

Data Path : Z:\HPCHEM1\BNA G\DATA\BG060717\  
 Data File : BG027299.D  
 Acq On : 8 Jun 2017 1:11  
 Operator : SJ/MA  
 Sample : I3479-14  
 Misc :  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 SB-4(7-9)20170604

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 G\METHODS\8270-BG060517.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	3.815	15	21	35	rVB3	26736	62232	1.31%	0.241%
2	5.701	337	342	352	rBV	120989	201552	4.24%	0.781%
3	6.141	409	417	430	rBV	1230904	2103536	44.22%	8.150%
4	7.693	671	681	695	rBV	1279715	2376281	49.96%	9.207%
5	8.092	740	749	761	rBV	1201201	2182886	45.89%	8.458%
6	8.556	821	828	839	rVB	164484	300860	6.32%	1.166%
7	8.885	875	884	894	rBV	782529	1451711	30.52%	5.625%
8	9.720	1016	1026	1040	rBV	667215	1304898	27.43%	5.056%
9	11.376	1300	1308	1317	rBV	250908	488349	10.27%	1.892%
10	13.768	1705	1715	1722	rBV	1947241	3234199	67.99%	12.531%
11	14.573	1844	1852	1858	rBV	269193	414622	8.72%	1.607%
12	15.137	1941	1948	1957	rVB3	421461	722970	15.20%	2.801%
13	16.623	2194	2201	2213	rBV	1726539	2778673	58.42%	10.766%
14	16.805	2226	2232	2236	rBV	41322	59925	1.26%	0.232%
15	17.887	2409	2416	2428	rVB2	566830	922340	19.39%	3.574%
16	18.727	2555	2559	2570	rBV2	89048	137951	2.90%	0.535%
17	20.466	2848	2855	2863	rBV	3454712	4756713	100.00%	18.431%
18	21.829	3082	3087	3102	rBV3	106585	215605	4.53%	0.835%
19	22.270	3155	3162	3174	rVB	562195	1087142	22.85%	4.212%
20	25.959	3779	3790	3805	rVB2	298285	1006301	21.16%	3.899%

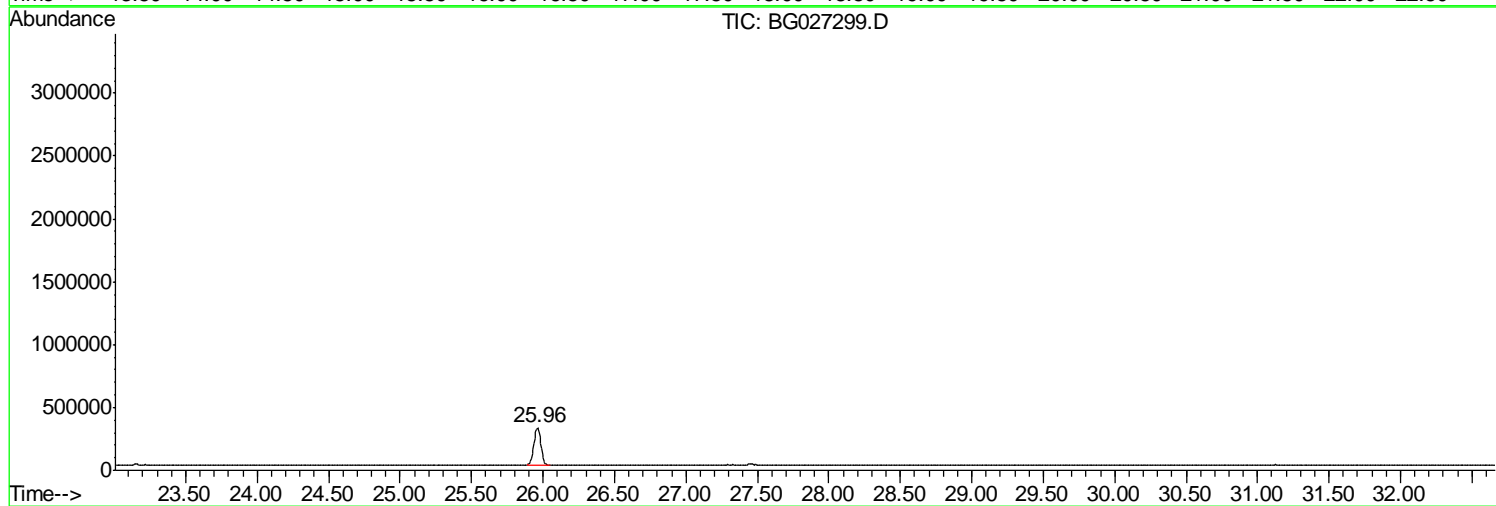
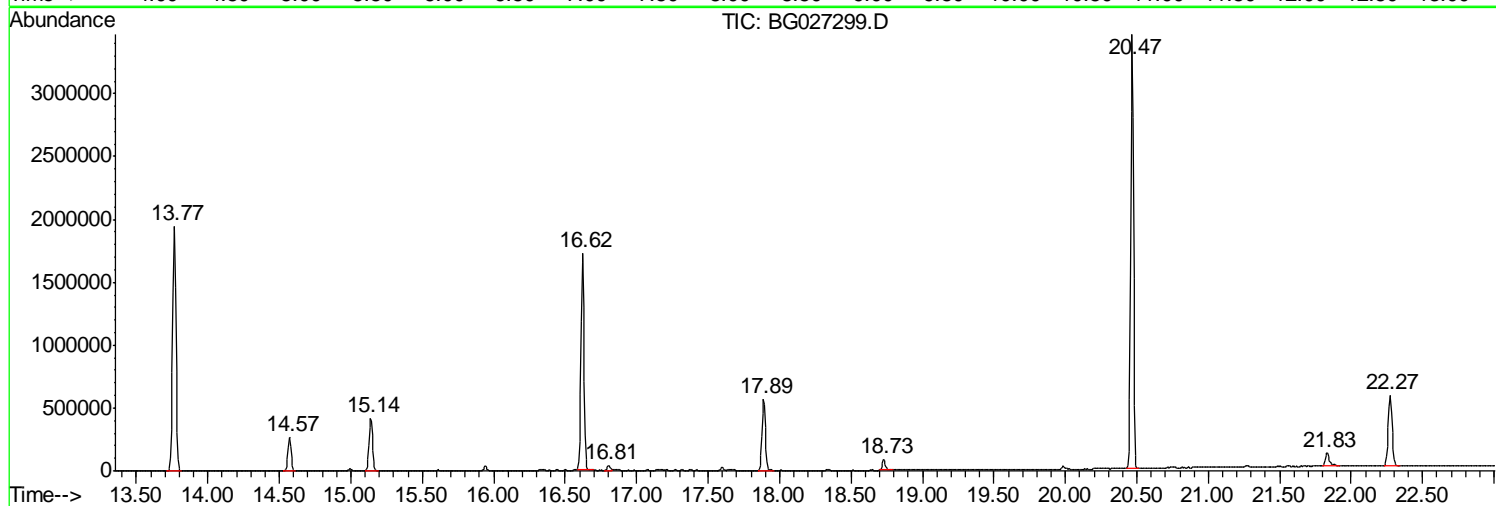
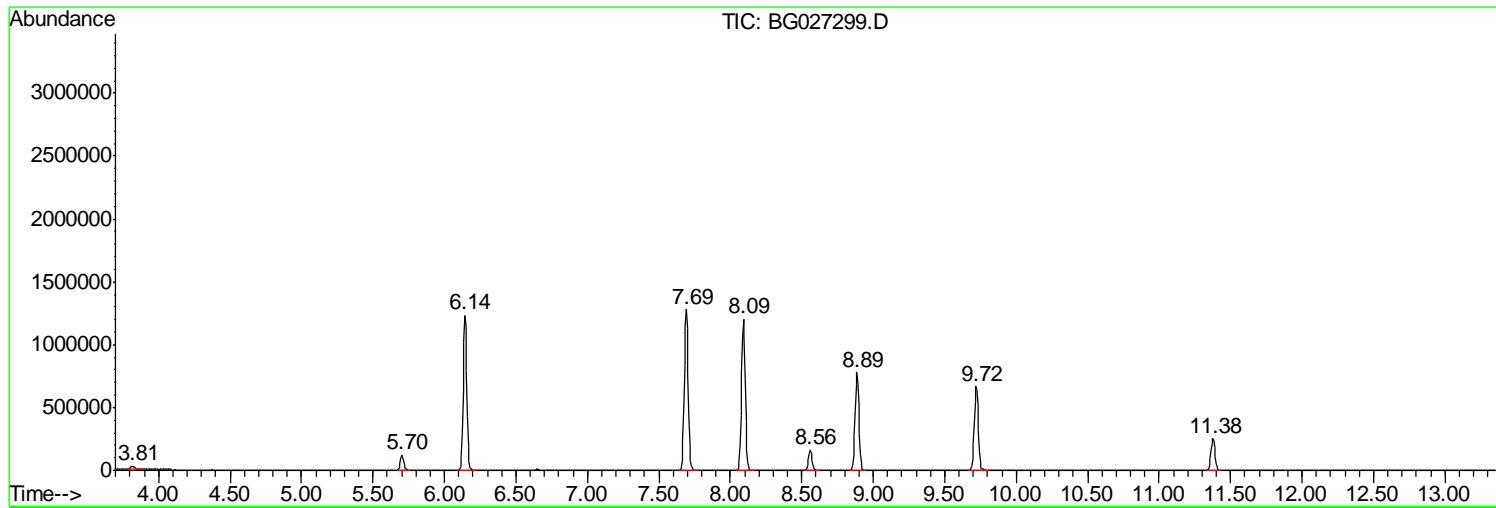
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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P



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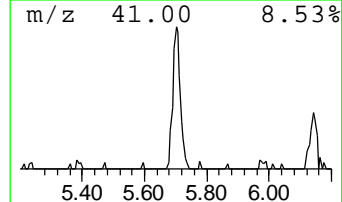
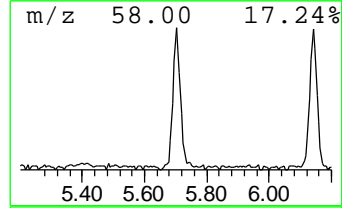
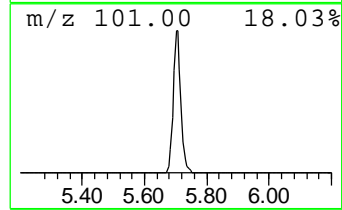
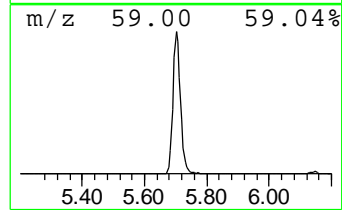
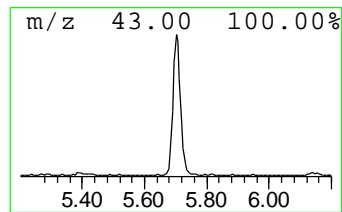
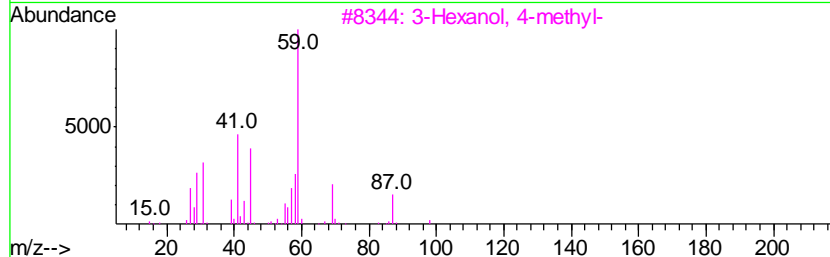
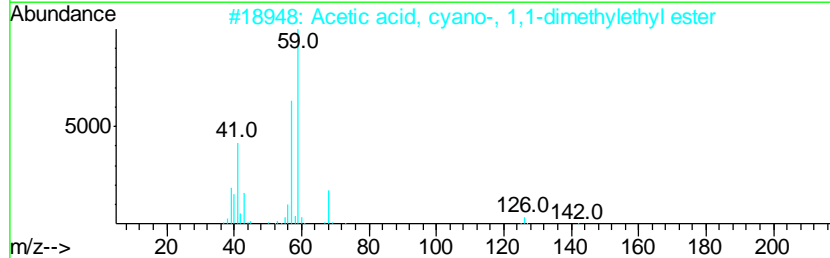
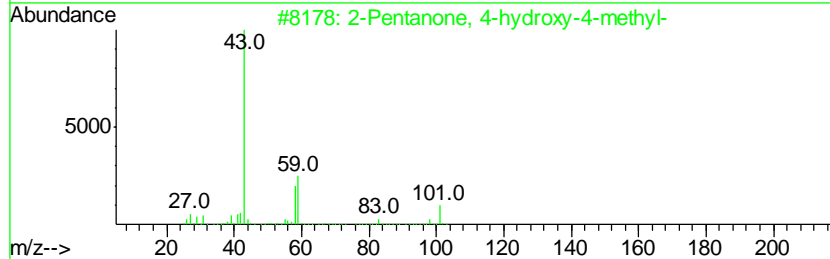
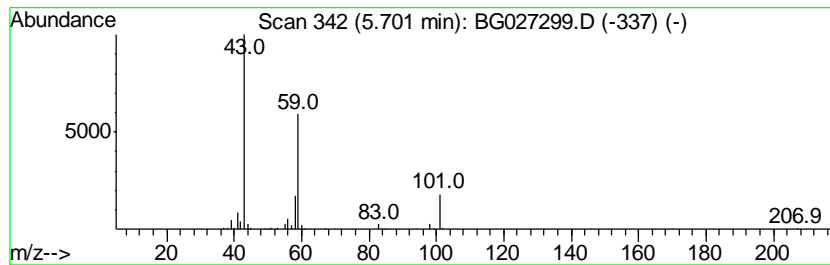
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.70	13.40 ng	201552	1,4-Dichlorobenzene-d4	8.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	37
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



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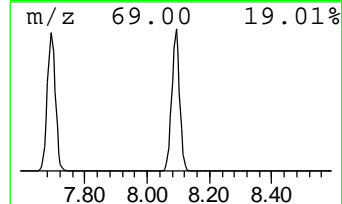
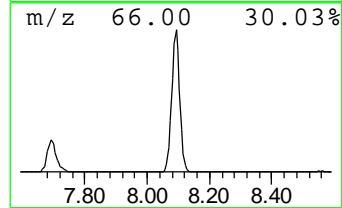
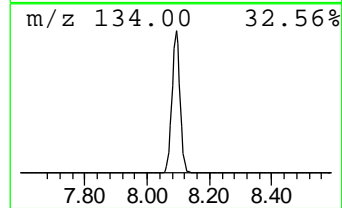
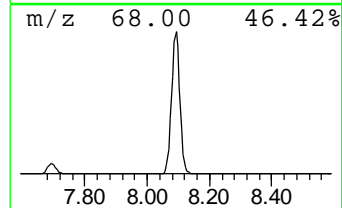
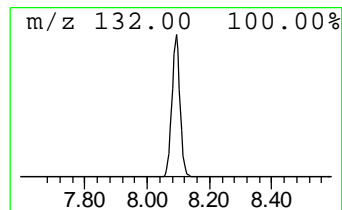
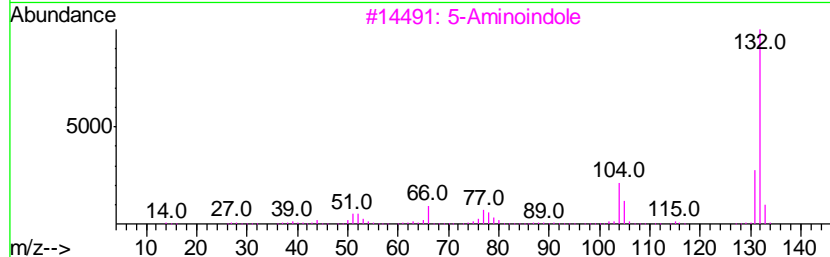
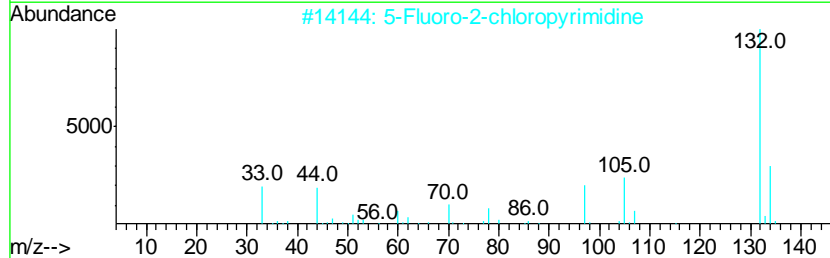
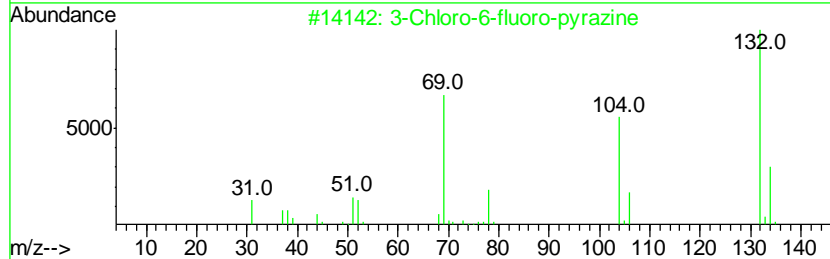
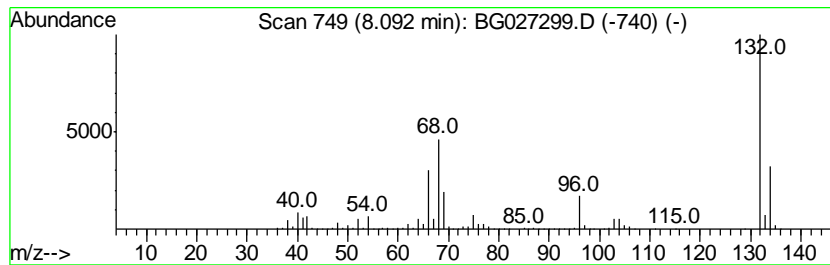
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 Peak Number 3 unknown8.09 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.09	145.11 ng	2182890	1,4-Dichlorobenzene-d4	8.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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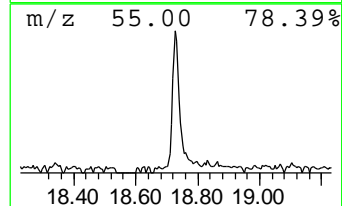
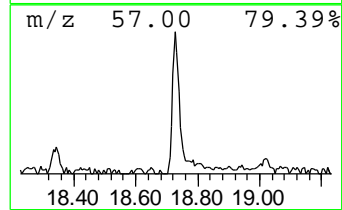
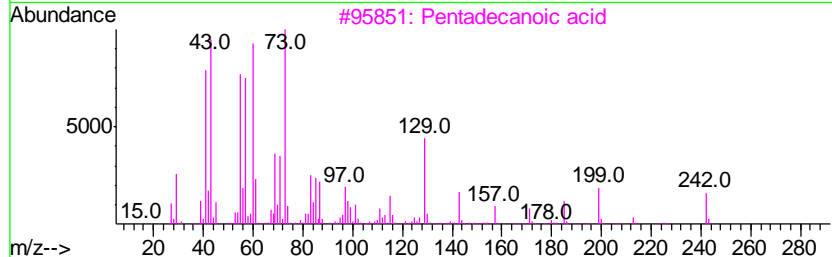
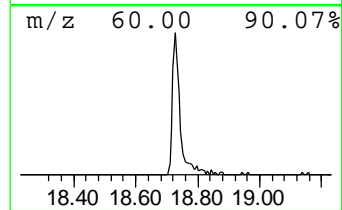
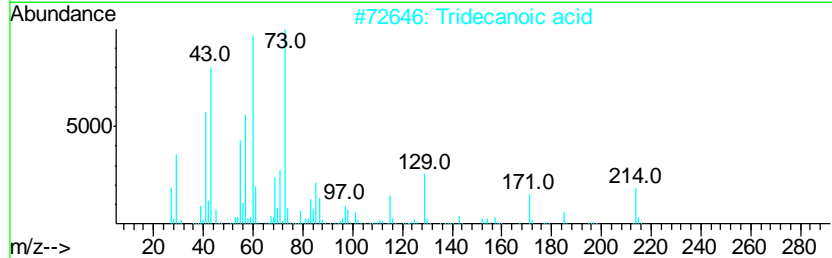
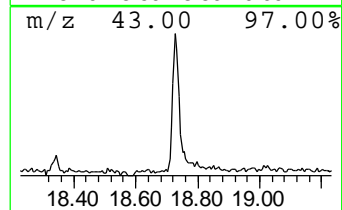
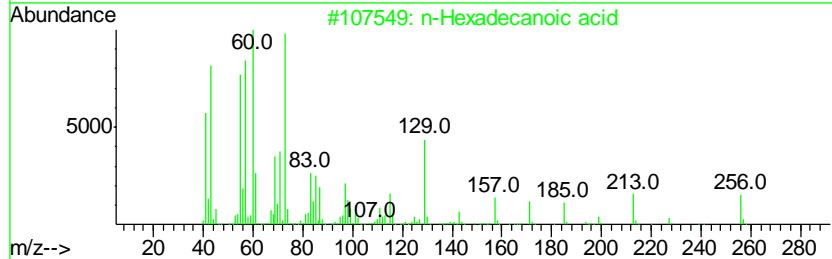
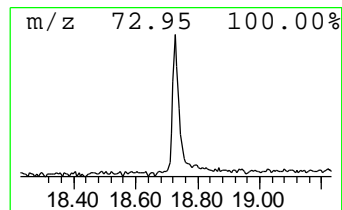
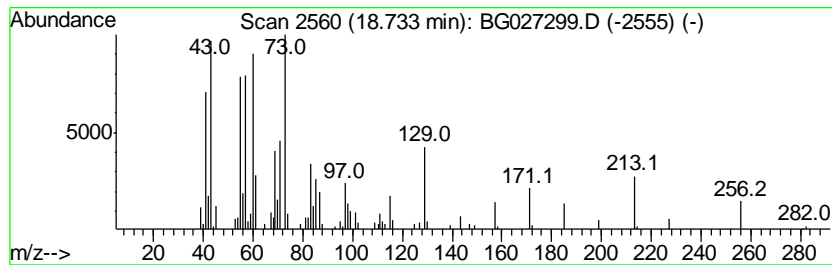
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.73	2.99 ng	137951	Phenanthrene-d10	17.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	76
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5		Dodecanoic acid	200	C12H24O2	000143-07-7	50



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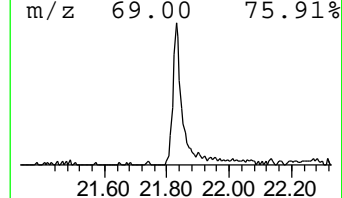
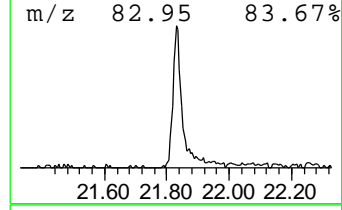
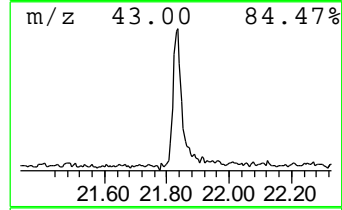
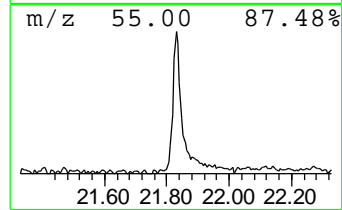
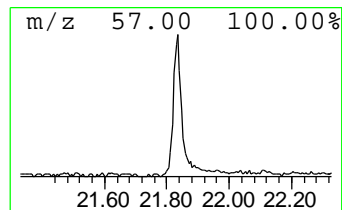
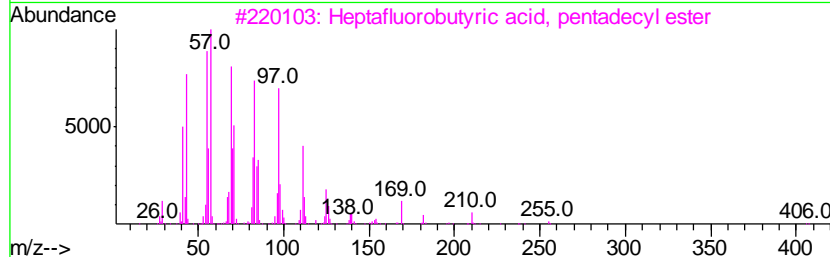
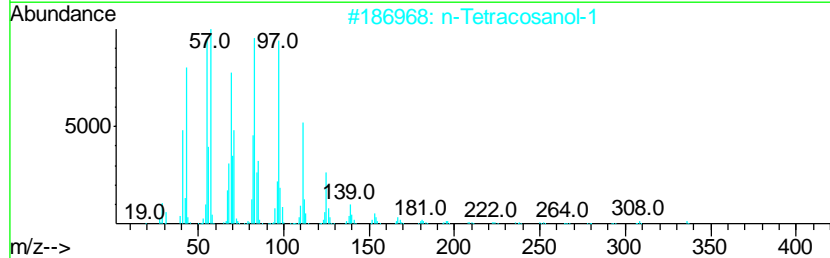
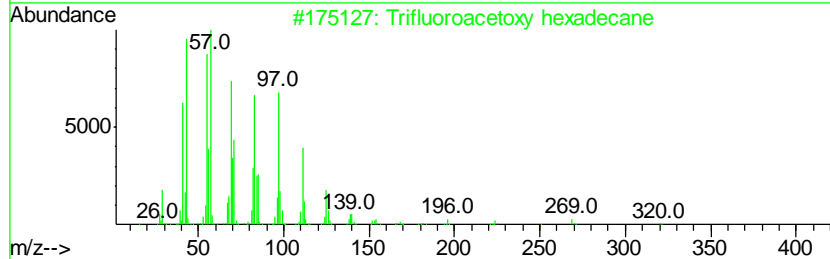
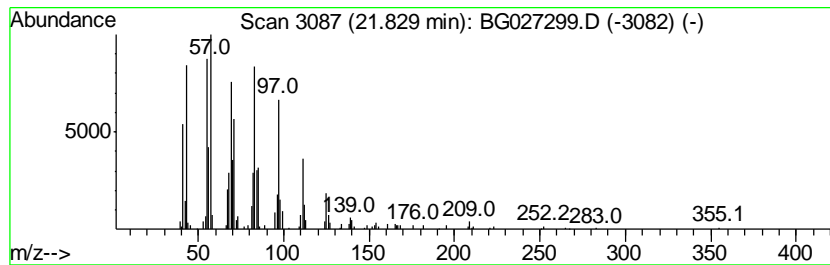
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 Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.83	3.97 ng	215605	Chrysene-d12	22.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3		Heptafluorobutyric acid, pentadec...	424	C19H31F7O2	959261-23-5	94
4		2-Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
5		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.70	13.4	ng	201552	1	8.56	300860	20.0
unknown8.09	8.09	145.1	ng	2182890	1	8.56	300860	20.0
n-Hexadecanoic acid	18.73	3.0	ng	137951	4	17.89	922340	20.0
Trifluoroacetoxy ...	21.83	4.0	ng	215605	5	22.27	1087140	20.0