

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081518\
 Data File : BF108185.D
 Acq On : 16 Aug 2018 00:18
 Operator : JU/SJ
 Sample : J4471-13
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-4

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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	2.402	5	11	34	rVB	492535	820505	11.98%	1.561%
2	3.678	226	228	241	rBV	37576	75661	1.10%	0.144%
3	5.266	493	498	511	rBV	817030	1220111	17.81%	2.321%
4	5.648	558	563	566	rBV	4939085	5603288	81.80%	10.659%
5	6.642	725	732	735	rBV	5153118	6049264	88.31%	11.508%
6	6.789	751	757	760	rBV	5670676	5877185	85.80%	11.180%
7	7.013	792	795	799	rVB	1401814	1248117	18.22%	2.374%
8	7.172	818	822	826	rVB	4692131	4543774	66.33%	8.644%
9	7.578	885	891	894	rBV	3526775	3985900	58.19%	7.583%
10	8.301	1009	1014	1017	rBV	1636802	1592689	23.25%	3.030%
11	9.372	1190	1196	1200	rBV	6408858	6849921	100.00%	13.031%
12	9.760	1258	1262	1267	rBV	459685	374297	5.46%	0.712%
13	10.060	1308	1313	1317	rBV2	2038347	1778473	25.96%	3.383%
14	10.854	1443	1448	1451	rBV	3552178	3220192	47.01%	6.126%
15	11.554	1563	1567	1571	rBV	1794066	1530715	22.35%	2.912%
16	13.142	1833	1837	1841	rBV	4773091	4866555	71.05%	9.258%
17	14.048	1984	1991	2001	rBV	98229	259977	3.80%	0.495%
18	14.207	2014	2018	2022	rBV	1331895	1204790	17.59%	2.292%
19	15.771	2278	2284	2292	rVB	902791	1273049	18.58%	2.422%
20	16.236	2359	2363	2369	rVB	58448	84456	1.23%	0.161%
21	16.795	2453	2458	2466	rBV4	51088	107703	1.57%	0.205%

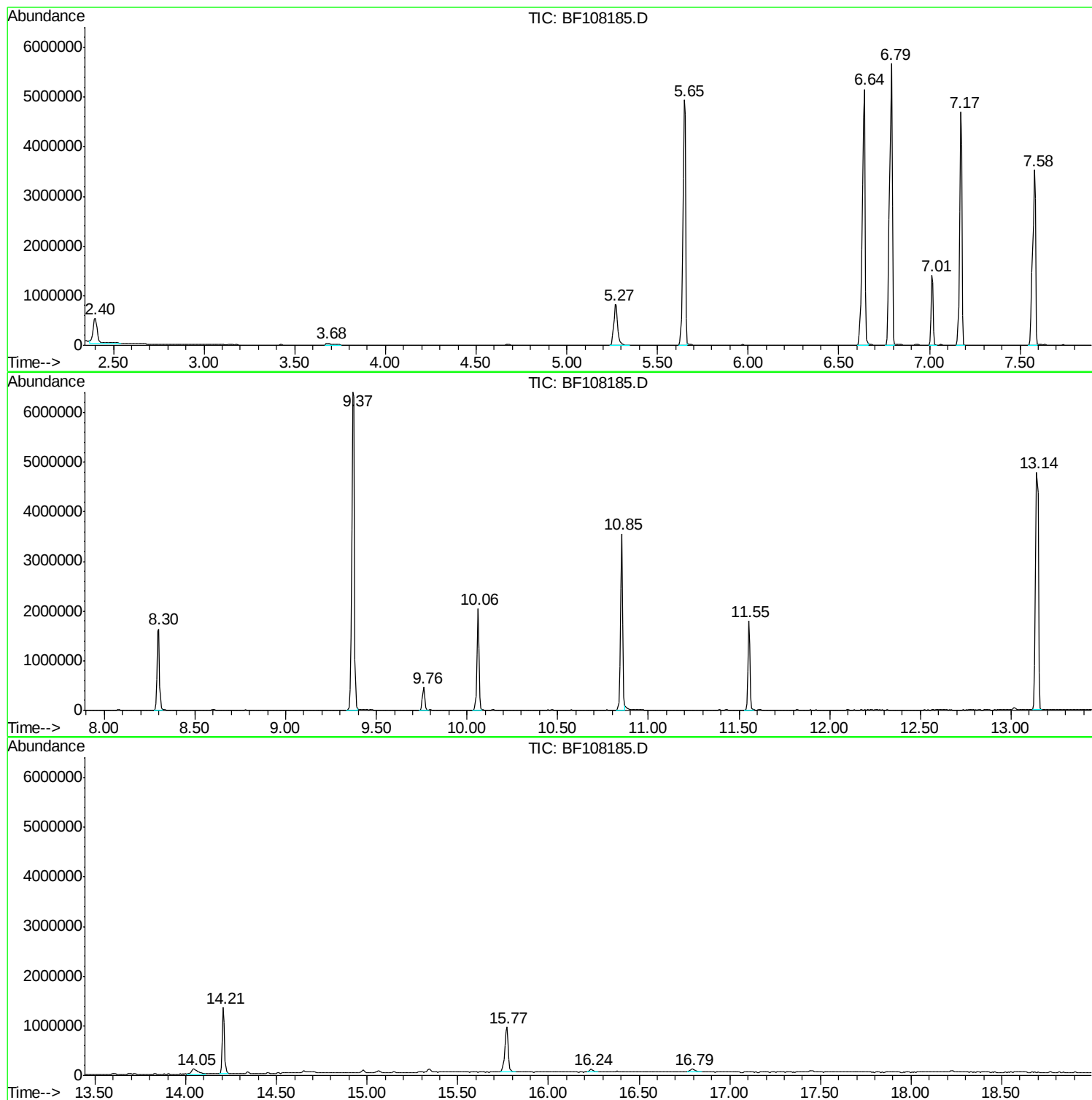
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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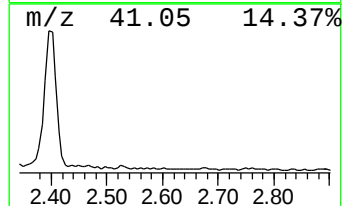
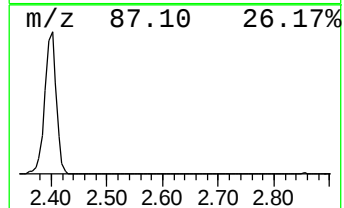
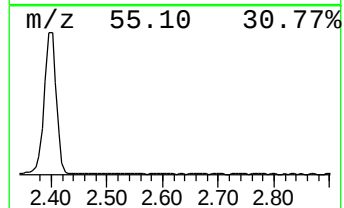
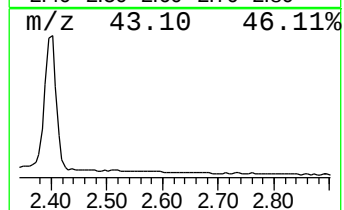
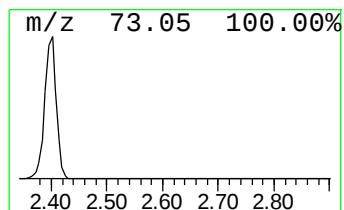
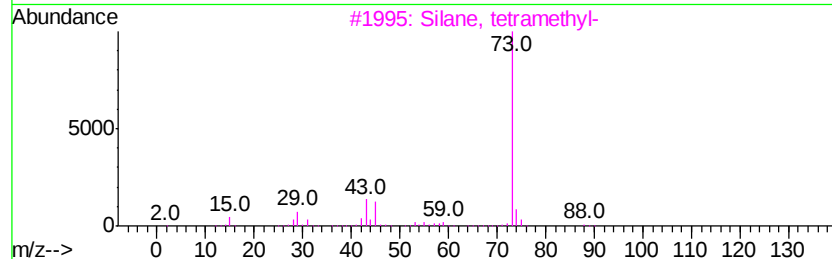
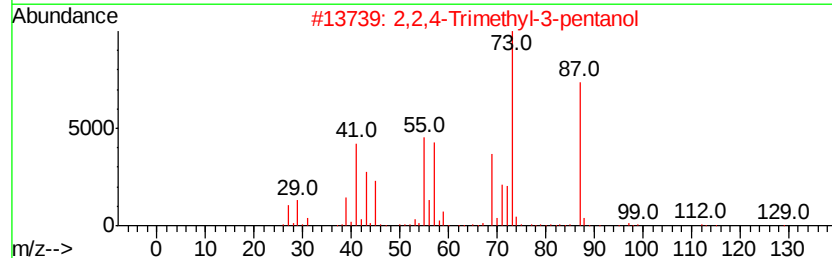
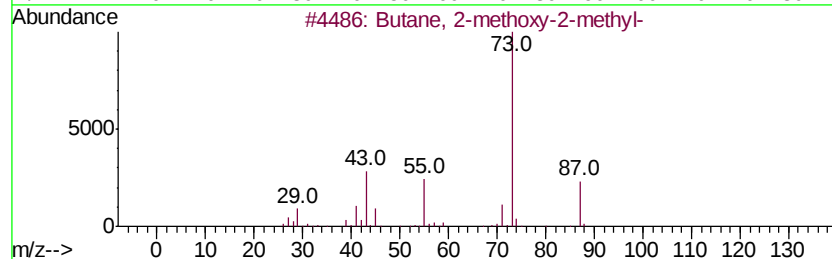
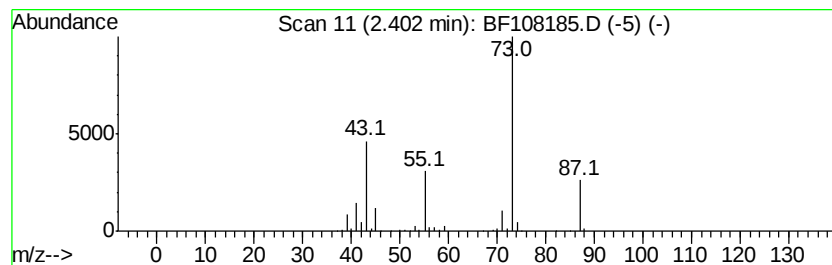
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.40	13.15 ng	820505	1,4-Dichlorobenzene-d4	7.01

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	39
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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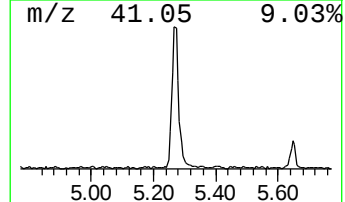
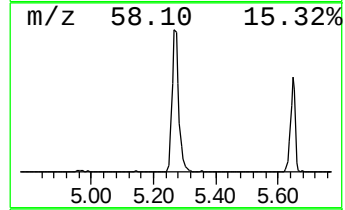
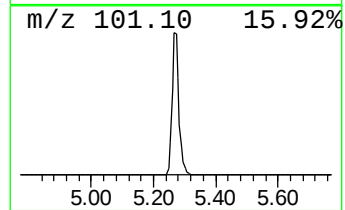
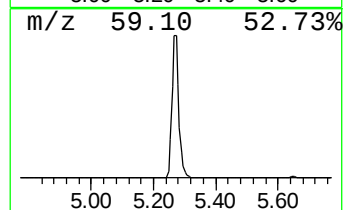
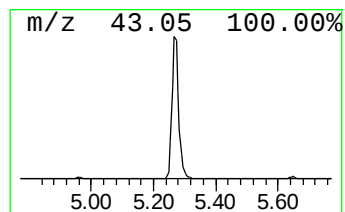
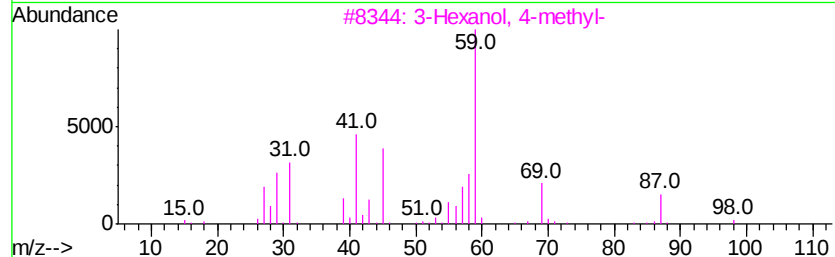
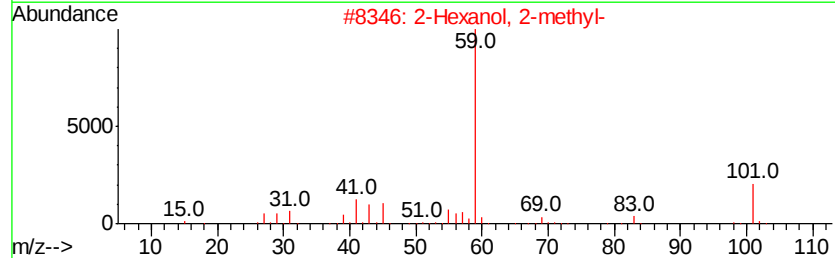
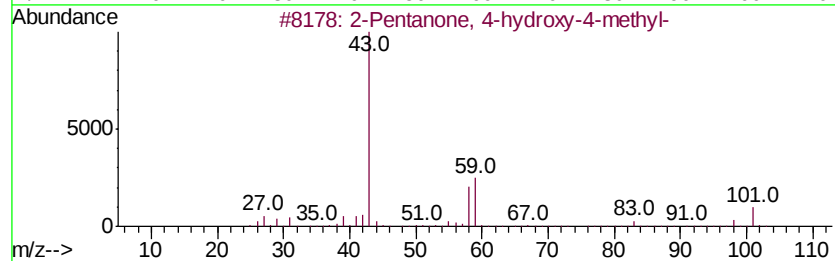
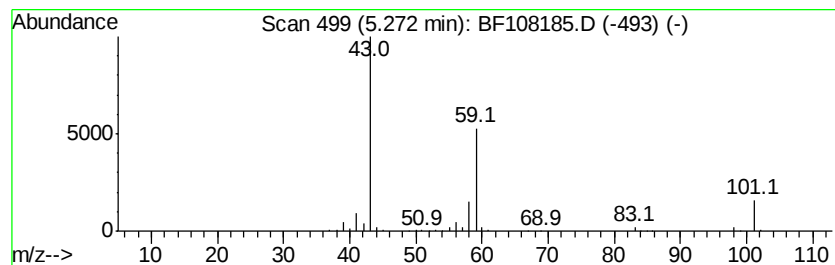
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.27	19.55 ng	1220110	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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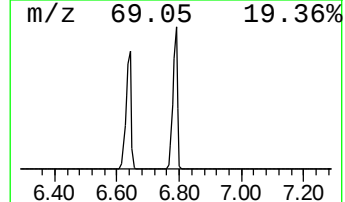
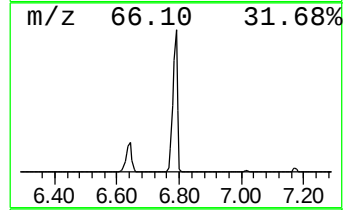
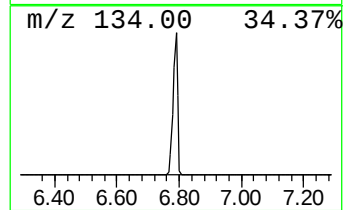
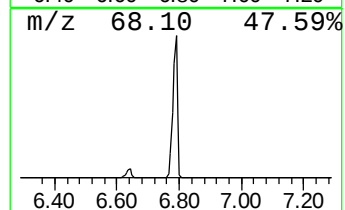
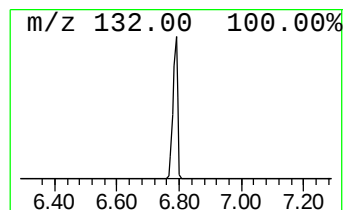
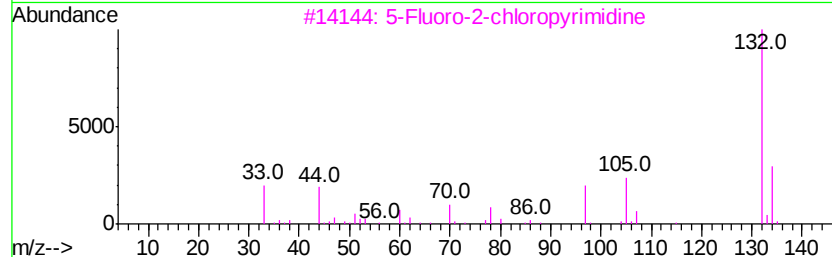
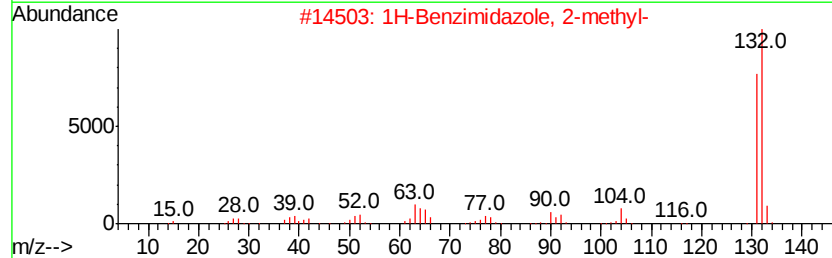
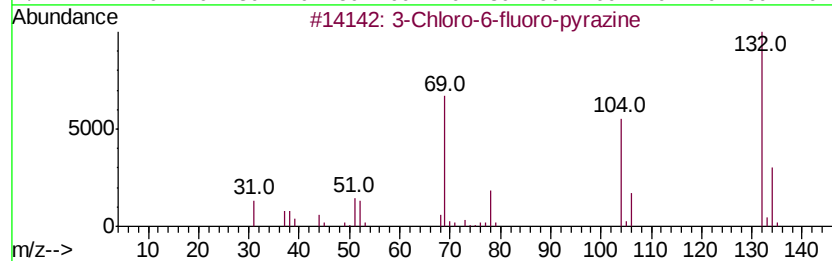
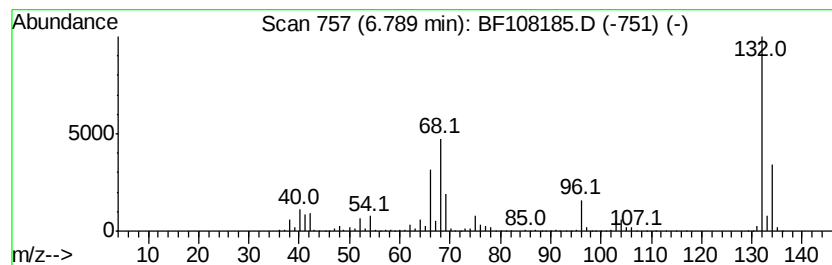
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Peak Number 3 unknown6.79 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.79	94.18 ng	5877190	1,4-Dichlorobenzene-d4	7.01

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5			(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10



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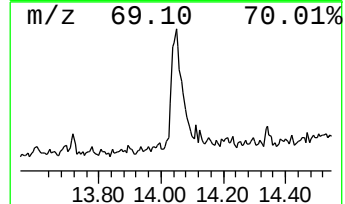
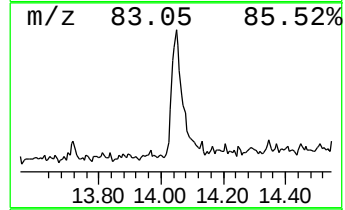
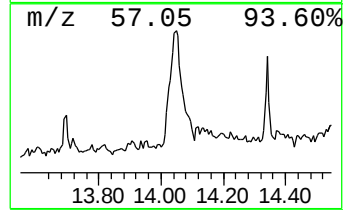
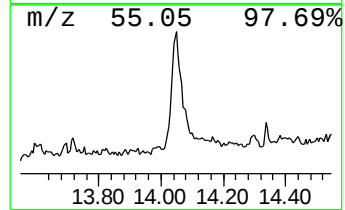
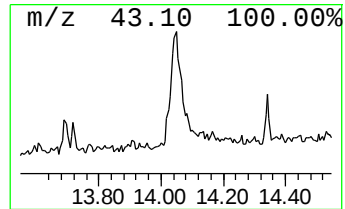
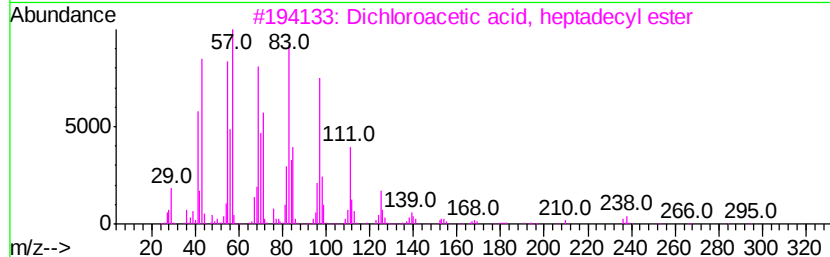
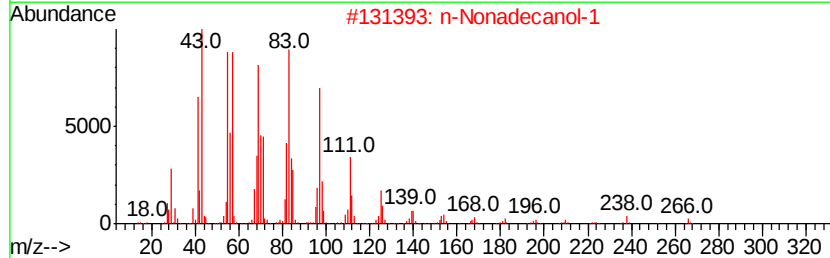
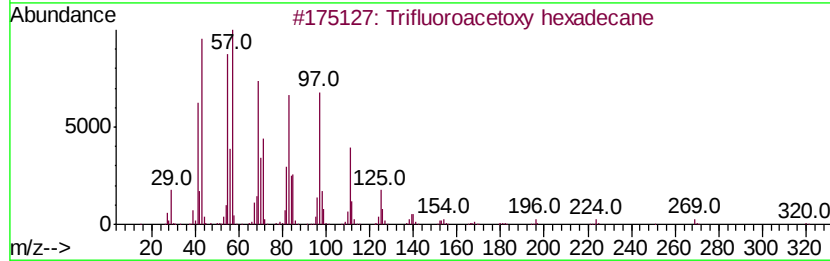
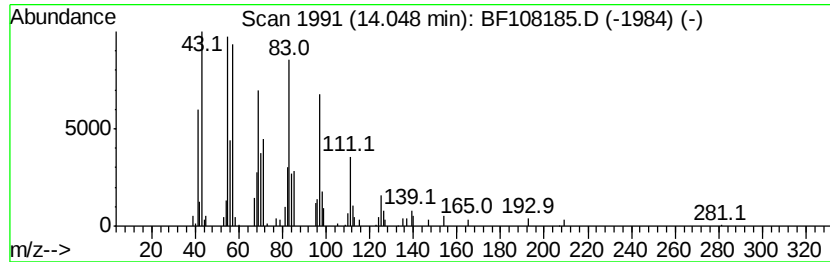
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.05	4.32 ng	259977	Chrysene-d12		14.21	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.40	13.2	ng	820505	1	7.01	1248120	20.0
2-Pentanone, 4-hy...	5.27	19.6	ng	1220110	1	7.01	1248120	20.0
unknown6.79	6.79	94.2	ng	5877190	1	7.01	1248120	20.0
Trifluoroacetoxy ...	14.05	4.3	ng	259977	5	14.21	1204790	20.0