

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF113016\
 Data File : BF091358.D
 Acq On : 30 Nov 2016 17:00
 Operator : UM/SJ
 Sample : H5767-02
 Misc :
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 112216-DSDC-E-D-S

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-BF112916.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	5.041	238	241	243	rBV	467625	534149	8.48%	1.491%
2	5.453	275	277	280	rBV	1211029	1529791	24.29%	4.269%
3	6.481	365	367	371	rVB	1246975	1096950	17.42%	3.061%
4	6.630	377	380	382	rBV	3076658	2915907	46.30%	8.137%
5	6.859	398	400	403	rBV	1048481	1184805	18.81%	3.306%
6	7.019	412	414	416	rVB	3985846	4346177	69.01%	12.129%
7	7.430	446	450	452	rBV	3853984	4067011	64.57%	11.350%
8	8.150	510	513	515	rBV	1741147	1573977	24.99%	4.392%
9	9.225	604	607	610	rBV	4846038	6298172	100.00%	17.576%
10	9.613	639	641	643	rBV	187105	181449	2.88%	0.506%
11	9.899	664	666	669	rBV	1736752	1513126	24.02%	4.223%
12	10.688	732	735	737	rBV	2044428	2040730	32.40%	5.695%
13	10.813	744	746	751	rVB	56928	69361	1.10%	0.194%
14	11.385	793	796	798	rBV	1361058	1318329	20.93%	3.679%
15	11.910	840	842	844	rBV	136117	147621	2.34%	0.412%
16	12.699	909	911	918	rBV	116471	156889	2.49%	0.438%
17	12.802	918	920	922	rVB	56374	71214	1.13%	0.199%
18	12.973	932	935	937	rBV	3900146	4617862	73.32%	12.887%
19	13.876	1011	1014	1022	rBV2	48666	83772	1.33%	0.234%
20	14.014	1023	1026	1028	rBV	1102497	1096928	17.42%	3.061%
21	15.442	1148	1151	1154	rBV	823221	989860	15.72%	2.762%

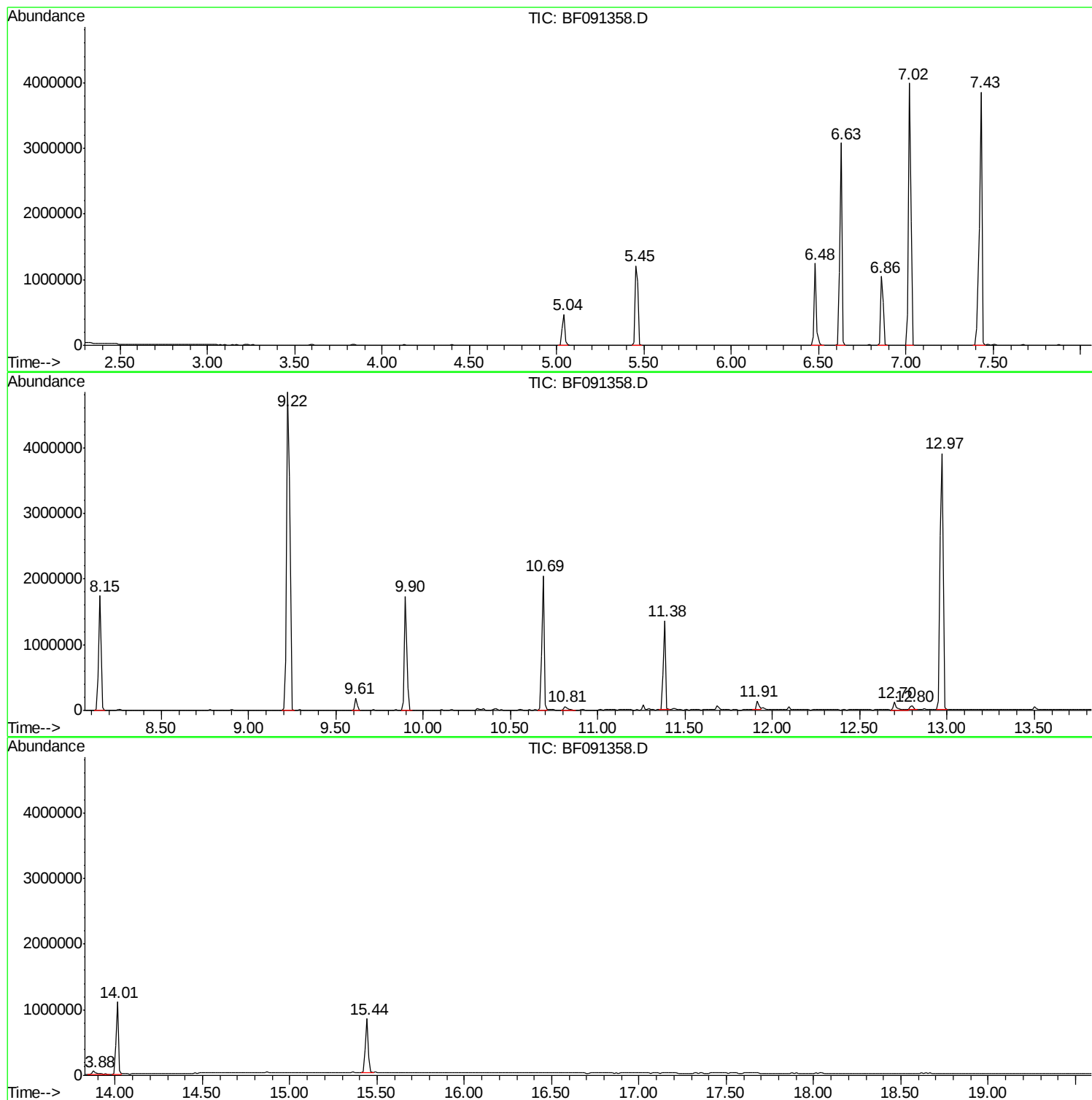
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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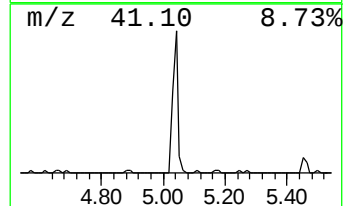
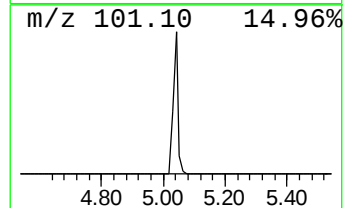
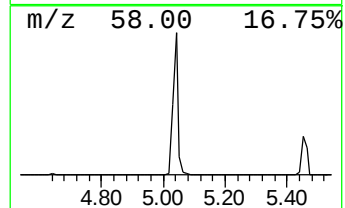
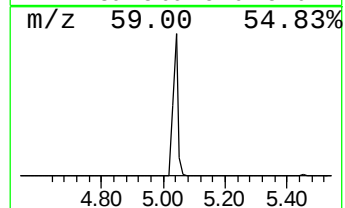
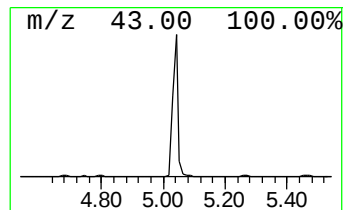
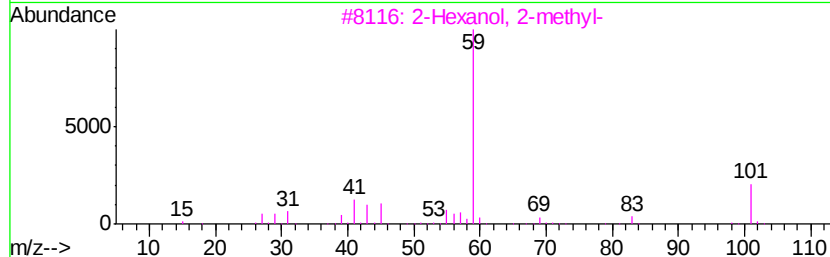
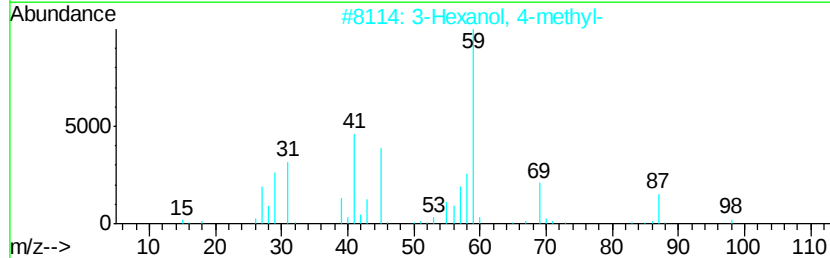
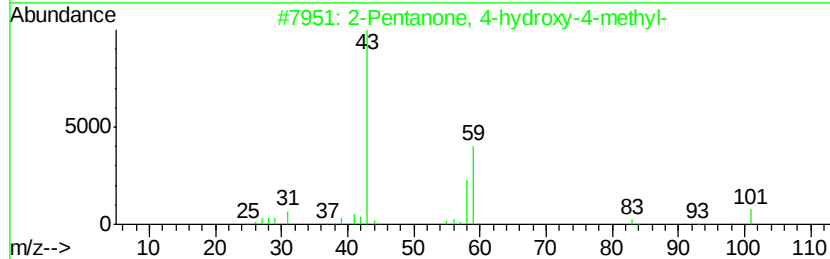
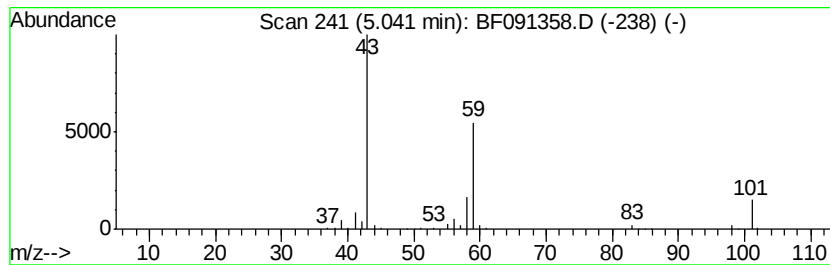
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
5.04	9.02 ng	534149	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17



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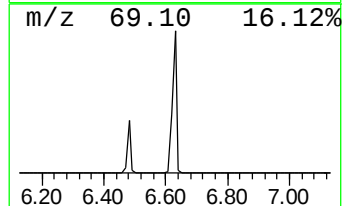
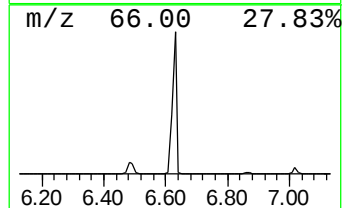
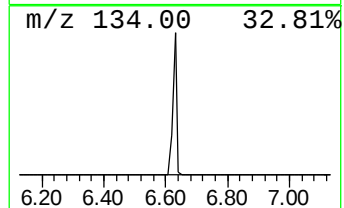
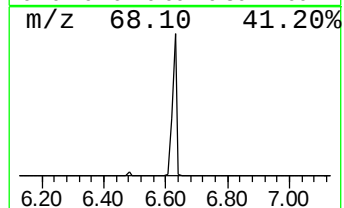
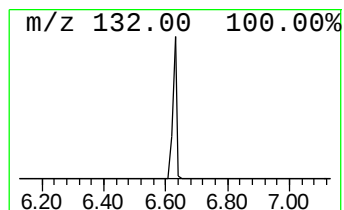
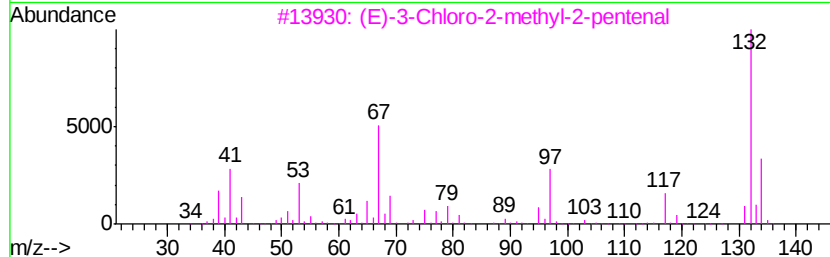
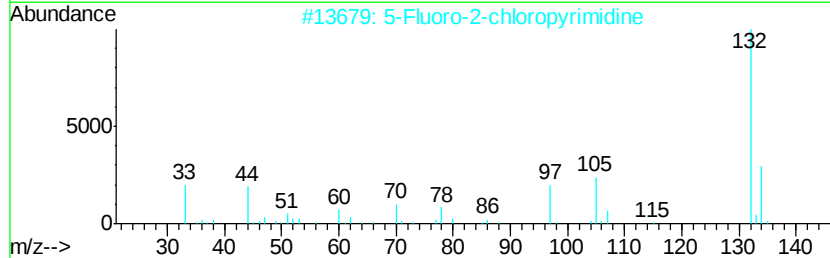
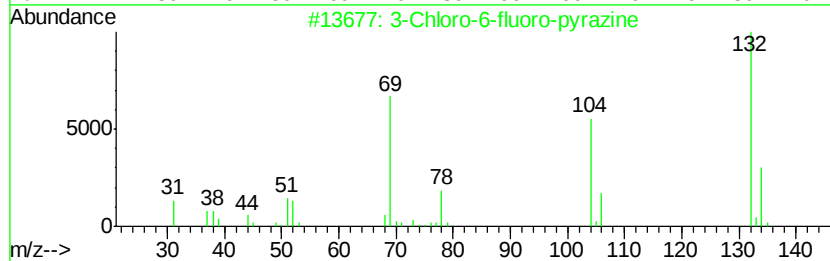
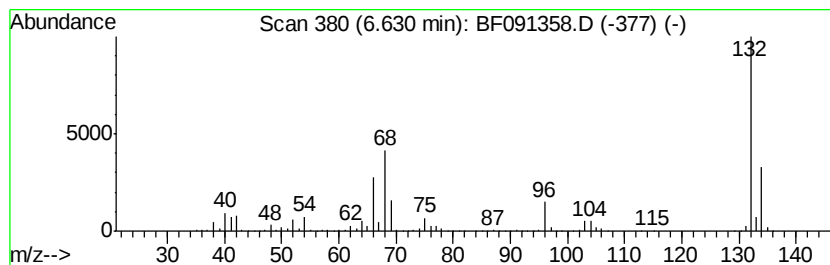
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Peak Number 2 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	49.22 ng	2915910	1,4-Dichlorobenzene-d4	6.86

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	16
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9



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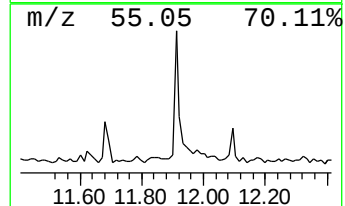
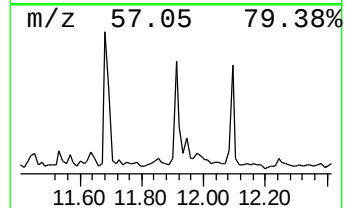
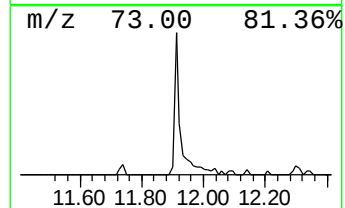
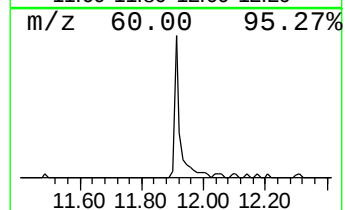
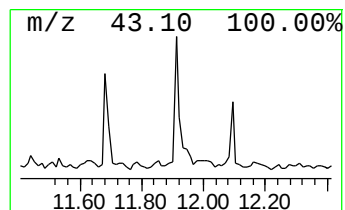
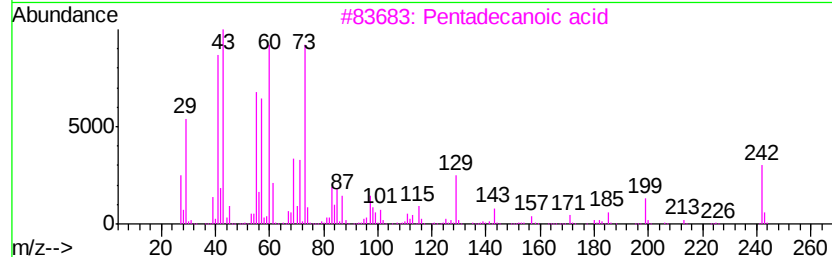
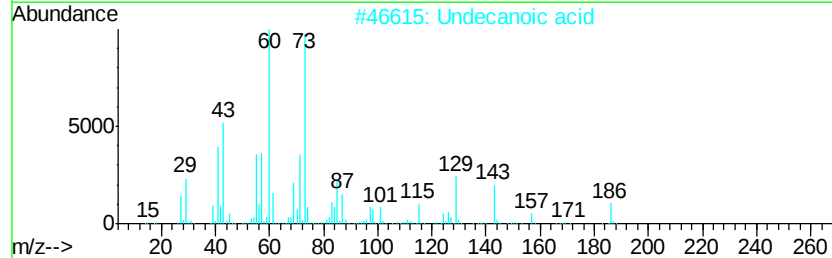
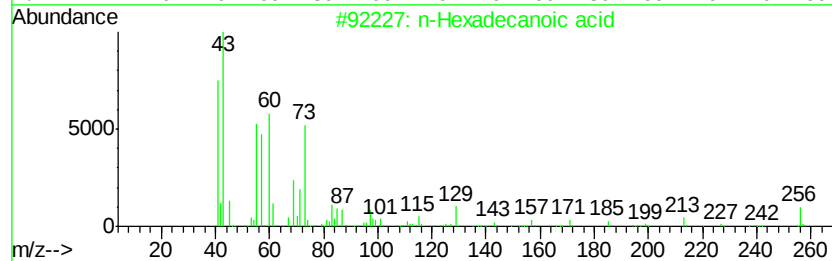
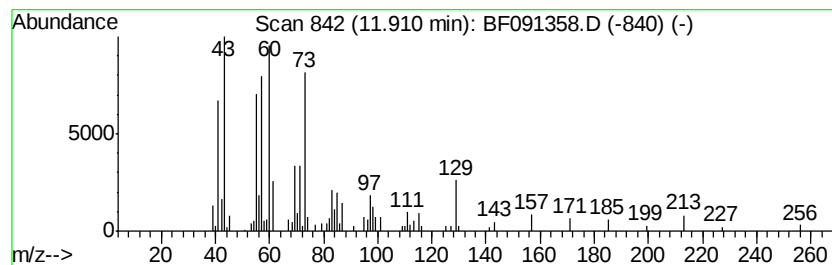
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	2.24 ng	147621	Phenanthrene-d10	11.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2		Undecanoic acid	186	C11H22O2	000112-37-8	80
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4		Tridecanoic acid	214	C13H26O2	000638-53-9	59
5		Dodecanoic acid	200	C12H24O2	000143-07-7	59



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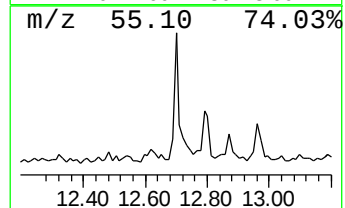
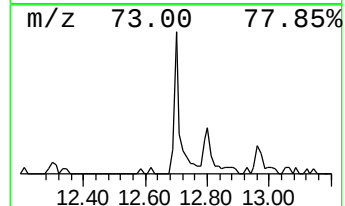
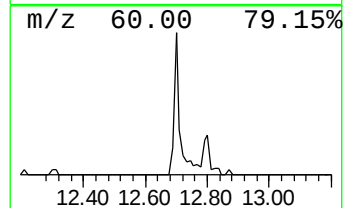
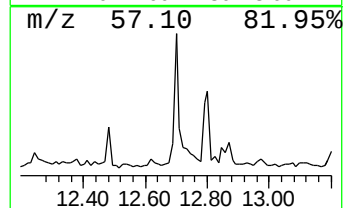
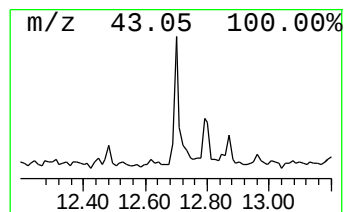
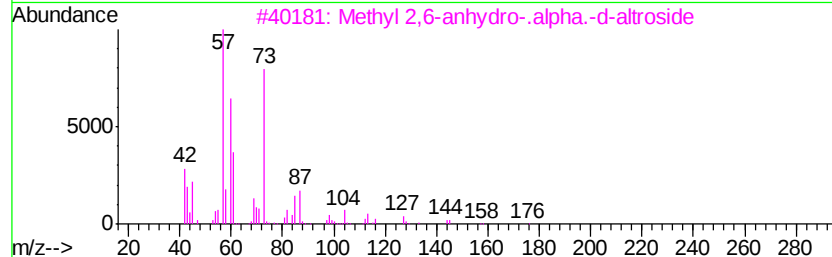
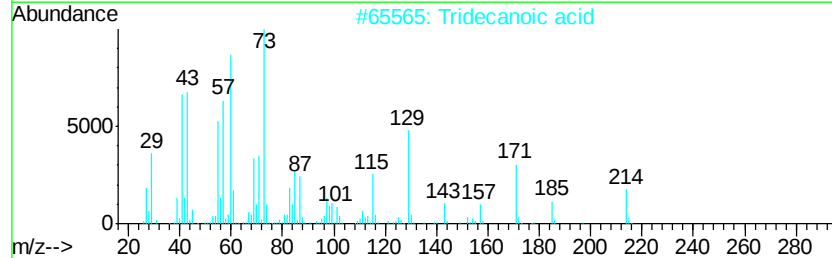
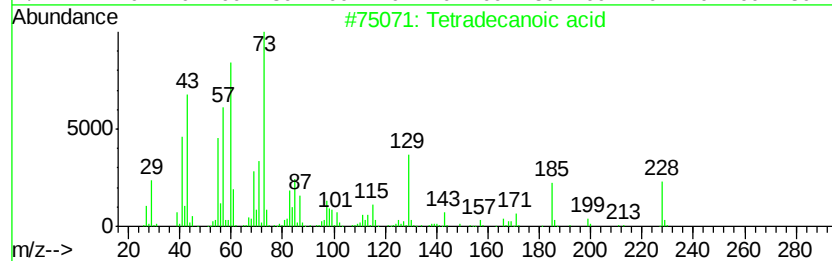
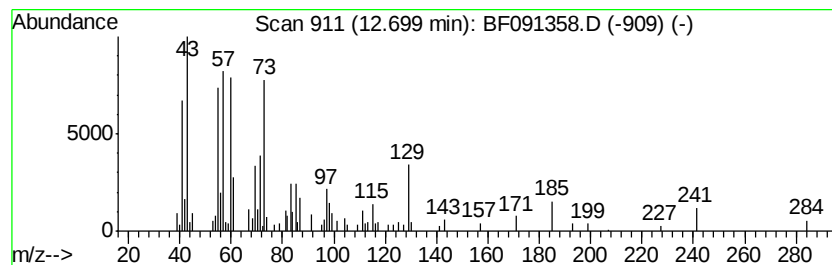
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Peak Number 5 Tetradecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	2.86 ng	156889	Chrysene-d12	14.01

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
2		Tridecanoic acid	214	C13H26O2	000638-53-9	35
3		Methyl 2,6-anhydro-.alpha.-d-alt...	176	C7H12O5	1000130-02-0	22
4		Octadecane, 2-methyl-	268	C19H40	001560-88-9	11
5		Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	11



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.04	9.0	ng	534149	1	6.86	1184810	20.0
unknown6.63	6.63	49.2	ng	2915910	1	6.86	1184810	20.0
n-Hexadecanoic acid	11.91	2.2	ng	147621	4	11.38	1318330	20.0
Tetradecanoic acid	12.70	2.9	ng	156889	5	14.01	1096930	20.0