

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110617\
 Data File : BF100255.D
 Acq On : 6 Nov 2017 17:18
 Operator : SJ/JU
 Sample : PB103997TB
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB103997TB

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-BF102317.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	4.992	491	494	514	rBV	125499	256058	11.08%	1.297%
2	5.392	559	562	601	rBV	1236624	1906642	82.47%	9.661%
3	6.410	732	735	753	rBV	1362582	1773775	76.72%	8.987%
4	6.534	753	756	767	rVB	1917138	1962834	84.90%	9.945%
5	6.757	791	794	810	rVB	518384	530730	22.96%	2.689%
6	6.910	817	820	835	rBV	1588930	1578383	68.27%	7.997%
7	7.334	888	892	920	rBV	1031932	1149361	49.71%	5.824%
8	8.039	1009	1012	1030	rBV	687400	723809	31.31%	3.667%
9	9.110	1190	1194	1206	rBV	2331443	2311901	100.00%	11.714%
10	9.792	1307	1310	1320	rBV	883517	820540	35.49%	4.158%
11	10.592	1442	1446	1463	rBV	1172302	1193674	51.63%	6.048%
12	11.286	1561	1564	1575	rBV	860953	855034	36.98%	4.332%
13	11.798	1642	1651	1663	rBV2	108709	203441	8.80%	1.031%
14	12.039	1681	1692	1703	rBV2	95592	300169	12.98%	1.521%
15	12.498	1765	1770	1771	rBV3	16669	25006	1.08%	0.127%
16	12.580	1779	1784	1798	rBV	286837	511835	22.14%	2.593%
17	12.868	1829	1833	1836	rBV	2369320	2229744	96.45%	11.298%
18	13.945	2012	2016	2028	rBV	633059	771000	33.35%	3.906%
19	14.510	2105	2112	2116	rBV6	13239	23189	1.00%	0.117%
20	15.339	2250	2253	2260	rVB3	18587	23753	1.03%	0.120%
21	15.404	2260	2264	2280	rBV	300909	534369	23.11%	2.708%
22	16.227	2399	2404	2409	rVB4	14420	23442	1.01%	0.119%
23	17.439	2603	2610	2617	rBV9	10884	27652	1.20%	0.140%

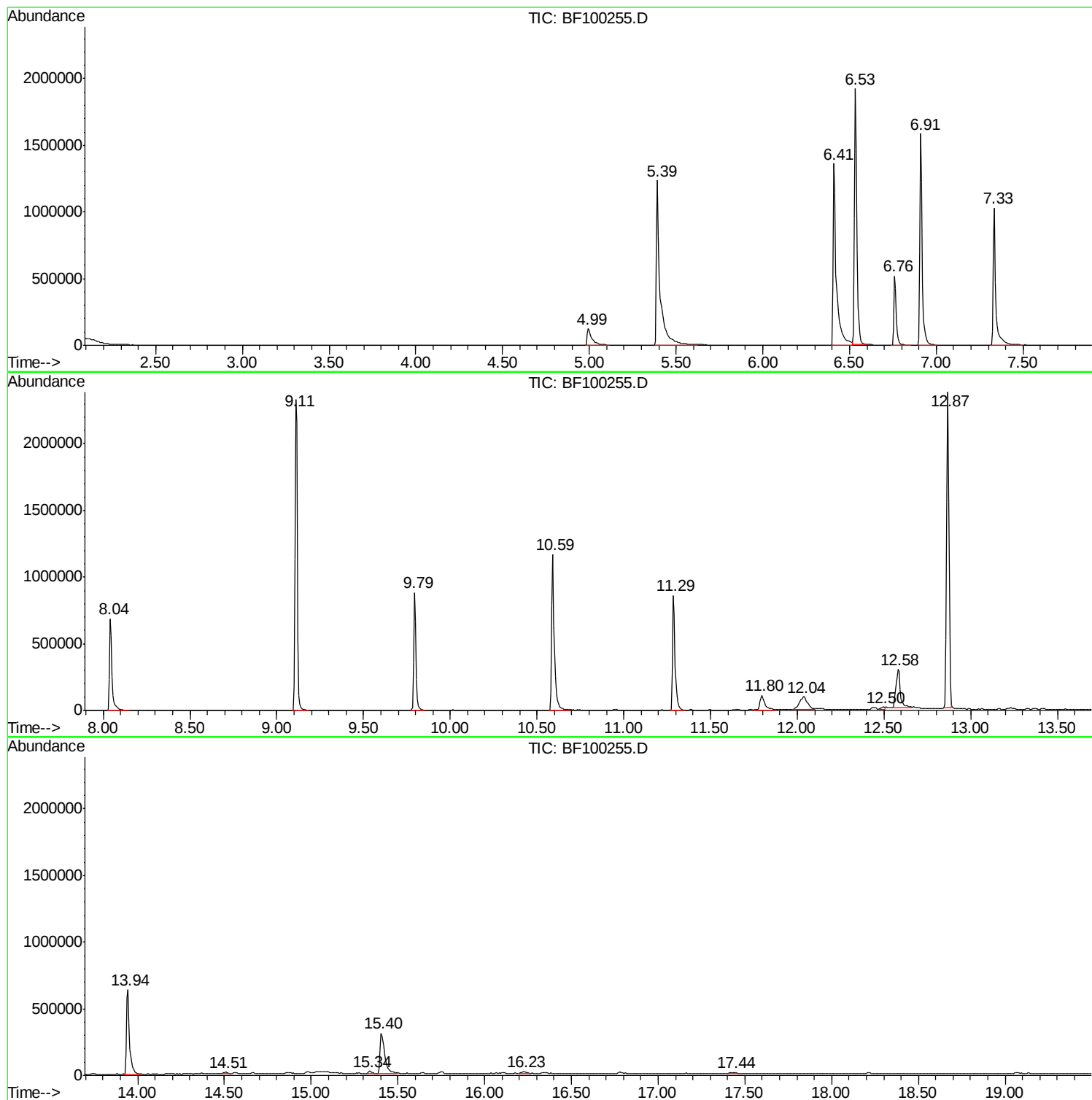
Sum of corrected areas: 19736341

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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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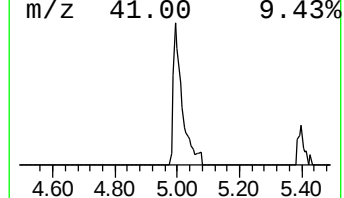
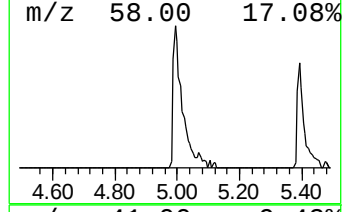
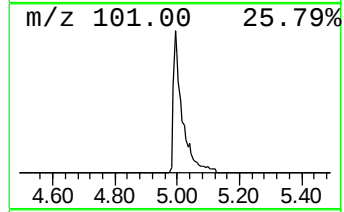
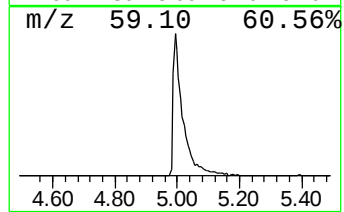
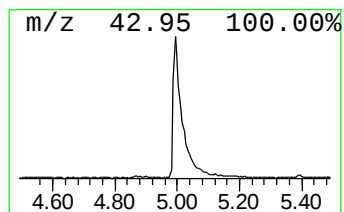
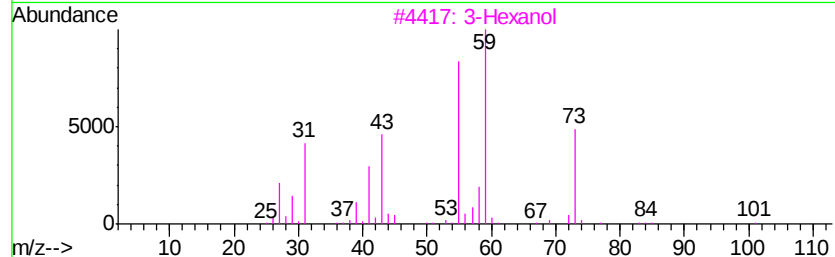
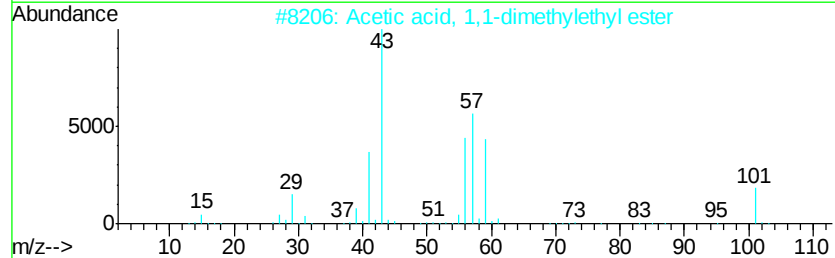
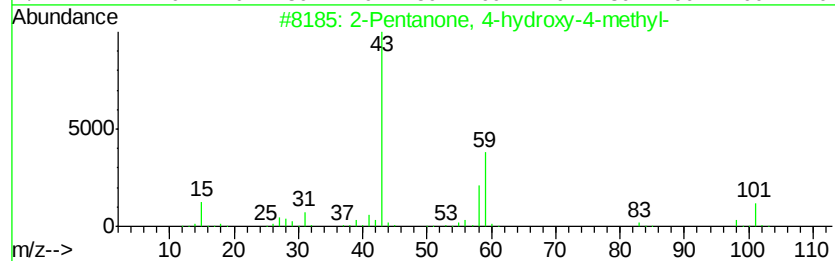
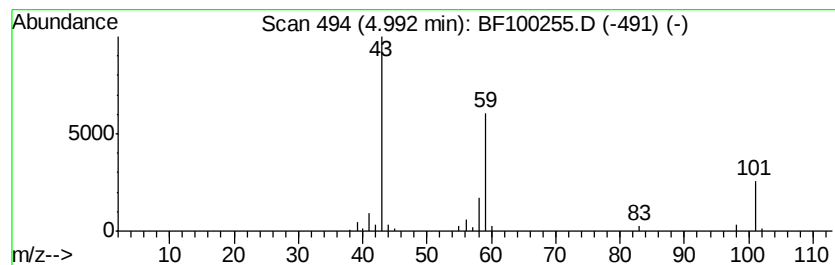
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	9.65 ng	256058	1,4-Dichlorobenzene-d4	6.76

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	102	C6H14O	000623-37-0	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			Acetone	58	C3H6O	000067-64-1	9



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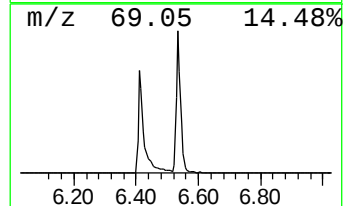
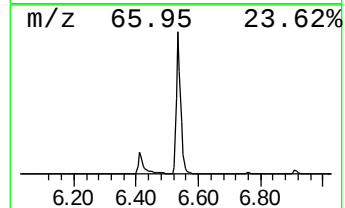
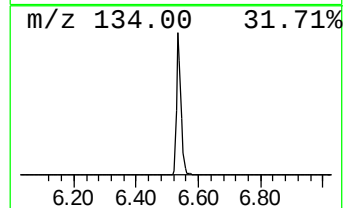
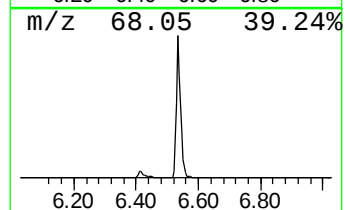
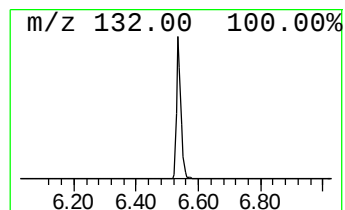
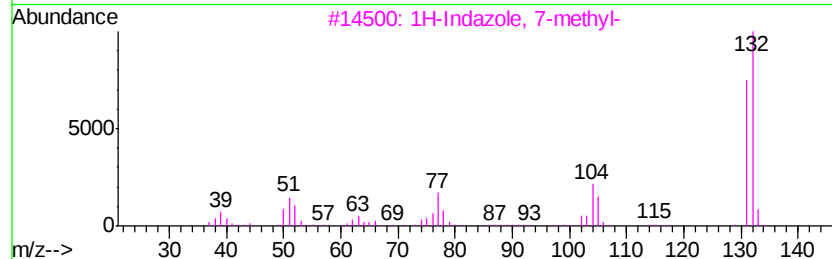
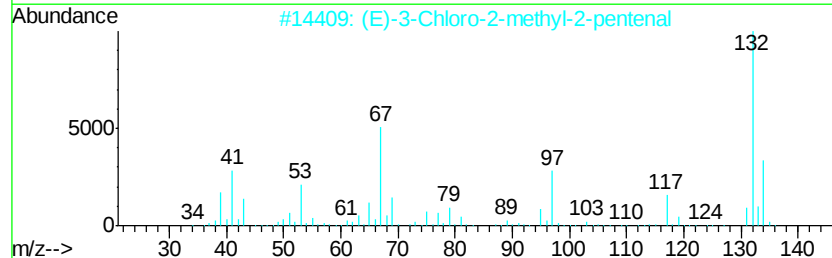
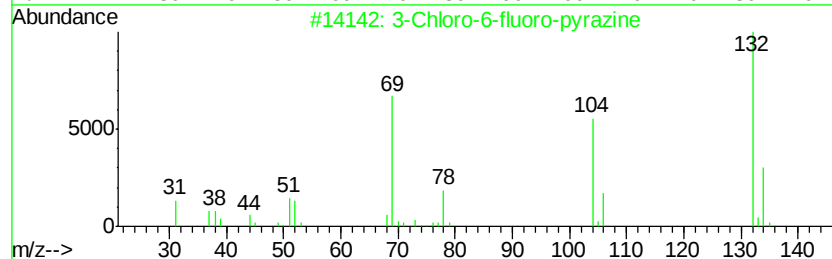
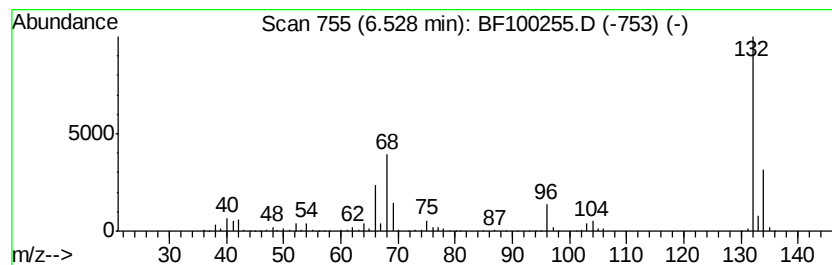
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	73.97 ng	1962830	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		1-Aminoindan	133	C9H11N	034698-41-4	9



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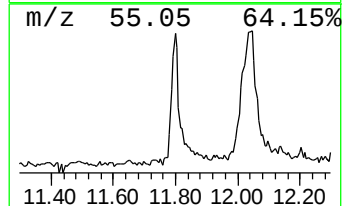
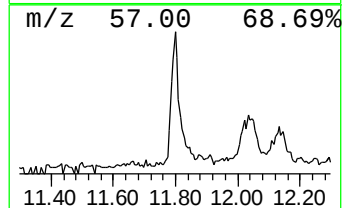
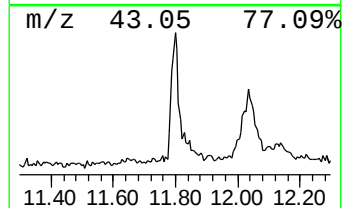
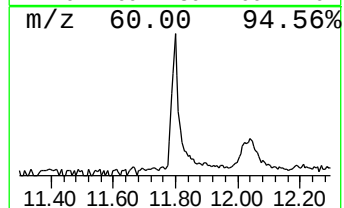
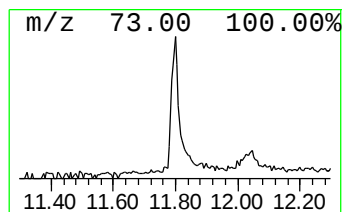
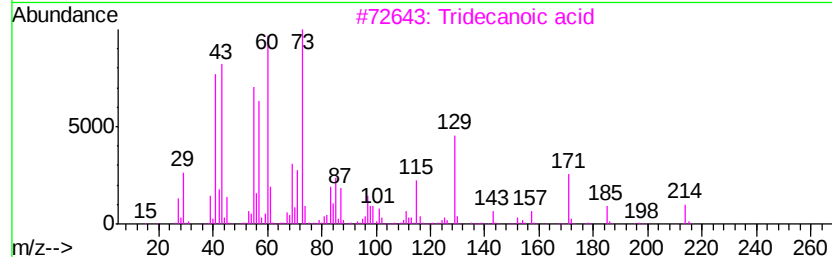
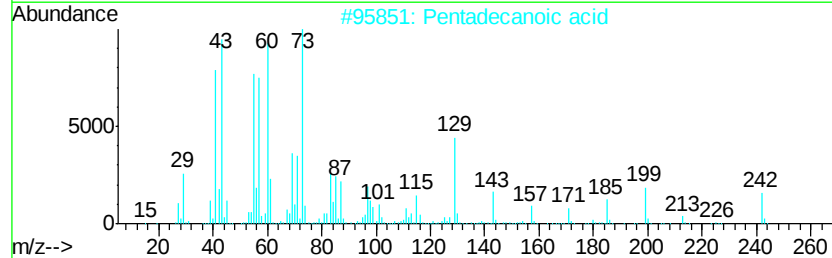
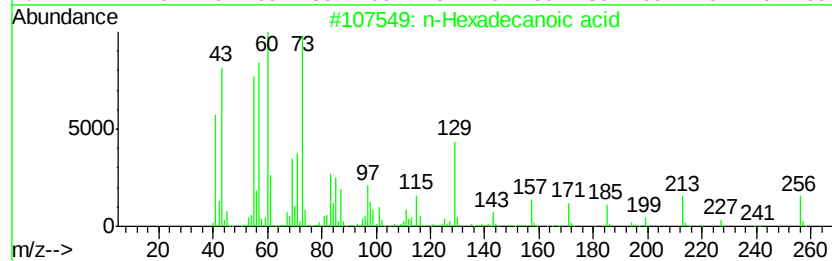
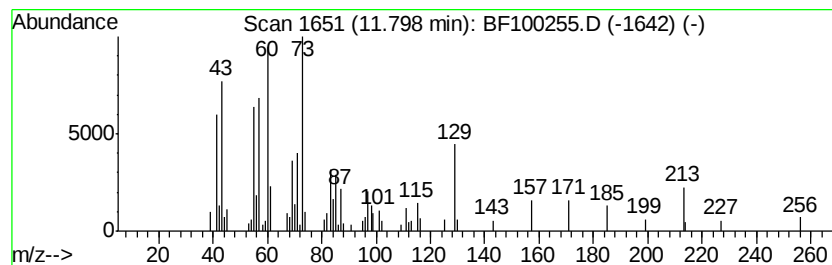
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TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.80	4.76 ng	203441	Phenanthrene-d10	11.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	25
5	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	18



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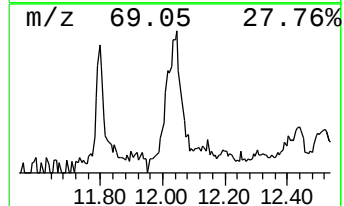
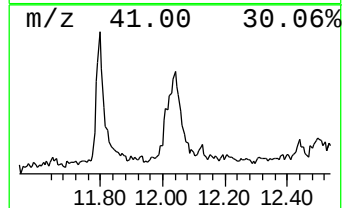
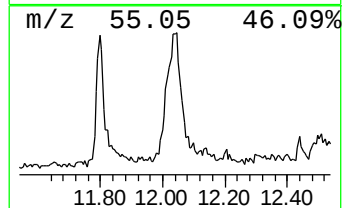
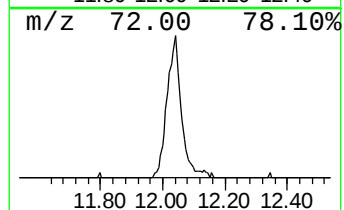
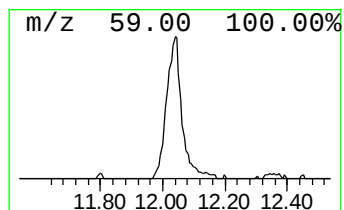
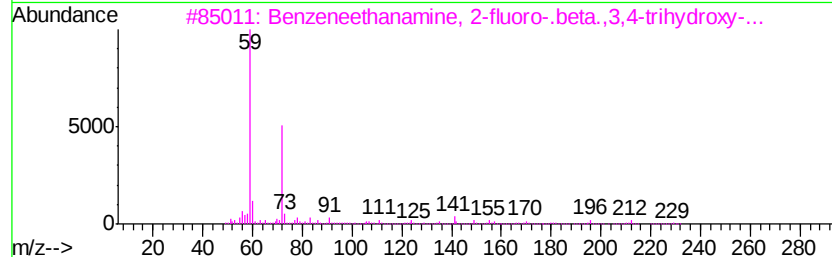
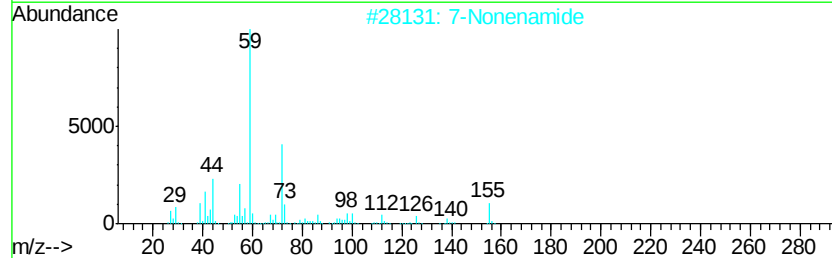
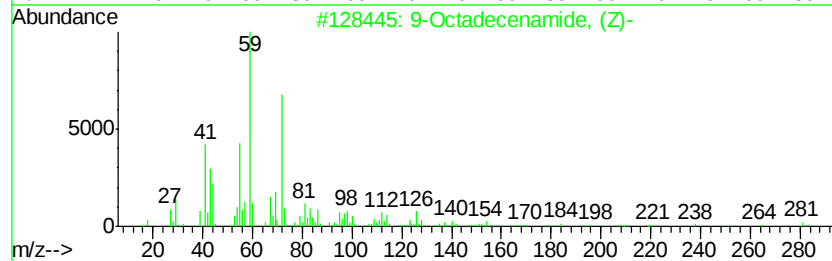
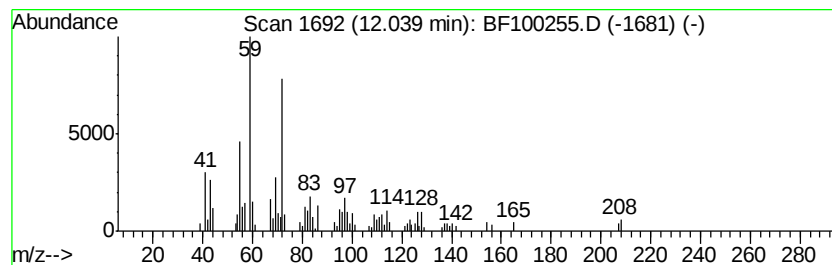
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.04	7.02 ng	300169	Phenanthrene-d10	11.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
2		7-Nonenamide	155	C9H17NO	090949-53-4	64
3		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	50
4		Tetradecanamide	227	C14H29NO	000638-58-4	43
5		Dodecanamide	199	C12H25NO	001120-16-7	38



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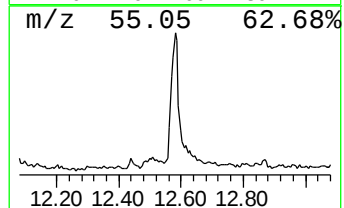
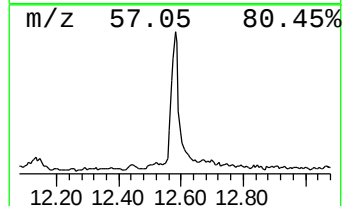
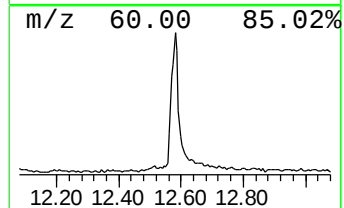
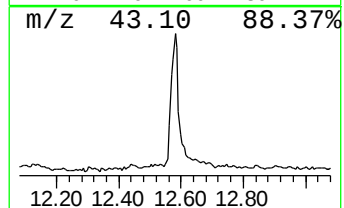
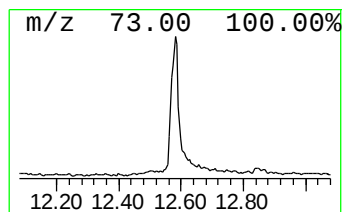
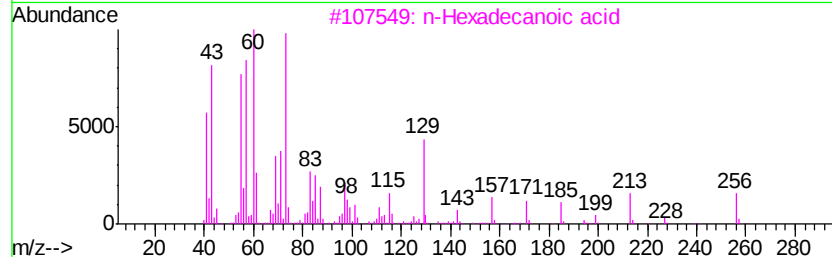
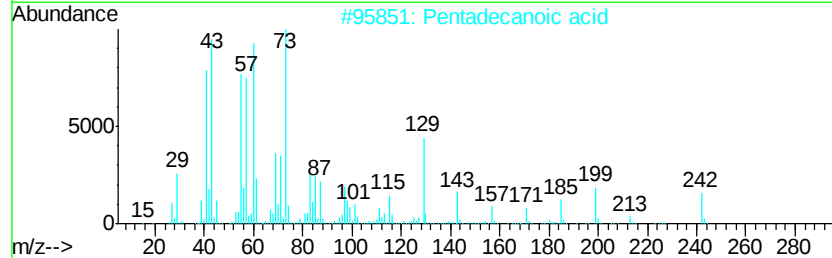
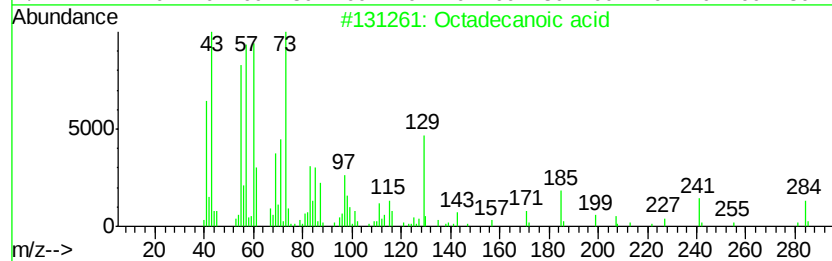
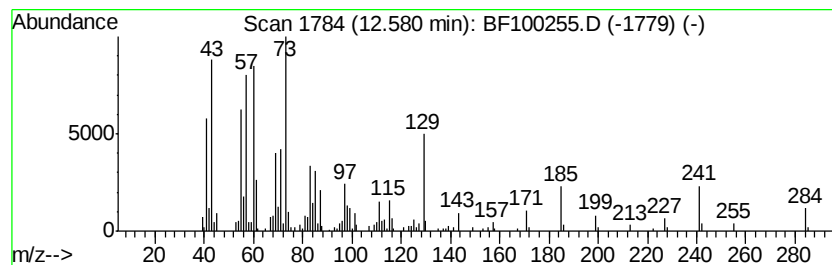
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Peak Number 6 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.58	11.97 ng	511835	Phenanthrene-d10		11.29	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.99	9.7	ng	256058	1	6.76	530730	20.0
unknown6.53	6.53	74.0	ng	1962830	1	6.76	530730	20.0
n-Hexadecanoic acid	11.80	4.8	ng	203441	4	11.29	855034	20.0
9-Octadecenamide,...	12.04	7.0	ng	300169	4	11.29	855034	20.0
Octadecanoic acid	12.58	12.0	ng	511835	4	11.29	855034	20.0