

Data Path : Z:\HPCHEM1\BNA F\Data\BF031617\
 Data File : BF093708.D
 Acq On : 16 Mar 2017 16:14
 Operator : SJ/MA
 Sample : I2255-05
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P-1

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-BF030717.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	4.847	257	259	268	rBV	75298	195501	4.01%	0.564%
2	5.293	296	298	318	rBV	1295242	2428768	49.80%	7.004%
3	6.367	390	392	399	rBV	796381	1574807	32.29%	4.542%
4	6.470	399	401	412	rVB	3112842	4213524	86.40%	12.151%
5	6.687	418	420	426	rBV	760354	1094679	22.45%	3.157%
6	6.847	432	434	443	rBV	3613815	3595388	73.72%	10.369%
7	7.270	469	471	480	rBV	2880466	3206086	65.74%	9.246%
8	7.990	531	534	536	rBV	1013410	1358787	27.86%	3.919%
9	9.065	625	628	630	rBV	4985074	4876840	100.00%	14.064%
10	9.465	661	663	666	rBV	138896	149719	3.07%	0.432%
11	9.739	684	687	689	rBV	1456172	1503993	30.84%	4.337%
12	10.162	723	724	726	rVB	134259	116242	2.38%	0.335%
13	10.253	730	732	736	rVB	91886	99403	2.04%	0.287%
14	10.528	754	756	759	rBV	2327227	2458033	50.40%	7.089%
15	10.631	763	765	768	rVV	75782	134712	2.76%	0.388%
16	10.676	768	769	773	rVB2	47200	54277	1.11%	0.157%
17	11.076	803	804	806	rBV	53809	78179	1.60%	0.225%
18	11.214	814	816	819	rBV2	1023868	1328777	27.25%	3.832%
19	11.751	861	863	872	rBV	71125	137581	2.82%	0.397%
20	12.802	952	955	957	rBV	3951277	3984400	81.70%	11.491%
21	13.705	1031	1034	1042	rBV7	17691	59450	1.22%	0.171%
22	13.854	1045	1047	1050	rBV	1069508	1179437	24.18%	3.401%
23	15.248	1167	1169	1176	rVB	520710	846800	17.36%	2.442%

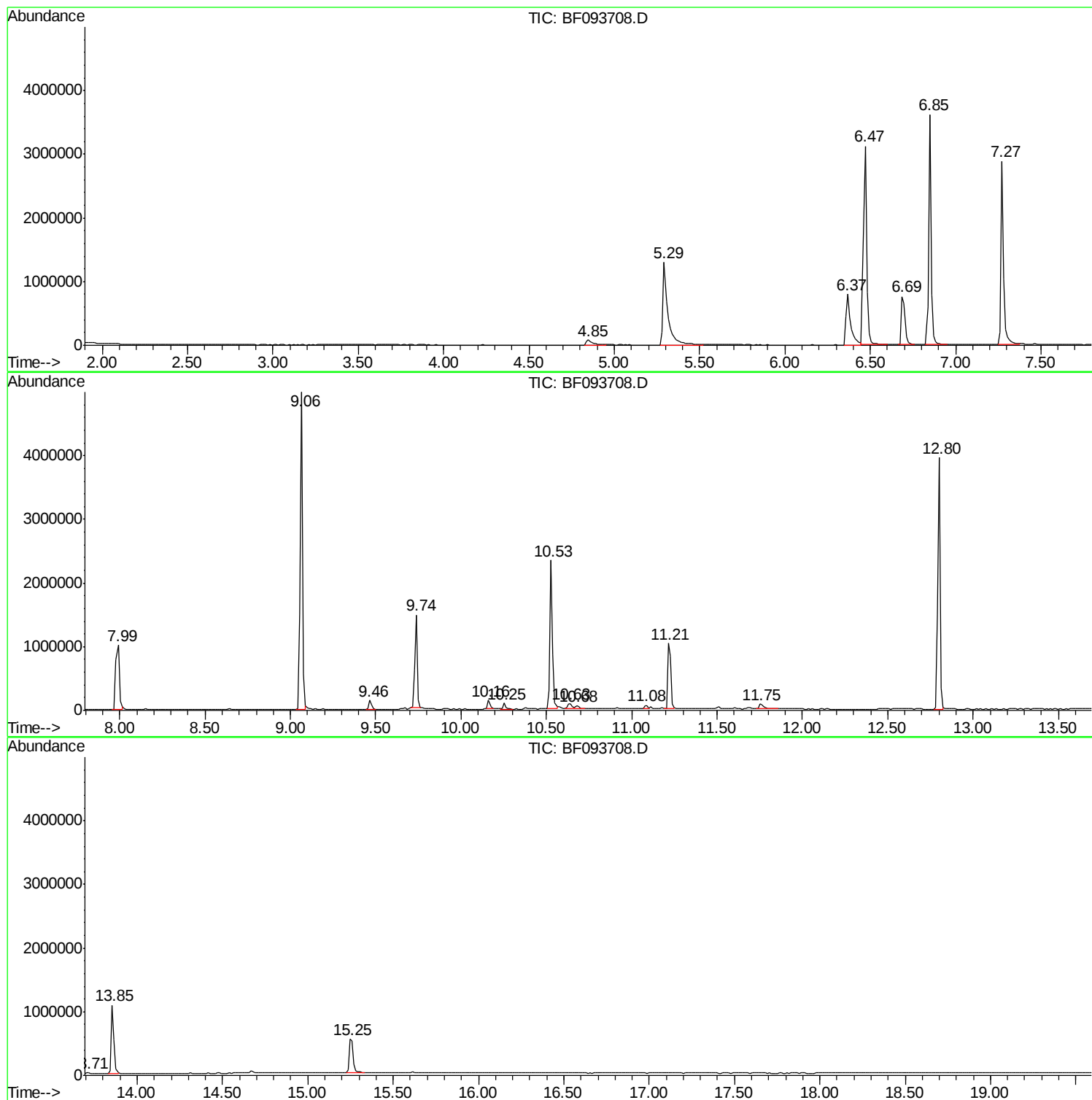
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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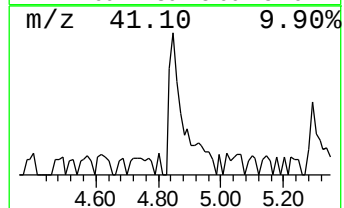
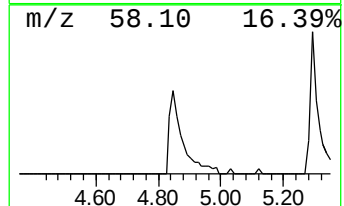
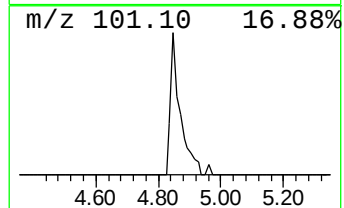
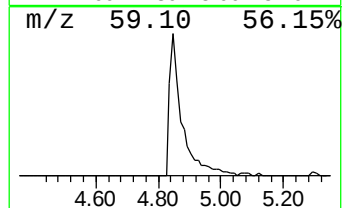
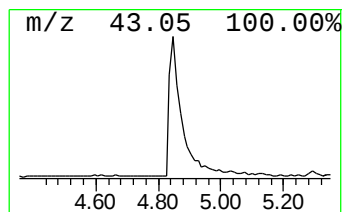
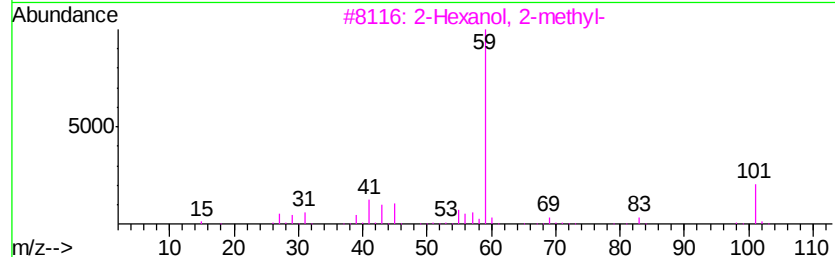
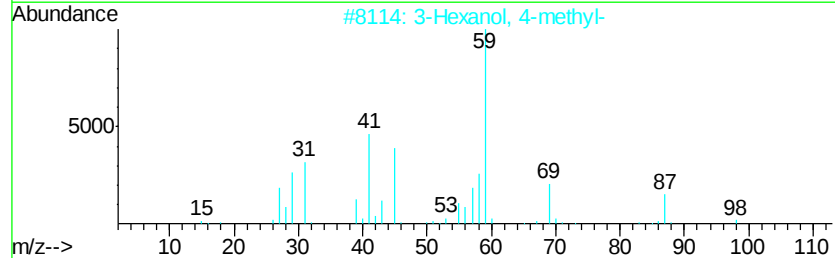
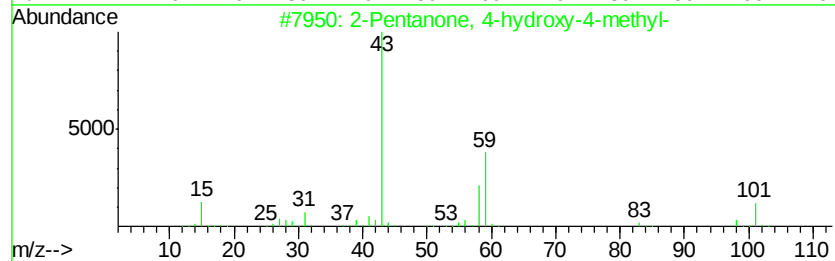
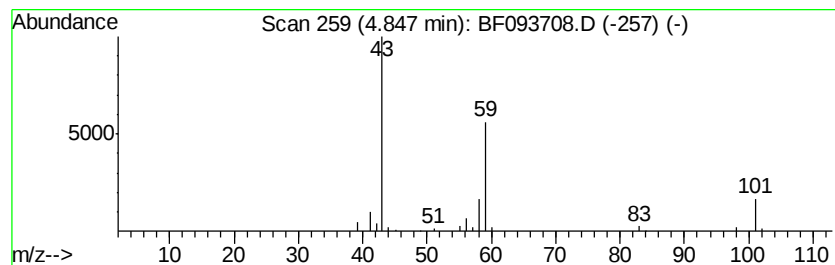
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.85	3.57 ng	195501	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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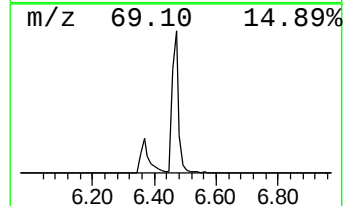
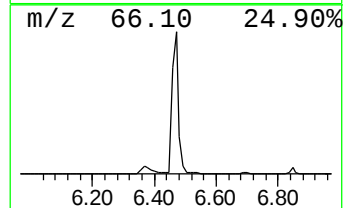
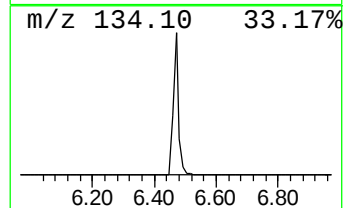
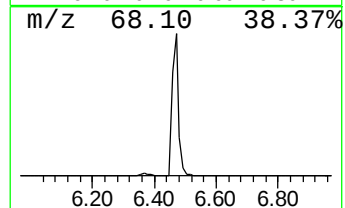
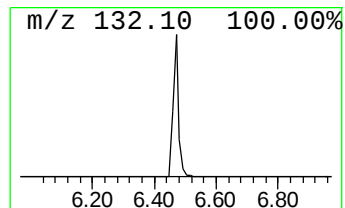
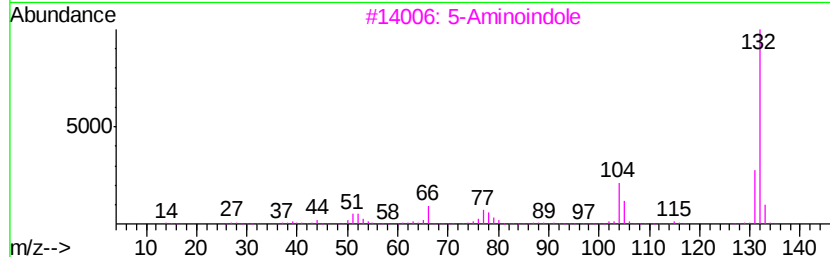
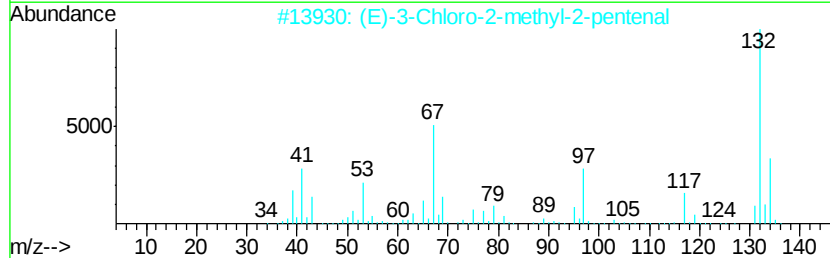
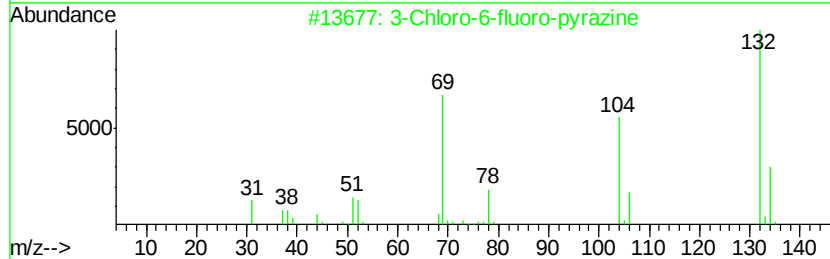
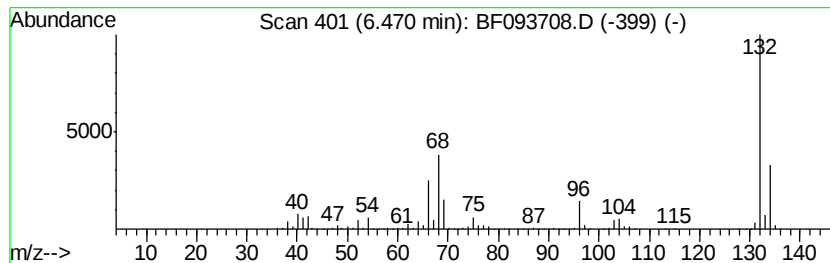
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Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	76.98 ng	4213520	1,4-Dichlorobenzene-d4	6.70

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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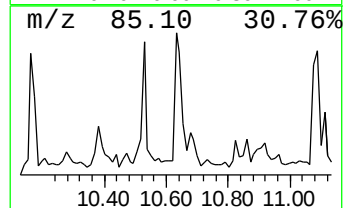
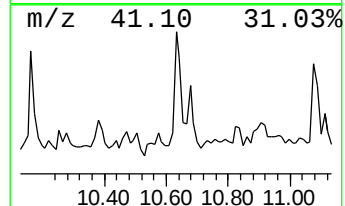
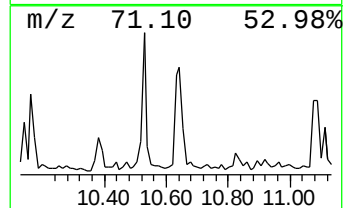
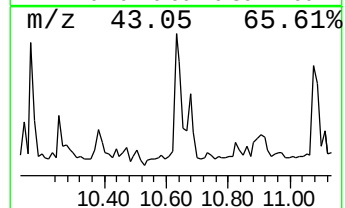
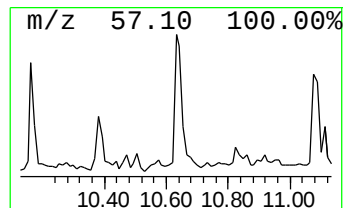
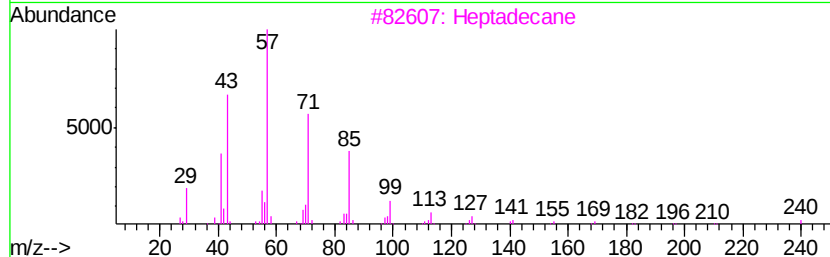
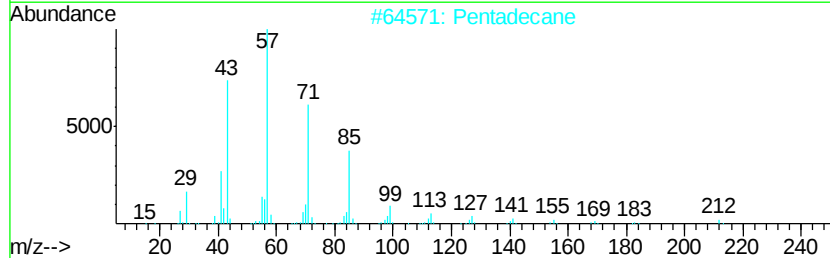
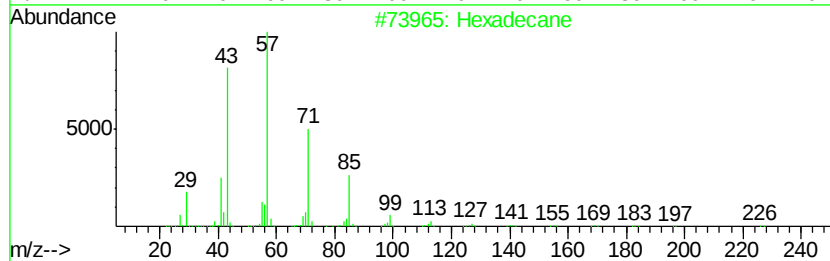
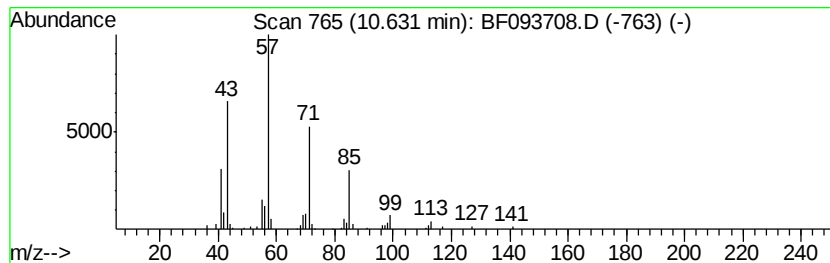
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Peak Number 4 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.63	2.03 ng	134712	Phenanthrene-d10	11.21	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Pentadecane	212	C15H32	000629-62-9	83
3	Heptadecane	240	C17H36	000629-78-7	83
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78
5	Tridecane	184	C13H28	000629-50-5	72



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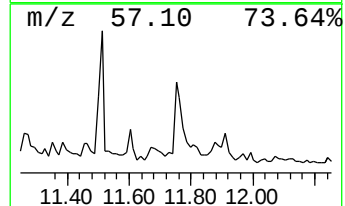
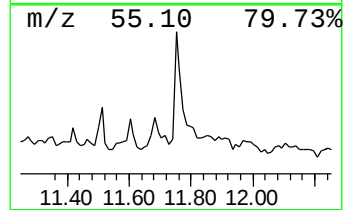
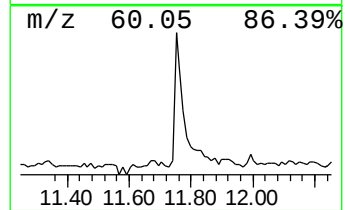
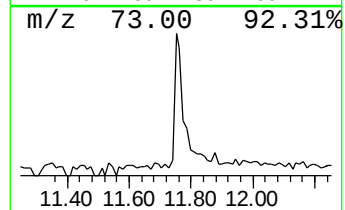
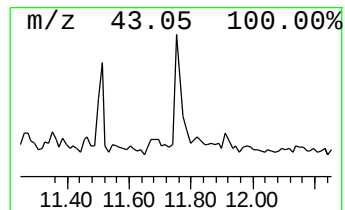
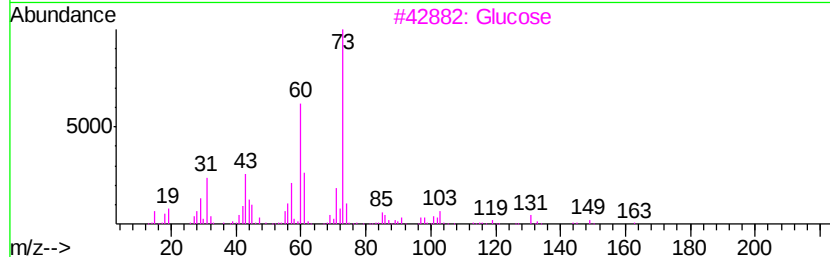
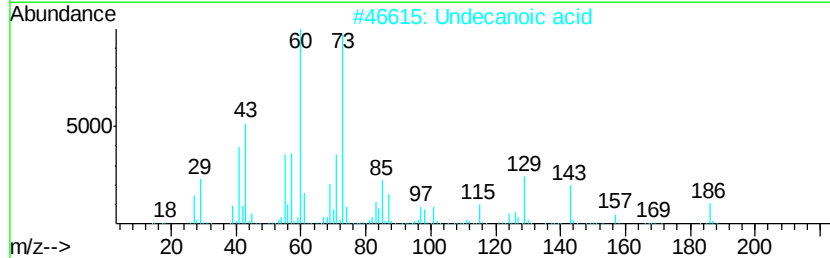
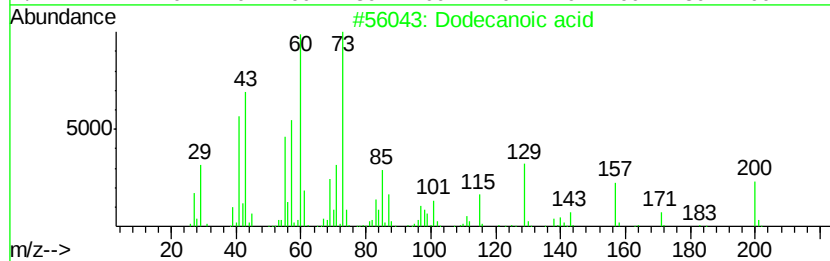
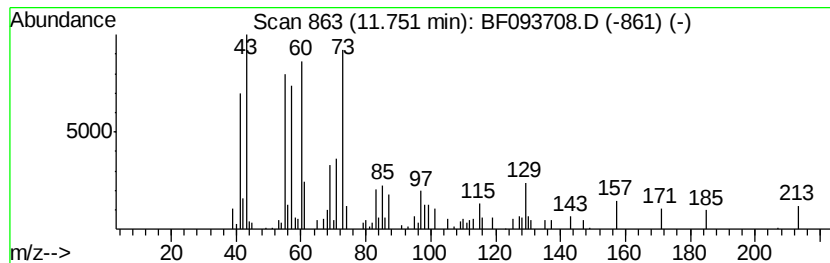
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Peak Number 5 Dodecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	2.07 ng	137581	Phenanthrene-d10	11.21

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	72
2			Undecanoic acid	186	C11H22O2	000112-37-8	53
3			Glucose	180	C6H12O6	000050-99-7	43
4			.alpha.-D-Glucopyranoside, .alph...	342	C12H22O11	000099-20-7	40
5			n-Decanoic acid	172	C10H20O2	000334-48-5	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.85	3.6	ng	195501	1	6.70	1094680	20.0
unknown6.47	6.47	77.0	ng	4213520	1	6.70	1094680	20.0
Hexadecane	10.63	2.0	ng	134712	4	11.21	1328780	20.0
Dodecanoic acid	11.75	2.1	ng	137581	4	11.21	1328780	20.0