

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092717\
 Data File : BF098858.D
 Acq On : 27 Sep 2017 12:53
 Operator : SJ/JU
 Sample : I5396-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PAMT-COMP-A

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	2.228	21	24	44	rVB4	135167	302728	7.96%	0.914%
2	5.146	516	520	531	rVB	550845	760457	20.00%	2.297%
3	5.540	581	587	590	rBV	3535577	3630251	95.46%	10.966%
4	6.540	751	757	760	rBV	3141029	3803047	100.00%	11.488%
5	6.687	777	782	785	rBV	3705411	3733855	98.18%	11.279%
6	6.916	817	821	824	rVB	995828	856282	22.52%	2.587%
7	7.069	843	847	851	rBV	2827167	2515141	66.13%	7.597%
8	7.475	911	916	919	rBV	2223898	2259610	59.42%	6.825%
9	7.545	924	928	931	rVB	47528	41833	1.10%	0.126%
10	8.192	1034	1038	1042	rBV	1339950	1174802	30.89%	3.549%
11	9.269	1216	1221	1224	rBV	3890946	3523470	92.65%	10.643%
12	9.657	1283	1287	1291	rBV	724027	623572	16.40%	1.884%
13	9.951	1333	1337	1341	rBV	1565873	1296382	34.09%	3.916%
14	10.375	1406	1409	1412	rVB	61660	53774	1.41%	0.162%
15	10.739	1466	1471	1474	rBV	2227894	2225404	58.52%	6.722%
16	10.845	1486	1489	1494	rBV	86959	78389	2.06%	0.237%
17	11.439	1586	1590	1593	rBV	1515751	1252261	32.93%	3.783%
18	13.022	1854	1859	1862	rBV	3134038	2991637	78.66%	9.037%
19	13.904	2005	2009	2017	rBV	299083	284222	7.47%	0.859%
20	14.074	2034	2038	2041	rBV	1016776	819497	21.55%	2.475%
21	14.539	2112	2117	2123	rBV4	24357	40018	1.05%	0.121%
22	14.692	2140	2143	2147	rBV	59383	49062	1.29%	0.148%
23	14.927	2180	2183	2188	rVB	56548	58489	1.54%	0.177%
24	15.563	2286	2291	2300	rVB	571116	731352	19.23%	2.209%

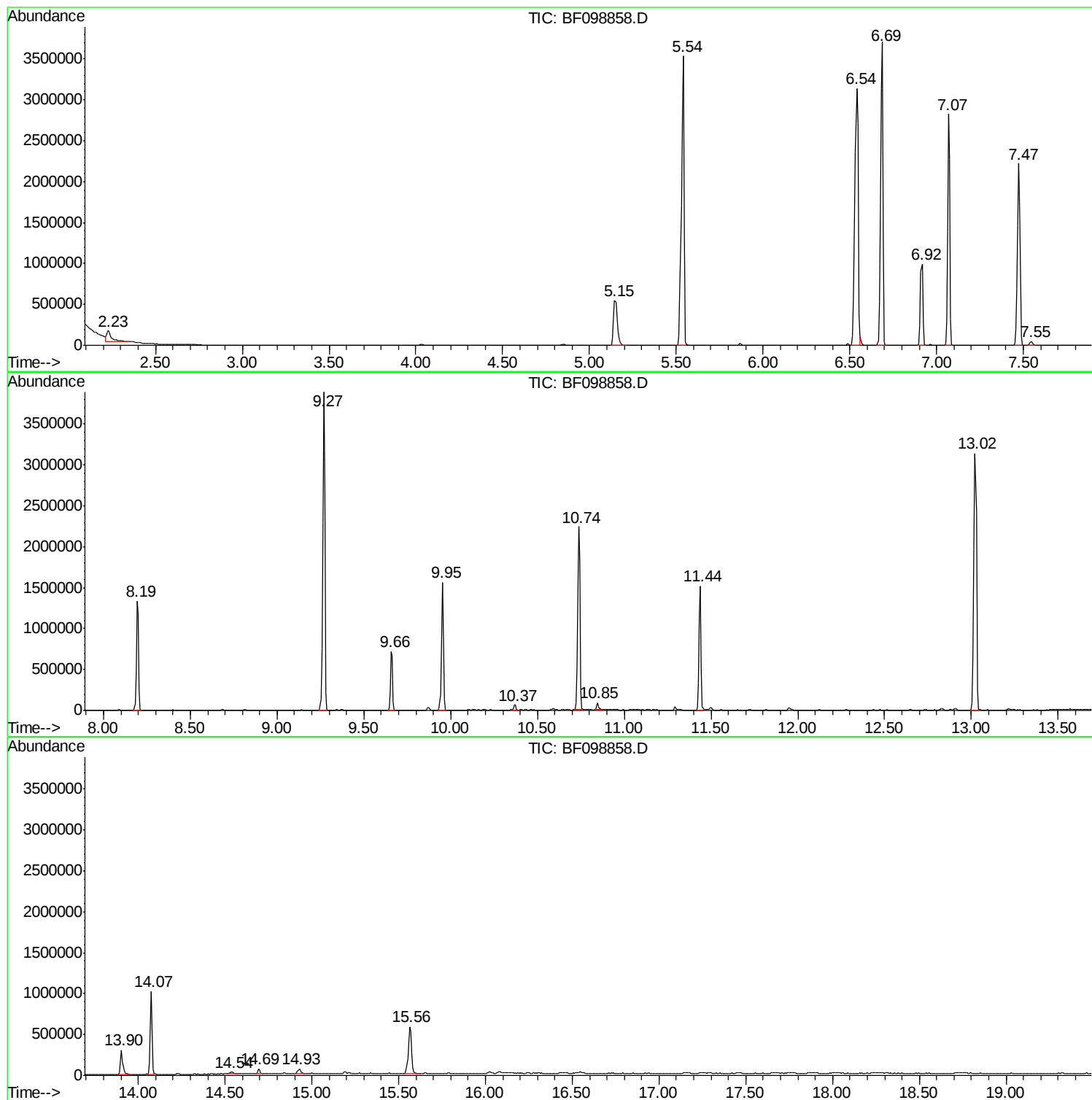
Sum of corrected areas: 33105535

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



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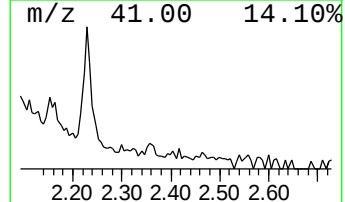
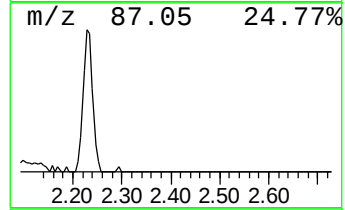
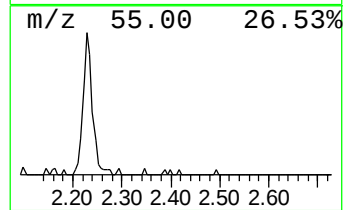
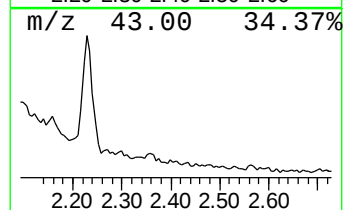
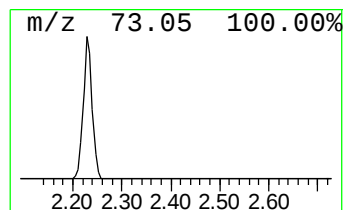
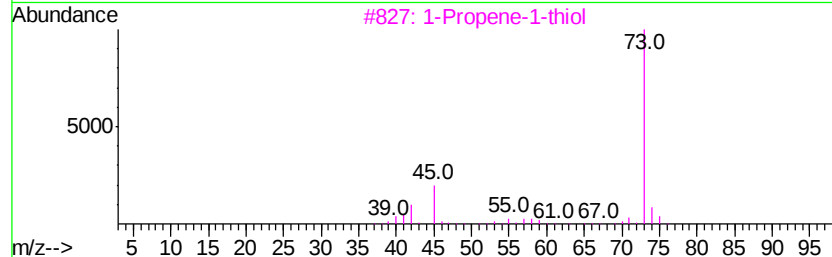
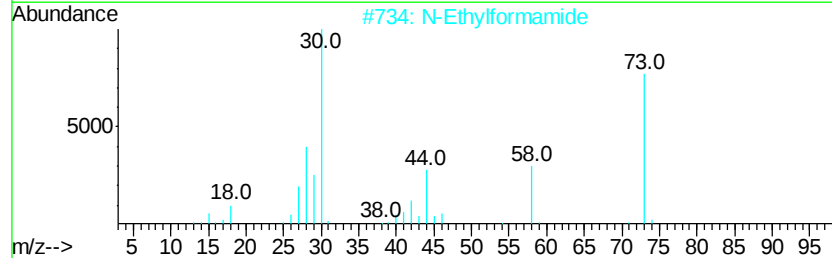
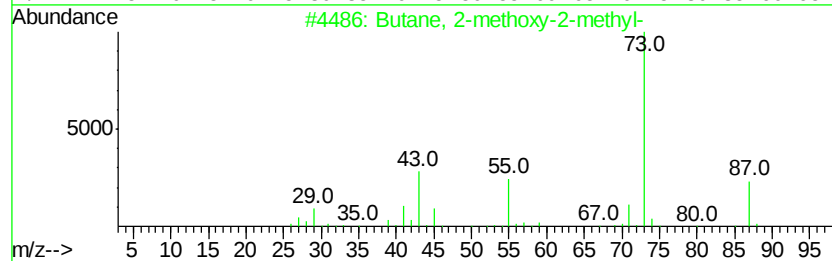
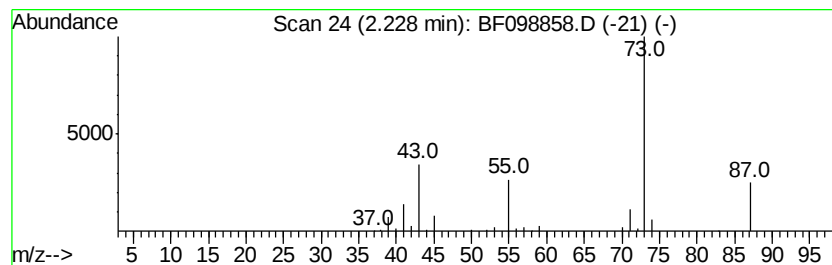
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	7.07 ng	302728	1,4-Dichlorobenzene-d4	6.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			N-Ethylformamide	73	C3H7NO	000627-45-2	9
3			1-Propene-1-thiol	74	C3H6S	000925-89-3	9
4			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	9
5			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	9



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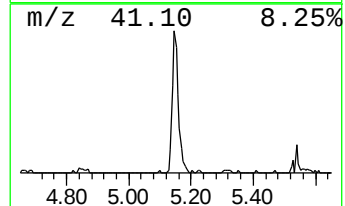
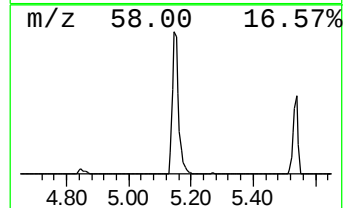
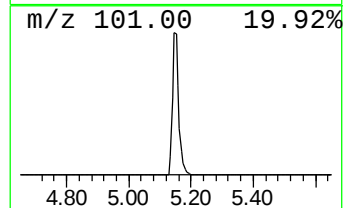
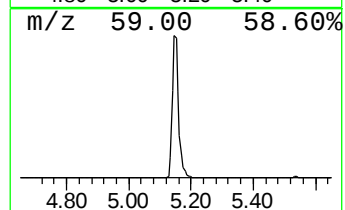
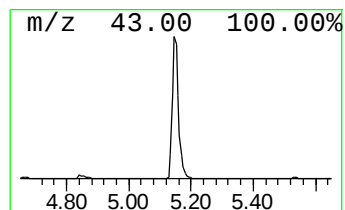
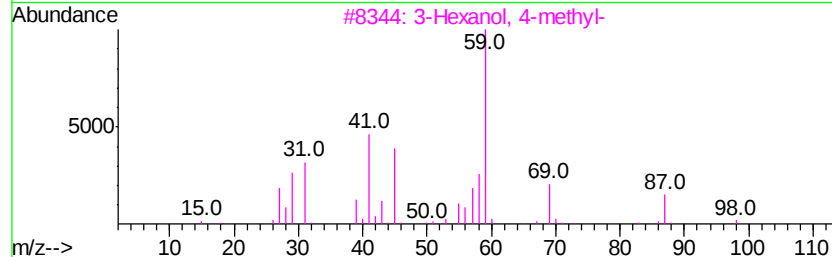
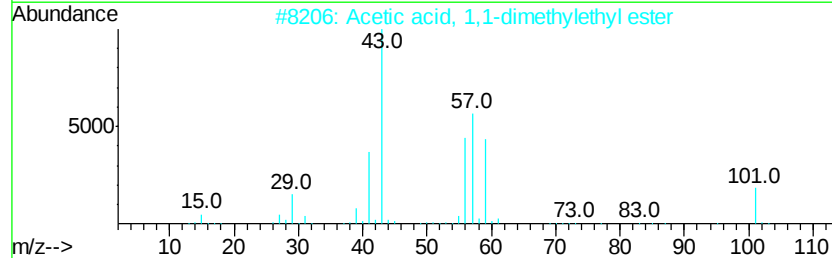
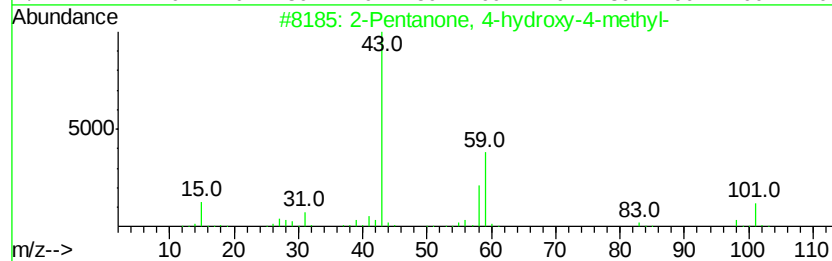
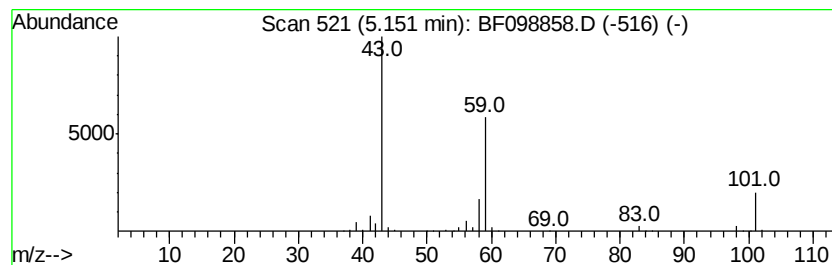
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	17.76 ng	760457	1,4-Dichlorobenzene-d4	6.92

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5		3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	9



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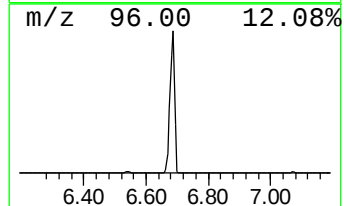
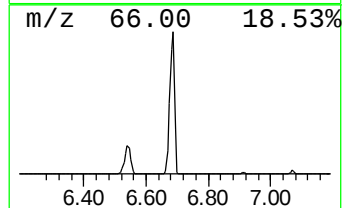
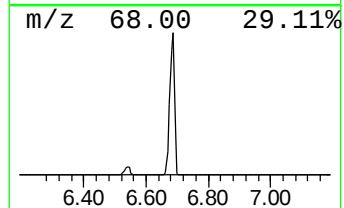
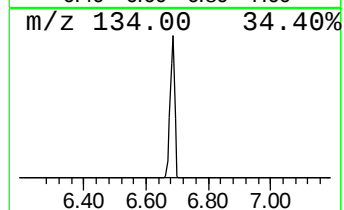
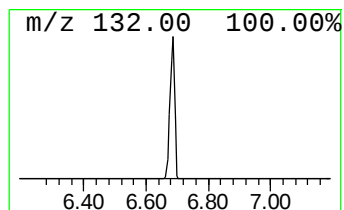
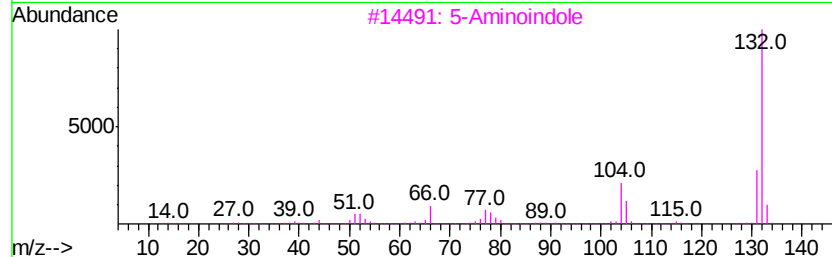
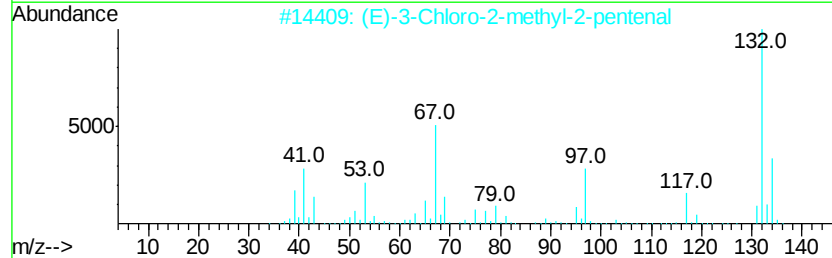
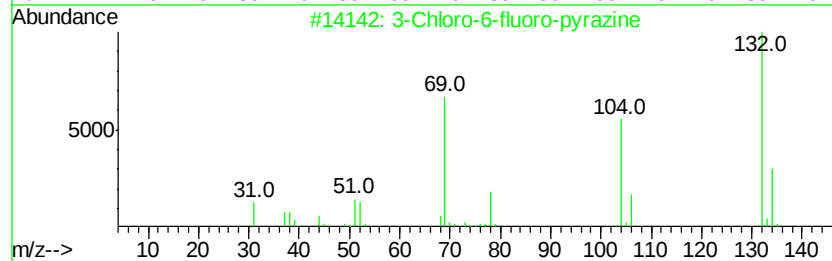
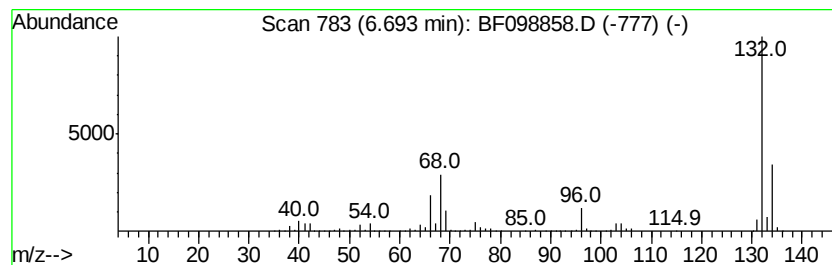
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Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	87.21 ng	3733860	1,4-Dichlorobenzene-d4	6.92

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		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9



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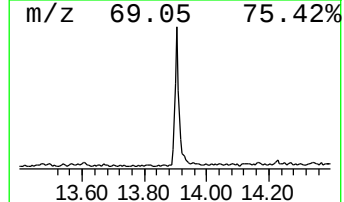
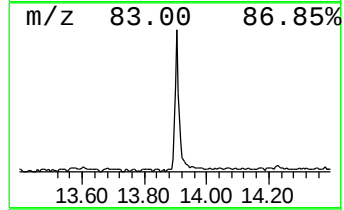
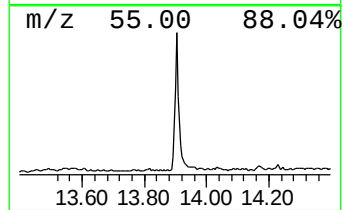
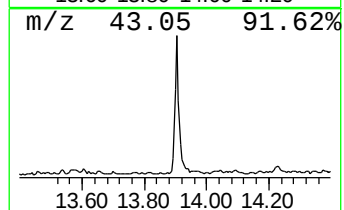
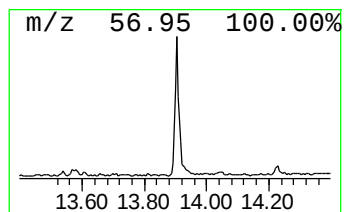
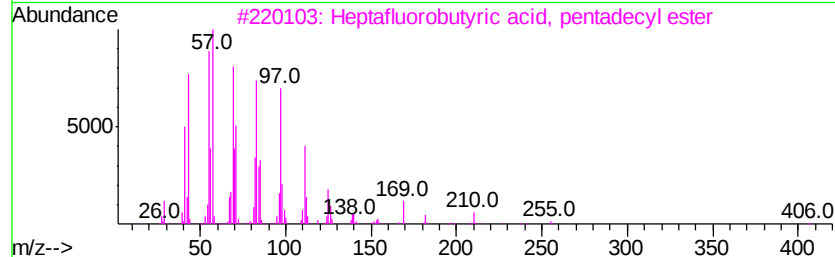
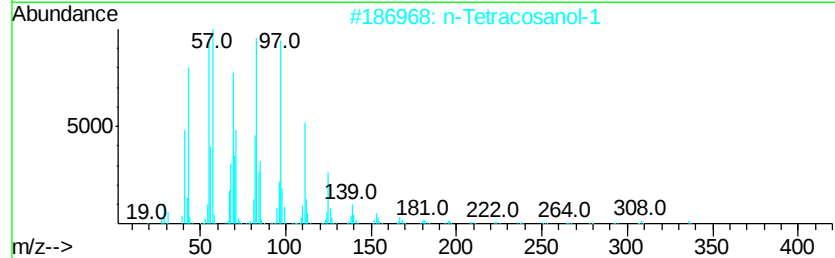
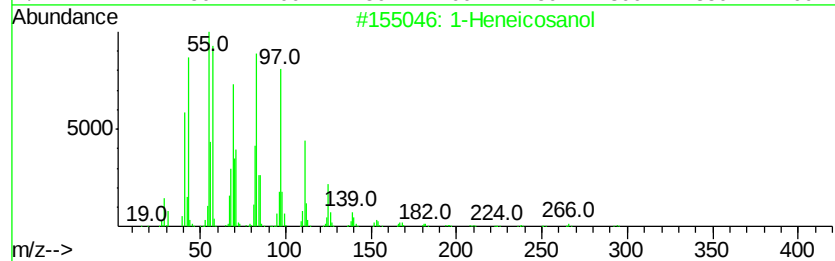
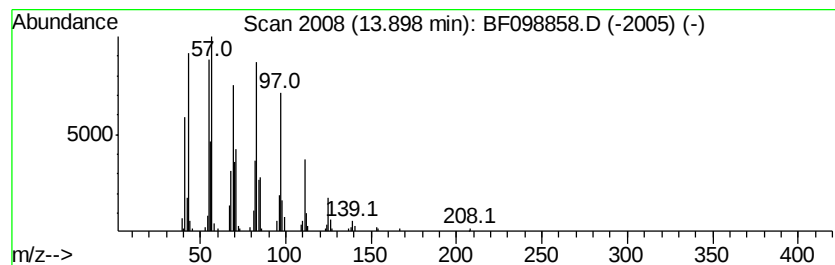
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Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.90	6.94 ng	284222	Chrysene-d12		14.07
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	94
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5	Behenic alcohol	326	C22H46O	000661-19-8	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.23	7.1	ng	302728	1	6.92	856282	20.0
2-Pentanone, 4-hy...	5.15	17.8	ng	760457	1	6.92	856282	20.0
unknown6.69	6.69	87.2	ng	3733860	1	6.92	856282	20.0
1-Heneicosanol	13.90	6.9	ng	284222	5	14.07	819497	20.0