

Data Path : V:\HPCHEM1\BNA F\DATA\BF112115\
 Data File : BF083139.D
 Acq On : 22 Nov 2015 5:31
 Operator : UM/IZ
 Sample : G4480-07
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LIBERTY SF_002-SPLPSVOC3

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-BF112115.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	4.810	244	247	264	rBV	904465	1279359	18.79%	2.604%
2	5.255	284	286	296	rBV	2676852	2785503	40.91%	5.670%
3	6.307	377	378	386	rBV	1188992	1814867	26.65%	3.694%
4	6.421	386	388	391	rBV	4008828	4638710	68.12%	9.442%
5	6.650	406	408	411	rBV	1356976	1226329	18.01%	2.496%
6	6.810	419	422	424	rBV	4848091	4602207	67.59%	9.367%
7	7.221	455	458	461	rBV	3367036	3730084	54.78%	7.592%
8	7.358	468	470	476	rVB2	67032	106516	1.56%	0.217%
9	7.941	518	521	523	rBV	1651638	1595937	23.44%	3.248%
10	9.016	613	615	618	rBV	4676399	6656455	97.76%	13.549%
11	9.347	641	644	646	rBV	39390	72572	1.07%	0.148%
12	9.427	649	651	653	rBV	129438	197760	2.90%	0.403%
13	9.690	671	674	676	rBV	1566019	1770495	26.00%	3.604%
14	10.113	706	711	712	rBV	46326	76386	1.12%	0.155%
15	10.479	740	743	745	rBV	3507567	4371510	64.20%	8.898%
16	10.604	752	754	758	rVB	106326	126879	1.86%	0.258%
17	11.050	791	793	795	rBV	108808	108010	1.59%	0.220%
18	11.165	800	803	805	rBV	1788881	1831225	26.89%	3.727%
19	11.656	842	846	849	rBV2	39791	102280	1.50%	0.208%
20	11.713	849	851	855	rBV3	641125	810770	11.91%	1.650%
21	12.399	907	911	916	rBV4	54546	159280	2.34%	0.324%
22	12.502	917	920	926	rVB	408197	597441	8.77%	1.216%
23	12.753	939	942	944	rBV	6241916	6809125	100.00%	13.859%
24	13.668	1019	1022	1030	rBV	276092	387925	5.70%	0.790%
25	13.782	1030	1032	1035	rBV	1701769	1744104	25.61%	3.550%
26	14.639	1105	1107	1109	rBV	82120	82759	1.22%	0.168%
27	15.153	1149	1152	1155	rBV	1097854	1445758	21.23%	2.943%

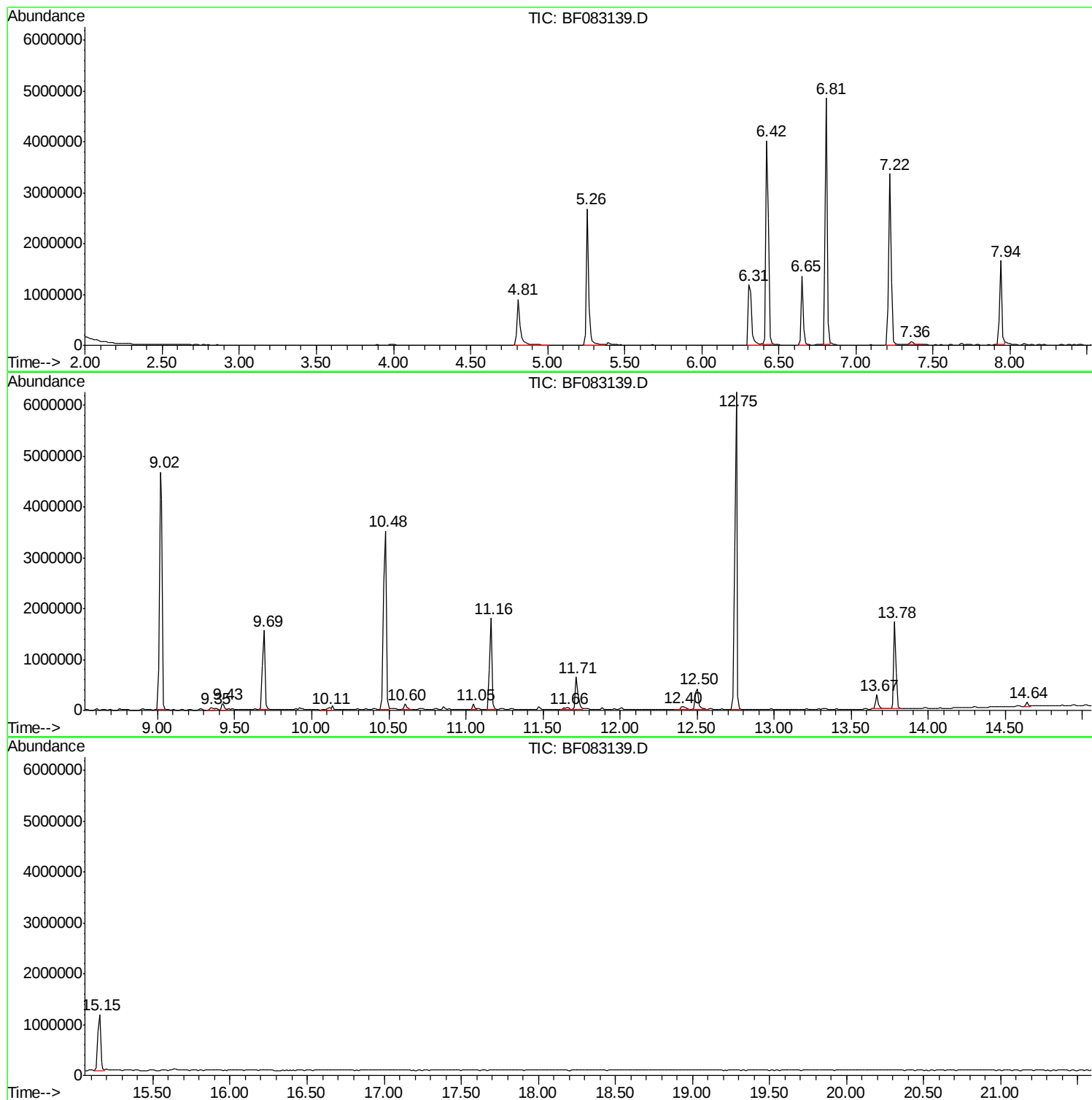
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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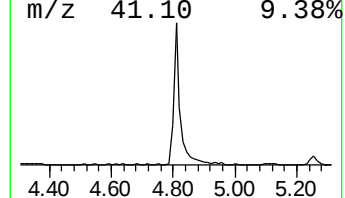
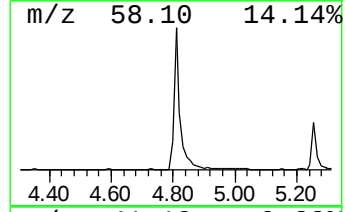
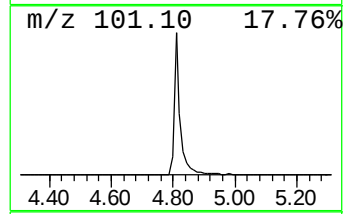
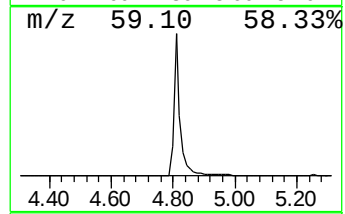
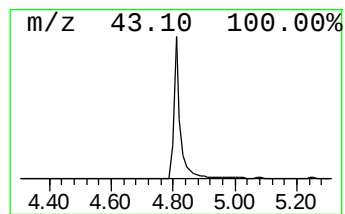
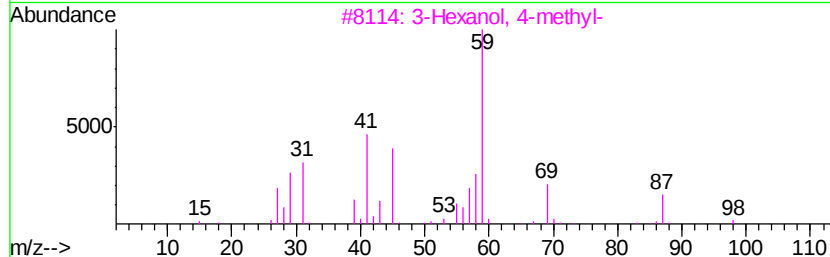
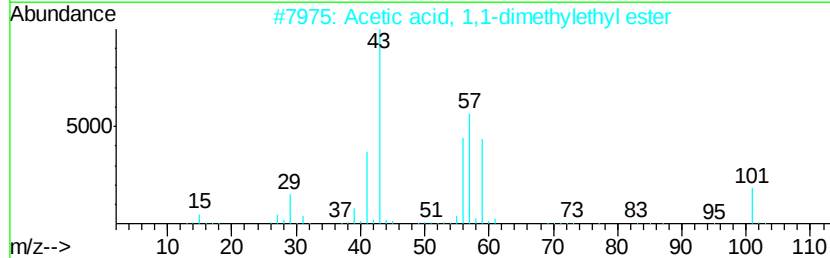
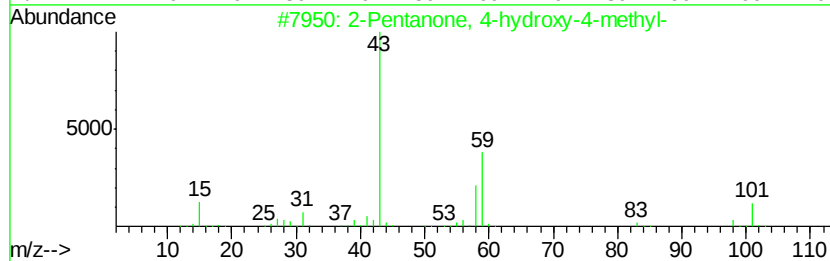
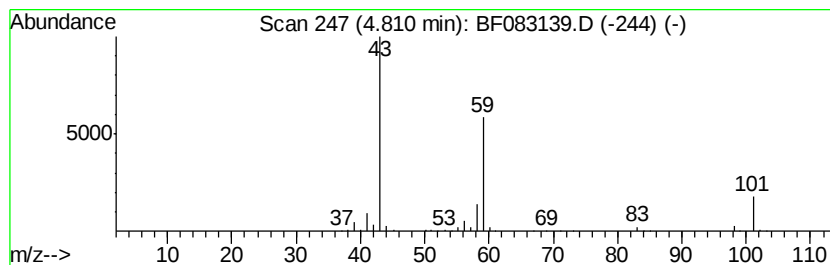
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.81	20.86 ng	1279360	1,4-Dichlorobenzene-d4	6.65

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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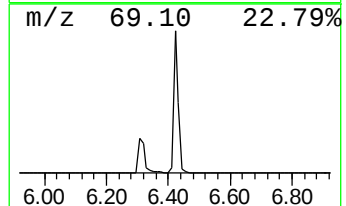
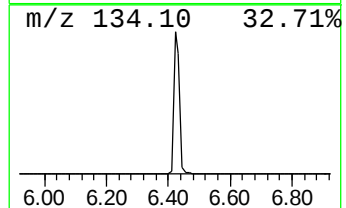
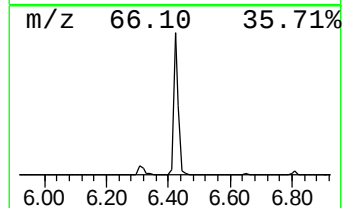
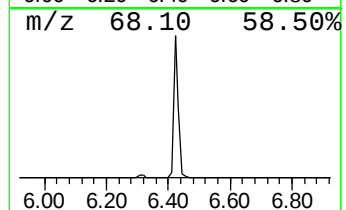
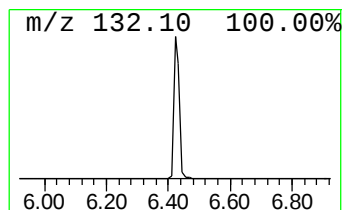
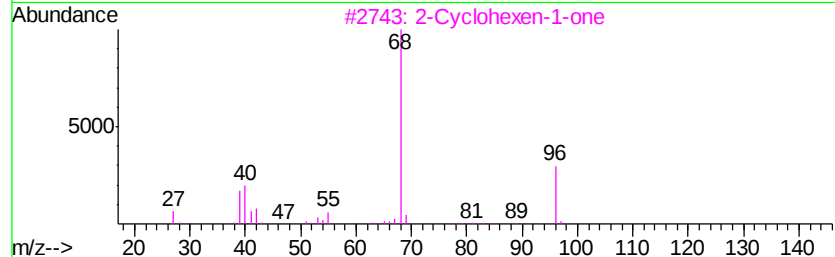
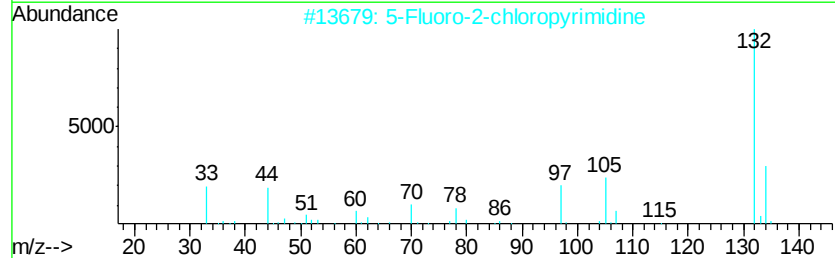
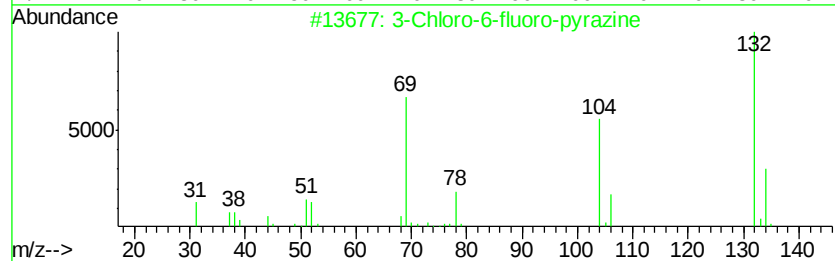
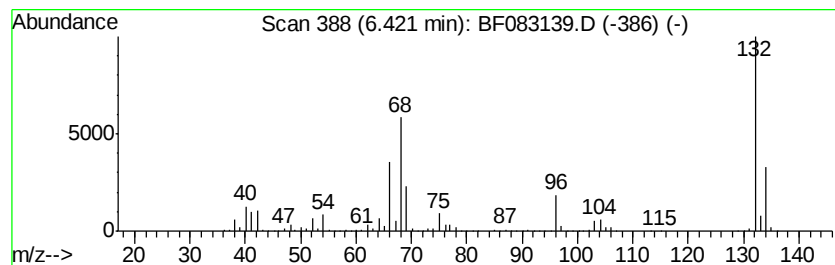
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	75.65 ng	4638710	1,4-Dichlorobenzene-d4	6.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11
4		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5		5-Aminoindole	132	C8H8N2	005192-03-0	10



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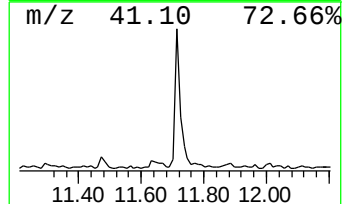
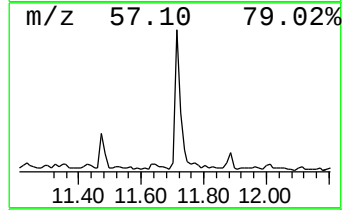
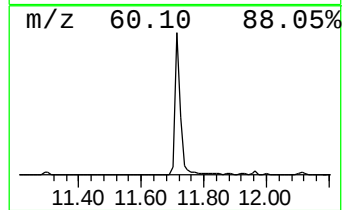
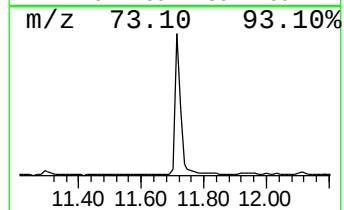
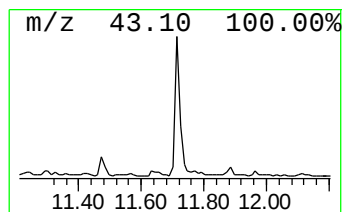
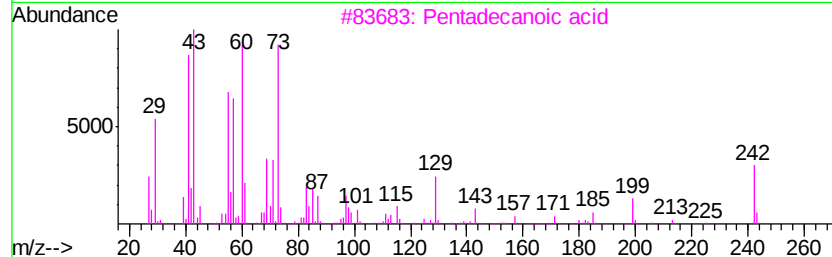
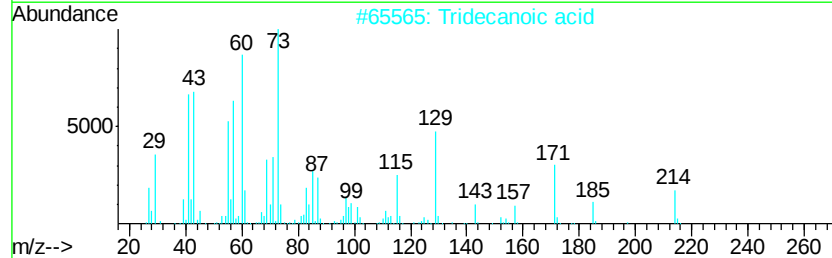
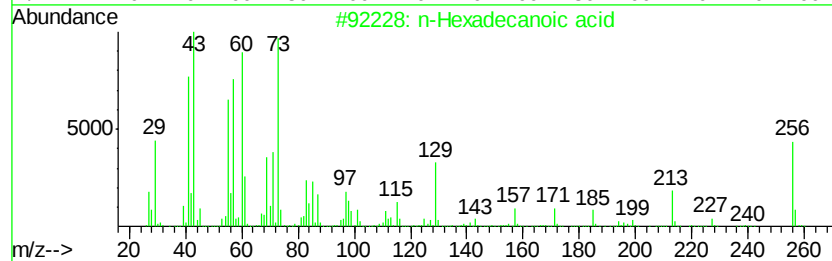
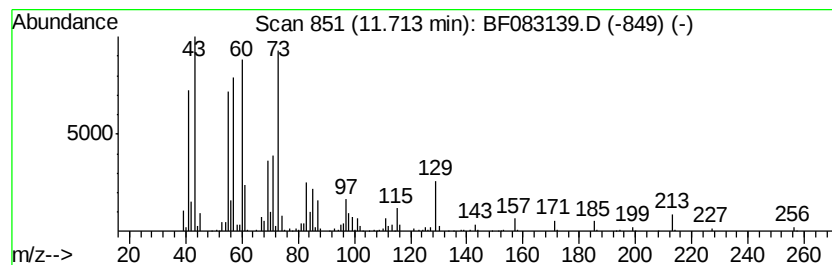
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TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.71	8.85 ng	810770	Phenanthrene-d10	11.16	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64



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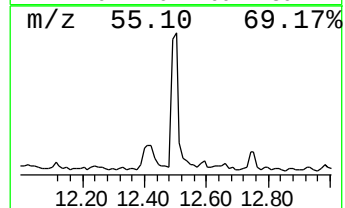
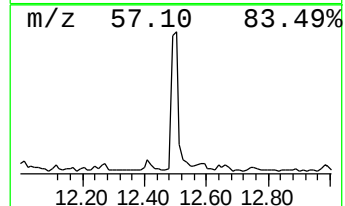
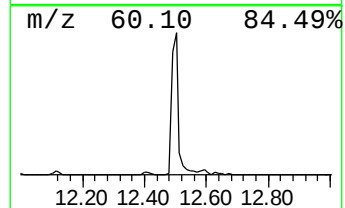
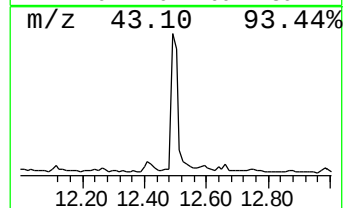
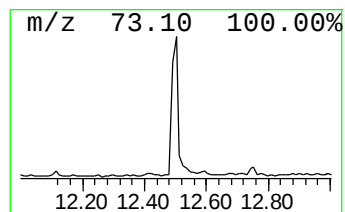
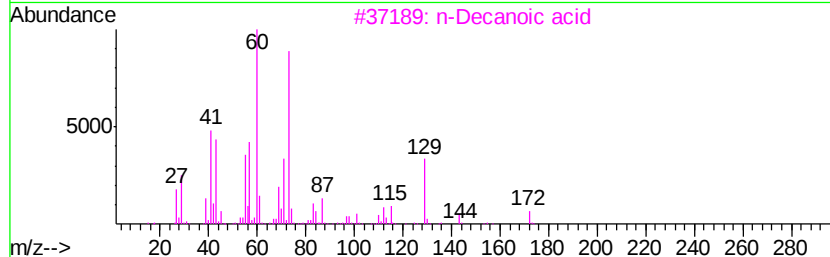
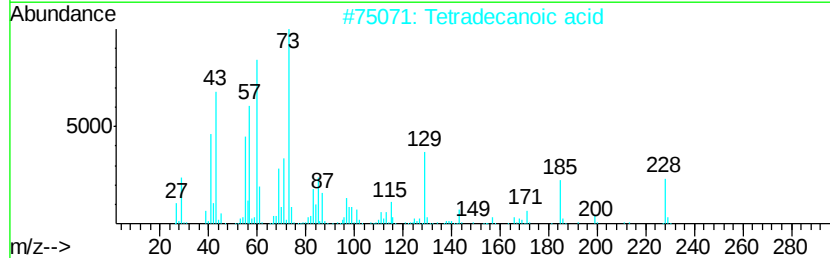
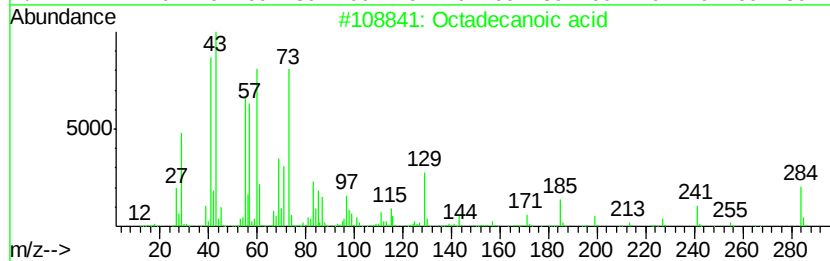
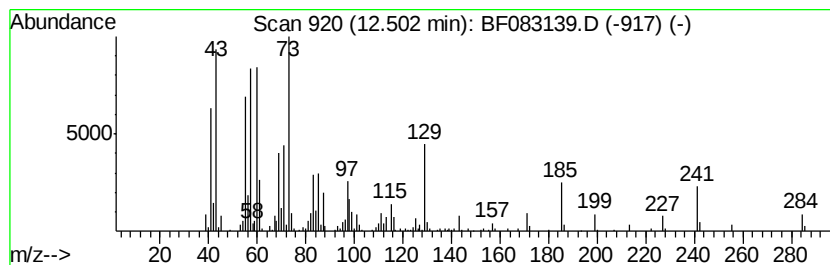
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.50	6.85 ng	597441	Chrysene-d12	13.78

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	98
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3		n-Decanoic acid	172	C10H20O2	000334-48-5	70
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	70
5		Undecanoic acid	186	C11H22O2	000112-37-8	38



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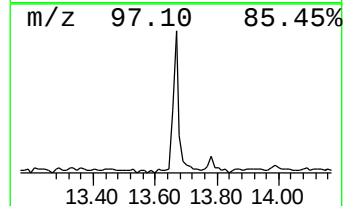
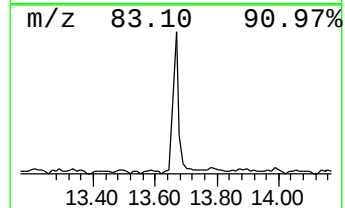
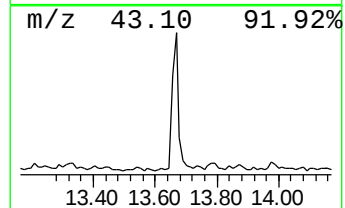
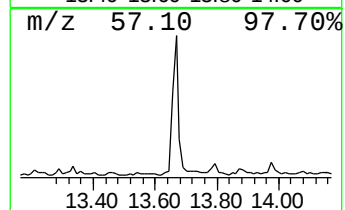
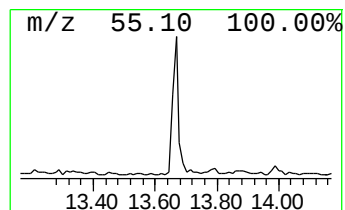
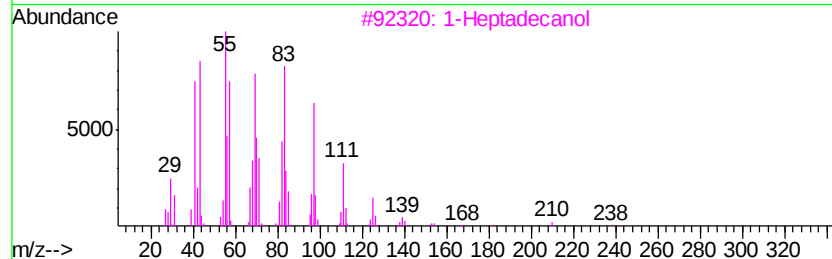
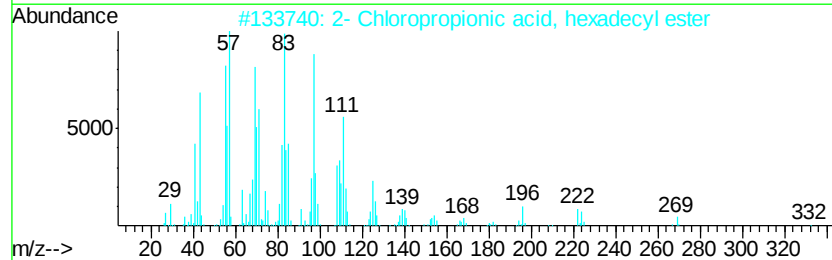
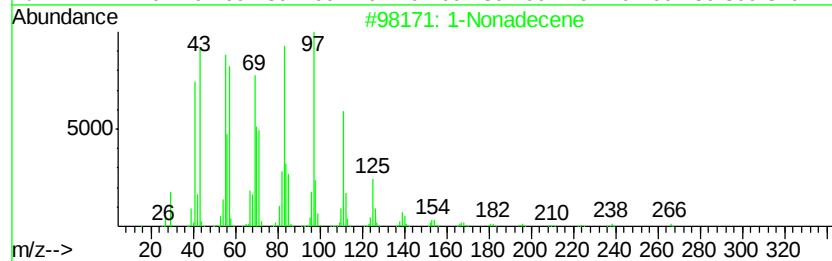
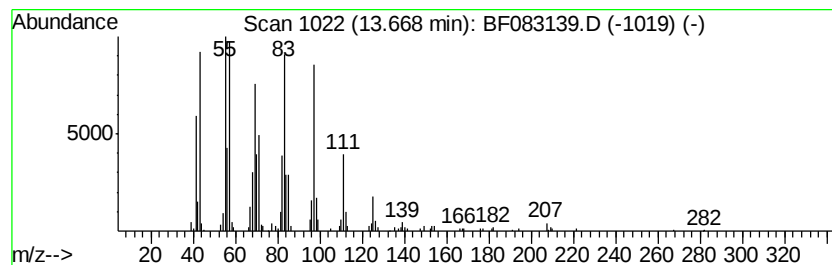
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Peak Number 6 1-Nonadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.67	4.45 ng	387925	Chrysene-d12	13.78
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Nonadecene	266 C19H38	018435-45-5	90
2	2- Chloropropionic acid, hexadec...	332 C19H37ClO2	086711-81-1	87
3	1-Heptadecanol	256 C17H36O	001454-85-9	83
4	Trichloroacetic acid, hexadecyl ...	386 C18H33Cl3O2	074339-54-1	83
5	Trichloroacetic acid, tetradecyl...	358 C16H29Cl3O2	074339-52-9	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.81	20.9	ng	1279360	1	6.65	1226330	20.0
unknown6.42	6.42	75.7	ng	4638710	1	6.65	1226330	20.0
n-Hexadecanoic acid	11.71	8.8	ng	810770	4	11.16	1831230	20.0
Octadecanoic acid	12.50	6.8	ng	597441	5	13.78	1744100	20.0
1-Nonadecene	13.67	4.5	ng	387925	5	13.78	1744100	20.0