

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111414\
 Data File : BF075540.D
 Acq On : 15 Nov 2014 14:25
 Operator : TP / JJ
 Sample : F4706-03
 Misc :
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-05(36-38)-111014

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-BF111214.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	1.613	43	46	49	rBV	4223692	4772826	100.00%	32.787%
2	1.761	56	59	62	rVB	147372	226114	4.74%	1.553%
3	1.967	73	77	84	rVB2	173524	347743	7.29%	2.389%
4	5.339	370	372	376	rVB	263167	277406	5.81%	1.906%
5	5.830	413	415	418	rBV	578658	801501	16.79%	5.506%
6	7.087	523	525	530	rBV	932152	854207	17.90%	5.868%
7	7.259	537	540	542	rBV	804354	831194	17.42%	5.710%
8	7.545	563	565	568	rBV	289246	328454	6.88%	2.256%
9	7.739	579	582	584	rVB	585644	570970	11.96%	3.922%
10	8.242	623	626	628	rBV	359714	453417	9.50%	3.115%
11	9.133	701	704	706	rBV	413933	467466	9.79%	3.211%
12	10.471	819	821	824	rVB	810556	767894	16.09%	5.275%
13	11.305	892	894	897	rBV	457418	506491	10.61%	3.479%
14	12.288	978	980	983	rBV	567079	535556	11.22%	3.679%
15	13.157	1054	1056	1058	rBV	557726	509848	10.68%	3.502%
16	14.962	1210	1214	1216	rBV2	51010	53121	1.11%	0.365%
17	15.145	1228	1230	1233	rBV	658171	889977	18.65%	6.114%
18	16.345	1331	1335	1342	rBV2	32167	119572	2.51%	0.821%
19	16.460	1342	1345	1347	rBV	523798	588372	12.33%	4.042%
20	18.231	1497	1500	1508	rBV	414842	654933	13.72%	4.499%

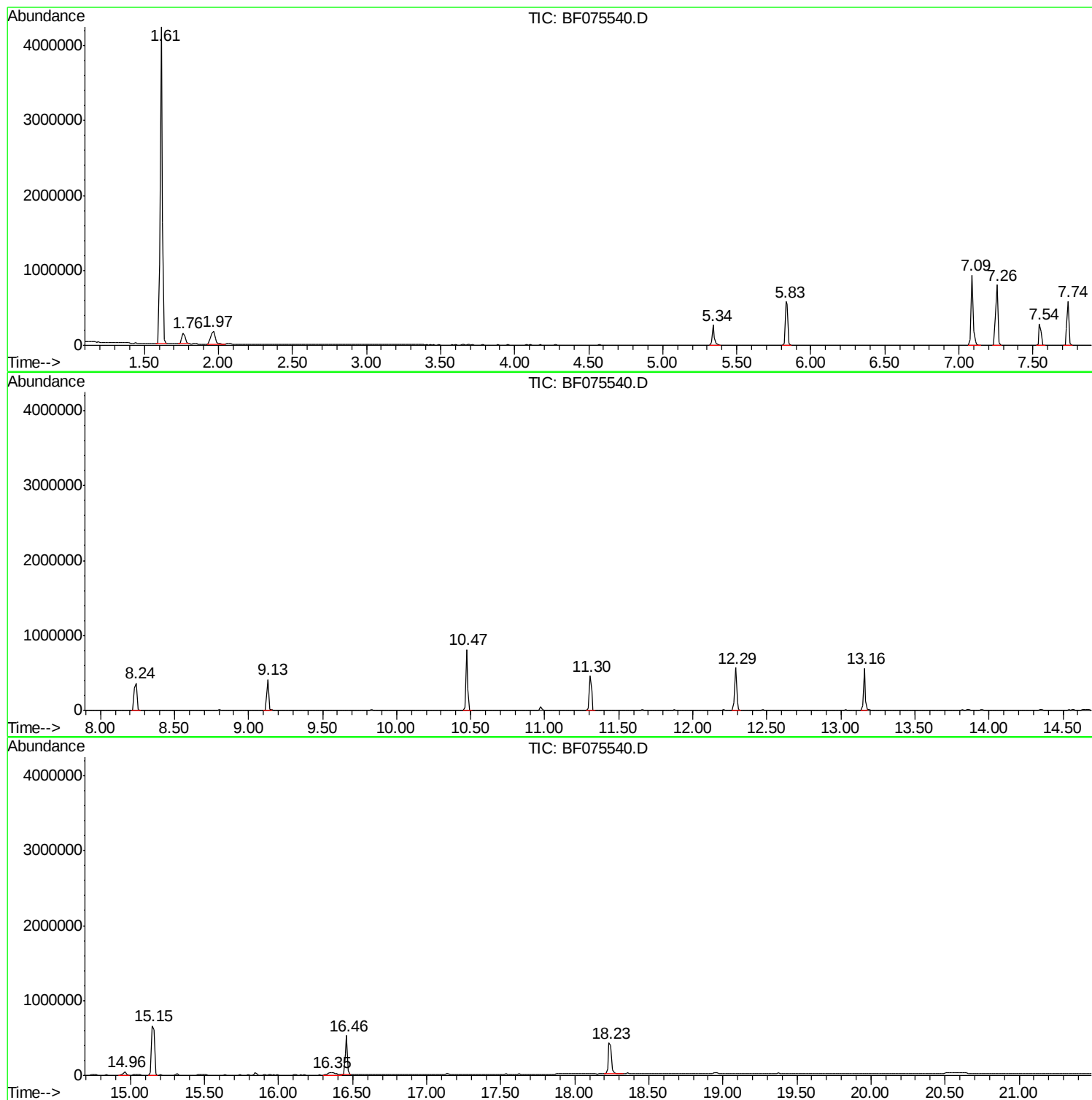
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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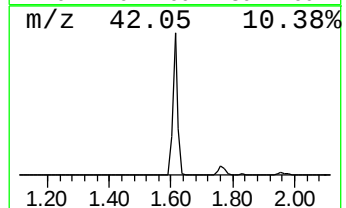
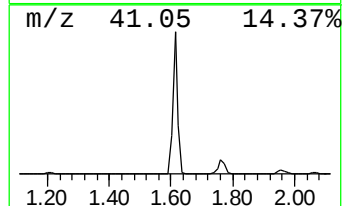
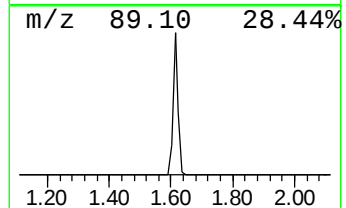
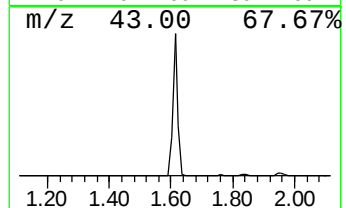
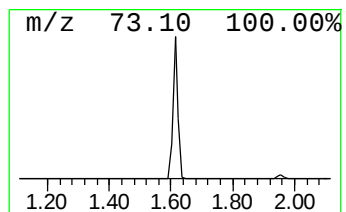
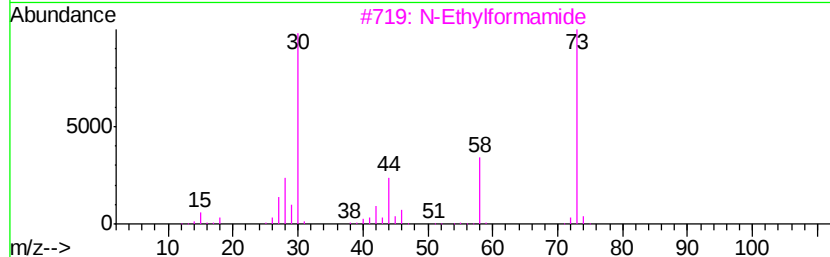
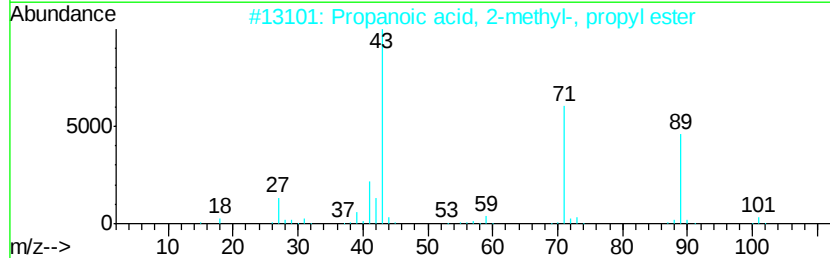
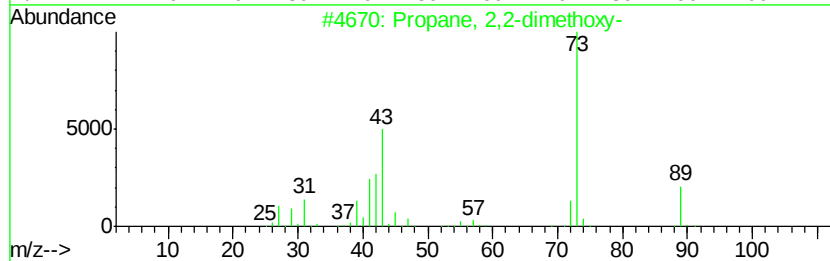
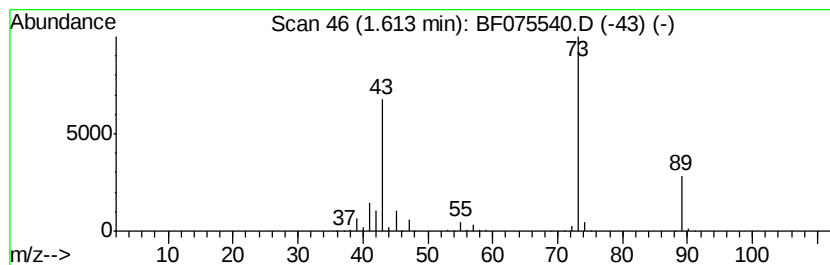
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF111214.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.61	290.62 ng	4772830	1,4-Dichlorobenzene-d4	7.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	50
2		Propanoic acid, 2-methyl-, propyl ester	130	C7H14O2	000644-49-5	23
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		1,3-Diaminoquanidine	89	CH7N5	004364-78-7	9
5		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9



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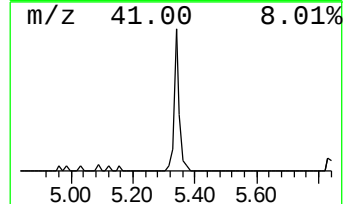
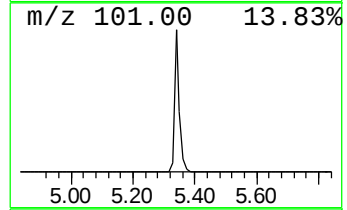
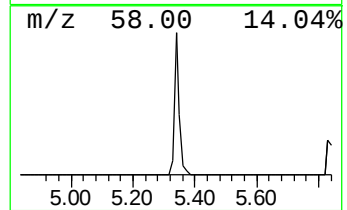
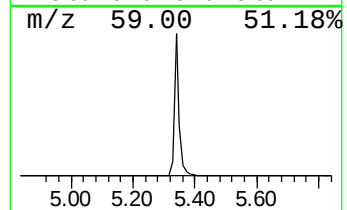
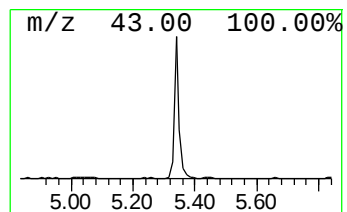
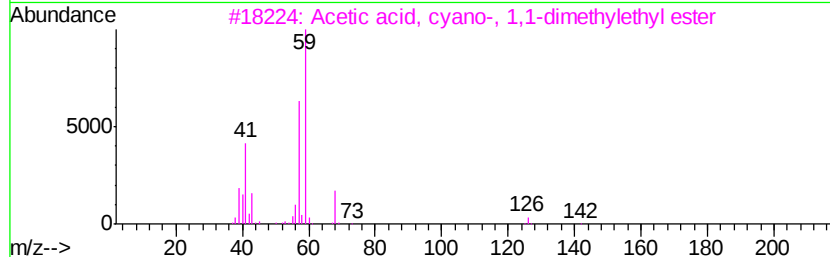
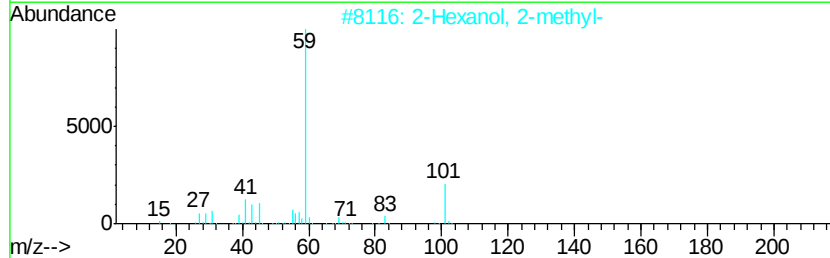
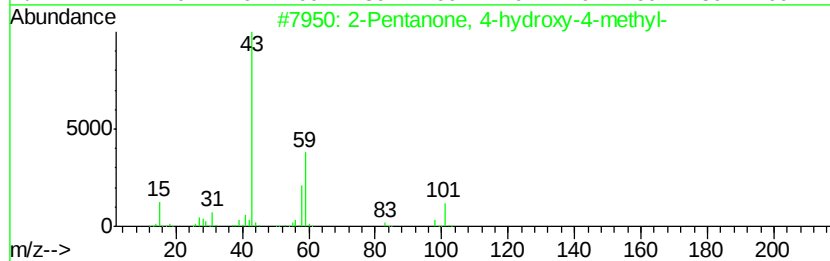
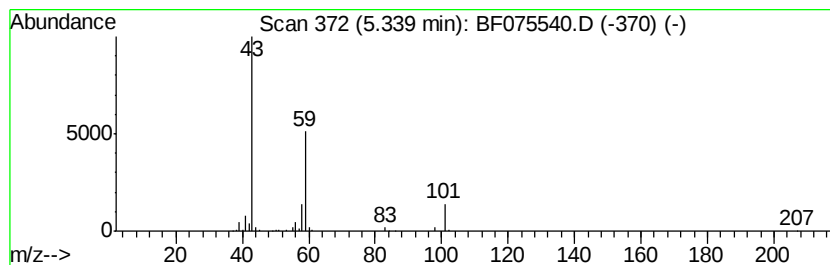
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.34	16.89 ng	277406	1,4-Dichlorobenzene-d4	7.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
5		3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	9



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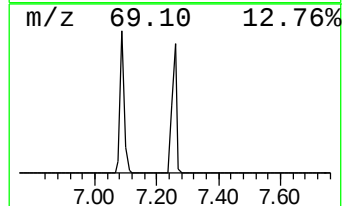
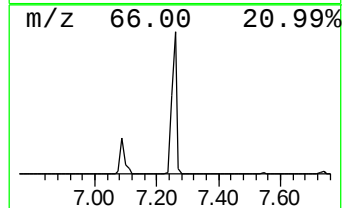
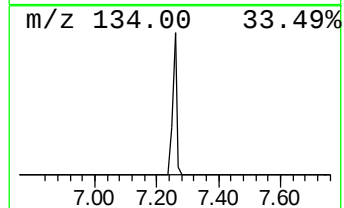
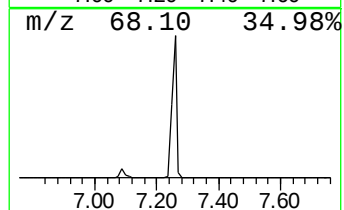
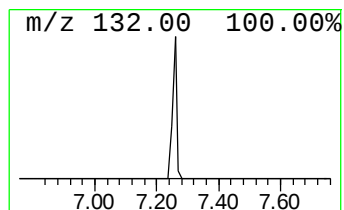
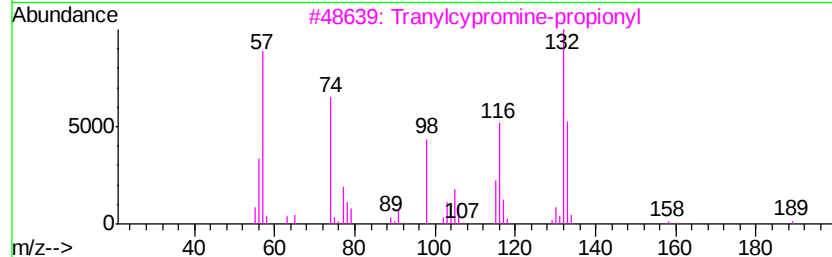
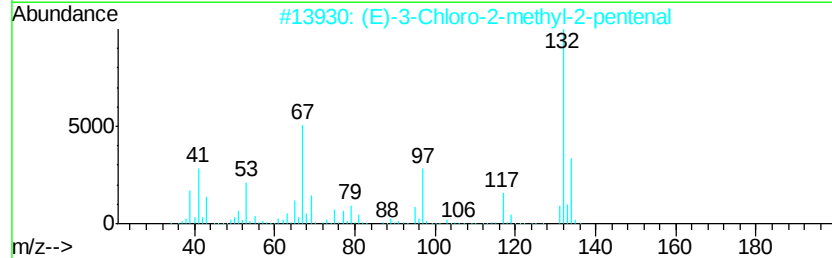
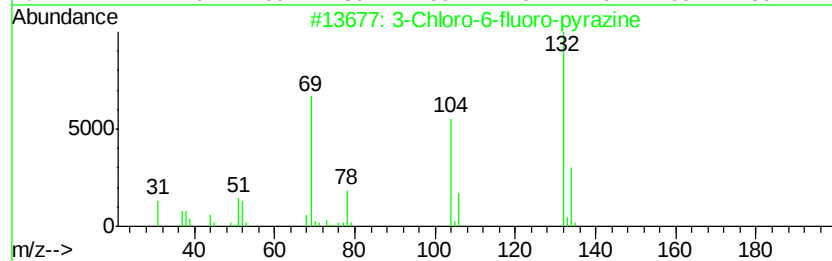
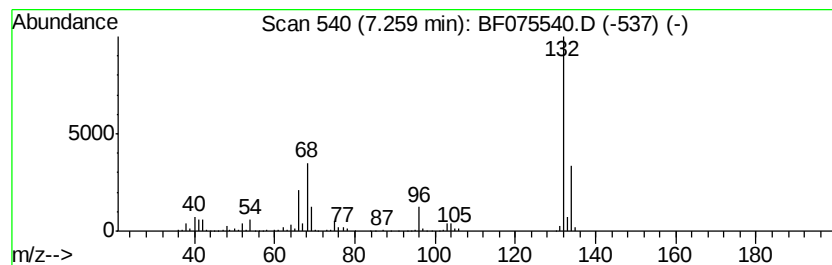
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Peak Number 5 unknown7.26 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.26	50.61 ng	831194	1,4-Dichlorobenzene-d4	7.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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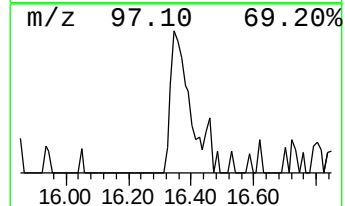
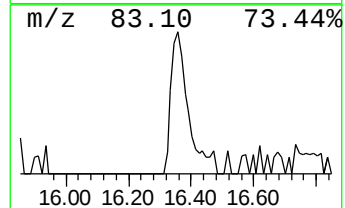
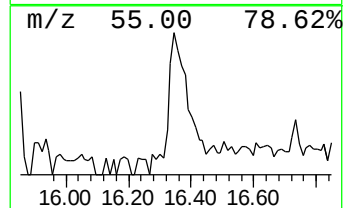
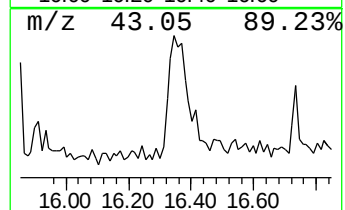
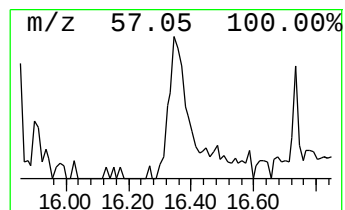
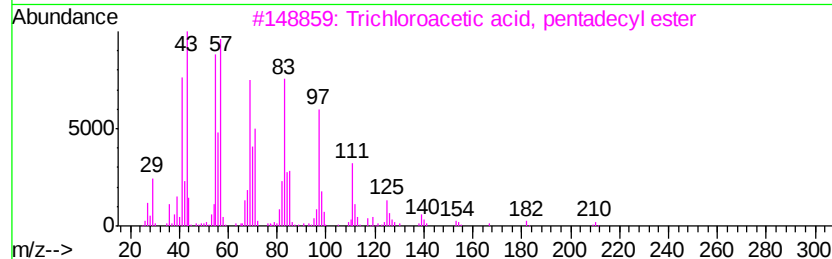
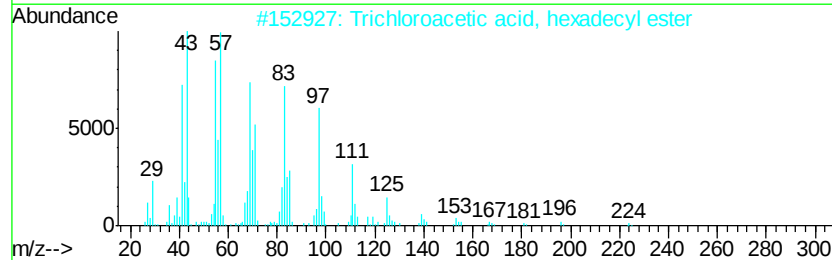
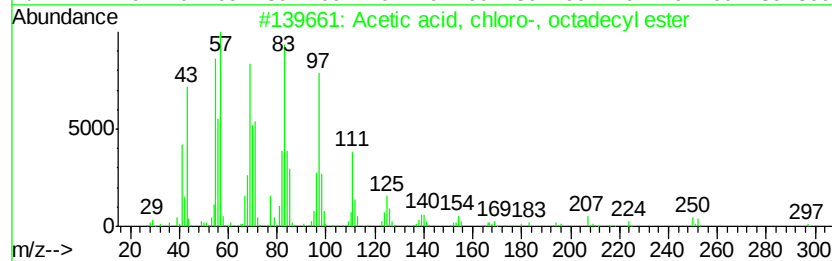
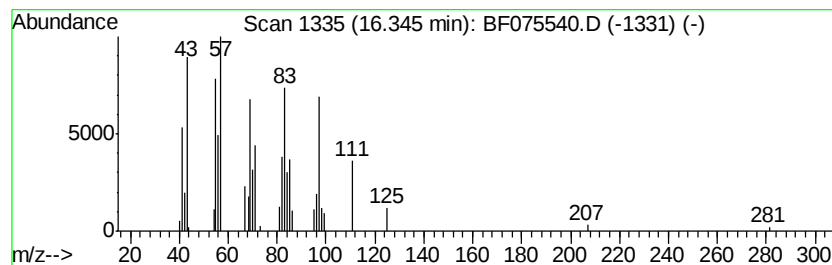
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Peak Number 7 Acetic acid, chloro-, octad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.35	4.06 ng	119572	Chrysene-d12	16.46

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	91
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	86
4		1-Hexacosanol	382	C26H54O	000506-52-5	80
5		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	78



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	1.61	290.6	ng	4772830	1	7.54	328454	20.0
2-Pentanone, 4-hy...	5.34	16.9	ng	277406	1	7.54	328454	20.0
unknown7.26	7.26	50.6	ng	831194	1	7.54	328454	20.0
Acetic acid, chlo...	16.35	4.1	ng	119572	5	16.46	588372	20.0