

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112319\
 Data File : BF117964.D
 Acq On : 23 Nov 2019 18:42
 Operator : JU
 Sample : K5951-03
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 IRONBOUND-8FT

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-BF111319.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	2.175	10	15	39	rVB	825494	1269954	26.67%	3.640%
2	5.116	510	515	524	rVB	518286	673339	14.14%	1.930%
3	5.516	578	583	586	rBV	3028228	3100284	65.11%	8.886%
4	6.528	749	755	758	rBV	3093413	3081233	64.71%	8.831%
5	6.669	775	779	783	rBV	3612580	3589934	75.40%	10.289%
6	6.904	815	819	822	rBV	742035	648128	13.61%	1.858%
7	7.063	841	846	849	rBV	2586242	2405996	50.53%	6.896%
8	7.463	909	914	917	rBV	1927666	1849168	38.84%	5.300%
9	8.186	1034	1037	1041	rBV	953571	826614	17.36%	2.369%
10	9.269	1216	1221	1224	rBV	4037809	3542773	74.41%	10.154%
11	9.663	1284	1288	1296	rBV	427491	385525	8.10%	1.105%
12	9.951	1333	1337	1348	rVB	1226880	1015792	21.33%	2.911%
13	10.745	1467	1472	1475	rBV	3118090	3020178	63.43%	8.656%
14	11.445	1587	1591	1598	rBV	1390722	1276846	26.82%	3.660%
15	11.510	1599	1602	1606	rVB3	64761	55027	1.16%	0.158%
16	11.963	1676	1679	1688	rBV	327809	355828	7.47%	1.020%
17	12.751	1810	1813	1822	rBV	84722	102856	2.16%	0.295%
18	13.039	1857	1862	1865	rBV	4978681	4761340	100.00%	13.647%
19	13.927	2009	2013	2023	rBV	245482	346408	7.28%	0.993%
20	14.092	2037	2041	2045	rBV	1463662	1282251	26.93%	3.675%
21	14.556	2116	2120	2124	rBV2	52259	60328	1.27%	0.173%
22	14.874	2167	2174	2177	rBV	55322	79216	1.66%	0.227%
23	15.221	2229	2233	2238	rBV2	56676	70571	1.48%	0.202%
24	15.592	2290	2296	2309	rBV	719256	1017222	21.36%	2.915%
25	16.074	2373	2378	2383	rBV2	47741	73466	1.54%	0.211%

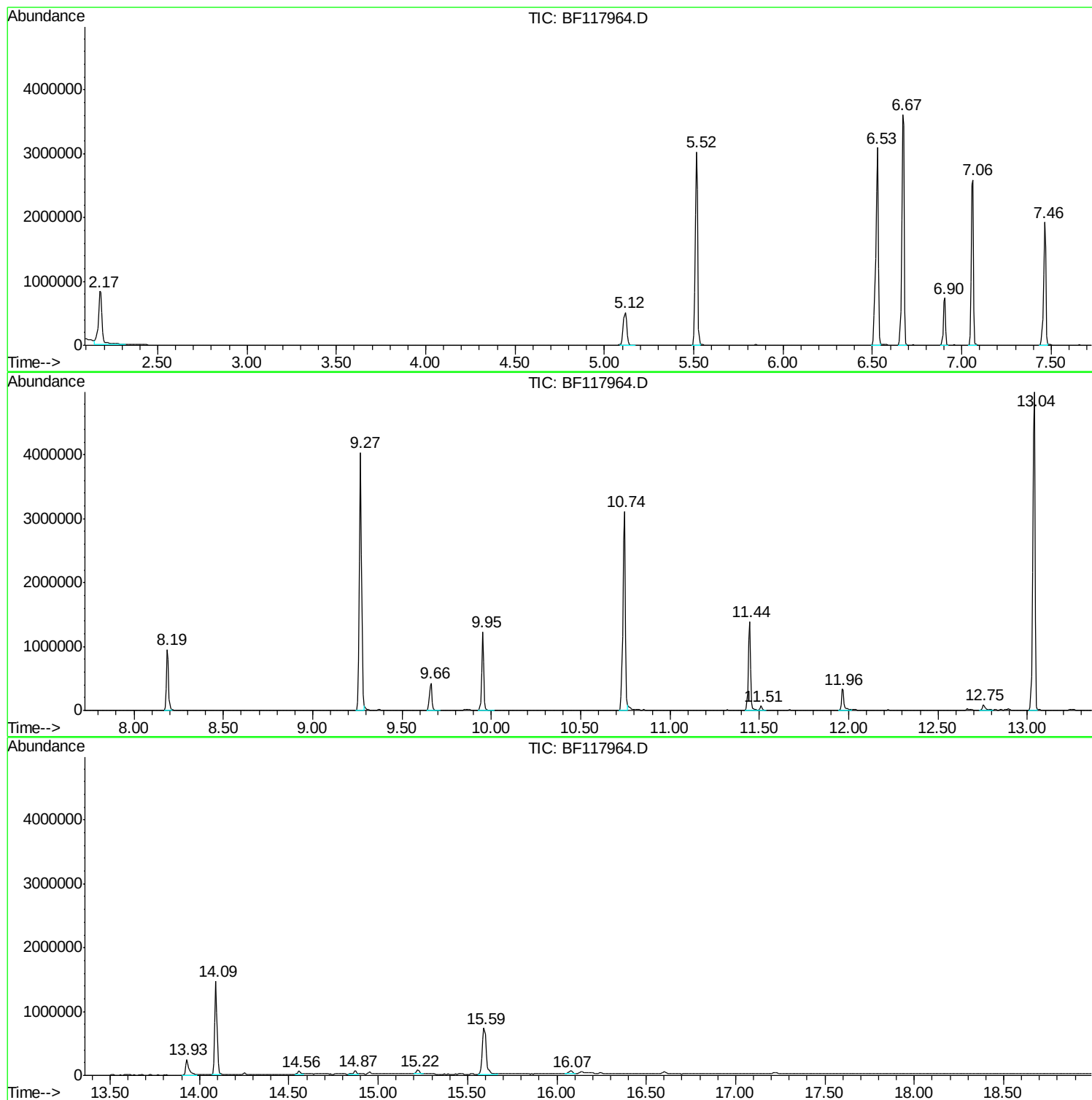
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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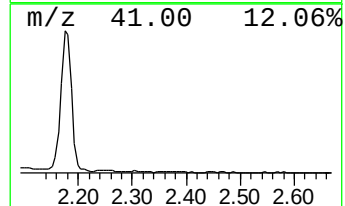
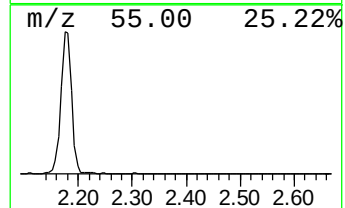
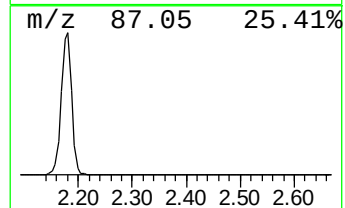
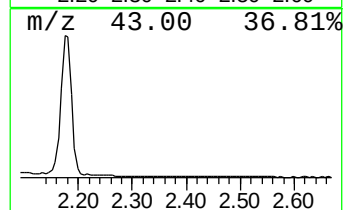
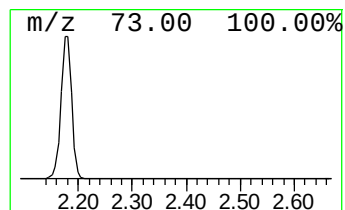
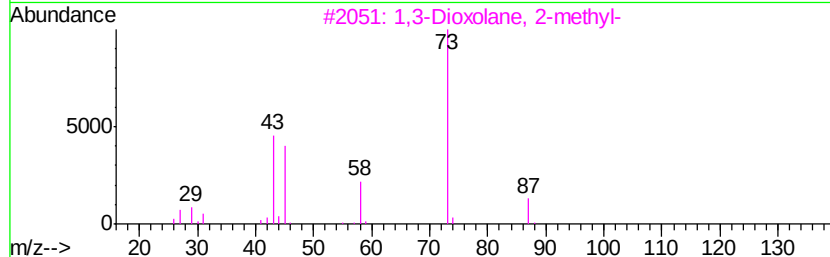
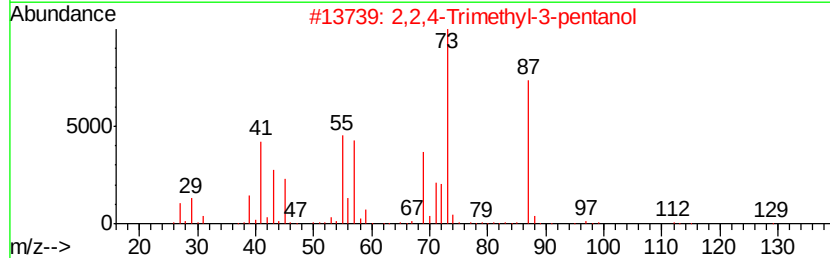
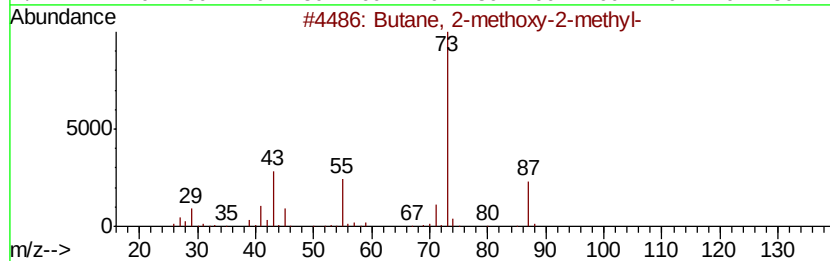
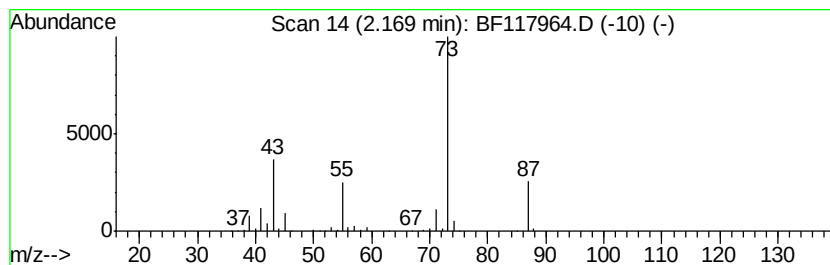
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.17	39.19 ng	1269950	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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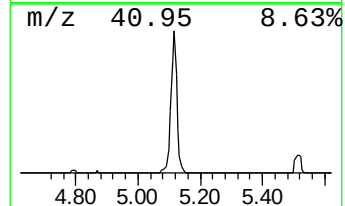
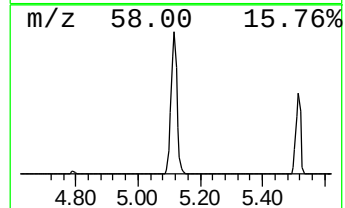
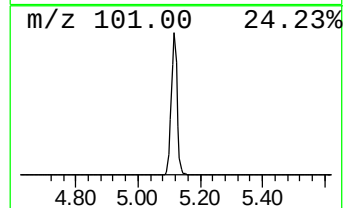
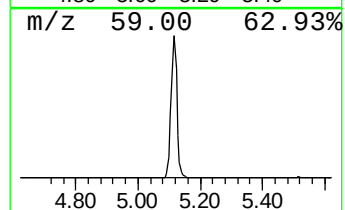
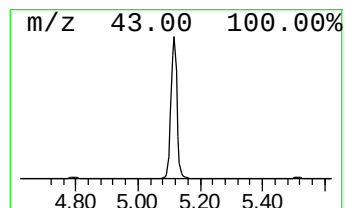
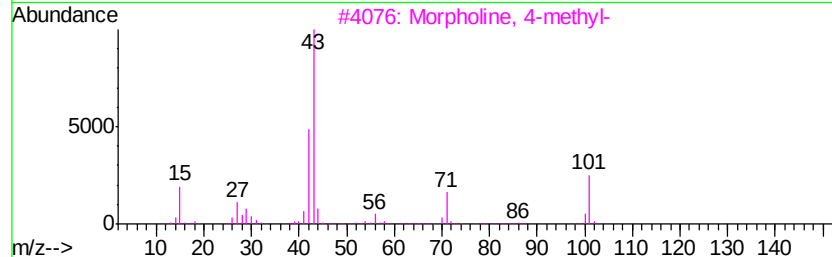
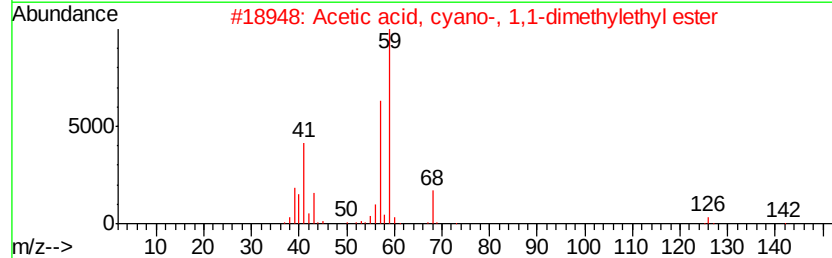
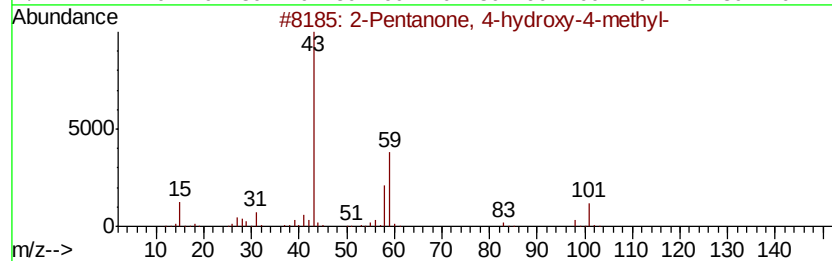
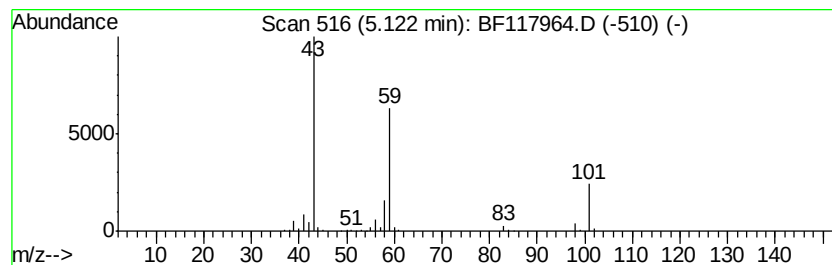
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	20.78 ng	673339	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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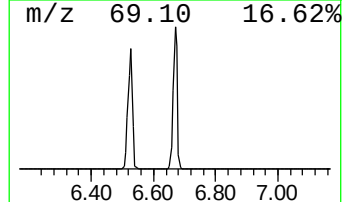
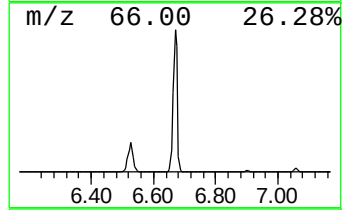
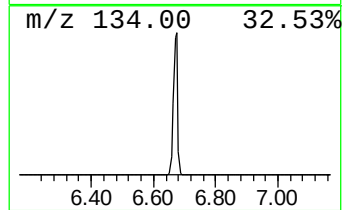
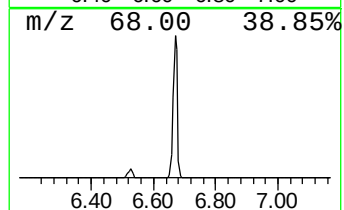
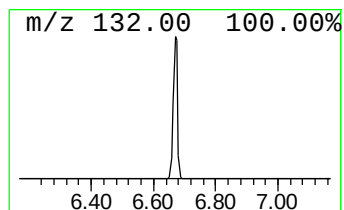
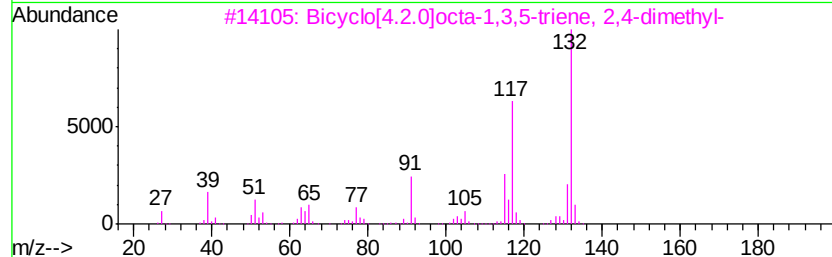
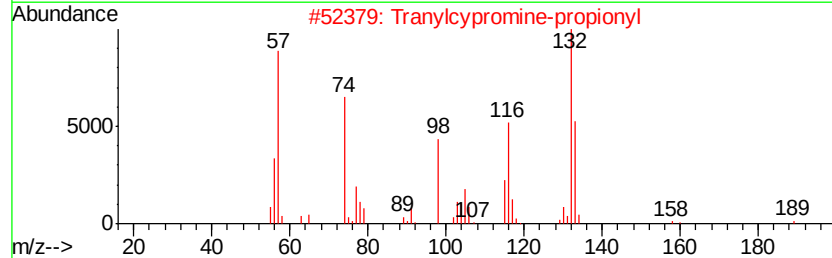
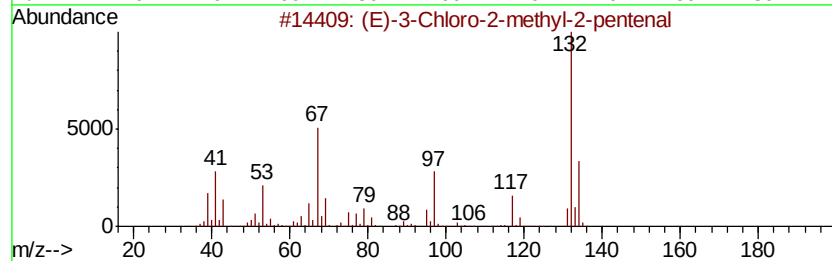
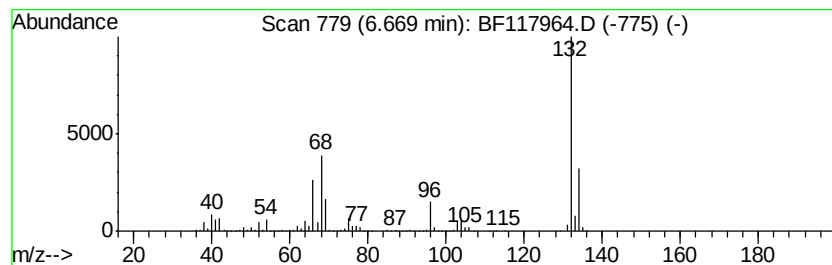
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	110.78 ng	3589930	1,4-Dichlorobenzene-d4	6.90

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17	
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10	
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9	
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9	
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9	



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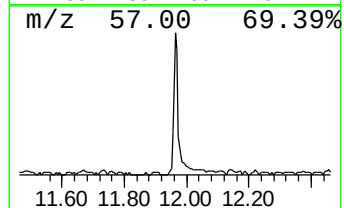
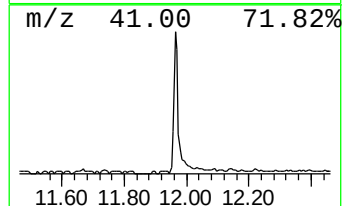
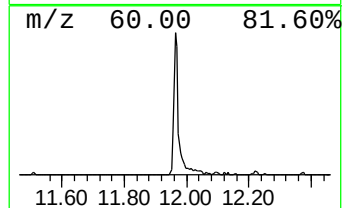
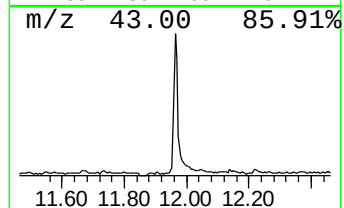
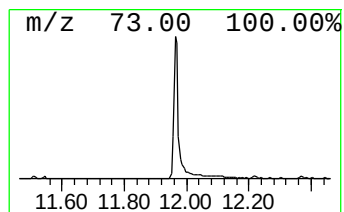
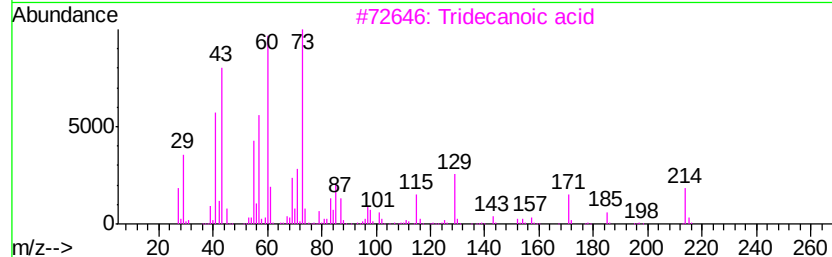
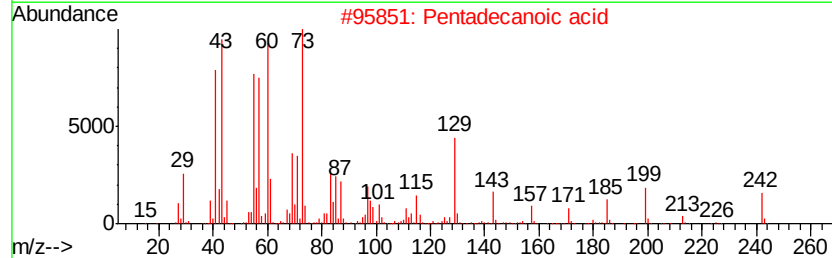
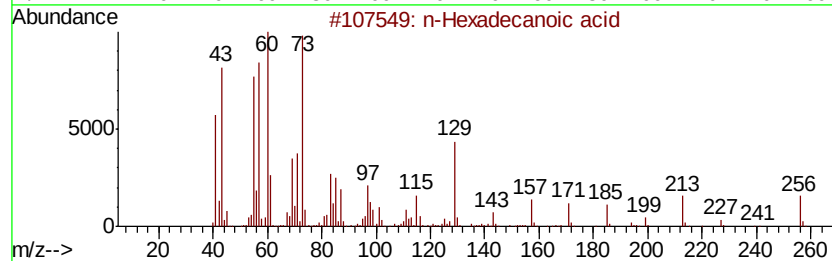
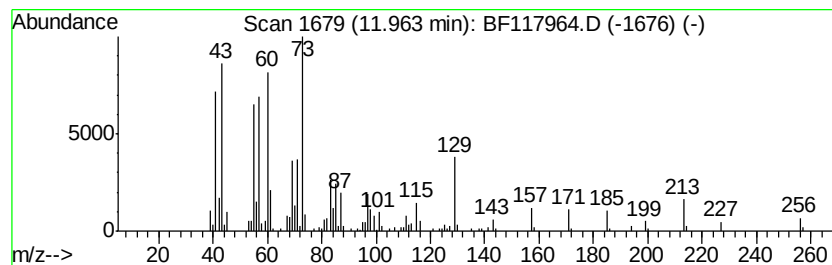
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	5.57 ng	355828	Phenanthrene-d10	11.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3		Tridecanoic acid	214	C13H26O2	000638-53-9	91
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5		Dodecanoic acid	200	C12H24O2	000143-07-7	58



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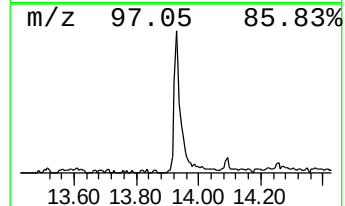
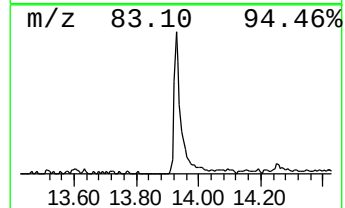
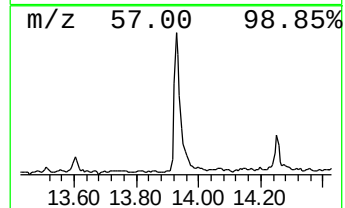
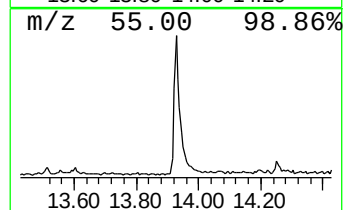
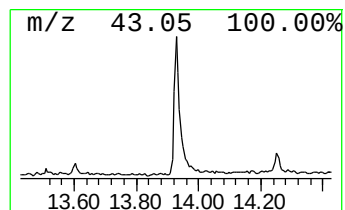
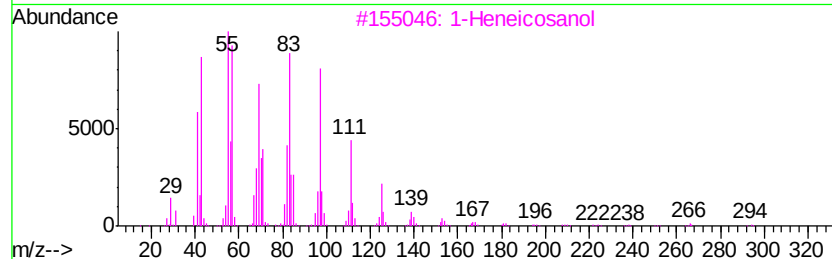
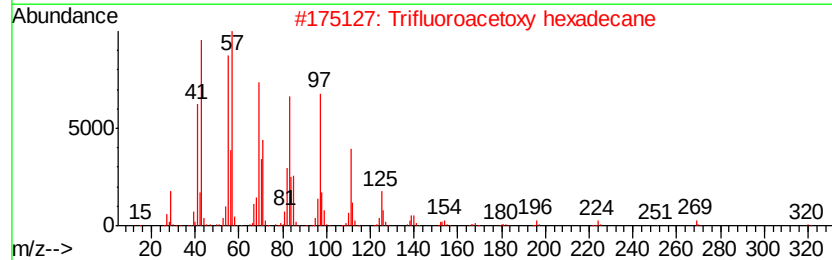
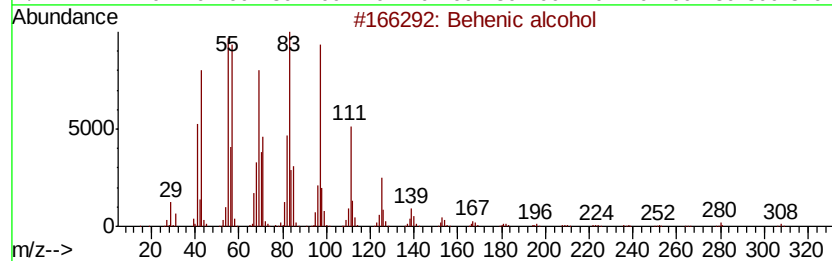
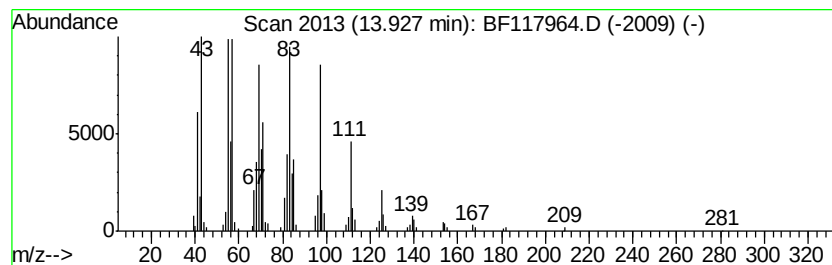
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Behenic alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.93	5.40 ng	346408	Chrysene-d12	14.09	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.17	39.2	ng	1269950	1	6.90	648128	20.0
2-Pentanone, 4-hy...	5.12	20.8	ng	673339	1	6.90	648128	20.0
unknown6.67	6.67	110.8	ng	3589930	1	6.90	648128	20.0
n-Hexadecanoic acid	11.96	5.6	ng	355828	4	11.44	1276850	20.0
Behenic alcohol	13.93	5.4	ng	346408	5	14.09	1282250	20.0