

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF101217\
 Data File : BF099390.D
 Acq On : 12 Oct 2017 12:42
 Operator : SJ/JU
 Sample : I5758-05
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB11

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	2.175	11	15	27	rVB	59496	95215	2.55%	0.315%
2	3.487	236	238	246	rBV2	16013	39765	1.07%	0.132%
3	5.092	507	511	528	rBV	410456	649104	17.41%	2.151%
4	5.487	573	578	581	rBV	3002804	3291587	88.26%	10.906%
5	6.498	743	750	767	rVB	2606011	3456906	92.70%	11.453%
6	6.628	767	772	775	rBV	3216470	3410528	91.45%	11.300%
7	6.851	806	810	814	rBV	869415	689492	18.49%	2.284%
8	7.010	832	837	840	rBV	2775519	2649509	71.05%	8.778%
9	7.422	901	907	910	rBV	2023551	2174185	58.30%	7.203%
10	8.133	1023	1028	1031	rBV	1130585	940156	25.21%	3.115%
11	9.210	1205	1211	1214	rBV	3720059	3729266	100.00%	12.356%
12	9.475	1252	1256	1263	rBV	85106	66112	1.77%	0.219%
13	9.598	1272	1277	1281	rBV	631845	526048	14.11%	1.743%
14	9.886	1321	1326	1330	rBV2	1175796	993081	26.63%	3.290%
15	10.680	1456	1461	1464	rBV	1942917	1936751	51.93%	6.417%
16	10.774	1474	1477	1486	rVB	41109	44519	1.19%	0.147%
17	11.374	1575	1579	1582	rBV	1096944	890802	23.89%	2.951%
18	12.957	1843	1848	1851	rBV	2623863	2577798	69.12%	8.541%
19	13.116	1870	1875	1879	rBV4	24970	38929	1.04%	0.129%
20	13.174	1882	1885	1888	rVB	57538	49731	1.33%	0.165%
21	13.833	1994	1997	2002	rBV	62031	67611	1.81%	0.224%
22	14.010	2024	2027	2031	rBV	612526	541369	14.52%	1.794%
23	14.621	2127	2131	2135	rVB	885332	745498	19.99%	2.470%
24	15.480	2272	2277	2287	rVB	458944	578812	15.52%	1.918%

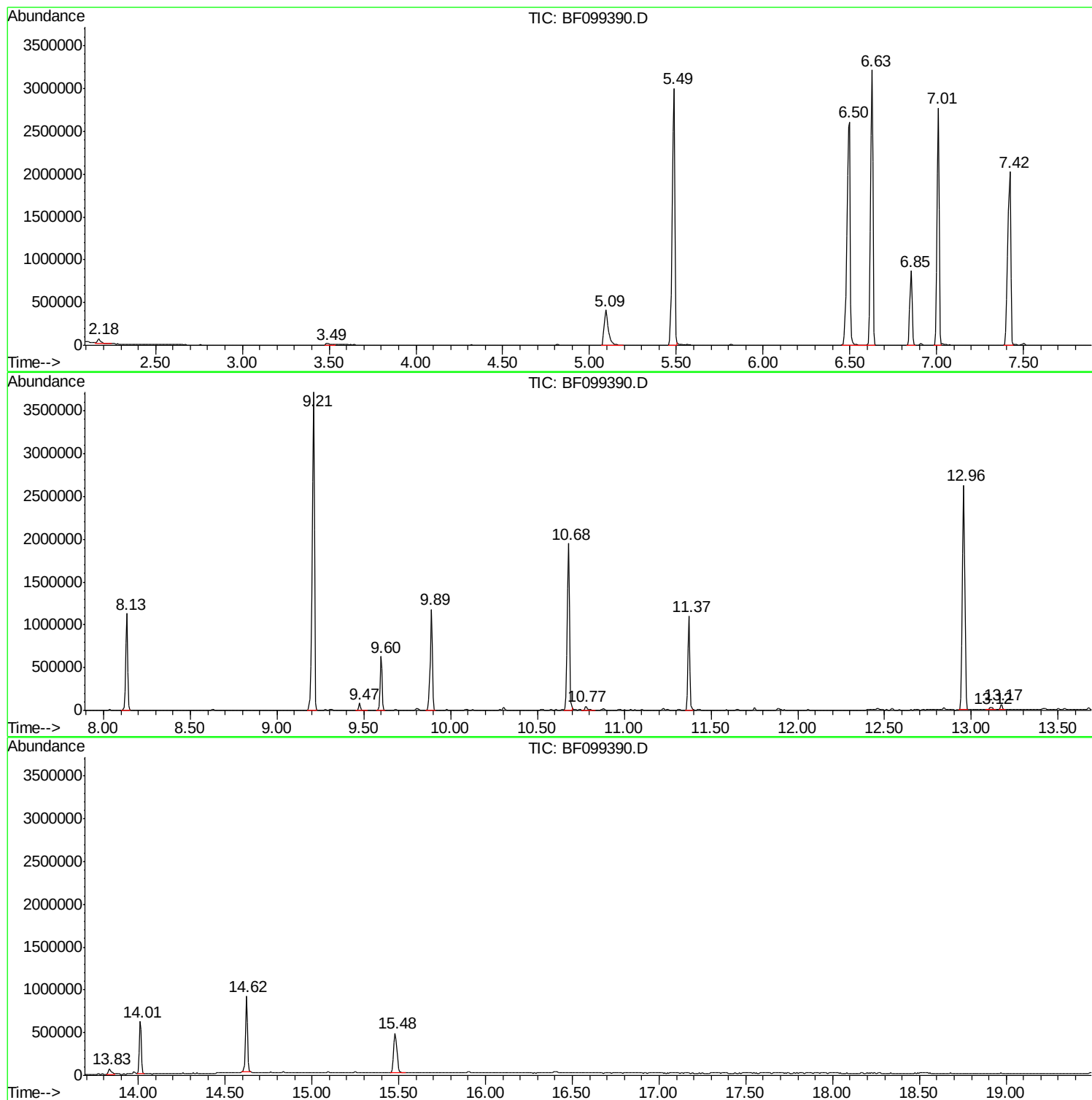
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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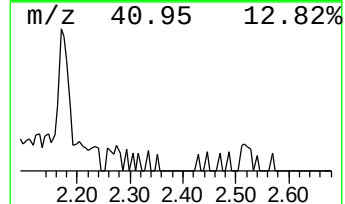
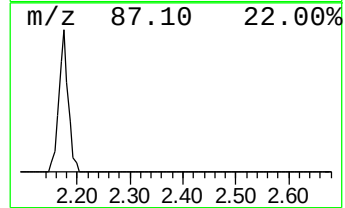
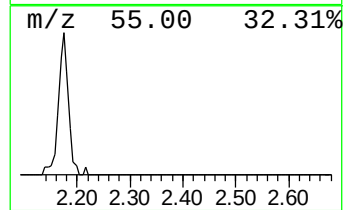
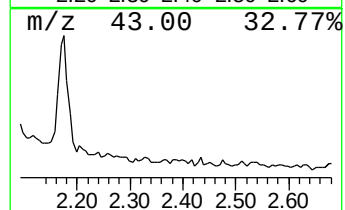
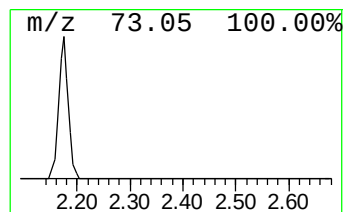
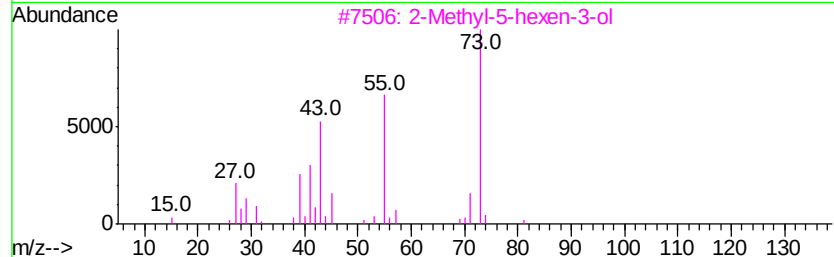
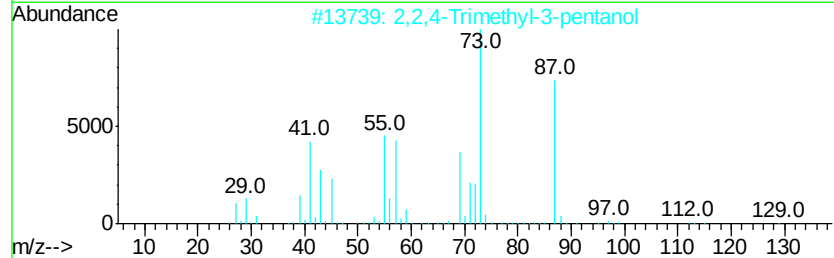
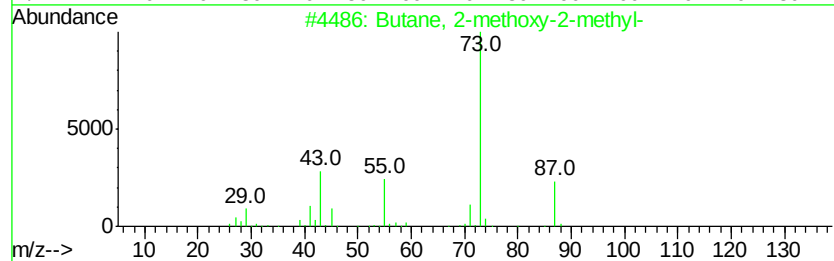
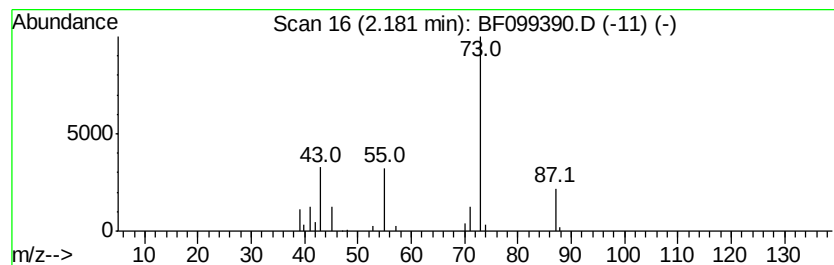
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	2.76 ng	95215	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	28
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	16
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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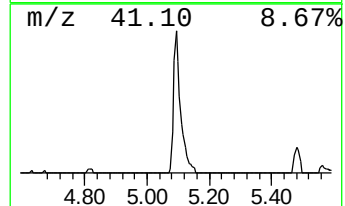
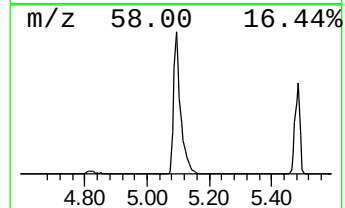
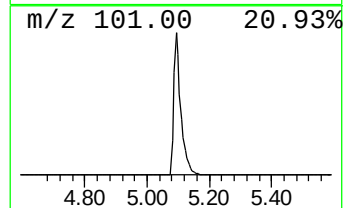
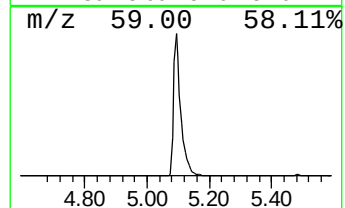
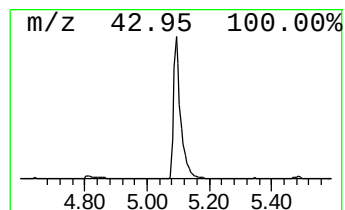
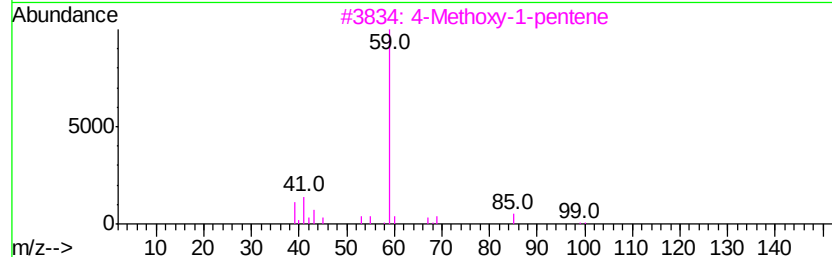
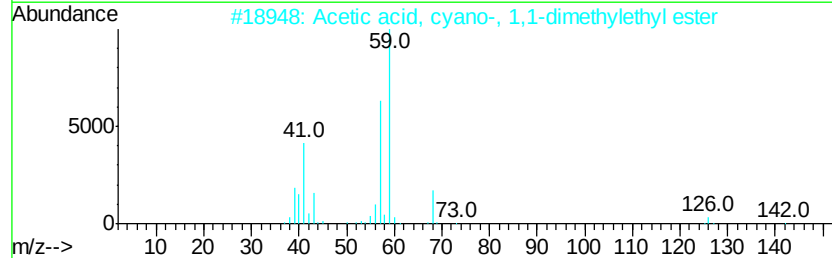
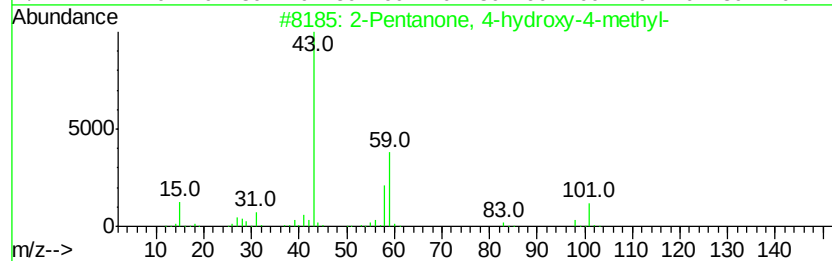
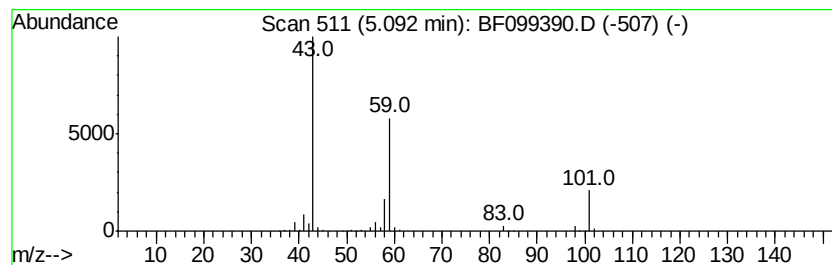
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	18.83 ng	649104	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	72
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3			4-Methoxy-1-pentene	100	C6H12O	098386-09-5	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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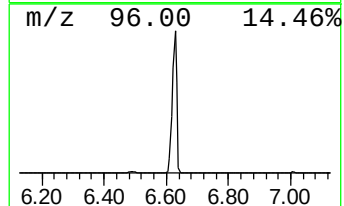
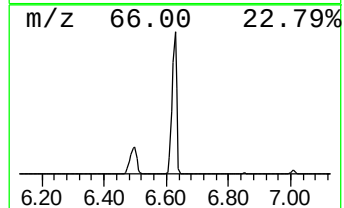
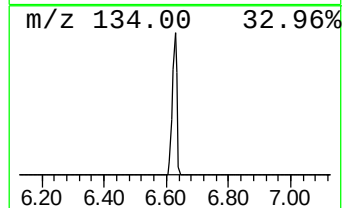
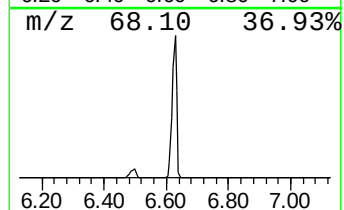
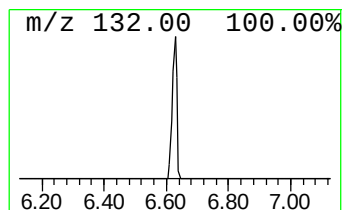
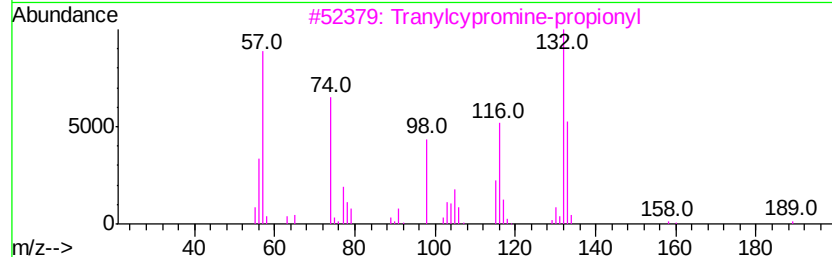
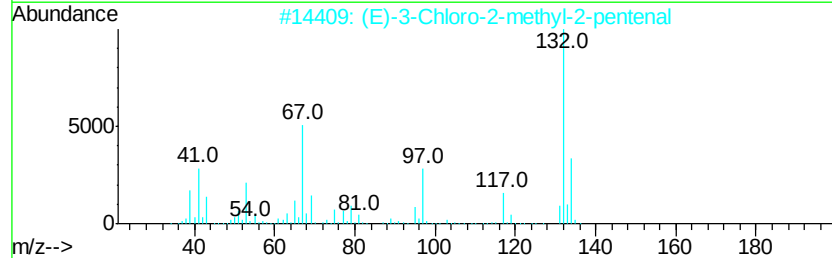
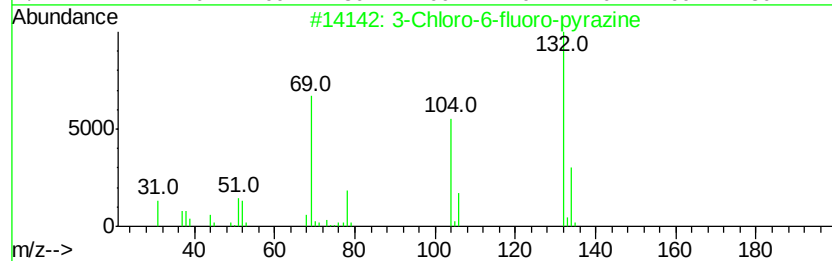
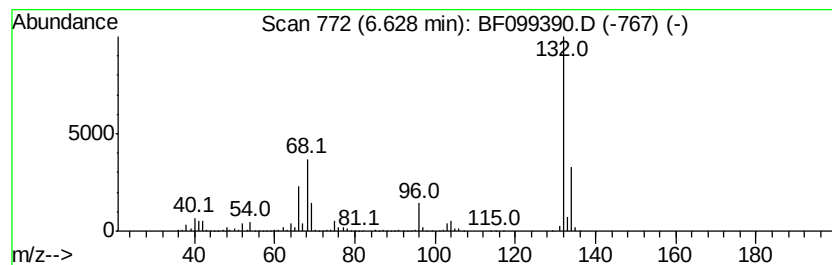
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Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	98.93 ng	3410530	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	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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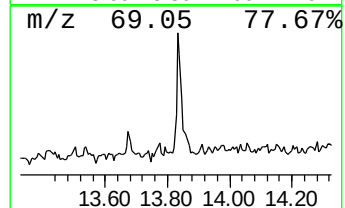
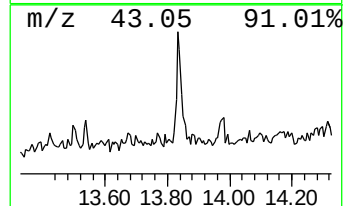
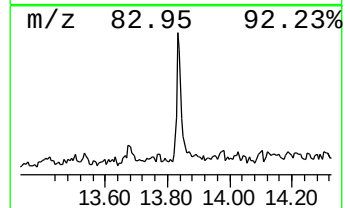
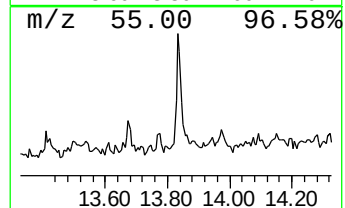
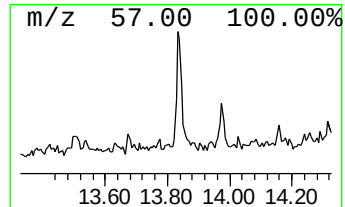
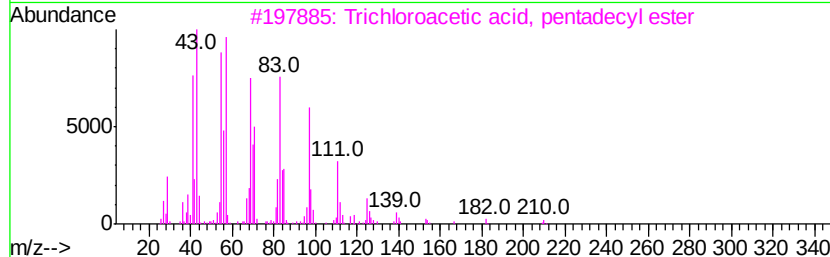
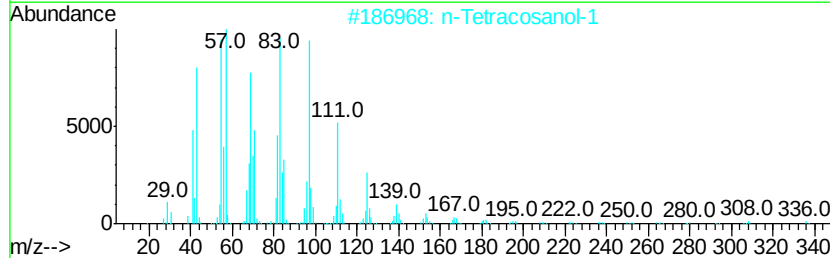
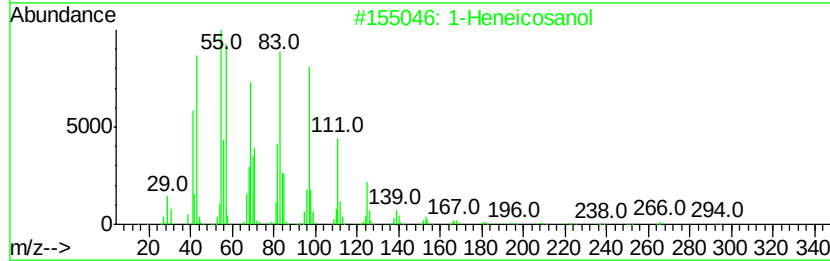
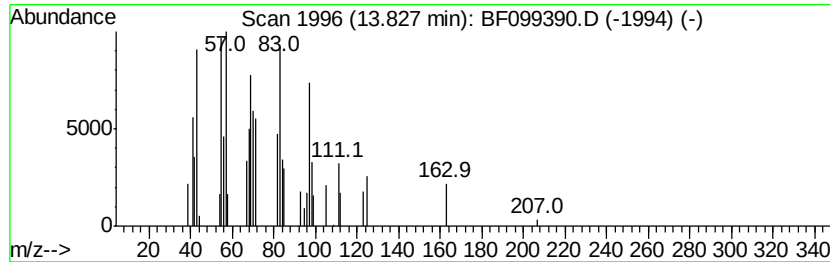
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Peak Number 5 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	2.50 ng	67611	Chrysene-d12	14.01

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	95
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	93
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	90
5		n-Heptadecanol-1	256	C17H36O	001454-85-9	90



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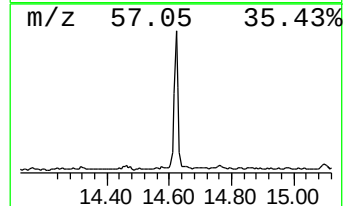
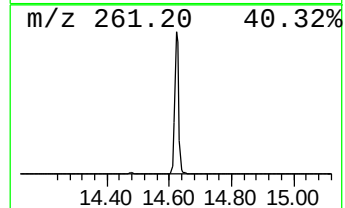
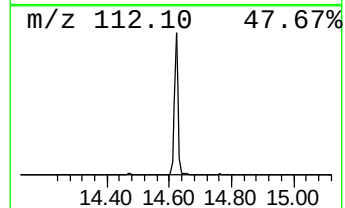
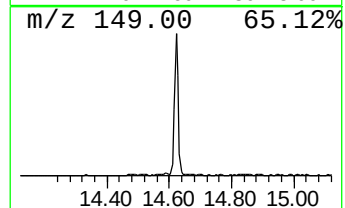
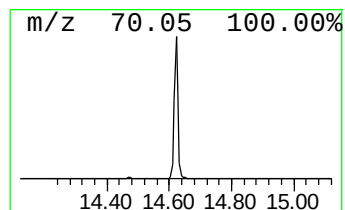
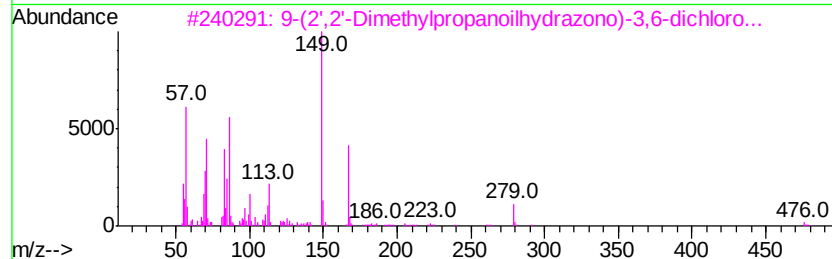
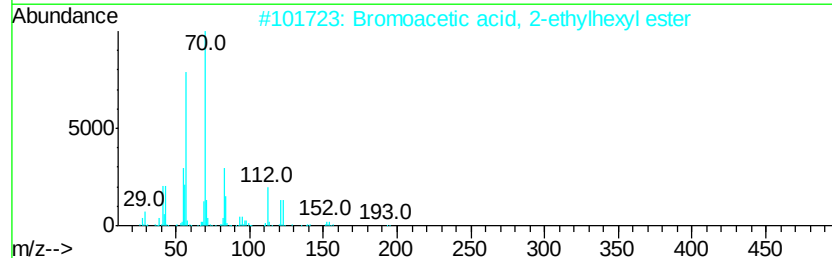
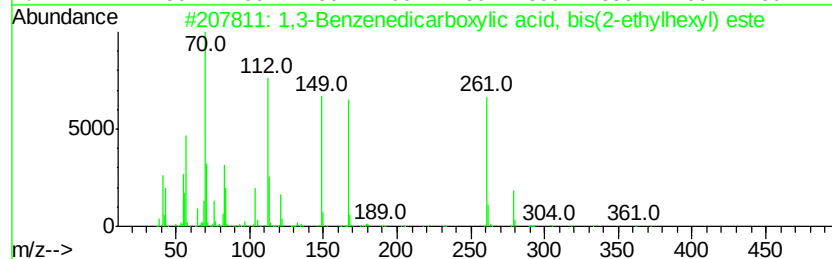
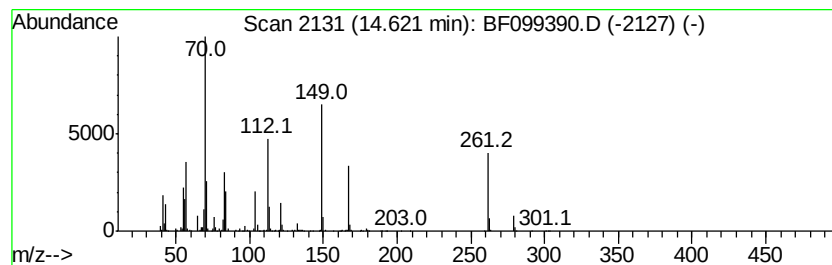
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Peak Number 6 1,3-Benzenedicarboxylic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	27.54 ng	745498	Chrysene-d12	14.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	52
2		Bromoacetic acid, 2-ethylhexyl e...	250	C10H19BrO2	068144-73-0	25
3		9-(2',2'-Dimethylpropanoilhydraz...	576	C30H42Cl2N4O3	1000111-04-6	18
4		Phthalic acid, 6-ethyloct-3-yl 2...	418	C26H42O4	1000315-53-8	14
5		Phthalic acid, 3-methylphenyl oc...	368	C23H28O4	1000314-86-2	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.18	2.8	ng	95215	1	6.85	689492	20.0
2-Pentanone, 4-hy...	5.09	18.8	ng	649104	1	6.85	689492	20.0
unknown6.63	6.63	98.9	ng	3410530	1	6.85	689492	20.0
1-Heneicosanol	13.83	2.5	ng	67611	5	14.01	541369	20.0
1,3-Benzenedicarb...	14.62	27.5	ng	745498	5	14.01	541369	20.0