

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF083118\
 Data File : BF108690.D
 Acq On : 31 Aug 2018 15:46
 Operator : JU/SJ
 Sample : J4712-08
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-07

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-BF083018.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	5.237	490	493	502	rBV	35570	53760	2.61%	0.331%
2	5.637	557	561	592	rBV	418796	1366640	66.27%	8.426%
3	6.631	727	730	750	rBV	606689	1581194	76.67%	9.748%
4	6.772	750	754	781	rVB	1184294	1988607	96.43%	12.260%
5	7.001	789	793	799	rBV	233451	397377	19.27%	2.450%
6	7.054	799	802	815	rVV	235664	714879	34.66%	4.407%
7	7.154	815	819	838	rVB	972014	1513218	73.38%	9.329%
8	7.566	885	889	911	rBV	522409	1131327	54.86%	6.975%
9	8.278	1007	1010	1033	rBV	367463	659876	32.00%	4.068%
10	9.348	1189	1192	1205	rBV	1604990	2062293	100.00%	12.715%
11	9.742	1255	1259	1269	rBV	167907	227939	11.05%	1.405%
12	10.036	1306	1309	1322	rVB	498227	593162	28.76%	3.657%
13	10.430	1373	1376	1381	rBV2	90576	98252	4.76%	0.606%
14	10.701	1419	1422	1424	rBV	63476	57548	2.79%	0.355%
15	10.836	1441	1445	1453	rBV	728894	1032912	50.09%	6.368%
16	11.248	1512	1515	1518	rBV	56306	62881	3.05%	0.388%
17	11.542	1561	1565	1572	rBV	414314	631804	30.64%	3.895%
18	12.048	1648	1651	1657	rBV	188377	302129	14.65%	1.863%
19	13.124	1831	1834	1840	rBV	1543217	1744132	84.57%	10.753%

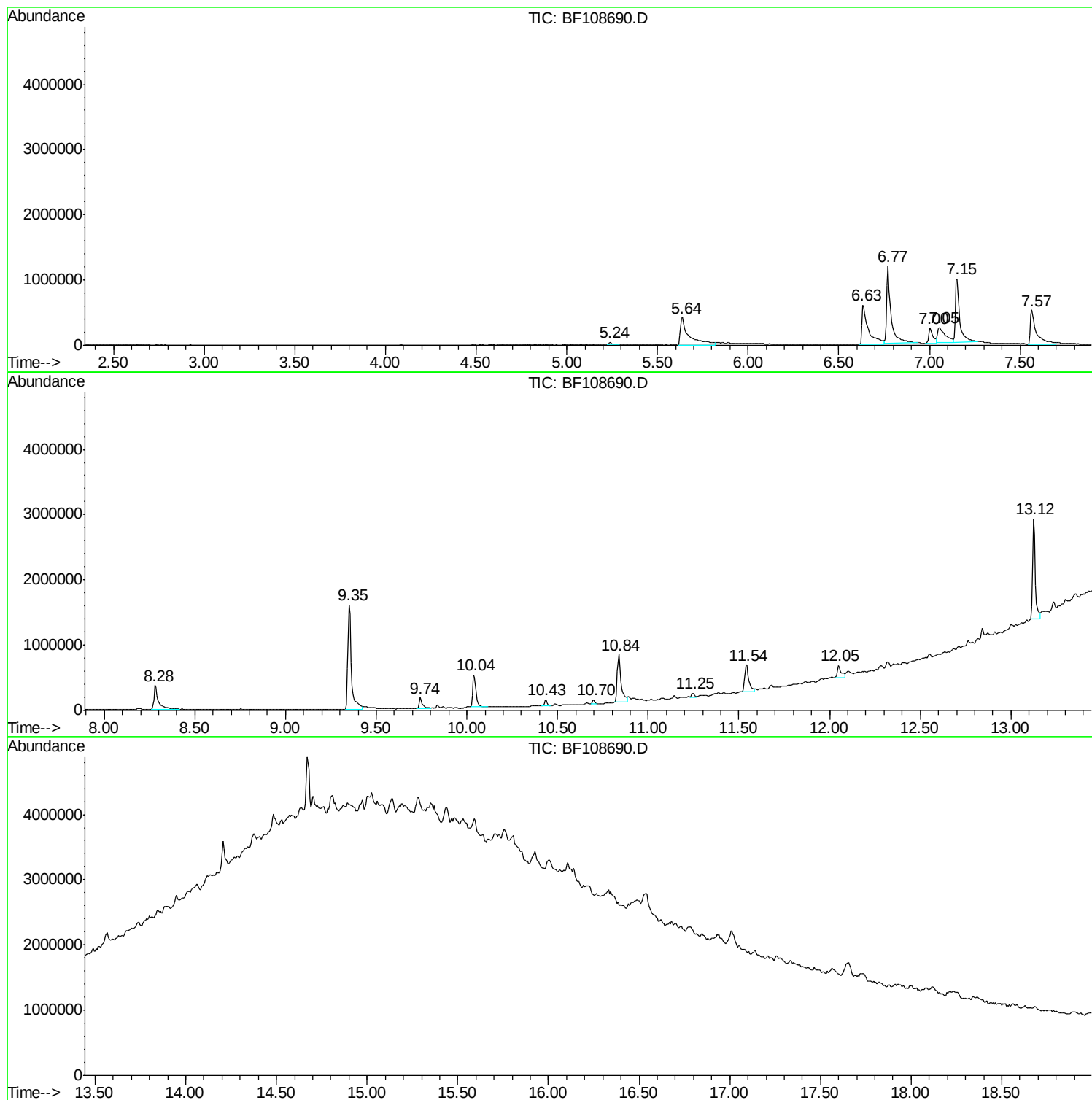
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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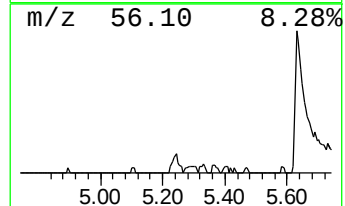
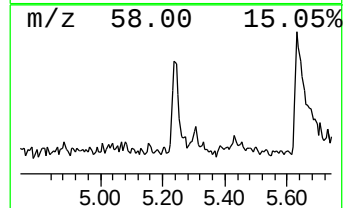
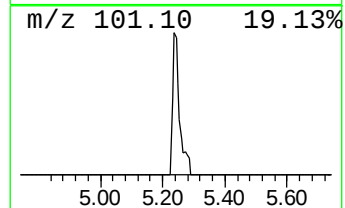
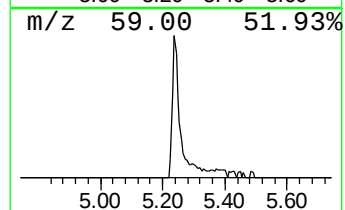
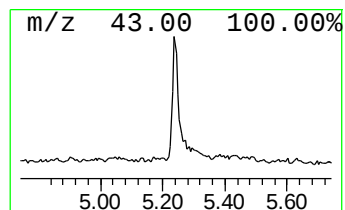
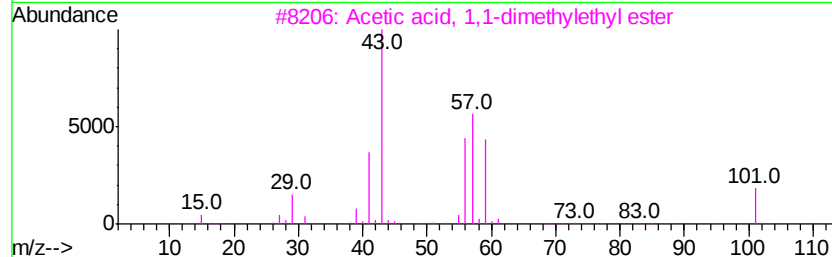
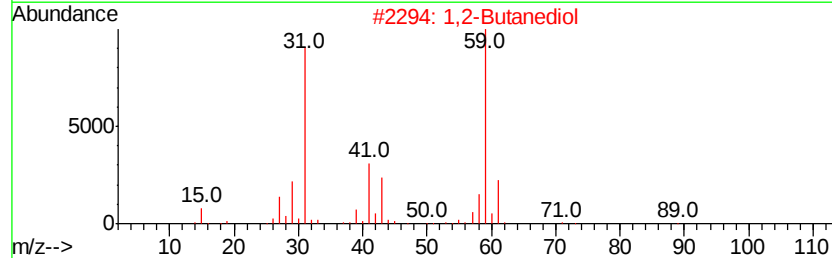
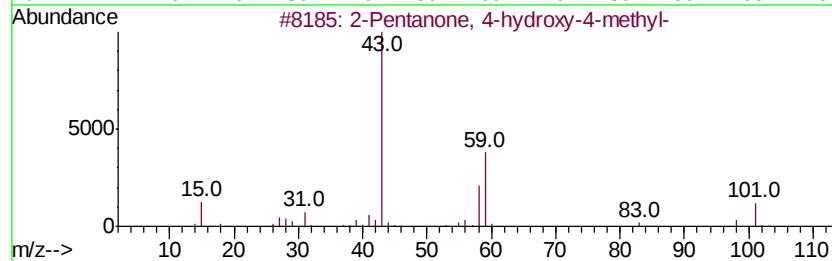
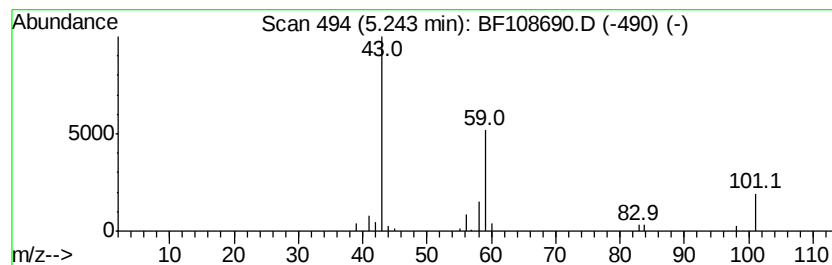
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.24	2.71 ng	53760	1,4-Dichlorobenzene-d4	7.00	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	1,2-Butanediol	90	C4H10O2	000584-03-2	28
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
4	Silane, ethyldimethyl-	88	C4H12Si	000758-21-4	9
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9



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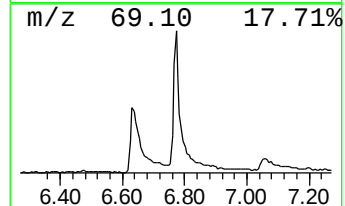
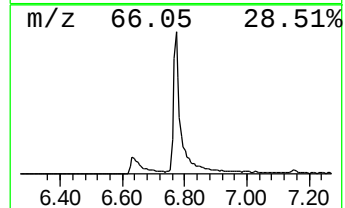
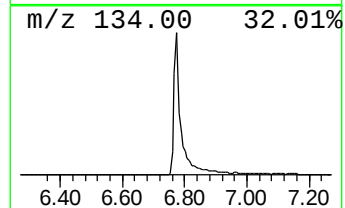
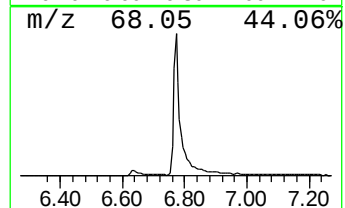
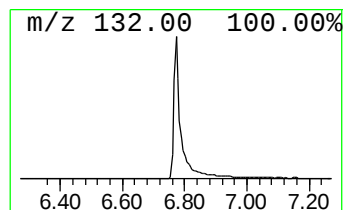
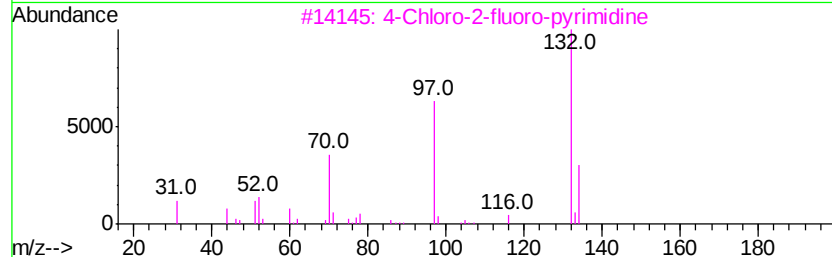
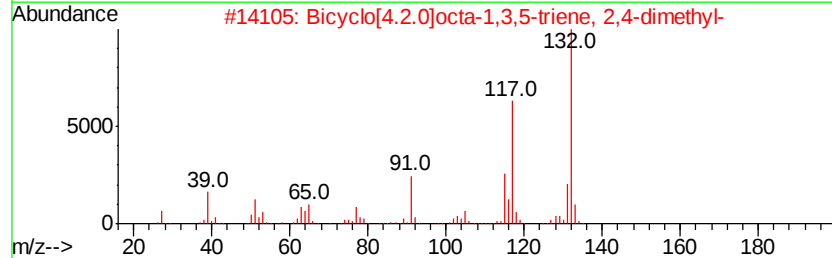
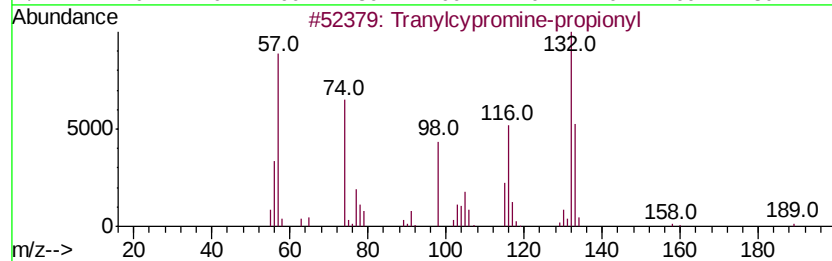
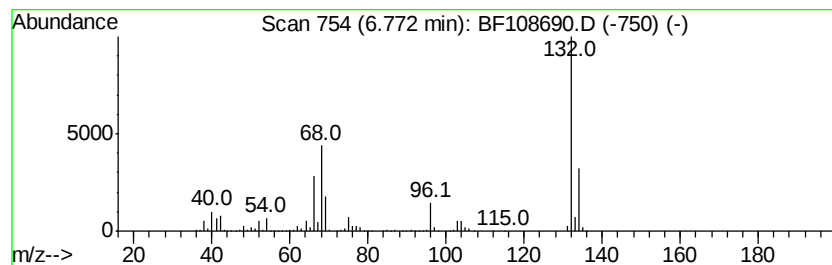
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Peak Number 2 unknown6.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	100.09 ng	1988610	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranvlcvpromine-propionyl	189	C12H15NO	1000123-86-3	10
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		5-Aminoindole	132	C8H8N2	005192-03-0	9



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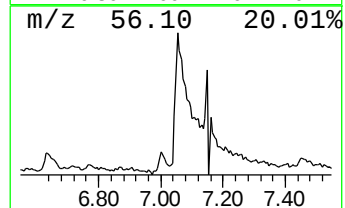
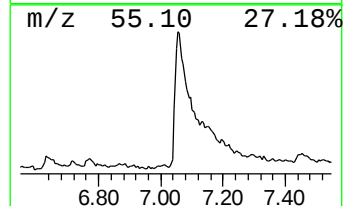
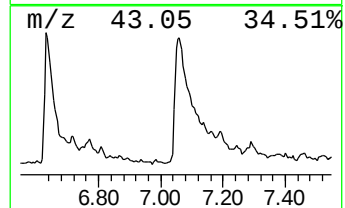
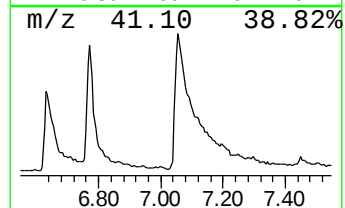
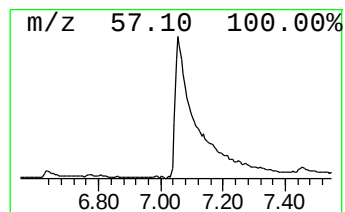
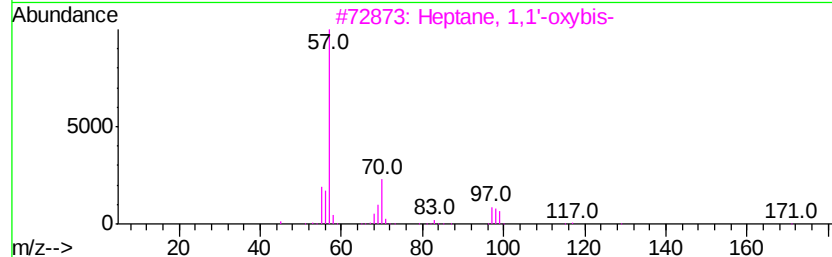
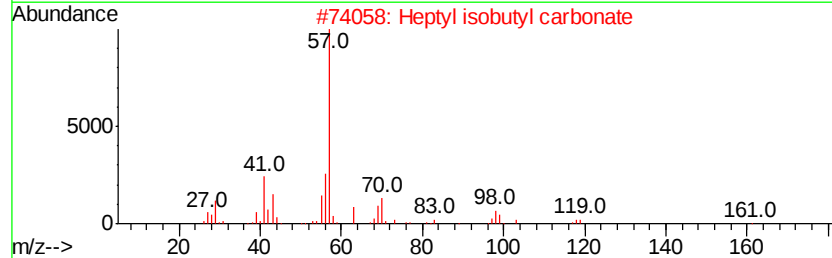
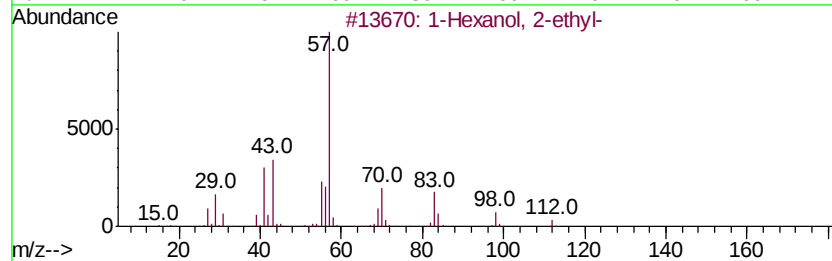
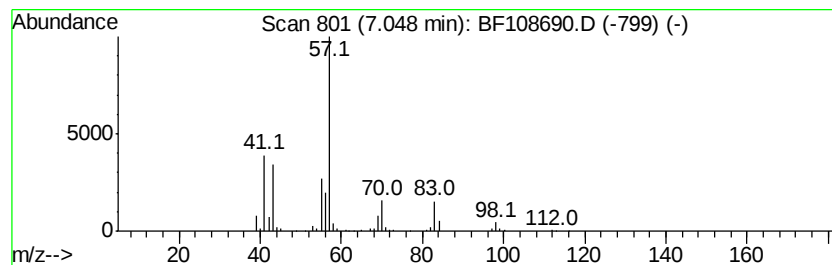
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Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.05	35.98 ng	714879	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2		Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	64
3		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	59
4		1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	47
5		1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	45



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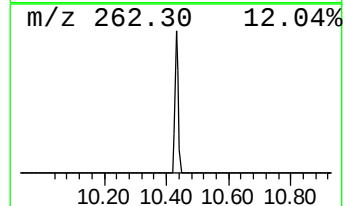
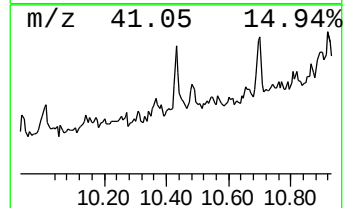
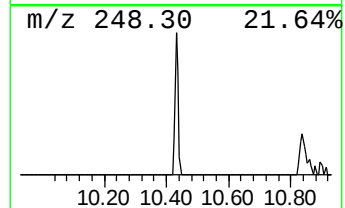
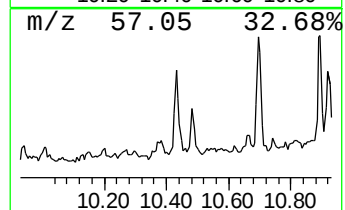
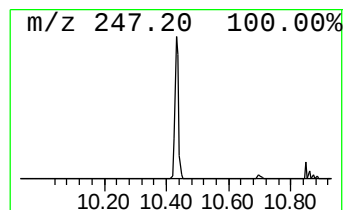
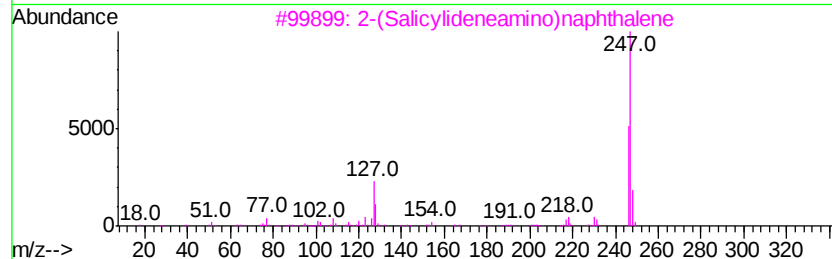
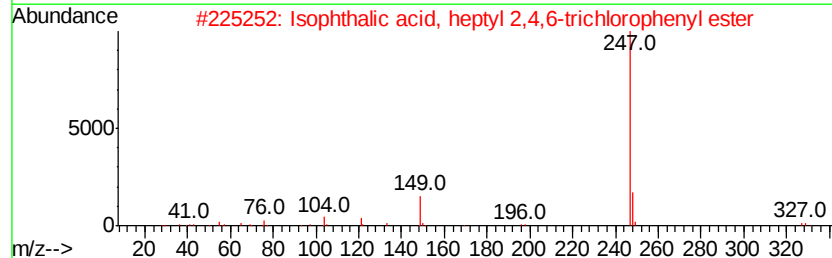
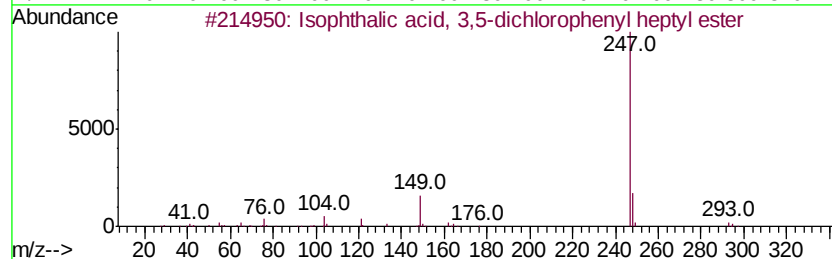
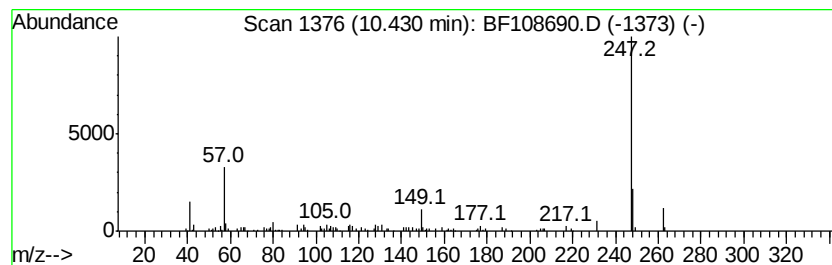
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Isophthalic acid, 3,5-dichl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.43	3.31 ng	98252	Acenaphthene-d10	10.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isophthalic acid, 3,5-dichloroph...	408	C21H22Cl2O4	1000356-58-6	64
2		Isophthalic acid, heptyl 2,4,6-t...	442	C21H21Cl3O4	1000344-57-1	64
3		2-(Salicylideneamino)naphthalene	247	C17H13NO	001689-72-1	64
4		Isophthalic acid, di(1-isopropyl...	362	C22H34O4	1000356-37-2	64
5		Isophthalic acid, heptyl 2,4,5-t...	442	C21H21Cl3O4	1000356-61-4	64



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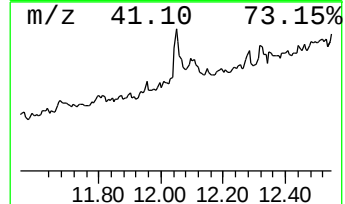
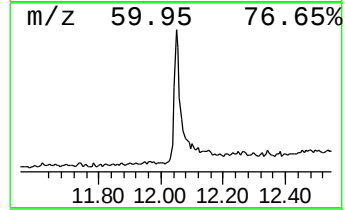
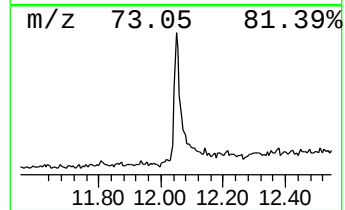
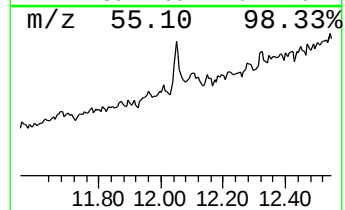
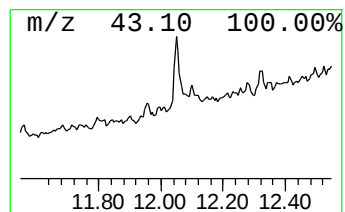
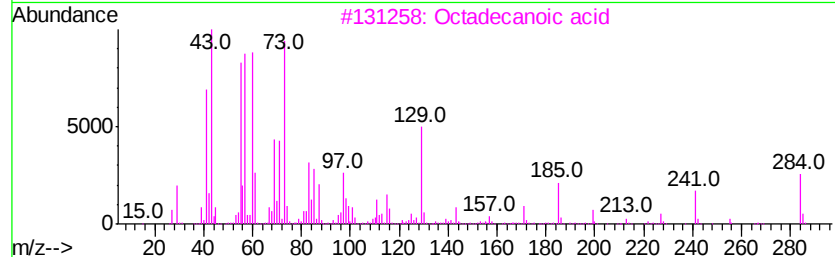
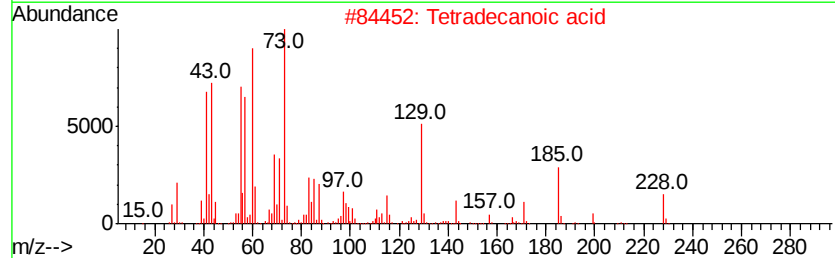
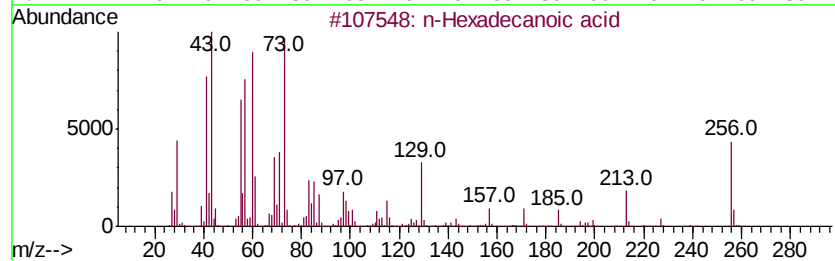
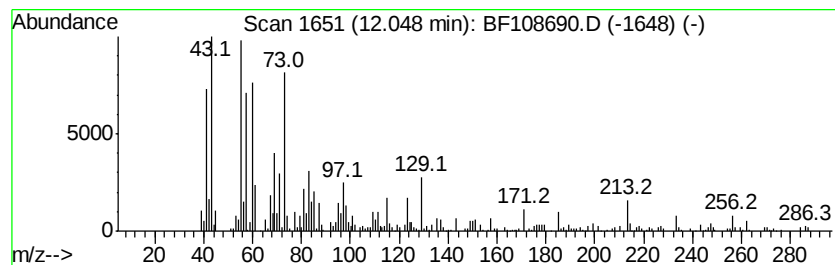
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	9.56 ng	302129	Phenanthrene-d10	11.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3		Octadecanoic acid	284	C18H36O2	000057-11-4	93
4		Heptadecanoic acid	270	C17H34O2	000506-12-7	91
5		Tridecanoic acid	214	C13H26O2	000638-53-9	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.24	2.7	ng	53760	1	7.00	397377	20.0
unknown6.77	6.77	100.1	ng	1988610	1	7.00	397377	20.0
1-Hexanol, 2-ethyl-	7.05	36.0	ng	714879	1	7.00	397377	20.0
Isophthalic acid,...	10.43	3.3	ng	98252	3	10.04	593162	20.0
n-Hexadecanoic acid	12.05	9.6	ng	302129	4	11.54	631804	20.0