

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120216\
 Data File : BF091395.D
 Acq On : 2 Dec 2016 18:01
 Operator : UM/SJ
 Sample : H5819-02
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 113016-02

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-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	248	rVB	1134888	1926366	32.25%	3.664%
2	5.464	275	278	280	rBV	4506786	4854893	81.28%	9.233%
3	6.493	364	368	370	rBV	4074894	5293157	88.62%	10.066%
4	6.630	377	380	382	rBV	3970187	4821277	80.72%	9.169%
5	6.859	397	400	402	rBV	1664052	1402480	23.48%	2.667%
6	7.019	411	414	416	rBV	3350485	3575182	59.86%	6.799%
7	7.419	446	449	451	rBV	2728654	2739945	45.87%	5.211%
8	8.139	510	512	515	rBV	1714942	1740445	29.14%	3.310%
9	9.225	603	607	609	rBV	5214337	5468922	91.56%	10.401%
10	9.613	638	641	643	rBV	684769	580443	9.72%	1.104%
11	9.796	655	657	659	rBV	47313	81264	1.36%	0.155%
12	9.899	663	666	668	rVB	2228513	2172347	36.37%	4.131%
13	10.333	703	704	706	rVB	123737	109389	1.83%	0.208%
14	10.551	721	723	727	rBV	35716	68457	1.15%	0.130%
15	10.688	732	735	737	rBV	3057723	3741828	62.65%	7.116%
16	10.813	744	746	749	rBV	120515	190736	3.19%	0.363%
17	11.259	783	785	786	rBV	135713	124558	2.09%	0.237%
18	11.385	793	796	798	rBV	1657028	2177946	36.46%	4.142%
19	11.682	820	822	825	rVB	82885	68826	1.15%	0.131%
20	11.911	840	842	855	rVB	443659	522309	8.74%	0.993%
21	12.619	900	904	909	rBV2	26342	64124	1.07%	0.122%
22	12.699	909	911	918	rBV	219558	259358	4.34%	0.493%
23	12.974	932	935	937	rBV	5055272	5972792	100.00%	11.359%
24	13.865	1010	1013	1021	rBV	343659	377359	6.32%	0.718%
25	14.014	1023	1026	1028	rBV	2488347	2326989	38.96%	4.425%
26	14.505	1061	1069	1072	rBV2	28883	72548	1.21%	0.138%
27	15.442	1148	1151	1154	rBV	1395084	1786542	29.91%	3.398%
28	15.957	1194	1196	1201	rBV3	31260	61593	1.03%	0.117%

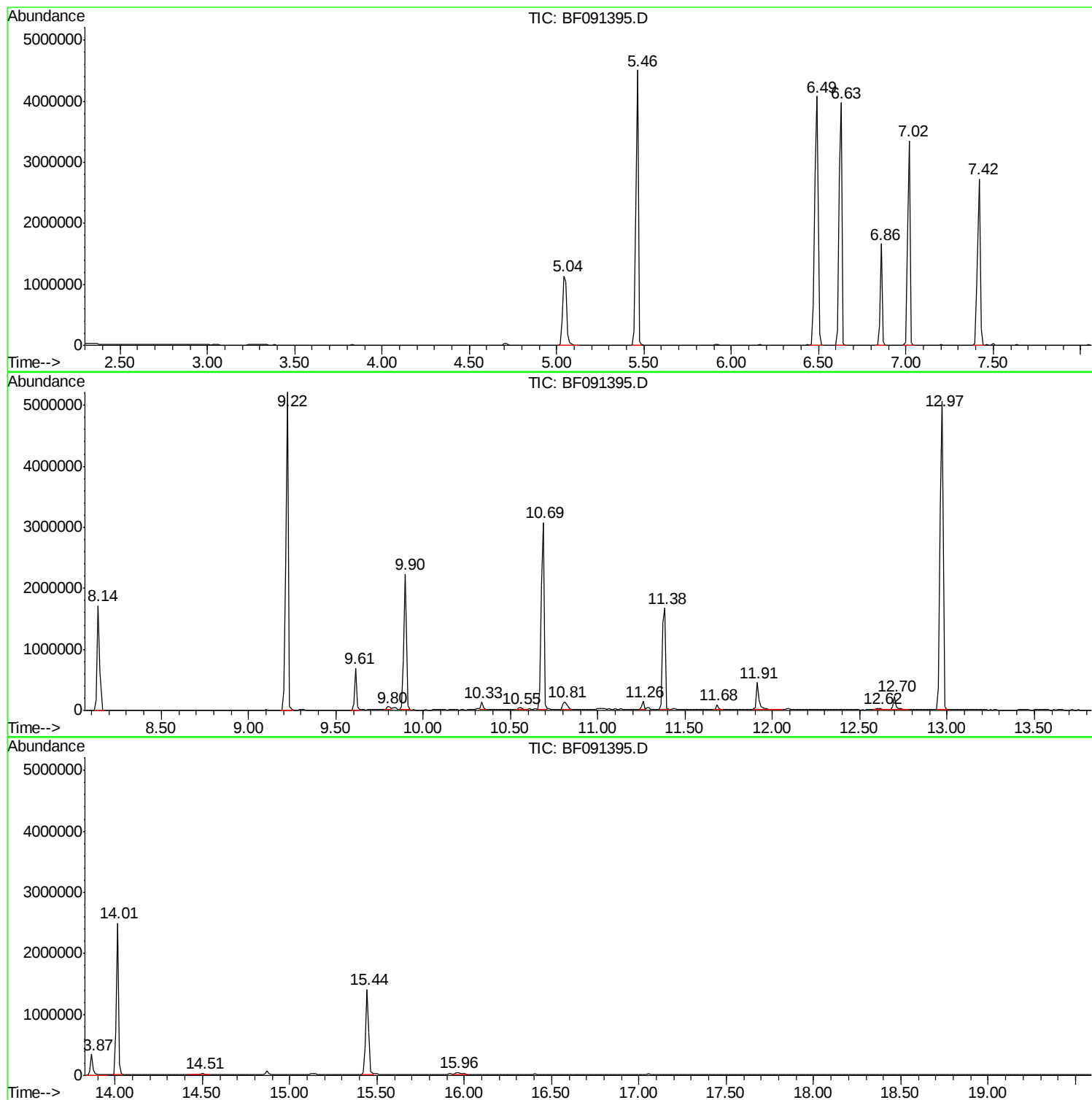
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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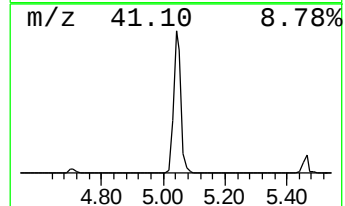
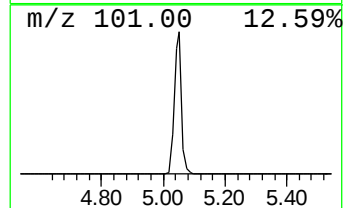
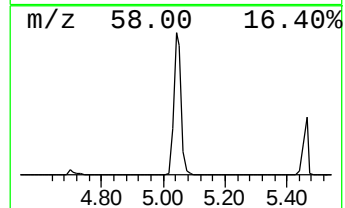
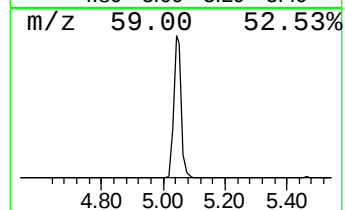
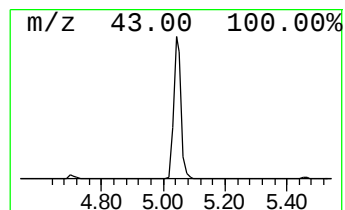
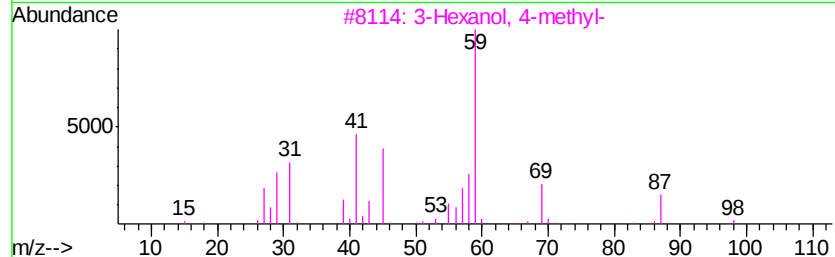
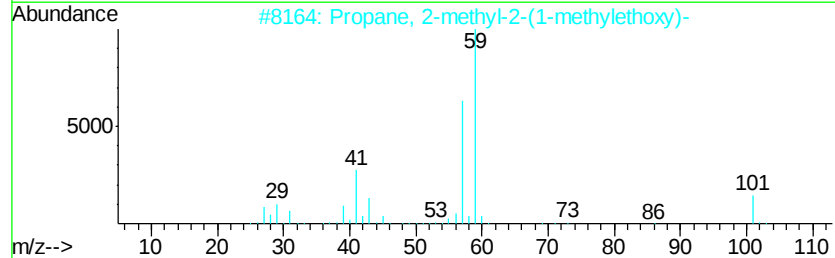
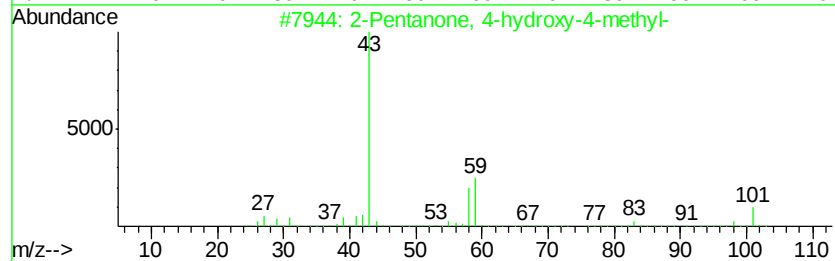
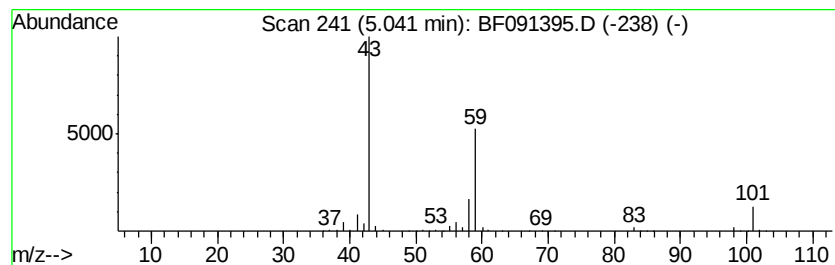
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	27.47 ng	1926370	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	59
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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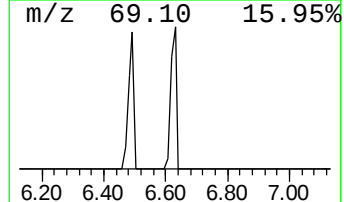
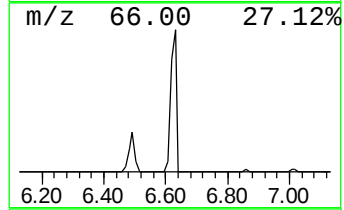
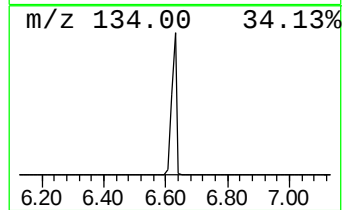
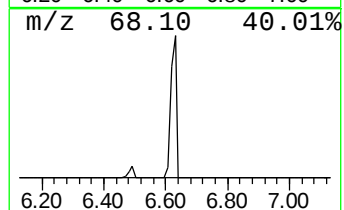
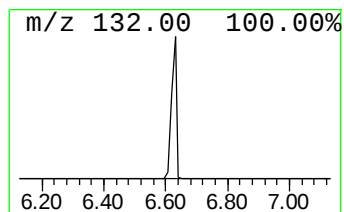
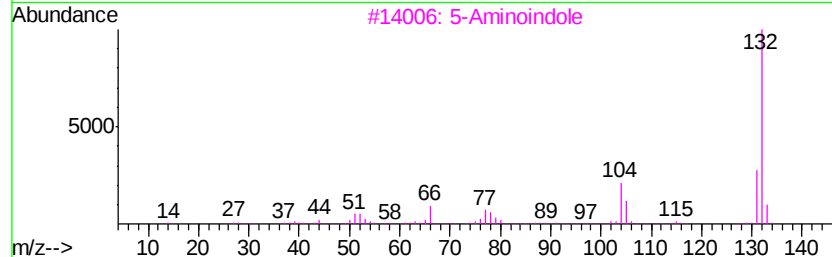
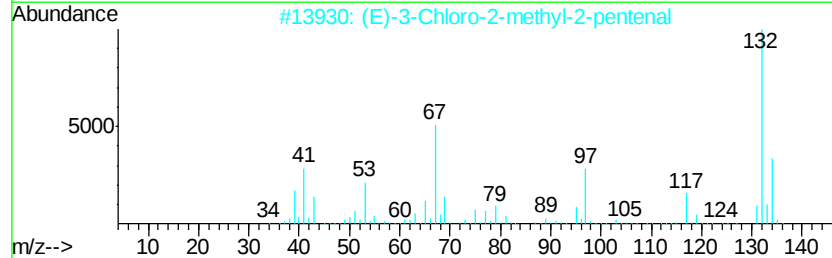
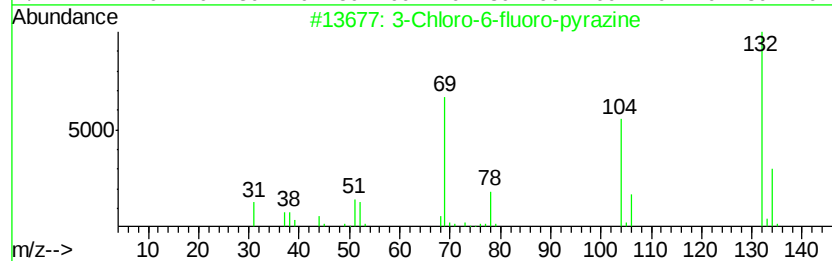
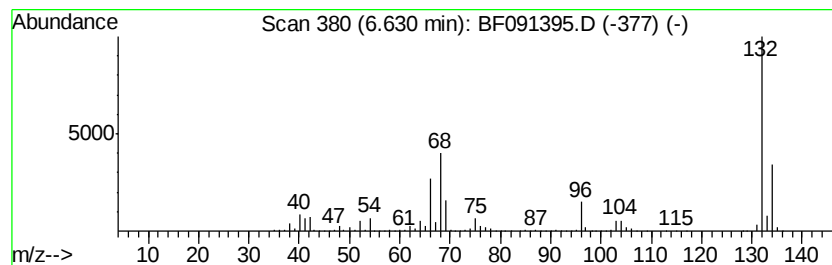
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Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	68.75 ng	4821280	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	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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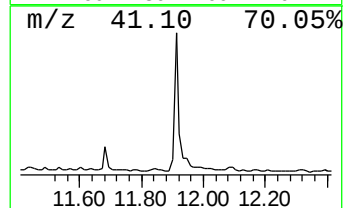
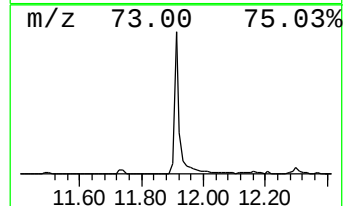
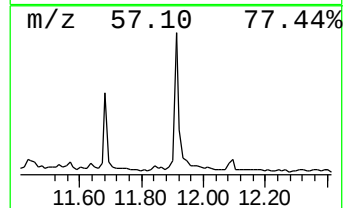
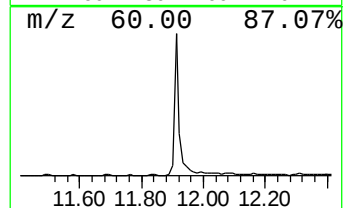
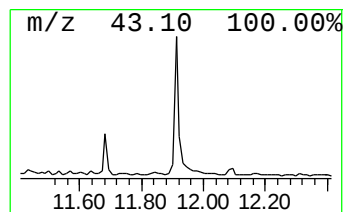
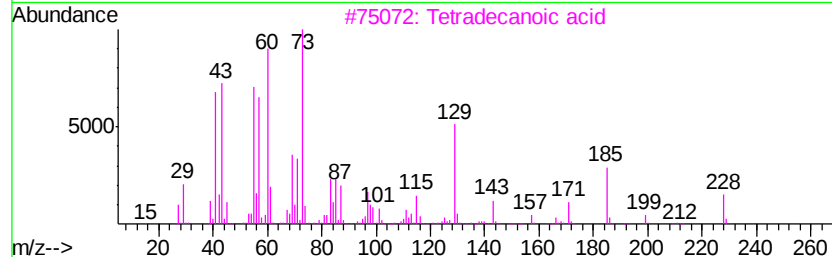
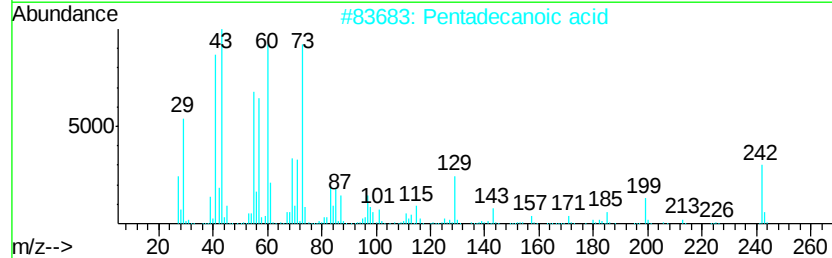
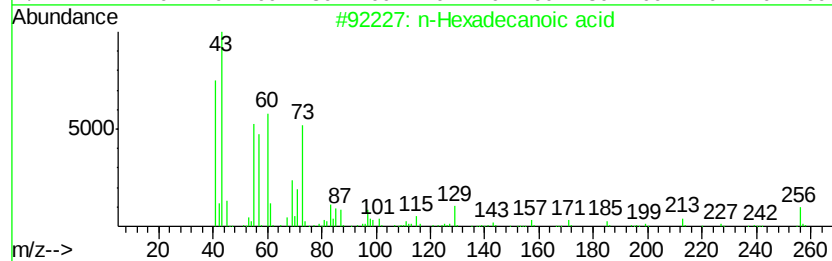
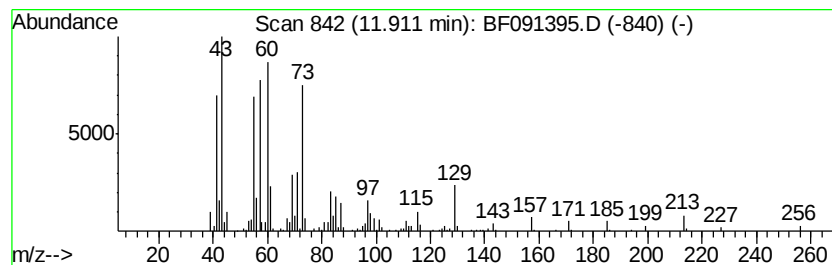
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.91	4.80 ng	522309	Phenanthrene-d10		11.38
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Undecanoic acid	186	C11H22O2	000112-37-8	80
5	Tridecanoic acid	214	C13H26O2	000638-53-9	80



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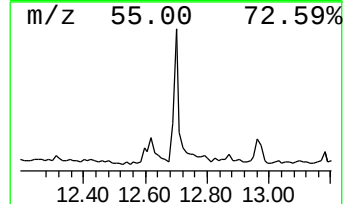
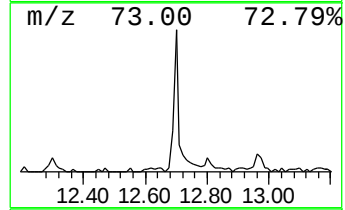
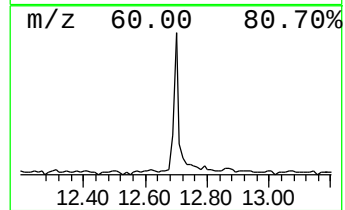
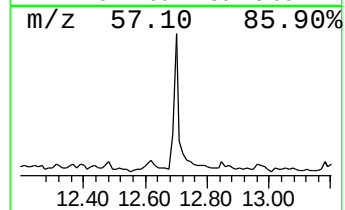
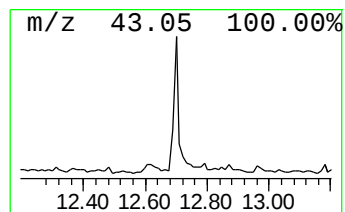
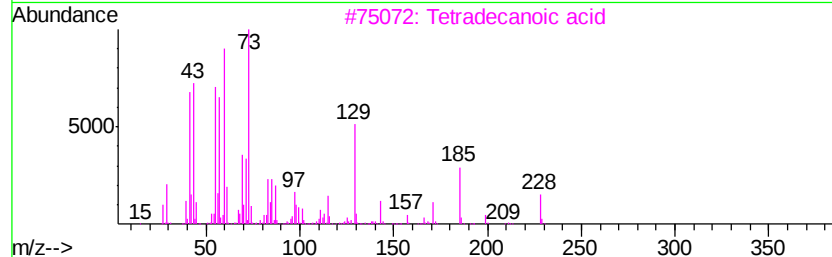
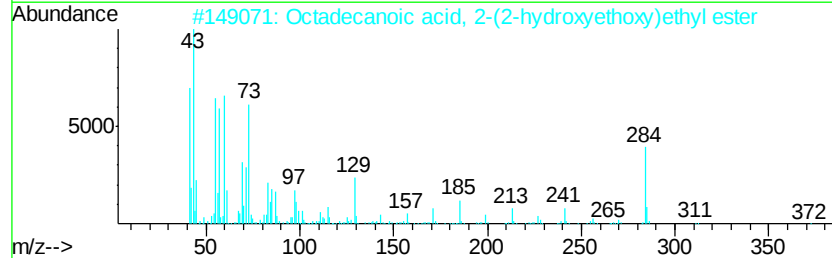
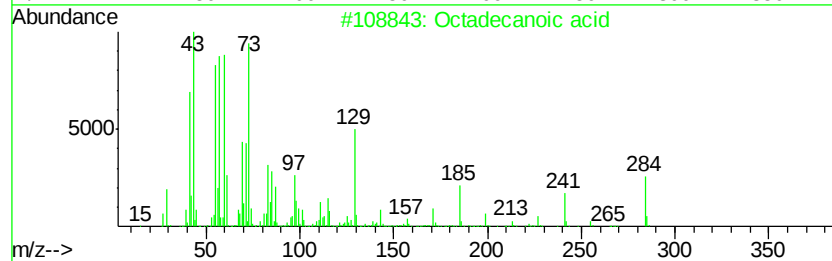
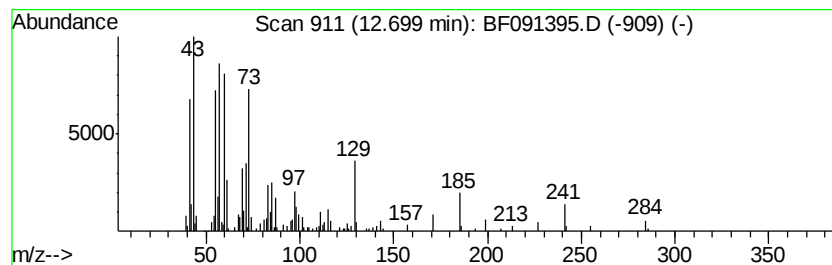
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Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	2.23 ng	259358	Chrysene-d12	14.01

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	94
2	Octadecanoic acid, 2-(2-hydroxye...		372	C22H44O4	000106-11-6	80
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	64
4	Tridecanoic acid		214	C13H26O2	000638-53-9	53
5	Undecanoic acid		186	C11H22O2	000112-37-8	47



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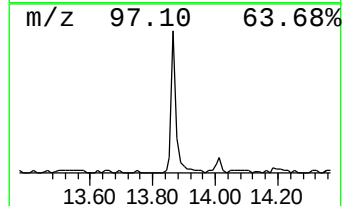
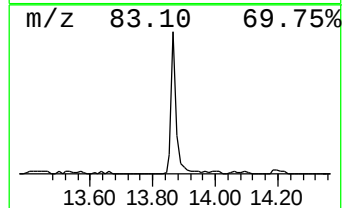
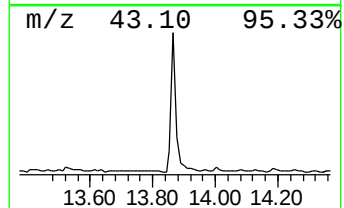
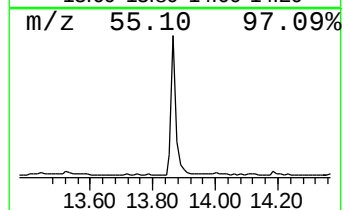
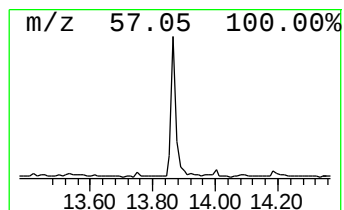
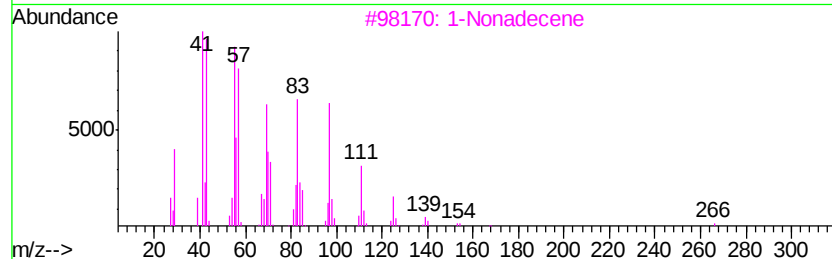
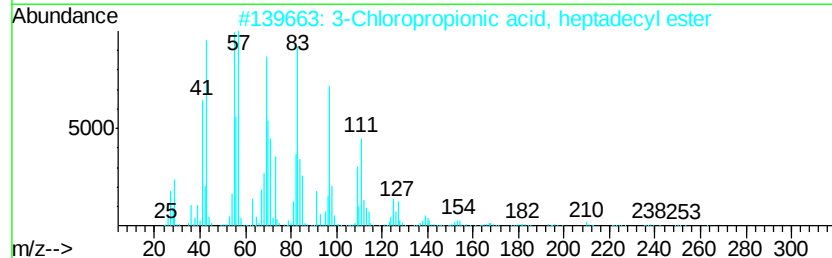
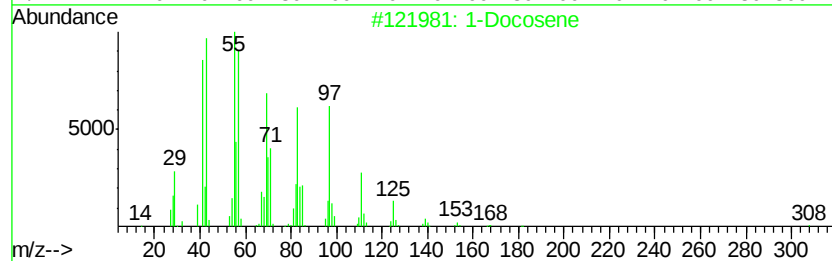
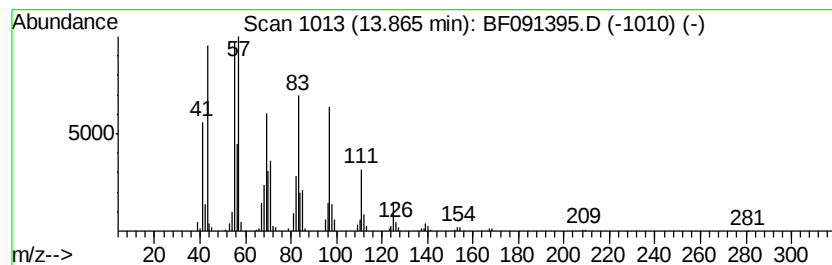
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Peak Number 6 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	3.24 ng	377359	Chrysene-d12	14.01

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene		308	C22H44	001599-67-3	94
2	3-Chloropropionic acid, heptadec...		346	C20H39ClO2	1000283-05-1	91
3	1-Nonadecene		266	C19H38	018435-45-5	91
4	9-Eicosene, (E)-		280	C20H40	074685-29-3	90
5	3-Eicosene, (E)-		280	C20H40	074685-33-9	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.04	27.5	ng	1926370	1	6.86	1402480	20.0
unknown6.63	6.63	68.8	ng	4821280	1	6.86	1402480	20.0
n-Hexadecanoic acid	11.91	4.8	ng	522309	4	11.38	2177950	20.0
Octadecanoic acid	12.70	2.2	ng	259358	5	14.01	2326990	20.0
1-Docosene	13.87	3.2	ng	377359	5	14.01	2326990	20.0