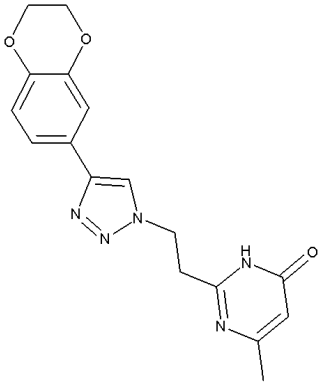
Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

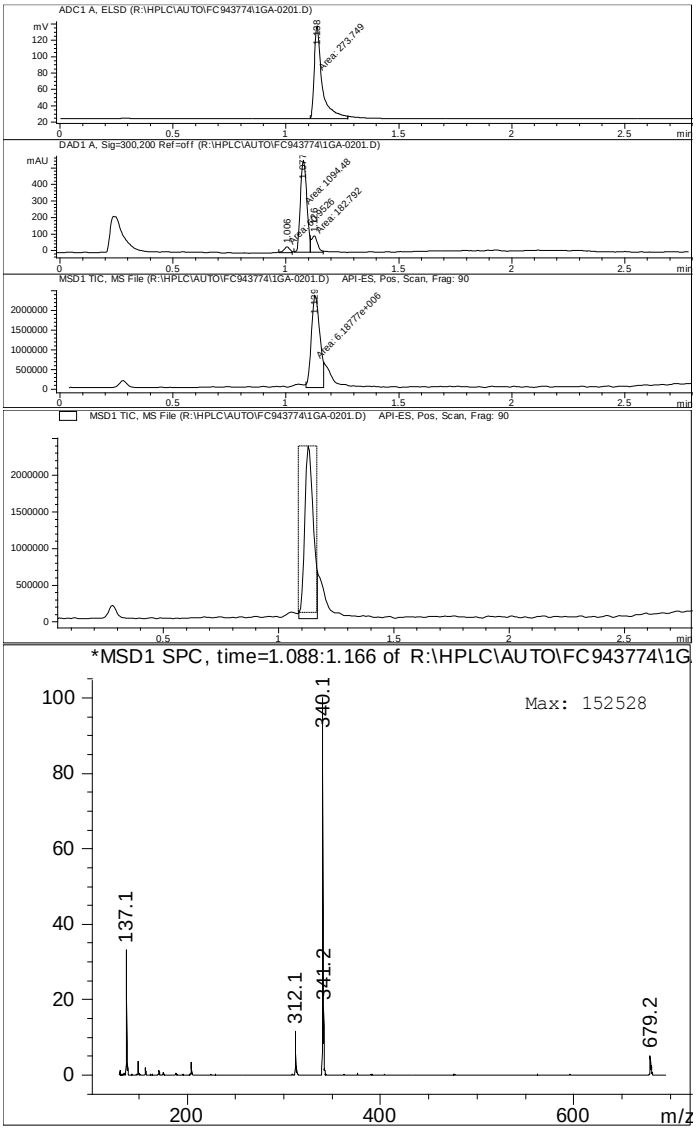
Compound	Supplier	Code	Analysis Method
3	ChemBridge	58238331	LCMS
4	ChemBridge	50509137	LCMS
10	ChemBridge	95652737	LCMS
15	ChemBridge	5304371	LCMS
17	ChemBridge	64993287	LCMS
25	ChemBridge	9048612	NMR
31	ChemBridge	9283033	LCMS
42	Enamine	Z167023036	LCMS
48	Enamine	Z1139229987	LCMS
50	Enamine	Z119631558	LCMS
56	Enamine	Z224851022	NMR
57	Enamine	Z30508852	LCMS
58	Enamine	Z281523990	LCMS
60	Enamine	Z237505970	LCMS
64	Enamine	Z1001812522	NMR
72	Enamine	Z24107796	LCMS
74	Enamine	Z226124130	NMR
80	Ambinter	Amb16766591	LCMS
84	Ambinter	Amb5367264	NMR
85	Ambinter	Amb13914491	NMR

Compound 3, Supplier: ChemBridge

FC94377407

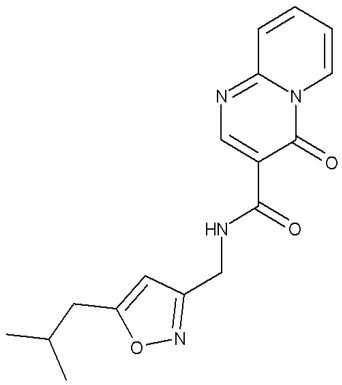


ID	58238331	339.3567	$C_{17}H_{17}N_5O_3$

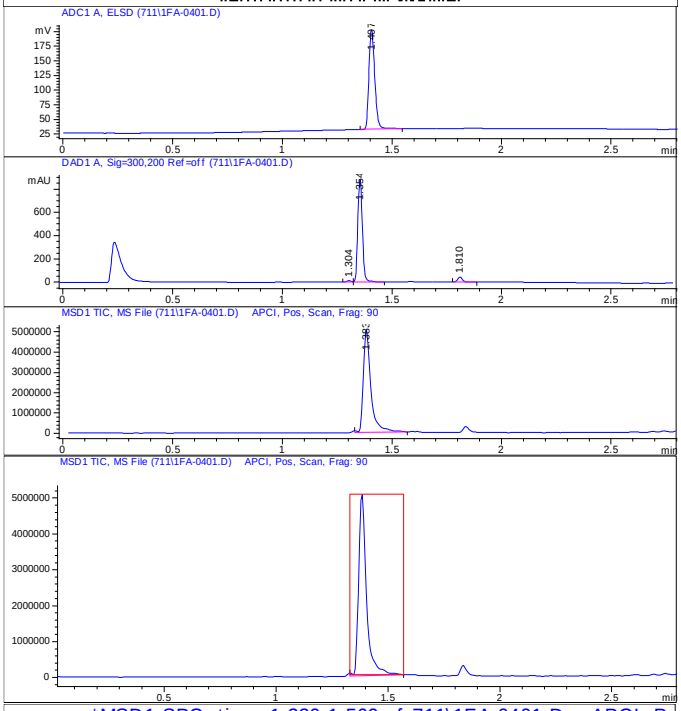


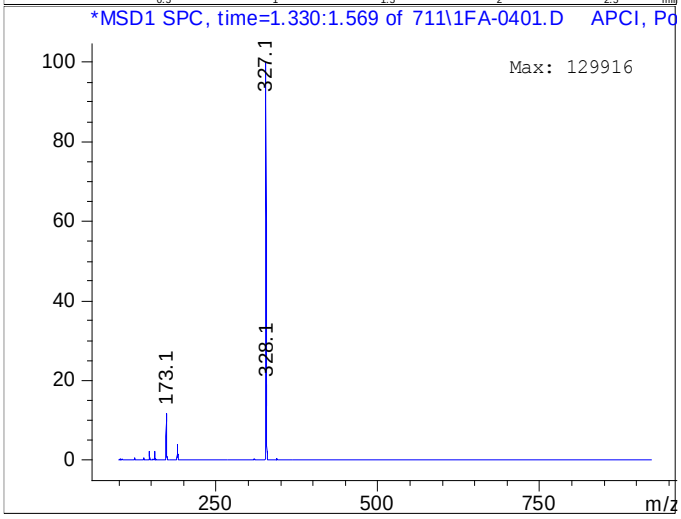
Compound 4

FC94194006



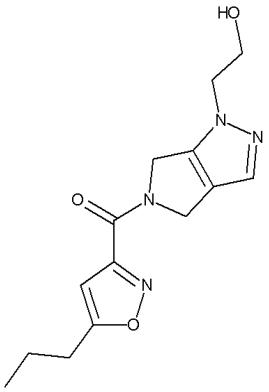
ID	50509137	326.3580	$C_{17}H_{18}N_4O_3$



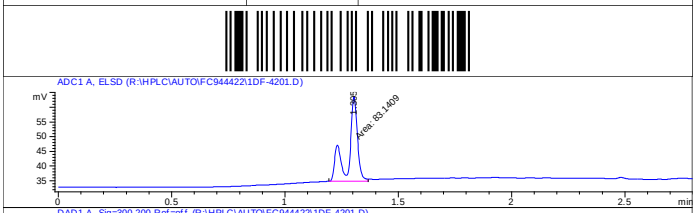


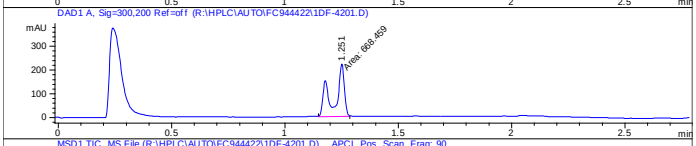
Compound 10

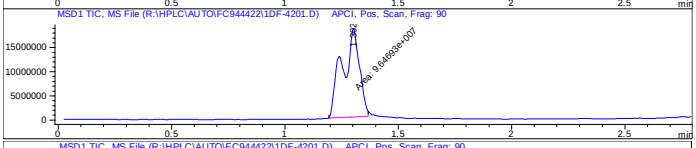
FC94442244

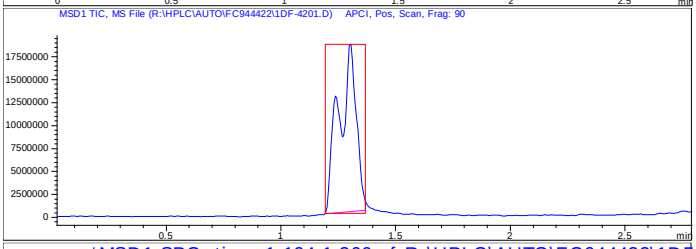


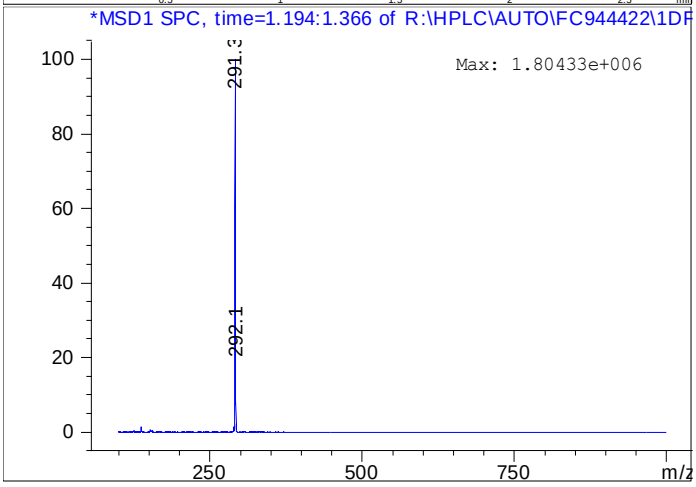
ID	95652737	290.3246	$C_{14}H_{18}N_4O_3$

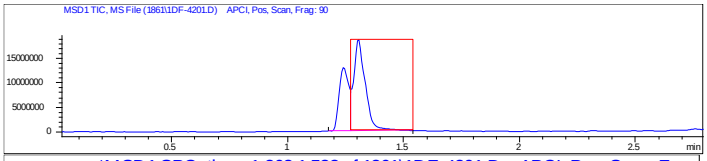


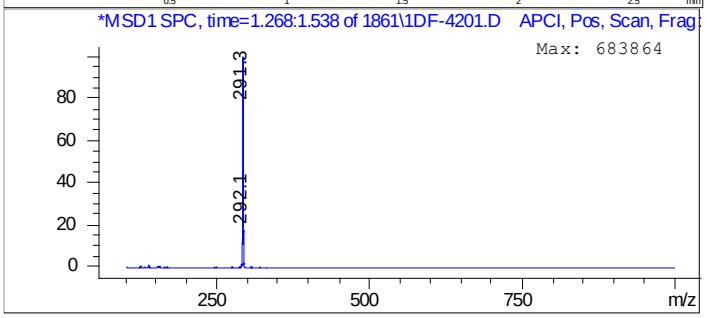




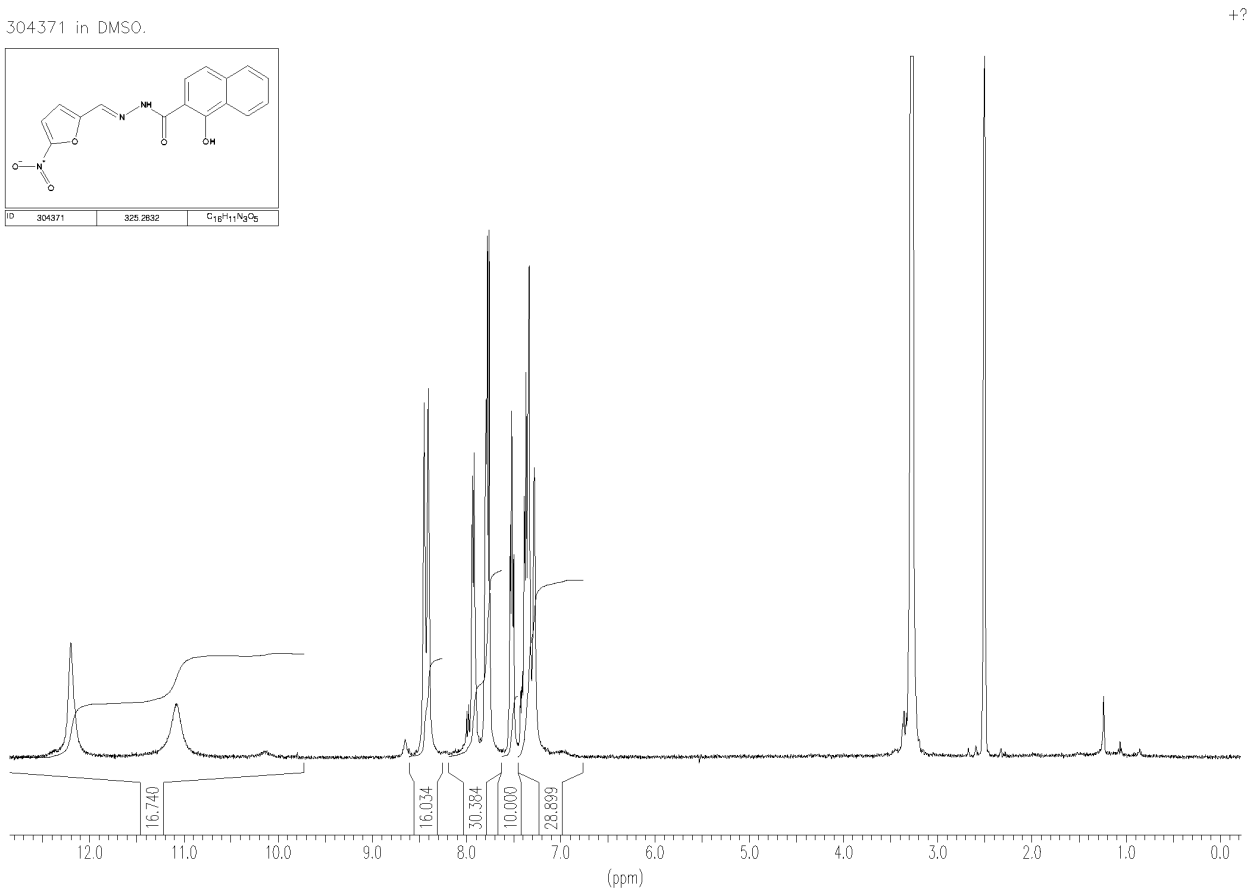






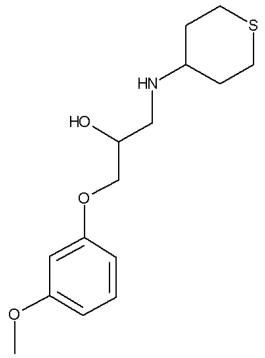


Compound 15, Supplier: ChemBridge

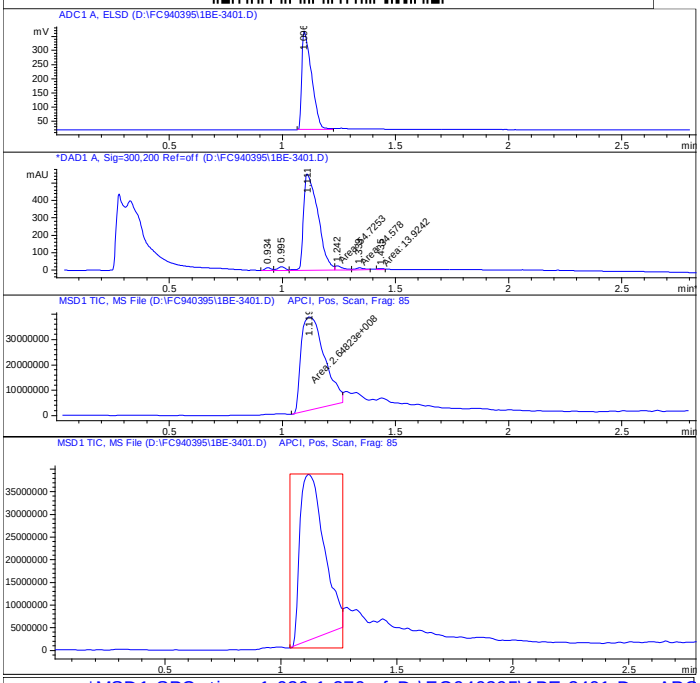


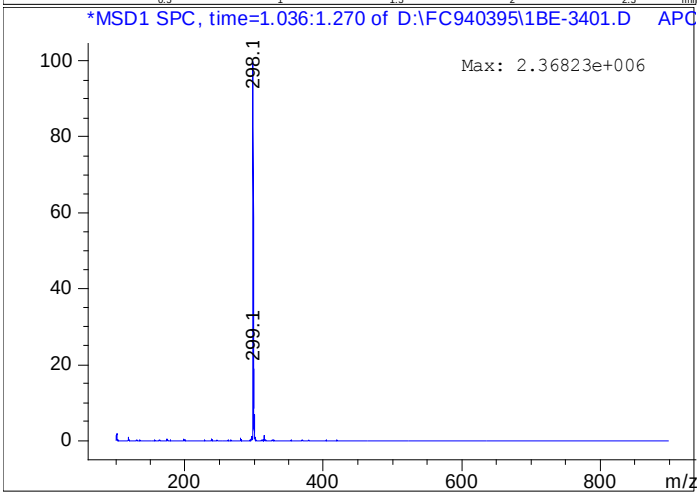
Compound 17

FC94039534

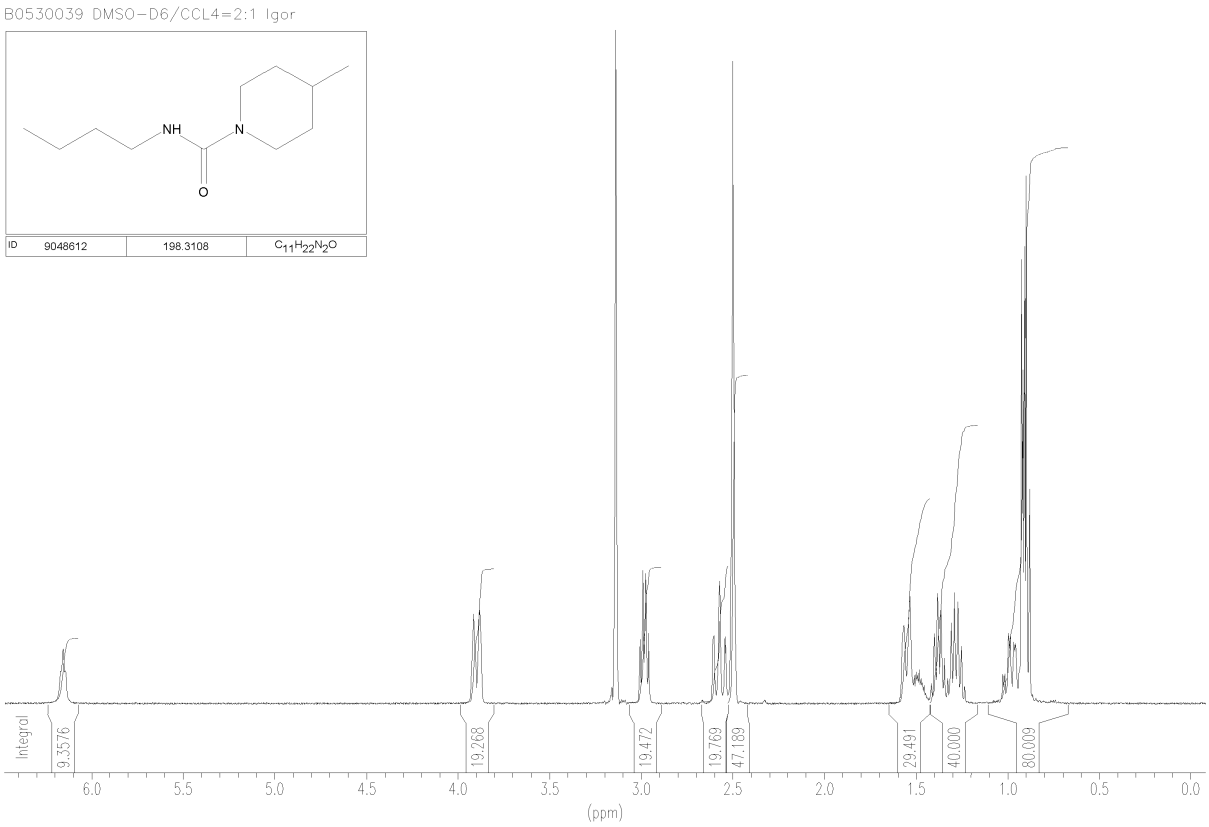


ID	64993287	297.4195	$C_{15}H_{23}NO_3S$



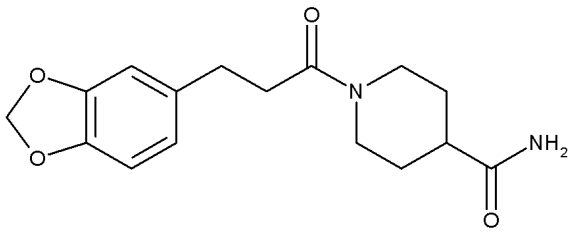


Compound 25

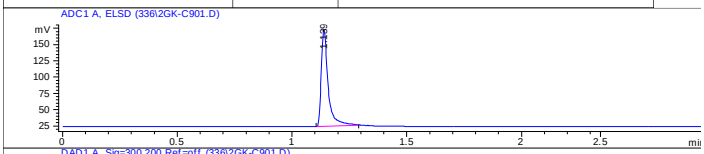

B0530039 DMSO-D6/CCL4=2:1 Igor
NH
N
O
ID 9048612
198.3108
$C_{11}H_{22}N_2O$
Integral
9.3576
19.268
19.472
19.769
47.189
29.491
40.000
80.009
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)

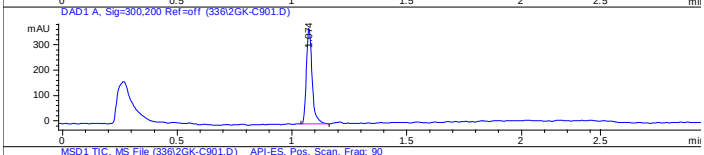
Compound 31

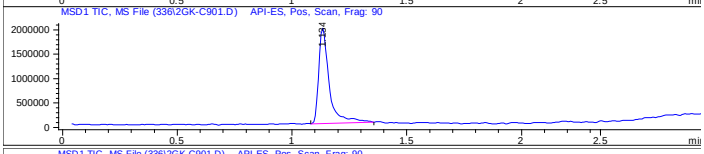
CH00676287

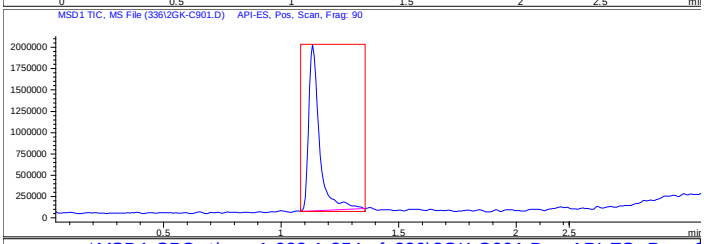


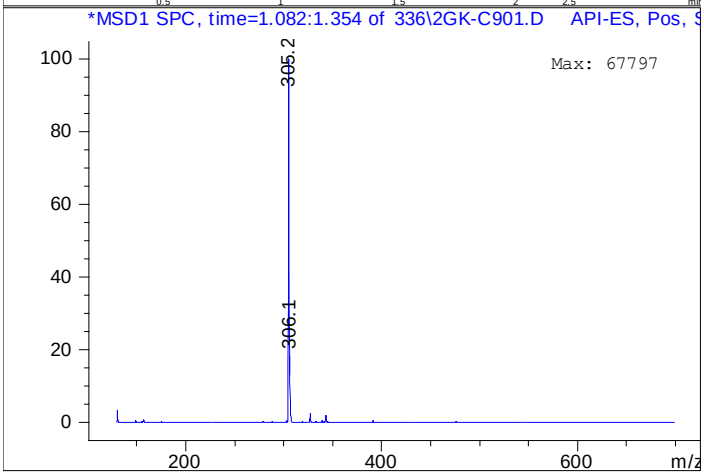
ID	9283033	304.3488	$C_{16}H_{20}N_2O_4$





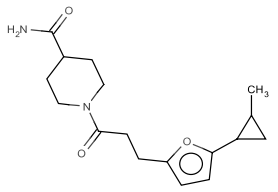






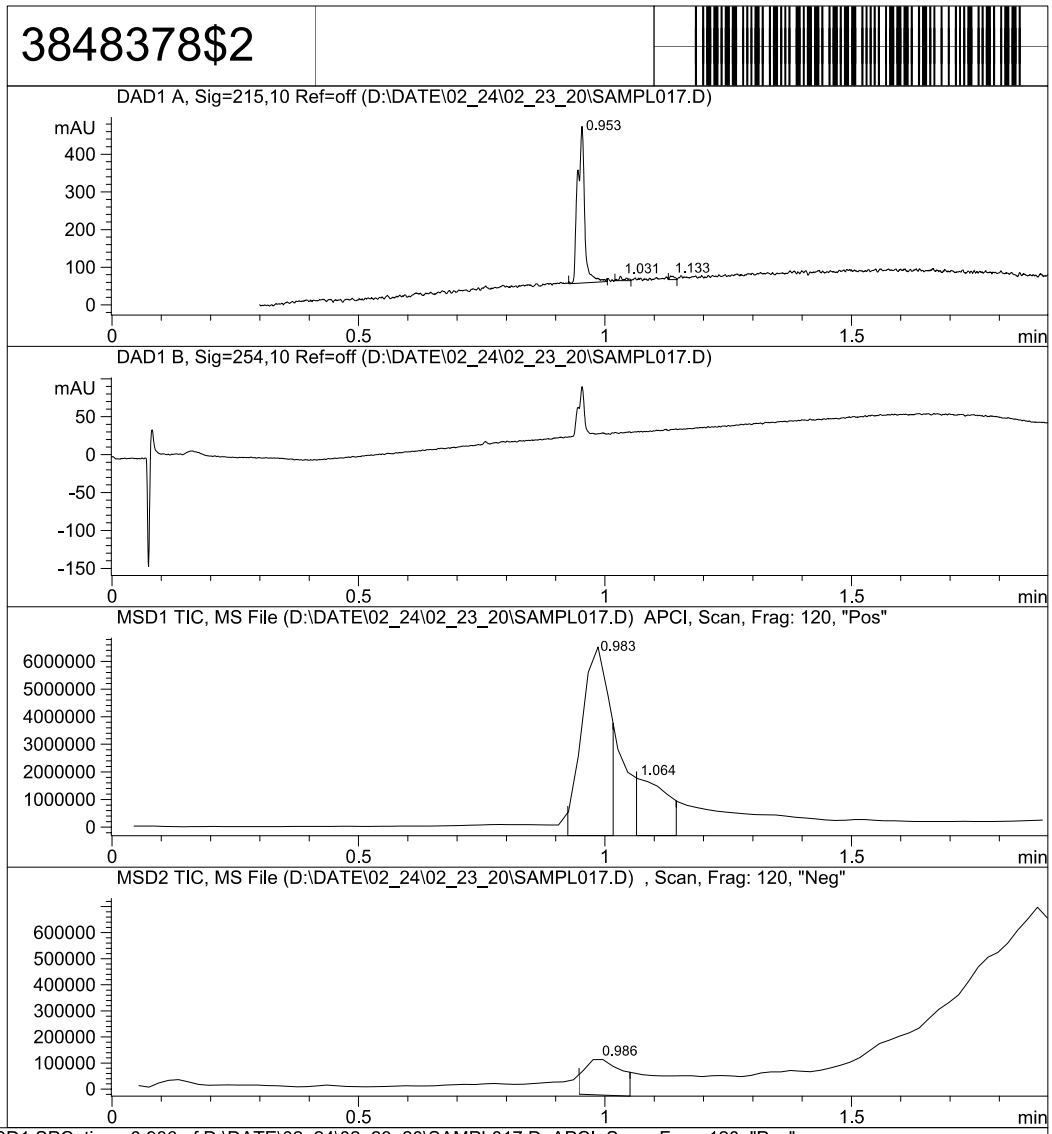
Compound 42

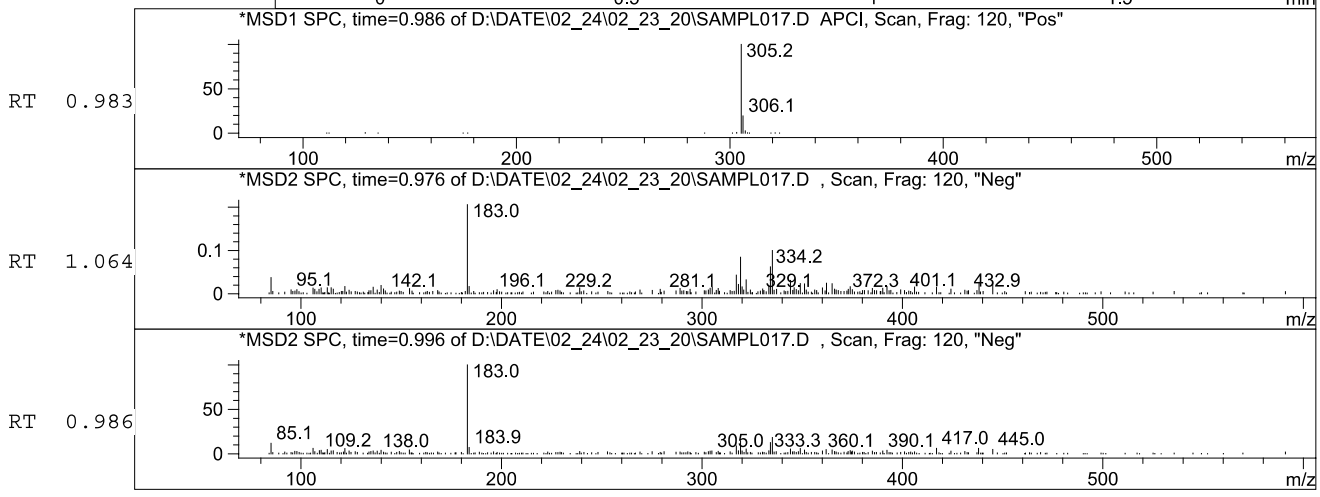
MaxPeak: 96.65%
Ret_Time: 0.953 min



Mol Wt **304.384**
Exact Mass **304.21**

#	Time	Area%
1	0.953	96.65
2	1.031	1.91
3	1.133	1.44

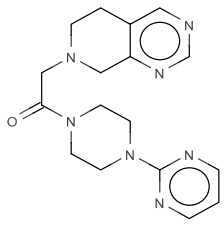




Inj.Date 2/24/2011 L P2-B-07 SL Acq. Method C:\HPCHEM\-> ->

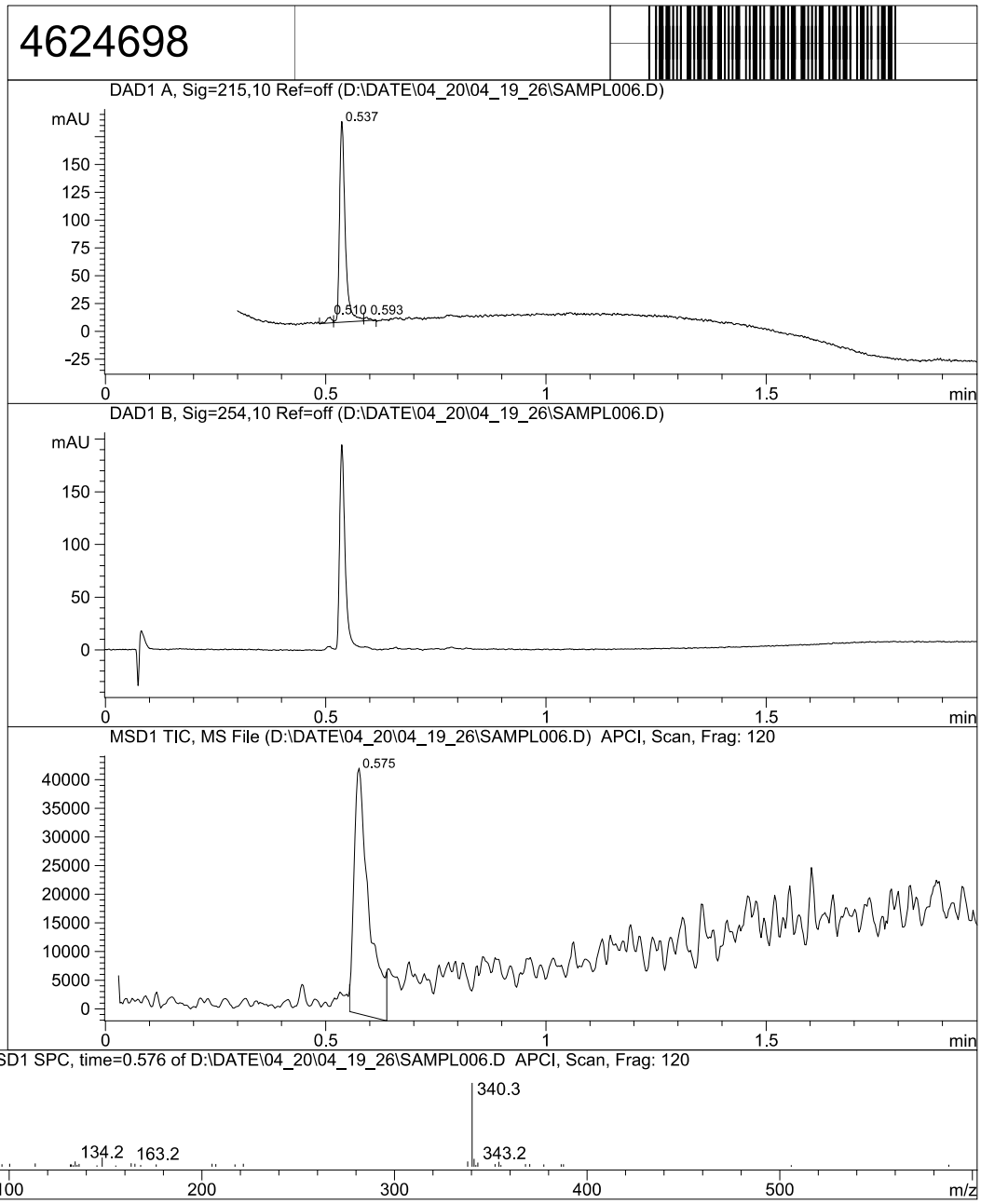
Compound 48

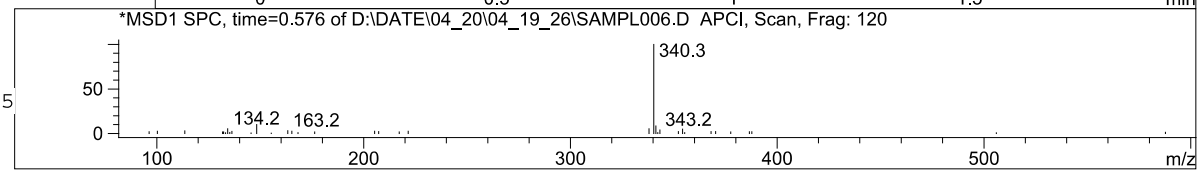
MaxPeak: 96.03%
Ret_Time: 0.537 min



Mol Wt **339.395**
Exact Mass **339.2**

#	Time	Area%
1	0.510	2.66
2	0.537	96.03
3	0.593	1.31



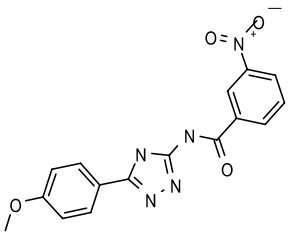


RT 0.575

Inj.Date 4/20/2011 L P2-A-05 VL Acq. Method C:\HPCHEM\-> ->

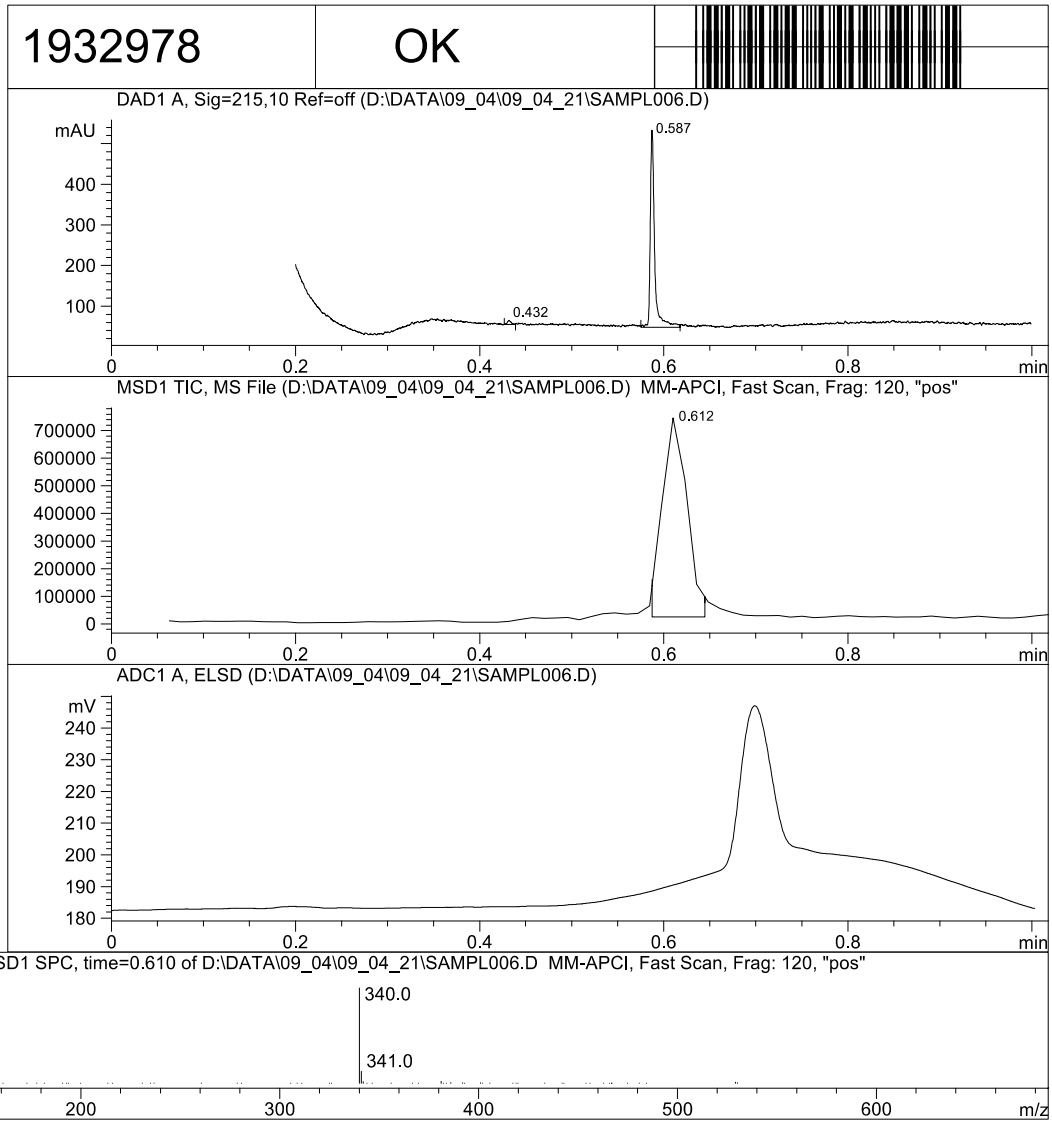
Compound 50

MaxPeak: 98.28%
Ret_Time: 0.587 min

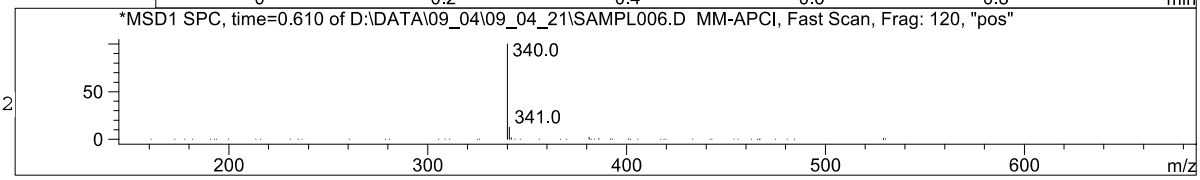


mw = 339.31

#	Time	Area%
1	0.432	1.72
2	0.587	98.28

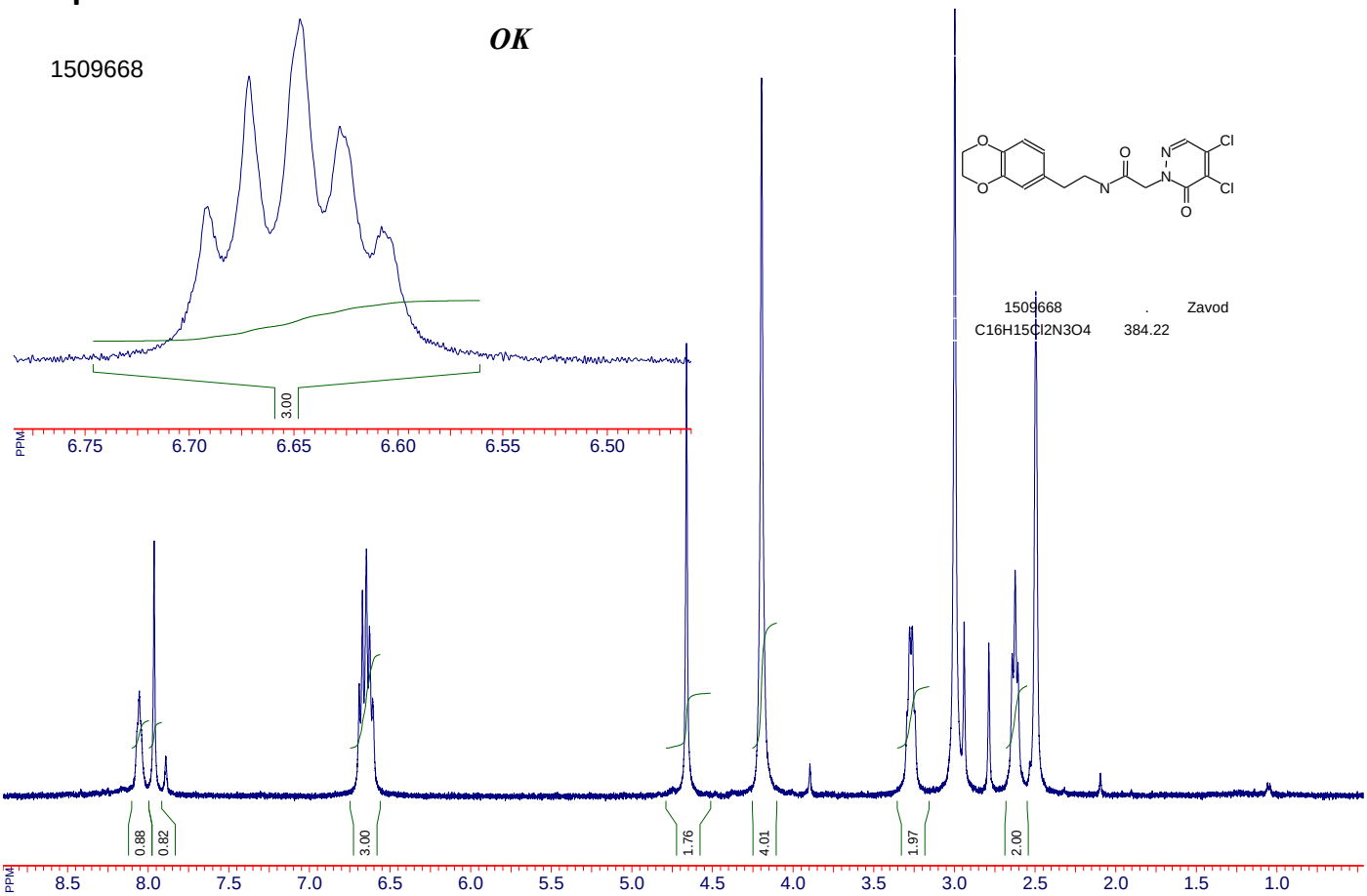


RT 0.612



Inj.Date 9/5/2007 O P2-A-08 Acq. Method C:\Chem32\->

Compound 56

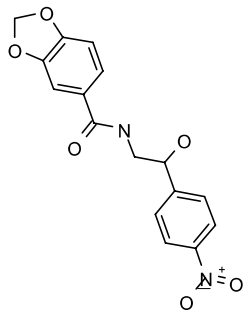


File name: 1509668	Operator: Roshina	SF: 399.9681 MHz	NSC: 0	PW: 14.80 usec, RG: 48	SI: 65536
Date: 01-Dec-2006	Solvent	SW: 6375 Hz	TE: 295 K	AQ: 2.00 sec, RD: 0.00 sec	*1509668*

Compound 57

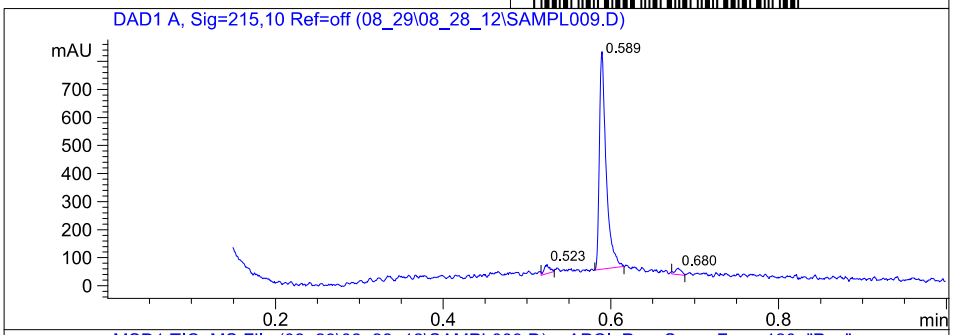
Sample Name: 1435105 OK

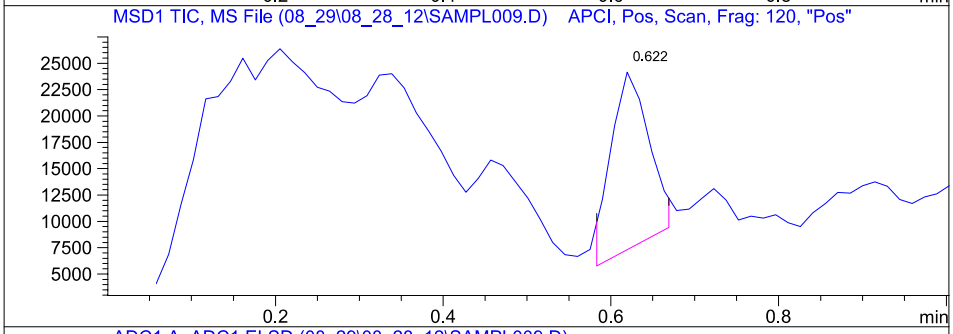
MaxPeak: 94.01%
Ret_Time: 0.589 min

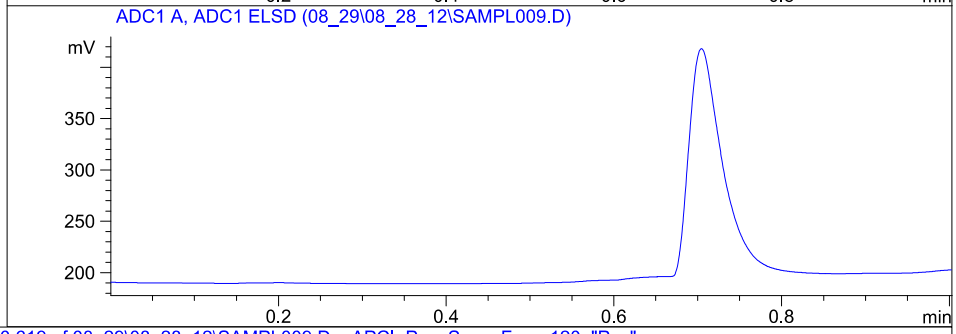


mw = 330,3

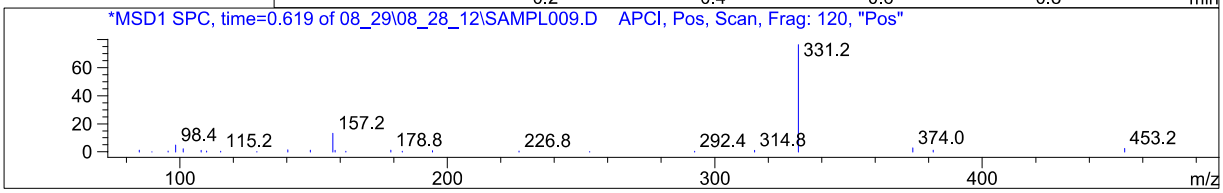
#	Time	Area%
1	0.523	3.34
2	0.589	94.01
3	0.680	2.65







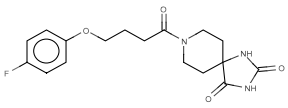
RT 0.622



Inj.Date 29.08.2006 T P2-B-01 Acq. Method SB15_3PN.M

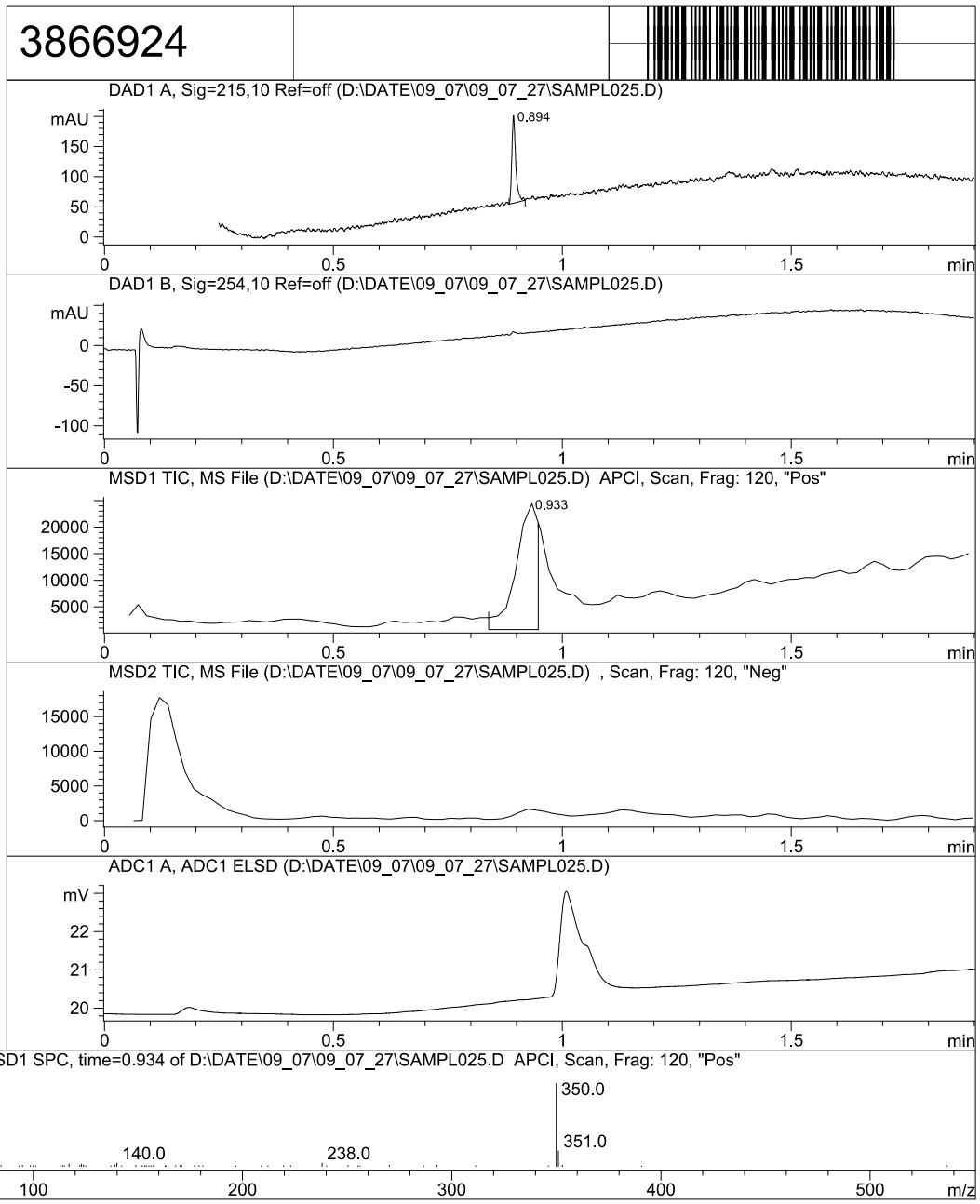
Compound 58

MaxPeak: 100.00%
Ret_Time: 0.894 min

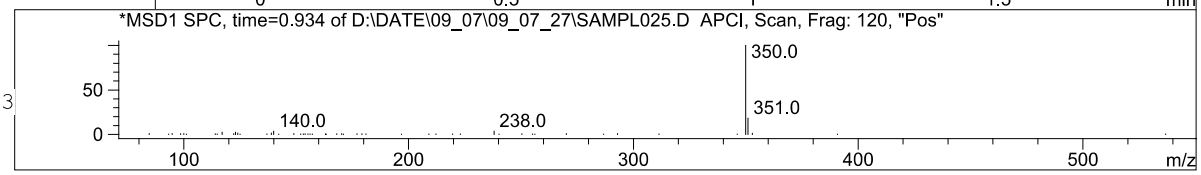


Mol Wt 349.357
Exact Mass 349.16

#	Time	Area%
1	0.894	100.00



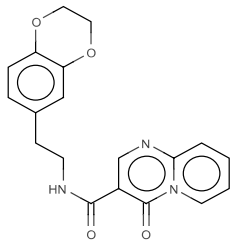
RT 0.933



Inj.Date 9/8/2010 O P2-C-07 SL Acq. Method C:\HPCHEM\-> ->

Compound 60

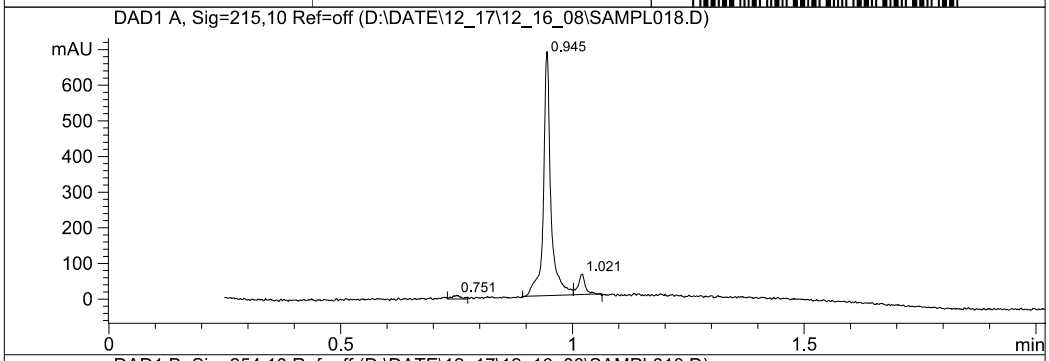
MaxPeak: 91.11%
Ret_Time: 0.945 min

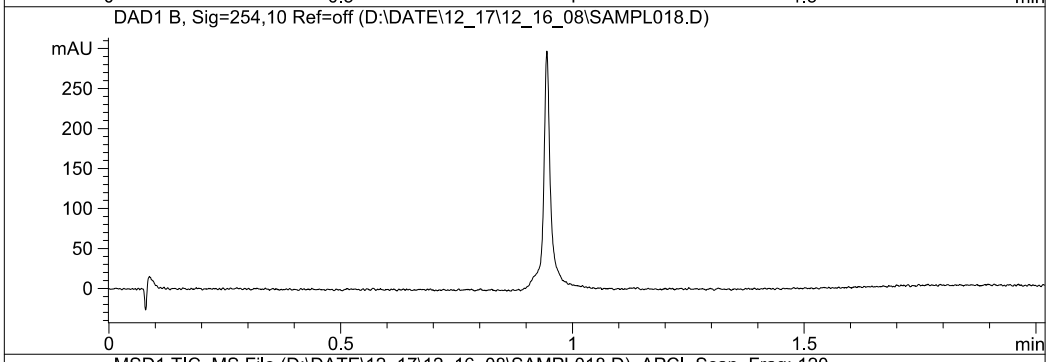


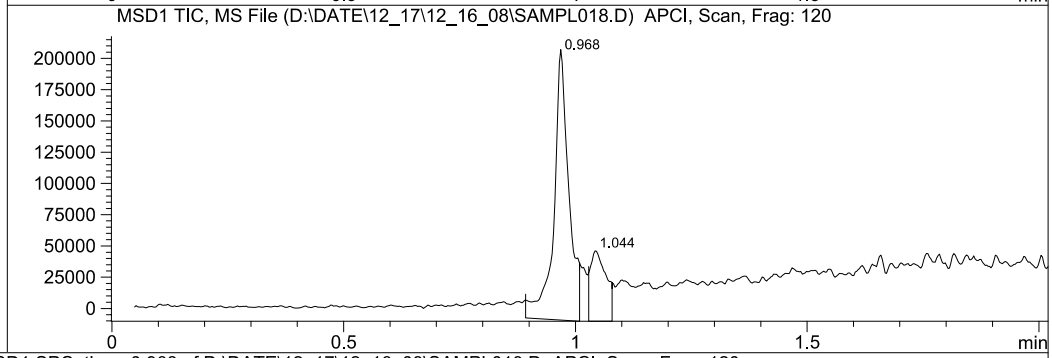
Mol Wt 351.356
Exact Mass 351.13

#	Time	Area%
1	0.751	1.69
2	0.945	91.11
3	1.021	7.20

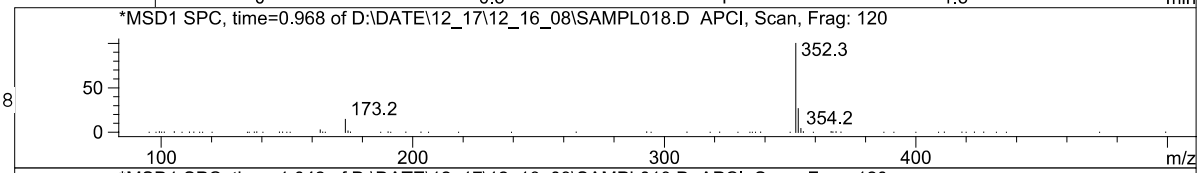
3105740



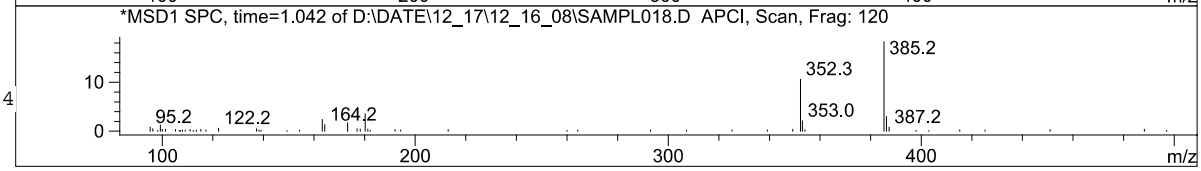




RT 0.968



RT 1.044

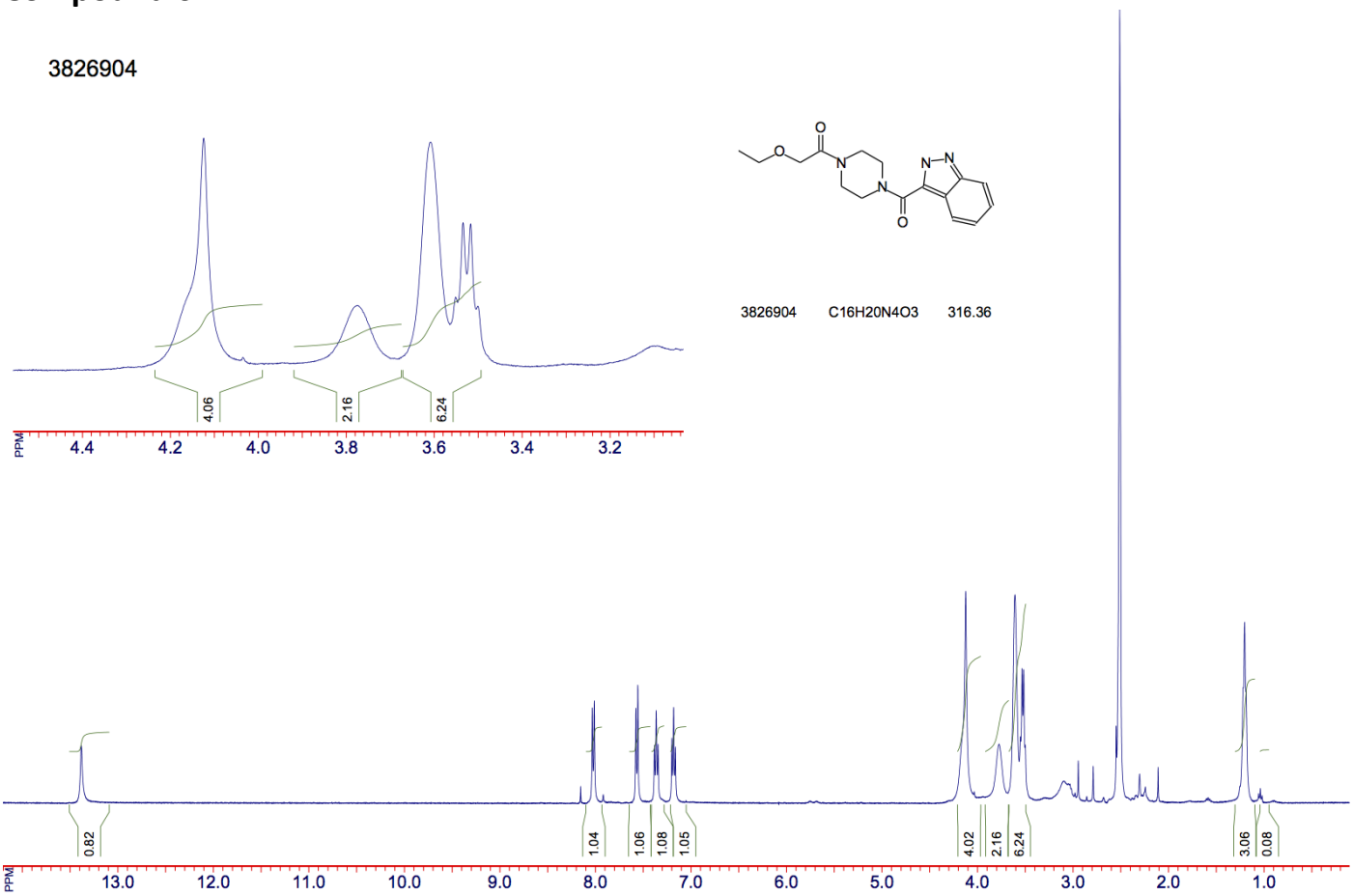


Inj.Date 12/17/2009 L P2-B-09 VL Acq. Method C:\HPCHEM\-> ->

Compound 64

3826904

3826904 C16H20N4O3 316.36



File name: 3826904	Kinder Tetyana	SF: 399.9703 MHz	NSC: 0	PW: 7.50 usec, RG: 32	SI: 65536
Date: 05-Mar-2011	Solvent: dmso-d6+ccl4	SW: 6803 Hz	TE: 293 K	AQ: 1.33 sec, RD: 0.00 sec	*3826904*

Compound 72

Sample Name: CV794 OK

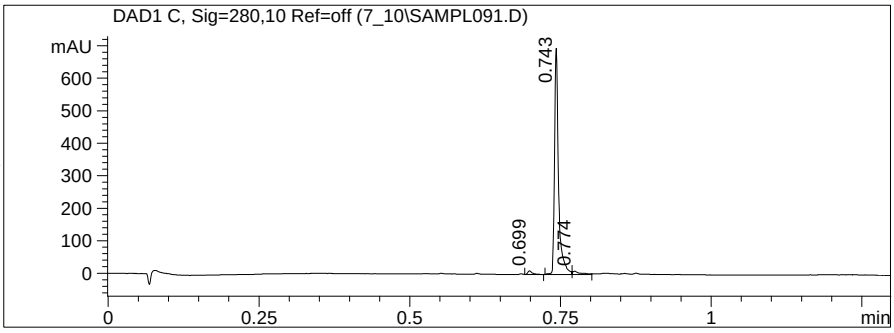
Data file : C:\HPCHEM\1\DATA\7_10\SAMPL091.D

Injection Date	: Sat, 10. Jul. 2004	Seq Line	: 90
Sample Name	: CV794	Location	: Vial 91
Acq Operator	: W	Inj. No.	: 1

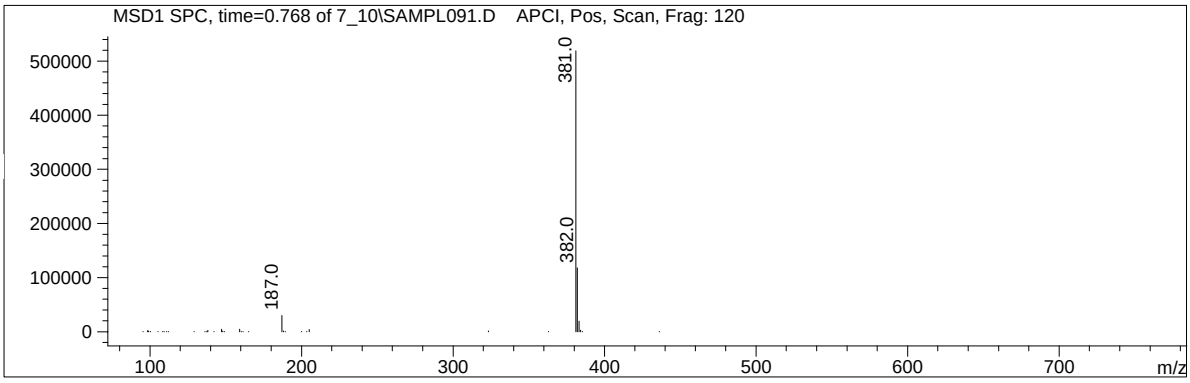
Acq. Method : SB3TFA_P.M
Analysis Method : C:\HPCHEM\1\METHODS\NITRIL_5.M
Last Changed : Sat, 10. Jul. 2004, 02:09:40 pm
(modified after loading)

The method for the Gradient Sample (DAD only) using short rapid resolution columns Eclipse XDB-C18 2.1 x 30mm (p/n 973700-932). For testing purity of syntez. With using pure water.

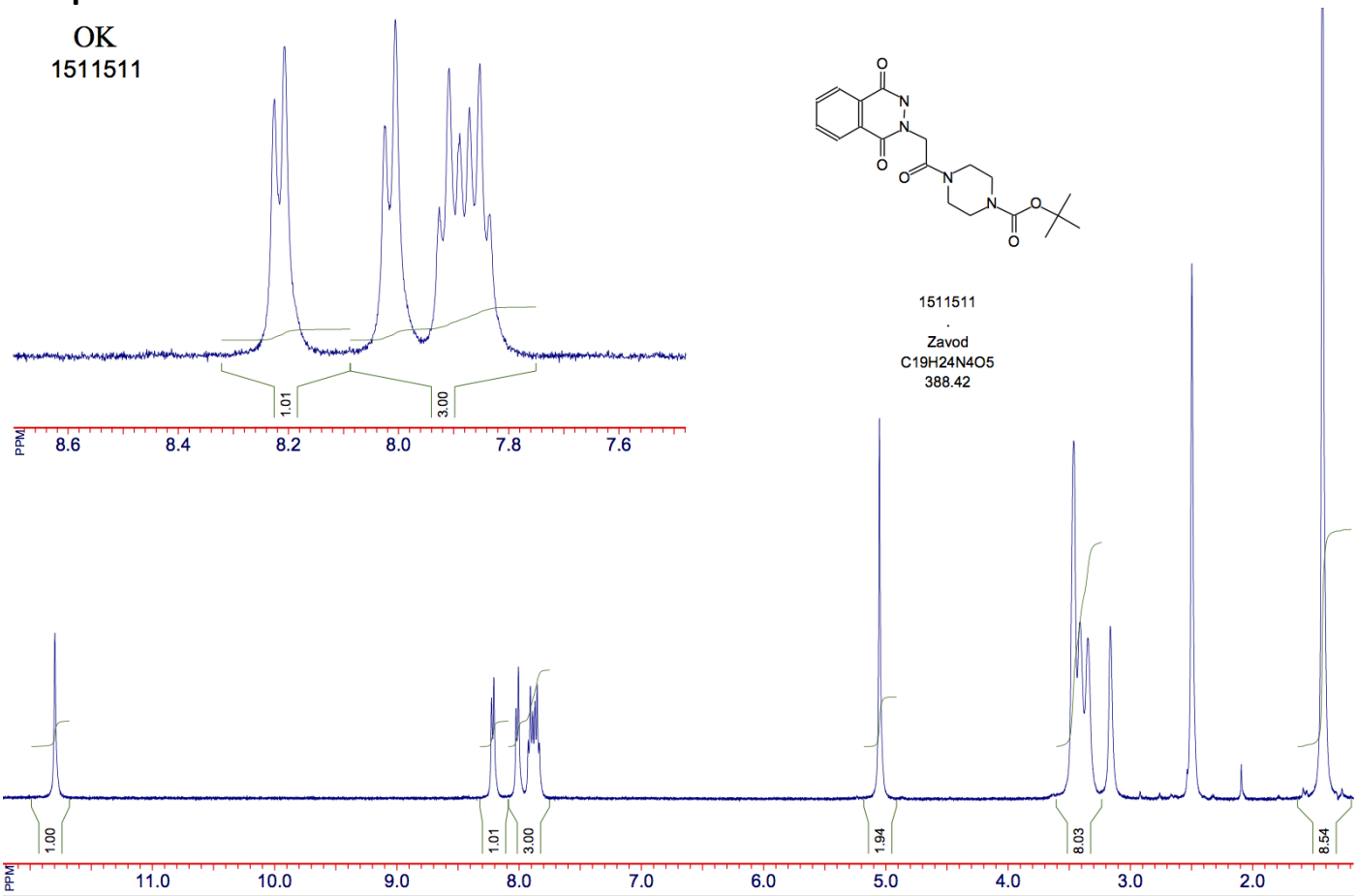
Peak #	RT [min]	Width [min]	Area %
1	0.699	0.008	1.788
2	0.743	0.007	95.337
3	0.774	0.012	2.876



RT (min)
0.768



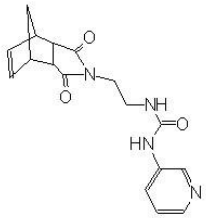
Compound 74



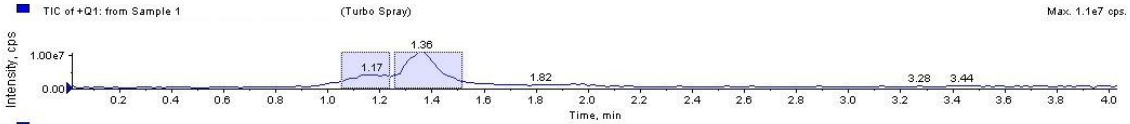
File name: 1511511	Operator: Turov	SF: 399.9602 MHz	NSC: 0	PW: 10.00 usec, RG: 50	SI: 65536
Date: 30-Oct-2006	Solvent: DMSO-d6+CCl4	SW: 6364 Hz	TE: 295 K	AQ: 1.50 sec, RD: 0.00 sec	1511511

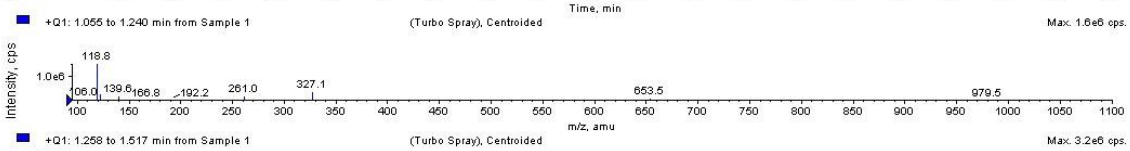
Compound 80

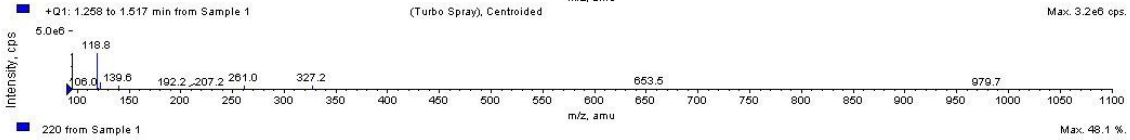
IDNUMBER
Amb16755507
09.09.14 12:37:06
C17 H18 N4 O3
M.W.=326.36

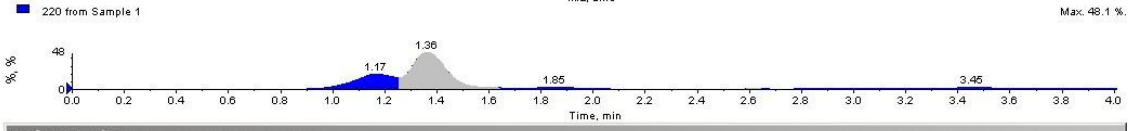


GRADE: OK[0]
EXPERT: AK
LIST: 1238





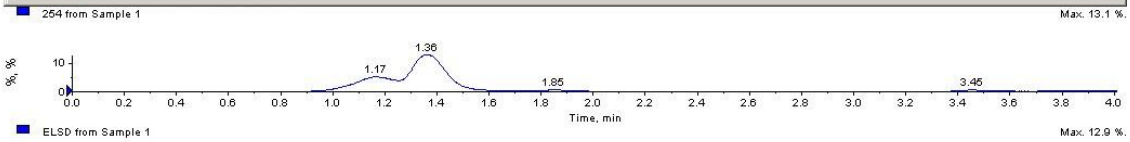


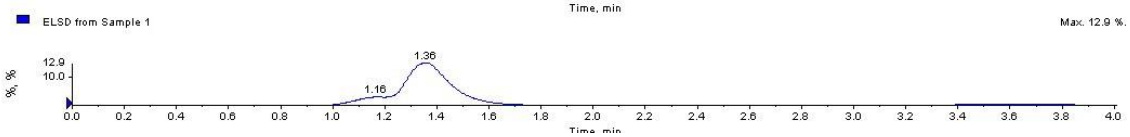


220 from Sample 1

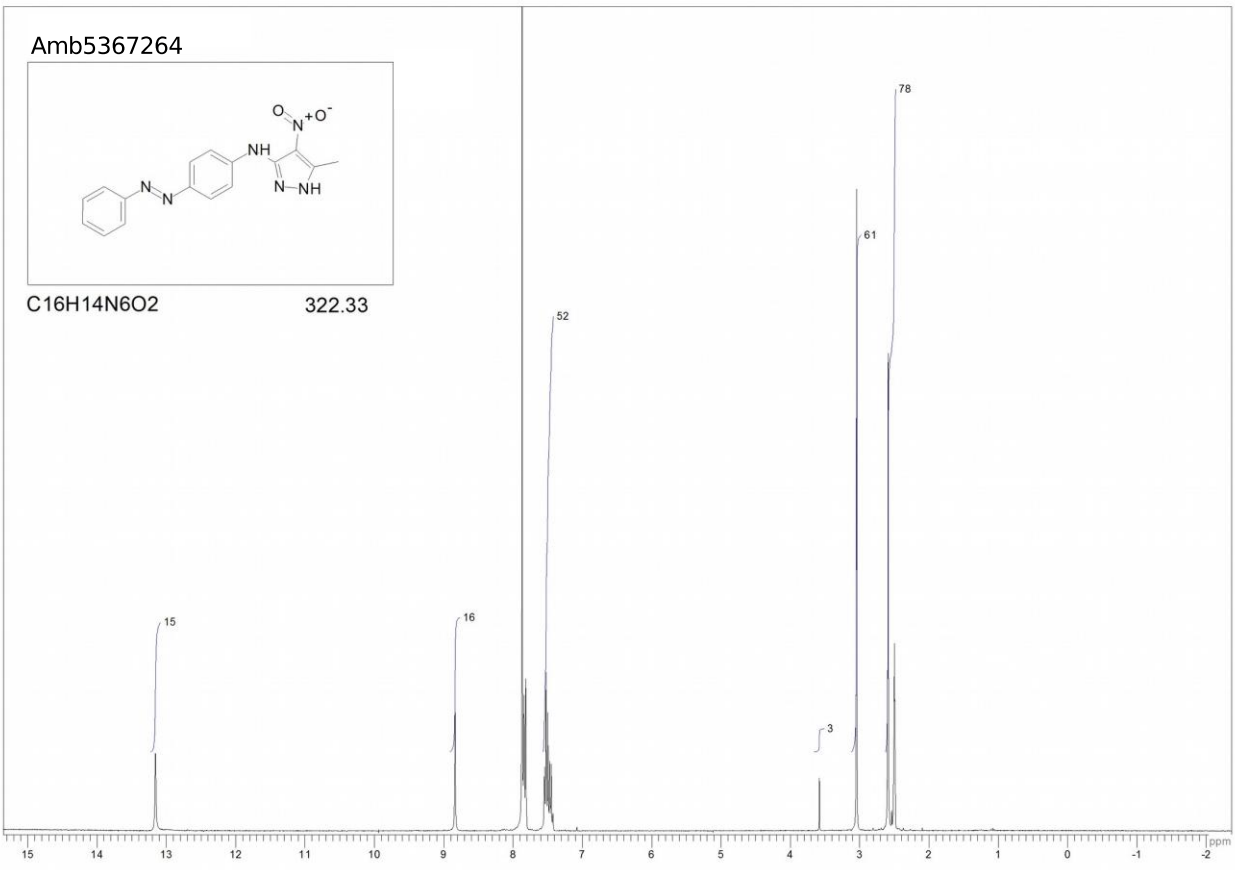
Data List | Peak List

	Time (min)	Area (counts)	% Area	Height (%)	% Height	Width (min)	Baseline Type
4	1.3627	429.6587	65.3202	46.3267	67.5046	0.3867	Valley
3	1.1663	206.9696	31.4652	18.8911	27.5271	0.4333	Valley

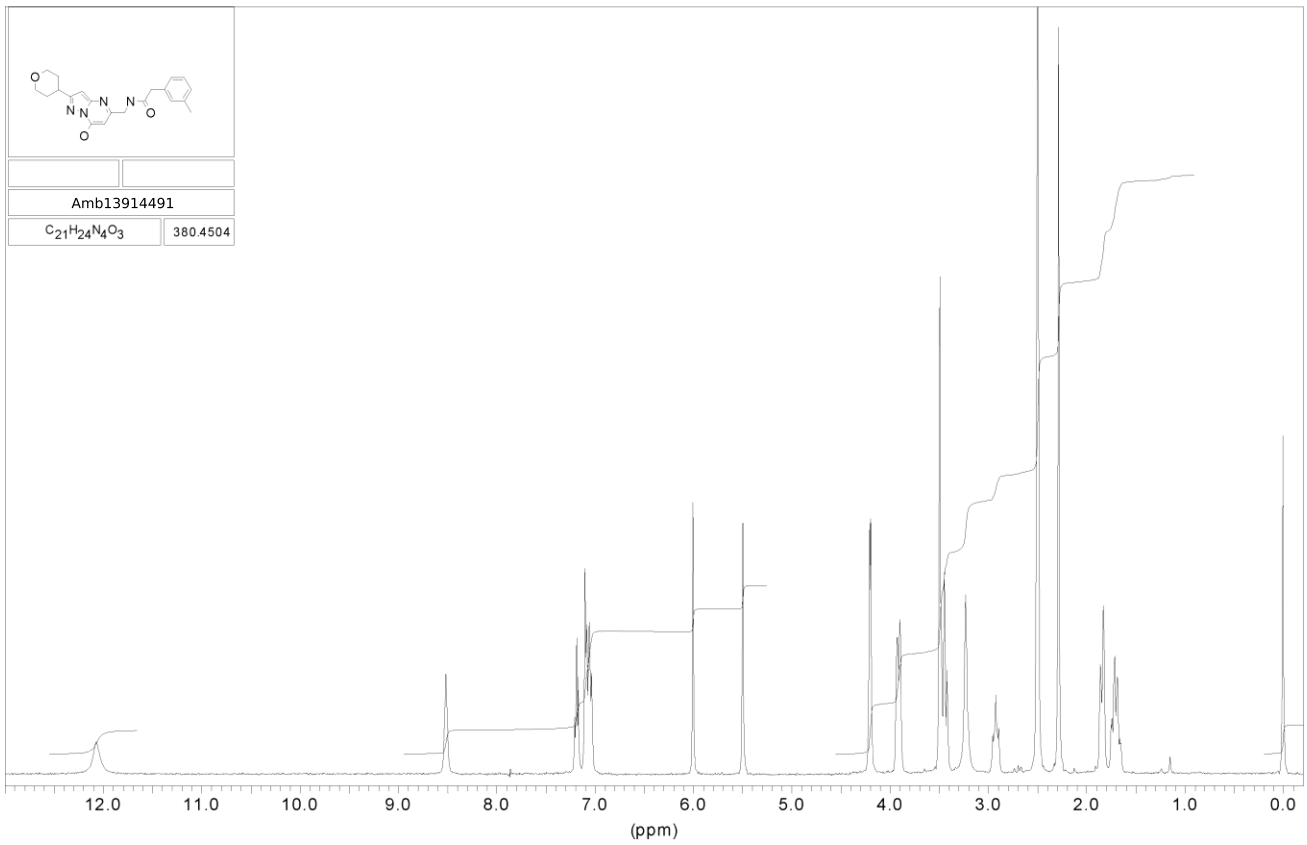




Compound 84



Compound 85


Amb13914491
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3.0
2.0
1.0
0.0
(ppm)