

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF101117\
 Data File : BF099380.D
 Acq On : 12 Oct 2017 8:39
 Operator : SJ/JU
 Sample : PB103152BL
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB103152BL

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	5.081	506	509	527	rBV	421960	514924	18.33%	2.656%
2	5.481	573	577	594	rBV	1794159	1648606	58.70%	8.503%
3	6.481	743	747	750	rBV	1643674	1595396	56.81%	8.228%
4	6.622	767	771	774	rBV	1961845	1713274	61.00%	8.836%
5	6.851	806	810	813	rBV	739940	595437	21.20%	3.071%
6	7.004	832	836	840	rBV	2025080	2005179	71.40%	10.341%
7	7.416	901	906	909	rBV	1511967	1505398	53.60%	7.764%
8	8.134	1023	1028	1031	rBV	907797	824275	29.35%	4.251%
9	9.210	1205	1211	1214	rBV	2754445	2808480	100.00%	14.484%
10	9.886	1321	1326	1335	rBB	1046569	898253	31.98%	4.633%
11	10.675	1456	1460	1475	rBB	1024136	870510	31.00%	4.490%
12	11.375	1575	1579	1582	rBV	982491	832279	29.63%	4.292%
13	12.763	1812	1815	1818	rBV	87005	64243	2.29%	0.331%
14	12.957	1843	1848	1851	rBV	2254847	2132431	75.93%	10.998%
15	13.469	1931	1935	1939	rBV	56865	49430	1.76%	0.255%
16	14.010	2023	2027	2032	rBV	619278	525264	18.70%	2.709%
17	15.480	2271	2277	2285	rBV	470089	596773	21.25%	3.078%
18	15.904	2344	2349	2354	rBV3	32450	46540	1.66%	0.240%
19	16.404	2429	2434	2441	rVB2	36844	64646	2.30%	0.333%
20	16.992	2528	2534	2541	rVB	25926	50751	1.81%	0.262%
21	17.686	2646	2652	2660	rVB5	19698	47556	1.69%	0.245%

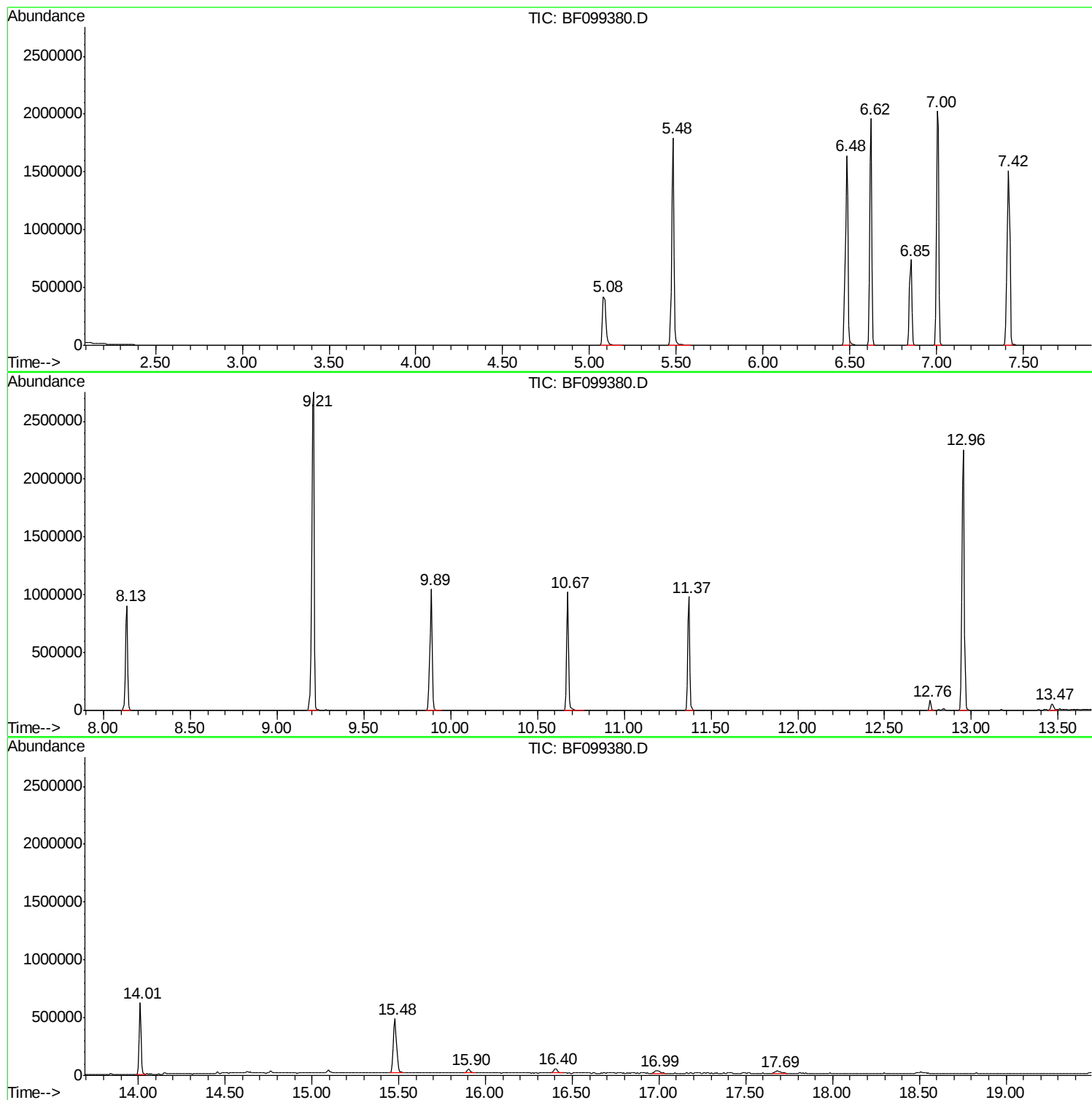
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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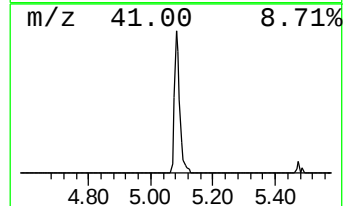
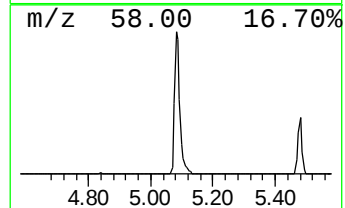
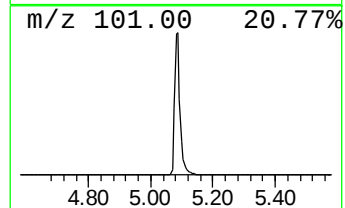
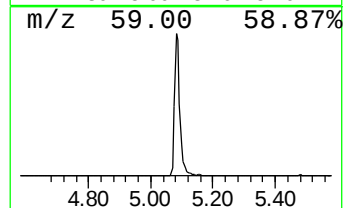
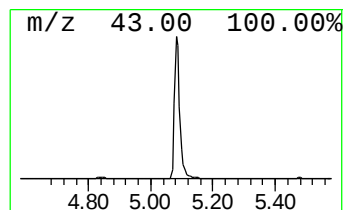
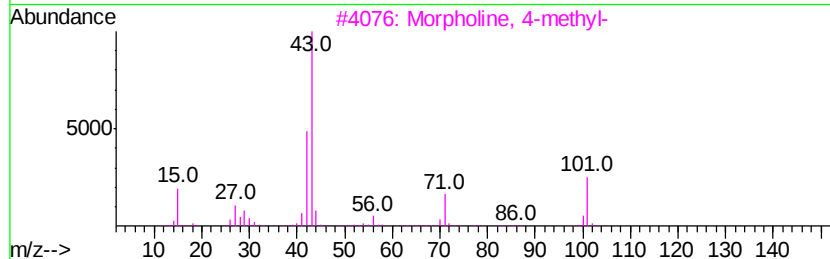
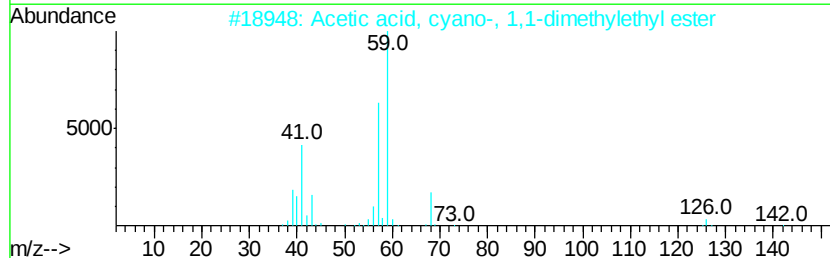
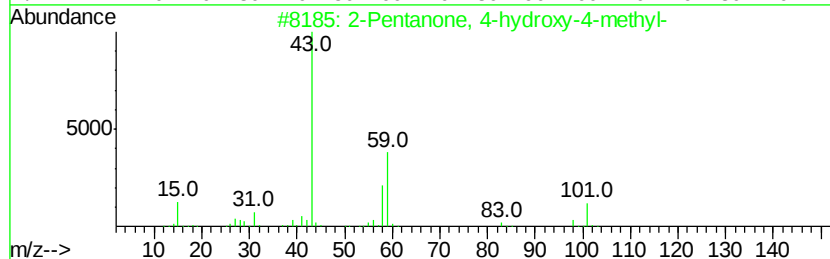
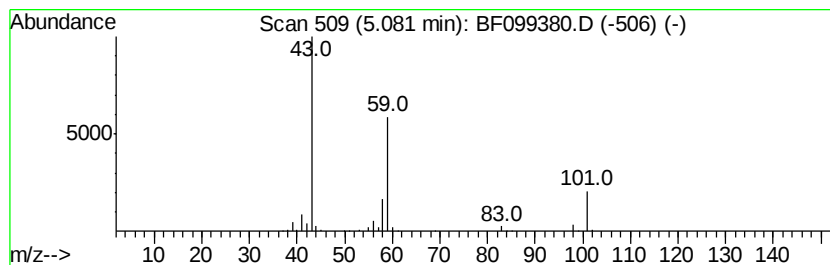
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	17.30 ng	514924	1,4-Dichlorobenzene-d4	6.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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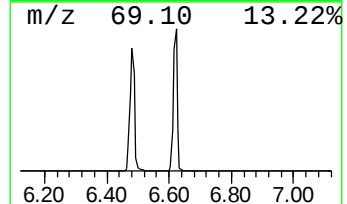
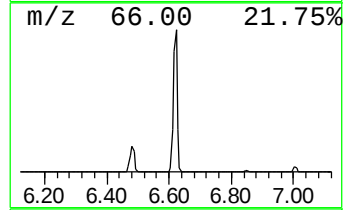
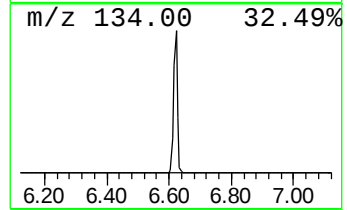
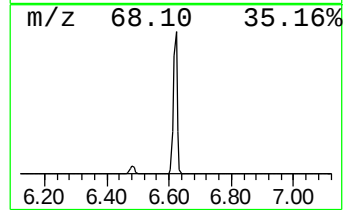
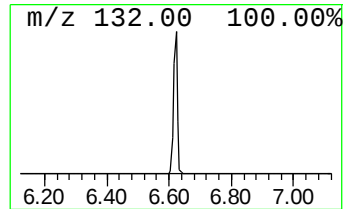
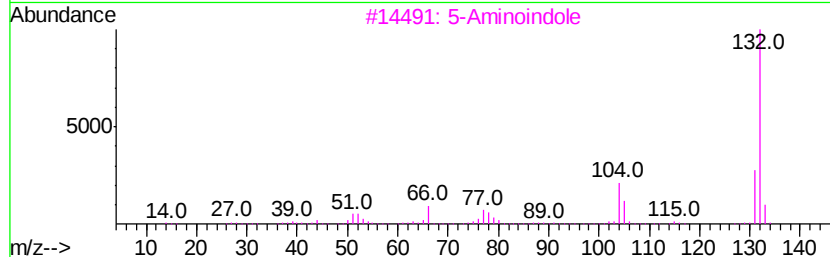
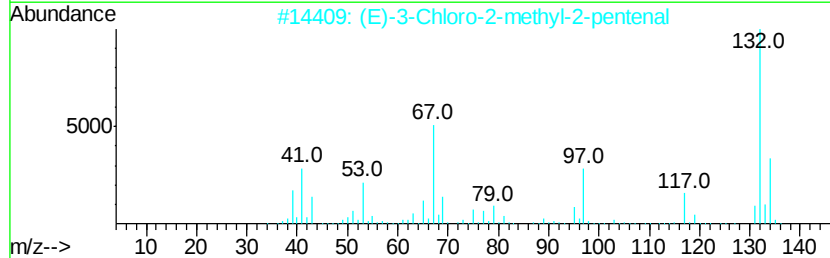
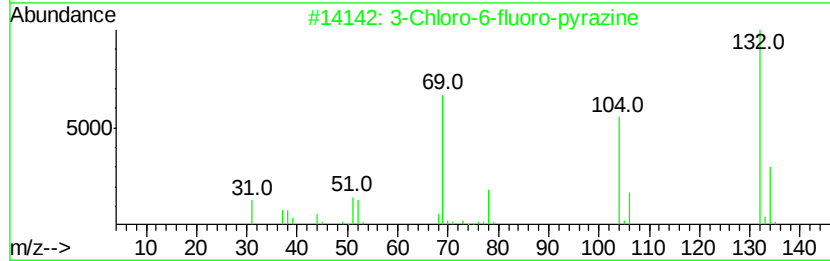
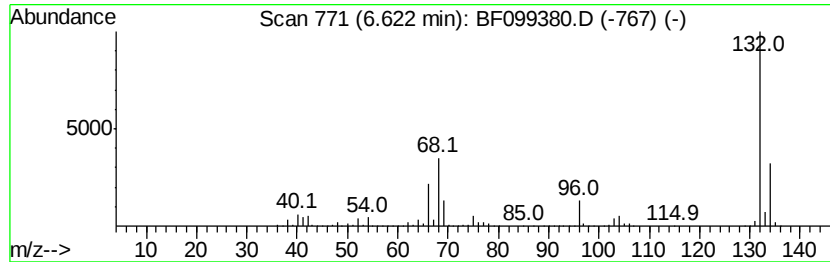
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Peak Number 2 unknown6.62 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	57.55 ng	1713270	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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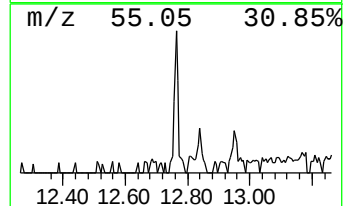
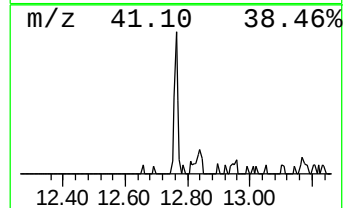
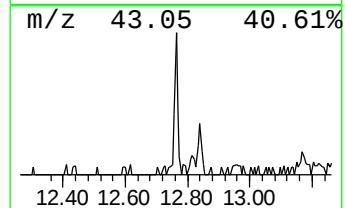
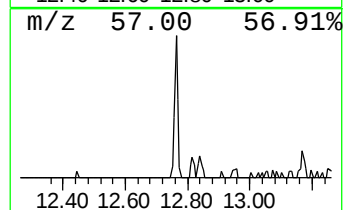
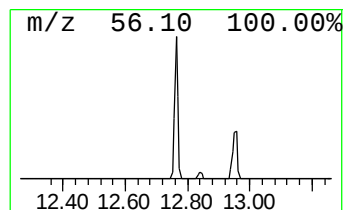
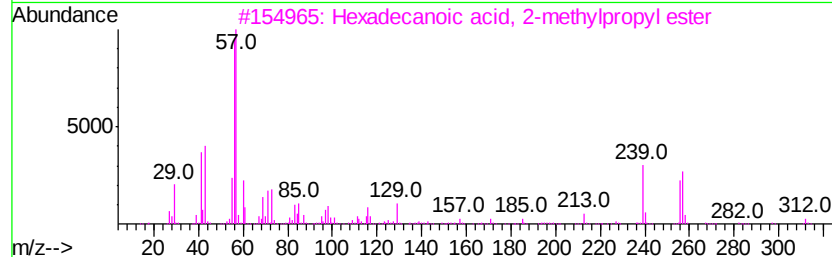
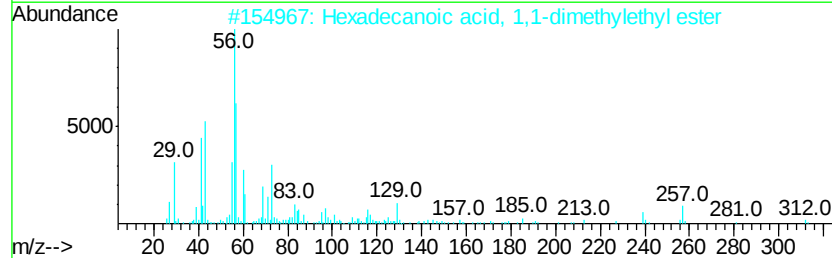
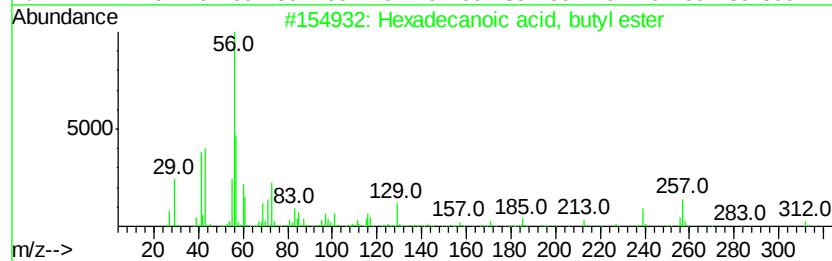
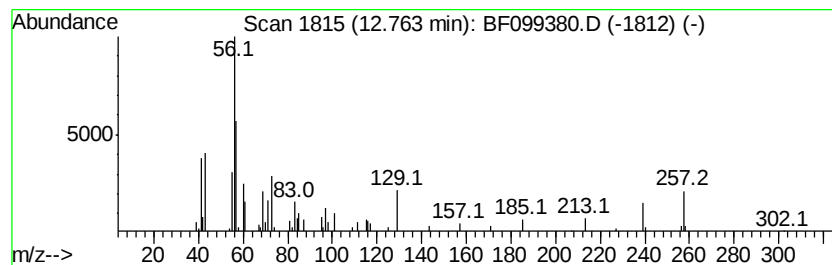
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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.76	2.45 ng	64243	Chrysene-d12	14.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	74
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	50
4		Nipecotic acid	129	C6H11NO2	000498-95-3	38
5		1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27



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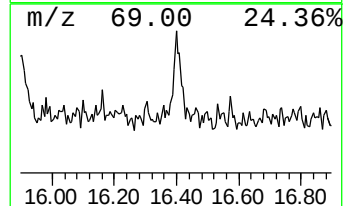
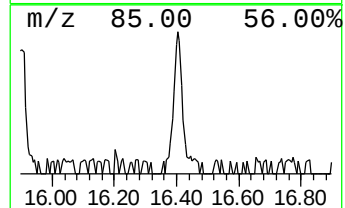
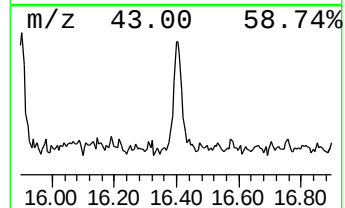
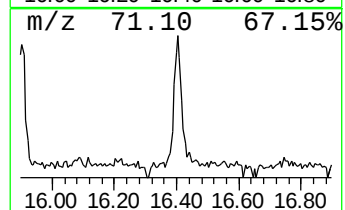
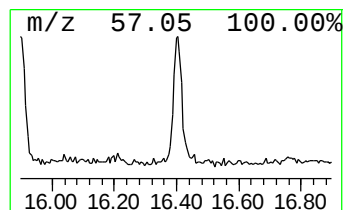
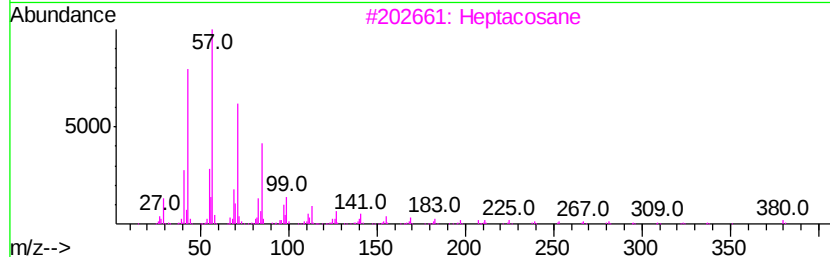
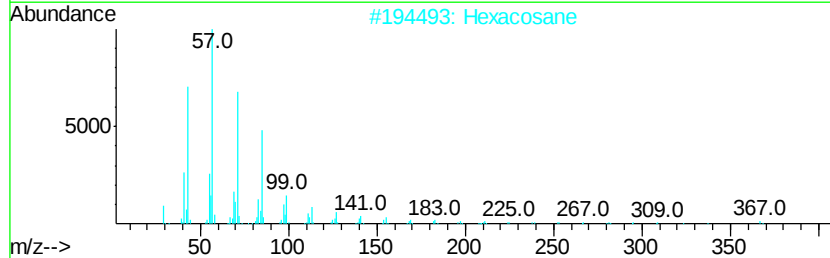
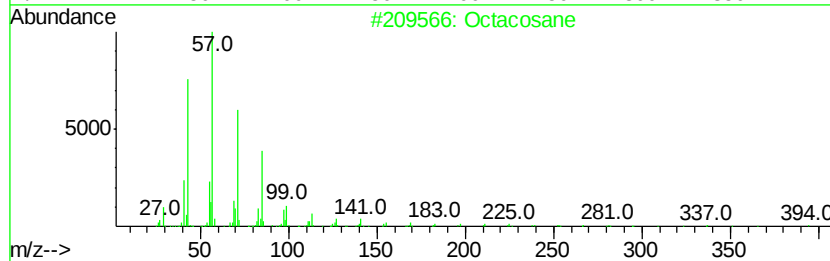
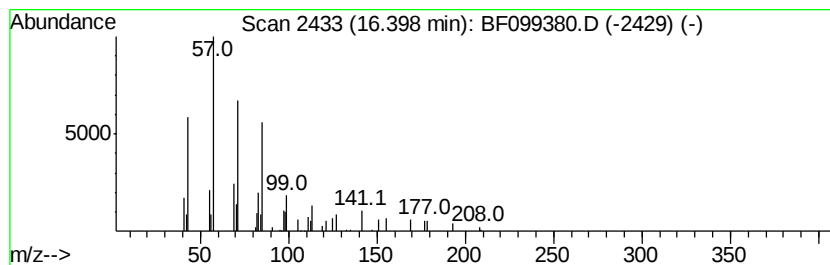
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Peak Number 5 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.40	2.17 ng	64646	Perylene-d12	15.48

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	91
2	Hexacosane		366	C26H54	000630-01-3	91
3	Heptacosane		380	C27H56	000593-49-7	91
4	2-methyloctacosane		408	C29H60	1000376-72-8	90
5	Heneicosane, 11-(1-ethylpropyl)-		366	C26H54	055282-11-6	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.08	17.3	ng	514924	1	6.85	595437	20.0
unknown6.62	6.62	57.5	ng	1713270	1	6.85	595437	20.0
Hexadecanoic acid...	12.76	2.5	ng	64243	5	14.01	525264	20.0
Octacosane	16.40	2.2	ng	64646	6	15.48	596773	20.0