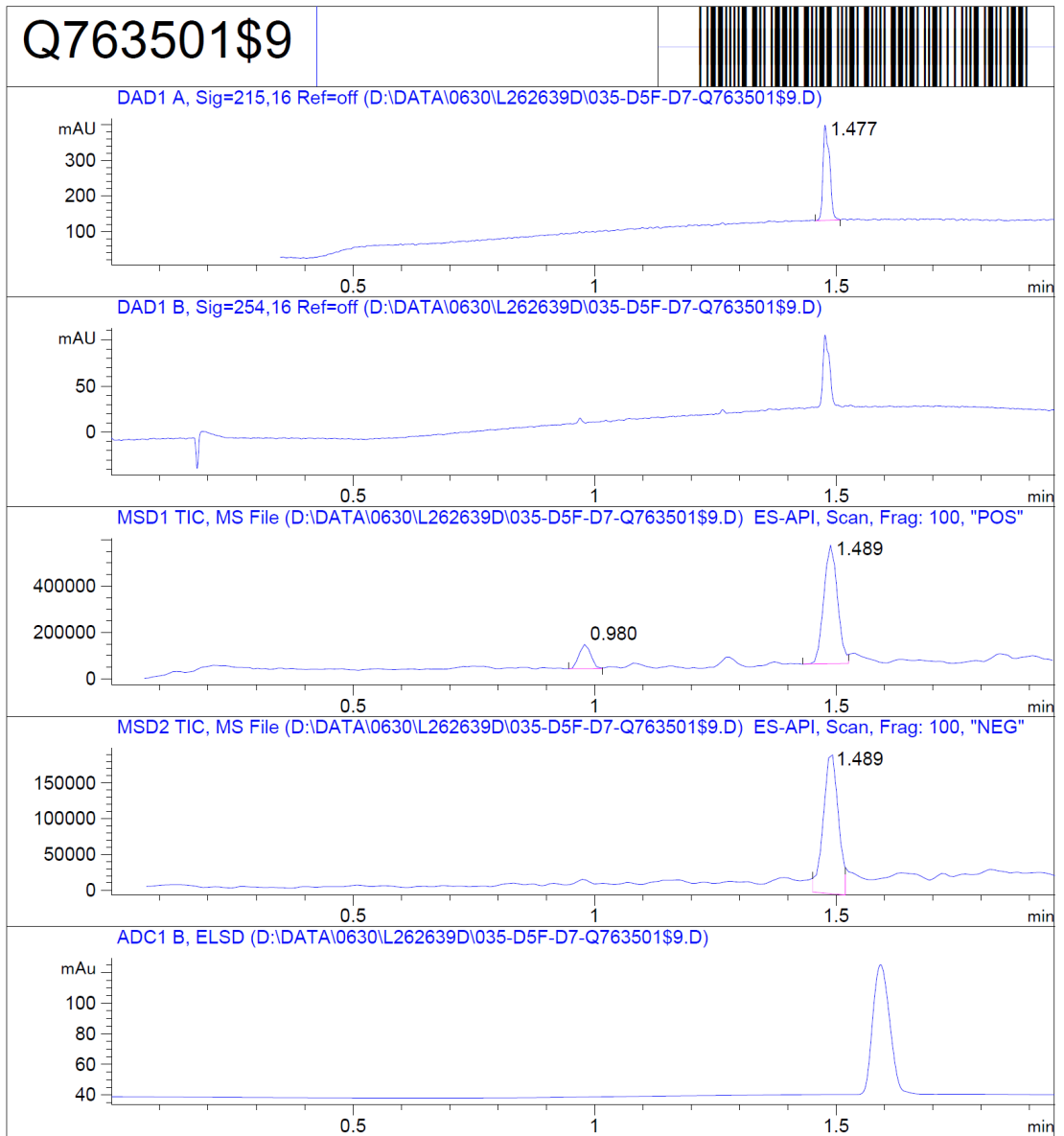
MaxPeak: 100.00%  
Ret\_Time: 1.477 min

# Q763501\$9

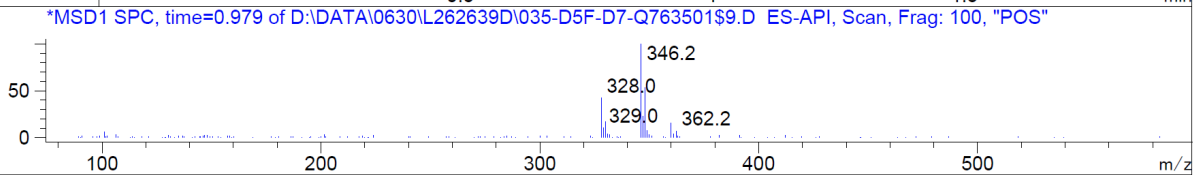


**Mol Wt** 337.82  
**Exact Mass** 337.07

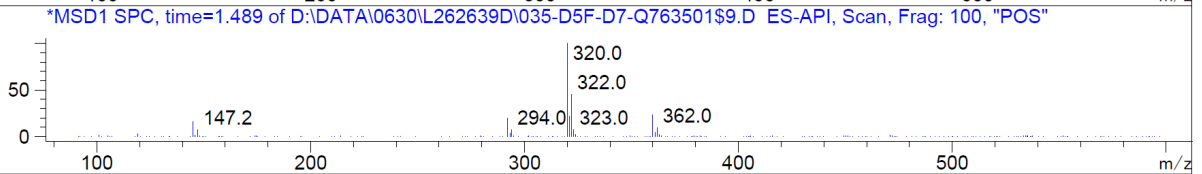
#	Time	Area%
1	1.477	100.00



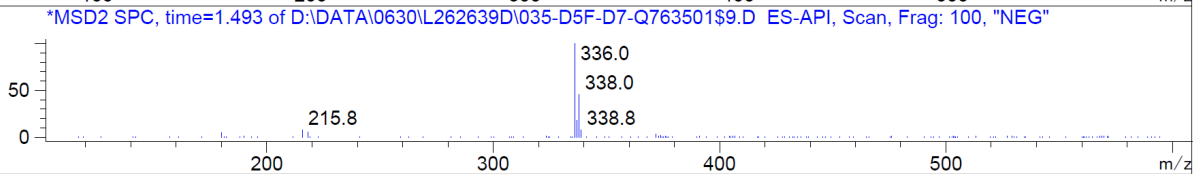
RT 0.980



RT 1.489

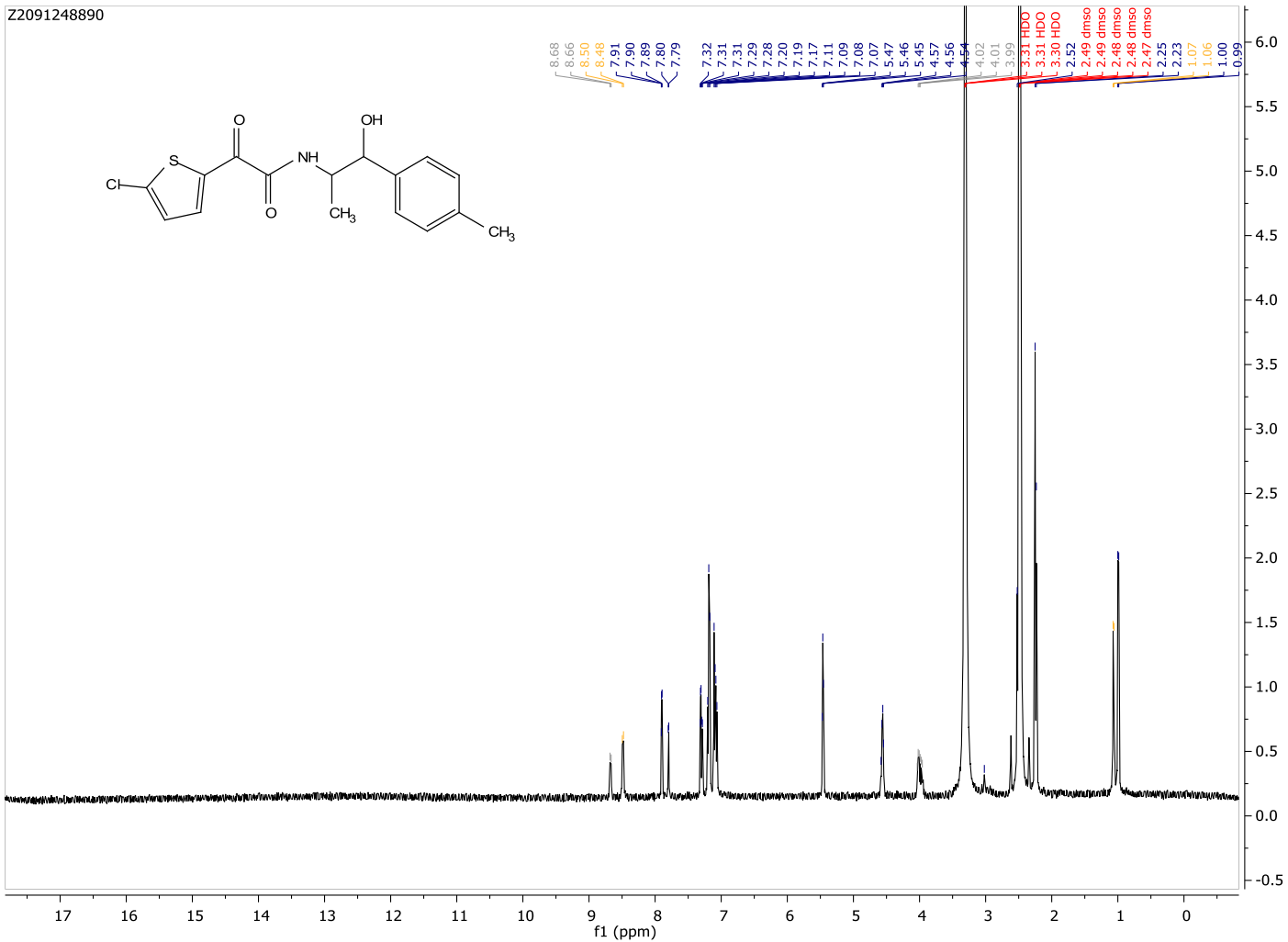
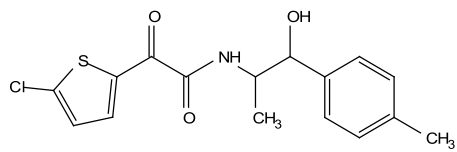


RT 1.489



Z2091248890

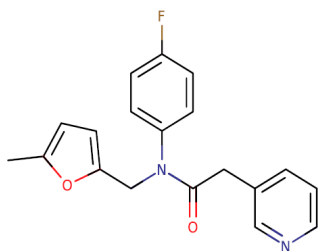
Z2091248890





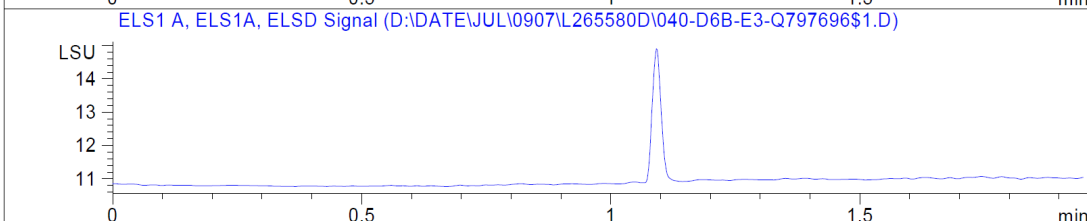
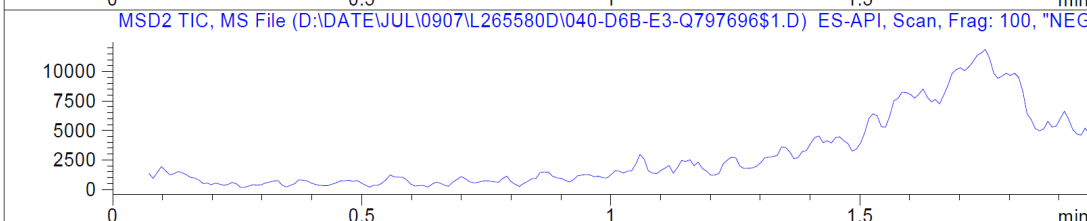
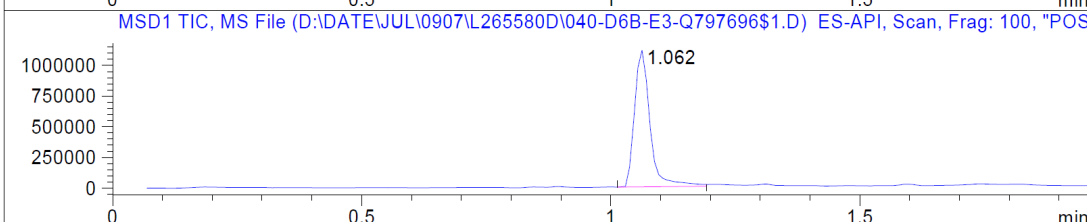
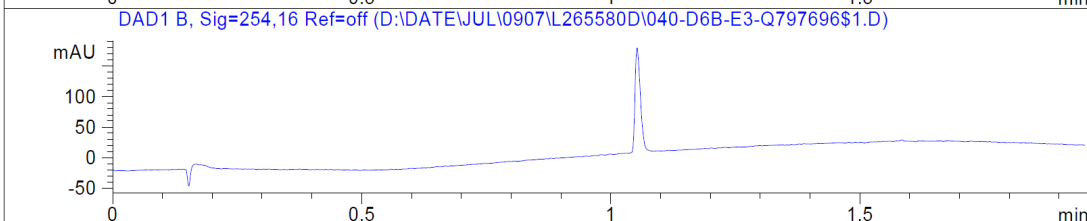
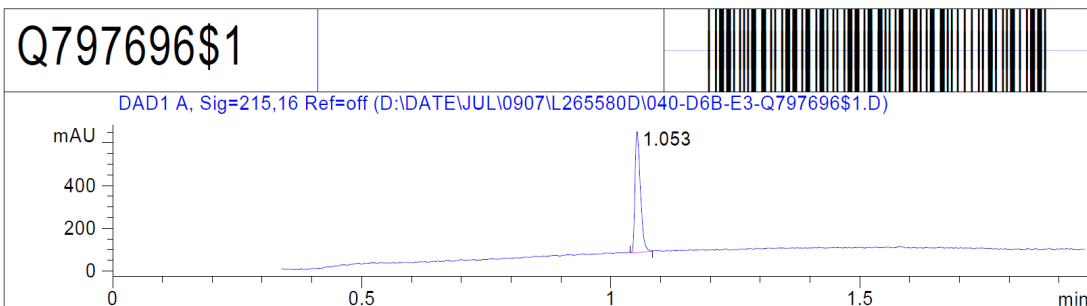
MaxPeak: 100.00%  
Ret\_Time: 1.053 min

# Q797696\$1

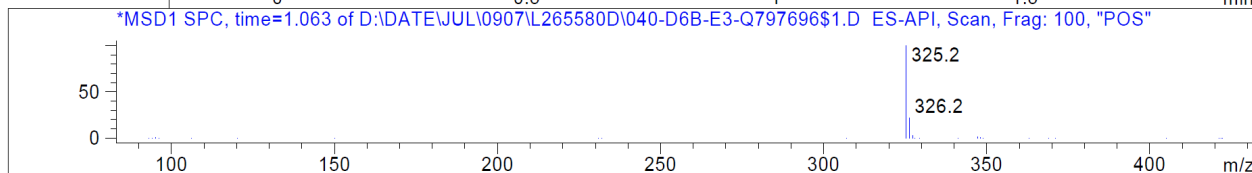


**Mol Wt** 324.35  
**Exact Mass** 324.15

#	Time	Area%
1	1.053	100.00

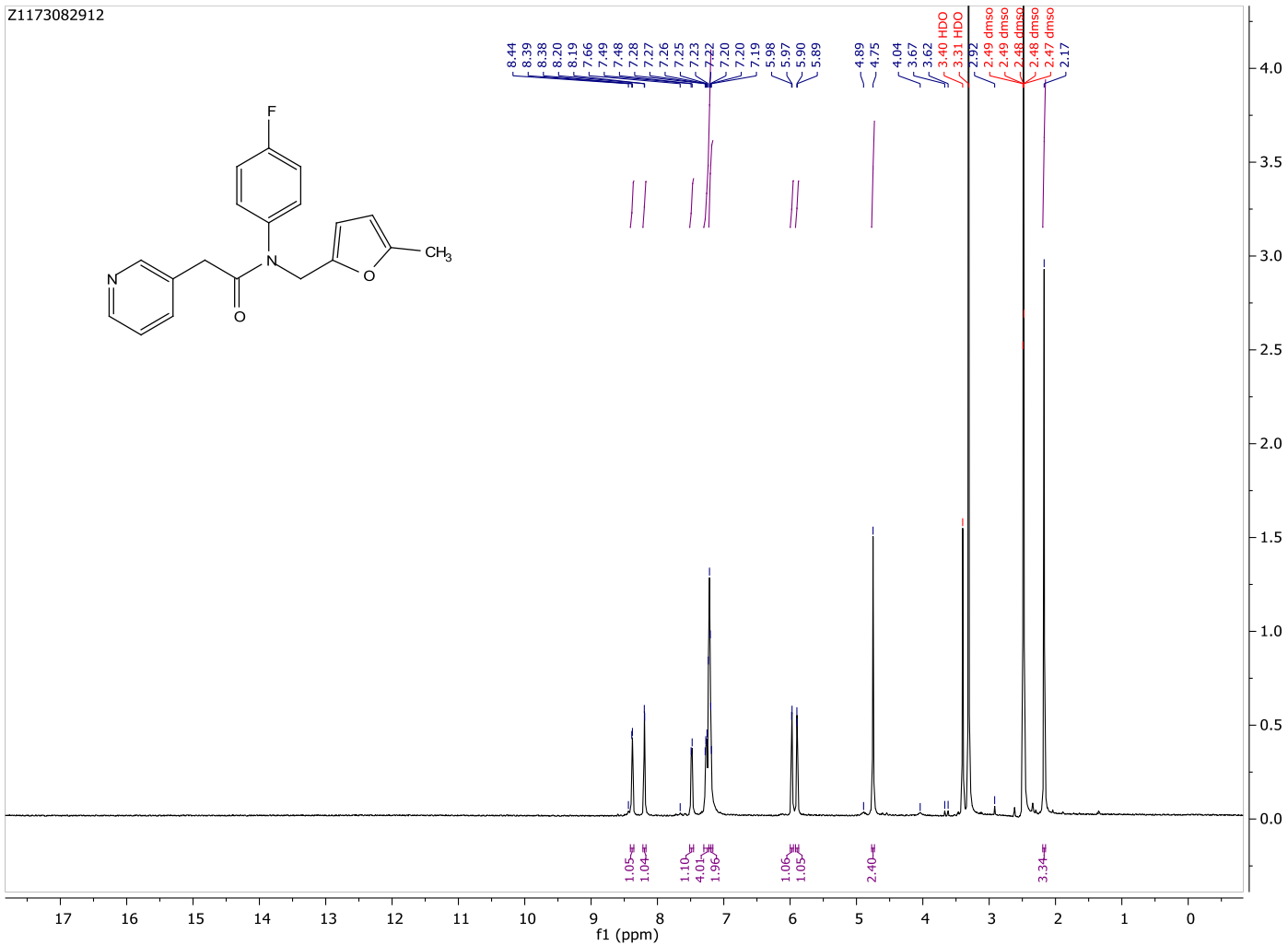
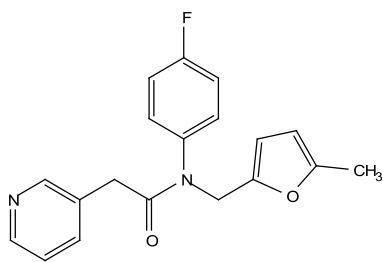


RT 1.062



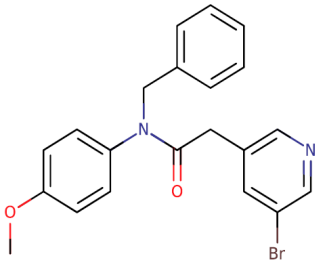
Z1173082912

Z1173082912



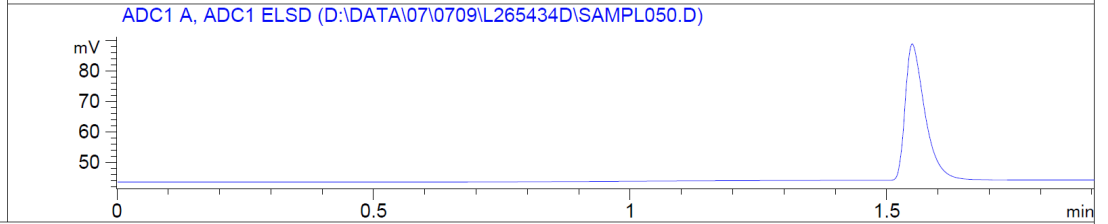
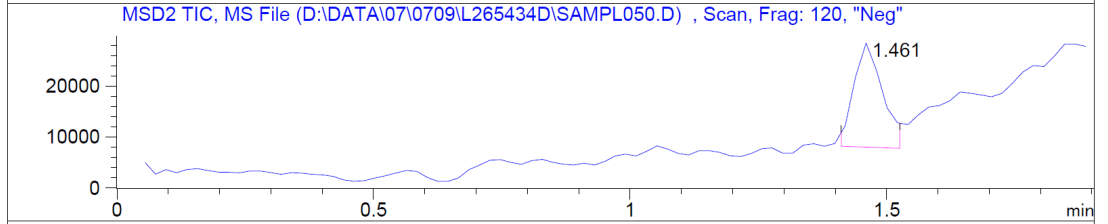
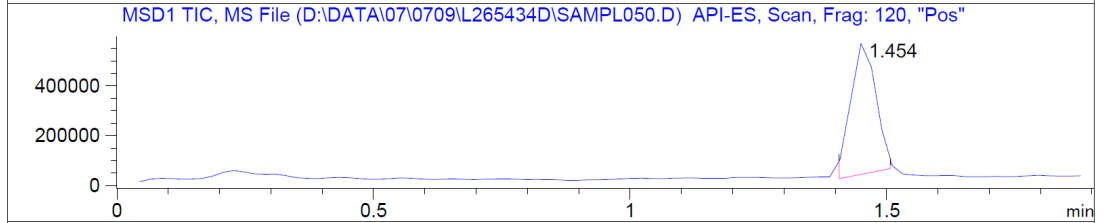
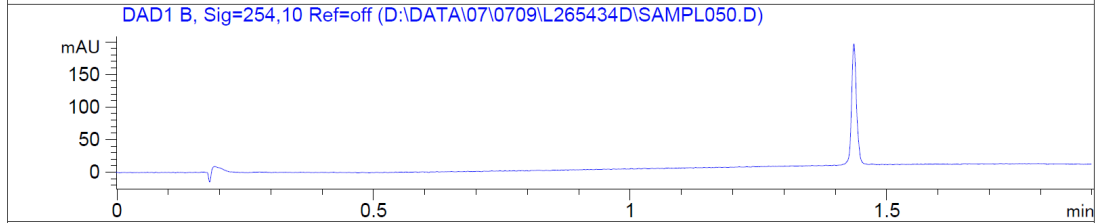
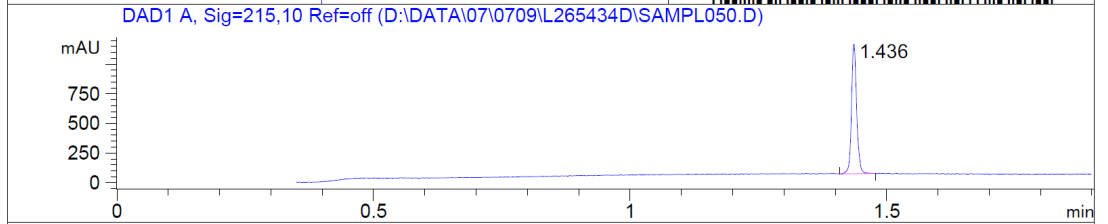
MaxPeak: 100.00%  
Ret\_Time: 1.436 min

Q797821\$2

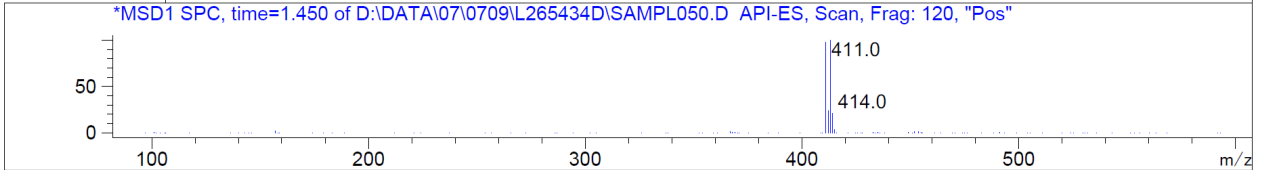


Mol Wt 411.29  
Exact Mass 412.09

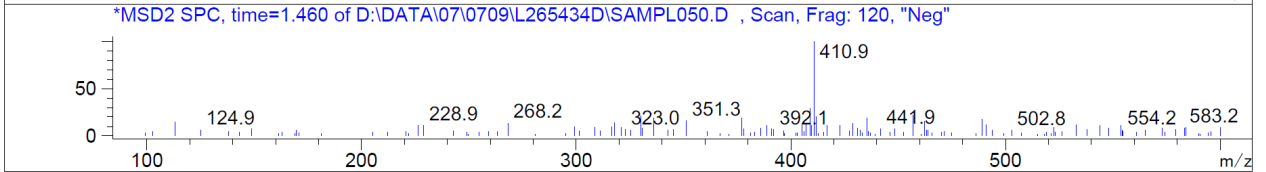
#	Time	Area%
1	1.436	100.00



RT 1.454

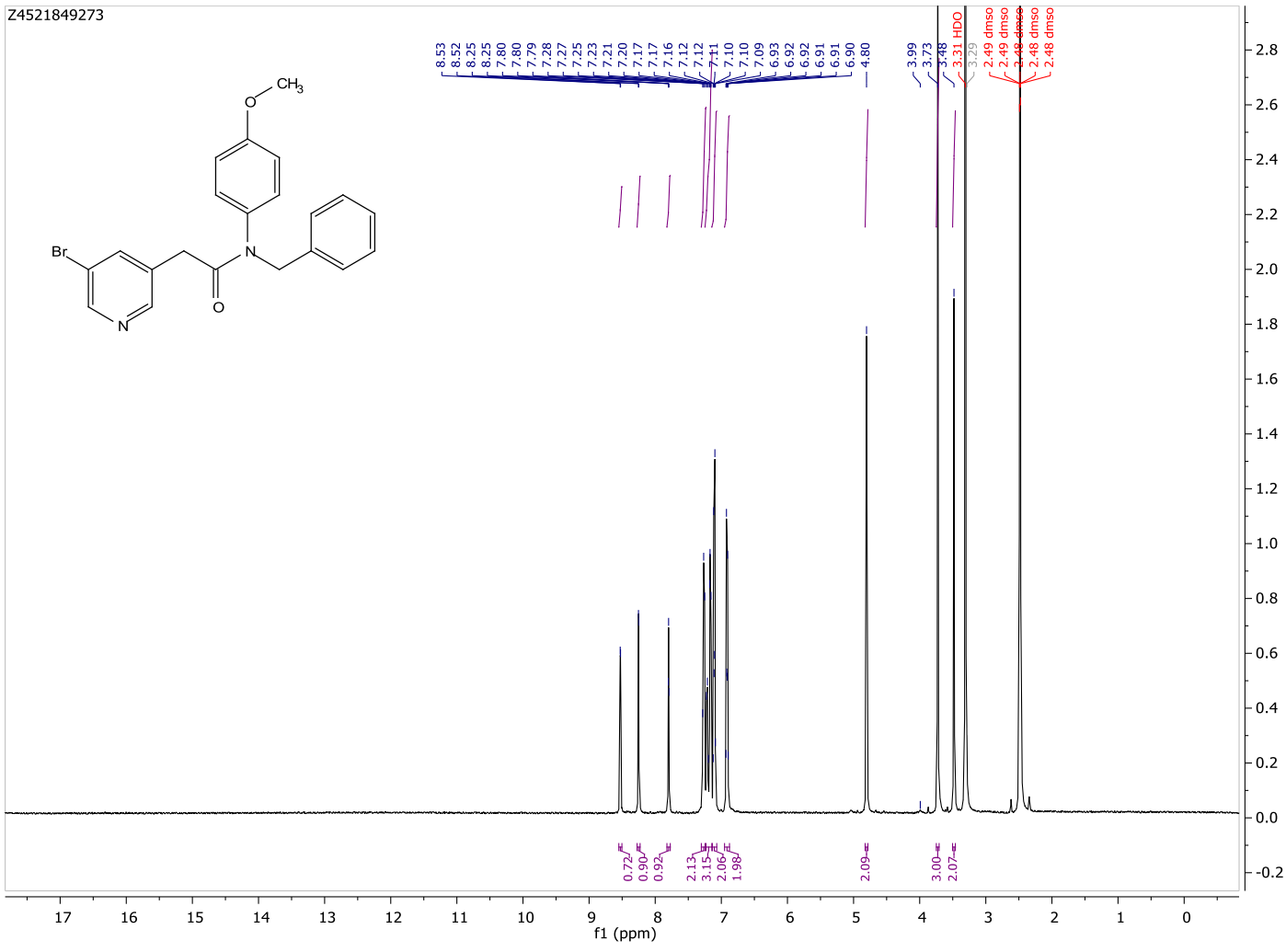
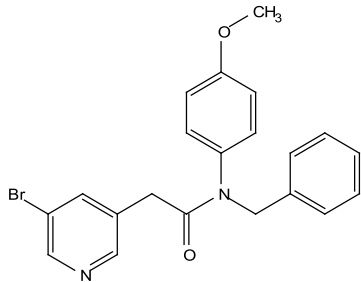


RT 1.461

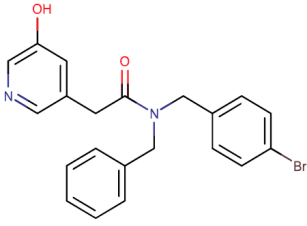


Z4521849273

Z4521849273



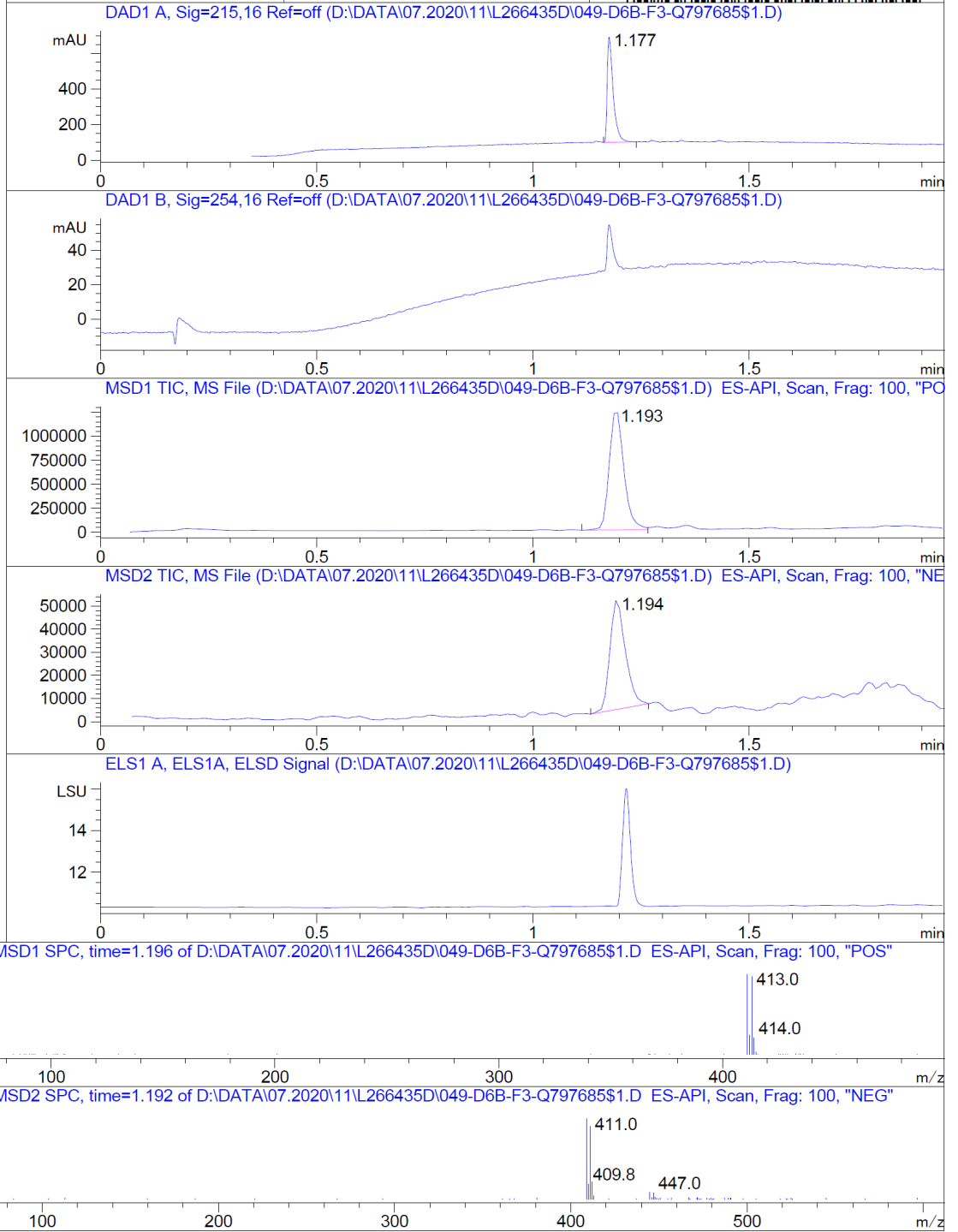
MaxPeak: 100.00%  
Ret\_Time: 1.177 min



Mol Wt 411.29  
Exact Mass 412.09

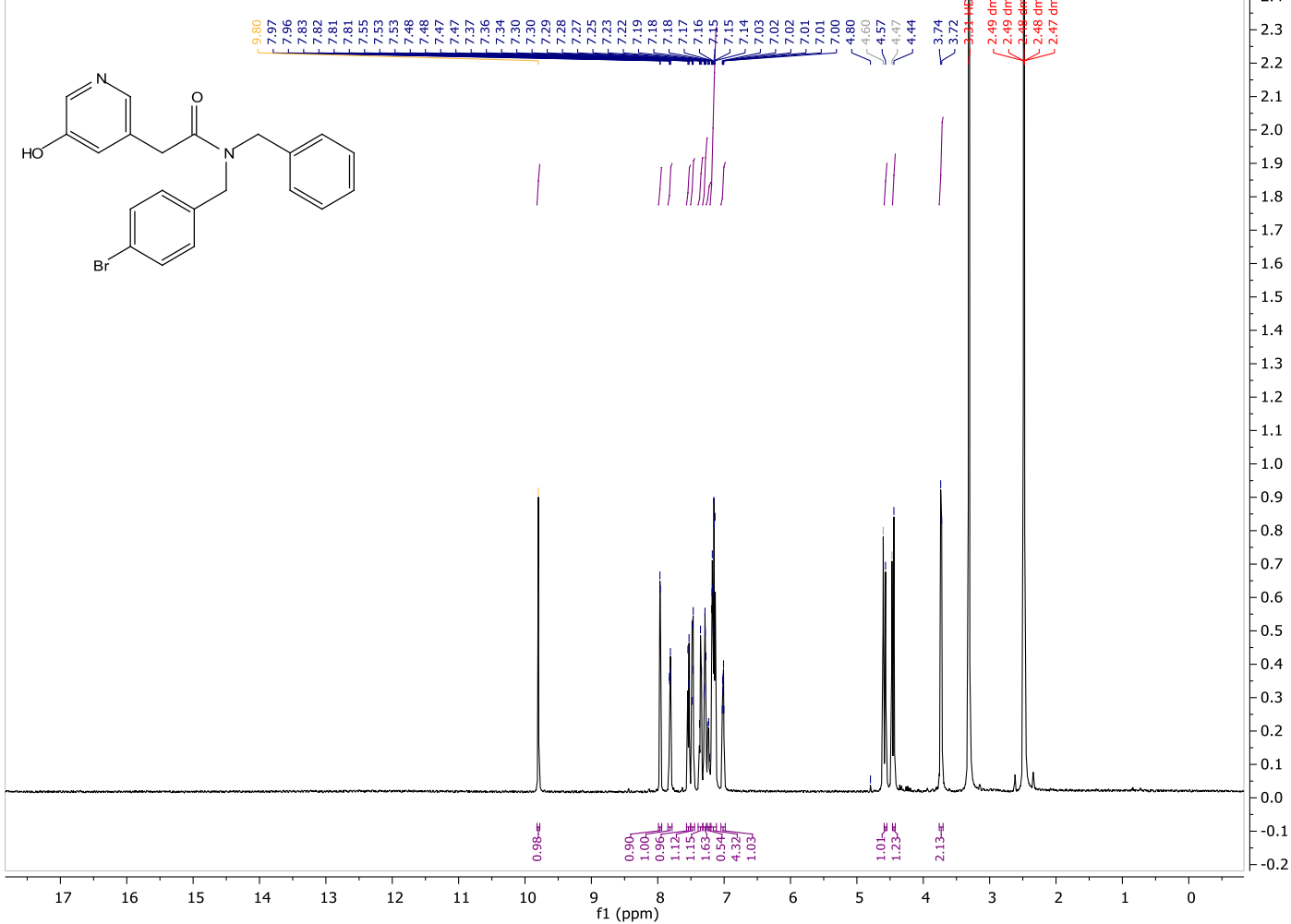
#	Time	Area%
1	1.177	100.00

Q797685\$1



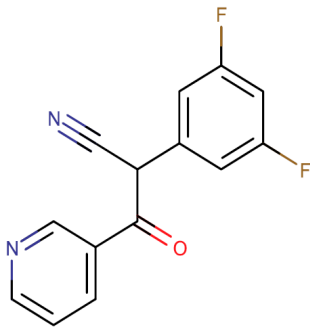
Z4521849300

Z4521849300



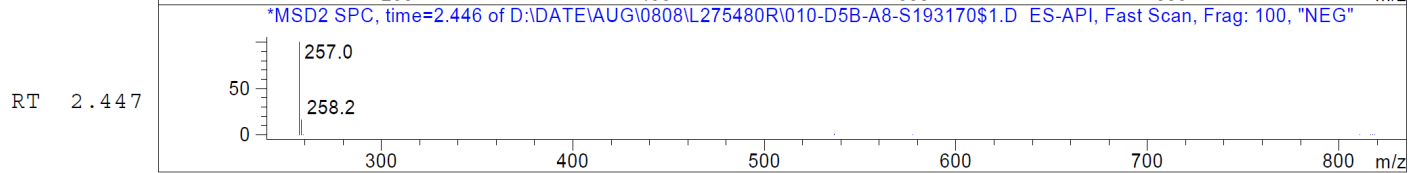
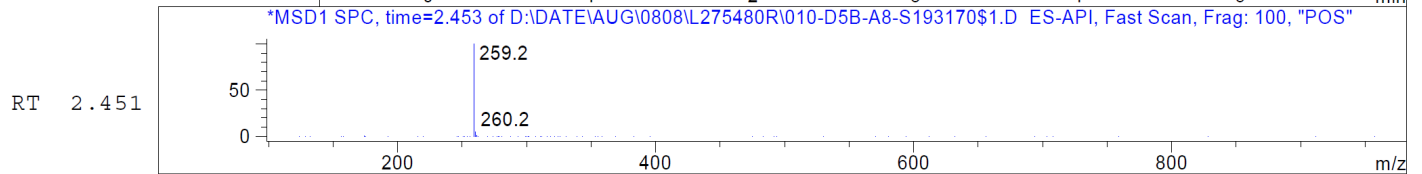
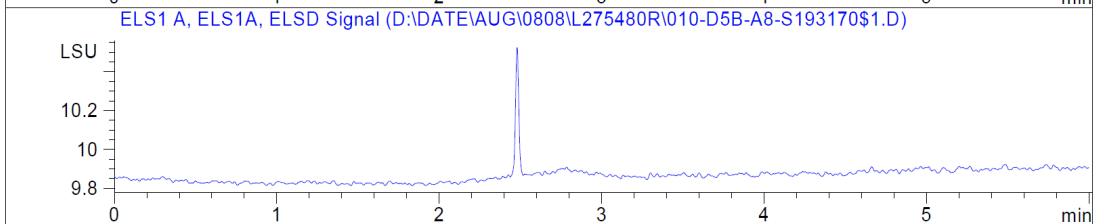
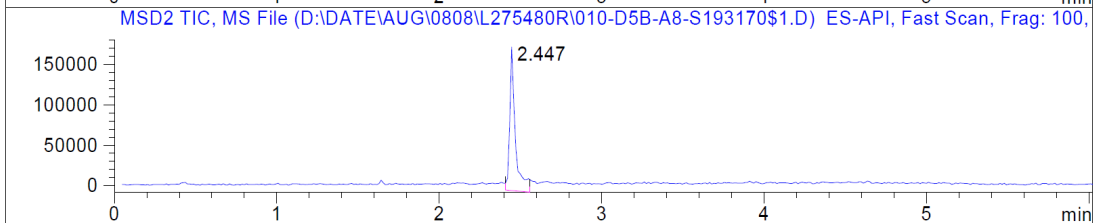
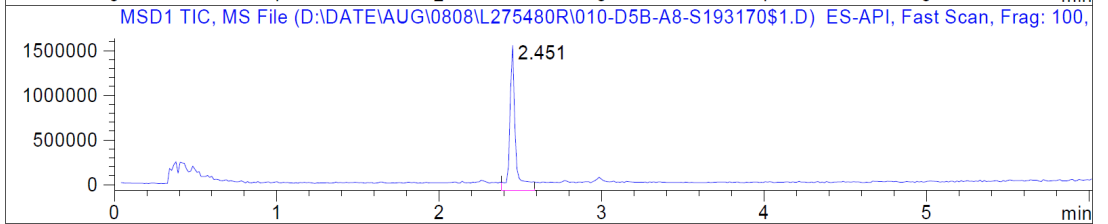
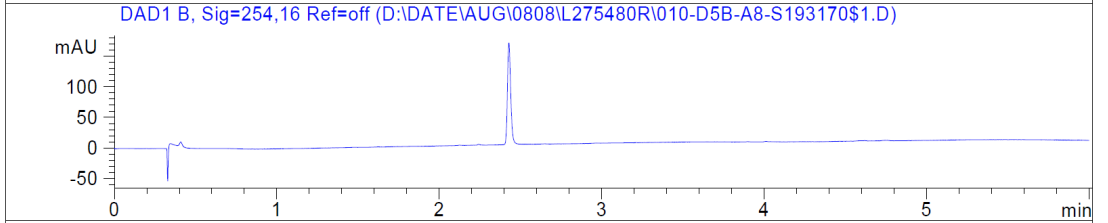
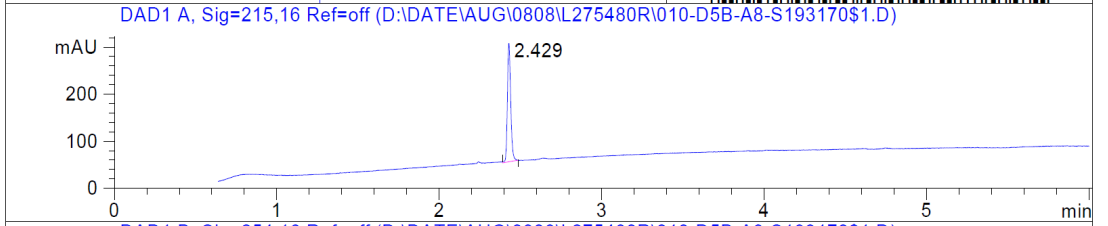
MaxPeak: 100.00%  
Ret\_Time: 2.429 min

# S193170\$1



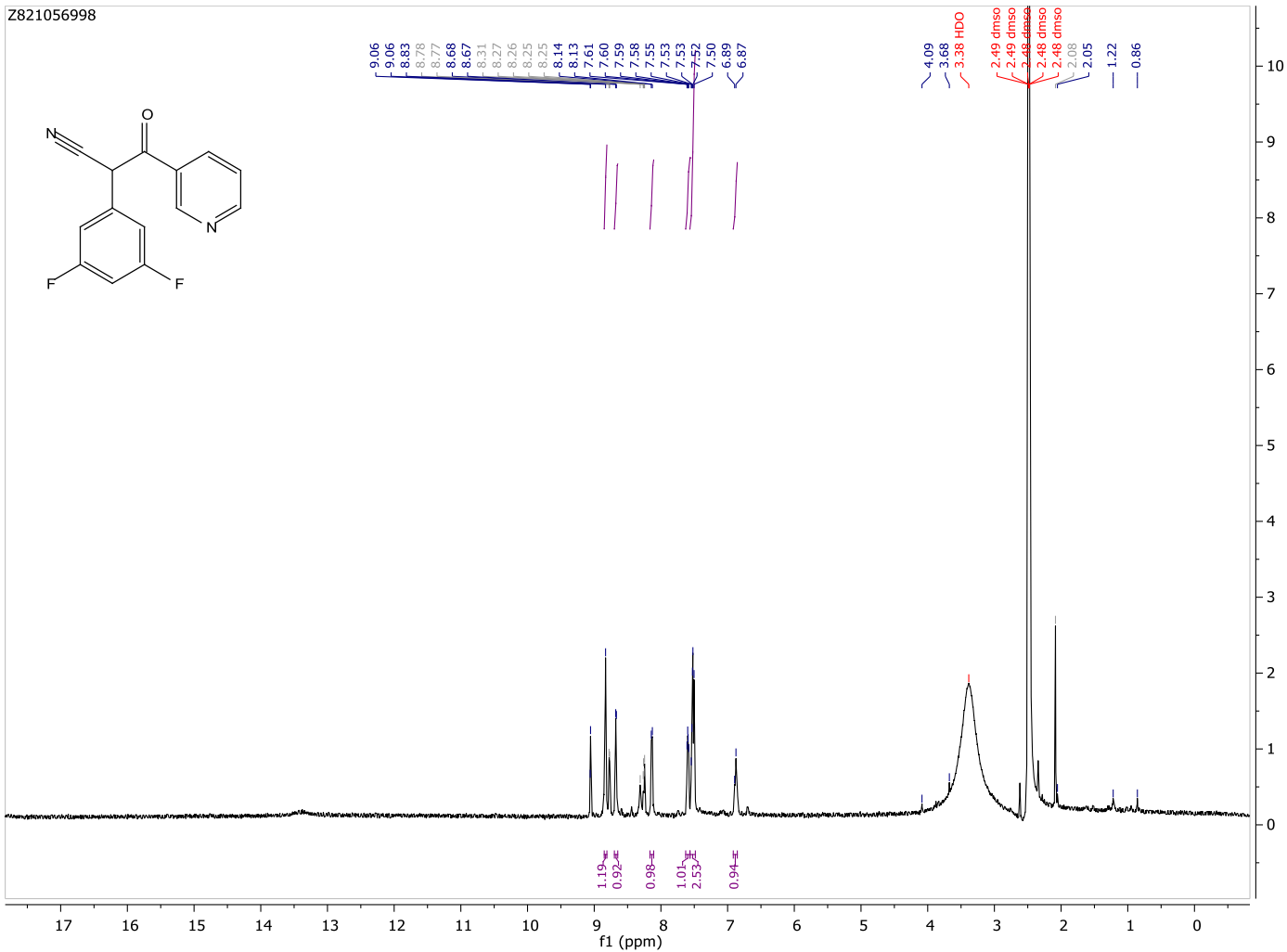
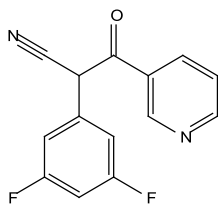
Mol Wt 258.22  
Exact Mass 258.07

#	Time	Area%
1	2.429	100.00



Z821056998

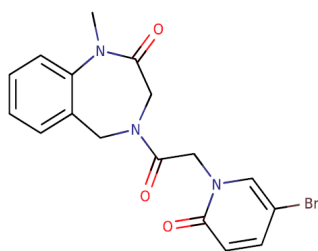
Z821056998





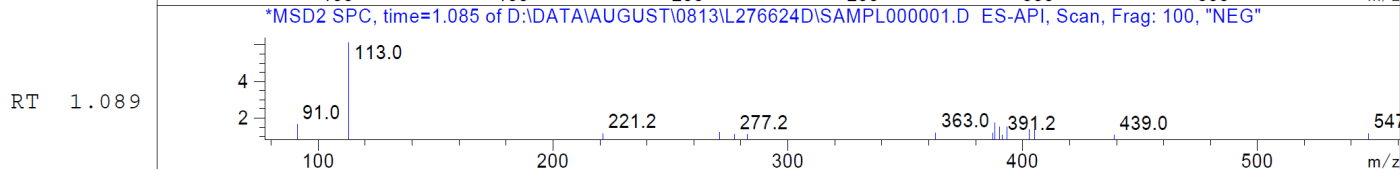
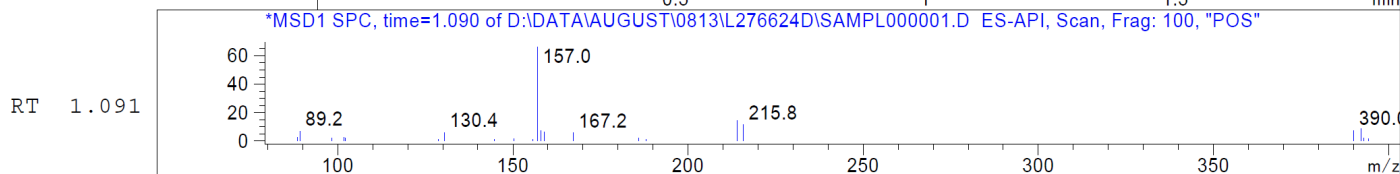
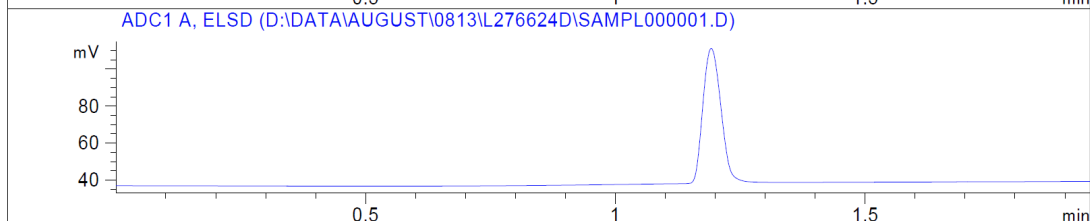
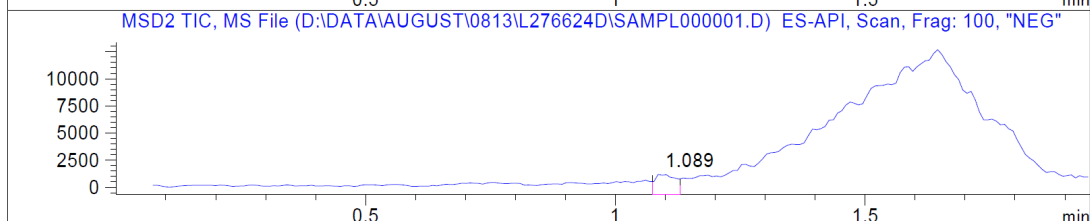
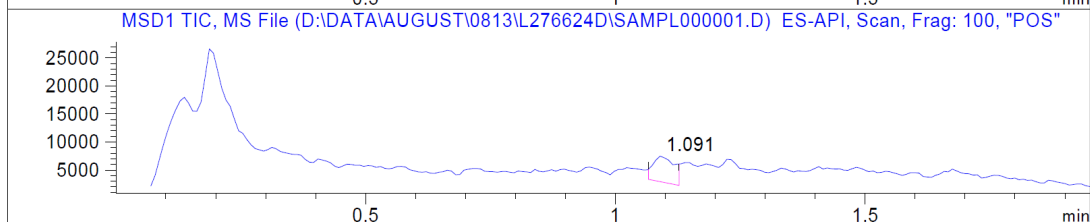
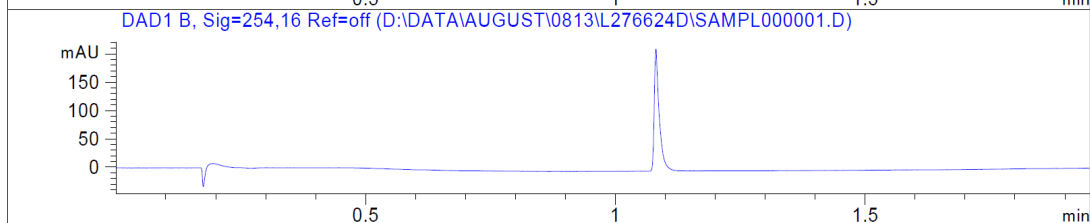
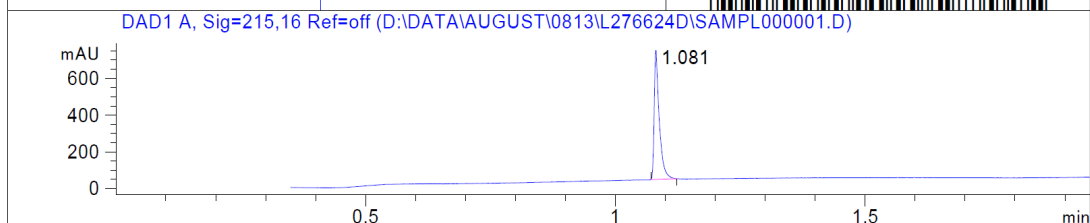
MaxPeak: 100.00%  
Ret\_Time: 1.081 min

# S081650\$1



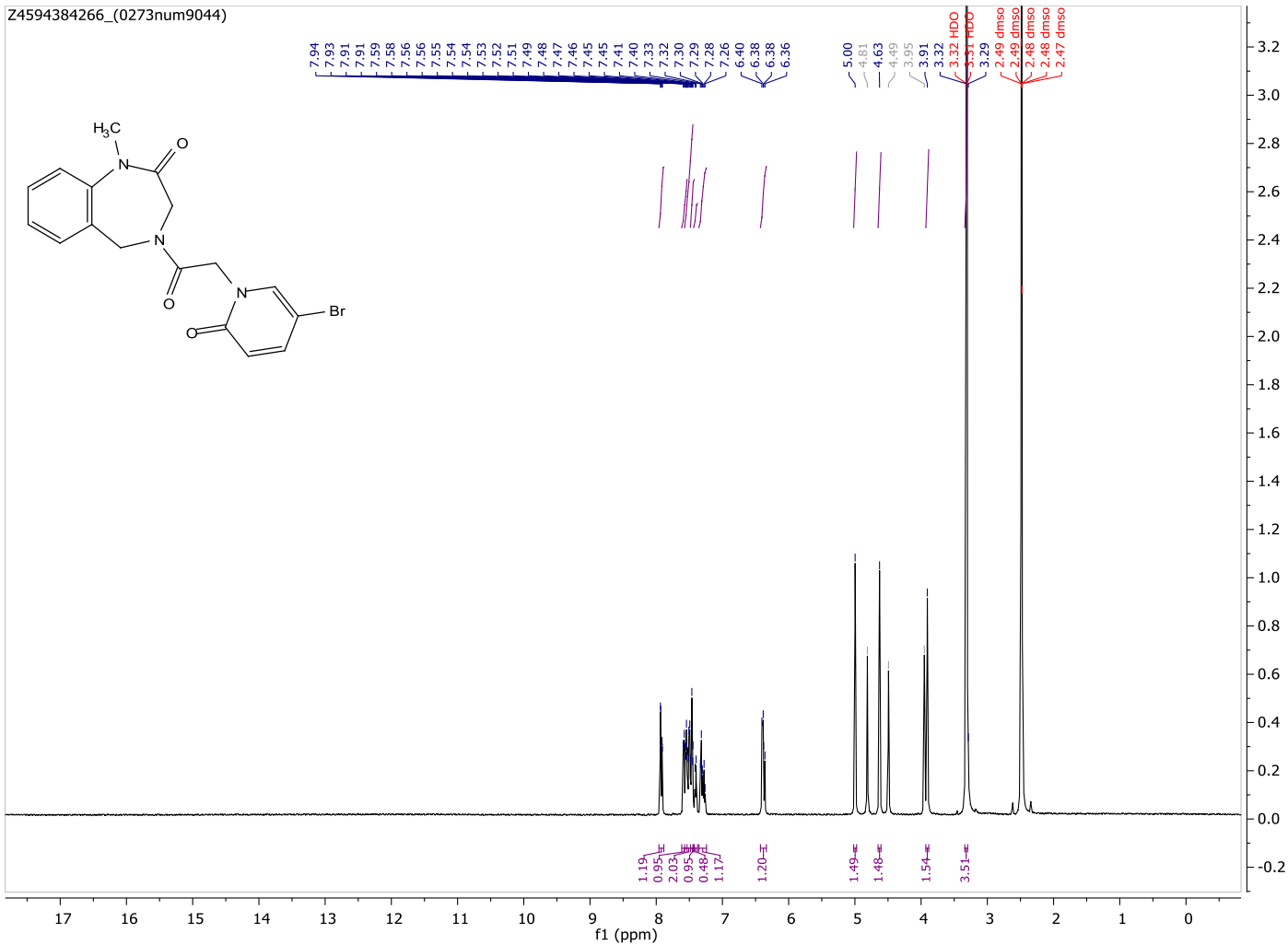
**Mol Wt** 390.23  
**Exact Mass** 389.05

#	Time	Area%
1	1.081	100.00



Z4594384266\_(0273num9044)

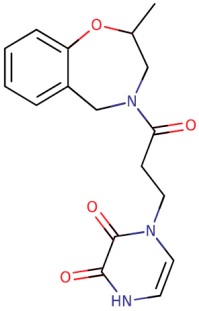
Z4594384266\_(0273num9044)



# S081659\$1

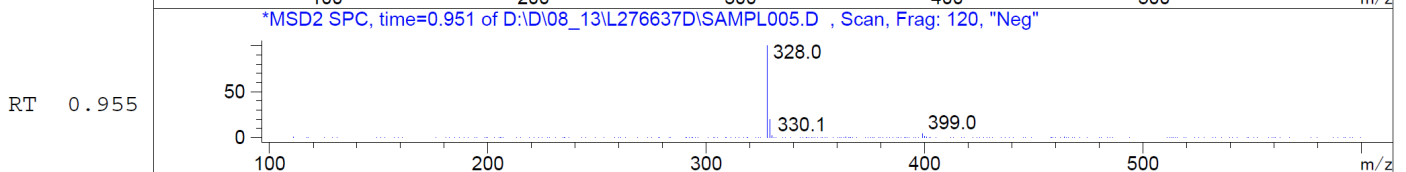
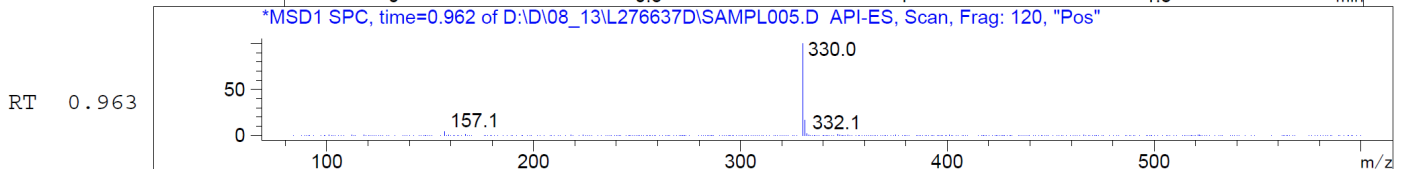
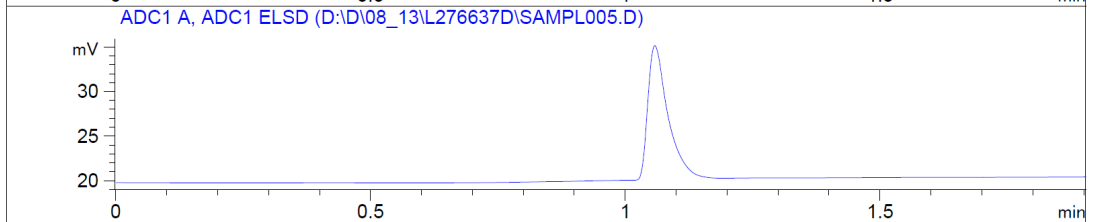
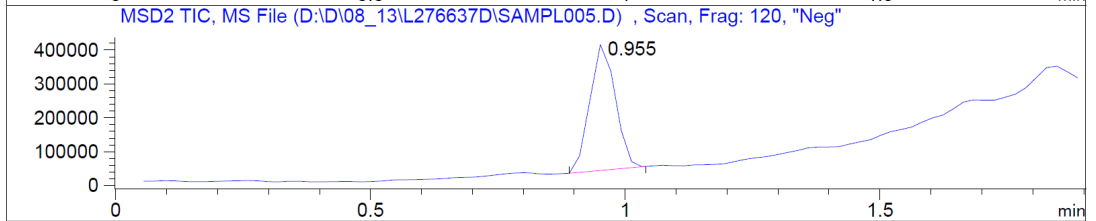
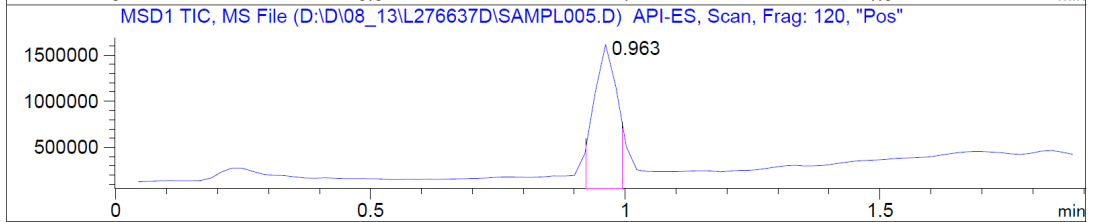
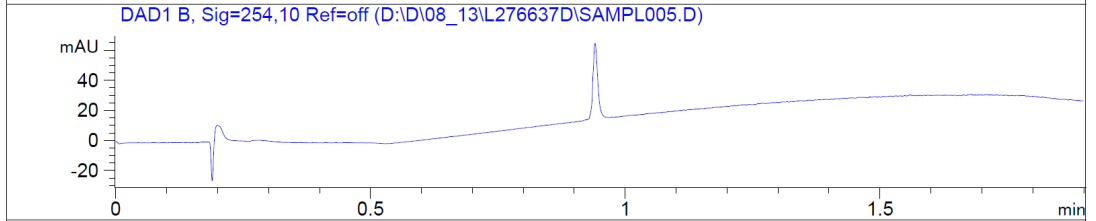
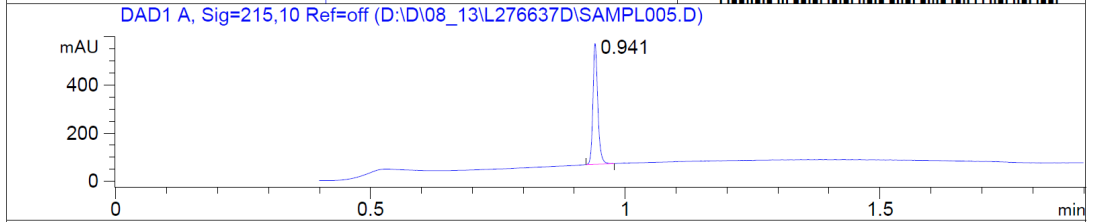


MaxPeak: 100.00%  
Ret\_Time: 0.941 min



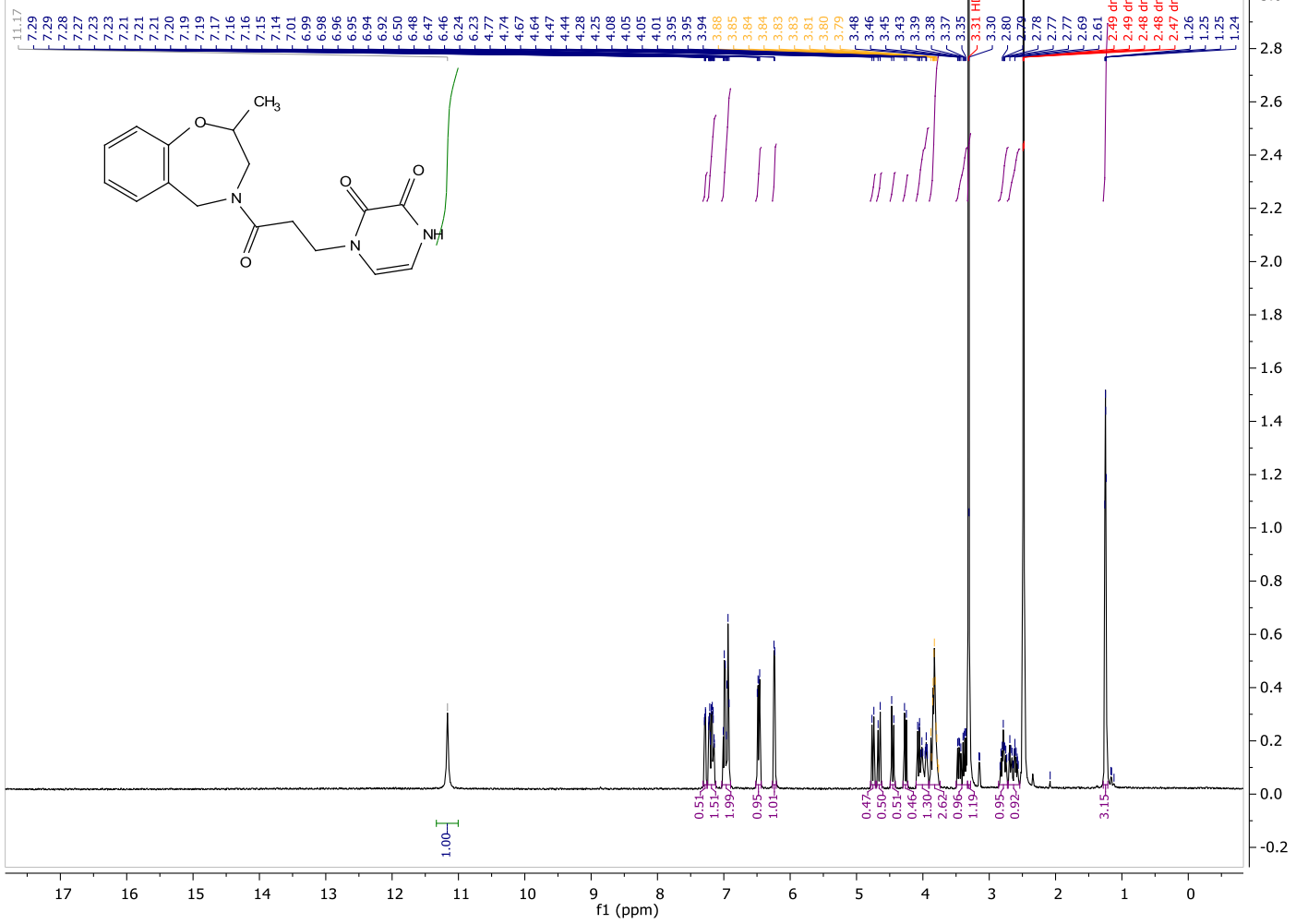
Mol Wt 329.35  
Exact Mass 329.15

#	Time	Area%
1	0.941	100.00

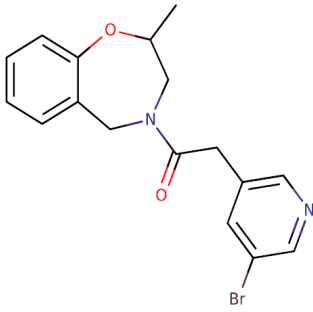


Z2230166392\_(0273num3613.2)

Z2230166392\_(0273num3613.2)



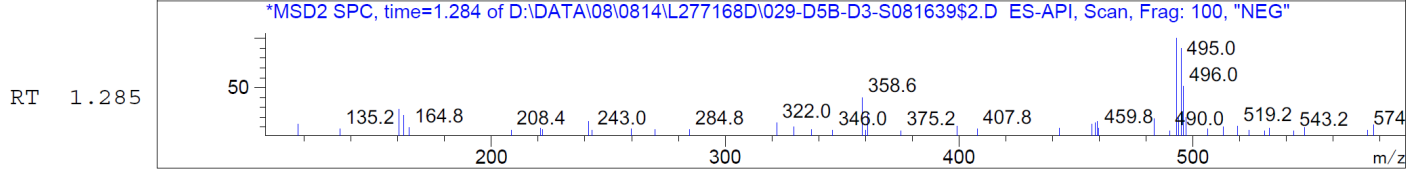
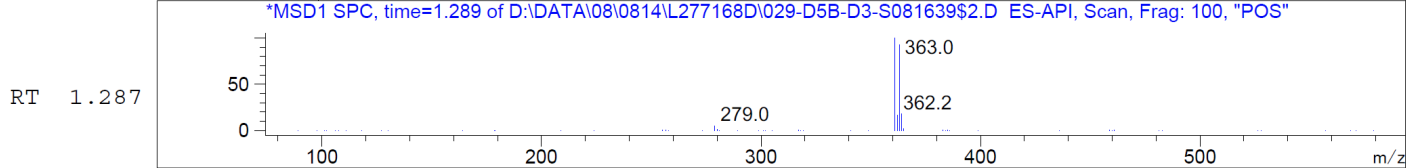
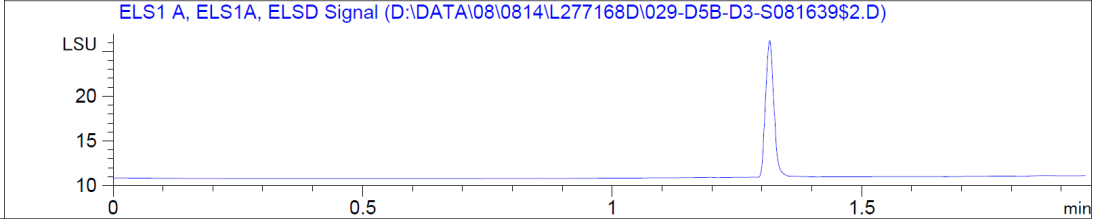
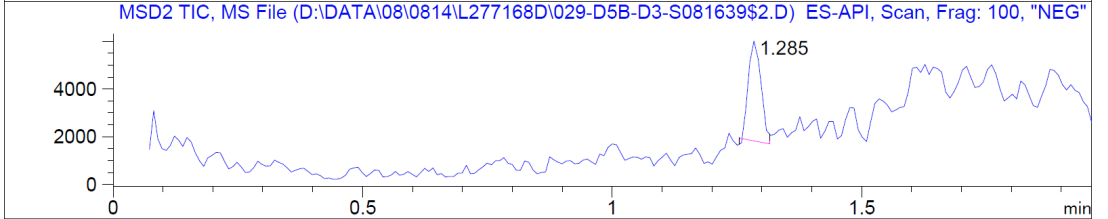
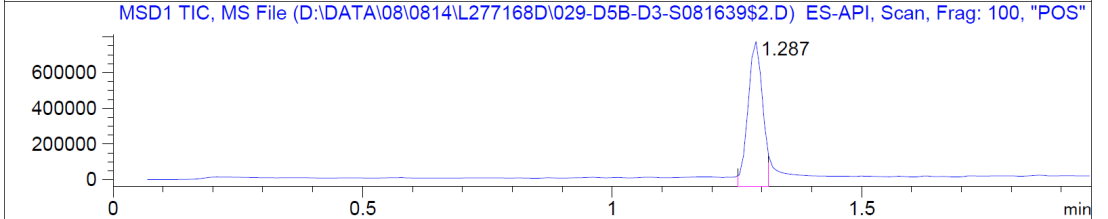
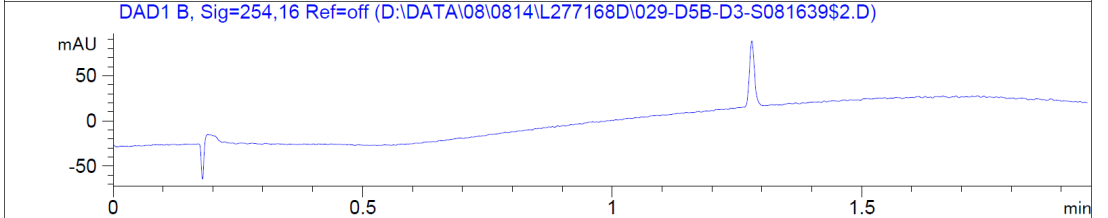
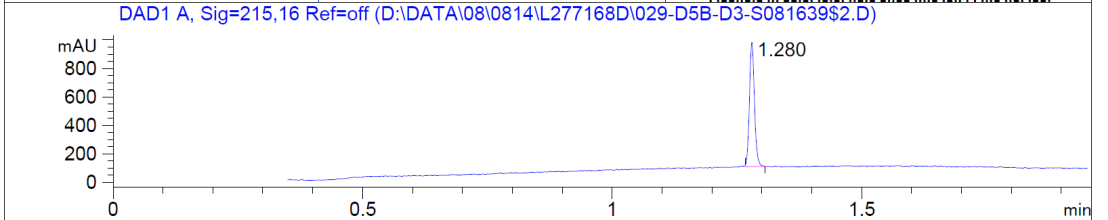
MaxPeak: 100.00%  
Ret\_Time: 1.280 min



Mol Wt 361.23  
Exact Mass 360.07

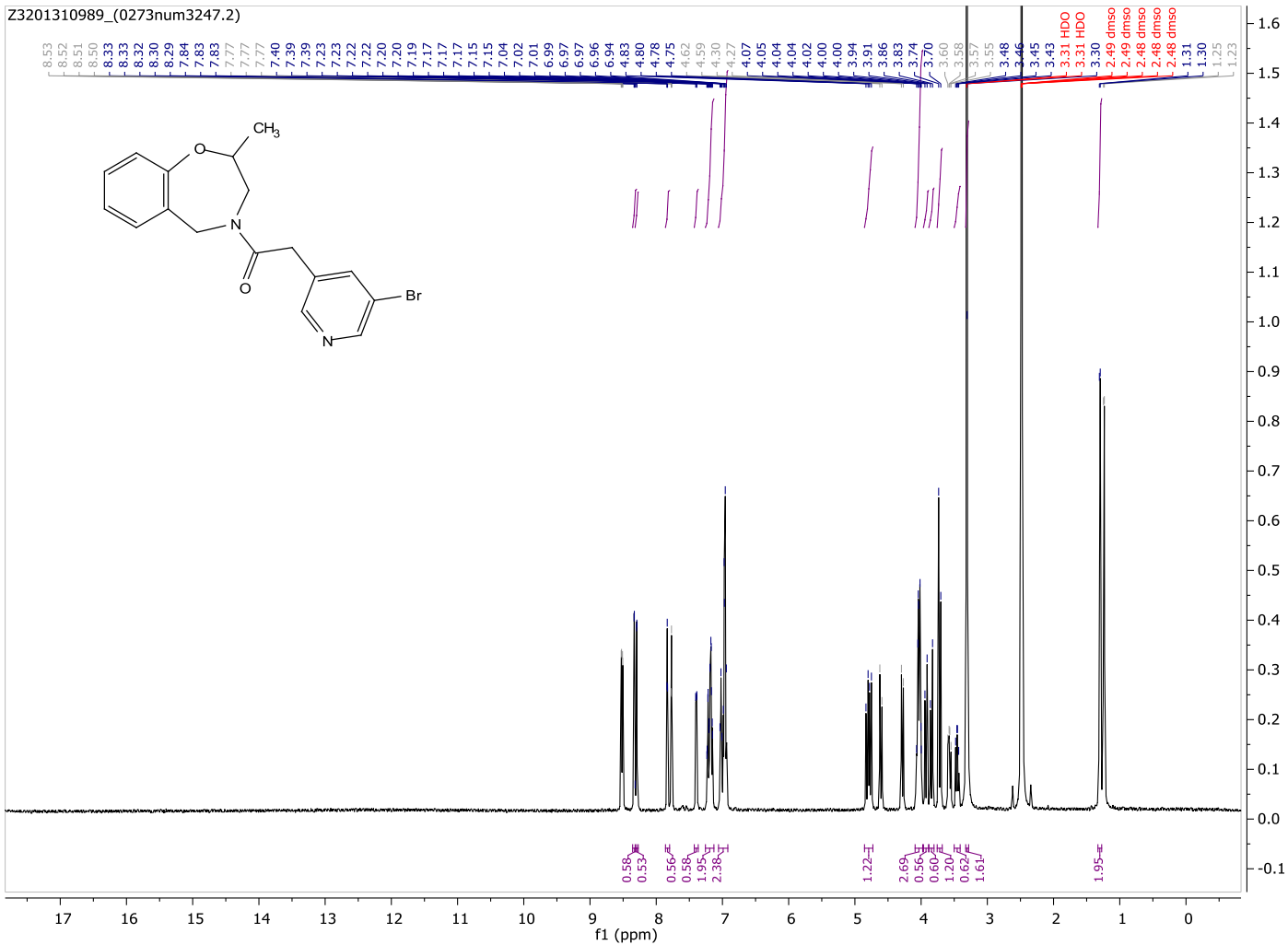
#	Time	Area%
1	1.280	100.00

S081639\$2

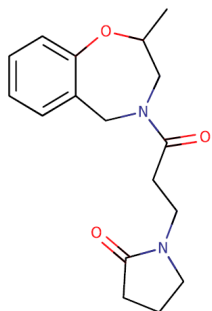


Z3201310989\_(0273num3247.2)

Z3201310989\_(0273num3247.2)



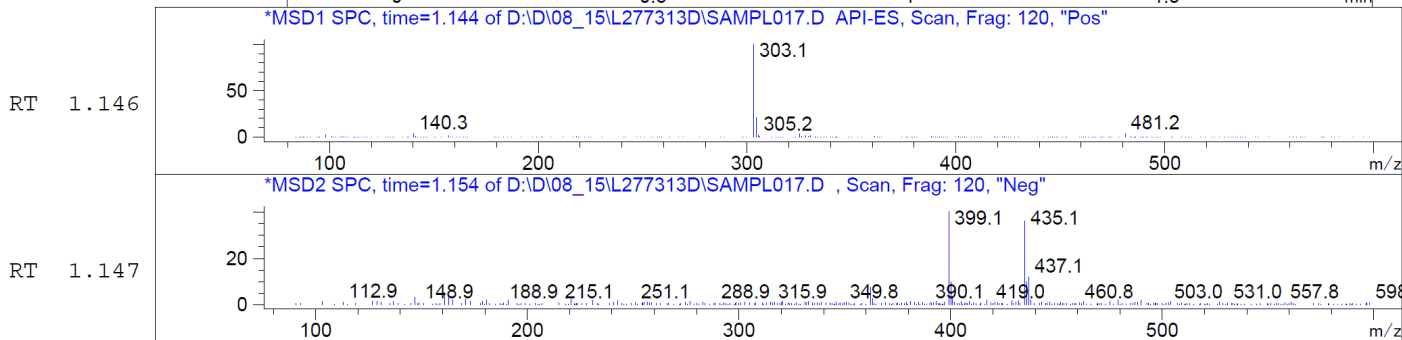
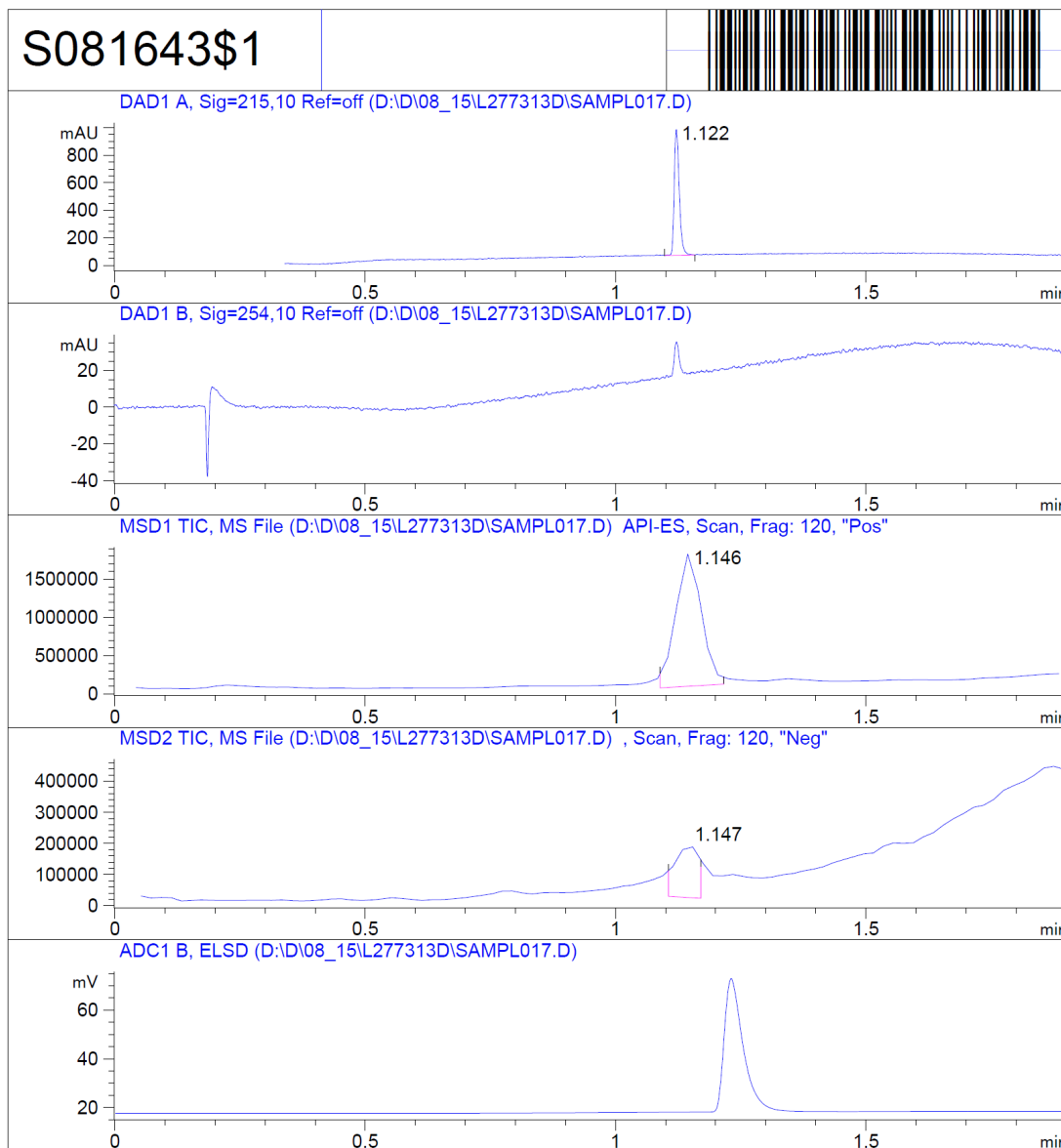
MaxPeak: 100.00%  
Ret\_Time: 1.122 min



Mol Wt 302.37  
Exact Mass 302.19

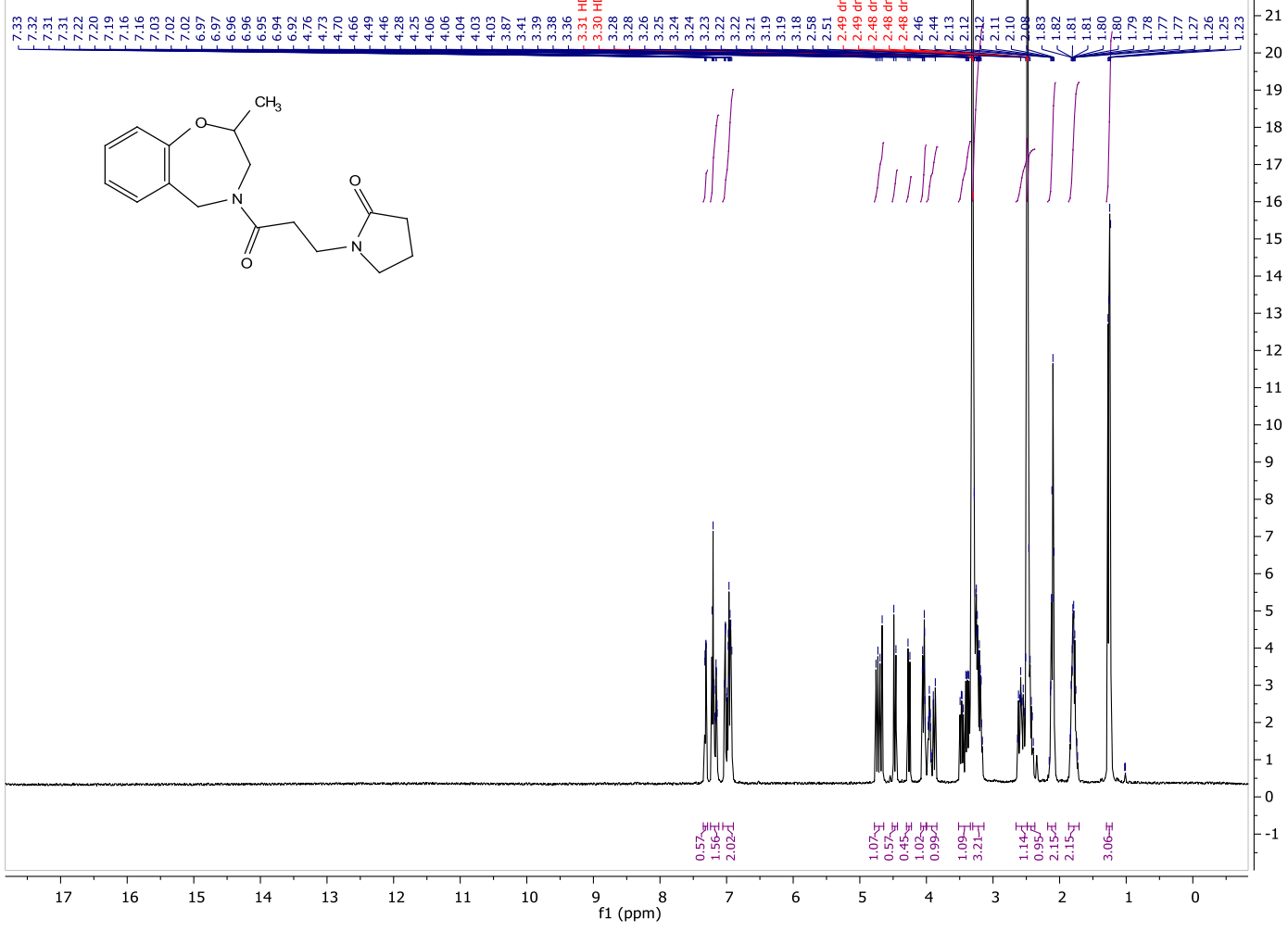
#	Time	Area%
1	1.122	100.00

# S081643\$1



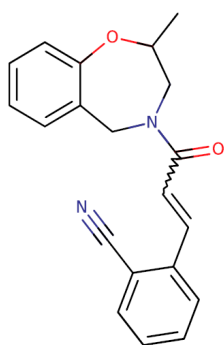
Z2227611595\_(0273num3604.2)

Z2227611595\_(0273num3604.2)





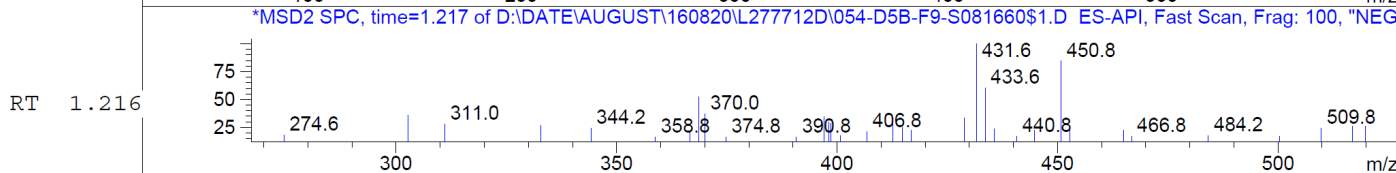
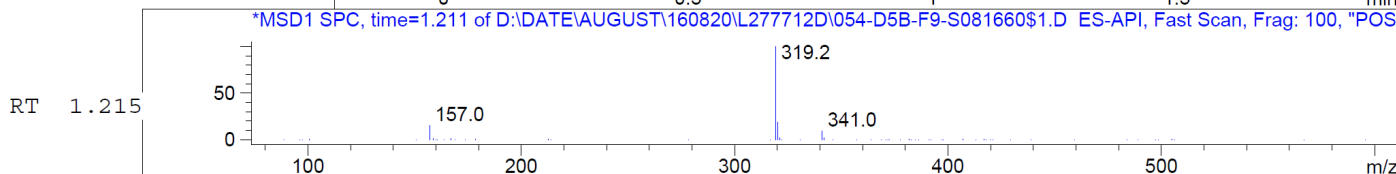
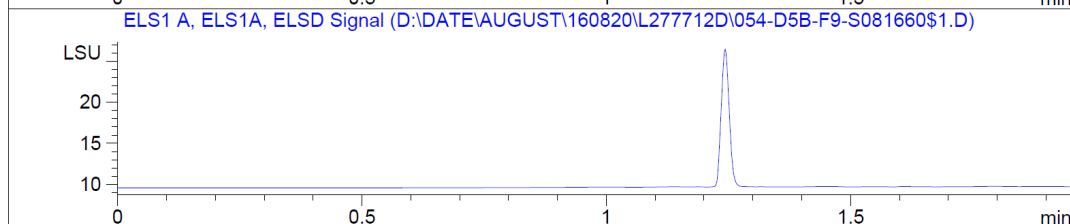
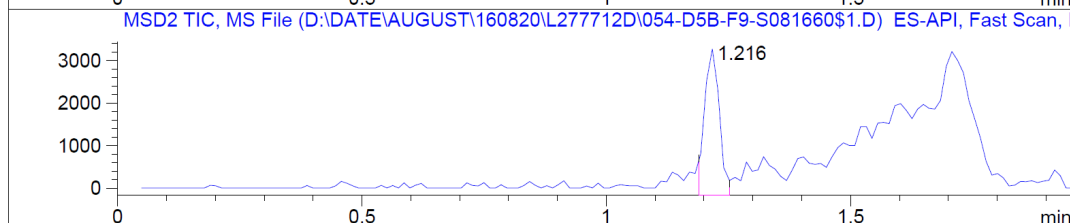
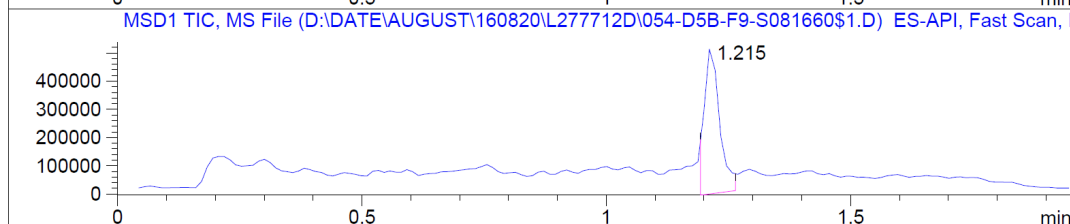
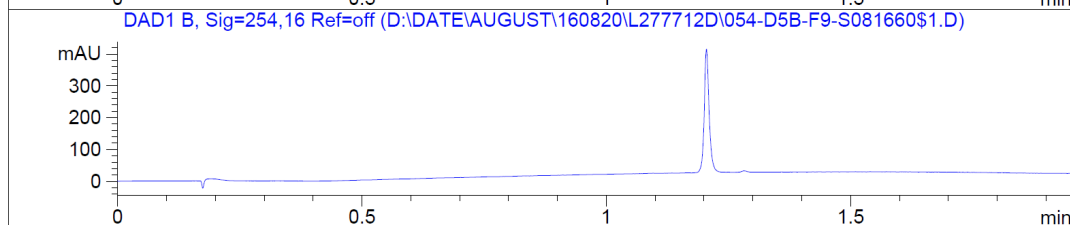
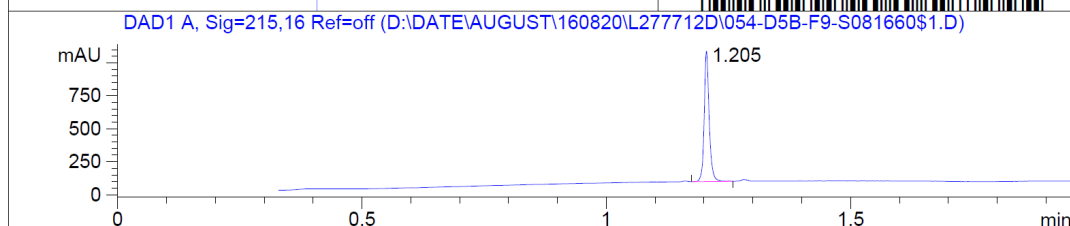
MaxPeak: 100.00%  
Ret\_Time: 1.205 min



Mol Wt 318.37  
Exact Mass 318.16

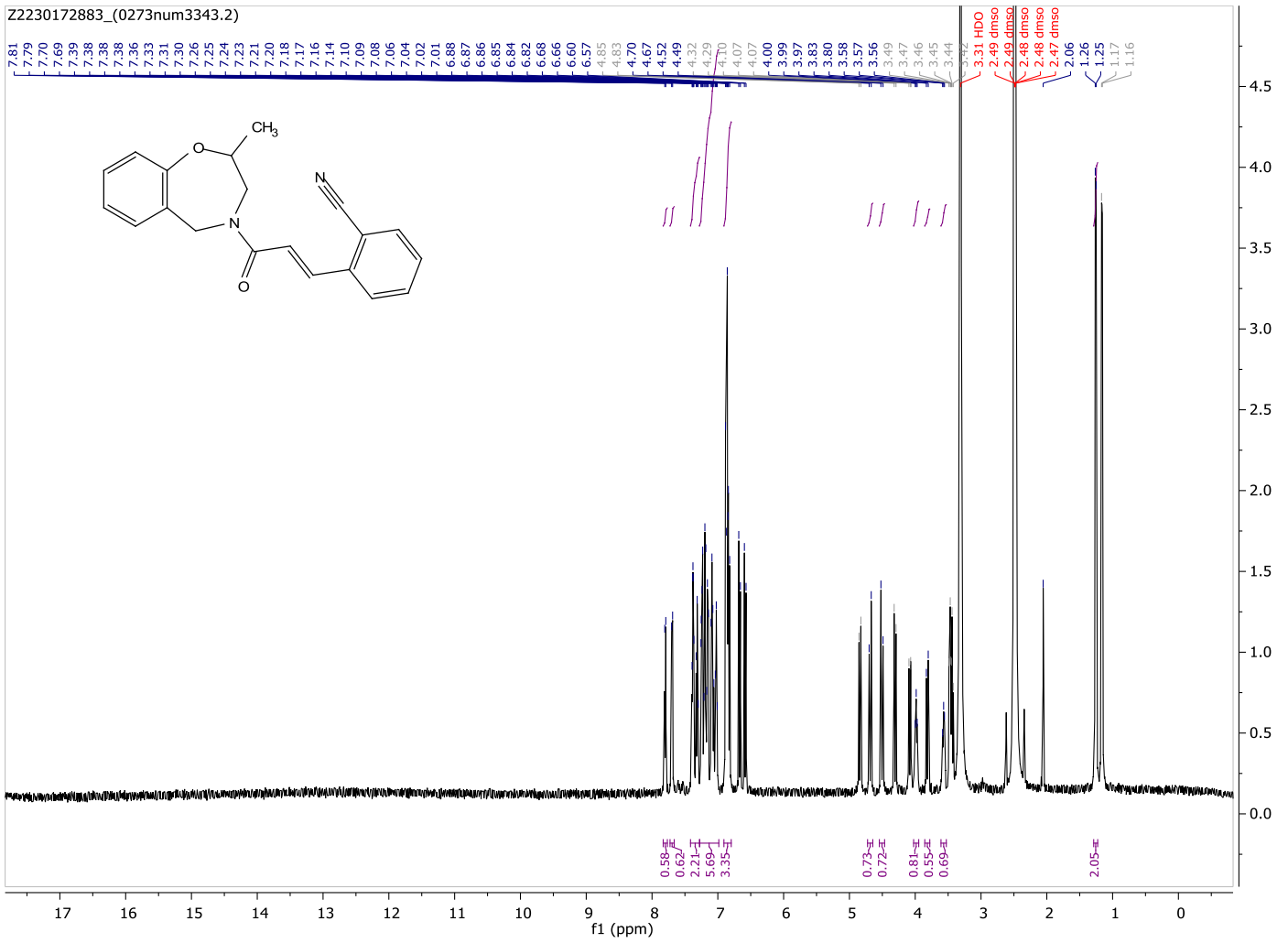
#	Time	Area%
1	1.205	100.00

# S081660\$1



Z2230172883\_(0273num3343.2)

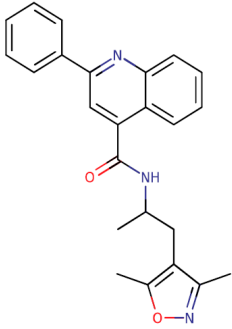
Z2230172883\_(0273num3343.2)



# S117856\$2

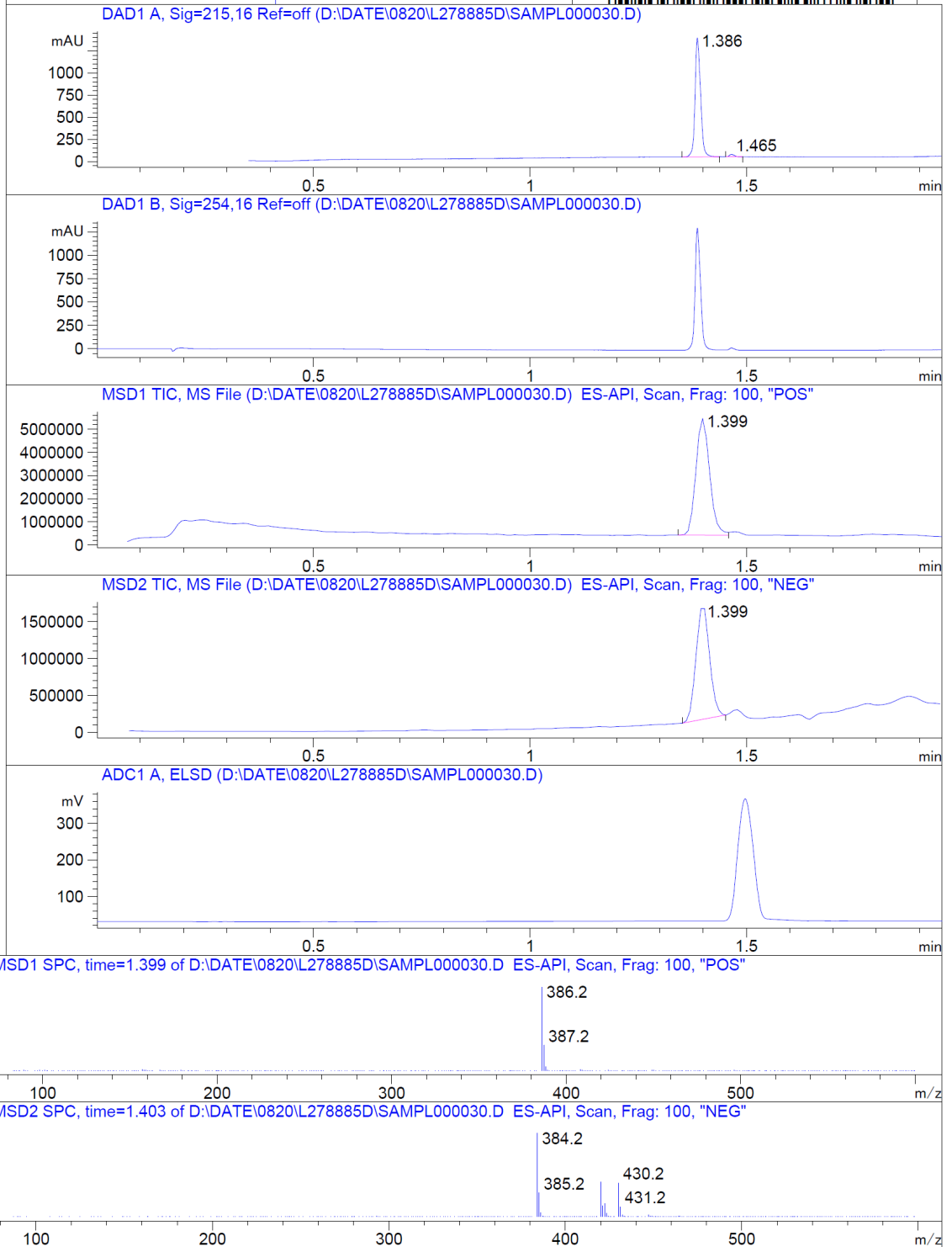


MaxPeak: 98.21%  
Ret\_Time: 1.386 min



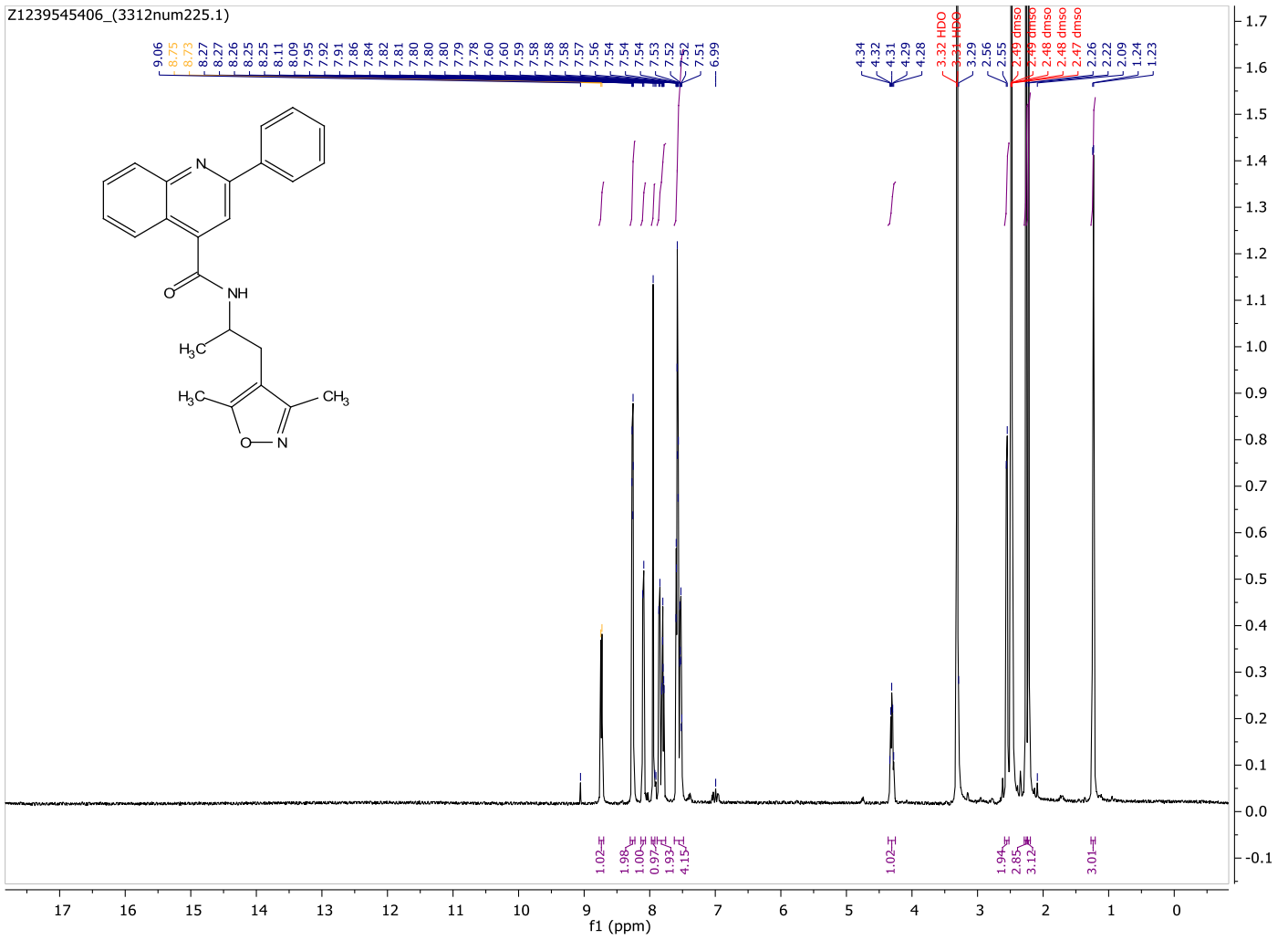
Mol Wt 385.46  
Exact Mass 385.21

#	Time	Area%
1	1.386	98.21
2	1.465	1.79



Z1239545406\_(3312num225.1)

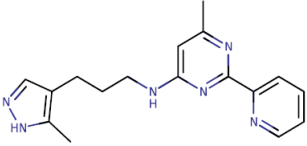
Z1239545406\_(3312num225.1)



# S117850\$4

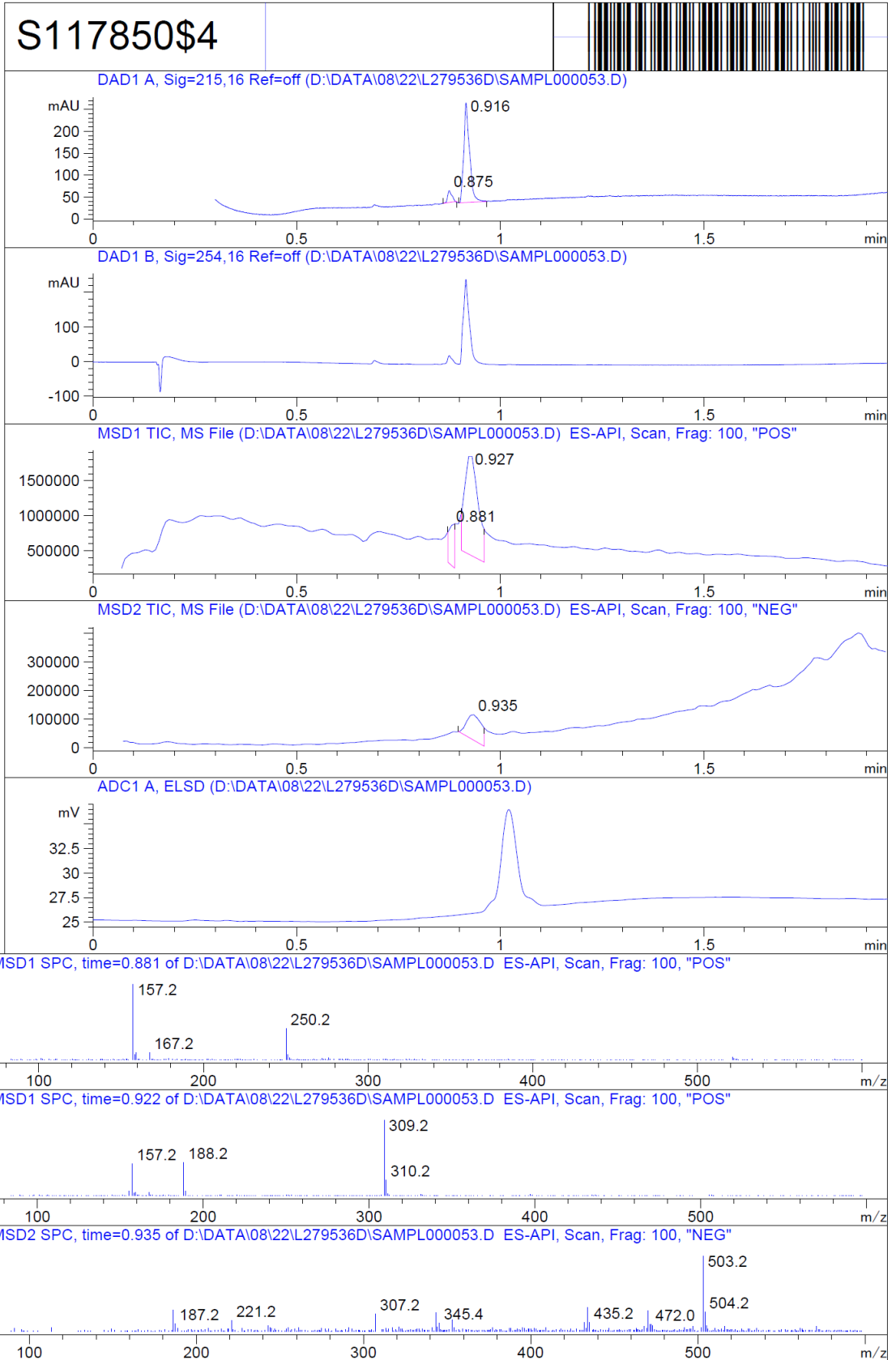


MaxPeak: 92.07%  
Ret\_Time: 0.916 min



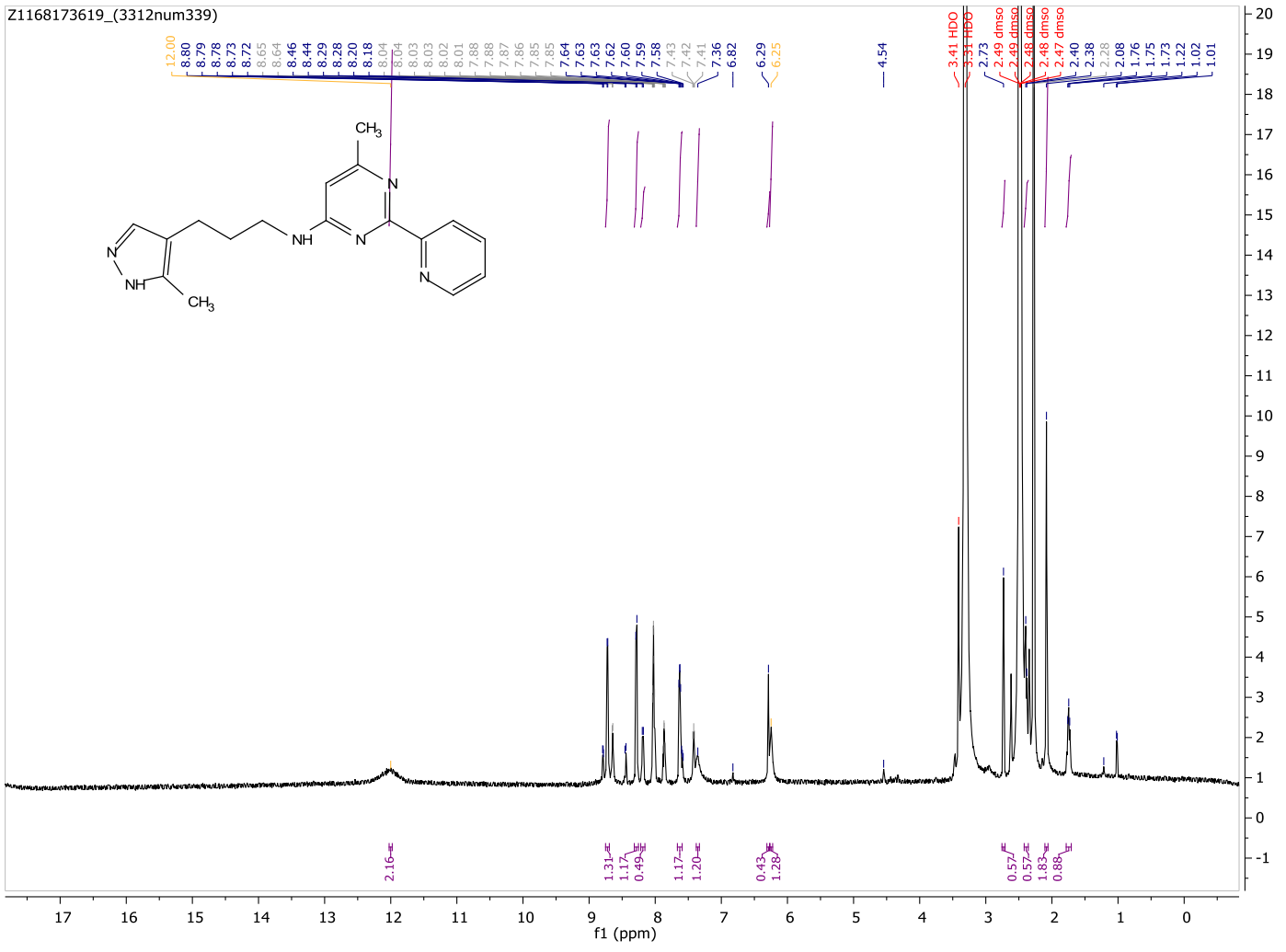
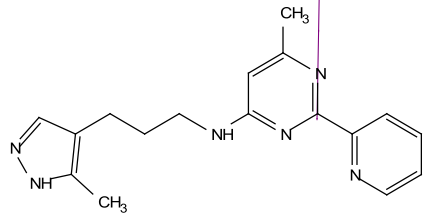
**Mol Wt** 308.38  
**Exact Mass** 308.2

#	Time	Area%
1	0.875	7.93
2	0.916	92.07

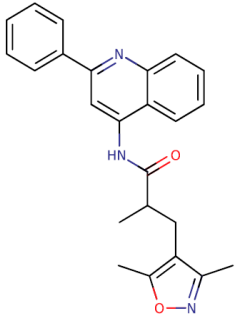


Z1168173619\_(3312num339)

Z1168173619\_(3312num339)



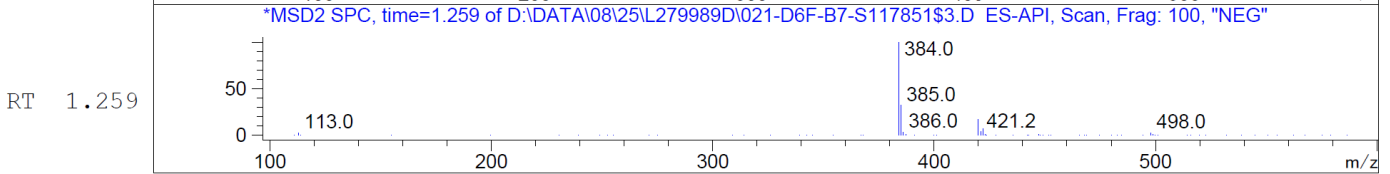
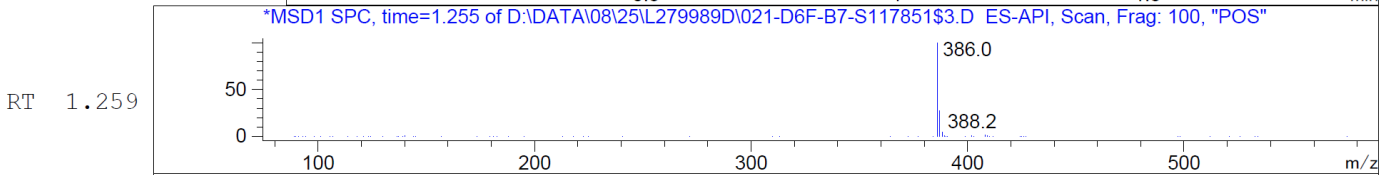
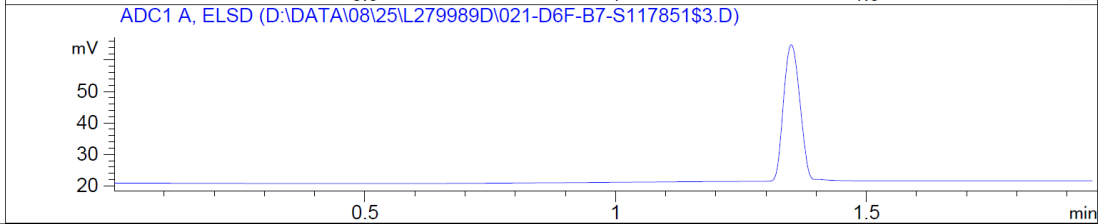
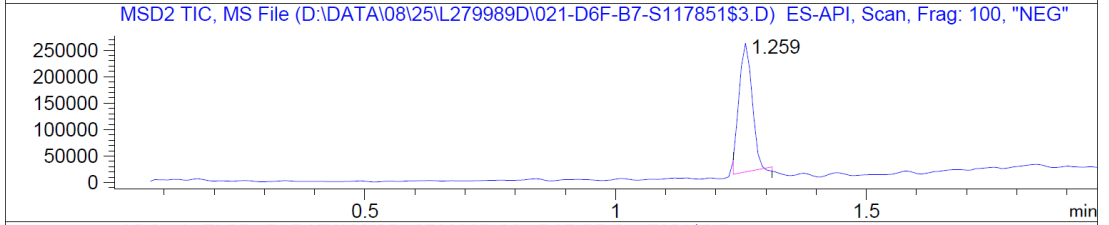
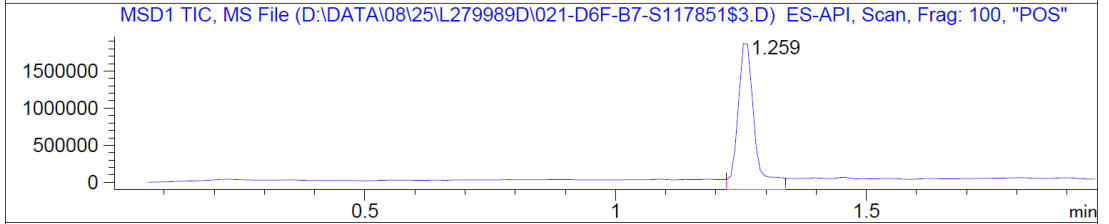
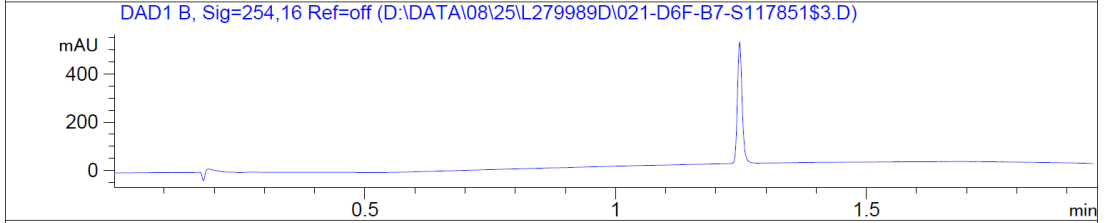
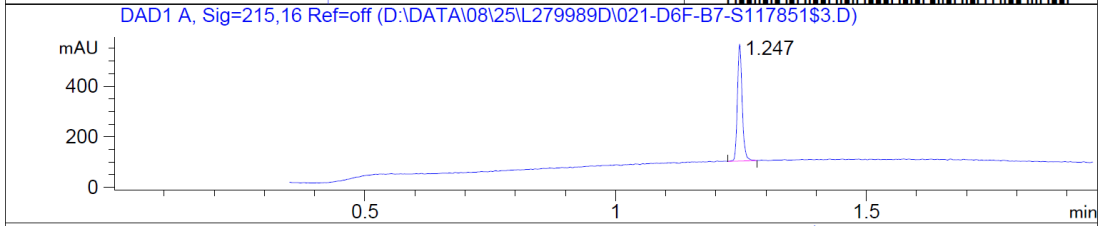
MaxPeak: 100.00%  
Ret\_Time: 1.247 min



Mol Wt 385.46  
Exact Mass 385.21

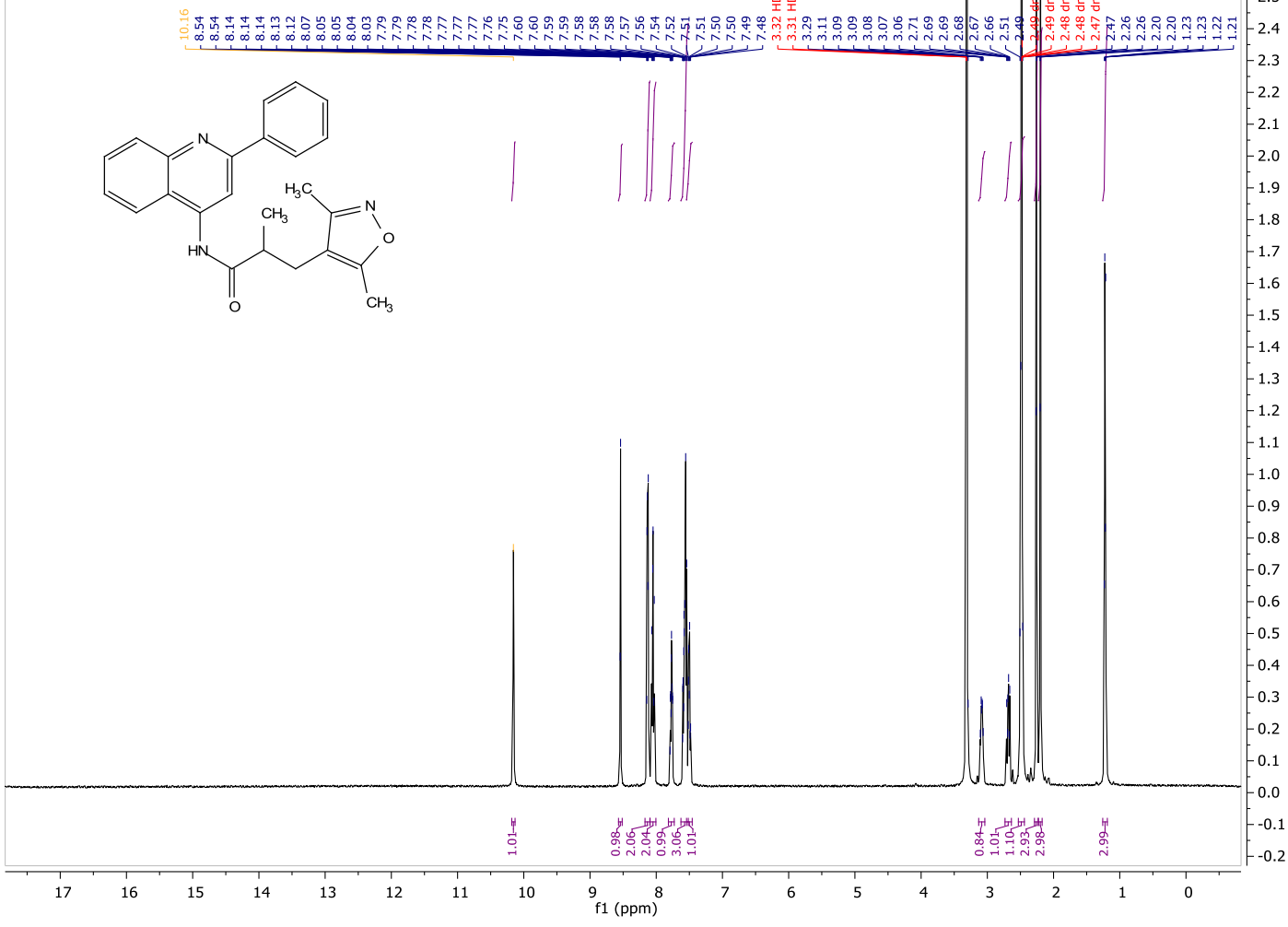
#	Time	Area%
1	1.247	100.00

# S117851\$3



Z4570447323\_(3312num215.1)

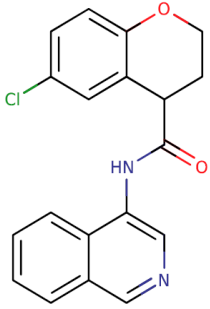
Z4570447323\_(3312num215.1)





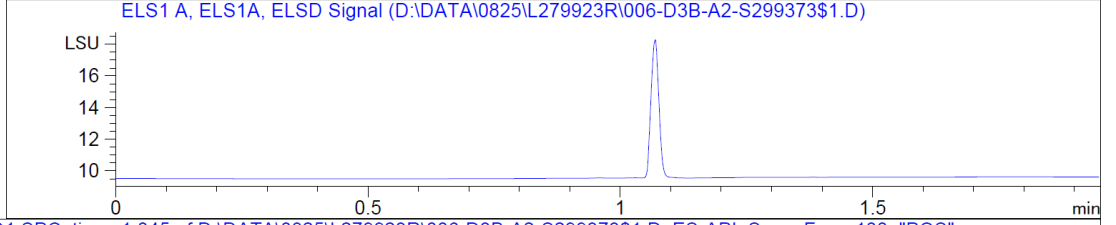
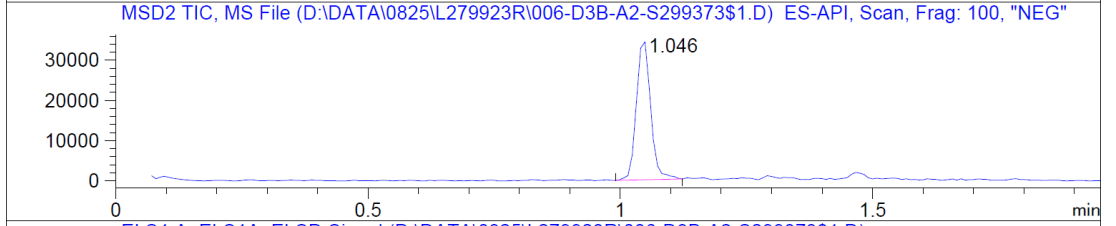
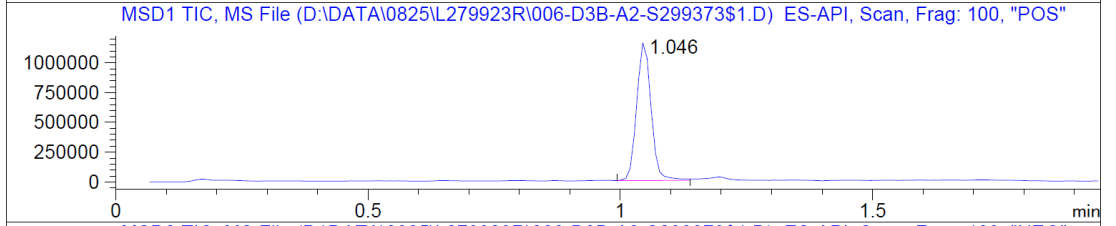
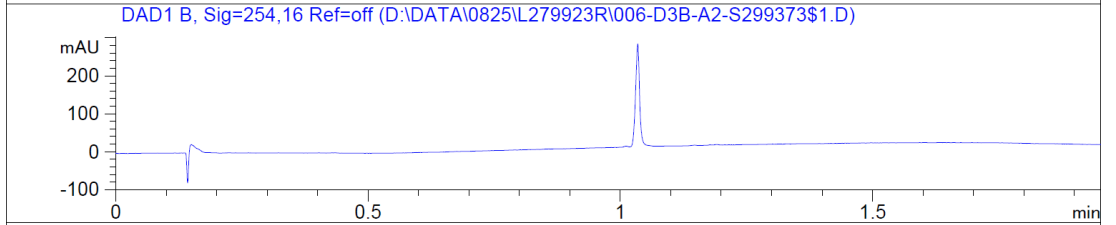
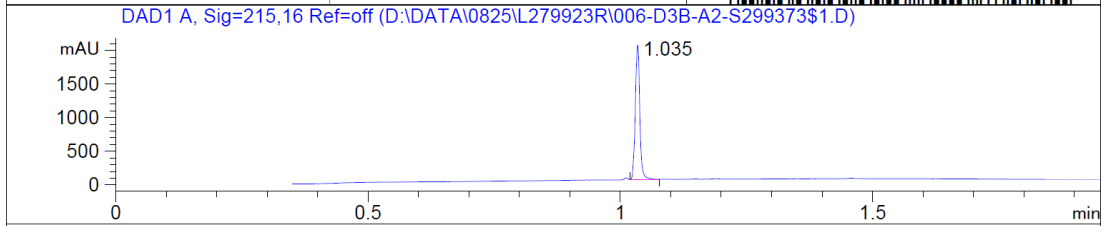
MaxPeak: 100.00%  
Ret\_Time: 1.035 min

# S299373\$1

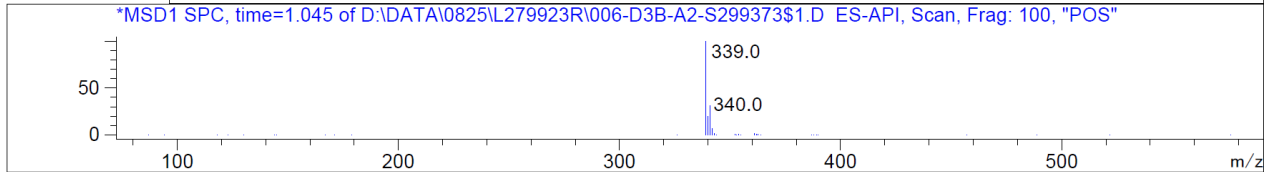


**Mol Wt** 338.79  
**Exact Mass** 338.1

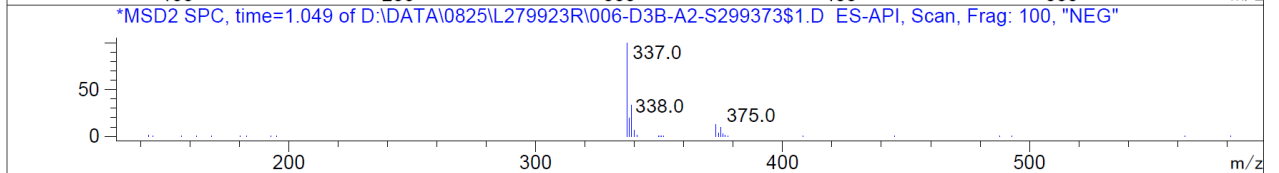
#	Time	Area%
1	1.035	100.00



RT 1.046

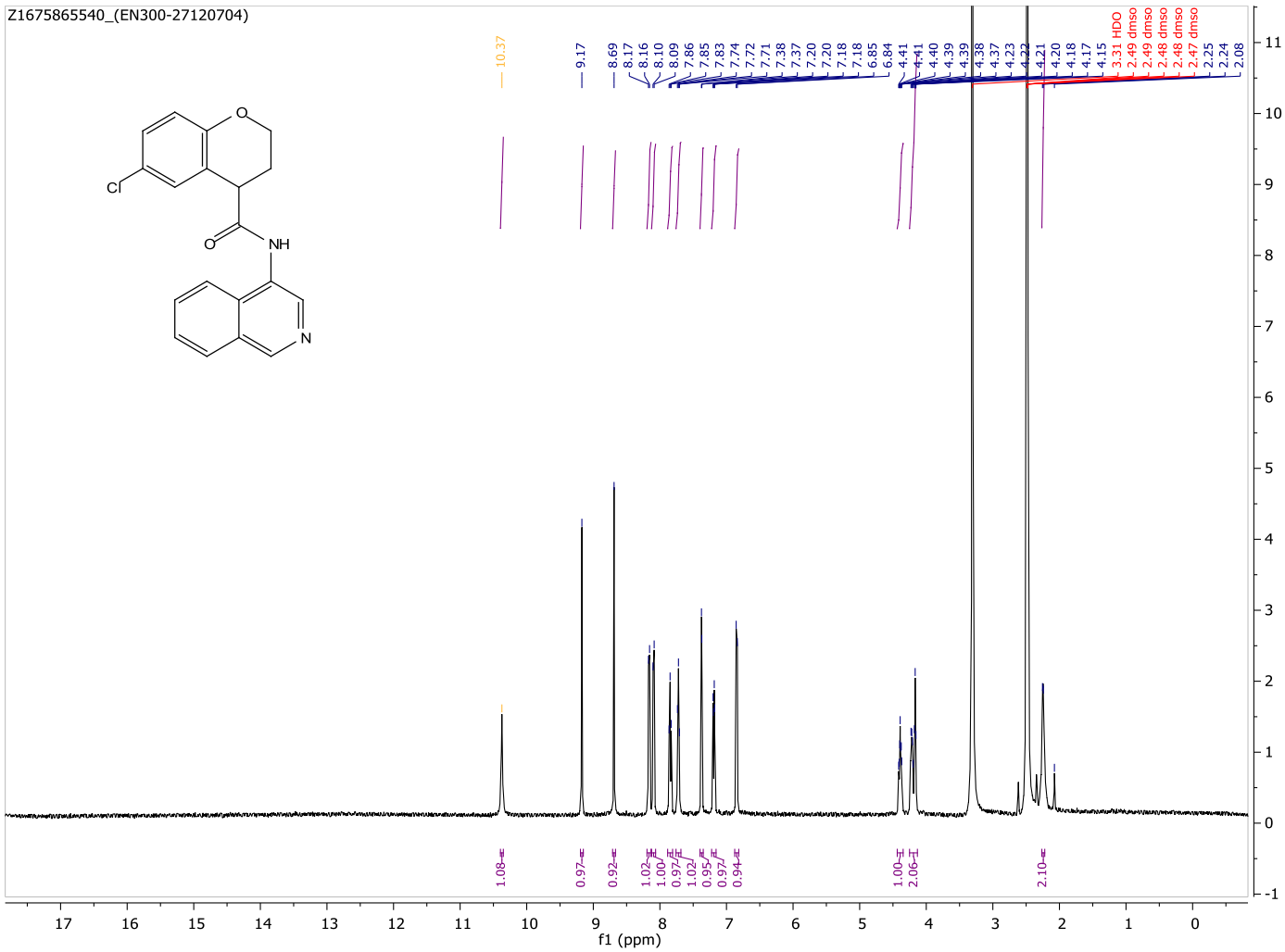
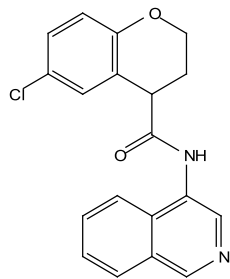


RT 1.046

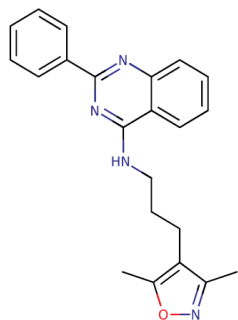


Z1675865540\_(EN300-27120704)

Z1675865540\_(EN300-27120704)



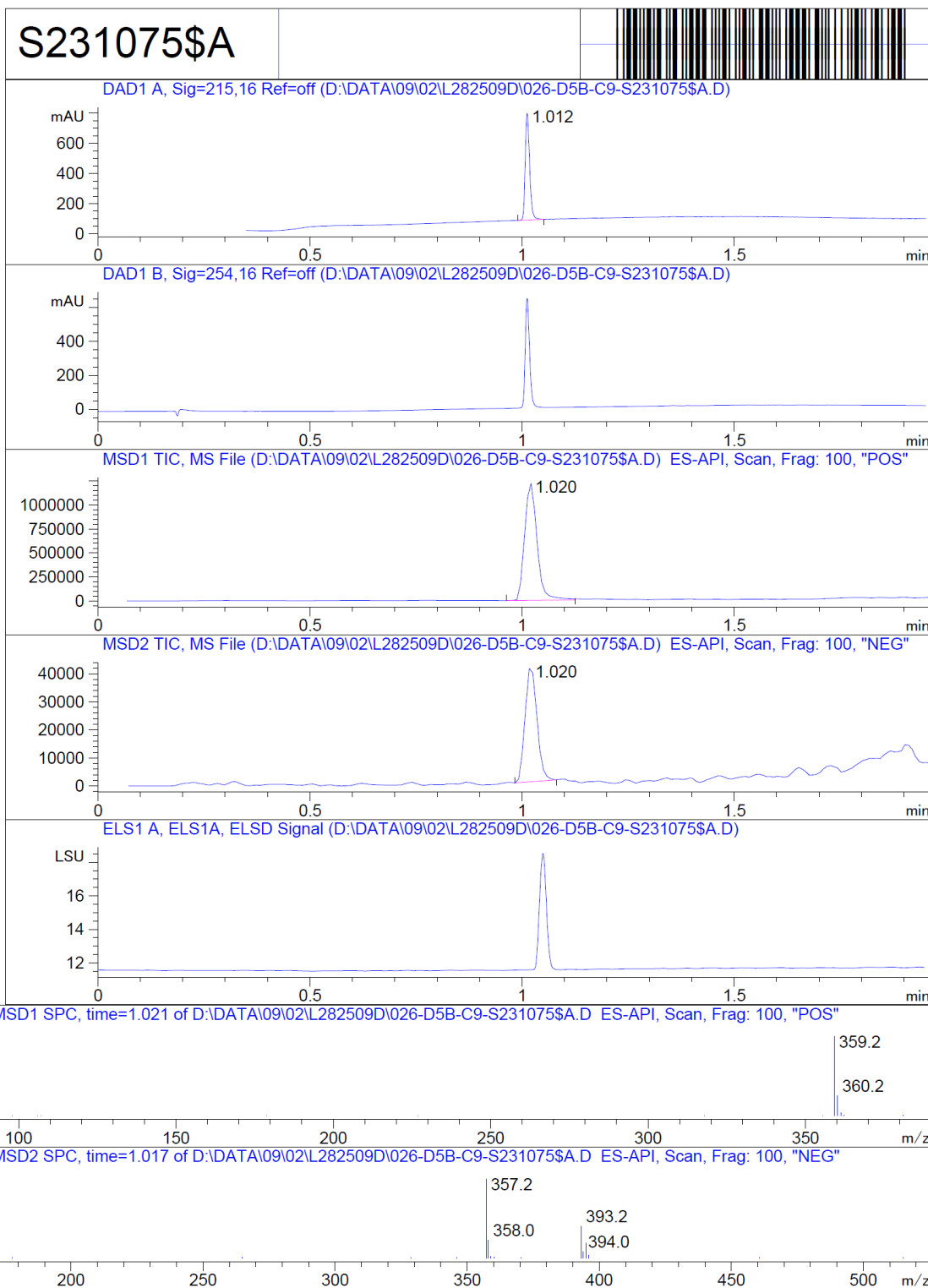
MaxPeak: 100.00%  
Ret\_Time: 1.012 min



Mol Wt 358.44

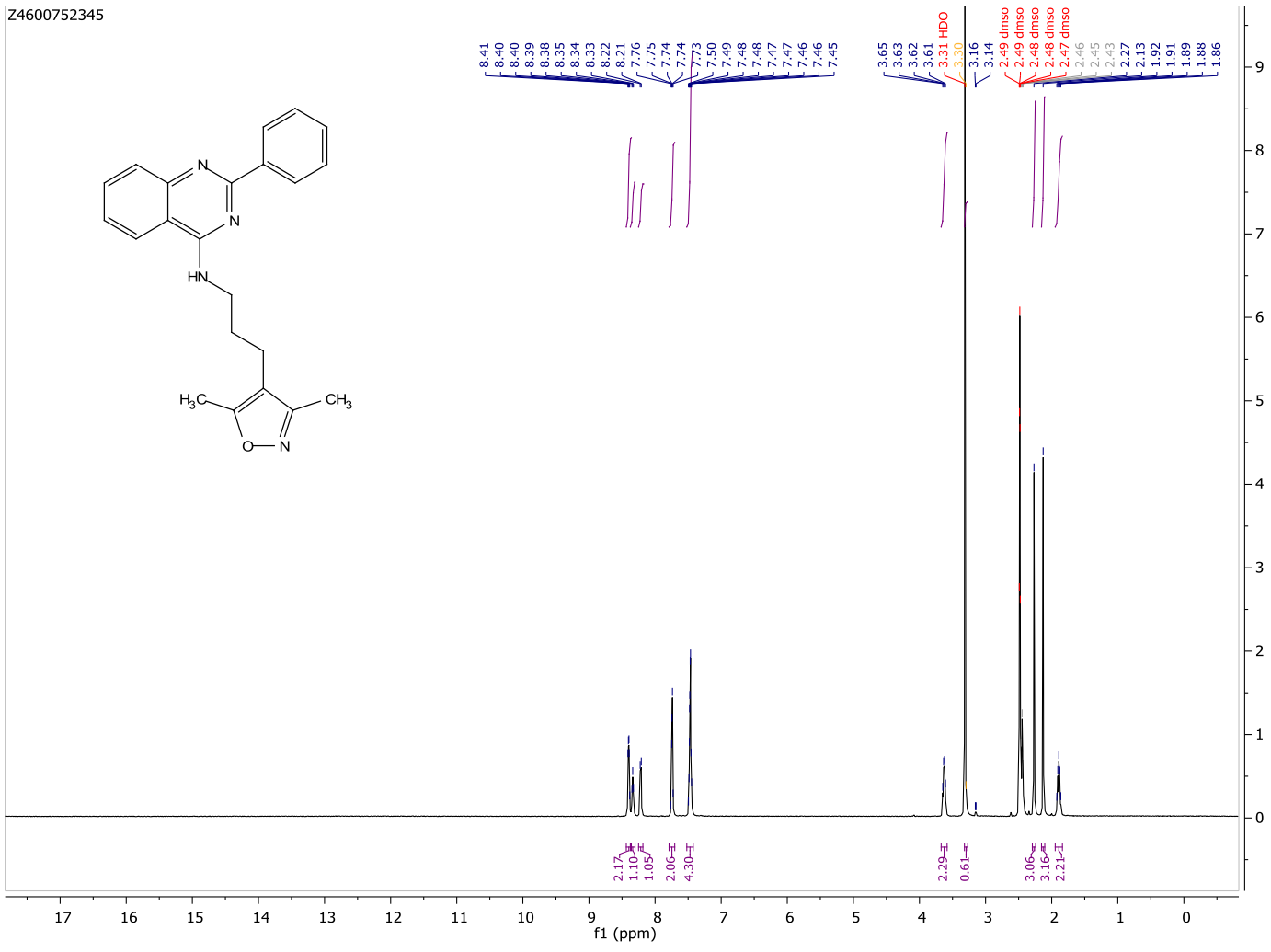
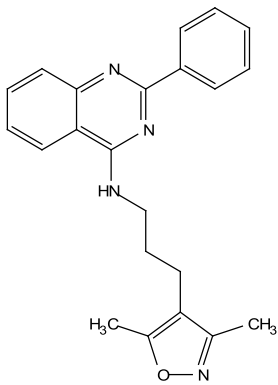
Exact Mass 358.21

#	Time	Area%
1	1.012	100.00

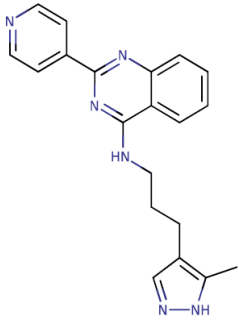


Z4600752345

Z4600752345

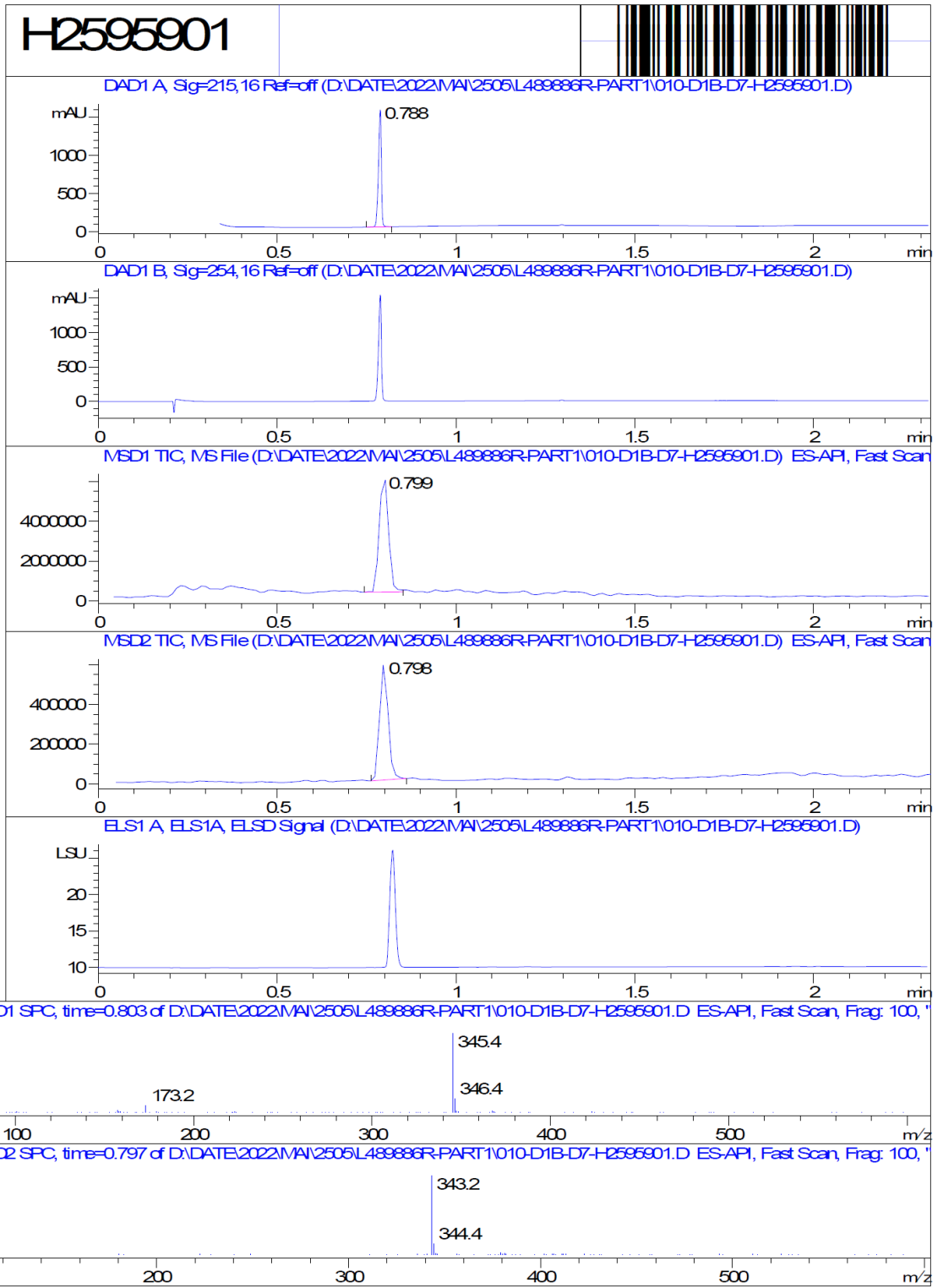


MaxPeak: 100.00%  
Ret\_Time: 0.788 min



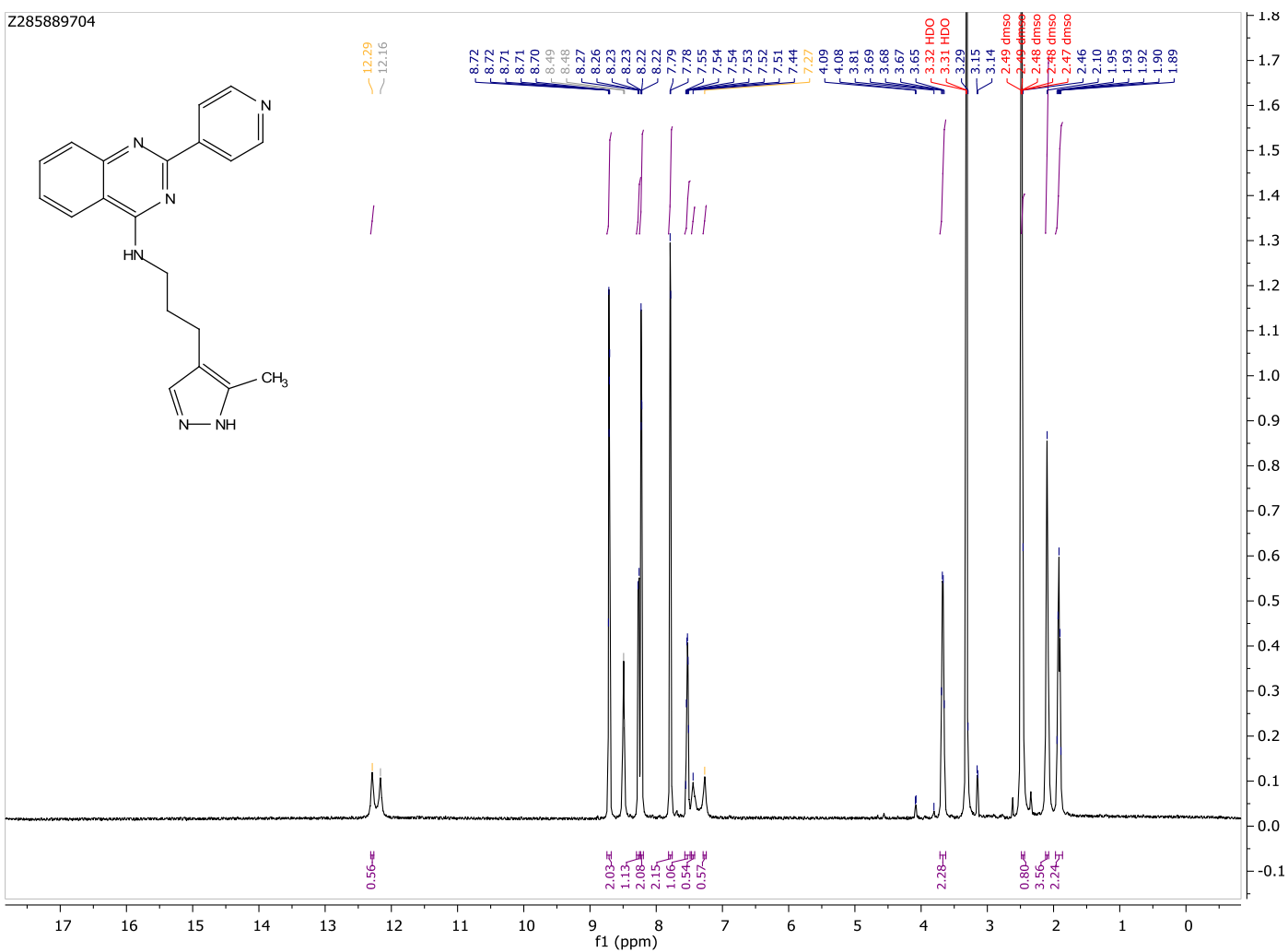
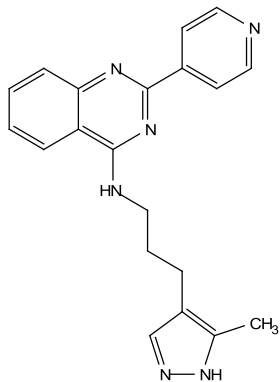
**Mol Wt** 344.41  
**Exact Mass** 344.2

#	Time	Area%
1	0.788	100.00



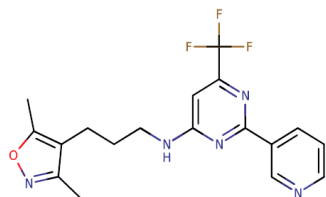
Z285889704

Z285889704



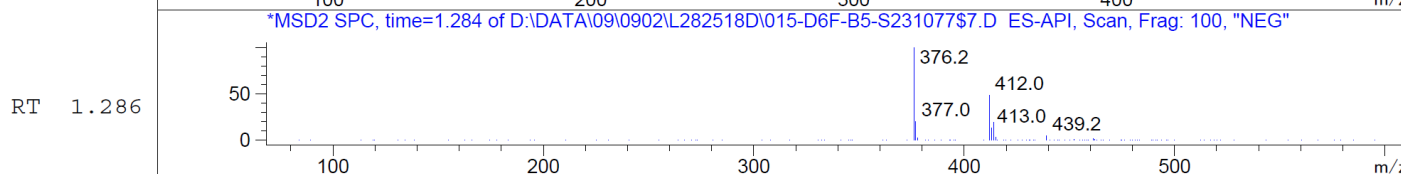
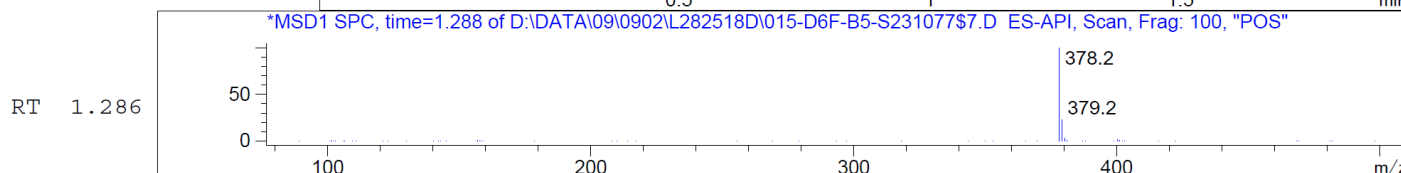
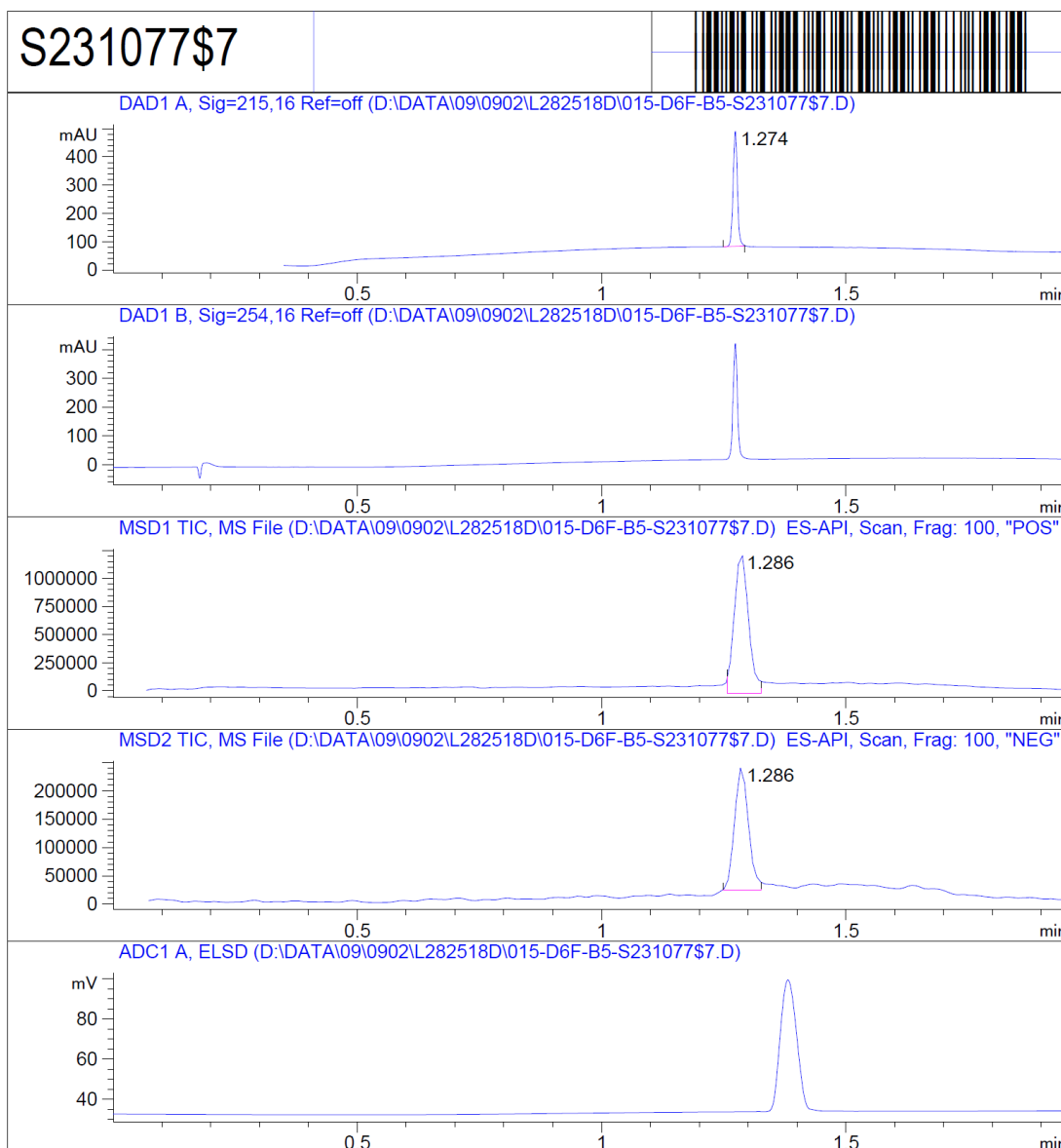
MaxPeak: 100.00%  
Ret\_Time: 1.274 min

# S231077\$7



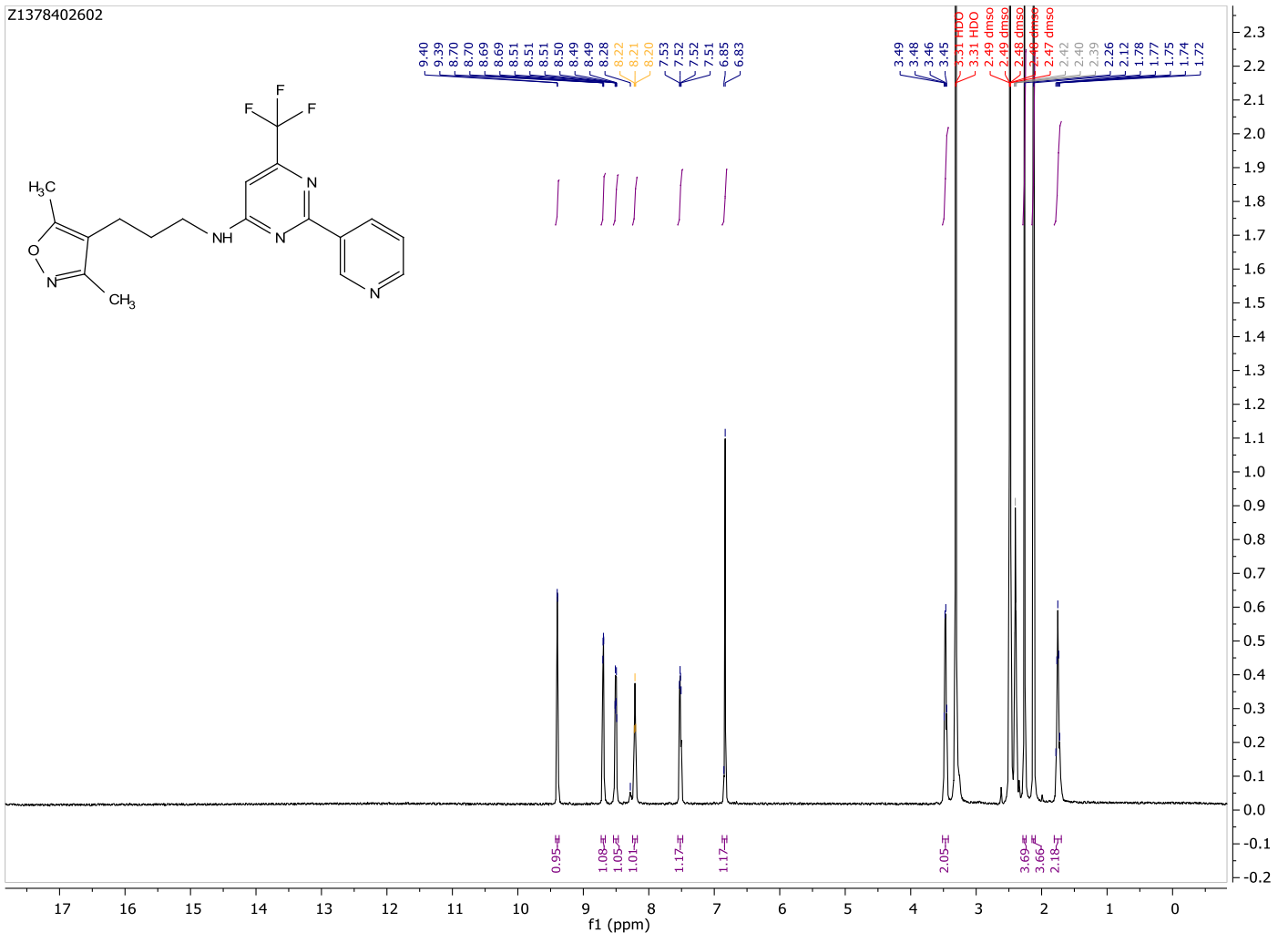
**Mol Wt** 377.36  
**Exact Mass** 377.17

#	Time	Area%
1	1.274	100.00



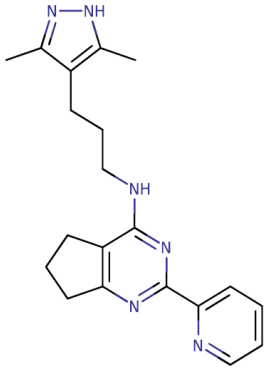
Z1378402602

Z1378402602





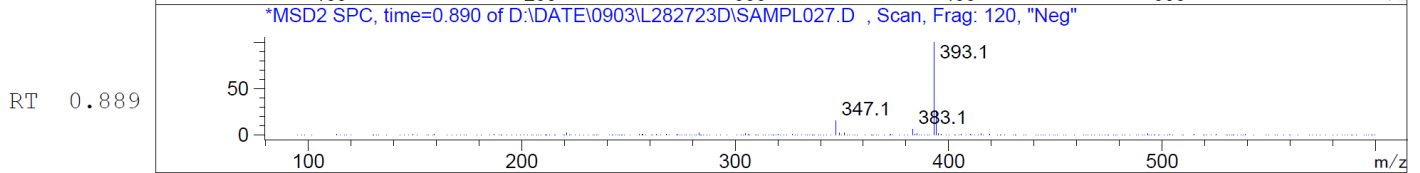
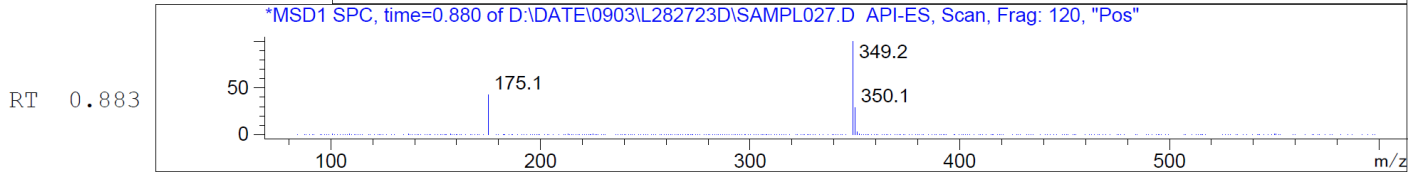
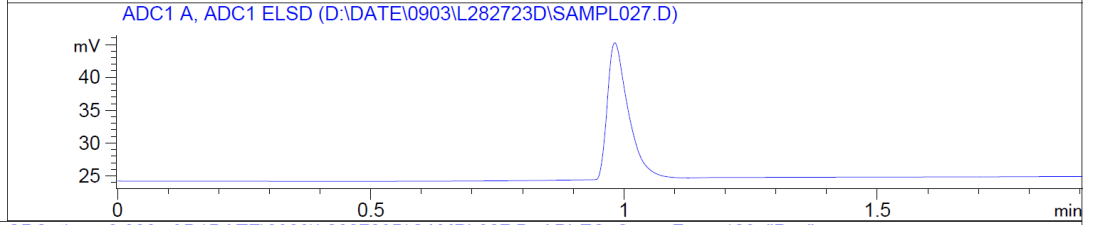
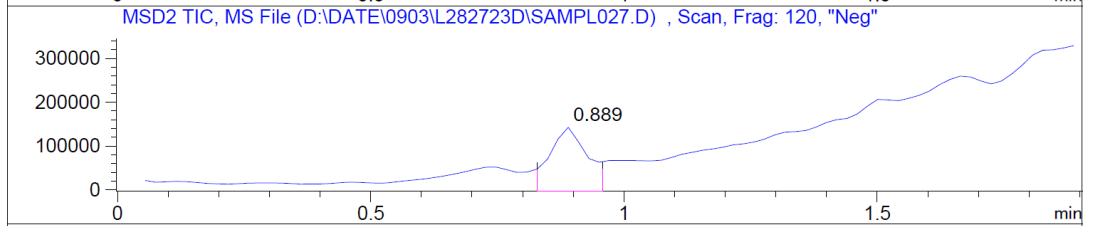
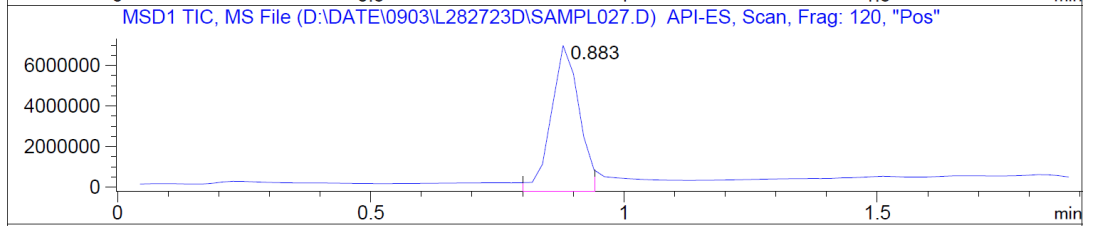
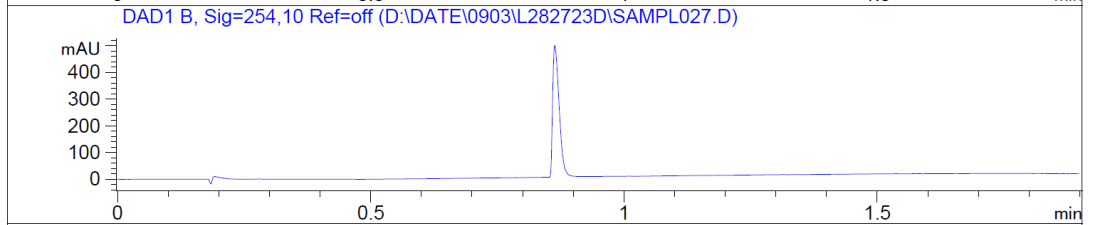
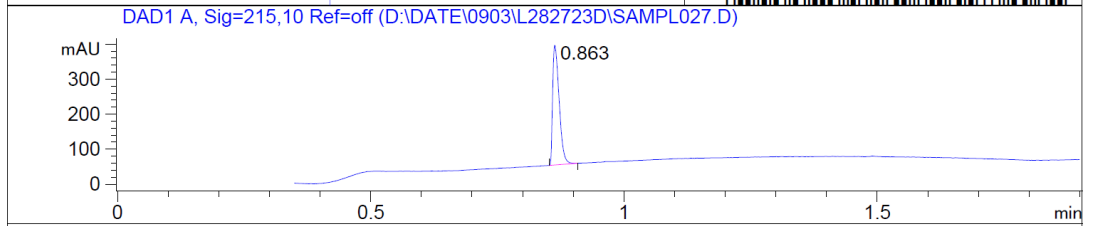
MaxPeak: 100.00%  
Ret\_Time: 0.863 min



Mol Wt 348.44  
Exact Mass 348.24

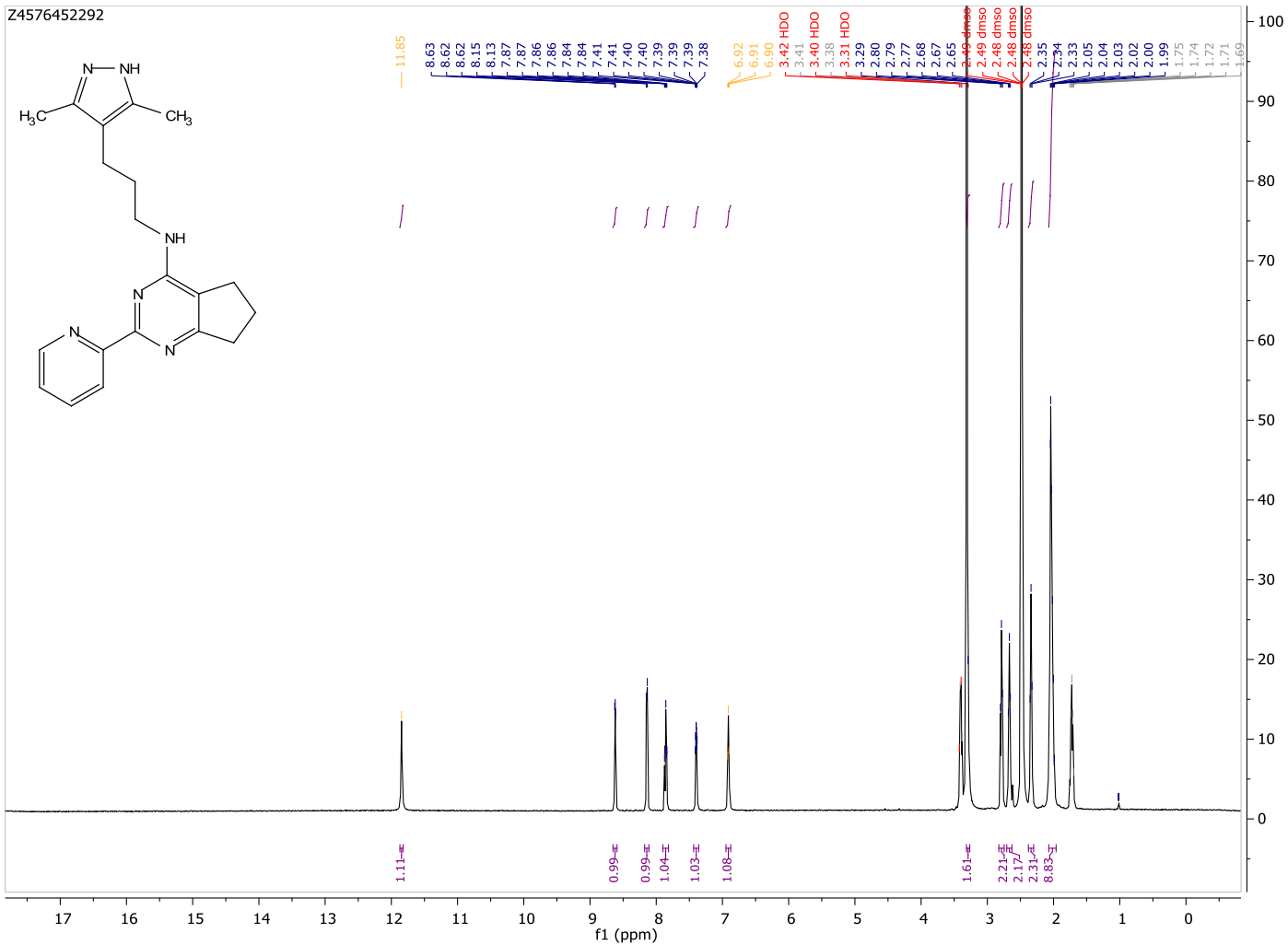
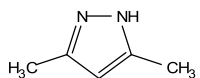
#	Time	Area%
1	0.863	100.00

S231074\$6

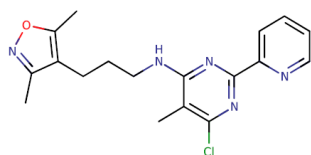


Z4576452292

Z4576452292



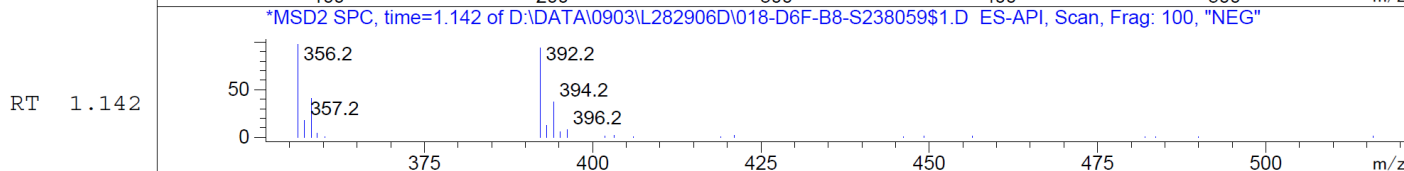
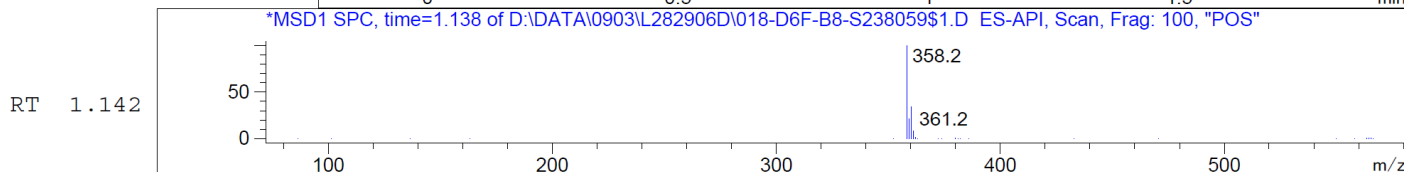
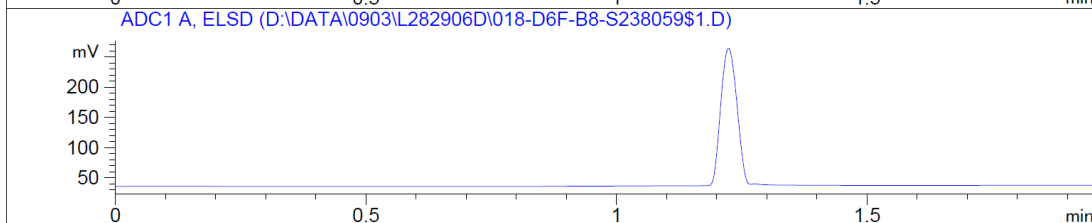
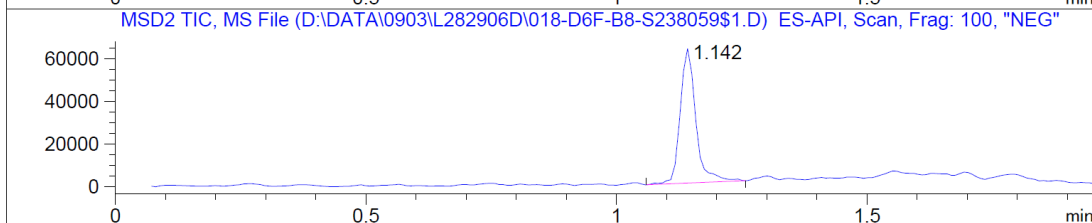
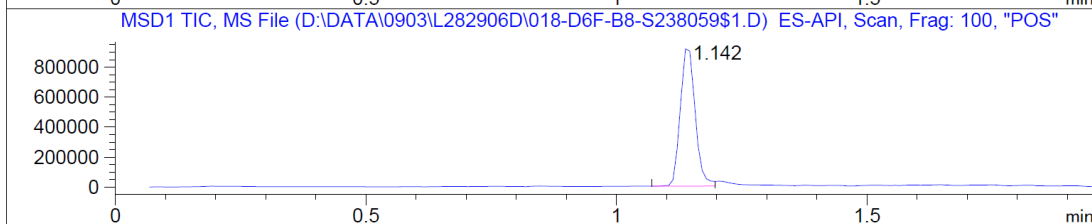
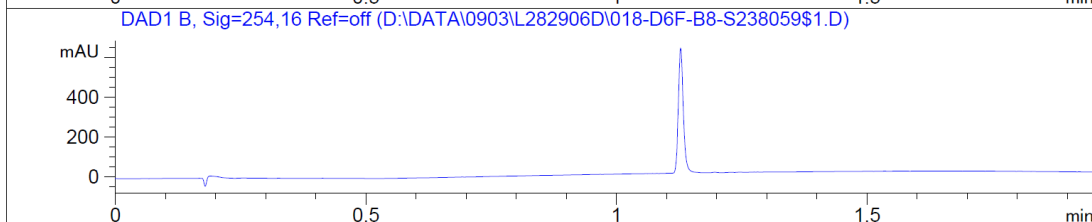
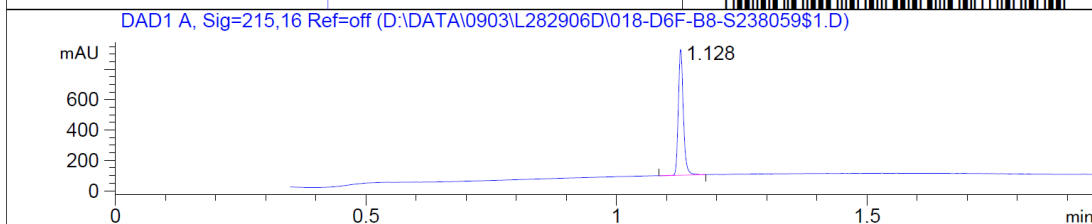
MaxPeak: 100.00%  
Ret\_Time: 1.128 min



Mol Wt 357.84  
Exact Mass 357.16

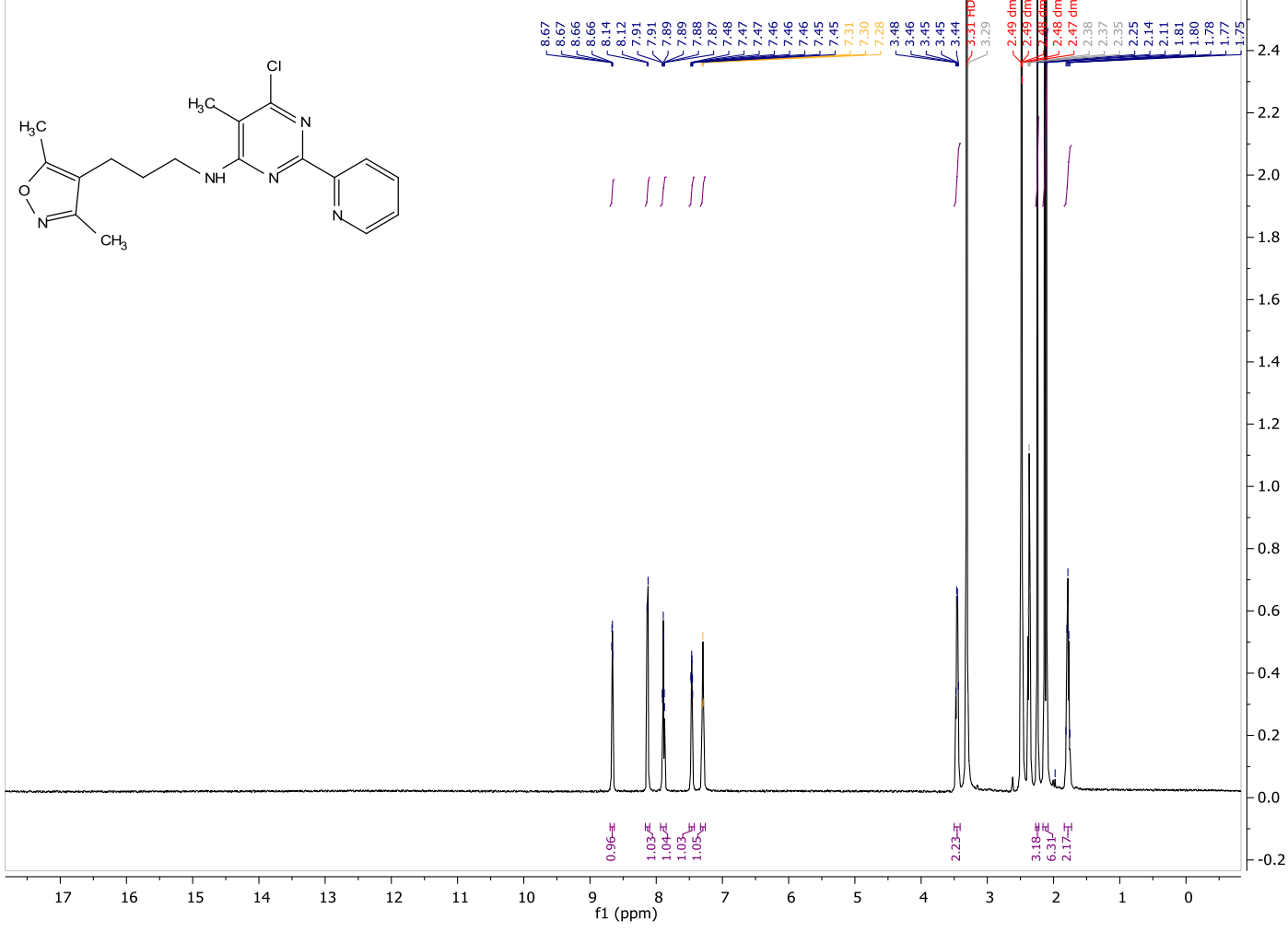
#	Time	Area%
1	1.128	100.00

# S238059\$1



Z4607408926

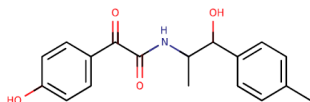
Z4607408926



# S568076\$2

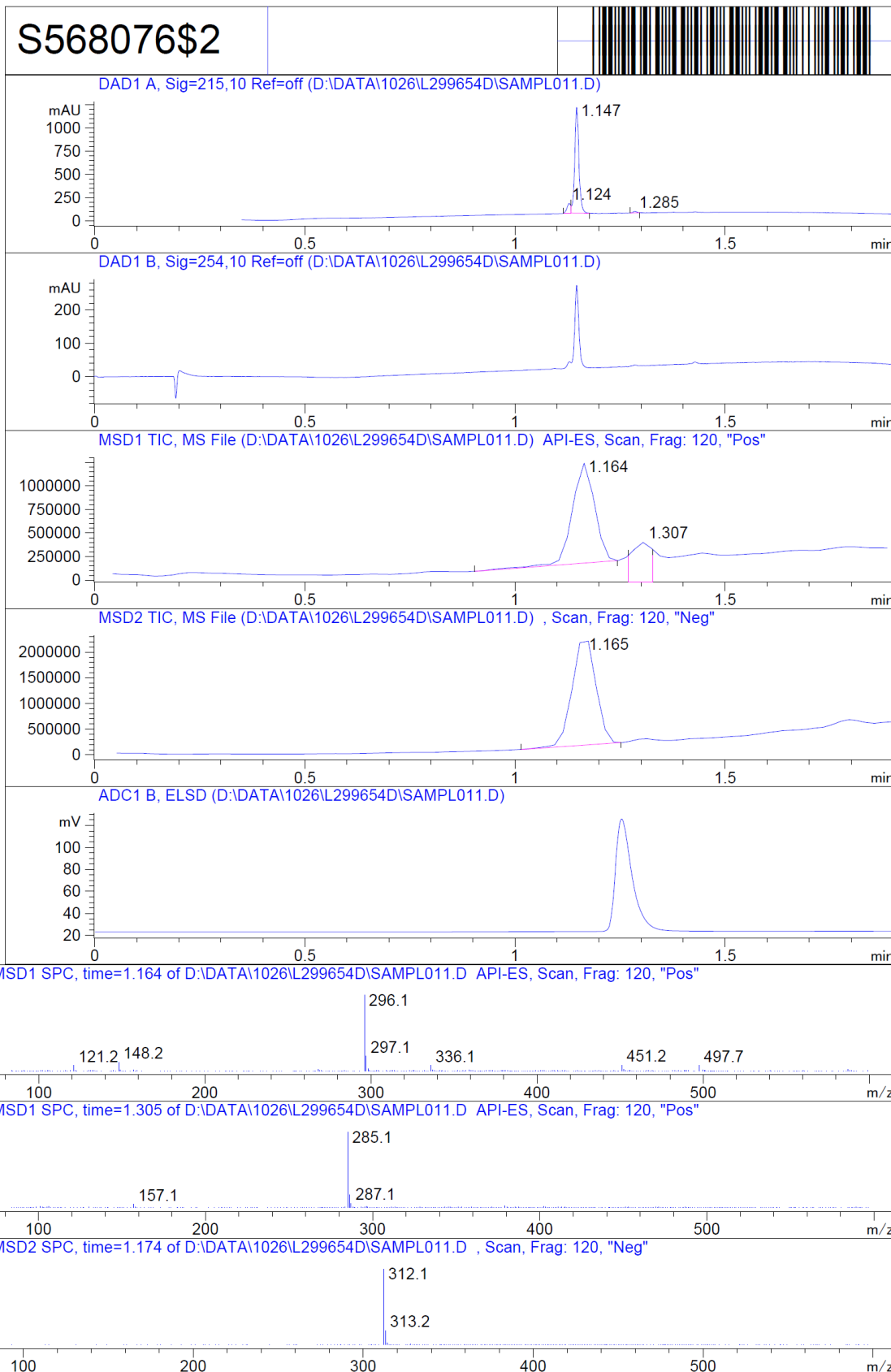


MaxPeak: 91.57%  
Ret\_Time: 1.147 min



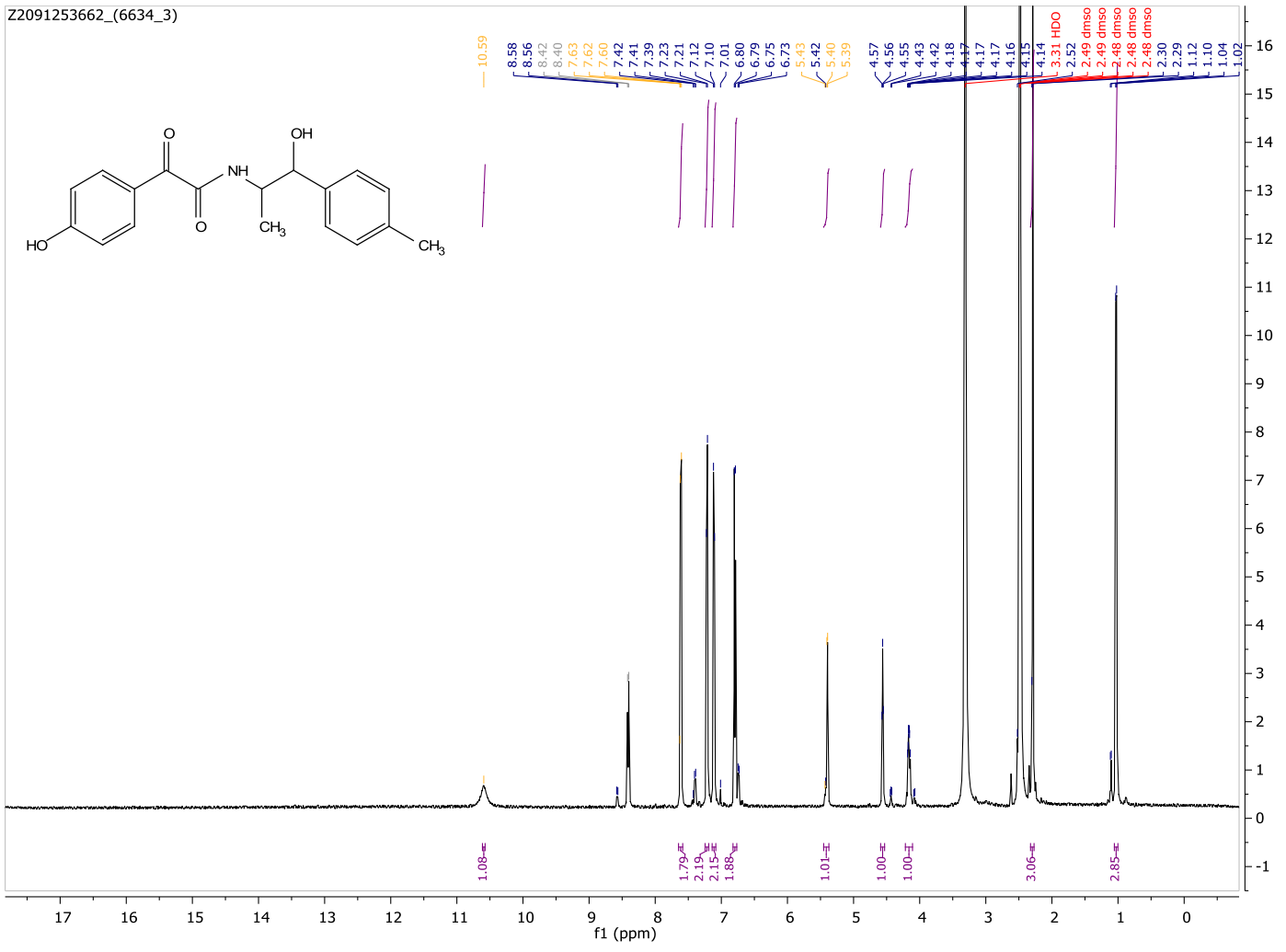
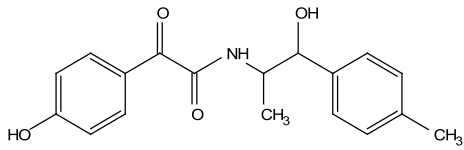
**Mol Wt** 313.35  
**Exact Mass** 313.15

#	Time	Area%
1	1.124	7.28
2	1.147	91.57
3	1.285	1.15



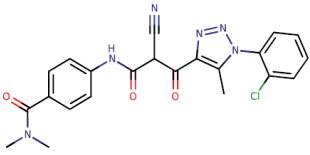
Z2091253662\_(6634\_3)

Z2091253662\_(6634\_3)



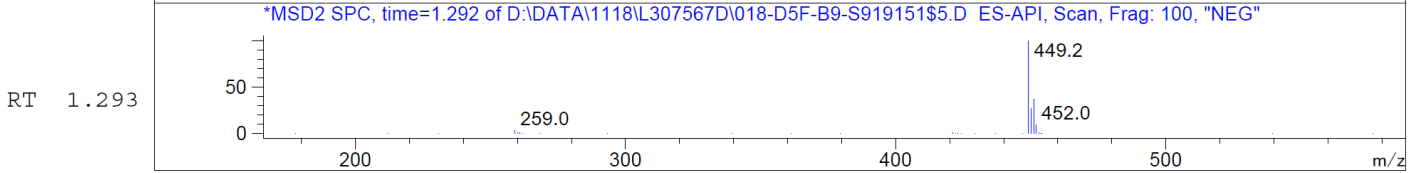
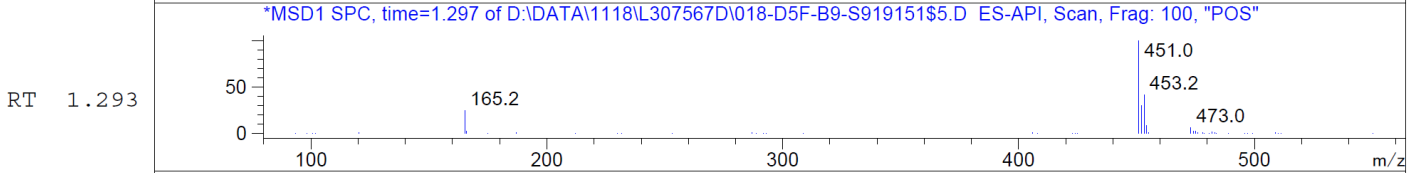
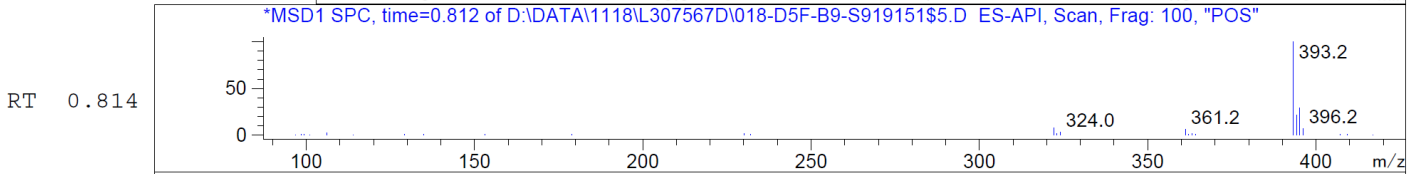
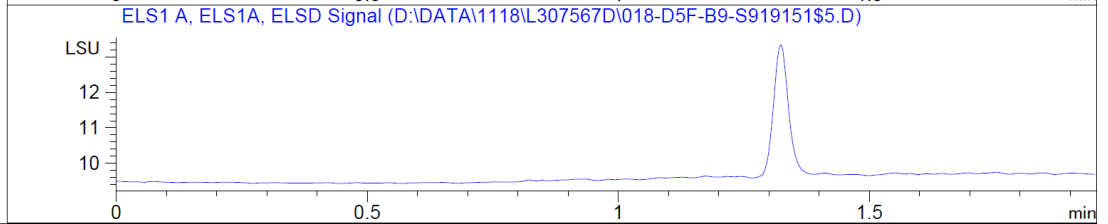
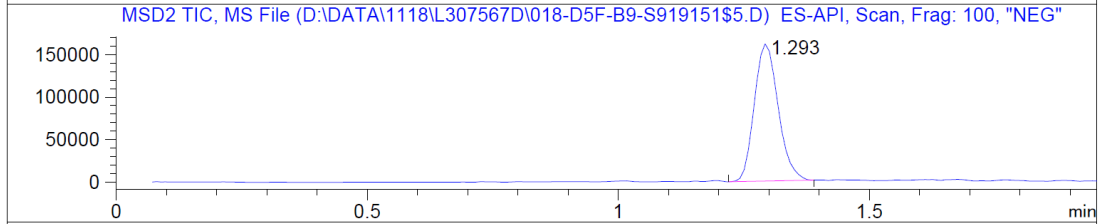
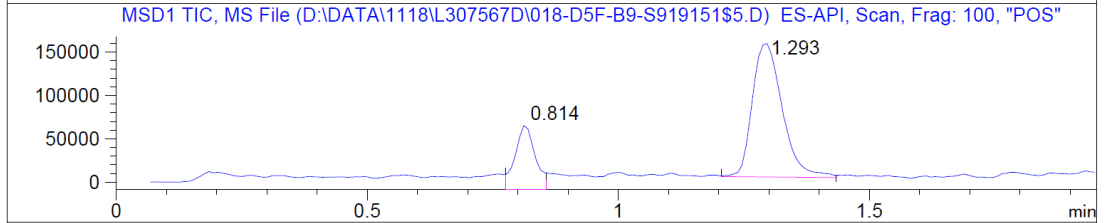
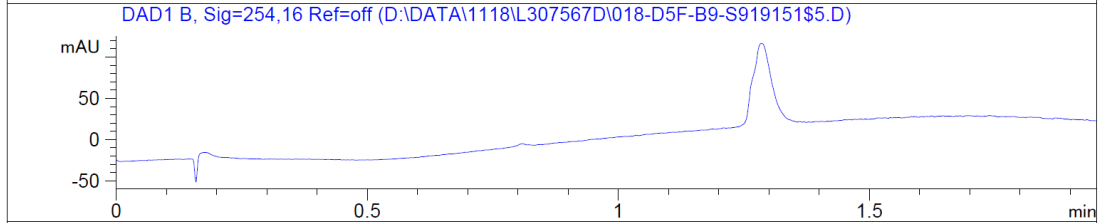
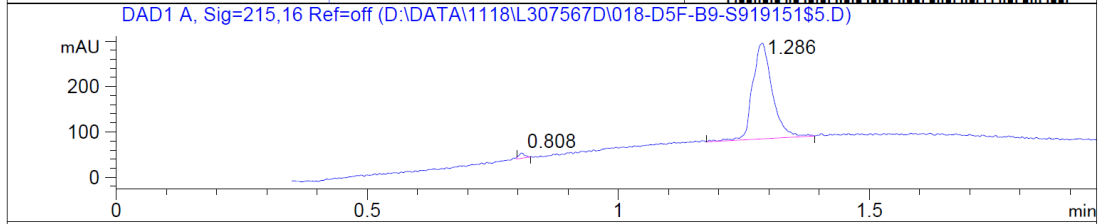
MaxPeak: 98.42%  
Ret\_Time: 1.286 min

# S919151\$5



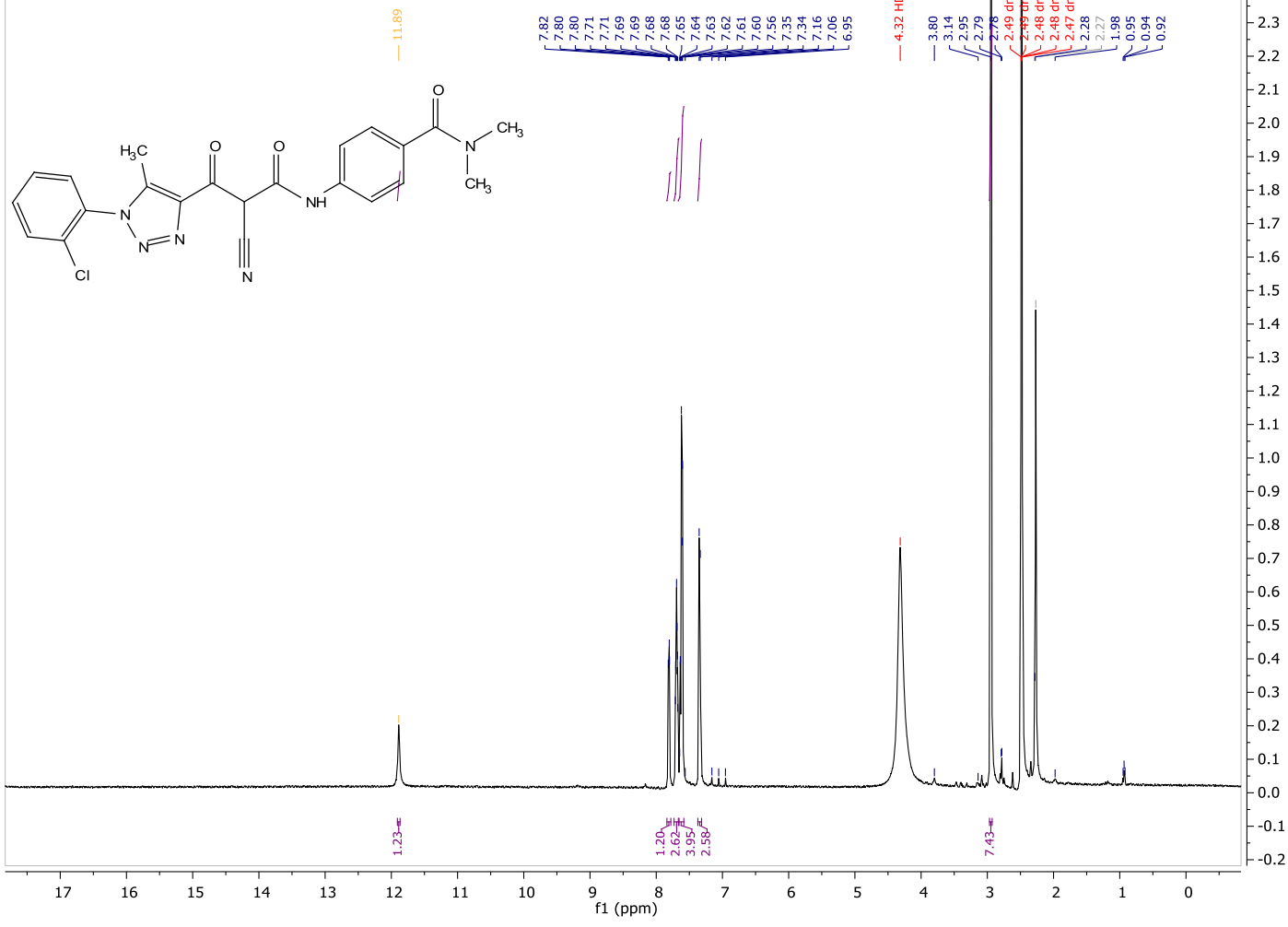
**Mol Wt** 450.88  
**Exact Mass** 450.13

#	Time	Area%
1	0.808	1.58
2	1.286	98.42



Z1123377193\_(6792\_6)

Z1123377193\_(6792\_6)

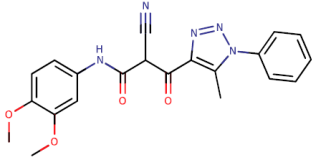




# S910024\$A

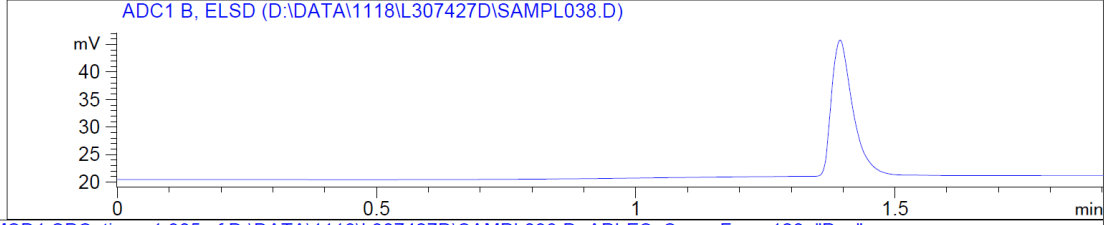
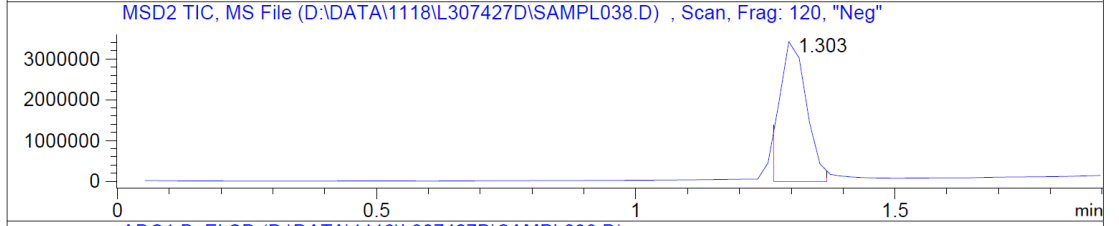
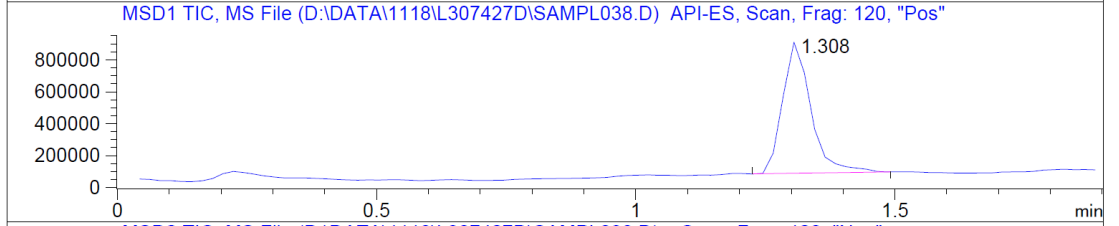
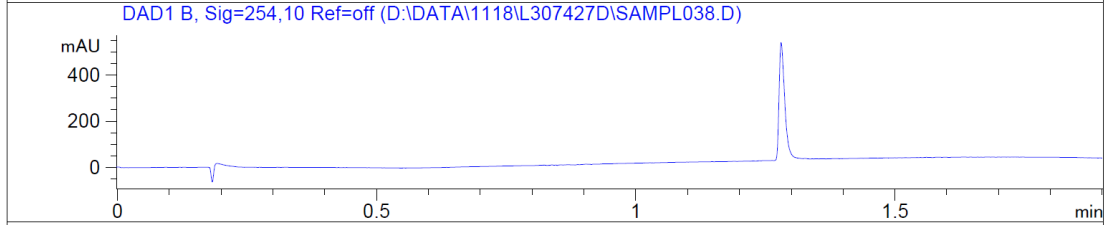
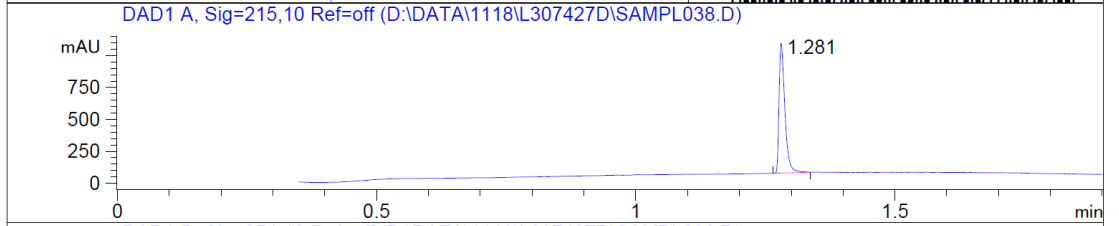


MaxPeak: 100.00%  
Ret\_Time: 1.281 min

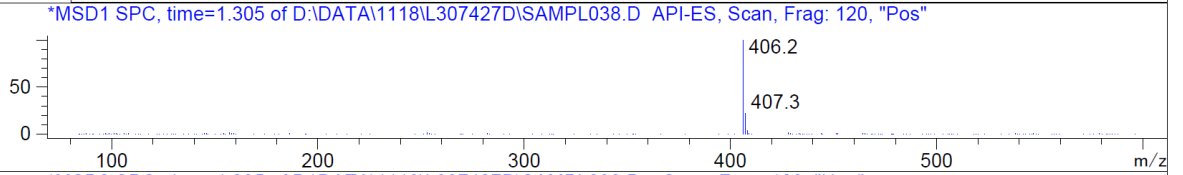


**Mol Wt** 405.41  
**Exact Mass** 405.15

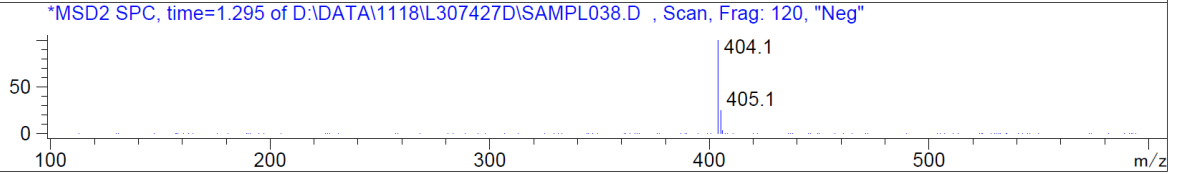
#	Time	Area%
1	1.281	100.00



RT 1.308

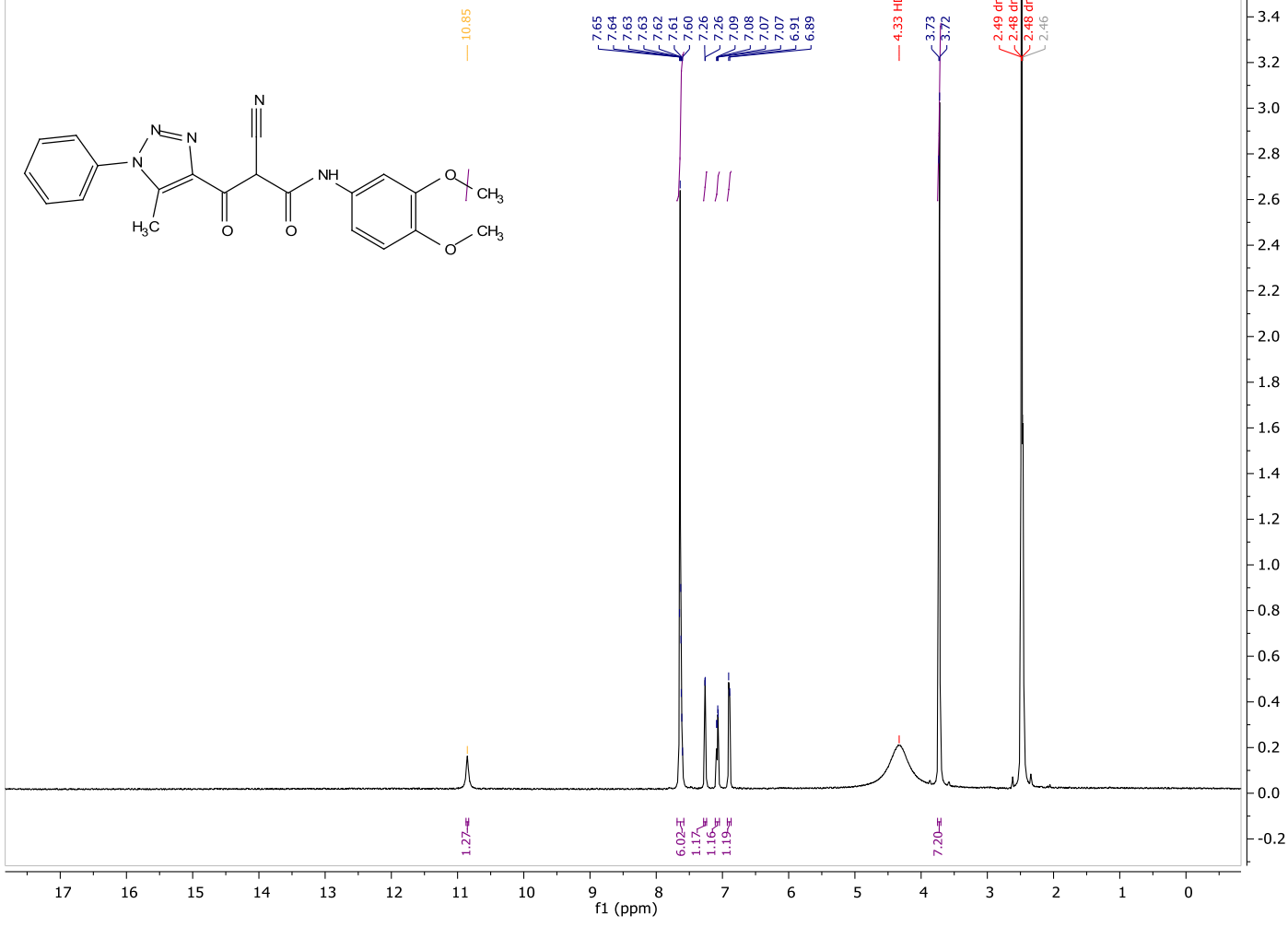


RT 1.303

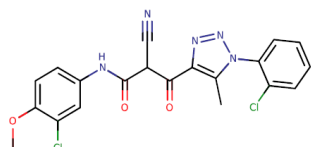


Z762211478\_(6792\_5)

Z762211478\_(6792\_5)



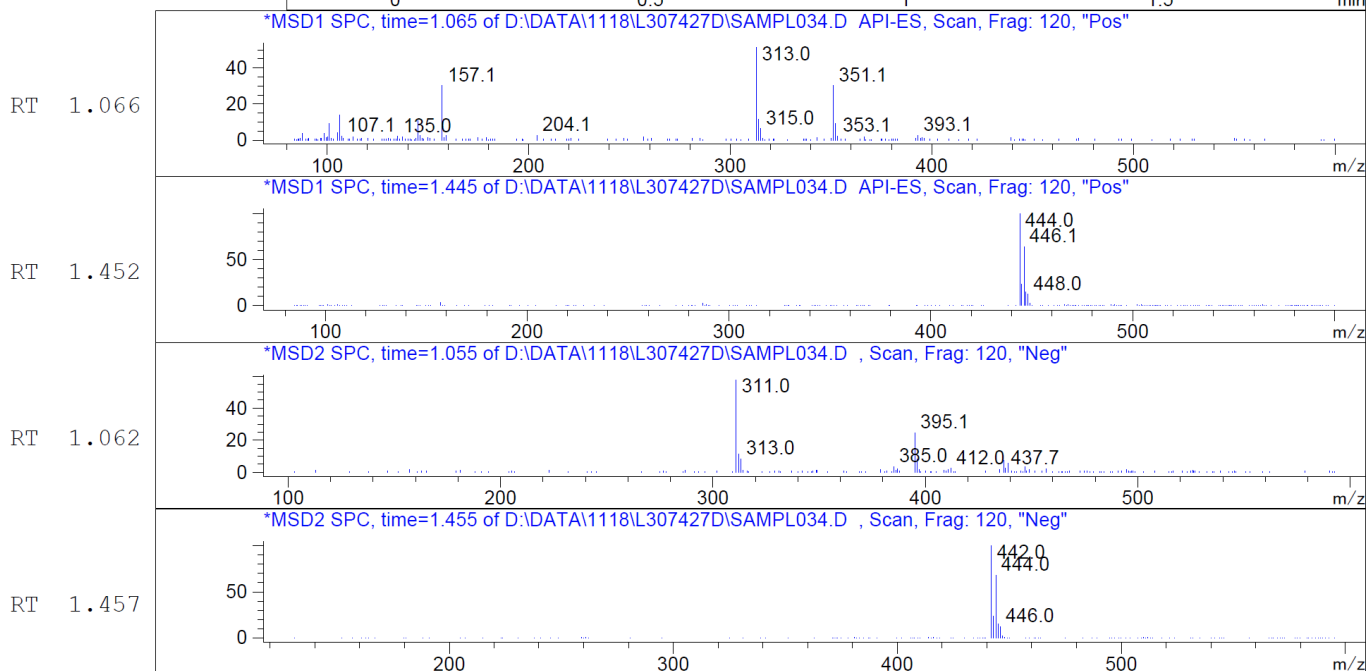
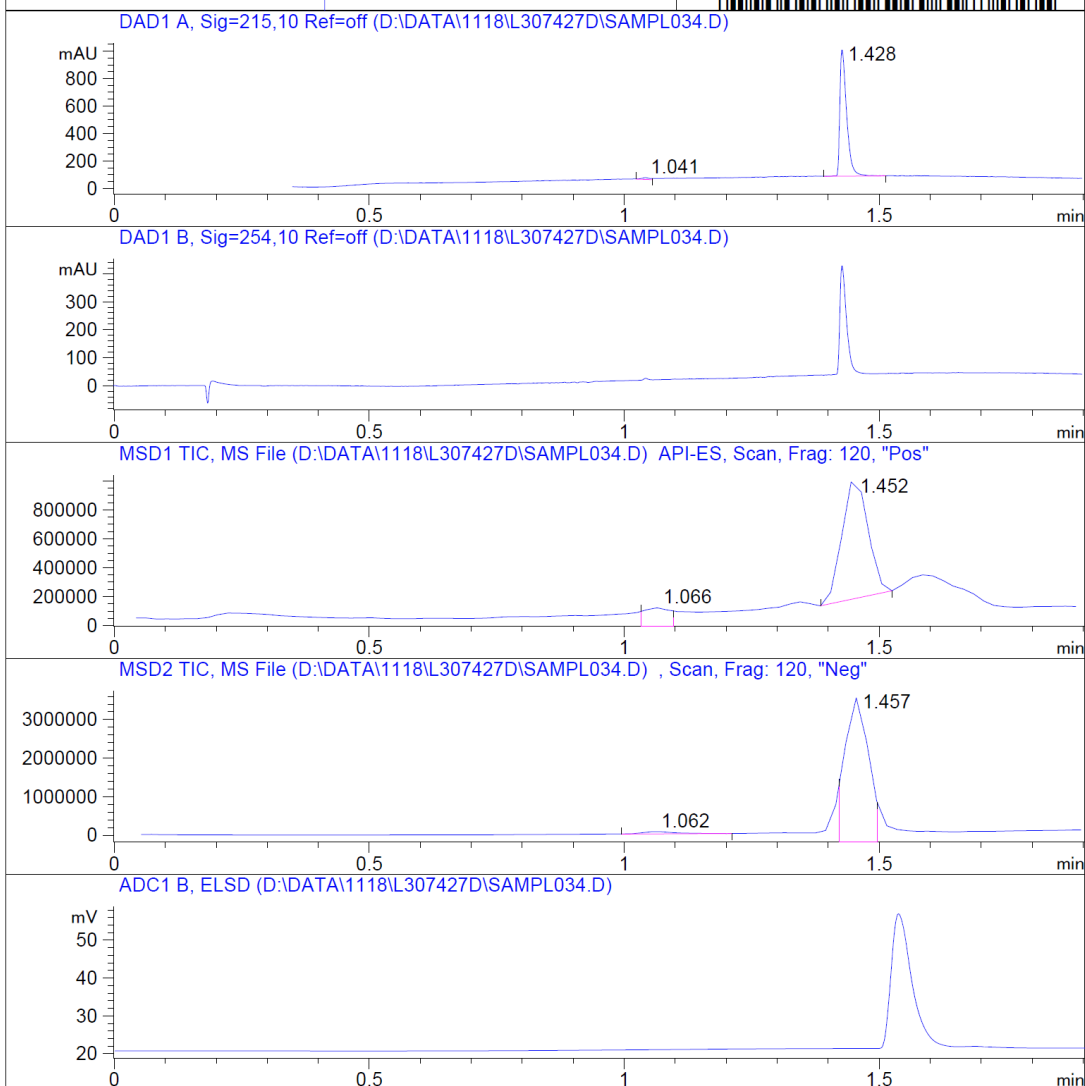
MaxPeak: 98.46%  
Ret\_Time: 1.428 min



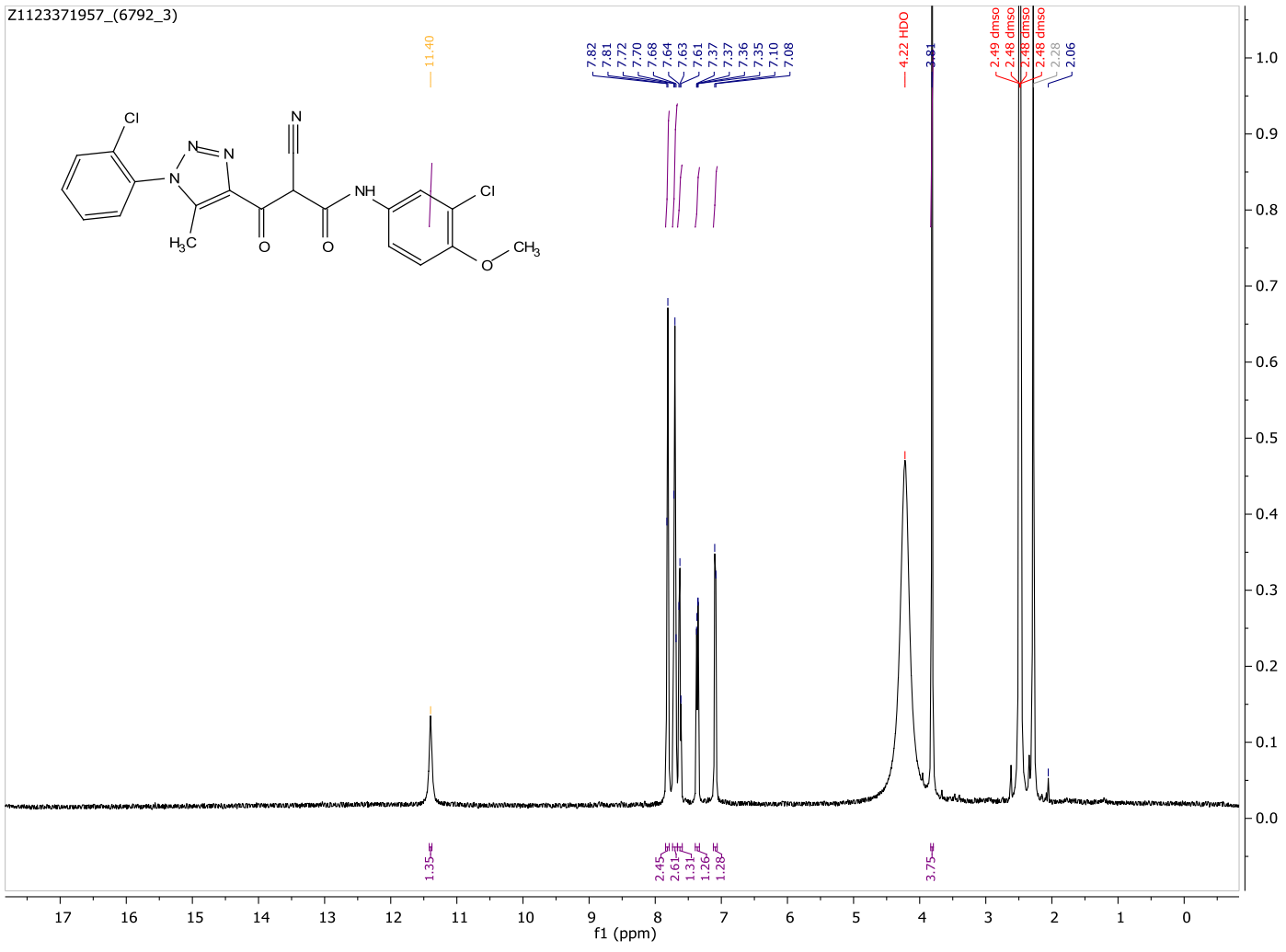
Mol Wt 444.27  
Exact Mass 443.06

#	Time	Area%
1	1.041	1.54
2	1.428	98.46

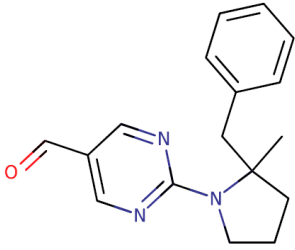
S917050\$B



Z1123371957\_(6792\_3)



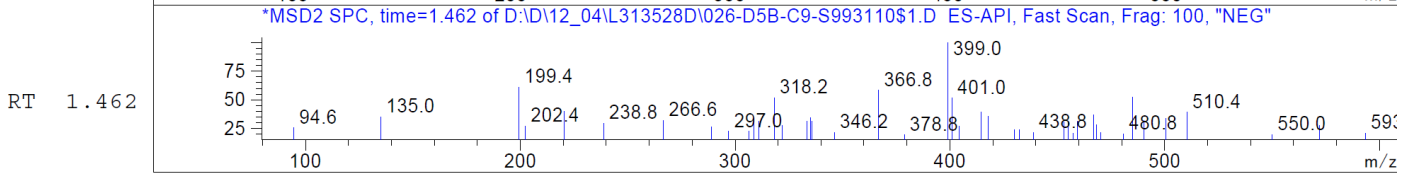
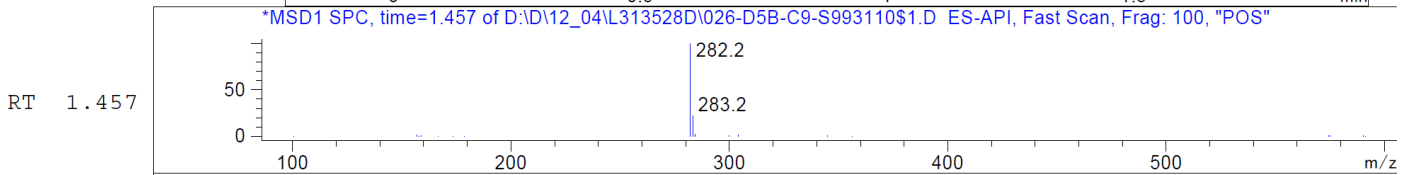
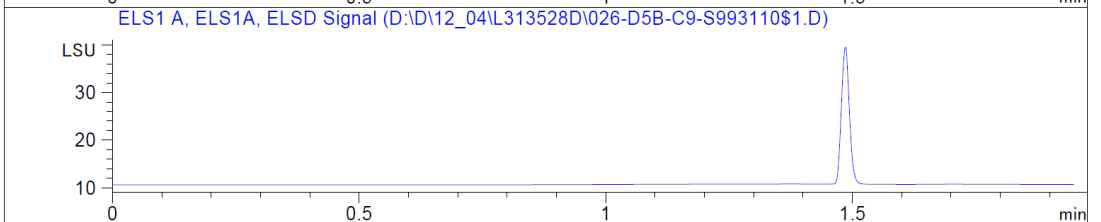
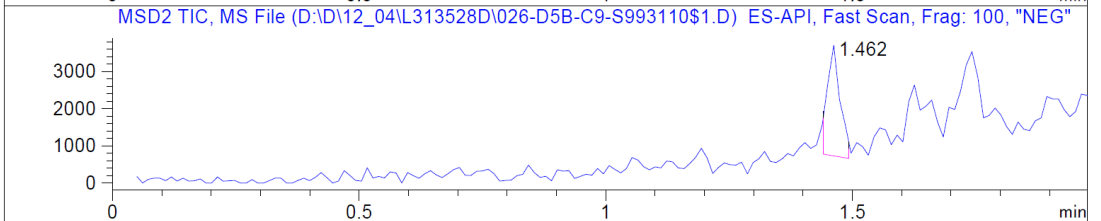
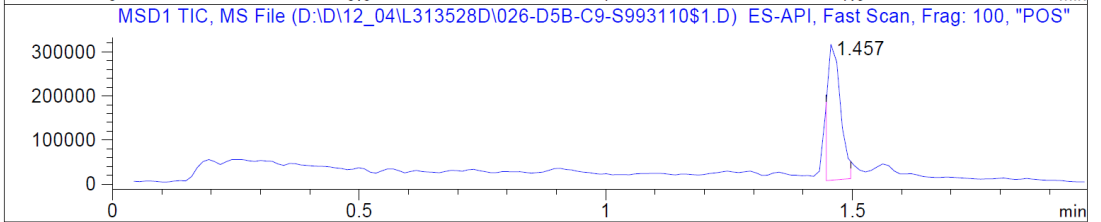
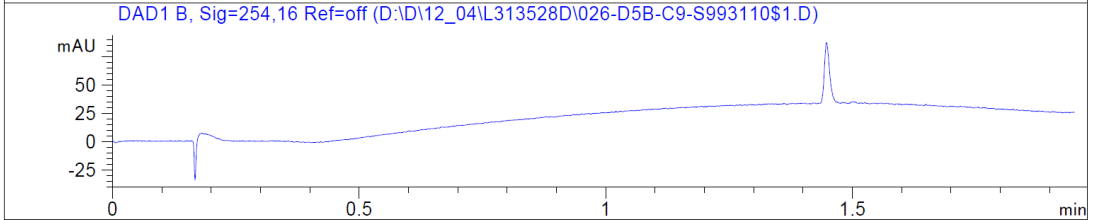
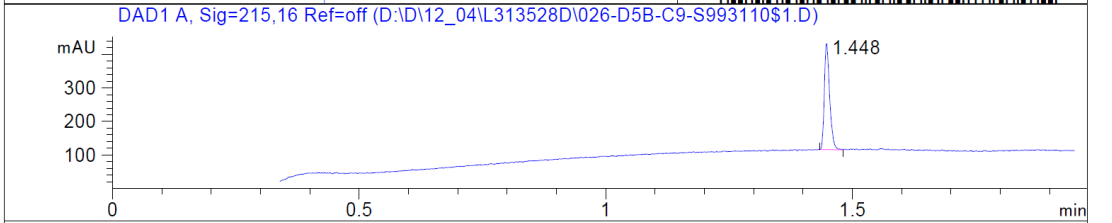
MaxPeak: 100.00%  
Ret\_Time: 1.448 min



Mol Wt 281.35  
Exact Mass 281.18

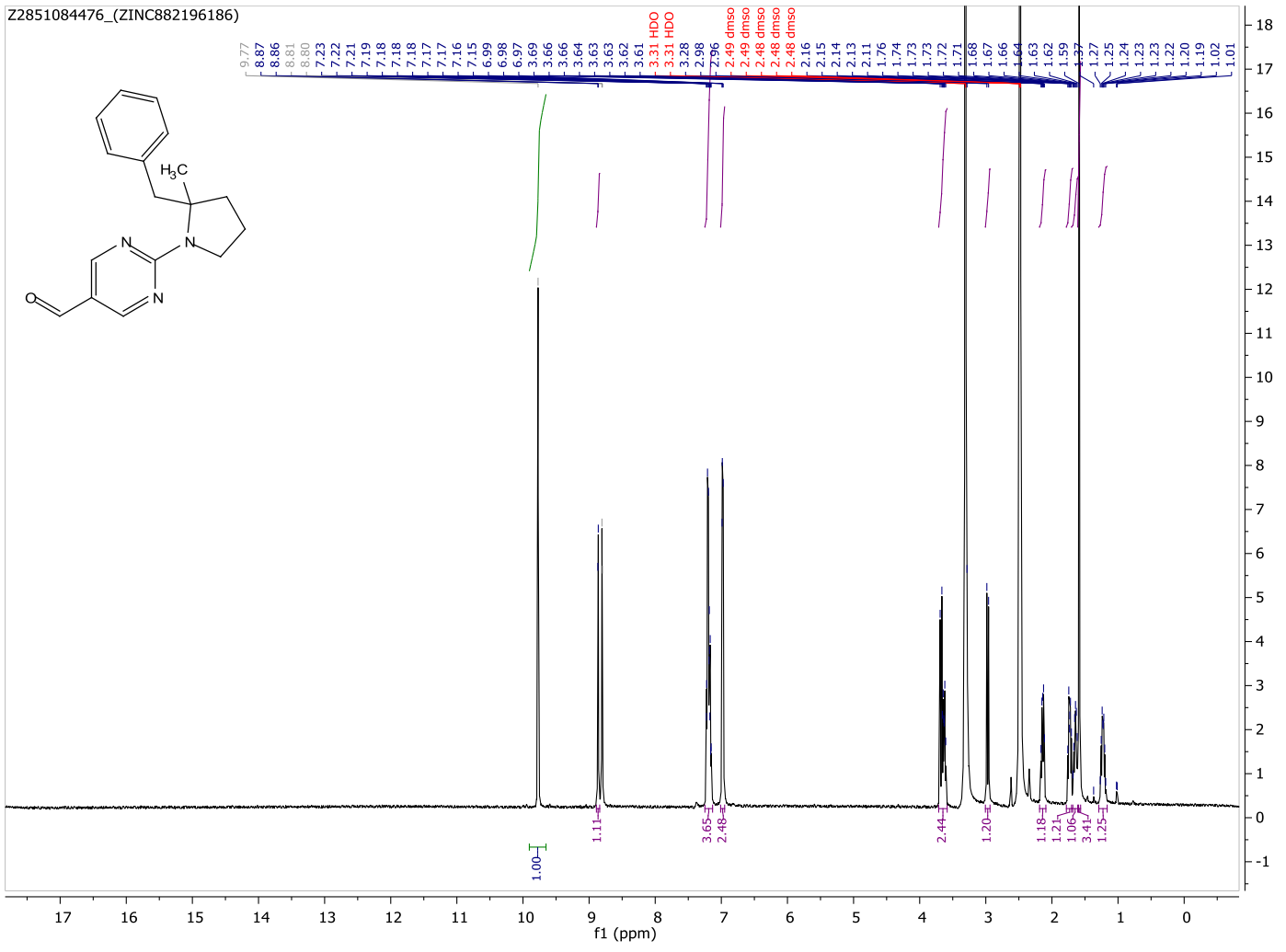
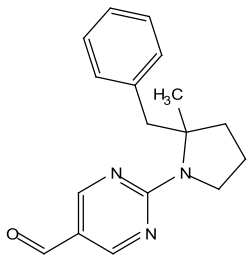
#	Time	Area%
1	1.448	100.00

# S993110\$1



Z2851084476\_(ZINC882196186)

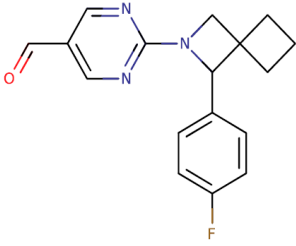
Z2851084476\_(ZINC882196186)



# S993119\$1

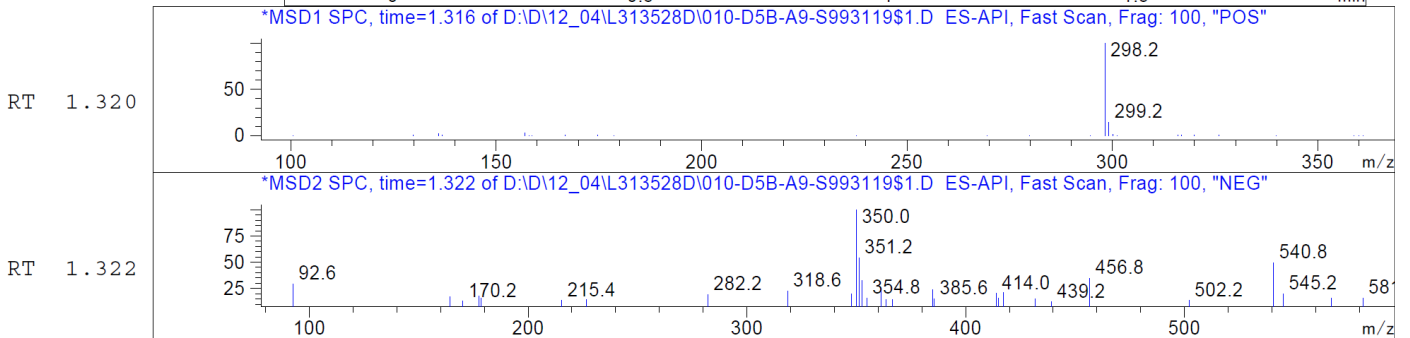
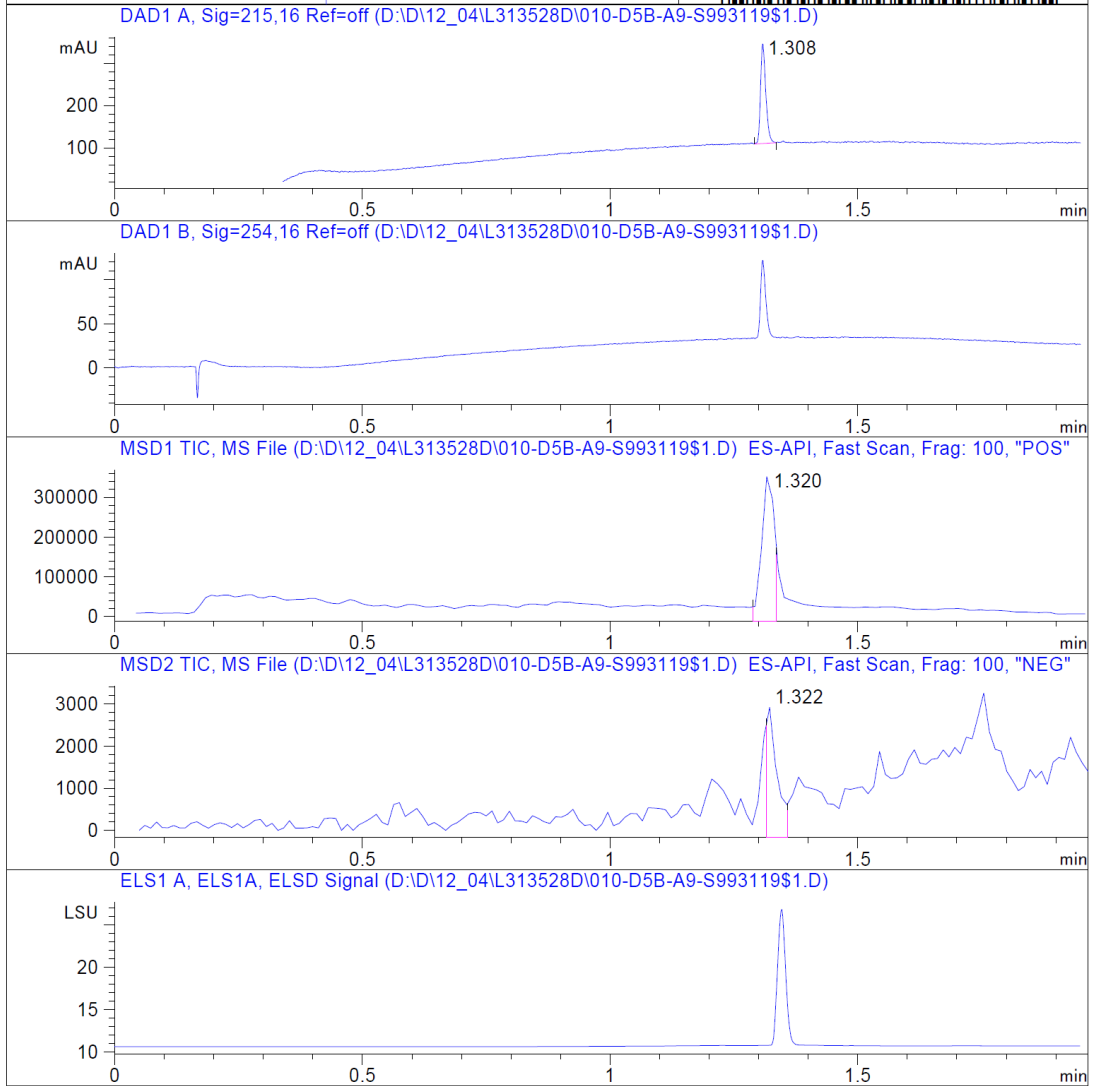


MaxPeak: 100.00%  
Ret\_Time: 1.308 min



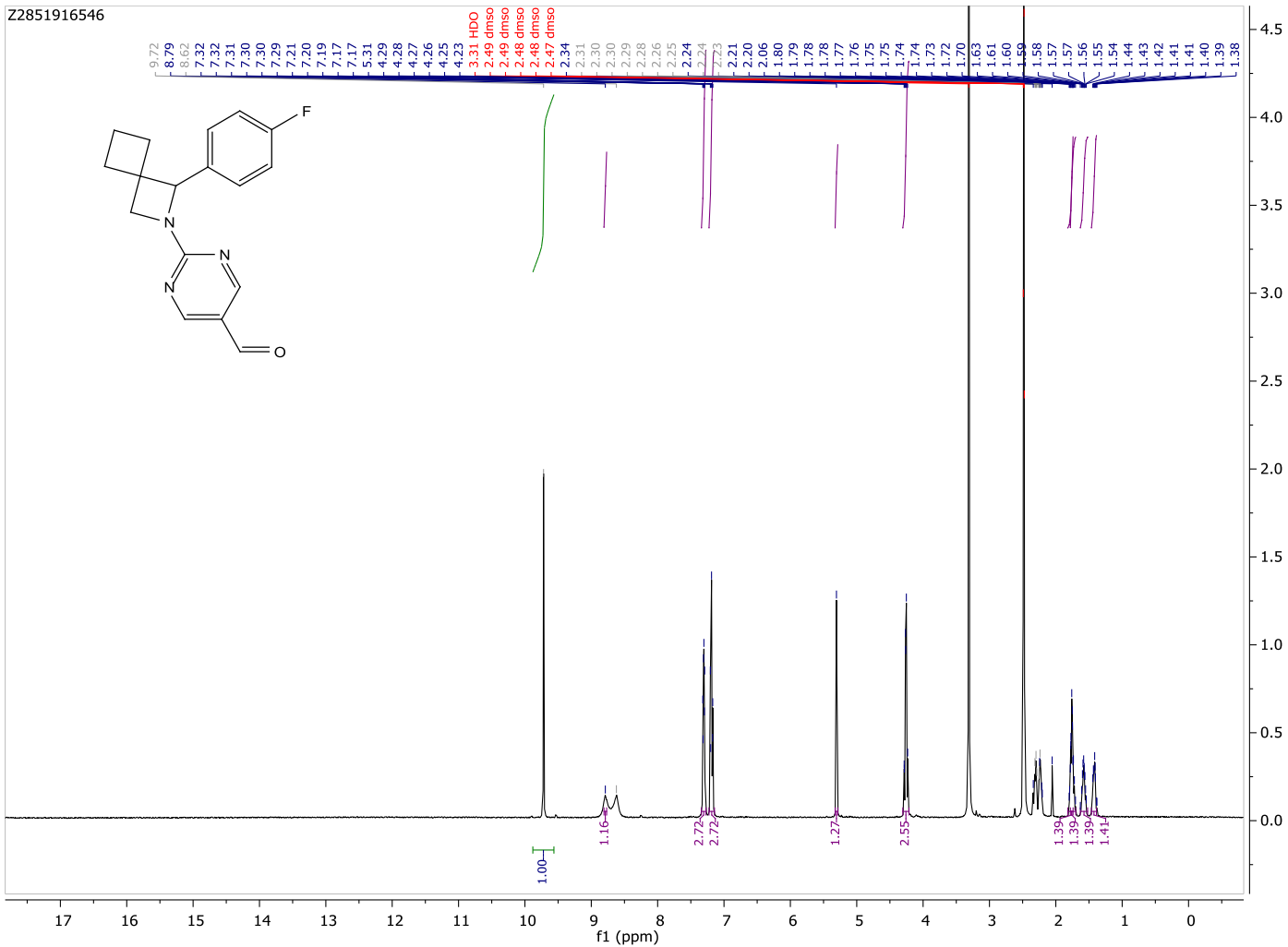
**Mol Wt** 297.33  
**Exact Mass** 297.15

#	Time	Area%
1	1.308	100.00



Z2851916546

Z2851916546

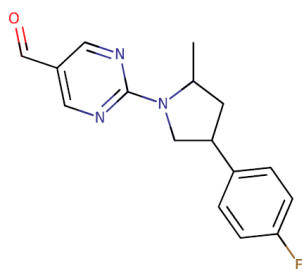




# S993127\$1

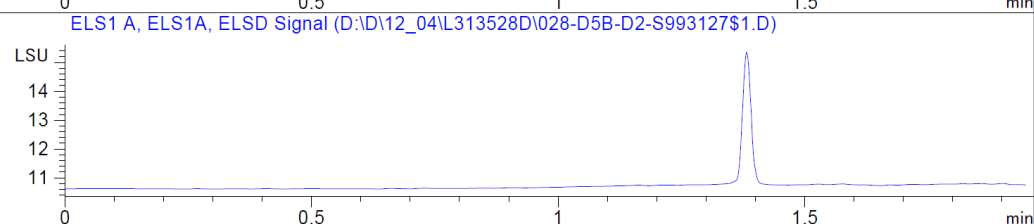
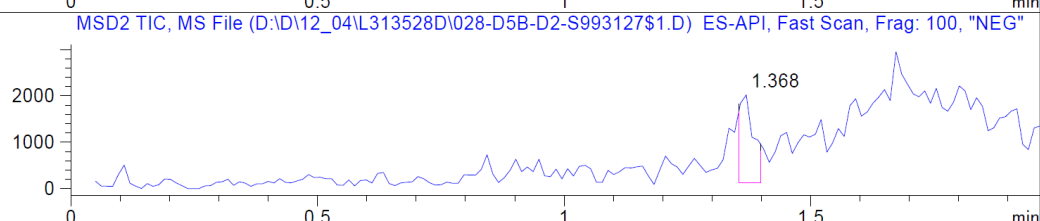
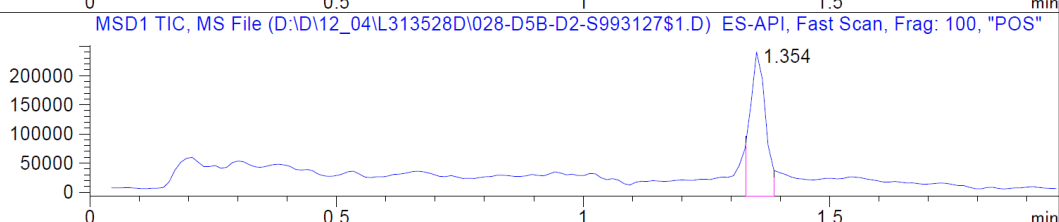
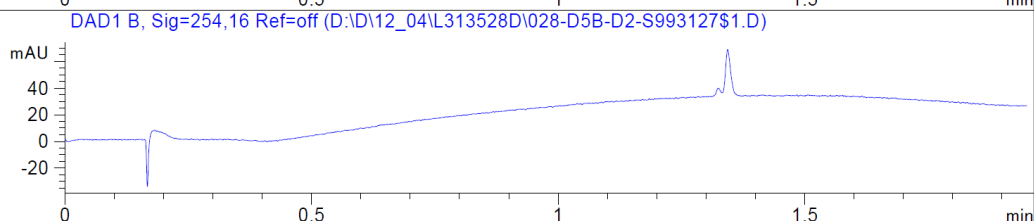
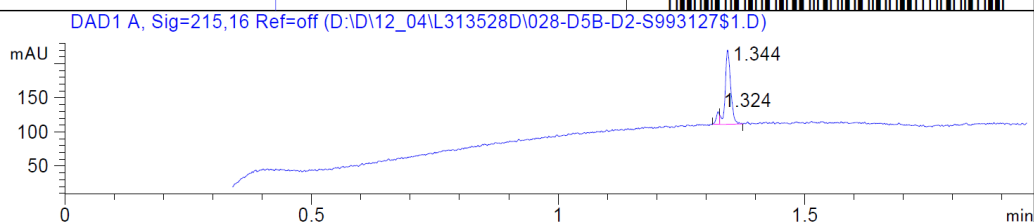


MaxPeak: 90.85%  
Ret\_Time: 1.344 min

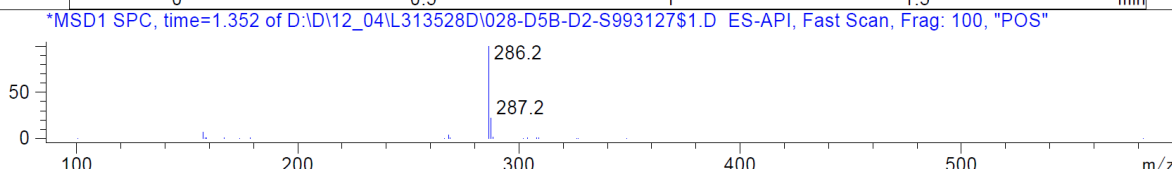


Mol Wt 285.32  
Exact Mass 285.15

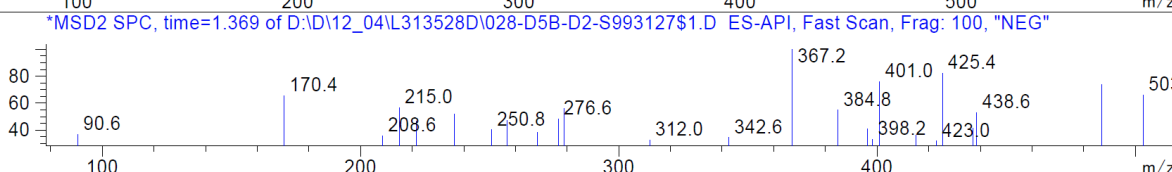
#	Time	Area%
1	1.324	9.15
2	1.344	90.85



RT 1.354

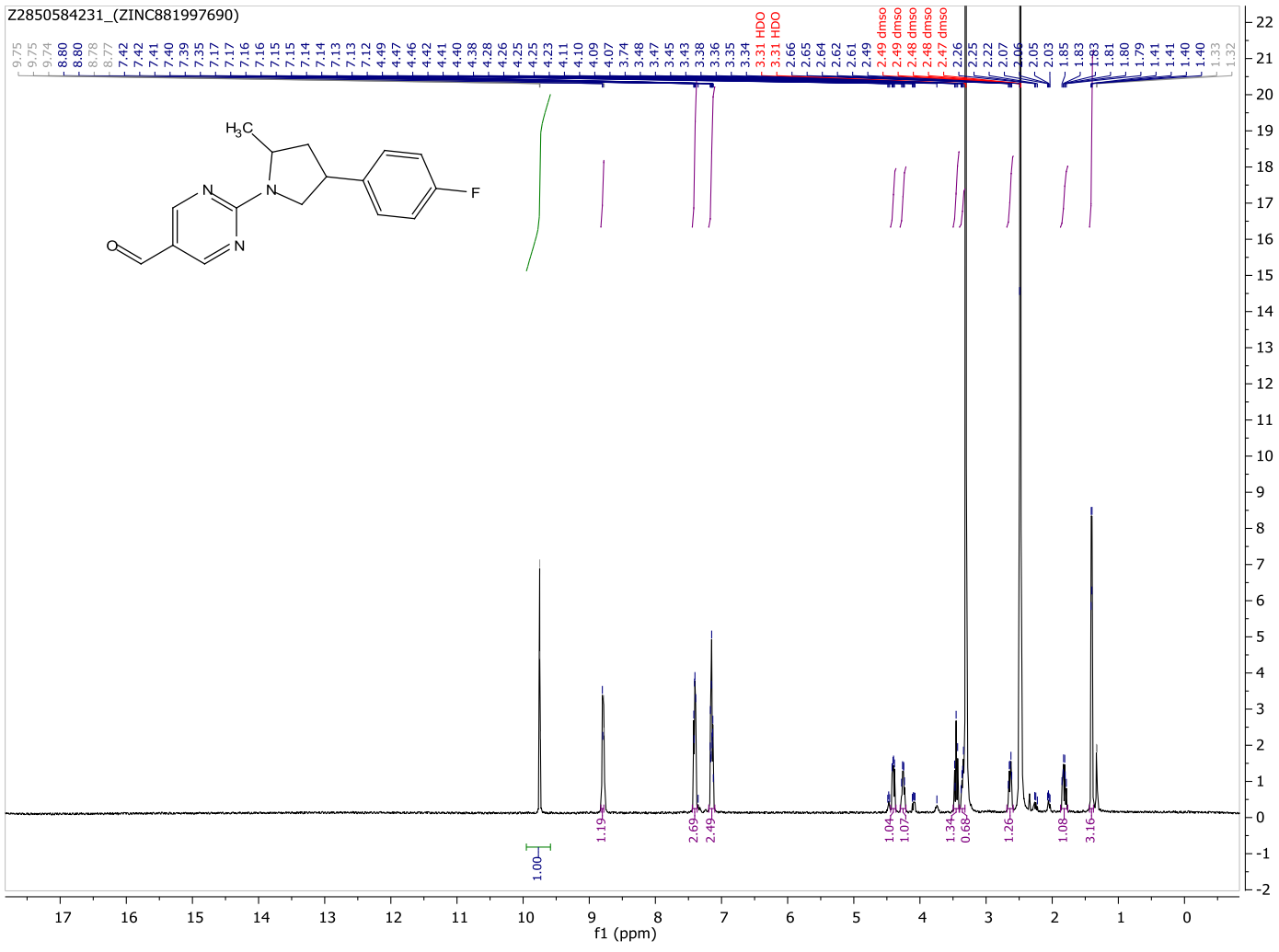
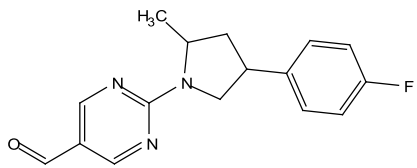


RT 1.368



Z2850584231\_(ZINC881997690)

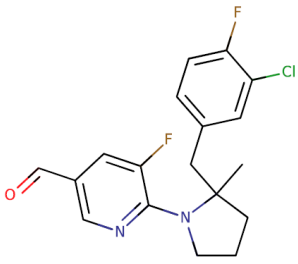
Z2850584231\_(ZINC881997690)



# S999646\$1

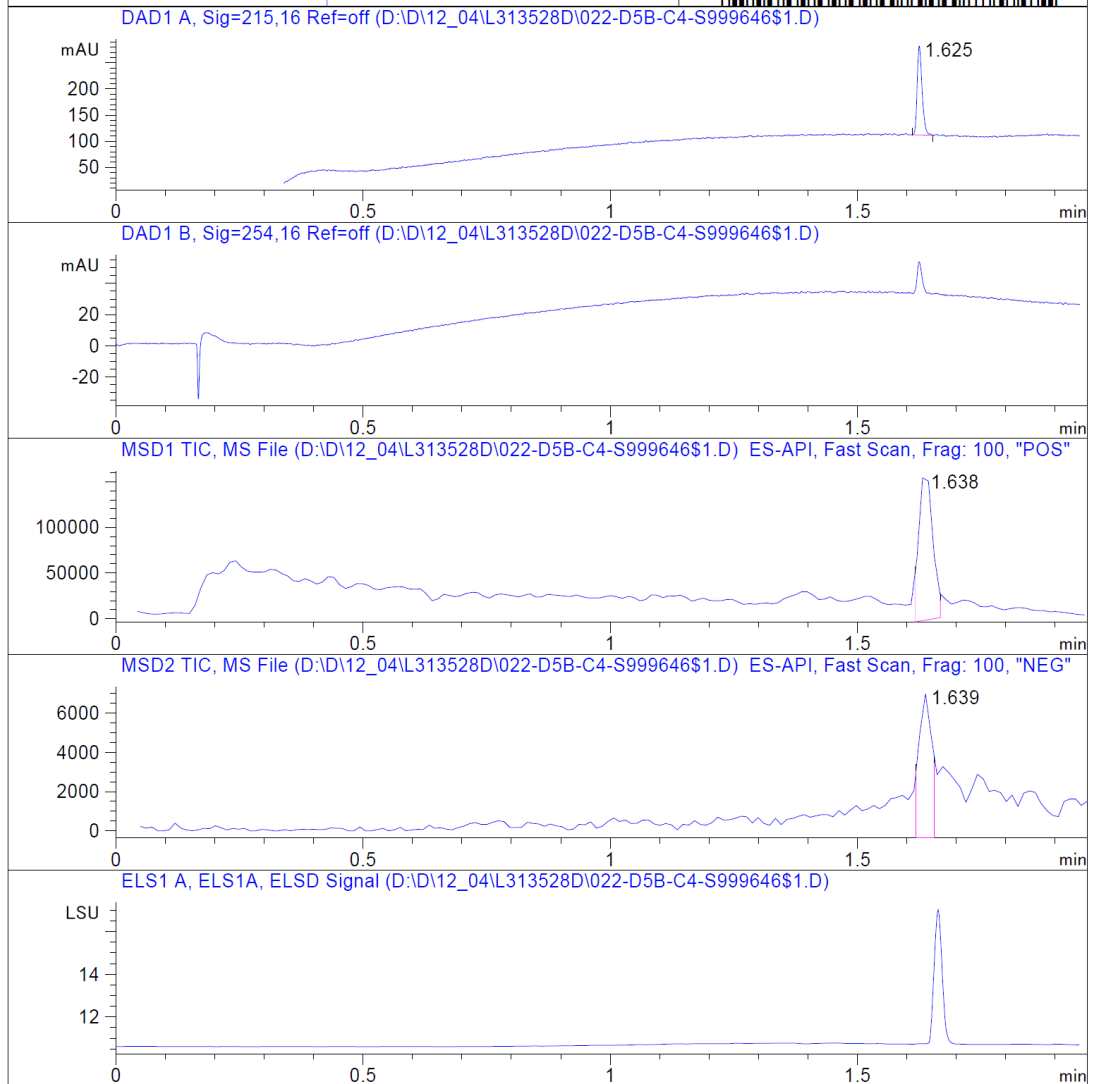


MaxPeak: 100.00%  
Ret\_Time: 1.625 min

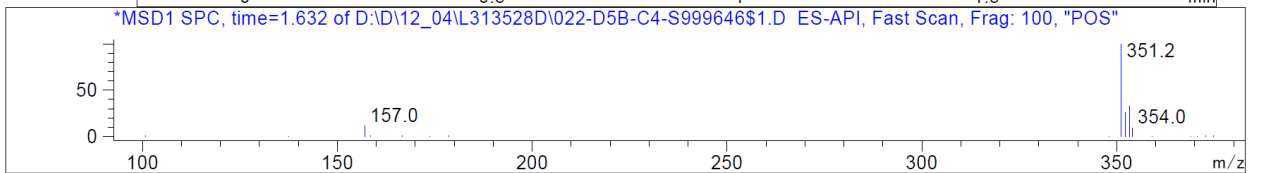


**Mol Wt** 350.79  
**Exact Mass** 350.13

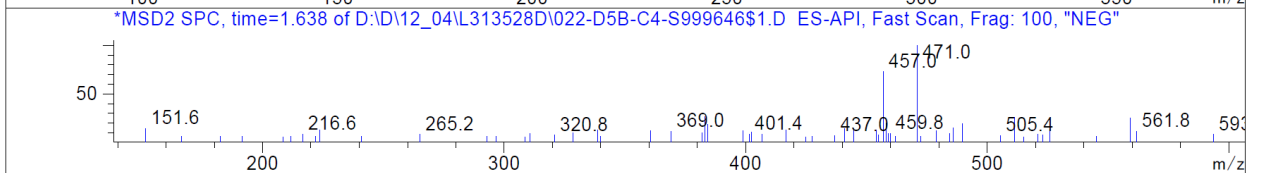
#	Time	Area%
1	1.625	100.00



RT 1.638

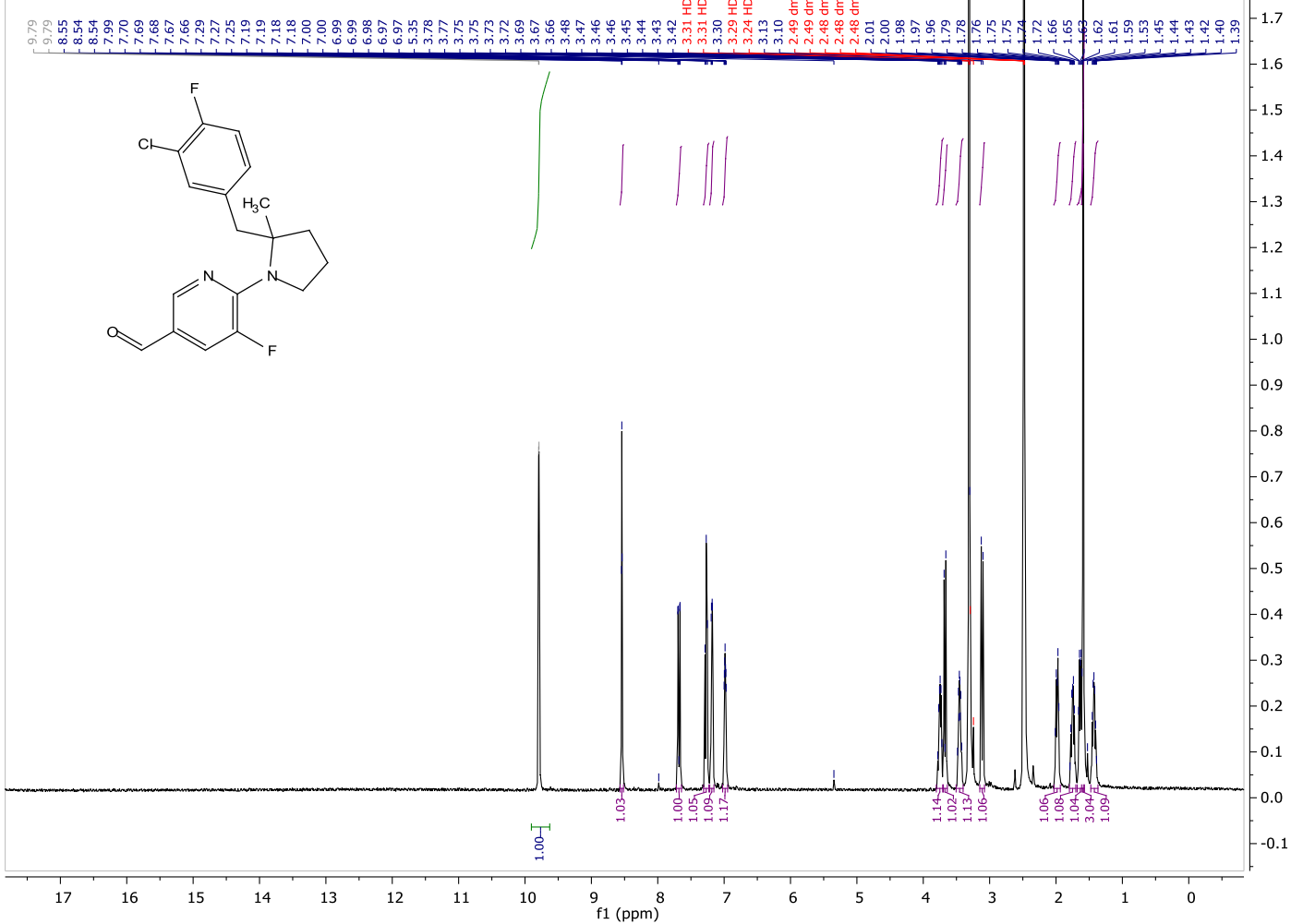


RT 1.639

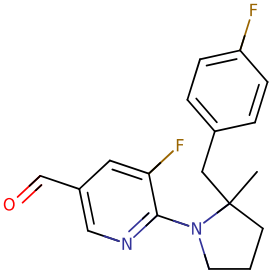


Z4767502333

Z4767502333



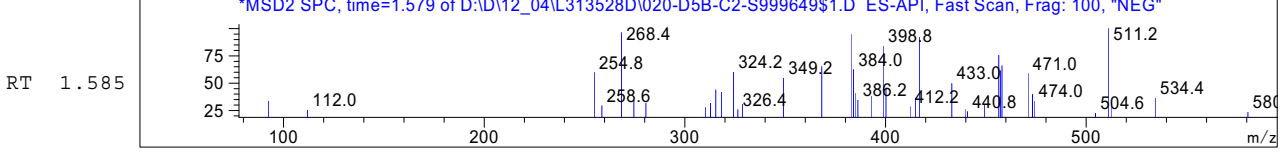
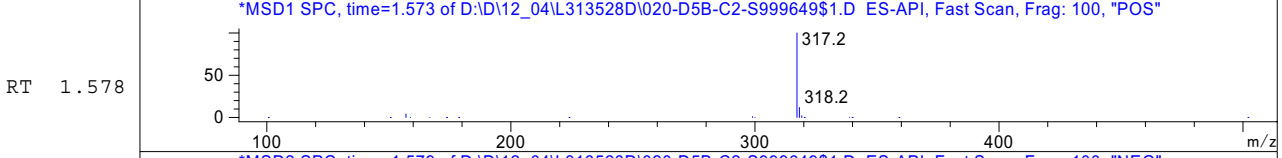
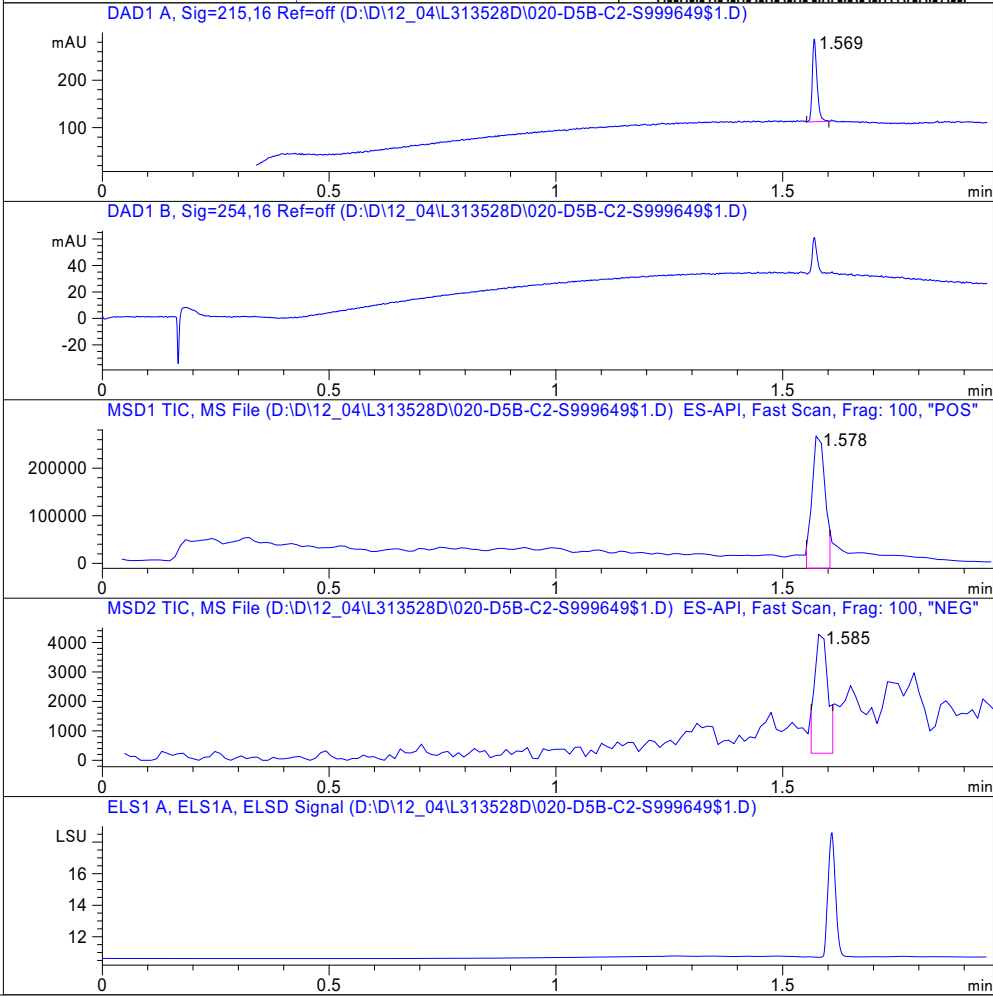
MaxPeak: 100.00%  
Ret\_Time: 1.569 min



Mol Wt 316.35  
Exact Mass 316.17

#	Time	Area%
1	1.569	100.00

S999649\$1



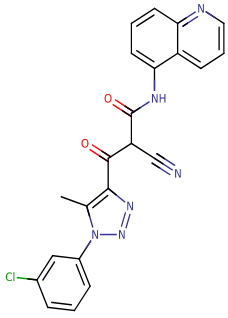
Inj.Date 12/3/2020

N

Acq. Method C:\Users\ -> ->

Z4767502336\_

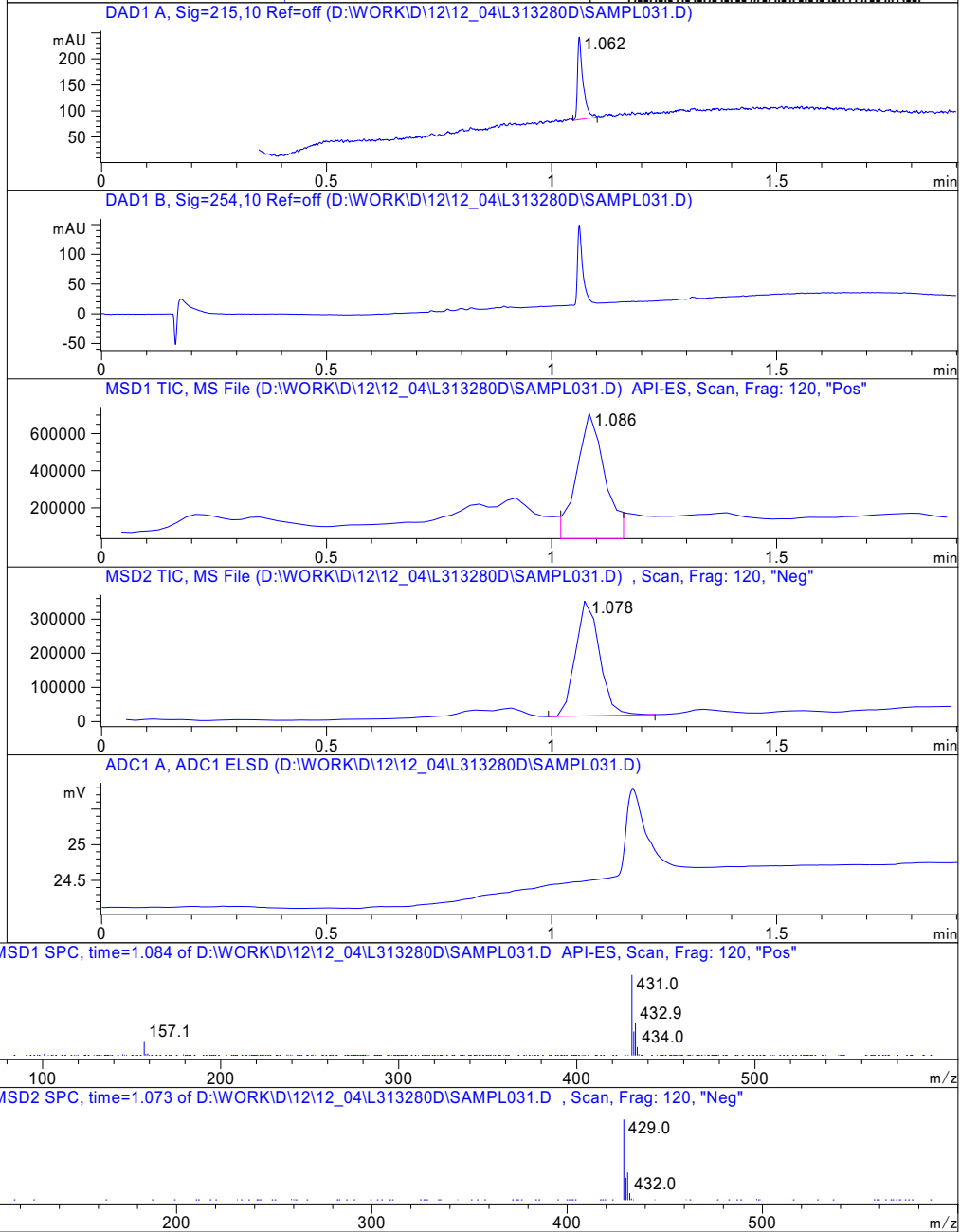
MaxPeak: 100.00%  
Ret\_Time: 1.062 min



Mol Wt 430.85  
Exact Mass 430.1

#	Time	Area%
1	1.062	100.00

S993149\$3



RT 1.086

RT 1.078

Inj.Date 12/4/2020

K

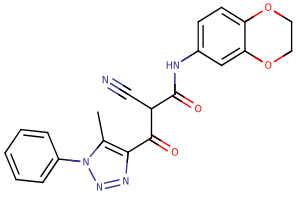
-VL-

Acq. Method C:\HPCHEM\ -> ->

Z762205396\_

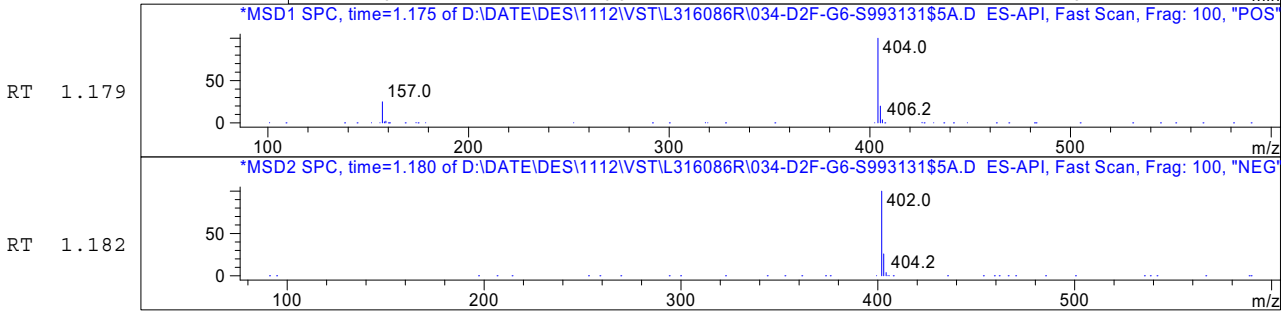
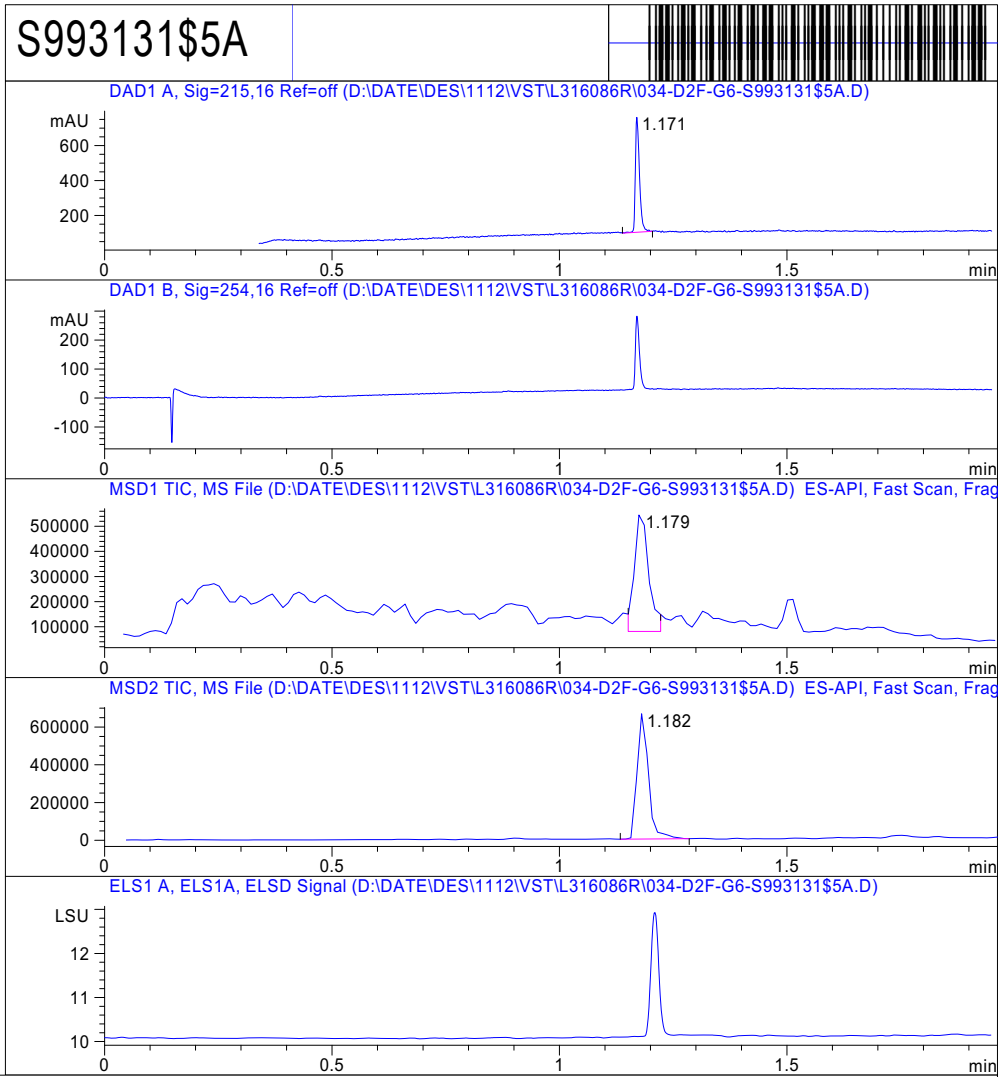
MaxPeak: 100.00%  
Ret\_Time: 1.171 min

S993131\$5A



Mol Wt 403.39  
Exact Mass 403.13

#	Time	Area%
1	1.171	100.00



Inj.Date 12/11/2020

Y

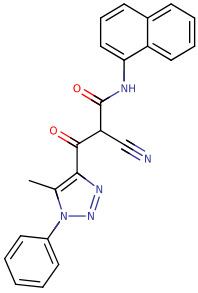
Acq. Method C:\Users\ -> ->

Z762217606\_

# S993150\$56

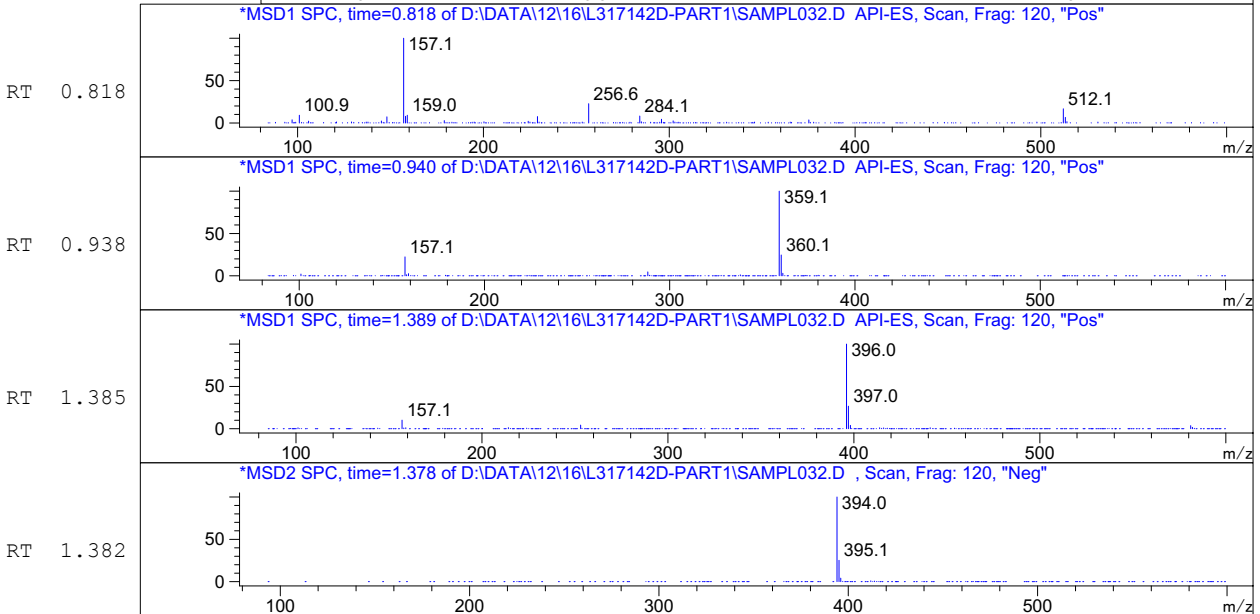
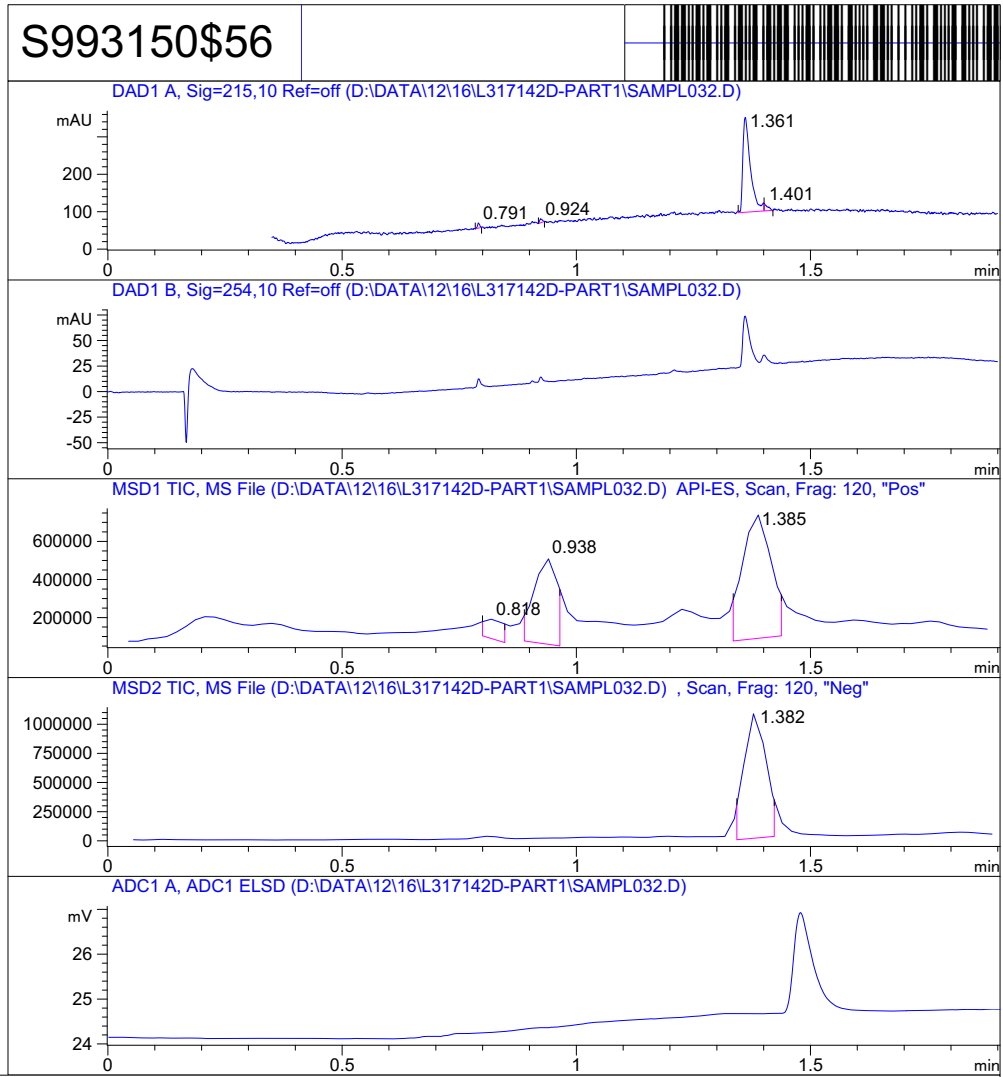


MaxPeak: 94.15%  
Ret\_Time: 1.361 min



**Mol Wt** 395.41  
**Exact Mass** 395.15

#	Time	Area%
1	0.791	1.38
2	0.924	1.34
3	1.361	94.15
4	1.401	3.13



Inj.Date 12/16/2020

LB

-VL-

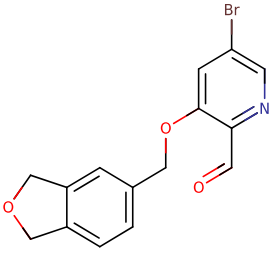
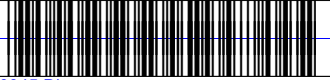
Acq. Method C:\HPCHEM\ -> ->

Z762209308\_



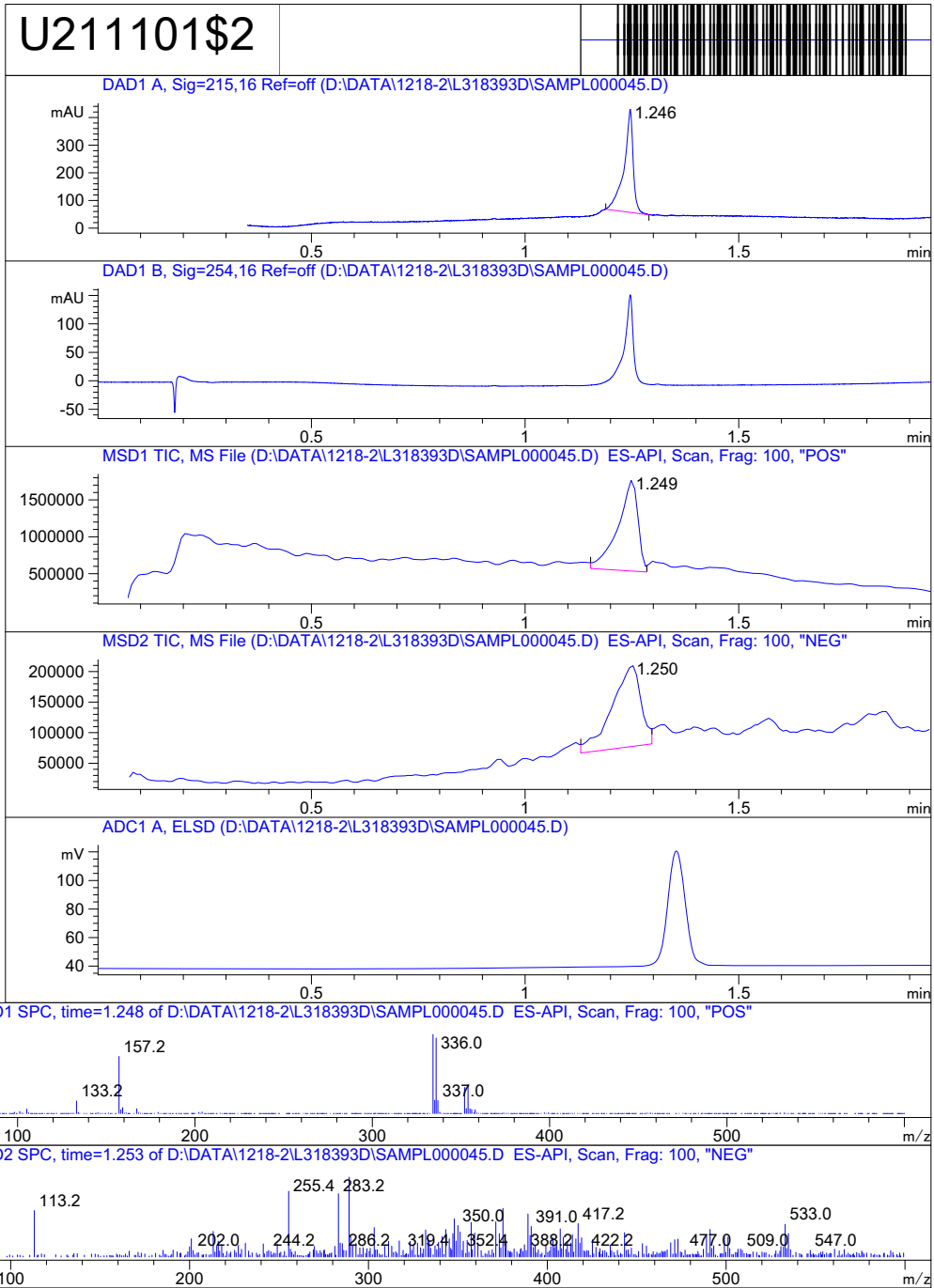
MaxPeak: 100.00%  
Ret\_Time: 1.246 min

U211101\$2



Mol Wt 334.16  
Exact Mass 333.01

#	Time	Area%
1	1.246	100.00

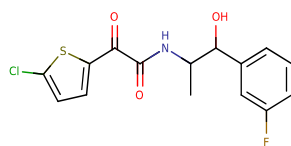
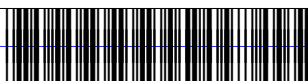


RT 1.249

RT 1.250

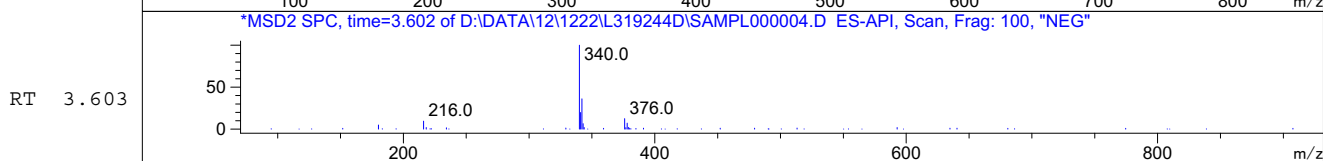
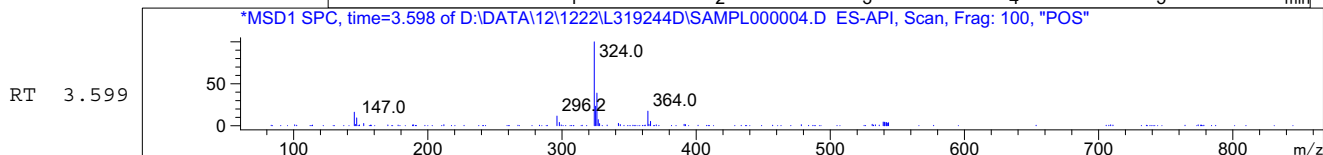
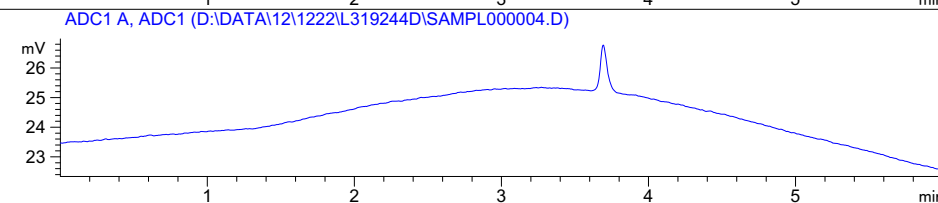
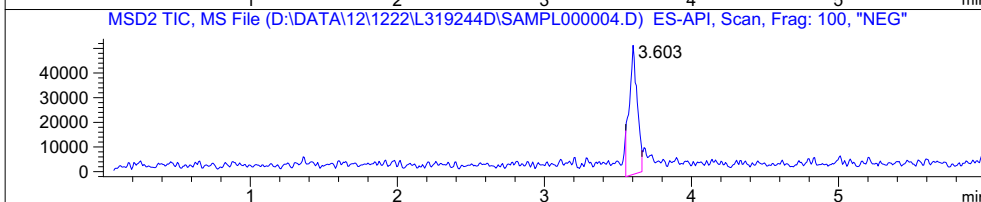
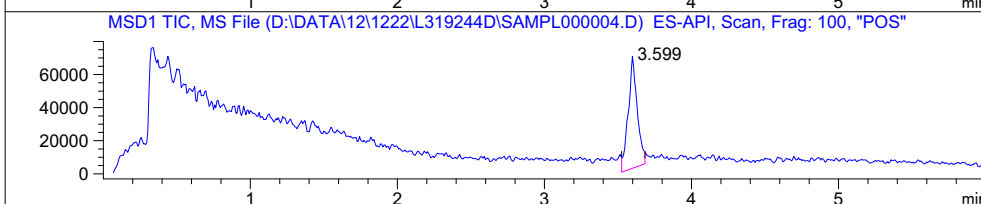
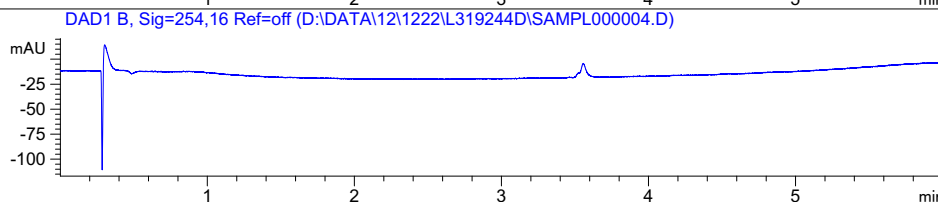
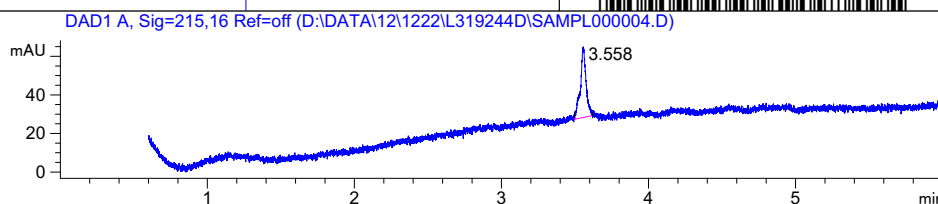
MaxPeak: 100.00%  
Ret\_Time: 3.558 min

U211102\$9

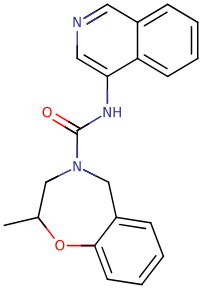


Mol Wt 341.78  
Exact Mass 341.04

#	Time	Area%
1	3.558	100.00



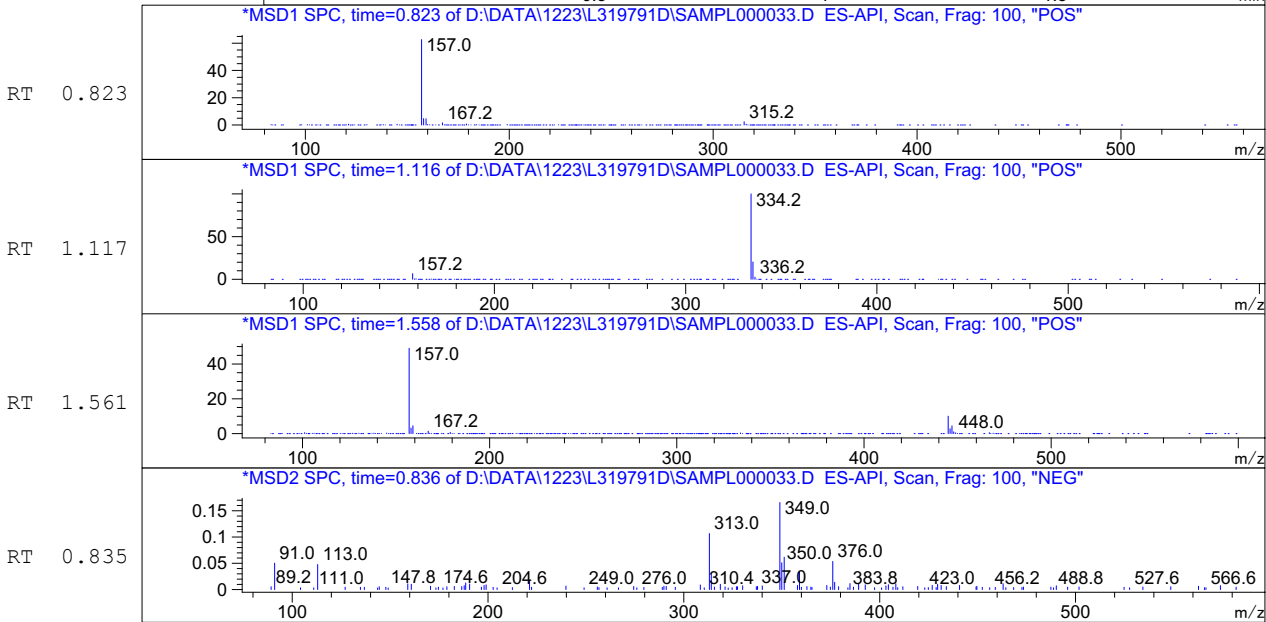
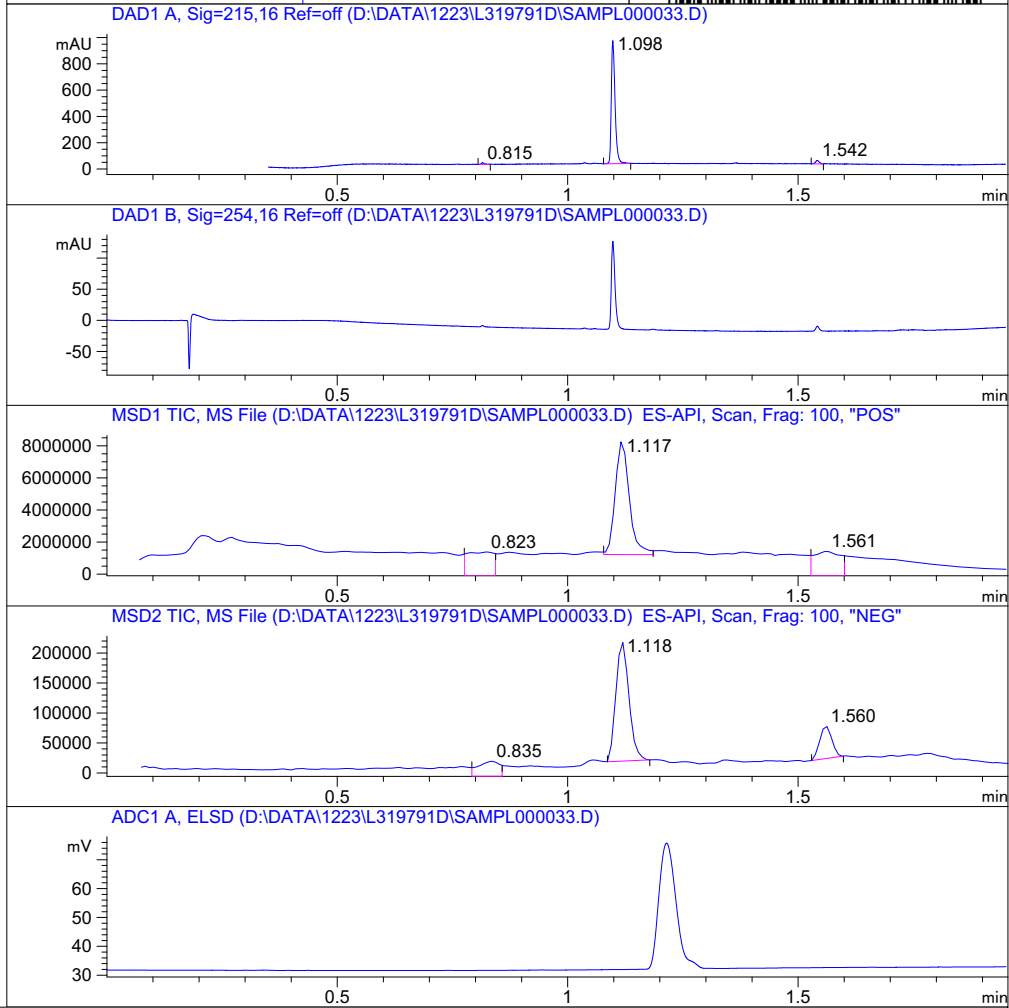
MaxPeak: 96.04%  
Ret\_Time: 1.098 min



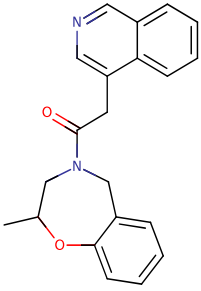
Mol Wt 333.38  
Exact Mass 333.17

#	Time	Area%
1	0.815	1.16
2	1.098	96.04
3	1.542	2.79

U173081\$3



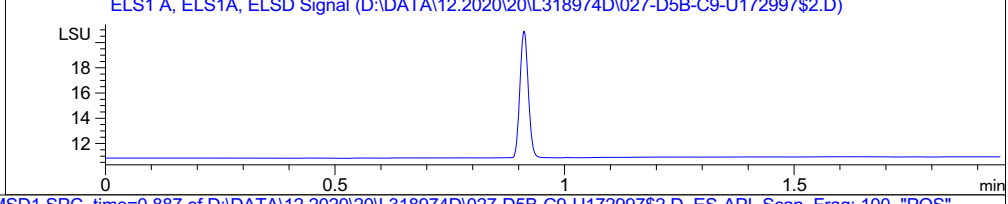
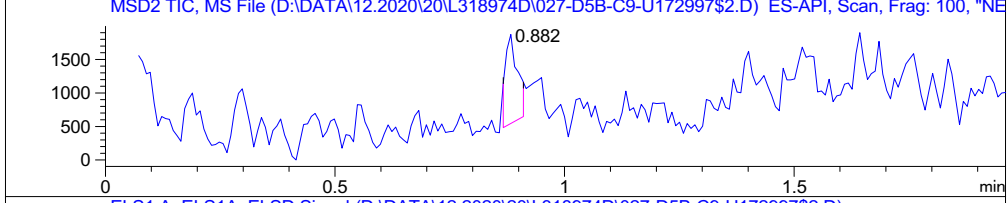
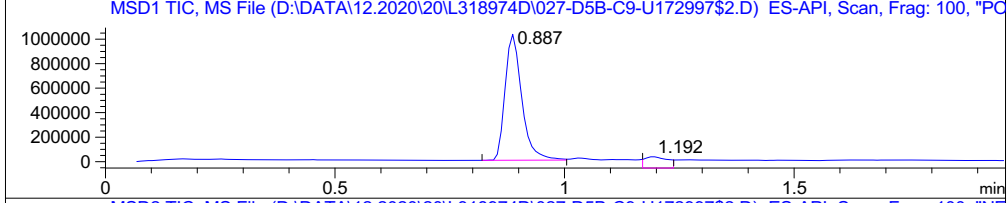
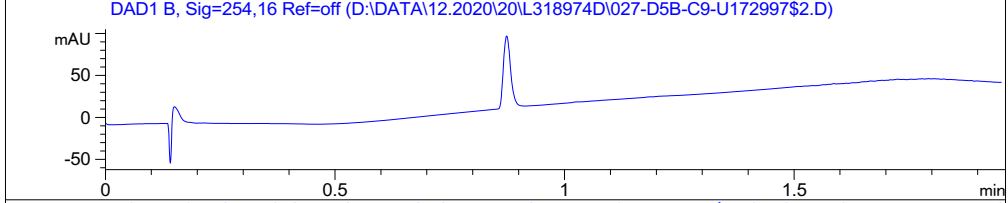
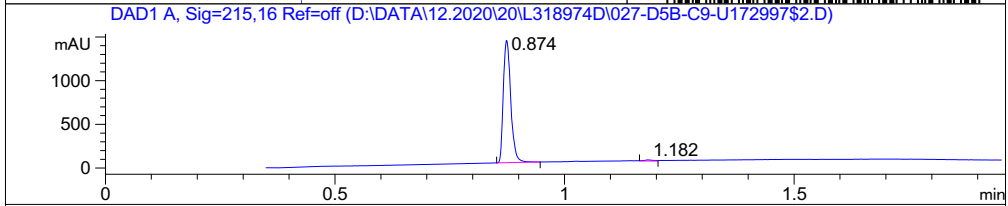
MaxPeak: 98.86%  
Ret\_Time: 0.874 min



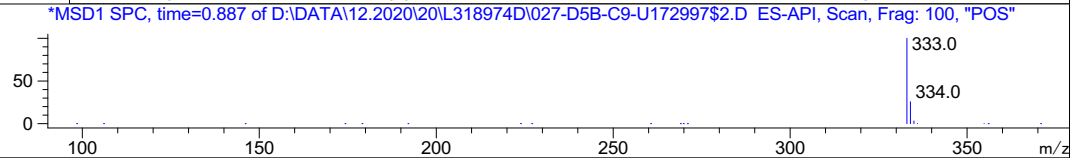
Mol Wt 332.4  
Exact Mass 332.18

#	Time	Area%
1	0.874	98.86
2	1.182	1.14

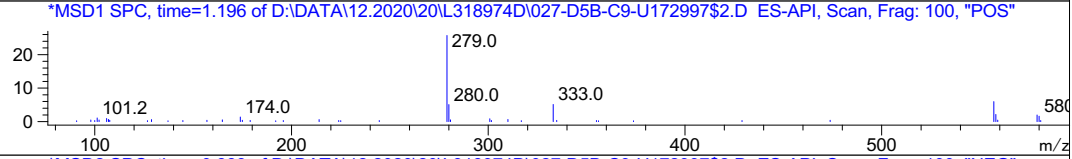
U172997\$2



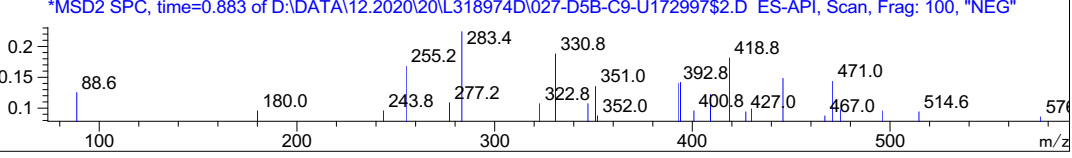
RT 0.887



RT 1.192



RT 0.882



Inj.Date 12/19/2020

CH <invalid> 13

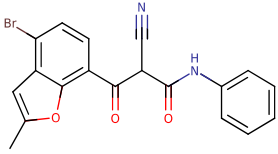
Acq. Method C:\Chem32\ -> ->

Z4872561612\_

# U217010\$A

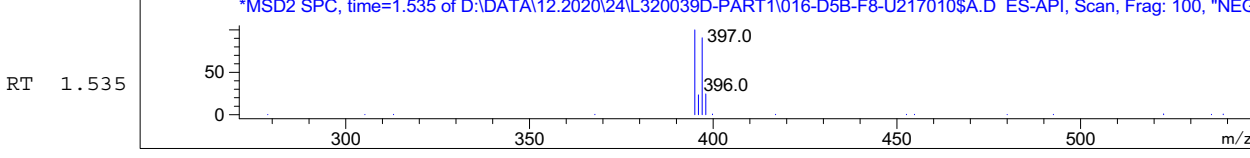
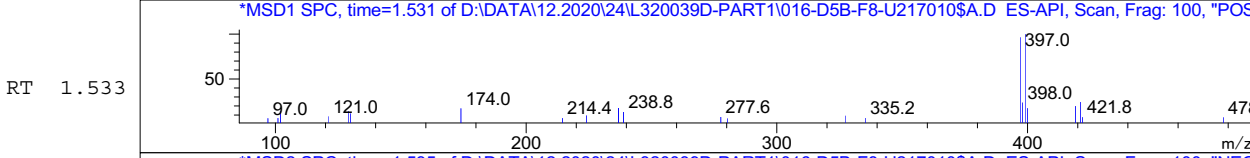
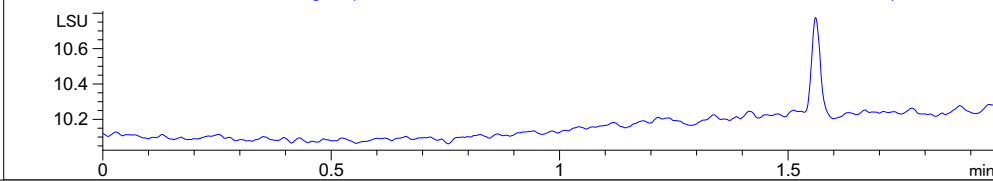
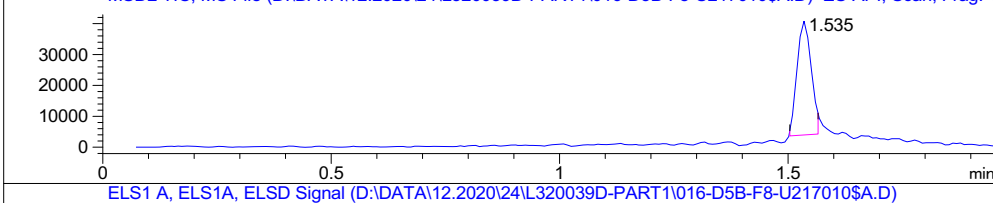
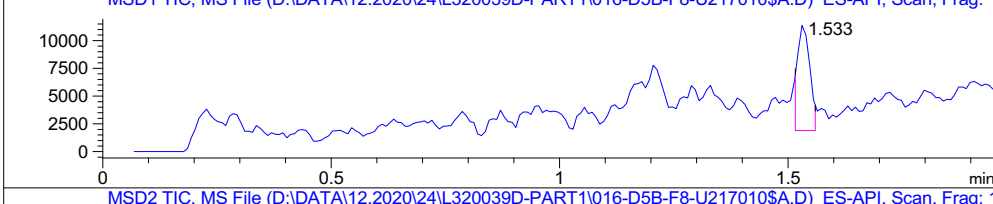
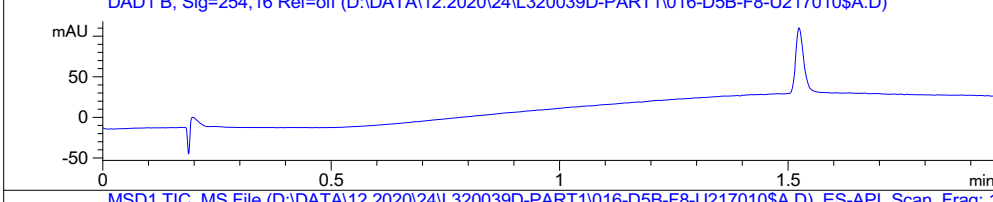
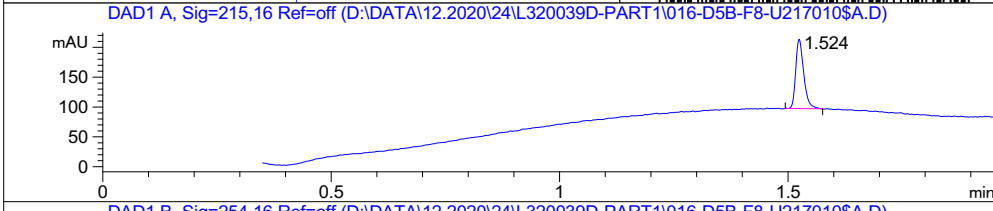


MaxPeak: 100.00%  
Ret\_Time: 1.524 min



Mol Wt 397.22  
Exact Mass 396.02

#	Time	Area%
1	1.524	100.00



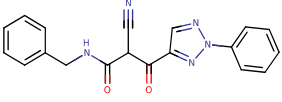
Inj.Date 12/24/2020

CH <invalid> -15-

Acq. Method C:\Chem32\ -> ->

Z1798873704\_

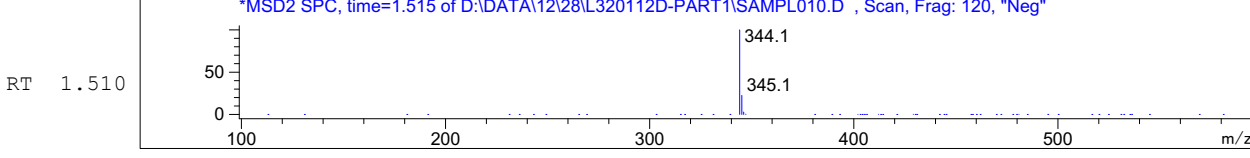
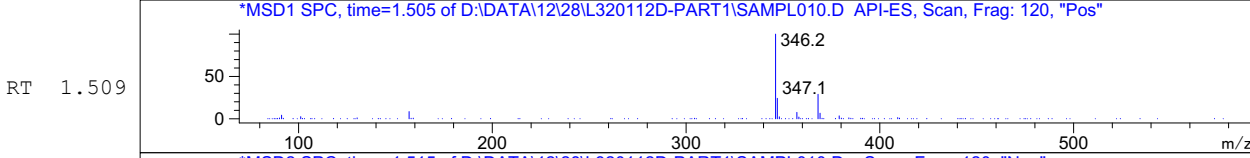
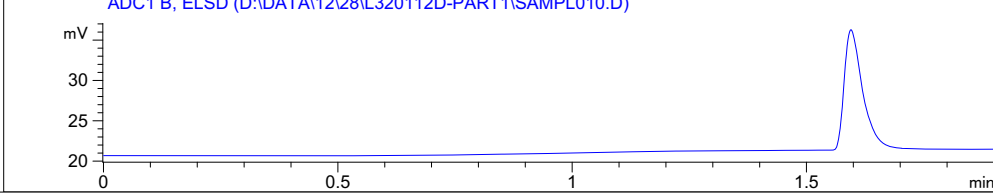
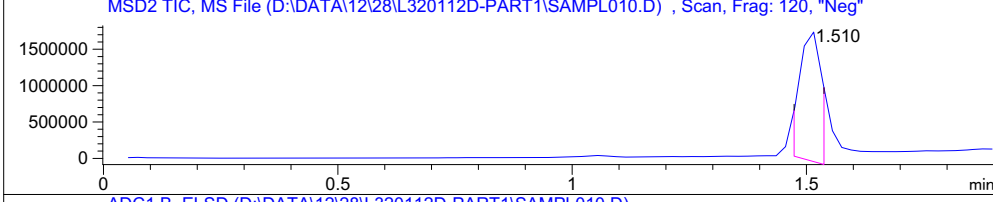
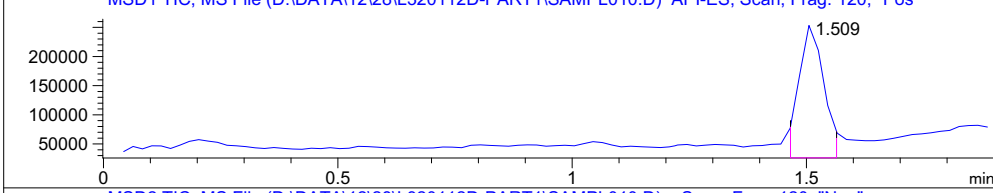
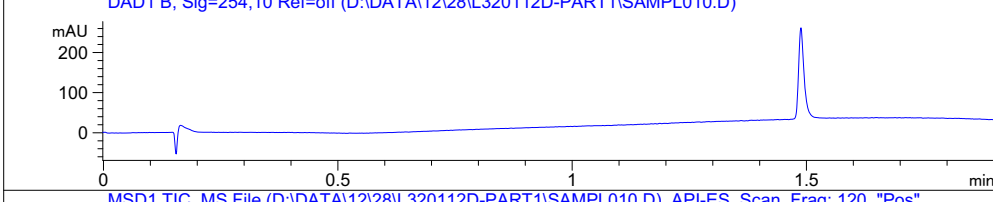
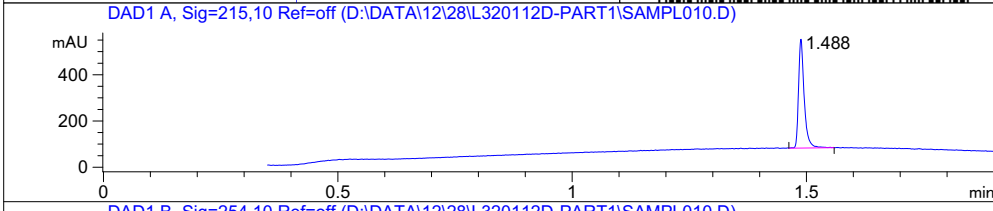
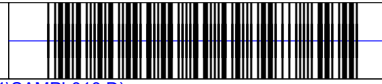
MaxPeak: 100.00%  
Ret\_Time: 1.488 min



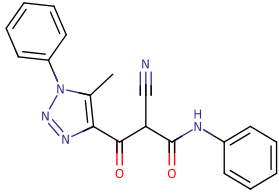
Mol Wt 345.36  
Exact Mass 345.13

#	Time	Area%
1	1.488	100.00

U253697\$G



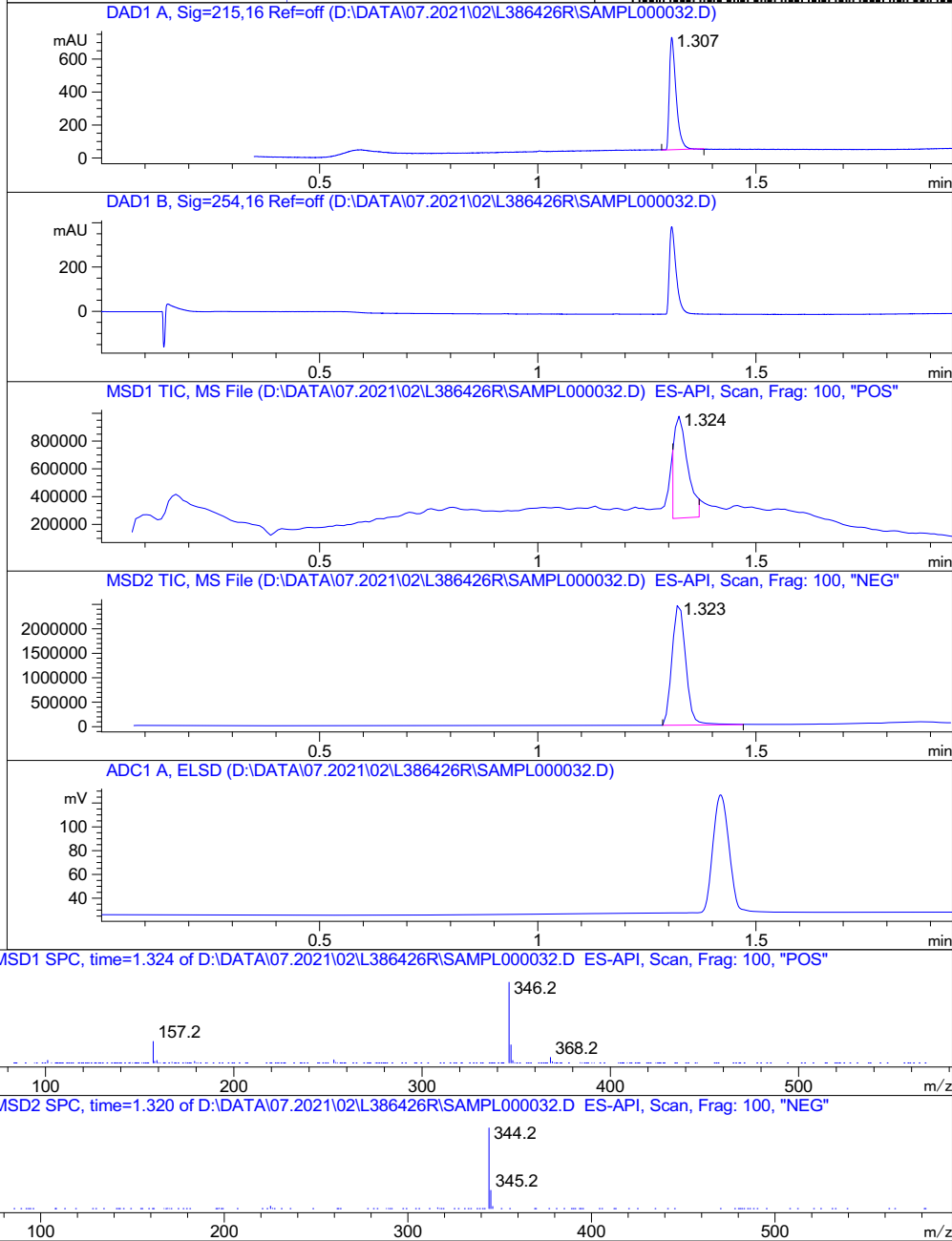
MaxPeak: 100.00%  
Ret\_Time: 1.307 min



Mol Wt 345.36  
Exact Mass 345.13

#	Time	Area%
1	1.307	100.00

7165188710



RT 1.324

RT 1.323

Inj.Date 7/2/2021

CH

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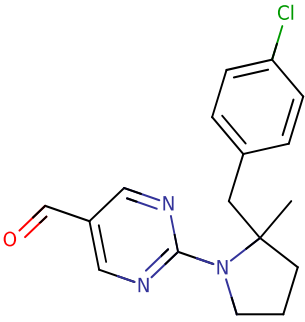
-5-

Acq. Method C:\CHEM32\ ->

->

Z762207984\_

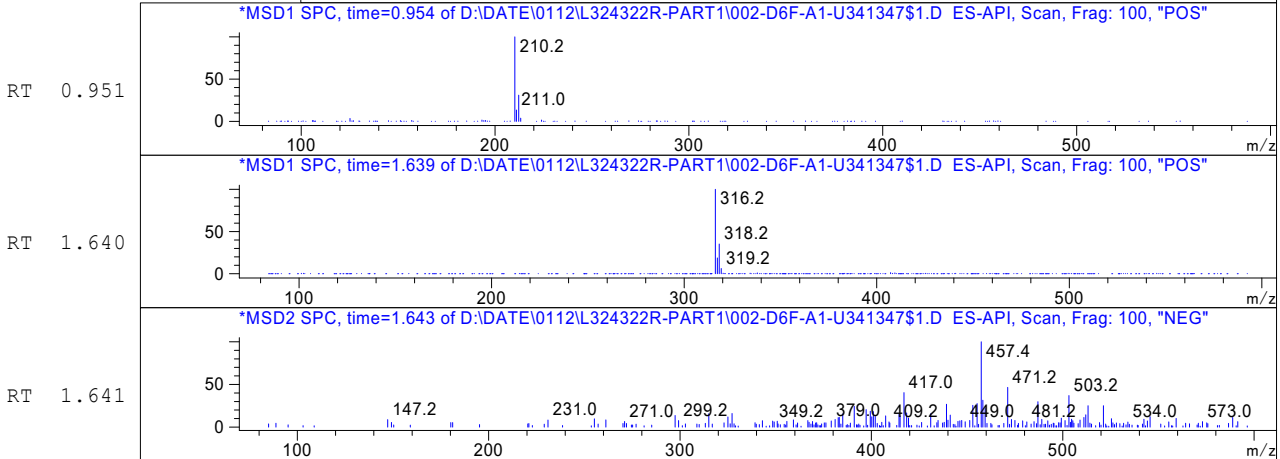
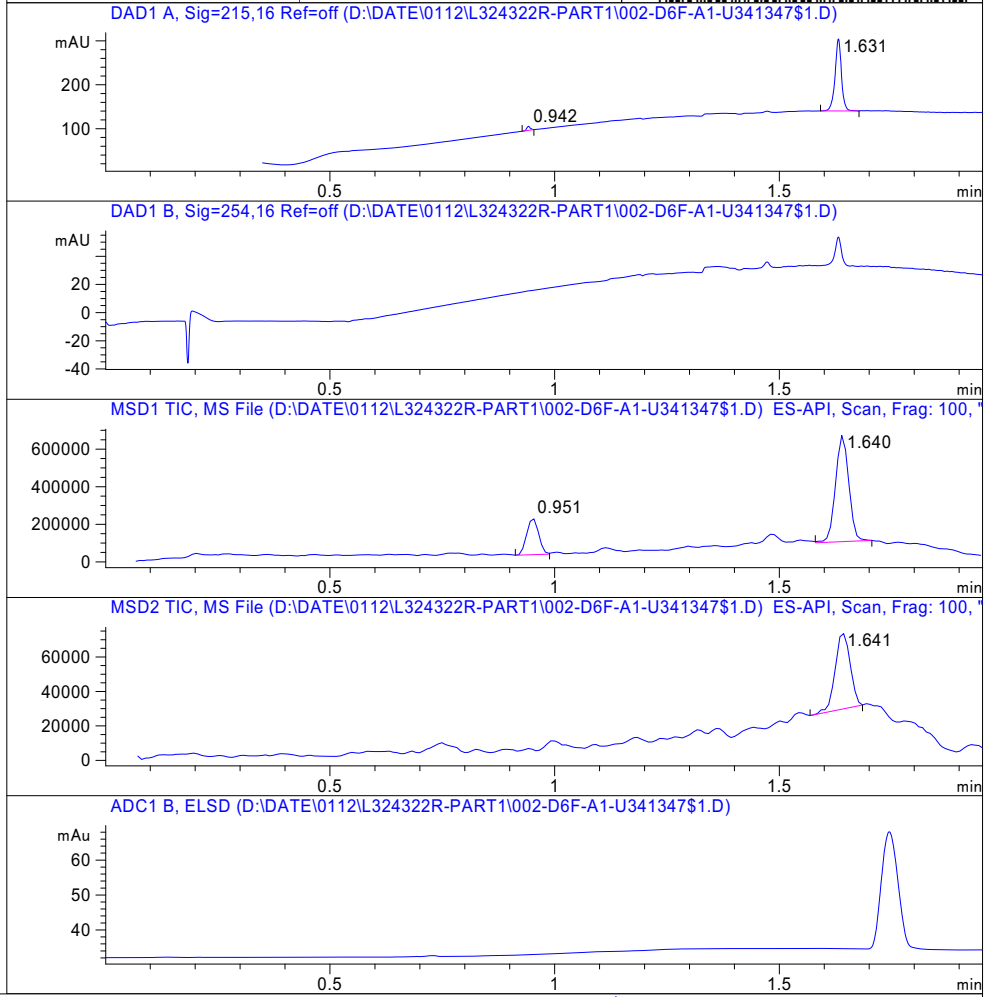
MaxPeak: 97.01%  
Ret\_Time: 1.631 min



Mol Wt 315.8  
Exact Mass 315.14

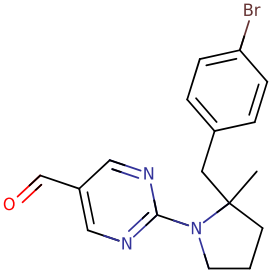
#	Time	Area%
1	0.942	2.99
2	1.631	97.01

U341347\$1





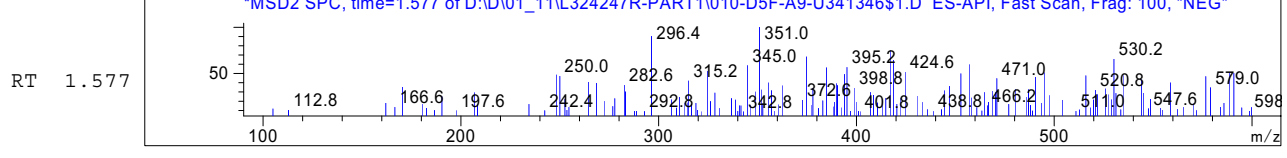
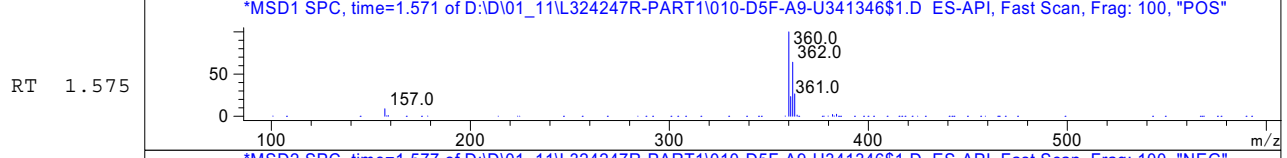
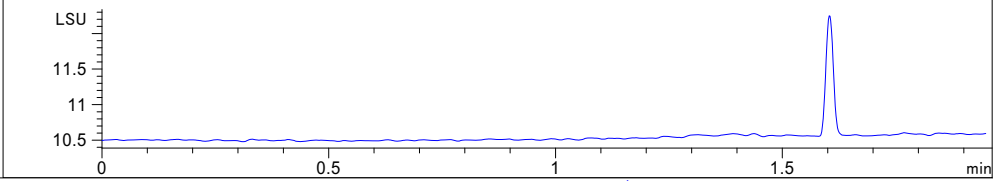
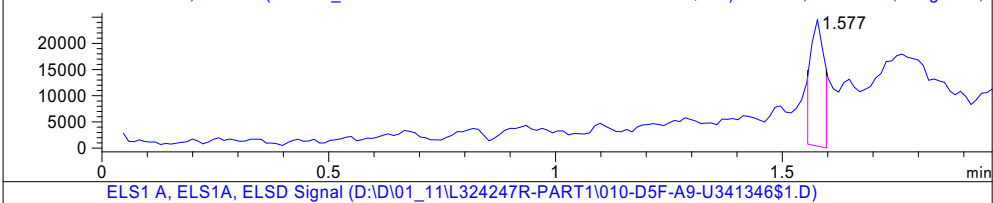
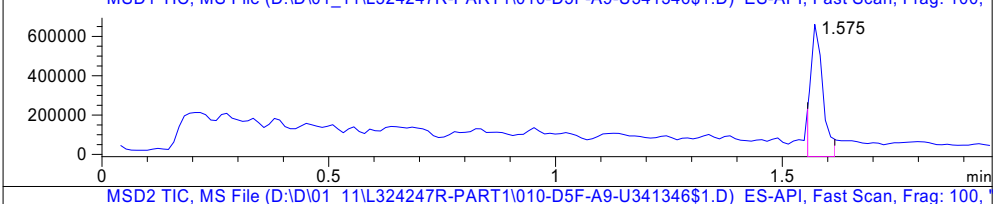
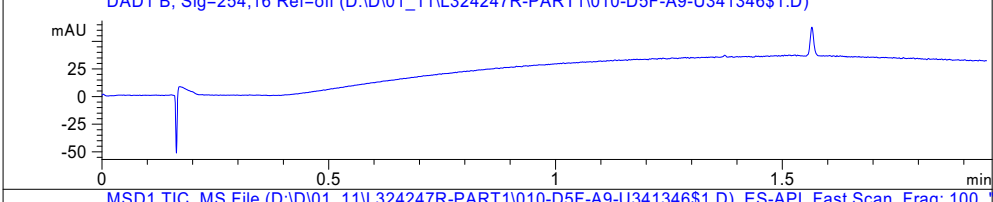
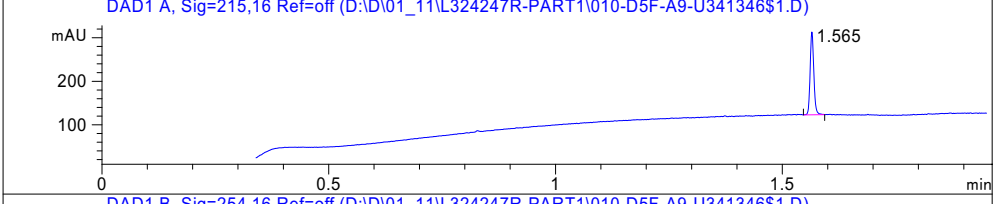
MaxPeak: 100.00%  
Ret\_Time: 1.565 min



Mol Wt 360.25  
Exact Mass 359.09

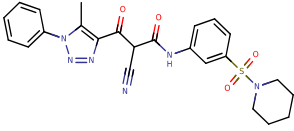
#	Time	Area%
1	1.565	100.00

# U341346\$1



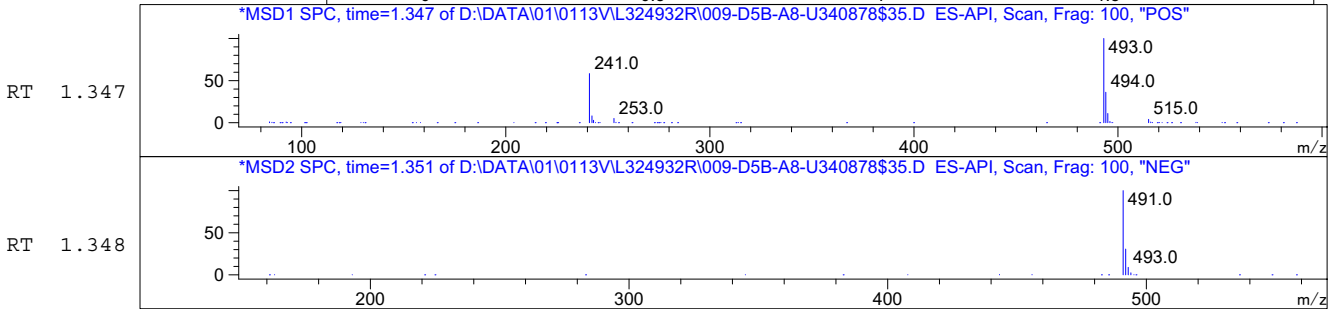
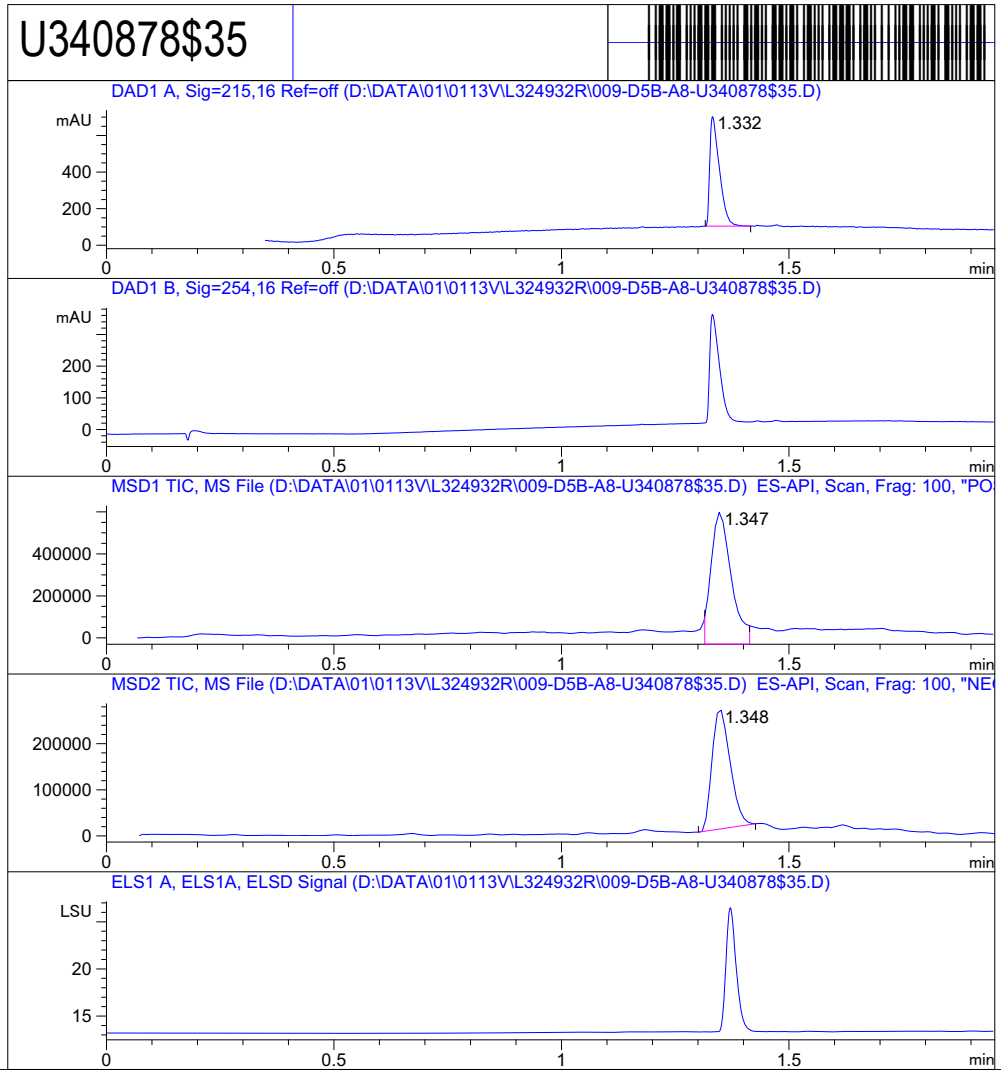
MaxPeak: 100.00%  
Ret\_Time: 1.332 min

U340878\$35



Mol Wt 492.55  
Exact Mass 492.17

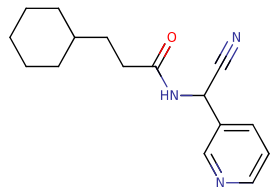
#	Time	Area%
1	1.332	100.00



U804751\$32



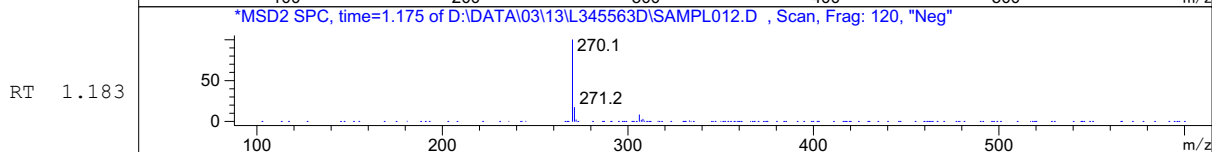
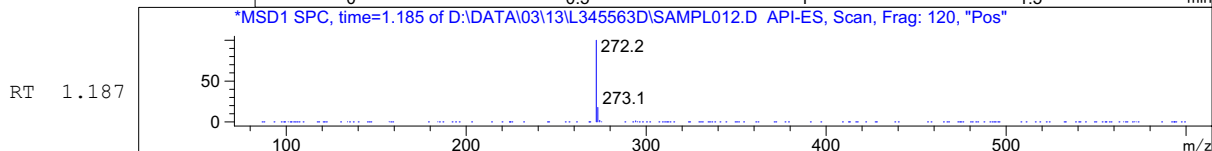
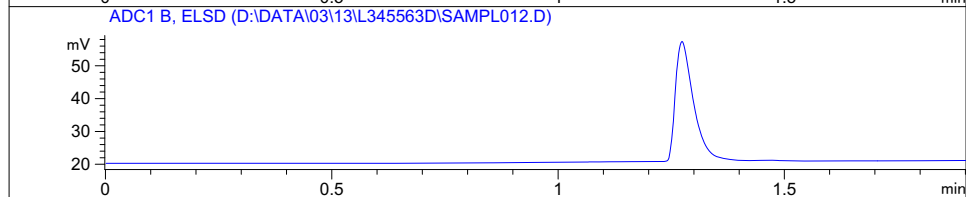
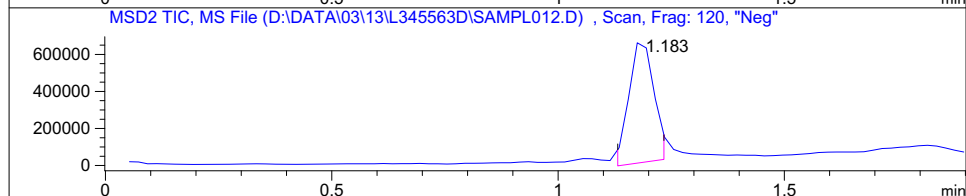
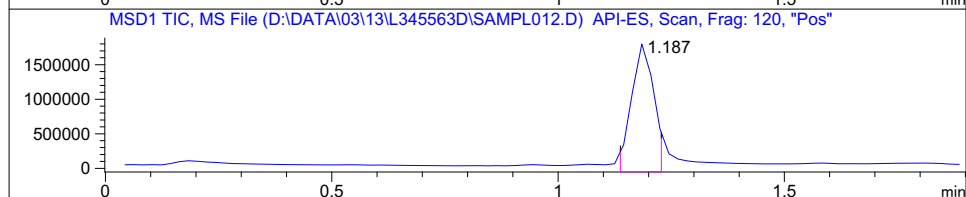
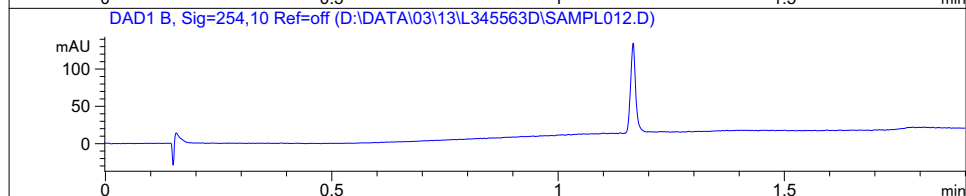
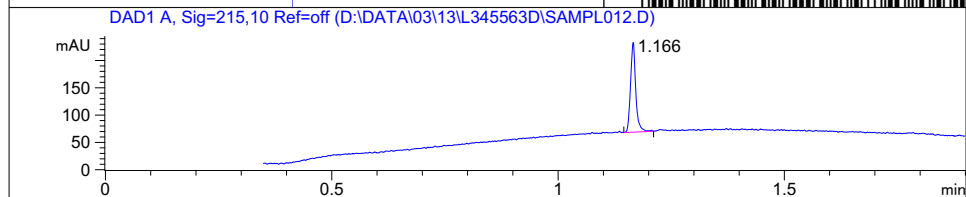
MaxPeak: 100.00%  
Ret\_Time: 1.166 min



Mol Wt 271.36

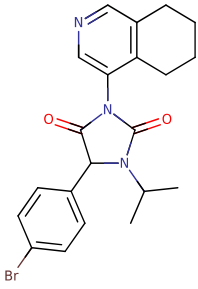
Exact Mass 271.2

#	Time	Area%
1	1.166	100.00



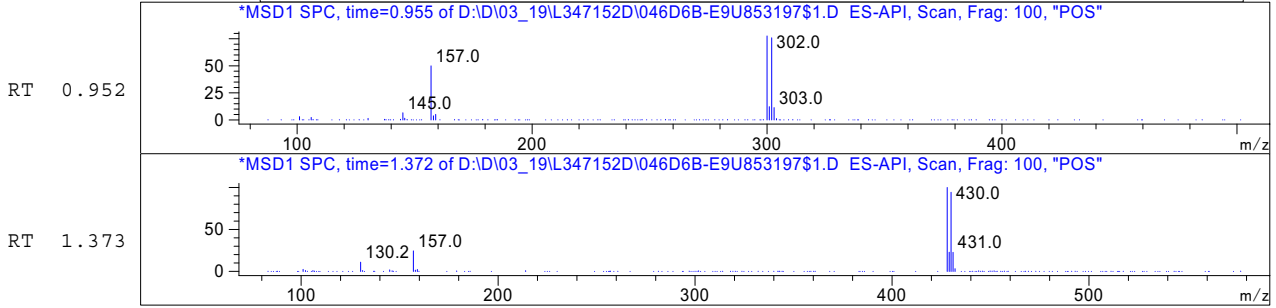
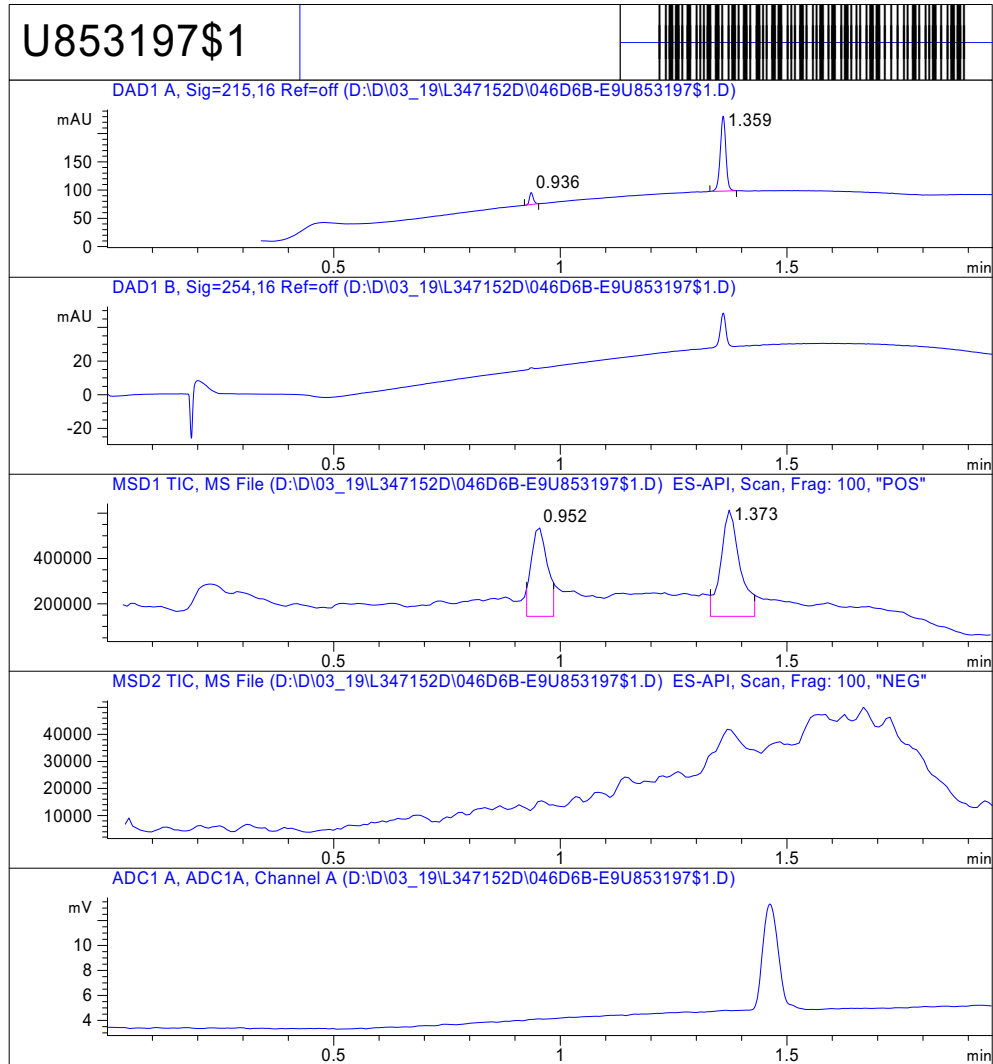
# U853197\$1

MaxPeak: 90.21%  
Ret\_Time: 1.359 min



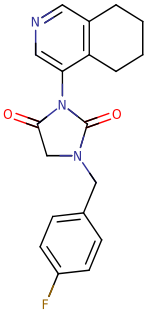
Mol Wt 428.32  
Exact Mass 429.12

#	Time	Area%
1	0.936	9.79
2	1.359	90.21



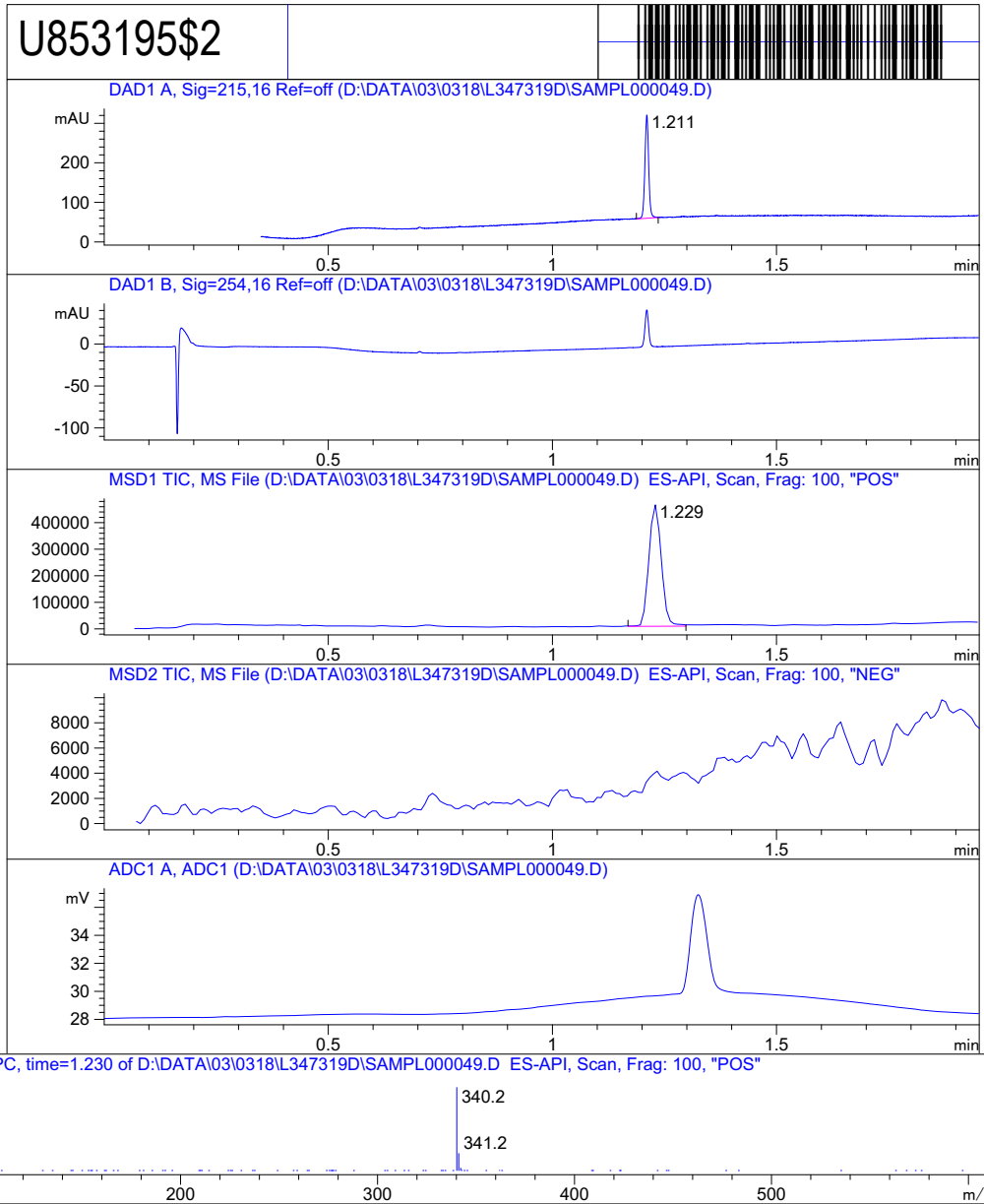
MaxPeak: 100.00%  
Ret\_Time: 1.211 min

U853195\$2



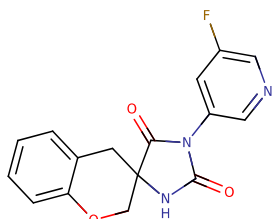
Mol Wt 339.36  
Exact Mass 339.16

#	Time	Area%
1	1.211	100.00



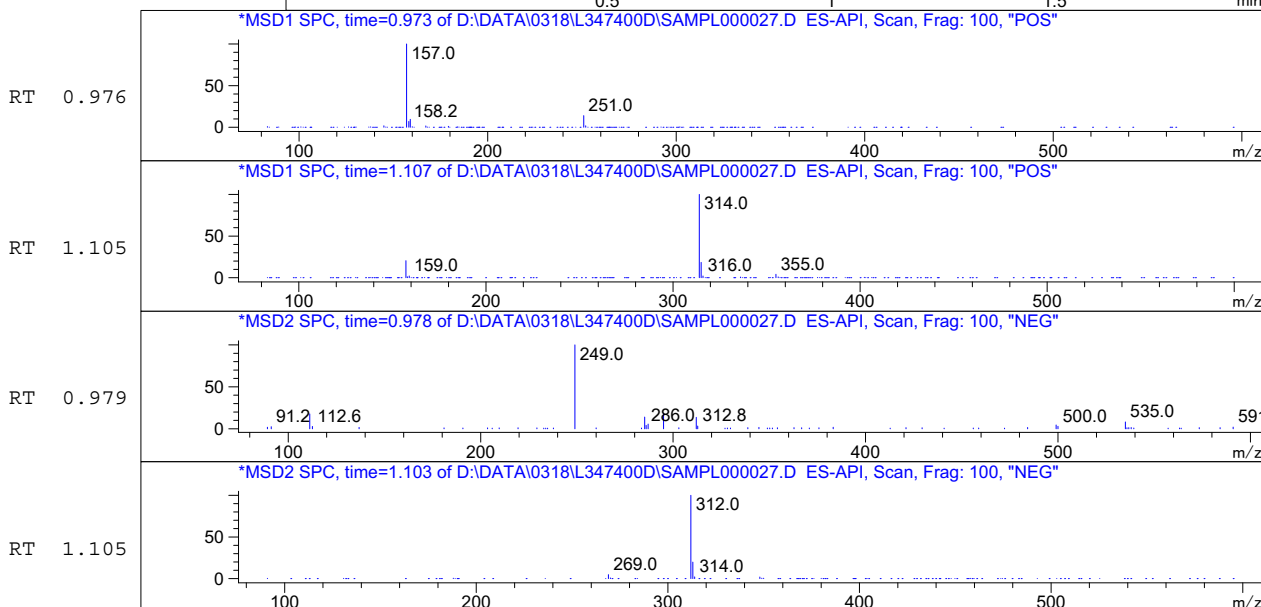
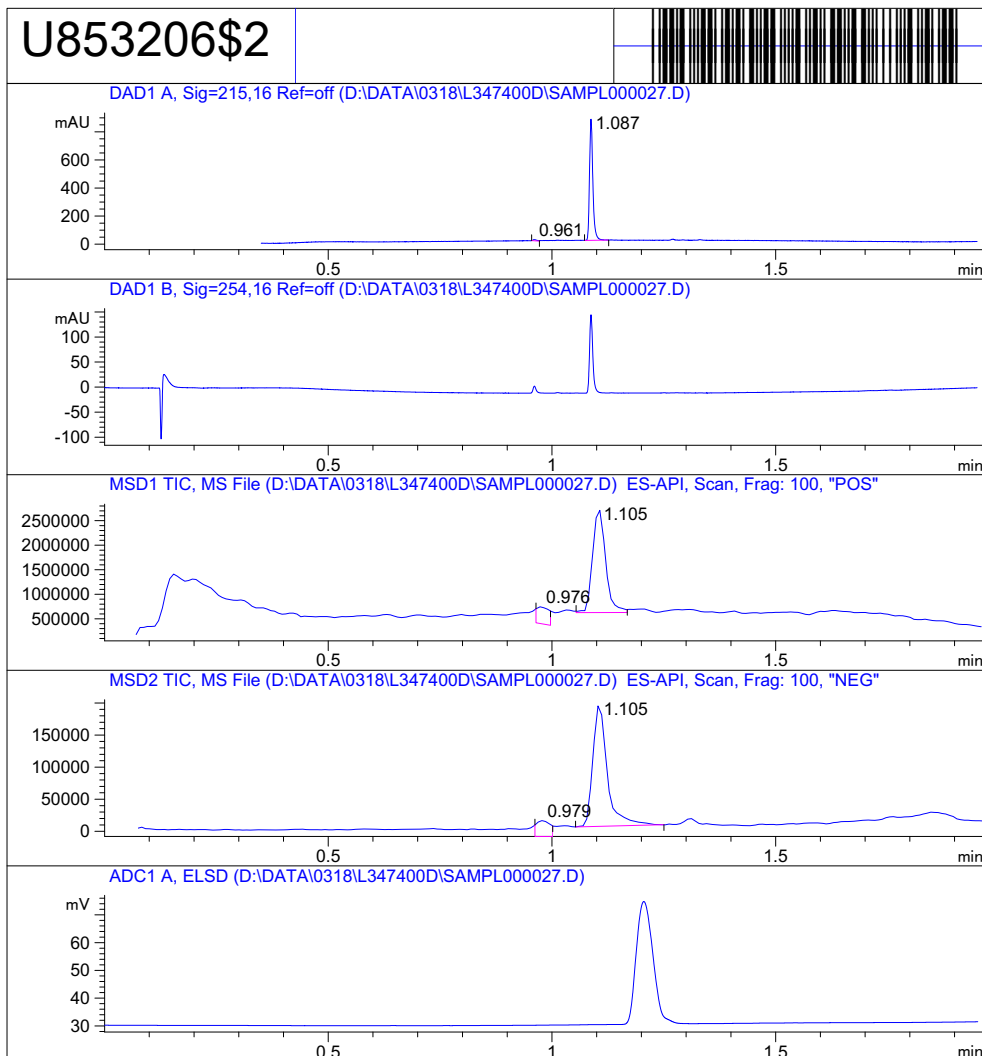
MaxPeak: 98.91%  
Ret\_Time: 1.087 min

# U853206\$2



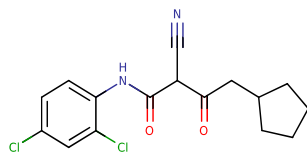
Mol Wt 313.28  
Exact Mass 313.09

#	Time	Area%
1	0.961	1.09
2	1.087	98.91



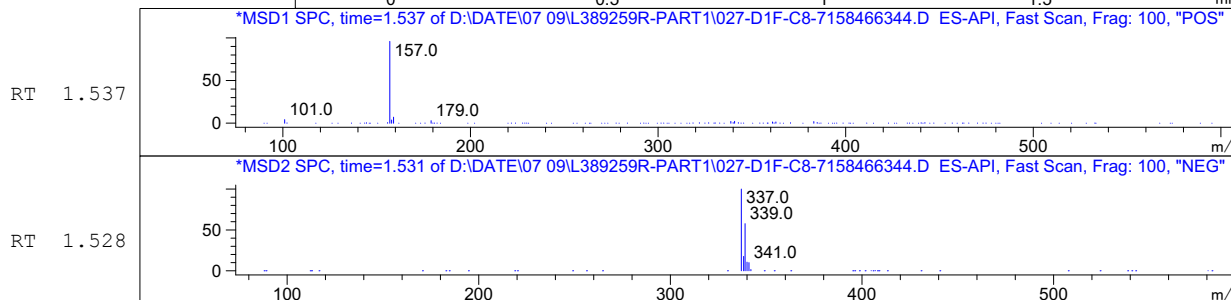
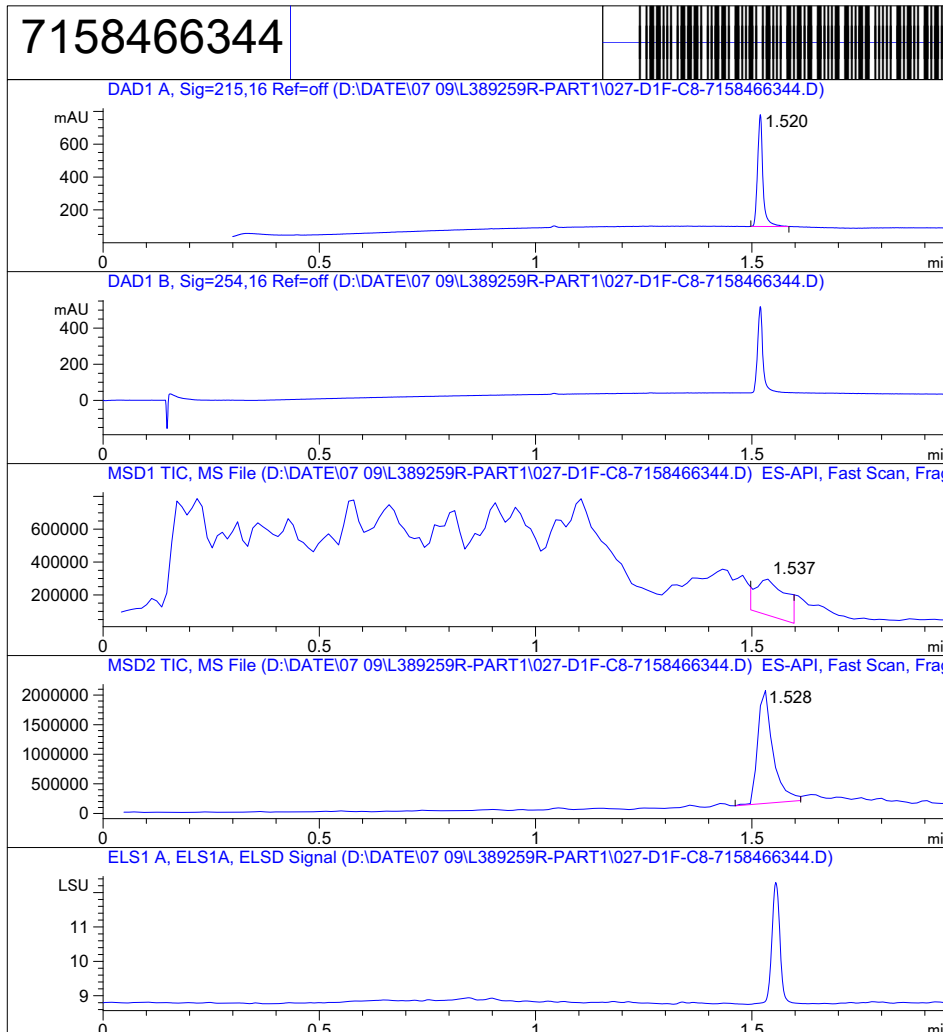
MaxPeak: 100.00%  
Ret\_Time: 1.520 min

7158466344



Mol Wt 339.22  
Exact Mass 338.08

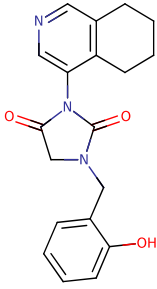
#	Time	Area%
1	1.520	100.00



# U853196\$2

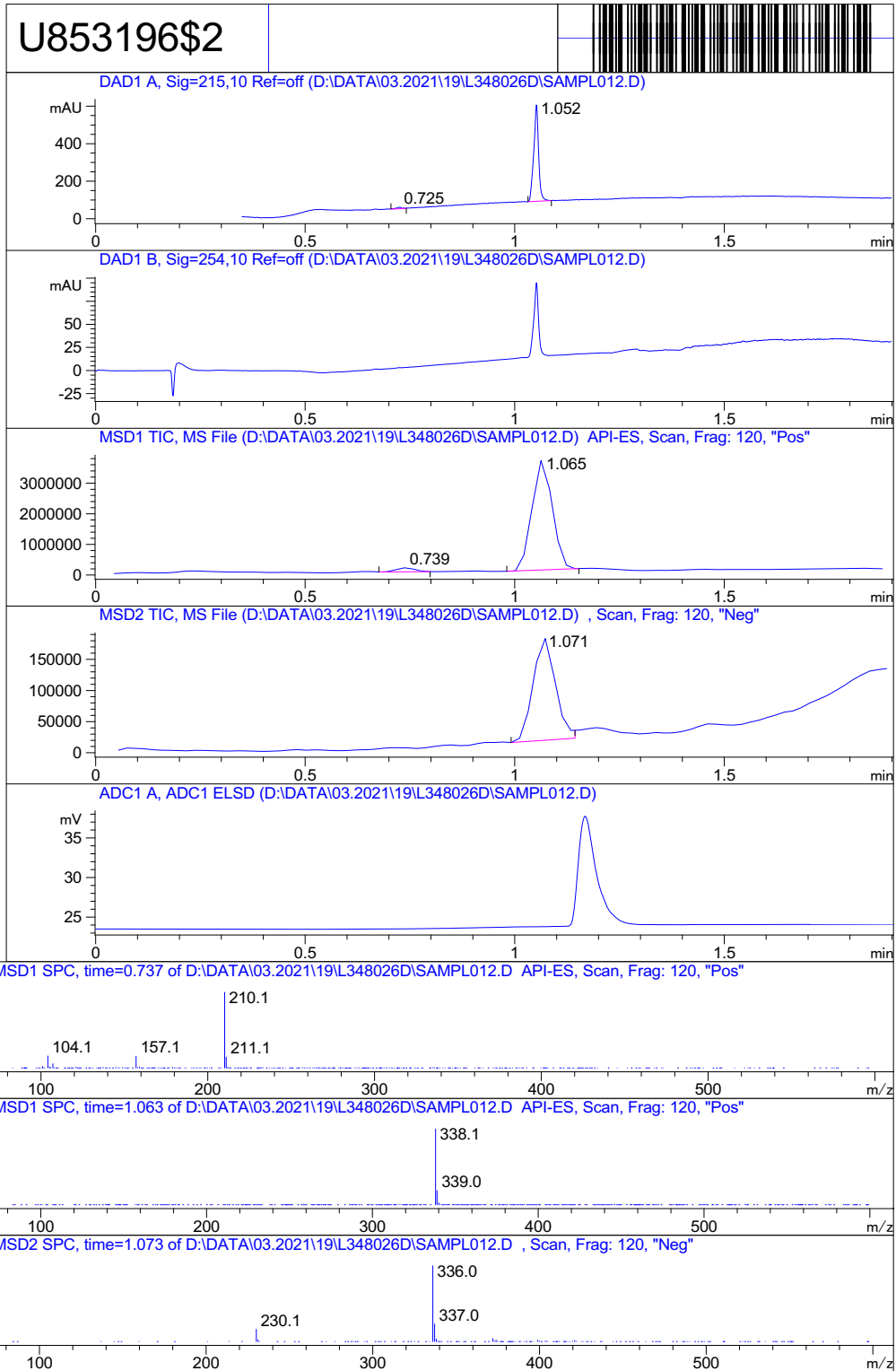


MaxPeak: 98.16%  
Ret\_Time: 1.052 min



Mol Wt 337.37  
Exact Mass 337.16

#	Time	Area%
1	0.725	1.84
2	1.052	98.16



Inj.Date 3/19/2021

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P2-B-03

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Acq. Method C:\HPCHEM\ ->

->

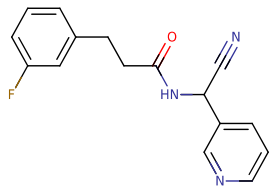
Z4929616577\_



U812291\$23

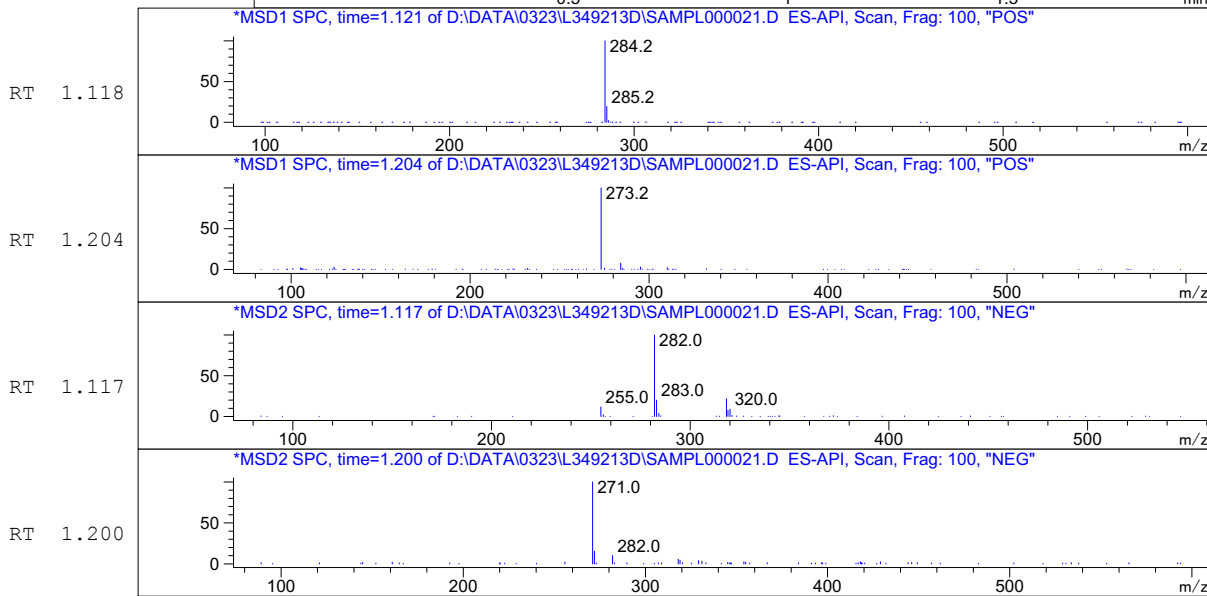
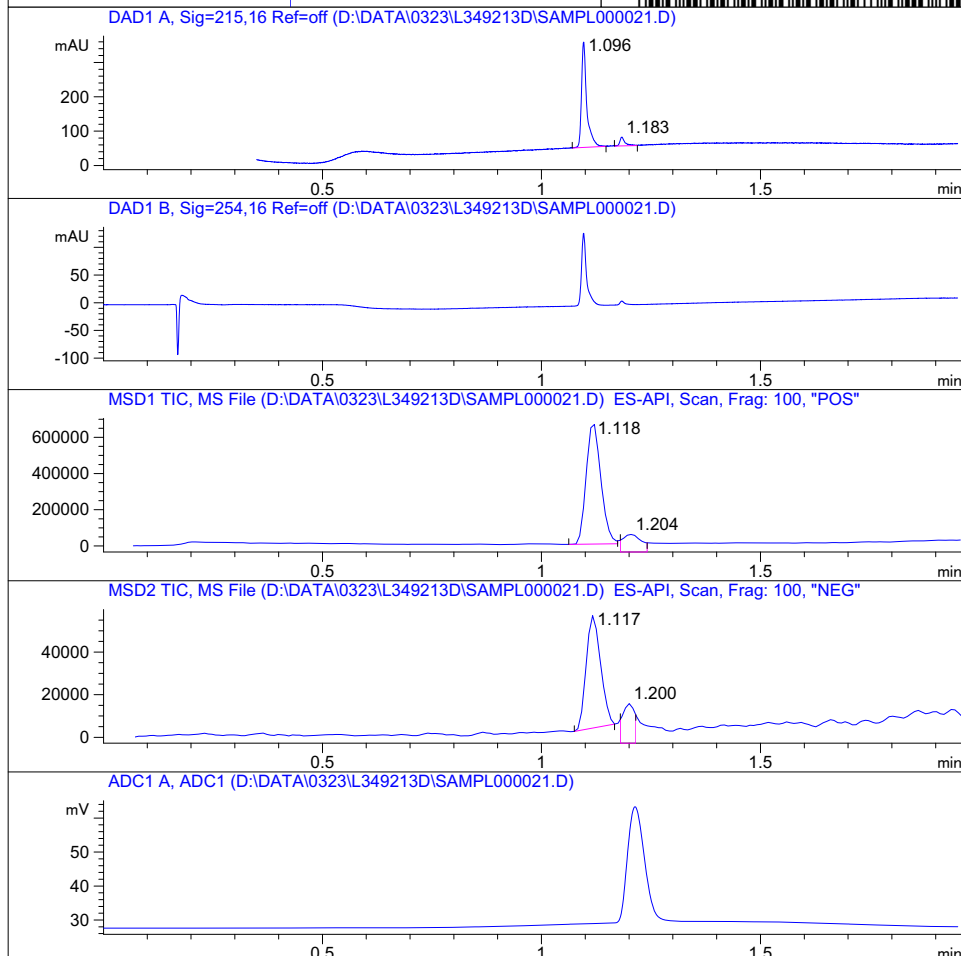


MaxPeak: 92.69%  
Ret\_Time: 1.096 min



Mol Wt 283.3  
Exact Mass 283.13

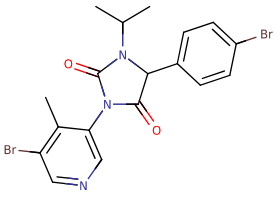
#	Time	Area%
1	1.096	92.69
2	1.183	7.31



U853208\$2

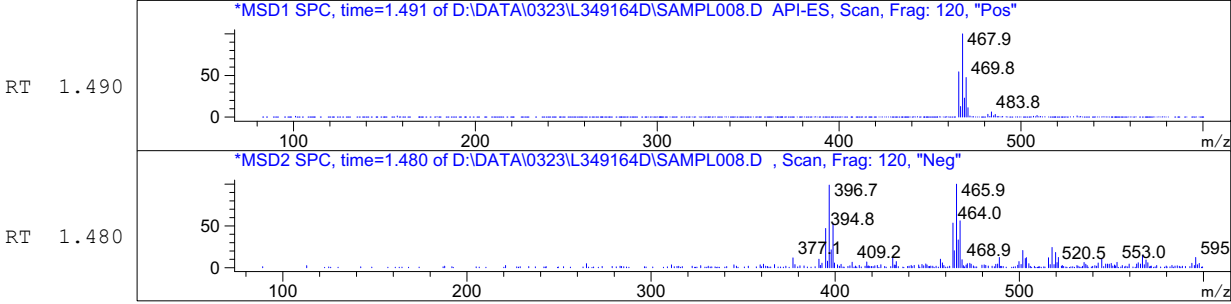
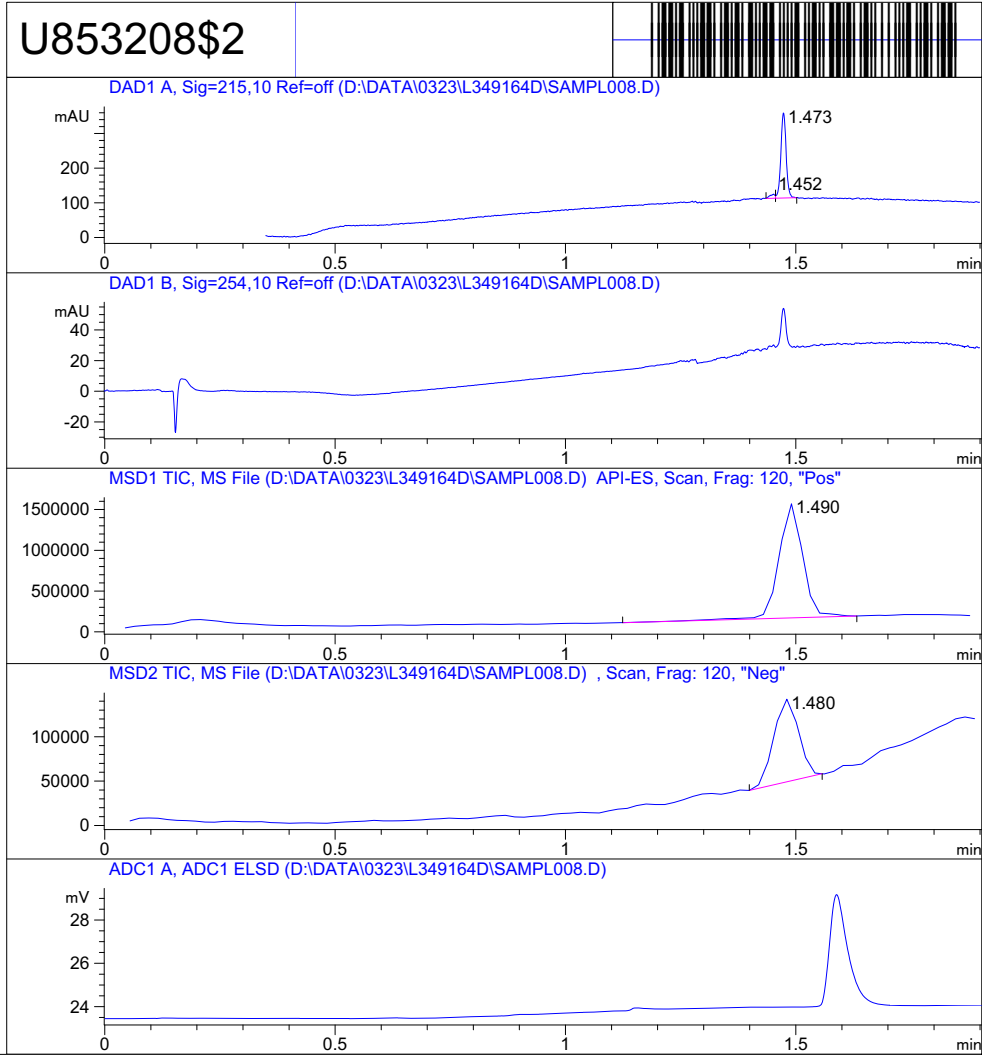


MaxPeak: 95.50%  
Ret\_Time: 1.473 min



Mol Wt 467.15  
Exact Mass 466.99

#	Time	Area%
1	1.452	4.50
2	1.473	95.50



Inj.Date 3/23/2021

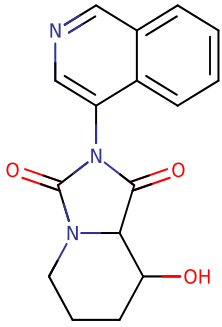
OA

-VL-

Acq. Method C:\HPCHEM\ -> ->

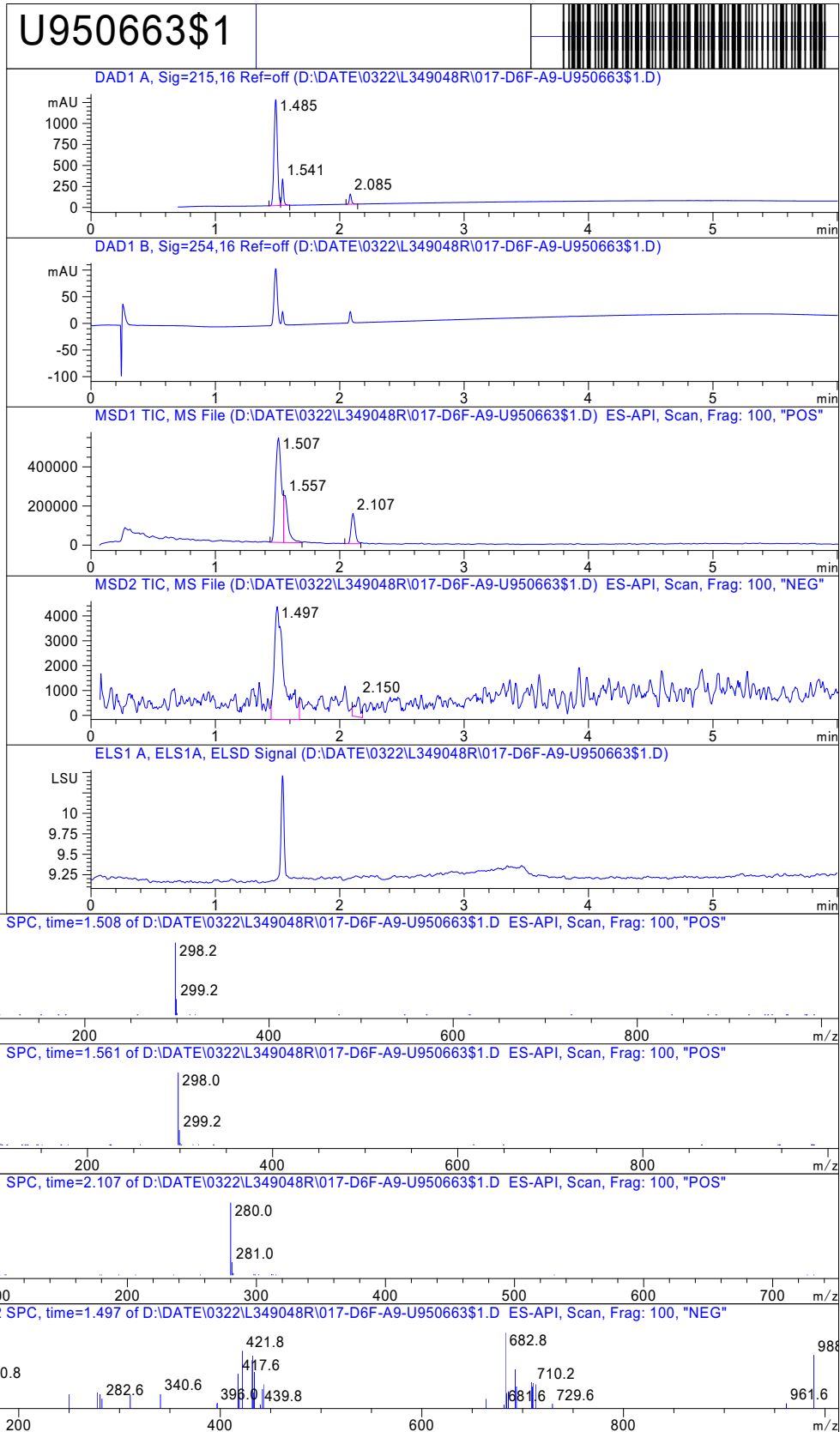
Z4927215427\_

MaxPeak: 83.37%  
Ret\_Time: 1.485 min



Mol Wt 297.31  
Exact Mass 297.12

#	Time	Area%
1	1.485	83.37
2	1.541	11.66
3	2.085	4.97



Inj.Date 3/22/2021

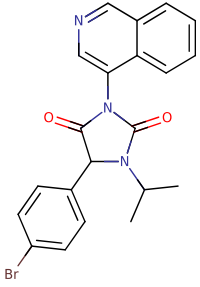
E

13

Acq. Method C:\Chem32\> >

Z4929616088\_

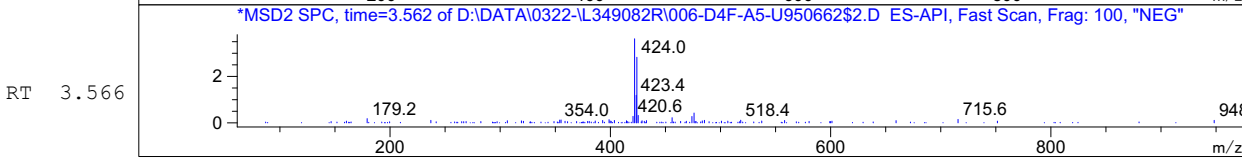
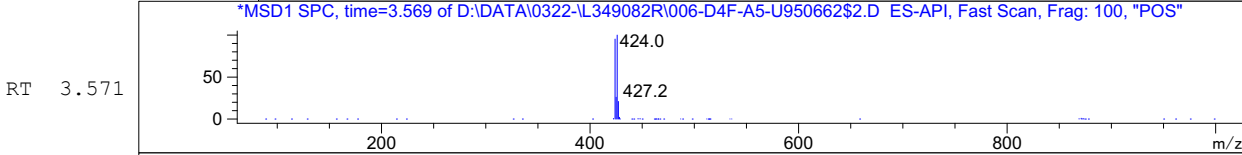
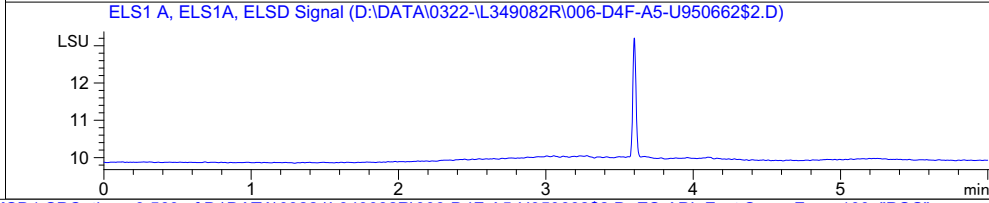
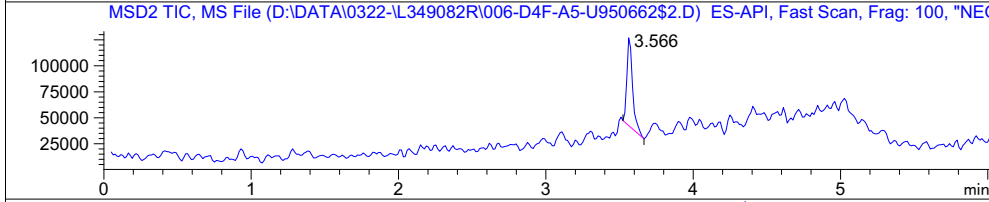
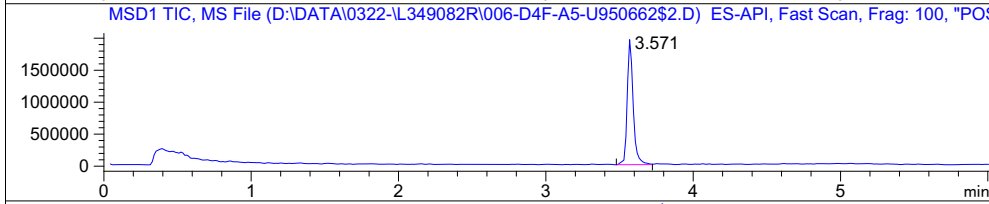
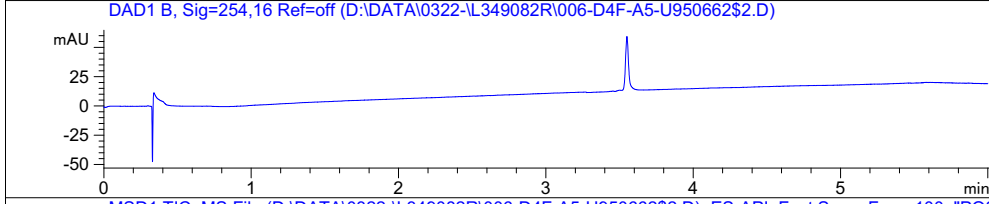
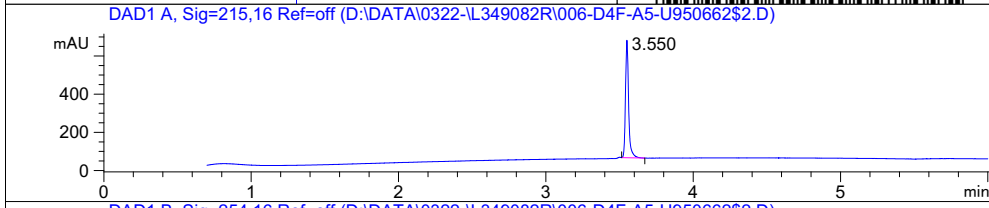
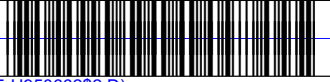
MaxPeak: 100.00%  
Ret\_Time: 3.550 min



Mol Wt 424.29  
Exact Mass 425.08

#	Time	Area%
1	3.550	100.00

U950662\$2



Inj.Date 3/22/2021

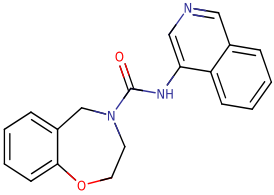
OA

Acq. Method C:\Users\ -> ->

Z4925123630\_

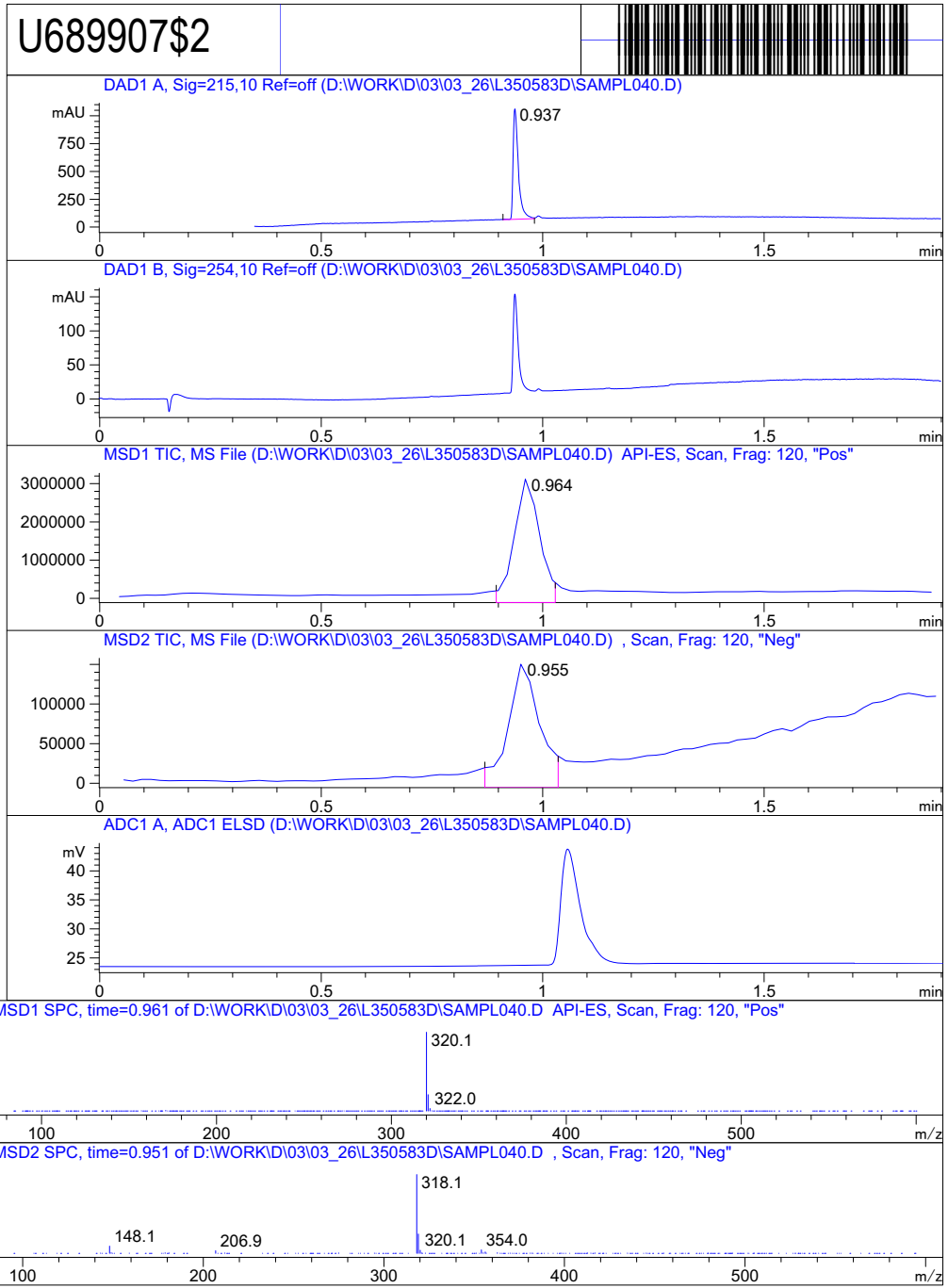
MaxPeak: 100.00%  
Ret\_Time: 0.937 min

U689907\$2



Mol Wt 319.36  
Exact Mass 319.15

#	Time	Area%
1	0.937	100.00



RT 0.964

RT 0.955

Inj.Date 3/26/2021

K

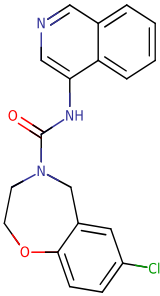
-VL-

Acq. Method C:\HPCHEM\ -> ->

Z1531604940\_

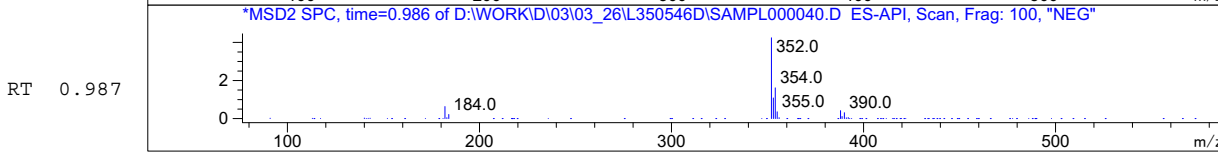
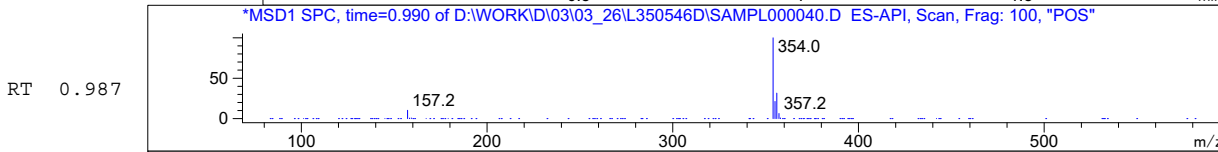
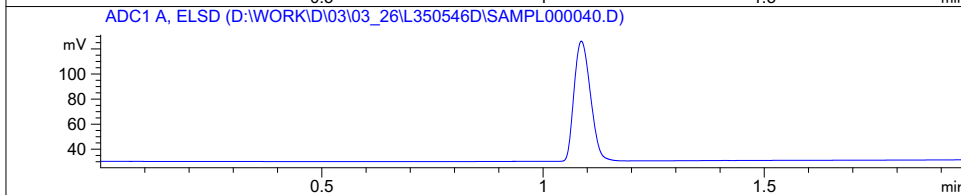
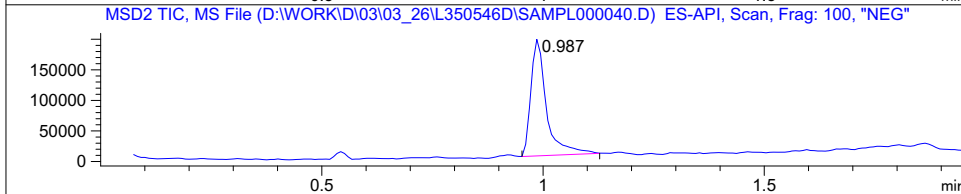
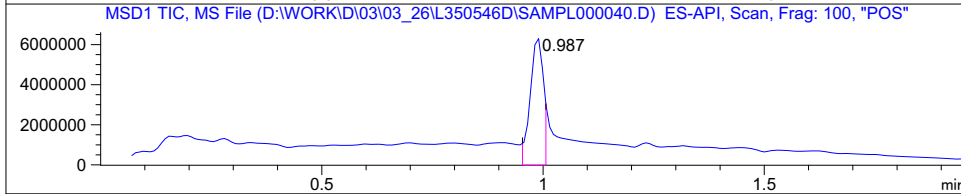
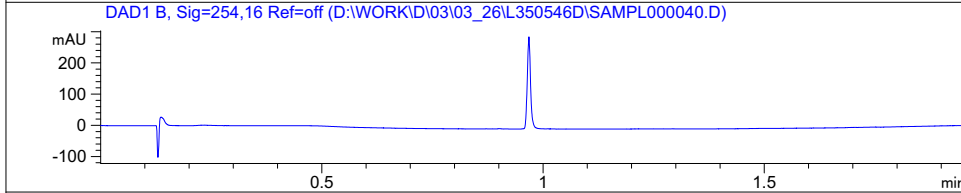
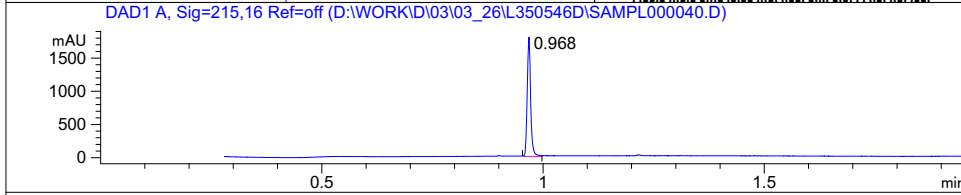
MaxPeak: 100.00%  
Ret\_Time: 0.968 min

U693154\$1

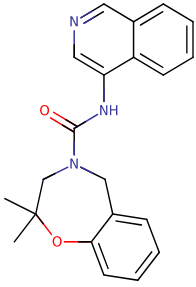


Mol Wt 353.8  
Exact Mass 353.11

#	Time	Area%
1	0.968	100.00



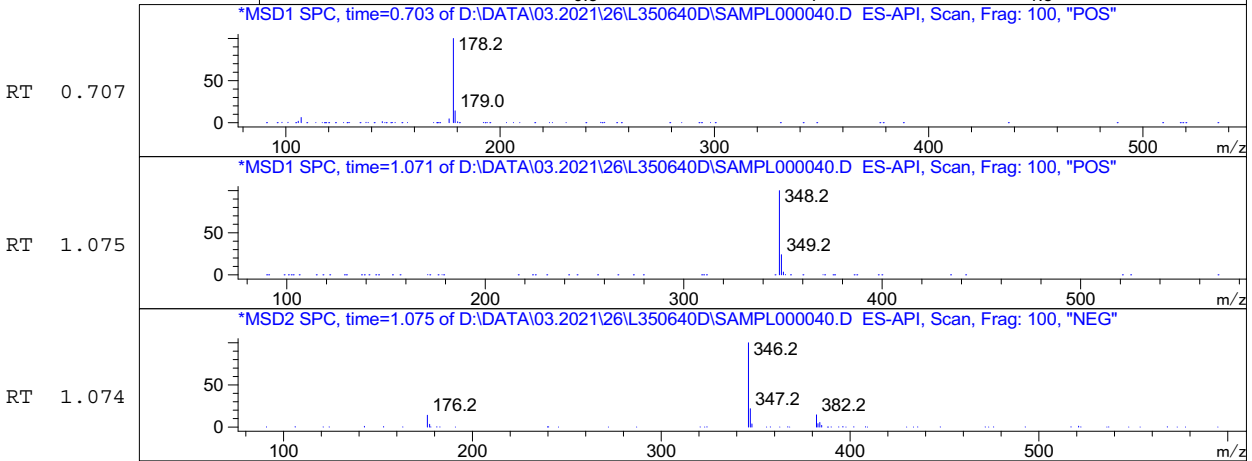
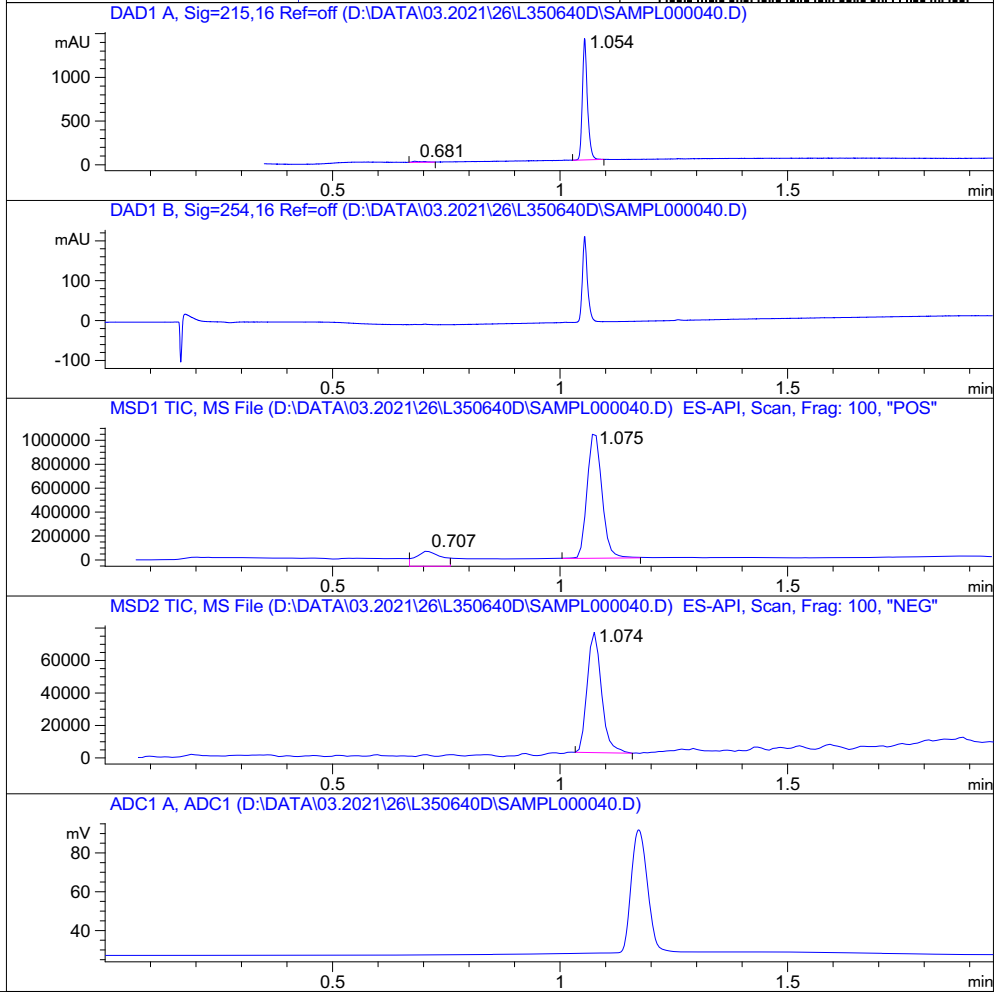
MaxPeak: 98.19%  
Ret\_Time: 1.054 min



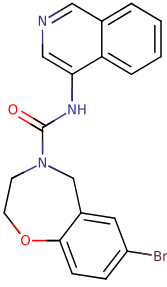
Mol Wt 347.41  
Exact Mass 347.19

#	Time	Area%
1	0.681	1.81
2	1.054	98.19

U689906\$3



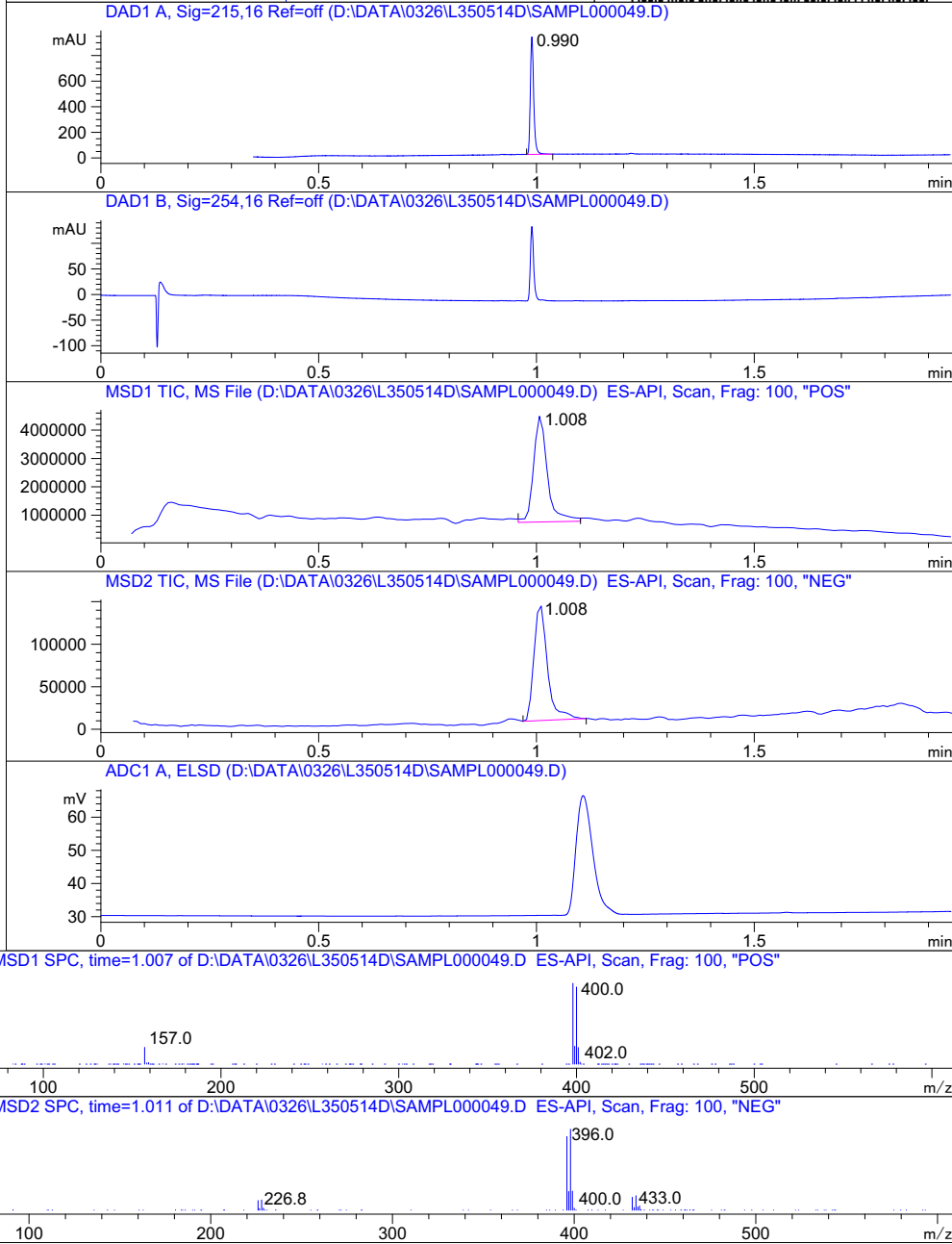
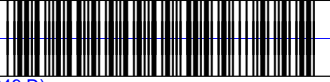
MaxPeak: 100.00%  
Ret\_Time: 0.990 min



Mol Wt 398.25  
Exact Mass 397.06

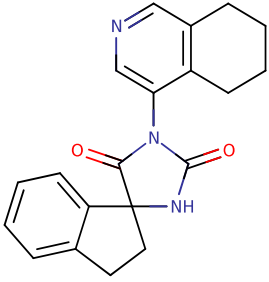
#	Time	Area%
1	0.990	100.00

U689908\$1





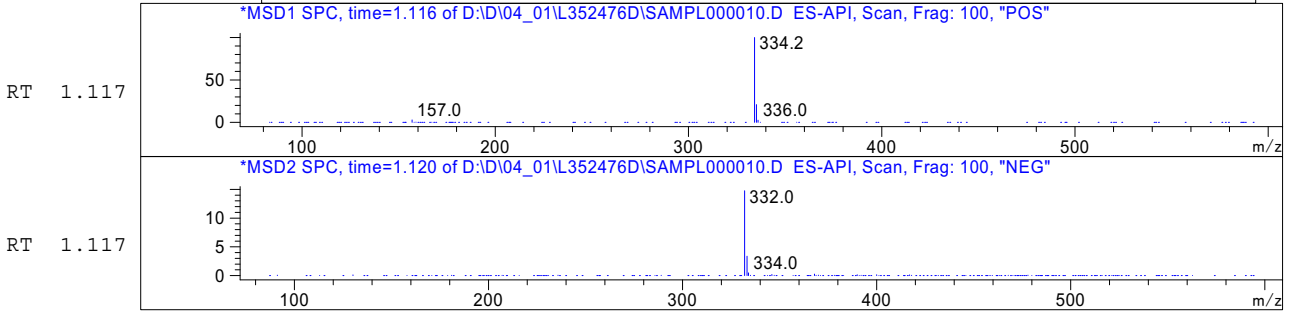
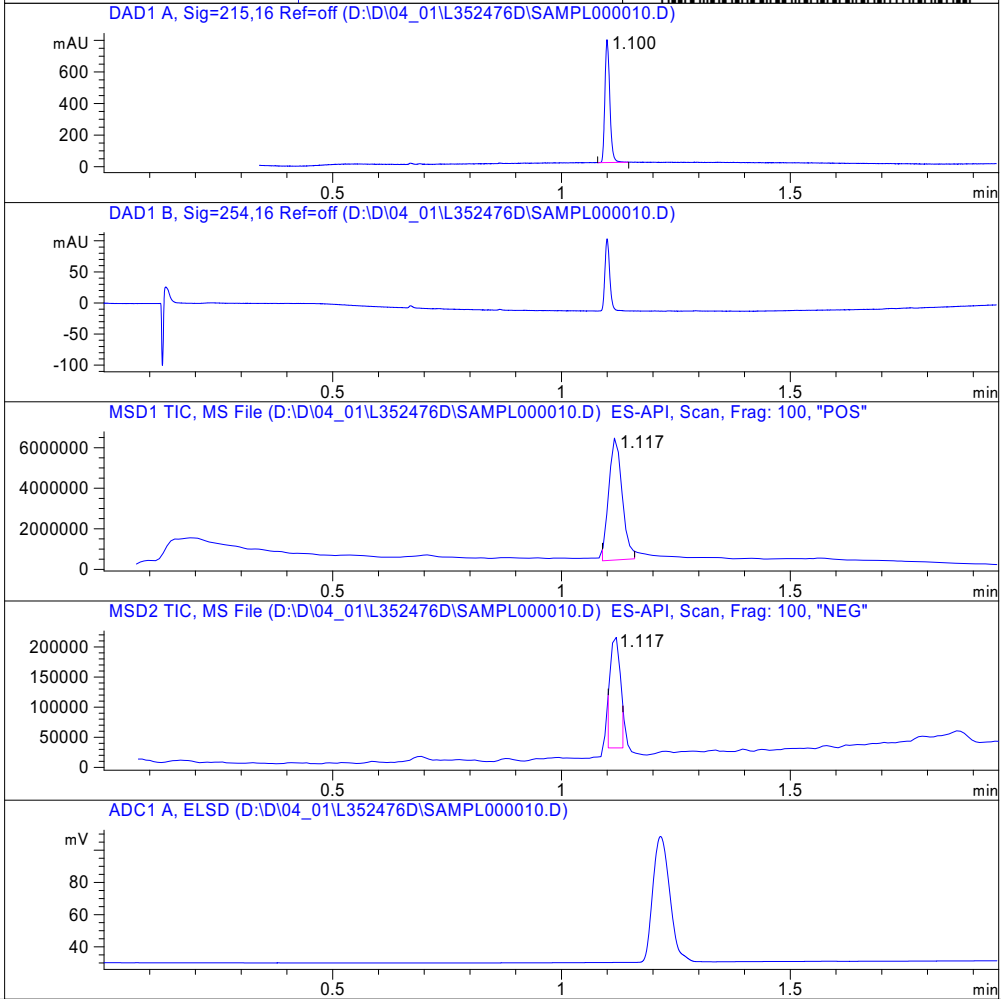
MaxPeak: 100.00%  
Ret\_Time: 1.100 min



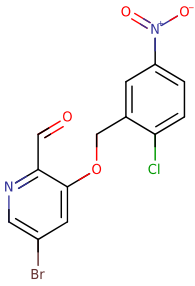
Mol Wt 333.38  
Exact Mass 333.17

#	Time	Area%
1	1.100	100.00

U963858\$1



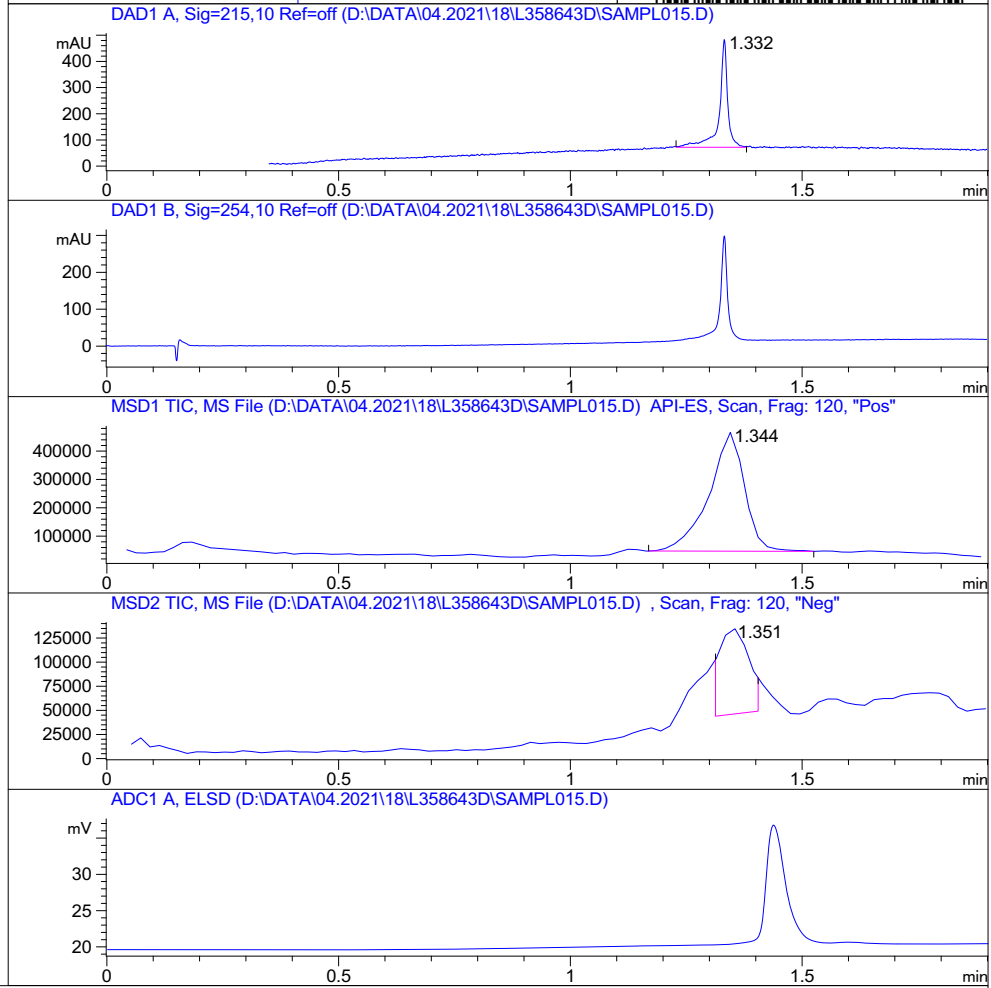
MaxPeak: 100.00%  
Ret\_Time: 1.332 min



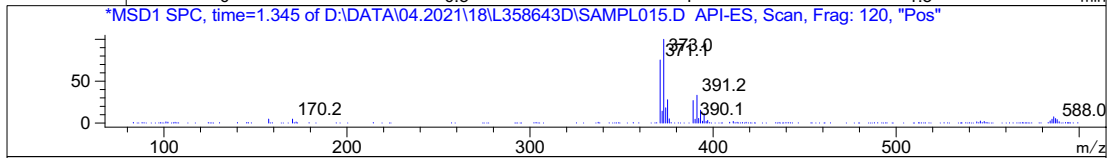
Mol Wt 371.57  
Exact Mass 371.93

#	Time	Area%
1	1.332	100.00

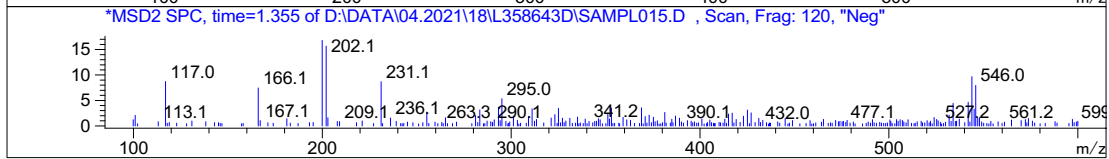
U920096\$2



RT 1.344



RT 1.351



Inj.Date 4/18/2021

CH

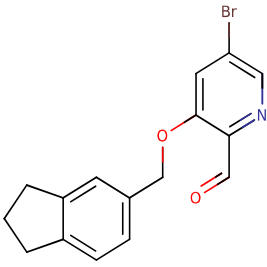
P2-B-06

-SL-

Acq. Method C:\HPCHEM\--> -->

Z4954569105\_

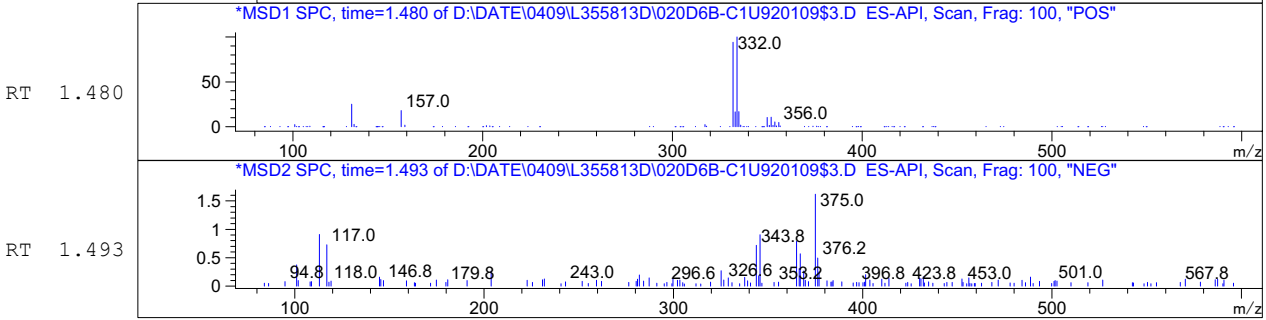
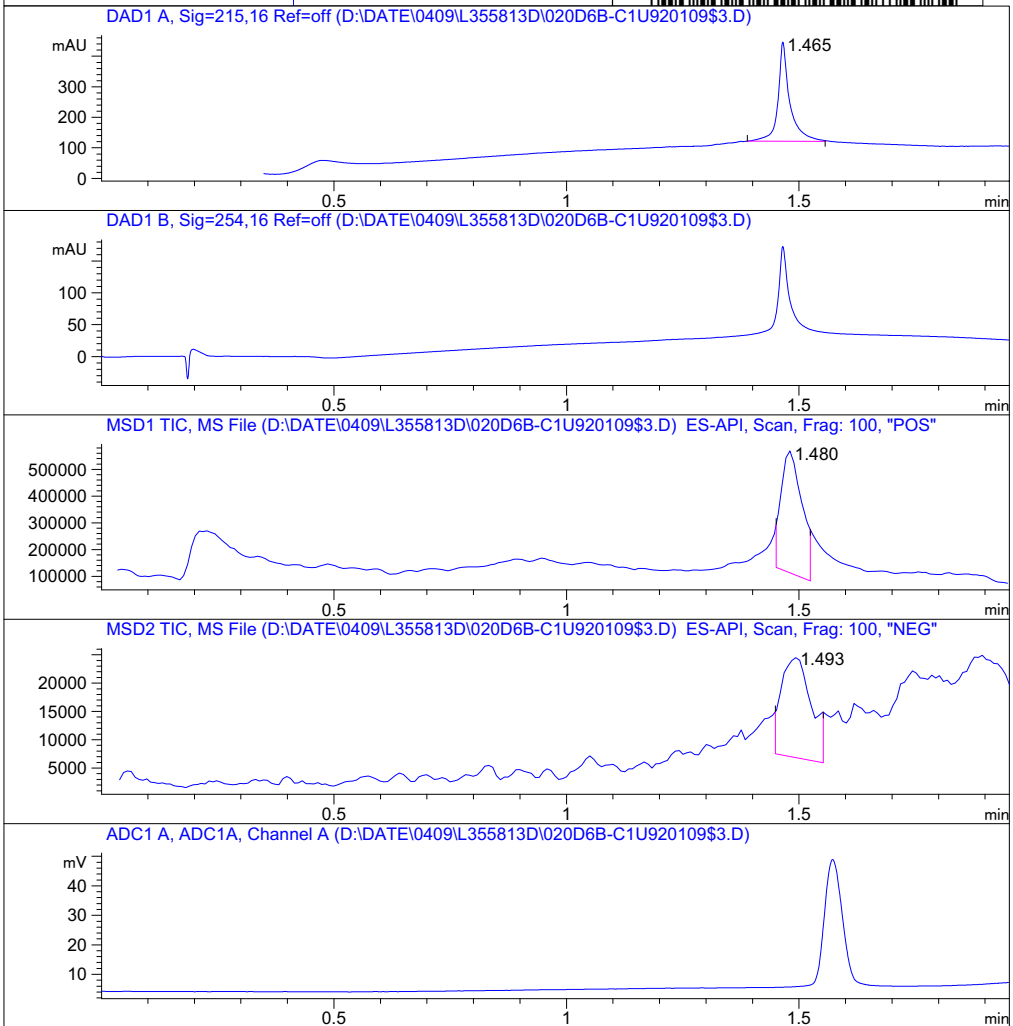
MaxPeak: 100.00%  
Ret\_Time: 1.465 min



Mol Wt 332.19  
Exact Mass 331.04

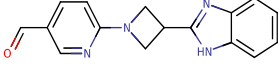
#	Time	Area%
1	1.465	100.00

# U920109\$3



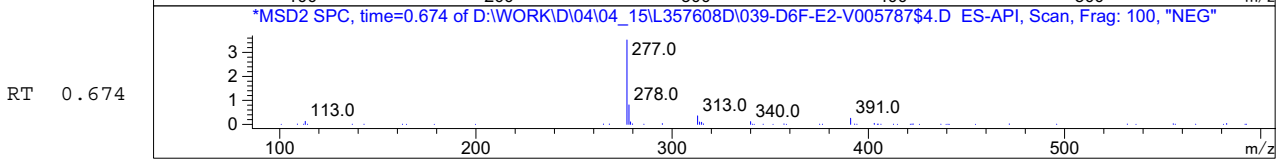
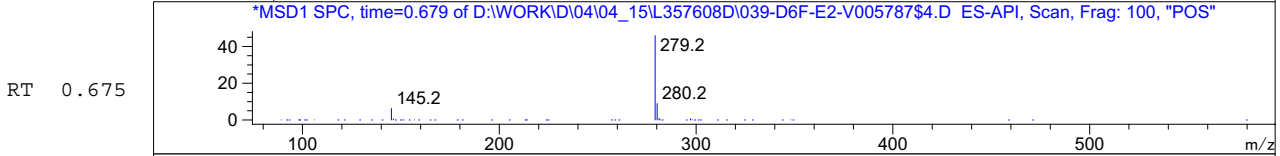
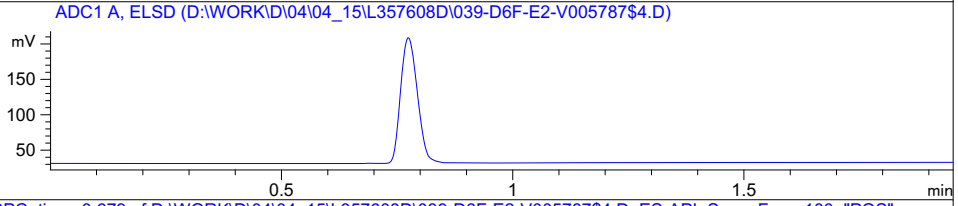
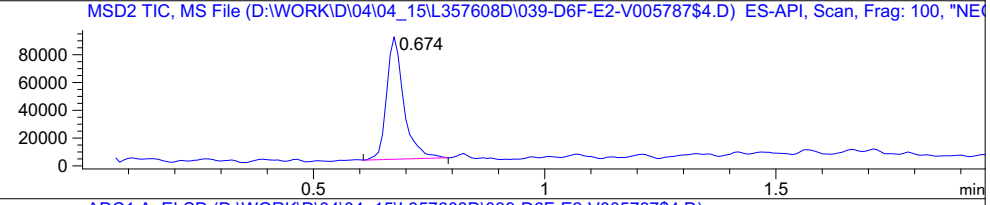
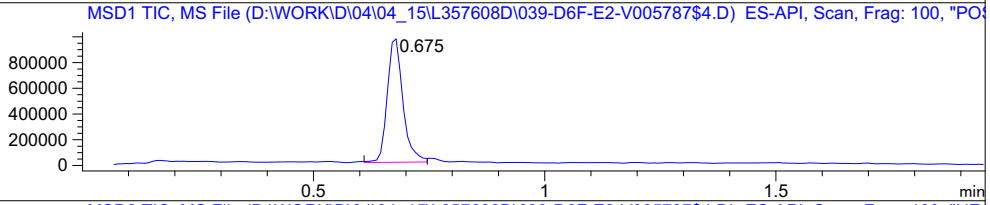
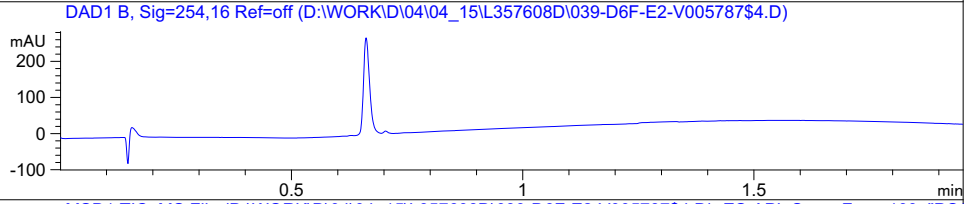
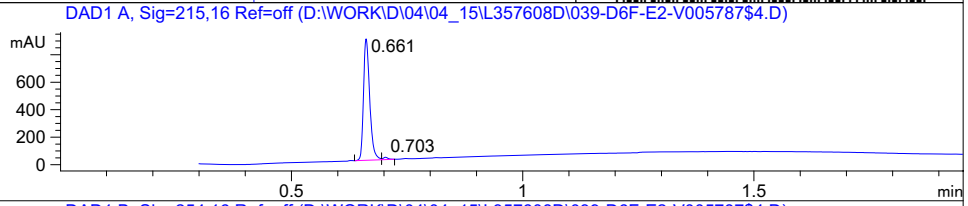
MaxPeak: 98.52%  
Ret\_Time: 0.661 min

V005787\$4



Mol Wt 278.31  
Exact Mass 278.13

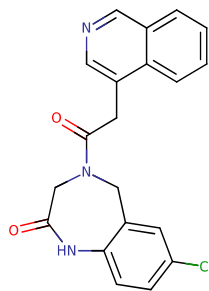
#	Time	Area%
1	0.661	98.52
2	0.703	1.48



V123973\$1

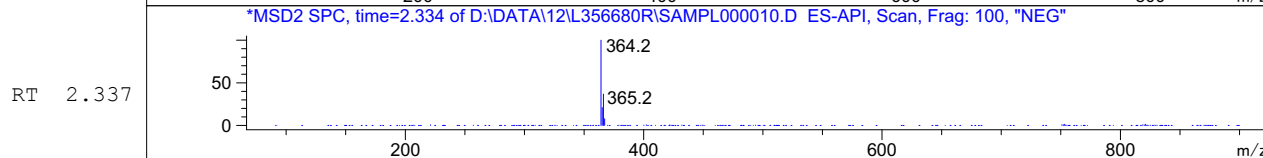
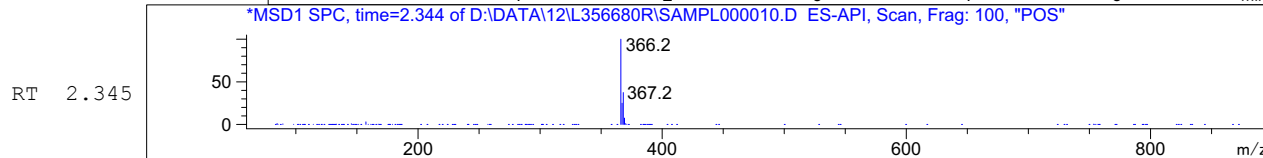
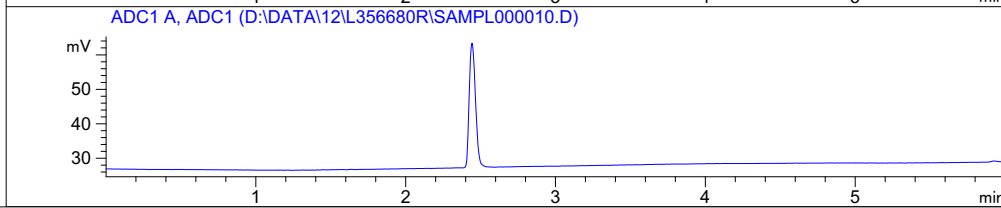
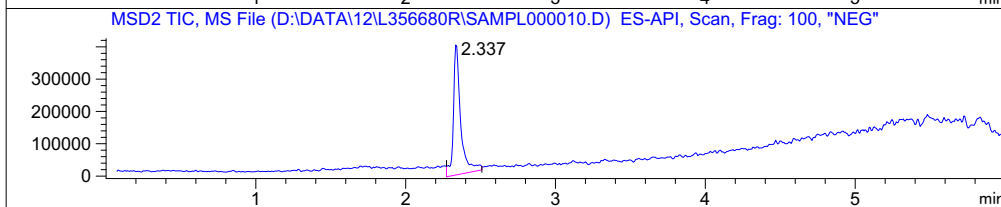
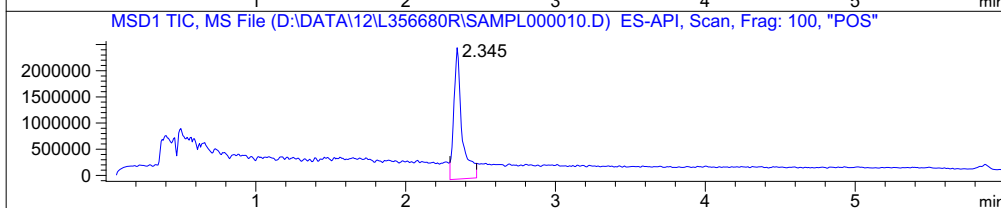
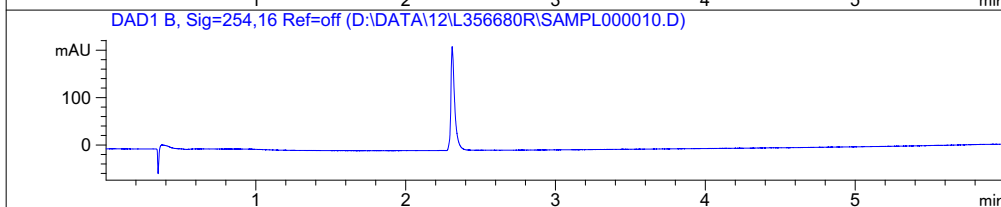
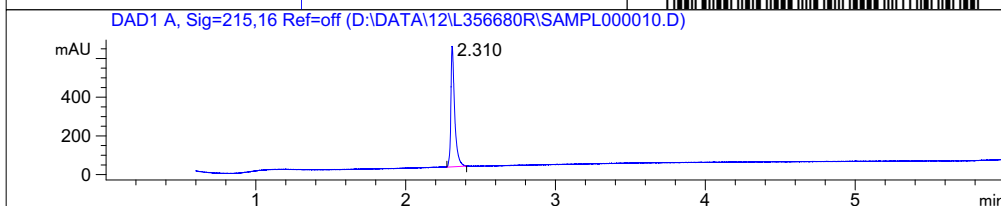


MaxPeak: 100.00%  
Ret\_Time: 2.310 min



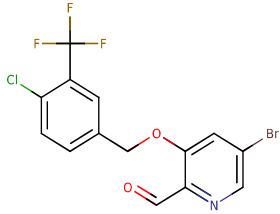
Mol Wt 365.81  
Exact Mass 365.11

#	Time	Area%
1	2.310	100.00



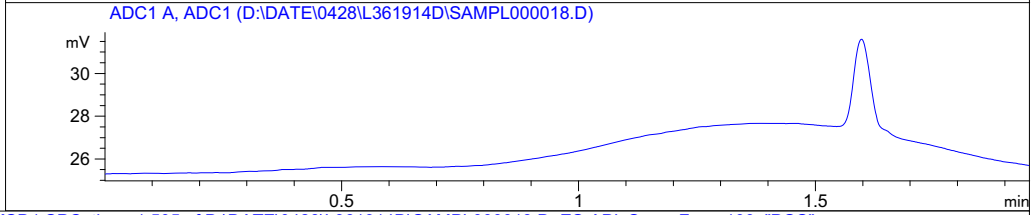
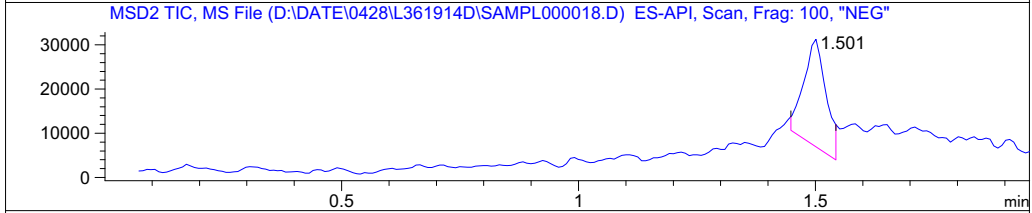
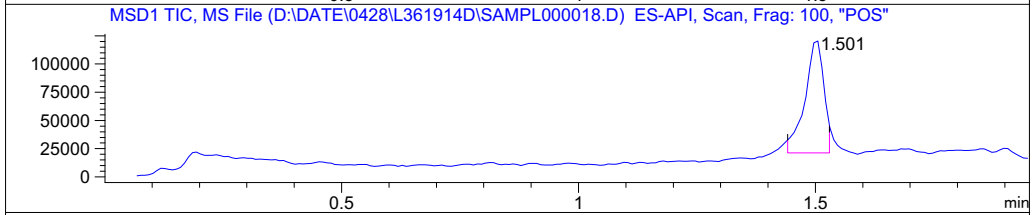
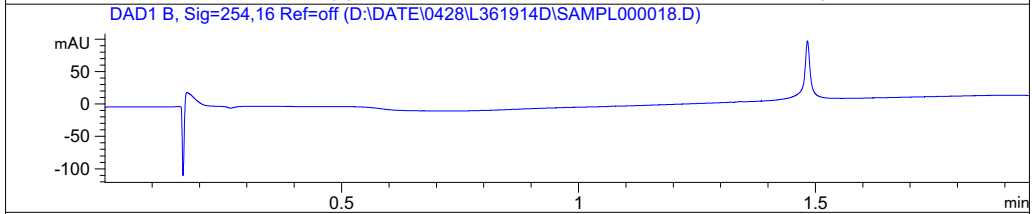
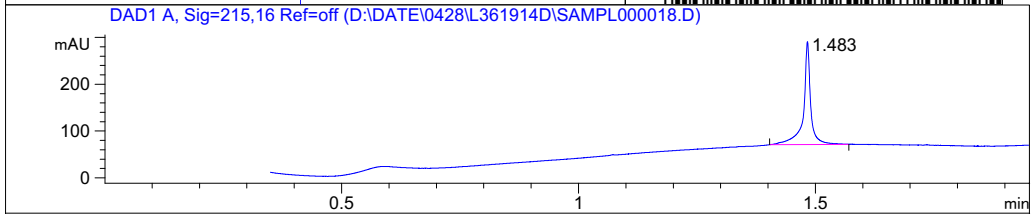
MaxPeak: 100.00%  
Ret\_Time: 1.483 min

U920101\$22

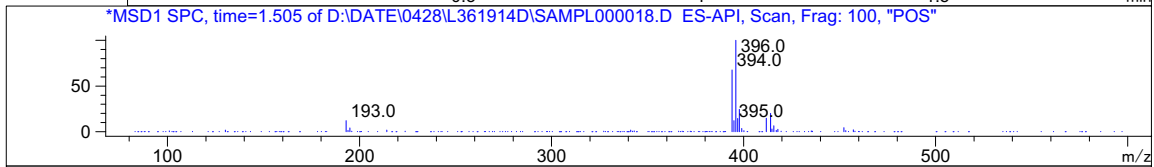


Mol Wt 394.57  
Exact Mass 394.95

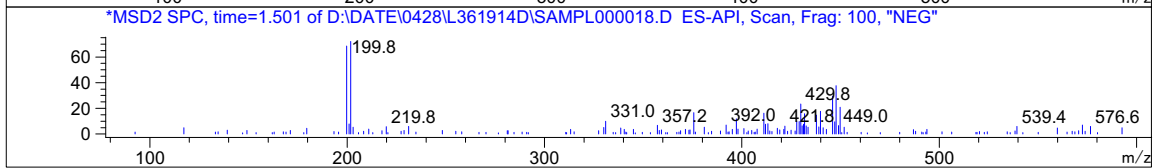
#	Time	Area%
1	1.483	100.00



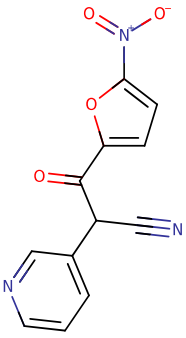
RT 1.501



RT 1.501



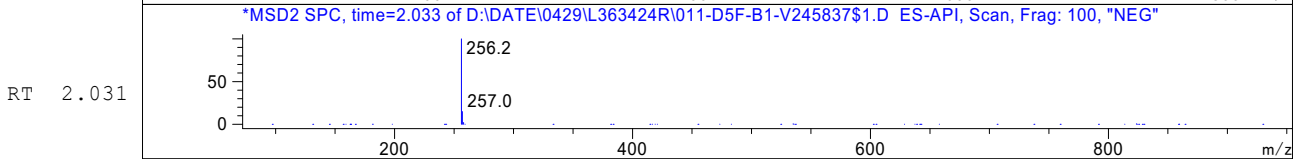
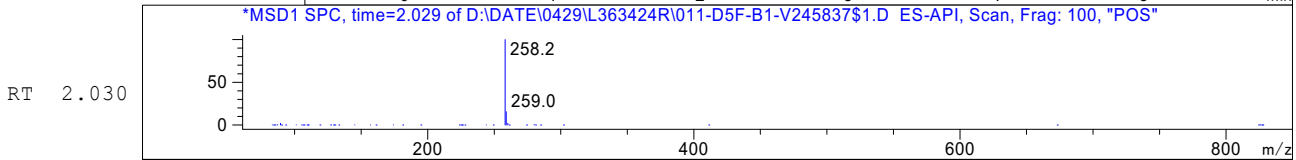
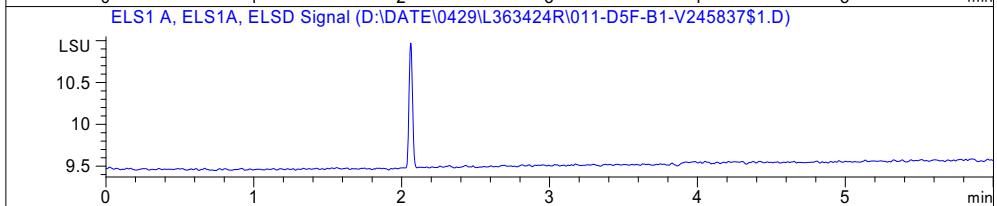
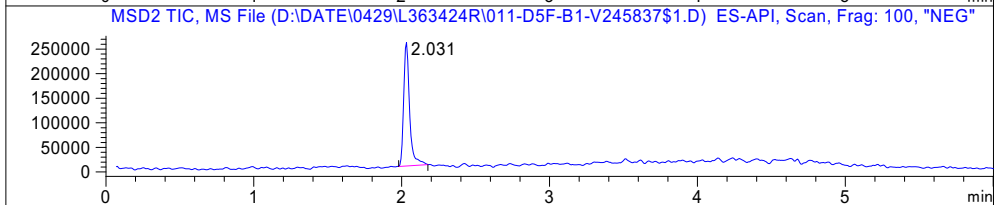
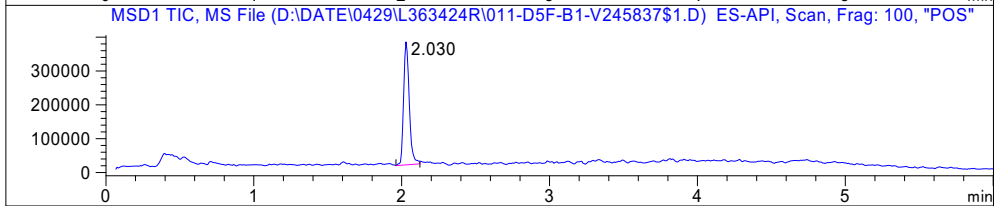
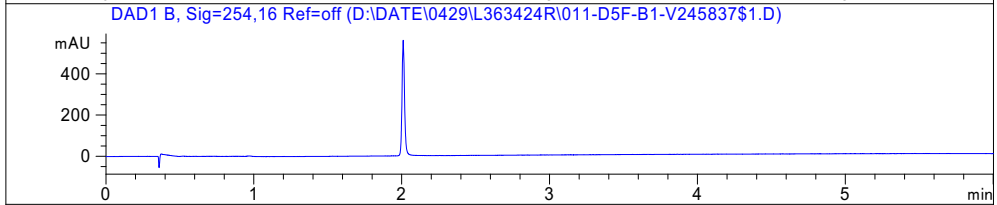
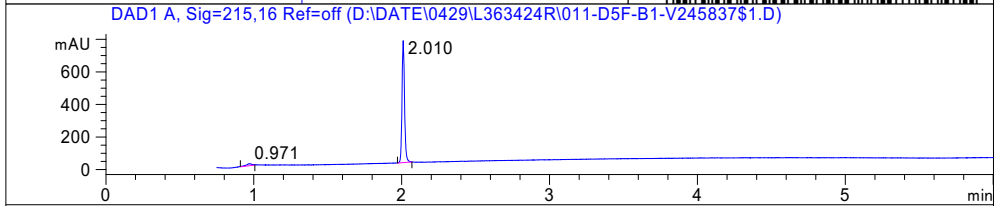
MaxPeak: 96.26%  
Ret\_Time: 2.010 min



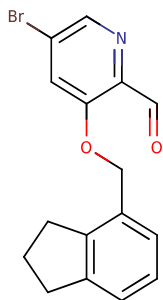
Mol Wt 257.2  
Exact Mass 257.03

#	Time	Area%
1	0.971	3.74
2	2.010	96.26

# V245837\$1

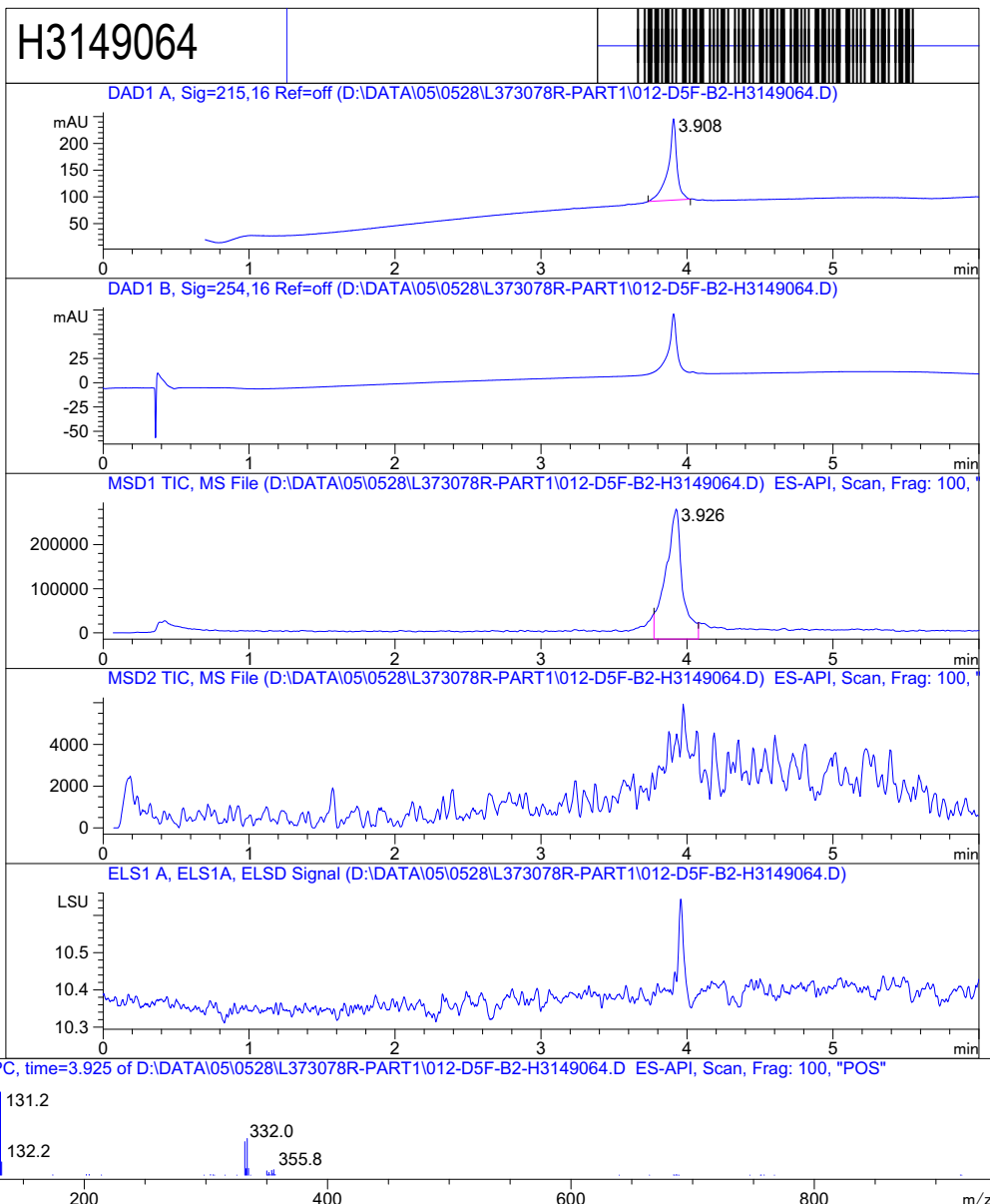


MaxPeak: 100.00%  
Ret\_Time: 3.908 min



Mol Wt 332.19  
Exact Mass 331.04

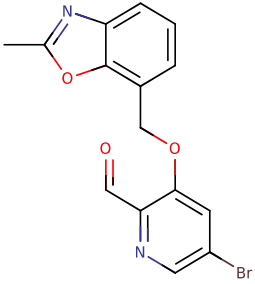
#	Time	Area%
1	3.908	100.00



RT 3.926



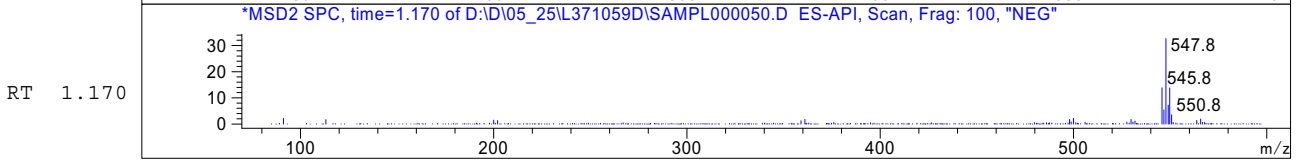
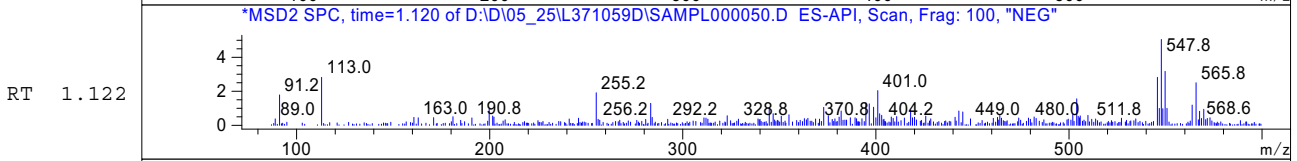
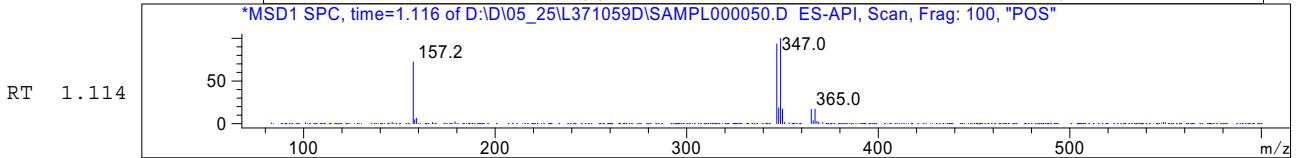
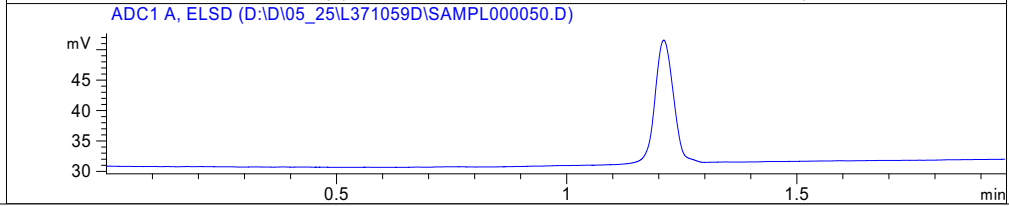
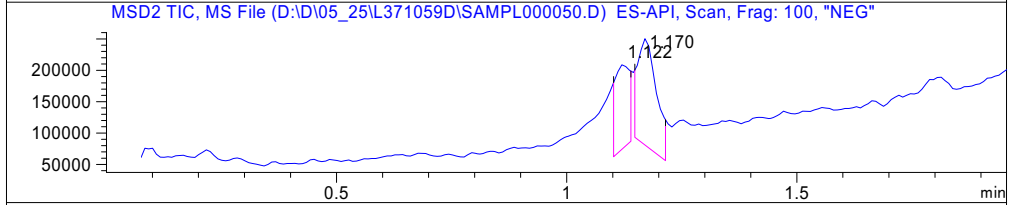
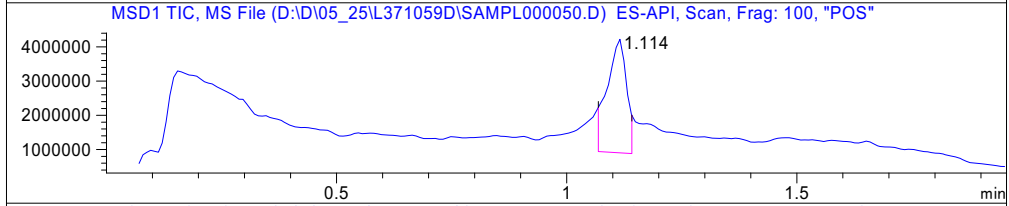
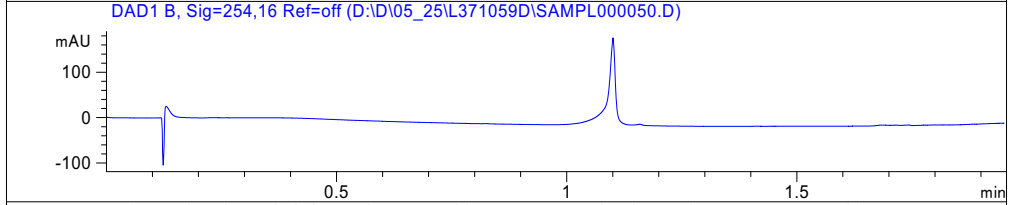
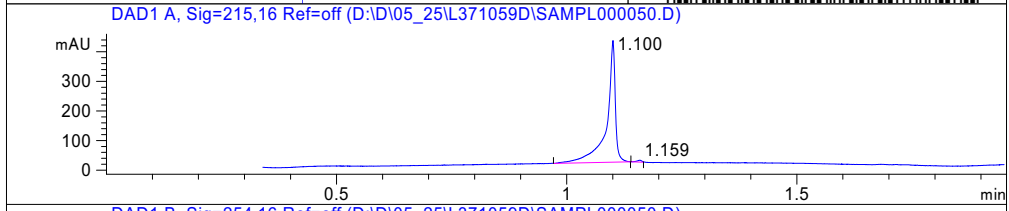
MaxPeak: 99.08%  
Ret\_Time: 1.100 min



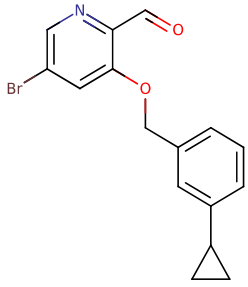
Mol Wt 347.16  
Exact Mass 346

#	Time	Area%
1	1.100	99.08
2	1.159	0.92

V296344\$7



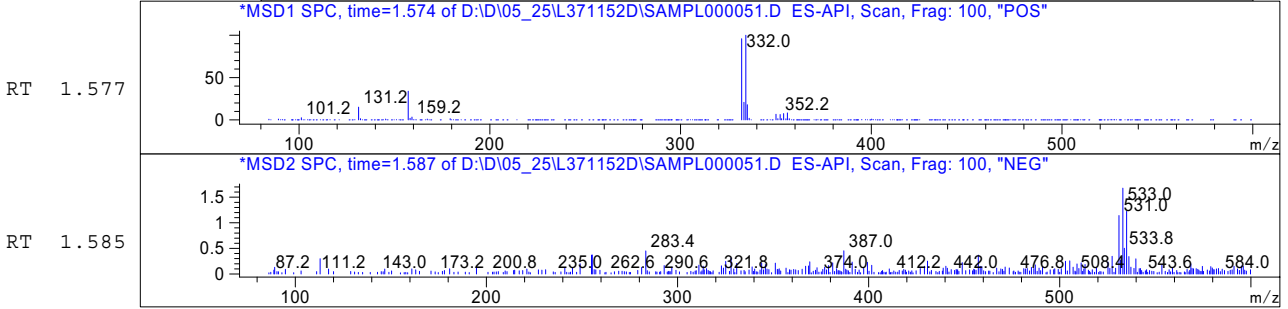
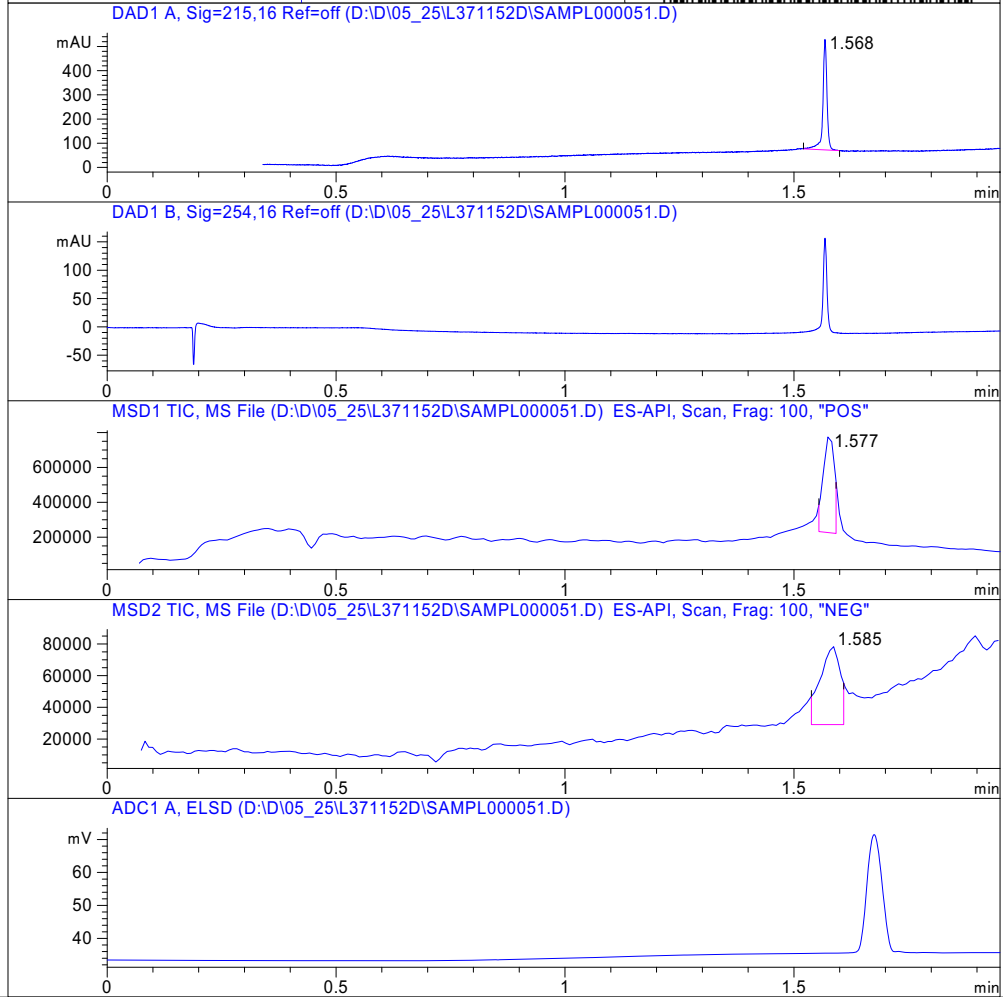
MaxPeak: 100.00%  
Ret\_Time: 1.568 min



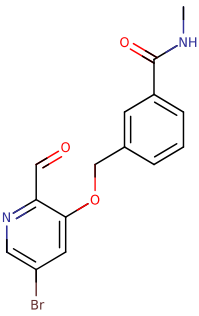
Mol Wt 332.19  
Exact Mass 331.04

#	Time	Area%
1	1.568	100.00

V211811\$A

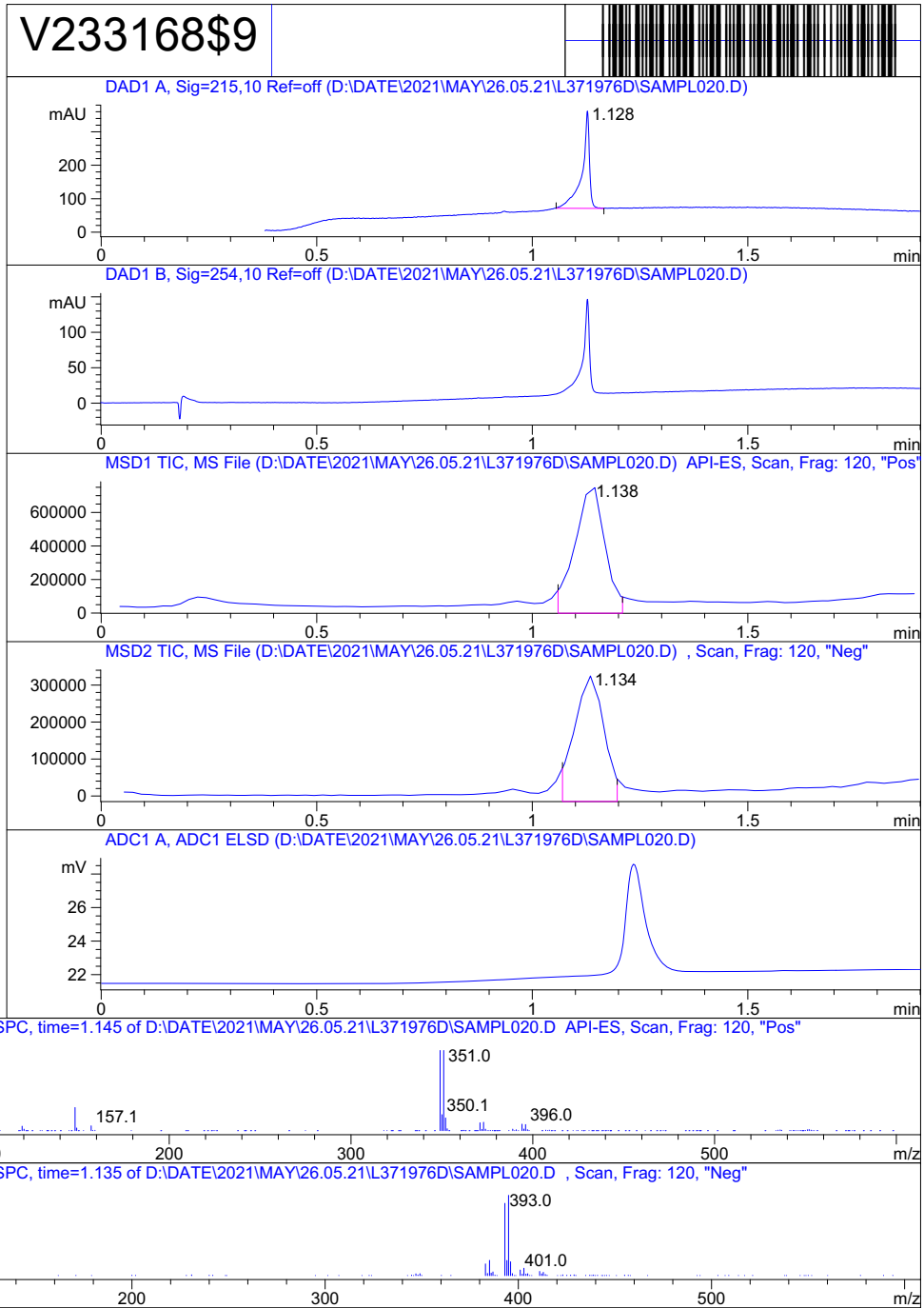


MaxPeak: 100.00%  
Ret\_Time: 1.128 min



Mol Wt 349.18  
Exact Mass 348.02

#	Time	Area%
1	1.128	100.00



Inj.Date 5/26/2021

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P2-C-03

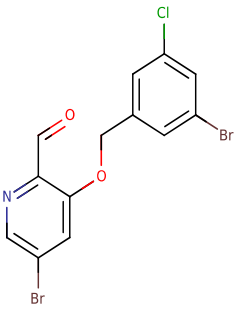
-SL-

Acq. Method C:\HPCHEM\ ->

->

Z5009000157\_

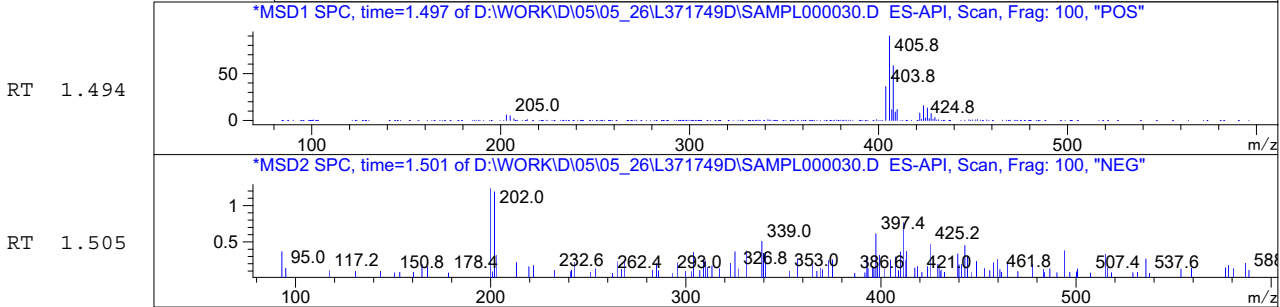
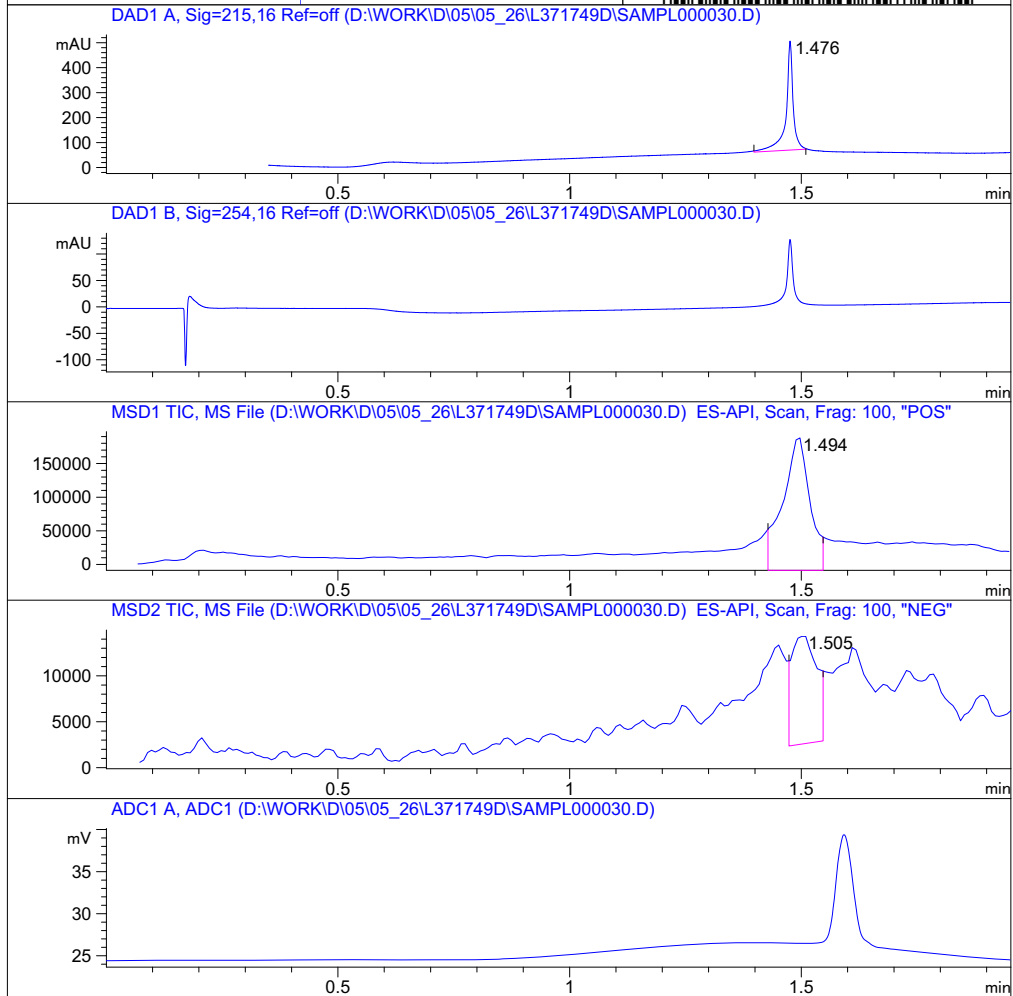
MaxPeak: 100.00%  
Ret\_Time: 1.476 min



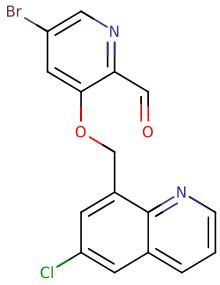
Mol Wt 405.47  
Exact Mass 404.87

#	Time	Area%
1	1.476	100.00

V233167\$2



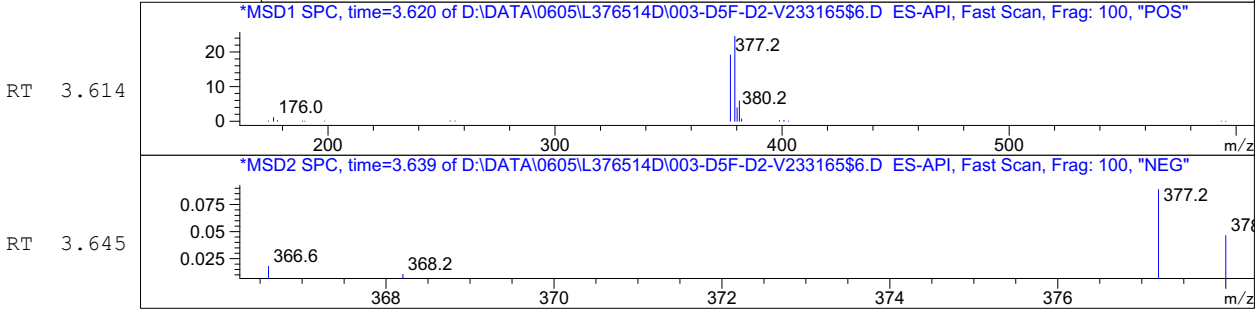
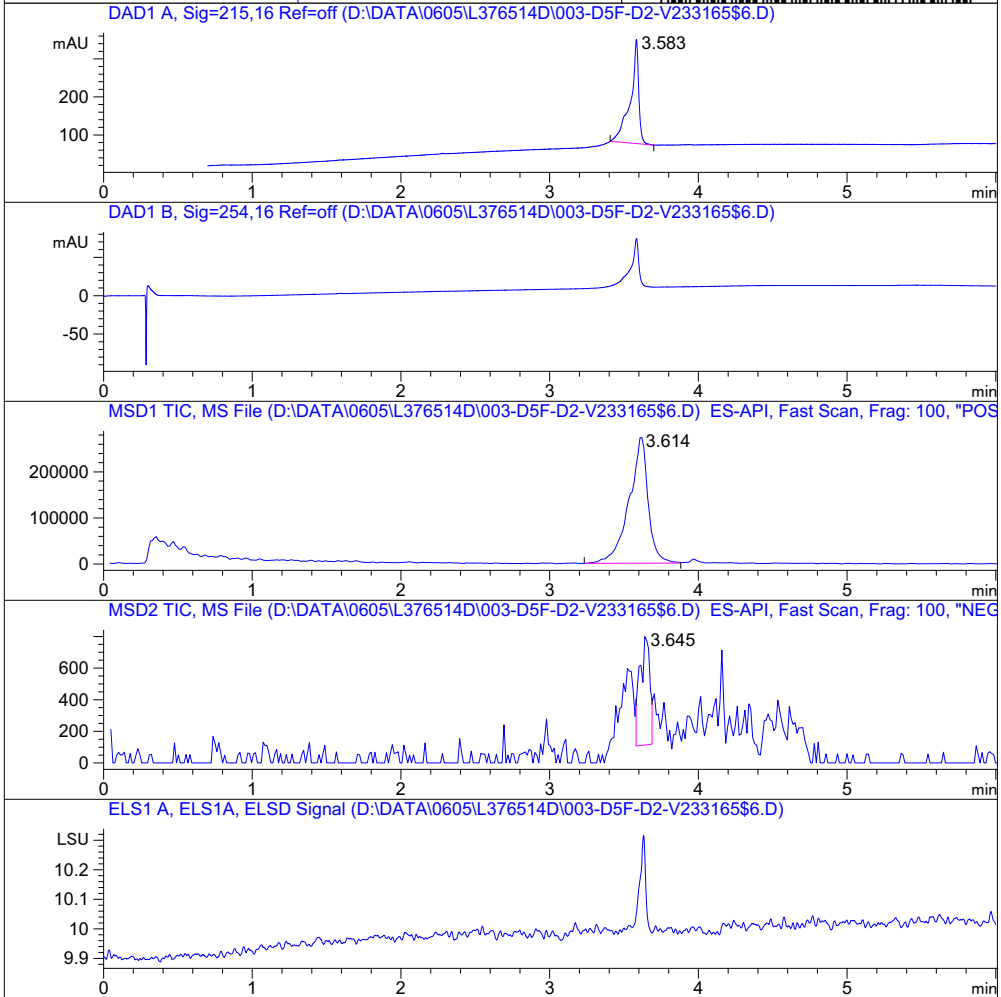
MaxPeak: 100.00%  
Ret\_Time: 3.583 min



Mol Wt 377.62  
Exact Mass 377.97

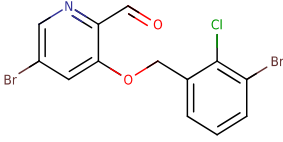
#	Time	Area%
1	3.583	100.00

V233165\$6



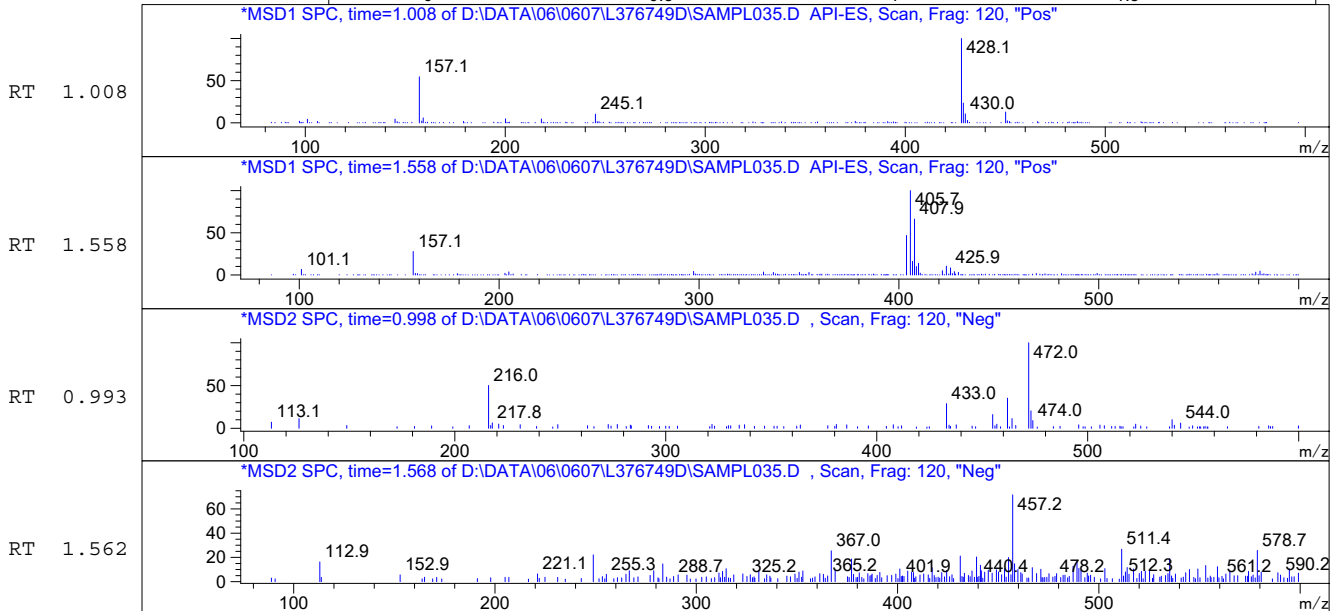
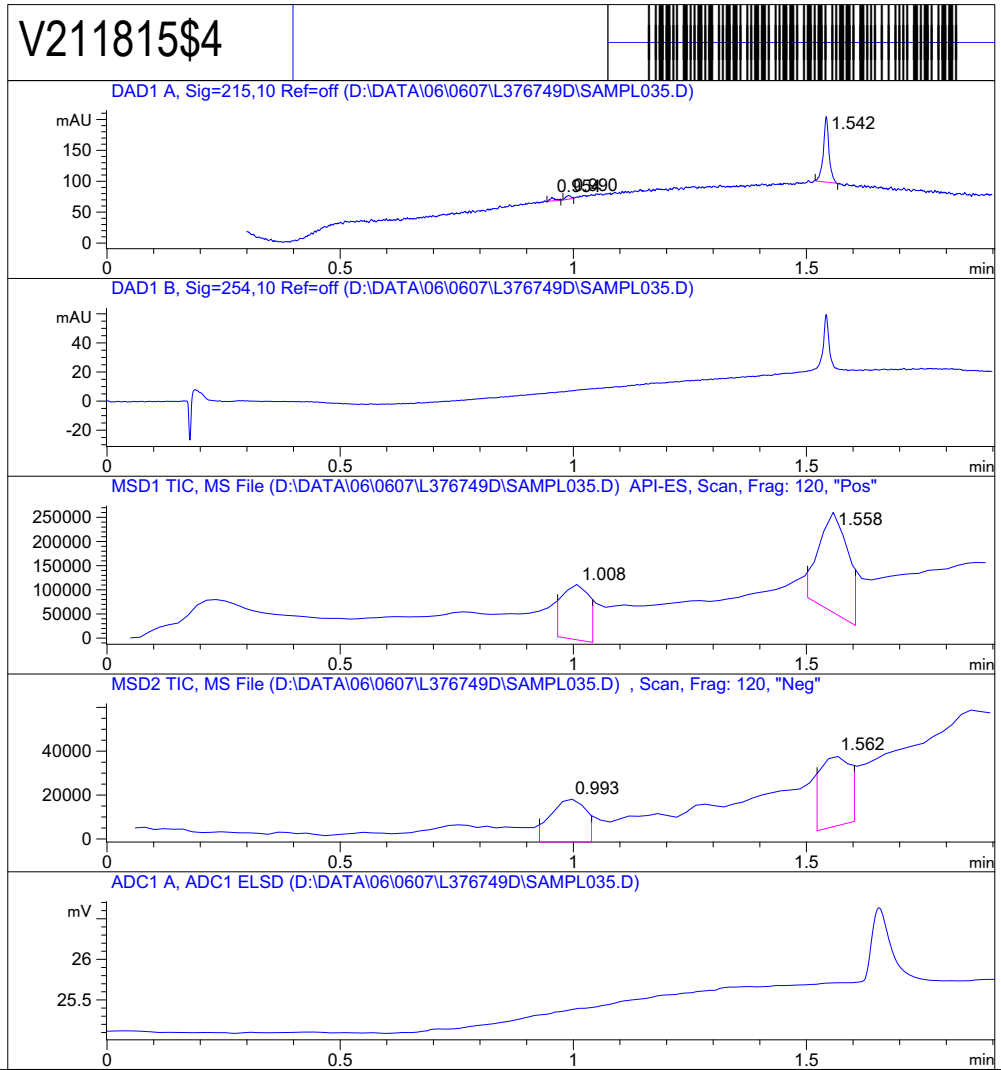
MaxPeak: 90.89%  
Ret\_Time: 1.542 min

V211815\$4



Mol Wt 405.47  
Exact Mass 404.87

#	Time	Area%
1	0.954	4.30
2	0.990	4.81
3	1.542	90.89



Inj.Date 6/6/2021

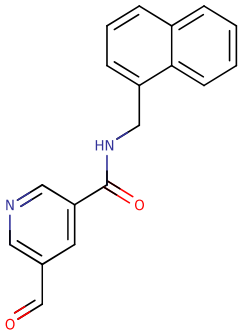
LT

-VL-

Acq. Method C:\HPCHEM\ -> ->

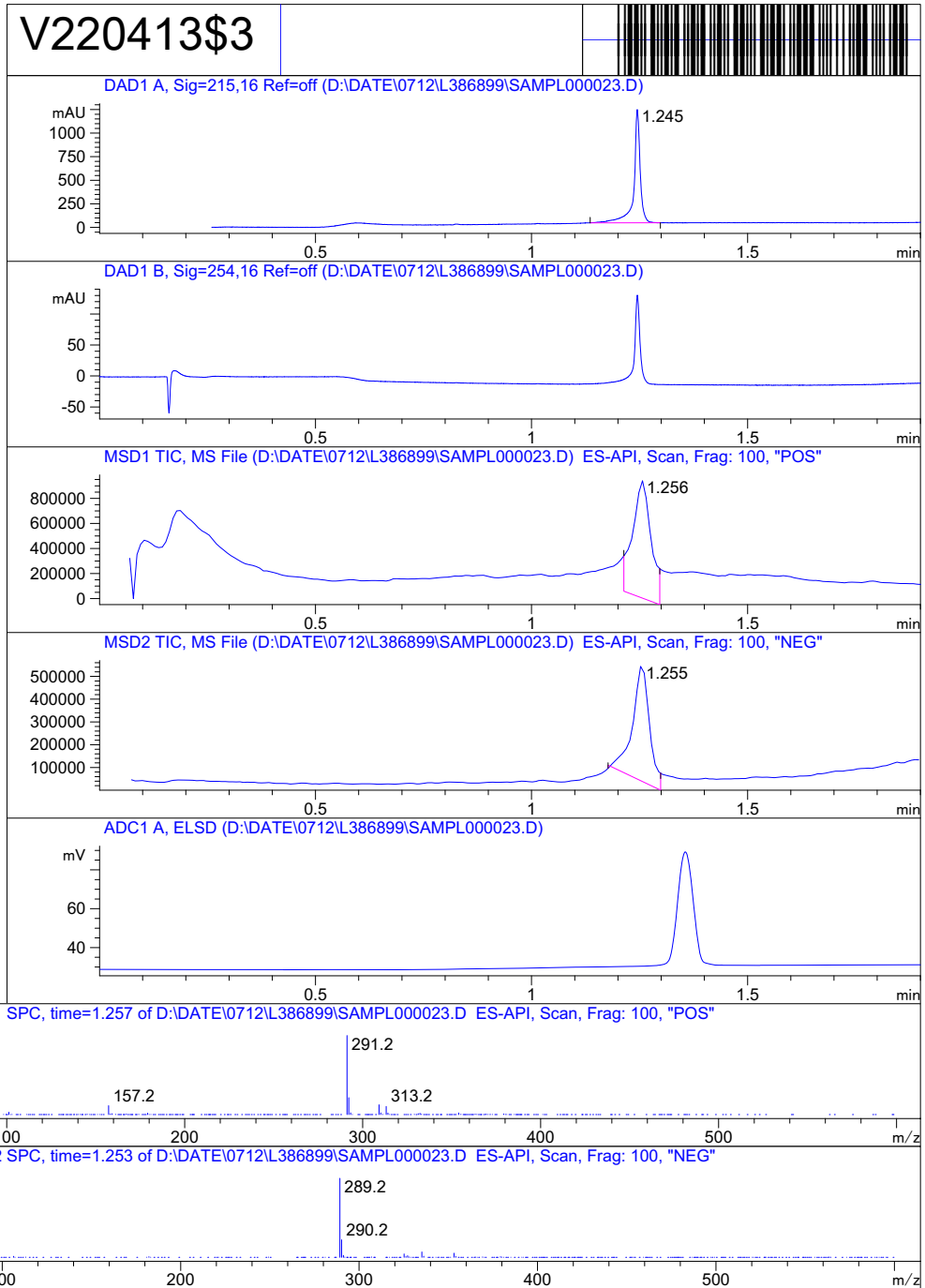
Z4989203260\_

MaxPeak: 100.00%  
Ret\_Time: 1.245 min



Mol Wt 290.32  
Exact Mass 290.12

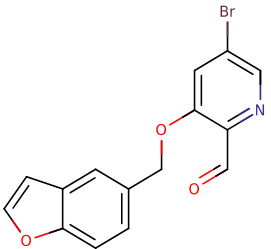
#	Time	Area%
1	1.245	100.00



V816207\$5

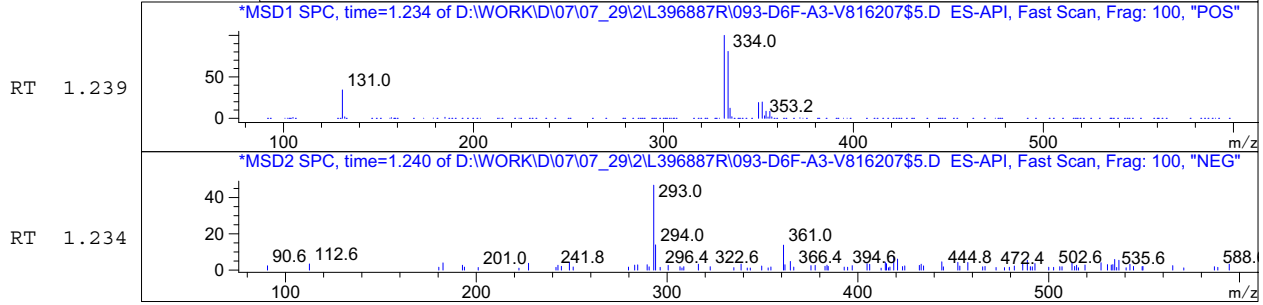
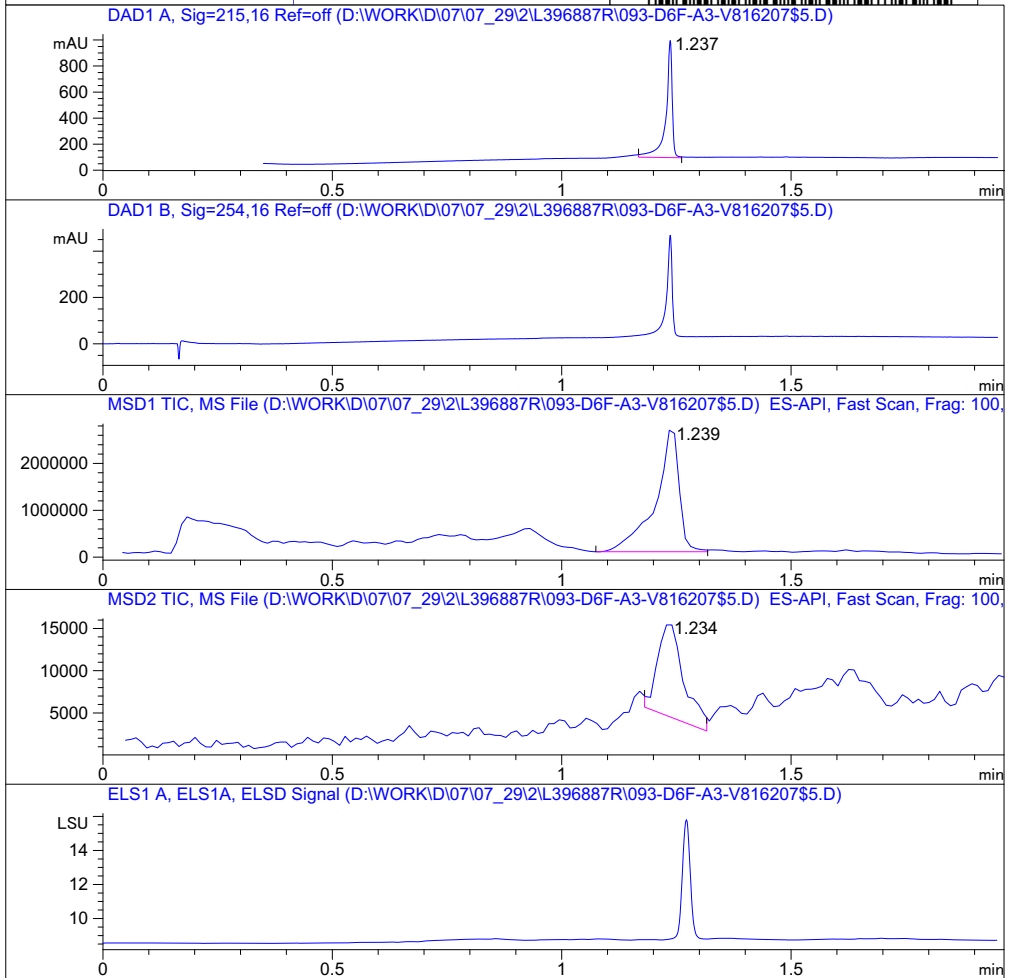


MaxPeak: 100.00%  
Ret\_Time: 1.237 min



Mol Wt 332.15  
Exact Mass 330.99

#	Time	Area%
1	1.237	100.00



Inj.Date 7/29/2021

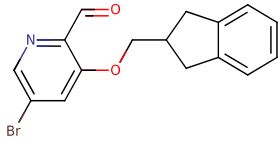
K <invalid>

Acq. Method C:\Users\ -> ->

Z5084954212\_



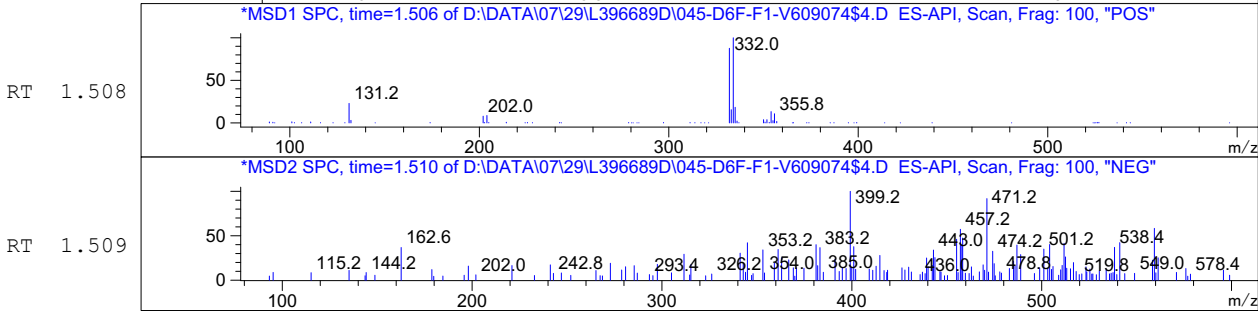
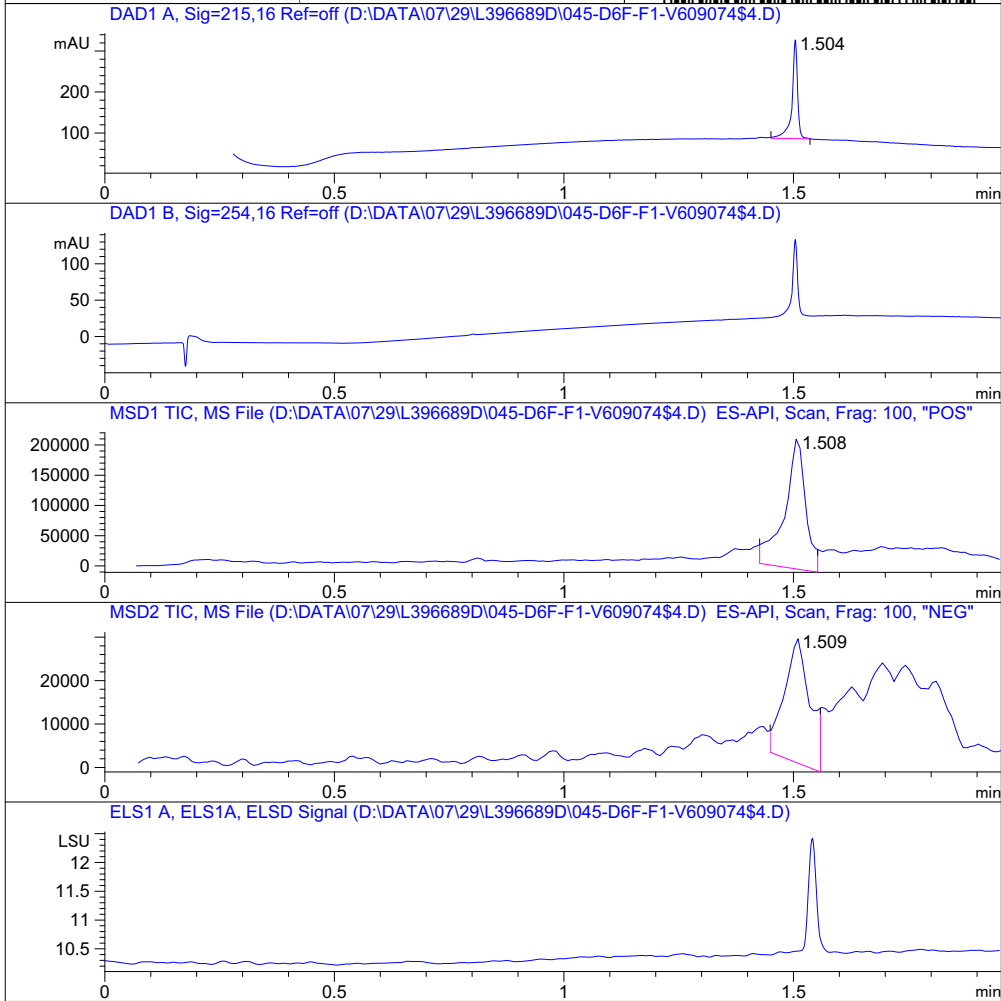
MaxPeak: 100.00%  
Ret\_Time: 1.504 min



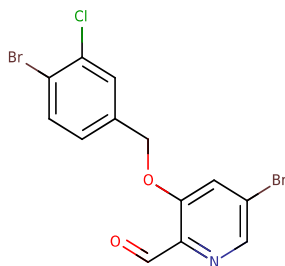
Mol Wt 332.19  
Exact Mass 331.04

#	Time	Area%
1	1.504	100.00

V609074\$4



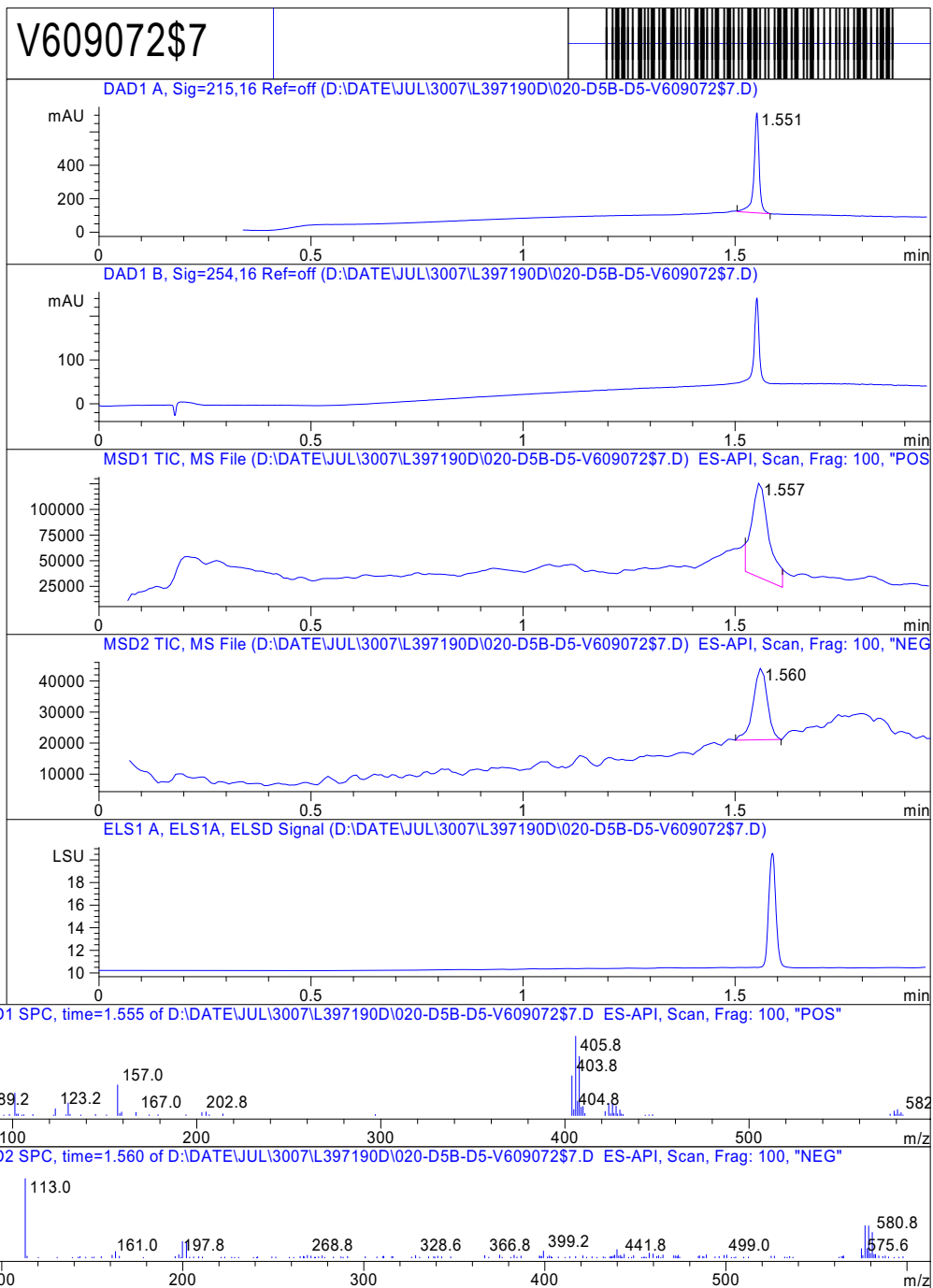
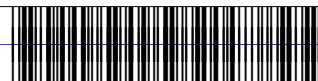
MaxPeak: 100.00%  
Ret\_Time: 1.551 min



Mol Wt 405.47  
Exact Mass 404.87

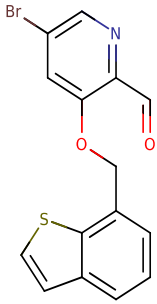
#	Time	Area%
1	1.551	100.00

V609072\$7



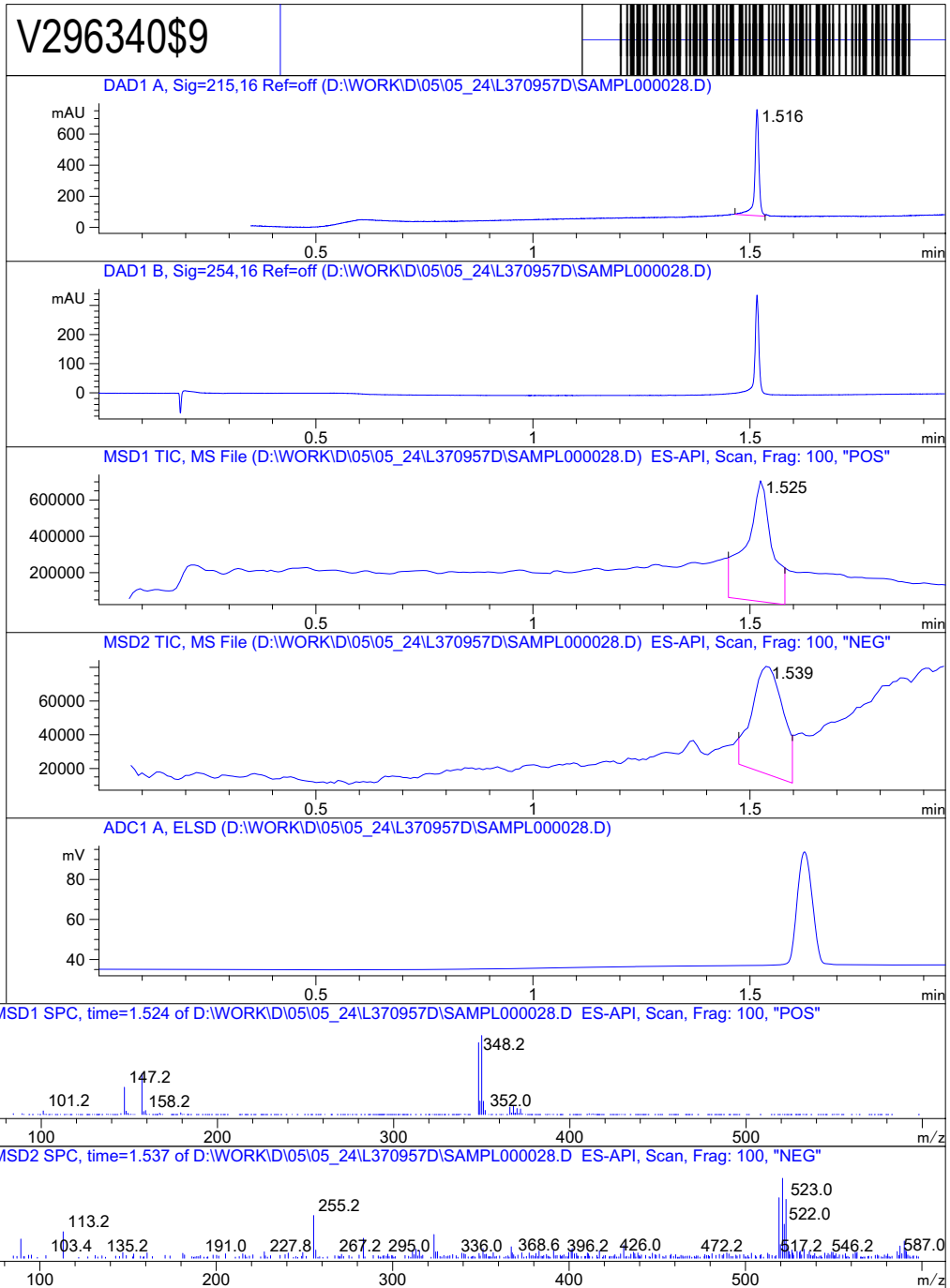
MaxPeak: 100.00%  
Ret\_Time: 1.516 min

V296340\$9



Mol Wt 348.21  
Exact Mass 348.97

#	Time	Area%
1	1.516	100.00



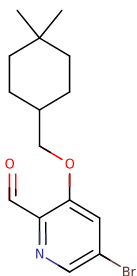
RT 1.525

RT 1.539

# W179753\$3



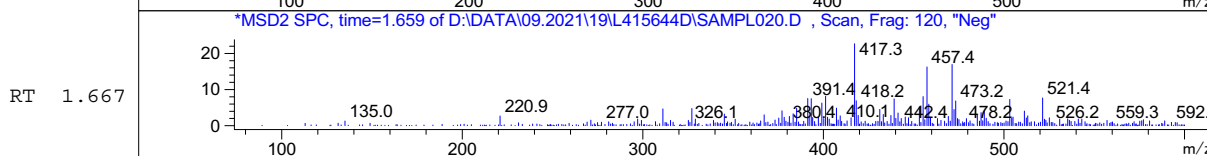
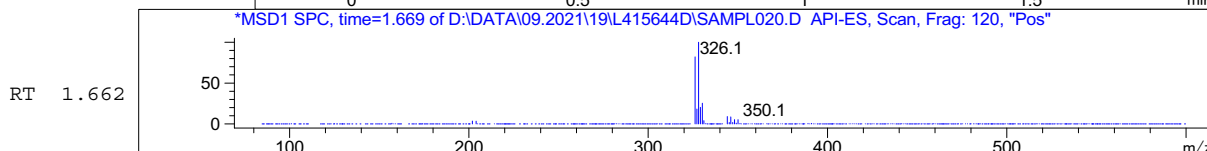
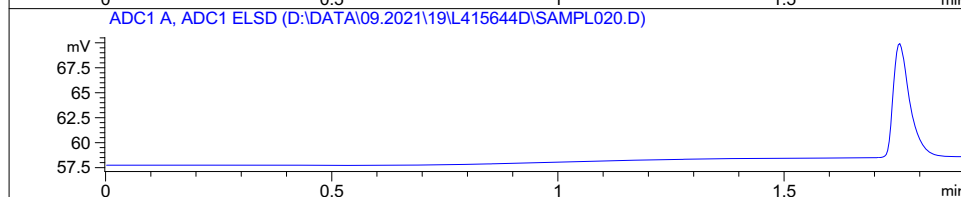
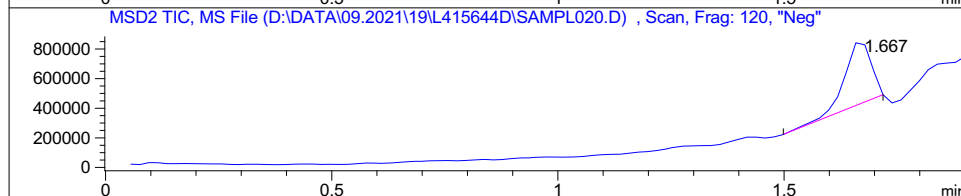
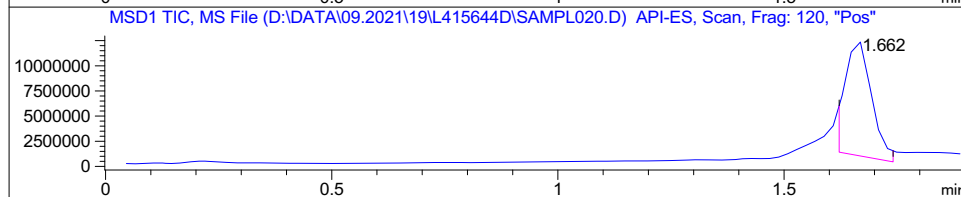
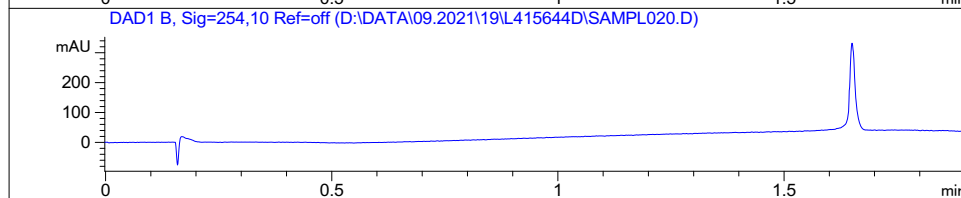
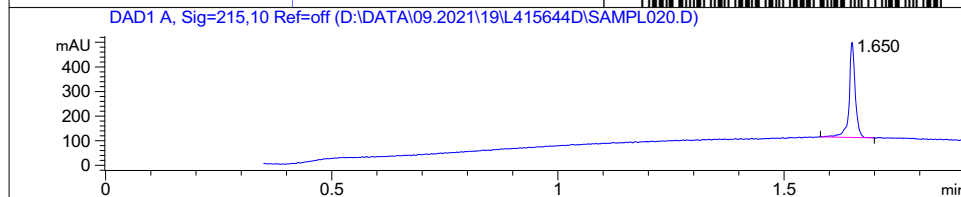
MaxPeak: 100.00%  
Ret\_Time: 1.650 min



Mol Wt 326.23

Exact Mass 325.1

#	Time	Area%
1	1.650	100.00



Inj.Date 9/19/2021

CH

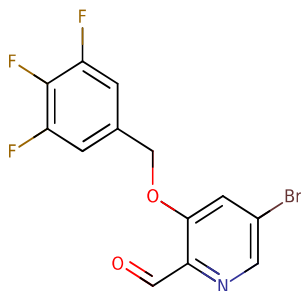
P2-C-03

-SL-

Acq. Method C:\HPCHEM\ -> ->

Z5192779009\_

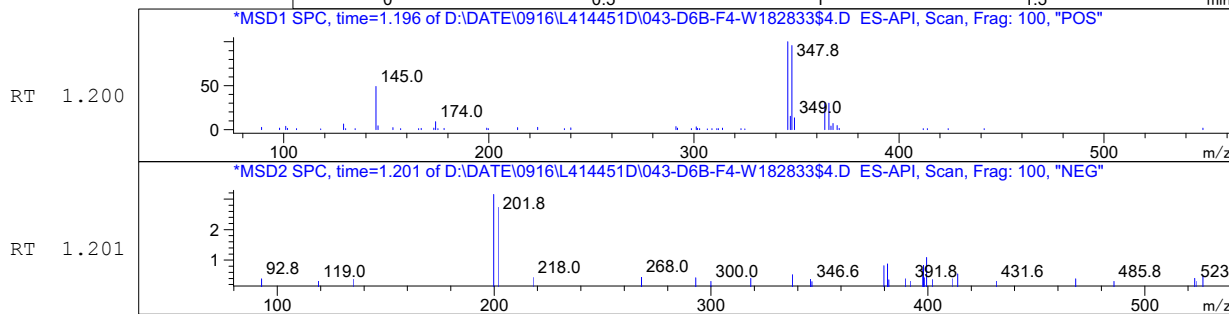
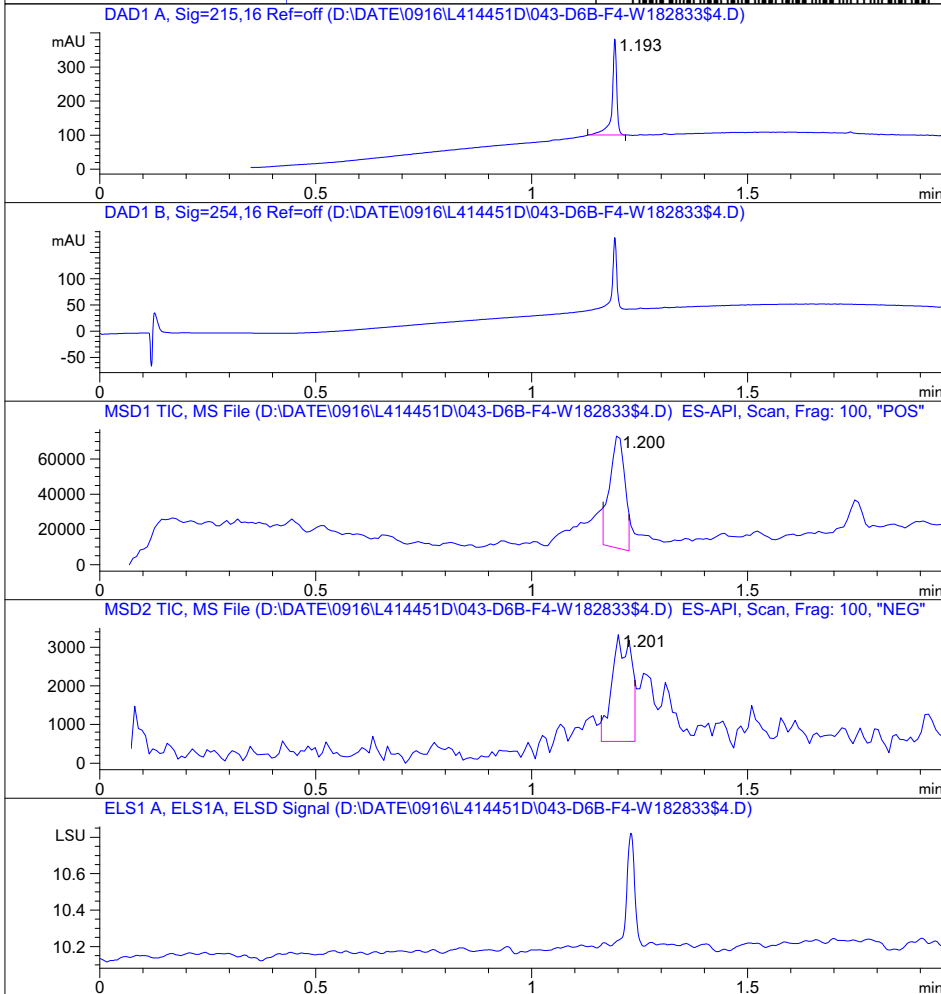
MaxPeak: 100.00%  
Ret\_Time: 1.193 min



Mol Wt 346.1  
Exact Mass 344.97

#	Time	Area%
1	1.193	100.00

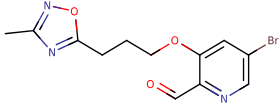
# W182833\$4



# W557252\$2

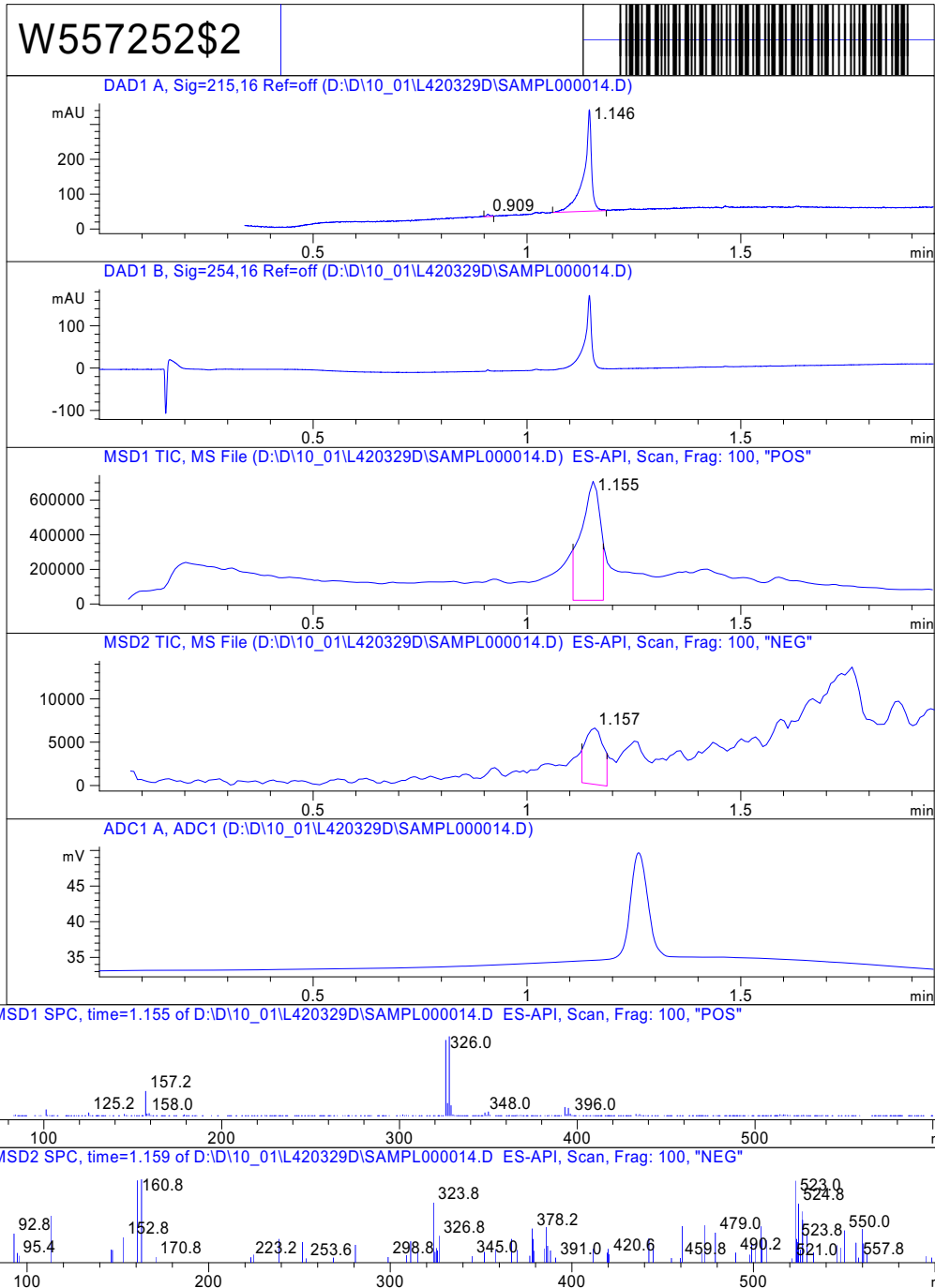


MaxPeak: 98.96%  
Ret\_Time: 1.146 min



Mol Wt 326.15  
Exact Mass 325.01

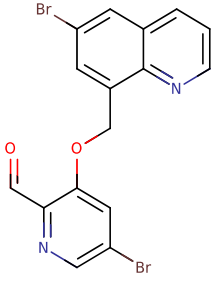
#	Time	Area%
1	0.909	1.04
2	1.146	98.96



RT 1.155

RT 1.157

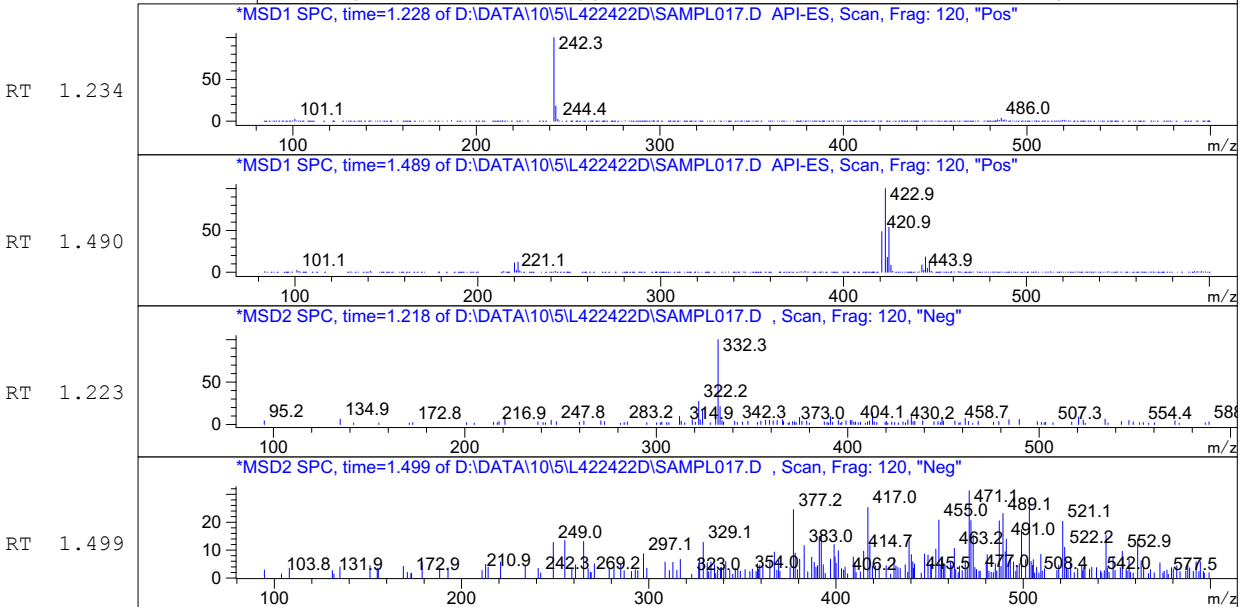
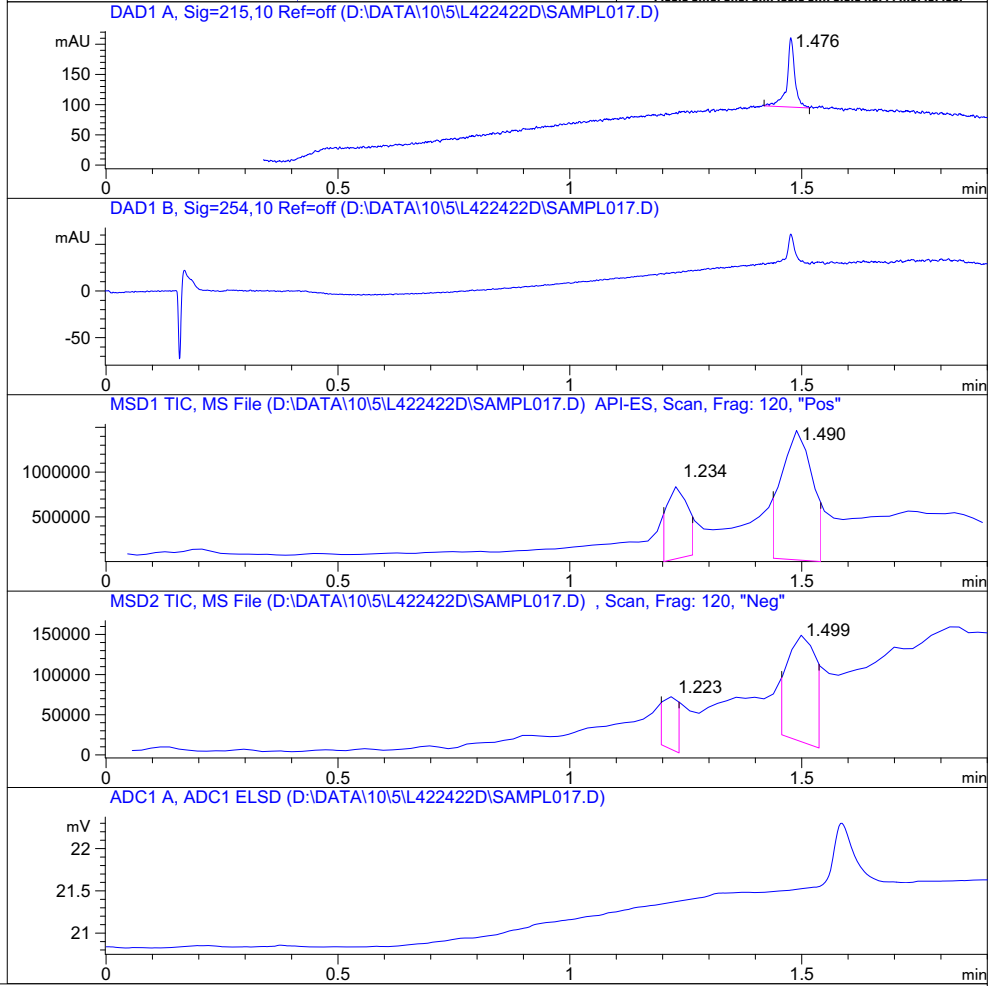
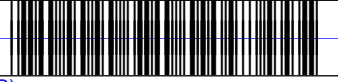
MaxPeak: 100.00%  
Ret\_Time: 1.476 min



Mol Wt 422.07  
Exact Mass 421.92

#	Time	Area%
1	1.476	100.00

W557642\$B



Inj.Date 10/6/2021

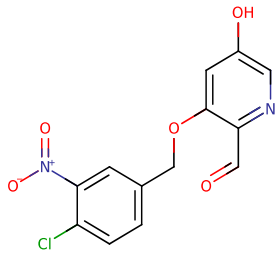
LB

-SL-

Acq. Method C:\HPCHEM\--> -->

Z5192779150\_

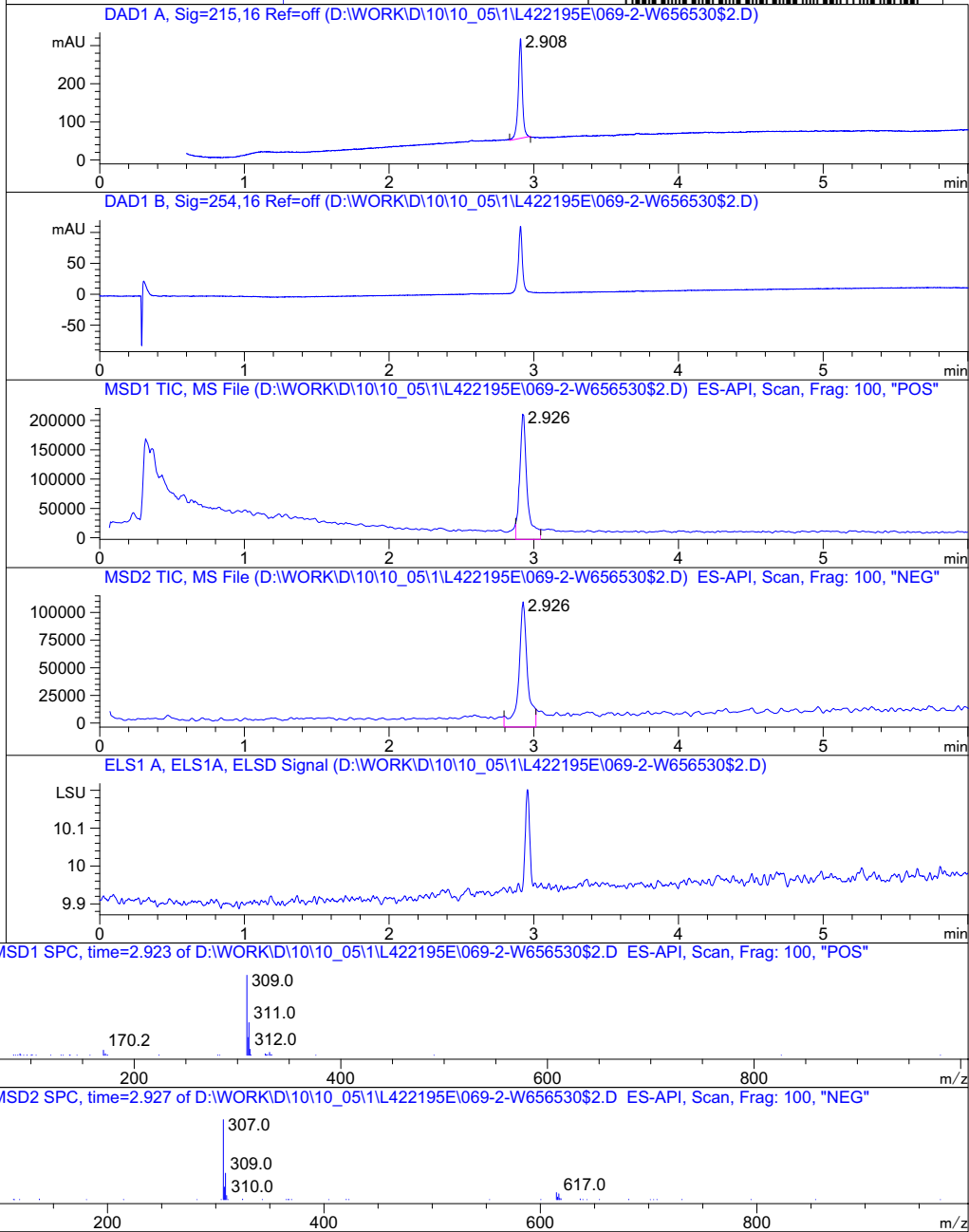
MaxPeak: 100.00%  
Ret\_Time: 2.908 min



Mol Wt 308.67  
Exact Mass 308.01

#	Time	Area%
1	2.908	100.00

W656530\$2

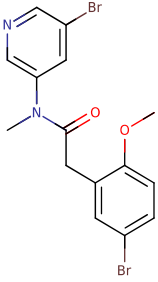




# W847046\$2

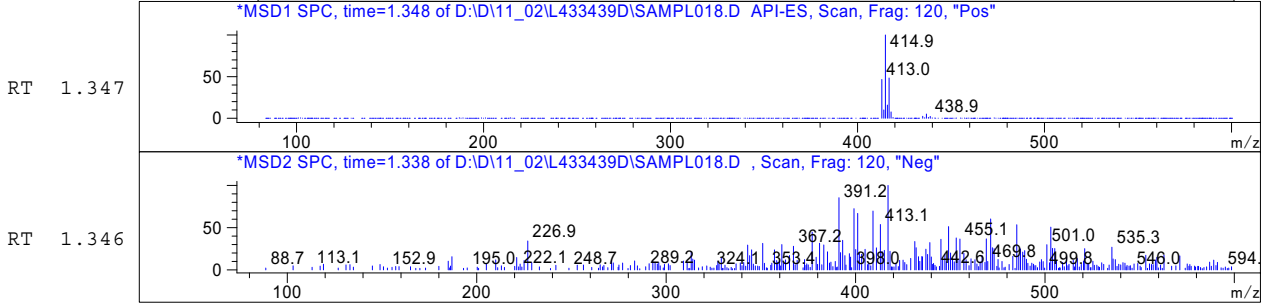
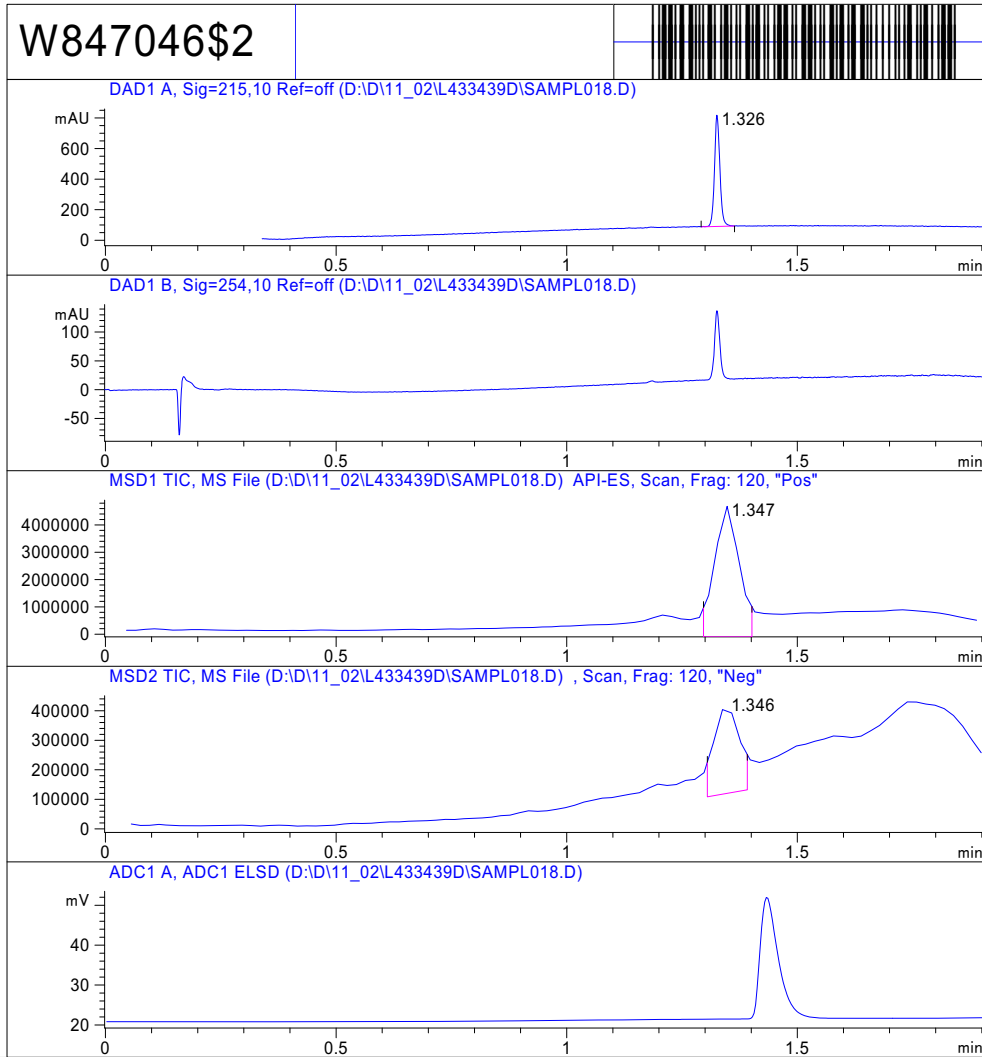


MaxPeak: 100.00%  
Ret\_Time: 1.326 min



Mol Wt 414.09  
Exact Mass 413.96

#	Time	Area%
1	1.326	100.00



Inj.Date 11/2/2021

N

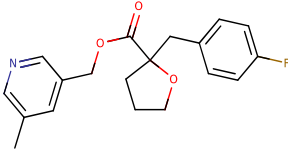
-SL-

Acq. Method C:\HPCHEM\ -> ->

Z5385490967\_

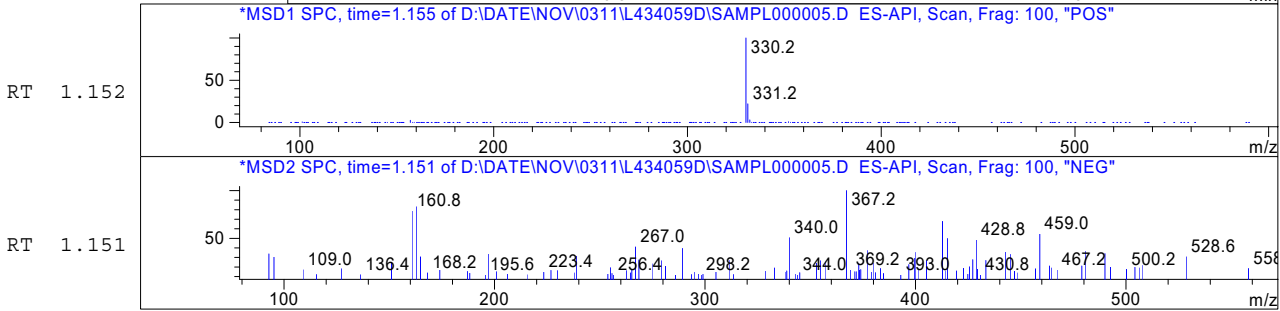
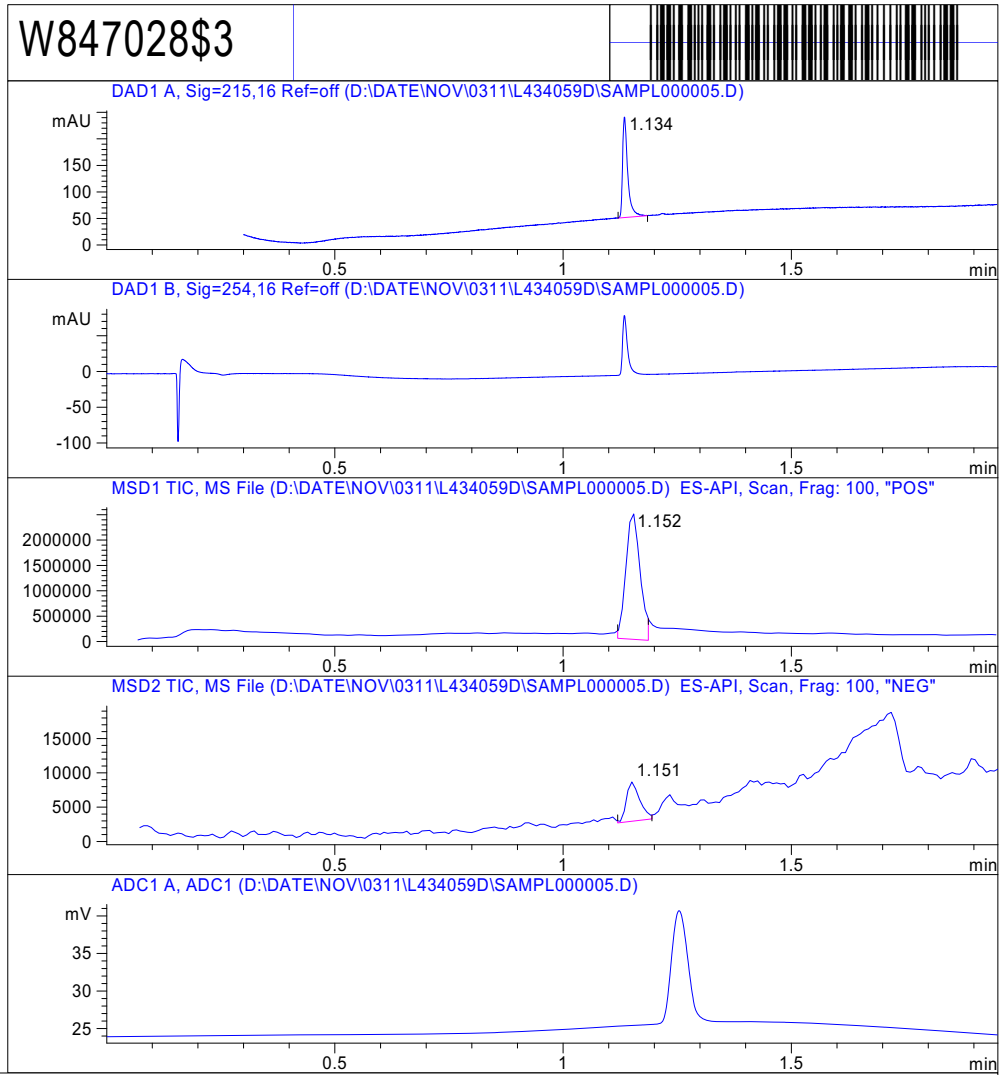
MaxPeak: 100.00%  
Ret\_Time: 1.134 min

W847028\$3

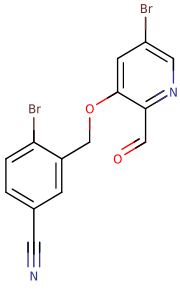


Mol Wt 329.36  
Exact Mass 329.17

#	Time	Area%
1	1.134	100.00



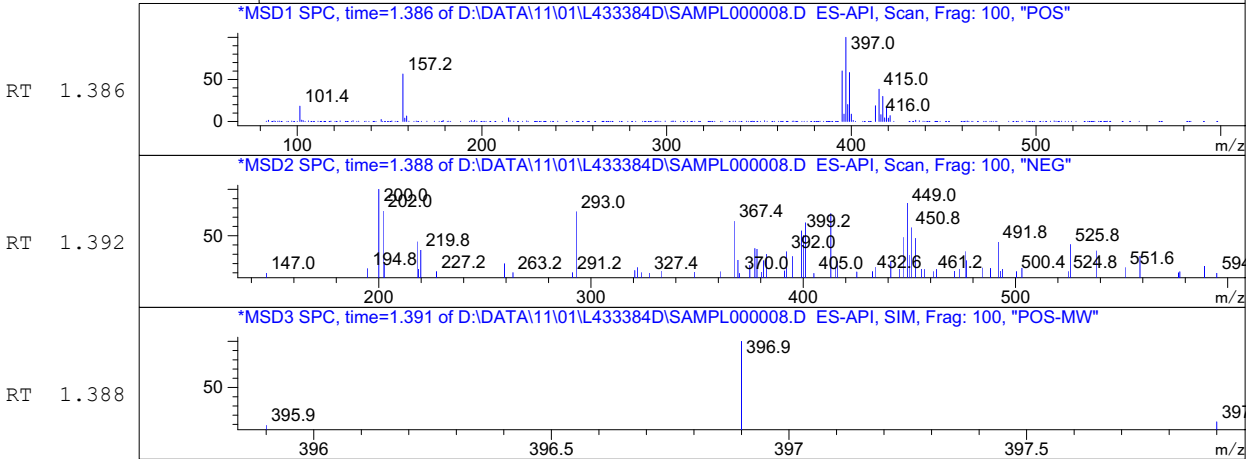
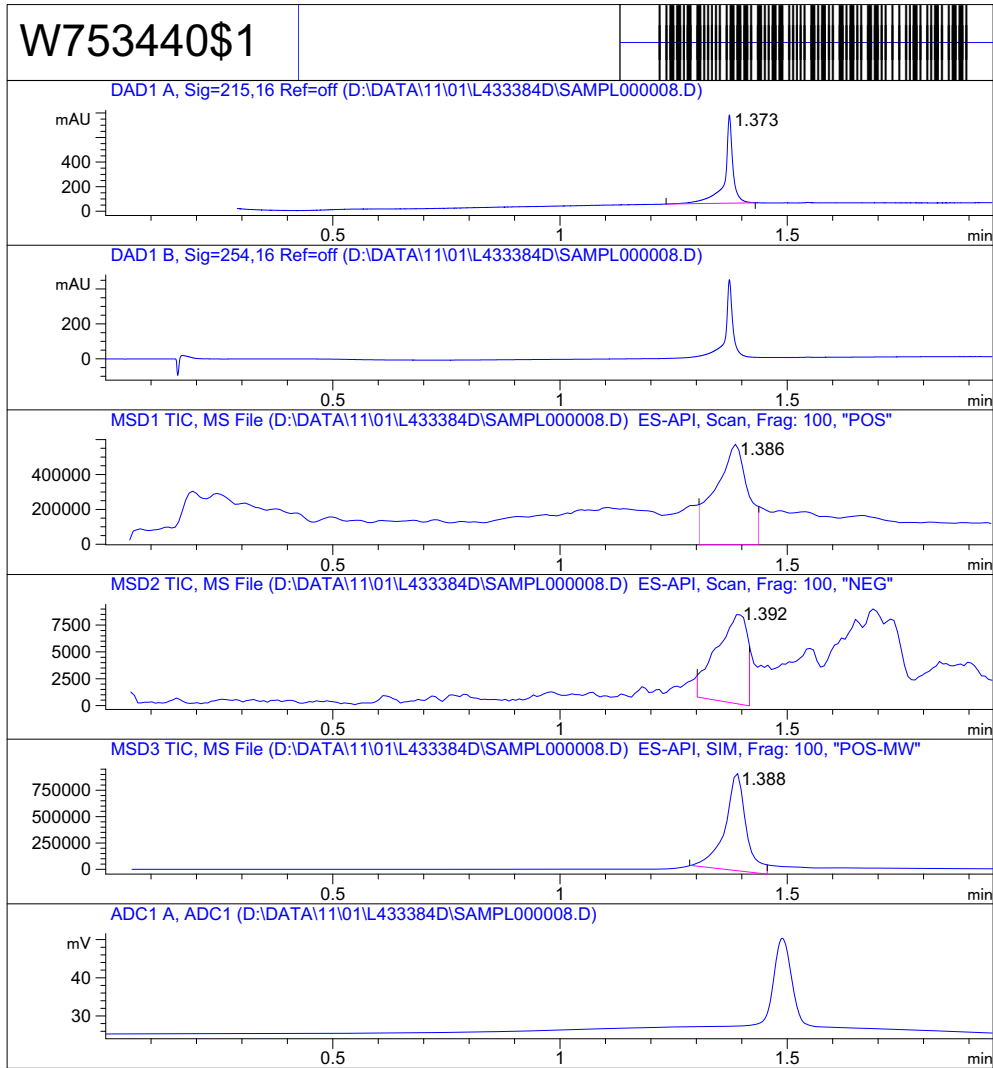
MaxPeak: 100.00%  
Ret\_Time: 1.373 min



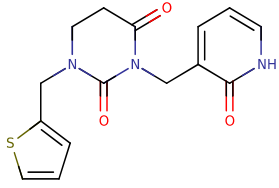
**Mol Wt** 396.03  
**Exact Mass** 395.9

#	Time	Area%
1	1.373	100.00

W753440\$1



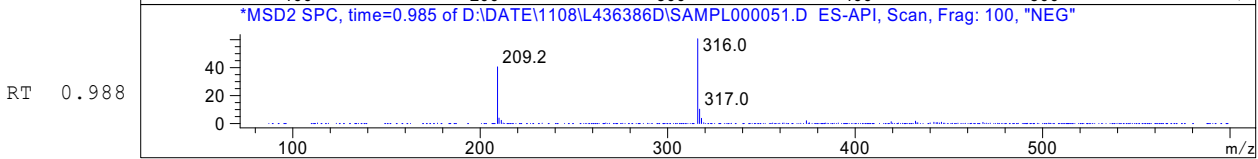
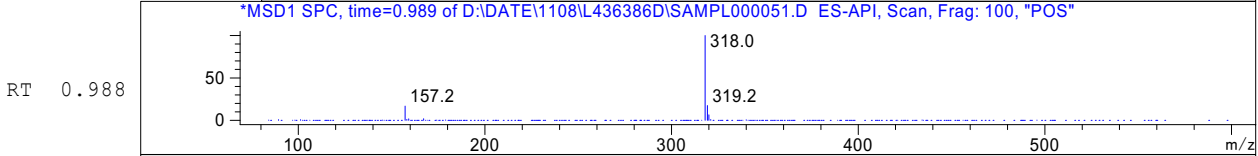
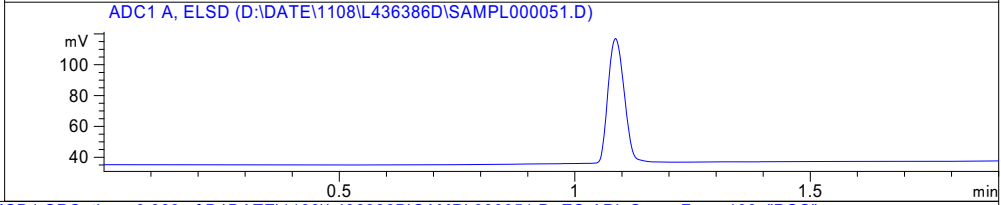
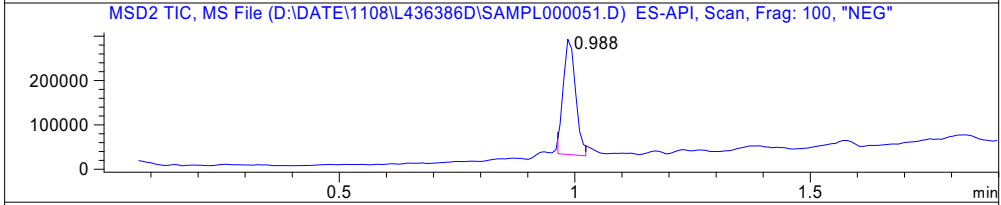
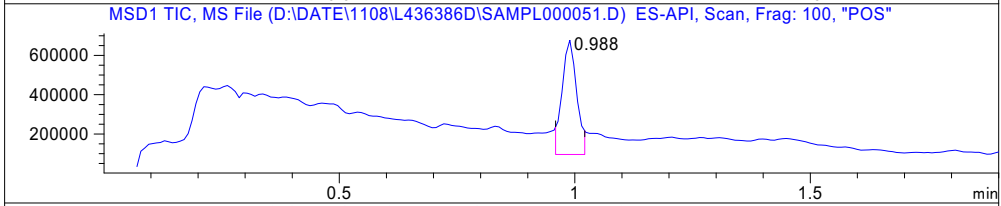
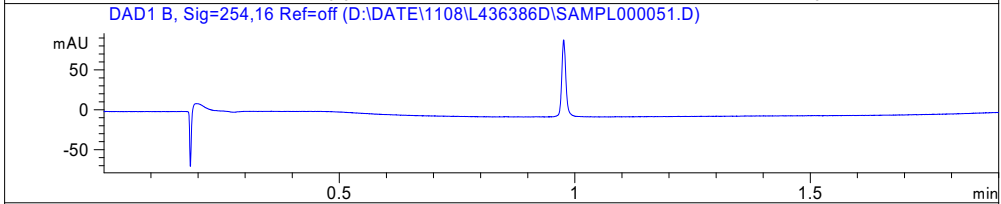
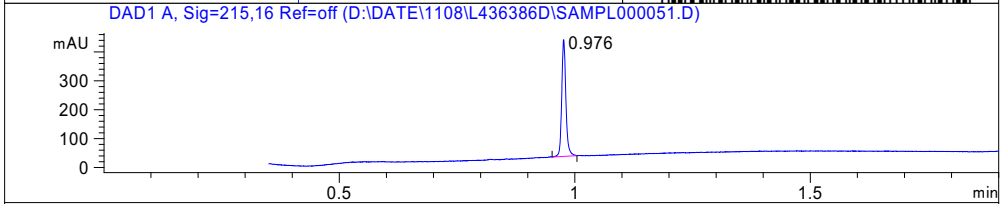
MaxPeak: 100.00%  
Ret\_Time: 0.976 min



Mol Wt 317.36  
Exact Mass 317.09

#	Time	Area%
1	0.976	100.00

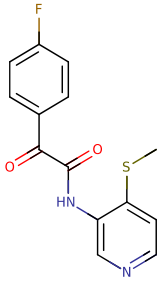
W847029\$1



W980739\$2

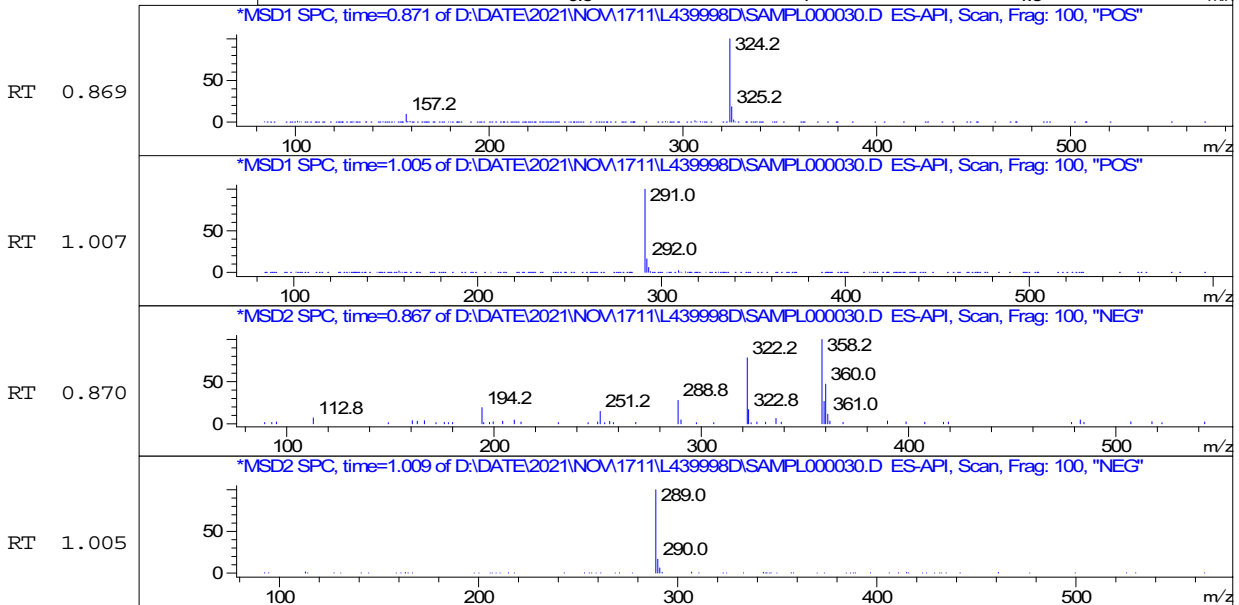
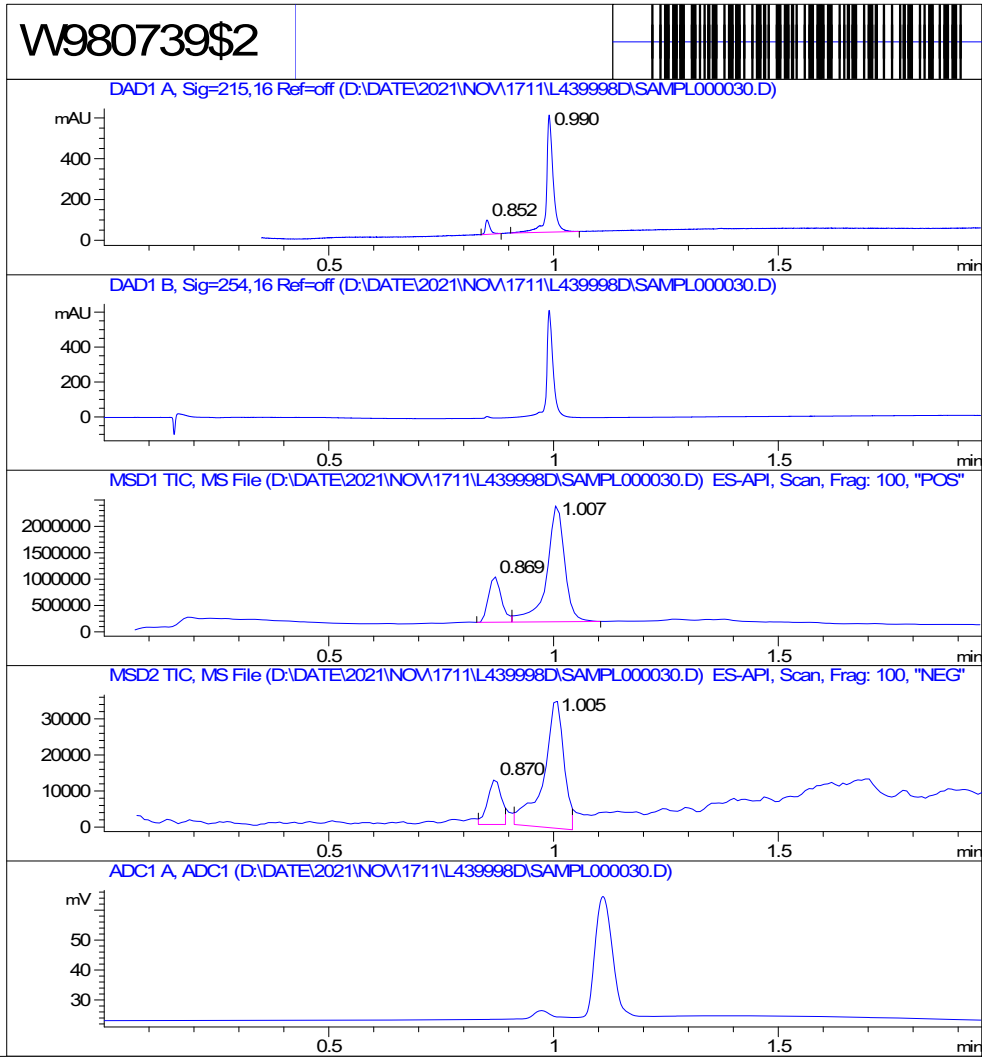


MaxPeak: 92.20%  
Ret\_Time: 0.990 min



Mol Wt 290.31  
Exact Mass 290.06

#	Time	Area%
1	0.852	7.80
2	0.990	92.20



Inj.Date 17-Nov-21

A

P2-D-03

- 4 -

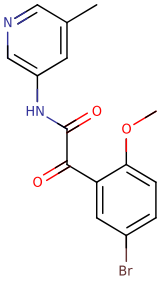
Acq. Method C:\CHEM32\ -> ->

Z1669286714\_

W980702\$6

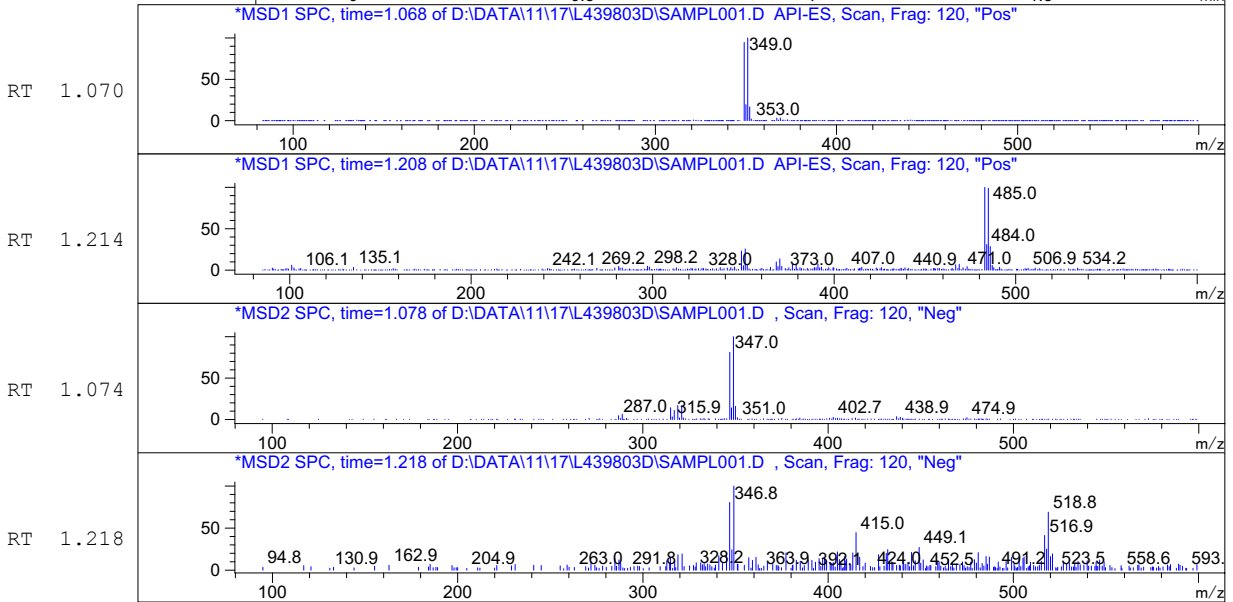
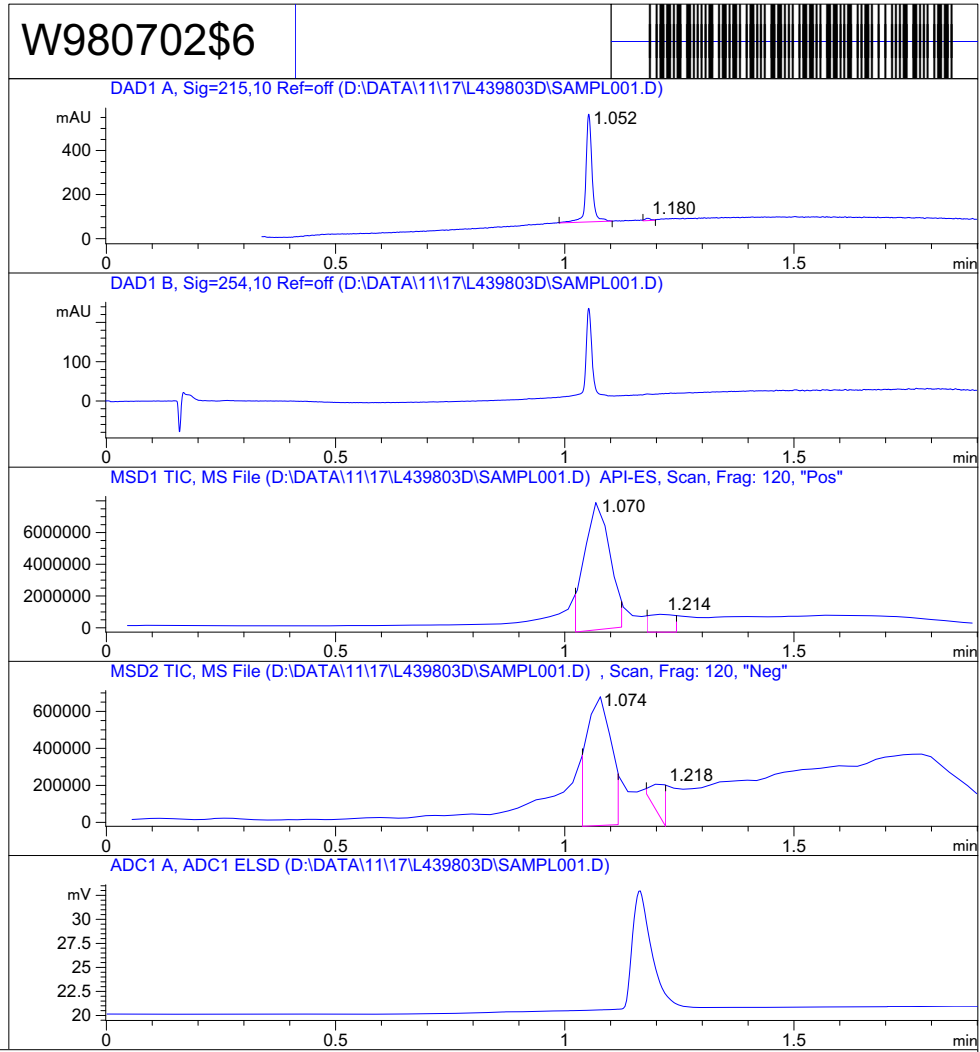


MaxPeak: 97.88%  
Ret\_Time: 1.052 min



Mol Wt 349.18  
Exact Mass 348.02

#	Time	Area%
1	1.052	97.88
2	1.180	2.12



Inj.Date 11/17/2021

LB

-SL-

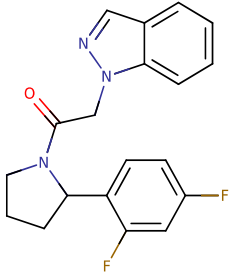
Acq. Method C:\HPCHEM\> >

Z1355254448\_

W980607\$1

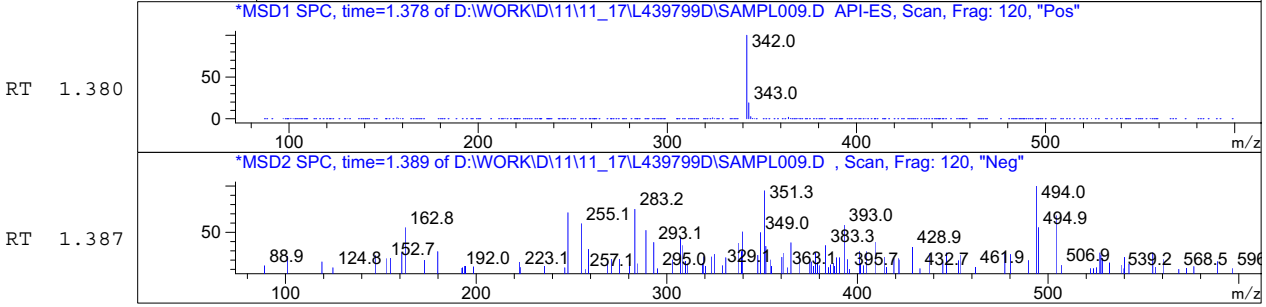
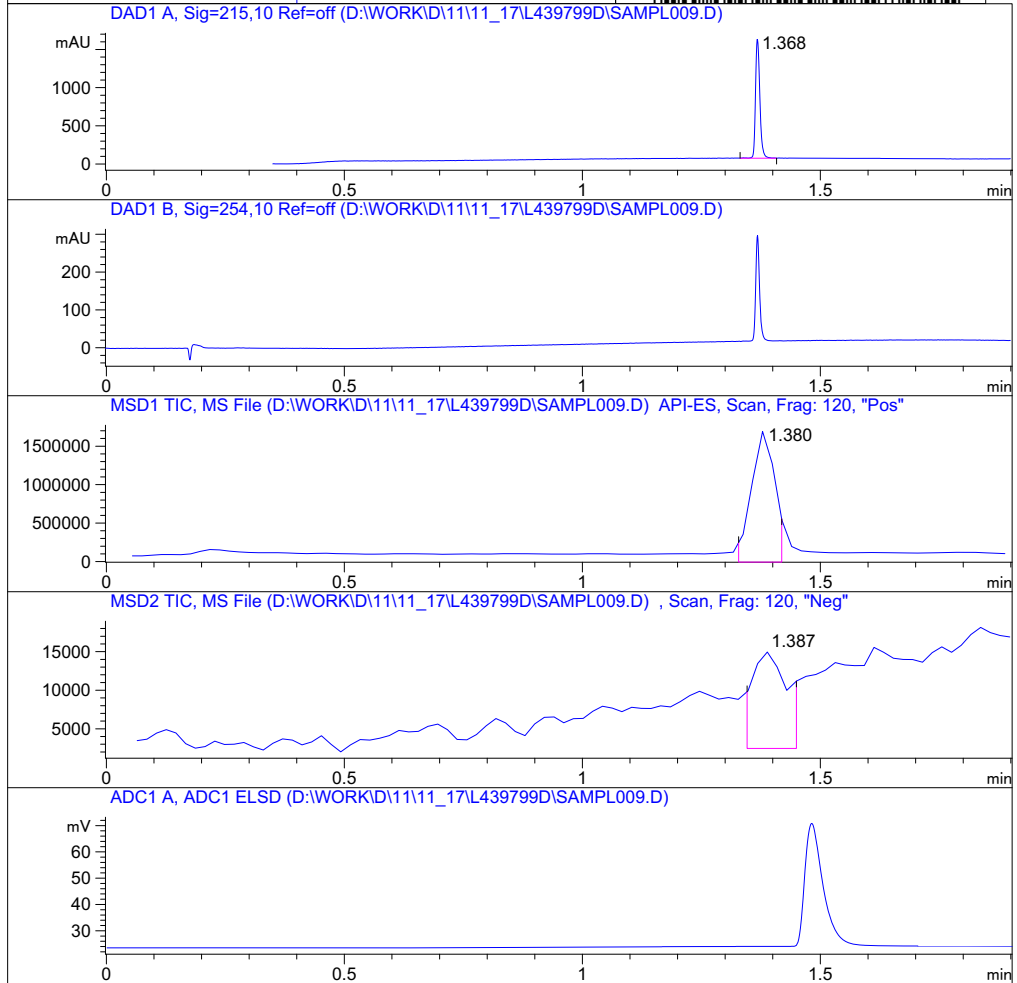


MaxPeak: 100.00%  
Ret\_Time: 1.368 min



Mol Wt 341.36  
Exact Mass 341.16

#	Time	Area%
1	1.368	100.00



Inj.Date 11/17/2021

K

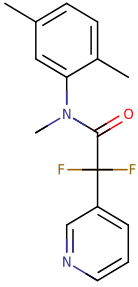
P2-A-09

-VL-

Acq. Method C:\HPCHEM\ -> ->

Z2298806057\_

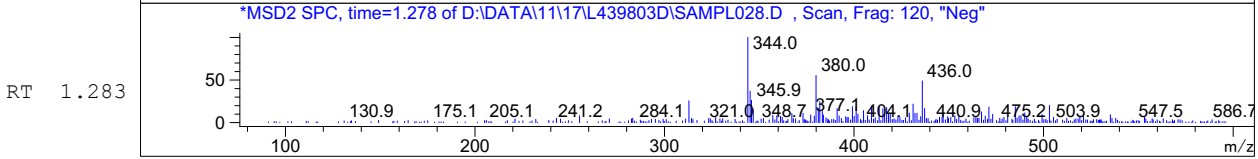
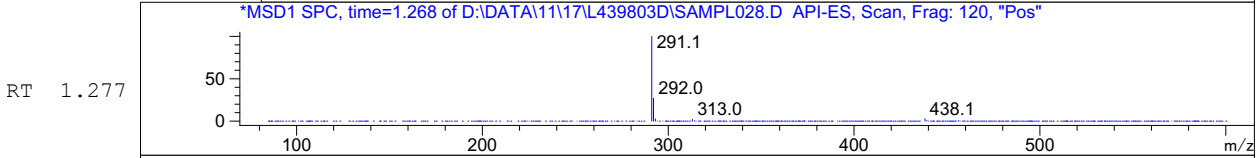
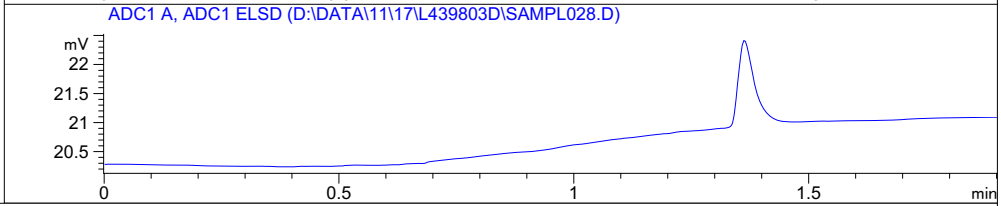
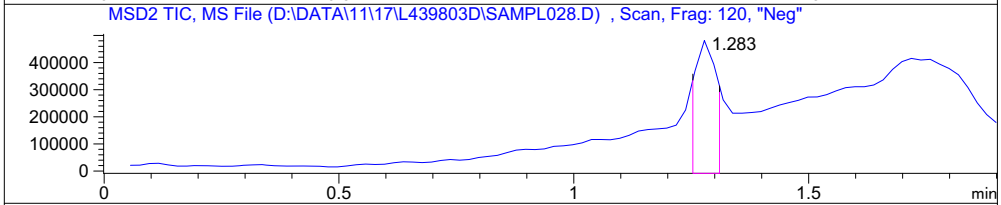
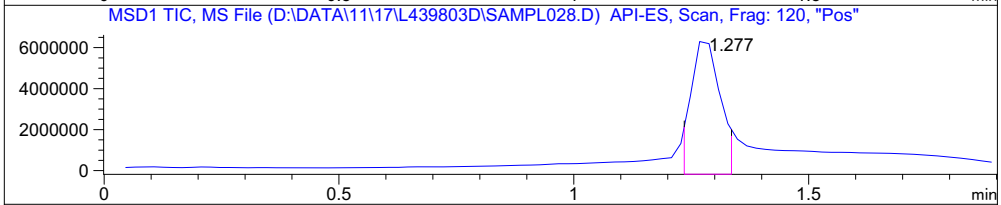
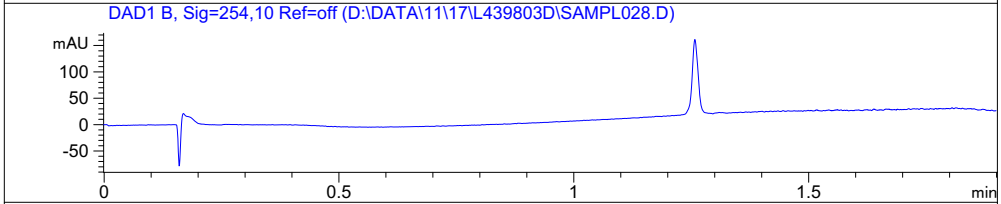
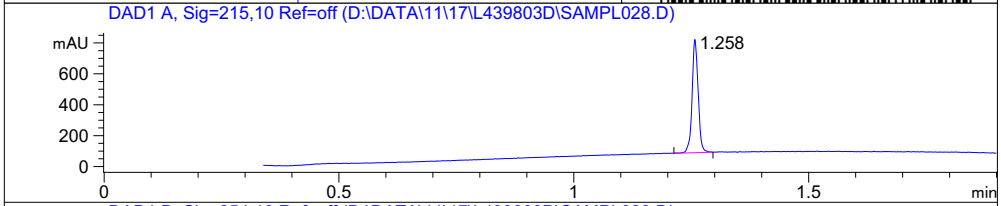
MaxPeak: 100.00%  
Ret\_Time: 1.258 min



Mol Wt 290.31  
Exact Mass 290.15

#	Time	Area%
1	1.258	100.00

W980611\$2



Inj.Date 11/17/2021

LB

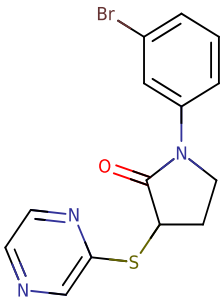
-SL-

Acq. Method C:\HPCHEM\ -> ->

Z3079159560\_



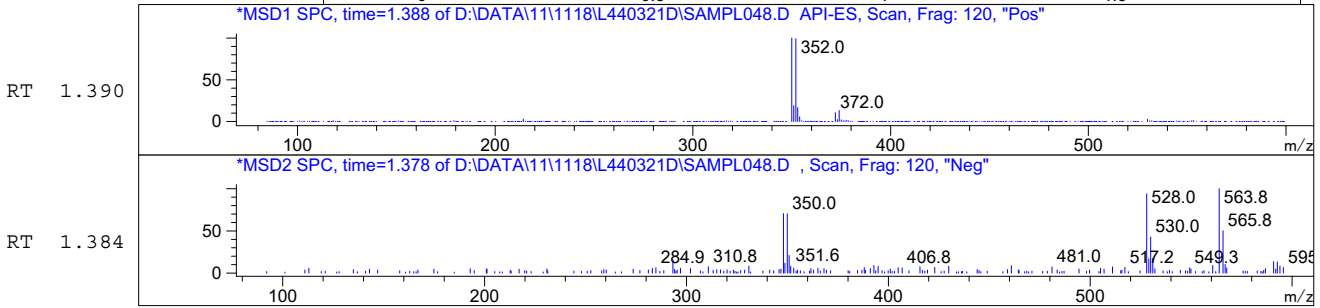
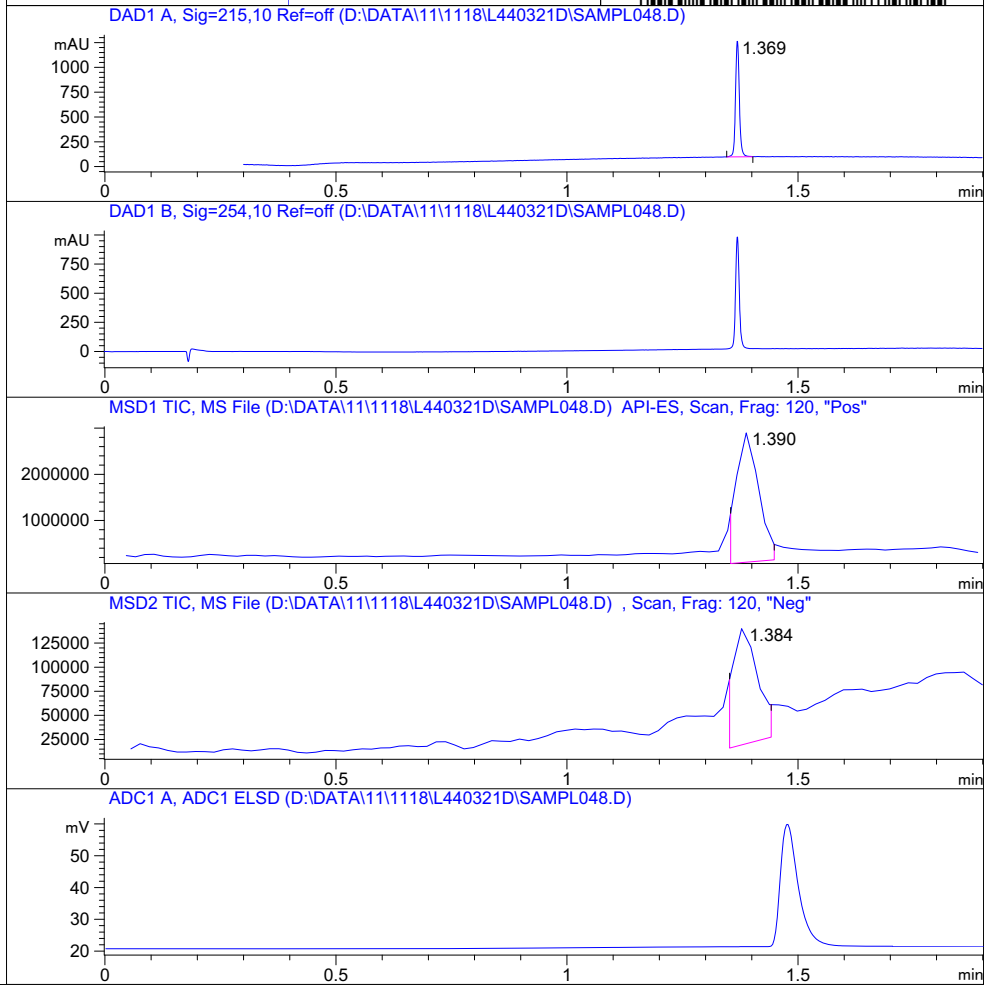
MaxPeak: 100.00%  
Ret\_Time: 1.369 min



Mol Wt 350.23  
Exact Mass 351

#	Time	Area%
1	1.369	100.00

W980703\$1



Inj.Date 11/18/2021

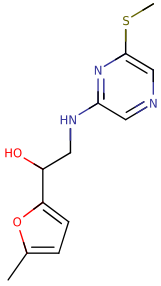
LT

-SL-

Acq. Method C:\HPCHEM\ -> ->

Z1872042935\_

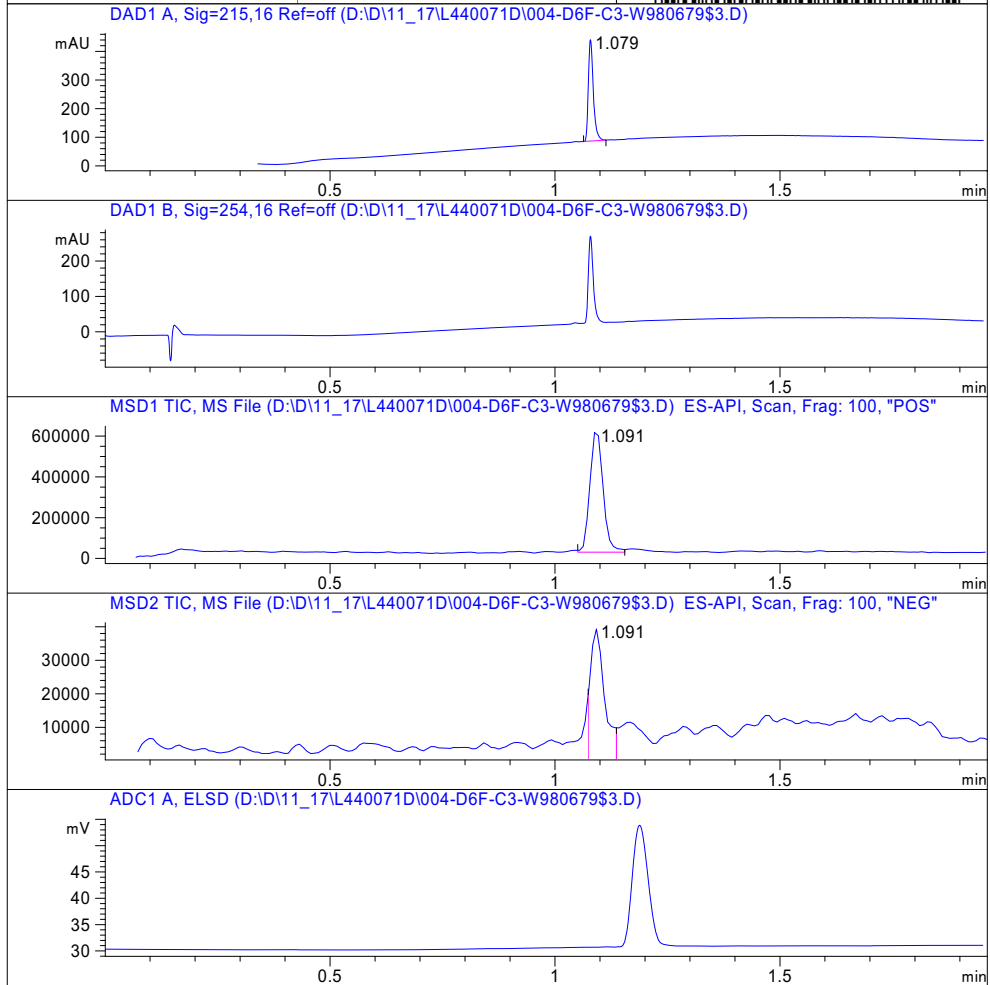
MaxPeak: 100.00%  
Ret\_Time: 1.079 min



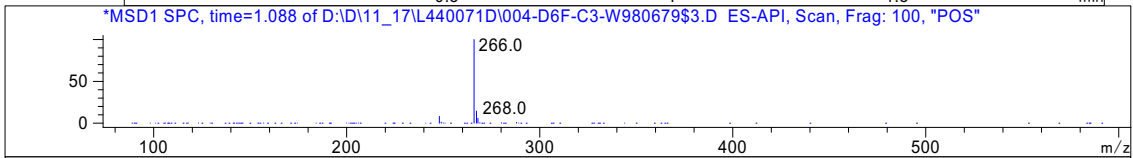
Mol Wt 265.33  
Exact Mass 265.1

#	Time	Area%
1	1.079	100.00

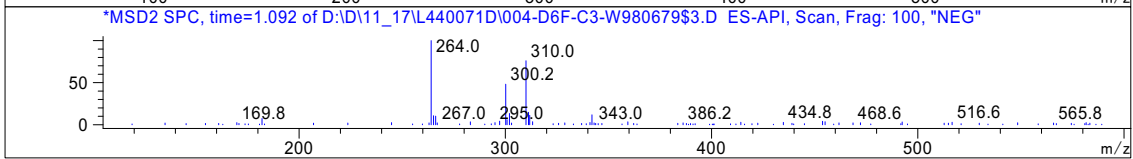
W980679\$3



RT 1.091

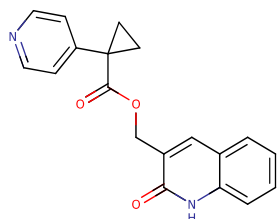


RT 1.091



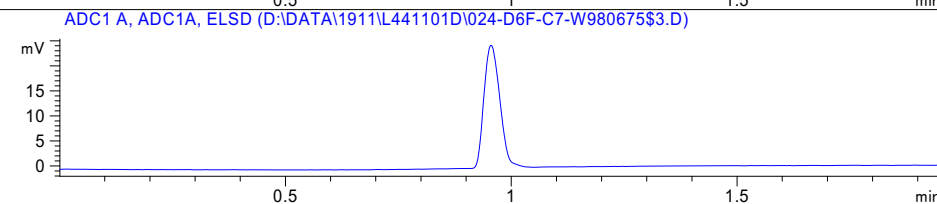
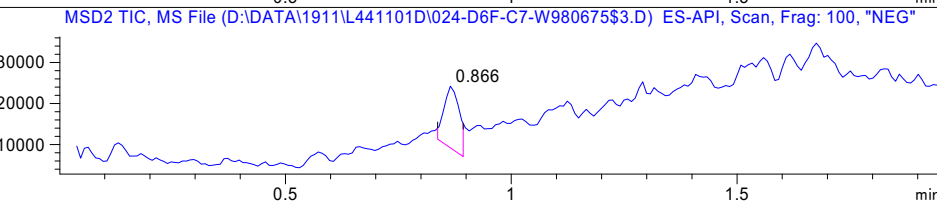
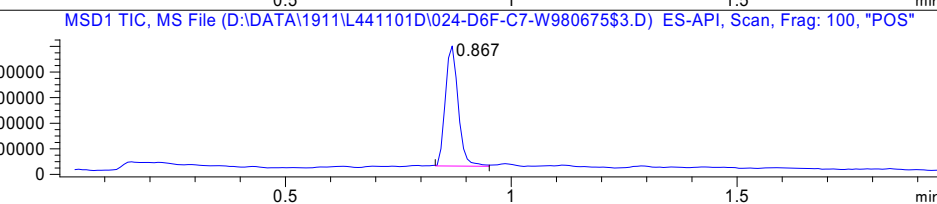
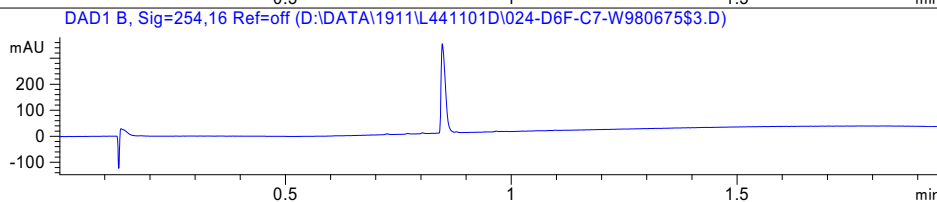
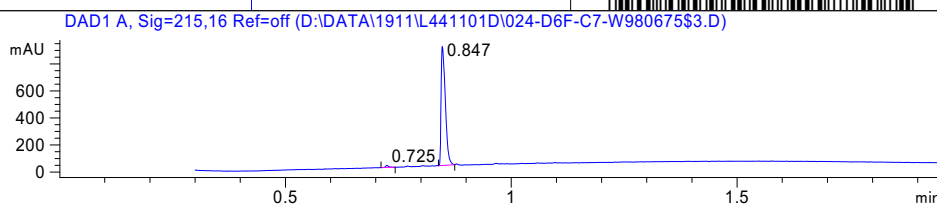
MaxPeak: 98.67%  
Ret\_Time: 0.847 min

# W980675\$3

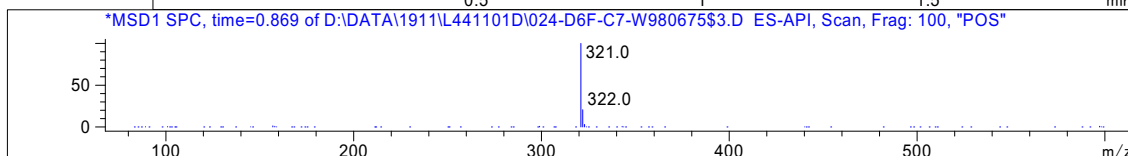


**Mol Wt** 320.34  
**Exact Mass** 320.13

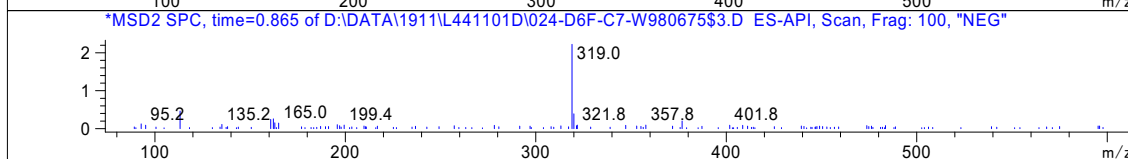
#	Time	Area%
1	0.725	1.33
2	0.847	98.67



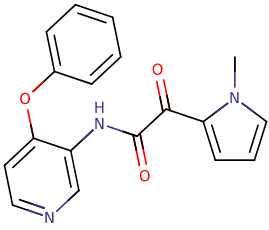
RT 0.867



RT 0.866



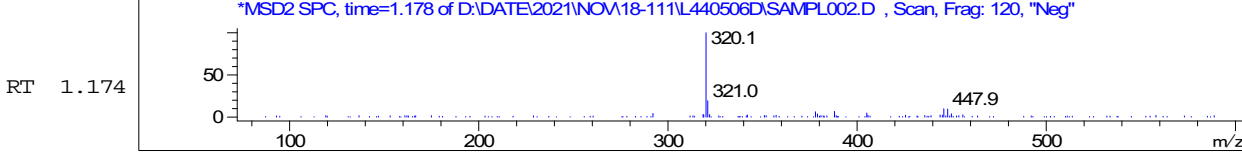
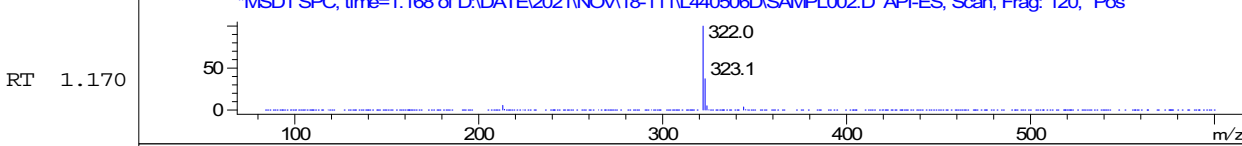
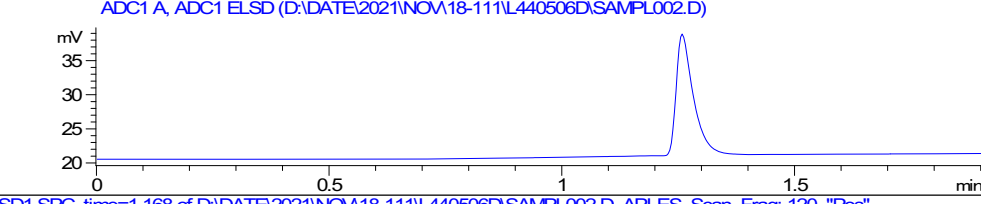
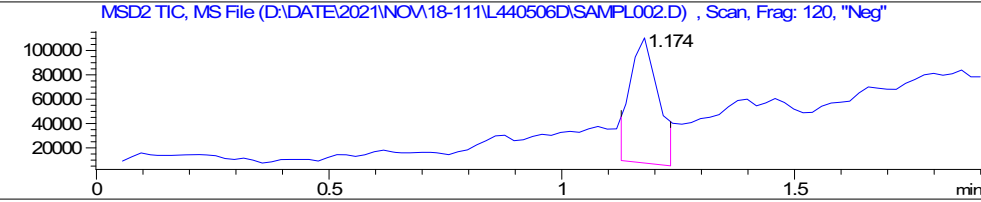
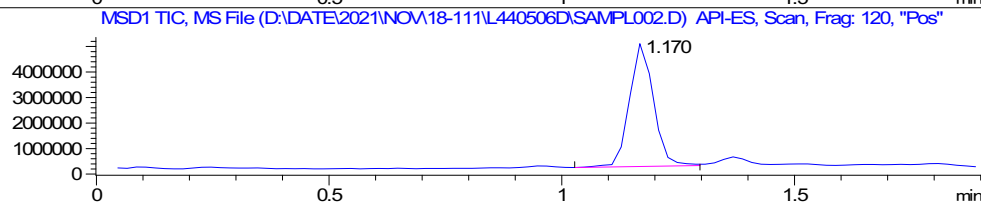
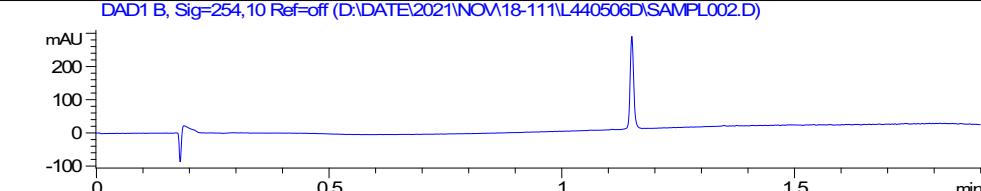
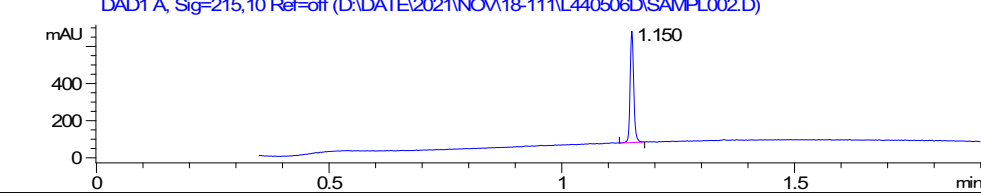
MaxPeak: 100.00%  
Ret\_Time: 1.150 min



Mol Wt 321.33  
Exact Mass 321.12

#	Time	Area%
1	1.150	100.00

W980606\$8



Inj.Date 18-Nov-21

A

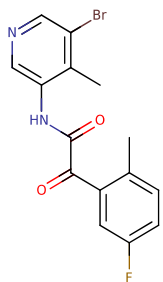
P2-A-02

-SL-

Acq. Method C:\HPCHEM\ -> ->

Z2195811405\_

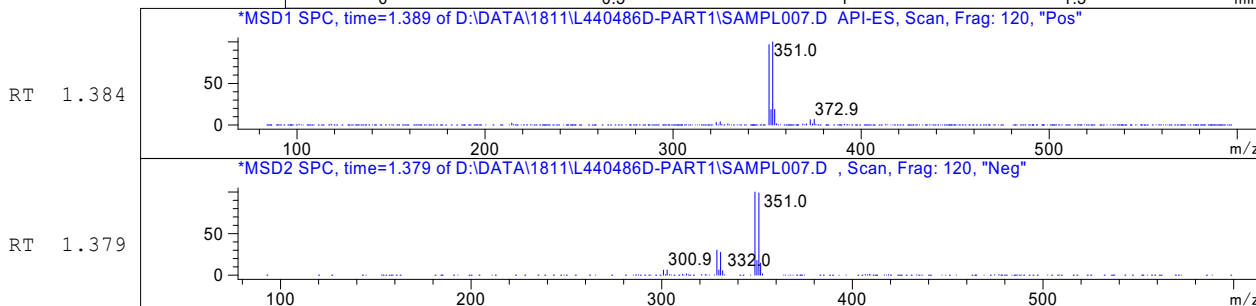
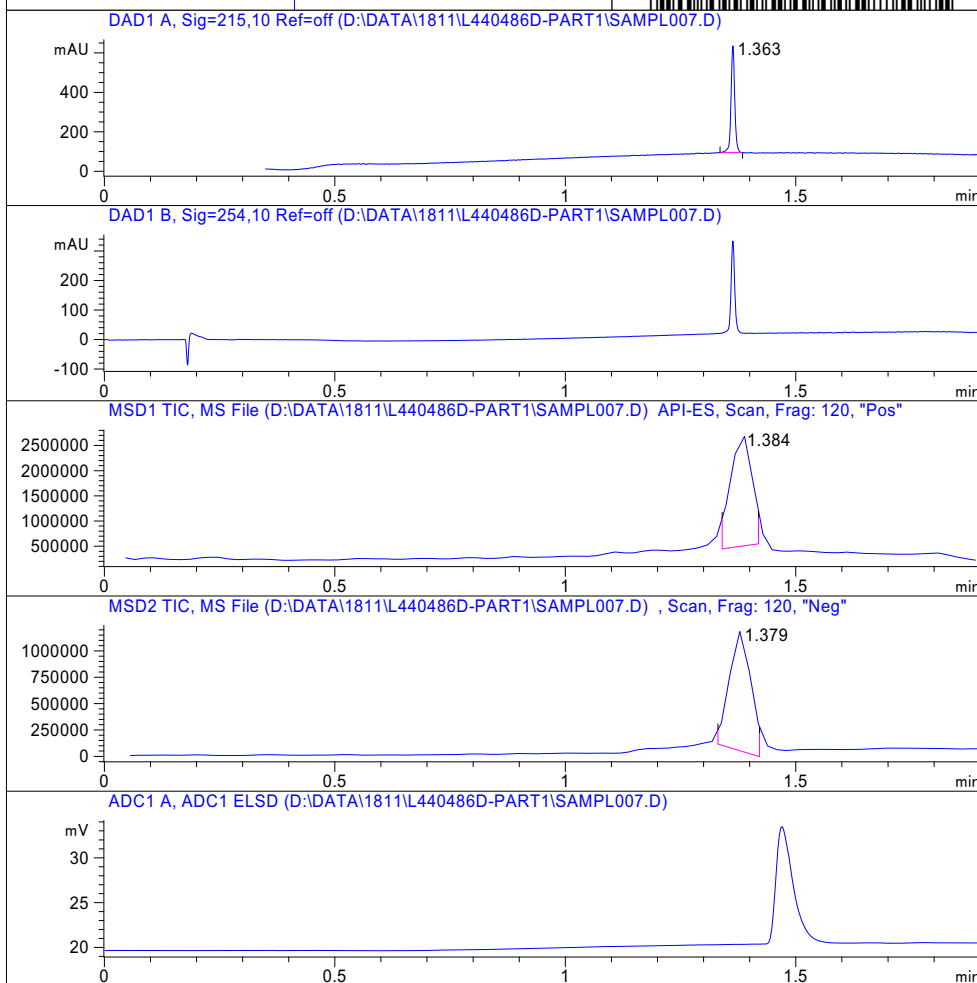
MaxPeak: 100.00%  
Ret\_Time: 1.363 min



Mol Wt 351.17  
Exact Mass 350.02

#	Time	Area%
1	1.363	100.00

W980620\$3



Inj.Date 11/18/2021

H

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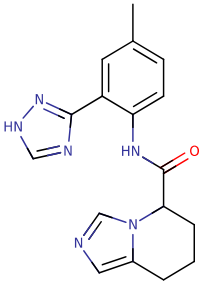
Acq. Method C:\HPCHEM\ ->

Z5420225795\_

W980749\$4

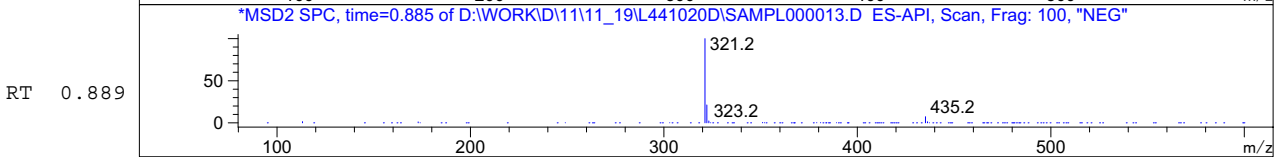
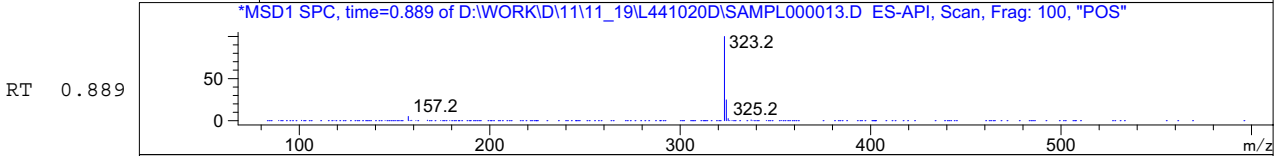
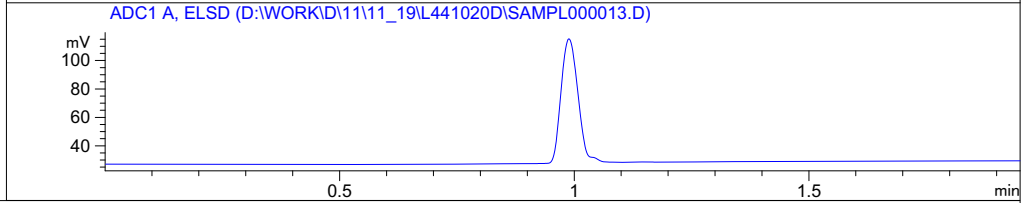
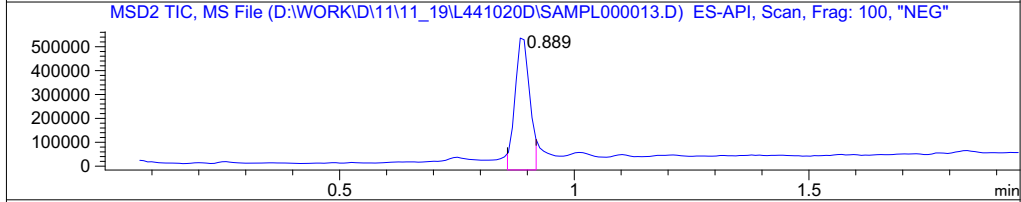
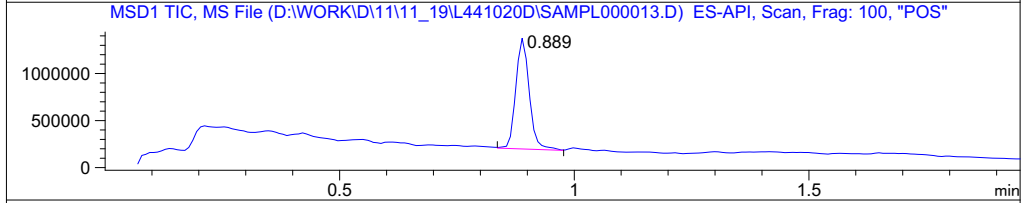
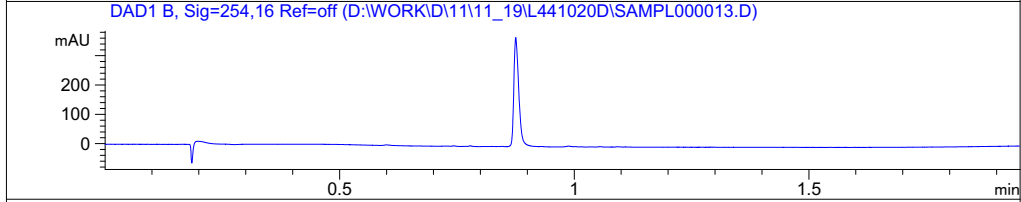
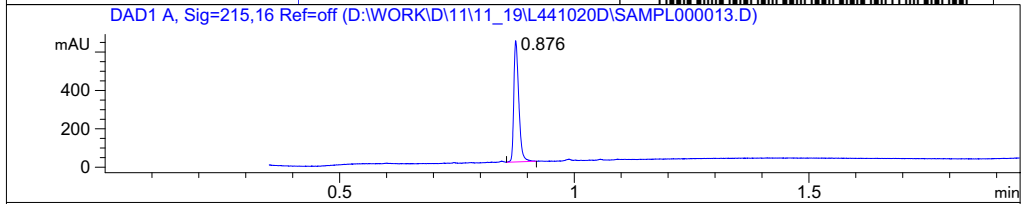


MaxPeak: 100.00%  
Ret\_Time: 0.876 min

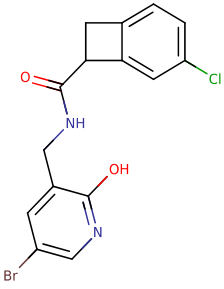


Mol Wt 322.36  
Exact Mass 322.17

#	Time	Area%
1	0.876	100.00

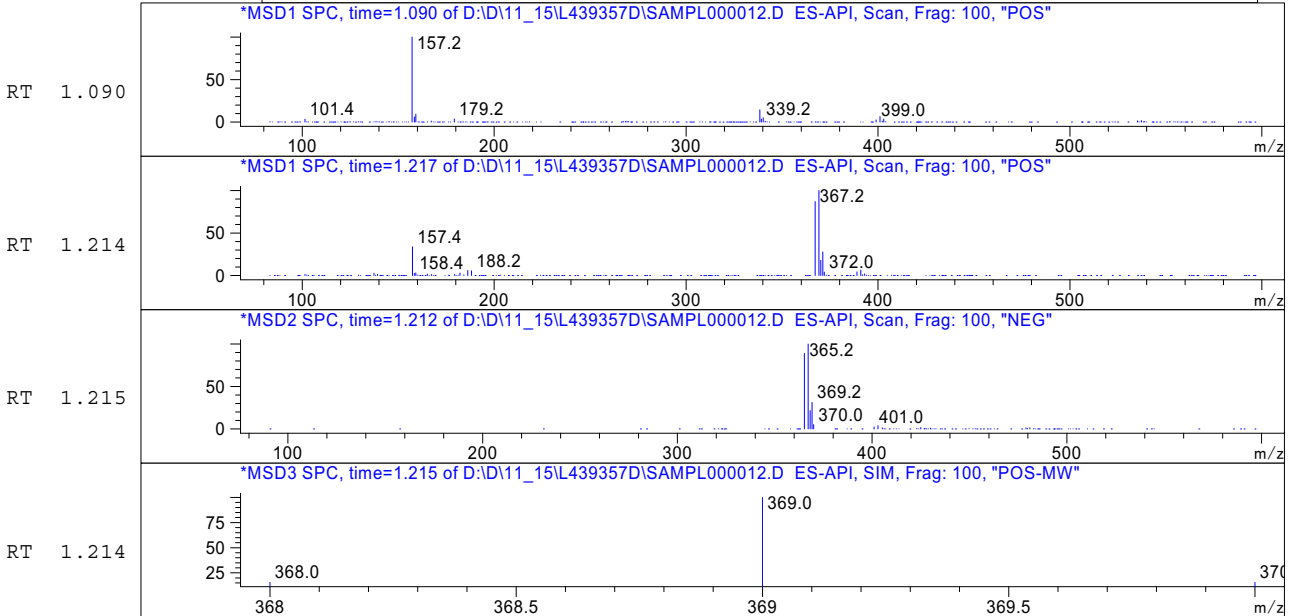
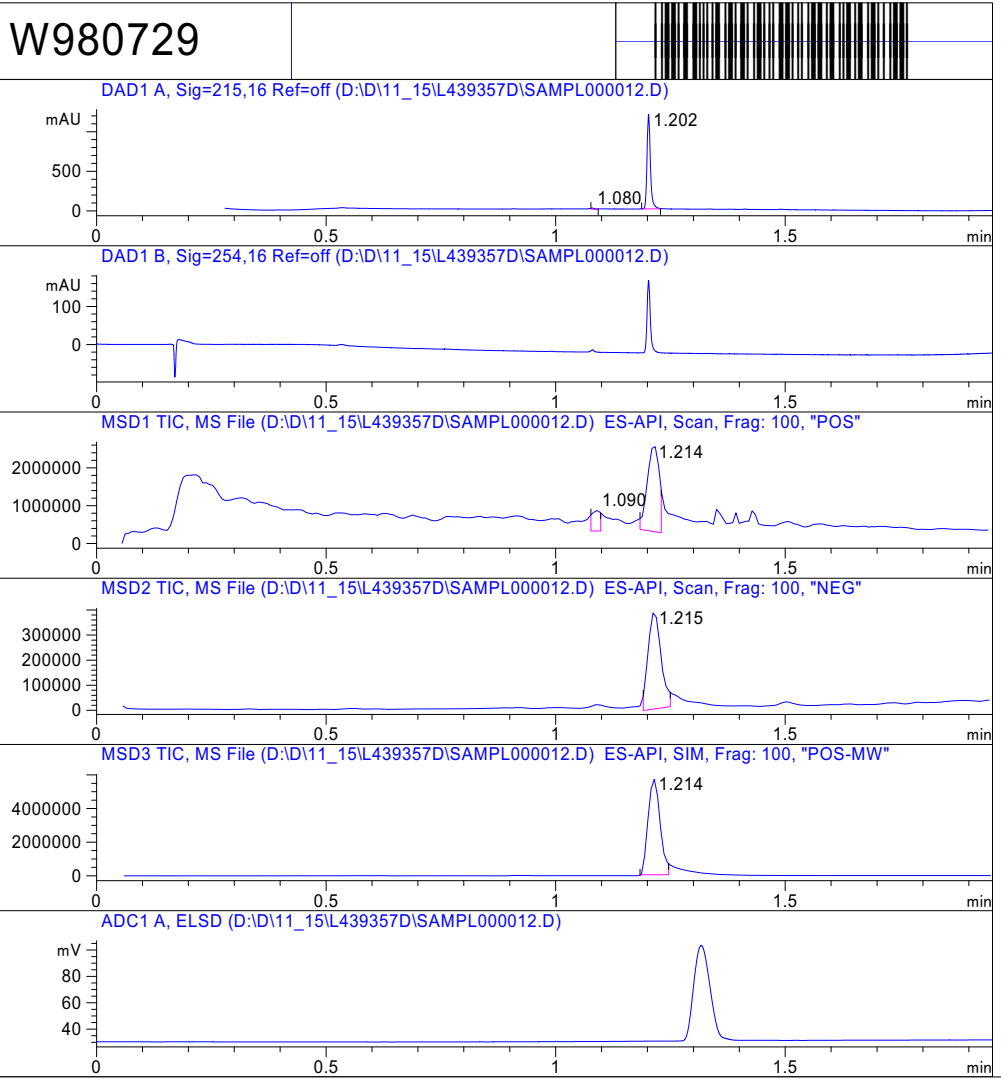


MaxPeak: 98.55%  
Ret\_Time: 1.202 min

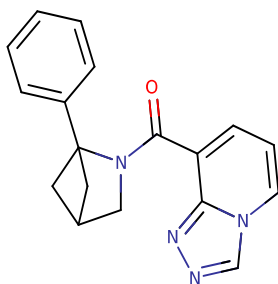


Mol Wt 367.62  
Exact Mass 367.99

#	Time	Area%
1	1.080	1.45
2	1.202	98.55



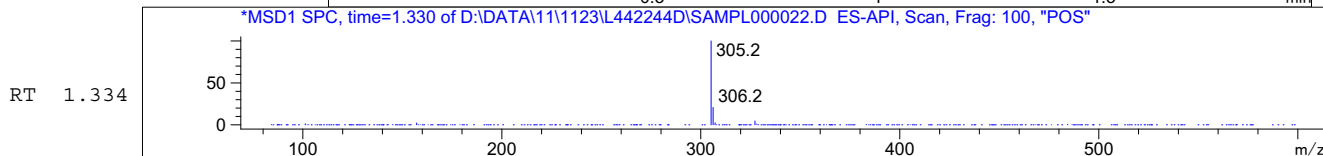
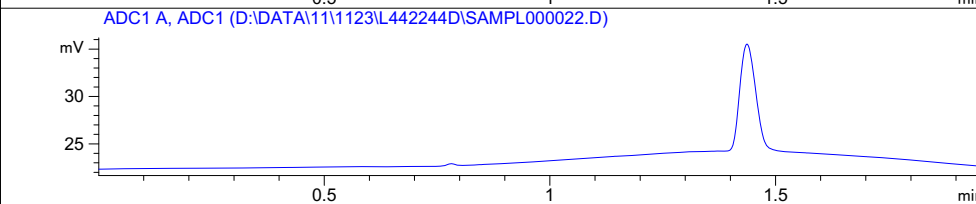
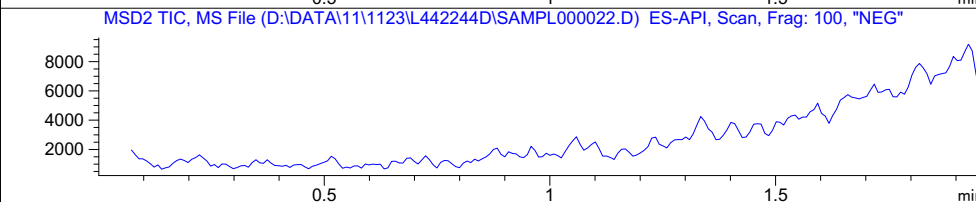
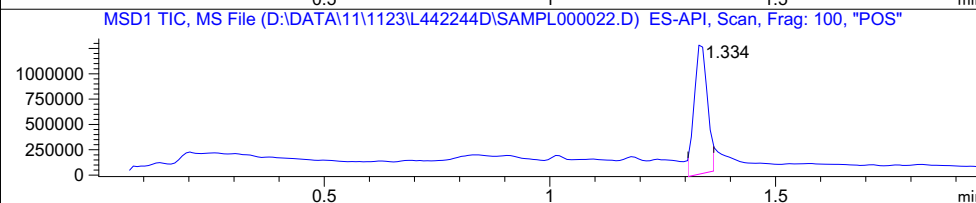
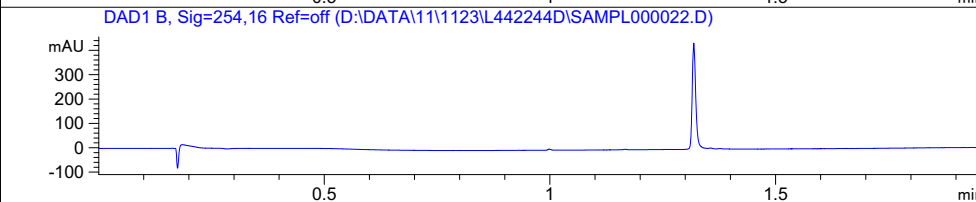
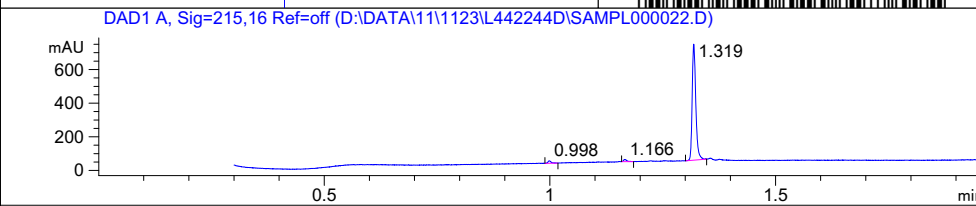
MaxPeak: 96.28%  
Ret\_Time: 1.319 min



Mol Wt 304.35  
Exact Mass 304.15

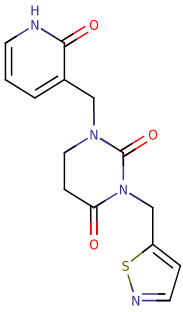
#	Time	Area%
1	0.998	1.94
2	1.166	1.79
3	1.319	96.28

X175457\$4





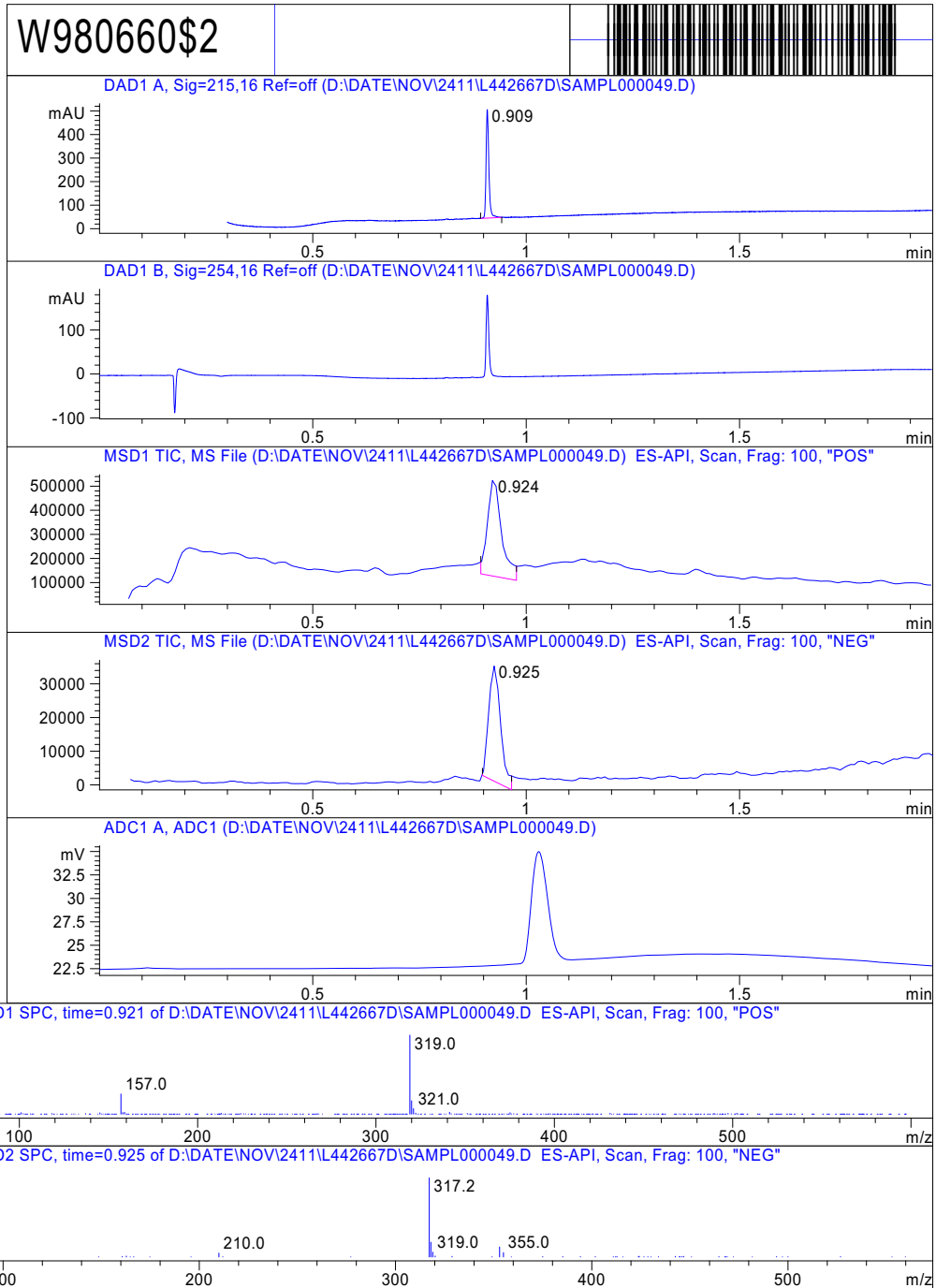
MaxPeak: 100.00%  
Ret\_Time: 0.909 min



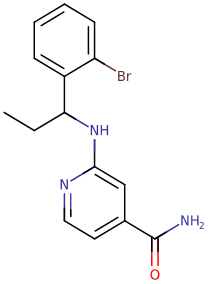
Mol Wt 318.35  
Exact Mass 318.08

#	Time	Area%
1	0.909	100.00

W980660\$2



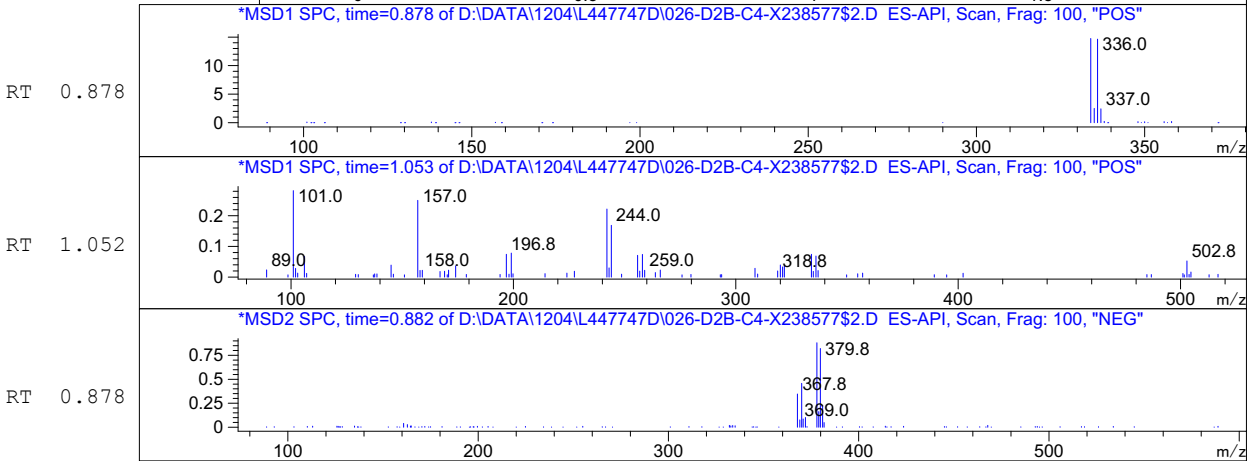
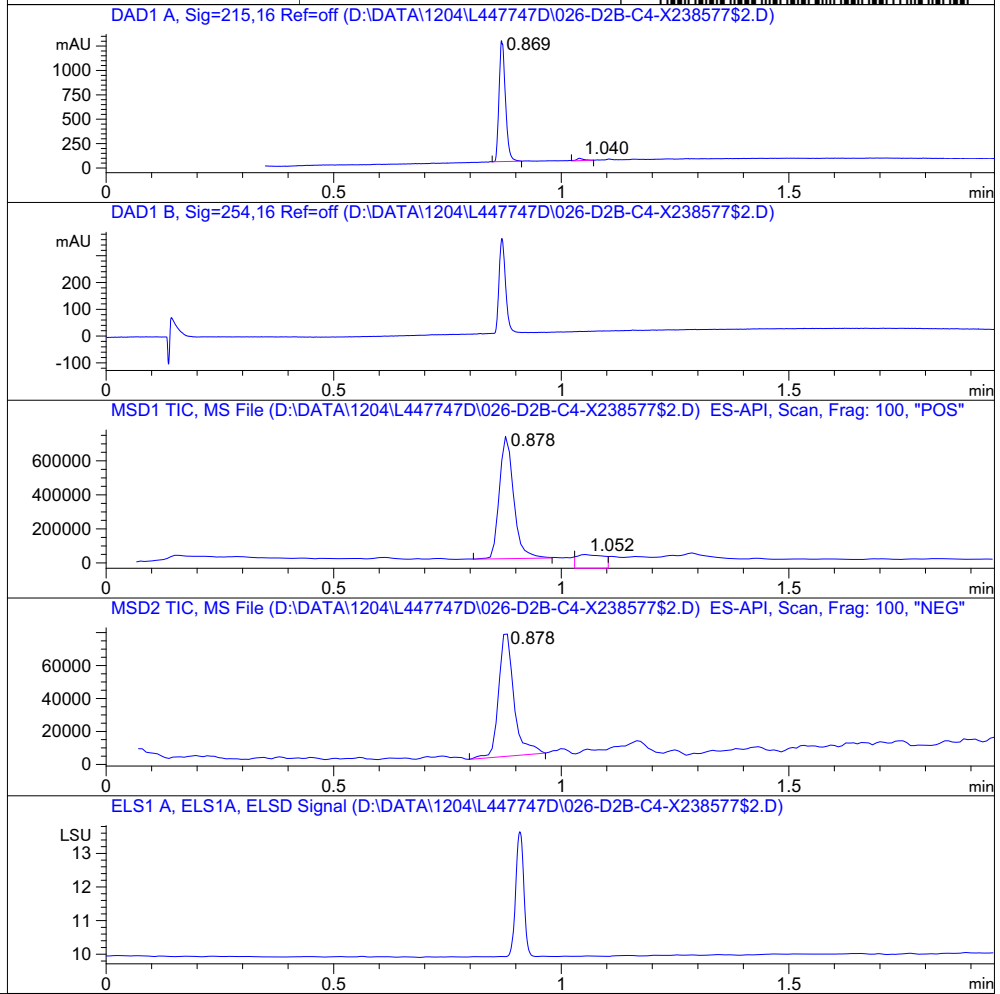
MaxPeak: 98.00%  
Ret\_Time: 0.869 min



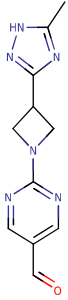
Mol Wt 334.21  
Exact Mass 333.07

#	Time	Area%
1	0.869	98.00
2	1.040	2.00

X238577\$2



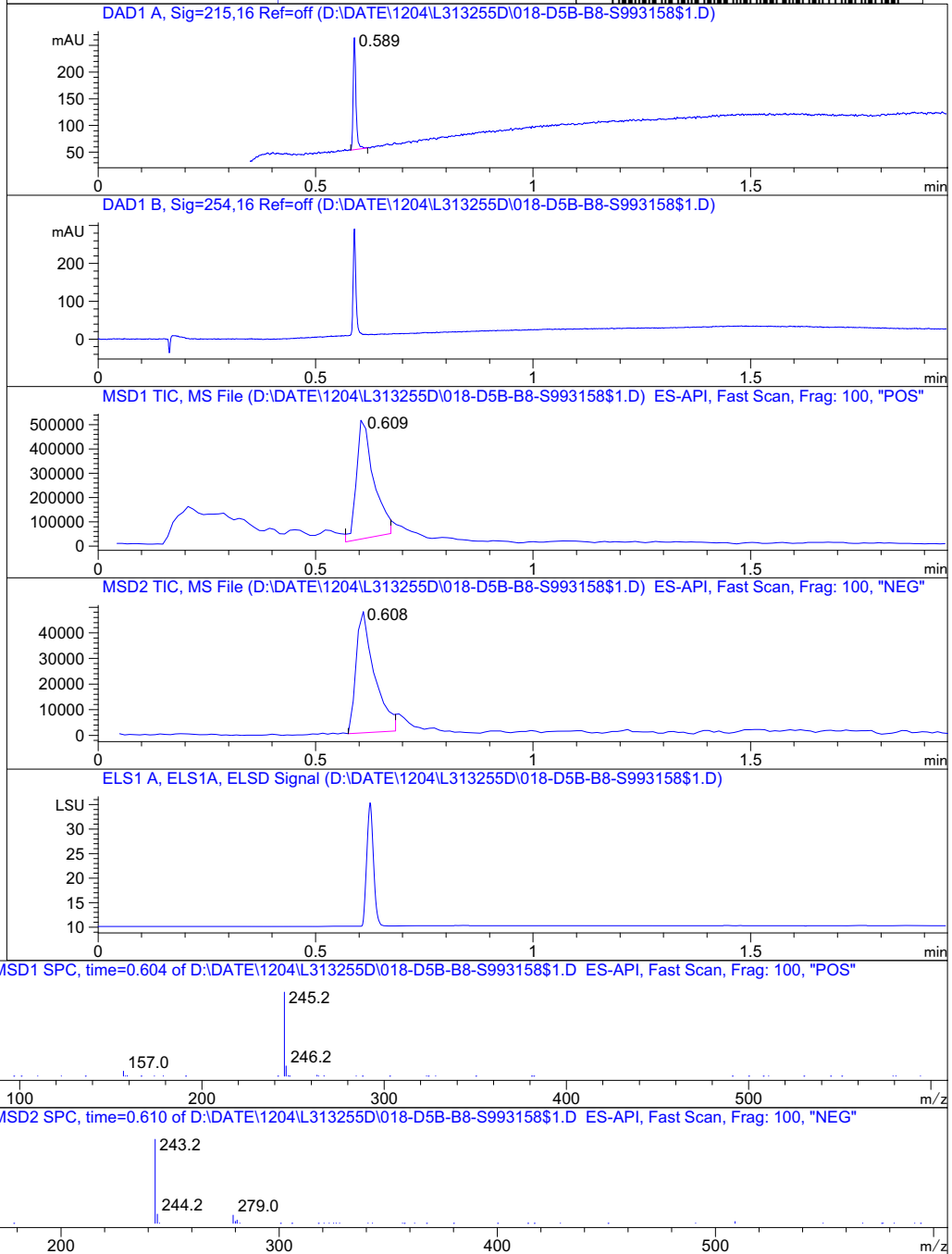
MaxPeak: 100.00%  
Ret\_Time: 0.589 min



Mol Wt 244.25  
Exact Mass 244.11

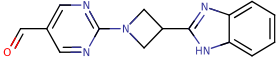
#	Time	Area%
1	0.589	100.00

S993158\$1



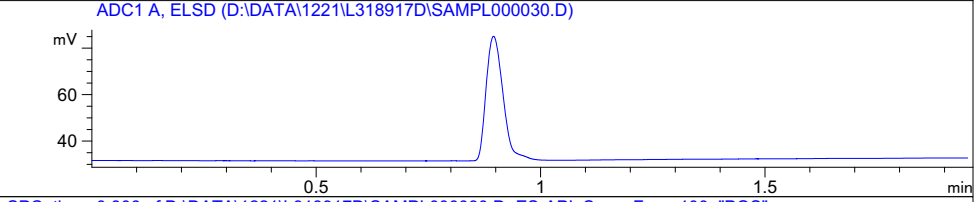
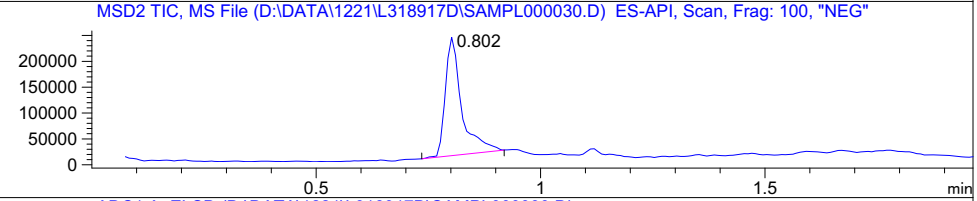
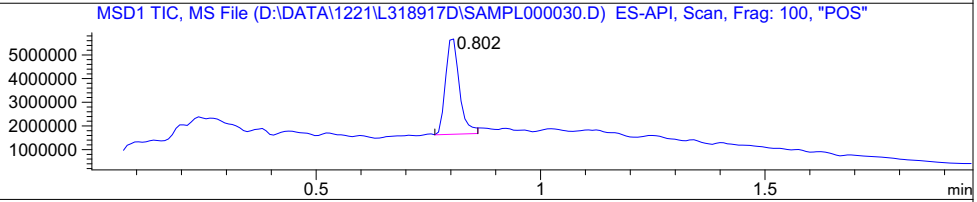
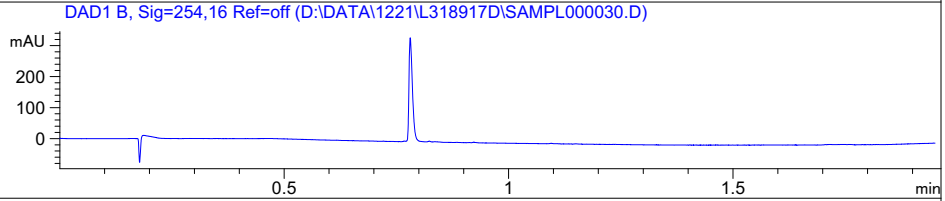
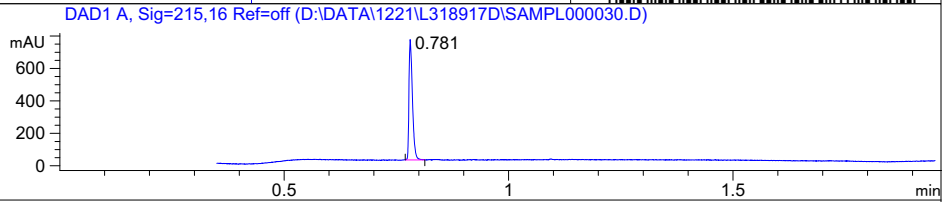
MaxPeak: 100.00%  
Ret\_Time: 0.781 min

U211096\$2

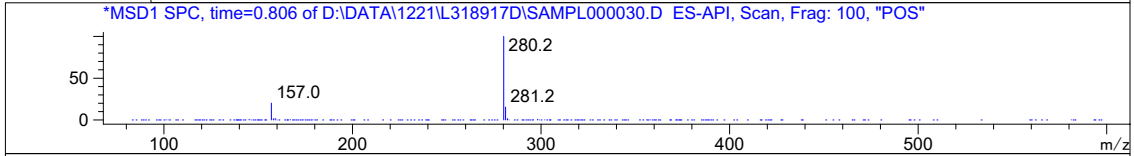


Mol Wt 279.3  
Exact Mass 279.12

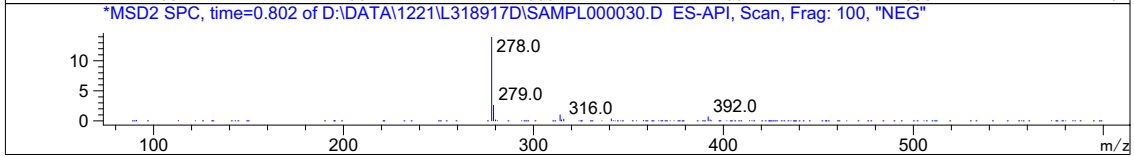
#	Time	Area%
1	0.781	100.00



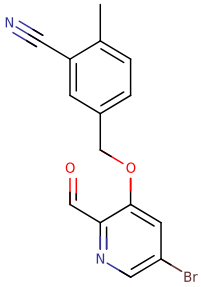
RT 0.802



RT 0.802



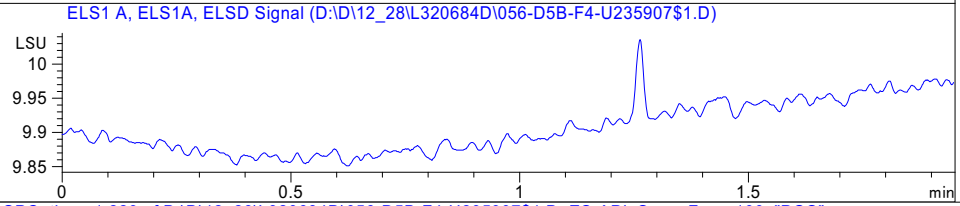
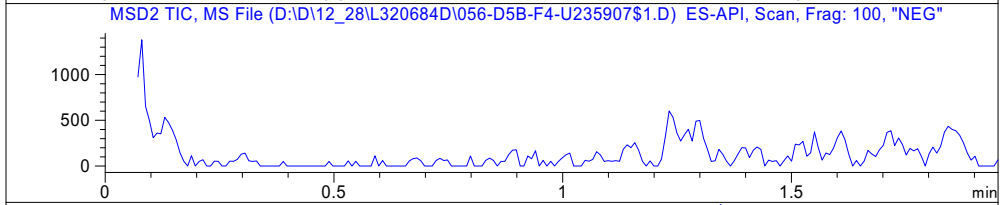
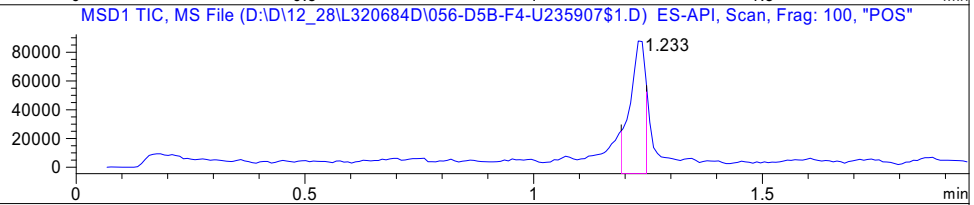
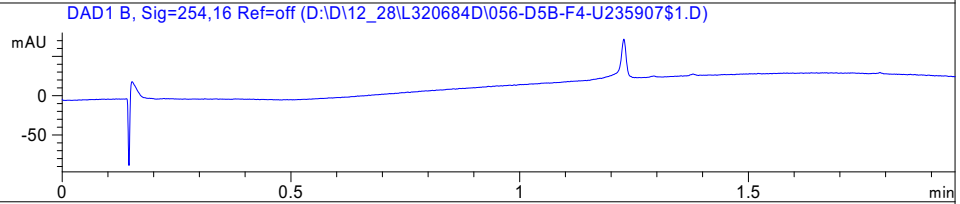
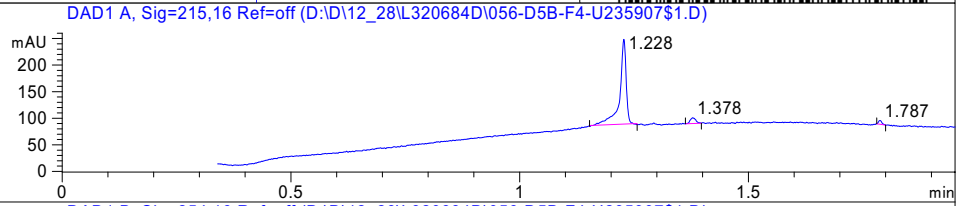
MaxPeak: 92.45%  
Ret\_Time: 1.228 min



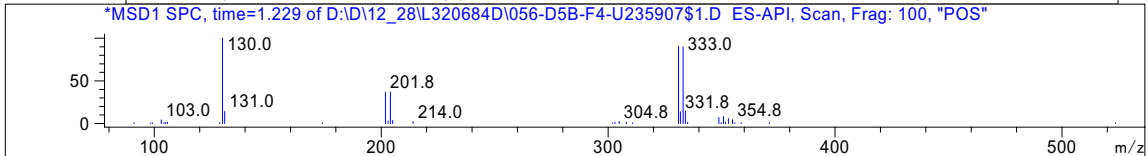
Mol Wt 331.16  
Exact Mass 330.01

#	Time	Area%
1	1.228	92.45
2	1.378	5.40
3	1.787	2.15

U235907\$1

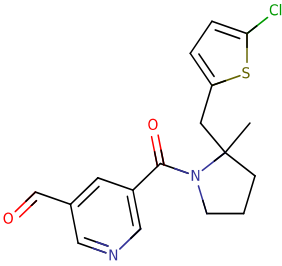


RT 1.233



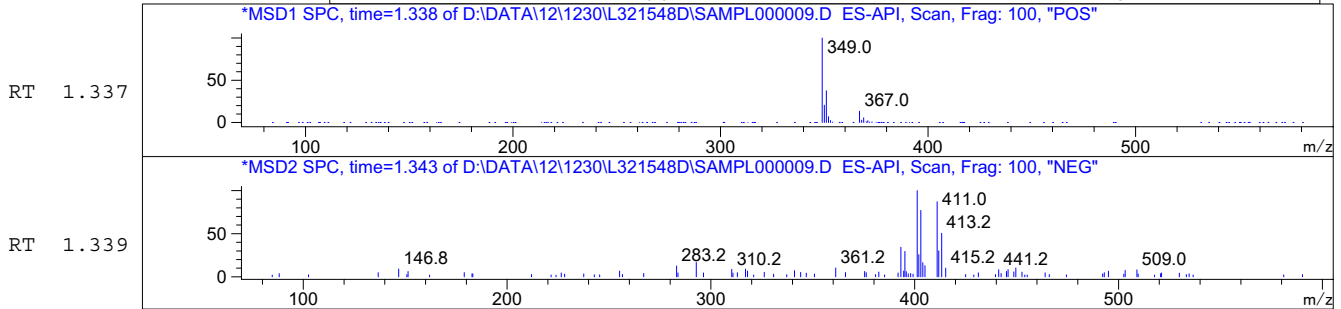
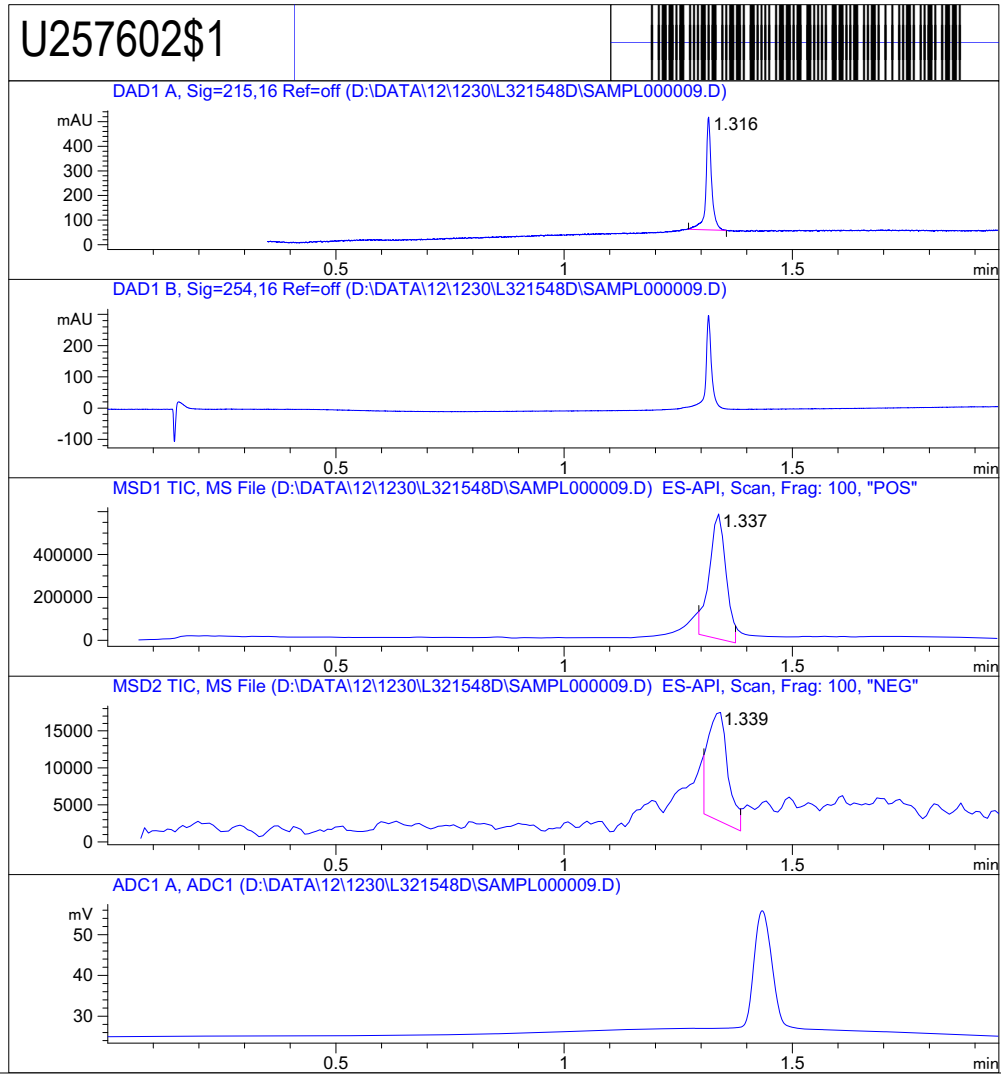
MaxPeak: 100.00%  
Ret\_Time: 1.316 min

U257602\$1

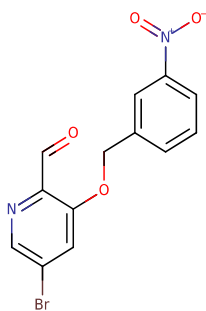


Mol Wt 348.85  
Exact Mass 348.09

#	Time	Area%
1	1.316	100.00



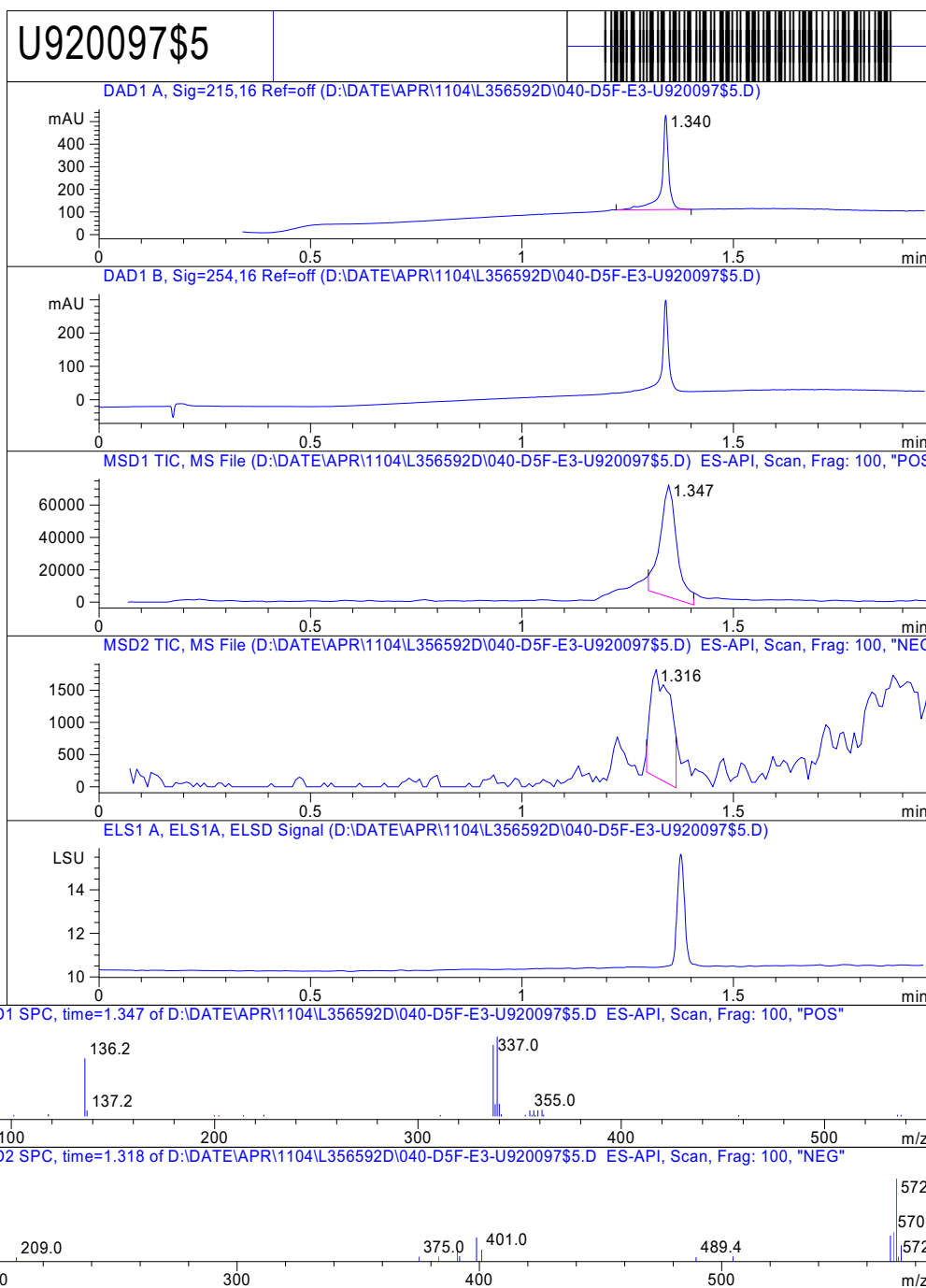
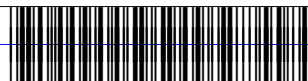
MaxPeak: 100.00%  
Ret\_Time: 1.340 min



Mol Wt 337.13  
Exact Mass 335.97

#	Time	Area%
1	1.340	100.00

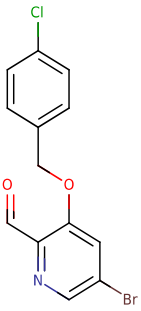
U920097\$5



RT 1.347

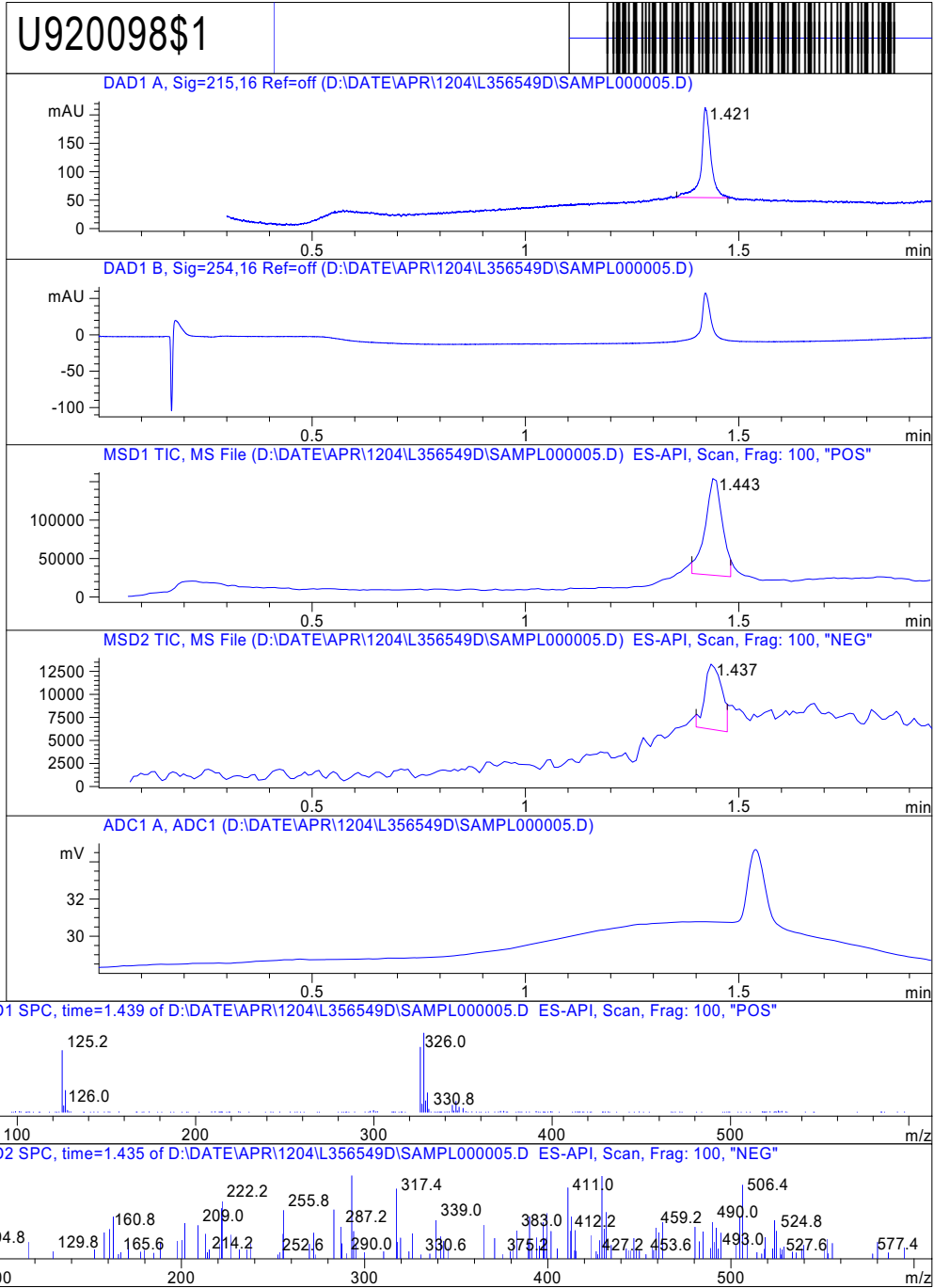
RT 1.316

MaxPeak: 100.00%  
Ret\_Time: 1.421 min



Mol Wt 326.57  
Exact Mass 326.96

#	Time	Area%
1	1.421	100.00



Inj.Date 4/11/2021

Y

- 4 -

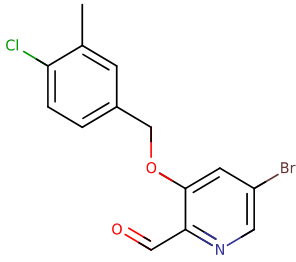
Acq. Method C:\CHEM32\ -> ->

Z4954569113\_



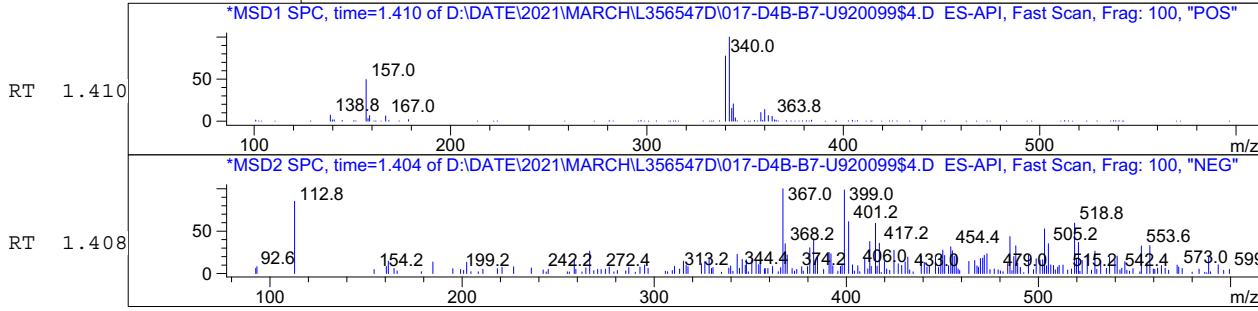
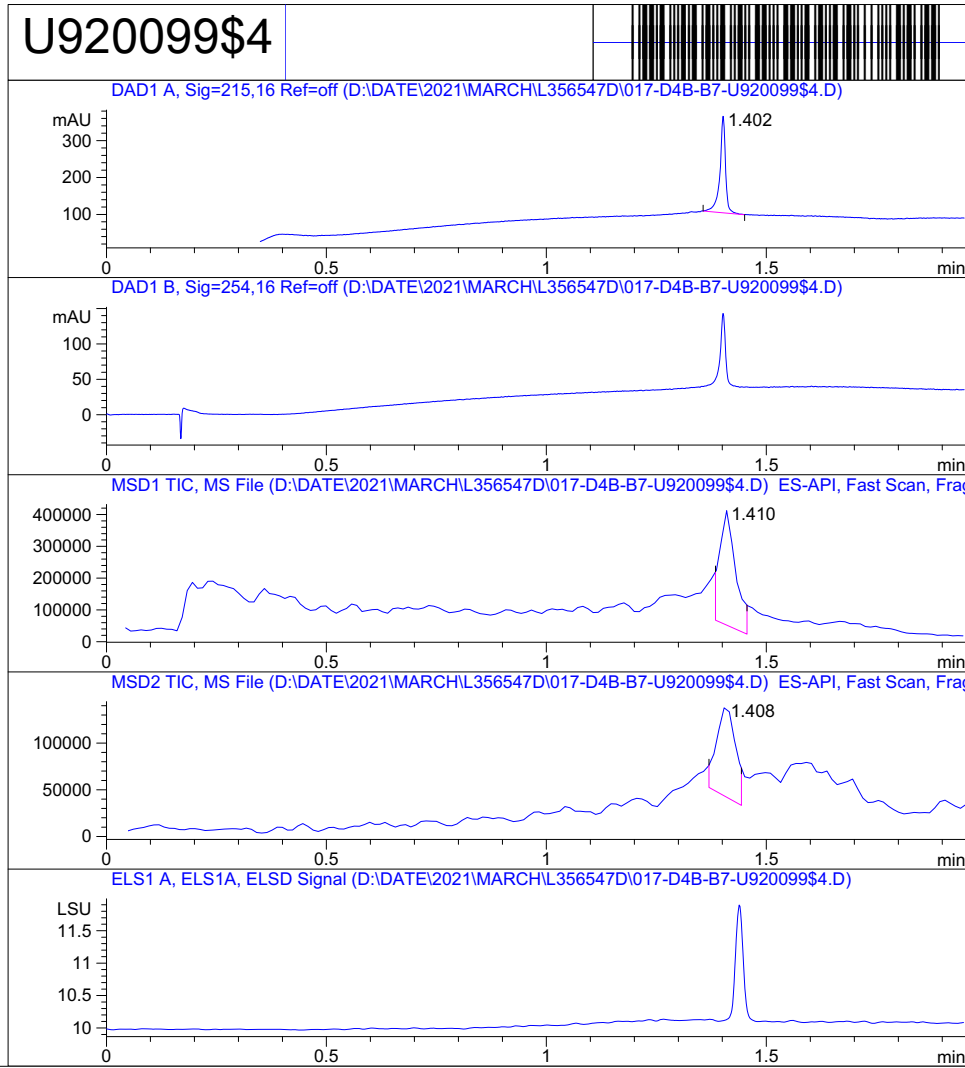
MaxPeak: 100.00%  
Ret\_Time: 1.402 min

U920099\$4



Mol Wt 340.6  
Exact Mass 340.98

#	Time	Area%
1	1.402	100.00



Inj.Date 4/11/2021

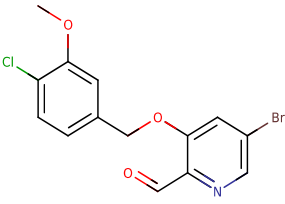
T <invalid>

Acq. Method C:\Users\ -> ->

Z4954569120\_

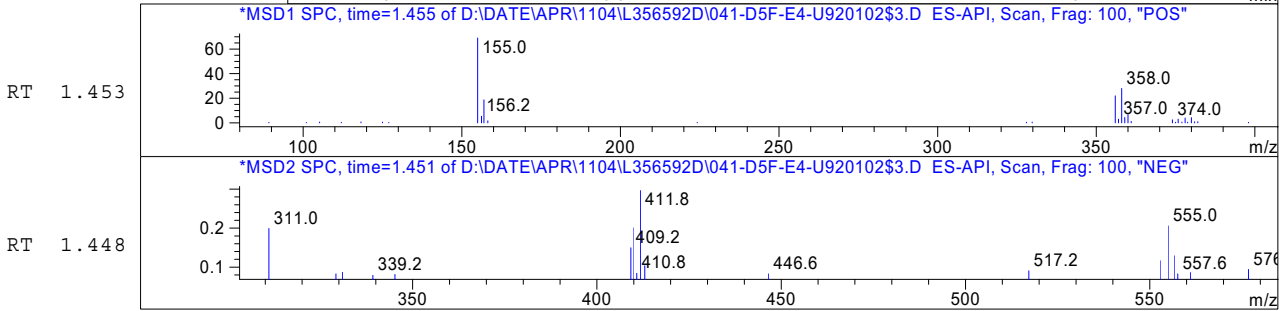
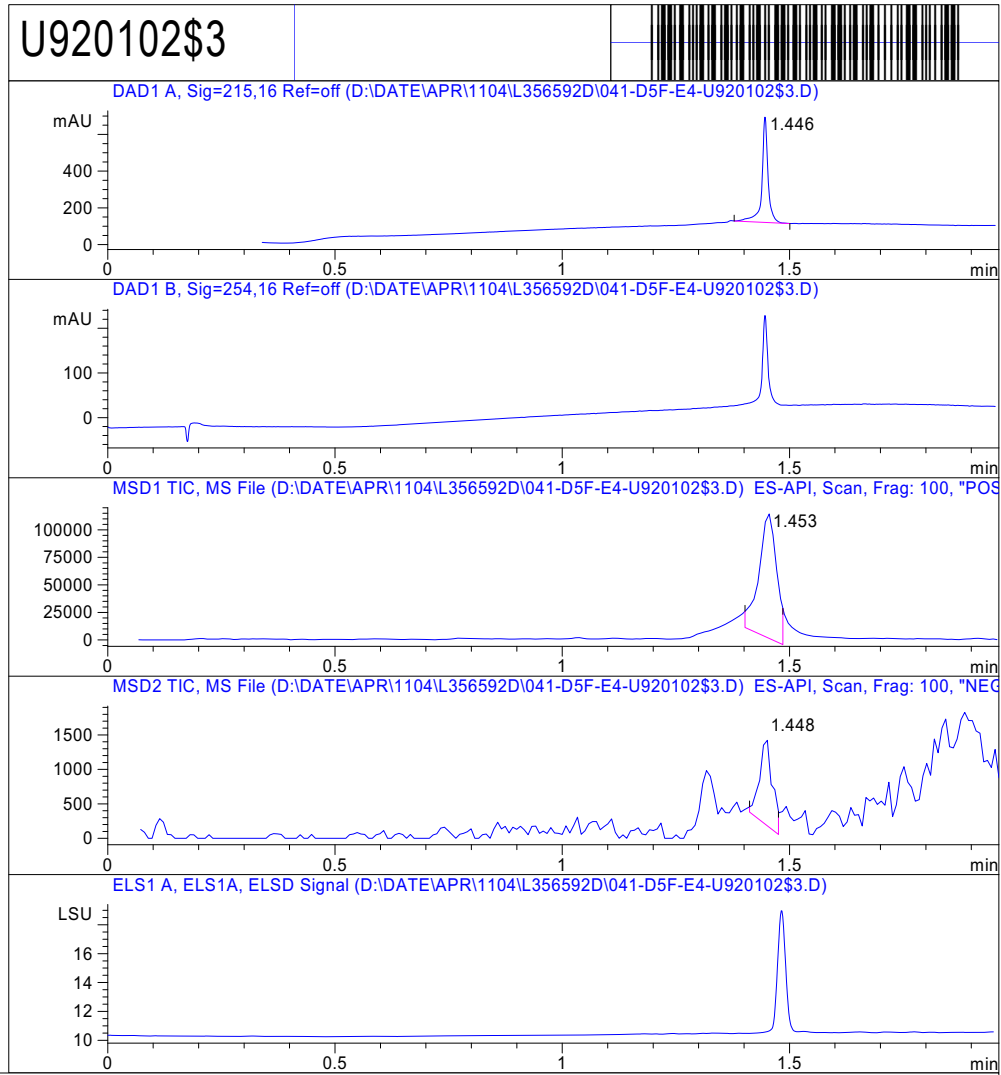
MaxPeak: 100.00%  
Ret\_Time: 1.446 min

# U920102\$3



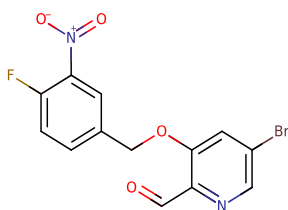
**Mol Wt** 356.6  
**Exact Mass** 356.97

#	Time	Area%
1	1.446	100.00



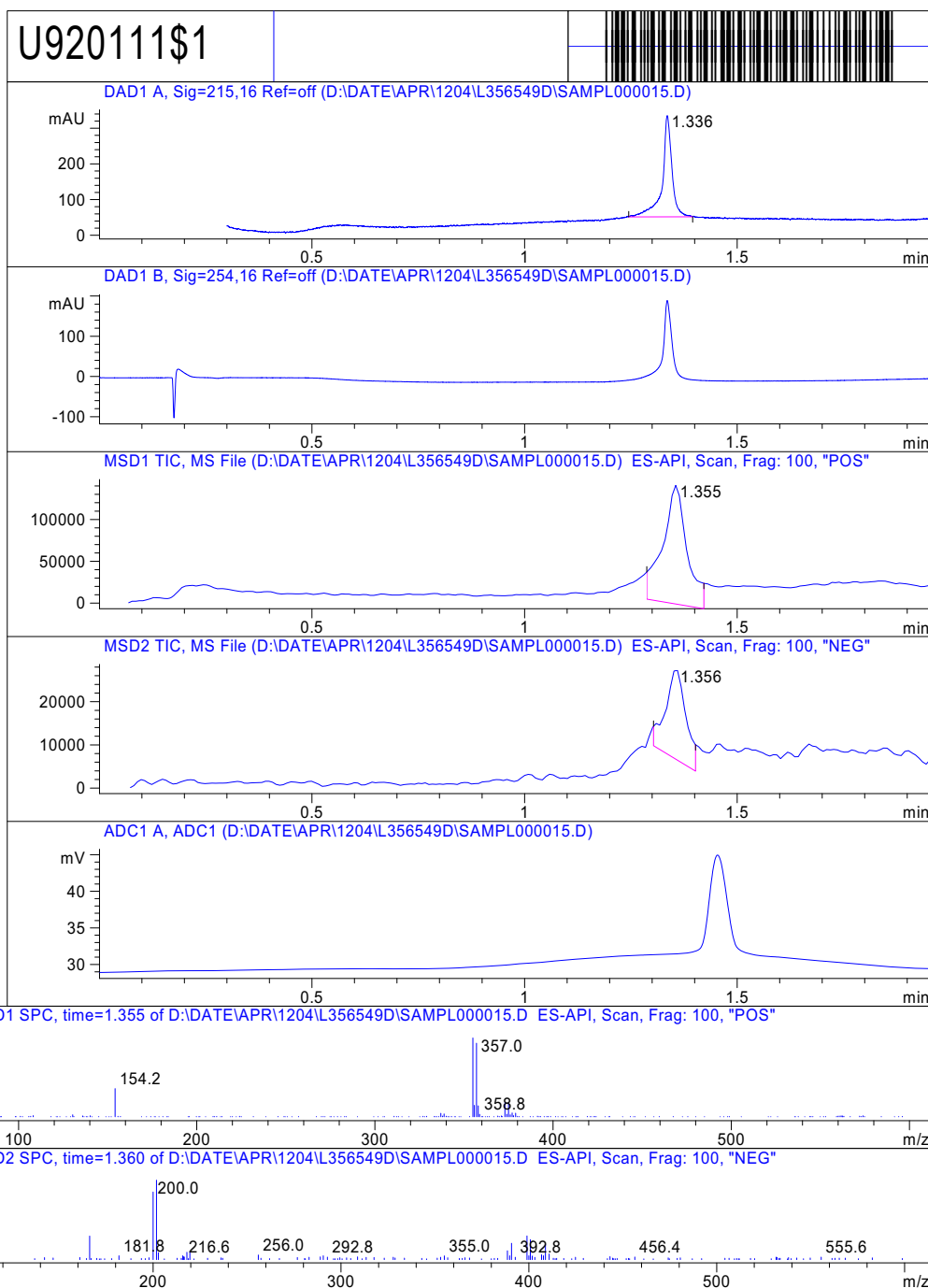
MaxPeak: 100.00%  
Ret\_Time: 1.336 min

U920111\$1



Mol Wt 355.12  
Exact Mass 353.96

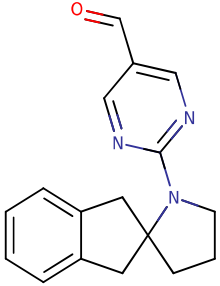
#	Time	Area%
1	1.336	100.00



RT 1.355

RT 1.356

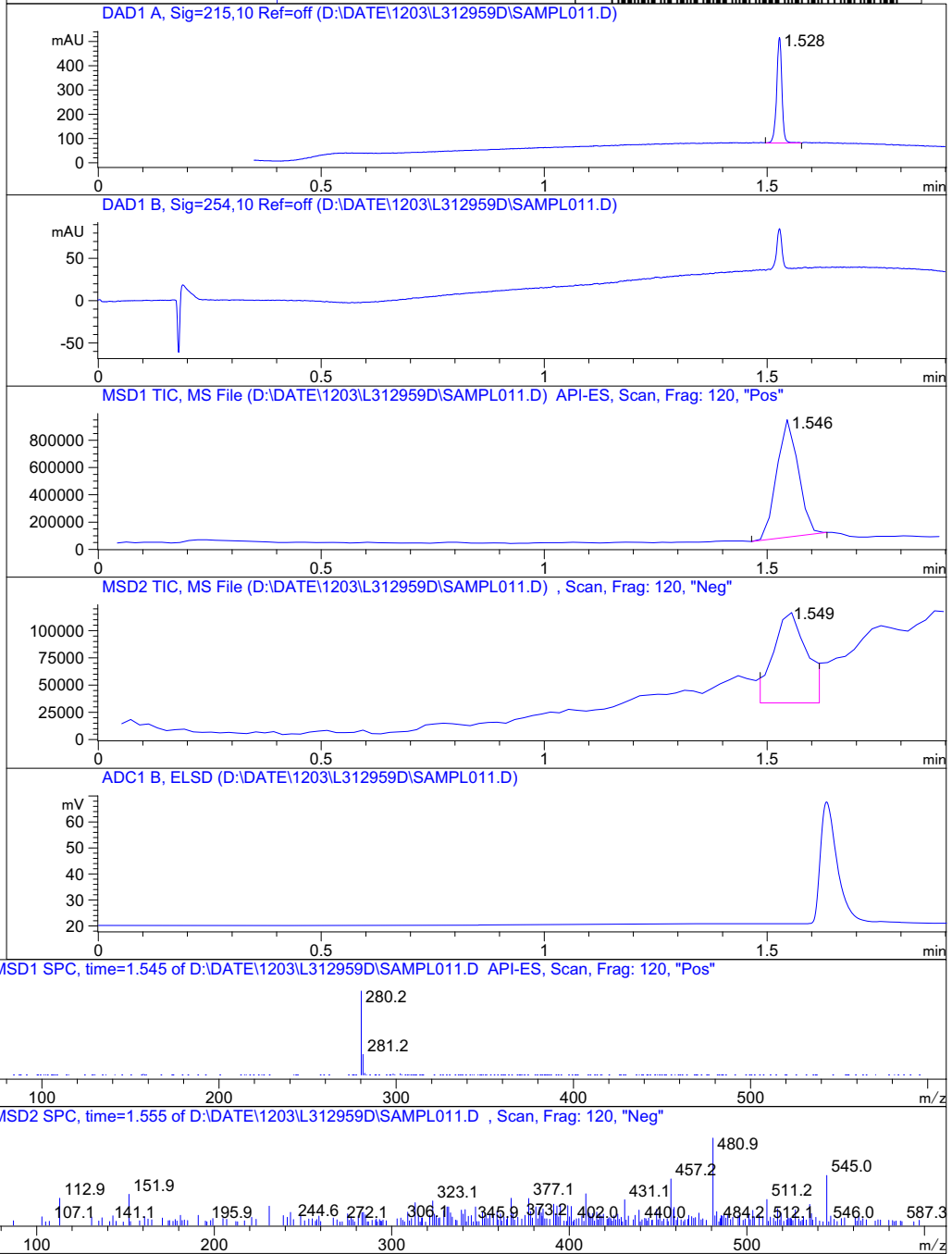
MaxPeak: 100.00%  
Ret\_Time: 1.528 min



Mol Wt 279.34  
Exact Mass 279.16

#	Time	Area%
1	1.528	100.00

S993138\$1



RT 1.546

RT 1.549

Inj.Date 12/3/2020

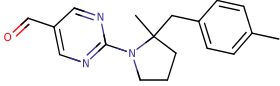
O

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Acq. Method C:\HPCHEM\ -> ->

Z2851996828\_

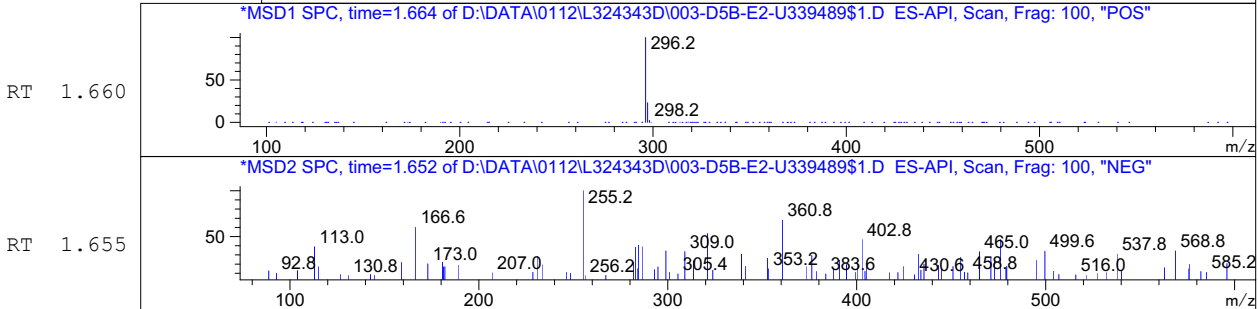
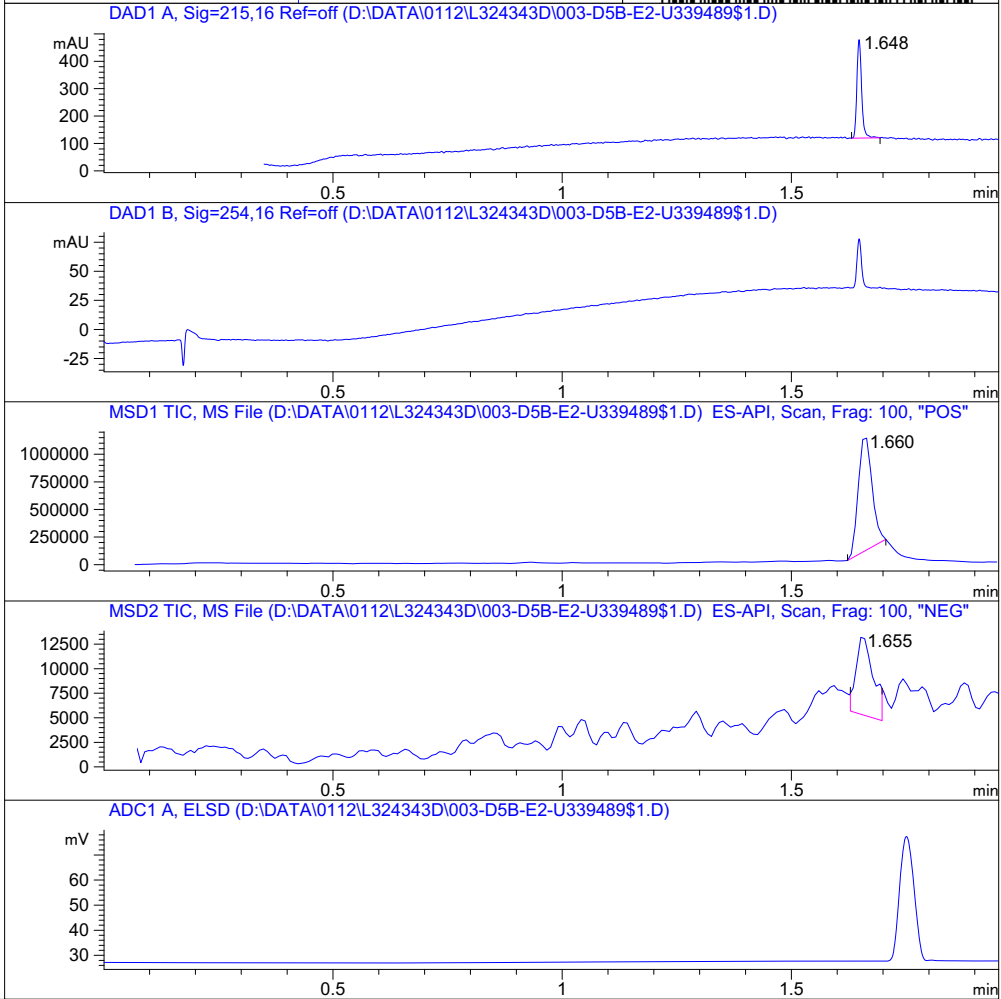
MaxPeak: 100.00%  
Ret\_Time: 1.648 min



Mol Wt 295.38  
Exact Mass 295.2

#	Time	Area%
1	1.648	100.00

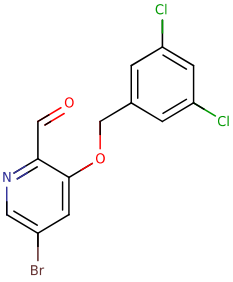
U339489\$1



W179754\$4

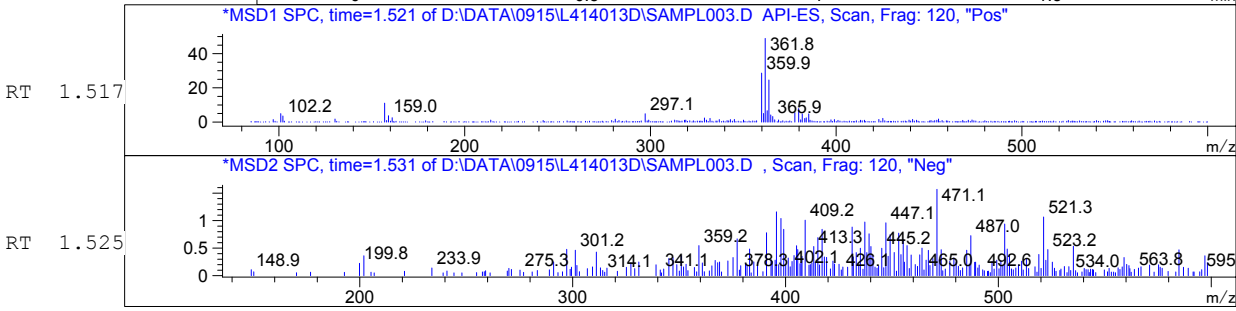
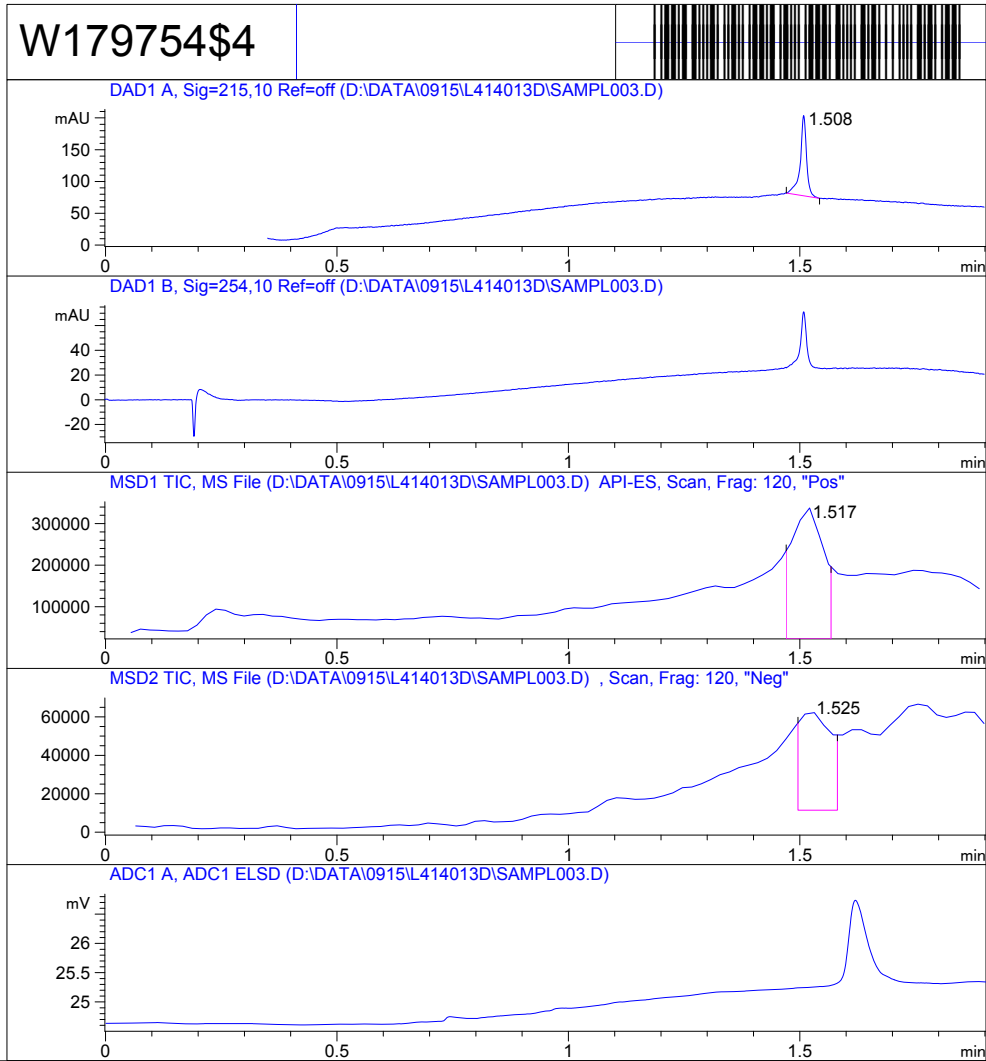


MaxPeak: 100.00%  
Ret\_Time: 1.508 min



Mol Wt 361.02  
Exact Mass 360.92

#	Time	Area%
1	1.508	100.00



Inj.Date 9/16/2021

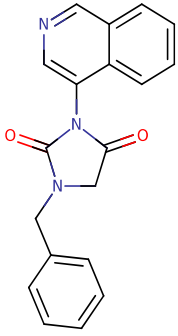
OA

-VL-

Acq. Method C:\HPCHEM\ -> ->

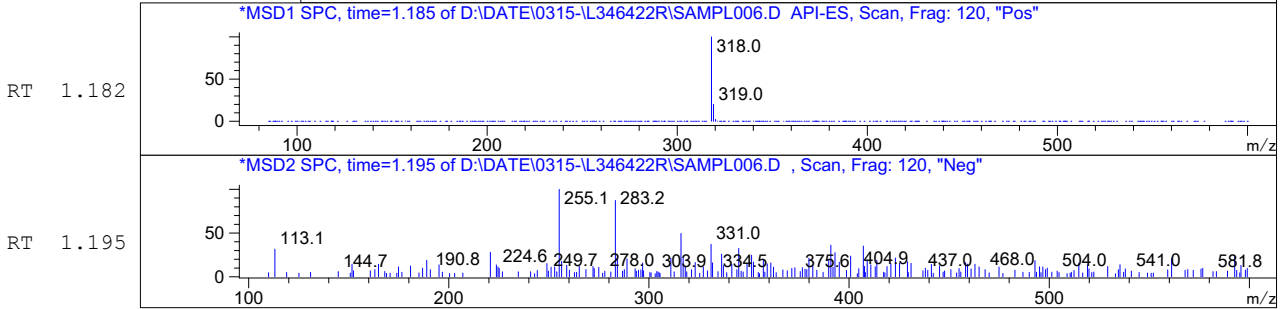
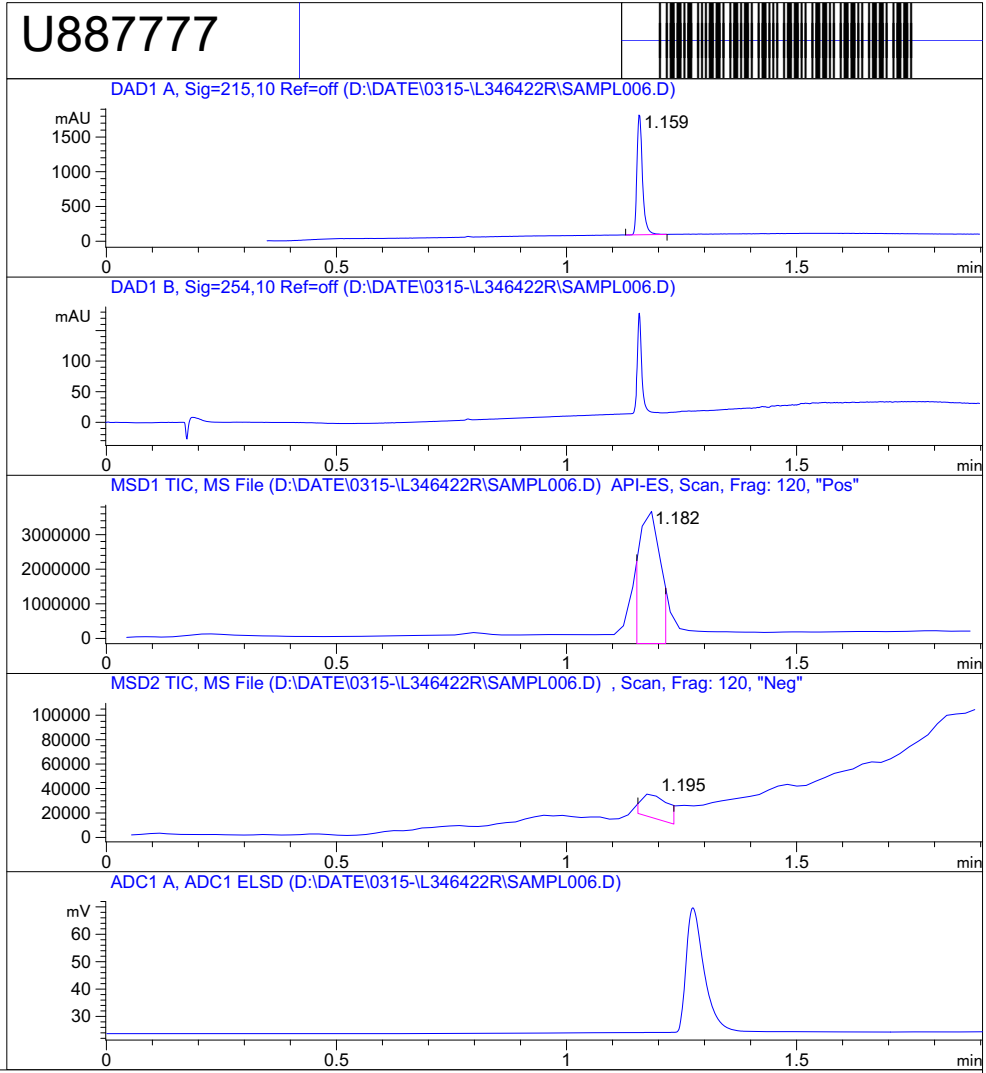
Z5192779033\_

MaxPeak: 100.00%  
Ret\_Time: 1.159 min

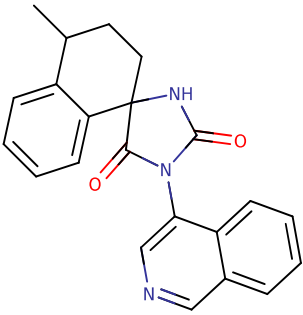


Mol Wt 317.34  
Exact Mass 317.13

#	Time	Area%
1	1.159	100.00

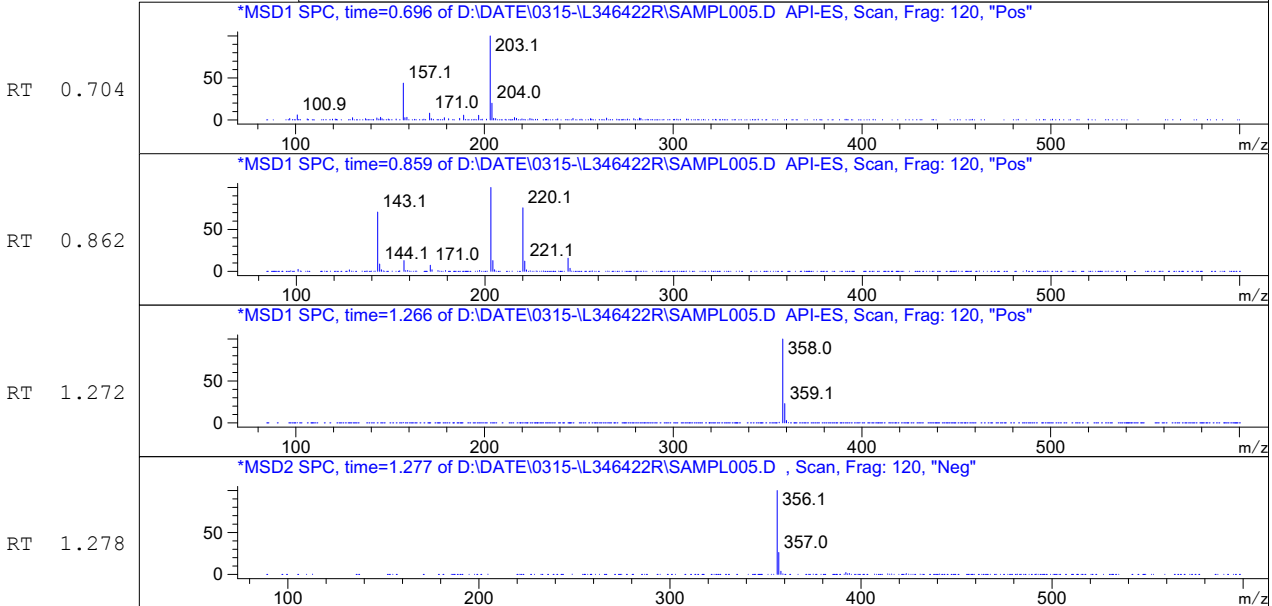
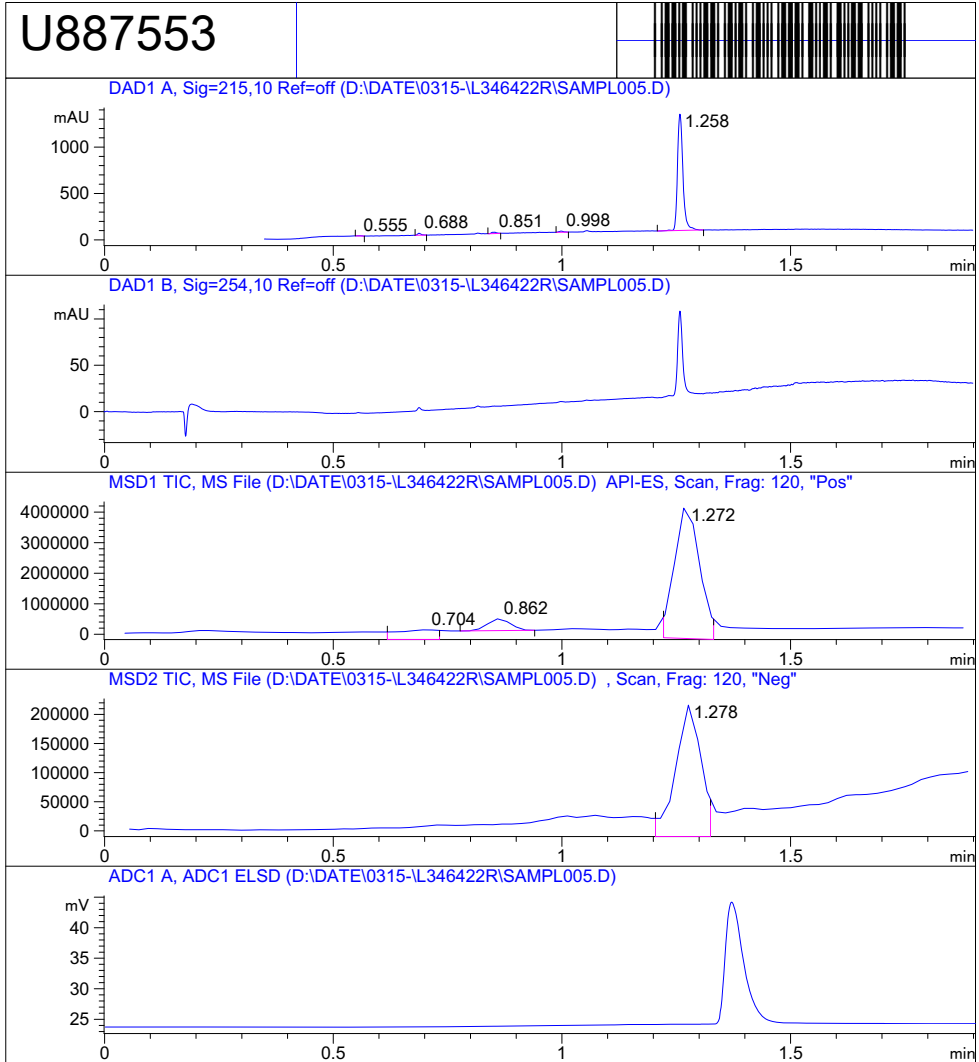


MaxPeak: 96.82%  
Ret\_Time: 1.258 min



Mol Wt 357.4  
Exact Mass 357.17

#	Time	Area%
1	0.555	0.19
2	0.688	1.05
3	0.851	1.12
4	0.998	0.81
5	1.258	96.82



Inj.Date 3/16/2021

E

-VL-

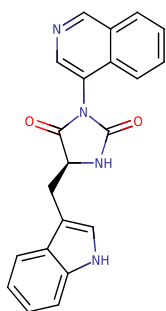
Acq. Method C:\HPCHEM\> >

Z4929616137\_



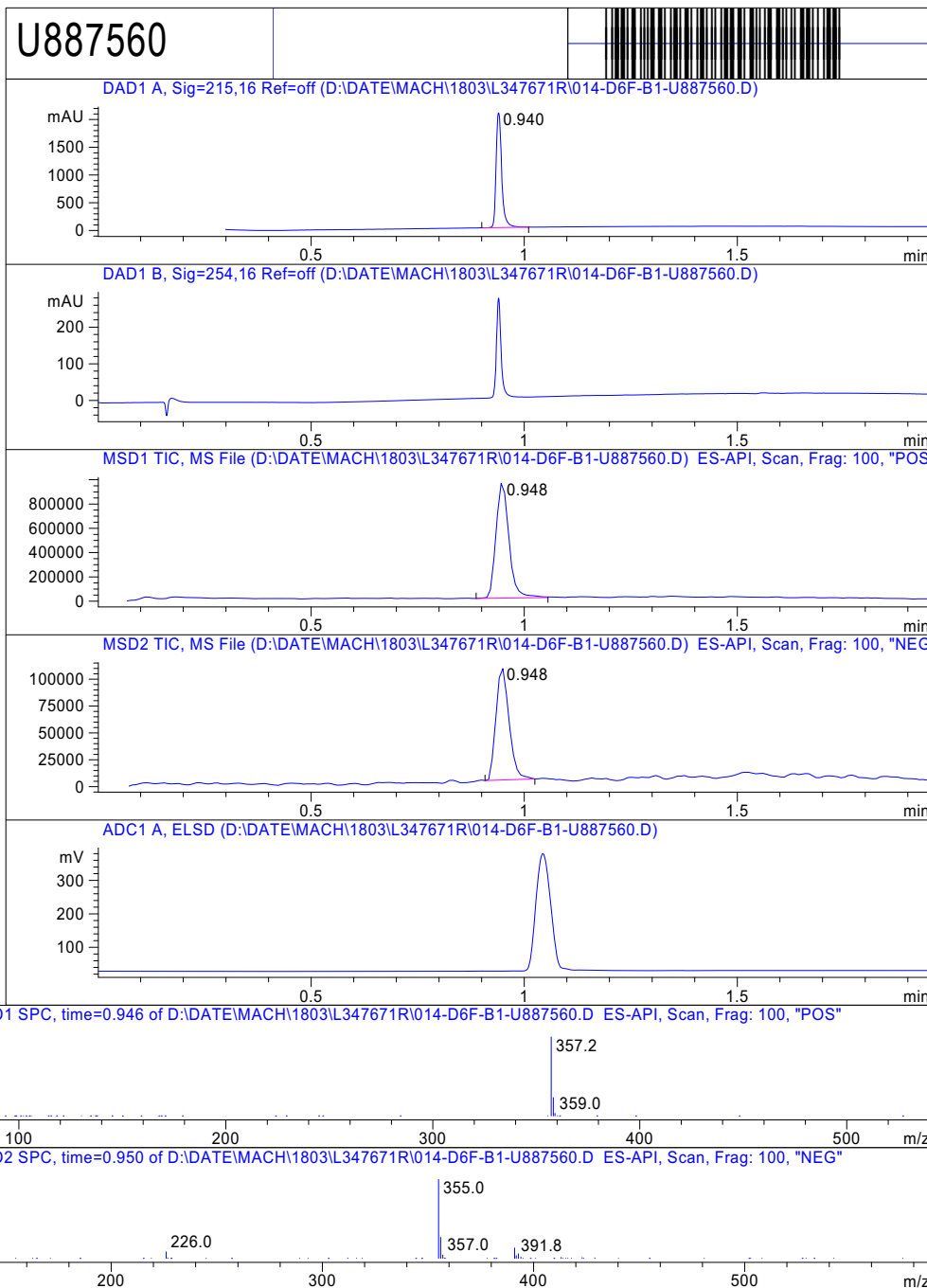


MaxPeak: 100.00%  
Ret\_Time: 0.940 min

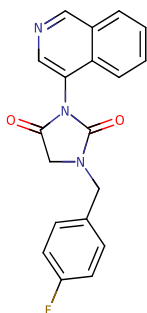


Mol Wt 356.38  
Exact Mass 356.14

#	Time	Area%
1	0.940	100.00



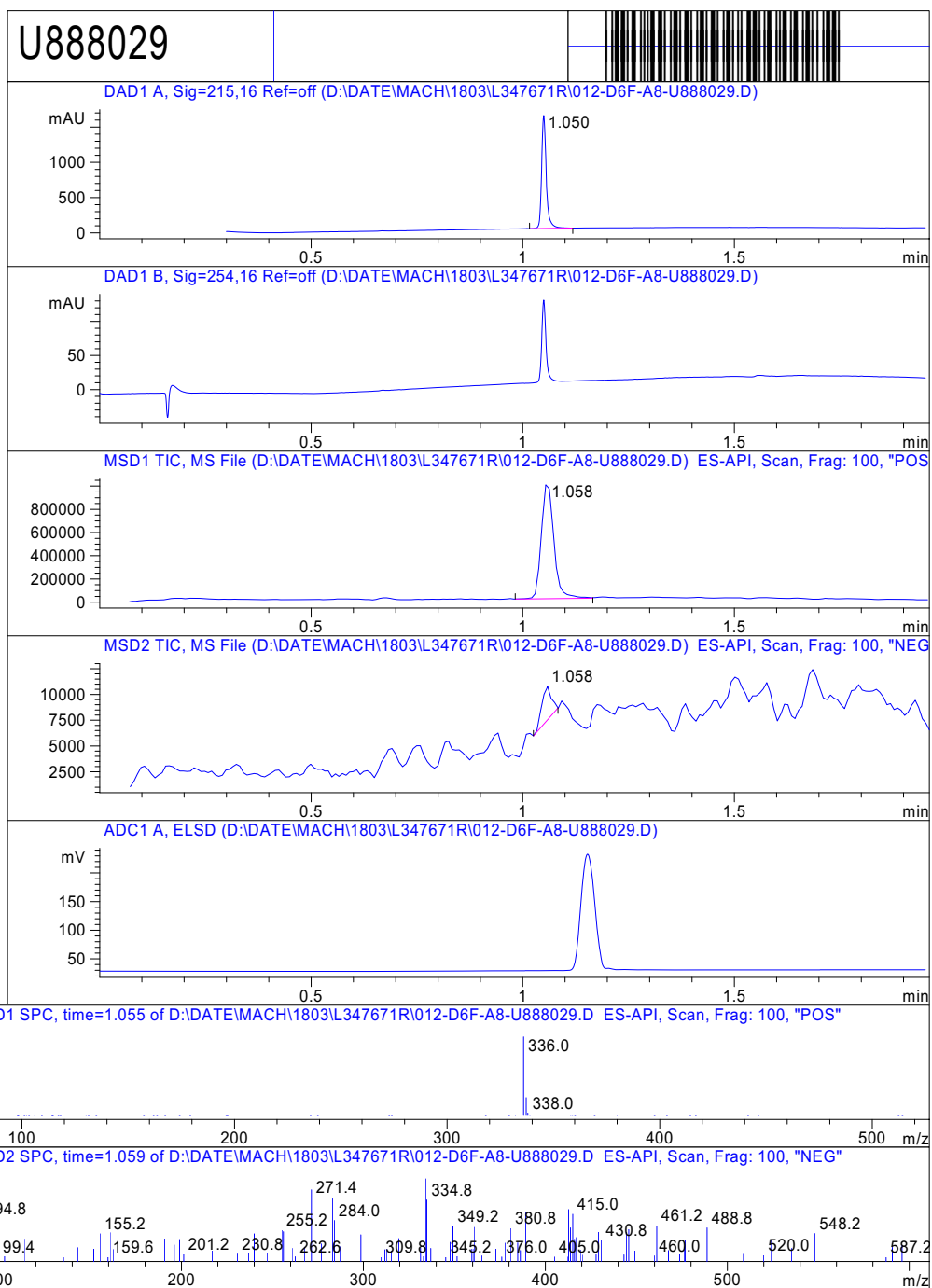
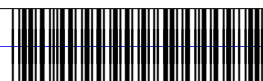
MaxPeak: 100.00%  
Ret\_Time: 1.050 min



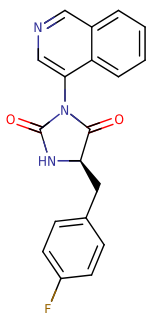
Mol Wt 335.33  
Exact Mass 335.12

#	Time	Area%
1	1.050	100.00

U888029



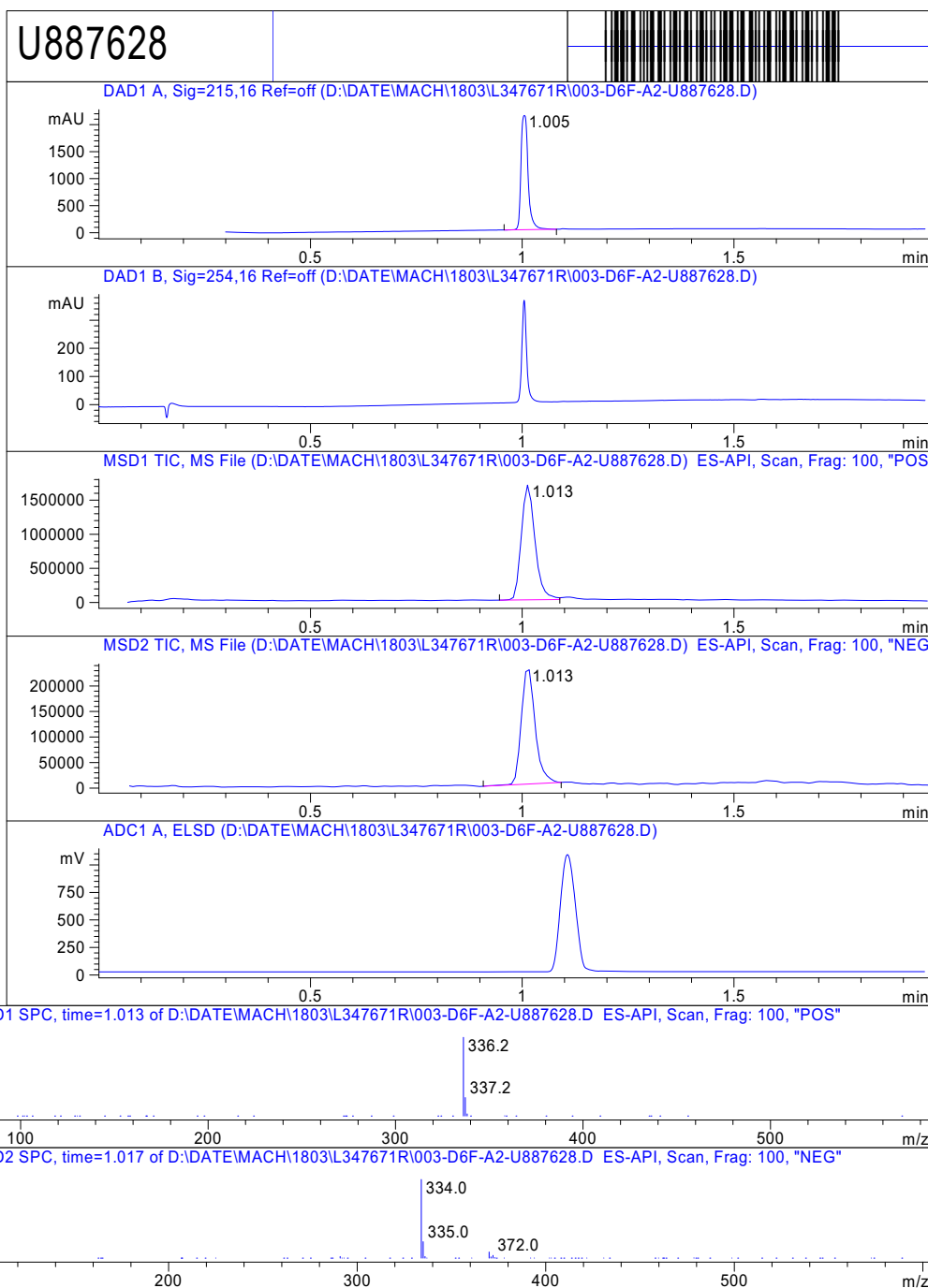
MaxPeak: 100.00%  
Ret\_Time: 1.005 min



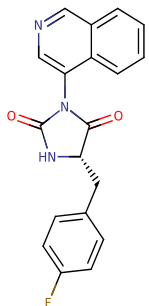
Mol Wt 335.33  
Exact Mass 335.12

#	Time	Area%
1	1.005	100.00

# U887628



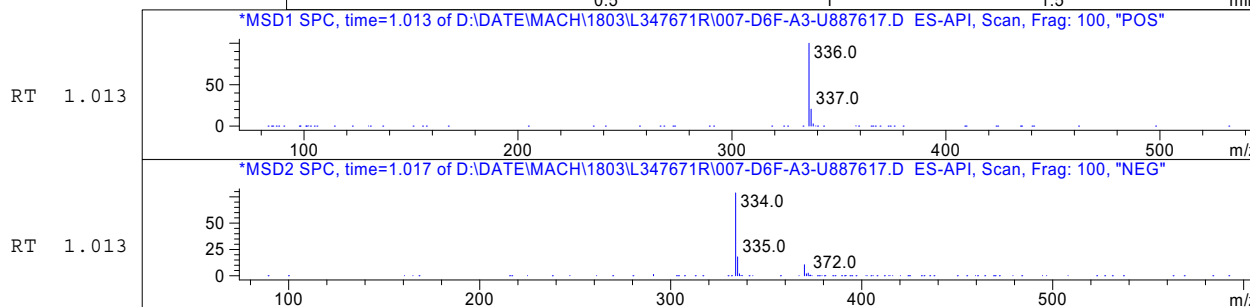
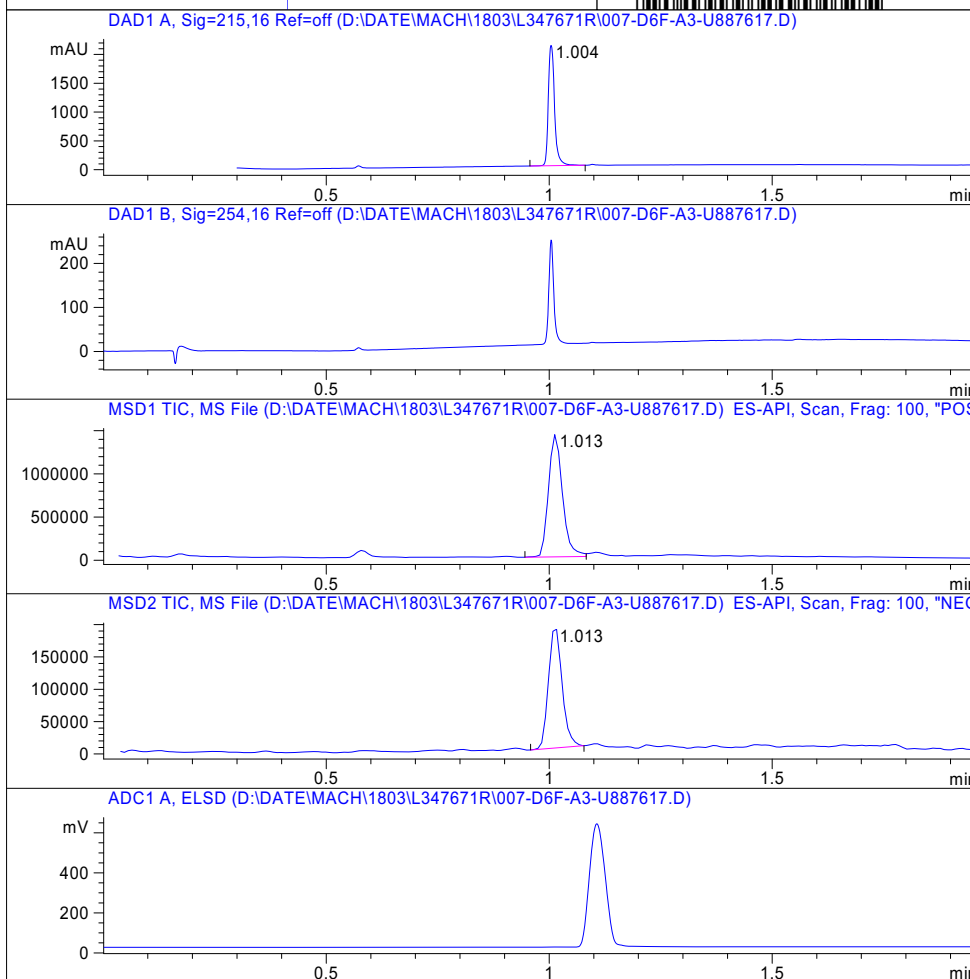
MaxPeak: 100.00%  
Ret\_Time: 1.004 min



Mol Wt 335.33  
Exact Mass 335.12

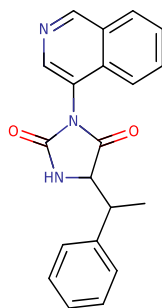
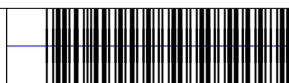
#	Time	Area%
1	1.004	100.00

# U887617



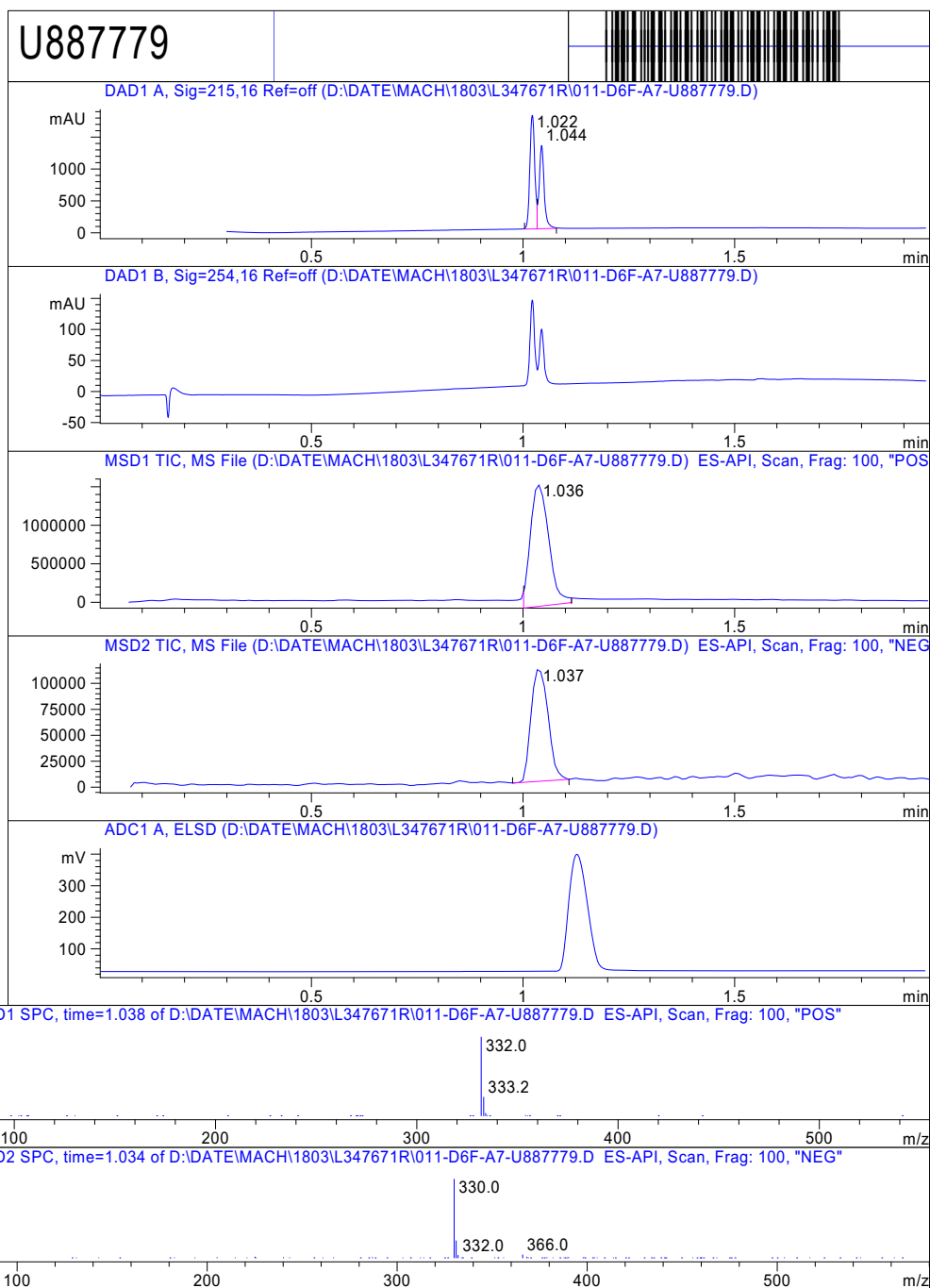
MaxPeak: 57.60%  
Ret\_Time: 1.022 min

# U887779

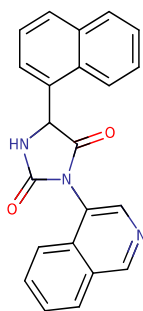


**Mol Wt** 331.37  
**Exact Mass** 331.15

#	Time	Area%
1	1.022	57.60
2	1.044	42.40

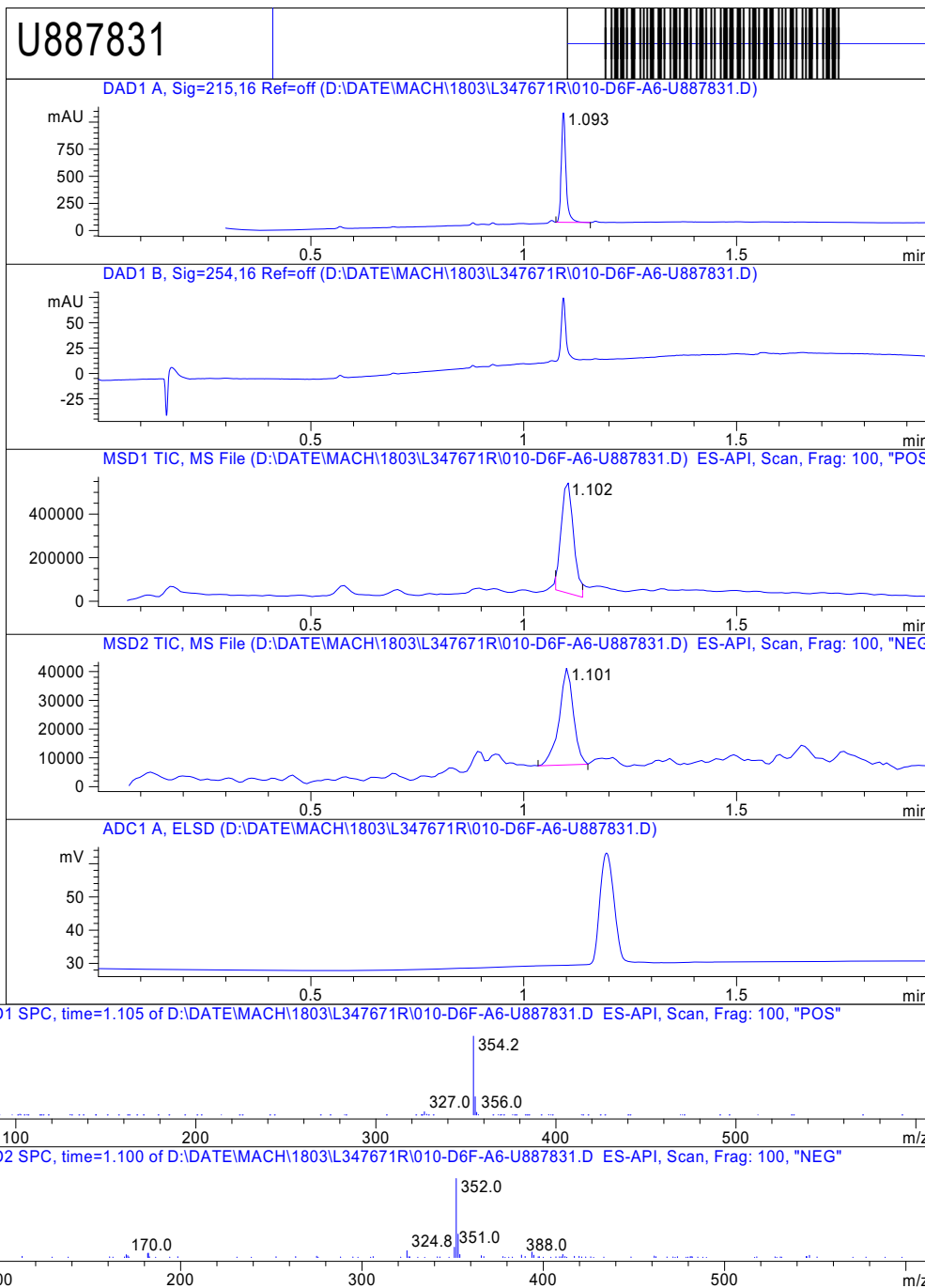


MaxPeak: 100.00%  
Ret\_Time: 1.093 min

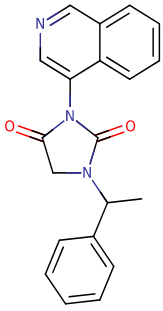


Mol Wt 353.37  
Exact Mass 353.13

#	Time	Area%
1	1.093	100.00

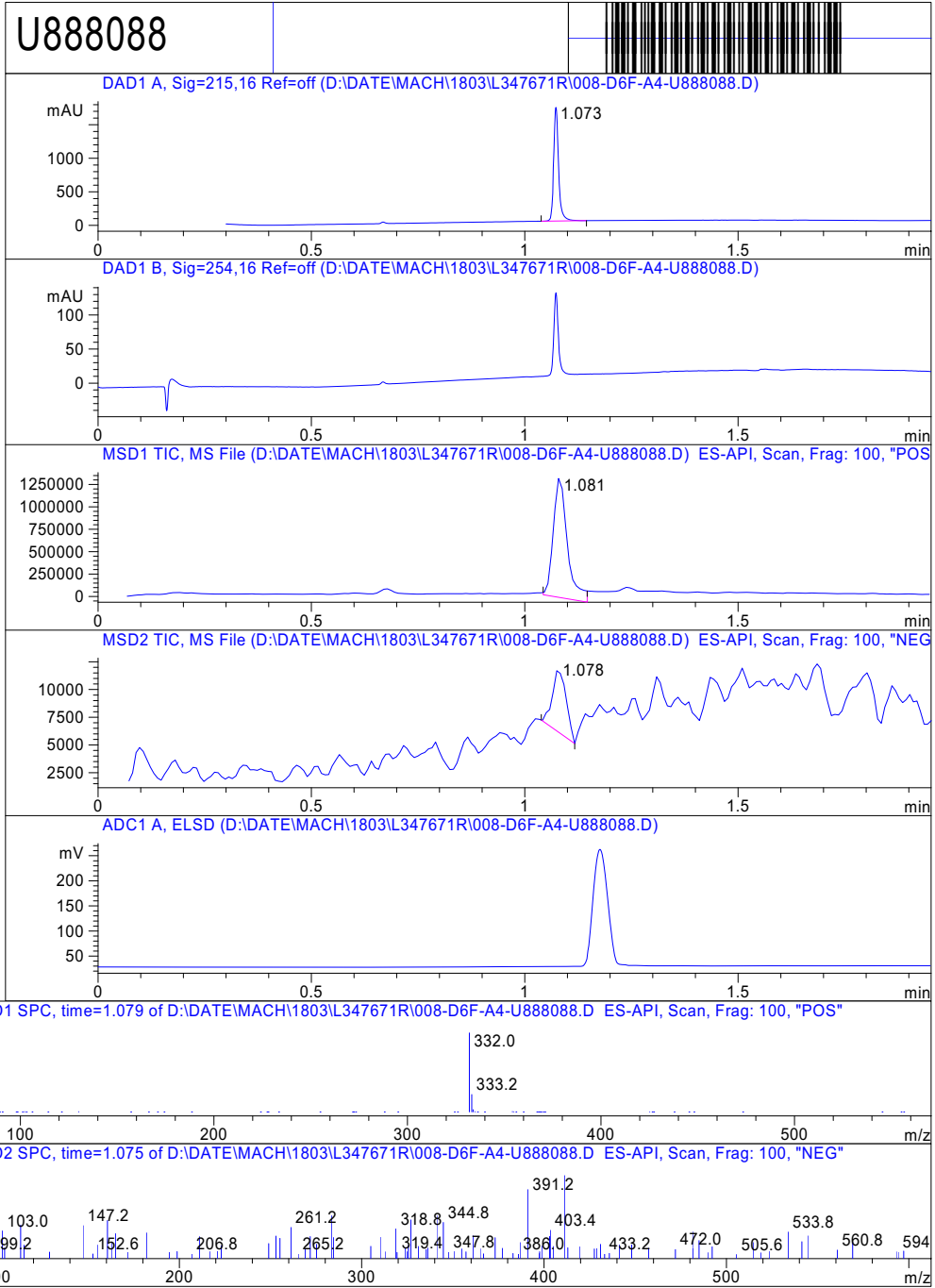


MaxPeak: 100.00%  
Ret\_Time: 1.073 min



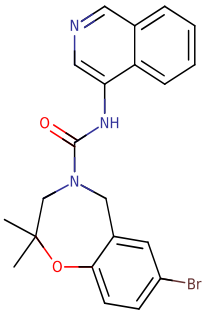
Mol Wt 331.37  
Exact Mass 331.15

#	Time	Area%
1	1.073	100.00





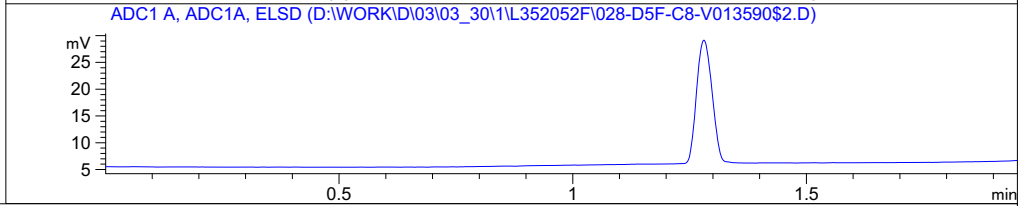
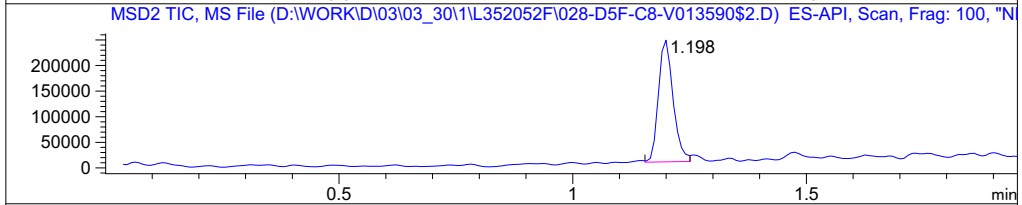
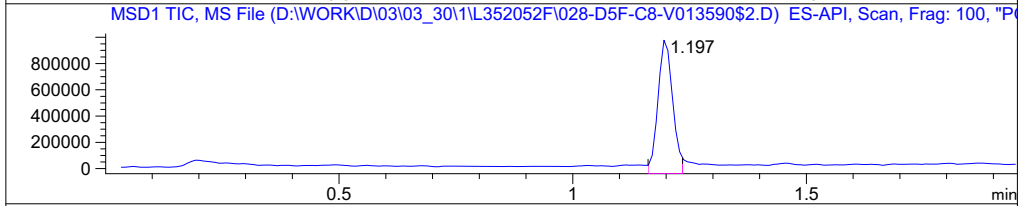
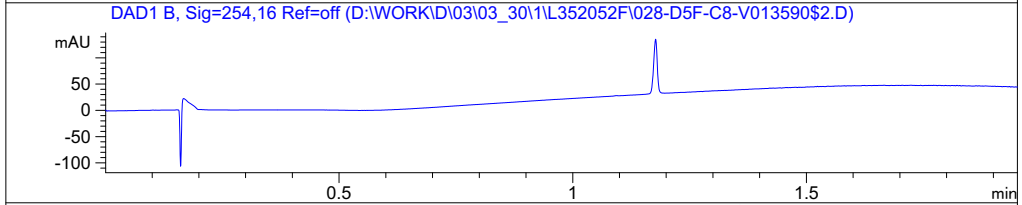
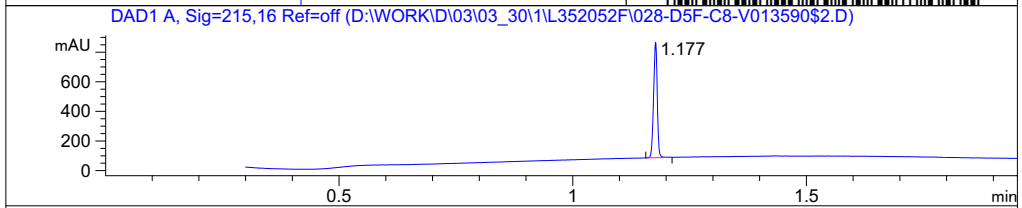
MaxPeak: 100.00%  
Ret\_Time: 1.177 min



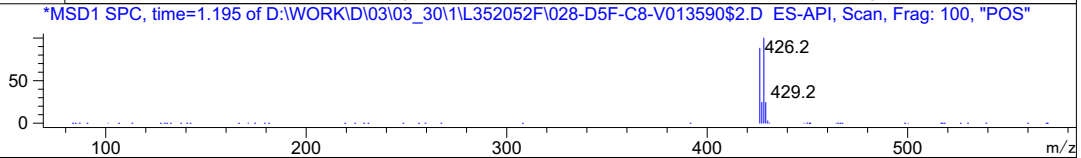
Mol Wt 426.31  
Exact Mass 427.1

#	Time	Area%
1	1.177	100.00

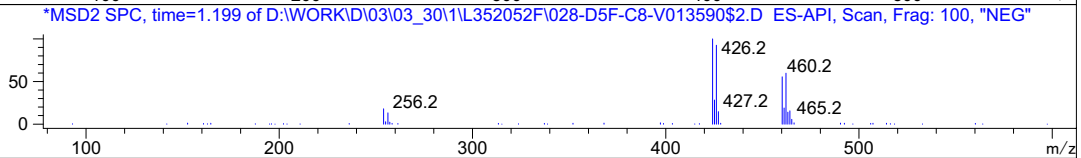
V013590\$2



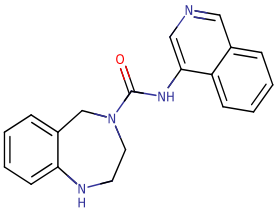
RT 1.197



RT 1.198



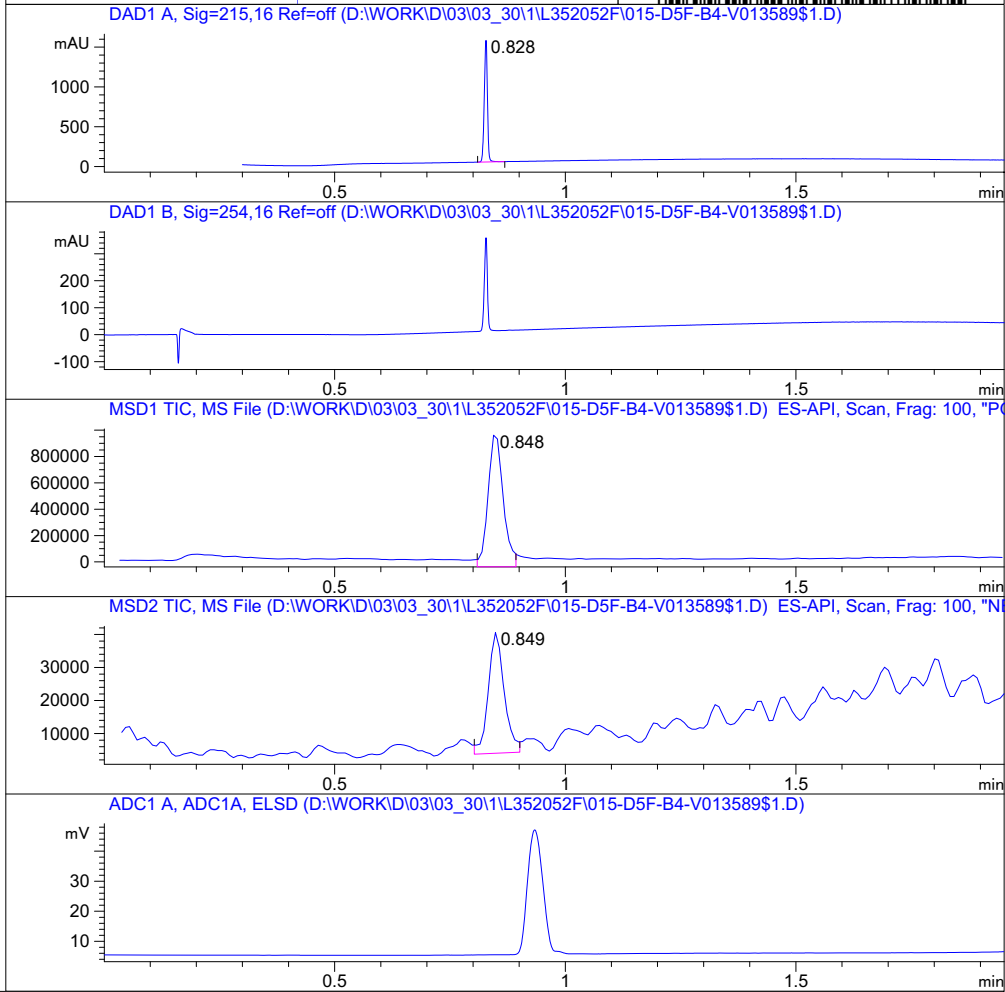
MaxPeak: 100.00%  
Ret\_Time: 0.828 min



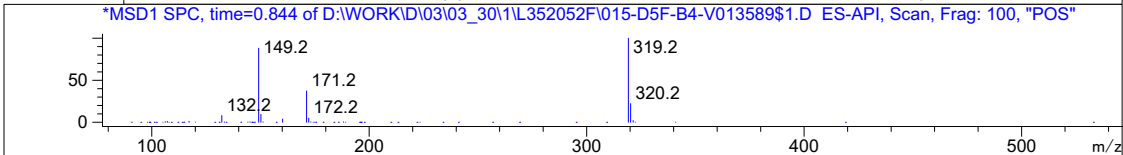
Mol Wt 318.37  
Exact Mass 318.17

#	Time	Area%
1	0.828	100.00

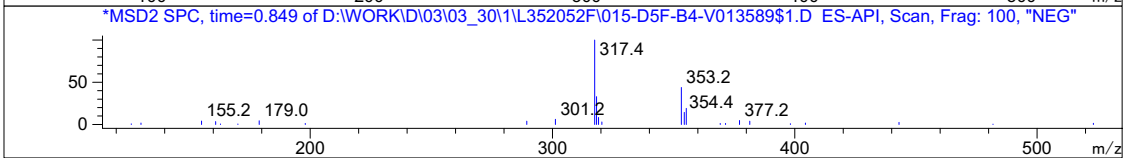
V013589\$1



RT 0.848



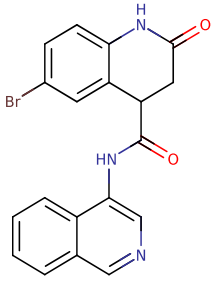
RT 0.849



V048775\$2

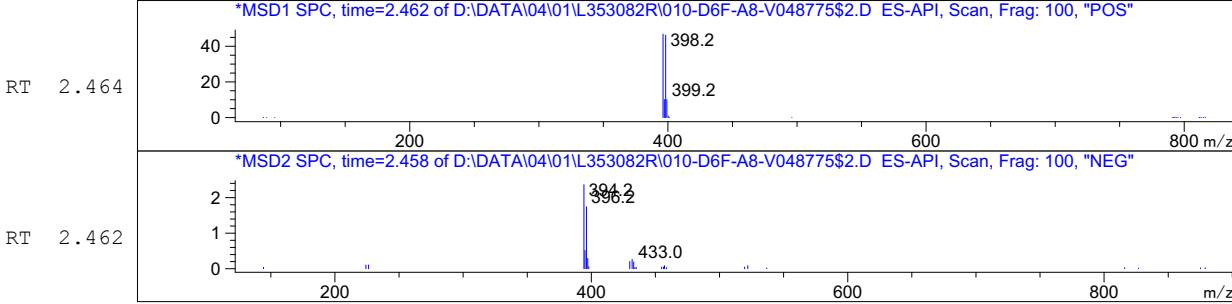
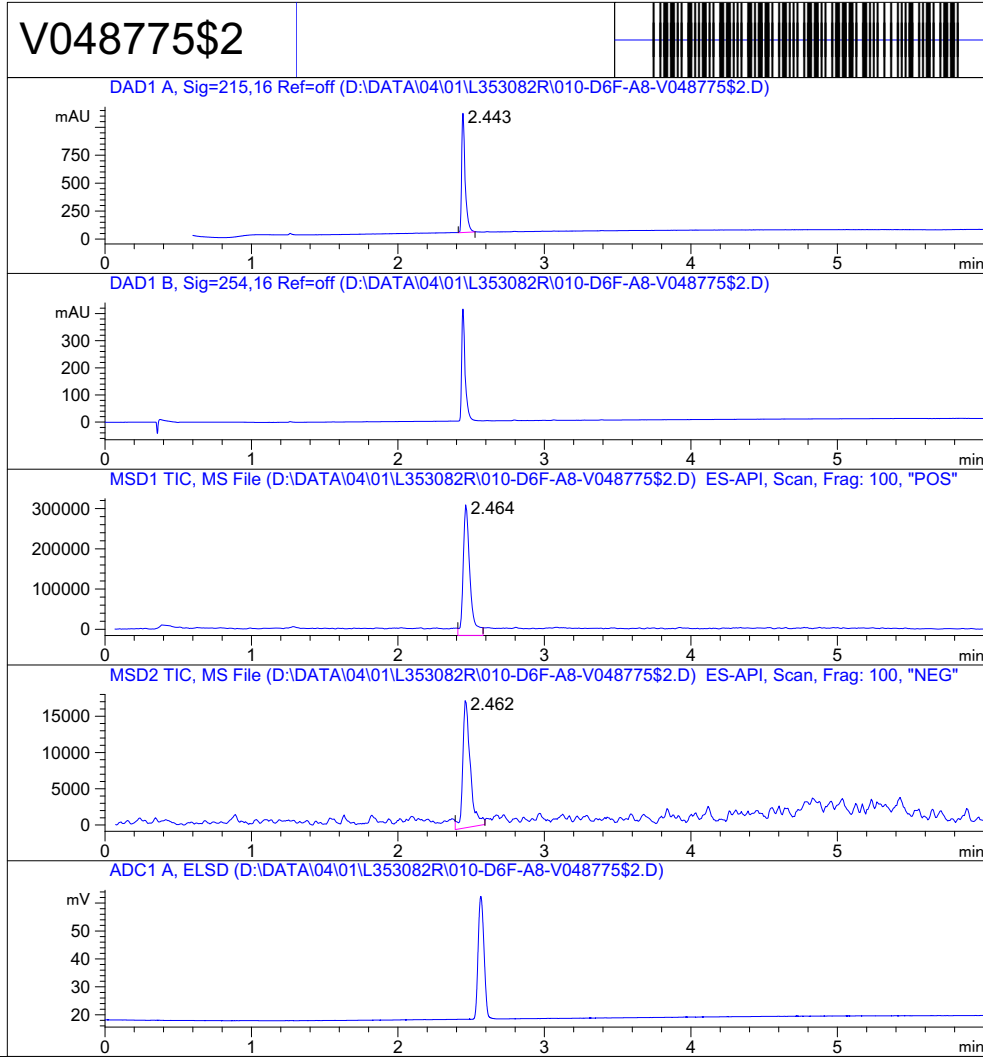


MaxPeak: 100.00%  
Ret\_Time: 2.443 min

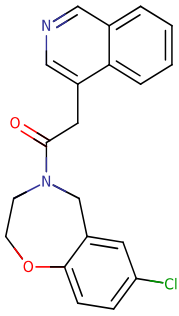


Mol Wt 396.24  
Exact Mass 395.04

#	Time	Area%
1	2.443	100.00



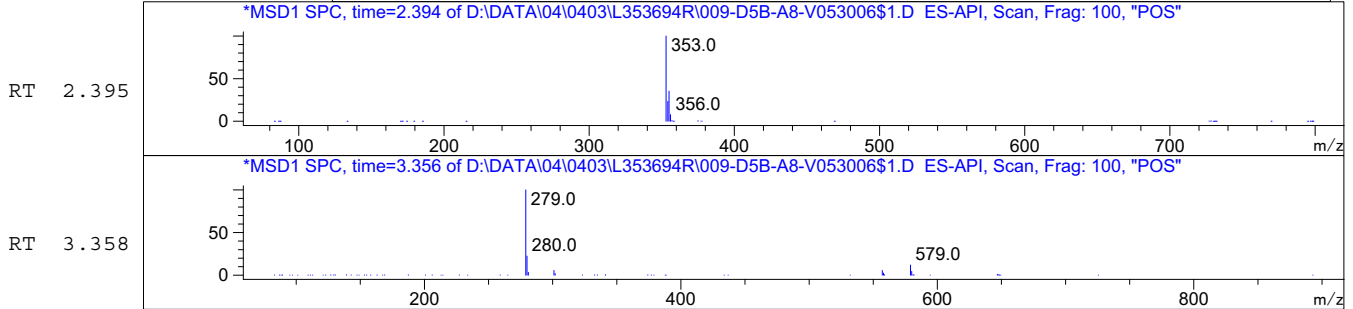
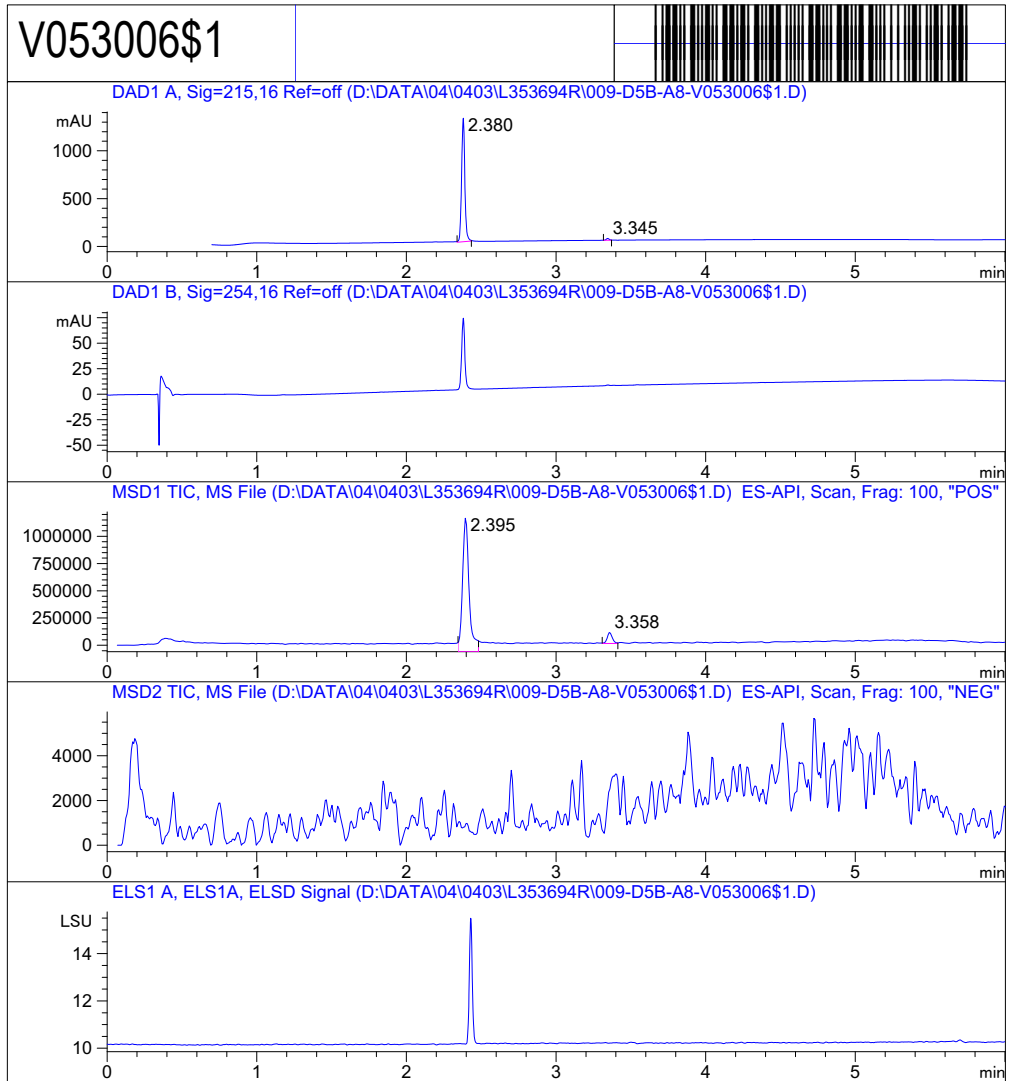
MaxPeak: 98.67%  
Ret\_Time: 2.380 min



Mol Wt 352.81  
Exact Mass 352.12

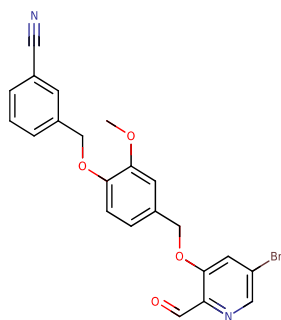
#	Time	Area%
1	2.380	98.67
2	3.345	1.33

V053006\$1



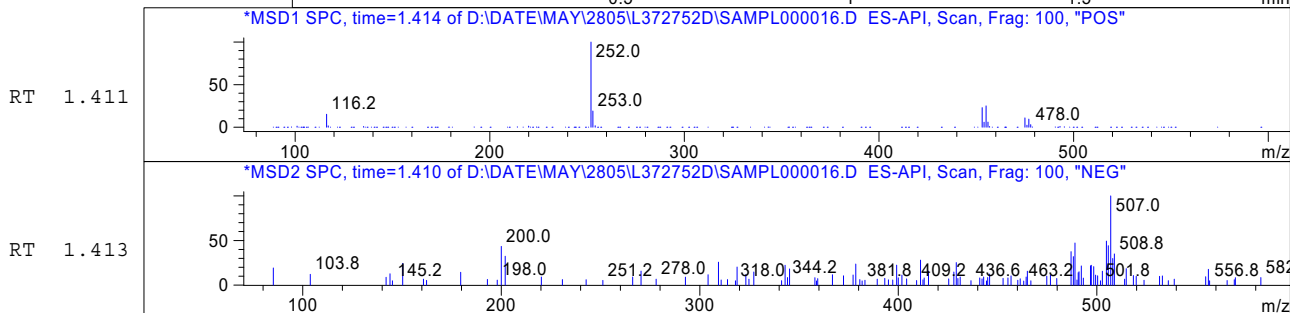
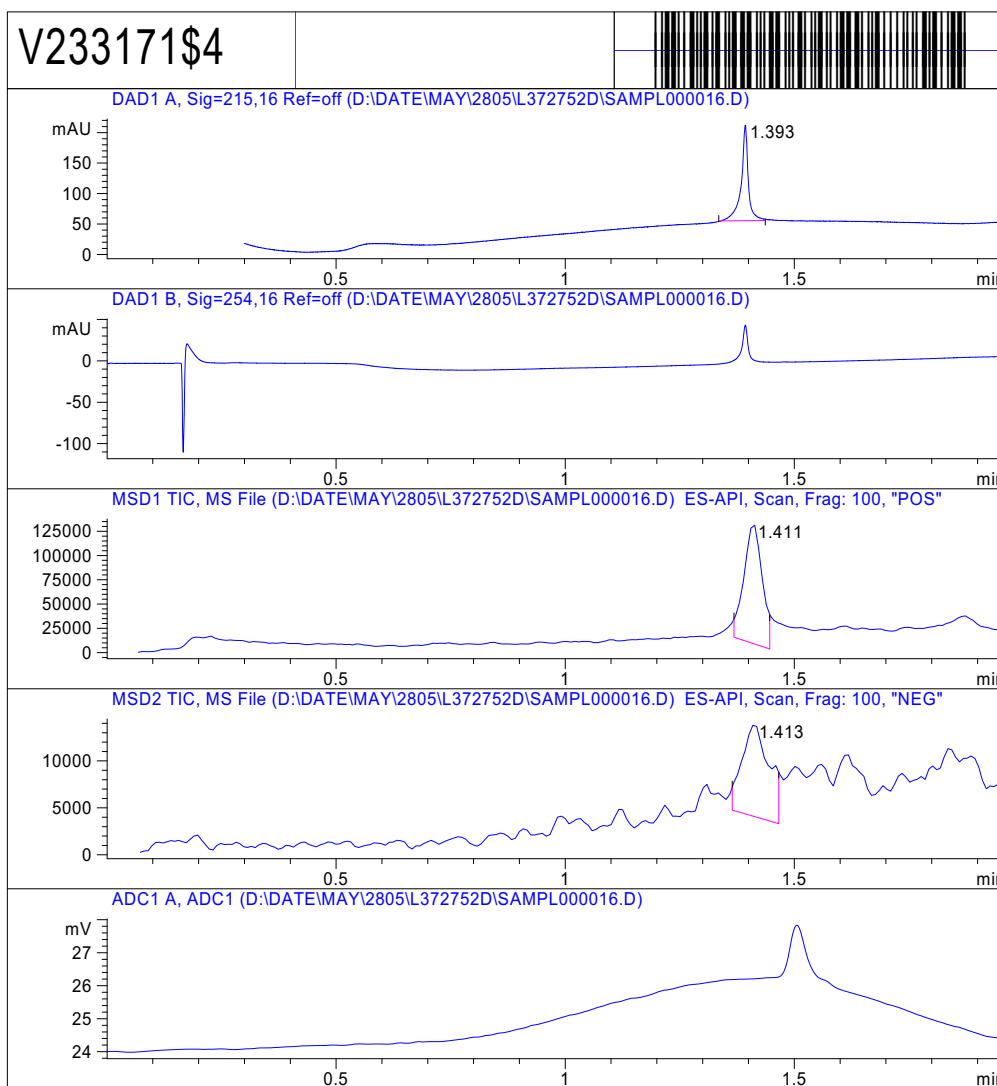
MaxPeak: 100.00%  
Ret\_Time: 1.393 min

V233171\$4



Mol Wt 453.28  
Exact Mass 454.05

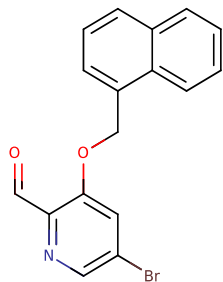
#	Time	Area%
1	1.393	100.00



# V608763\$7

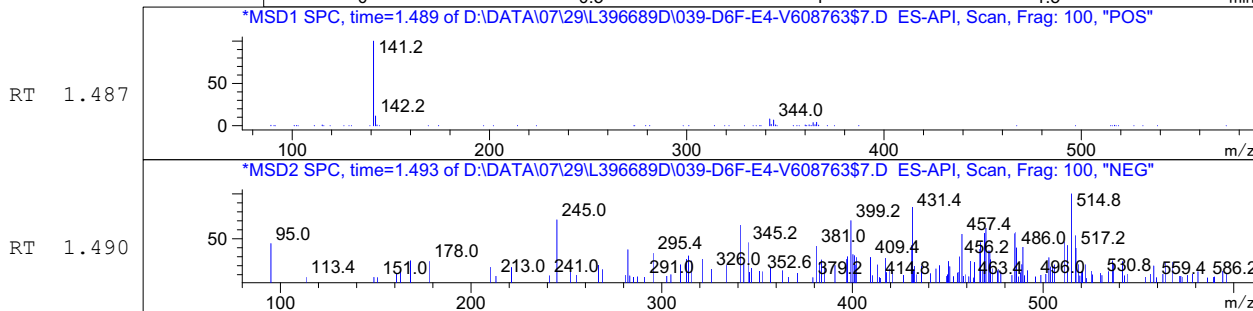
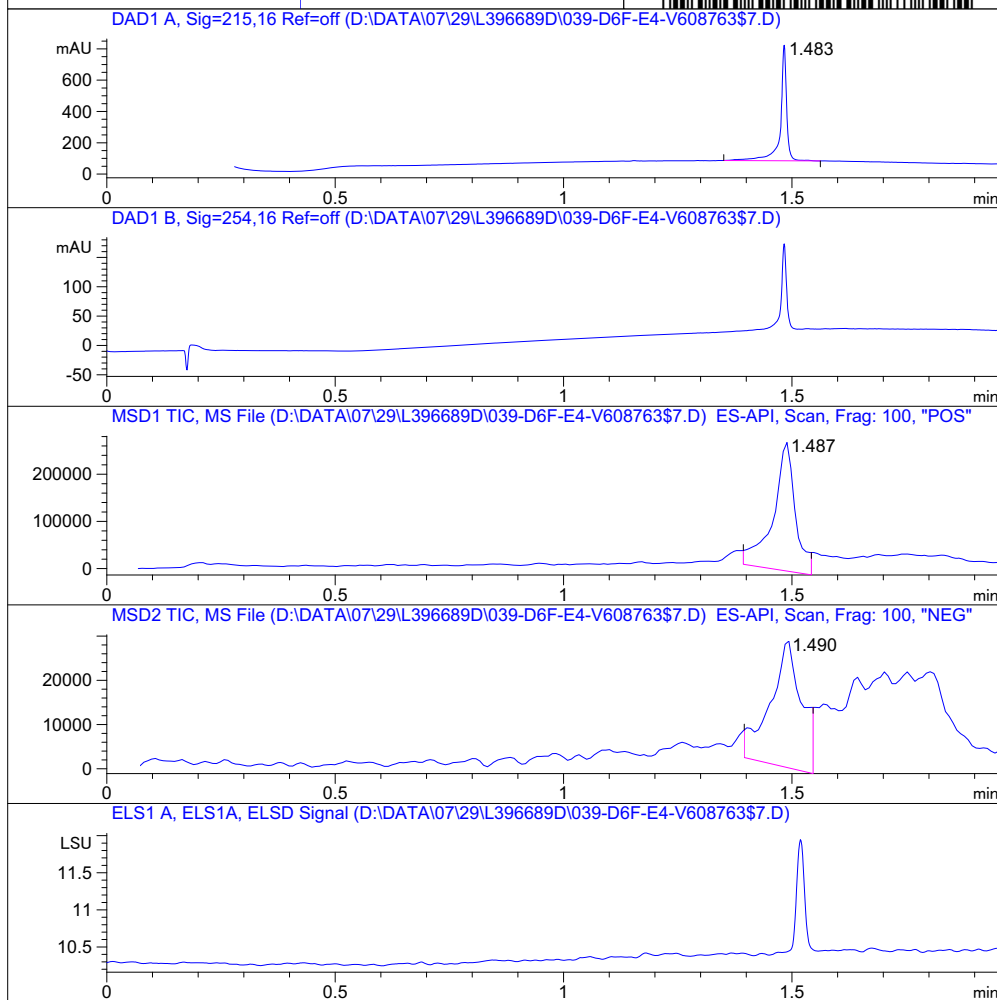


MaxPeak: 100.00%  
Ret\_Time: 1.483 min

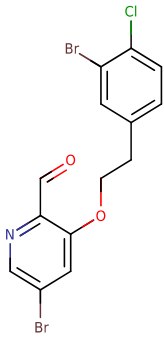


Mol Wt 342.19  
Exact Mass 341.02

#	Time	Area%
1	1.483	100.00

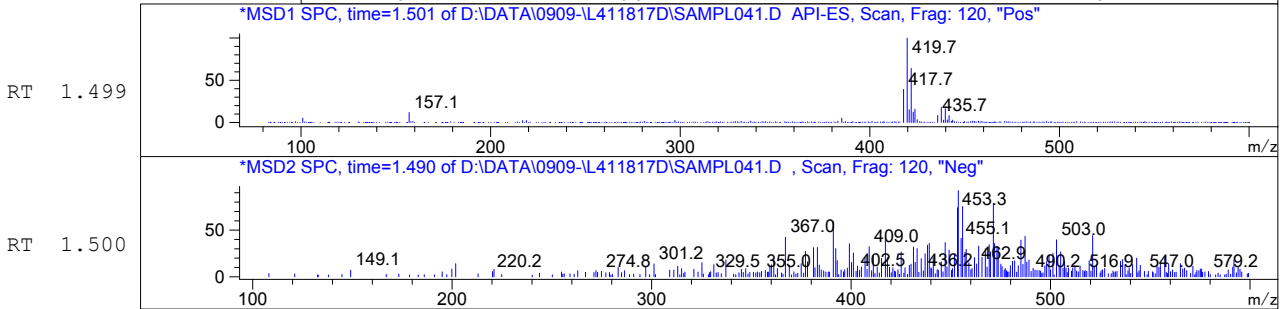
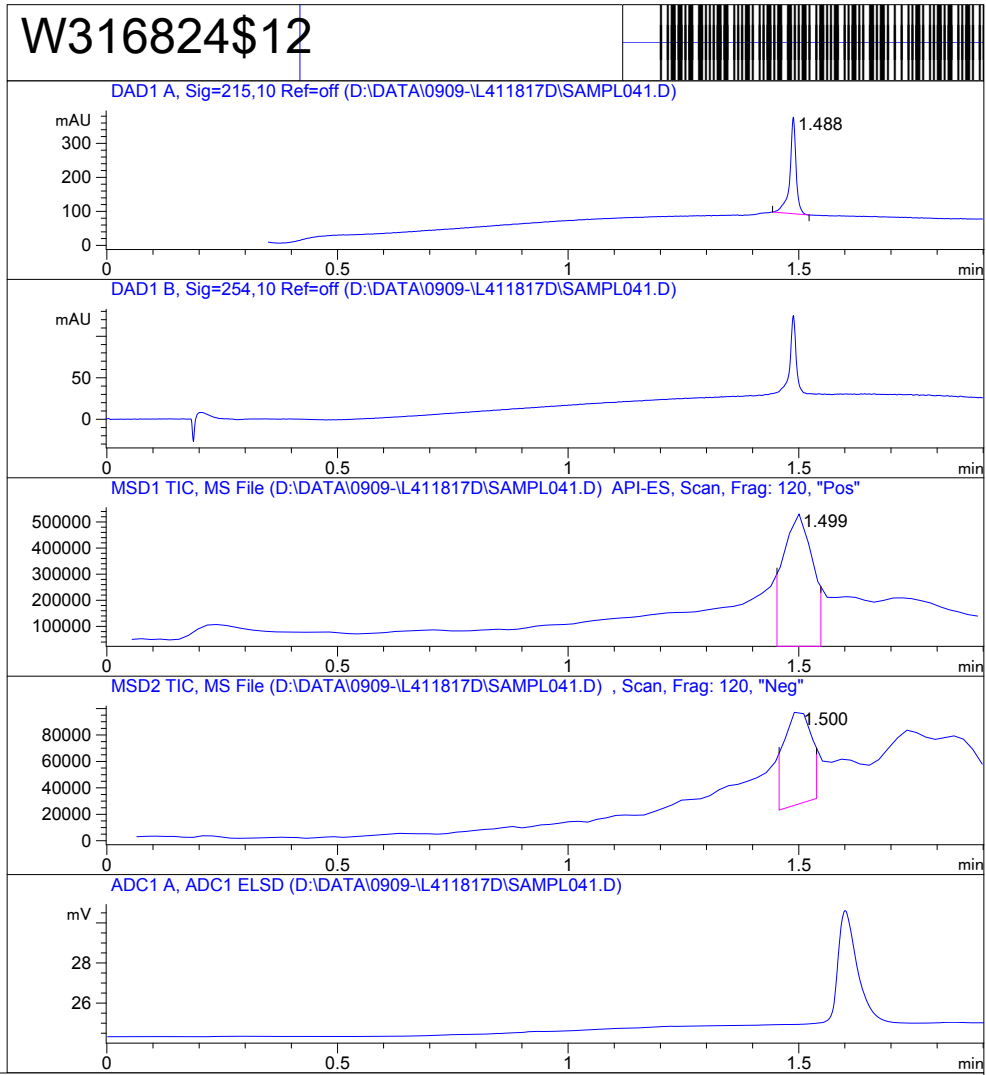


MaxPeak: 100.00%  
Ret\_Time: 1.488 min



Mol Wt 419.5  
Exact Mass 418.89

#	Time	Area%
1	1.488	100.00



Inj.Date 9/9/2021

OA

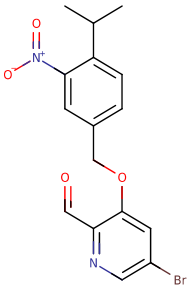
-VL-

Acq. Method C:\HPCHEM\ ->

->

Z5192779061\_

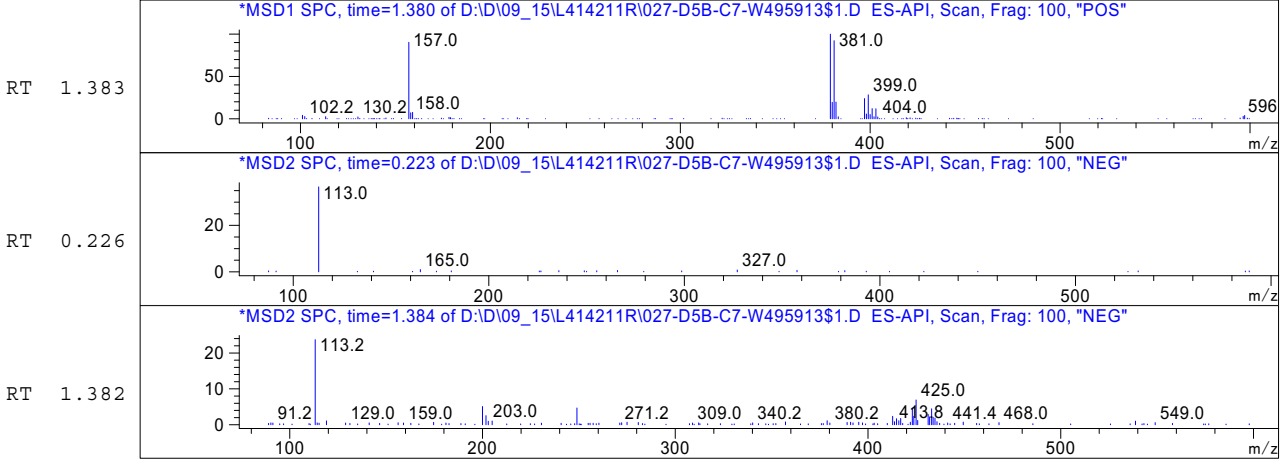
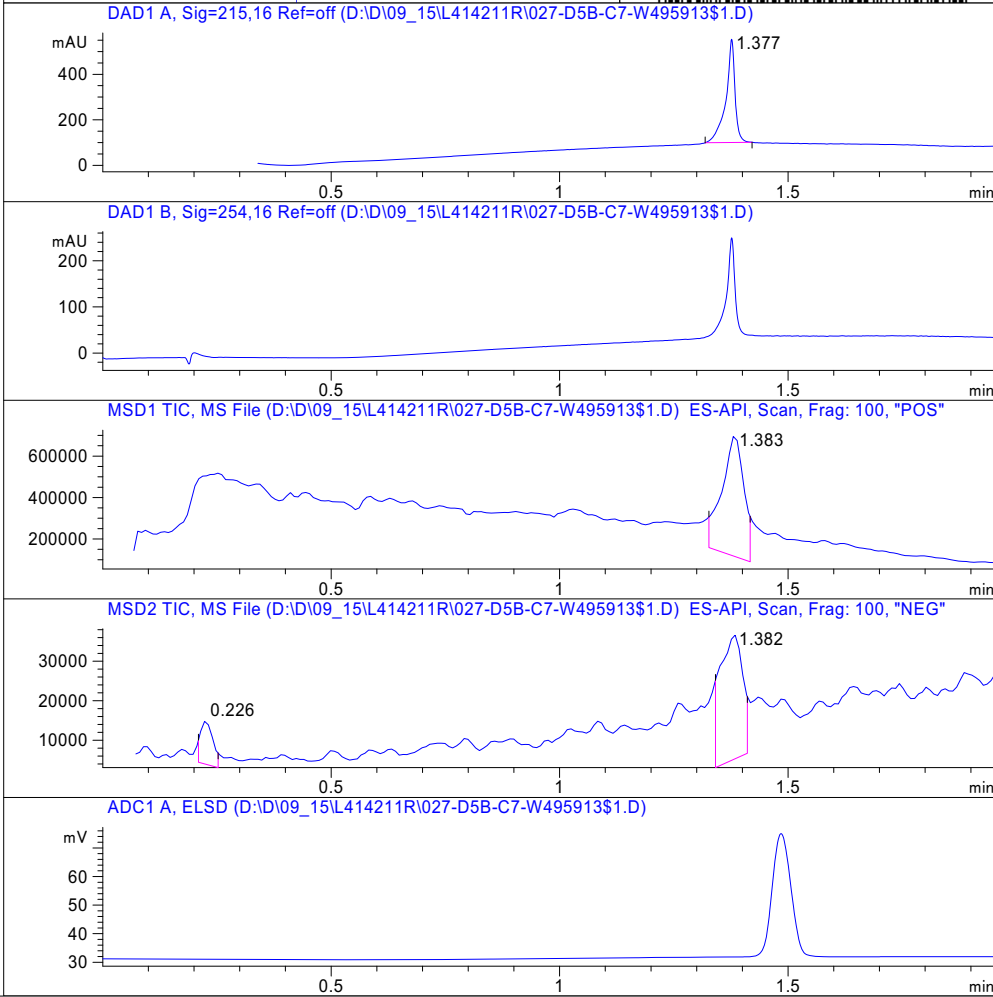
MaxPeak: 100.00%  
Ret\_Time: 1.377 min



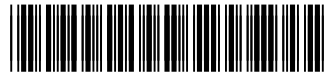
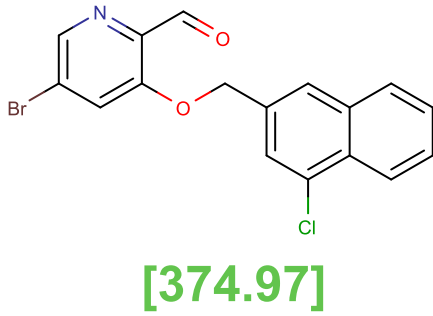
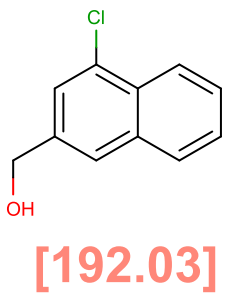
Mol Wt 379.2  
Exact Mass 378.03

#	Time	Area%
1	1.377	100.00

W495913\$1



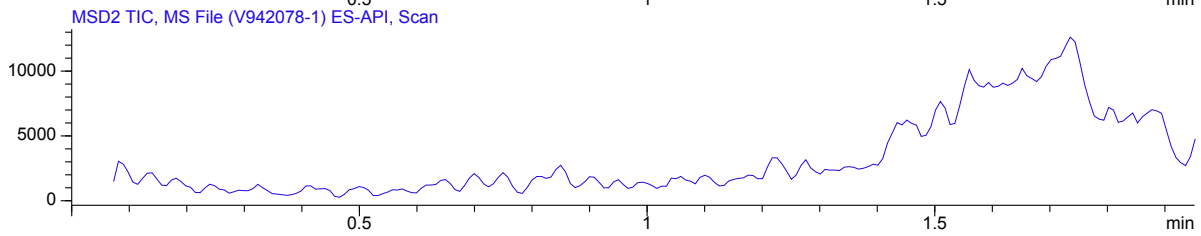
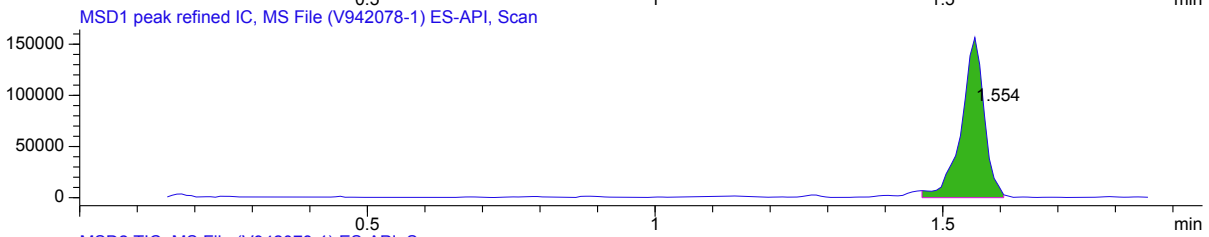
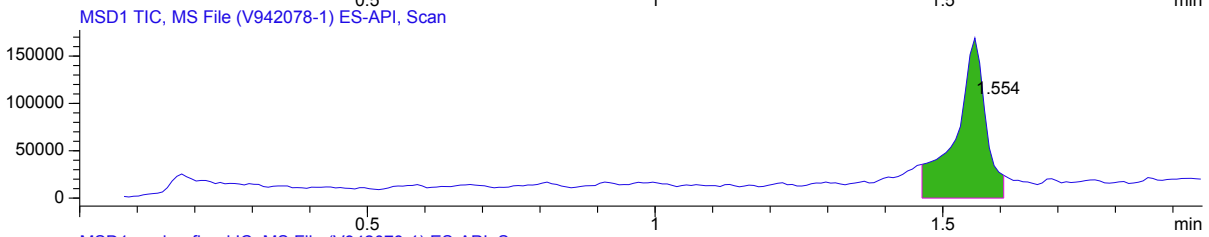
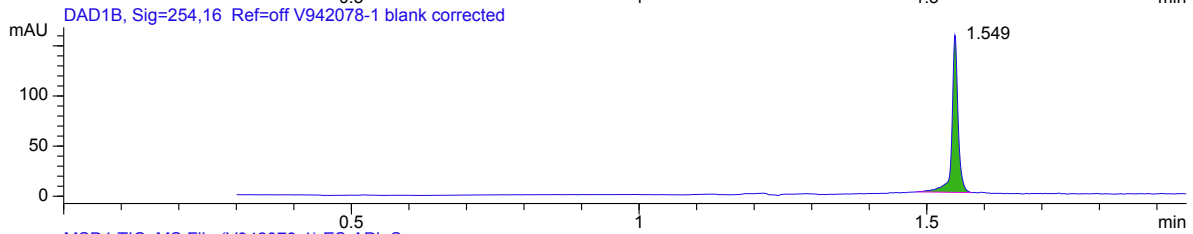
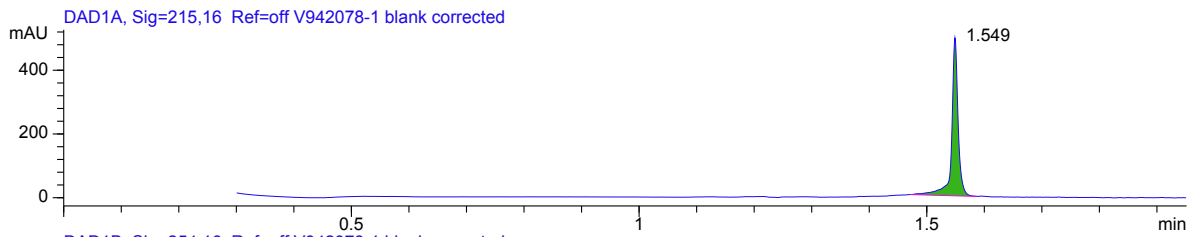




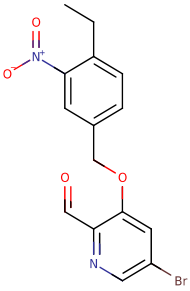
V942078-1

L411799F  
 LCMS-16  
 SUPOR\_30.M  
 09:49 09.09.2021  
 MaxPeak: 100.0%

#	RT	DAD1A	DAD1B	MSD1	MSD2	ELSD	MSD1 ions	MSD1 rt	MSD2 ions	MSD2 rt	Info
1	1.549	100.0%	100.0%	100.0%	---	100.0%	175.0(51),377.8(26),375.8(16)	1.554	---	---	Reagent1 -OH,P +H+



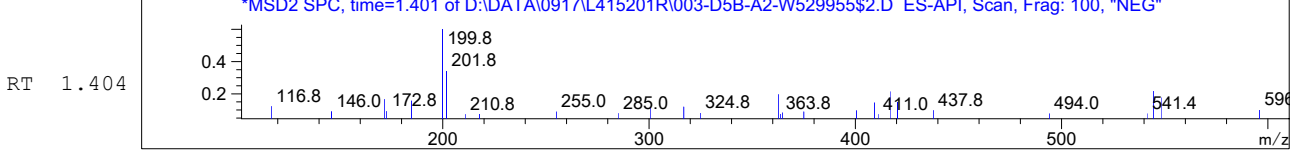
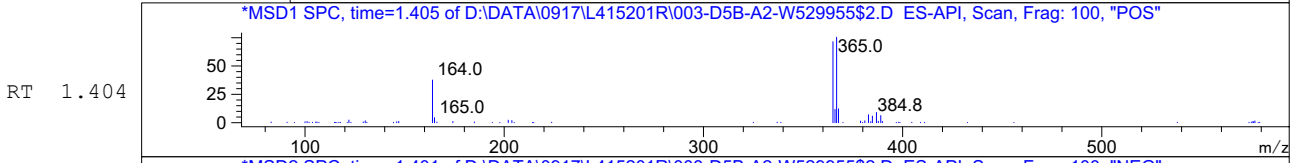
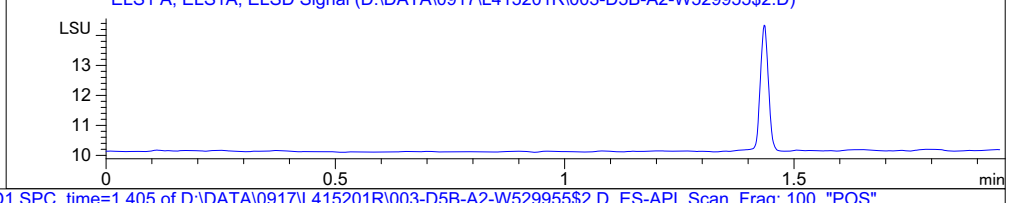
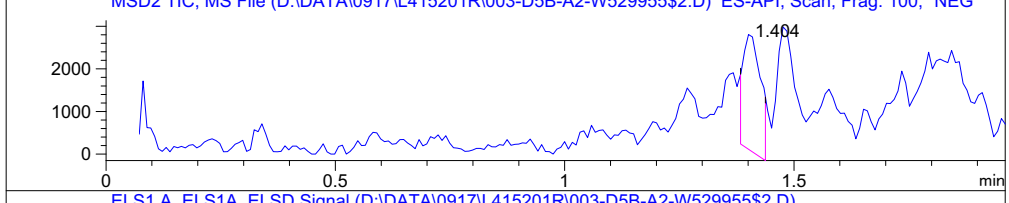
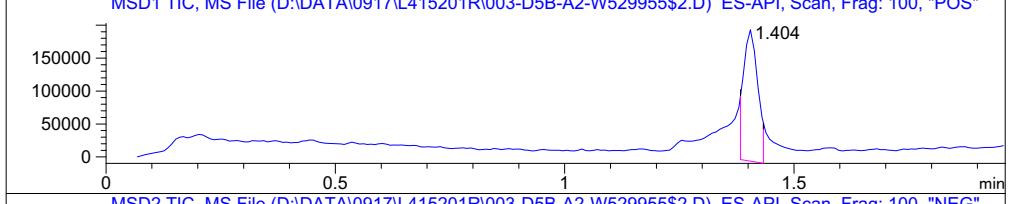
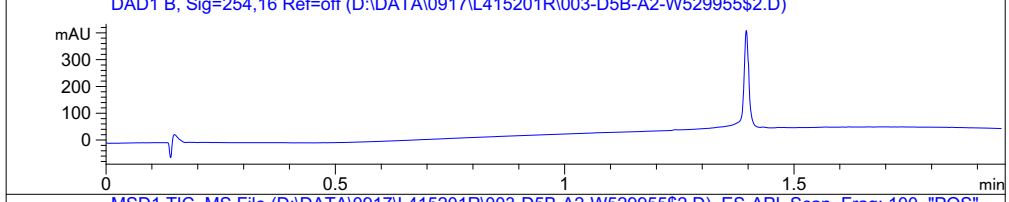
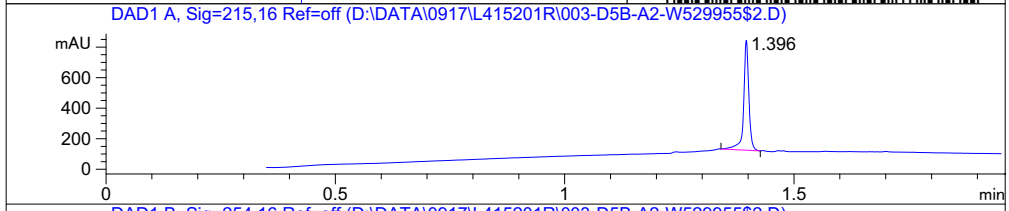
MaxPeak: 100.00%  
Ret\_Time: 1.396 min



Mol Wt 365.18  
Exact Mass 364.01

#	Time	Area%
1	1.396	100.00

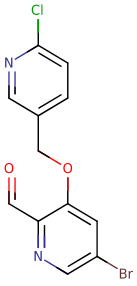
# W529955\$2



U920104\$26

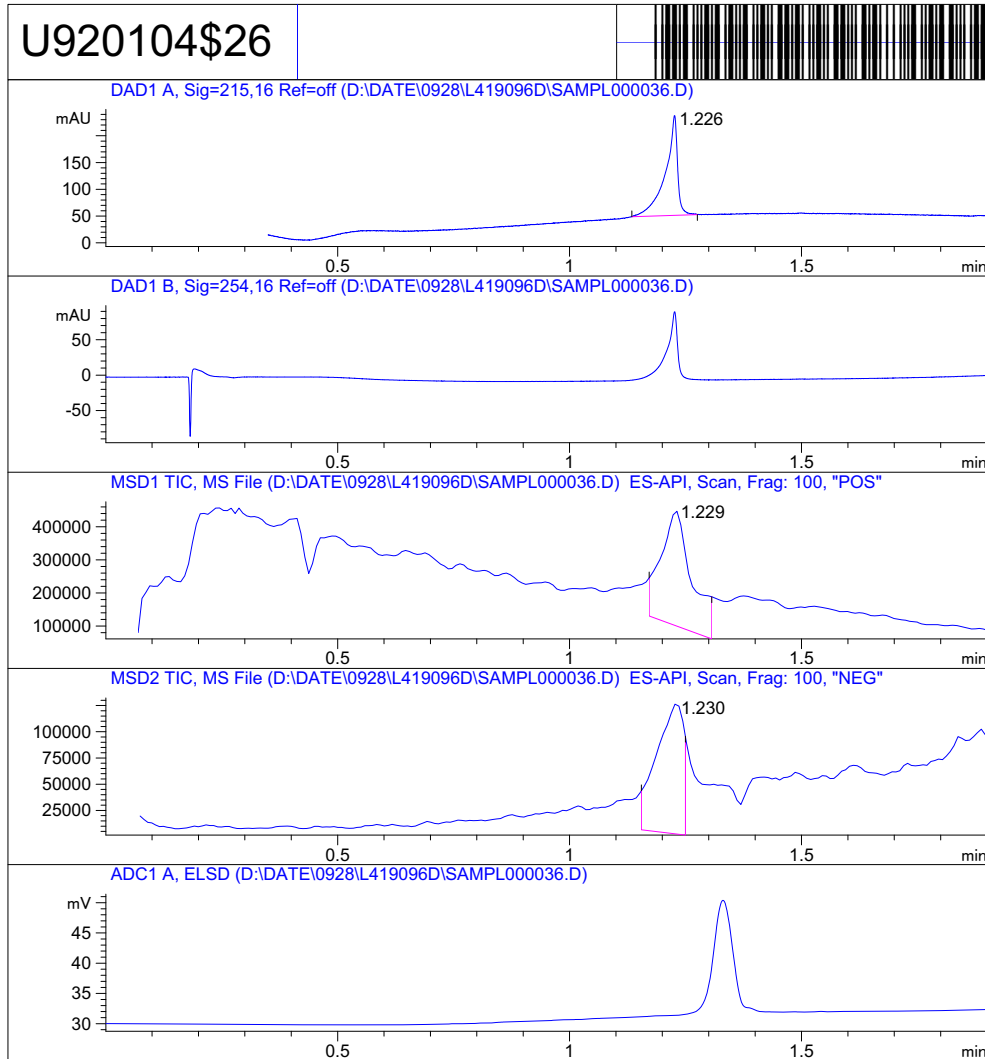


MaxPeak: 100.00%  
Ret\_Time: 1.226 min

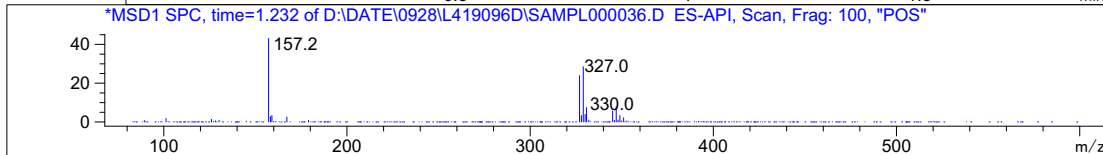


Mol Wt 327.56  
Exact Mass 327.95

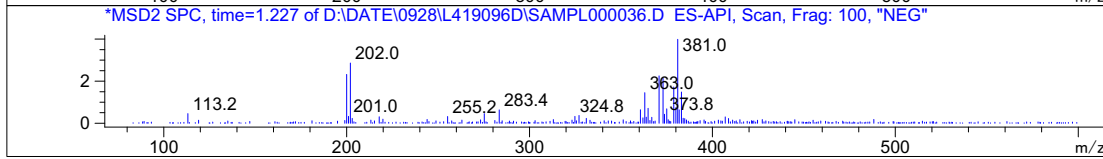
#	Time	Area%
1	1.226	100.00



RT 1.229

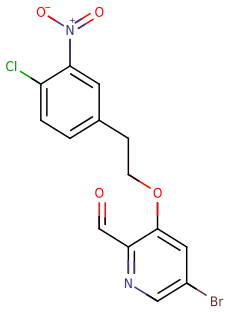


RT 1.230



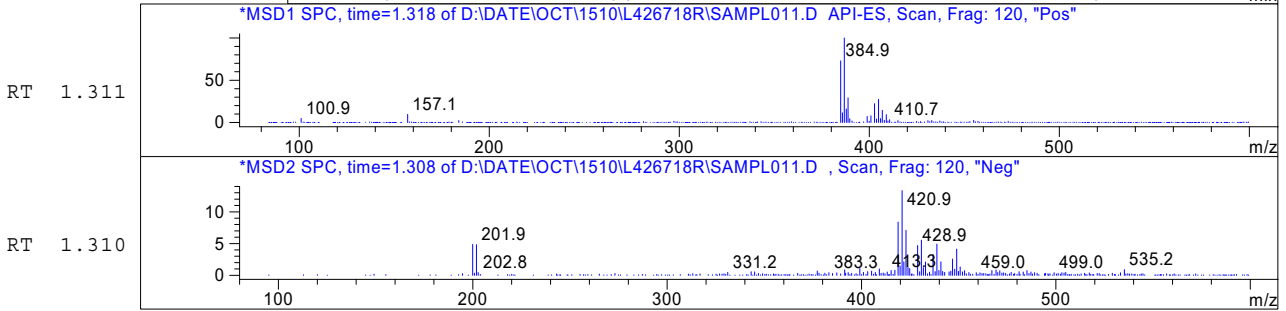
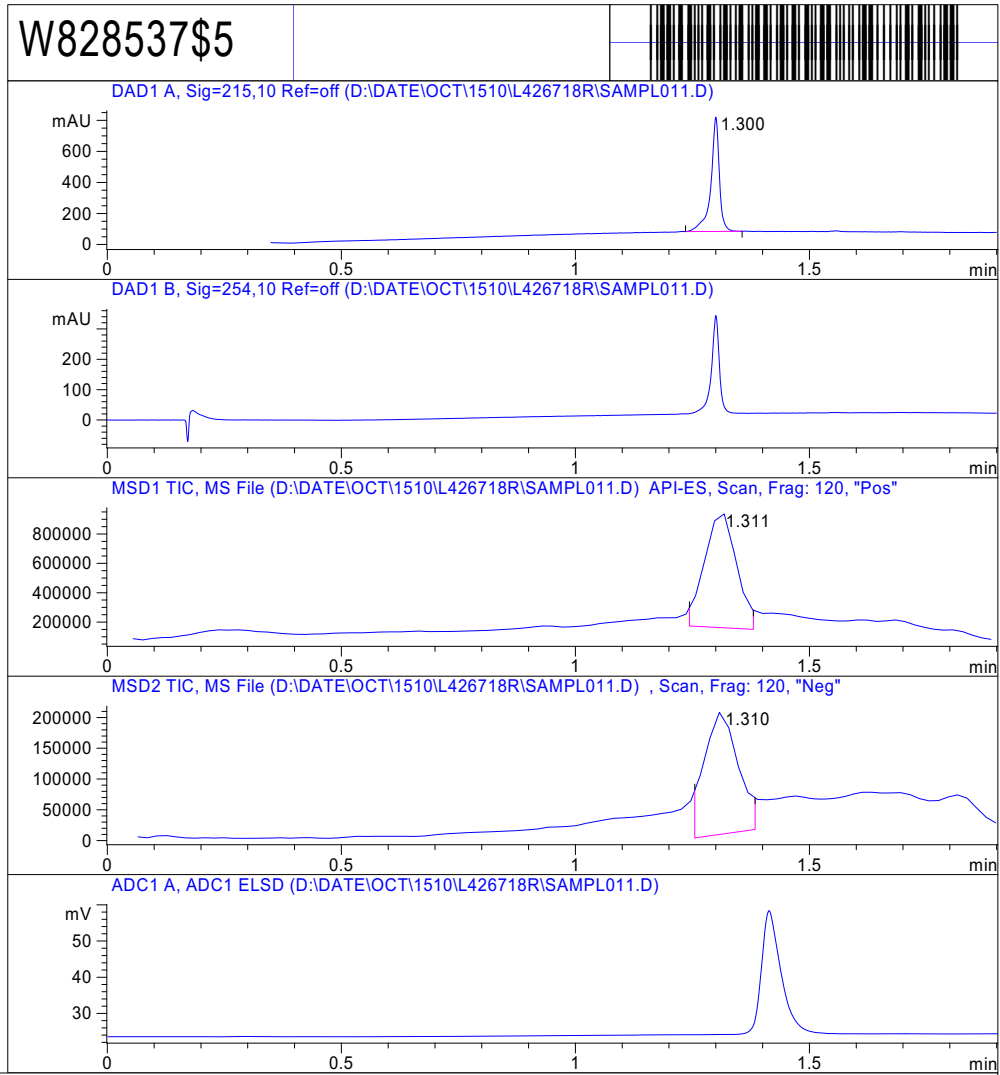
MaxPeak: 100.00%  
Ret\_Time: 1.300 min

W828537\$5



Mol Wt 385.6  
Exact Mass 385.95

#	Time	Area%
1	1.300	100.00



Inj.Date 10/15/2021

Y

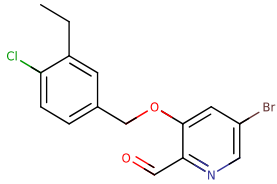
-VL-

Acq. Method C:\HPCHEM\ ->

->

Z5192779054\_

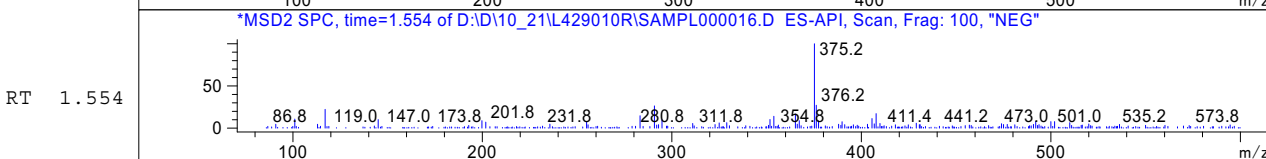
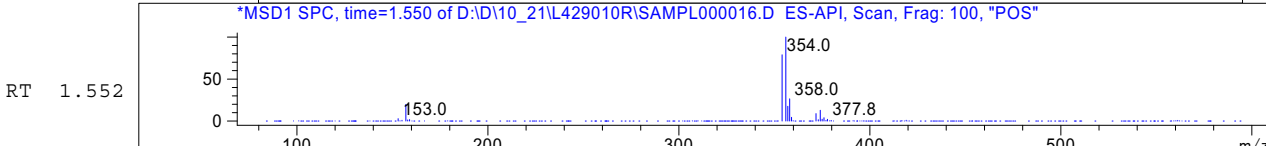
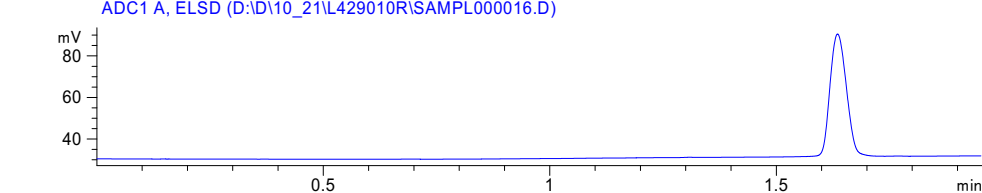
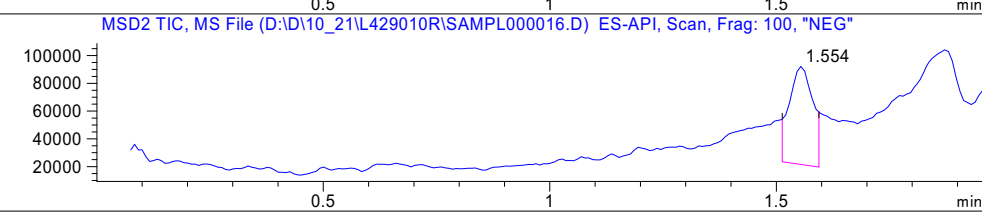
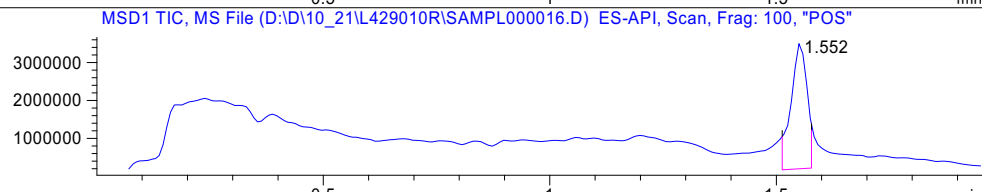
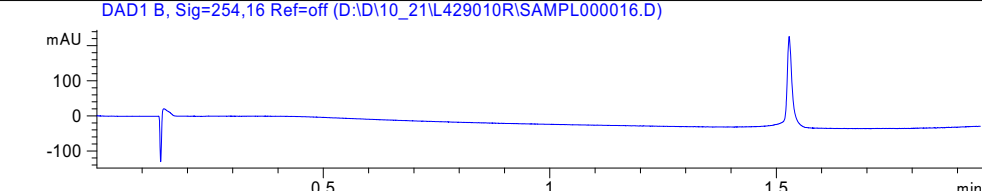
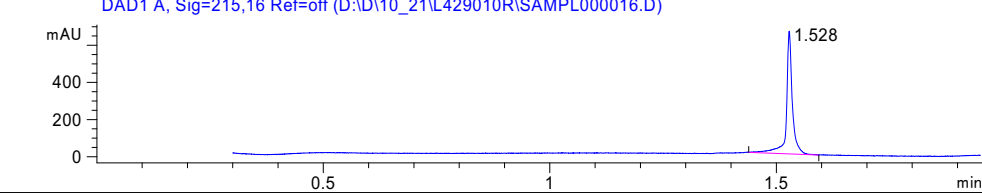
MaxPeak: 100.00%  
Ret\_Time: 1.528 min



Mol Wt 354.63  
Exact Mass 355

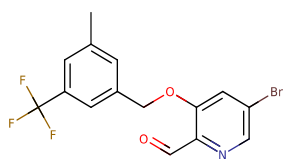
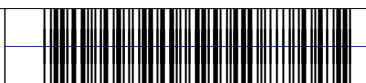
#	Time	Area%
1	1.528	100.00

W938418\$2



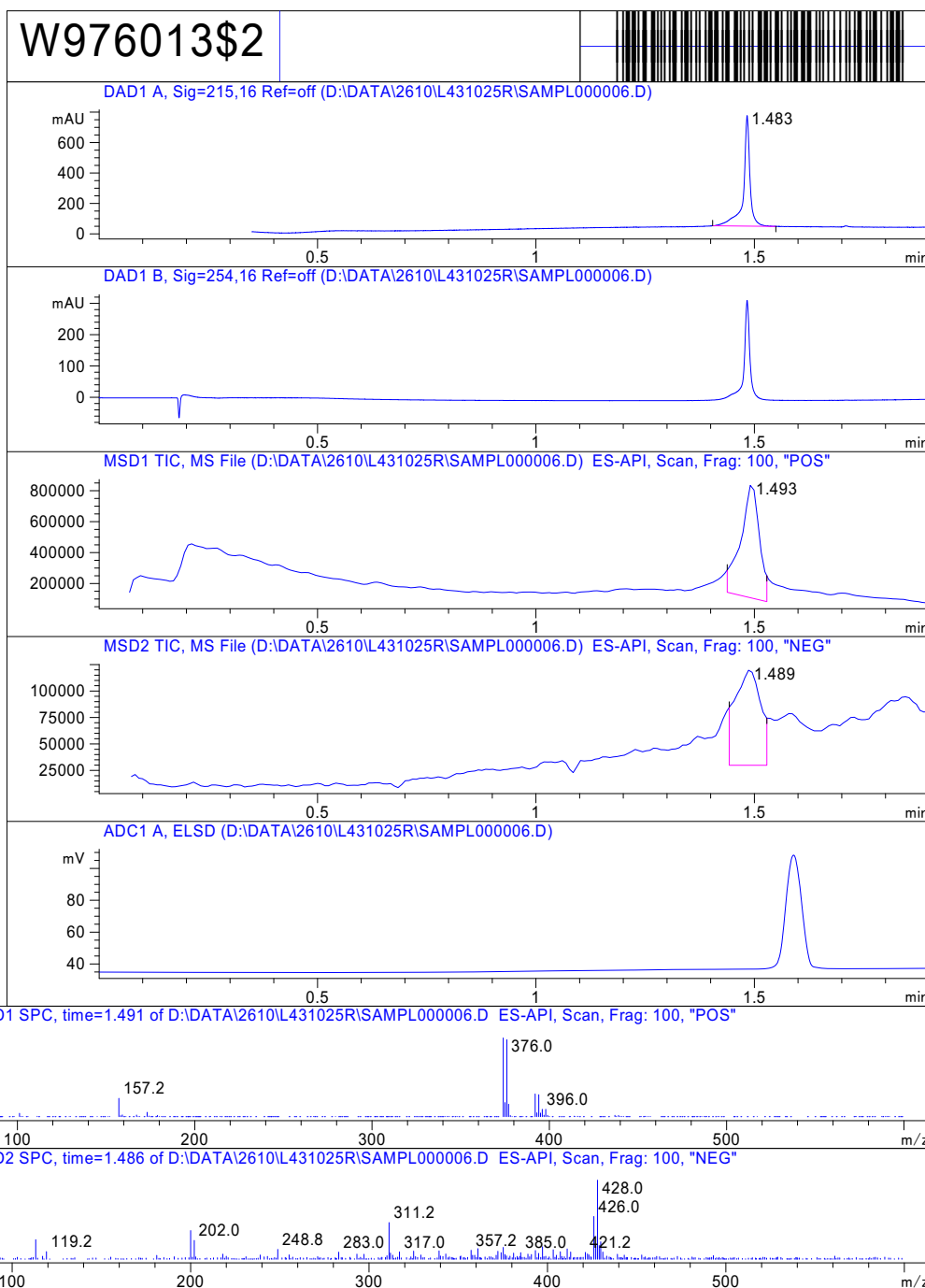
MaxPeak: 100.00%  
Ret\_Time: 1.483 min

W976013\$2

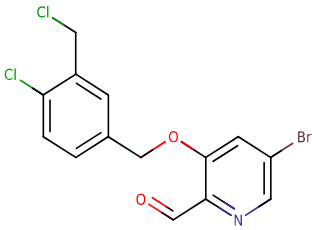


Mol Wt 374.15  
Exact Mass 373.01

#	Time	Area%
1	1.483	100.00



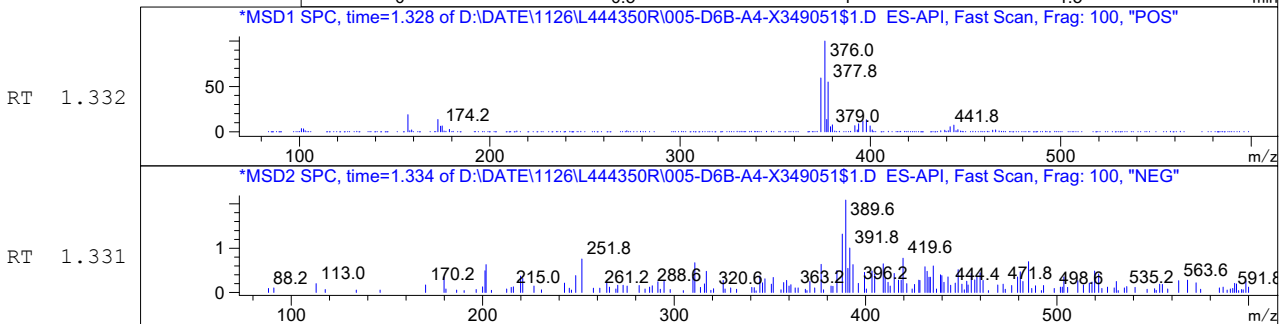
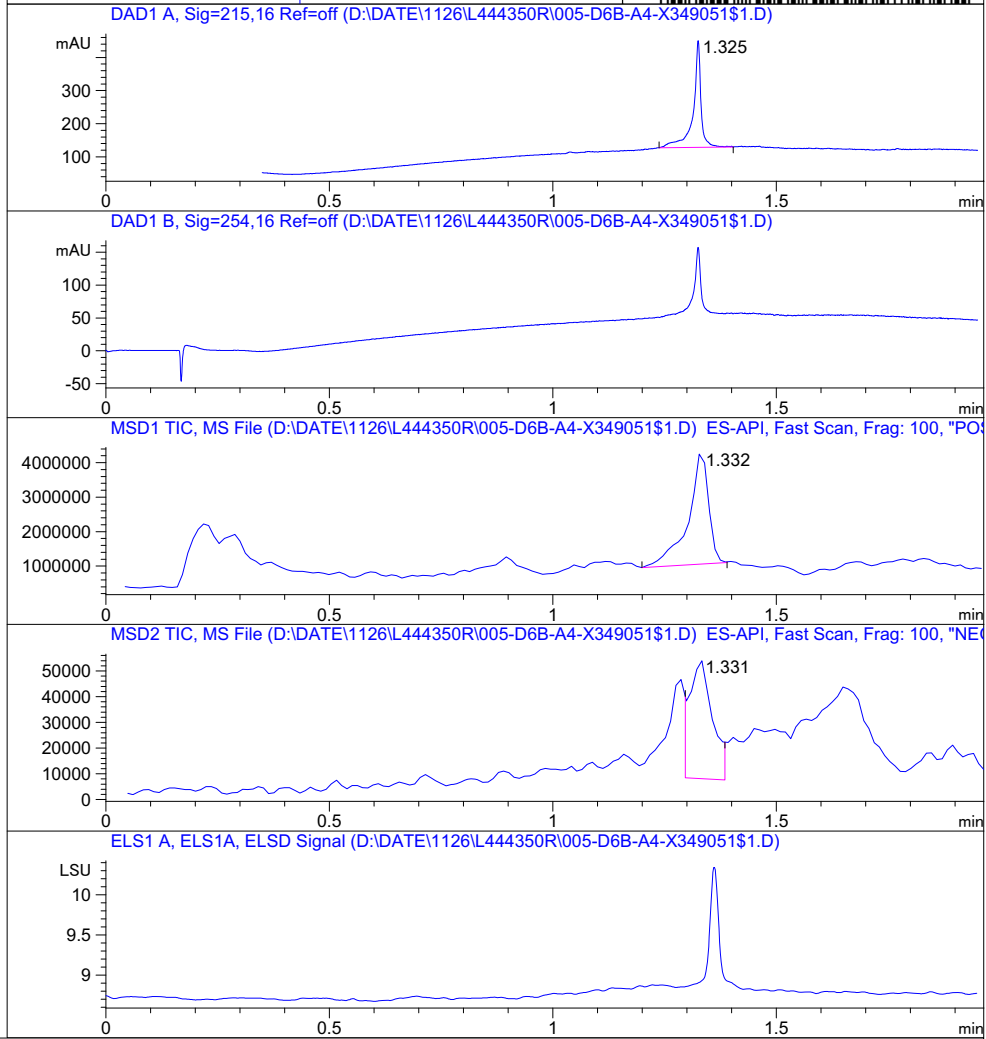
MaxPeak: 100.00%  
Ret\_Time: 1.325 min



Mol Wt 375.04  
Exact Mass 374.94

#	Time	Area%
1	1.325	100.00

# X349051\$1



Inj.Date 11/26/2021

E

Acq. Method C:\Users\ -> ->

Z5247643558\_

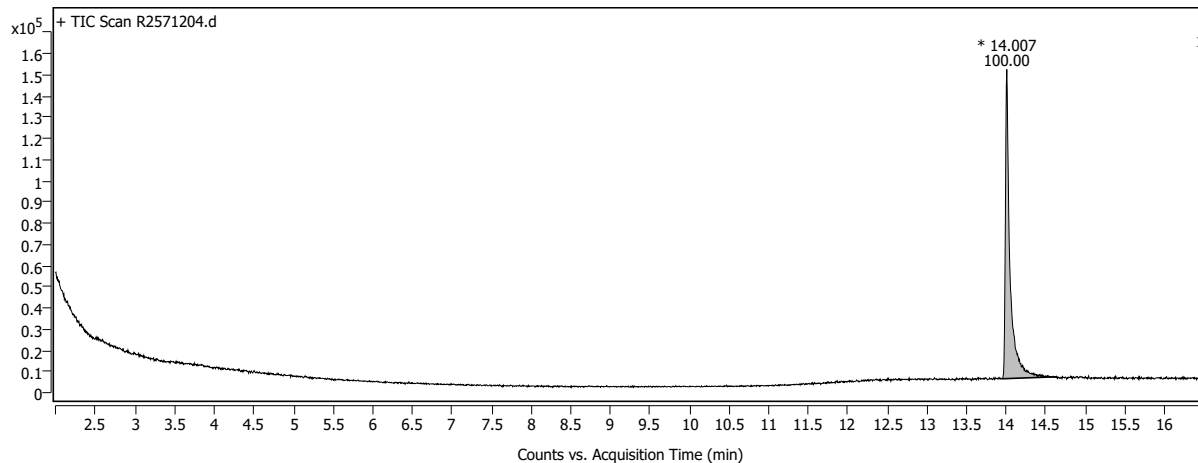
# Analysis Report



## Sample Information

Name	R2571204	Data File Path	D:\MassHunter\GCMS\1\data\04_20\R2571204.D
Comment	CH3CN	Acq. Time (Local)	20-Apr-21 22:22:08 (UTC+03:00)
Instrument	GCMS-5	Method Path (Acq)	D:\MassHunter\GCMS\1\methods\UNIV_ACN.M
Position	33		

## Sample Chromatograms



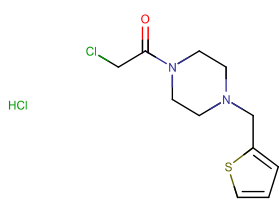
Chromatogram Peaks			
Peak	RT	Area	Area Sum %
1	14.007	594625	100.00

MassHunter Qual 10.0  
(End of Report)



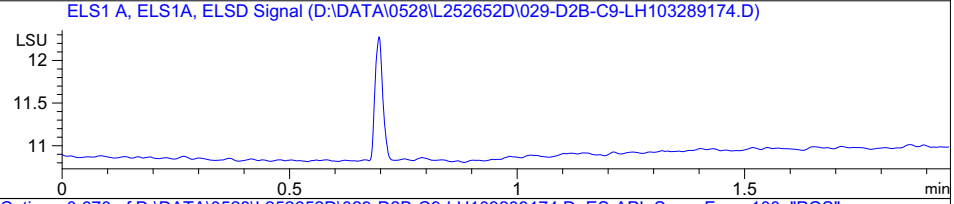
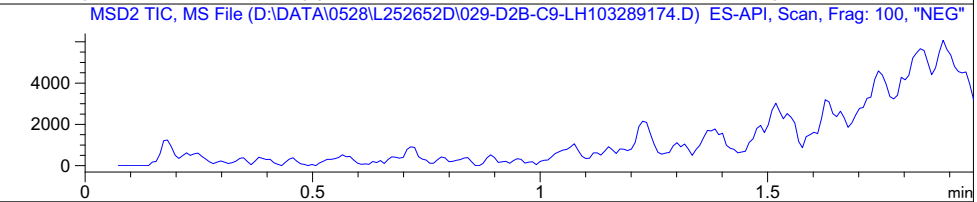
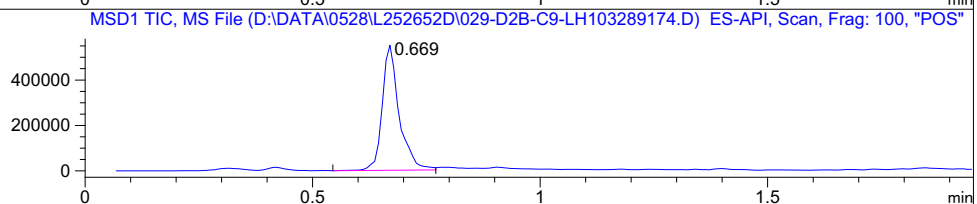
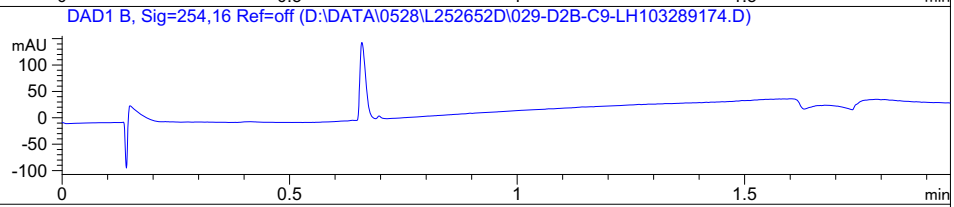
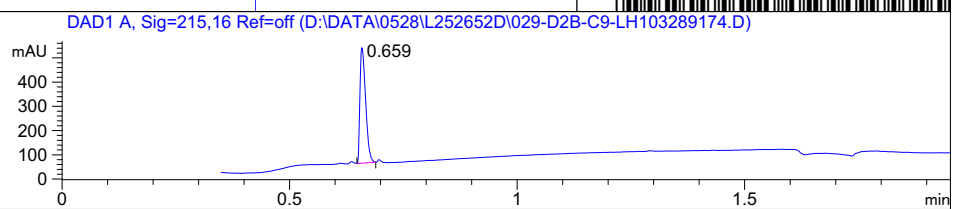
MaxPeak: 100.00%  
Ret\_Time: 0.659 min

# LH103289174

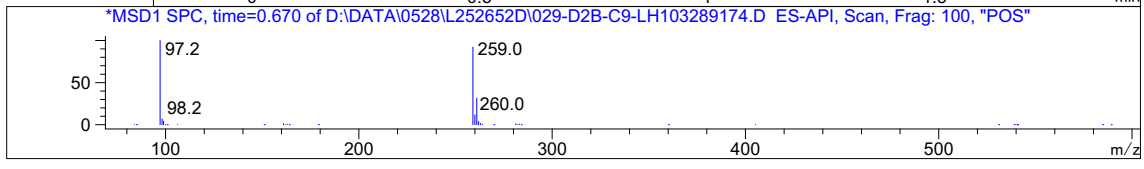


**Mol Wt** 295.23  
**Exact Mass** 258.08

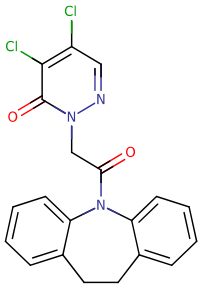
#	Time	Area%
1	0.659	100.00



RT 0.669



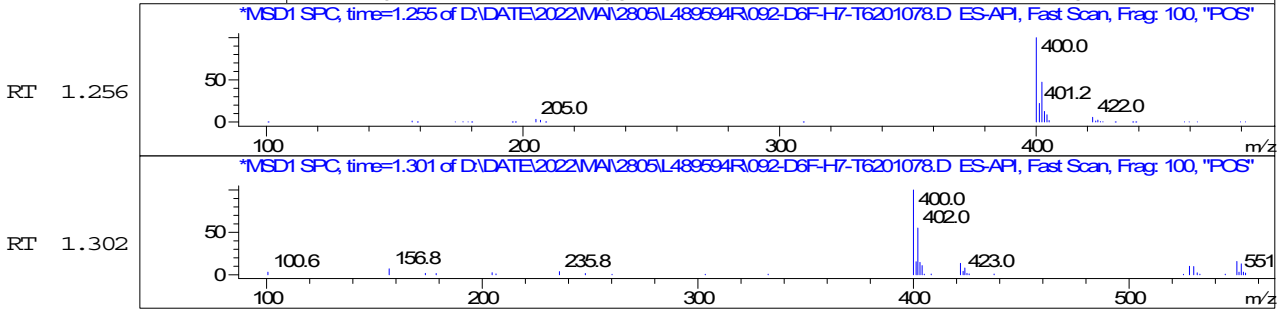
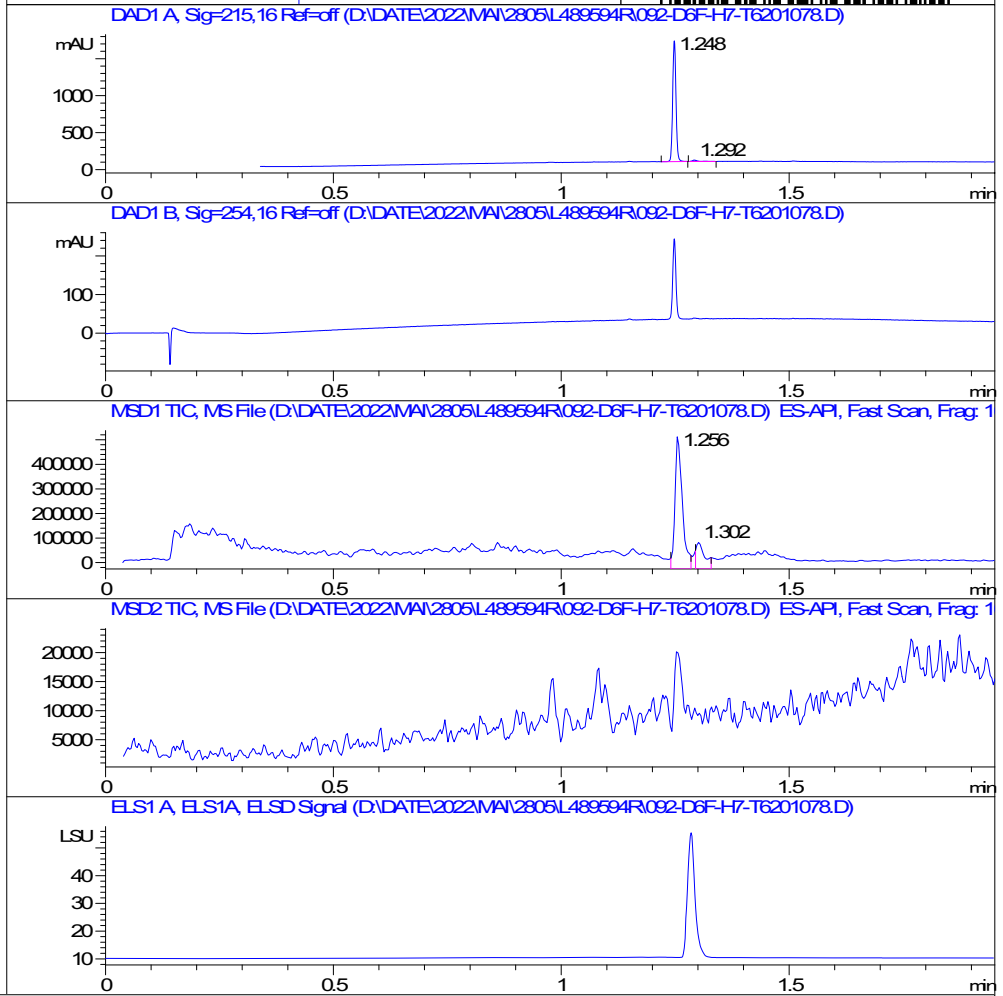
MaxPeak: 98.15%  
Ret\_Time: 1.248 min



Mol Wt 400.26  
Exact Mass 399.07

#	Time	Area%
1	1.248	98.15
2	1.292	1.85

# T6201078



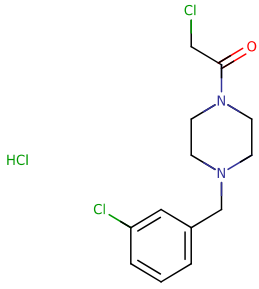
Inj.Date 28-May-22

Z <invalid>

Acq. Method C:\Users\ -> ->

Z335721330\_

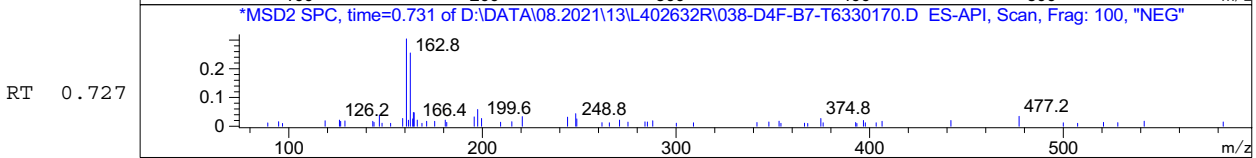
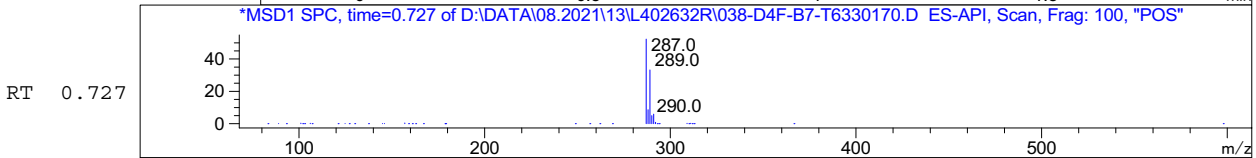
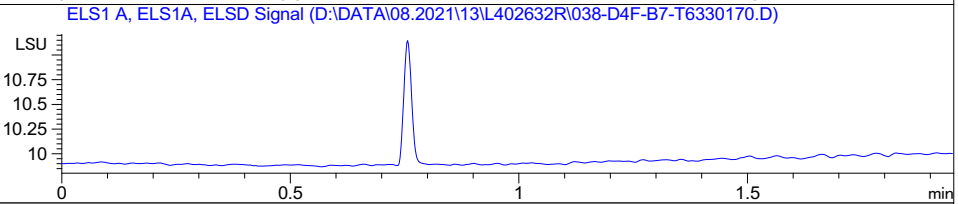
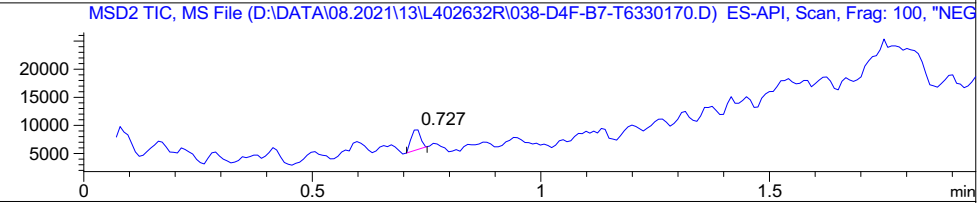
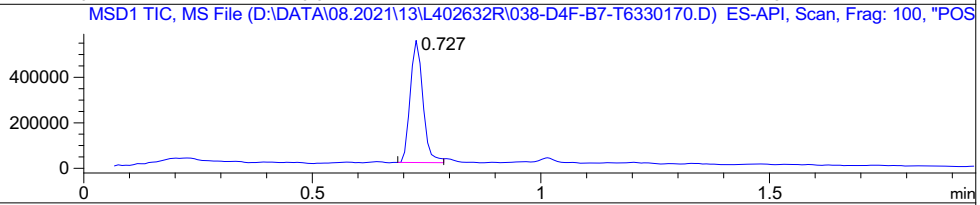
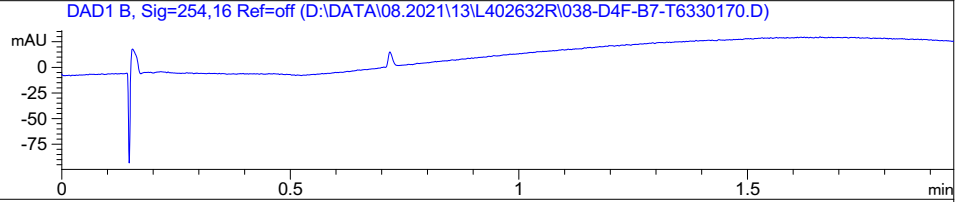
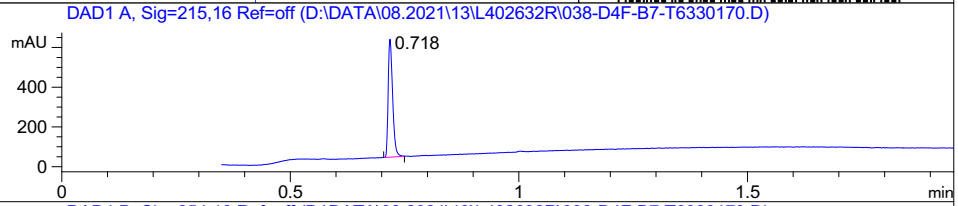
MaxPeak: 100.00%  
Ret\_Time: 0.718 min



Mol Wt 323.65  
Exact Mass 286.09

#	Time	Area%
1	0.718	100.00

T6330170



Inj.Date 8/13/2021

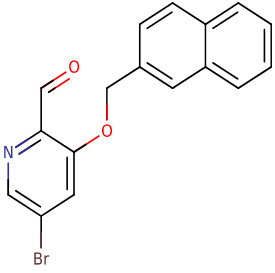
CH <invalid> -18-

Acq. Method C:\Chem32\ -> ->

Z147647726\_

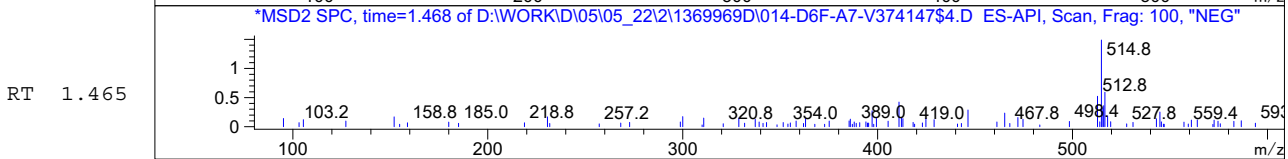
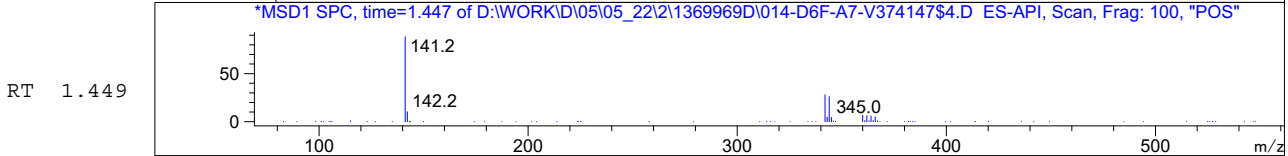
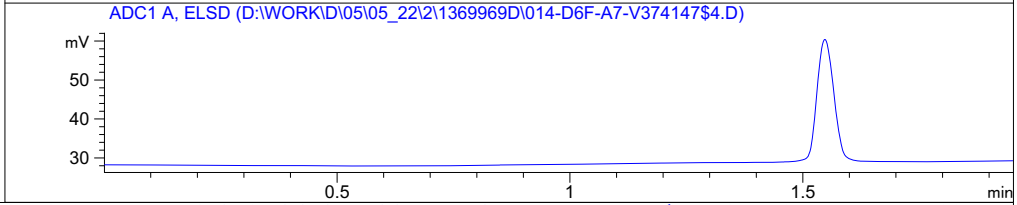
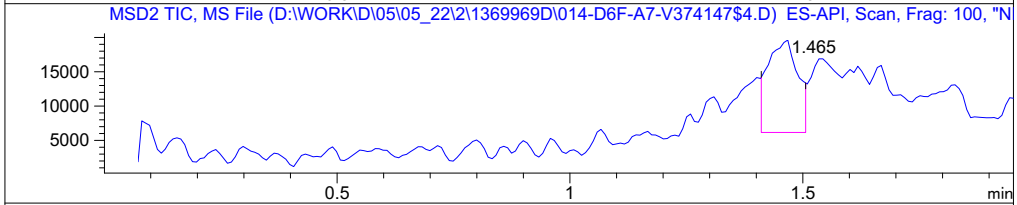
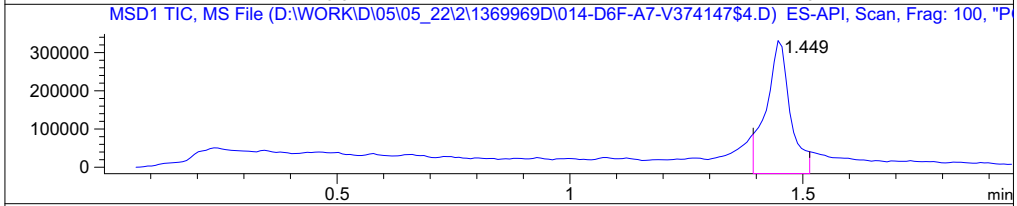
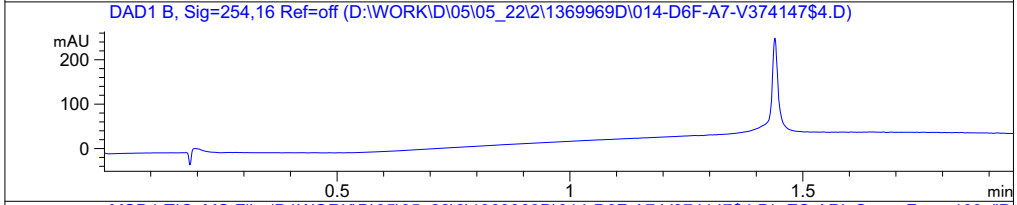
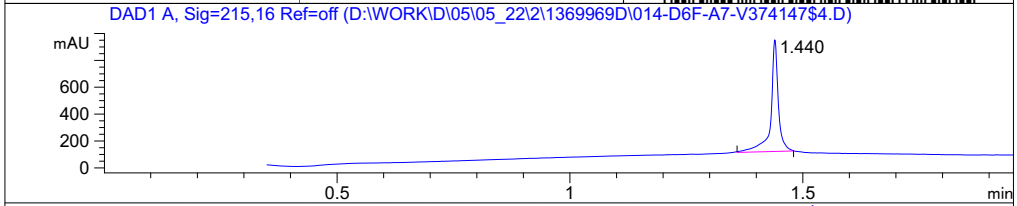
MaxPeak: 100.00%  
Ret\_Time: 1.440 min

V374147\$4



Mol Wt 342.19  
Exact Mass 341.02

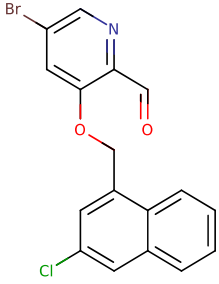
#	Time	Area%
1	1.440	100.00



# W557422\$R

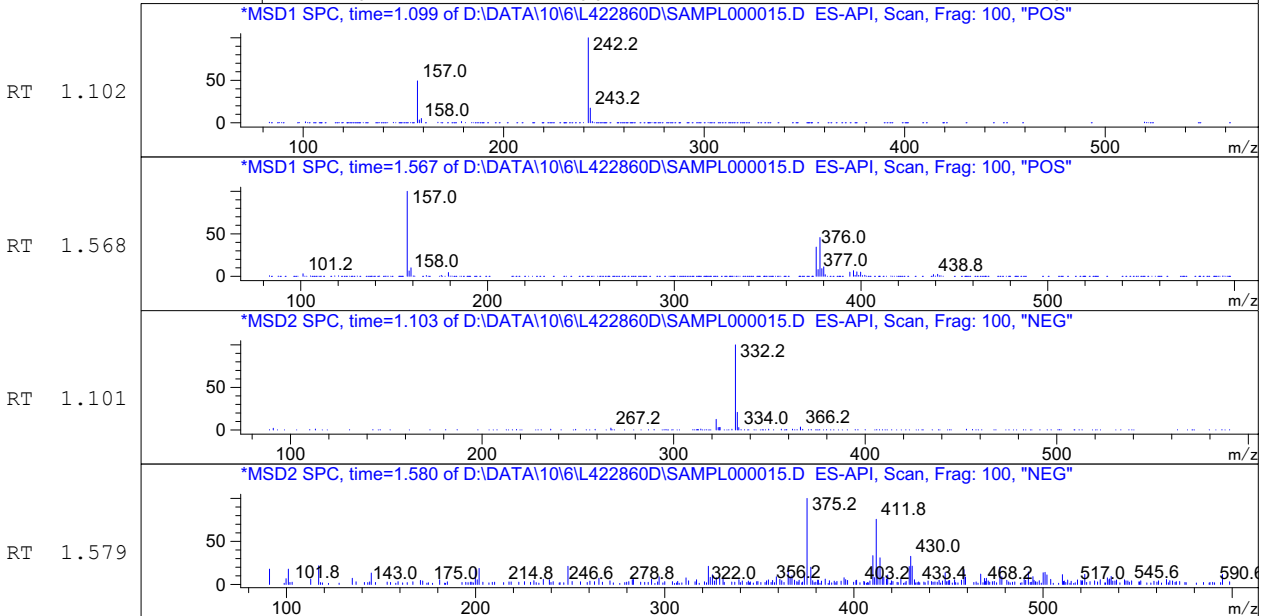
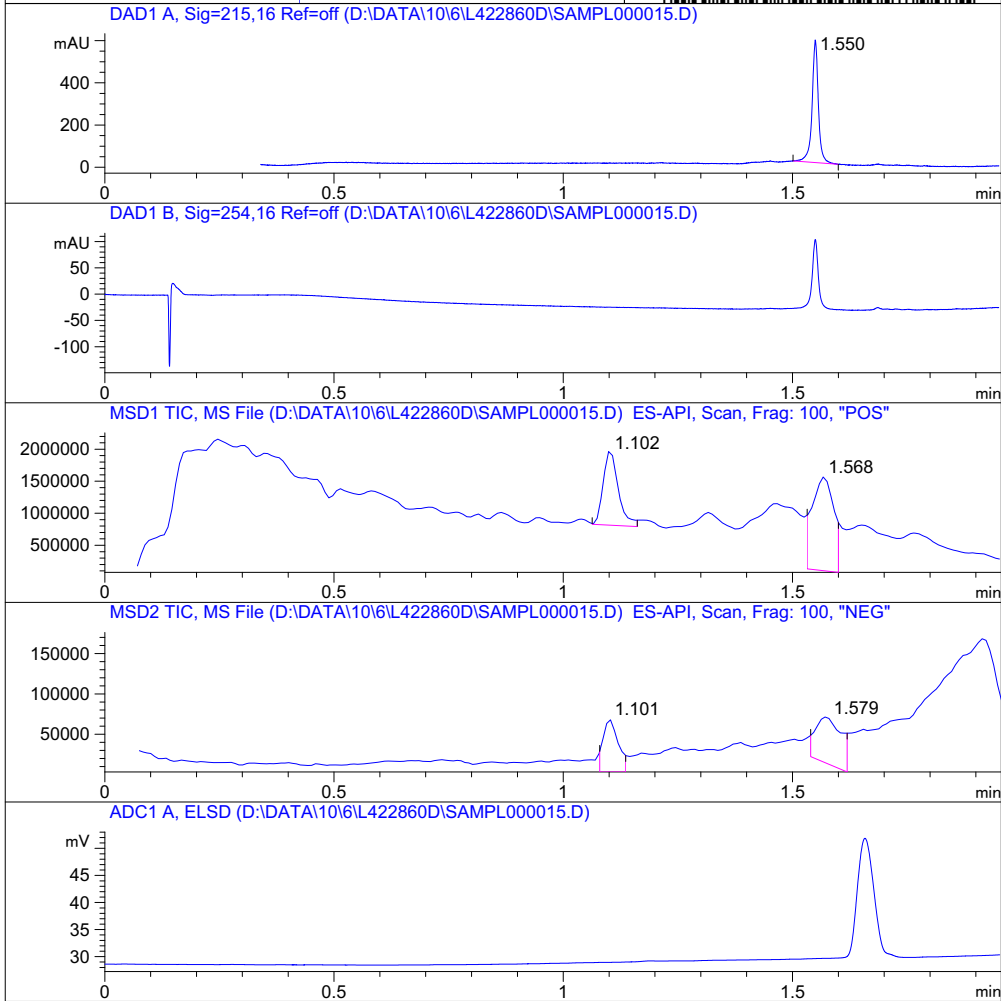


MaxPeak: 100.00%  
Ret\_Time: 1.550 min

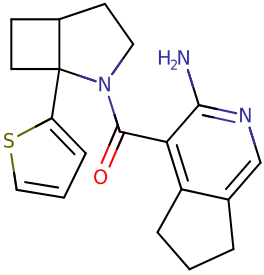


Mol Wt 376.63  
Exact Mass 376.98

#	Time	Area%
1	1.550	100.00



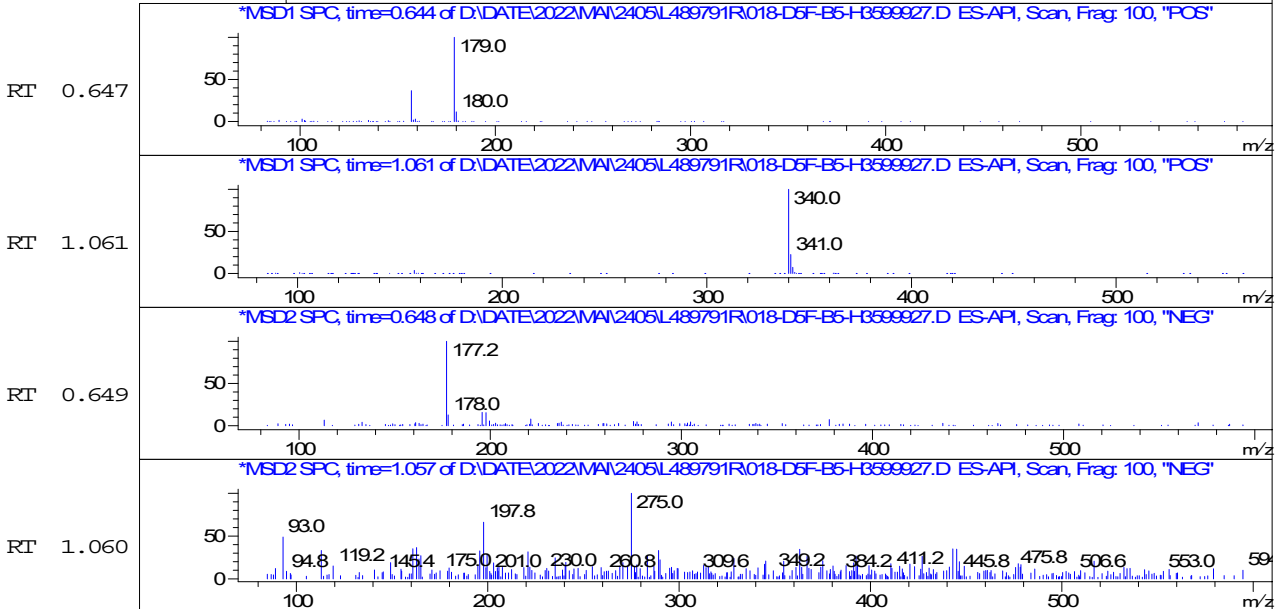
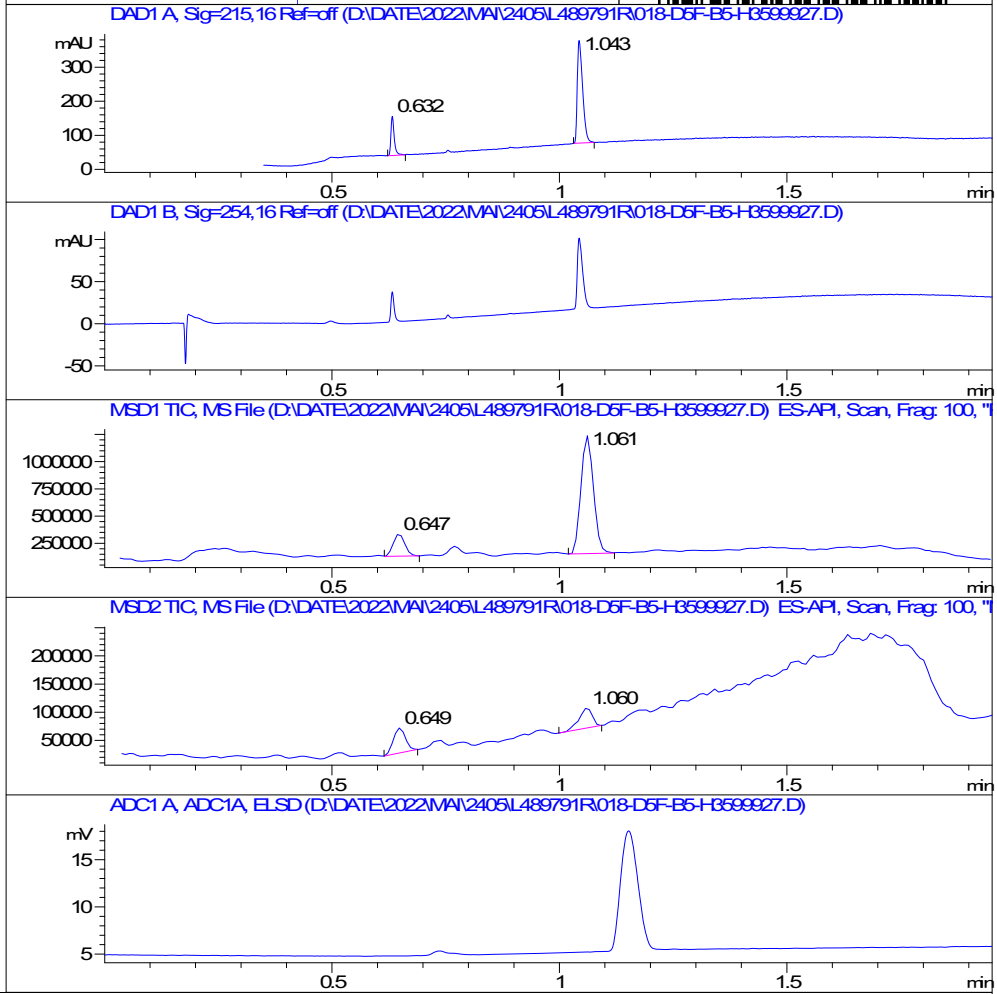
MaxPeak: 80.83%  
Ret\_Time: 1.043 min



Mol Wt 339.46  
Exact Mass 339.17

#	Time	Area%
1	0.632	19.17
2	1.043	80.83

# H3599927



Inj.Date 24-May-22

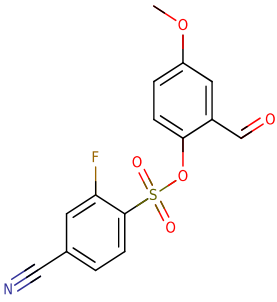
Z

<invalid> -25-

Acq. Method C:\Users\ -> ->

Z4124468376\_

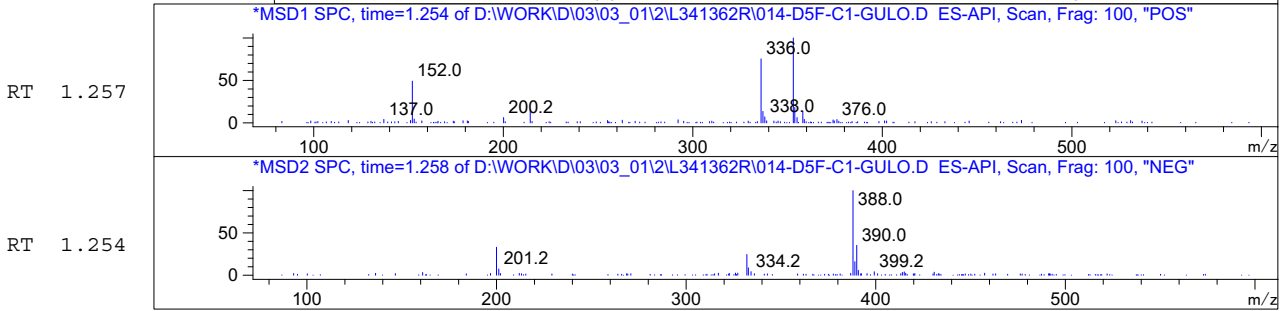
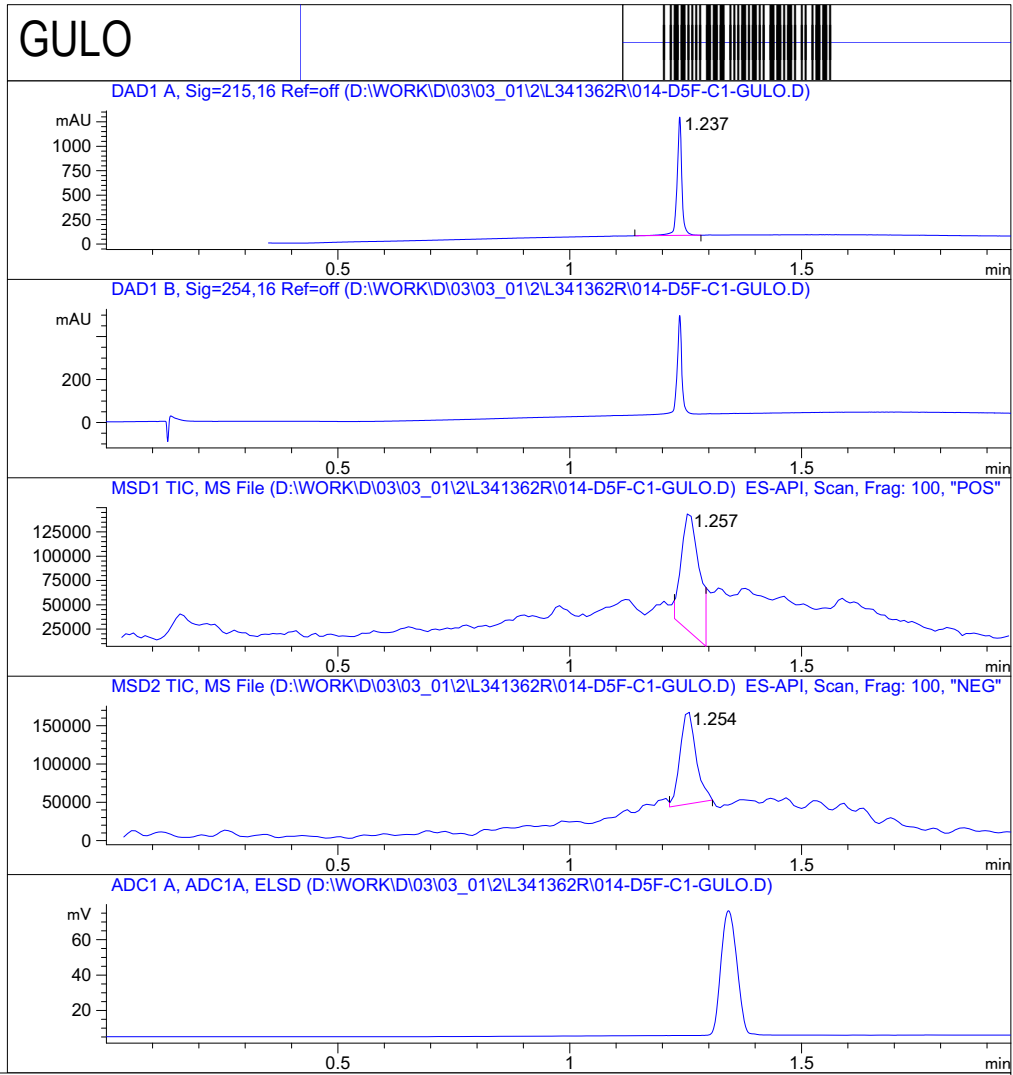
MaxPeak: 100.00%  
Ret\_Time: 1.237 min



Mol Wt 335.31  
Exact Mass 335.02

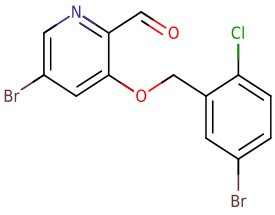
#	Time	Area%
1	1.237	100.00

# GULO



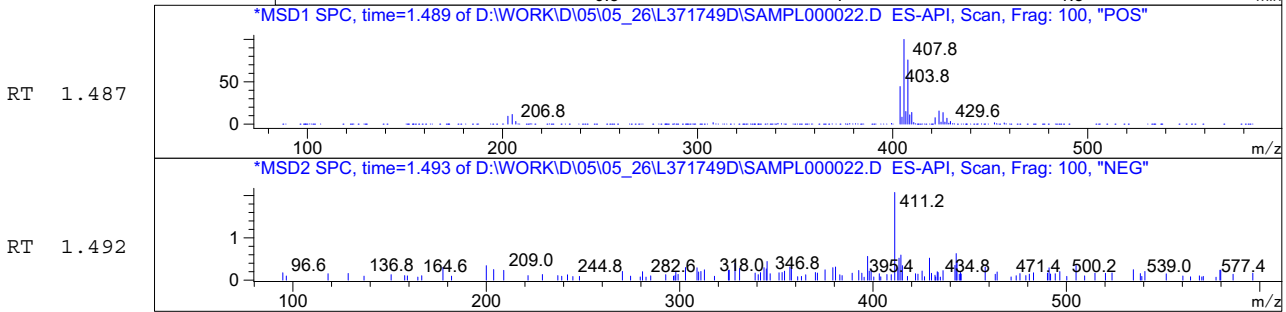
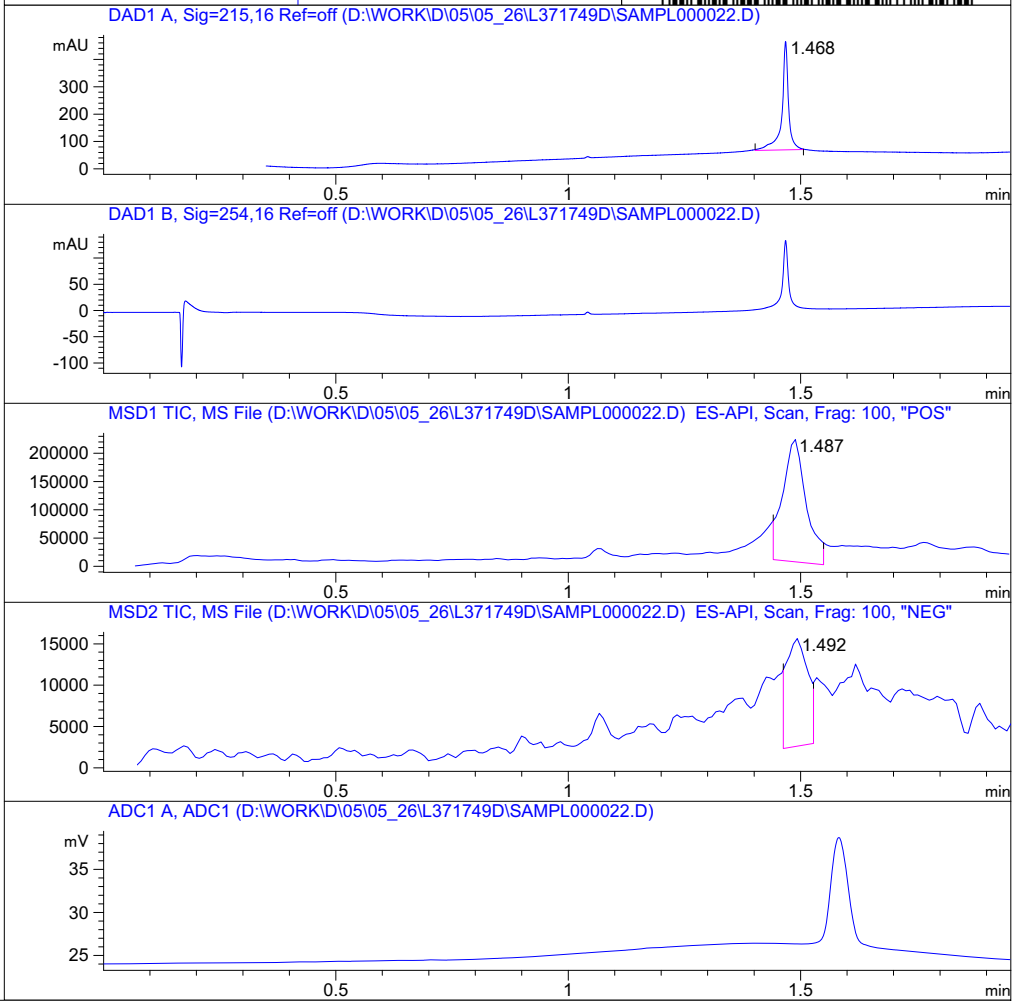
MaxPeak: 100.00%  
Ret\_Time: 1.468 min

V233166\$4



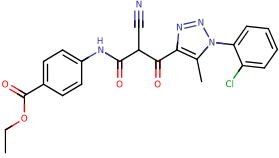
Mol Wt 405.47  
Exact Mass 404.87

#	Time	Area%
1	1.468	100.00





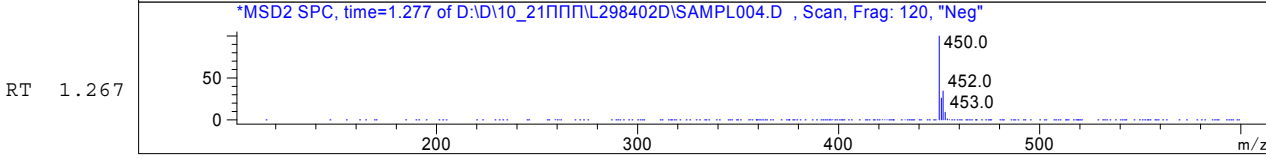
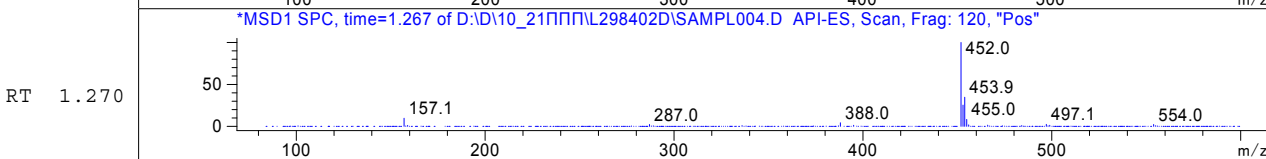
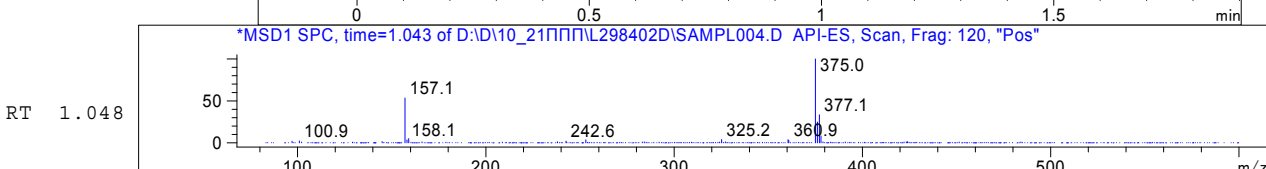
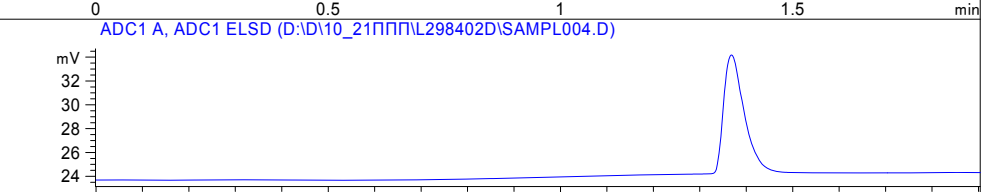
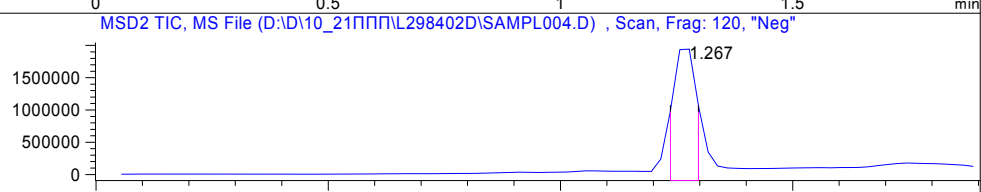
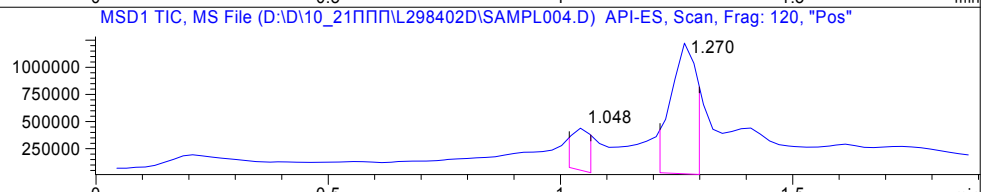
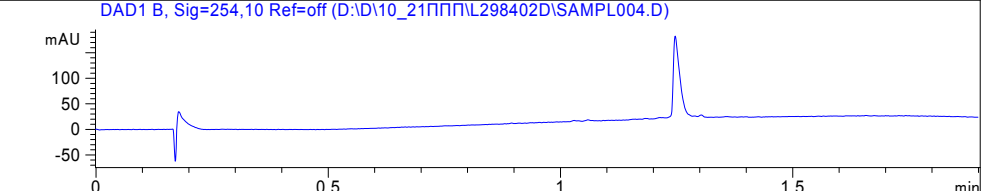
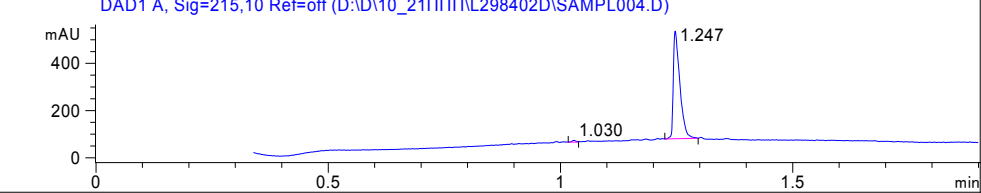
MaxPeak: 98.93%  
Ret\_Time: 1.247 min



Mol Wt 451.86  
Exact Mass 451.11

#	Time	Area%
1	1.030	1.07
2	1.247	98.93

S568083\$4



Inj.Date 10/22/2020

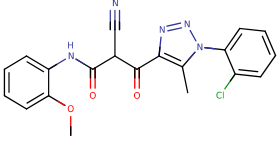
N

-VL-

Acq. Method C:\HPCHEM\ -> ->

Z1123372000\_

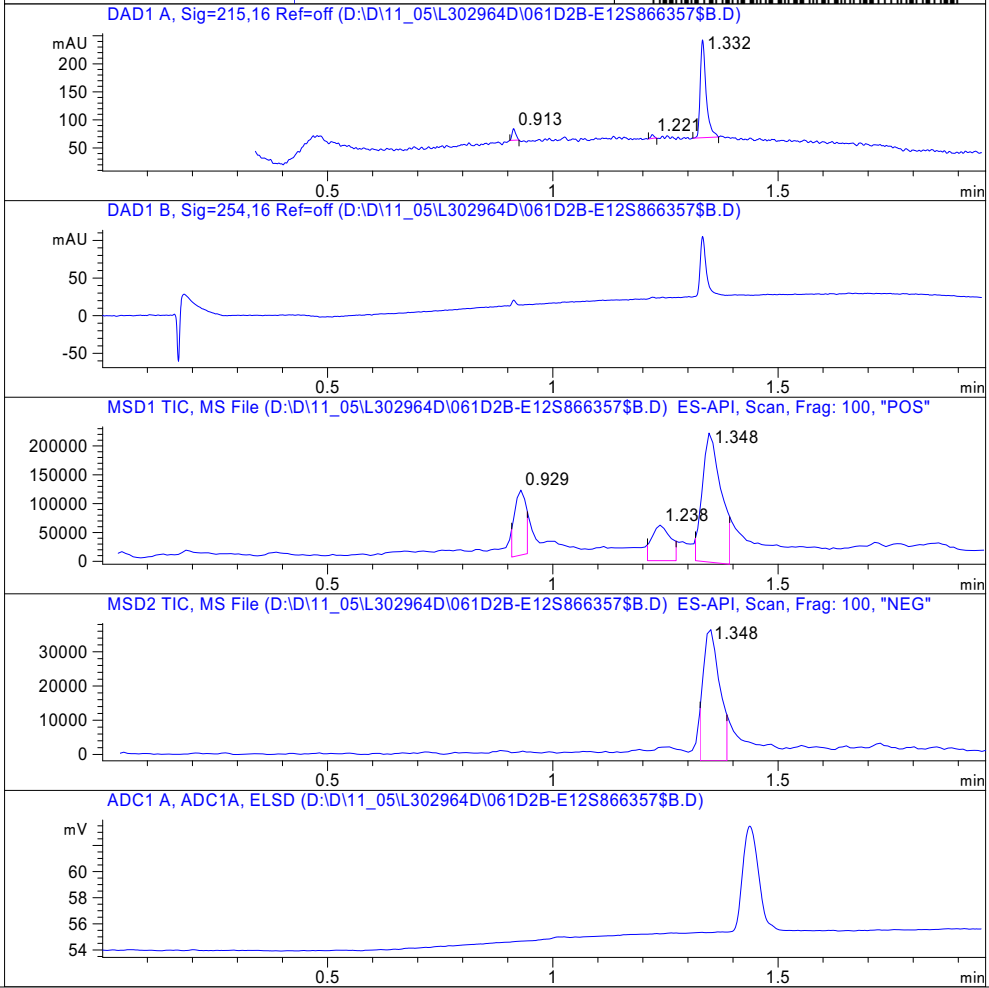
MaxPeak: 91.40%  
Ret\_Time: 1.332 min



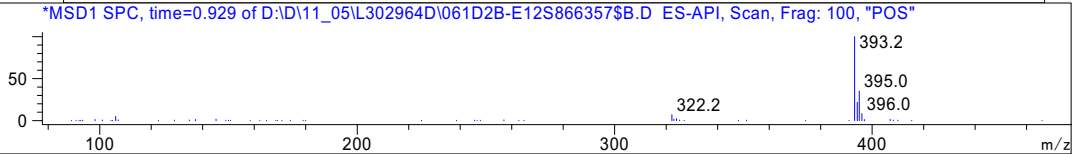
Mol Wt 409.83  
Exact Mass 409.1

#	Time	Area%
1	0.913	6.77
2	1.221	1.83
3	1.332	91.40

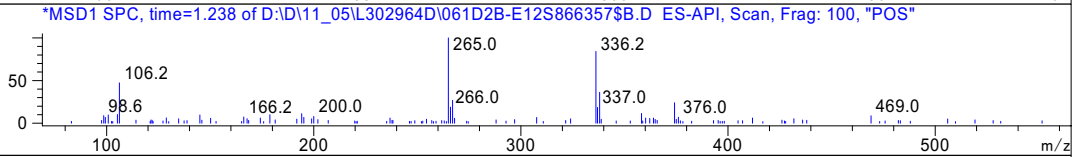
S866357\$B



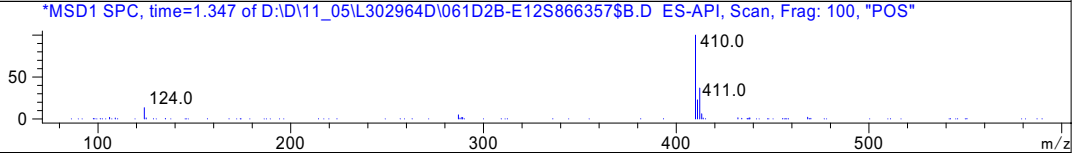
RT 0.929



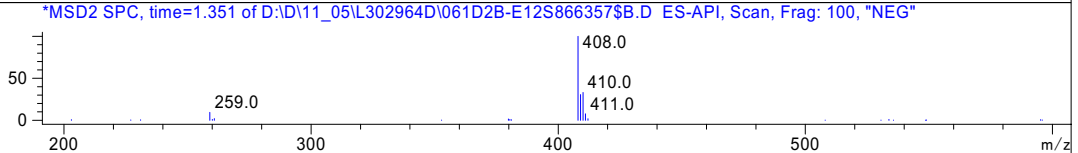
RT 1.238



RT 1.348

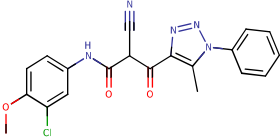


RT 1.348



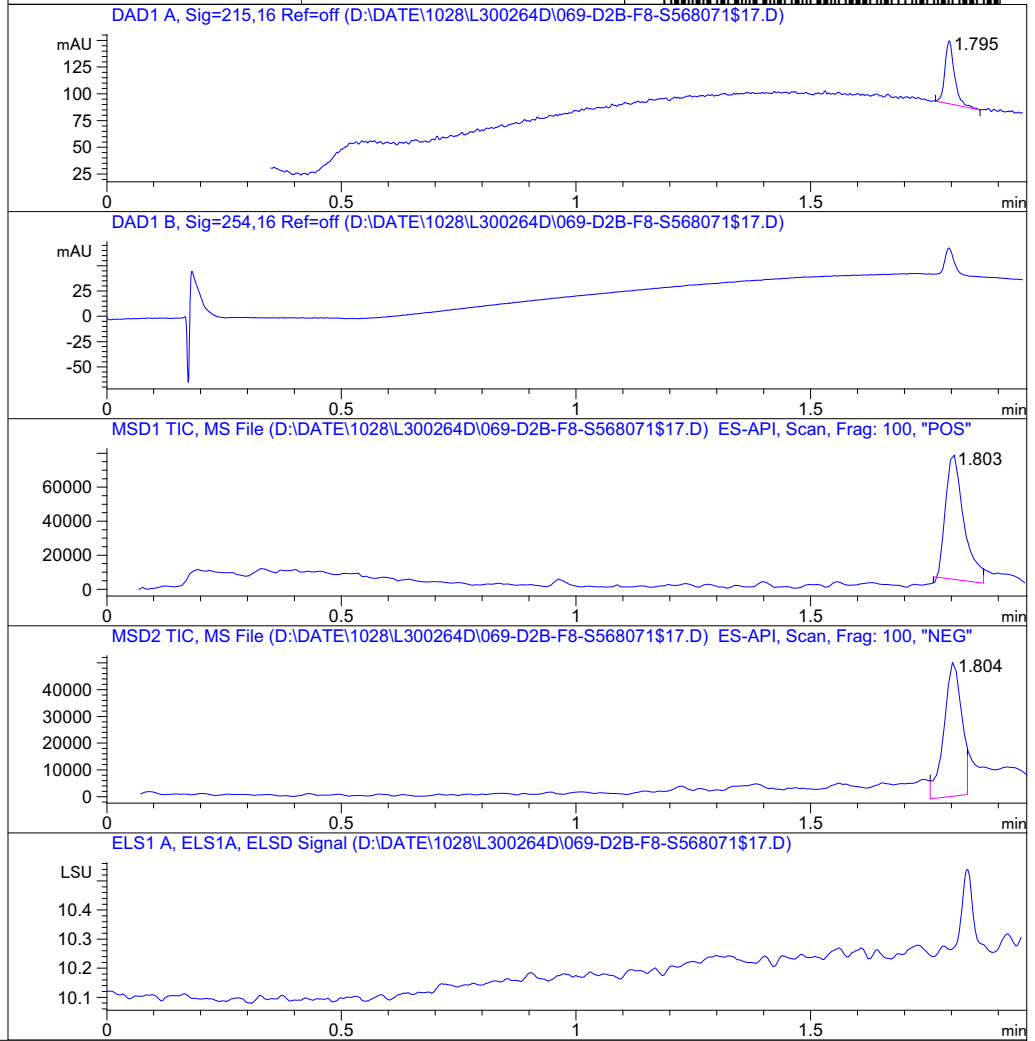
MaxPeak: 100.00%  
Ret\_Time: 1.795 min

S568071\$17

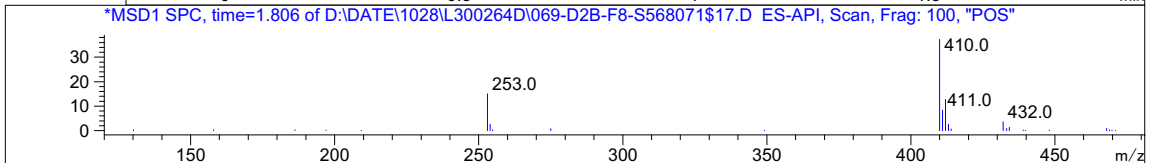


Mol Wt 409.83  
Exact Mass 409.1

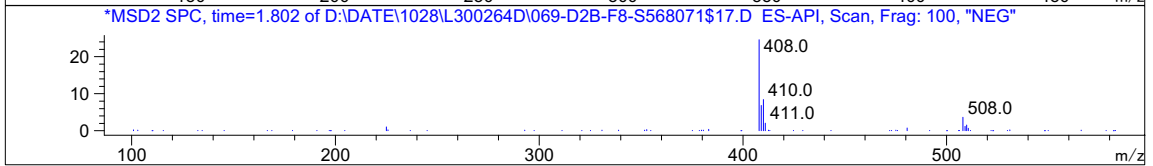
#	Time	Area%
1	1.795	100.00



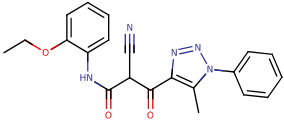
RT 1.803



RT 1.804



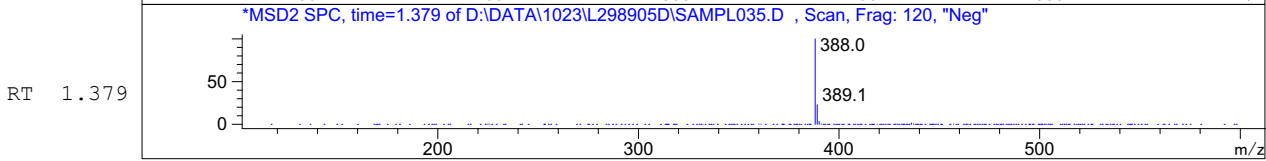
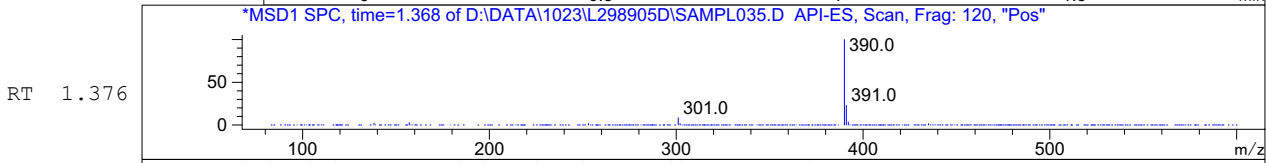
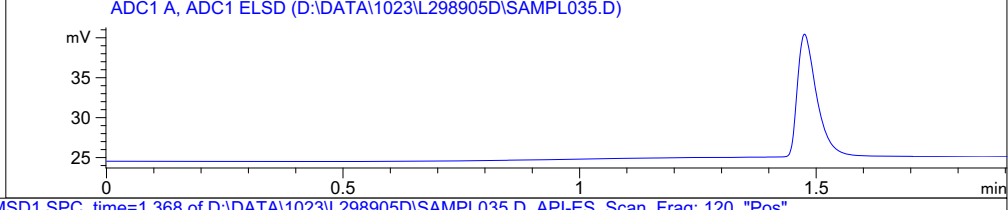
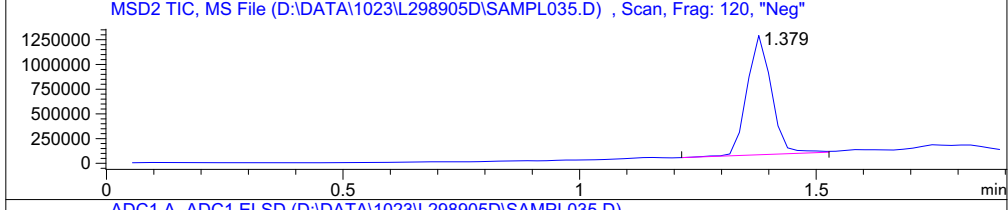
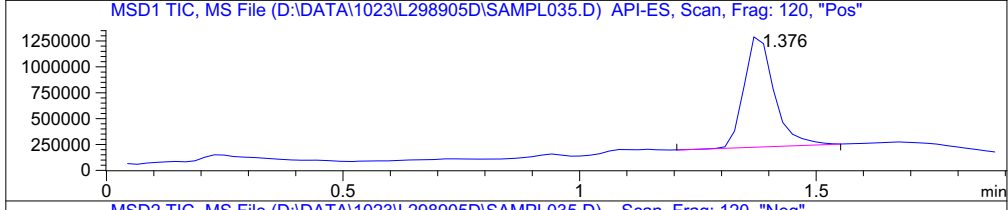
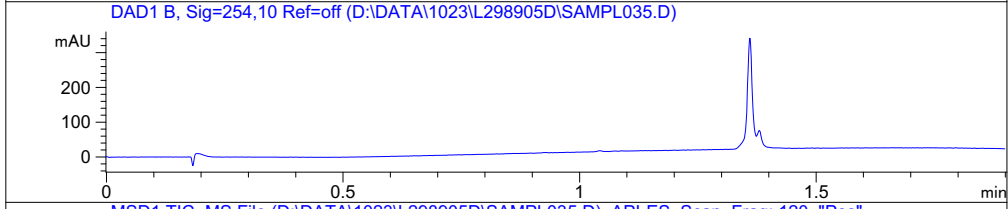
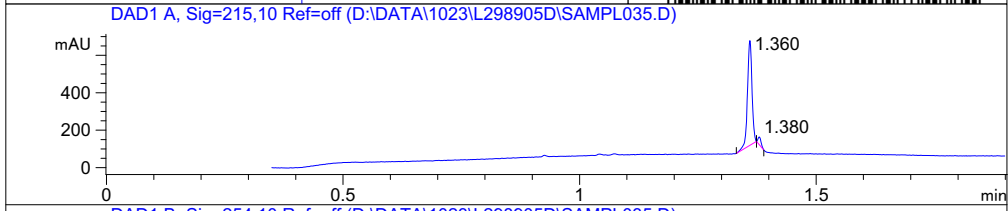
MaxPeak: 95.28%  
Ret\_Time: 1.360 min



Mol Wt 389.41  
Exact Mass 389.16

#	Time	Area%
1	1.360	95.28
2	1.380	4.72

S568078\$C



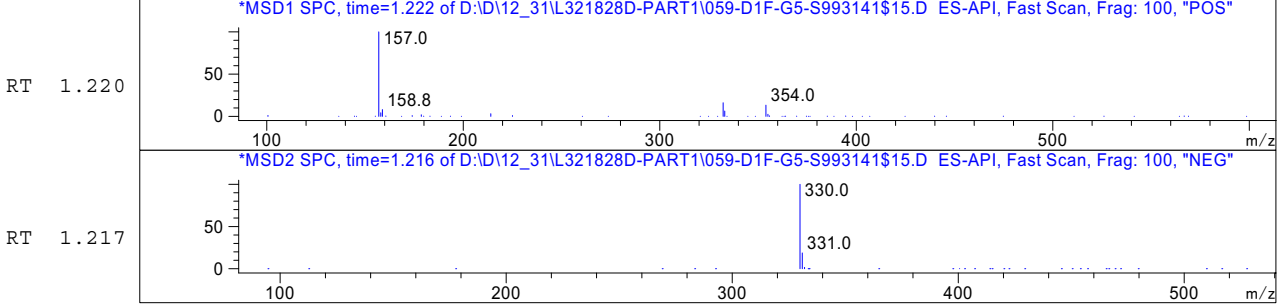
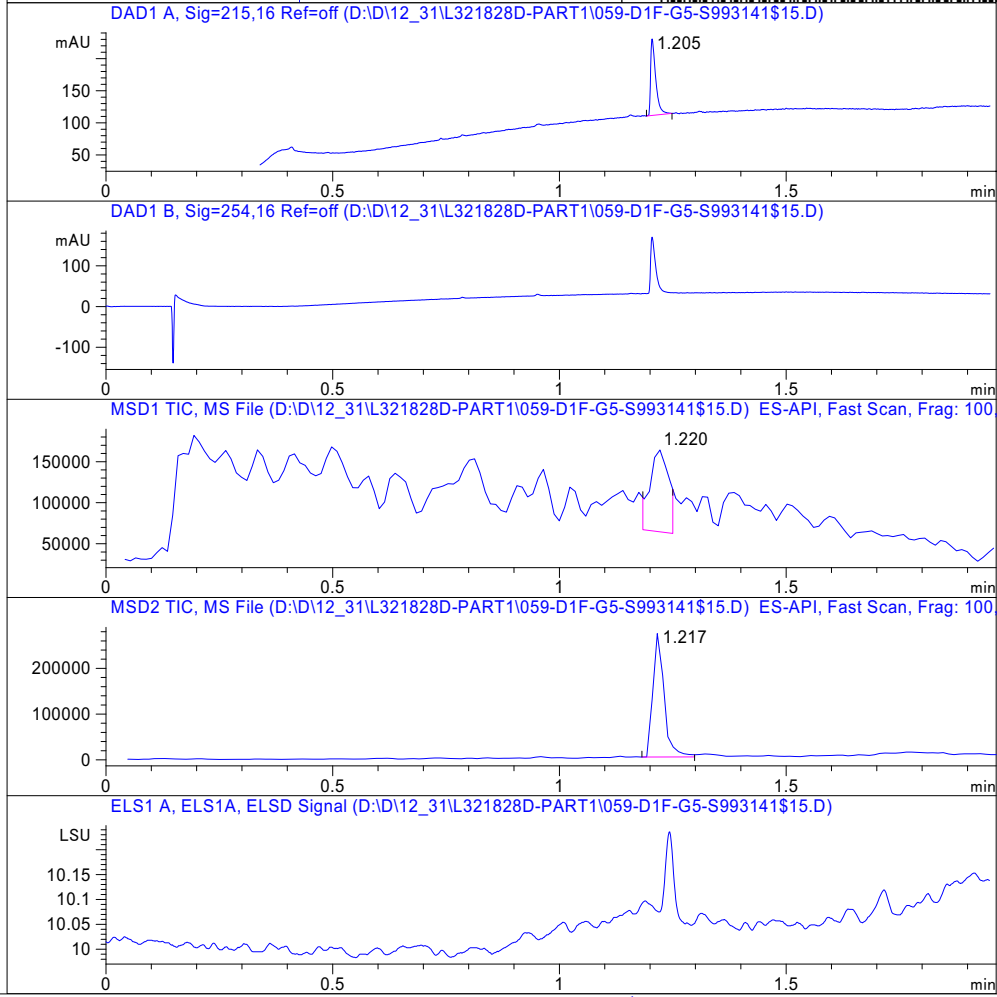
MaxPeak: 100.00%  
Ret\_Time: 1.205 min



Mol Wt 331.33  
Exact Mass 331.11

#	Time	Area%
1	1.205	100.00

S993141\$15



Inj.Date 12/30/2020

N

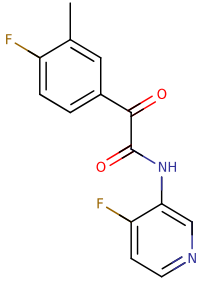
Acq. Method C:\Users\ -> ->

Z638927484\_

# H3659984

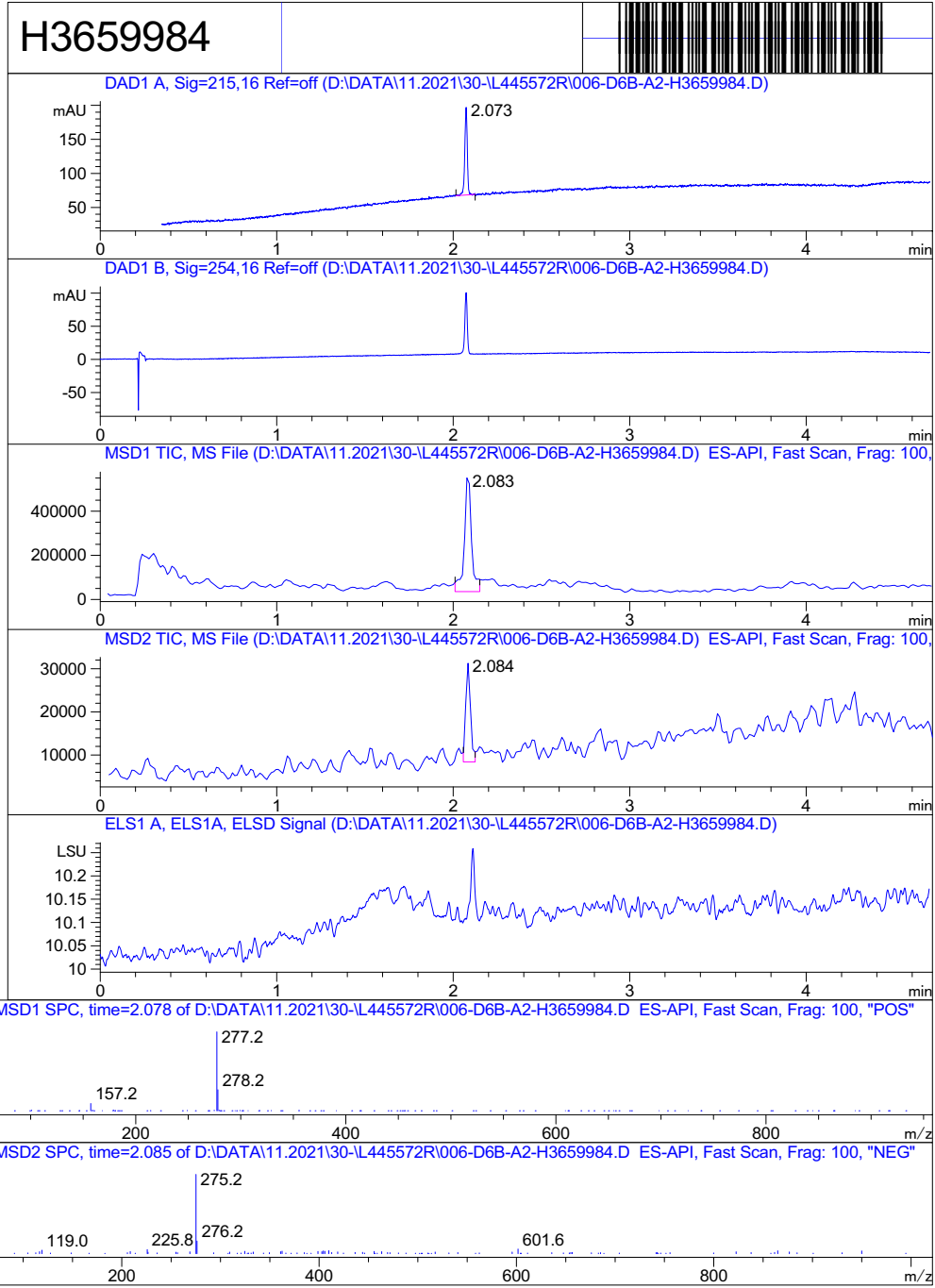


MaxPeak: 100.00%  
Ret\_Time: 2.073 min



Mol Wt 276.24  
Exact Mass 276.08

#	Time	Area%
1	2.073	100.00



Inj.Date 11/30/2021

CH <invalid>

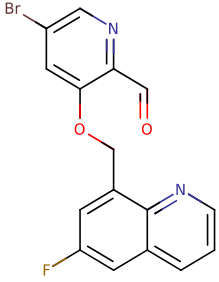
Acq. Method C:\Users\ -> ->

Z5420738300\_

# W179756\$55

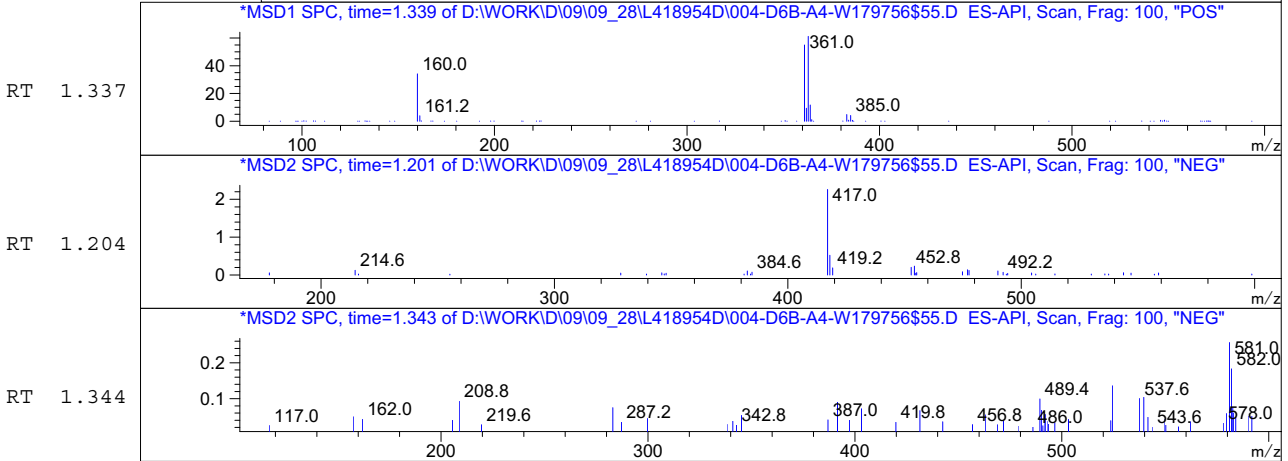
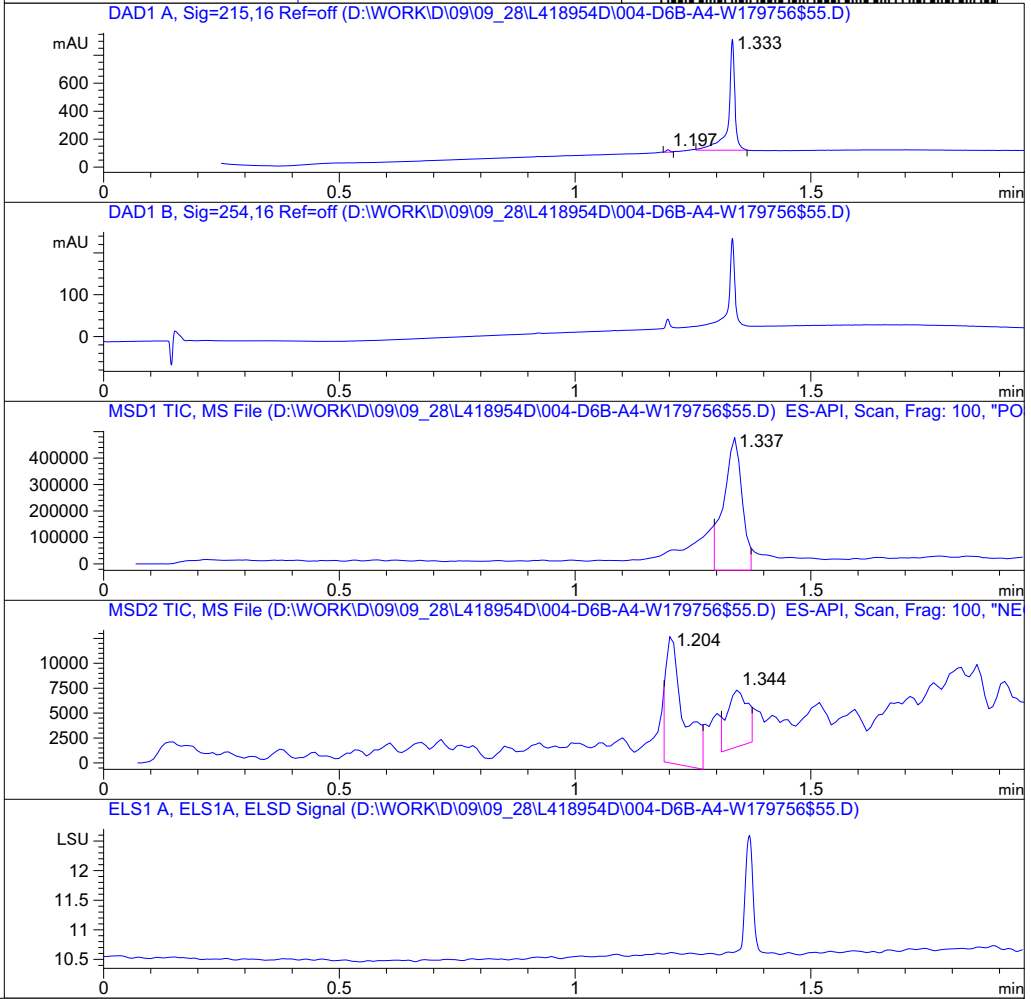


MaxPeak: 98.62%  
Ret\_Time: 1.333 min



Mol Wt 361.16  
Exact Mass 360

#	Time	Area%
1	1.197	1.38
2	1.333	98.62



Inj.Date 9/28/2021

K

<invalid> -15-

Acq. Method C:\Chem32\--> -->

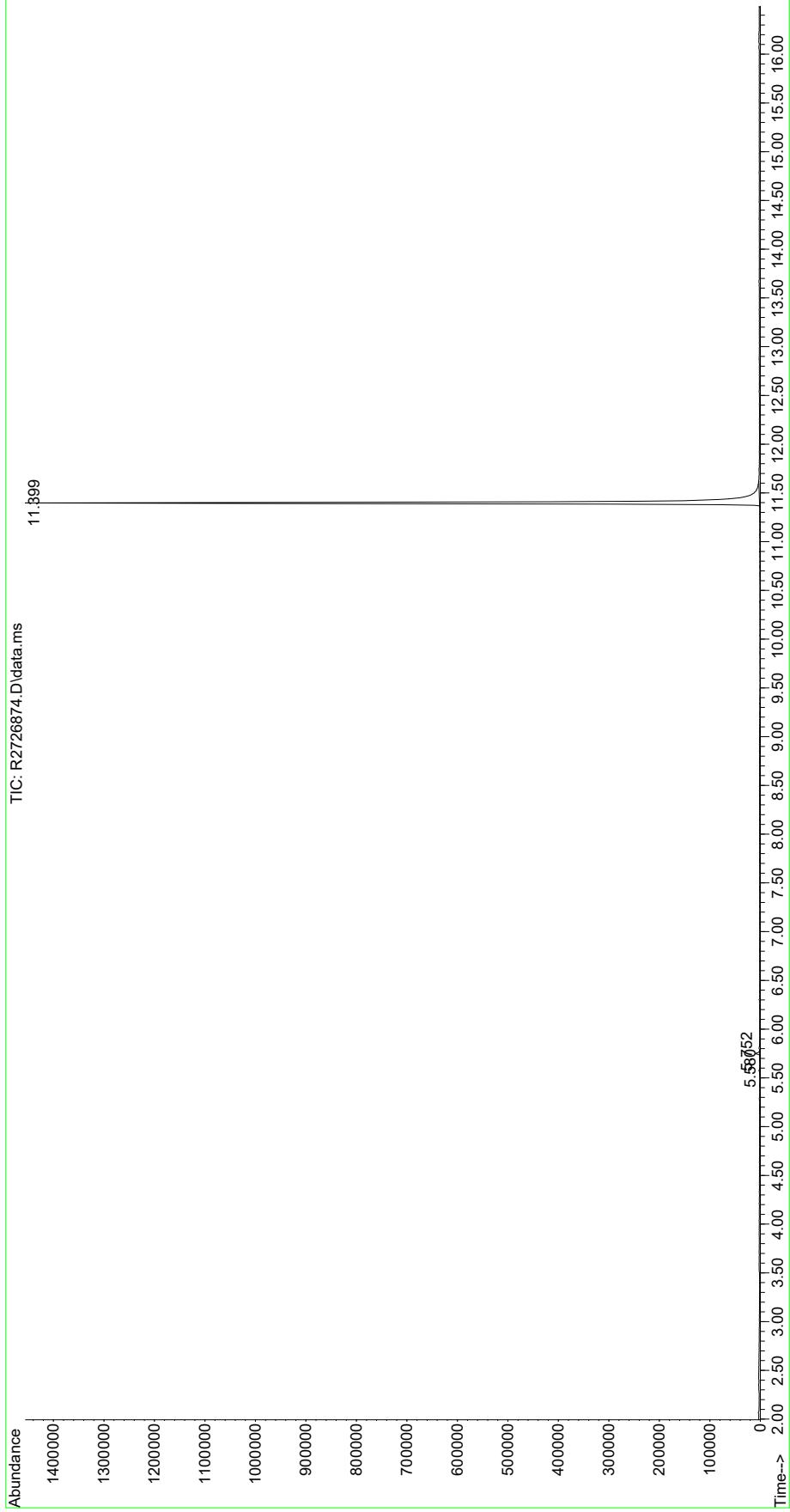
Z5192779144\_

Library Search Report

Data Path : D:\MassHunter\GCMS\1\data\09\_22\  
Data File : R2726874.D  
Acq On : 22 Sep 2021 15:10  
Operator :  
Sample : R2726874  
Misc : CH3CN  
ALS Vial : 77 Sample Multiplier: 1

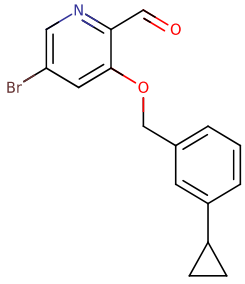
Search Libraries: C:\Database\EMPTY.L Minimum Quality: 0

Unknown Spectrum: Apex  
Integration Events: ChemStation Integrator - autoint1.e





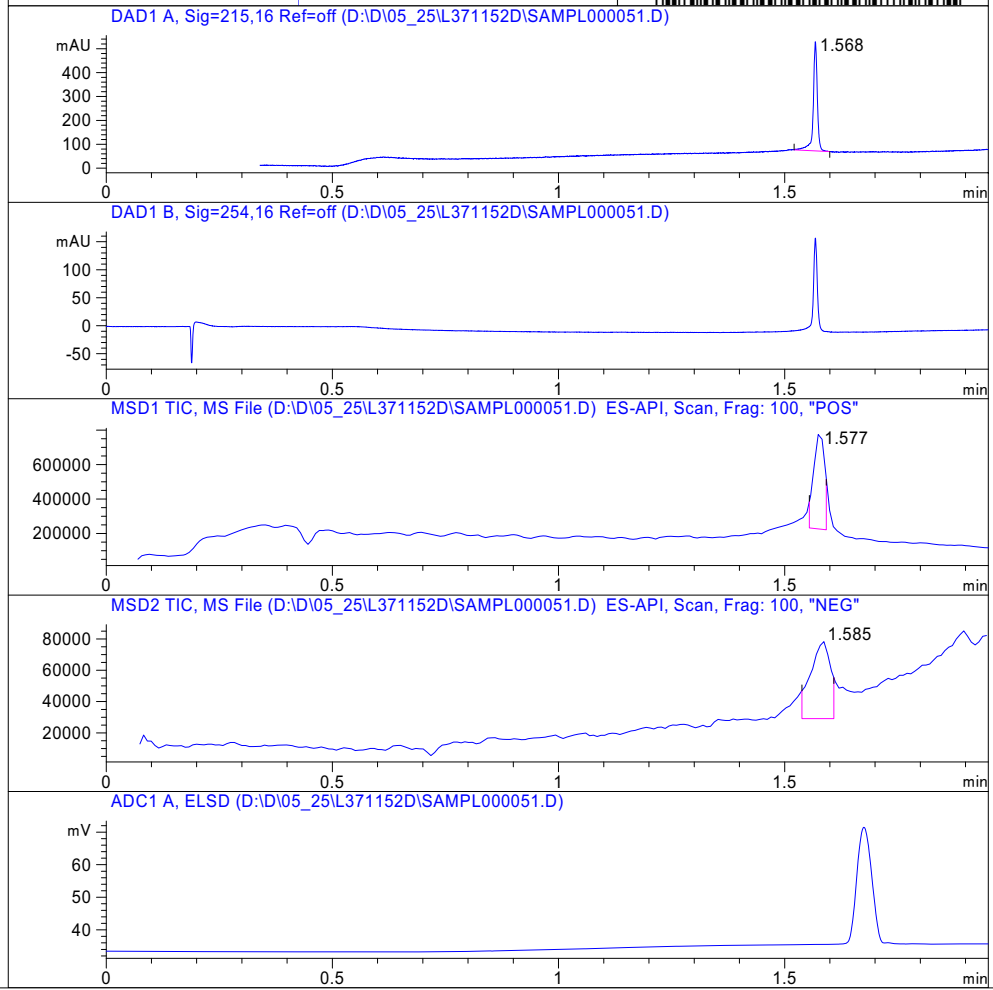
MaxPeak: 100.00%  
Ret\_Time: 1.568 min



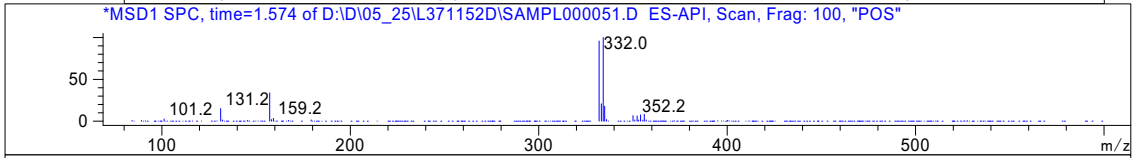
Mol Wt 332.19  
Exact Mass 331.04

#	Time	Area%
1	1.568	100.00

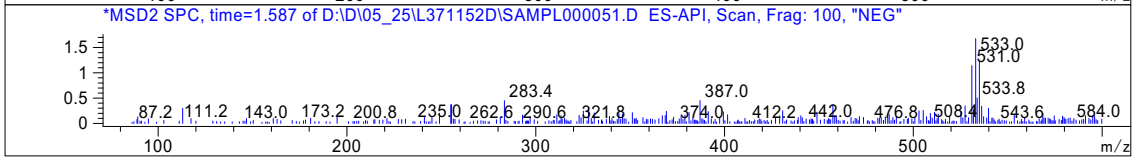
V211811\$A



RT 1.577



RT 1.585



Inj.Date 5/23/2021

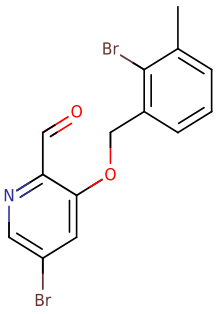
N

-5-

Acq. Method C:\CHEM32\--> -->

Z4989203264\_

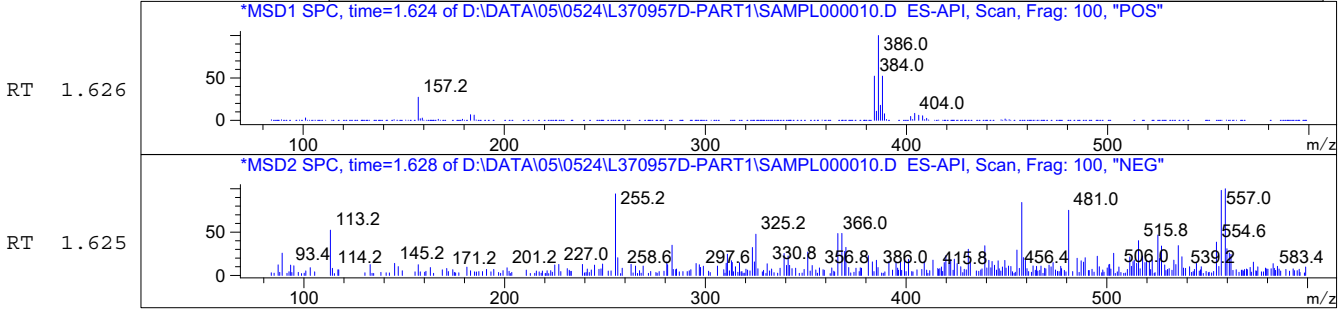
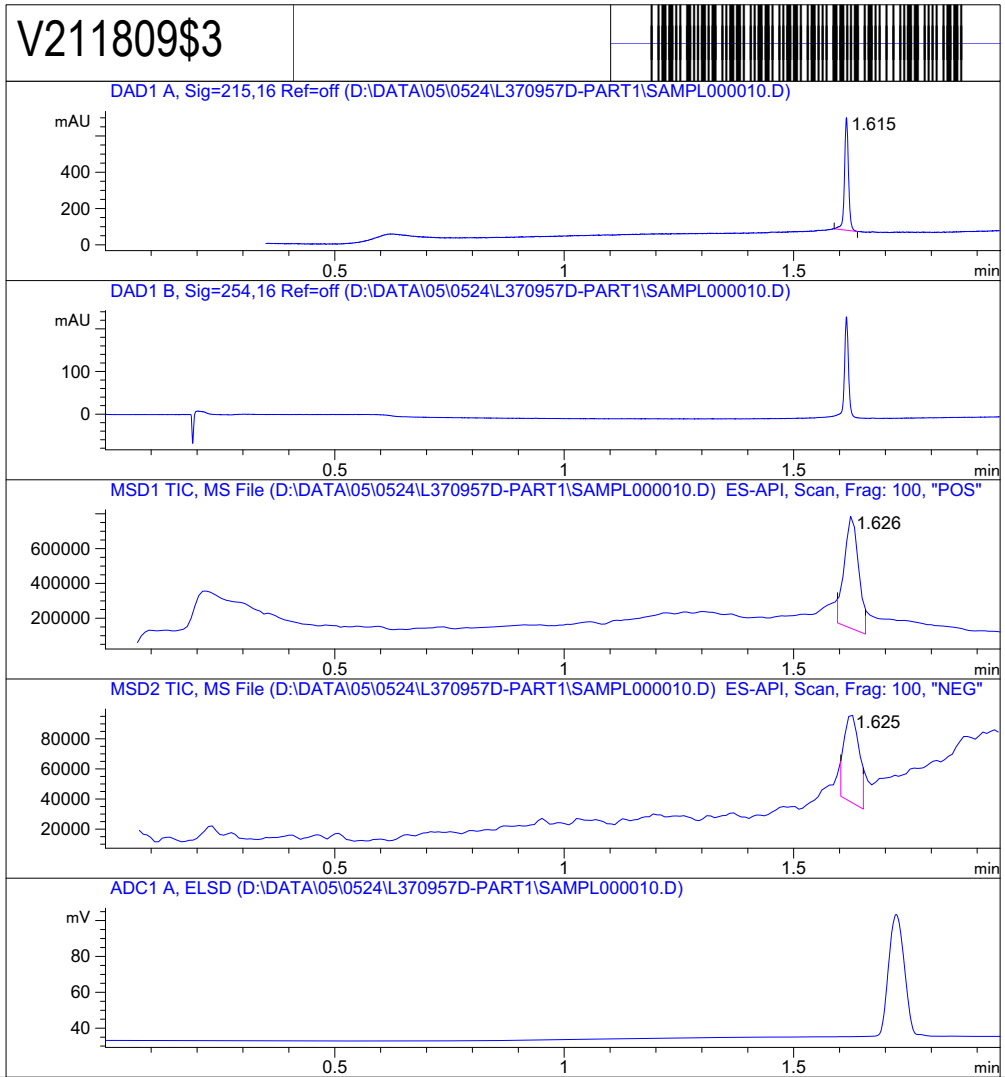
MaxPeak: 100.00%  
Ret\_Time: 1.615 min



Mol Wt 385.05  
Exact Mass 384.93

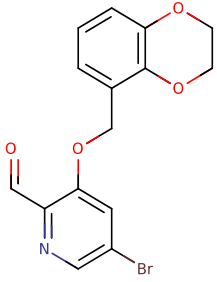
#	Time	Area%
1	1.615	100.00

V211809\$3



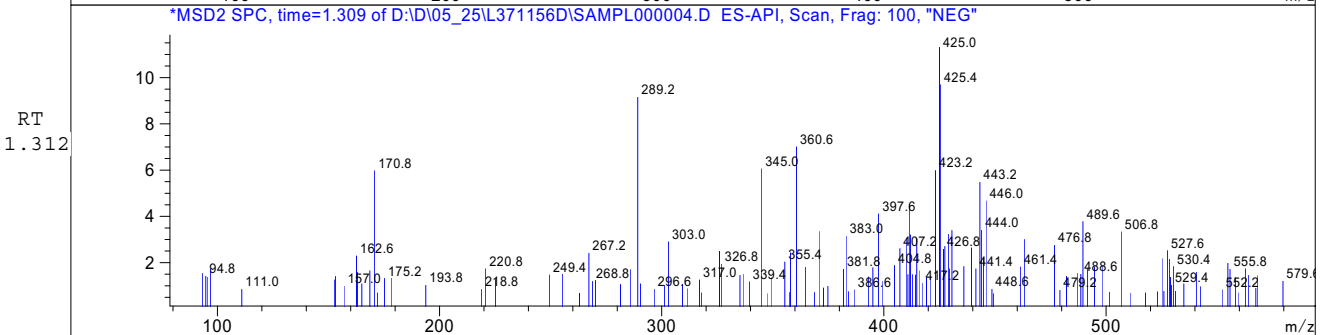
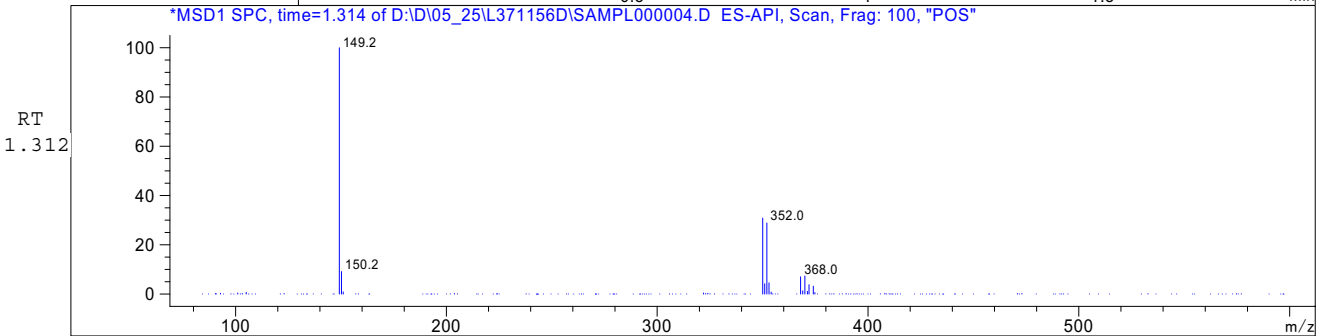
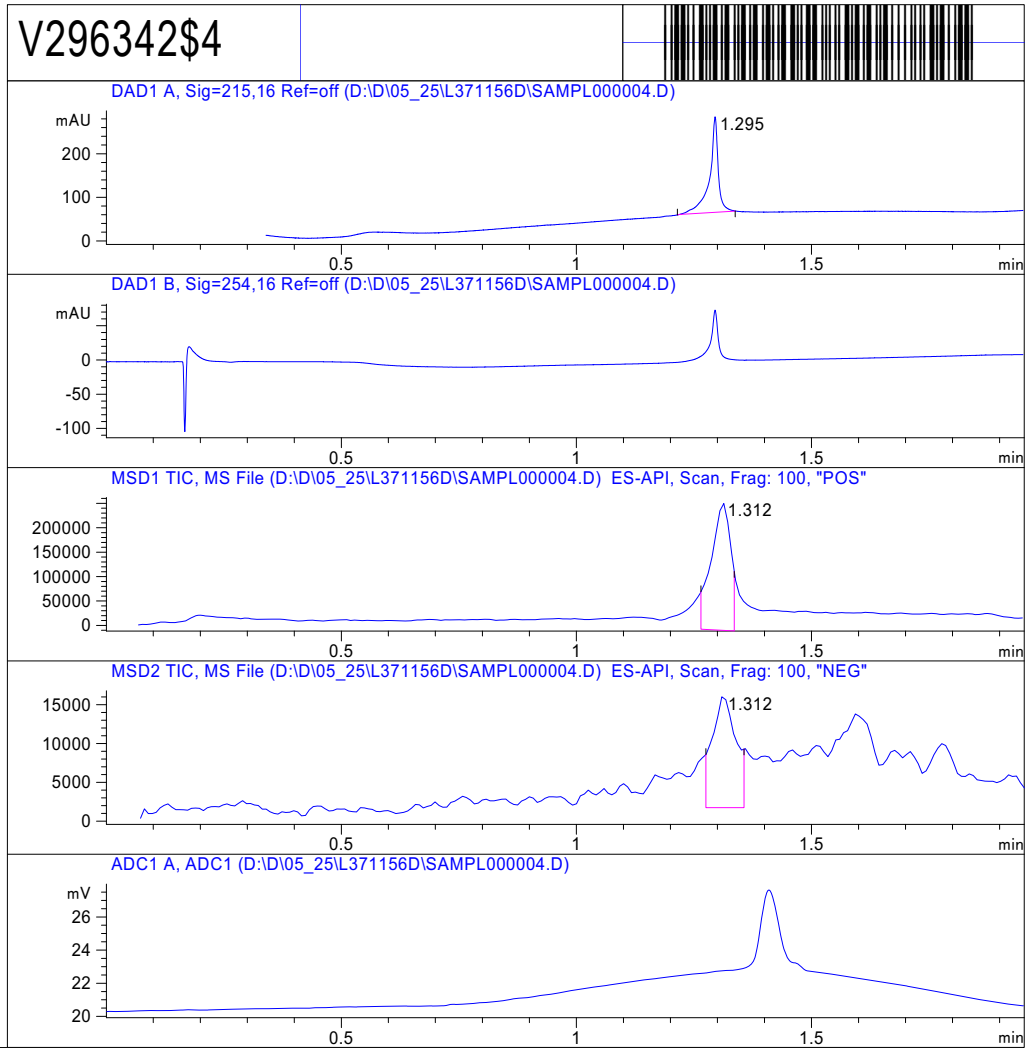
MaxPeak: 100.00%  
Ret\_Time: 1.295 min

V296342\$4



Mol Wt 350.16  
Exact Mass 349

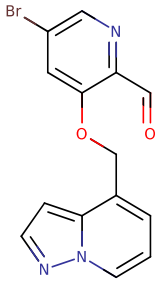
#	Time	Area%
1	1.295	100.00



V296341\$6

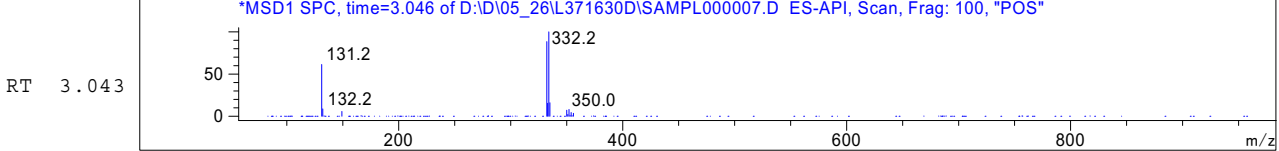
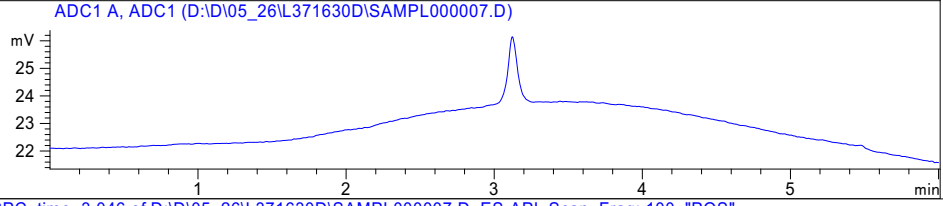
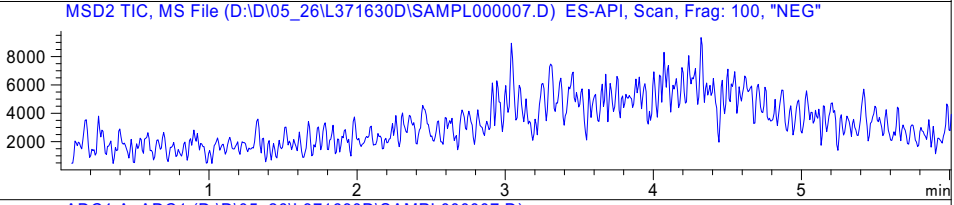
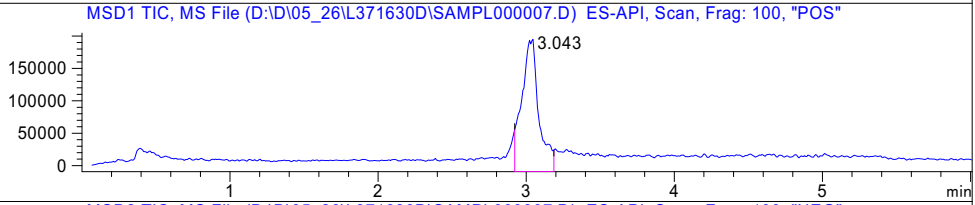
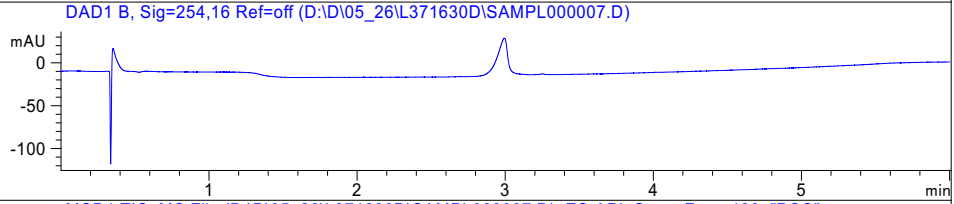
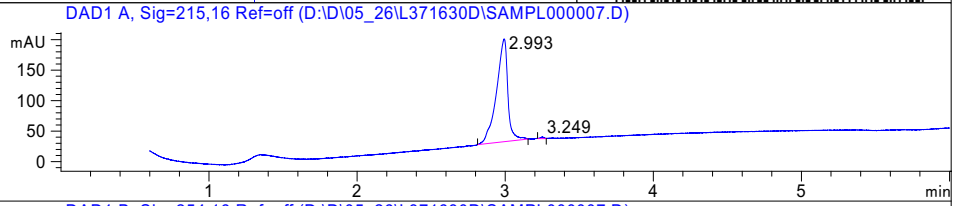


MaxPeak: 99.47%  
Ret\_Time: 2.993 min



Mol Wt 332.15  
Exact Mass 331

#	Time	Area%
1	2.993	99.47
2	3.249	0.53



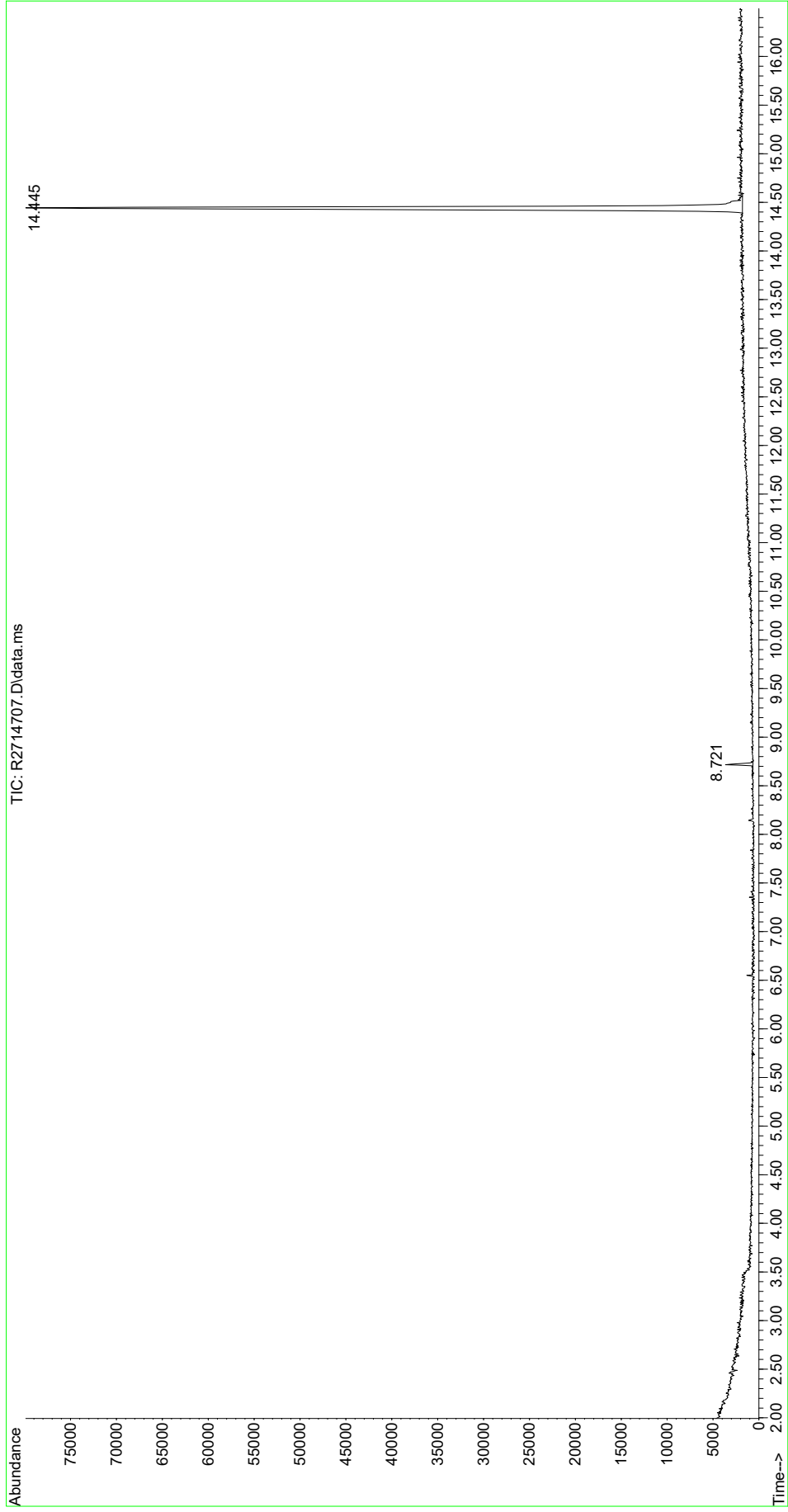
RT 3.043

Library Search Report

Data Path : D:\MassHunter\GCMS\1\data\09\_09\  
Data File : R2714707.D  
Acq On : 09 Sep 2021 17:49  
Operator :  
Sample : R2714707  
Misc : CH3CN  
ALS Vial : 126 Sample Multiplier: 1

Search Libraries: C:\Database\EMPTY.L Minimum Quality: 0

Unknown Spectrum: Apex  
Integration Events: ChemStation Integrator - autoint1.e

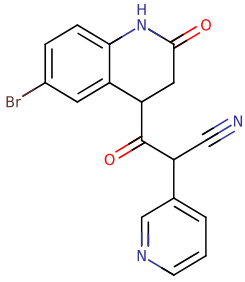


Z4954569231\_

# R2539922

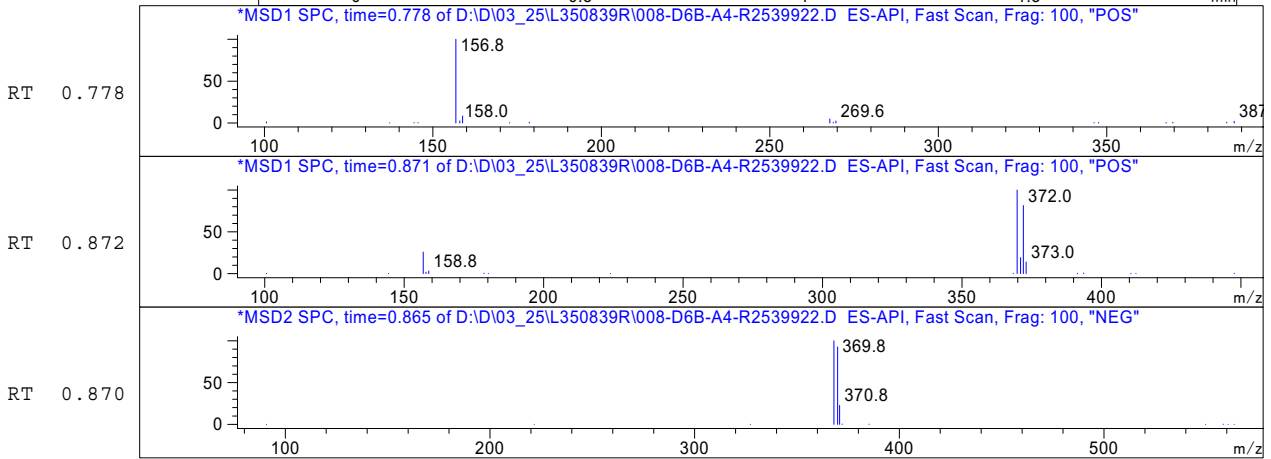
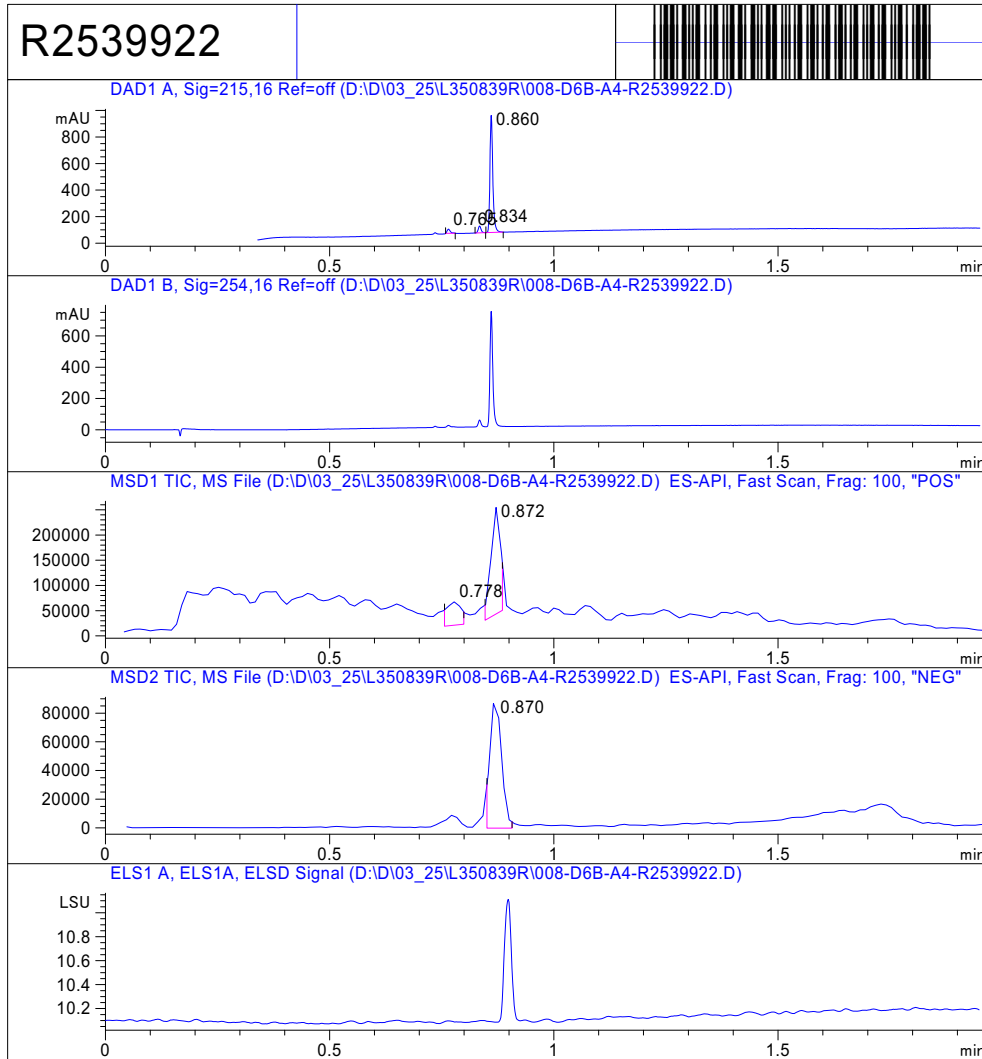


MaxPeak: 91.30%  
Ret\_Time: 0.860 min



Mol Wt 370.2  
Exact Mass 369.02

#	Time	Area%
1	0.765	3.46
2	0.834	5.24
3	0.860	91.30



Inj.Date 3/25/2021

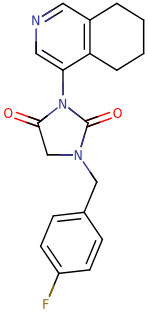
N

Acq. Method C:\Users\ -> ->

Z4934489646\_

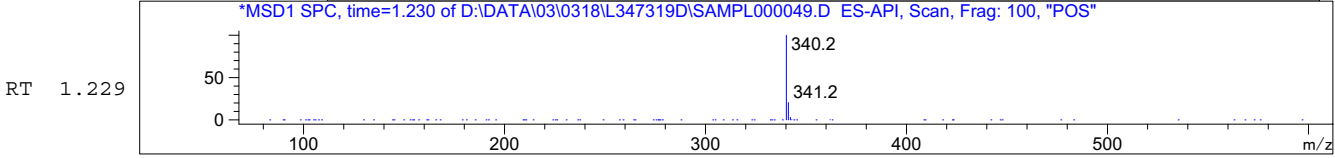
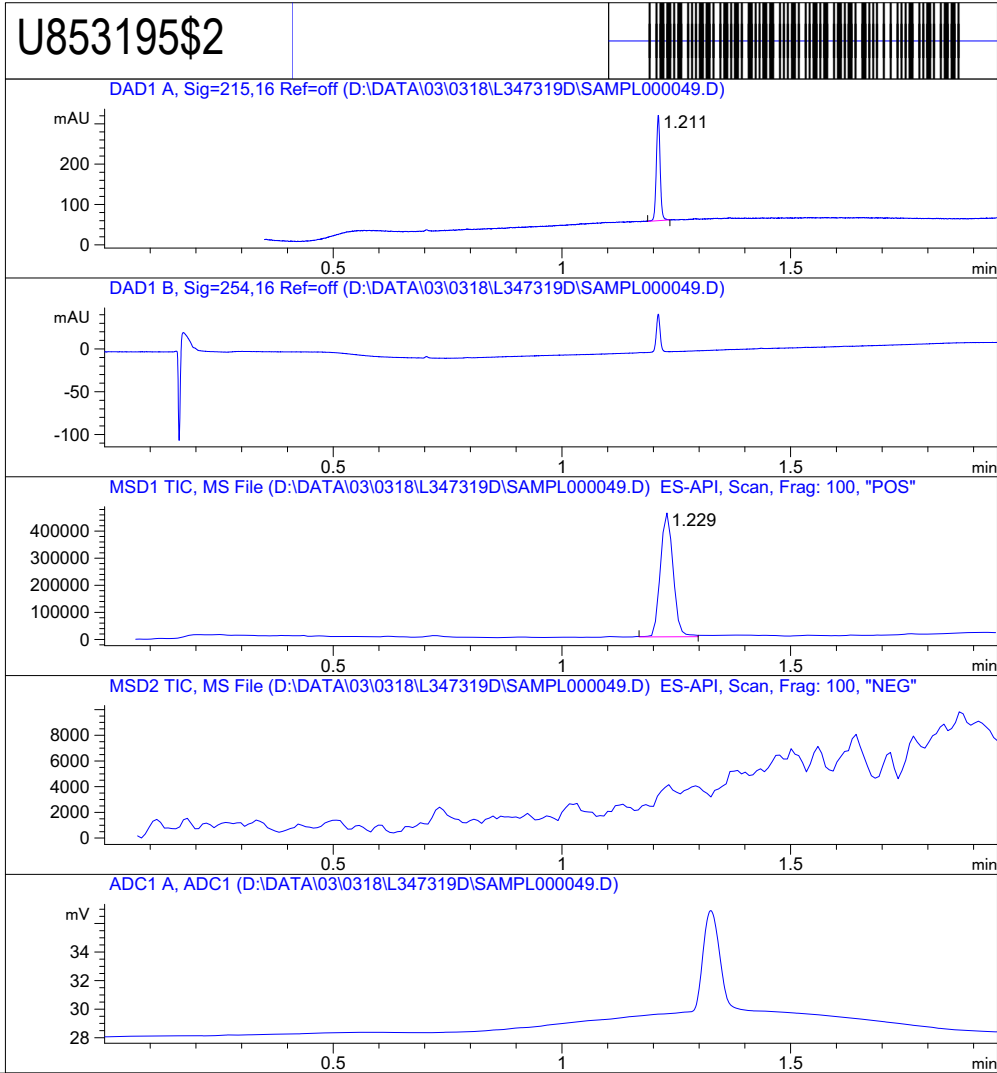
MaxPeak: 100.00%  
Ret\_Time: 1.211 min

U853195\$2



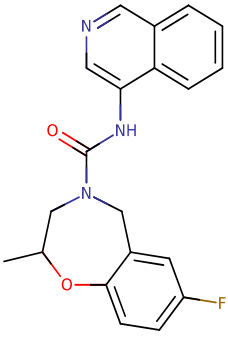
Mol Wt 339.36  
Exact Mass 339.16

#	Time	Area%
1	1.211	100.00



RT 1.229

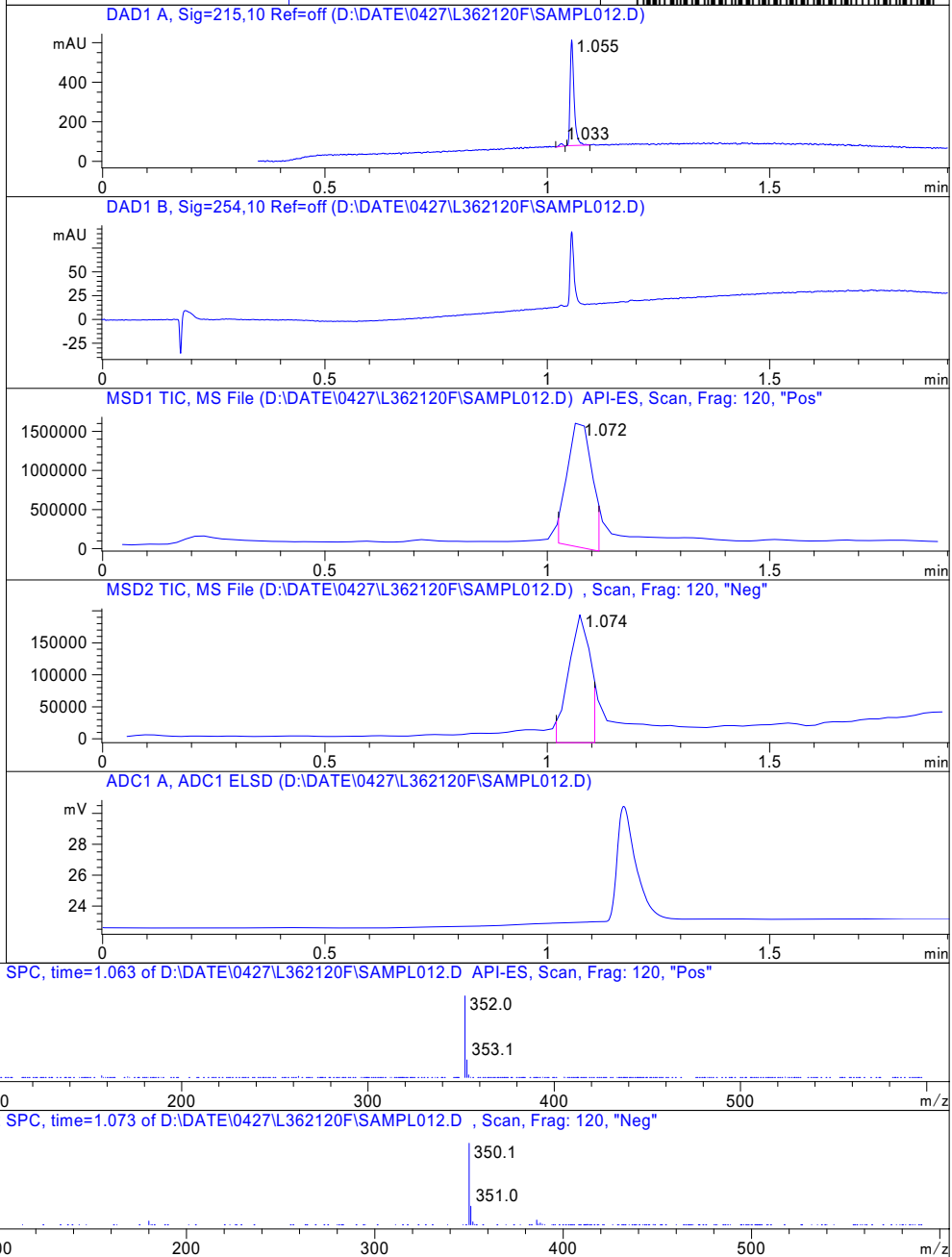
MaxPeak: 97.64%  
Ret\_Time: 1.055 min



Mol Wt 351.37  
Exact Mass 351.16

#	Time	Area%
1	1.033	2.36
2	1.055	97.64

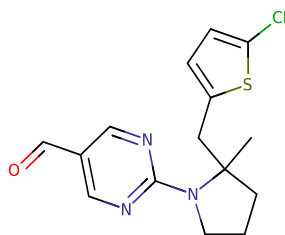
V218888\$1





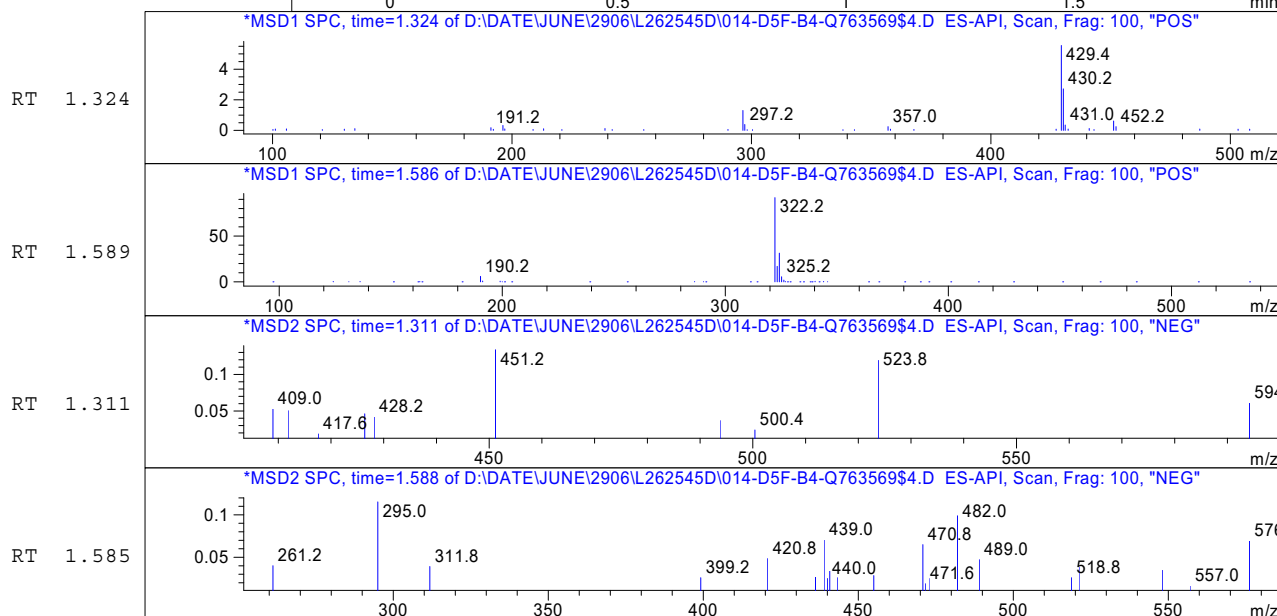
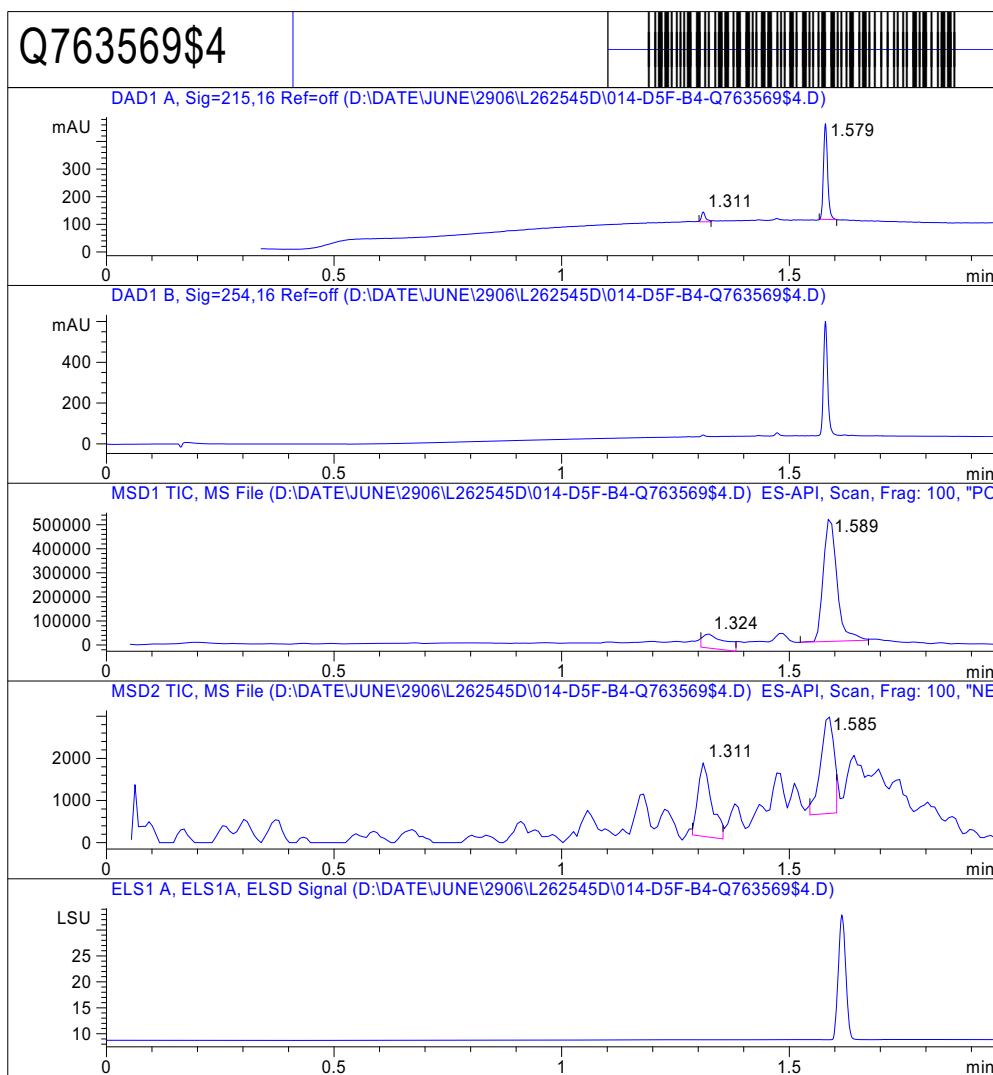
MaxPeak: 90.44%  
Ret\_Time: 1.579 min

Q763569\$4



Mol Wt 321.82  
Exact Mass 321.09

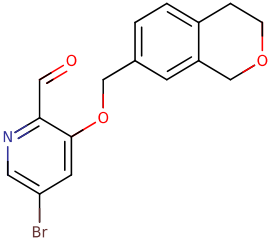
#	Time	Area%
1	1.311	9.56
2	1.579	90.44



S993128\$9

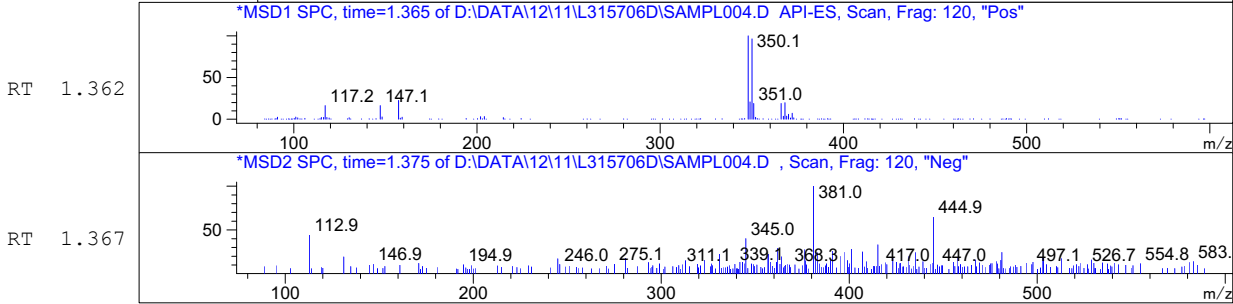
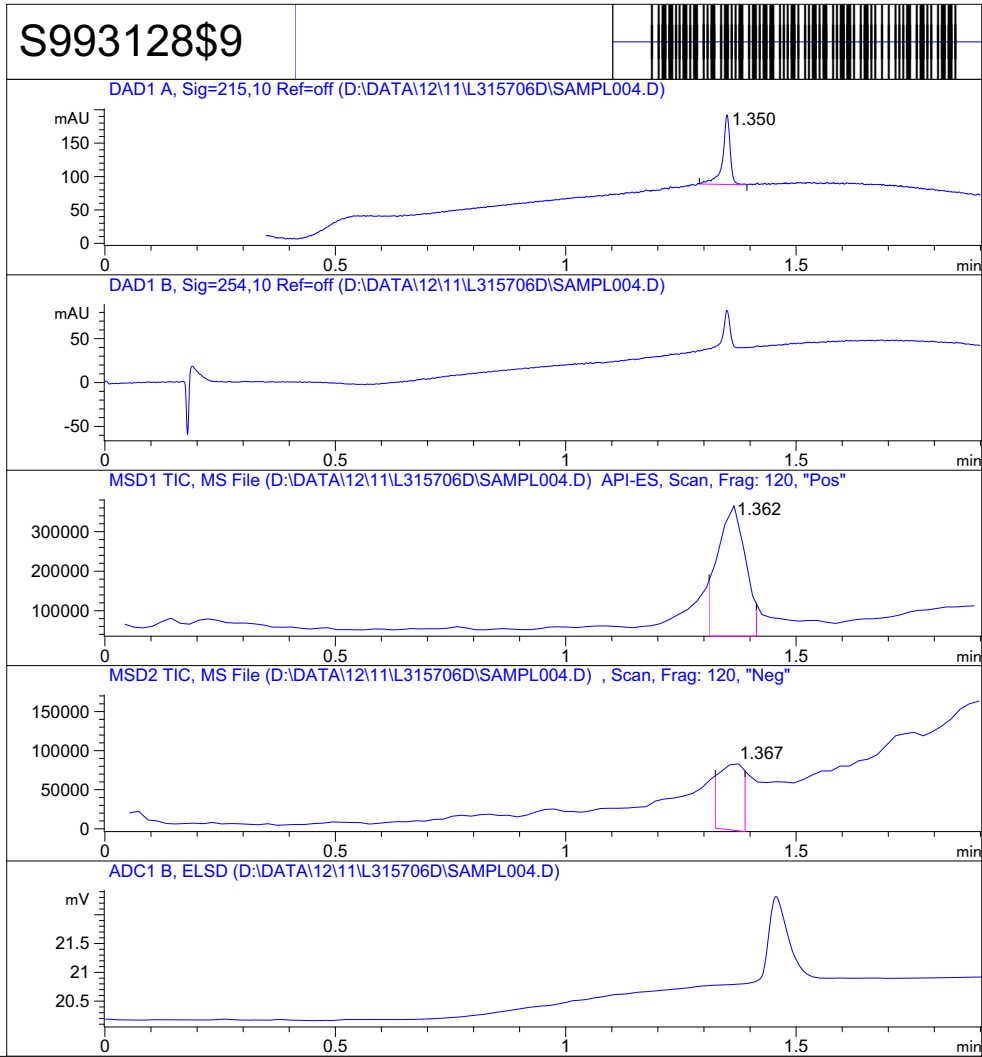


MaxPeak: 100.00%  
Ret\_Time: 1.350 min



Mol Wt 348.19  
Exact Mass 347.03

#	Time	Area%
1	1.350	100.00



Inj.Date 12/11/2020

LB

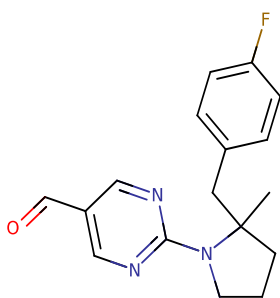
-SL-

Acq. Method C:\HPCHEM\ -> ->

Z3339728474\_

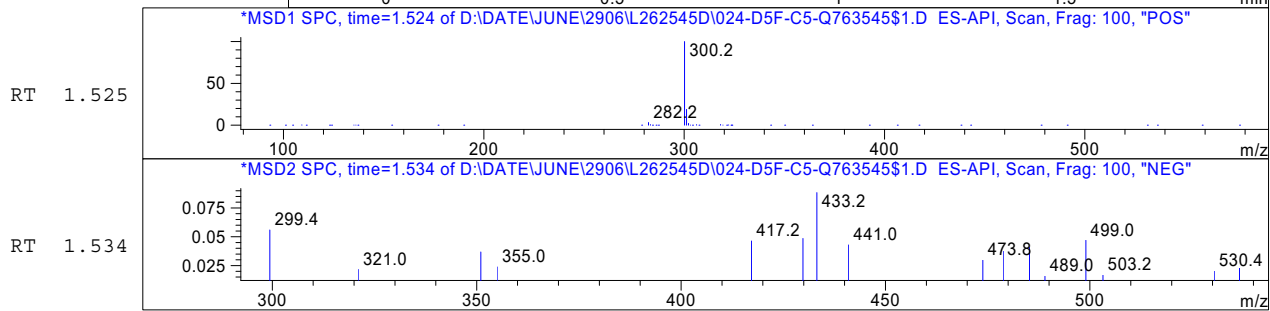
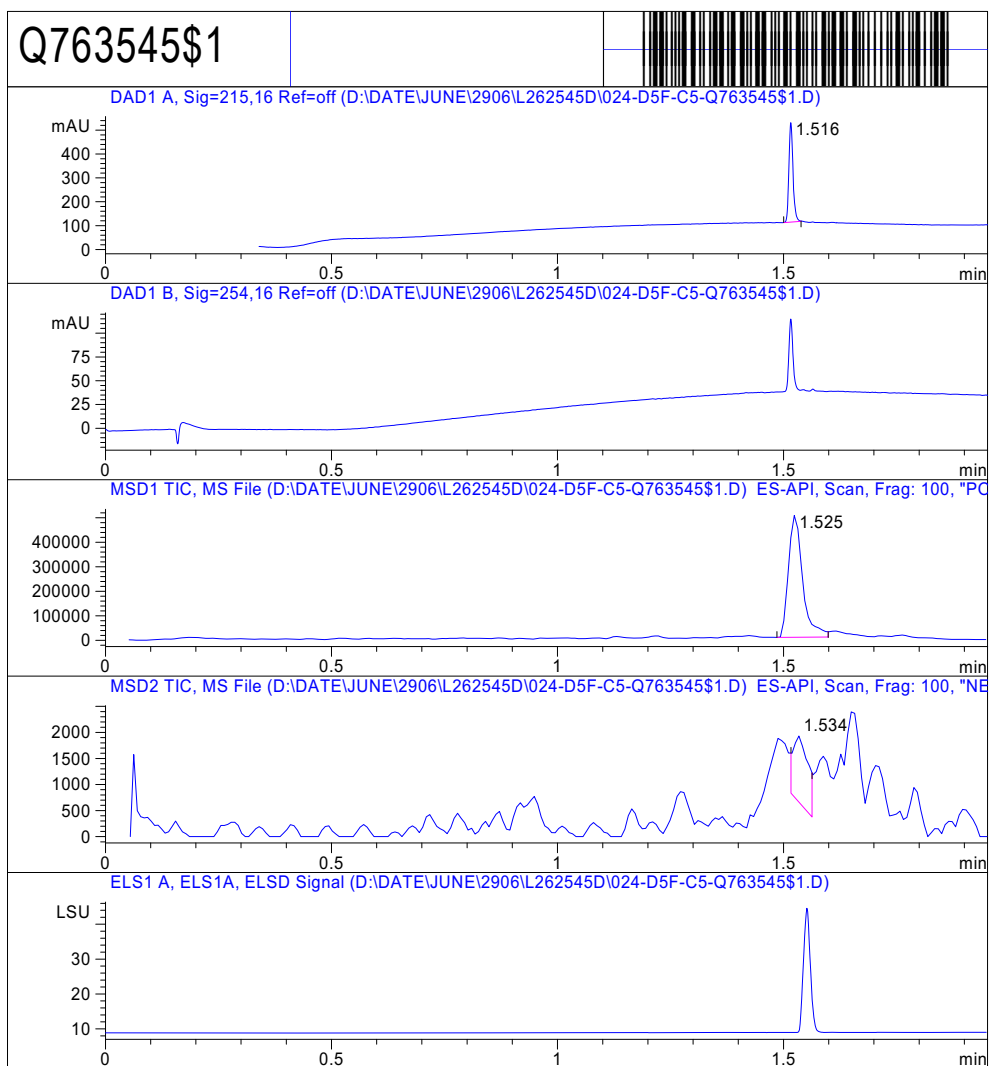
MaxPeak: 100.00%  
Ret\_Time: 1.516 min

# Q763545\$1



**Mol Wt** 299.34  
**Exact Mass** 299.17

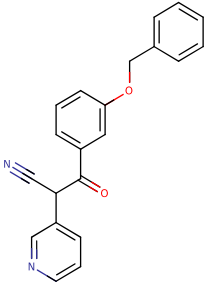
#	Time	Area%
1	1.516	100.00



# R2541405

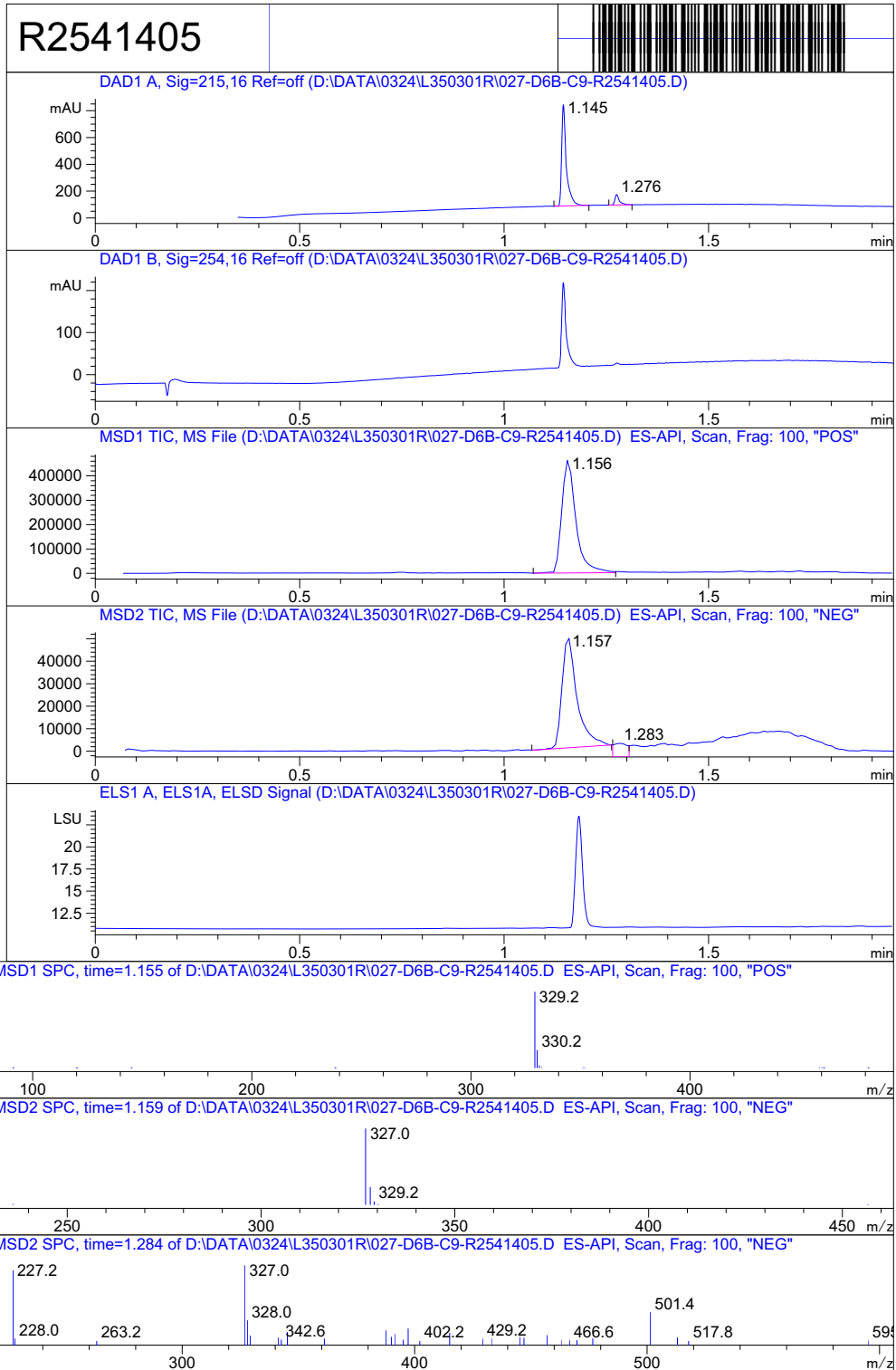


MaxPeak: 90.89%  
Ret\_Time: 1.145 min

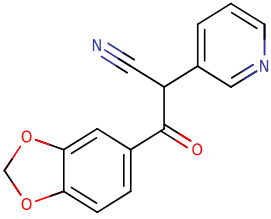


**Mol Wt** 328.36  
**Exact Mass** 328.14

#	Time	Area%
1	1.145	90.89
2	1.276	9.11

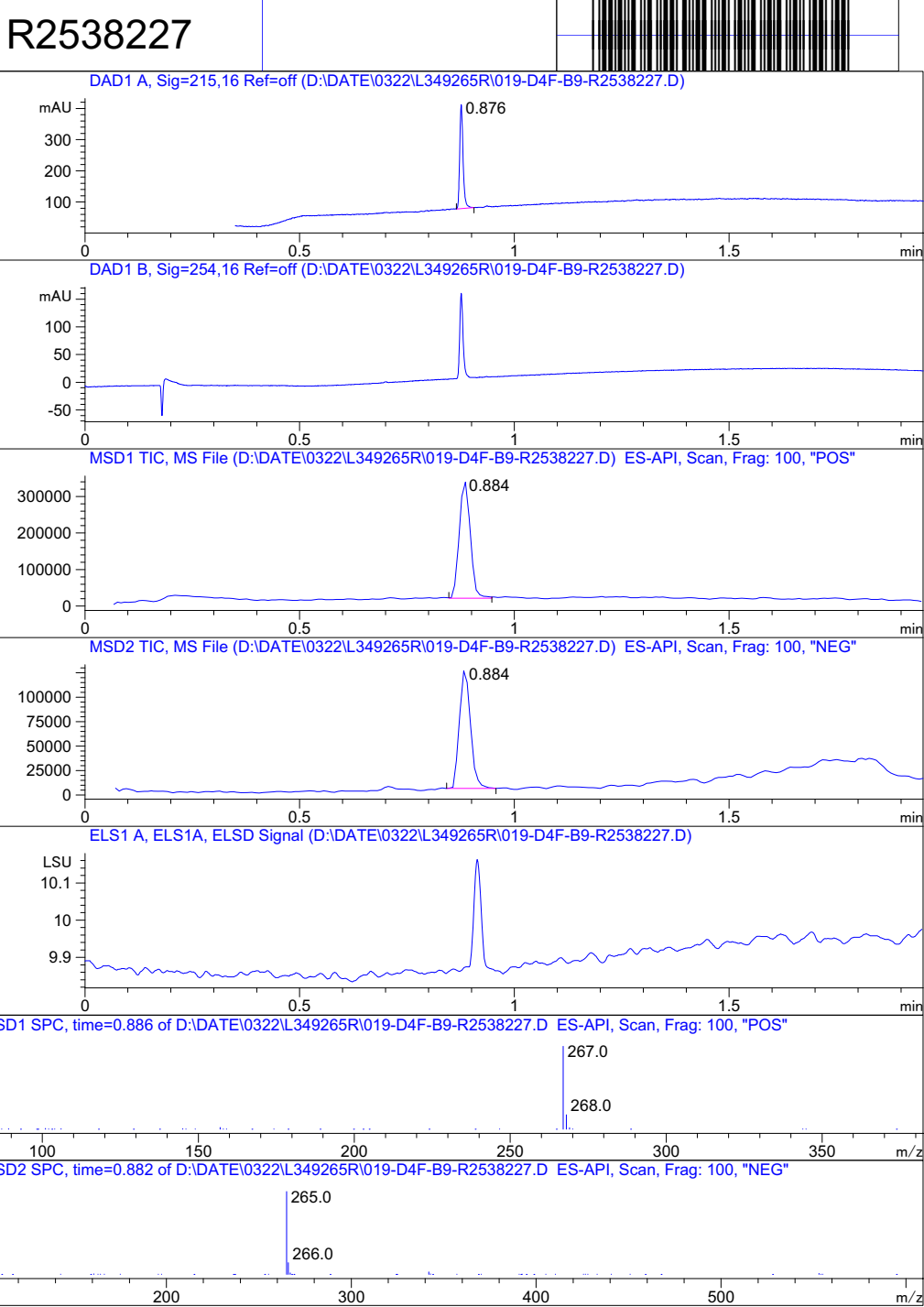


MaxPeak: 100.00%  
Ret\_Time: 0.876 min

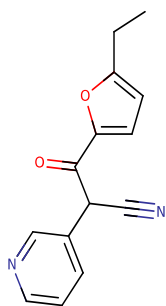


Mol Wt 266.25  
Exact Mass 266.07

#	Time	Area%
1	0.876	100.00



MaxPeak: 100.00%  
Ret\_Time: 0.964 min

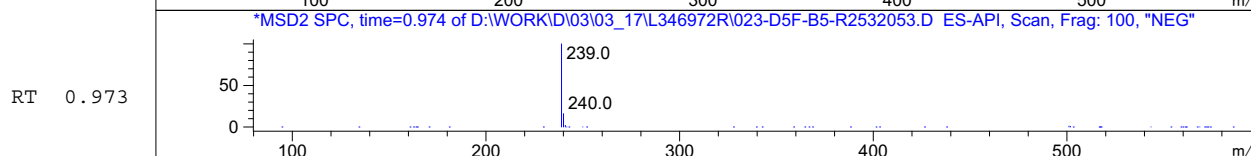
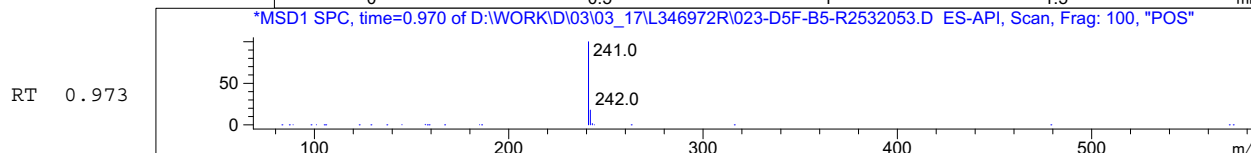
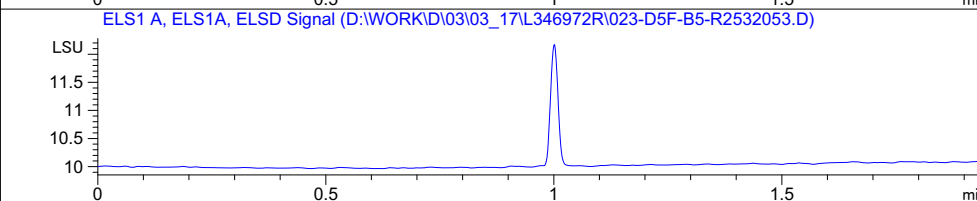
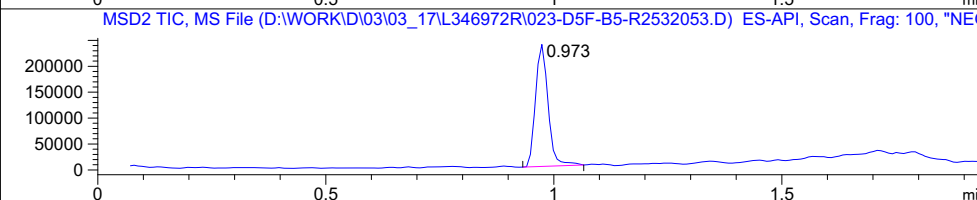
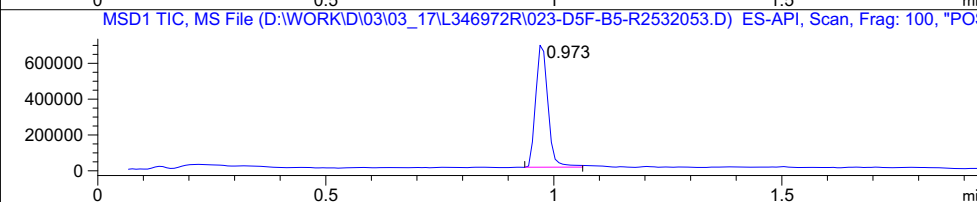
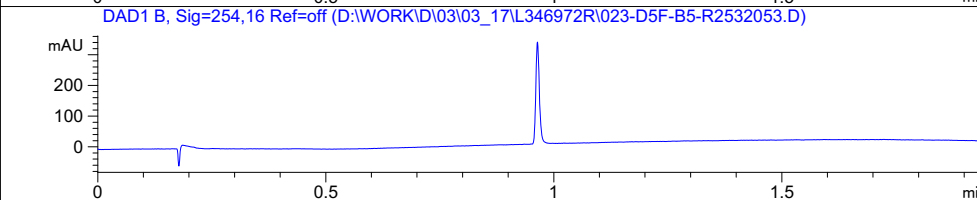
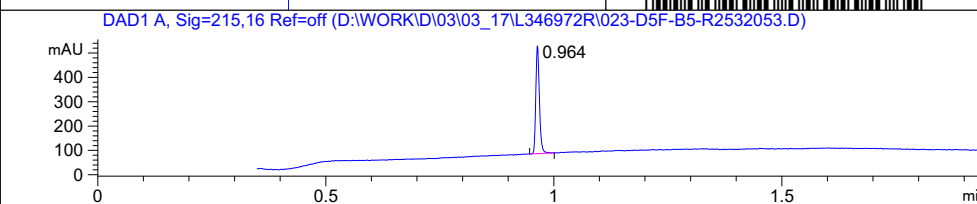


Mol Wt 240.26

Exact Mass 240.1

#	Time	Area%
1	0.964	100.00

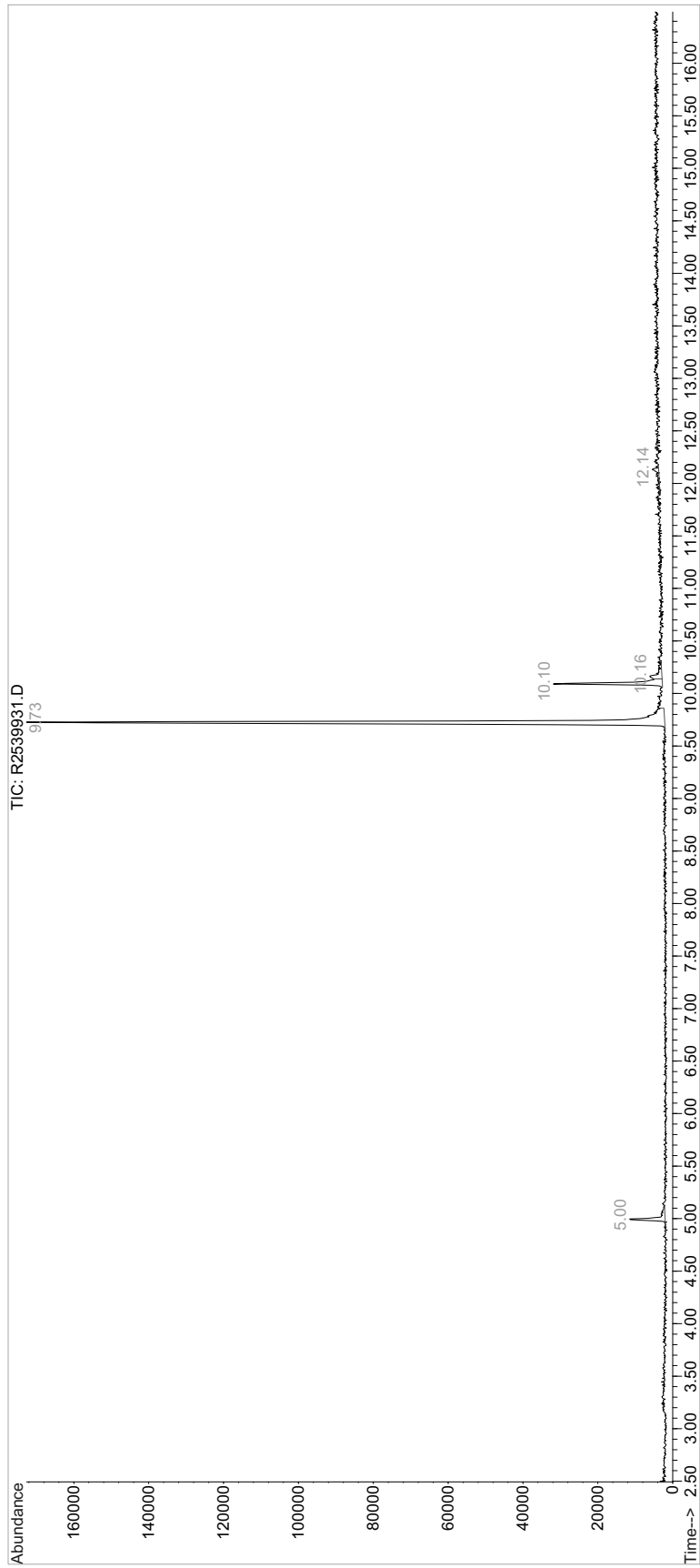
R2532053



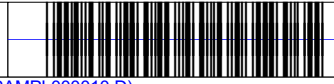
Library Search Report

Data File : C:\MSDCHEM\1\DATA\03\_23\R2539931.D  
Acq On : 24 Mar 2021 4:20 Vial: 16  
Sample : R2539931 Operator:  
Misc : CH3CN+CH2Cl2 Inst : GCMS2 #1  
Sample Amount: 0.00 Multiplr: 1.00

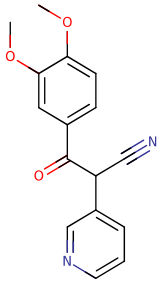
MS Integration Params: autoint1.e  
Method : C:\MSDCHEM\1\METHODS\UNIVERS.M (Chemstation Integrator)  
Title :



# R2535275

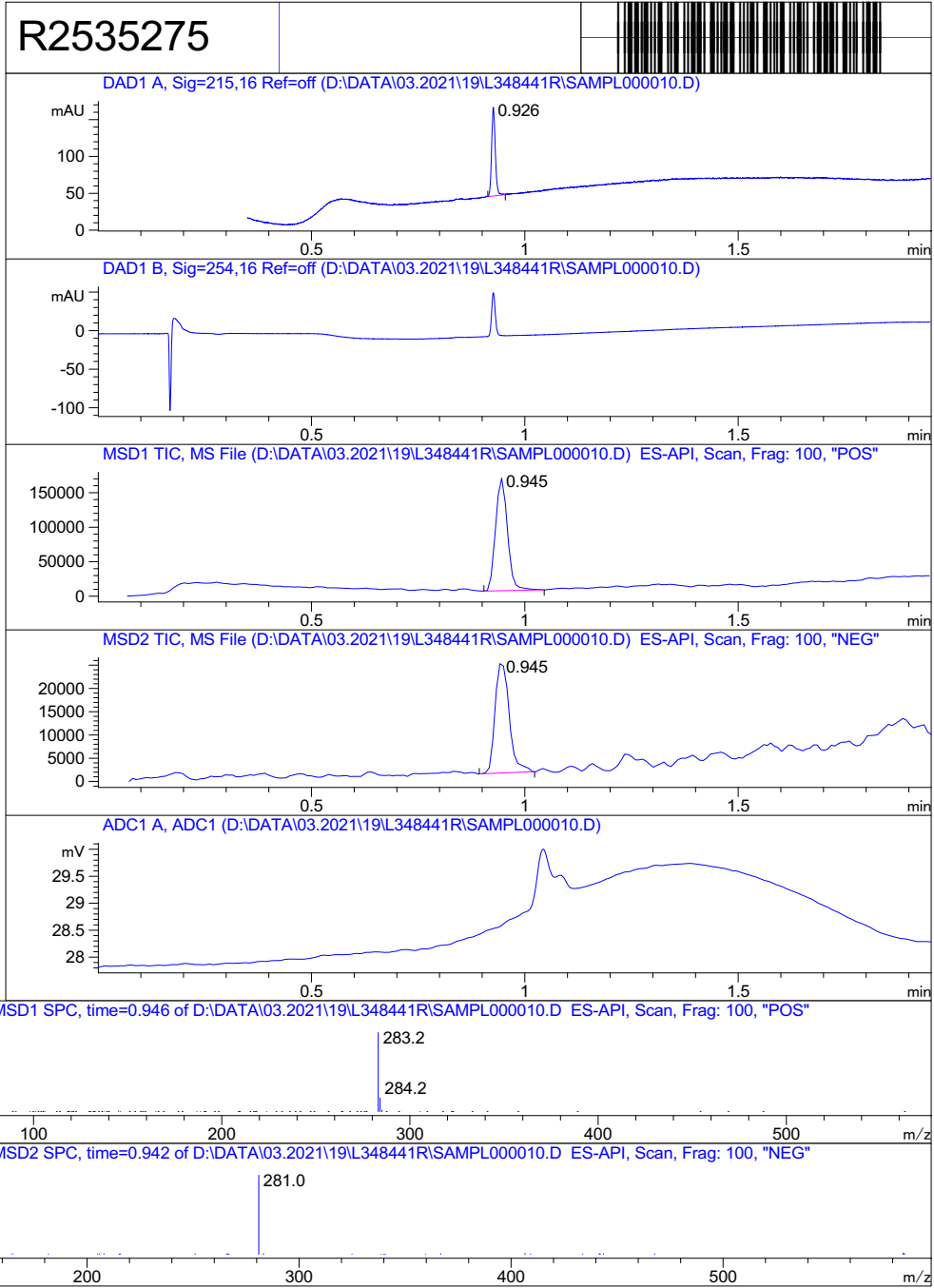


MaxPeak: 100.00%  
Ret\_Time: 0.926 min



Mol Wt 282.29  
Exact Mass 282.11

#	Time	Area%
1	0.926	100.00

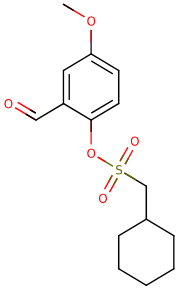


RT 0.945

RT 0.945



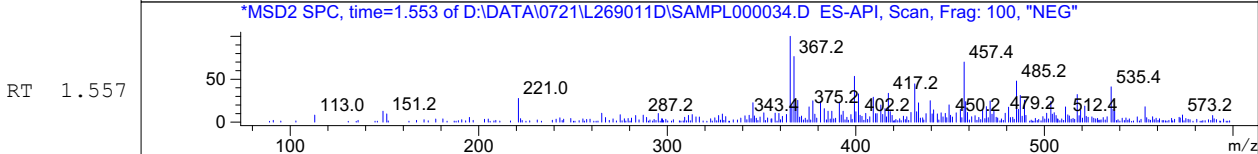
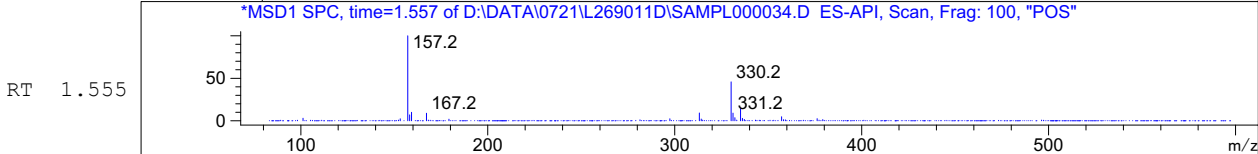
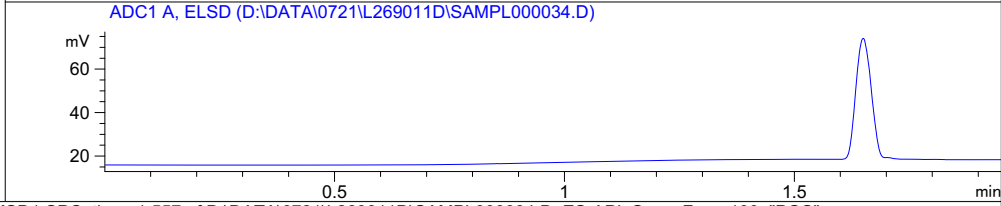
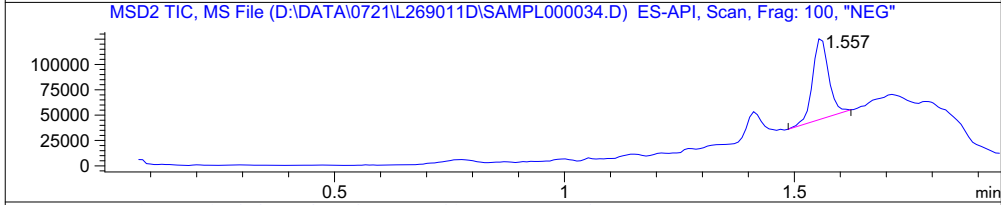
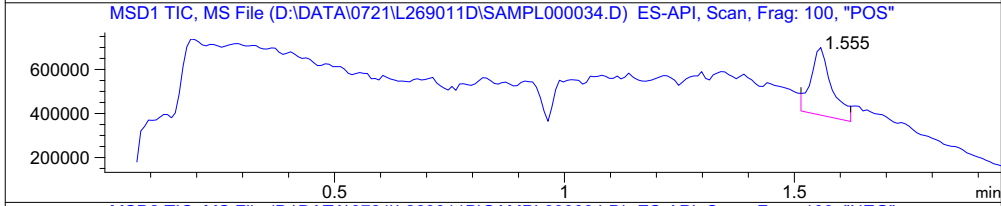
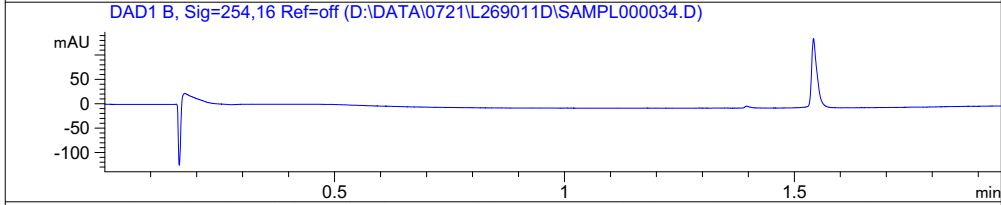
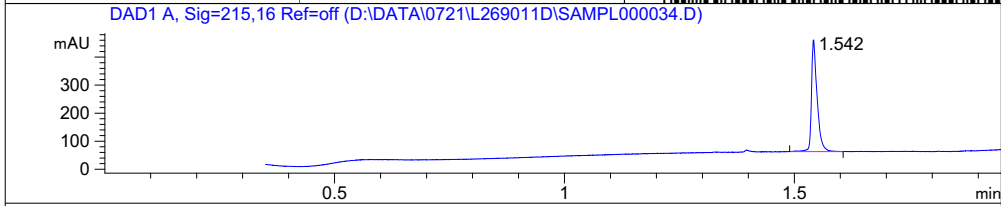
MaxPeak: 100.00%  
Ret\_Time: 1.542 min



Mol Wt 312.38  
Exact Mass 312.12

#	Time	Area%
1	1.542	100.00

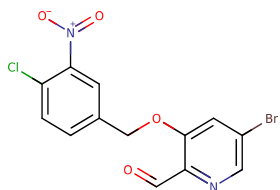
Q786891\$71



# V498758\$I

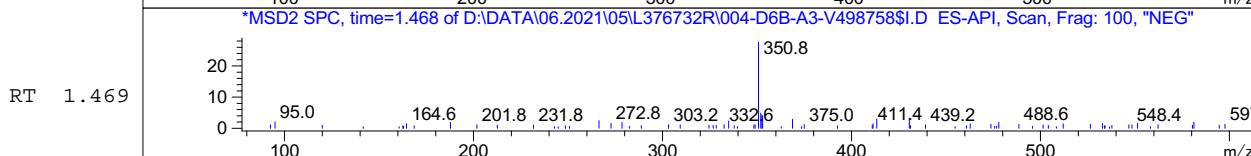
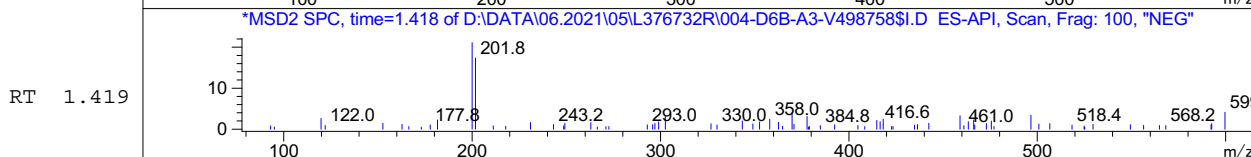
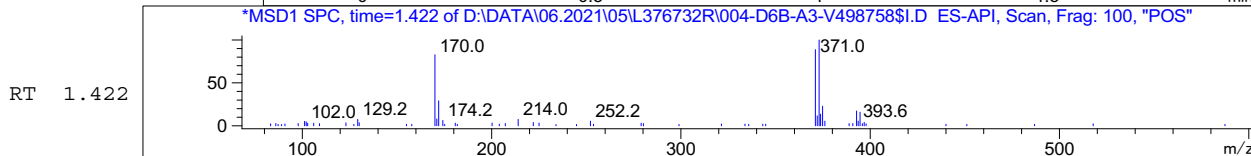
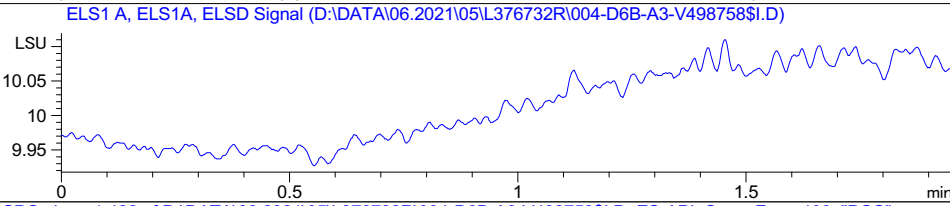
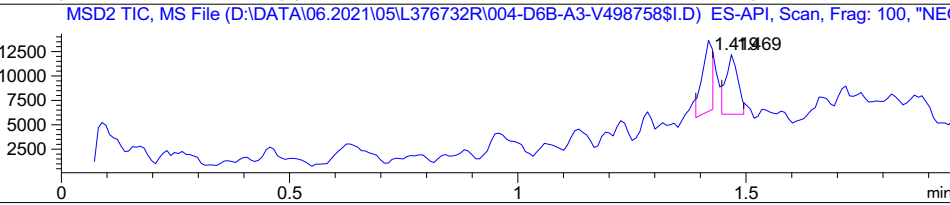
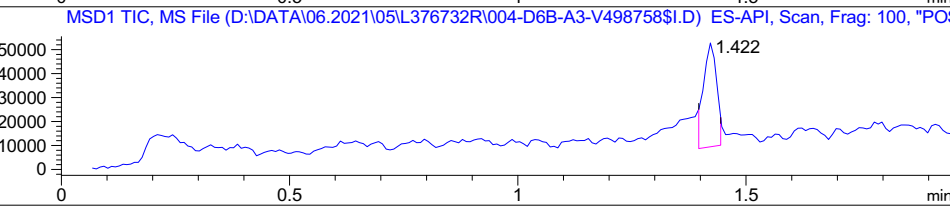
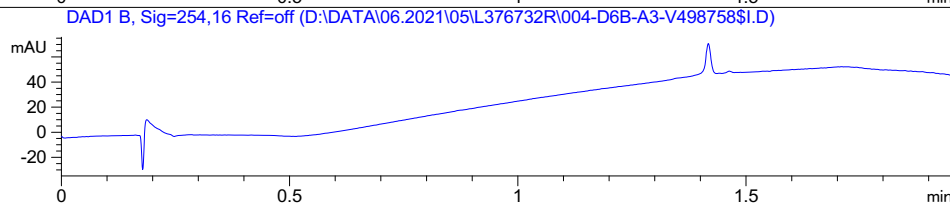
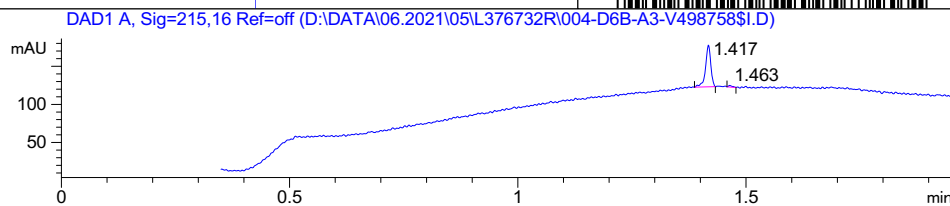


MaxPeak: 97.18%  
Ret\_Time: 1.417 min



Mol Wt 371.57  
Exact Mass 371.93

#	Time	Area%
1	1.417	97.18
2	1.463	2.82



Inj.Date 6/5/2021

CH <invalid> -17-

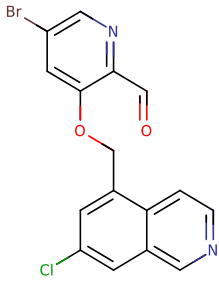
Acq. Method C:\Chem32\ -> ->

Z4767502618\_

# R2794156

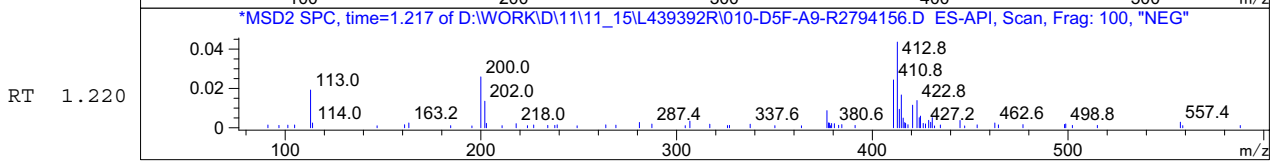
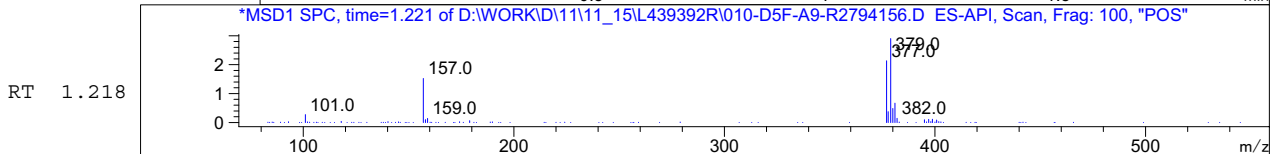
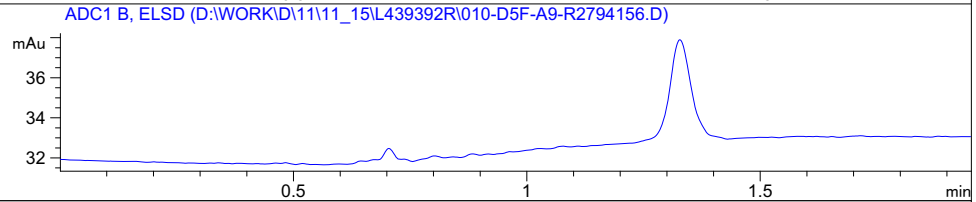
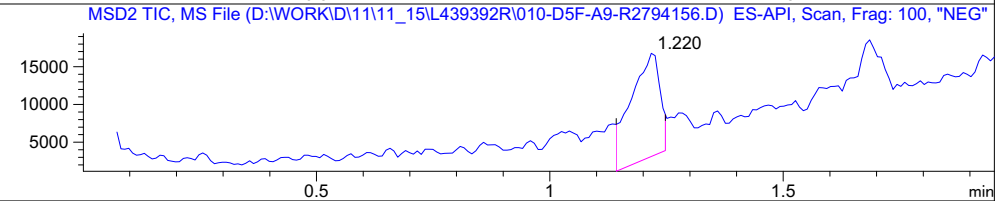
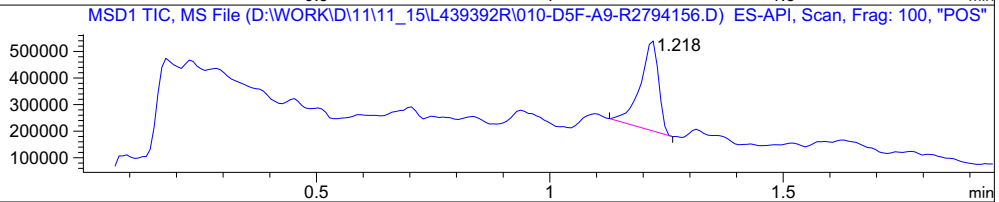
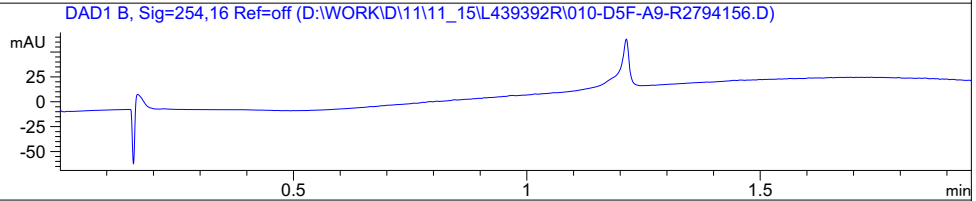
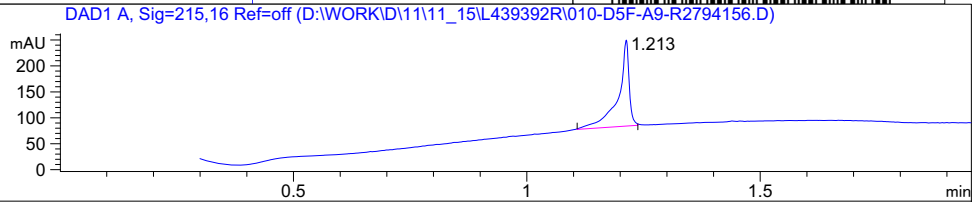


MaxPeak: 100.00%  
Ret\_Time: 1.213 min



Mol Wt 377.62  
Exact Mass 377.97

#	Time	Area%
1	1.213	100.00



Inj.Date 11/15/2021

K

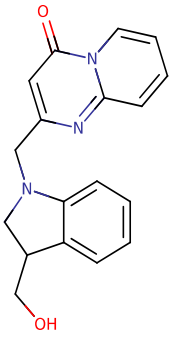
<invalid> -10-

Acq. Method C:\Chem32\ -> ->

Z5192779138\_

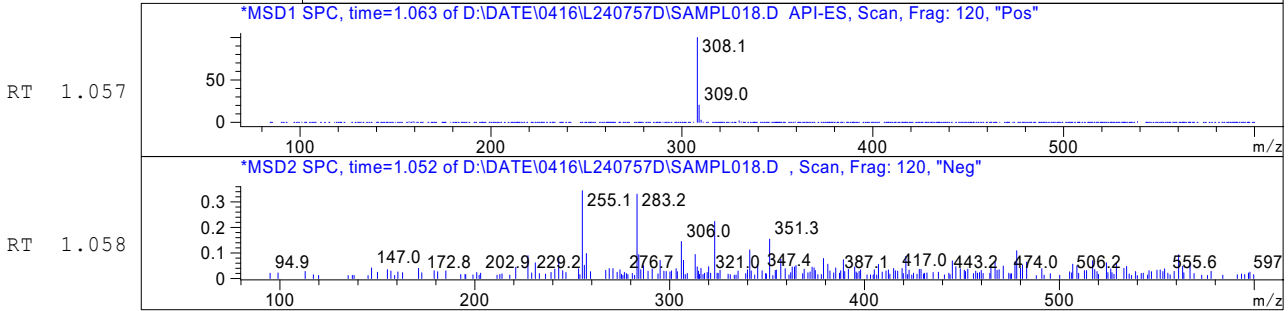
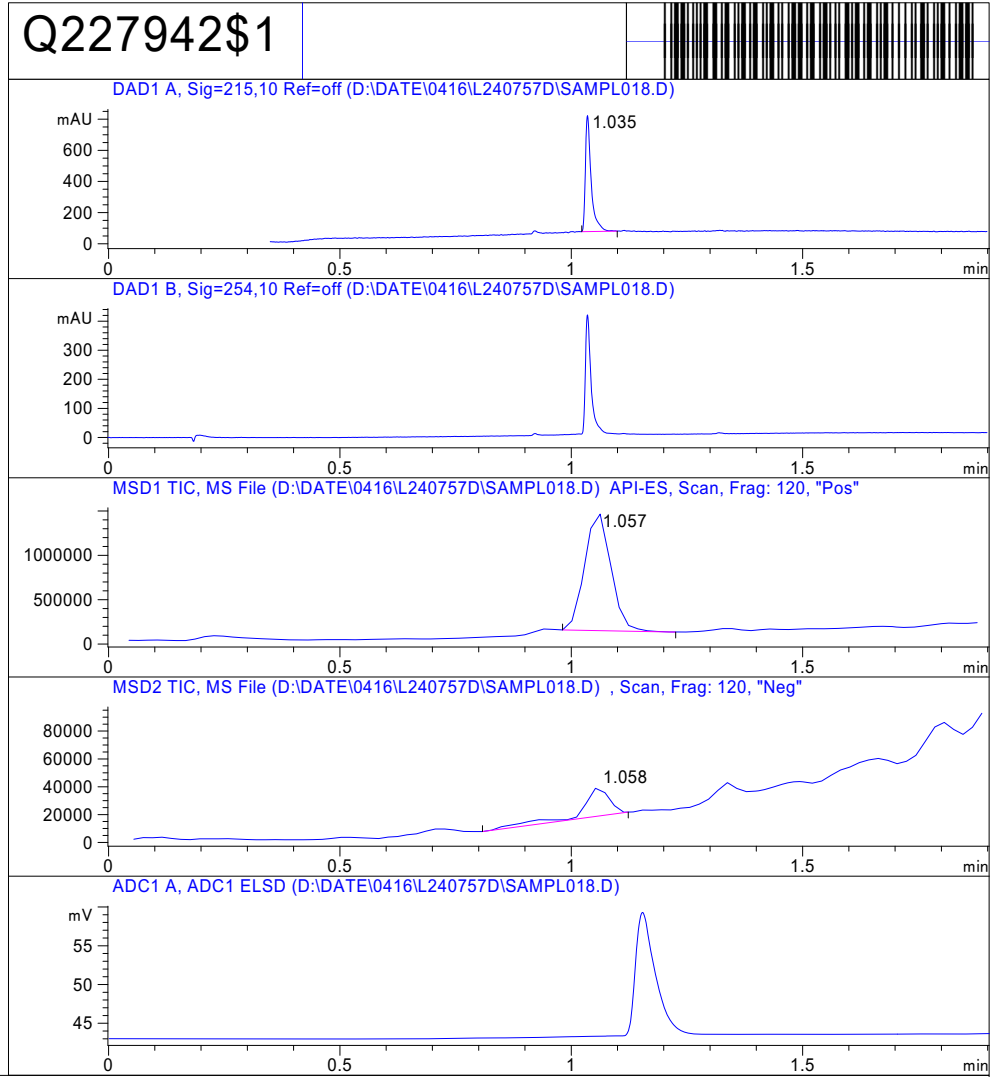
MaxPeak: 100.00%  
Ret\_Time: 1.035 min

Q227942\$1

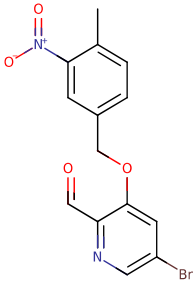


Mol Wt 307.35  
Exact Mass 307.15

#	Time	Area%
1	1.035	100.00



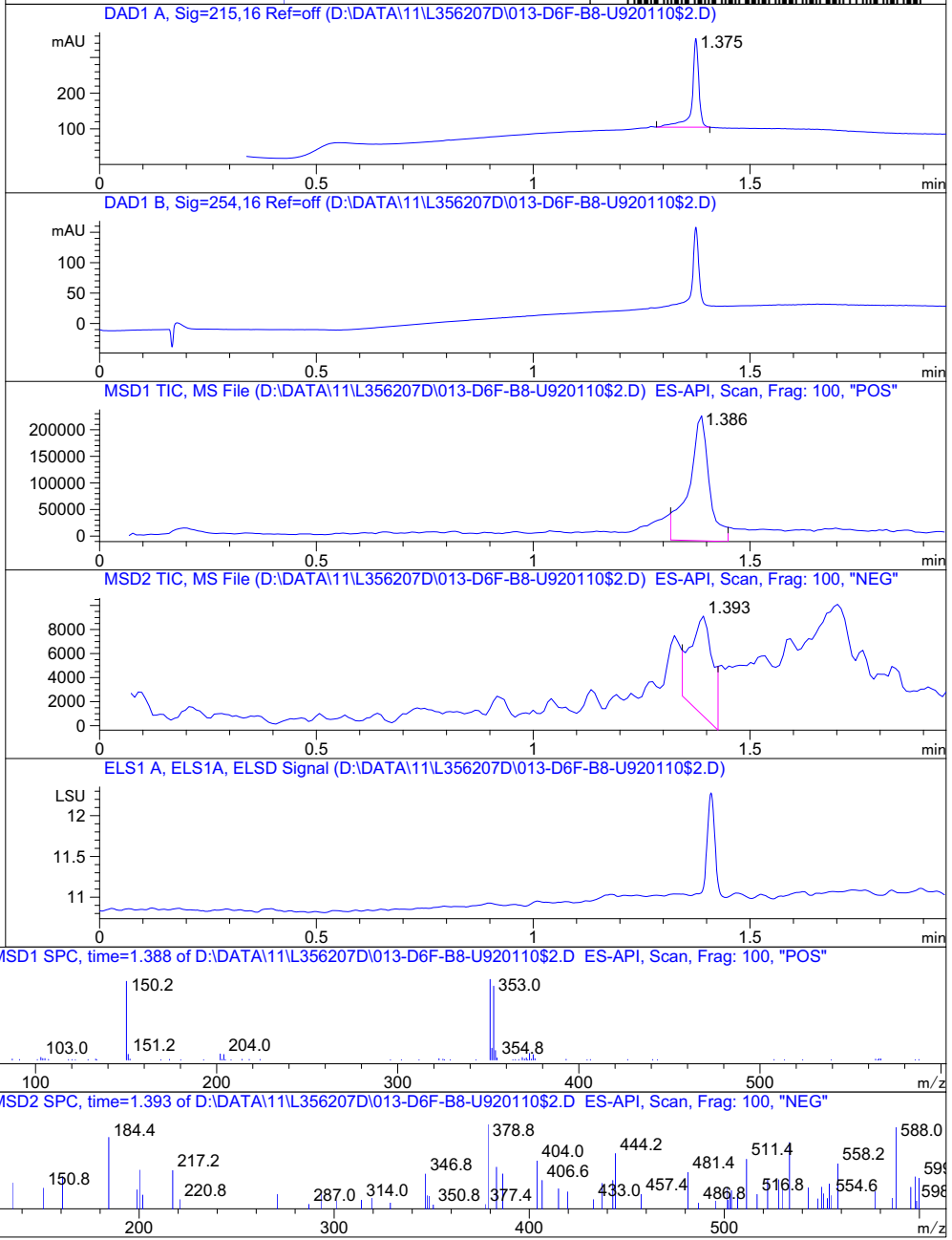
MaxPeak: 100.00%  
Ret\_Time: 1.375 min



Mol Wt 351.15  
Exact Mass 349.99

#	Time	Area%
1	1.375	100.00

# U920110\$2

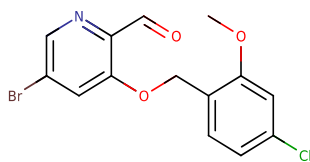
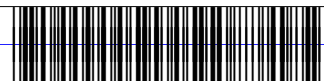


RT 1.386

RT 1.393

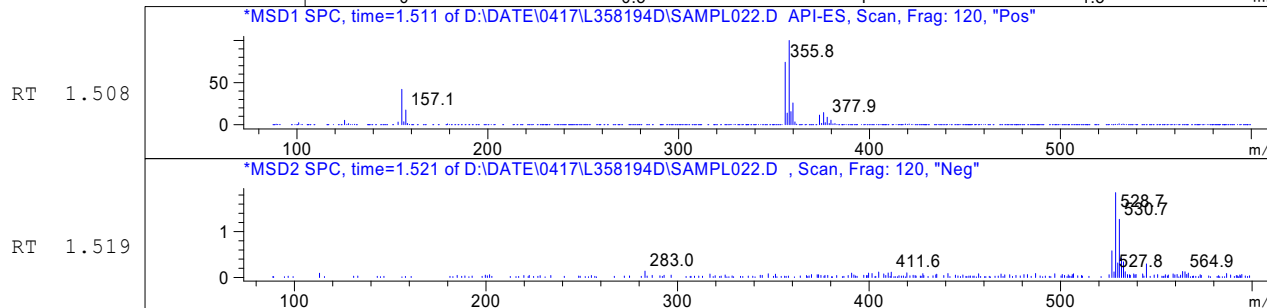
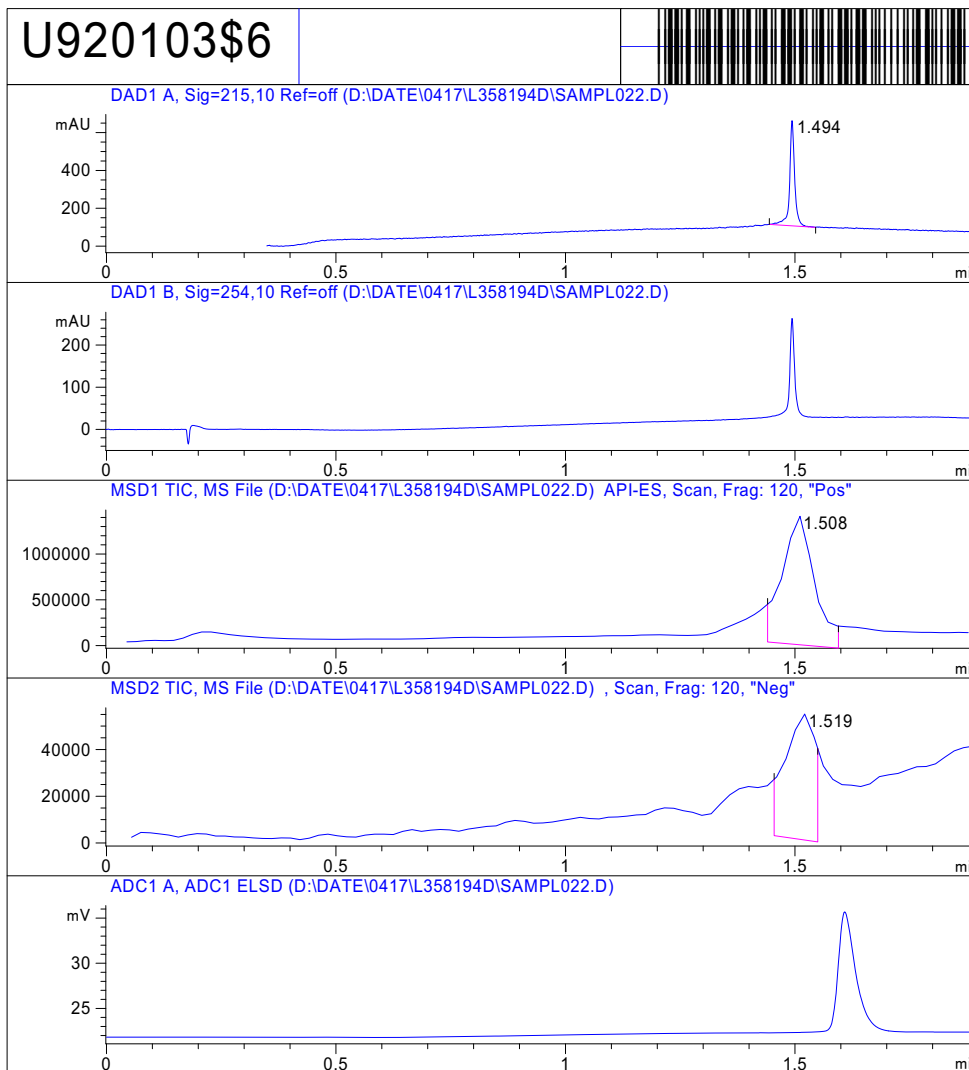
MaxPeak: 100.00%  
Ret\_Time: 1.494 min

U920103\$6



Mol Wt 356.6  
Exact Mass 356.97

#	Time	Area%
1	1.494	100.00



Inj.Date 4/17/2021

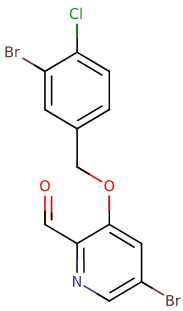
E

-VL-

Acq. Method C:\HPCHEM\ -> ->

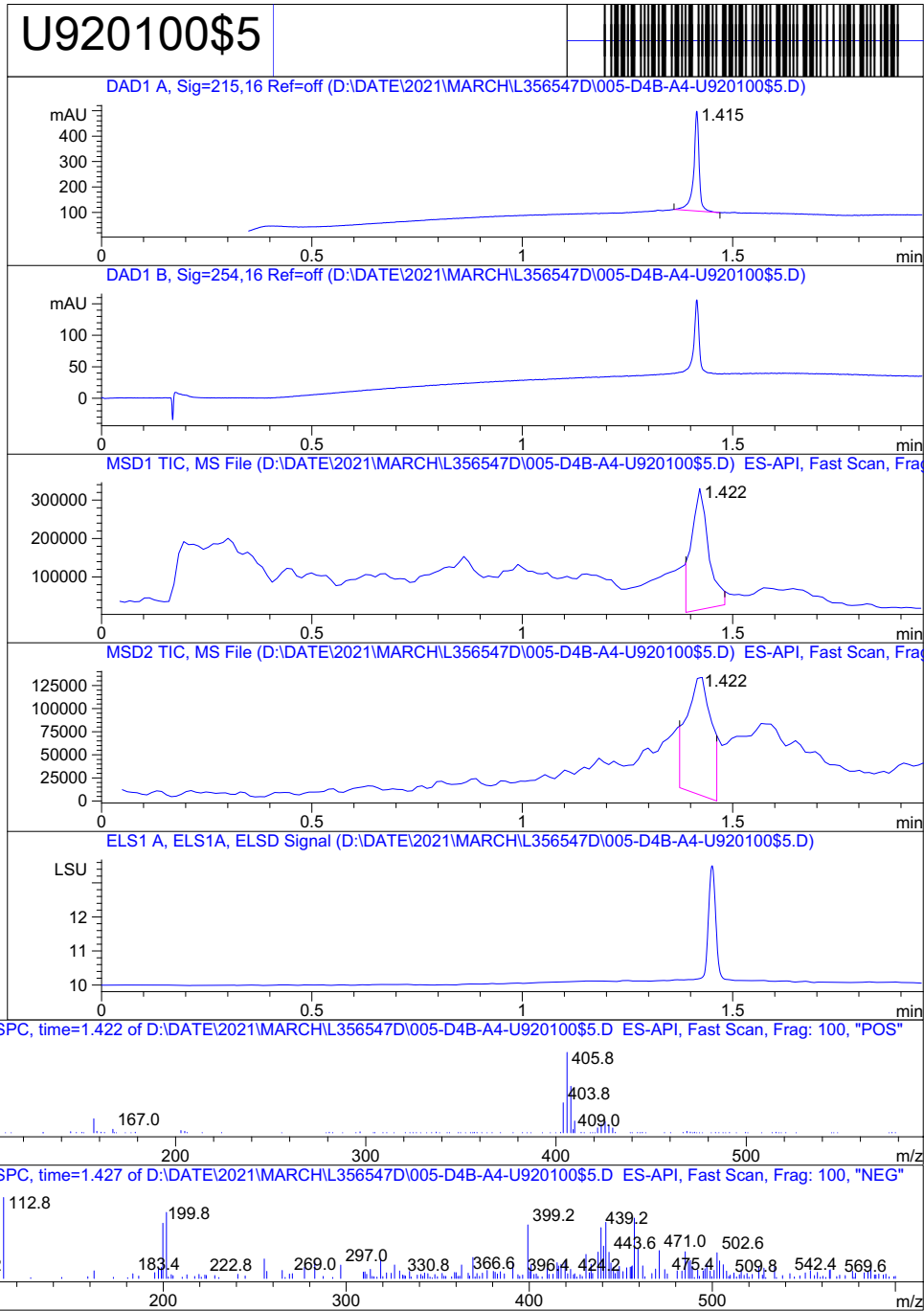
Z4954569127\_

MaxPeak: 100.00%  
Ret\_Time: 1.415 min



Mol Wt 405.47  
Exact Mass 404.87

#	Time	Area%
1	1.415	100.00

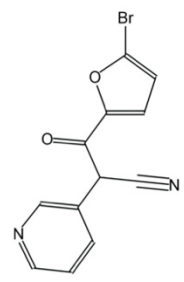
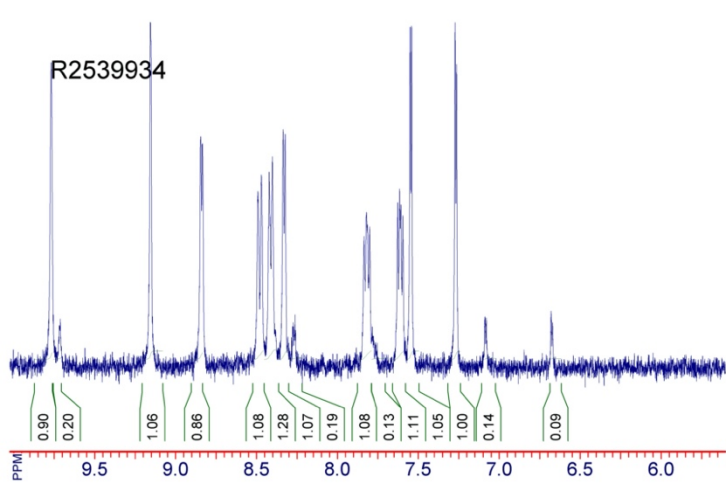


Inj.Date 4/11/2021

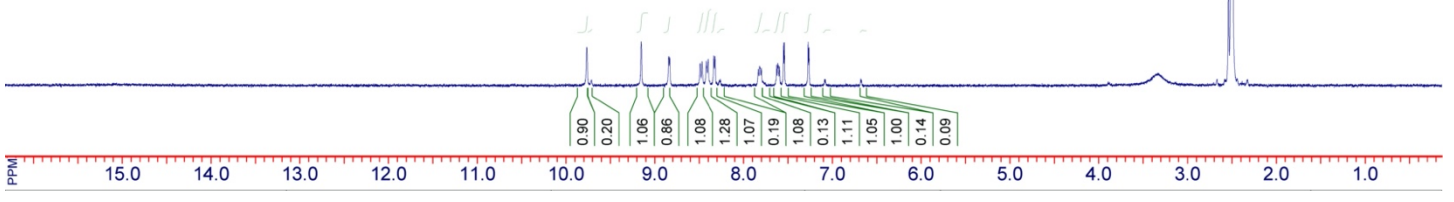
T <invalid>

Acq. Method C:\Users\ -> ->

Z4954569121\_



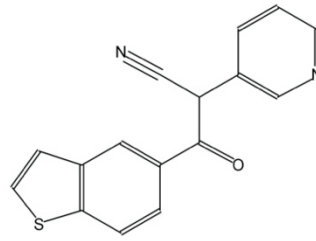
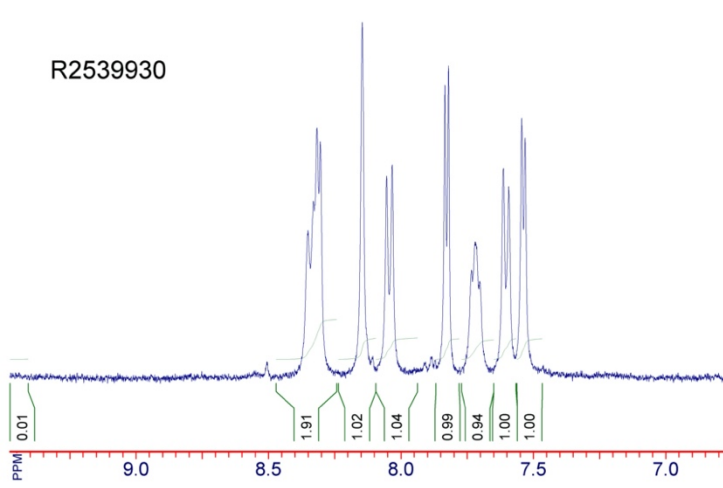
R2539934 C<sub>12</sub>H<sub>7</sub>BrN<sub>2</sub>O<sub>2</sub> 291.10



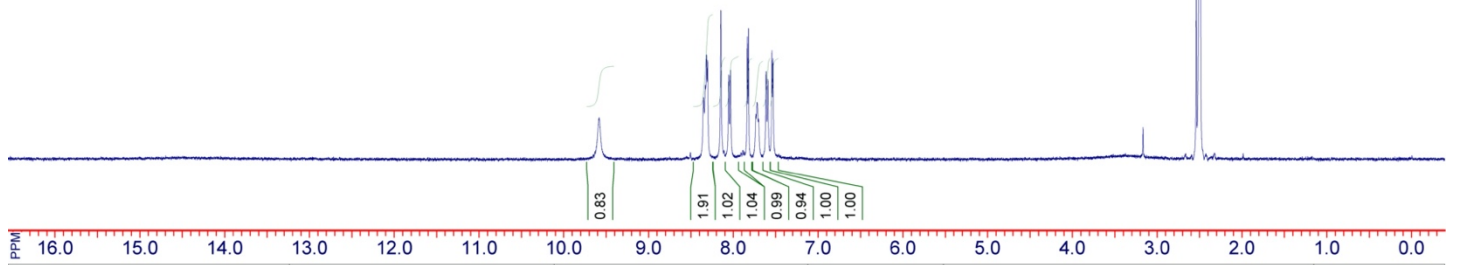
Z1410957817\_



R2539930



R2539930 C16H10N2OS 278.33



Z3302062818\_