

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040918\
 Data File : BF104364.D
 Acq On : 9 Apr 2018 11:46
 Operator : JU/SJ
 Sample : J2184-03
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-2-1(1-3)

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-BF040618.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	3.234	192	195	203	rBV	22825	38790	1.08%	0.120%
2	5.022	494	499	507	rVB	189956	260638	7.24%	0.807%
3	5.416	560	566	569	rBV	3182946	3372432	93.73%	10.443%
4	6.434	732	739	742	rBV	3105279	3305764	91.87%	10.237%
5	6.575	757	763	766	rBV	3248340	3412240	94.83%	10.567%
6	6.804	798	802	805	rBV	1084636	866164	24.07%	2.682%
7	6.963	824	829	832	rVB	2712605	2630746	73.11%	8.147%
8	7.369	892	898	901	rBV	2211095	2127110	59.12%	6.587%
9	8.086	1016	1020	1023	rBV	1455039	1178966	32.77%	3.651%
10	9.163	1198	1203	1206	rBV	3805187	3598159	100.00%	11.142%
11	9.557	1266	1270	1273	rBV	263632	229836	6.39%	0.712%
12	9.769	1303	1306	1310	rVB	105535	84178	2.34%	0.261%
13	9.839	1314	1318	1322	rVB2	1466690	1297910	36.07%	4.019%
14	10.269	1388	1391	1395	rVB	122928	105223	2.92%	0.326%
15	10.492	1422	1429	1432	rBV	32527	46118	1.28%	0.143%
16	10.633	1446	1453	1456	rBV	2221592	2290200	63.65%	7.092%
17	10.745	1469	1472	1481	rVB	103144	99545	2.77%	0.308%
18	11.327	1567	1571	1573	rBV	1503539	1233080	34.27%	3.818%
19	11.351	1573	1575	1578	rVB	151591	110390	3.07%	0.342%
20	11.857	1658	1661	1664	rBV	268818	238574	6.63%	0.739%
21	12.539	1774	1777	1780	rBV	193220	164320	4.57%	0.509%
22	12.639	1791	1794	1802	rBV3	67880	78871	2.19%	0.244%
23	12.768	1808	1816	1819	rBV	137950	143586	3.99%	0.445%
24	12.921	1837	1842	1845	rBV	3175526	3088636	85.84%	9.564%
25	13.810	1990	1993	1997	rBV	297678	272770	7.58%	0.845%
26	13.968	2015	2020	2023	rBV	979839	893539	24.83%	2.767%
27	13.992	2023	2024	2027	rVB	60408	41014	1.14%	0.127%
28	15.004	2193	2196	2200	rBV	42553	58817	1.63%	0.182%
29	15.304	2244	2247	2252	rVB	34288	45174	1.26%	0.140%
30	15.362	2254	2257	2261	rBV	38487	44825	1.25%	0.139%
31	15.433	2263	2269	2273	rBV	657058	849150	23.60%	2.630%
32	15.951	2353	2357	2370	rBV	32393	86179	2.40%	0.267%

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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
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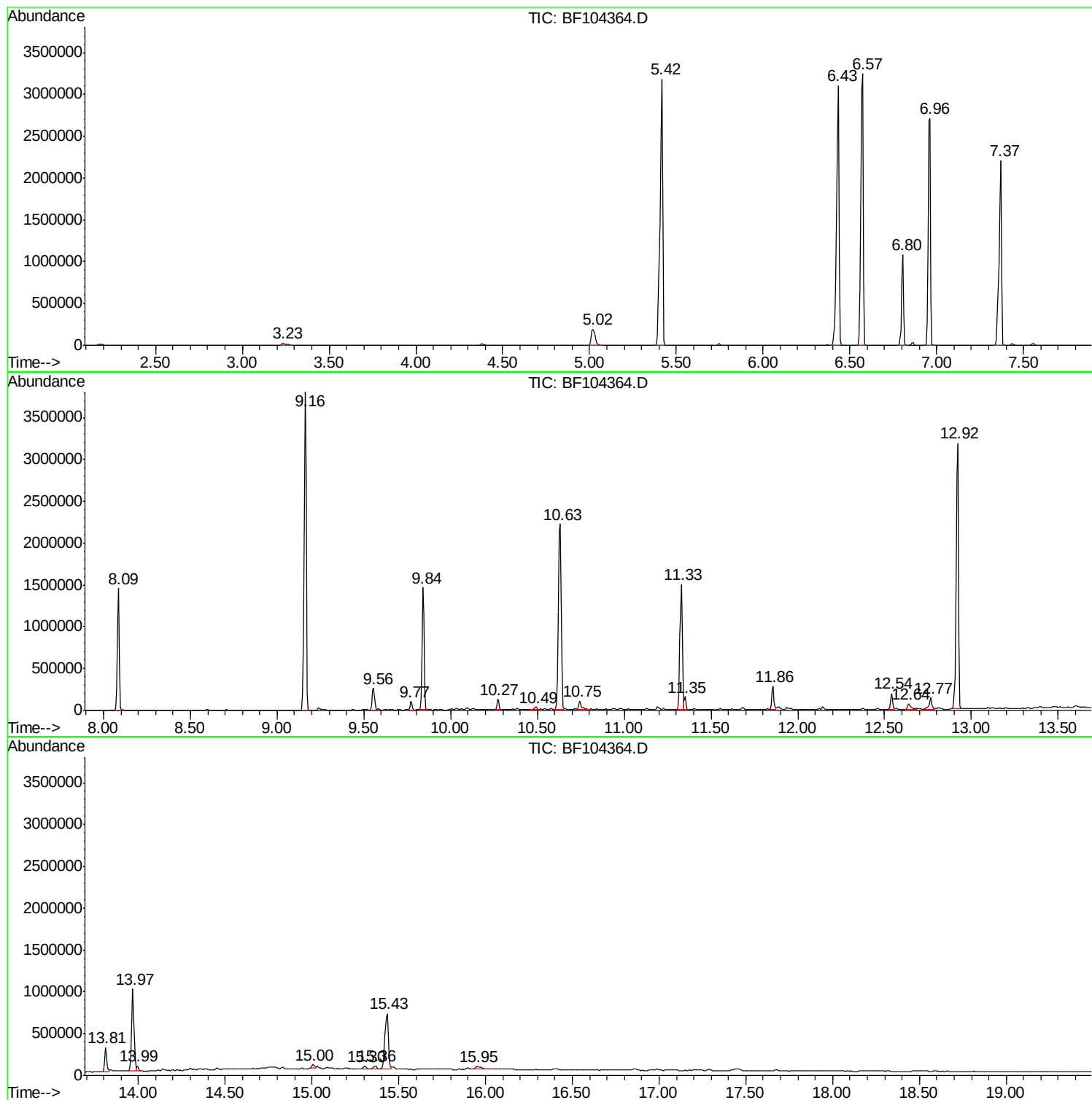
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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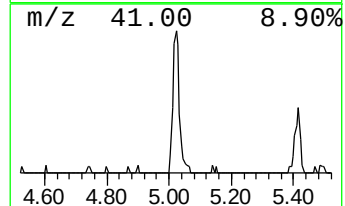
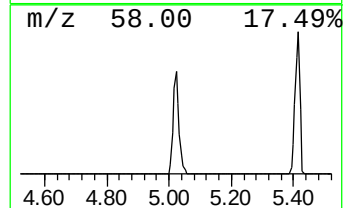
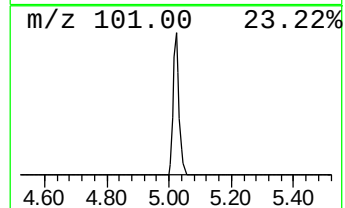
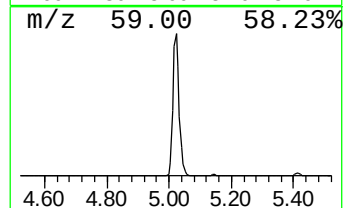
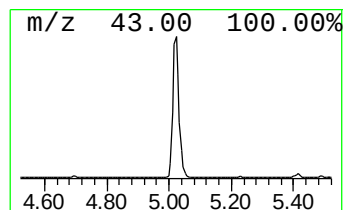
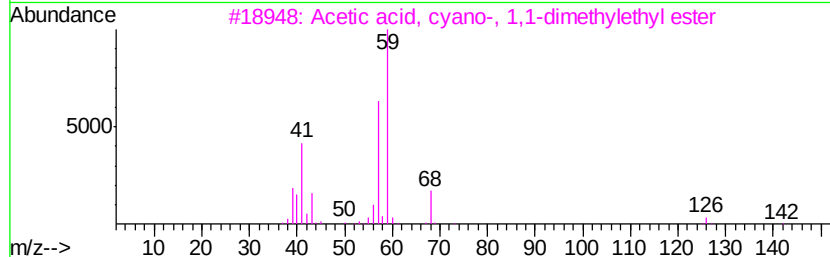
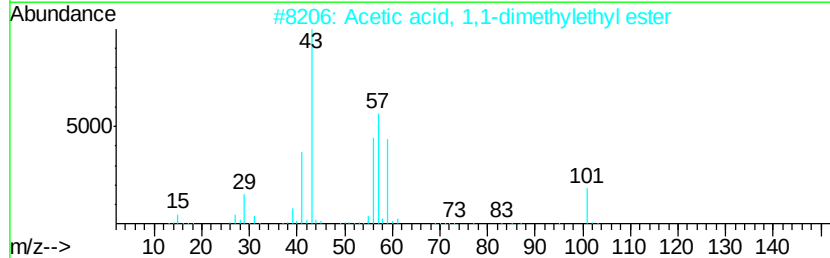
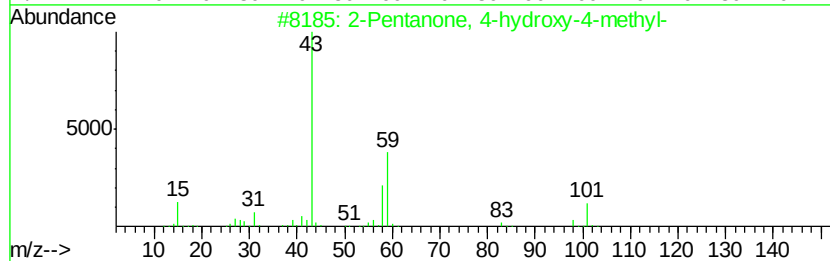
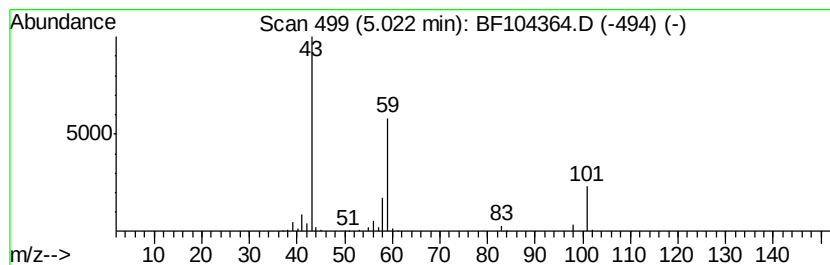
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	6.02 ng	260638	1,4-Dichlorobenzene-d4	6.80

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39	
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17	
4	Butane	58	C4H10	000106-97-8	9	
5	Acetone	58	C3H6O	000067-64-1	9	



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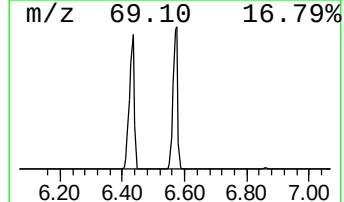
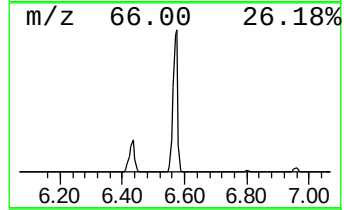
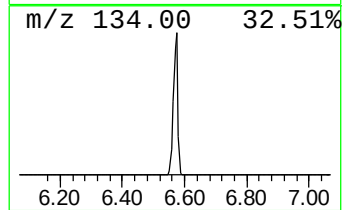
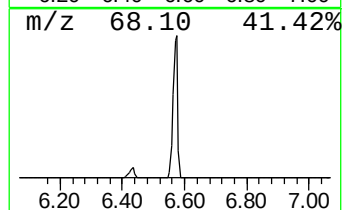
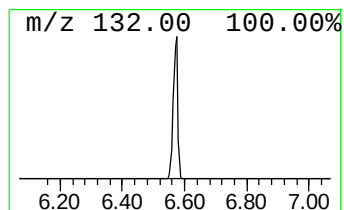
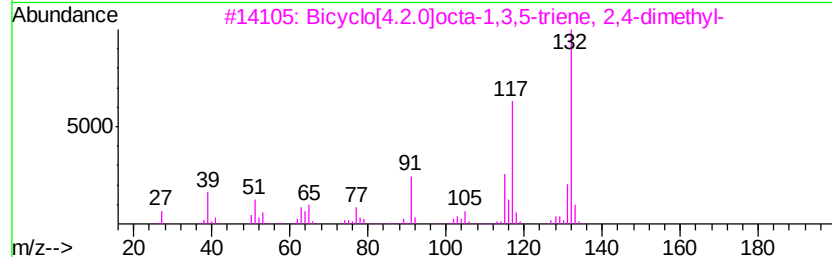
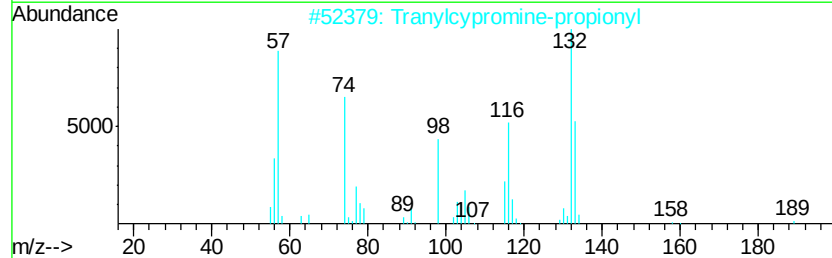
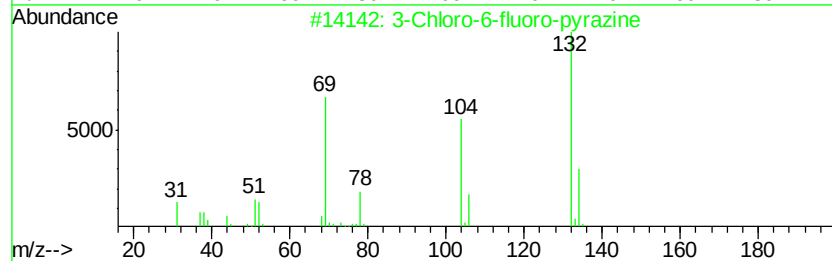
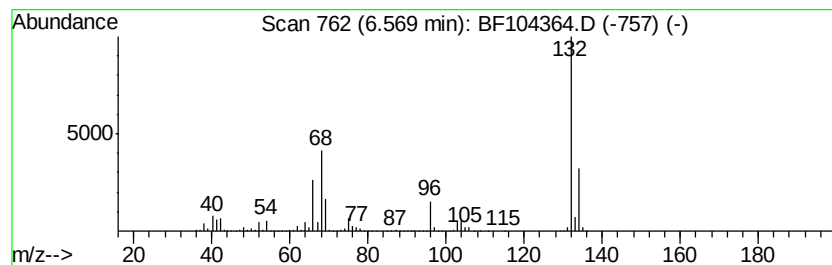
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	78.79 ng	3412240	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
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		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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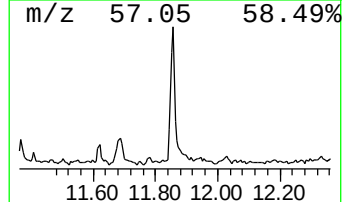
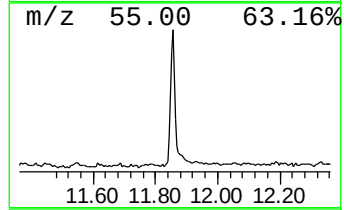
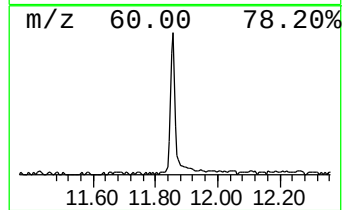
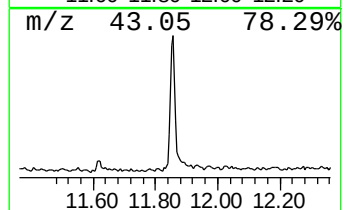
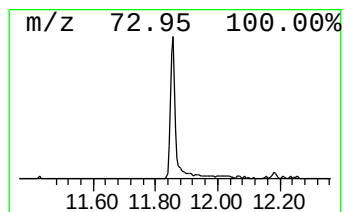
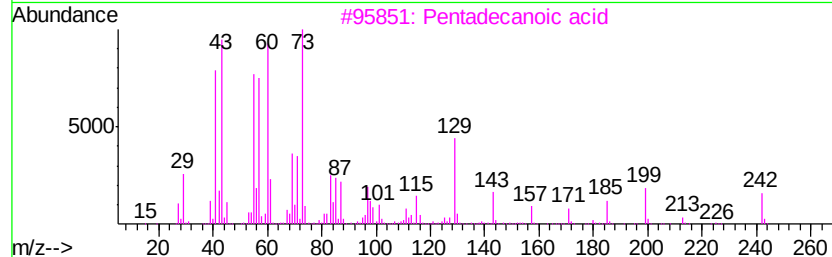
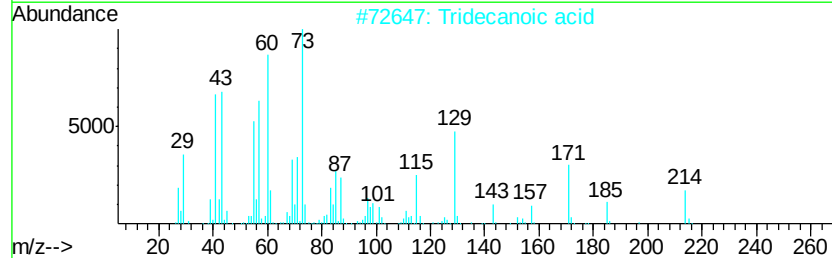
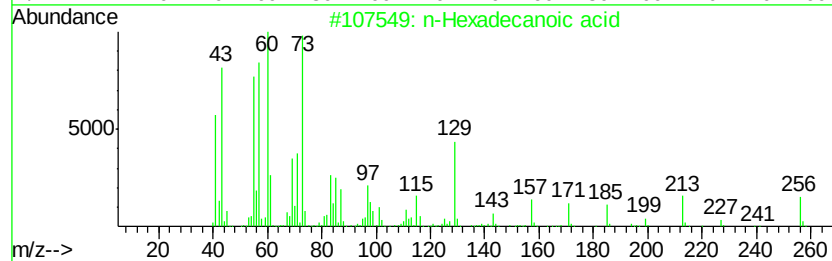
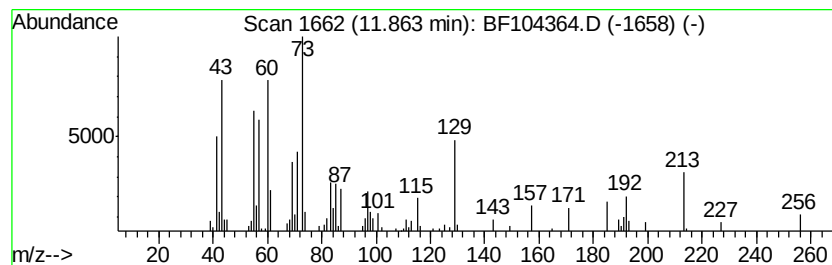
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.86	3.87 ng	238574	Phenanthrene-d10		11.33
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	91
4	Undecanoic acid	186	C11H22O2	000112-37-8	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62



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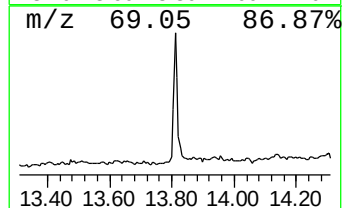
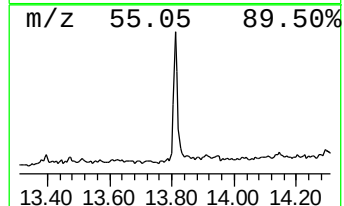
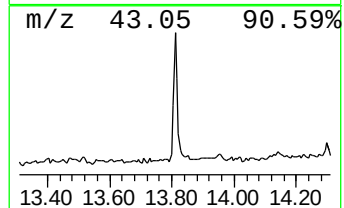
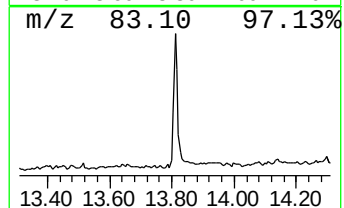
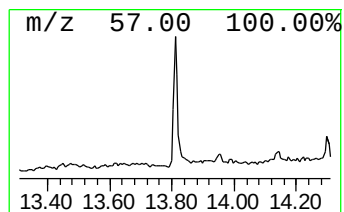
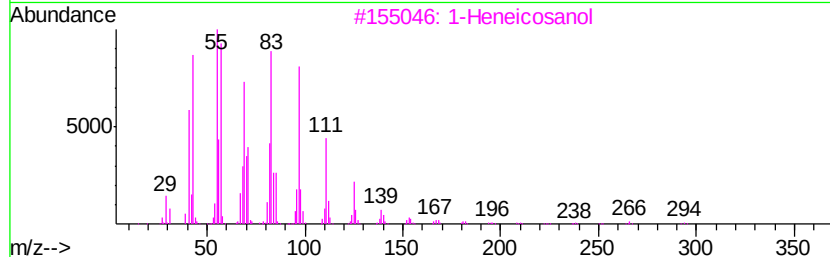
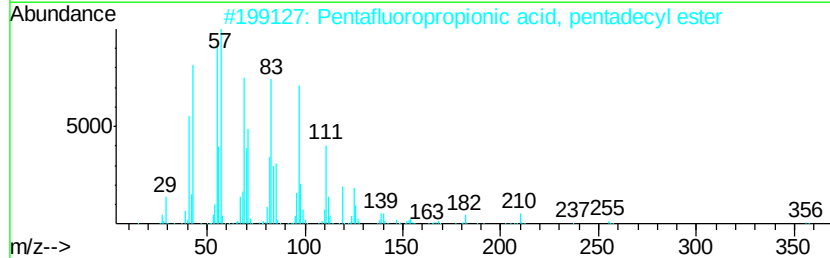
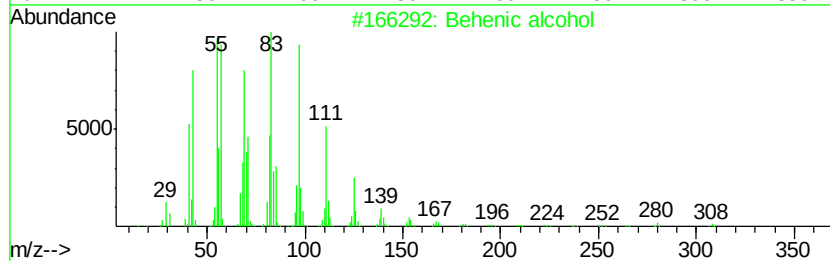
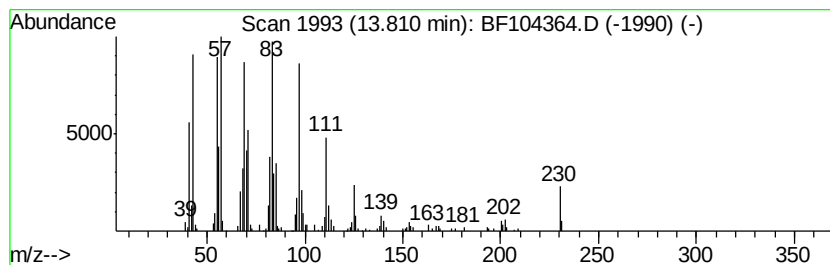
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Behenic alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.81	6.11 ng	272770	Chrysene-d12	13.97	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
5	Trifluoroacetoxyl hexadecane	338	C18H33F3O2	006222-03-3	94



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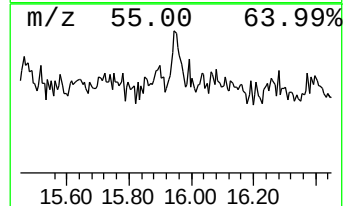
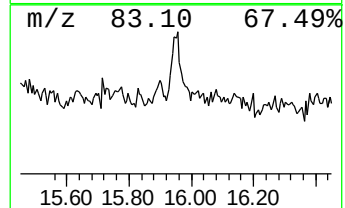
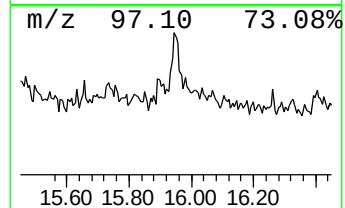
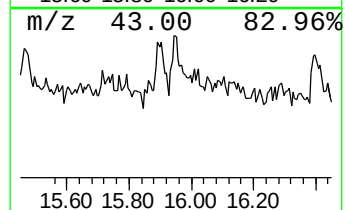
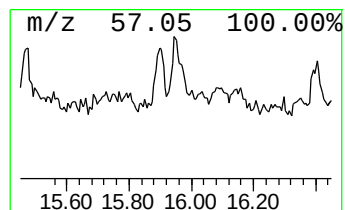
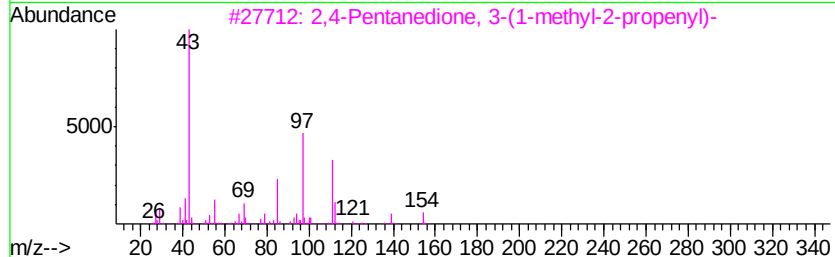
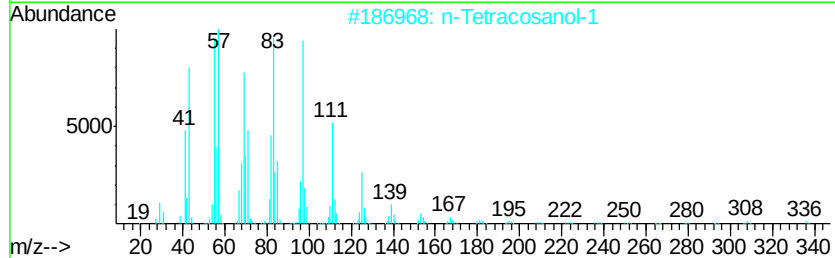
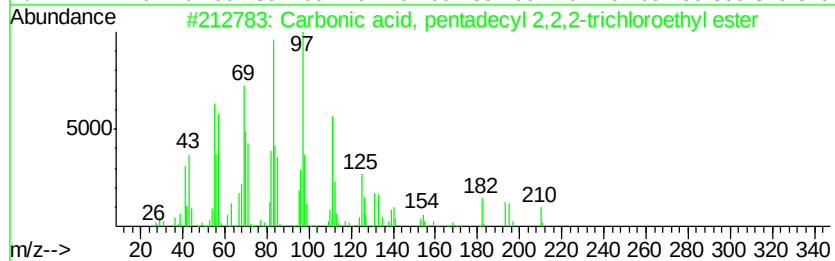
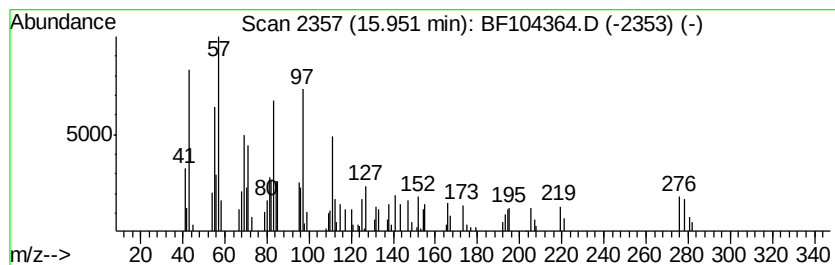
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Peak Number 6 unknown15.95 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	2.03 ng	86179	Perylene-d12	15.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Carbonic acid, pentadecyl 2,2,2-...	402	C18H33Cl3O3	1000314-56-1	49
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	43
3		2,4-Pentanedione, 3-(1-methyl-2-...	154	C9H14O2	029149-83-5	43
4		1-Heptacosanol	396	C27H56O	002004-39-9	41
5		Octacosyl acetate	452	C30H60O2	018206-97-8	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.02	6.0	ng	260638	1	6.80	866164	20.0
unknown6.57	6.57	78.8	ng	3412240	1	6.80	866164	20.0
n-Hexadecanoic acid	11.86	3.9	ng	238574	4	11.33	1233080	20.0
Behenic alcohol	13.81	6.1	ng	272770	5	13.97	893539	20.0
unknown15.95	15.95	2.0	ng	86179	6	15.43	849150	20.0