

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092517\
 Data File : BF098782.D
 Acq On : 25 Sep 2017 14:40
 Operator : SJ/JU
 Sample : I5364-02
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SASP2P-ENV-118-5(5-10)

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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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	2.228	20	24	30	rVB	62249	82559	2.38%	0.273%
2	5.145	516	520	532	rVB	464211	608368	17.53%	2.014%
3	5.540	581	587	590	rBV	3398009	3380173	97.39%	11.190%
4	6.540	751	757	760	rBV	3037087	3470759	100.00%	11.490%
5	6.687	777	782	785	rBV	3650802	3437492	99.04%	11.380%
6	6.916	817	821	824	rVB	1251539	983450	28.34%	3.256%
7	7.075	843	848	851	rVB	2782067	2570114	74.05%	8.508%
8	7.475	911	916	919	rBV	2049420	2108919	60.76%	6.982%
9	8.198	1034	1039	1042	rBV	1584984	1299600	37.44%	4.302%
10	9.269	1216	1221	1225	rBV	3488275	3441879	99.17%	11.394%
11	9.657	1283	1287	1291	rBV	392296	347606	10.02%	1.151%
12	9.951	1333	1337	1341	rVB	1417884	1251614	36.06%	4.143%
13	10.375	1406	1409	1412	rVB	66404	50326	1.45%	0.167%
14	10.739	1467	1471	1474	rBV	1822024	1610339	46.40%	5.331%
15	10.845	1486	1489	1494	rBV	85858	80346	2.31%	0.266%
16	11.292	1563	1565	1568	rBV	43165	38050	1.10%	0.126%
17	11.439	1586	1590	1593	rBV	1237976	1004748	28.95%	3.326%
18	11.951	1673	1677	1686	rBV4	120914	138321	3.99%	0.458%
19	12.651	1793	1796	1800	rBV	79490	67214	1.94%	0.223%
20	12.880	1832	1835	1839	rVB	70673	57980	1.67%	0.192%
21	13.021	1855	1859	1863	rVB	2411402	2218938	63.93%	7.346%
22	13.904	2006	2009	2016	rBV2	209272	207878	5.99%	0.688%
23	14.080	2035	2039	2042	rBV	912288	876787	25.26%	2.903%
24	14.927	2180	2183	2187	rVB	137025	131547	3.79%	0.435%
25	15.127	2214	2217	2221	rBV3	42304	78730	2.27%	0.261%
26	15.568	2288	2292	2301	rVB	495491	663459	19.12%	2.196%

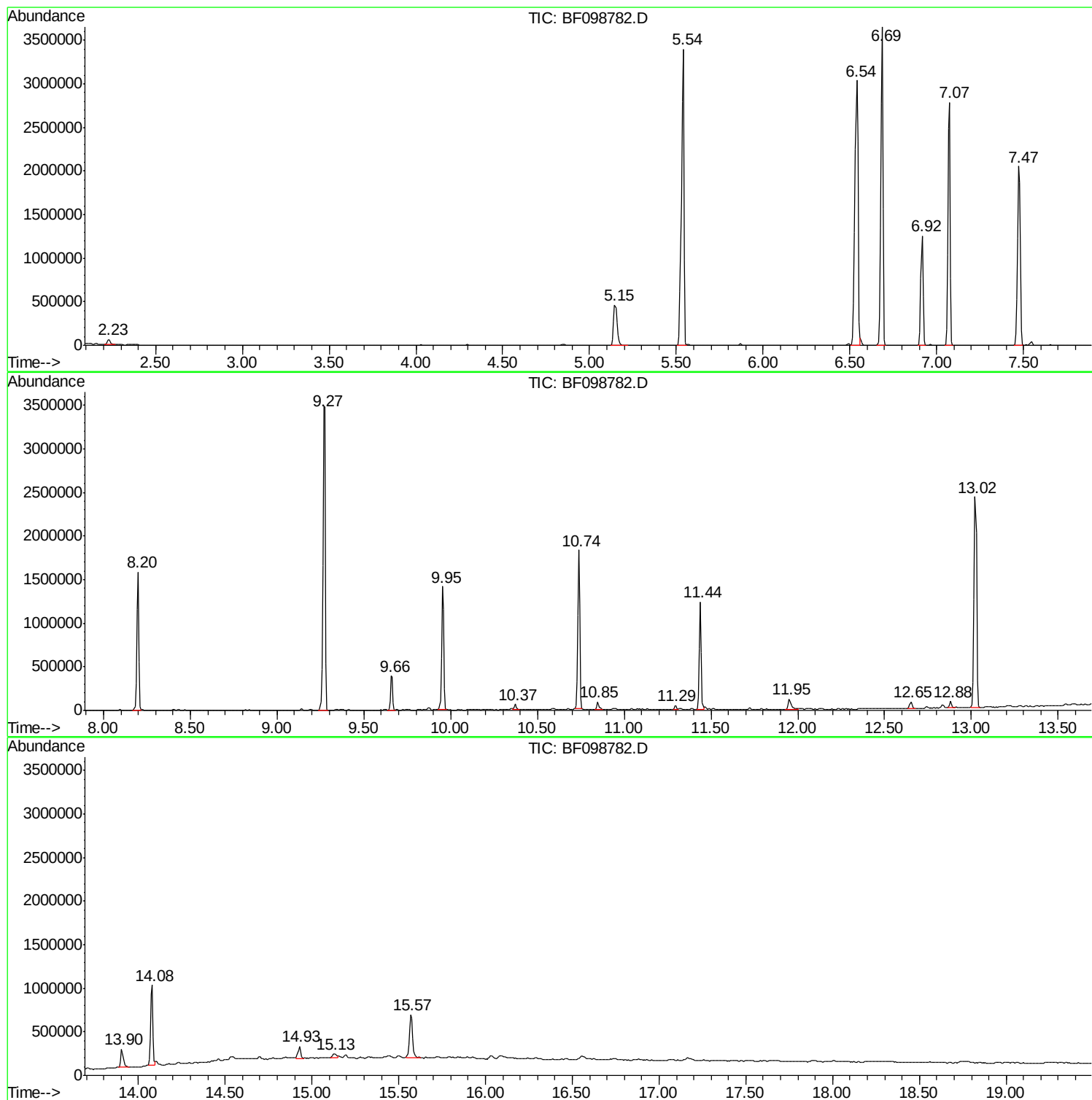
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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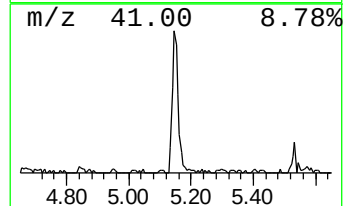
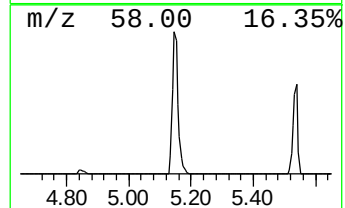
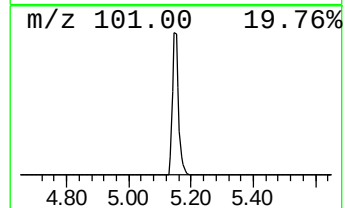
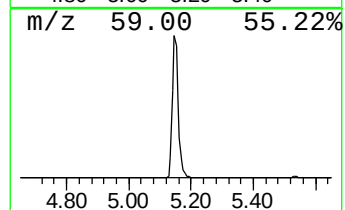
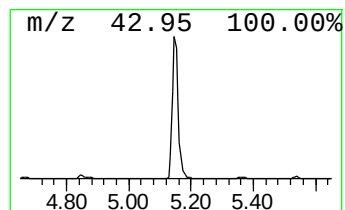
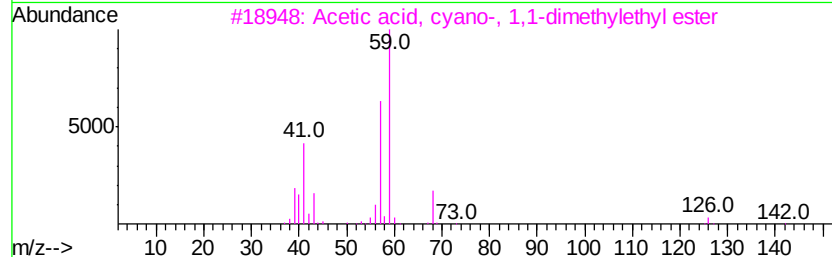
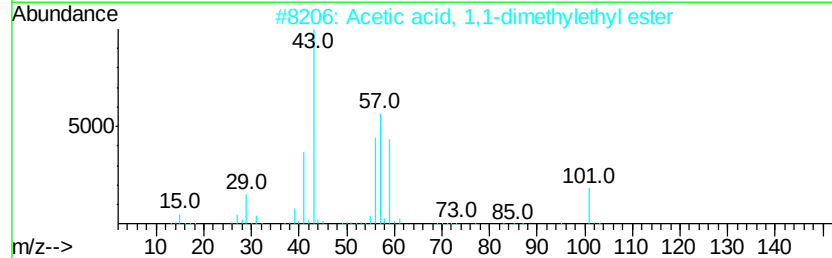
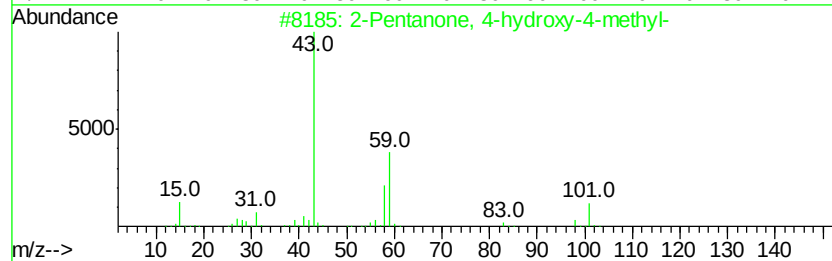
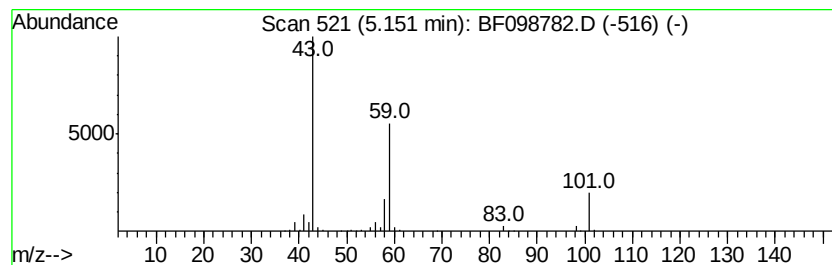
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	12.37 ng	608368	1,4-Dichlorobenzene-d4	6.92

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
4		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



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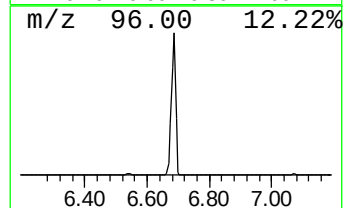
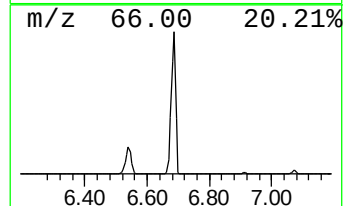
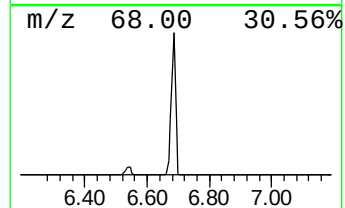
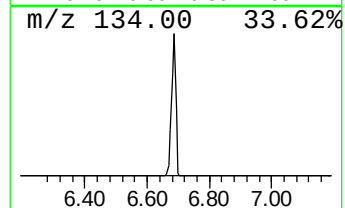
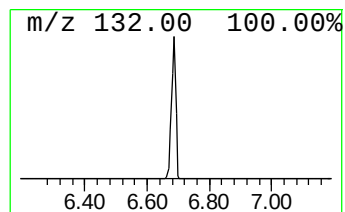
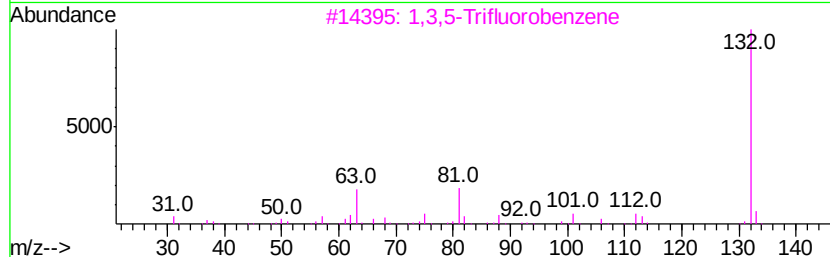
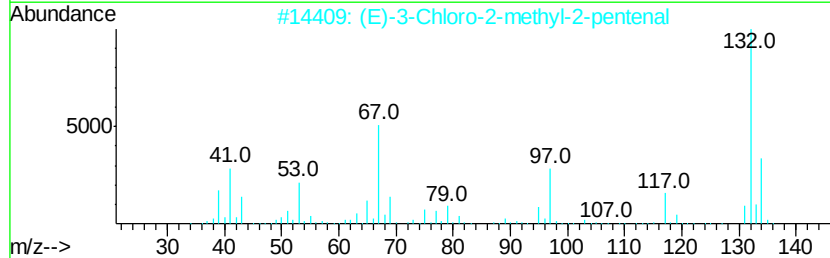
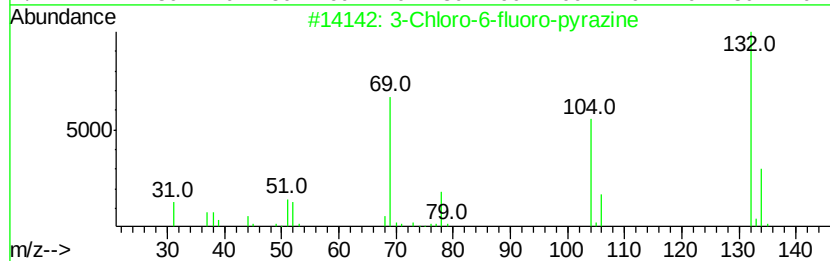
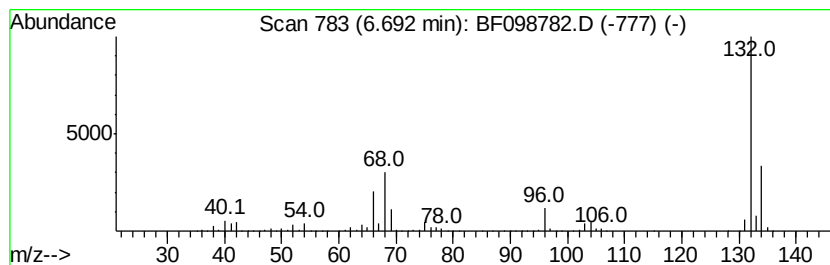
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	69.91 ng	3437490	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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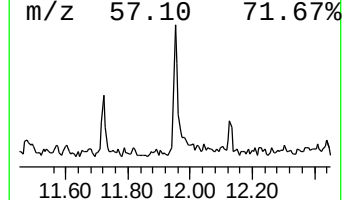
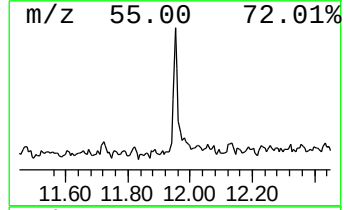
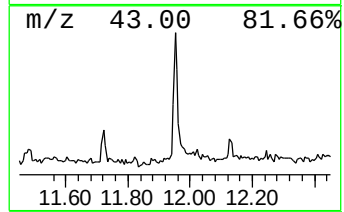
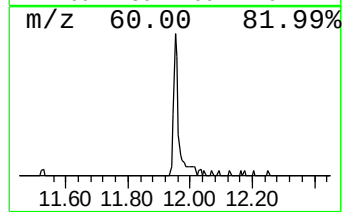
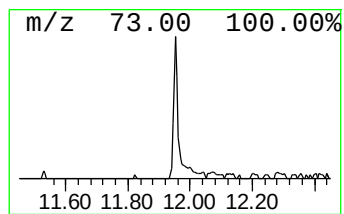
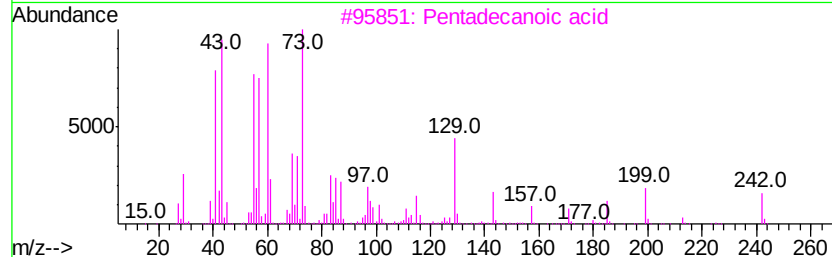
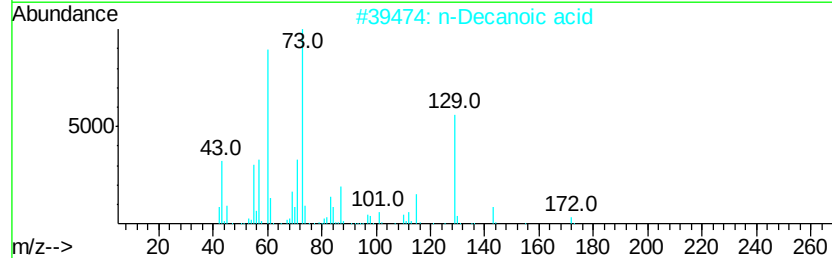
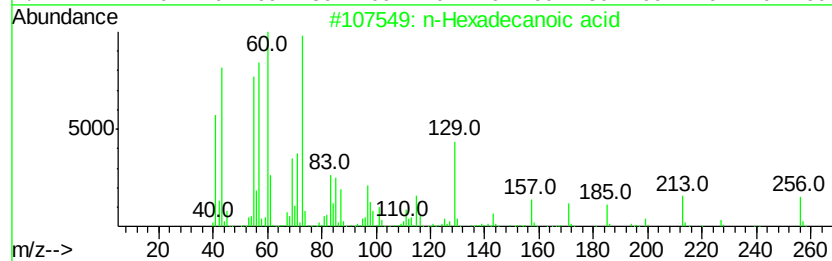
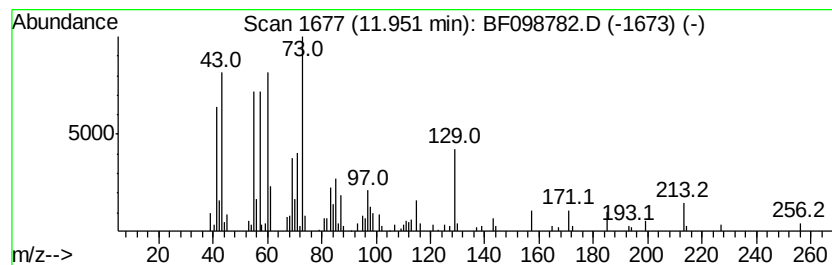
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.95	2.75 ng	138321	Phenanthrene-d10		11.44
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	n-Decanoic acid	172	C10H20O2	000334-48-5	92
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	90
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	83



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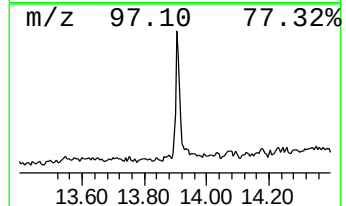
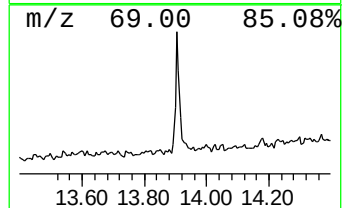
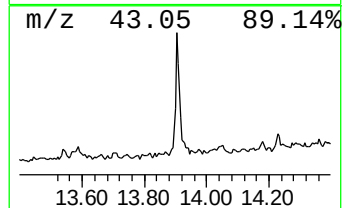
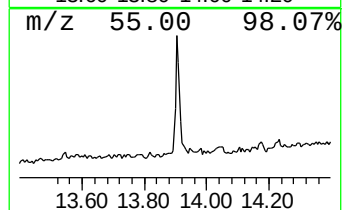
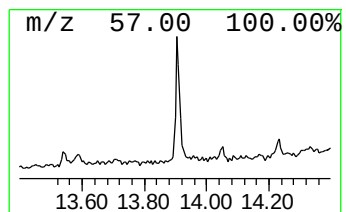
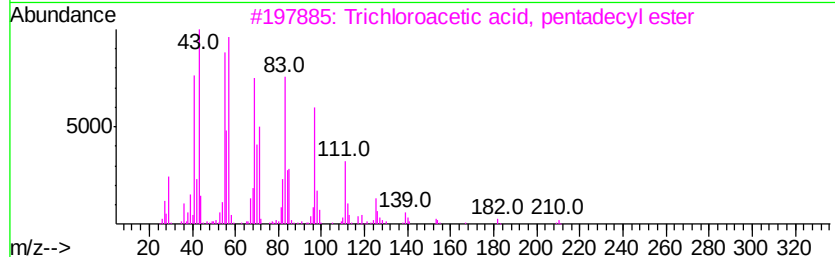
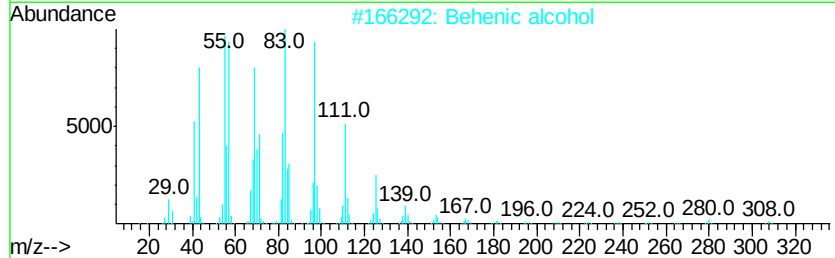
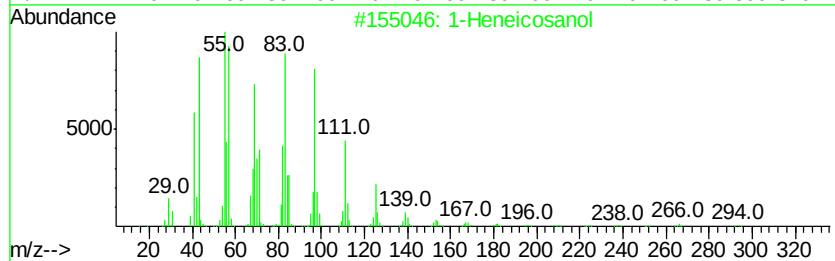
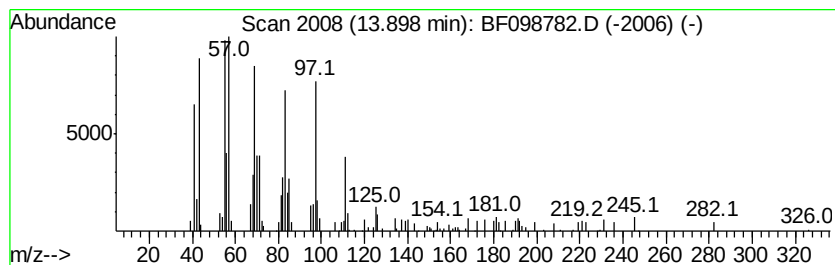
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Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.90	4.74 ng	207878	Chrysene-d12	14.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94



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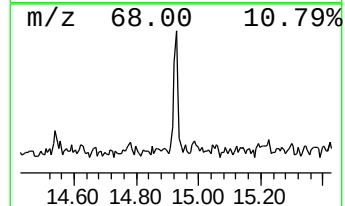
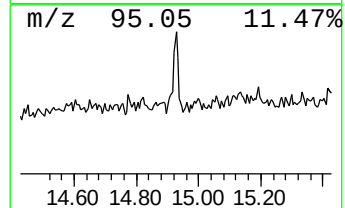
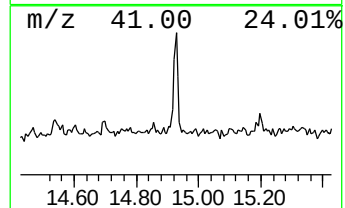
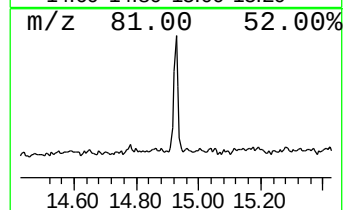
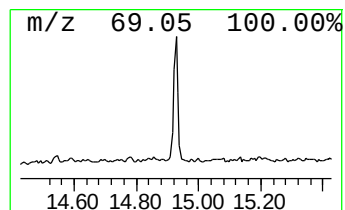
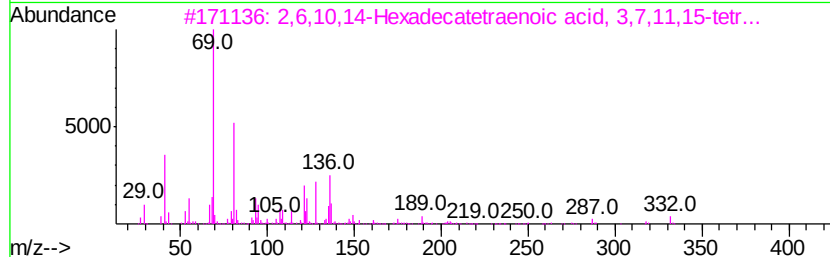
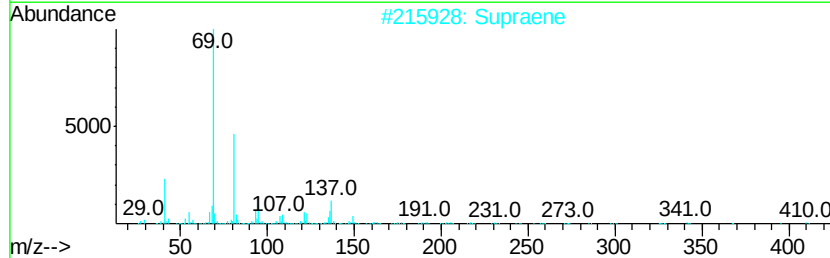
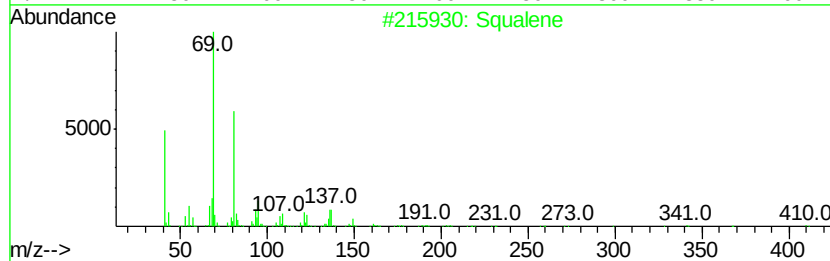
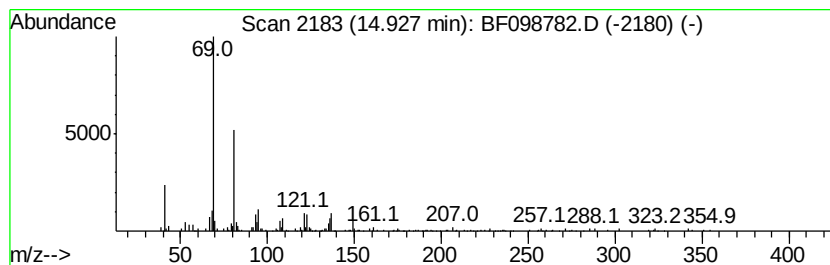
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Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	3.97 ng	131547	Perylene-d12	15.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	90
2		Supraene	410	C30H50	007683-64-9	83
3		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64
4		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	56
5		2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.15	12.4	ng	608368	1	6.92	983450	20.0
unknown6.69	6.69	69.9	ng	3437490	1	6.92	983450	20.0
n-Hexadecanoic acid	11.95	2.8	ng	138321	4	11.44	1004750	20.0
1-Heneicosanol	13.90	4.7	ng	207878	5	14.08	876787	20.0
Squalene	14.93	4.0	ng	131547	6	15.57	663459	20.0