

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101017\
 Data File : BF099318.D
 Acq On : 10 Oct 2017 23:44
 Operator : SJ/JU
 Sample : I5691-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ENV-115-8(0-5)

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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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	2.128	4	7	18	rVB2	49930	97847	5.51%	0.646%
2	5.087	506	510	523	rVB	213506	269801	15.19%	1.781%
3	5.487	574	578	589	rBV	1656729	1591091	89.56%	10.500%
4	6.492	745	749	764	rBV	1529017	1603101	90.23%	10.580%
5	6.634	769	773	776	rBV	1954617	1669514	93.97%	11.018%
6	6.863	809	812	816	rBV	674117	527380	29.68%	3.480%
7	7.022	835	839	842	rBV	1441730	1326883	74.68%	8.757%
8	7.428	903	908	911	rBV	1129659	959006	53.98%	6.329%
9	8.145	1026	1030	1033	rBV	825573	656574	36.96%	4.333%
10	9.216	1208	1212	1222	rBV	2014398	1776661	100.00%	11.725%
11	9.292	1222	1225	1228	rVB2	26354	25609	1.44%	0.169%
12	9.610	1275	1279	1285	rBV	288268	244299	13.75%	1.612%
13	9.822	1310	1315	1317	rBV2	18969	26365	1.48%	0.174%
14	9.898	1324	1328	1332	rVB	742011	616098	34.68%	4.066%
15	10.316	1394	1399	1403	rVB3	31899	33719	1.90%	0.223%
16	10.686	1459	1462	1472	rBV	766688	674703	37.98%	4.453%
17	10.792	1477	1480	1485	rBV2	44184	51259	2.89%	0.338%
18	11.386	1577	1581	1584	rBV	637529	517687	29.14%	3.416%
19	12.968	1845	1850	1853	rBV	1525813	1347379	75.84%	8.892%
20	13.851	1997	2000	2010	rBV3	47647	73160	4.12%	0.483%
21	14.027	2026	2030	2037	rBV	616317	575588	32.40%	3.799%
22	15.504	2276	2281	2287	rBV	360549	465865	26.22%	3.074%
23	16.621	2467	2471	2475	rBV7	13983	23026	1.30%	0.152%

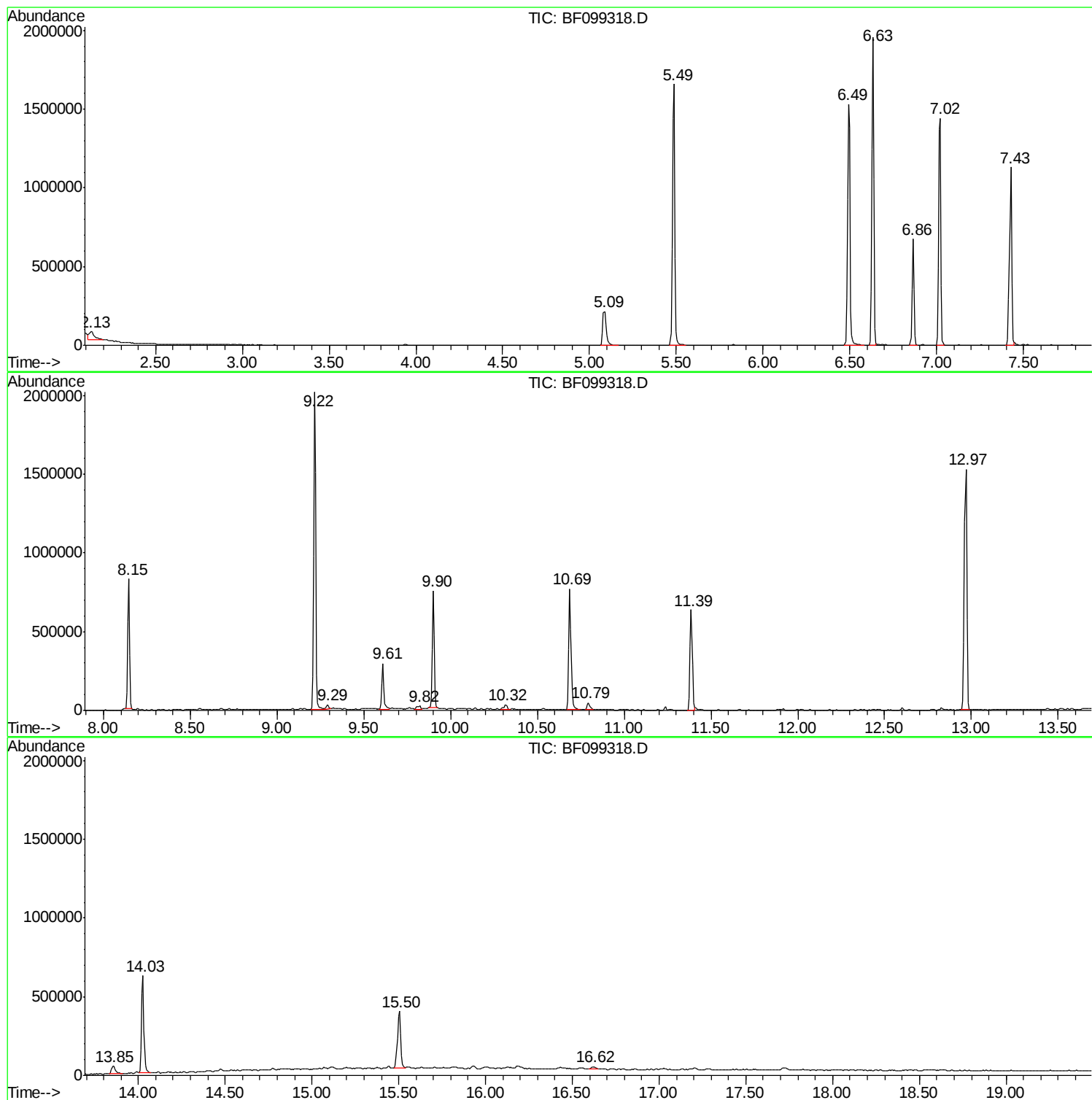
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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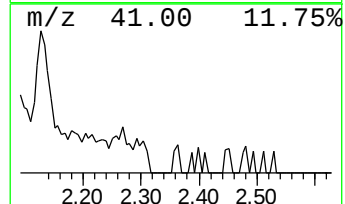
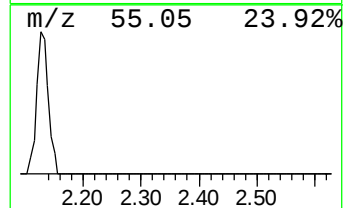
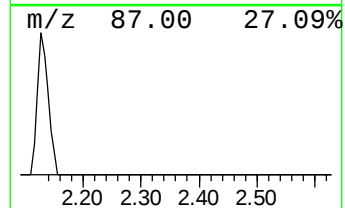
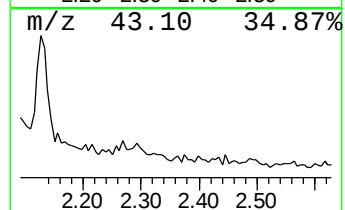
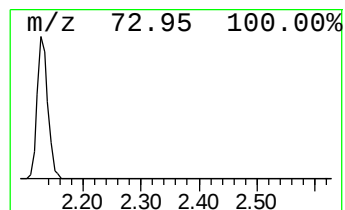
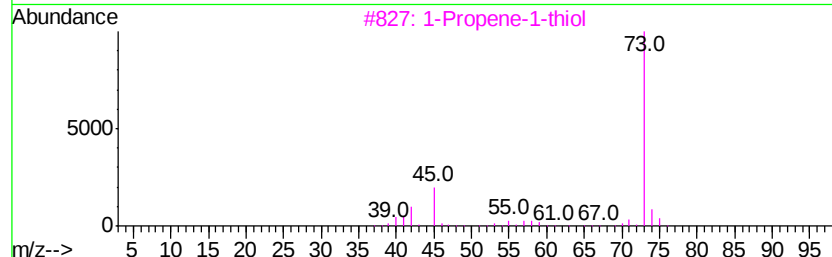
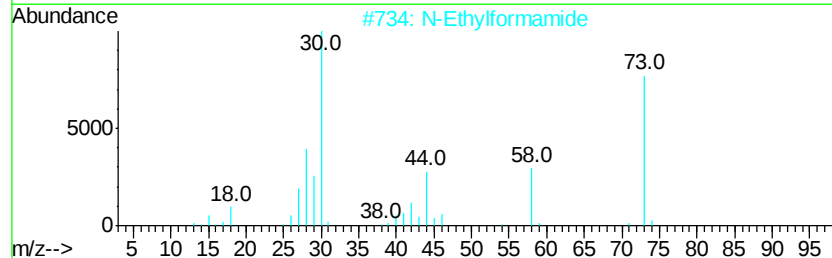
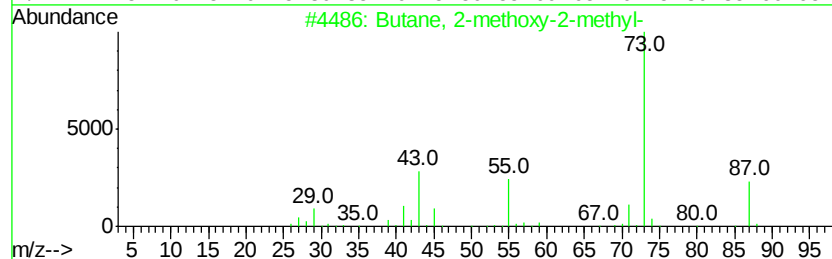
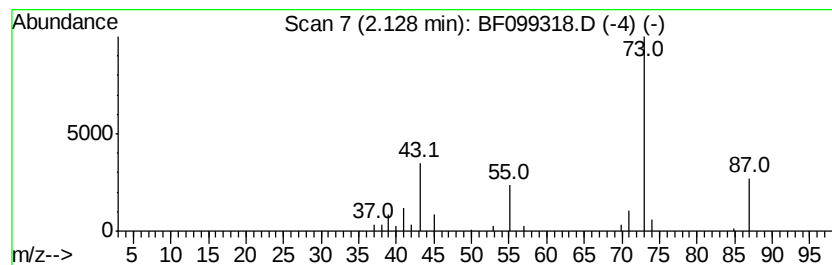
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	3.71 ng	97847	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	56
2			N-Ethylformamide	73	C3H7NO	000627-45-2	5
3			1-Propene-1-thiol	74	C3H6S	000925-89-3	4
4			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	4
5			Isobutylamine	73	C4H11N	000078-81-9	4



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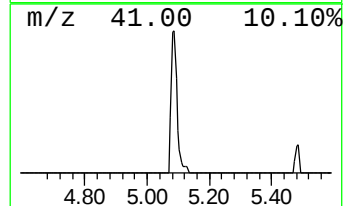
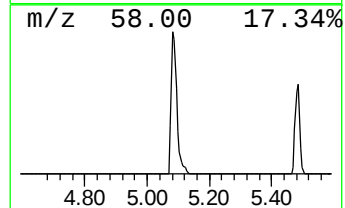
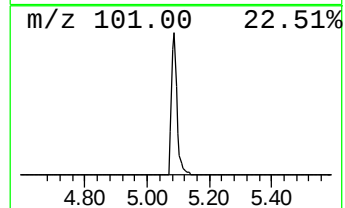
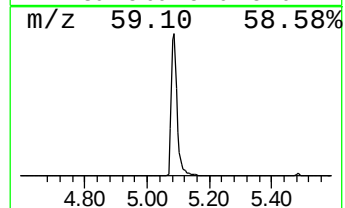
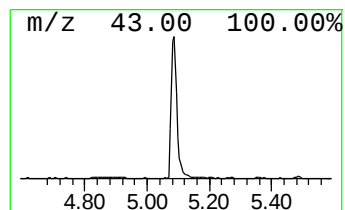
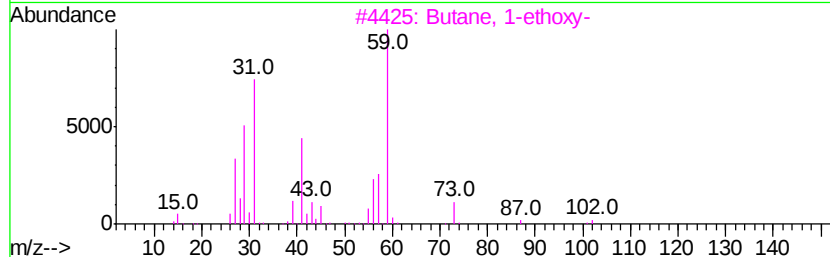
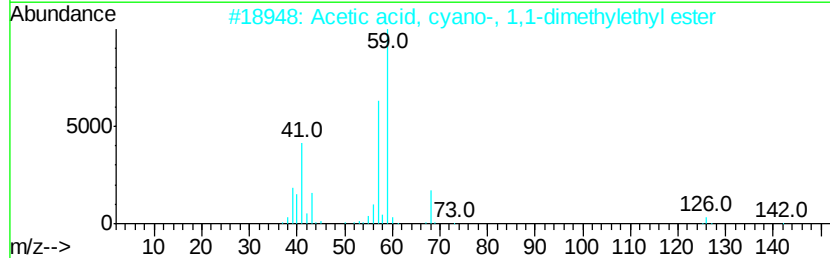
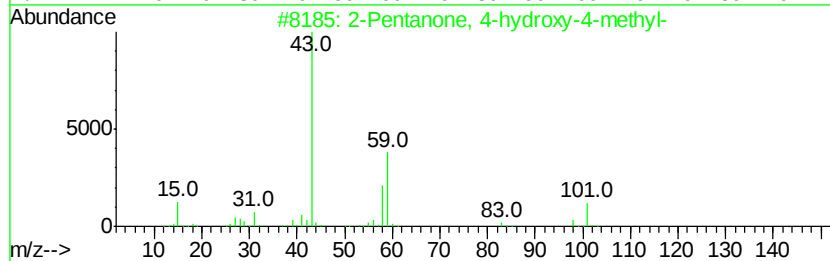
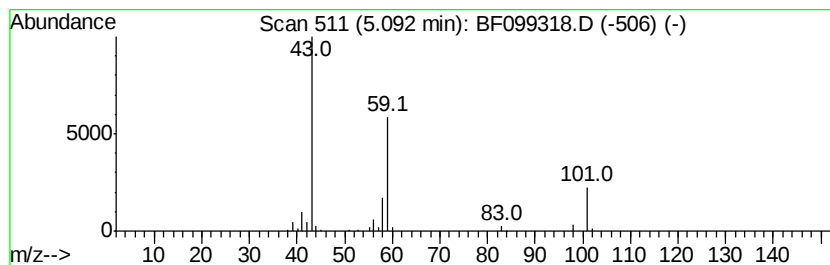
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	10.23 ng	269801	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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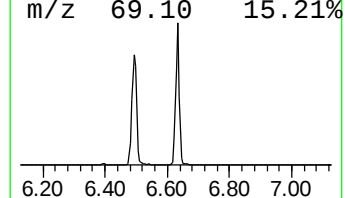
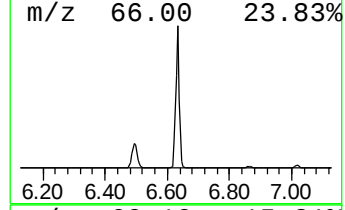
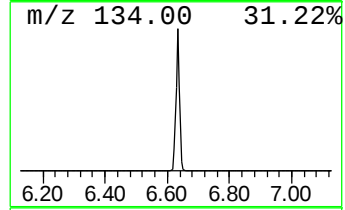
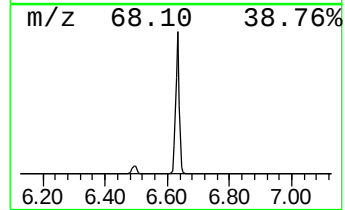
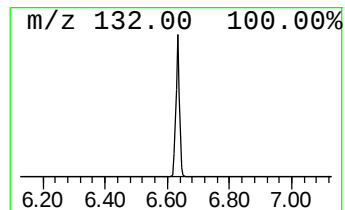
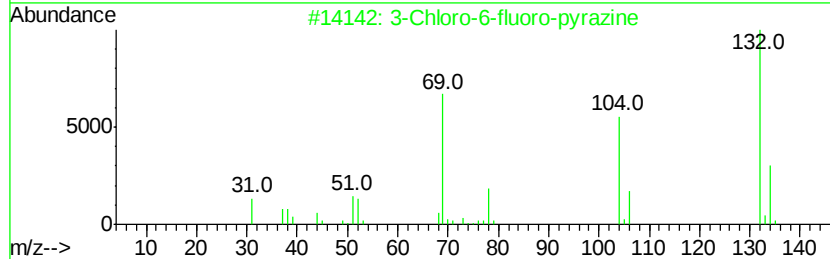
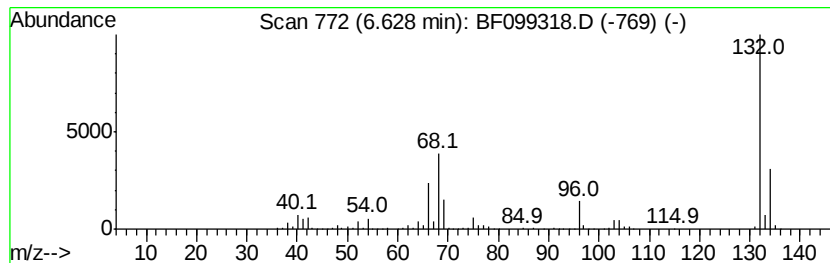
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Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	63.31 ng	1669510	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal			132	C6H9ClO	031357-76-3	35
3	5-Aminoindole			132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl			189	C12H15NO	1000123-86-3	12
5	4-Chloro-2-fluoro-pyrimidine			132	C4H2ClFN2	051422-00-5	9



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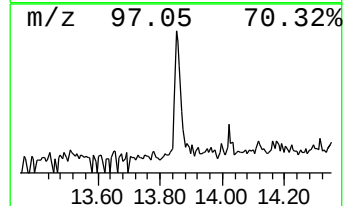
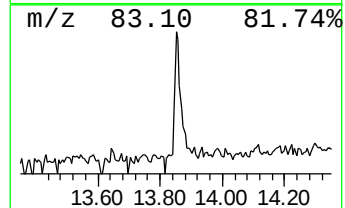
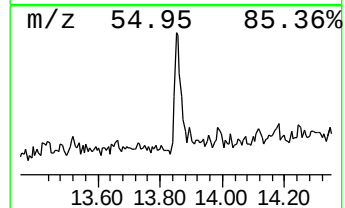
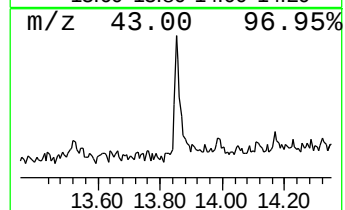
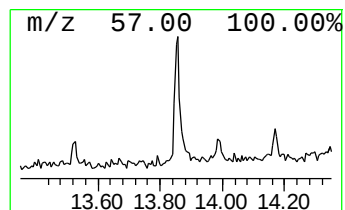
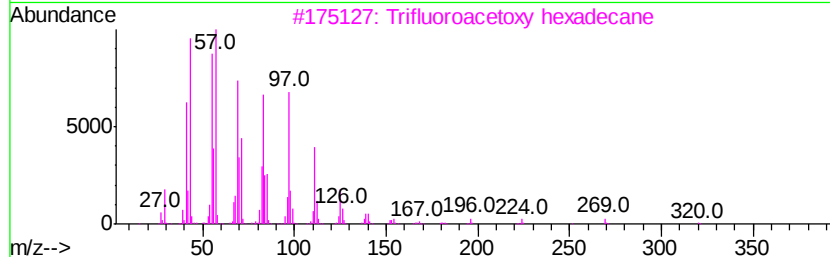
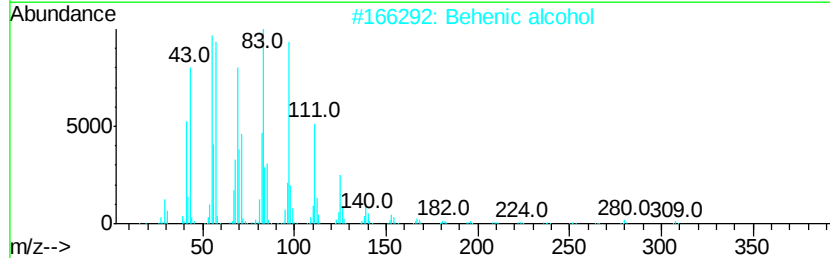
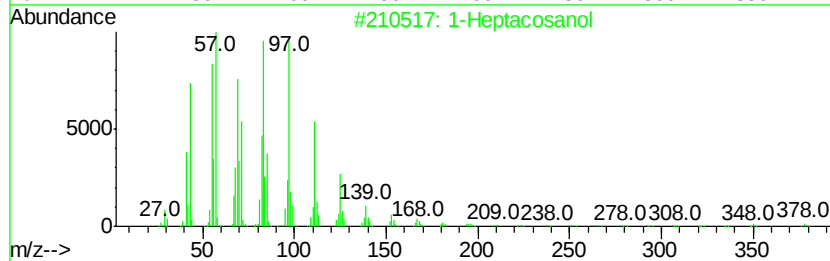
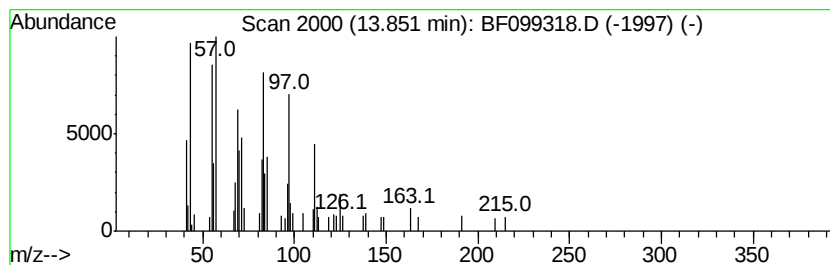
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Peak Number 5 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	2.54 ng	73160	Chrysene-d12	14.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heptacosanol	396	C27H56O	002004-39-9	93
2		Behenic alcohol	326	C22H46O	000661-19-8	93
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
4		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	90
5		1-Docosene	308	C22H44	001599-67-3	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.13	3.7	ng	97847	1	6.86	527380	20.0
2-Pentanone, 4-hy...	5.09	10.2	ng	269801	1	6.86	527380	20.0
unknown6.63	6.63	63.3	ng	1669510	1	6.86	527380	20.0
1-Heptacosanol	13.85	2.5	ng	73160	5	14.03	575588	20.0