

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011915\
 Data File : BF076930.D
 Acq On : 19 Jan 2015 15:23
 Operator : IZ / TP
 Sample : G1101-13
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TE-PMW-11S

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-BF011415.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	1.464	31	33	41	rVB	24937	55570	4.82%	0.714%
2	4.104	262	264	275	rVB	46694	105704	9.16%	1.357%
3	5.030	342	345	355	rBV	232869	426267	36.95%	5.474%
4	7.362	546	549	555	rBV	153647	257457	22.32%	3.306%
5	7.465	555	558	563	rVB	496790	786601	68.19%	10.101%
6	7.967	599	602	608	rVB	108160	175064	15.18%	2.248%
7	8.287	627	630	634	rBV	413825	728240	63.13%	9.351%
8	9.270	712	716	719	rBV	395428	584384	50.66%	7.504%
9	10.882	853	857	860	rBV	165735	249702	21.65%	3.206%
10	13.534	1085	1089	1092	rBV	795714	1153499	100.00%	14.812%
11	15.008	1215	1218	1222	rBV	170850	270501	23.45%	3.474%
12	16.677	1361	1364	1367	rBV	537104	688226	59.66%	8.838%
13	17.774	1457	1460	1463	rBV	238359	275327	23.87%	3.535%
14	19.466	1605	1608	1611	rVB	20260	23876	2.07%	0.307%
15	19.900	1643	1646	1649	rBV	79974	76531	6.63%	0.983%
16	20.003	1653	1655	1658	rVV	1032851	1083980	93.97%	13.919%
17	20.792	1722	1724	1727	rBV	49190	54478	4.72%	0.700%
18	20.929	1734	1736	1738	rVB	10521	12612	1.09%	0.162%
19	21.272	1761	1766	1769	rBV	286671	358940	31.12%	4.609%
20	21.660	1797	1800	1804	rVB2	12462	18350	1.59%	0.236%
21	22.037	1831	1833	1837	rBV	13830	18393	1.59%	0.236%
22	22.415	1863	1866	1869	rBV2	10959	19162	1.66%	0.246%
23	22.769	1895	1897	1899	rVB	13469	15468	1.34%	0.199%
24	22.917	1907	1910	1913	rBV	190992	250085	21.68%	3.211%
25	23.123	1926	1928	1932	rBV3	9728	16500	1.43%	0.212%
26	23.512	1960	1962	1965	rVB3	7662	12809	1.11%	0.164%
27	23.843	1987	1991	1994	rVB5	7579	20388	1.77%	0.262%
28	23.923	1994	1998	2000	rBV3	4917	12289	1.07%	0.158%
29	24.460	2042	2045	2049	rBV5	15400	37106	3.22%	0.476%

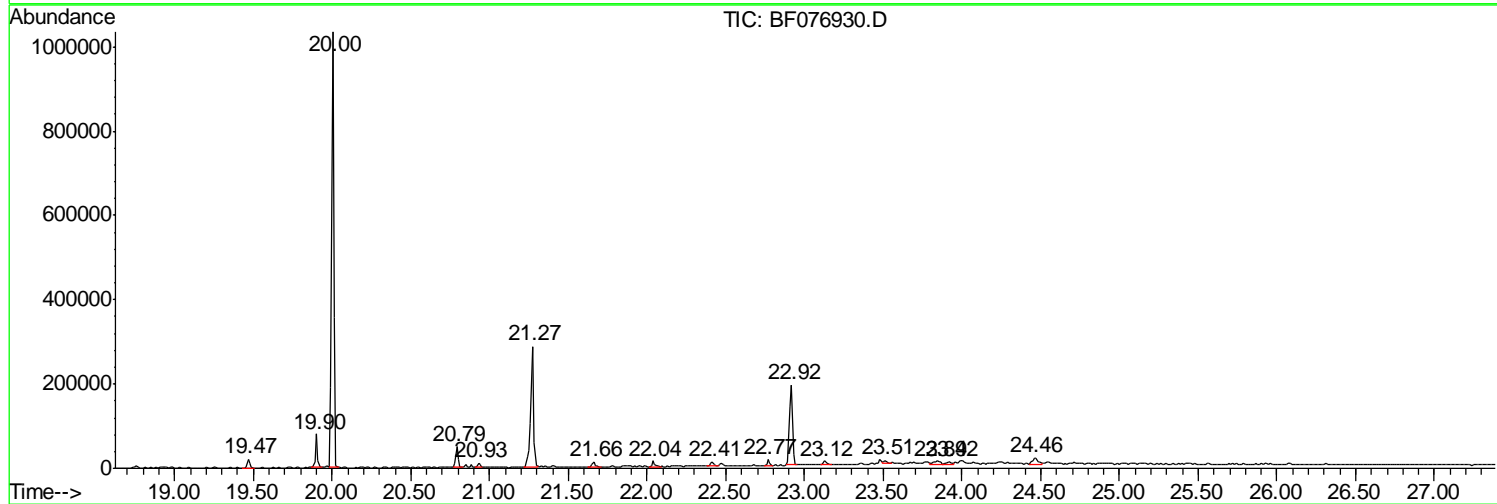
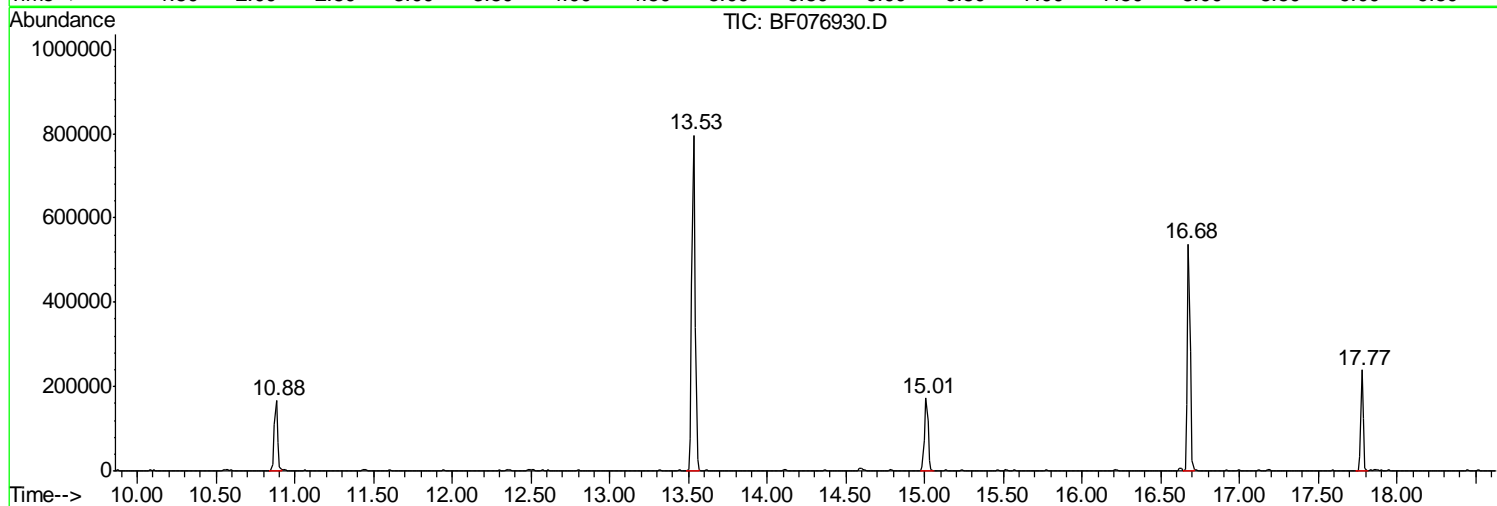
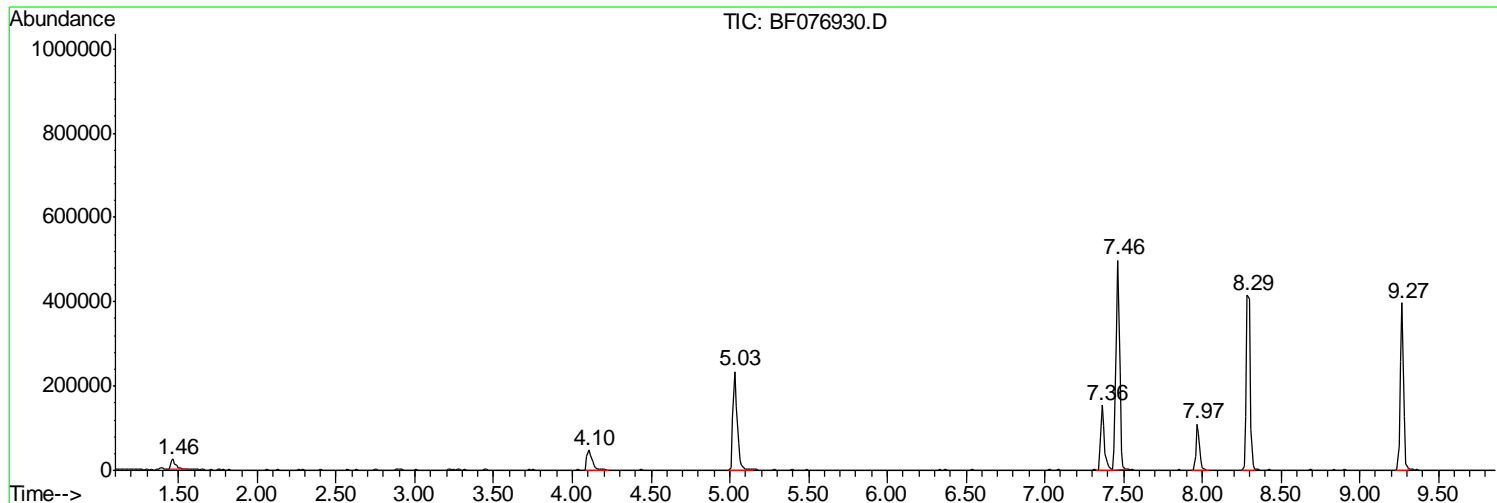
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 ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF011415.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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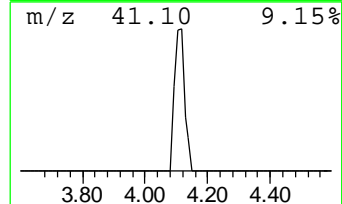
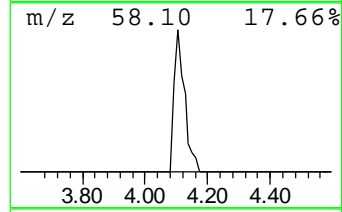
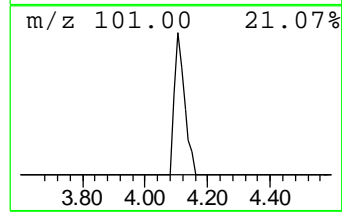
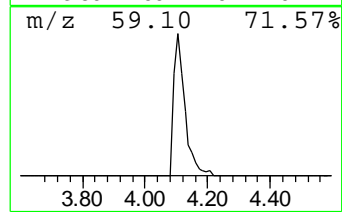
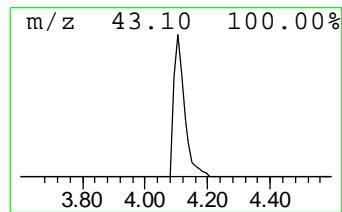
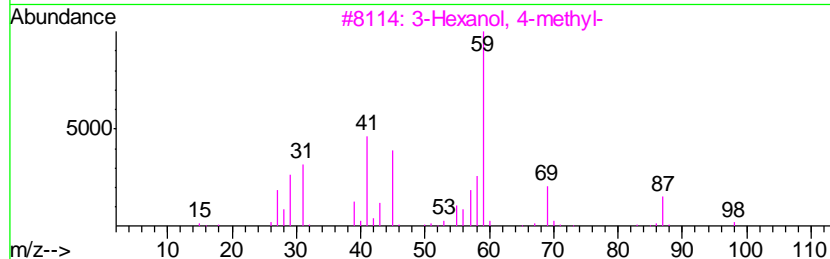
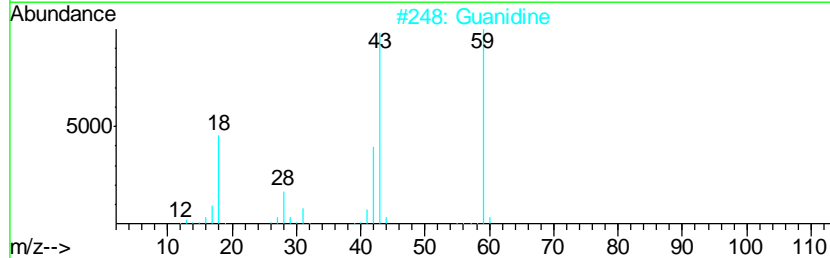
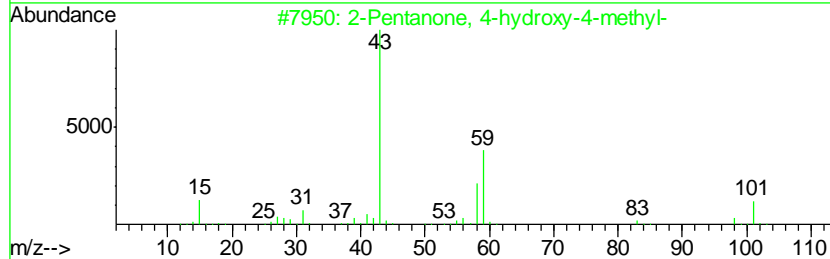
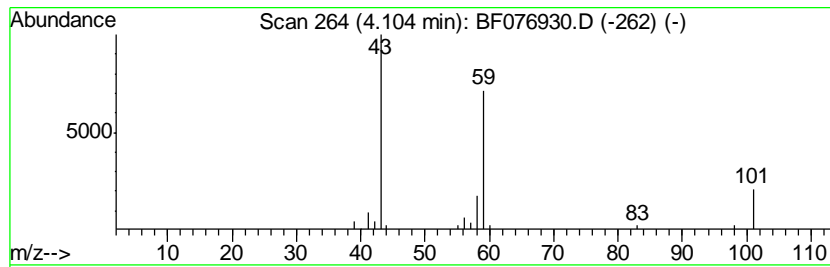
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TIC Library : C:\DATABASE\NIST02.L
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 Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.10	12.08 ng	105704	1,4-Dichlorobenzene-d4	7.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Guanidine	59	CH5N3	000113-00-8	43
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25
4		3-Hexanol	102	C6H14O	000623-37-0	9
5		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9



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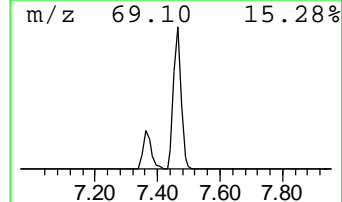
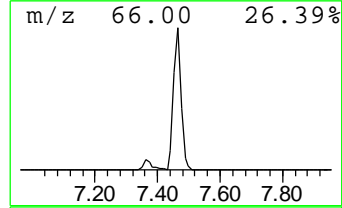
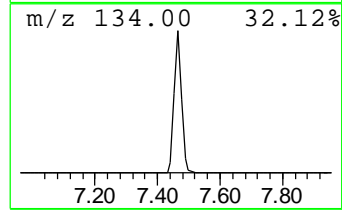
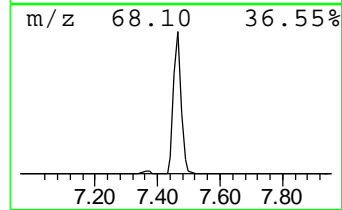
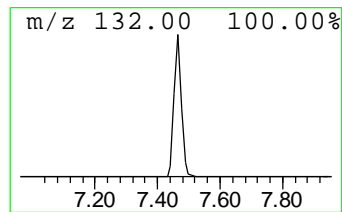
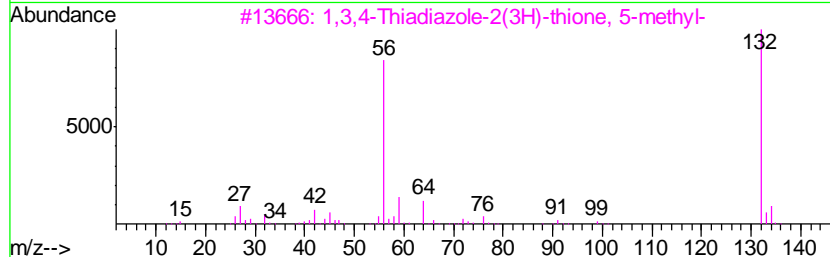
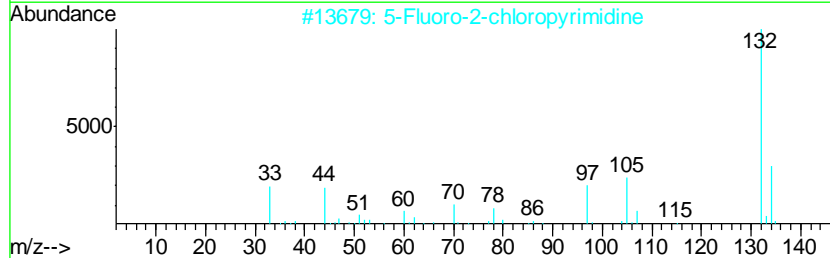
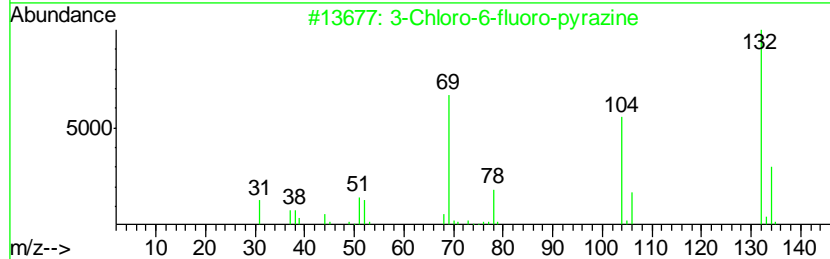
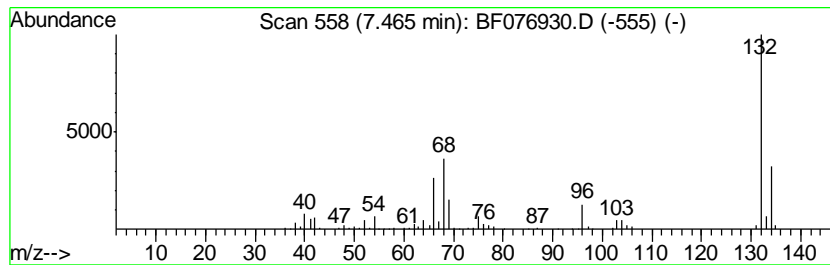
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 Peak Number 3 unknown7.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.46	89.86 ng	786601	1,4-Dichlorobenzene-d4	7.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	25
3		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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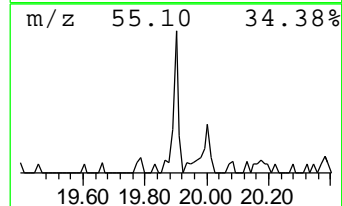
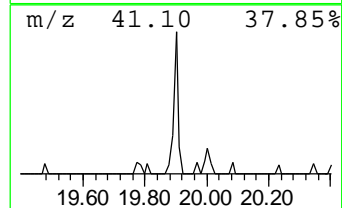
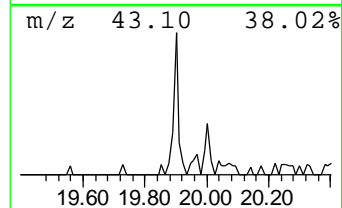
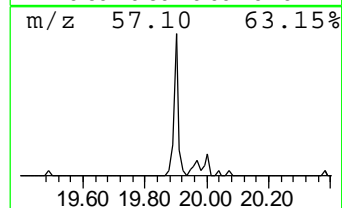
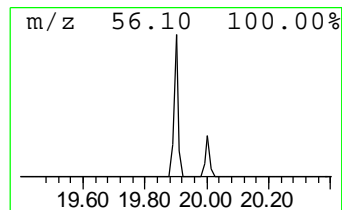
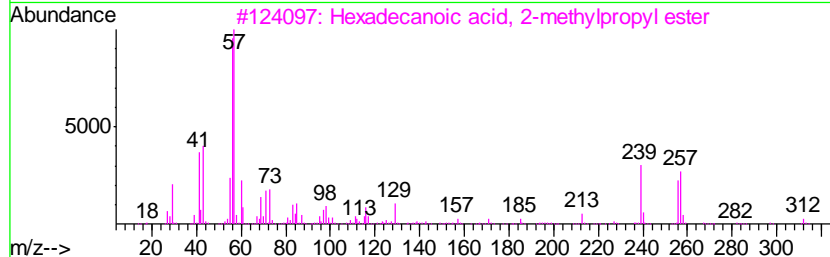
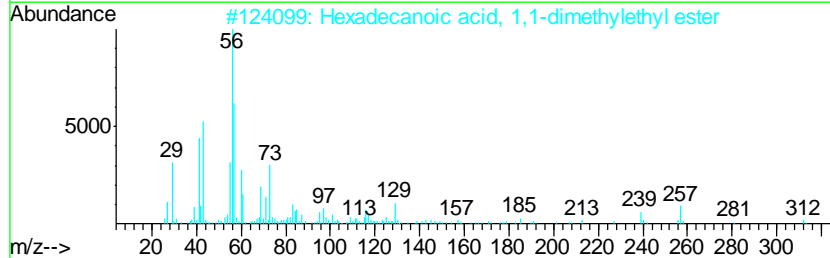
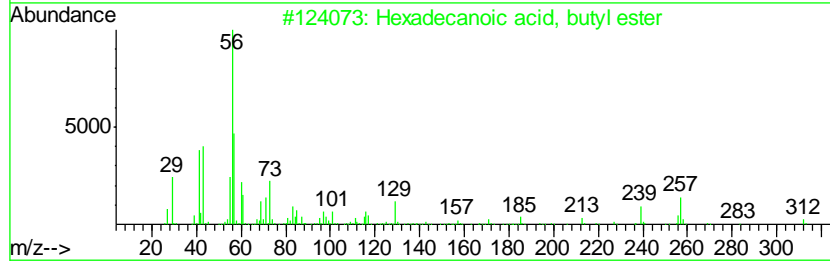
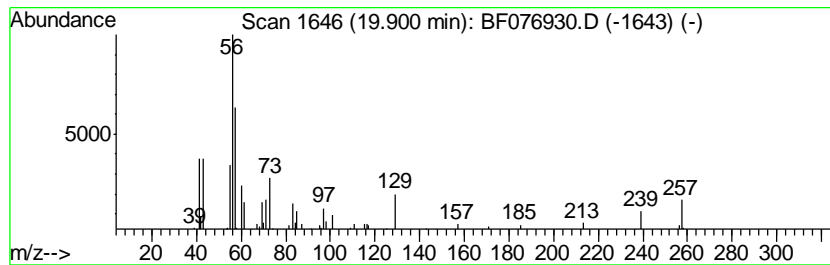
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 Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.90	4.26 ng	76531	Chrysene-d12	21.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	91
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	35
4		Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32
5		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	32



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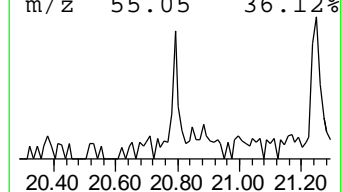
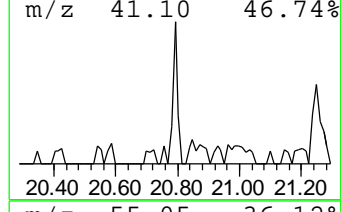
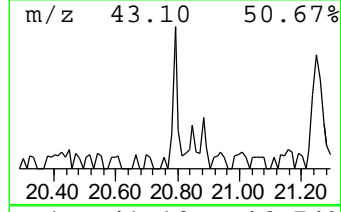
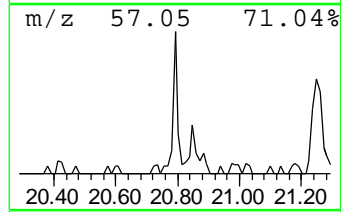
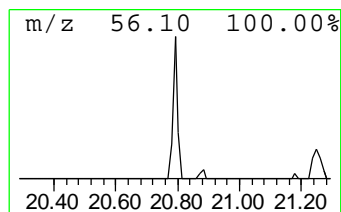
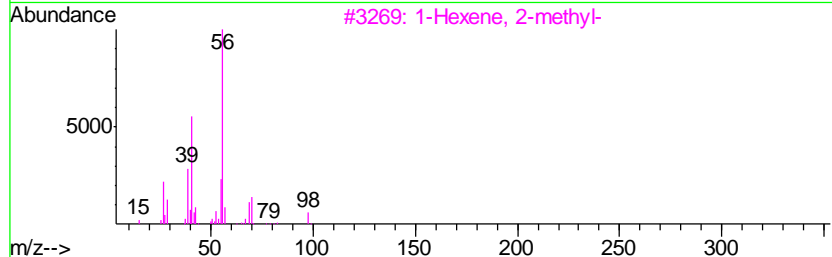
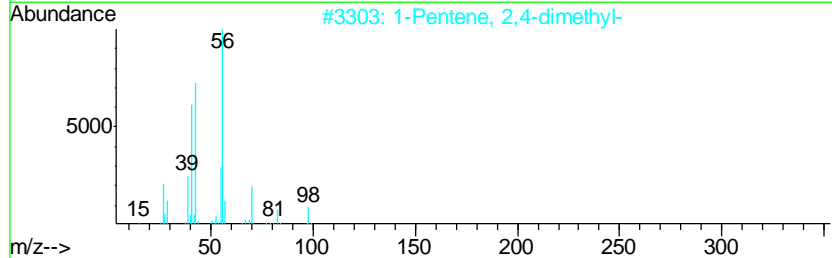
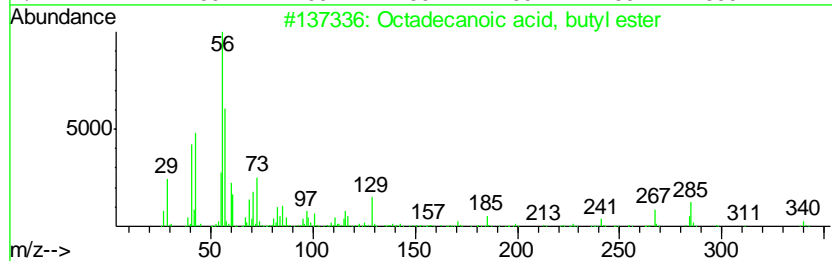
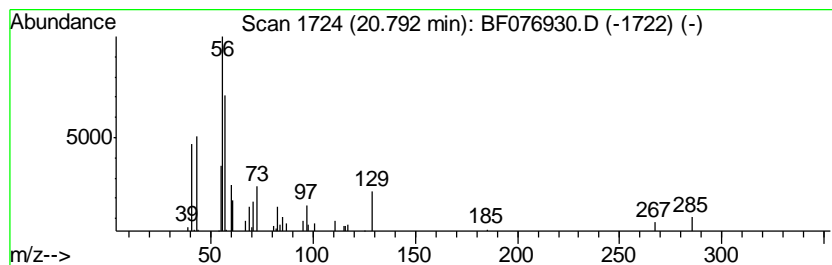
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TIC Library : C:\DATABASE\NIST02.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.79	3.04 ng	54478	Chrysene-d12	21.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	80
2		1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27
3		1-Hexene, 2-methyl-	98	C7H14	006094-02-6	27
4		2,4-Dimethyl-1-hexene	112	C8H16	016746-87-5	27
5		2-Methyl-1-octadecene	266	C19H38	061868-20-0	25



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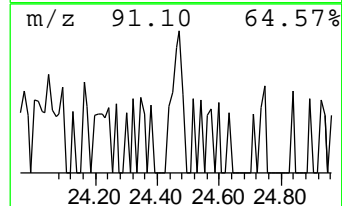
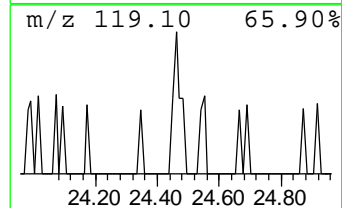
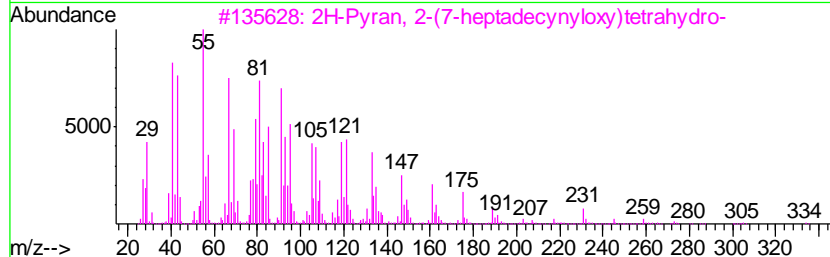
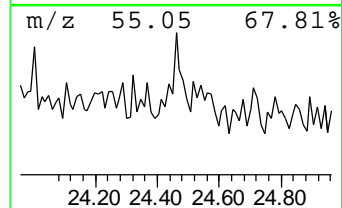
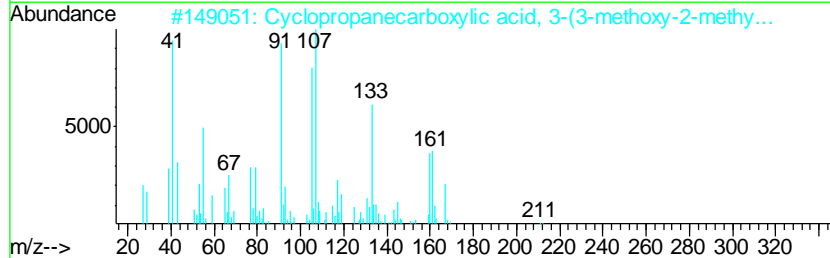
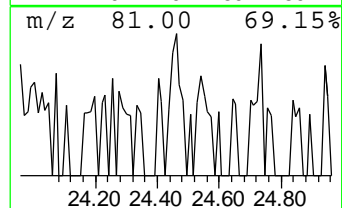
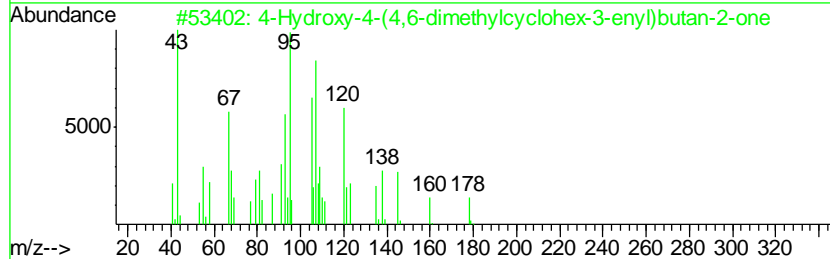
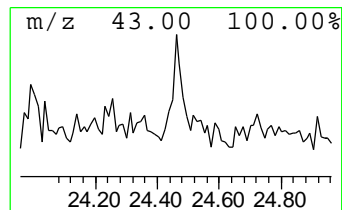
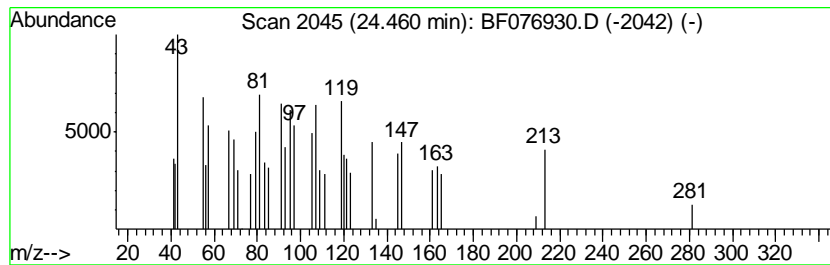
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TIC Library : C:\DATABASE\NIST02.L
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 Peak Number 7 unknown24.46 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.46	2.97 ng	37106	Perylene-d12	22.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Hydroxy-4-(4,6-dimethylcyclohe...	196	C12H20O2	002316-79-2	12
2		Cyclopropanecarboxylic acid, 3-(...	372	C22H28O5	000121-29-9	10
3		2H-Pyran, 2-(7-heptadecynyl)oxy)t...	336	C22H40O2	056599-50-9	10
4		7-Hydroxy-3-(1,1-dimethylprop-2-...	230	C14H14O3	056881-08-4	10
5		benz[d]isoxazole, 3-ethyl-	147	C9H9NO	066033-77-0	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.10	12.1	ng	105704	1	7.97	175064	20.0
unknown7.46	7.46	89.9	ng	786601	1	7.97	175064	20.0
Hexadecanoic acid...	19.90	4.3	ng	76531	5	21.27	358940	20.0
Octadecanoic acid...	20.79	3.0	ng	54478	5	21.27	358940	20.0
unknown24.46	24.46	3.0	ng	37106	6	22.92	250085	20.0