

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022718\
 Data File : BF103285.D
 Acq On : 28 Feb 2018 2:02
 Operator : SJ/JU
 Sample : J1690-01
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DSN001

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-BF022218.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	2.128	3	7	16	rVB	890407	1115156	27.76%	3.722%
2	2.263	26	30	45	rVB2	34969	69732	1.74%	0.233%
3	5.093	508	511	523	rBV	80345	106246	2.64%	0.355%
4	5.492	575	579	596	rBV	2065473	2127397	52.96%	7.100%
5	6.504	747	751	771	rBV	1203235	1442619	35.91%	4.815%
6	6.645	771	775	778	rBV	3718557	3457459	86.07%	11.539%
7	6.875	810	814	821	rBV	1041052	969508	24.13%	3.236%
8	7.034	836	841	844	rBV	3278338	3345220	83.27%	11.164%
9	7.439	905	910	913	rBV	2873157	2880027	71.69%	9.612%
10	8.157	1028	1032	1047	rBV	1292288	1238745	30.84%	4.134%
11	9.233	1210	1215	1218	rBV	4069367	4017118	100.00%	13.407%
12	9.622	1275	1281	1288	rBV	187849	192504	4.79%	0.642%
13	9.828	1313	1316	1320	rBV	115779	102310	2.55%	0.341%
14	9.910	1327	1330	1339	rBV	1109183	1122840	27.95%	3.747%
15	10.327	1398	1401	1404	rVB2	225766	181973	4.53%	0.607%
16	10.551	1433	1439	1441	rBV	57606	77553	1.93%	0.259%
17	10.704	1461	1465	1474	rBV	1702841	1870870	46.57%	6.244%
18	10.804	1479	1482	1489	rVB	169793	175063	4.36%	0.584%
19	10.957	1504	1508	1512	rVB	52178	52537	1.31%	0.175%
20	11.251	1555	1558	1561	rBV	75001	60136	1.50%	0.201%
21	11.404	1580	1584	1593	rBV	967214	944547	23.51%	3.152%
22	12.792	1817	1820	1824	rBV	67658	57183	1.42%	0.191%
23	12.992	1849	1854	1857	rBV	2523899	2628800	65.44%	8.773%
24	13.868	2000	2003	2017	rBV	228090	322670	8.03%	1.077%
25	14.051	2030	2034	2043	rBV	751284	774594	19.28%	2.585%
26	14.139	2046	2049	2052	rVB	45514	44397	1.11%	0.148%
27	15.551	2284	2289	2298	rBV	398168	586645	14.60%	1.958%

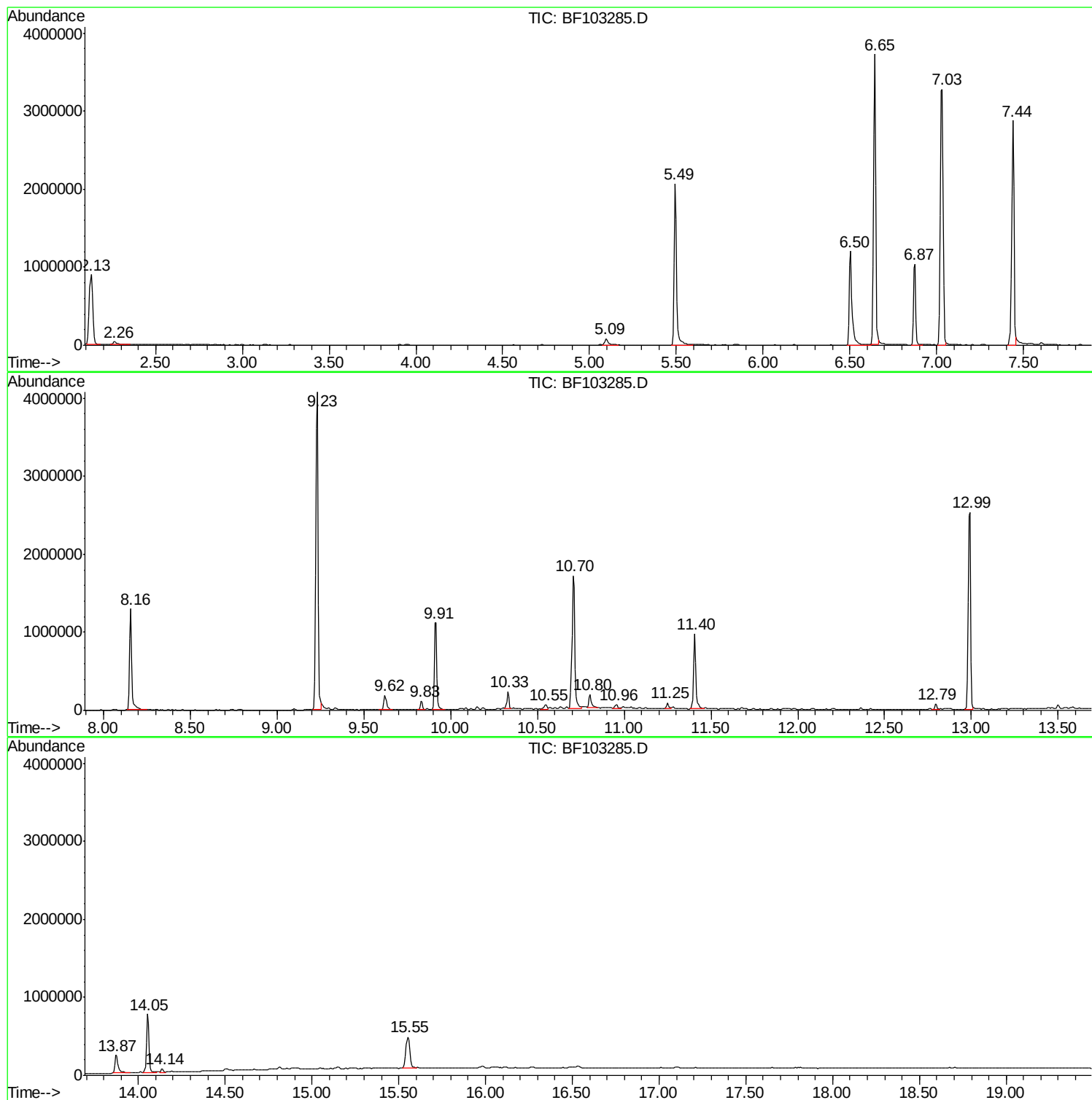
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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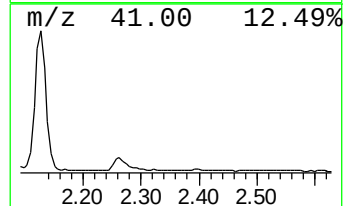
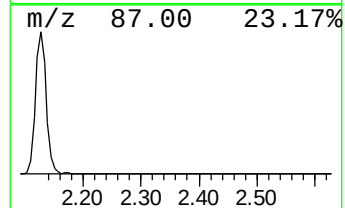
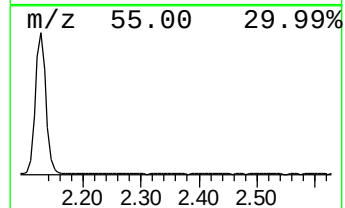
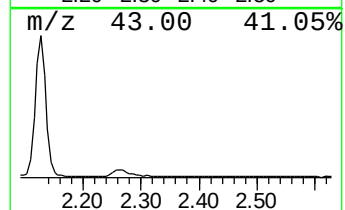
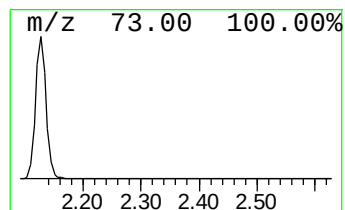
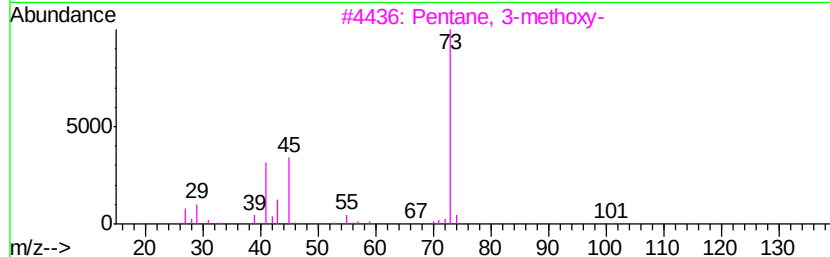
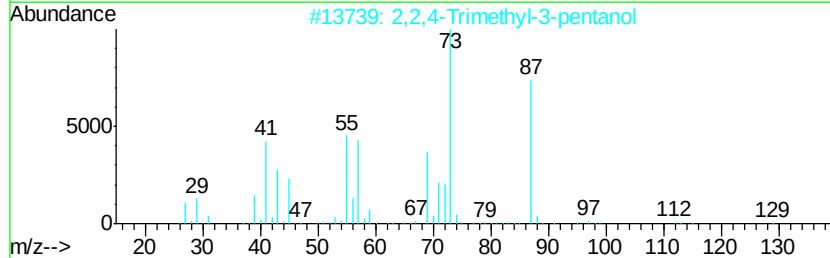
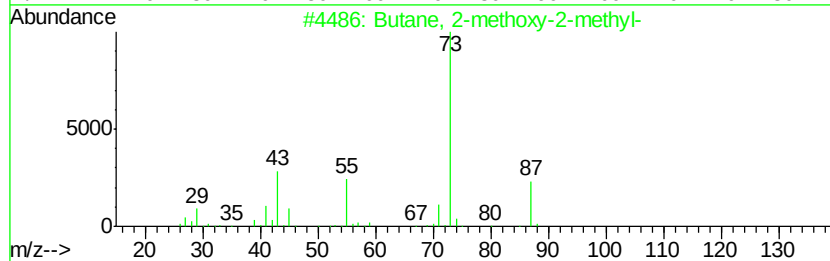
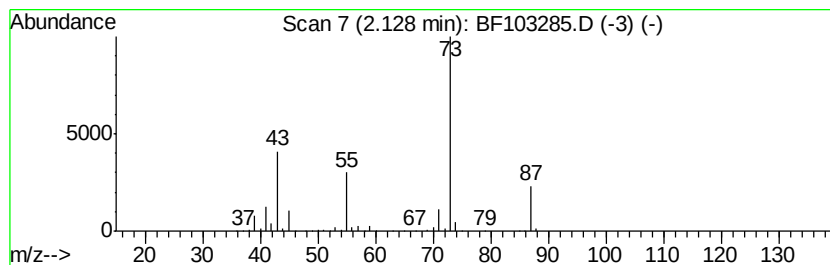
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	23.00 ng	1115160	1,4-Dichlorobenzene-d4	6.87

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	40
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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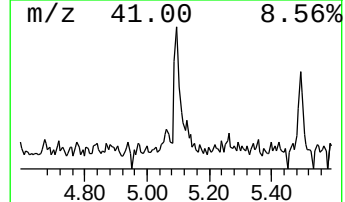
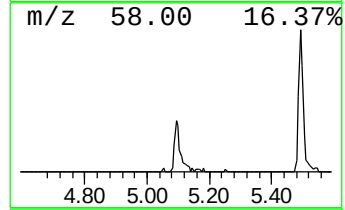
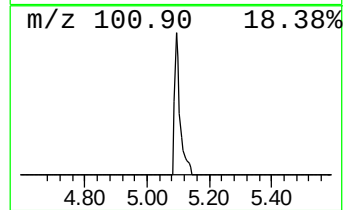
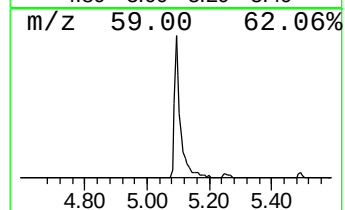
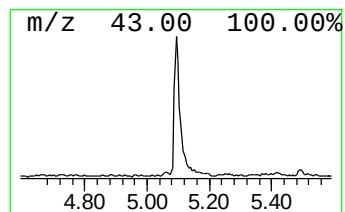
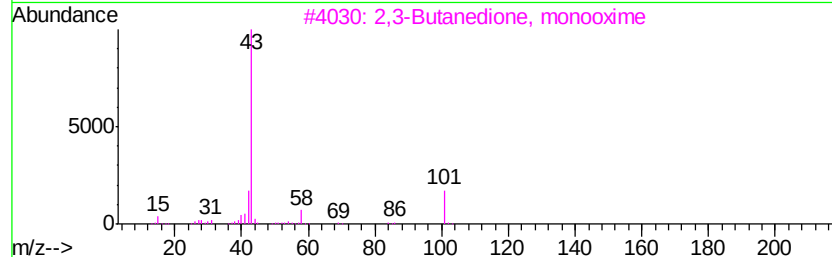
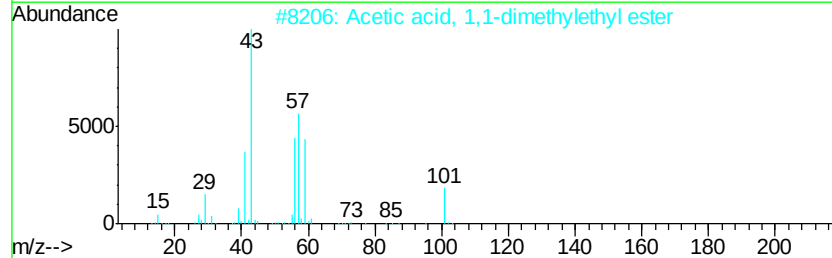
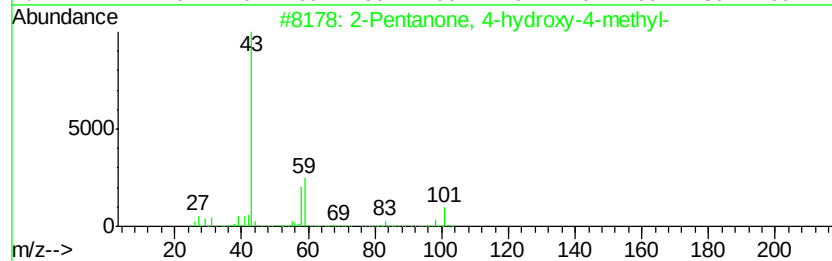
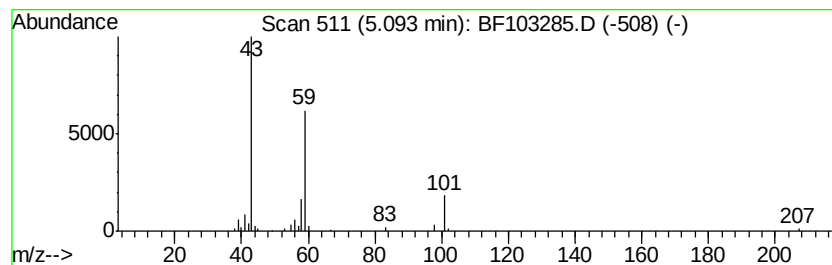
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	2.19 ng	106246	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Diacetamide	101	C4H7NO2	000625-77-4	9



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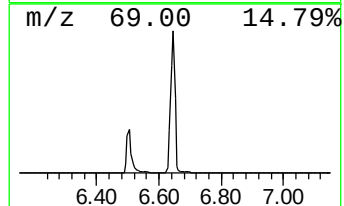
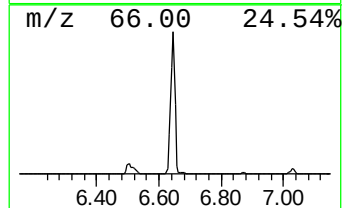
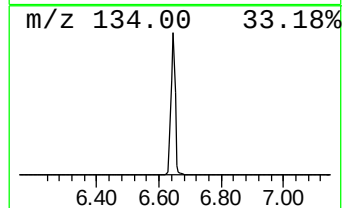
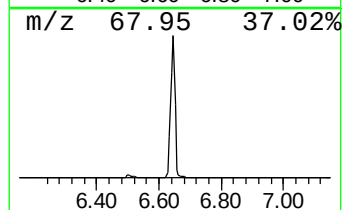
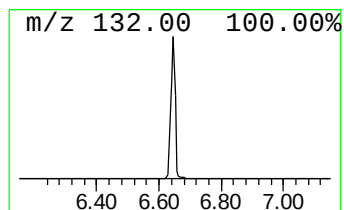
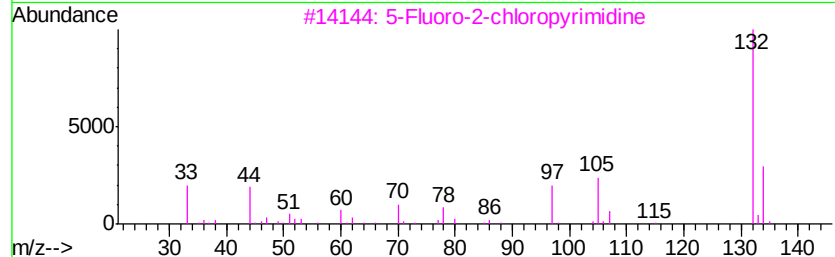
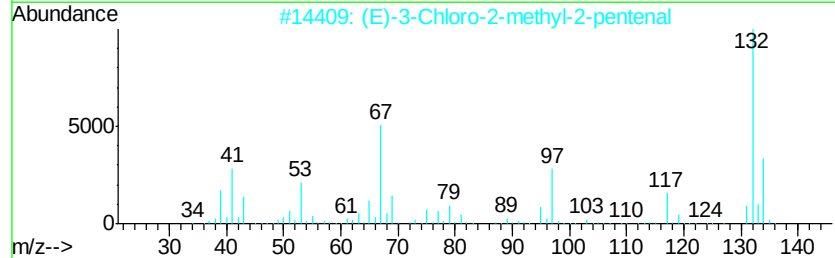
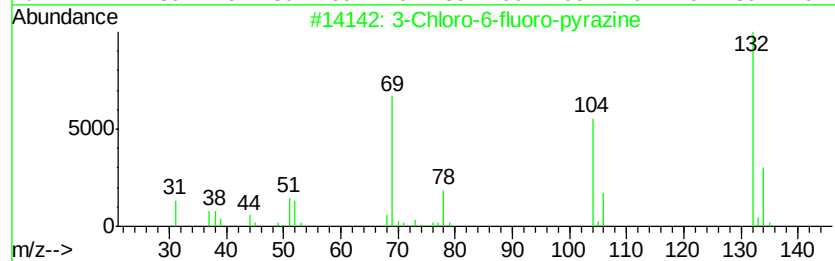
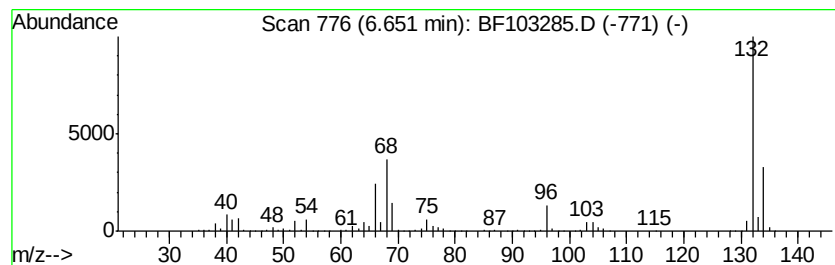
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	71.32 ng	3457460	1,4-Dichlorobenzene-d4	6.87

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	27
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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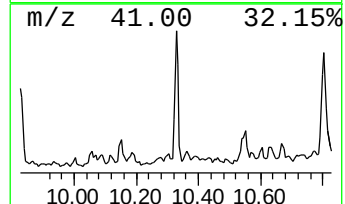
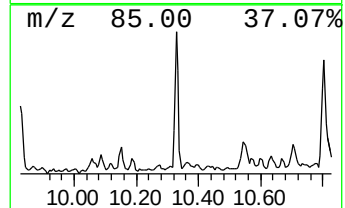
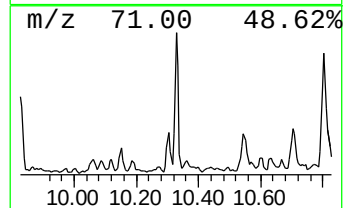
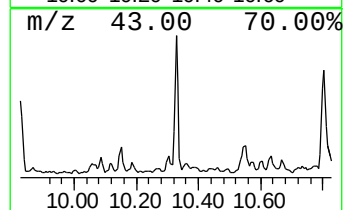
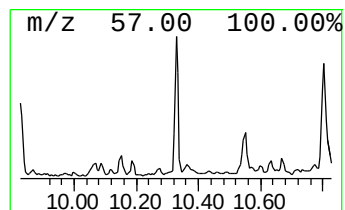
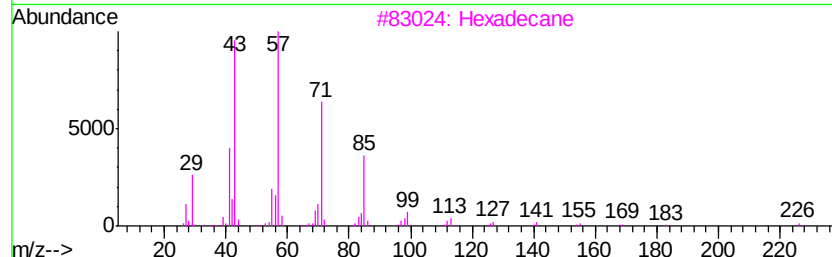
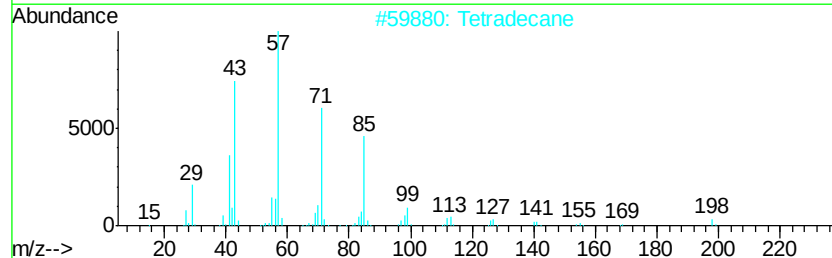
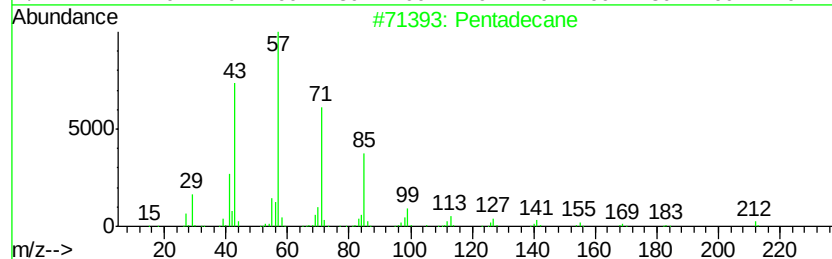
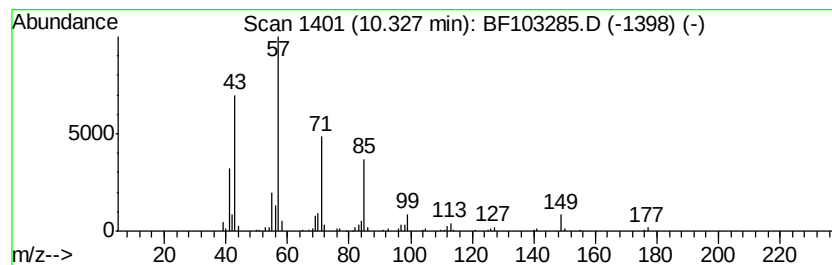
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Pentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.33	3.24 ng	181973	Acenaphthene-d10	9.91
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Pentadecane	212 C15H32	000629-62-9	86
2	Tetradecane	198 C14H30	000629-59-4	86
3	Hexadecane	226 C16H34	000544-76-3	86
4	Heneicosane	296 C21H44	000629-94-7	80
5	Decane, 2,3,5-trimethyl-	184 C13H28	062238-11-3	78



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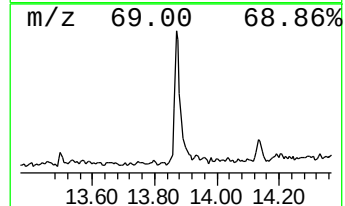
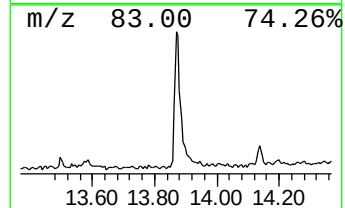
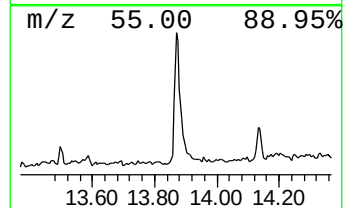
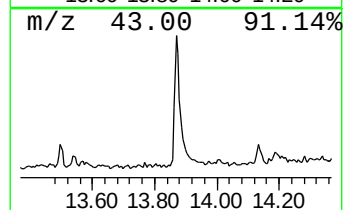
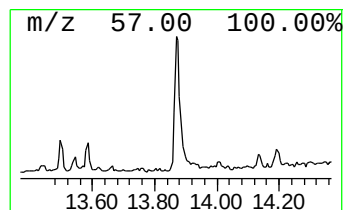
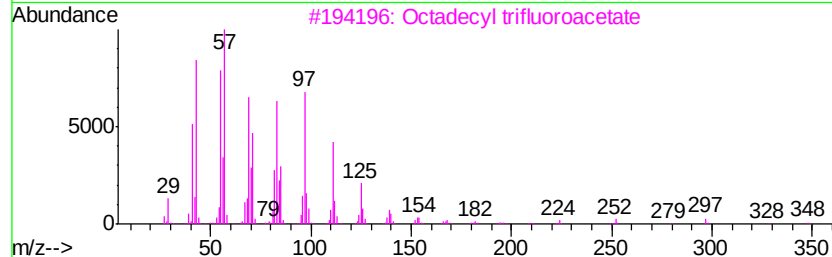
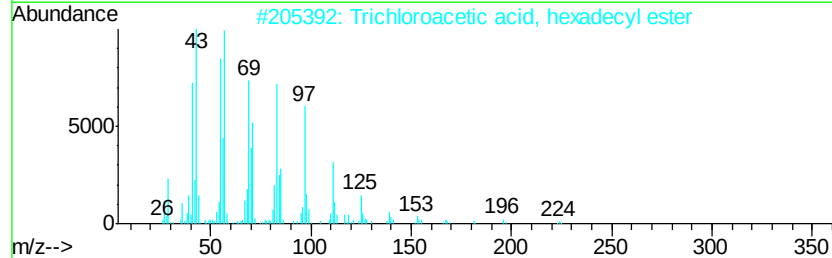
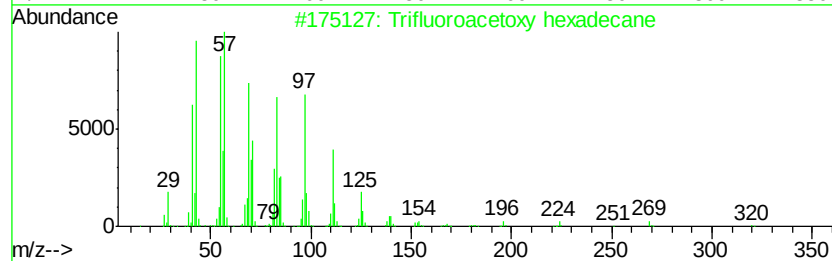
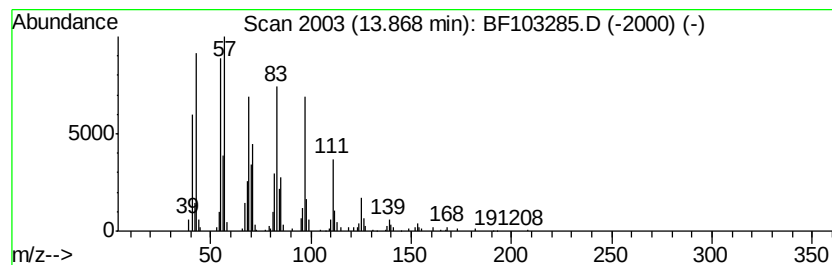
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	8.33 ng	322670	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
4		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
5		1-Heneicosanol	312	C21H44O	015594-90-8	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.13	23.0	ng	1115160	1	6.87	969508	20.0
2-Pentanone, 4-hy...	5.09	2.2	ng	106246	1	6.87	969508	20.0
unknown6.65	6.65	71.3	ng	3457460	1	6.87	969508	20.0
Pentadecane	10.33	3.2	ng	181973	3	9.91	1122840	20.0
Trifluoroacetoxy ...	13.87	8.3	ng	322670	5	14.05	774594	20.0