

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF080318\
 Data File : BF107948.D
 Acq On : 3 Aug 2018 20:00
 Operator : JU/SJ
 Sample : J4318-05
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BEEBEE-SITE-DEMO-2A

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-BF073018.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	5.184	480	484	502	rBV	219487	371199	12.51%	1.517%
2	5.596	551	554	584	rBV	677882	2064405	69.58%	8.434%
3	6.601	721	725	743	rBV	800684	2128103	71.73%	8.694%
4	6.725	743	746	776	rVB	1573464	2824343	95.19%	11.539%
5	6.954	782	785	807	rVB	263095	675232	22.76%	2.759%
6	7.101	807	810	834	rBV	1347180	2028034	68.36%	8.286%
7	7.519	878	881	905	rBV	534557	1471241	49.59%	6.011%
8	8.236	999	1003	1021	rBV	451299	902684	30.43%	3.688%
9	9.301	1181	1184	1212	rBV	2057588	2966913	100.00%	12.121%
10	9.701	1247	1252	1260	rBV	92418	137434	4.63%	0.561%
11	9.989	1297	1301	1313	rBV	777889	945878	31.88%	3.864%
12	10.789	1433	1437	1463	rBV	903181	1679578	56.61%	6.862%
13	11.489	1552	1556	1568	rBV	532760	933652	31.47%	3.814%
14	11.995	1638	1642	1646	rBV	415068	464568	15.66%	1.898%
15	12.542	1732	1735	1738	rBV2	33997	34879	1.18%	0.143%
16	12.707	1760	1763	1772	rBV	134987	219643	7.40%	0.897%
17	12.777	1772	1775	1782	rVV2	123414	158766	5.35%	0.649%
18	12.919	1796	1799	1800	rBV2	32304	35425	1.19%	0.145%
19	12.942	1800	1803	1808	rVB	102397	148470	5.00%	0.607%
20	13.071	1821	1825	1836	rBV	1753385	2246607	75.72%	9.179%
21	13.948	1971	1974	1979	rVB2	119991	150018	5.06%	0.613%
22	14.083	1995	1997	2001	rBV	46217	41962	1.41%	0.171%
23	14.142	2003	2007	2020	rBV	622080	1022546	34.46%	4.178%
24	15.671	2263	2267	2282	rVB	431698	824904	27.80%	3.370%

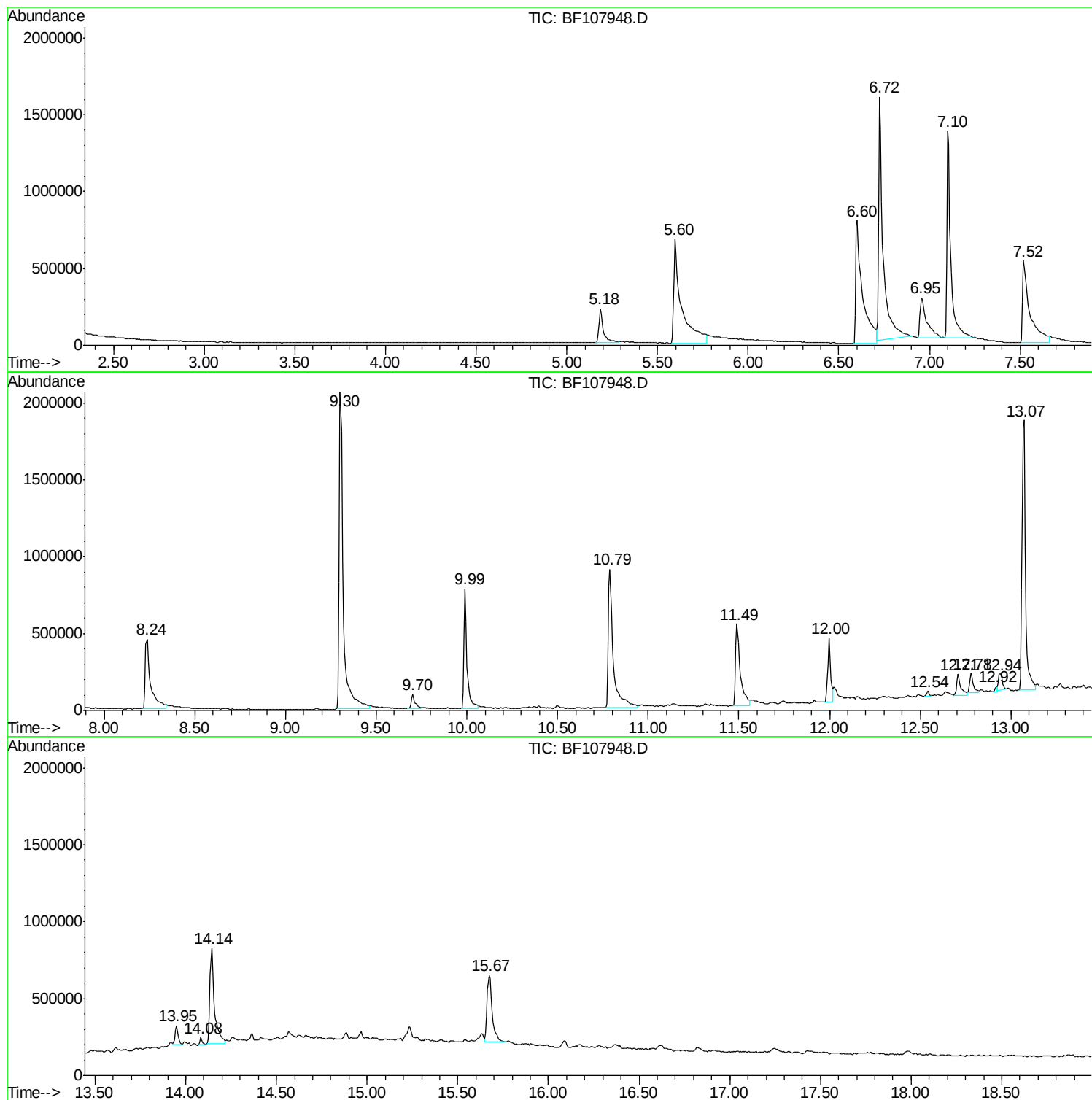
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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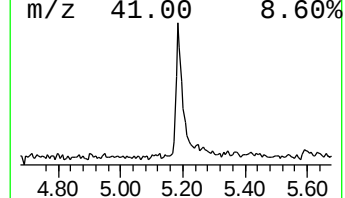
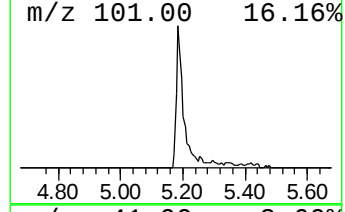
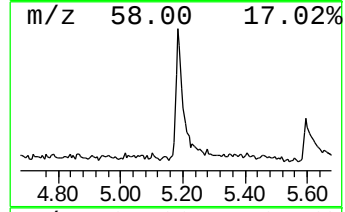
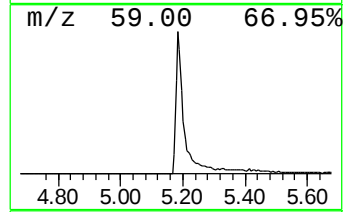
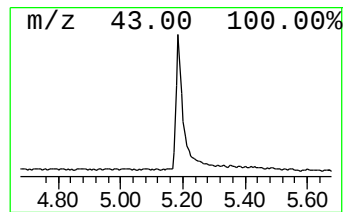
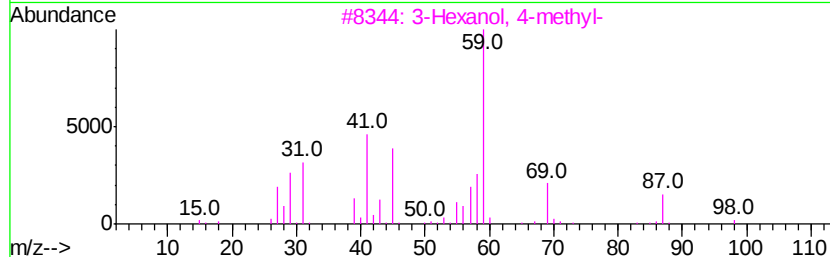
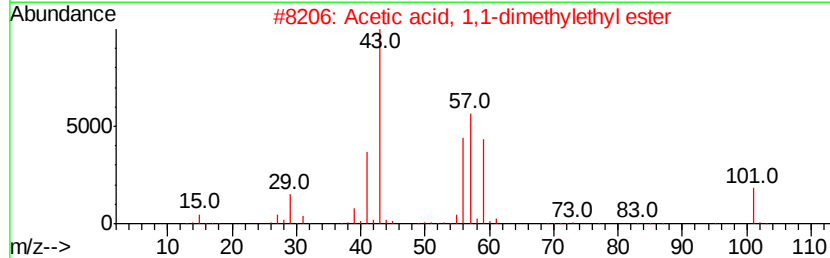
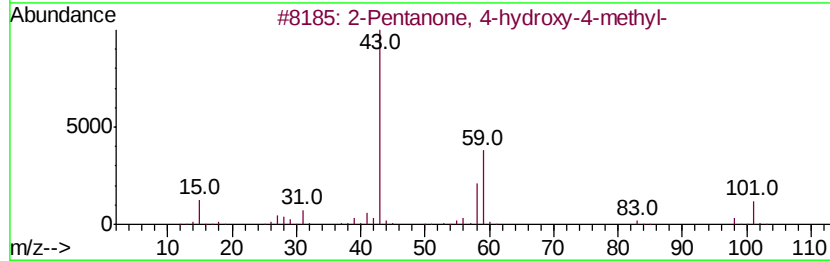
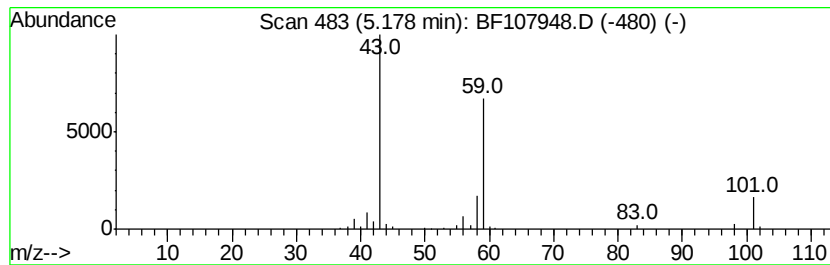
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.18	10.99 ng	371199	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5		Acetone	58	C3H6O	000067-64-1	9



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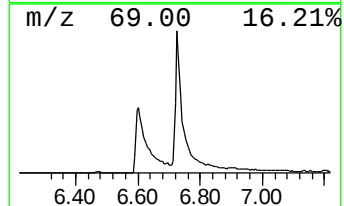
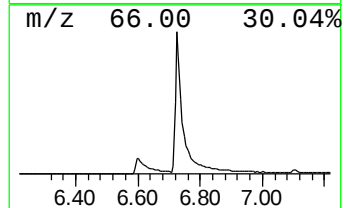
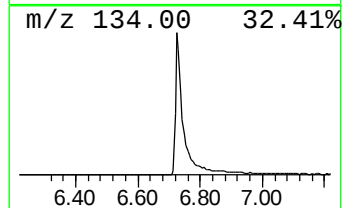
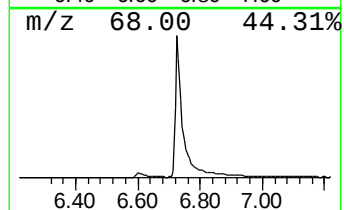
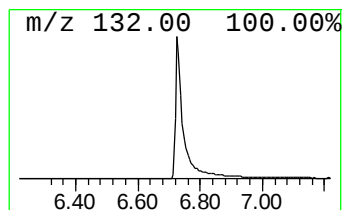
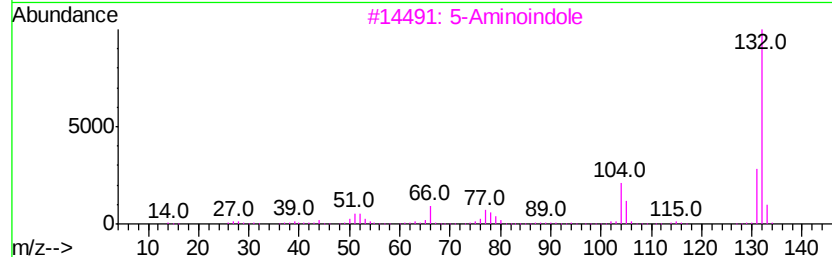
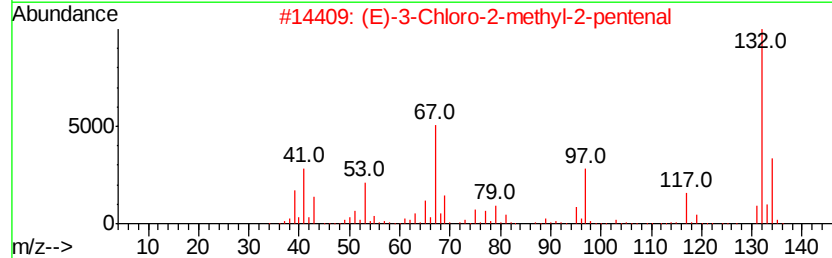
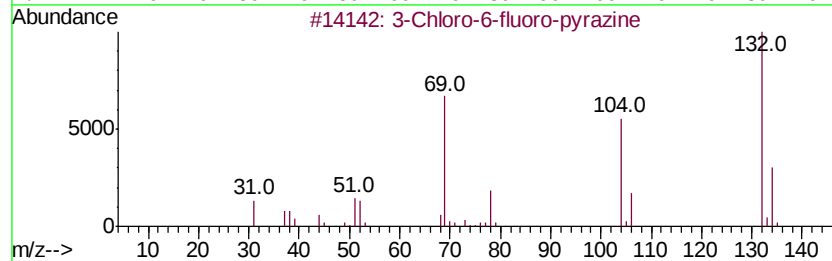
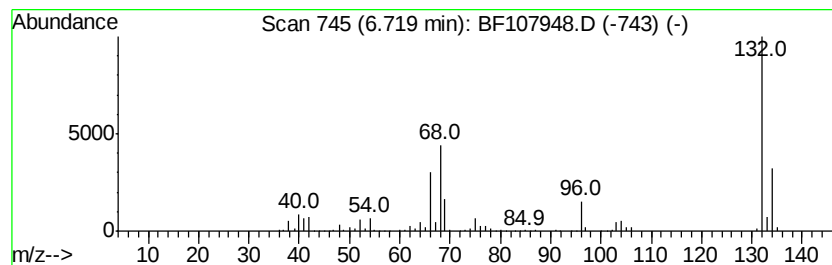
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	83.66 ng	2824340	1,4-Dichlorobenzene-d4	6.95

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	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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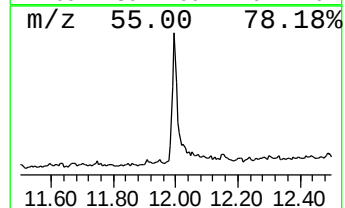
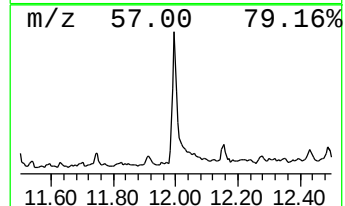
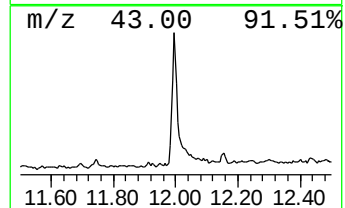
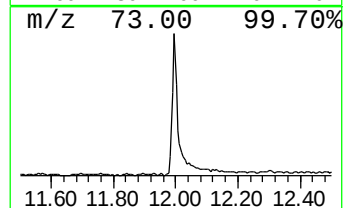
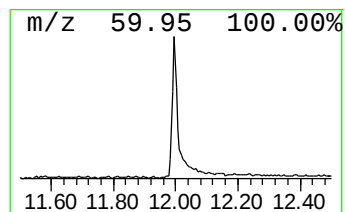
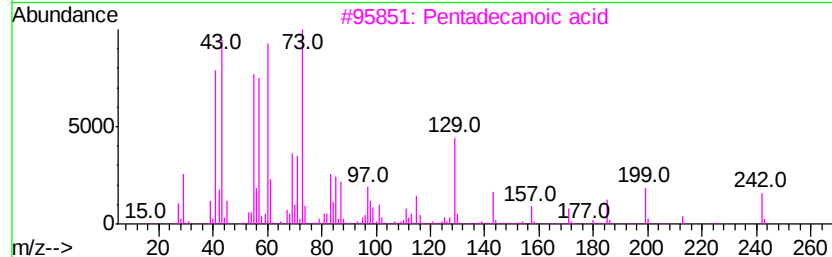
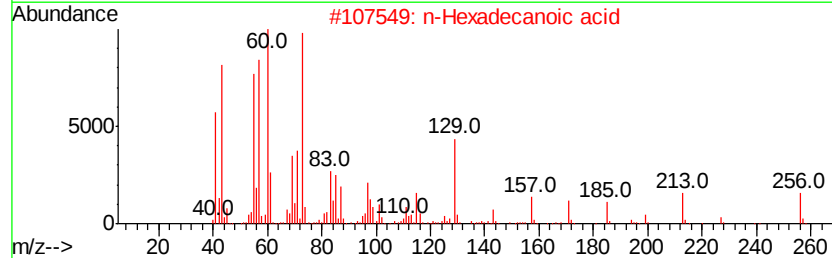
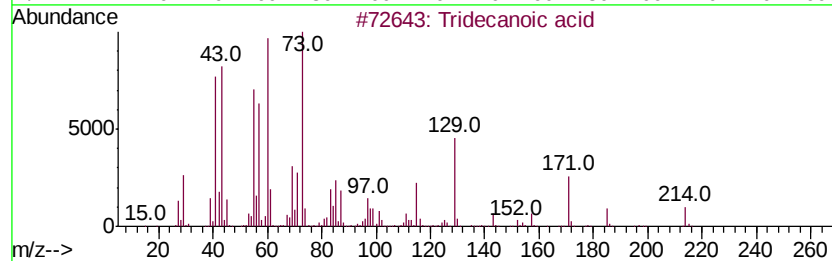
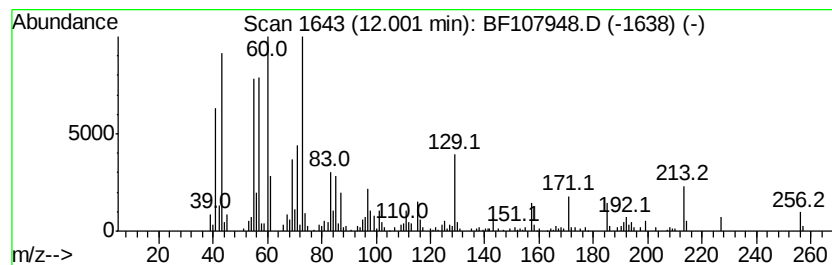
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	9.95 ng	464568	Phenanthrene-d10	11.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	94
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		n-Decanoic acid	172	C10H20O2	000334-48-5	70



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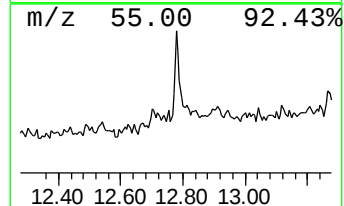
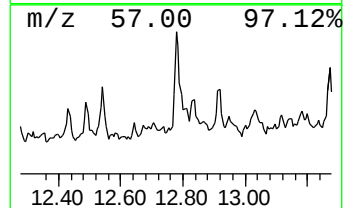
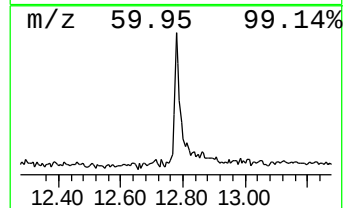
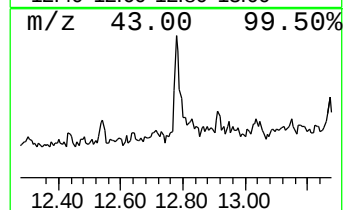
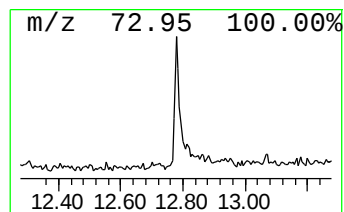
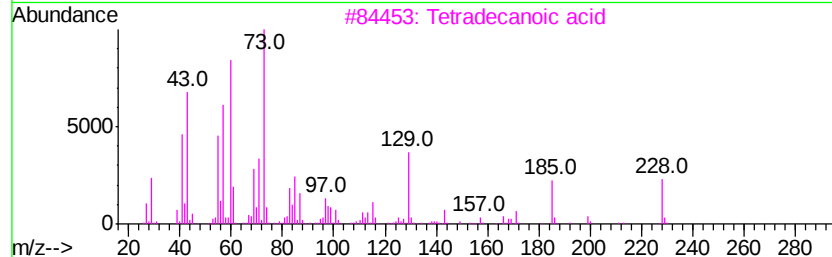
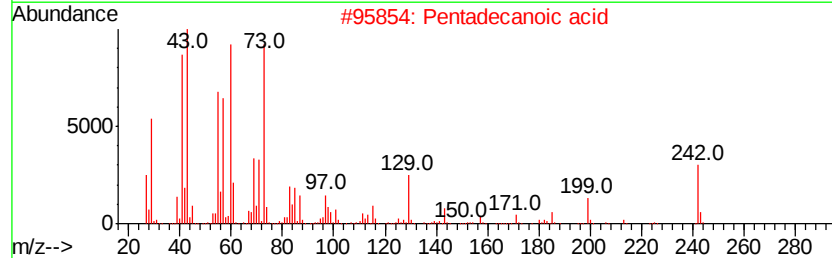
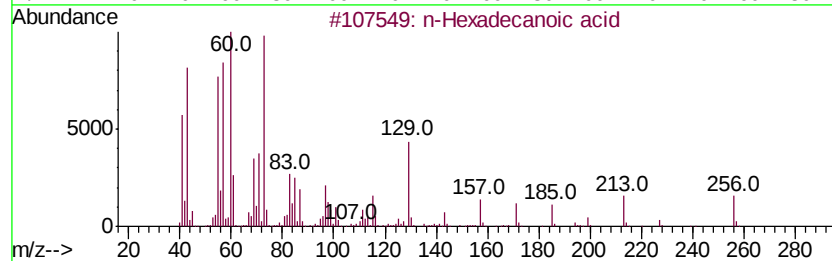
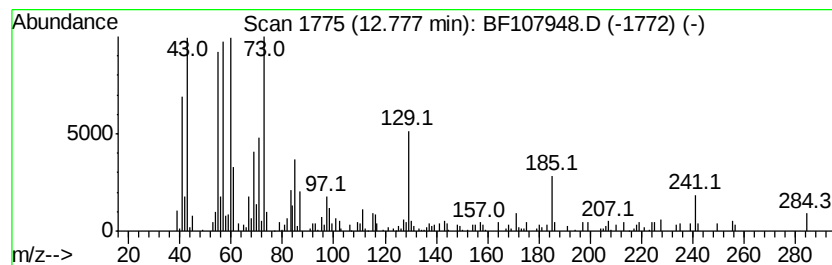
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	3.40 ng	158766	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Undecanoic acid	186	C11H22O2	000112-37-8	64
5	Octadecanoic acid	284	C18H36O2	000057-11-4	64



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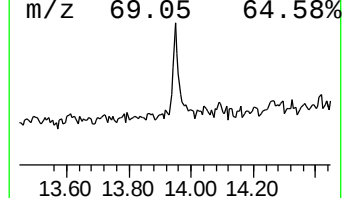
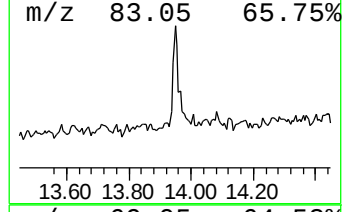
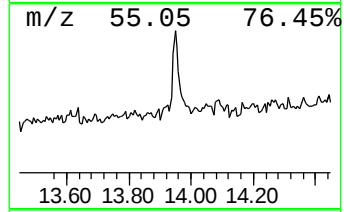
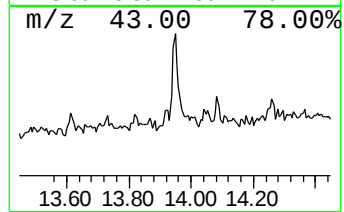
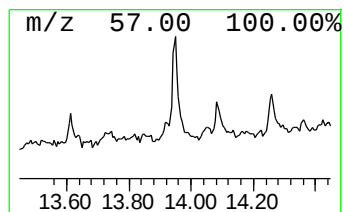
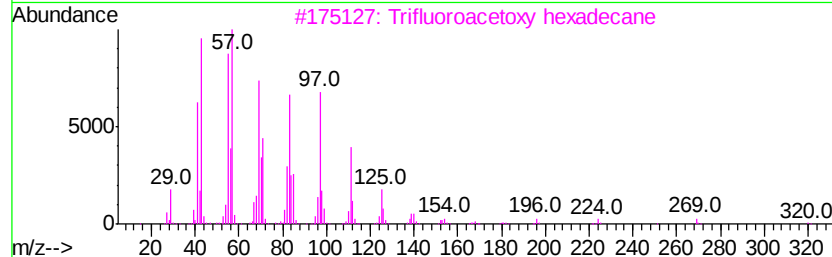
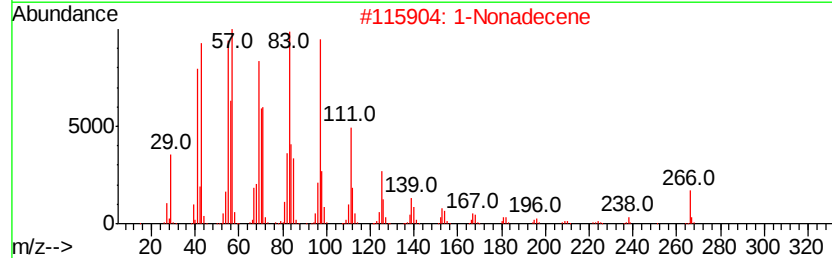
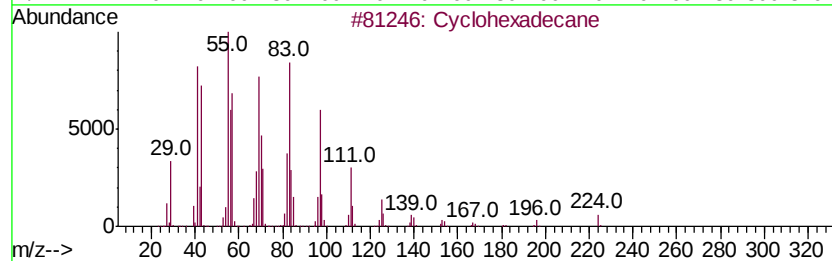
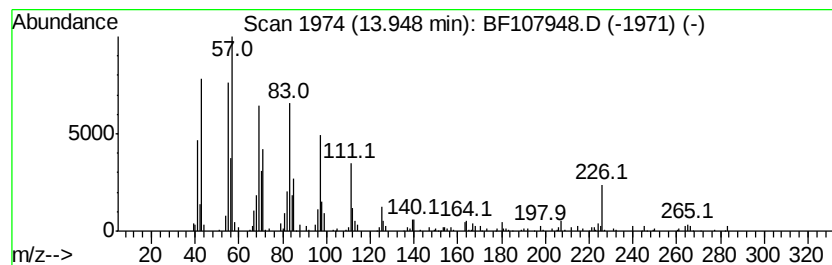
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclohexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	2.93 ng	150018	Chrysene-d12	14.14
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexadecane	224 C16H32	000295-65-8 95
2		1-Nonadecene	266 C19H38	018435-45-5 93
3		Trifluoroacetoxy hexadecane	338 C18H33F3O2	006222-03-3 93
4		Heptadecyl heptafluorobutyrat	452 C21H35F7O2	959085-66-6 90
5		Heptafluorobutyric acid, hexadec...	438 C20H33F7O2	006385-15-5 87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.18	11.0	ng	371199	1	6.95	675232	20.0
unknown6.72	6.72	83.7	ng	2824340	1	6.95	675232	20.0
Tridecanoic acid	12.00	9.9	ng	464568	4	11.49	933652	20.0
n-Hexadecanoic acid	12.78	3.4	ng	158766	4	11.49	933652	20.0
Cyclohexadecane	13.95	2.9	ng	150018	5	14.14	1022550	20.0