

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040918\
 Data File : BF104373.D
 Acq On : 9 Apr 2018 15:44
 Operator : JU/SJ
 Sample : J2104-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20180220-COMPOSITE-A

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.028	496	500	509	rVB	137784	193237	5.00%	0.595%
2	5.416	560	566	569	rBV	3121547	3801937	98.41%	11.700%
3	6.434	732	739	742	rBV	3125386	3863535	100.00%	11.890%
4	6.575	757	763	766	rBV	3661920	3795300	98.23%	11.680%
5	6.804	798	802	805	rBV	1015392	822259	21.28%	2.530%
6	6.963	824	829	832	rVB	2961605	2817063	72.91%	8.669%
7	7.369	892	898	901	rBV	2389503	2389110	61.84%	7.352%
8	8.087	1015	1020	1023	rBV	1293290	1115486	28.87%	3.433%
9	9.163	1198	1203	1206	rBV	3818550	3617371	93.63%	11.132%
10	9.557	1266	1270	1273	rBV	314349	261713	6.77%	0.805%
11	9.769	1303	1306	1309	rVB	57356	43725	1.13%	0.135%
12	9.839	1314	1318	1322	rVB	1383001	1212642	31.39%	3.732%
13	10.275	1389	1392	1394	rVB	78818	67962	1.76%	0.209%
14	10.633	1447	1453	1456	rBV	2477009	2461409	63.71%	7.575%
15	10.745	1468	1472	1481	rVB2	91982	109709	2.84%	0.338%
16	11.192	1545	1548	1551	rBV2	62609	57644	1.49%	0.177%
17	11.328	1567	1571	1574	rBV	1372682	1120849	29.01%	3.449%
18	11.857	1657	1661	1665	rBV	104087	108009	2.80%	0.332%
19	12.769	1813	1816	1819	rVB	58673	46830	1.21%	0.144%
20	12.922	1837	1842	1845	rBV	2855355	2793469	72.30%	8.597%
21	13.810	1990	1993	2001	rBV2	114557	119218	3.09%	0.367%
22	13.969	2015	2020	2023	rBV	919543	791034	20.47%	2.434%
23	15.427	2263	2268	2273	rBV	662446	817425	21.16%	2.516%
24	17.451	2604	2612	2619	rBV9	30227	67394	1.74%	0.207%

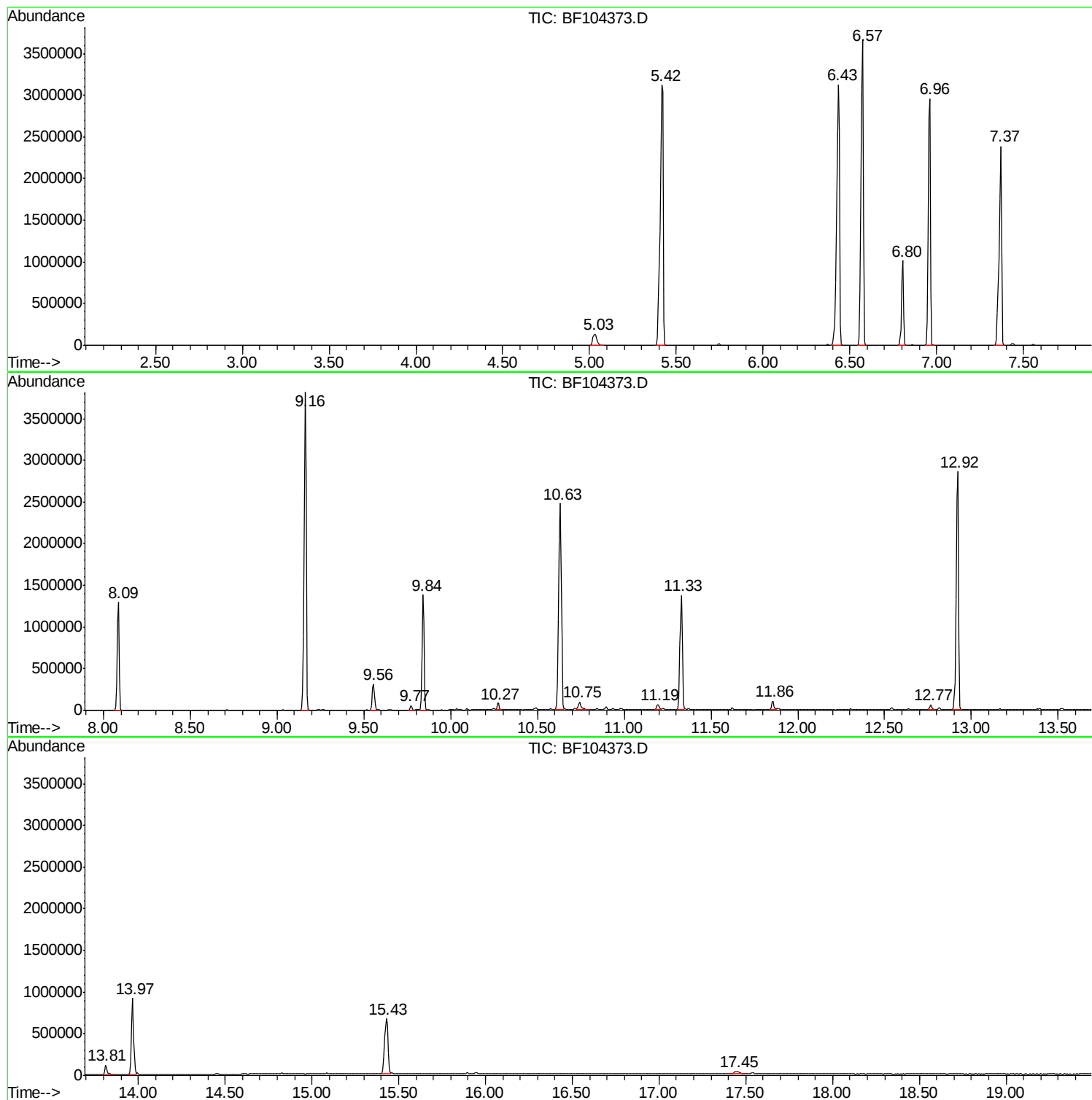
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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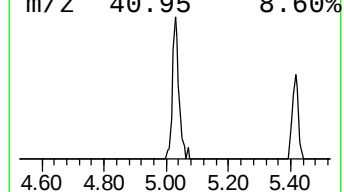
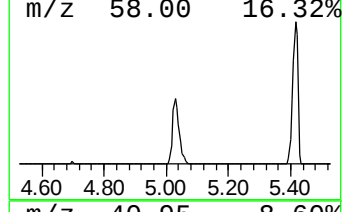
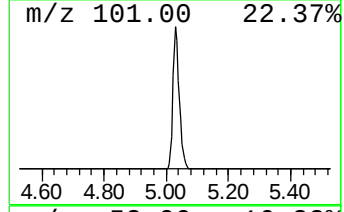
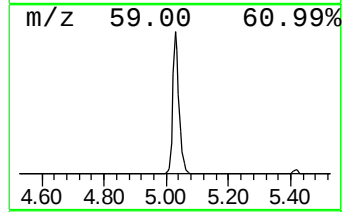
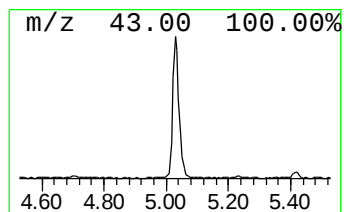
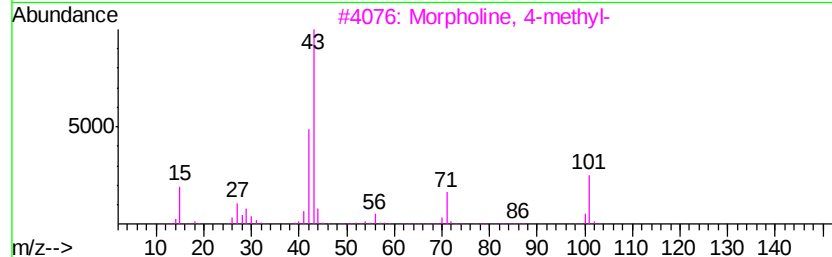
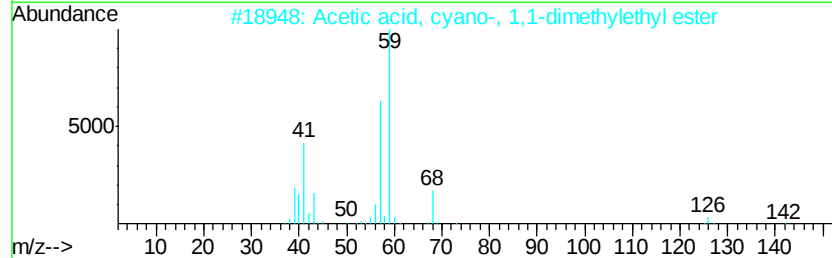
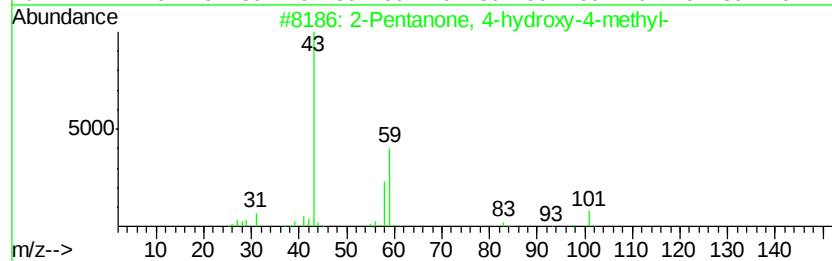
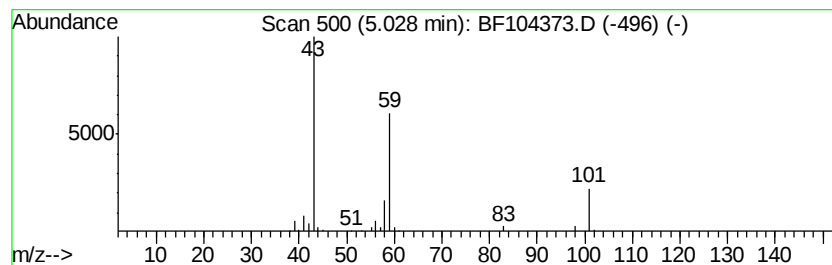
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.03	4.70 ng	193237	1,4-Dichlorobenzene-d4	6.80	
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-dimethyl...	141	C7H11NO2	001116-98-9	23
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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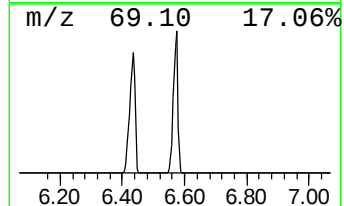
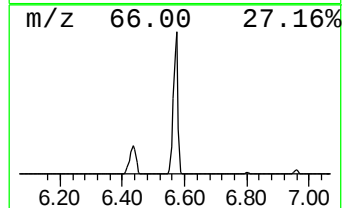
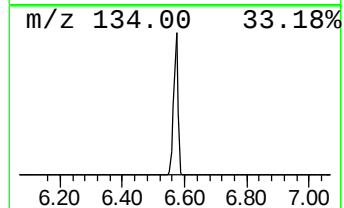
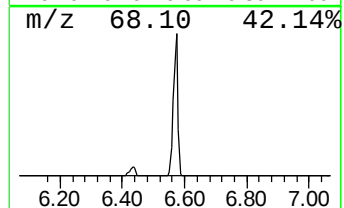
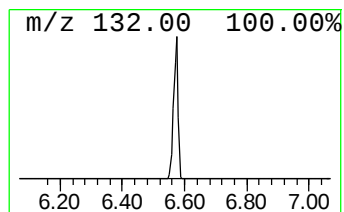
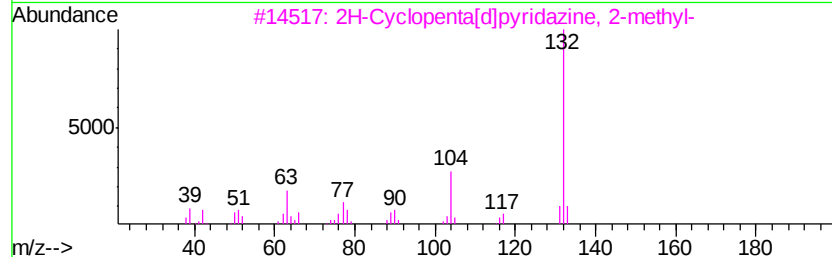
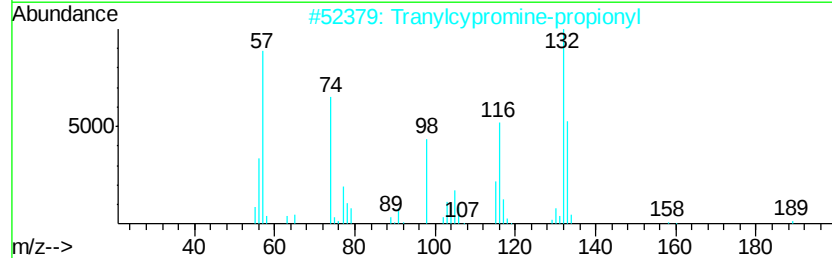
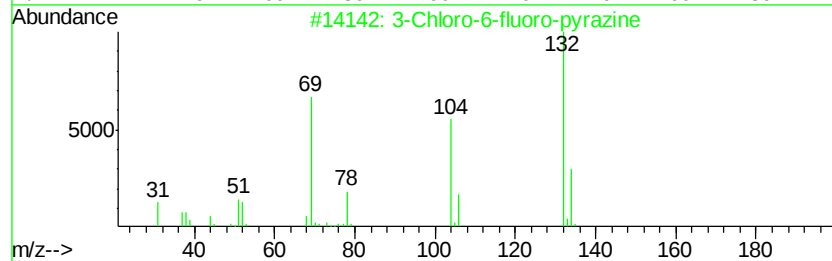
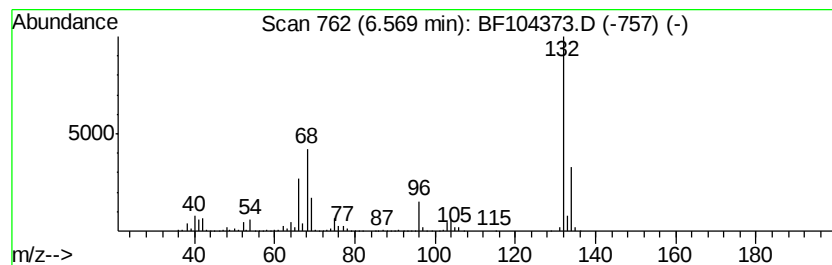
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Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	92.31 ng	3795300	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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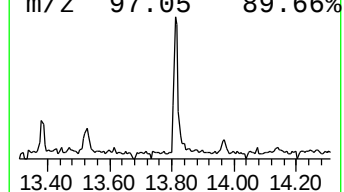
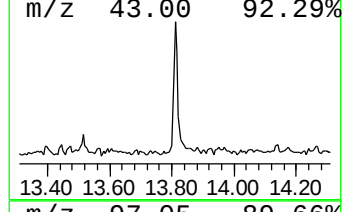
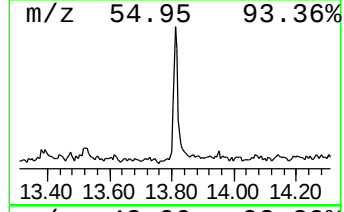
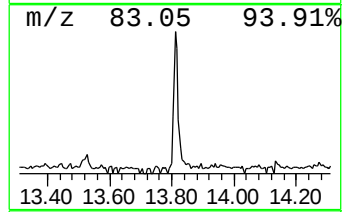
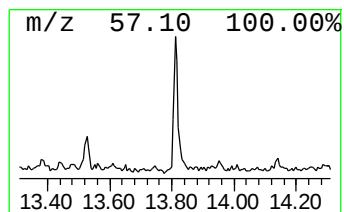
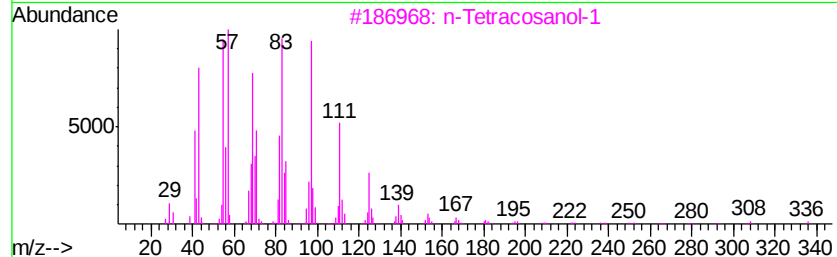
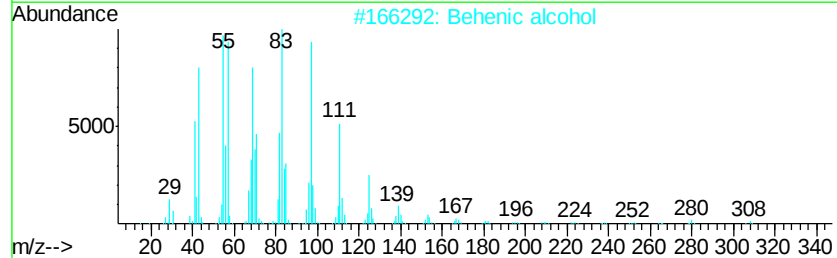
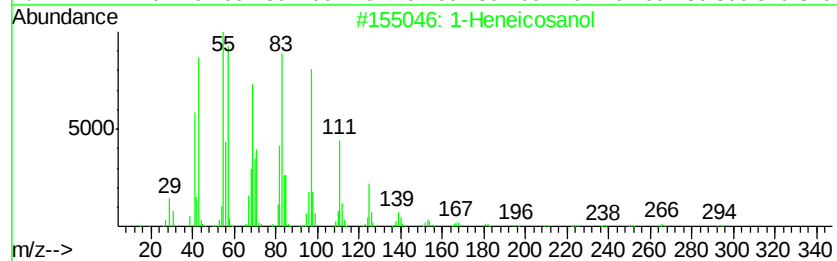
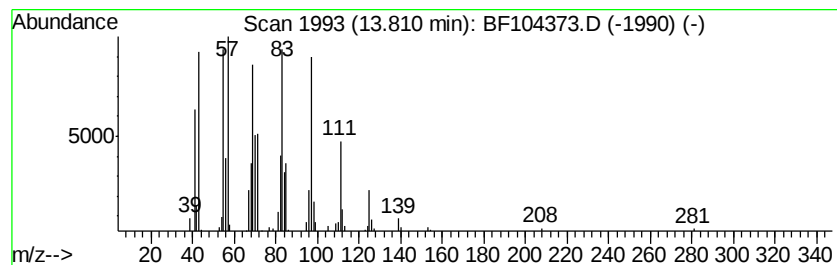
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Peak Number 4 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.81	3.01 ng	119218	Chrysene-d12		13.97
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5	1-Heptacosanol	396	C27H56O	002004-39-9	91



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.03	4.7	ng	193237	1	6.80	822259	20.0
unknown6.57	6.57	92.3	ng	3795300	1	6.80	822259	20.0
1-Heneicosanol	13.81	3.0	ng	119218	5	13.97	791034	20.0