

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061418\
 Data File : BF106467.D
 Acq On : 15 Jun 2018 2:51
 Operator : JU/SJ
 Sample : J3495-01
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DSN-002A-061318

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-BF061118.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	5.195	482	486	492	rVB	65459	71614	2.36%	0.358%
2	5.613	554	557	571	rVB	1402131	1381712	45.52%	6.907%
3	6.607	723	726	739	rVB	901162	947248	31.20%	4.735%
4	6.748	746	750	753	rBV	2407947	2080537	68.54%	10.400%
5	6.966	783	787	790	rBV	810430	621195	20.46%	3.105%
6	7.125	810	814	817	rBV	2300383	2010501	66.23%	10.050%
7	7.531	878	883	886	rBV	1616175	1546128	50.93%	7.728%
8	8.248	1001	1005	1008	rBV	847478	662930	21.84%	3.314%
9	9.325	1183	1188	1191	rBV	2554537	2449110	80.68%	12.242%
10	9.713	1250	1254	1259	rBV	141202	116369	3.83%	0.582%
11	10.007	1300	1304	1312	rVB2	742464	653992	21.54%	3.269%
12	10.419	1372	1374	1377	rVB	47189	36784	1.21%	0.184%
13	10.801	1434	1439	1442	rBV	1797216	1613717	53.16%	8.066%
14	10.895	1452	1455	1466	rVB	43846	50007	1.65%	0.250%
15	11.495	1554	1557	1561	rBV	853764	772114	25.43%	3.859%
16	13.083	1823	1827	1831	rBV	3034829	3035653	100.00%	15.174%
17	13.965	1974	1977	1983	rBV	104081	122921	4.05%	0.614%
18	14.148	2004	2008	2012	rBV	1013227	889344	29.30%	4.445%
19	15.007	2150	2154	2161	rVB	292987	307322	10.12%	1.536%
20	15.683	2264	2269	2274	rBV	497414	636378	20.96%	3.181%

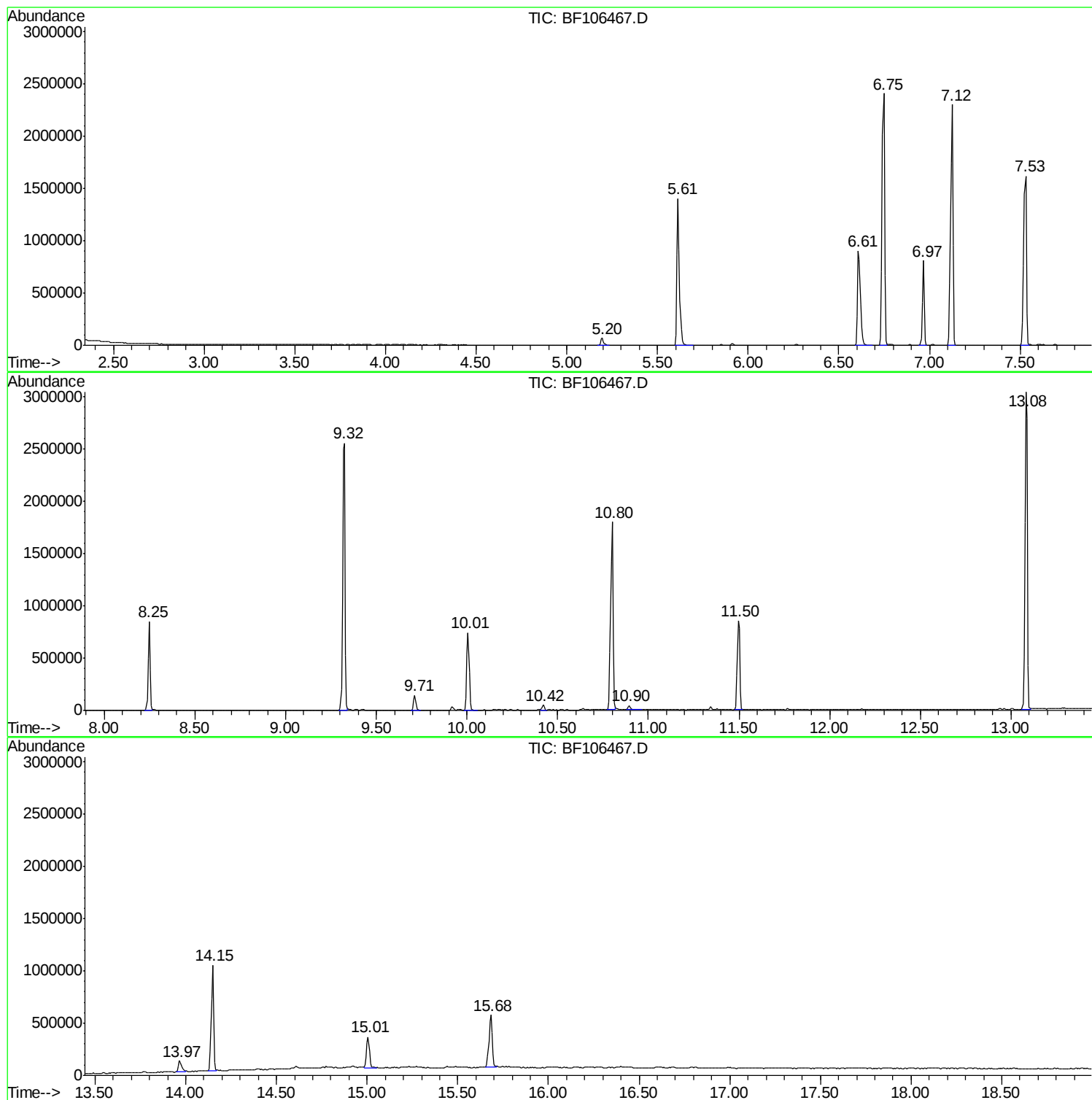
Sum of corrected areas: 20005576

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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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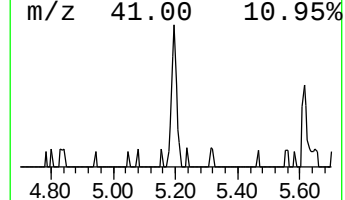
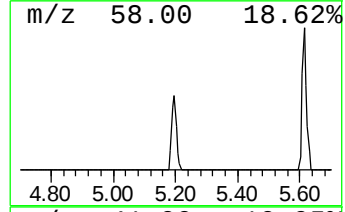
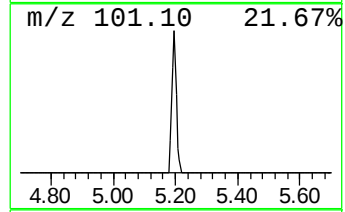
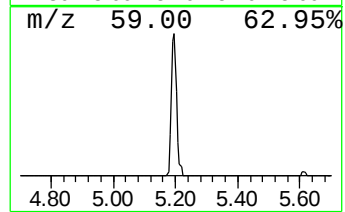
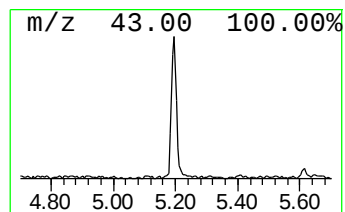
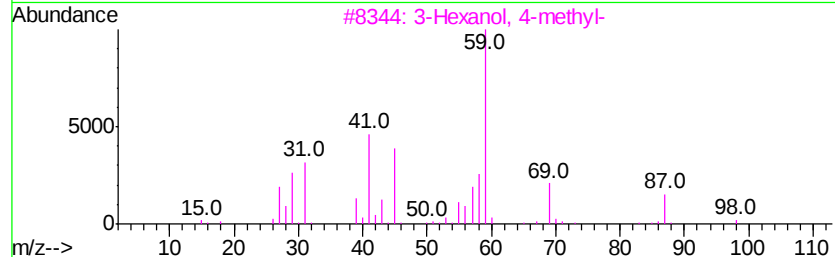
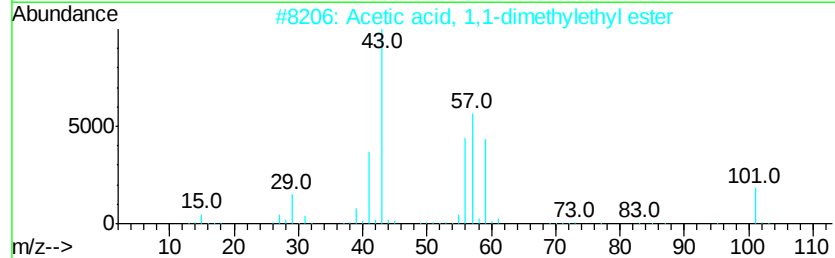
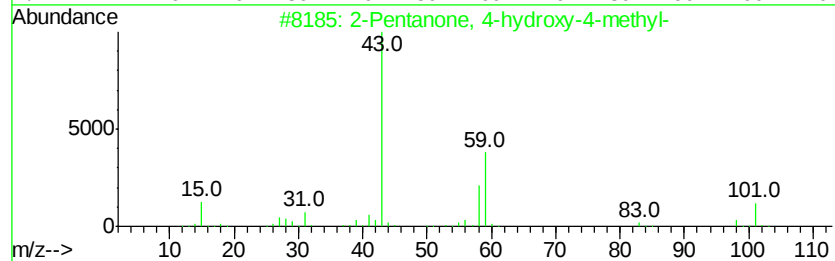
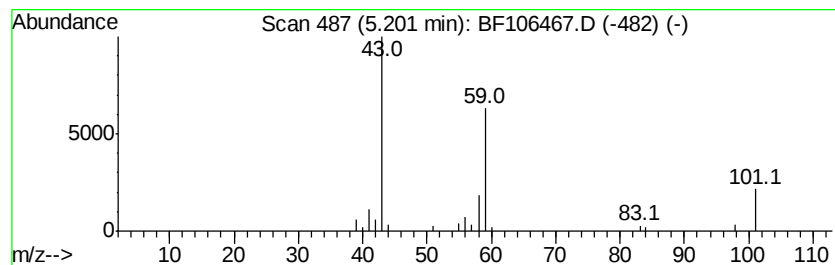
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	2.31 ng	71614	1,4-Dichlorobenzene-d4	6.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56	
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39	
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28	
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23	
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9	



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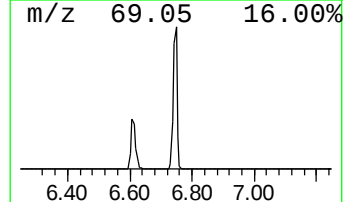
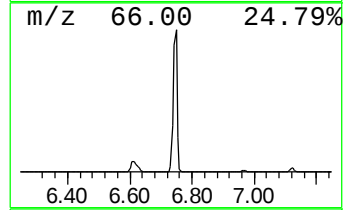
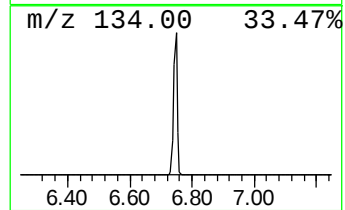
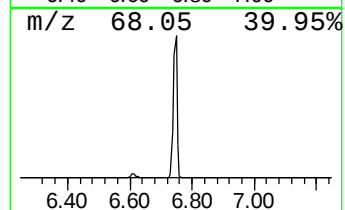
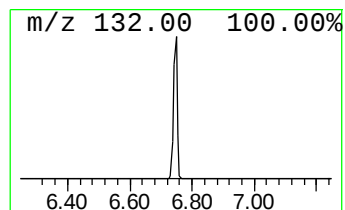
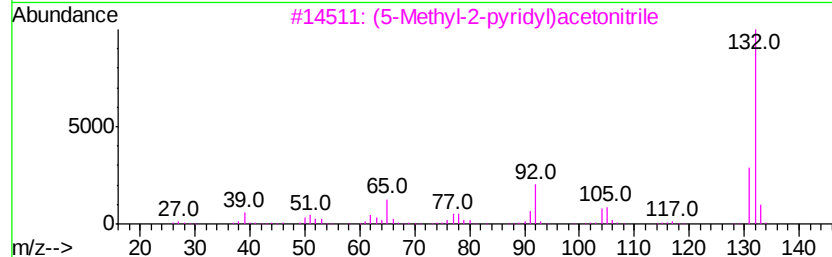
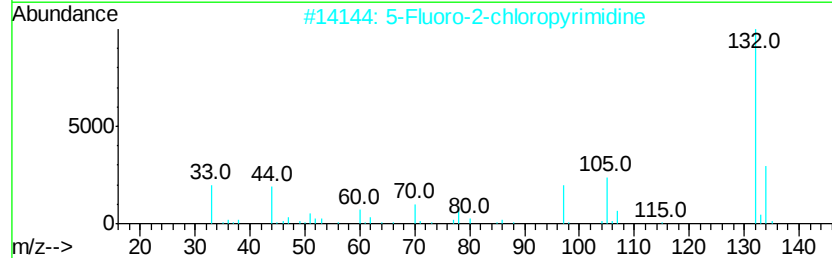
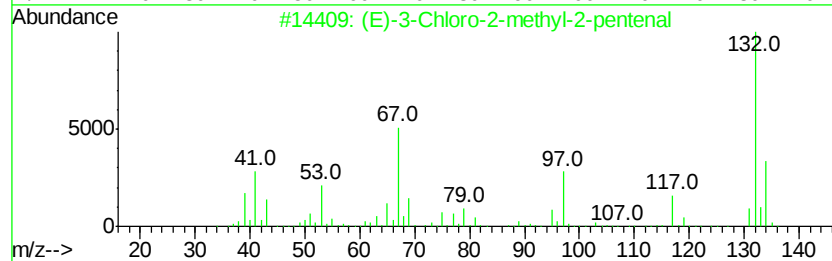
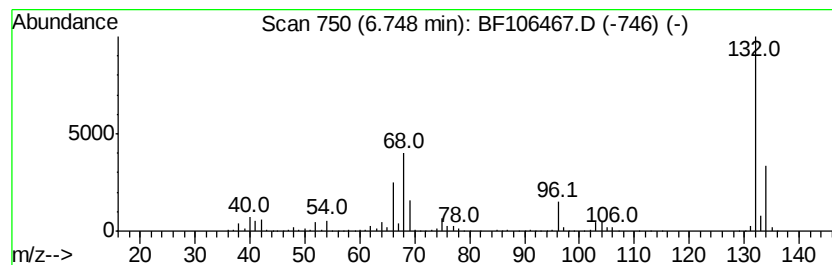
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Peak Number 2 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	66.99 ng	2080540	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
3		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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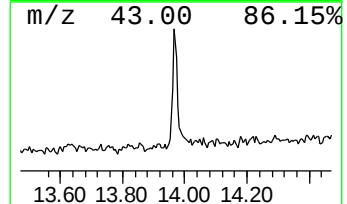
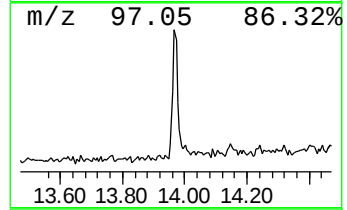
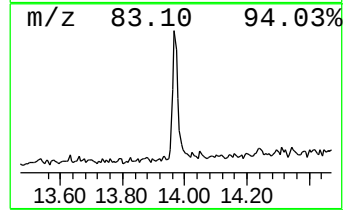
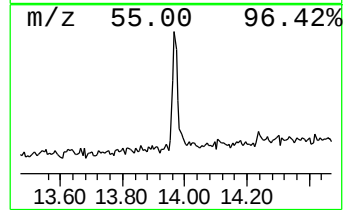
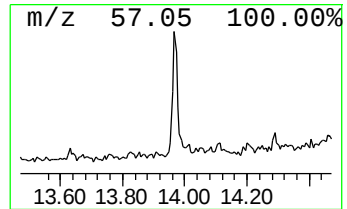
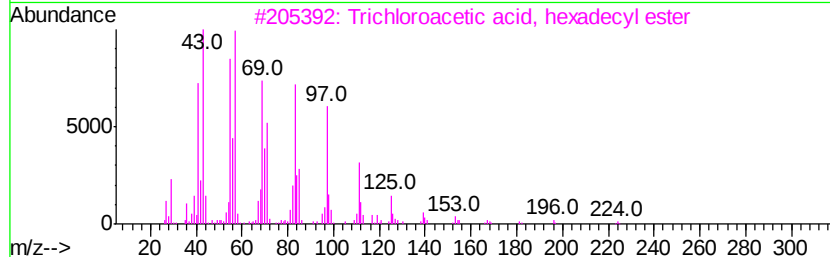
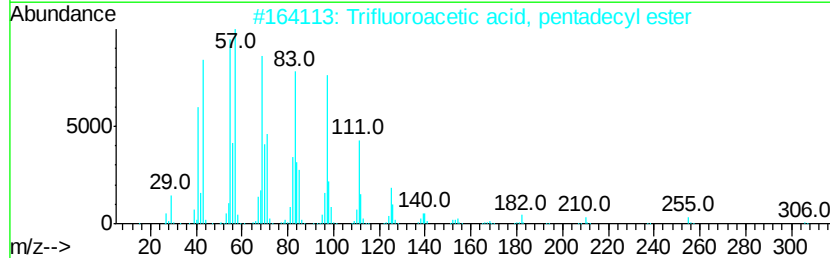
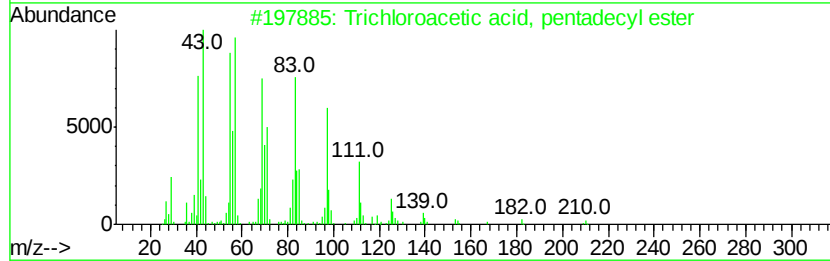
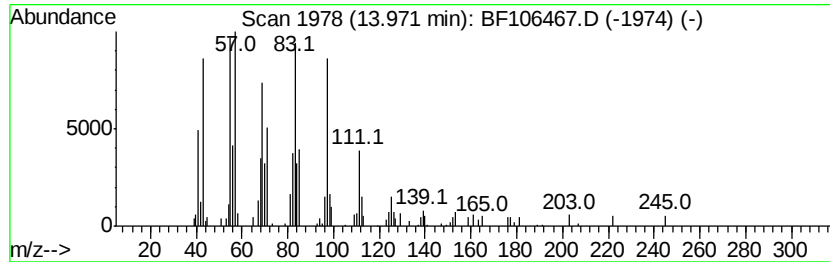
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Peak Number 4 Trichloroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	2.76 ng	122921	Chrysene-d12	14.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
2		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4		1-Heneicosanol	312	C21H44O	015594-90-8	94
5		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94



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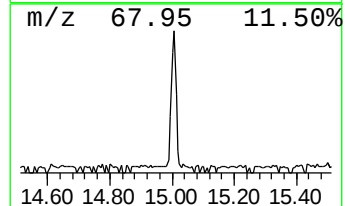
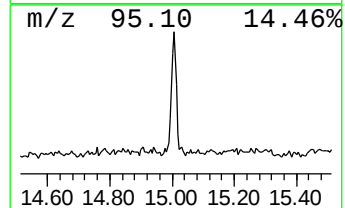
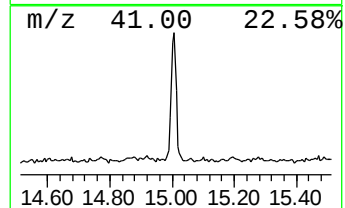
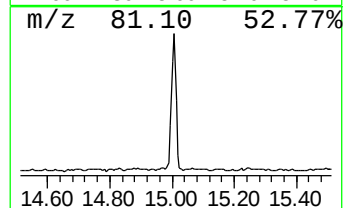
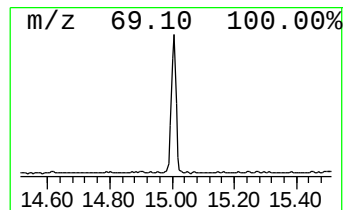
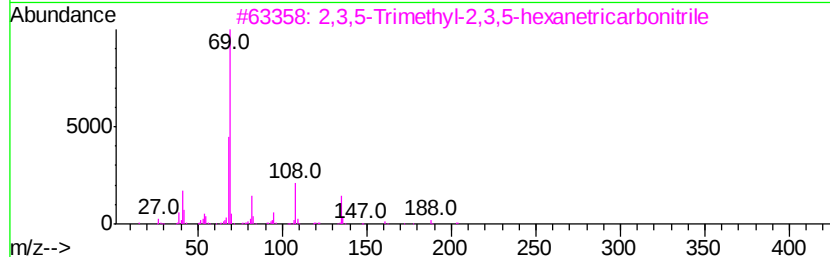
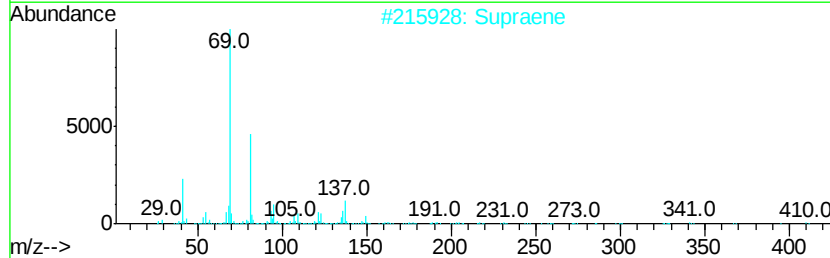
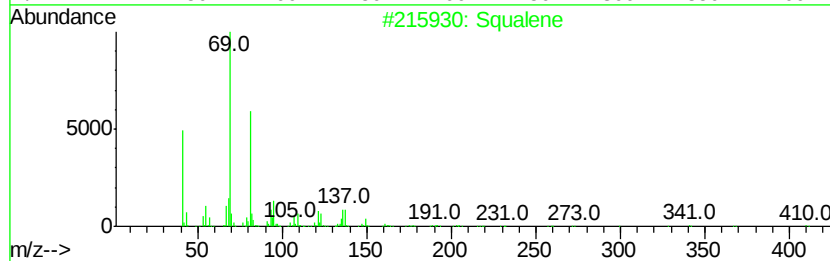
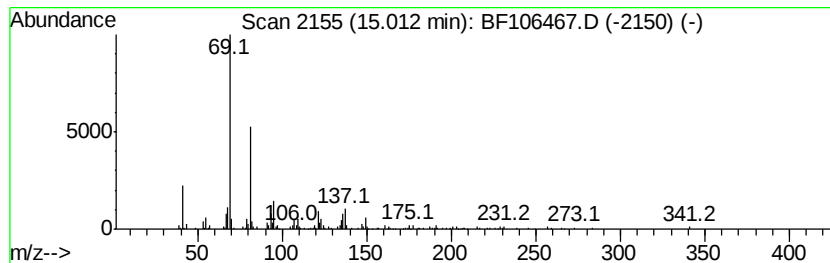
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Peak Number 5 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.01	9.66 ng	307322	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50
4		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	50
5		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.20	2.3	ng	71614	1	6.97	621195	20.0
unknown6.75	6.75	67.0	ng	2080540	1	6.97	621195	20.0
Trichloroacetic a...	13.97	2.8	ng	122921	5	14.15	889344	20.0
Squalene	15.01	9.7	ng	307322	6	15.68	636378	20.0