

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092217\  
 Data File : BF098688.D  
 Acq On : 22 Sep 2017 9:48  
 Operator : SJ/JU  
 Sample : I5313-01  
 Misc :  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 72-12000-R4-COMP

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-BF092117.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	2.234	22	25	43	rVB	114759	250703	6.93%	0.795%
2	3.528	242	245	252	rBV2	19563	51135	1.41%	0.162%
3	5.151	517	521	532	rVB	484043	622540	17.20%	1.974%
4	5.539	582	587	591	rBV	3111401	3374127	93.24%	10.700%
5	6.545	751	758	761	rBV	3296933	3618735	100.00%	11.476%
6	6.692	778	783	786	rBV	3585518	3528296	97.50%	11.189%
7	6.928	819	823	826	rBV	1032683	897339	24.80%	2.846%
8	7.081	845	849	852	rBV	2469550	2104781	58.16%	6.675%
9	7.486	912	918	921	rBV	2244302	2097064	57.95%	6.650%
10	8.204	1036	1040	1044	rBV	1440337	1208700	33.40%	3.833%
11	9.280	1218	1223	1226	rBV	4080292	3525904	97.43%	11.182%
12	9.386	1237	1241	1244	rVB2	73613	62229	1.72%	0.197%
13	9.669	1285	1289	1292	rBV	350277	256421	7.09%	0.813%
14	9.963	1334	1339	1342	rBV	1397444	1257433	34.75%	3.988%
15	10.745	1466	1472	1476	rBV	2266879	2133390	58.95%	6.766%
16	10.857	1488	1491	1498	rBV	53334	57929	1.60%	0.184%
17	11.445	1587	1591	1594	rBV	1460438	1181266	32.64%	3.746%
18	11.963	1673	1679	1683	rBV3	85588	112989	3.12%	0.358%
19	12.657	1793	1797	1801	rBV	113346	97079	2.68%	0.308%
20	12.745	1809	1812	1820	rBV2	37233	47688	1.32%	0.151%
21	12.886	1830	1836	1840	rBV	89149	85302	2.36%	0.271%
22	13.033	1856	1861	1864	rVB	2995091	2950618	81.54%	9.357%
23	13.915	2008	2011	2018	rVB2	78862	81015	2.24%	0.257%
24	14.057	2031	2035	2036	rBV	173386	139192	3.85%	0.441%
25	14.080	2036	2039	2042	rVB	908164	777786	21.49%	2.467%
26	14.704	2142	2145	2149	rBV	86486	93118	2.57%	0.295%
27	15.127	2214	2217	2226	rVB3	32635	66365	1.83%	0.210%
28	15.568	2287	2292	2301	rVB	619595	799484	22.09%	2.535%
29	17.686	2648	2652	2661	rVB9	27030	54269	1.50%	0.172%

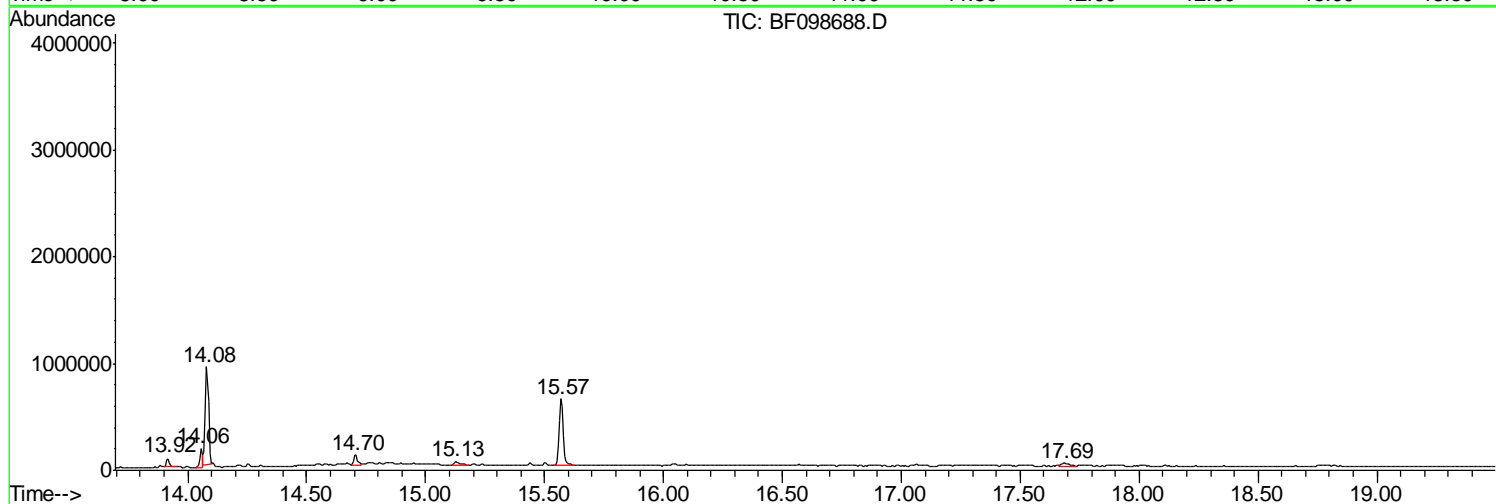
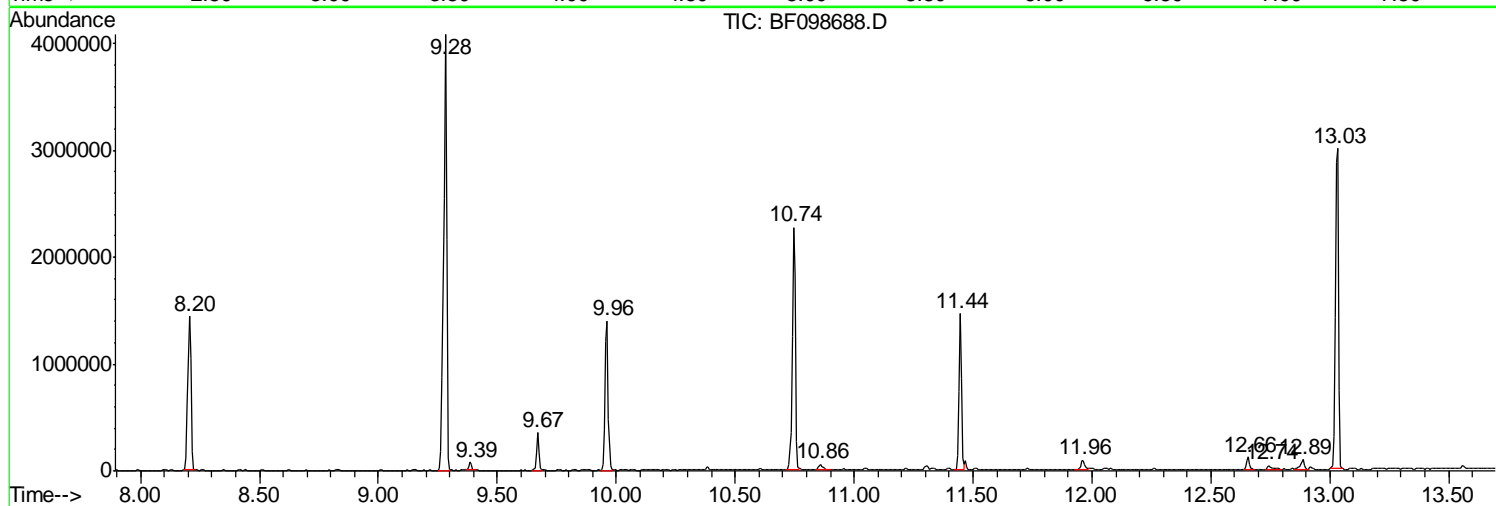
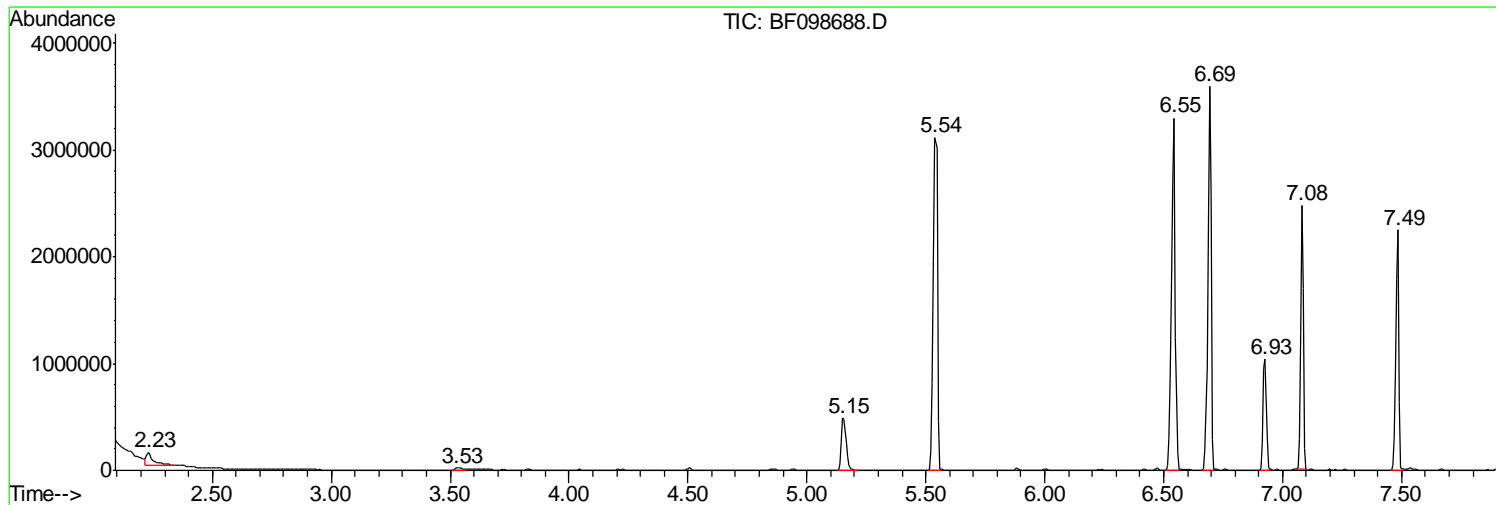
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72-12000-R4-COMP

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092117.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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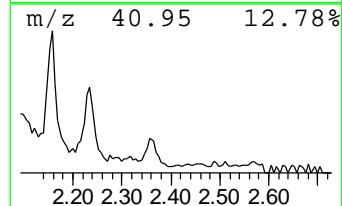
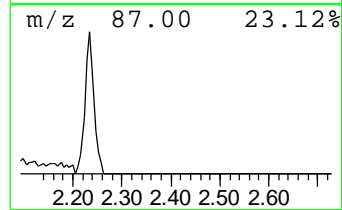
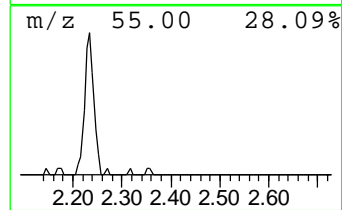
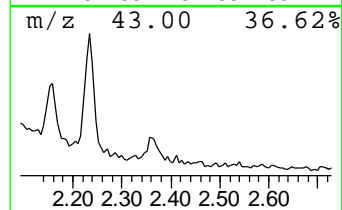
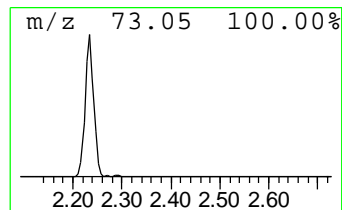
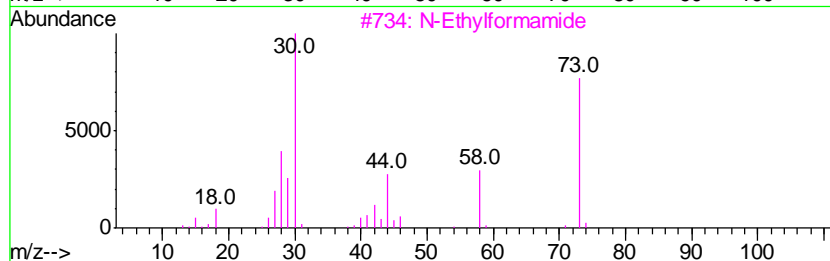
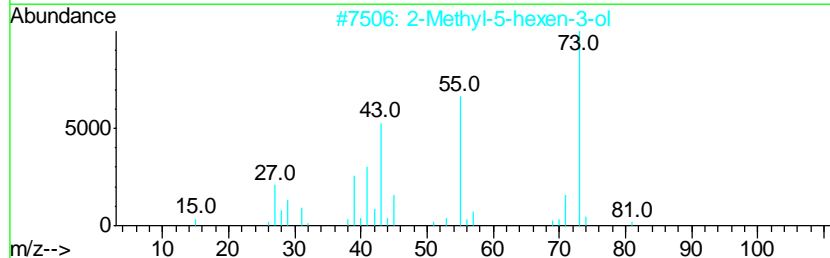
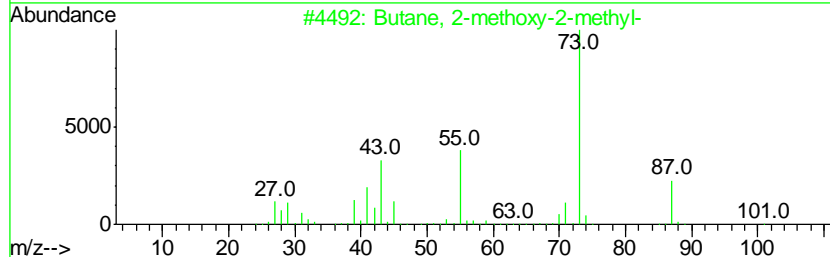
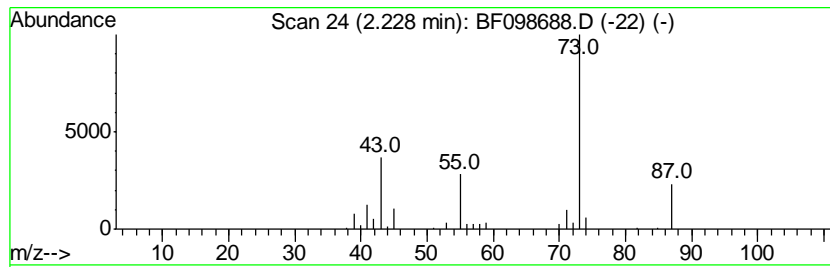
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TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	5.59 ng	250703	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		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	32
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5		1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	9



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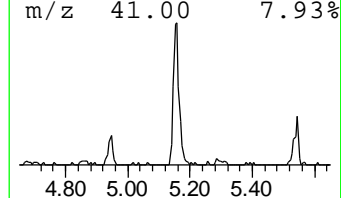
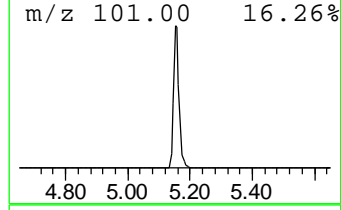
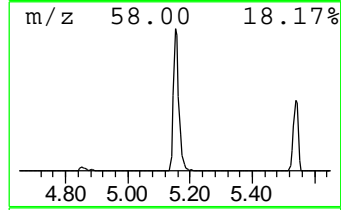
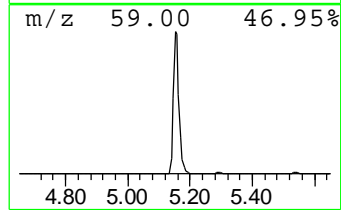
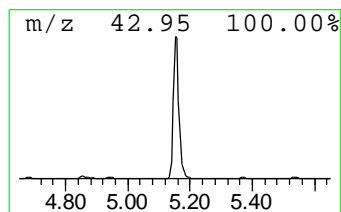
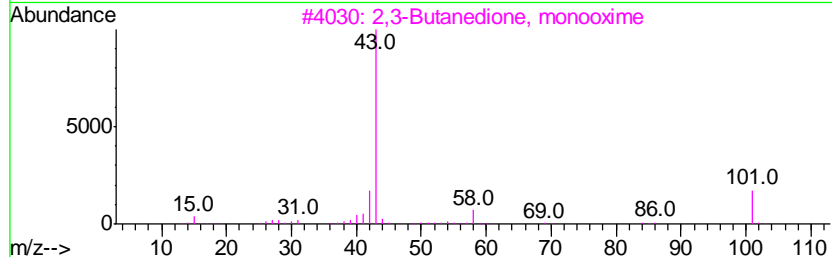
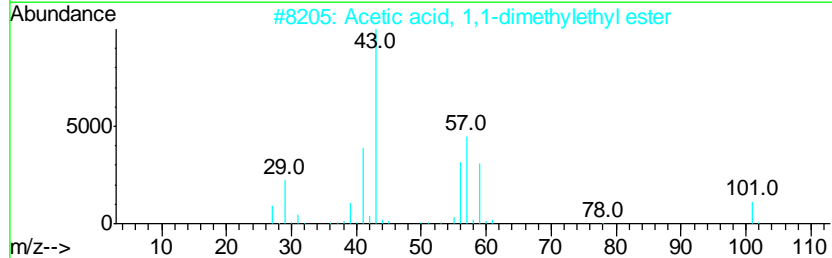
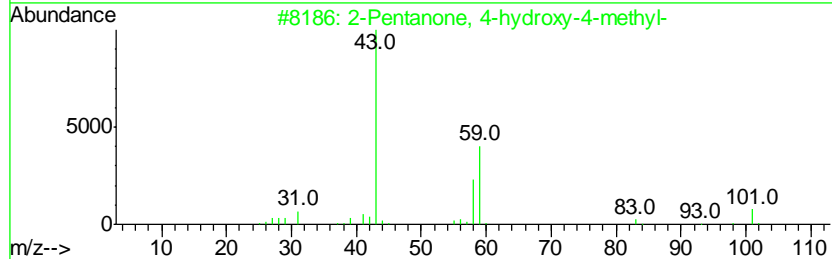
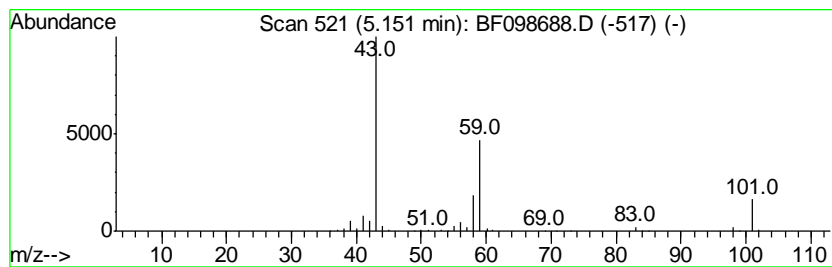
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 Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	13.88 ng	622540	1,4-Dichlorobenzene-d4	6.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4		Acetone	58	C3H6O	000067-64-1	12
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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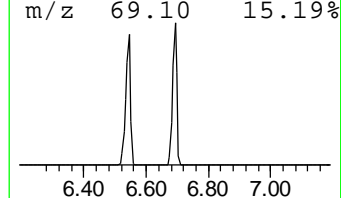
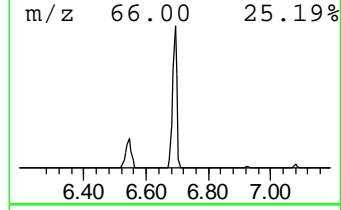
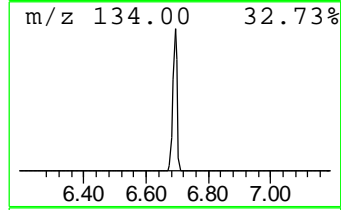
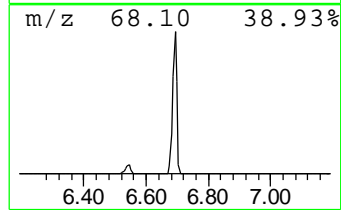
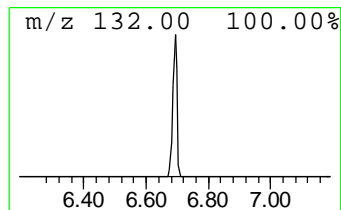
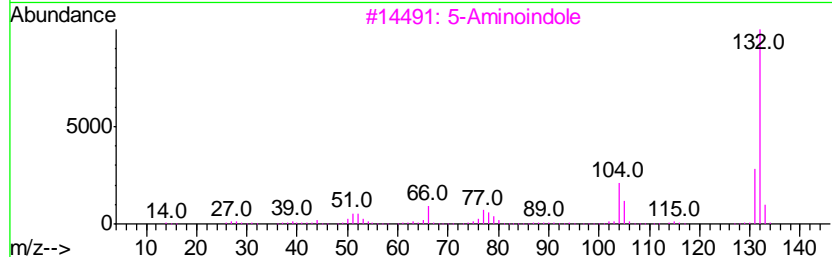
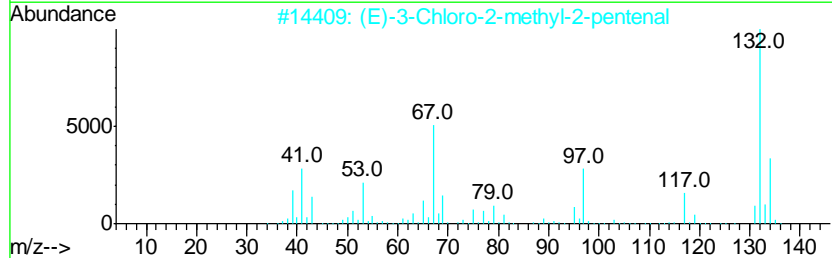
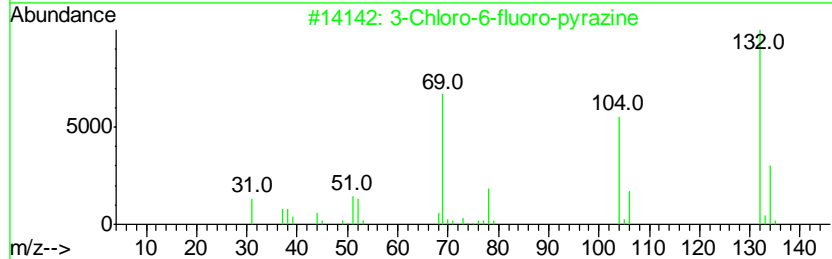
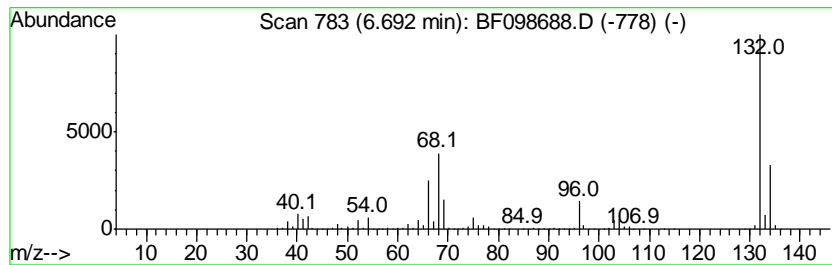
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TIC Library : C:\DATABASE\NIST11.L  
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 Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	78.64 ng	3528300	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	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



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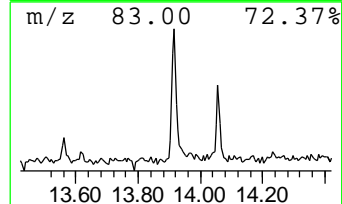
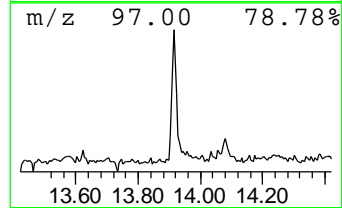
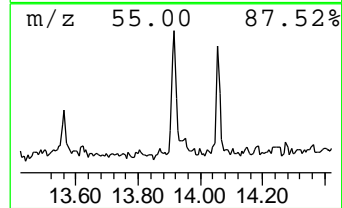
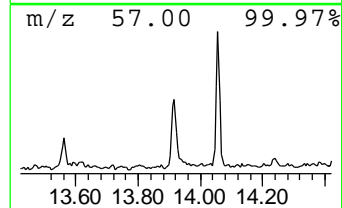
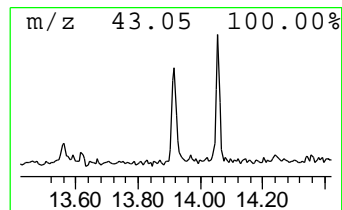
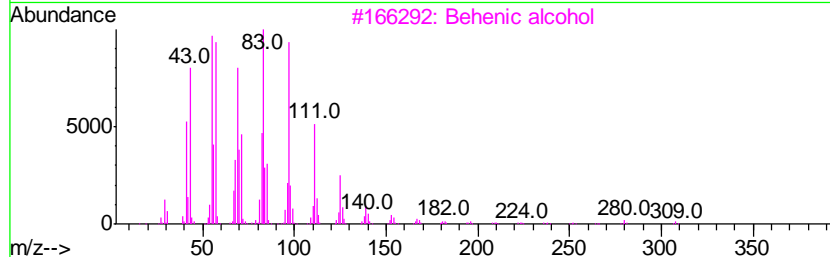
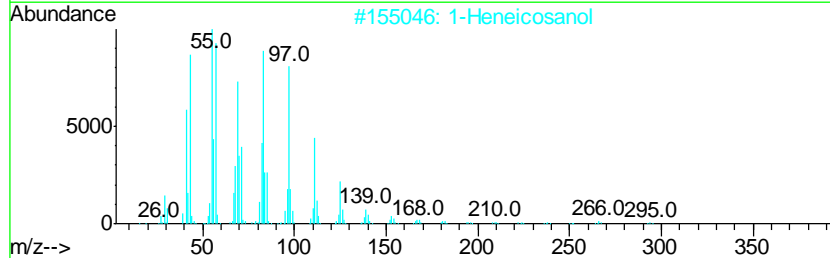
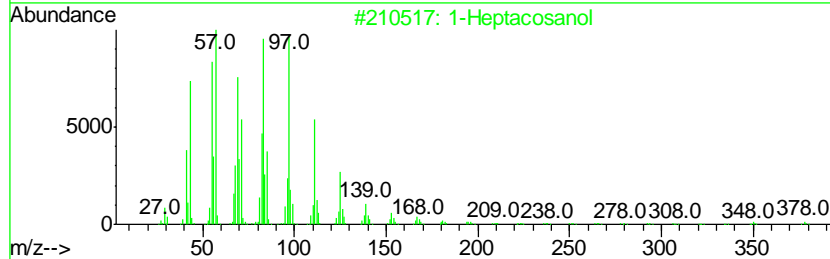
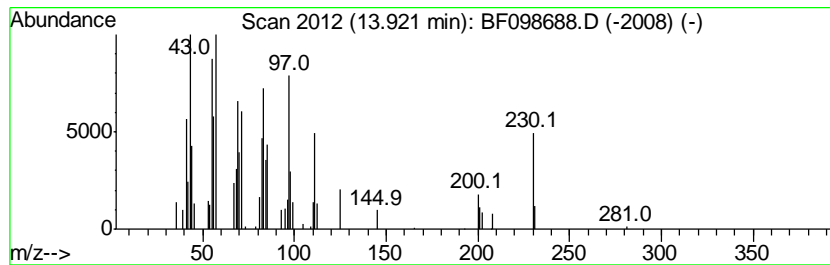
TIC Library : C:\DATABASE\NIST11.L  
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 Peak Number 6 1-Heptacosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	2.08 ng	81015	Chrysene-d12	14.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heptacosanol	396	C27H56O	002004-39-9	95
2		1-Heneicosanol	312	C21H44O	015594-90-8	93
3		Behenic alcohol	326	C22H46O	000661-19-8	93
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	90
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	90



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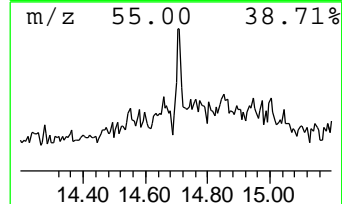
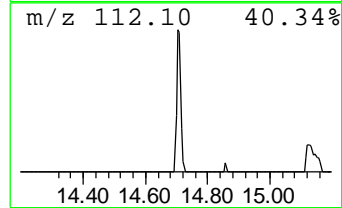
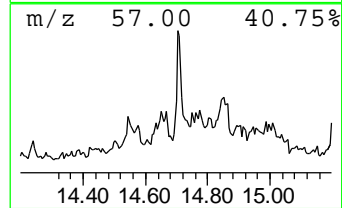
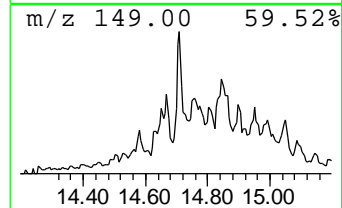
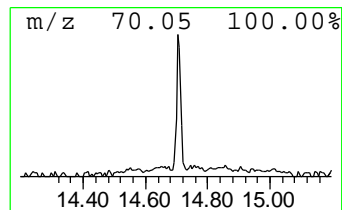
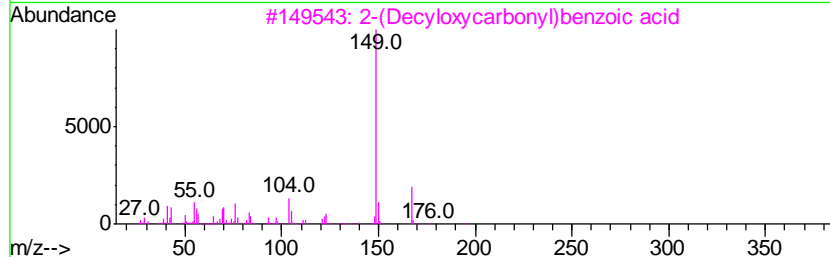
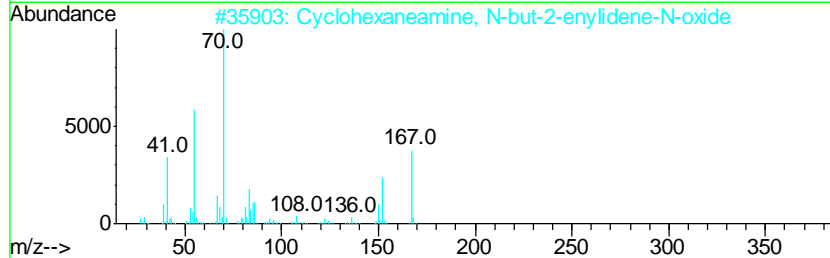
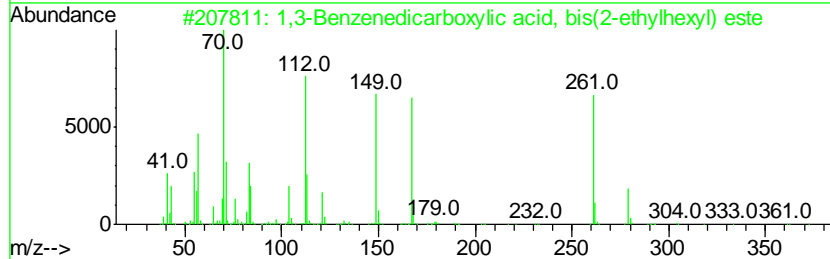
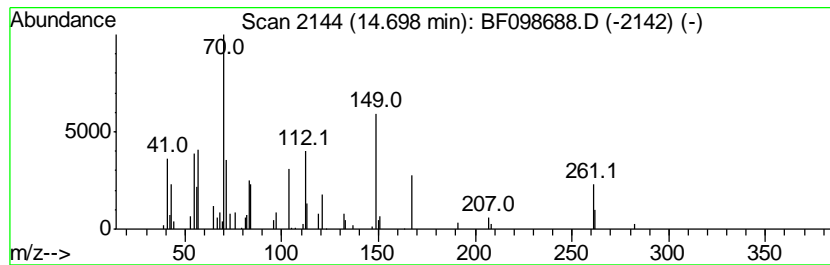
TIC Library : C:\DATABASE\NIST11.L  
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 Peak Number 7 1,3-Benzenedicarboxylic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	2.39 ng	93118	Chrysene-d12	14.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	52
2		Cyclohexaneamine, N-but-2-enylid...	167	C10H17NO	068048-01-1	35
3		2-(Decyloxy carbonyl)benzoic acid	306	C18H26O4	1000373-53-2	32
4		Diisooctyl phthalate	390	C24H38O4	000131-20-4	22
5		Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	22



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.23	5.6	ng	250703	1	6.93	897339	20.0
2-Pentanone, 4-hy...	5.15	13.9	ng	622540	1	6.93	897339	20.0
unknown6.69	6.69	78.6	ng	3528300	1	6.93	897339	20.0
1-Heptacosanol	13.92	2.1	ng	81015	5	14.08	777786	20.0
1,3-Benzenedicarb...	14.70	2.4	ng	93118	5	14.08	777786	20.0