

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111219\
 Data File : BF117758.D
 Acq On : 12 Nov 2019 14:41
 Operator : JU
 Sample : K5789-07
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-16B-S

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.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	2.216	17	22	39	rVB	1145142	1688420	29.72%	3.062%
2	5.140	512	519	529	rVB	944363	1077979	18.97%	1.955%
3	5.540	582	587	590	rBV	5047102	4672783	82.24%	8.475%
4	6.545	752	758	762	rBV	4751308	5098350	89.73%	9.247%
5	6.692	778	783	786	rBV	5612663	5034771	88.62%	9.131%
6	6.928	819	823	826	rBV	1921063	1687828	29.71%	3.061%
7	7.081	845	849	853	rBV	4553090	3979004	70.03%	7.217%
8	7.487	913	918	921	rBV	3320449	3095501	54.48%	5.614%
9	8.210	1037	1041	1045	rBV	2636289	2214100	38.97%	4.016%
10	9.286	1220	1224	1228	rBV	5809510	5681597	100.00%	10.305%
11	9.681	1287	1291	1295	rBV	814901	647957	11.40%	1.175%
12	9.975	1336	1341	1344	rBV	2805012	2544268	44.78%	4.614%
13	10.763	1470	1475	1478	rBV	4218725	3704114	65.19%	6.718%
14	11.463	1590	1594	1598	rBV	2995277	2550651	44.89%	4.626%
15	11.986	1677	1683	1693	rBV	444436	433110	7.62%	0.786%
16	12.774	1813	1817	1827	rBV	92835	111641	1.96%	0.202%
17	13.057	1860	1865	1868	rBV	6222090	5611143	98.76%	10.177%
18	13.963	2014	2019	2034	rBV2	274884	609426	10.73%	1.105%
19	14.110	2040	2044	2048	rBV	2207202	2033659	35.79%	3.688%
20	14.580	2121	2124	2127	rBV	61108	63511	1.12%	0.115%
21	14.904	2176	2179	2182	rVB	79746	77298	1.36%	0.140%
22	14.980	2189	2192	2196	rVB	122619	127780	2.25%	0.232%
23	15.263	2236	2240	2245	rVB	73060	90603	1.59%	0.164%
24	15.621	2296	2301	2305	rBV2	1653400	2044906	35.99%	3.709%
25	15.663	2305	2308	2314	rVB	79697	103953	1.83%	0.189%
26	16.121	2382	2386	2393	rVB2	51706	83814	1.48%	0.152%
27	16.657	2474	2477	2487	rVB4	35737	68364	1.20%	0.124%

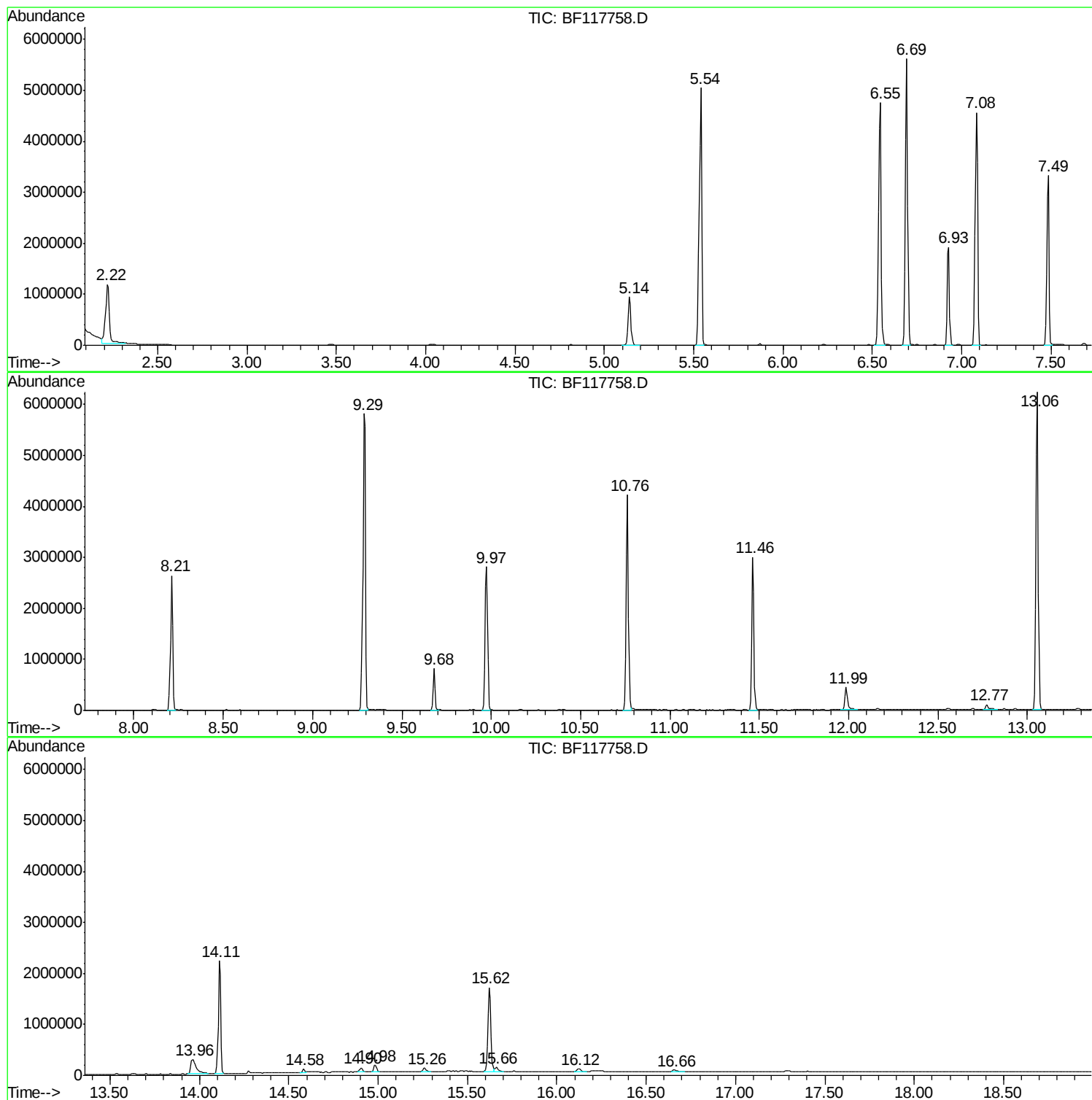
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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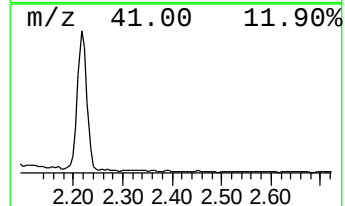
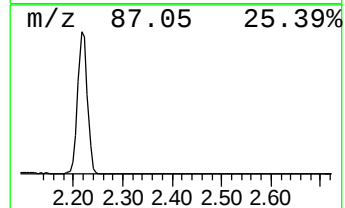
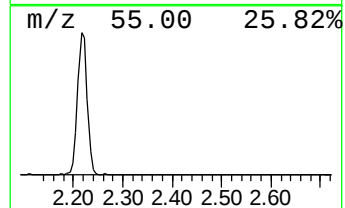
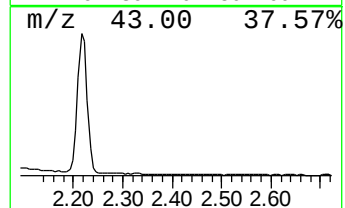
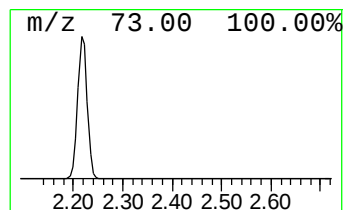
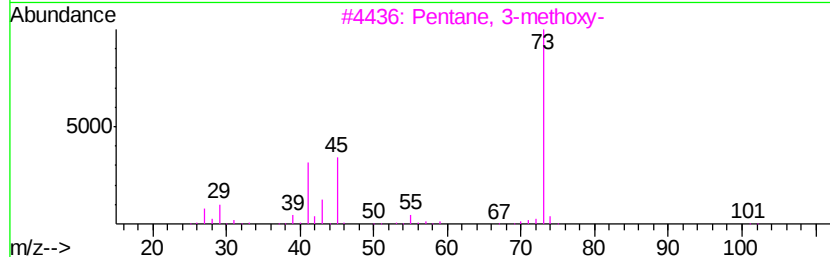
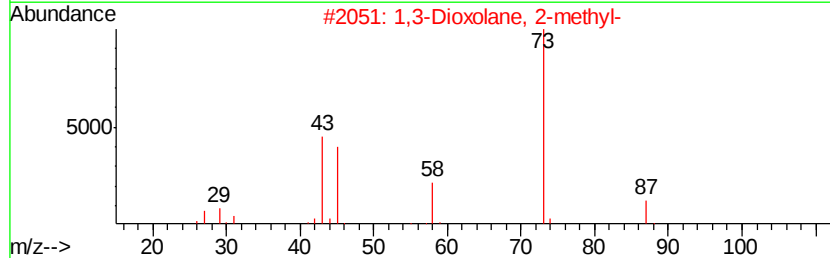
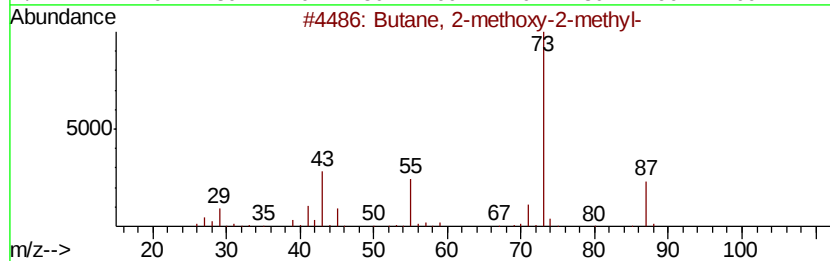
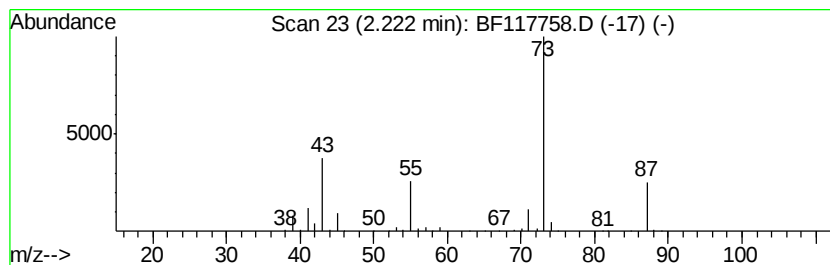
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	20.01 ng	1688420	1,4-Dichlorobenzene-d4	6.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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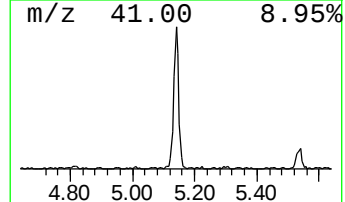
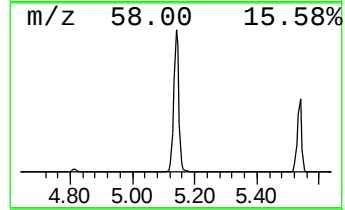
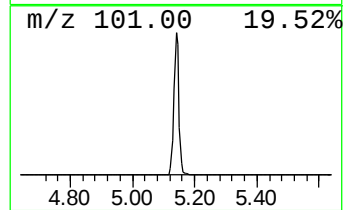
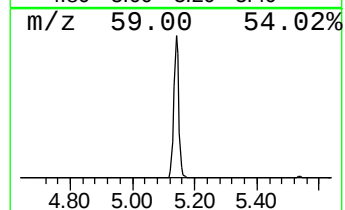
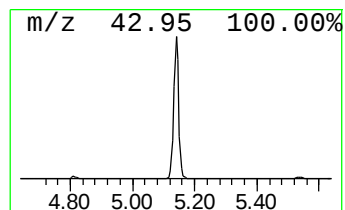
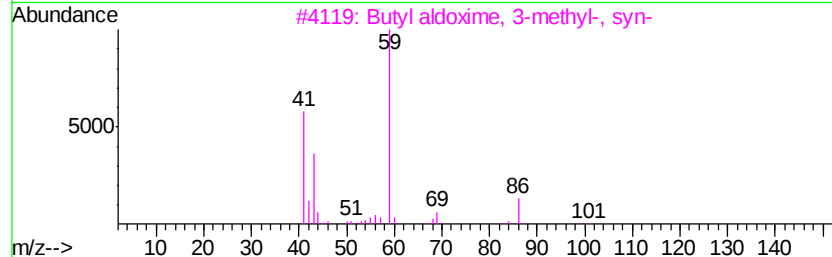
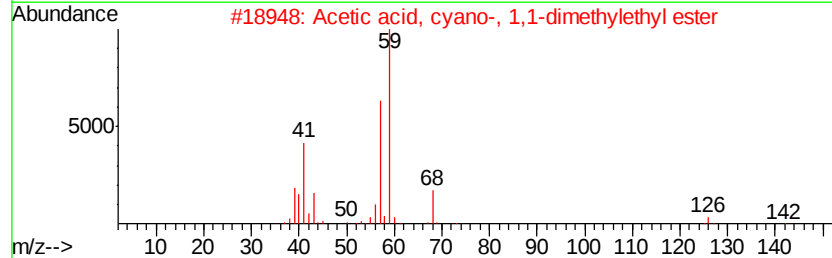
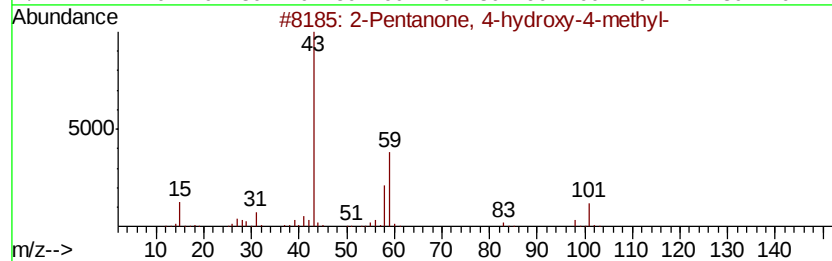
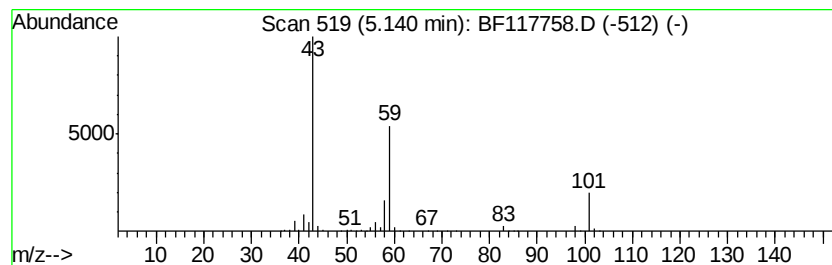
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	12.77 ng	1077980	1,4-Dichlorobenzene-d4	6.93

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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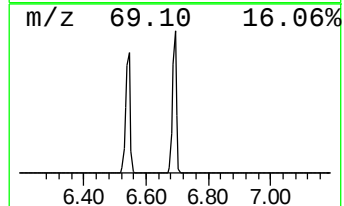
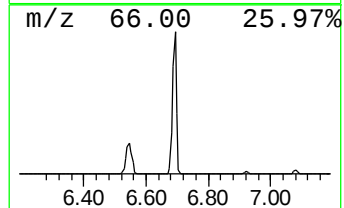
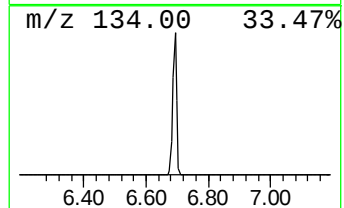
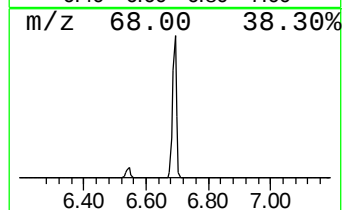
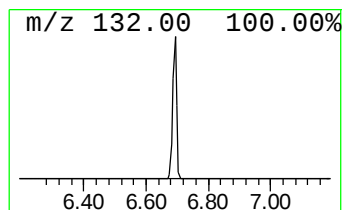
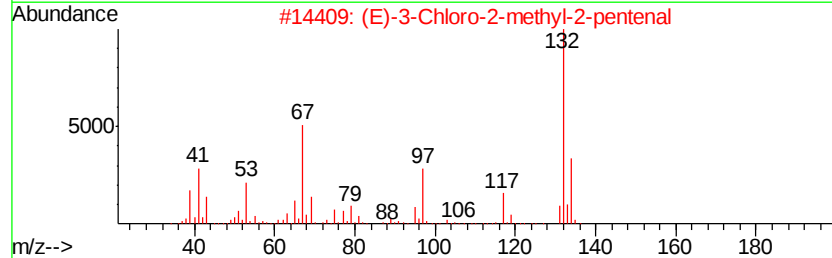
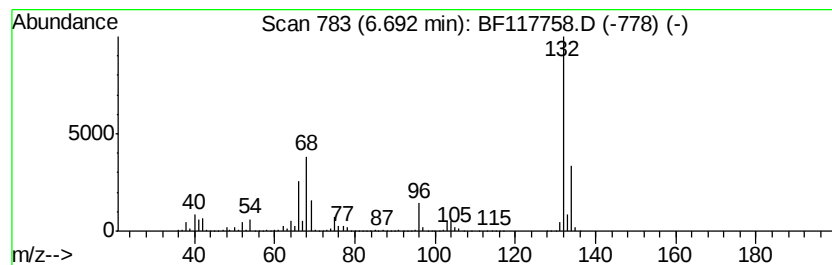
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	59.66 ng	5034770	1,4-Dichlorobenzene-d4	6.93

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	16
3		Tranvlcvpromine-propionyl	189	C12H15NO	1000123-86-3	12
4		Xenon	132	Xe	007440-63-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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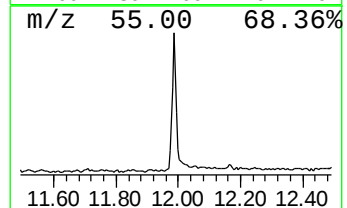
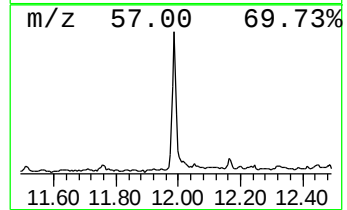
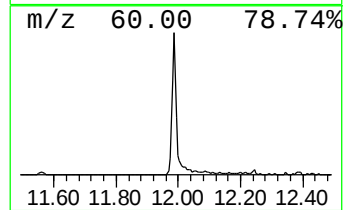
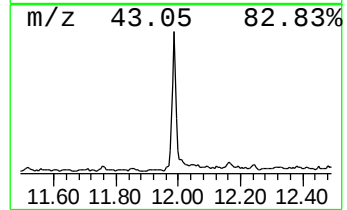
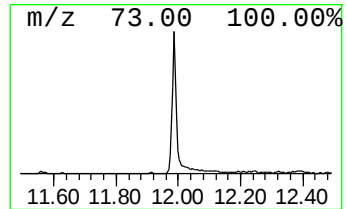
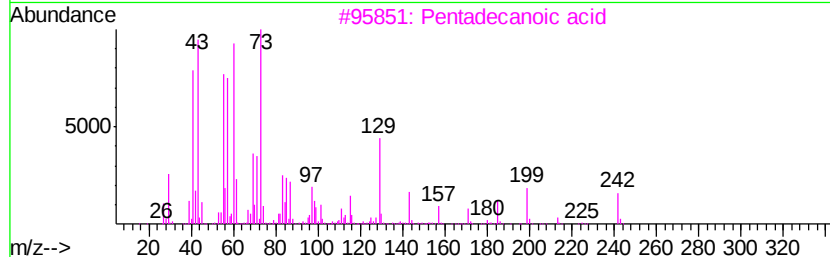
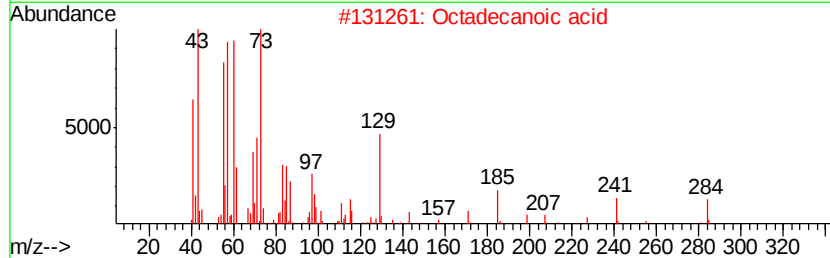
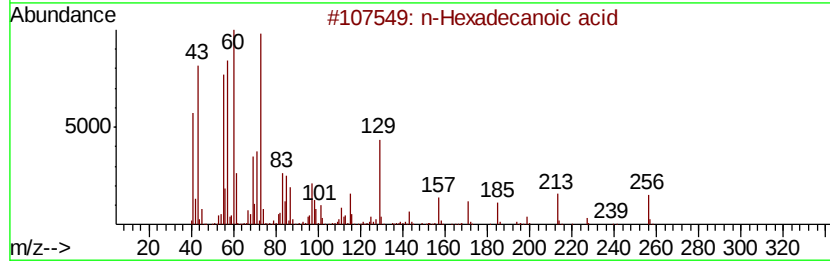
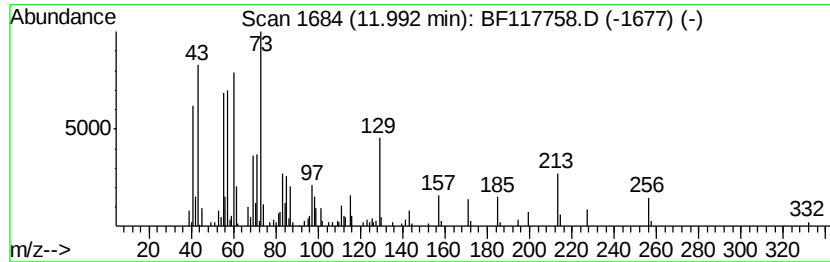
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.99	3.40 ng	433110	Phenanthrene-d10	11.46	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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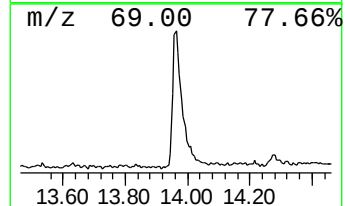
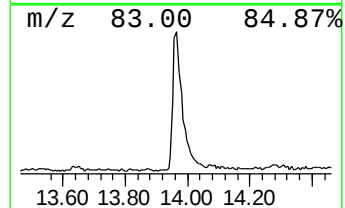
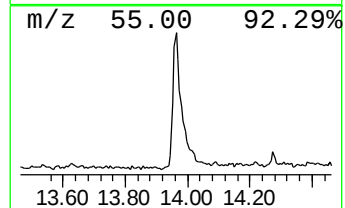
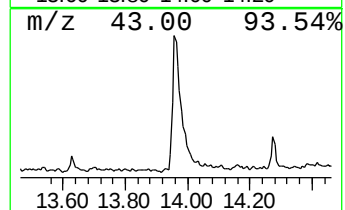
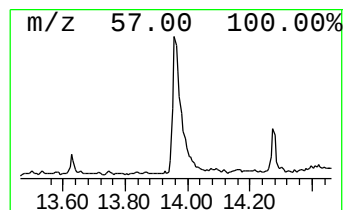
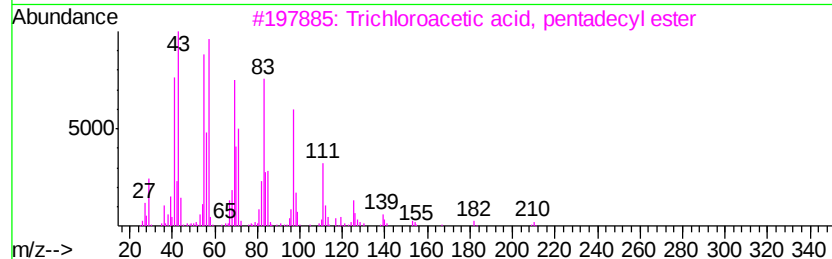
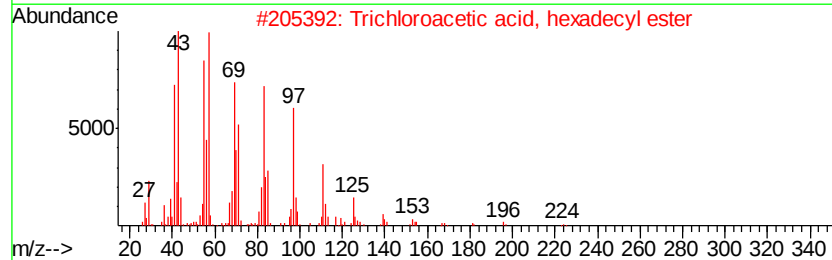
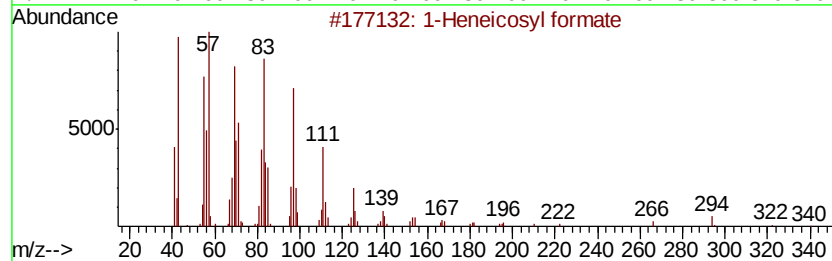
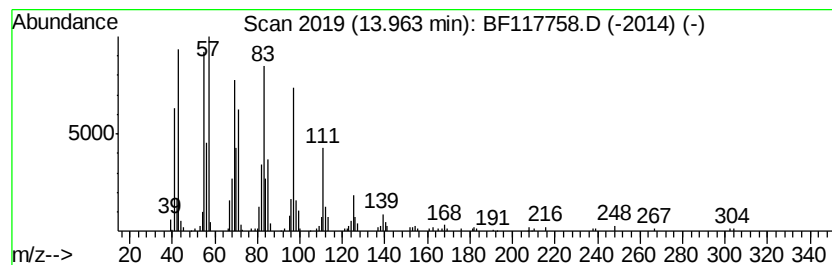
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TIC Library : C:\DATABASE\NIST11.L
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 Peak Number 6 1-Heneicosyl formate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	5.99 ng	609426	Chrysene-d12	14.11

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
4		1-Heneicosanol	312	C21H44O	015594-90-8	94
5		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.22	20.0	ng	1688420	1	6.93	1687830	20.0
2-Pentanone, 4-hy...	5.14	12.8	ng	1077980	1	6.93	1687830	20.0
unknown6.69	6.69	59.7	ng	5034770	1	6.93	1687830	20.0
n-Hexadecanoic acid	11.99	3.4	ng	433110	4	11.46	2550650	20.0
1-Heneicosyl formate	13.96	6.0	ng	609426	5	14.11	2033660	20.0