

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022417\
 Data File : BF093159.D
 Acq On : 24 Feb 2017 22:04
 Operator : SJ/MA
 Sample : I1957-11
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SRI-SB-7(8-9)20170222

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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	5.001	252	255	267	rBV	961180	1569510	42.65%	4.507%
2	5.424	289	292	295	rBV	3111047	3041019	82.64%	8.733%
3	6.476	381	384	386	rBV	2792850	3679717	100.00%	10.567%
4	6.602	392	395	397	rBV	3380913	3483974	94.68%	10.005%
5	6.830	413	415	418	rBV	1118445	928341	25.23%	2.666%
6	6.990	426	429	431	rBV	2758813	2691522	73.14%	7.729%
7	7.402	462	465	467	rBV	2272483	2169236	58.95%	6.230%
8	8.122	525	528	530	rBV	1420365	1245228	33.84%	3.576%
9	9.196	619	622	625	rBV	3292852	3611950	98.16%	10.373%
10	9.596	655	657	659	rBV	235519	196998	5.35%	0.566%
11	9.871	679	681	684	rBV	1107151	1325385	36.02%	3.806%
12	10.305	718	719	721	rVB	71552	54196	1.47%	0.156%
13	10.659	748	750	753	rBV2	1460041	1986062	53.97%	5.704%
14	10.773	759	760	765	rVB	77857	116711	3.17%	0.335%
15	11.231	798	800	801	rBV	63936	82861	2.25%	0.238%
16	11.356	809	811	814	rBV	1459489	1400650	38.06%	4.022%
17	11.654	835	837	839	rBV	60302	51286	1.39%	0.147%
18	12.945	947	950	953	rBV	3240114	3447749	93.70%	9.901%
19	13.425	990	992	997	rVB	360560	341808	9.29%	0.982%
20	13.505	997	999	1004	rVB2	23808	36971	1.00%	0.106%
21	13.837	1026	1028	1037	rBV	170692	283311	7.70%	0.814%
22	13.997	1040	1042	1045	rVB	1448587	1305719	35.48%	3.750%
23	14.465	1079	1083	1087	rBV4	15392	38829	1.06%	0.112%
24	14.740	1105	1107	1112	rBV2	151202	229320	6.23%	0.659%
25	14.831	1113	1115	1117	rVB	62269	59450	1.62%	0.171%
26	15.425	1164	1167	1174	rBV	806304	1060071	28.81%	3.044%
27	15.848	1201	1204	1207	rBV	48889	72153	1.96%	0.207%
28	16.328	1242	1246	1250	rBV	48550	88473	2.40%	0.254%
29	16.877	1291	1294	1299	rBV	30085	64088	1.74%	0.184%
30	17.540	1348	1352	1358	rVB	23240	53398	1.45%	0.153%
31	18.317	1416	1420	1427	rVB6	12513	44203	1.20%	0.127%
32	19.243	1495	1501	1506	rBV6	16361	61333	1.67%	0.176%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

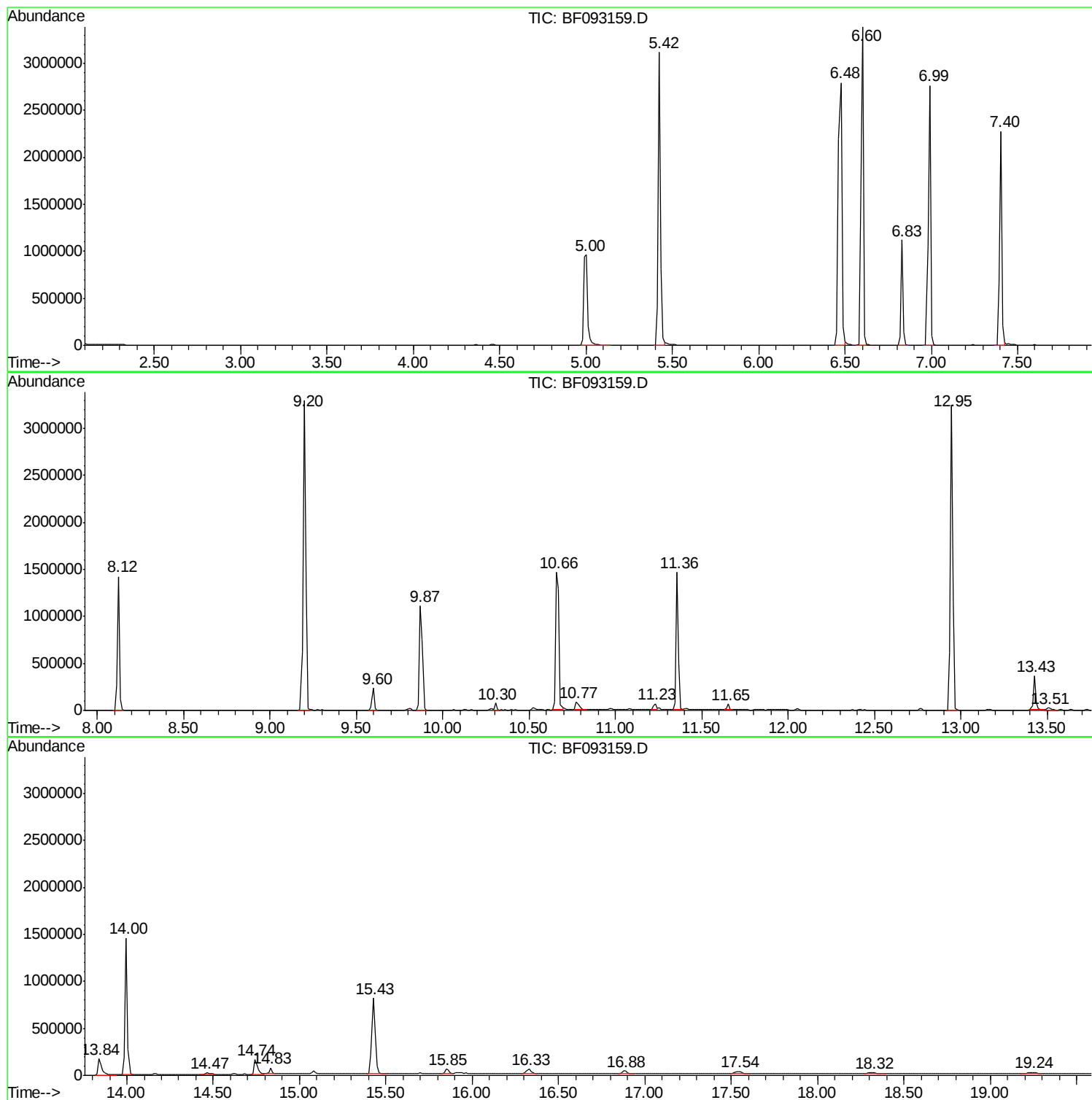
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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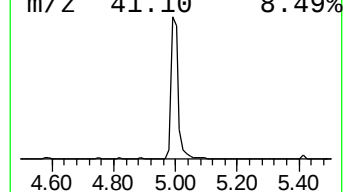
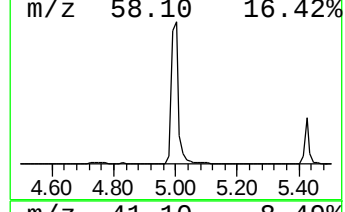
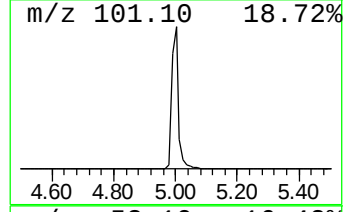
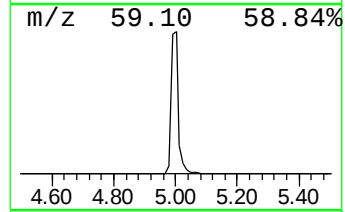
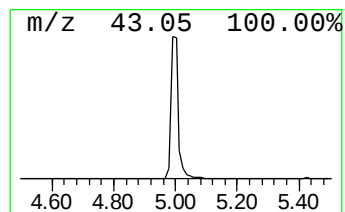
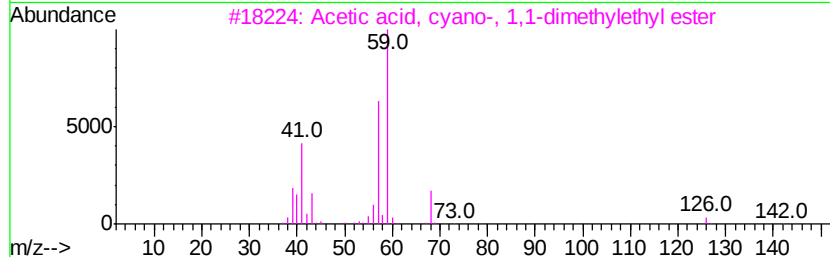
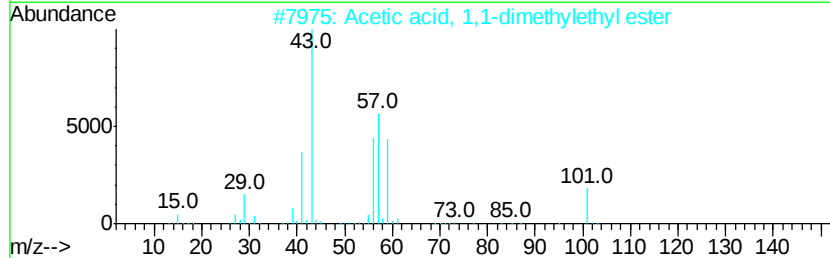
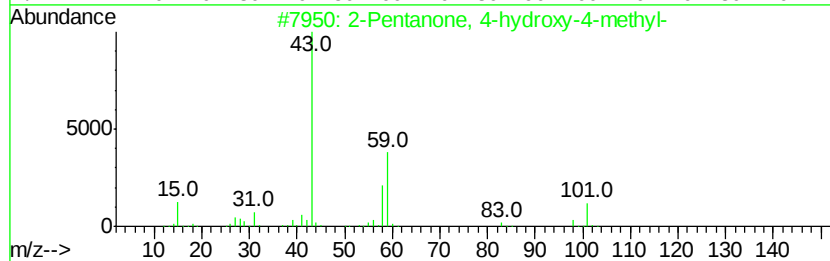
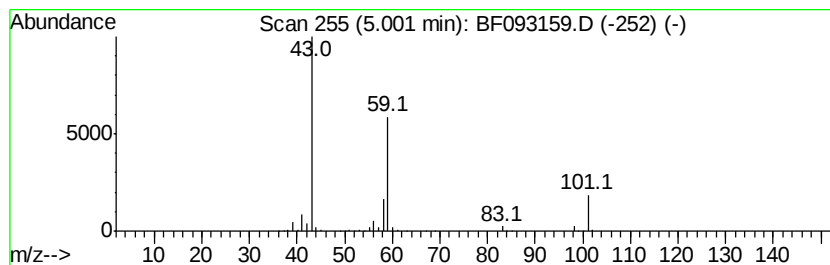
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	33.81 ng	1569510	1,4-Dichlorobenzene-d4	6.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9
5			1,2-Butanediol, (+/-)-	90	C4H10O2	026171-83-5	9



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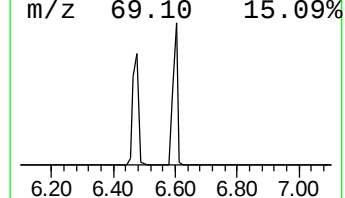
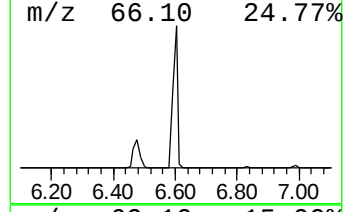
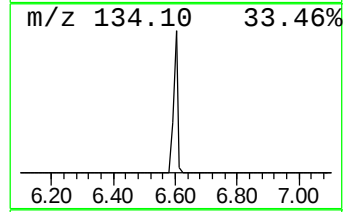
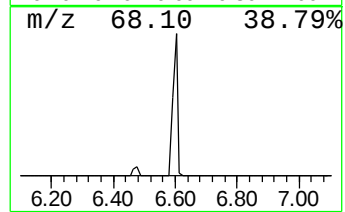
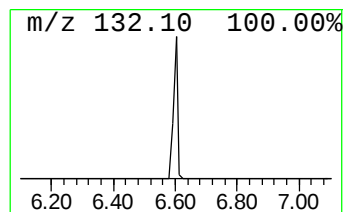
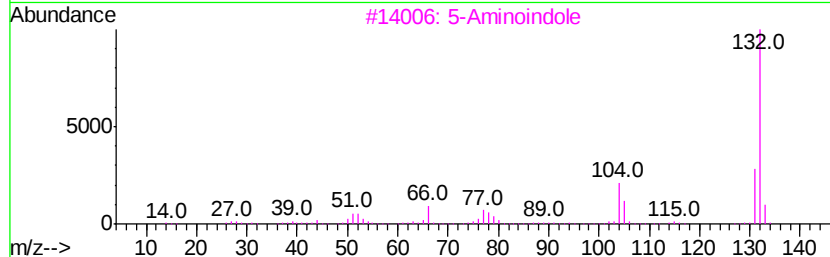
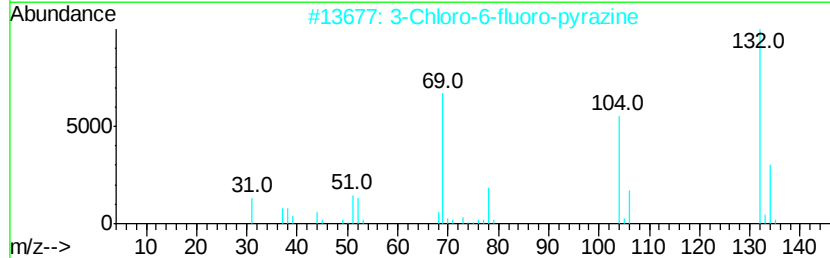
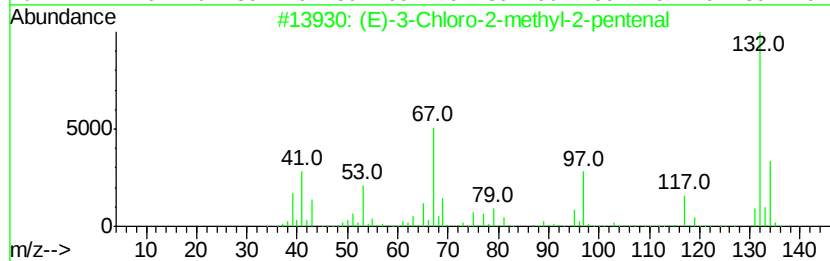
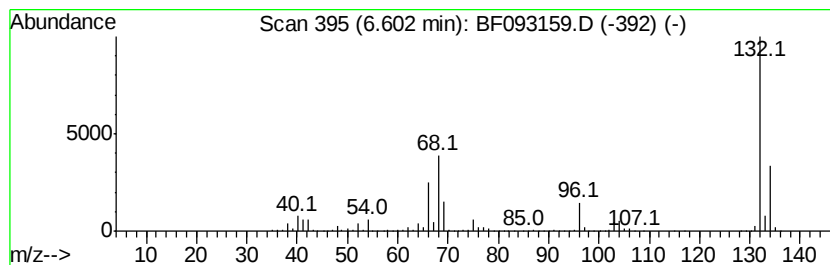
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Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	75.06 ng	3483970	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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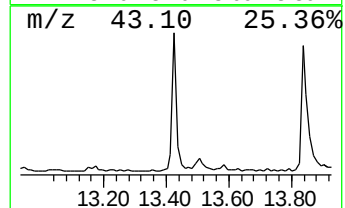
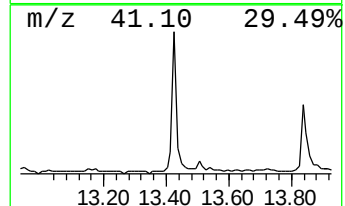
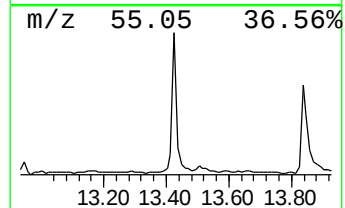
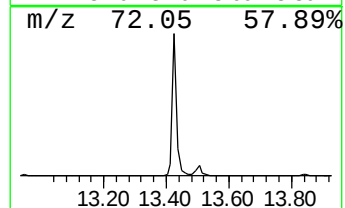
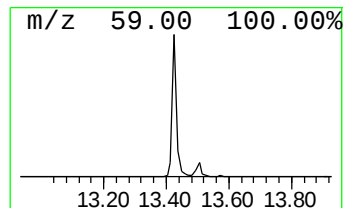
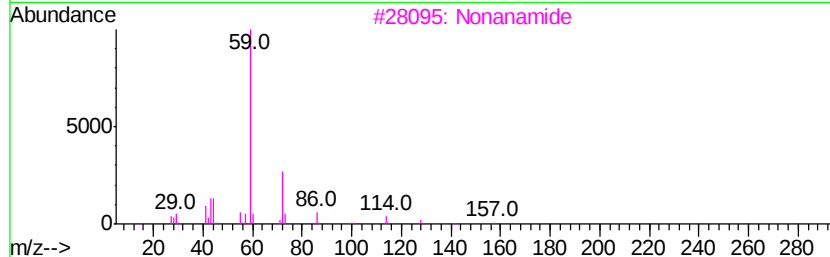
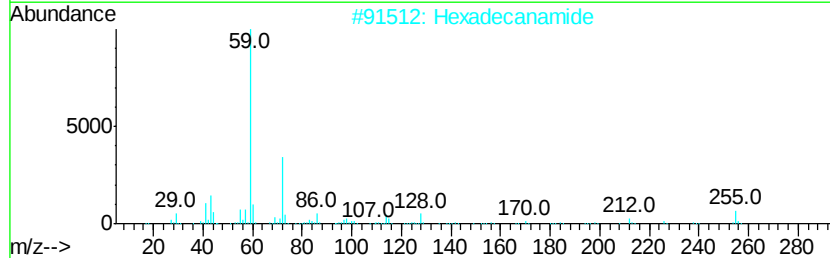
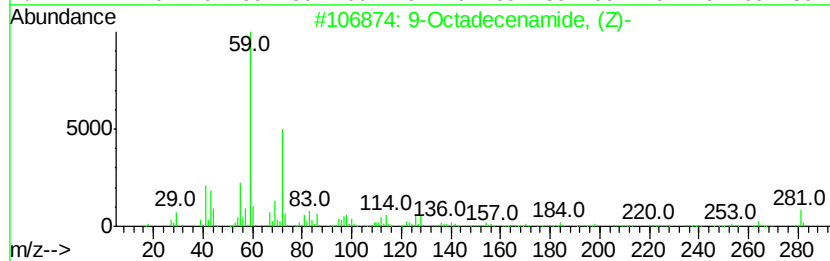
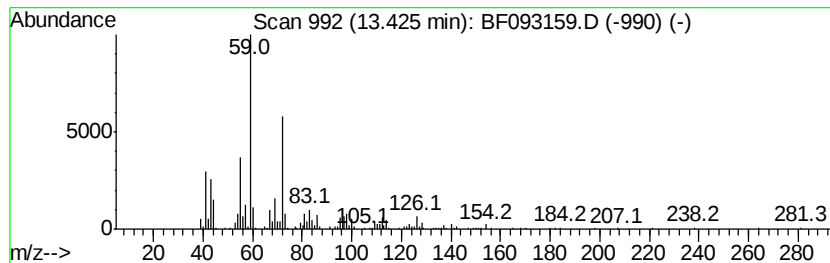
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.43	5.24 ng	341808	Chrysene-d12	14.00	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	78
2	Hexadecanamide	255	C16H33NO	000629-54-9	72
3	Nonanamide	157	C9H19NO	001120-07-6	50
4	Octanamide	143	C8H17NO	000629-01-6	50
5	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	50



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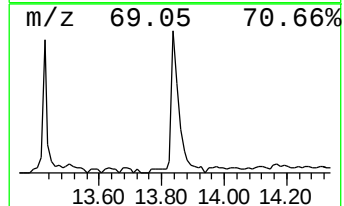
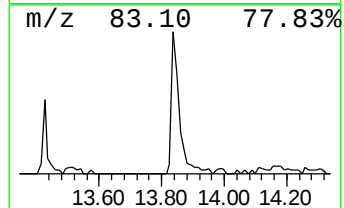
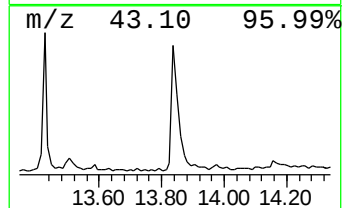
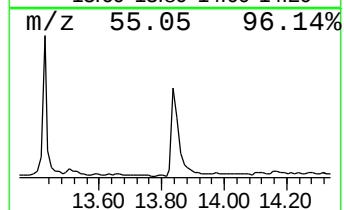
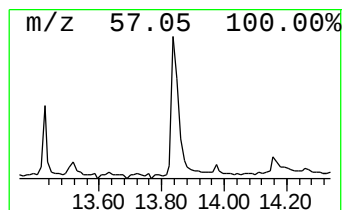
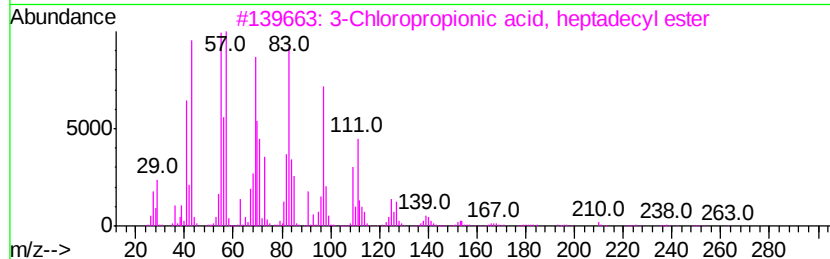
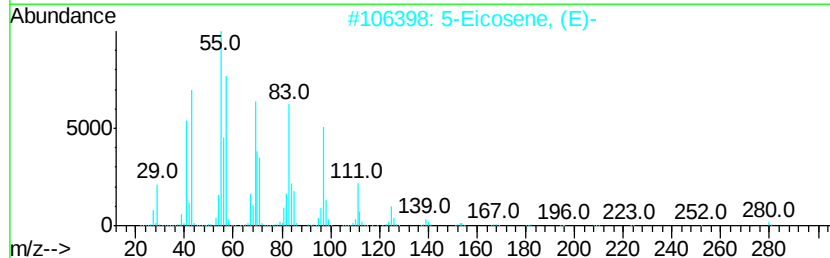
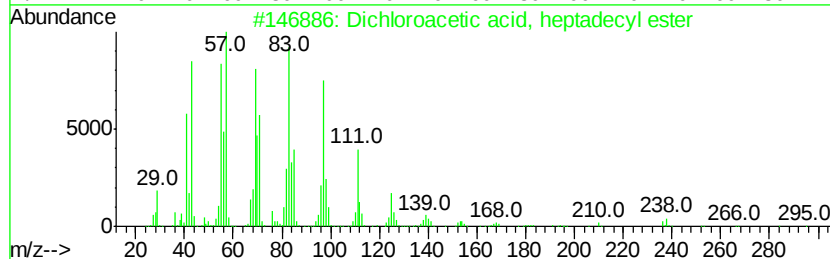
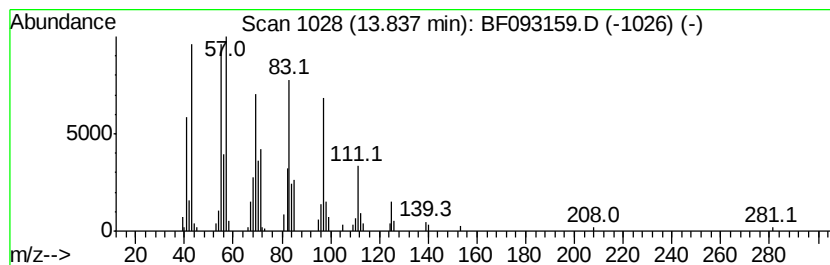
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Dichloroacetic acid, heptad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	4.34 ng	283311	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
2		5-Eicosene, (E)-	280	C20H40	074685-30-6	91
3		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
4		2-Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91
5		3-Eicosene, (E)-	280	C20H40	074685-33-9	91



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.00	33.8	ng	1569510	1	6.83	928341	20.0
unknown6.60	6.60	75.1	ng	3483970	1	6.83	928341	20.0
9-Octadecenamide, ...	13.43	5.2	ng	341808	5	14.00	1305720	20.0
Dichloroacetic ac...	13.84	4.3	ng	283311	5	14.00	1305720	20.0