LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100217\
Data File : BF099001.D
Acq On : 2 Oct 2017 15:59
Operator : SJ/JU
Sample : I5457-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-3_092717

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	2.216	17	22	34	rVB	369830	479384	11.69%	1.727%
2	5.128	513	517	529	rVB	235216	273054	6.66%	0.983%
3	5.522	579	584	587	rBV	1817088	1720852	41.98%	6.198%
4	6.522	749	754	757	rBV	1221571	1072067	26.15%	3.861%
5	6.669	774	779	782	rBV	2933501	2840706	69.29%	10.232%
6	6.898	814	818	822	rBV	904684	807497	19.70%	2.908%
7	7.057	841	845	848	rBV	2894809	2669052	65.11%	9.613%
8	7.463	909	914	917	rBV	2068073	2210259	53.92%	7.961%
9	8.181	1032	1036	1040	rBV	1194073	1061607	25.90%	3.824%
10	9.257	1213	1219	1223	rBV	3679437	4099499	100.00%	14.766%
11	9.645	1281	1285	1289	rBV	326593	280189	6.83%	1.009%
12	9.939	1330	1335	1339	rBV	1319511	1143672	27.90%	4.119%
13	10.133	1364	1368	1374	rBV	91871	83740	2.04%	0.302%
14	10.727	1464	1469	1473	rBV	1928236	2015845	49.17%	7.261%
15	10.822	1479	1485	1496	rVB	566765	859267	20.96%	3.095%
16	10.969	1506	1510	1517	rVB	75894	65584	1.60%	0.236%
17	11.427	1584	1588	1591	rBV	1343393	1111478	27.11%	4.003%
18	13.016	1853	1858	1861	rBV	3305595	3267109	79.70%	11.768%
19	13.892	2004	2007	2016	rBV	86514	101492	2.48%	0.366%
20	14.068	2033	2037	2040	rBV	909066	849763	20.73%	3.061%
21	15.557	2284	2290	2300	rBV	538372	706011	17.22%	2.543%
22	16.004	2361	2366	2372	rBV	29031	45685	1.11%	0.165%

Sum of corrected areas: 27763812

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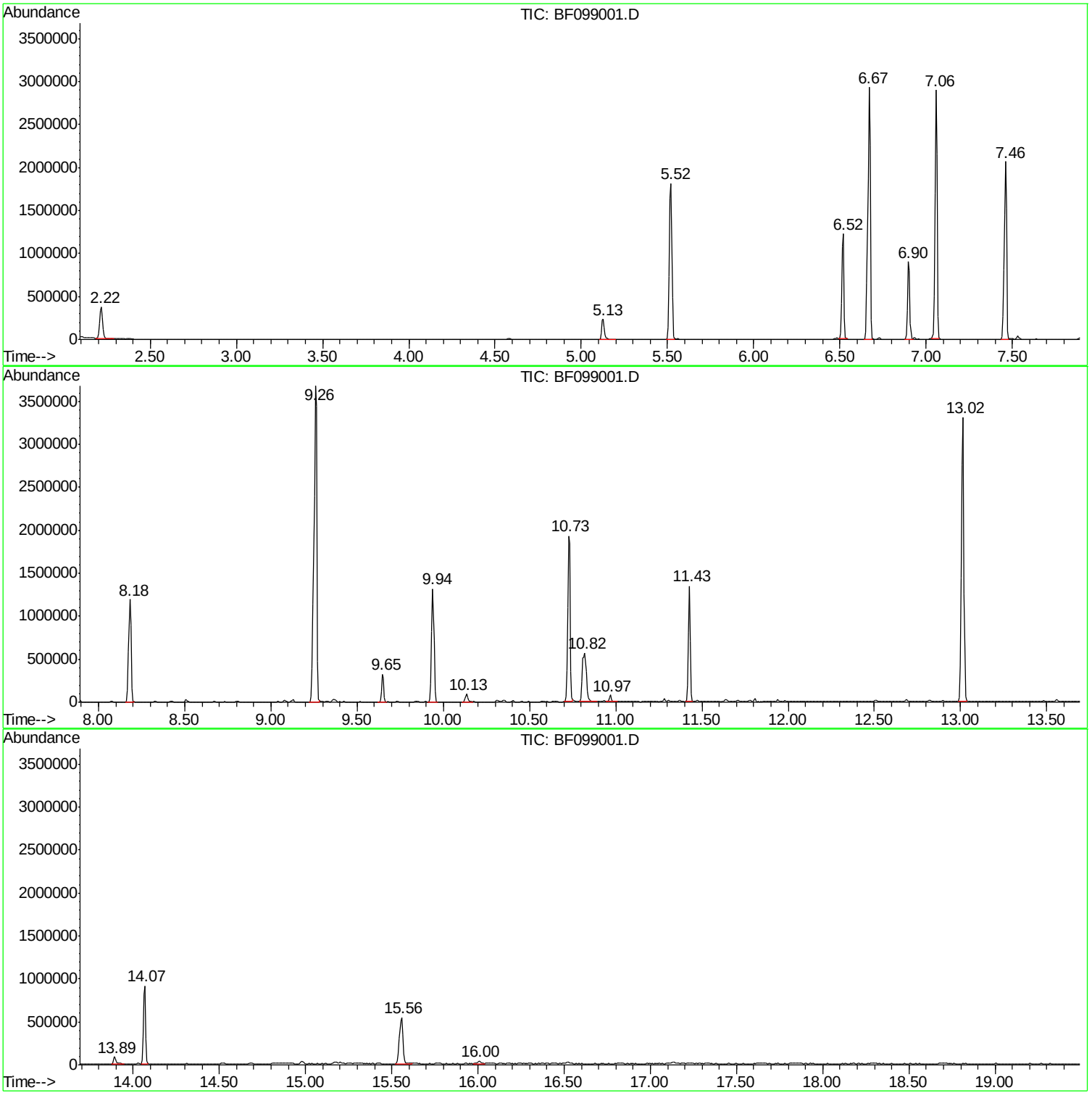
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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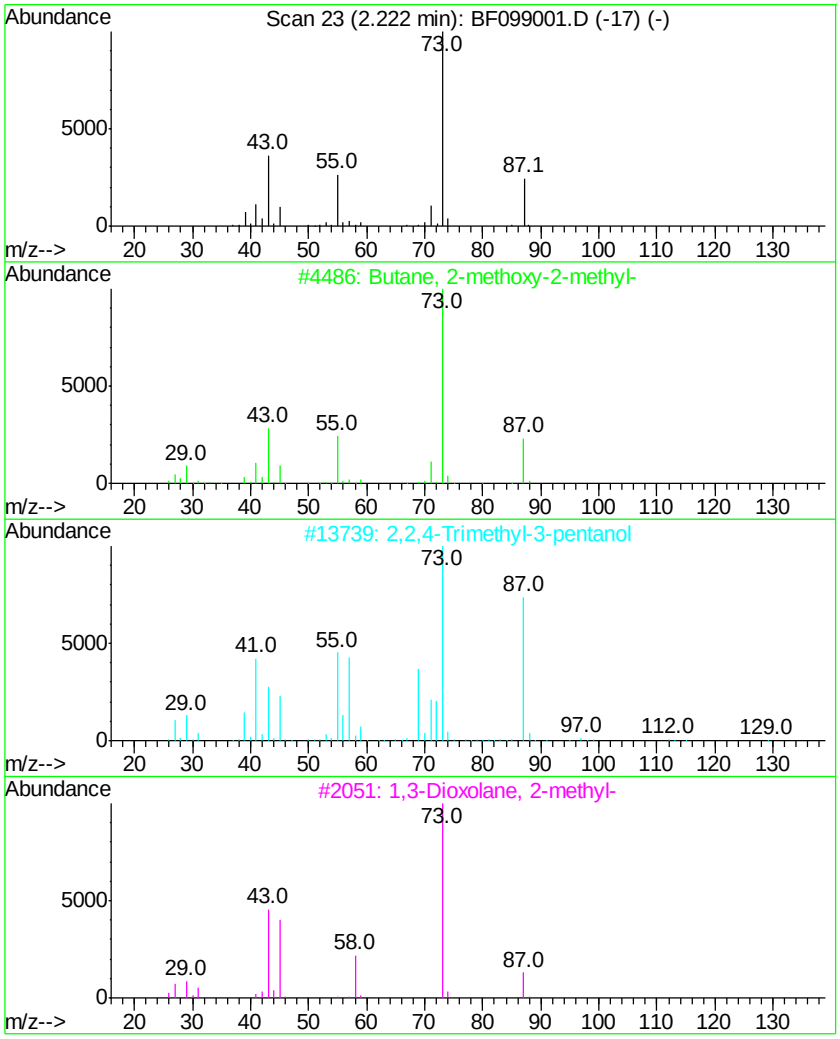
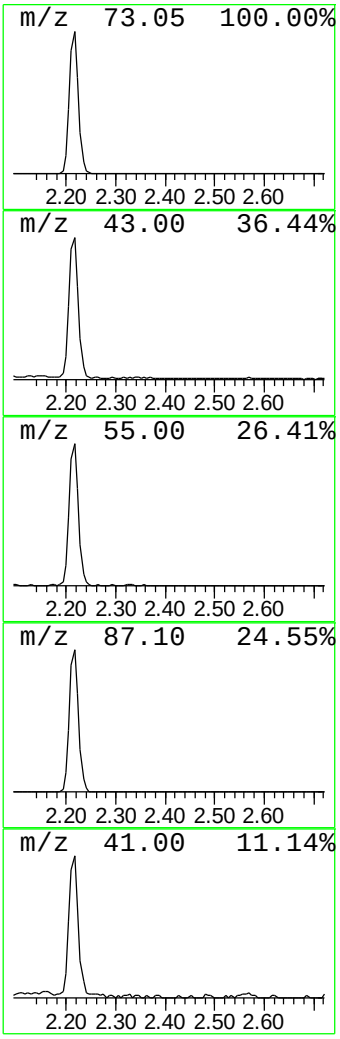
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	11.87 ng	479384	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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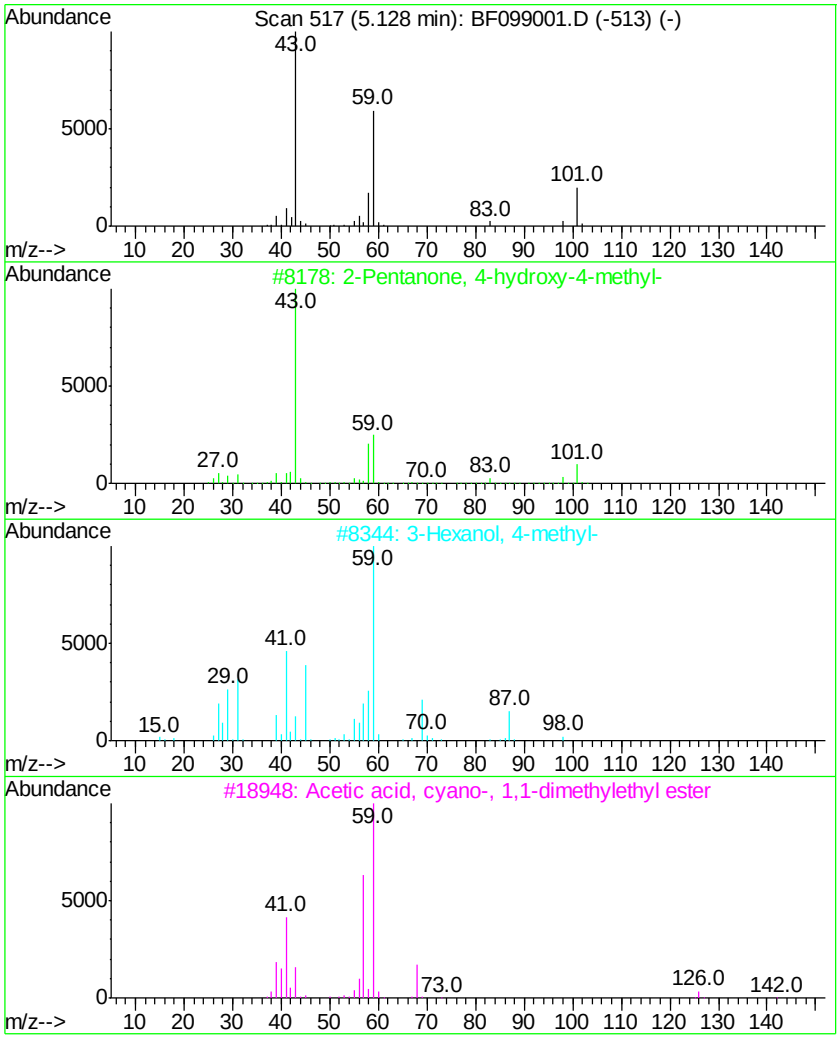
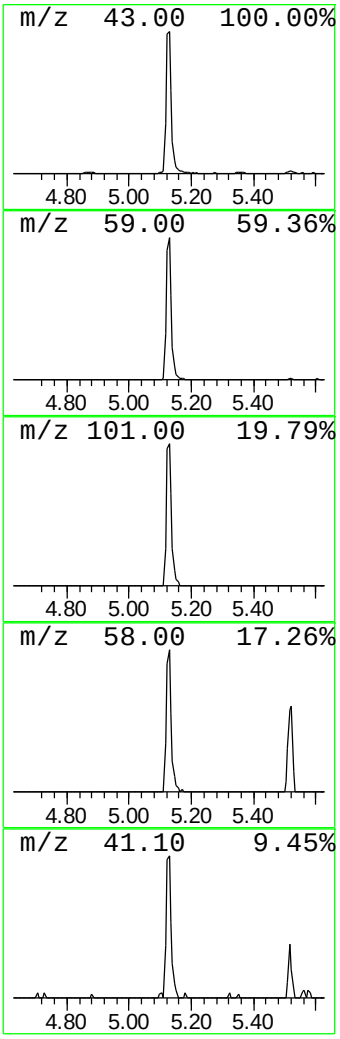
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	6.76 ng	273054	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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ClientSampleId : TW-3_092717

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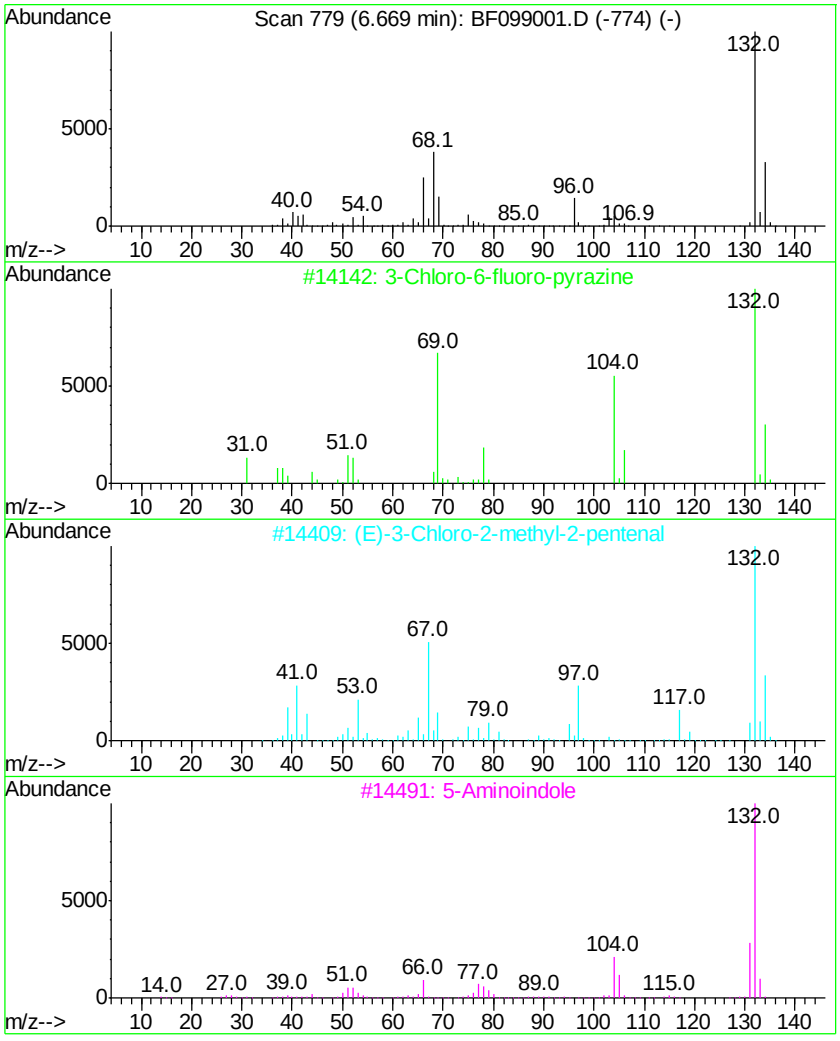
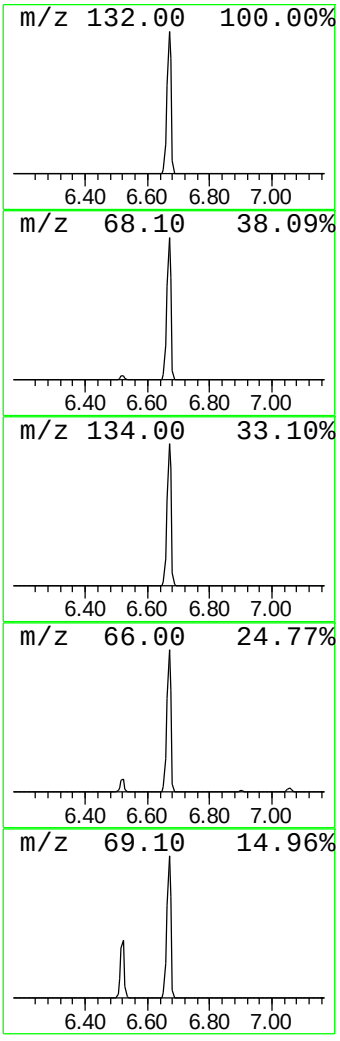
Peak Number 3 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	70.36 ng	2840710	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9





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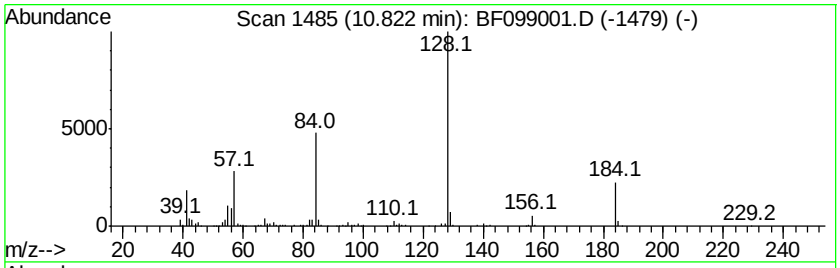
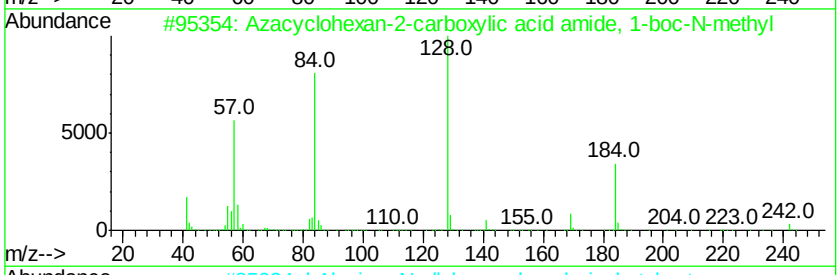
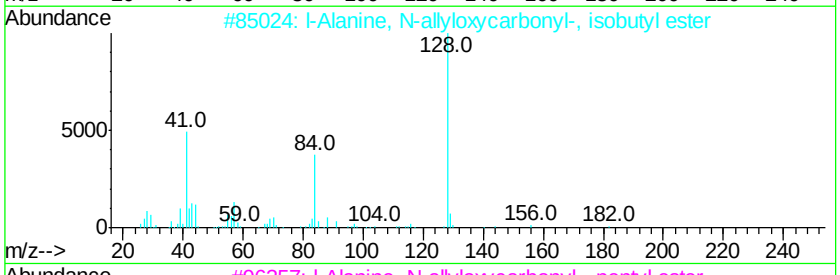
Peak Number 5 Azacyclohexan-2-carboxylic ... Concentration Rank 3

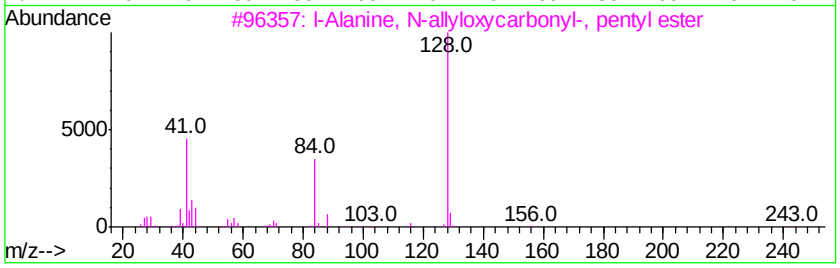
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	15.46 ng	859267	Phenanthrene-d10	11.43

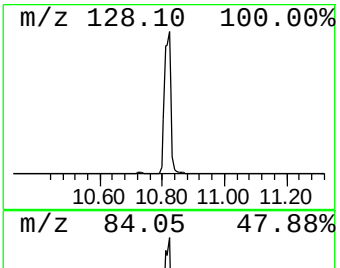
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Azacyclohexan-2-carboxylic acid ...	242	C12H22N2O3	184637-51-2	64
2	l-Alanine, N-allyloxycarbonyl-, ...	229	C11H19NO4	1000313-42-3	64
3	l-Alanine, N-allyloxycarbonyl-, ...	243	C12H21NO4	1000313-42-5	59
4	l-Alanine, N-allyloxycarbonyl-, ...	201	C9H15NO4	1000313-42-1	59
5	l-Alanine, N-allyloxycarbonyl-, ...	229	C11H19NO4	1000313-42-4	59

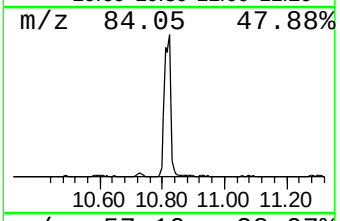


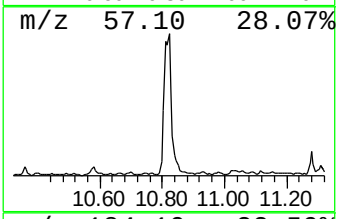


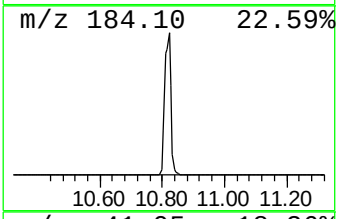


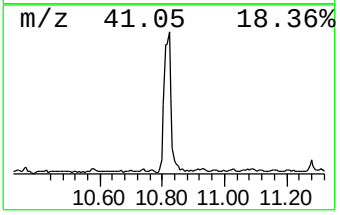












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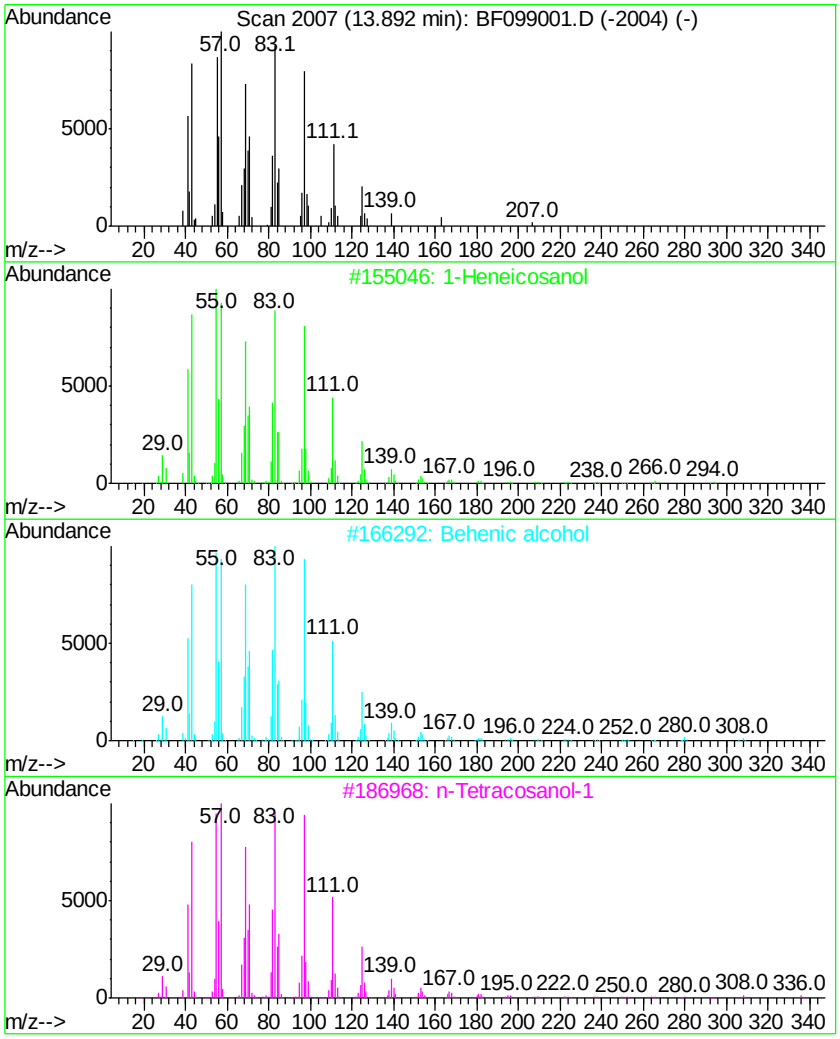
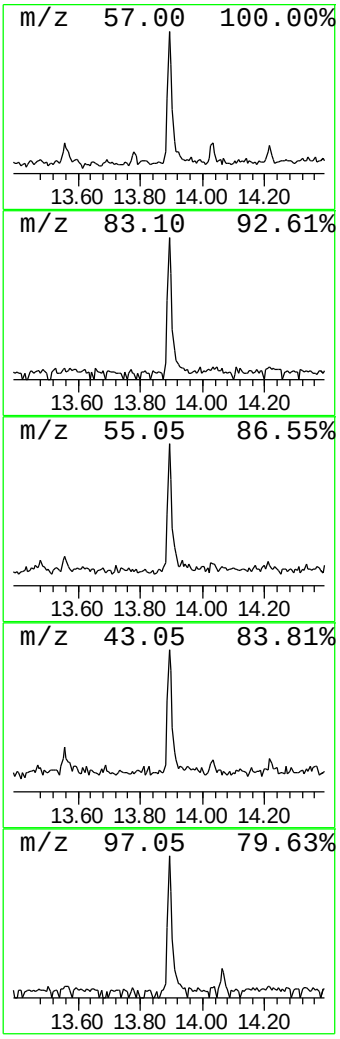
****

Peak Number 6 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	2.39 ng	101492	Chrysene-d12	14.07

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	93
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5	1-Heptacosanol	396	C27H56O	002004-39-9	91





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.22	11.9	ng	479384	1	6.90	807497	20.0
2-Pentanone, 4-hy...	5.13	6.8	ng	273054	1	6.90	807497	20.0
unknown6.67	6.67	70.4	ng	2840710	1	6.90	807497	20.0
Azacyclohexan-2-c...	10.82	15.5	ng	859267	4	11.43	1111480	20.0
1-Heneicosanol	13.89	2.4	ng	101492	5	14.07	849763	20.0