

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
 Data File : BF088946.D
 Acq On : 13 Jul 2016 5:50
 Operator : UM/SJ
 Sample : H3987-04
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-WALL-S-070816

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-BF063016.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	1.667	6	7	16	rVB	54637	96503	6.05%	0.723%
2	1.793	16	18	26	rVV	335587	467626	29.32%	3.504%
3	1.895	26	27	41	rVB	36557	65354	4.10%	0.490%
4	4.856	283	286	291	rBB	224899	302950	19.00%	2.270%
5	5.301	322	325	327	rBV	1458921	1404490	88.06%	10.524%
6	5.702	358	360	362	rBB	24072	20522	1.29%	0.154%
7	6.353	414	417	419	rBV	1425470	1459576	91.52%	10.936%
8	6.467	425	427	430	rBB	1140510	1564631	98.11%	11.724%
9	6.707	445	448	450	rBV	260842	347498	21.79%	2.604%
10	6.856	459	461	464	rVB	1103267	1068360	66.99%	8.005%
11	7.267	494	497	500	rBB	888386	866520	54.33%	6.493%
12	7.987	557	560	562	rBV	574014	472483	29.63%	3.540%
13	9.073	652	655	657	rBV	1238985	1594839	100.00%	11.950%
14	9.462	687	689	691	rVB	349939	270770	16.98%	2.029%
15	9.553	694	697	701	rBB	8239	19593	1.23%	0.147%
16	9.736	711	713	715	rBB	529983	445269	27.92%	3.336%
17	10.525	779	782	784	rBV	785600	766086	48.04%	5.740%
18	10.651	792	793	798	rVB	19427	24212	1.52%	0.181%
19	10.971	819	821	824	rVB	22592	32704	2.05%	0.245%
20	11.096	830	832	834	rBV	16981	18808	1.18%	0.141%
21	11.211	840	842	844	rVB	404367	344779	21.62%	2.583%
22	12.799	978	981	983	rBV	1075566	1011997	63.45%	7.583%
23	13.702	1057	1060	1066	rBV	43235	51731	3.24%	0.388%
24	13.839	1069	1072	1074	rBV	302210	343565	21.54%	2.574%
25	15.211	1189	1192	1194	rBV	231966	285228	17.88%	2.137%

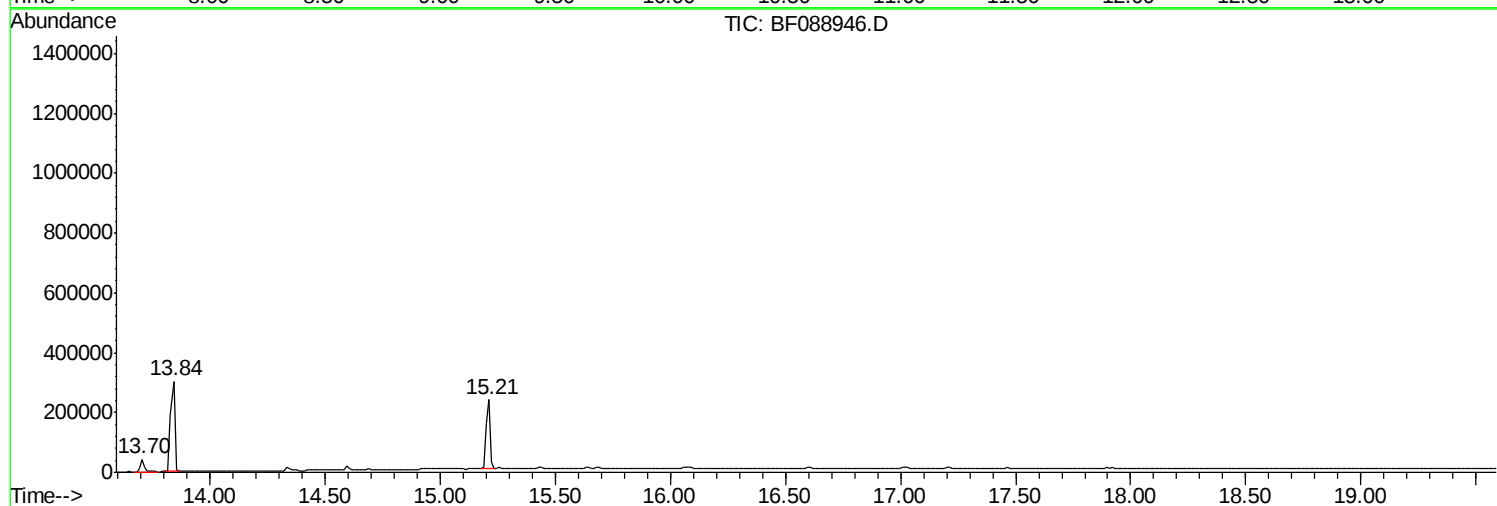
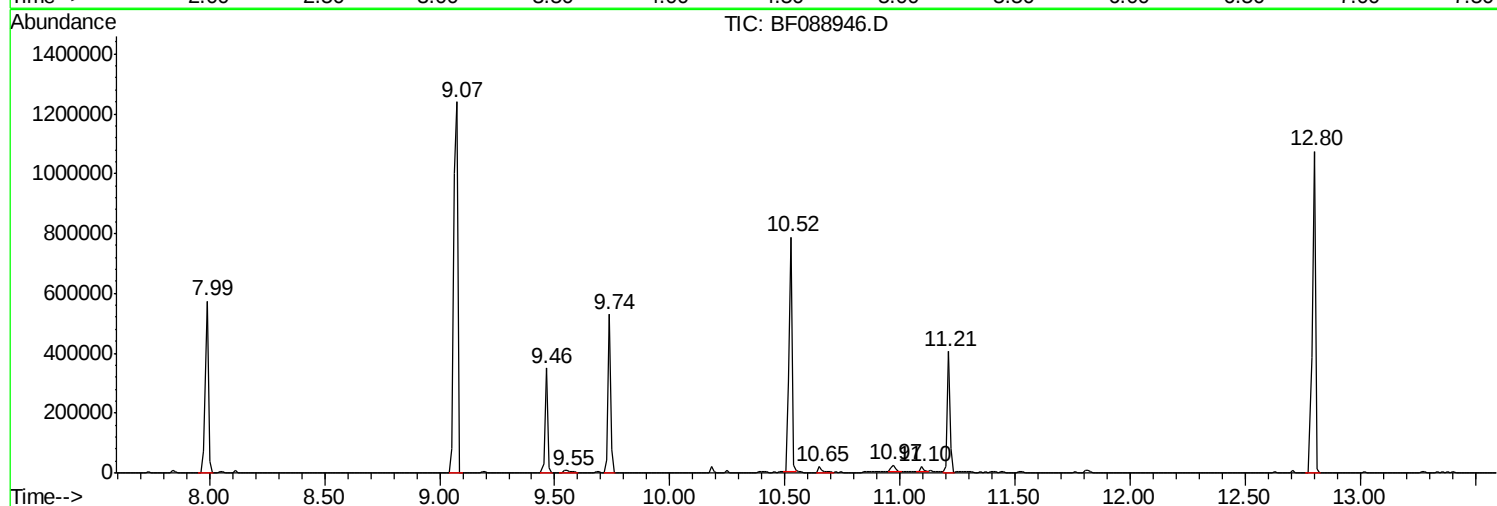
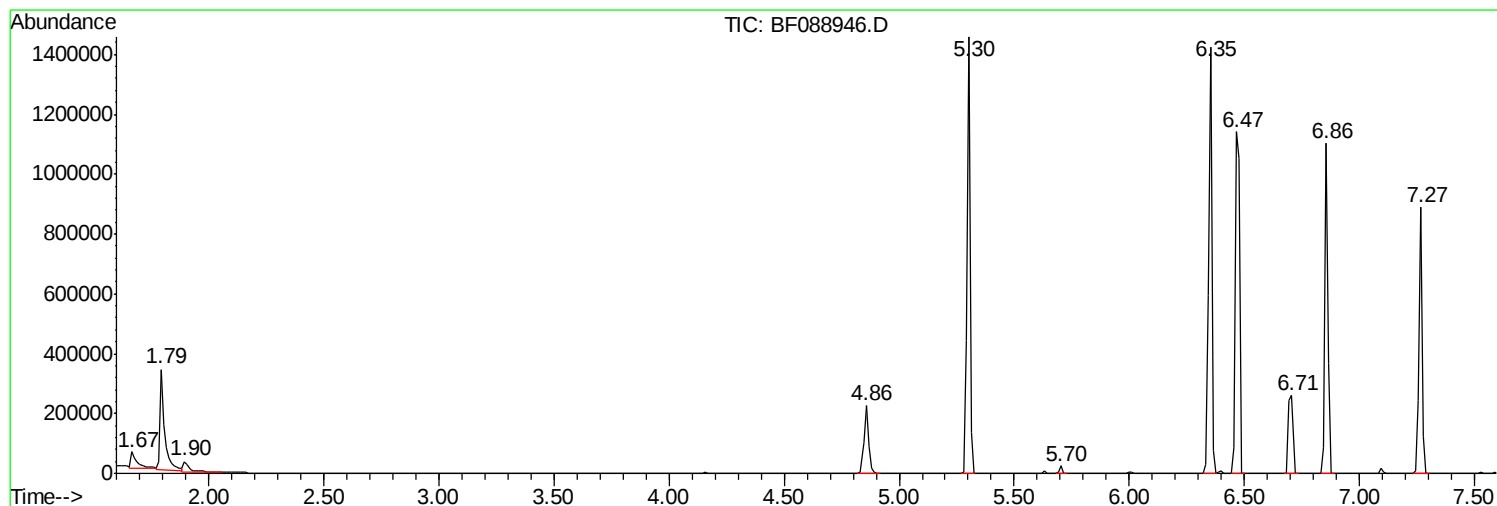
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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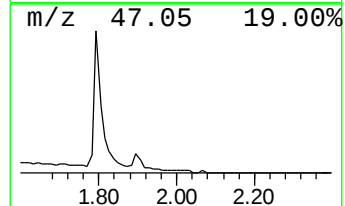
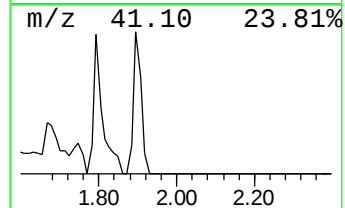
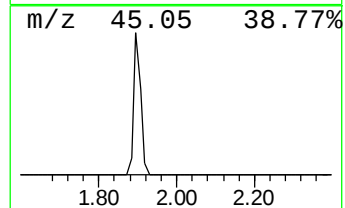
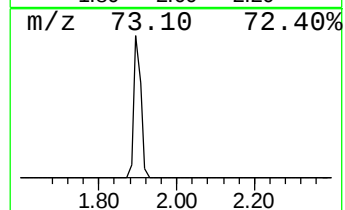
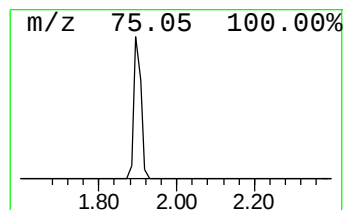
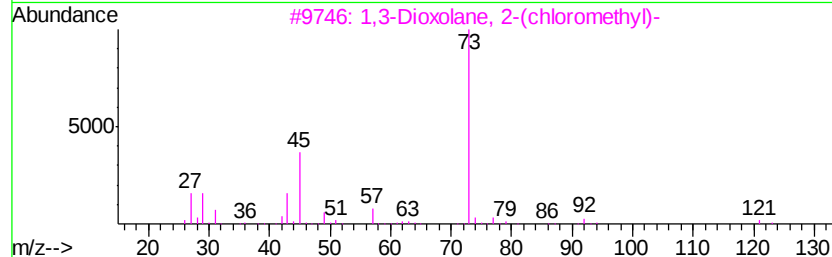
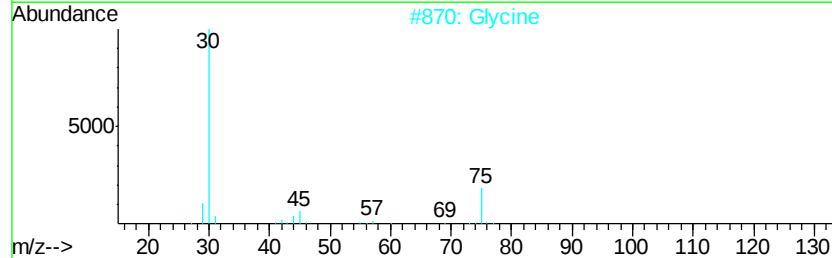
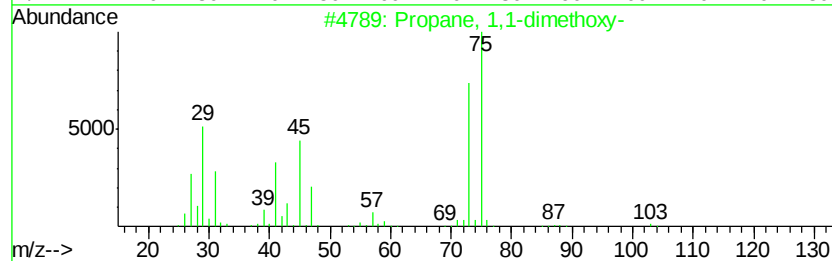
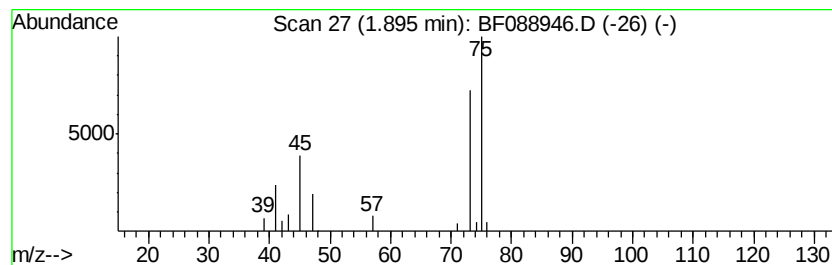
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.90	3.76 ng	65354	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2		Glycine	75	C2H5NO2	000056-40-6	9
3		1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	9
4		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9
5		1-Propene-1-thiol	74	C3H6S	000925-89-3	7



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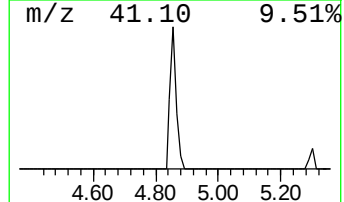
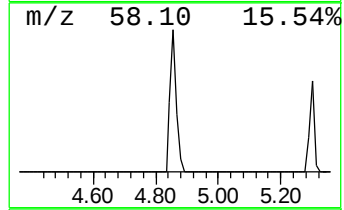
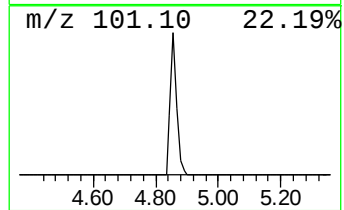
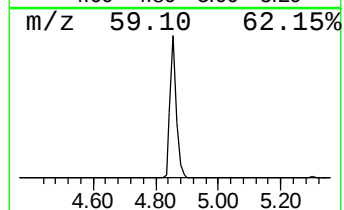
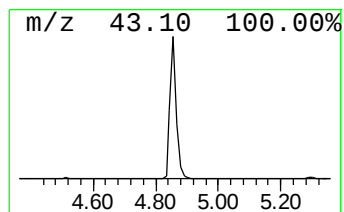
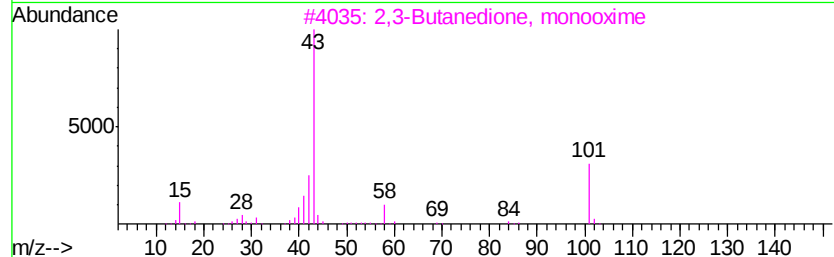
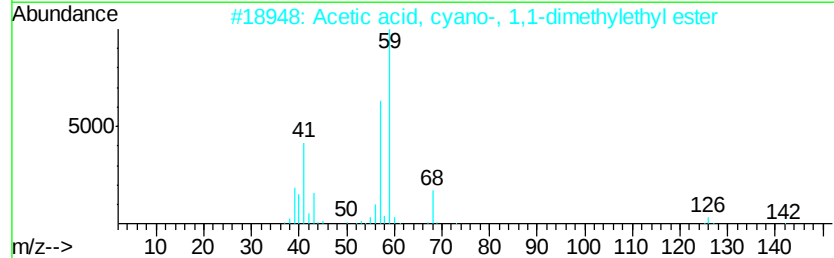
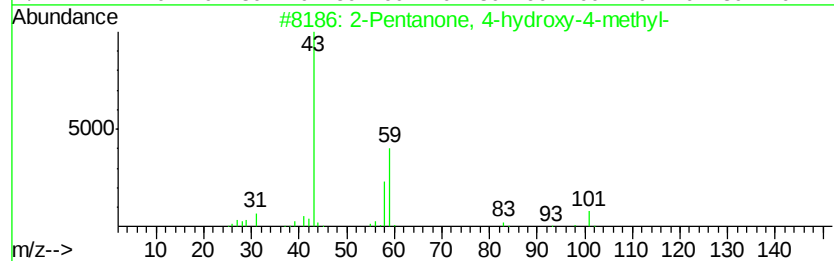
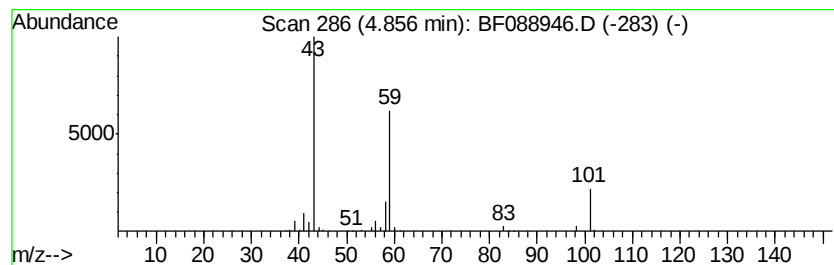
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	17.44 ng	302950	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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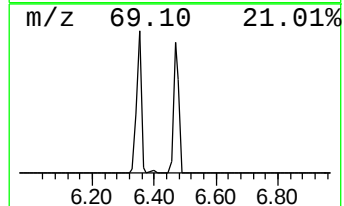
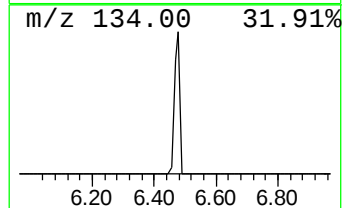
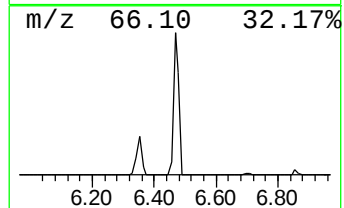
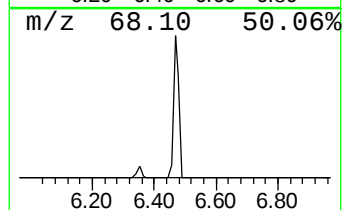
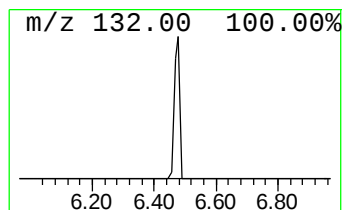
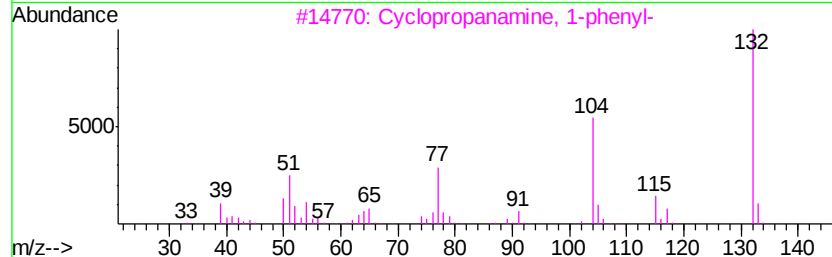
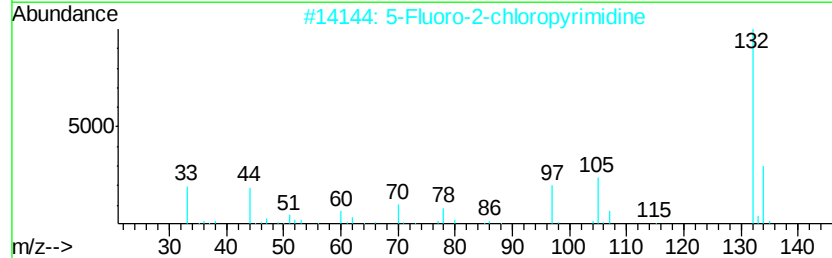
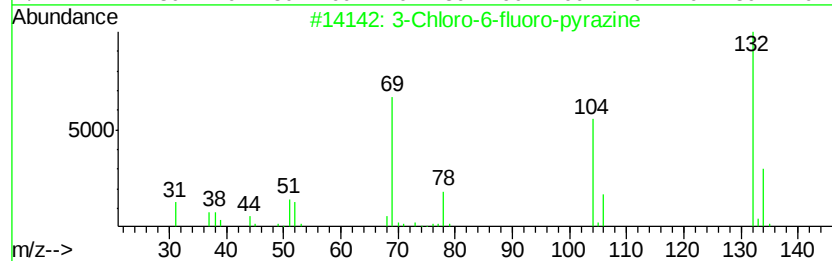
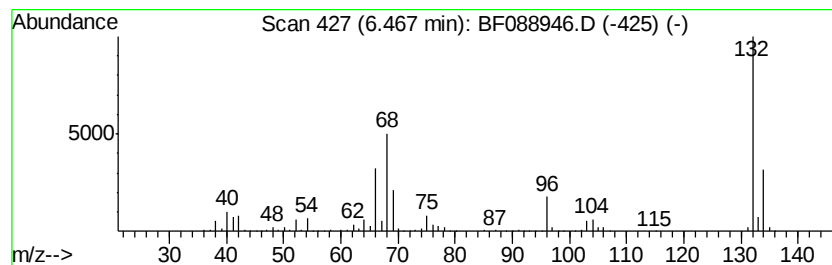
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Peak Number 5 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	90.05 ng	1564630	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10



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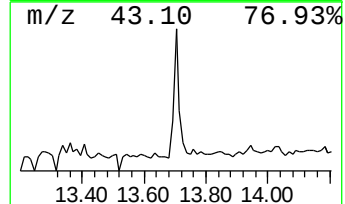
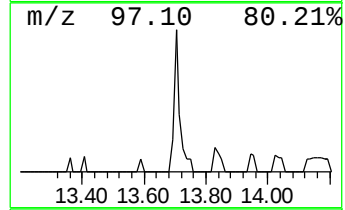
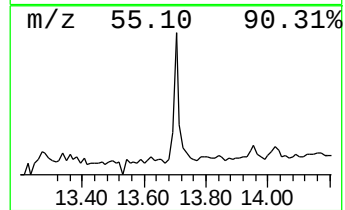
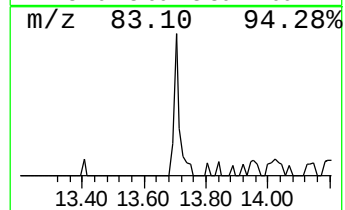
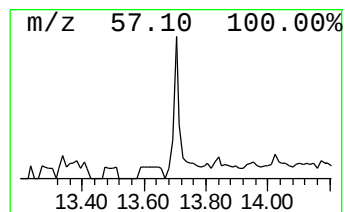
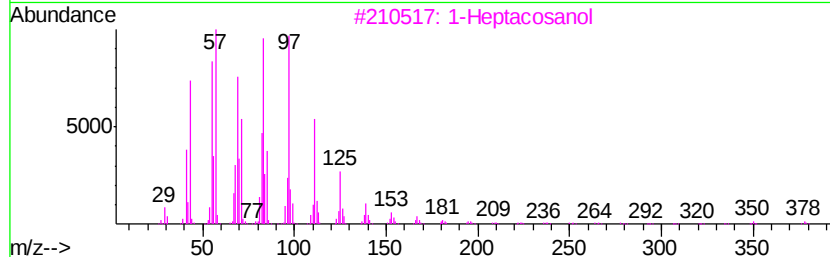
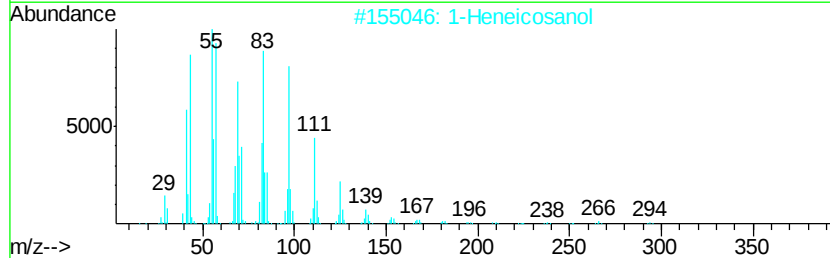
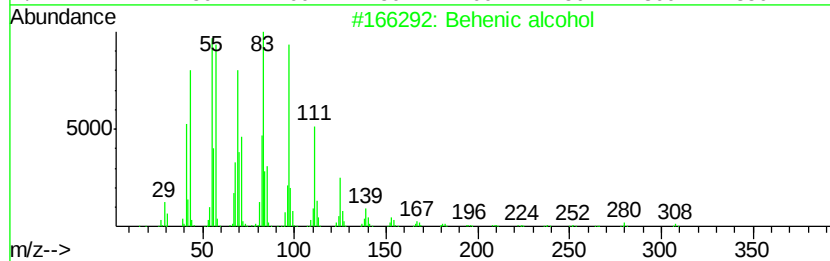
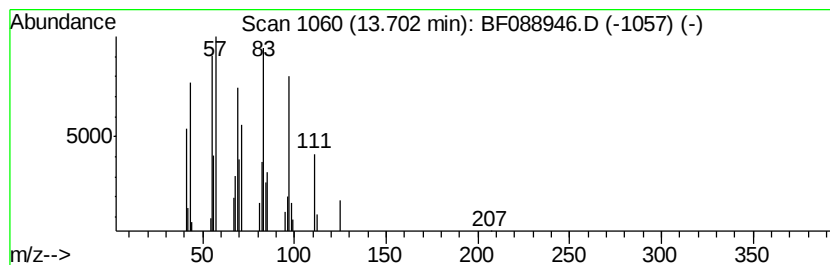
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Peak Number 7 Behenic alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	3.01 ng	51731	Chrysene-d12	13.84

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenic alcohol	326	C22H46O	000661-19-8	94
2		1-Heneicosanol	312	C21H44O	015594-90-8	94
3		1-Heptacosanol	396	C27H56O	002004-39-9	94
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	91
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	1.90	3.8	ng	65354	1	6.71	347498	20.0
2-Pentanone, 4-hy...	4.86	17.4	ng	302950	1	6.71	347498	20.0
unknown6.47	6.47	90.0	ng	1564630	1	6.71	347498	20.0
Behenic alcohol	13.70	3.0	ng	51731	5	13.84	343565	20.0