

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100622\
 Data File : BF130552.D
 Acq On : 06 Oct 2022 15:52
 Operator : CG\JU
 Sample : N4996-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 506D-1

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130552.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.787	454	459	465	rBV	244128	288182	10.18%	2.147%
2	5.216	529	532	542	rBV	1009151	995257	35.17%	7.413%
3	5.622	596	601	604	rBV	40055	35339	1.25%	0.263%
4	6.257	706	709	724	rVB	667579	598802	21.16%	4.460%
5	6.616	766	770	773	rBV	587087	467163	16.51%	3.480%
6	7.186	861	867	870	rBV	1684883	1540817	54.44%	11.477%
7	7.898	984	988	991	rVB	775656	620197	21.91%	4.620%
8	8.675	1117	1120	1128	rBV	25258	33033	1.17%	0.246%
9	8.975	1166	1171	1174	rBV	3066574	2830149	100.00%	21.081%
10	9.645	1281	1285	1289	rBV	830227	657823	23.24%	4.900%
11	10.433	1415	1419	1423	rBV	1599415	1399109	49.44%	10.422%
12	11.127	1533	1537	1540	rBV	702731	561584	19.84%	4.183%
13	11.669	1624	1629	1631	rBV	167236	148528	5.25%	1.106%
14	11.698	1631	1634	1638	rVB	620932	518252	18.31%	3.860%
15	12.451	1758	1762	1768	rBV2	62807	81130	2.87%	0.604%
16	12.715	1802	1807	1810	rBV	2173053	1776041	62.75%	13.229%
17	13.110	1864	1874	1876	rBV10	10240	29283	1.03%	0.218%
18	13.757	1980	1984	1988	rBV	424867	373128	13.18%	2.779%
19	14.033	2023	2031	2043	rVB	17676	52570	1.86%	0.392%
20	15.145	2215	2220	2224	rBV	358720	418689	14.79%	3.119%

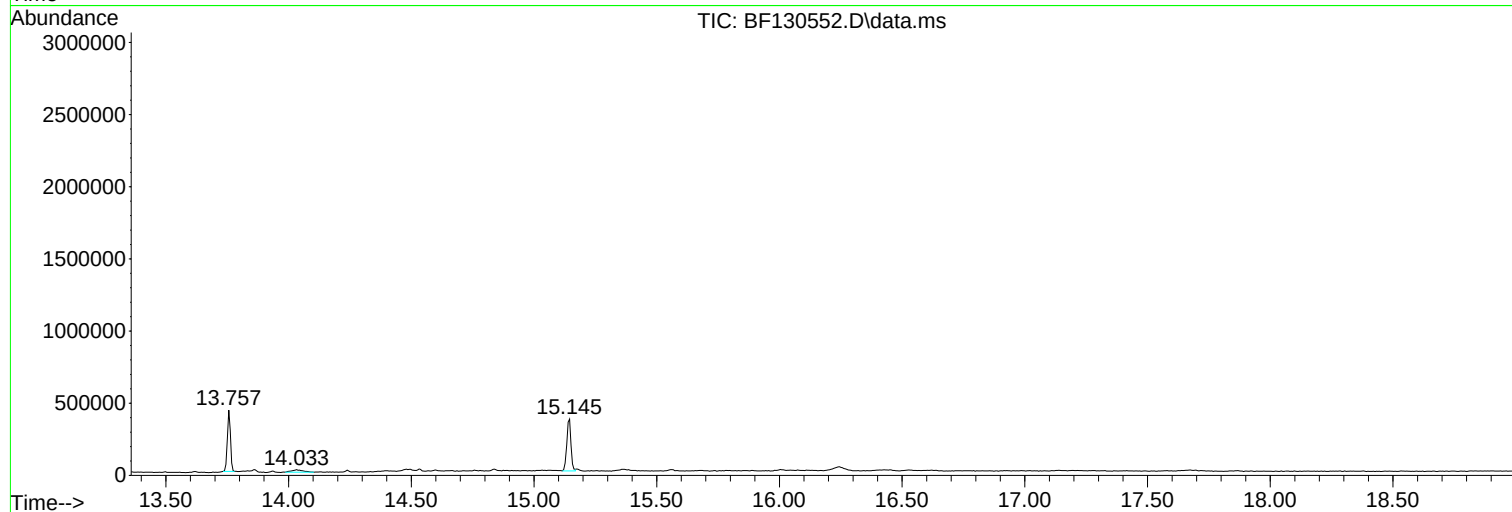
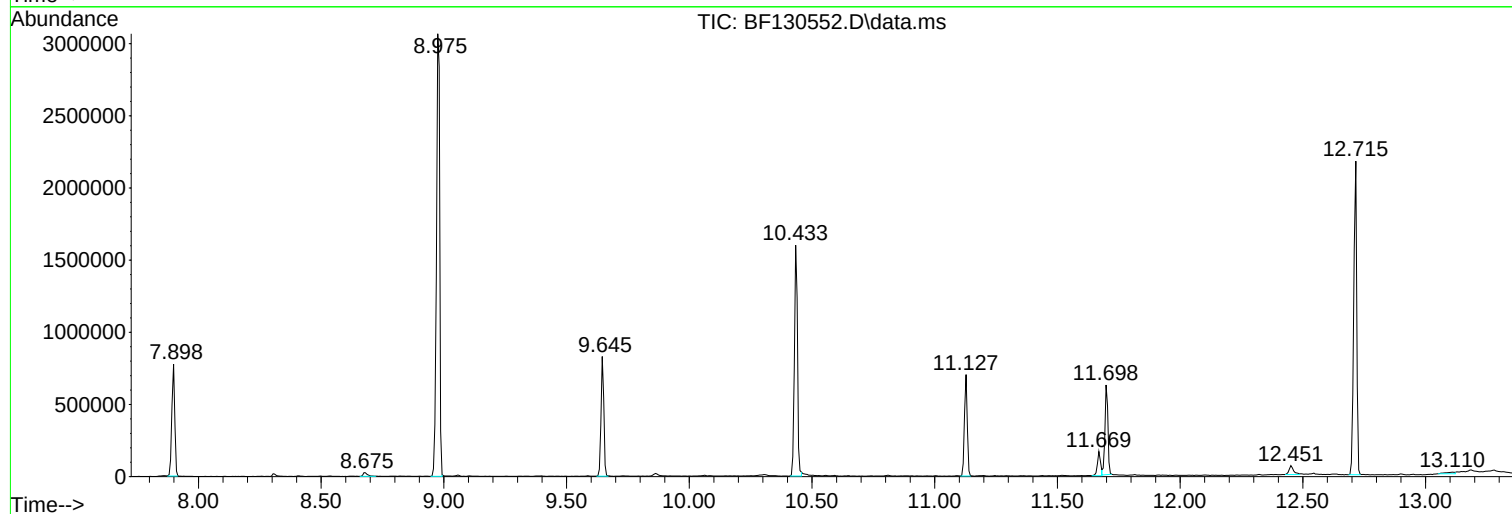
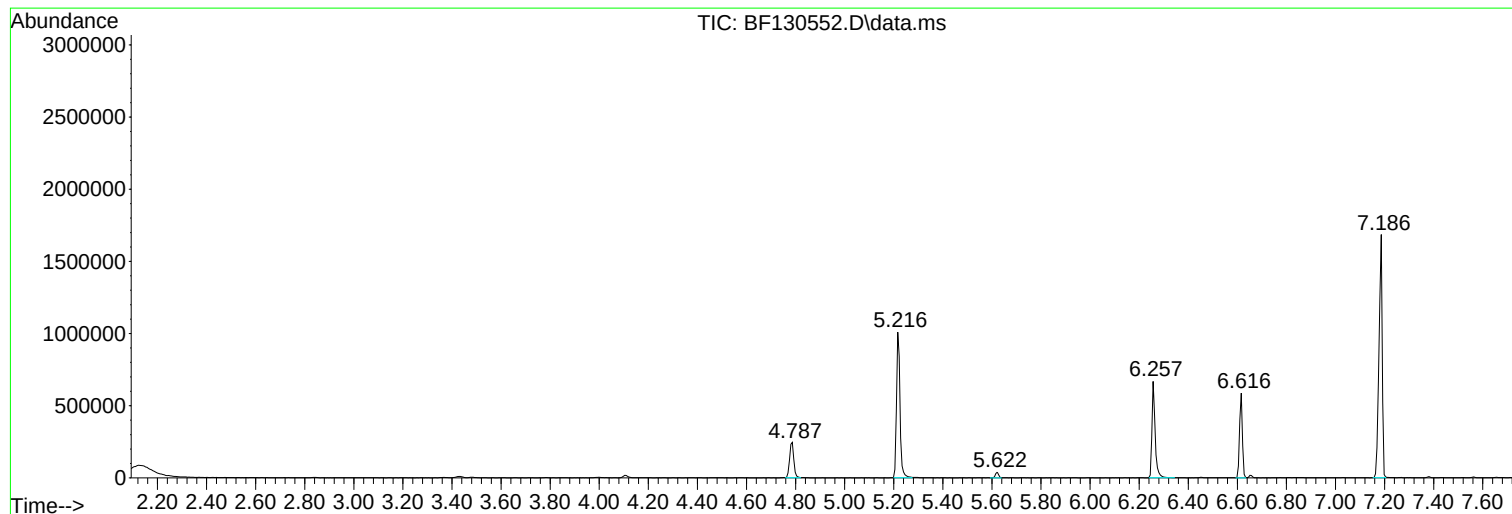
Sum of corrected areas: 13425076

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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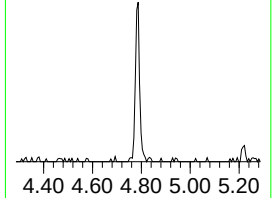
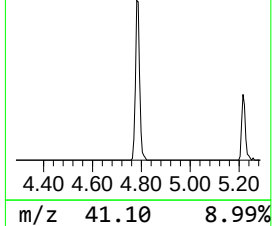
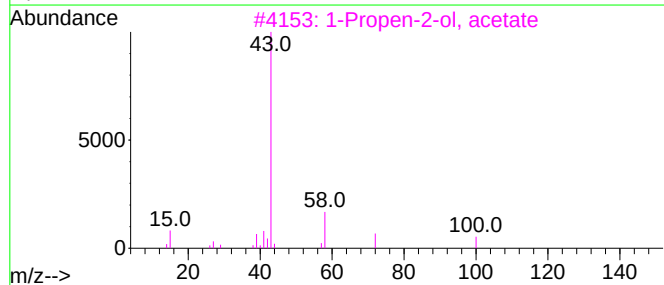
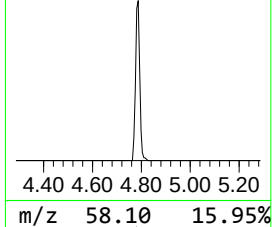
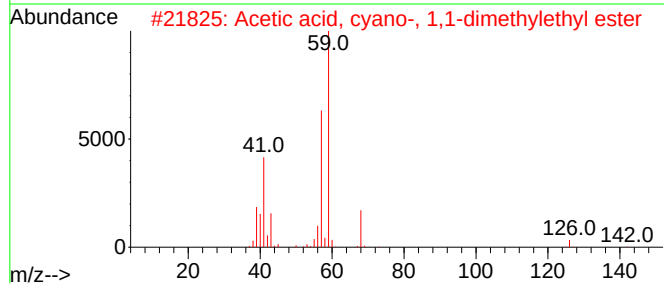
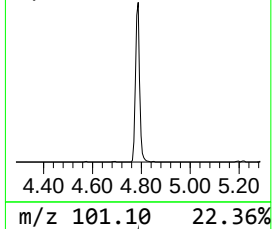
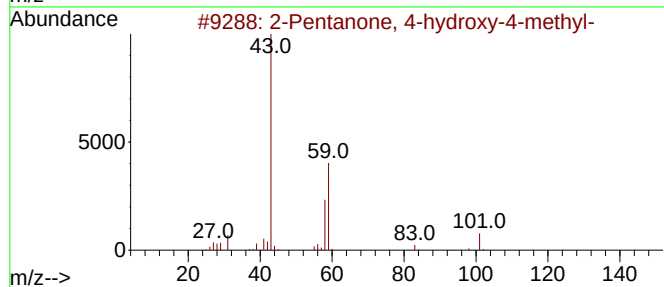
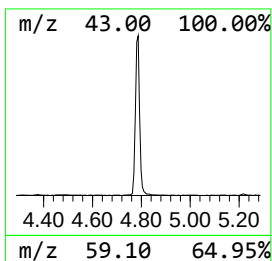
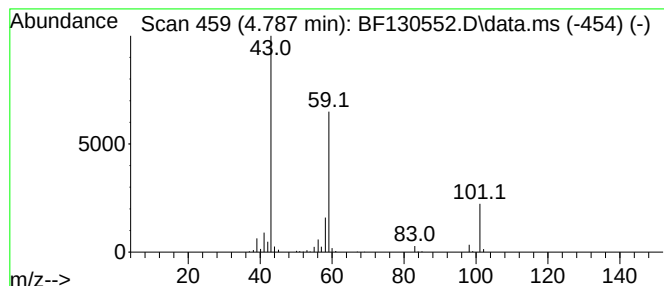
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.787	12.34 ng	288182	1,4-Dichlorobenzene-d4	6.616	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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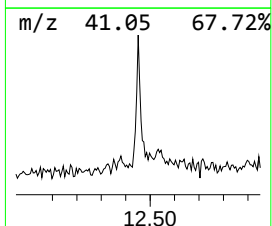
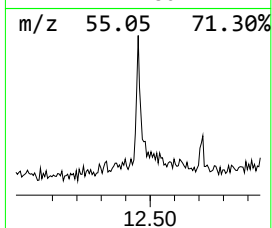
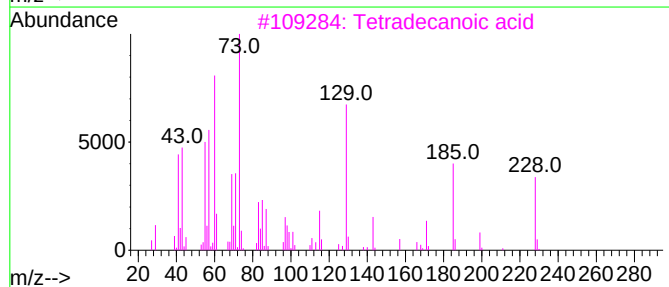
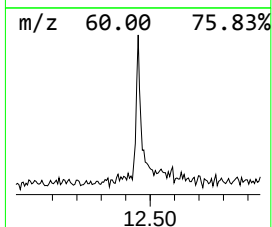
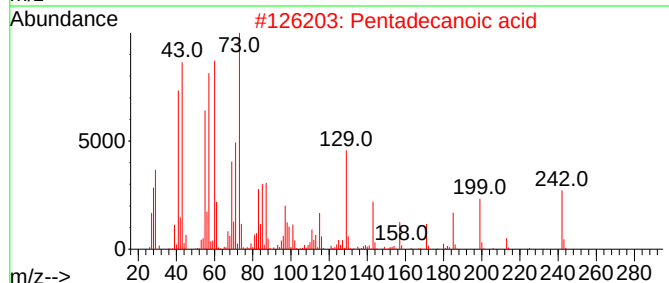
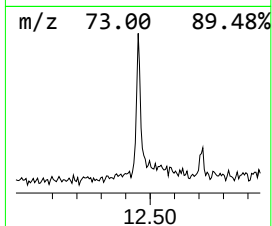
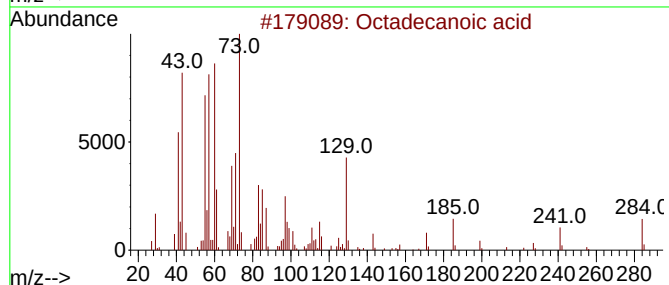
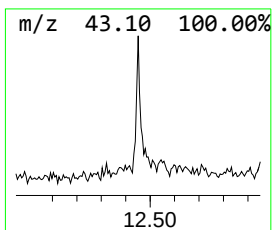
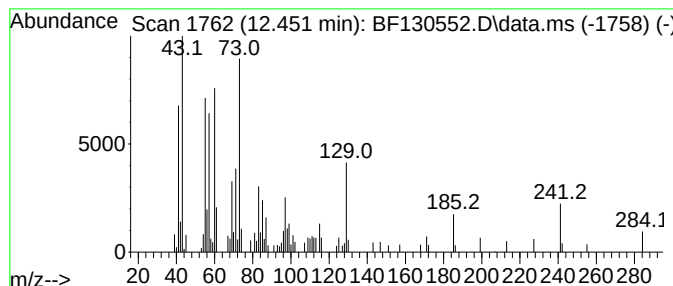
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.451	4.35 ng	81130	Chrysene-d12	13.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Tridecanoic acid	214	C13H26O2	000638-53-9	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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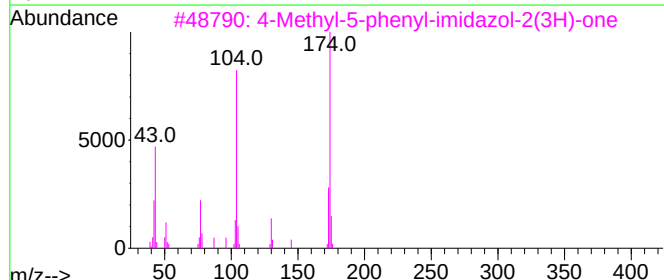
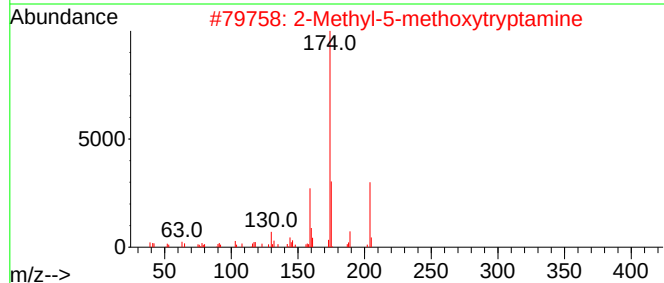
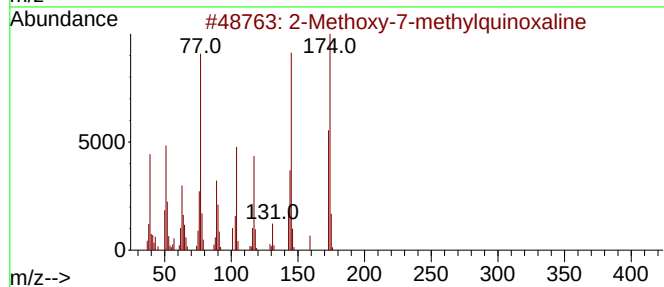
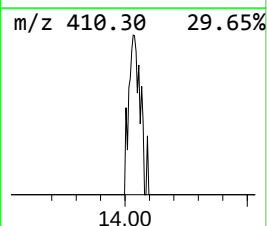
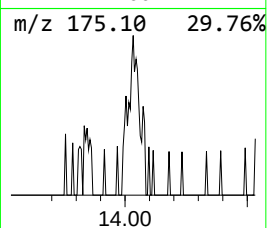
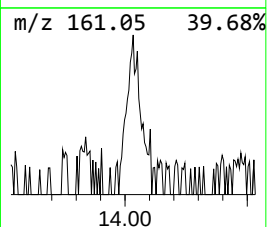
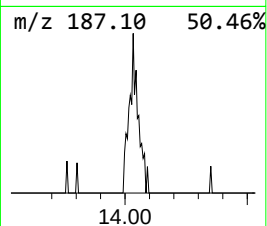
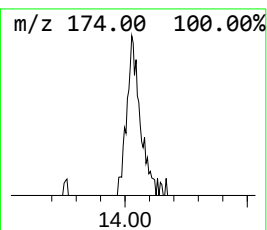
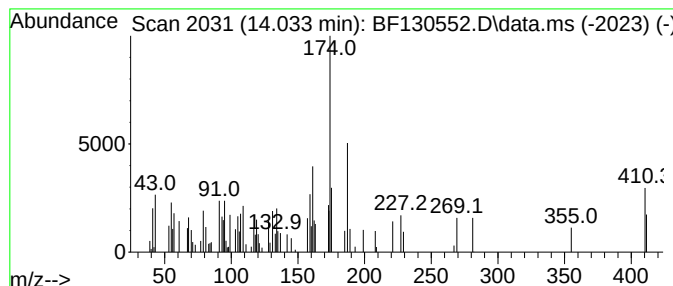
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Peak Number 3 unknown14.033 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.033	2.82 ng	52570	Chrysene-d12	13.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methoxy-7-methylquinoxaline	174	C10H10N2O	1000103-05-6	35		
2	2-Methyl-5-methoxytryptamine	204	C12H16N2O	003143-97-3	27		
3	4-Methyl-5-phenyl-imidazol-2(3H)...	174	C10H10N2O	1000147-06-1	27		
4	7-Amino-1H-indole, 3Me derivative	174	C11H14N2	1050234-37-1	25		
5	2-Fluoro-4-phenylpyrimidine	174	C10H7FN2	038953-34-3	25		



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.787	12.3	ng	288182	1	6.616	467163	20.0
Octadecanoic acid	12.451	4.3	ng	81130	5	13.757	373128	20.0
unknown14.033	14.033	2.8	ng	52570	5	13.757	373128	20.0