

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
 Data File : BF102259.D
 Acq On : 20 Jan 2018 12:16
 Operator : SJ/JU
 Sample : J1115-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-31-2.5-3.0

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-BF010918.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	4.922	477	482	490	rBV	169249	238505	7.38%	0.893%
2	5.334	547	552	555	rBV	3075272	3101131	95.99%	11.612%
3	6.363	721	727	731	rBV	2952814	3147009	97.41%	11.783%
4	6.492	744	749	752	rBV	3386708	3139757	97.19%	11.756%
5	6.716	784	787	791	rBV	854825	773430	23.94%	2.896%
6	6.875	810	814	817	rBV	2847934	2450554	75.85%	9.176%
7	7.287	879	884	887	rBV	2113524	1939336	60.03%	7.261%
8	8.004	1001	1006	1009	rBV	1112640	991301	30.68%	3.712%
9	9.081	1184	1189	1192	rBV	3585724	3230685	100.00%	12.097%
10	9.475	1252	1256	1259	rBV	301783	273568	8.47%	1.024%
11	9.686	1288	1292	1295	rVB	146835	109453	3.39%	0.410%
12	9.751	1300	1303	1307	rVB	1090776	963755	29.83%	3.609%
13	10.186	1373	1377	1380	rVB	151295	126403	3.91%	0.473%
14	10.404	1408	1414	1416	rBV	33962	44716	1.38%	0.167%
15	10.545	1431	1438	1441	rBV	1672478	1507065	46.65%	5.643%
16	10.657	1454	1457	1466	rBV	113415	110076	3.41%	0.412%
17	11.239	1552	1556	1559	rBV	883454	766282	23.72%	2.869%
18	12.821	1821	1825	1828	rBV	2326652	2093467	64.80%	7.839%
19	13.716	1973	1977	1980	rBV	132596	134813	4.17%	0.505%
20	13.868	1999	2003	2007	rBV	735859	732281	22.67%	2.742%
21	14.351	2081	2085	2089	rBV3	44476	53654	1.66%	0.201%
22	15.292	2240	2245	2257	rBV	570744	742536	22.98%	2.780%
23	16.204	2396	2400	2405	rBV5	24001	37444	1.16%	0.140%

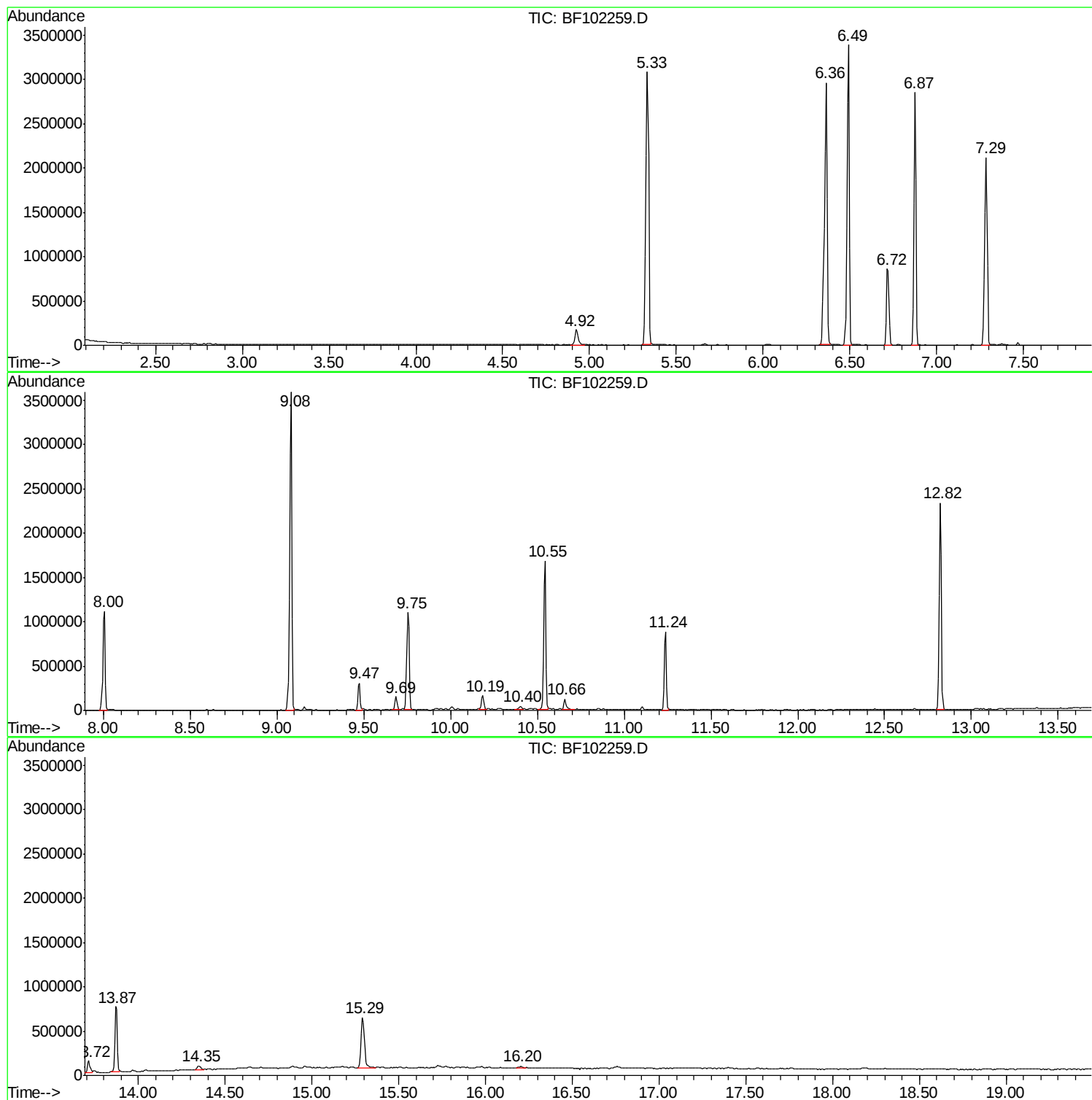
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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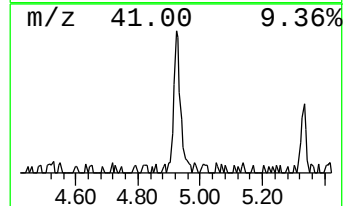
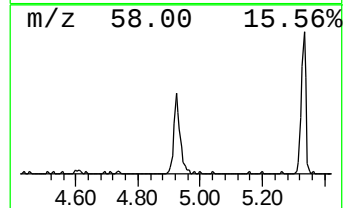
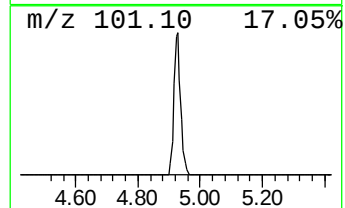
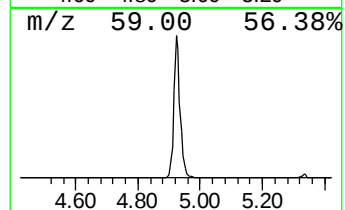
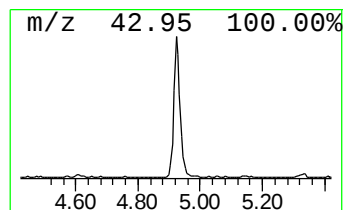
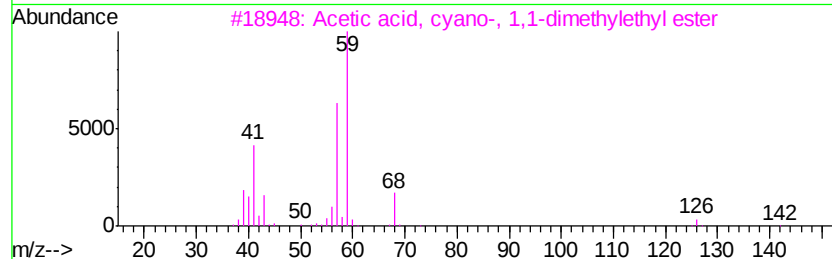
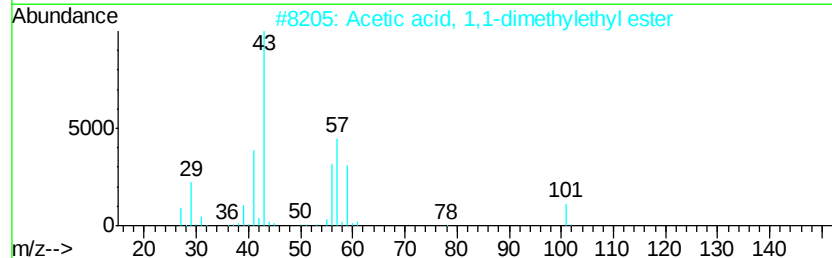
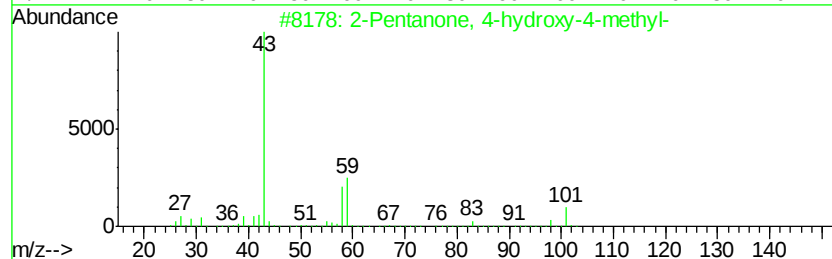
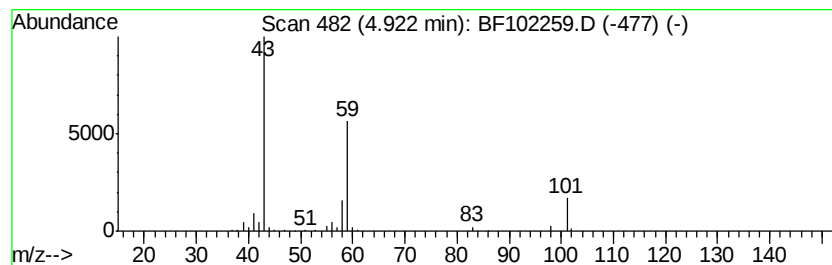
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.92	6.17 ng	238505	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	37
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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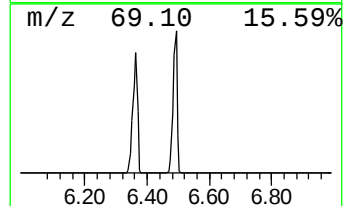
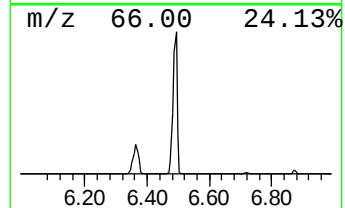
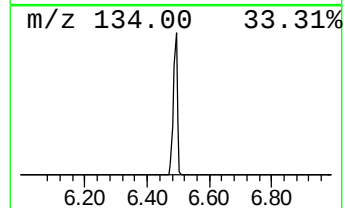
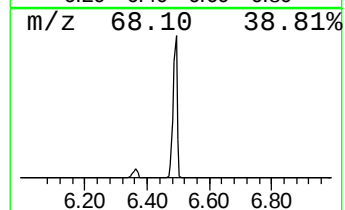
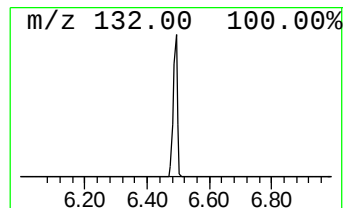
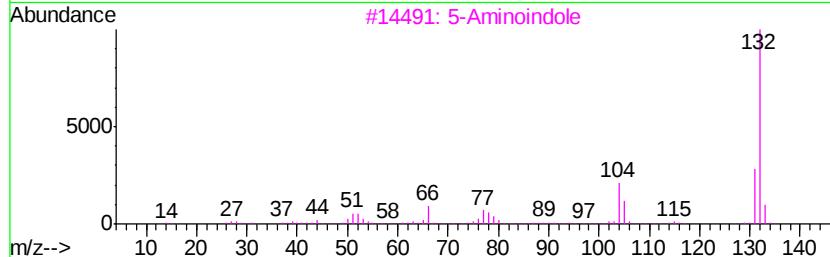
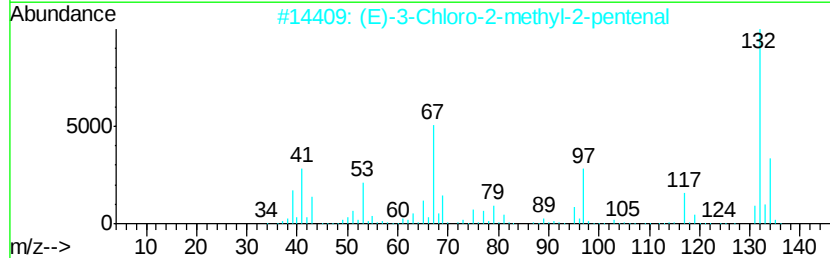
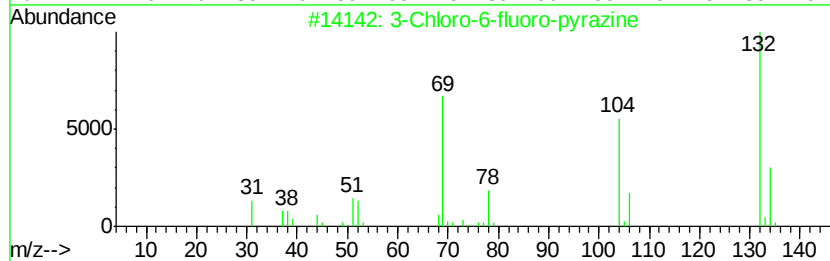
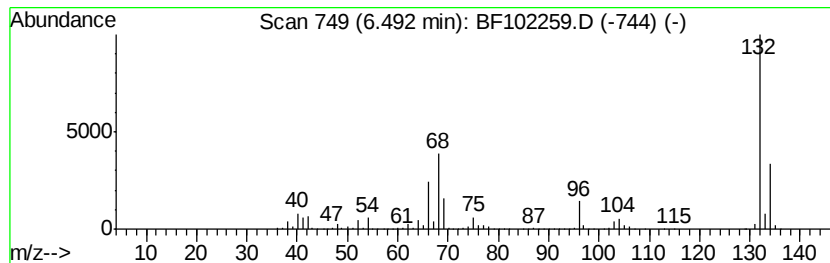
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	81.19 ng	3139760	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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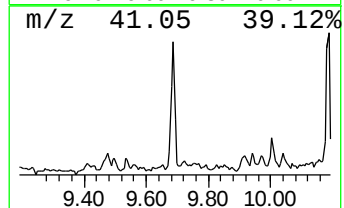
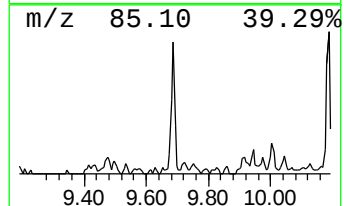
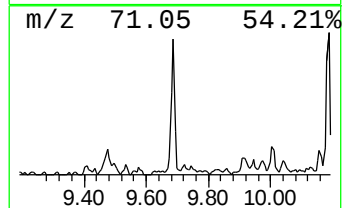
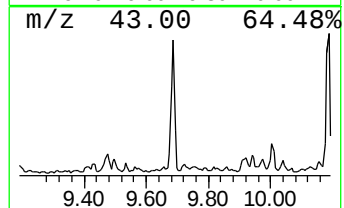
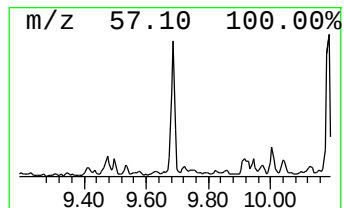
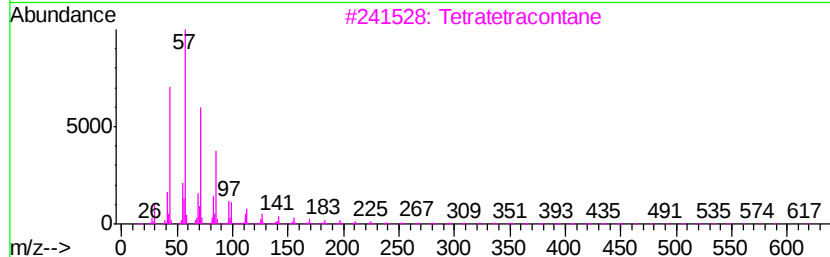
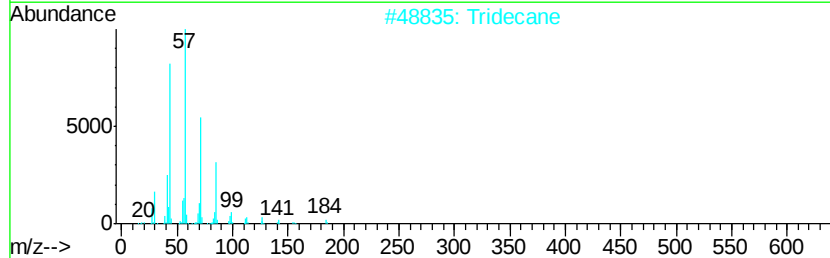
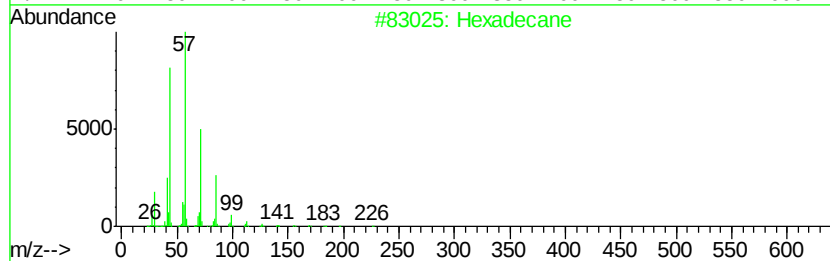
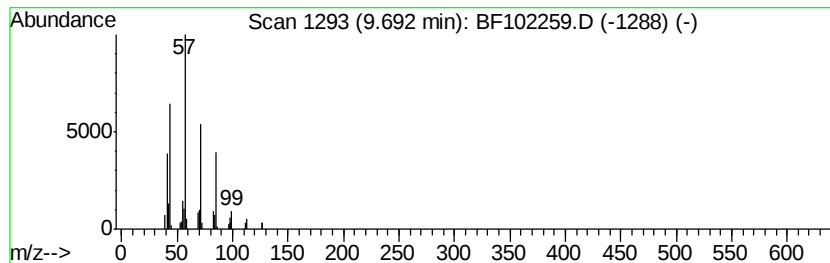
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Peak Number 4 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.69	2.27 ng	109453	Acenaphthene-d10	9.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	90
2	Tridecane		184	C13H28	000629-50-5	83
3	Tetratetracontane		619	C44H90	007098-22-8	78
4	Tetradecane		198	C14H30	000629-59-4	53
5	Octadecane		254	C18H38	000593-45-3	50



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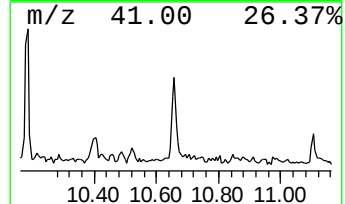
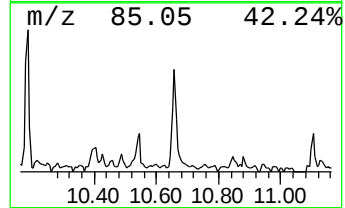
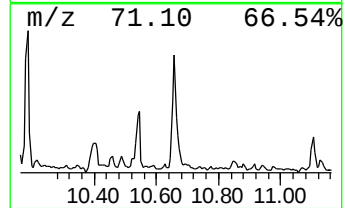
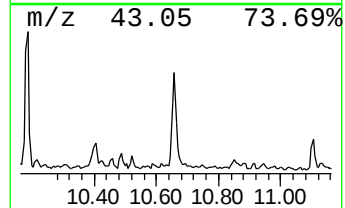
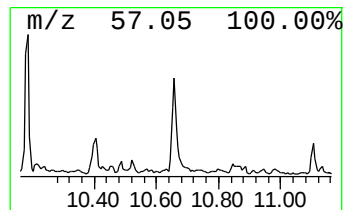
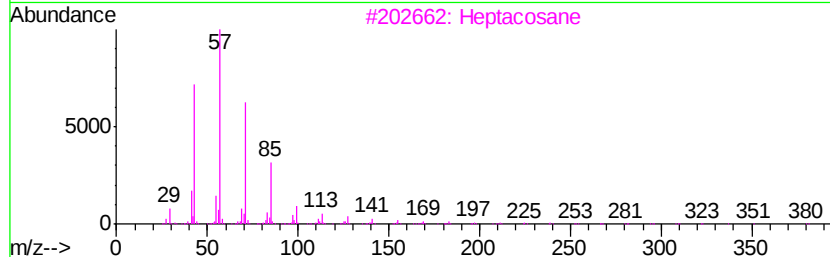
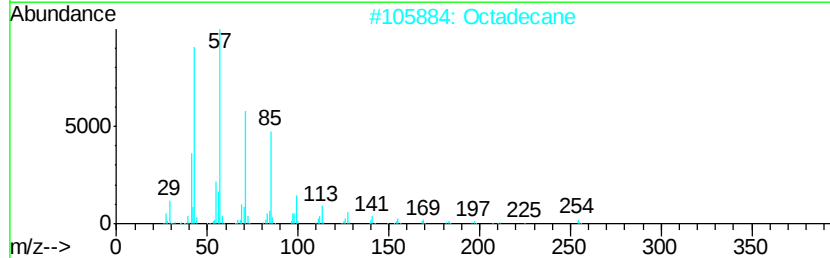
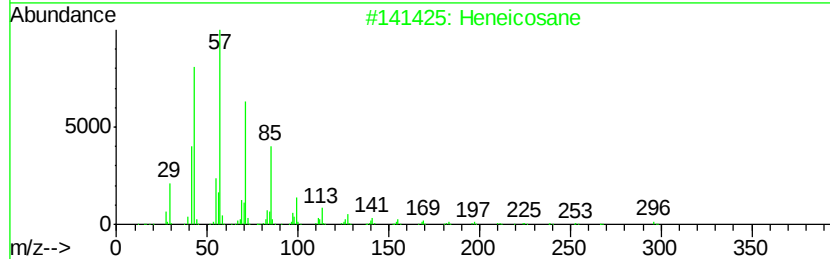
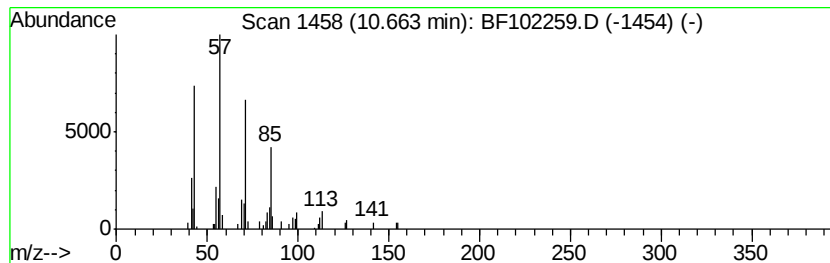
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Peak Number 6 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	2.87 ng	110076	Phenanthrene-d10	11.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Octadecane		254	C18H38	000593-45-3	90
3	Heptacosane		380	C27H56	000593-49-7	90
4	Tetracosane		338	C24H50	000646-31-1	90
5	Pentadecane		212	C15H32	000629-62-9	87



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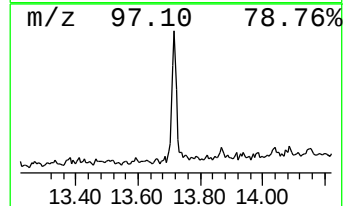
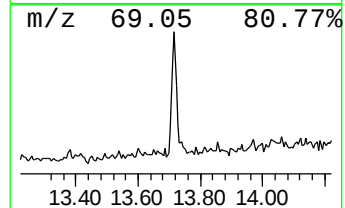
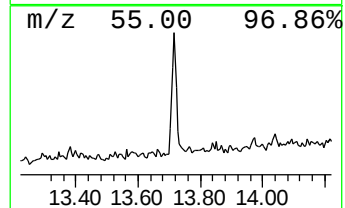
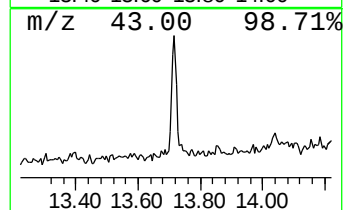
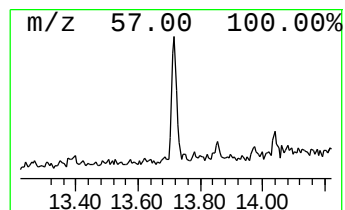
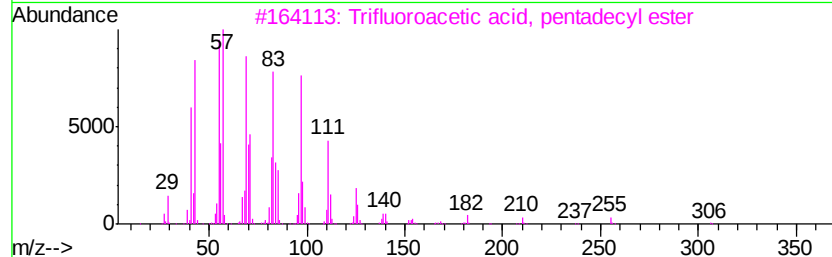
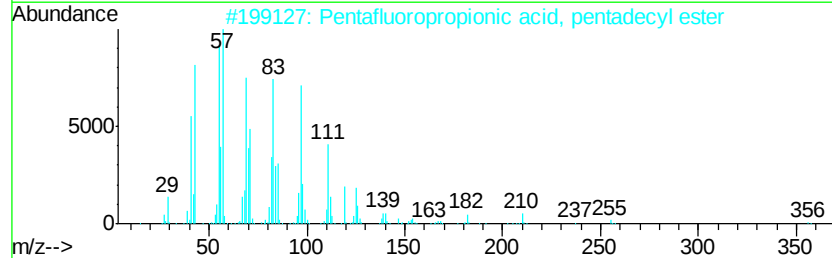
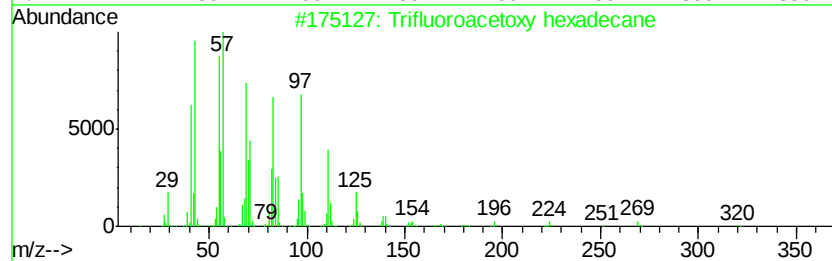
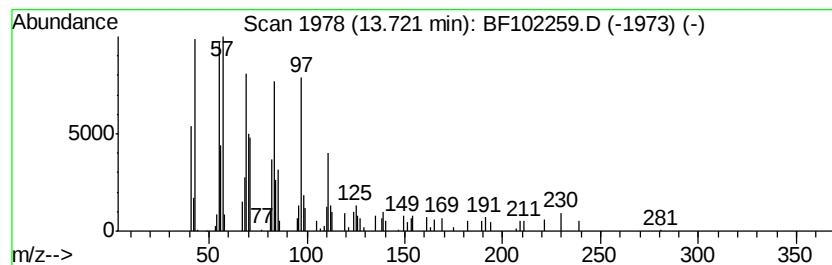
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 7 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	3.68 ng	134813	Chrysene-d12	13.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
3			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	93



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TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.92	6.2	ng	238505	1	6.72	773430	20.0
unknown6.49	6.49	81.2	ng	3139760	1	6.72	773430	20.0
Hexadecane	9.69	2.3	ng	109453	3	9.75	963755	20.0
Heneicosane	10.66	2.9	ng	110076	4	11.24	766282	20.0
Trifluoroacetoxy ...	13.72	3.7	ng	134813	5	13.87	732281	20.0