

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040618\
 Data File : BF104357.D
 Acq On : 7 Apr 2018 14:14
 Operator : JU/SJ
 Sample : J2255-12
 Misc :
 ALS Vial : 51 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 040418-DBRI-E-U-S

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-BF040618.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	4.998	491	495	503	rVB	143231	145740	3.67%	0.626%
2	5.404	559	564	567	rBV	1227356	1077984	27.14%	4.633%
3	6.416	732	736	745	rVB	829622	673266	16.95%	2.894%
4	6.569	757	762	765	rBV	2128366	2039911	51.36%	8.768%
5	6.804	798	802	805	rBV	963826	827852	20.84%	3.558%
6	6.957	824	828	832	rVB	2823601	2809283	70.74%	12.075%
7	7.369	892	898	901	rBV	2300640	2295790	57.81%	9.868%
8	8.087	1016	1020	1023	rVB	1357325	1096458	27.61%	4.713%
9	9.163	1198	1203	1206	rBV	4028884	3971531	100.00%	17.070%
10	9.551	1266	1269	1273	rBV	70178	69542	1.75%	0.299%
11	9.769	1303	1306	1309	rBV	72612	59186	1.49%	0.254%
12	9.839	1313	1318	1322	rVB2	1321625	1148841	28.93%	4.938%
13	10.269	1388	1391	1394	rVB	76450	64472	1.62%	0.277%
14	10.628	1447	1452	1455	rBV	1608396	1396218	35.16%	6.001%
15	10.745	1469	1472	1481	rVB	68775	68395	1.72%	0.294%
16	11.328	1567	1571	1574	rBV	1045861	882845	22.23%	3.795%
17	12.739	1807	1811	1814	rBV	195457	152180	3.83%	0.654%
18	12.922	1837	1842	1845	rBV	2709272	2762109	69.55%	11.872%
19	13.445	1928	1931	1934	rBV	120909	94928	2.39%	0.408%
20	13.816	1990	1994	2003	rBV	126111	132894	3.35%	0.571%
21	13.969	2016	2020	2023	rBV	857522	762059	19.19%	3.275%
22	15.421	2262	2267	2272	rBV	541114	688913	17.35%	2.961%
23	16.392	2425	2432	2440	rBV4	23386	45564	1.15%	0.196%

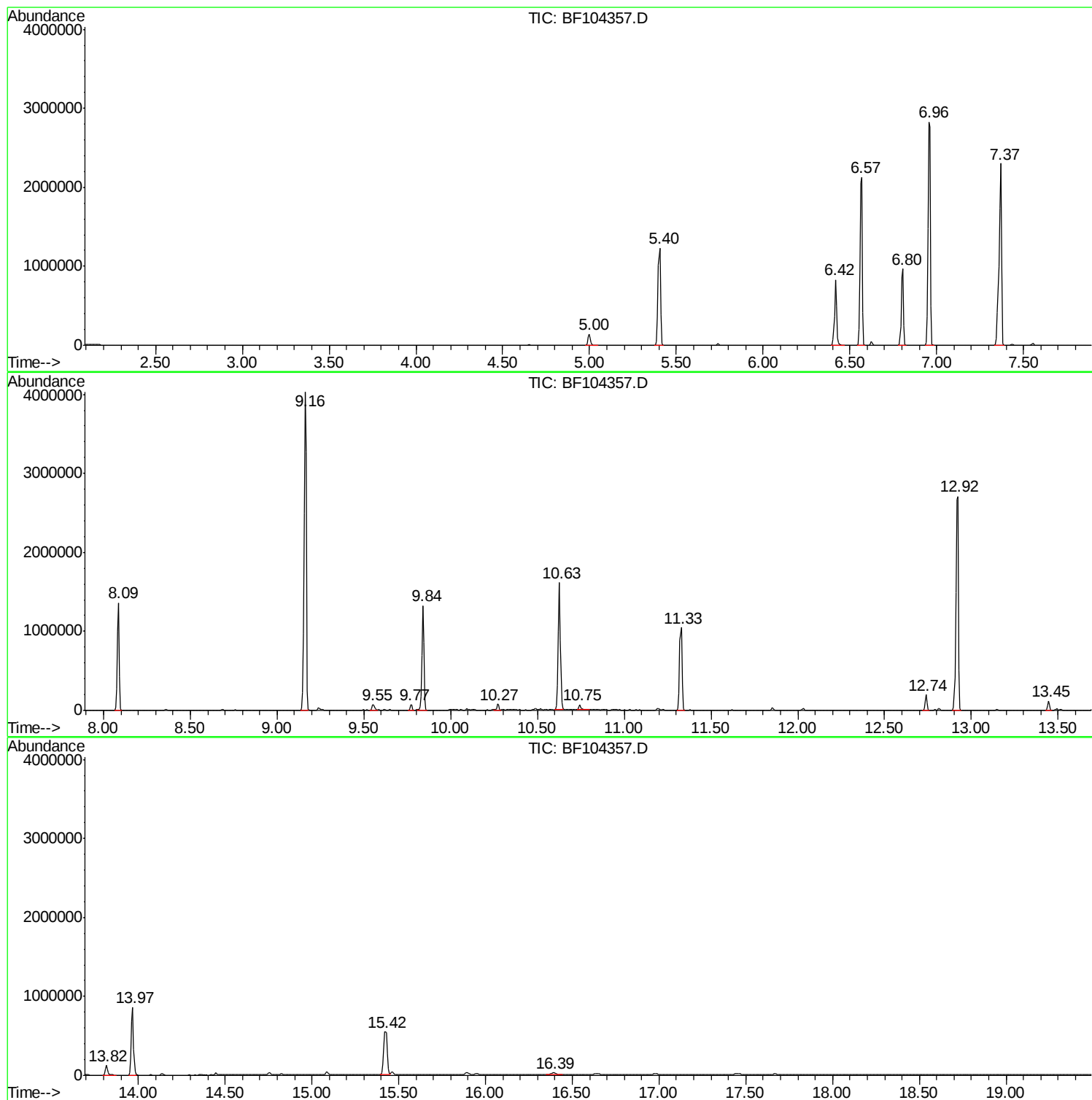
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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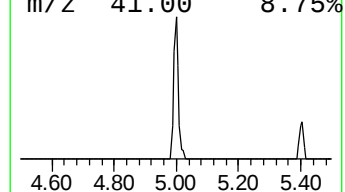
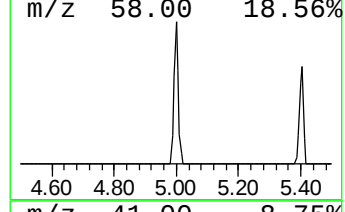
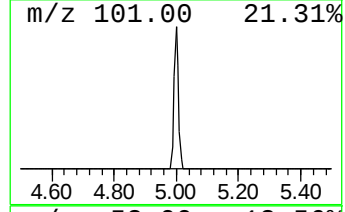
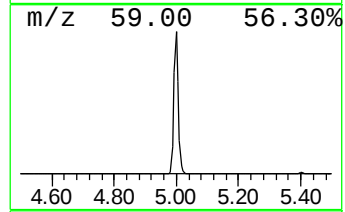
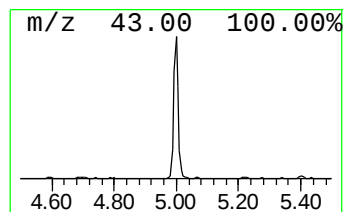
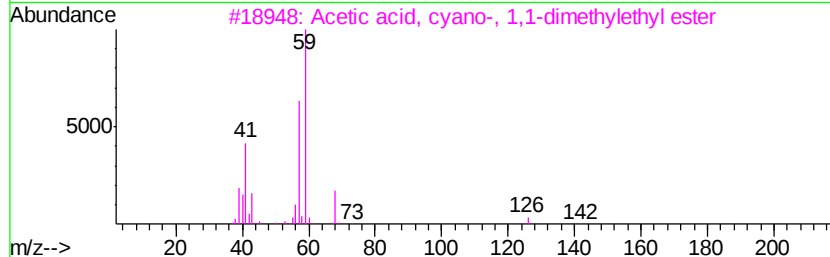
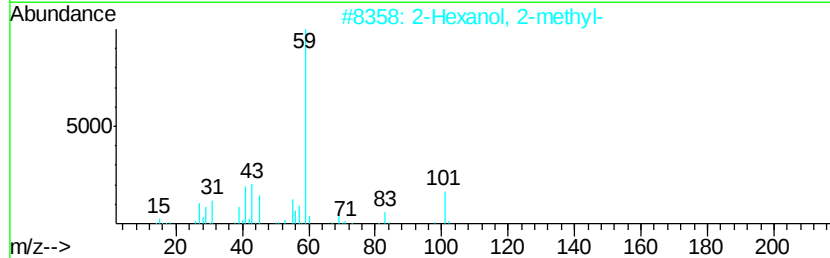
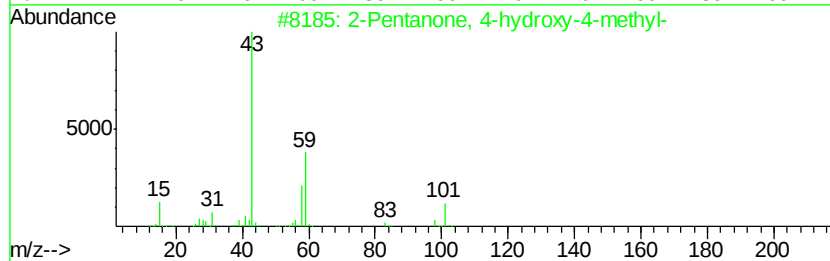
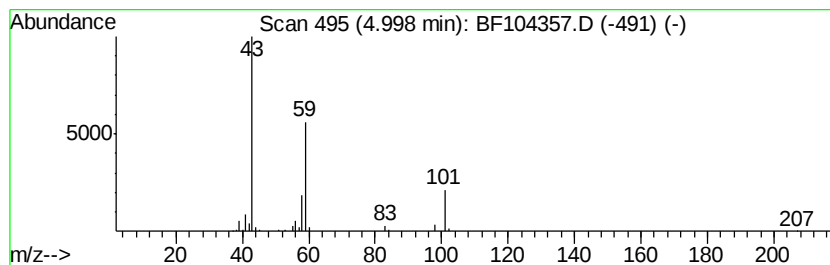
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ClientSampleId :
040418-DBRI-E-U-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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.	
5.00	3.52 ng	145740	1,4-Dichlorobenzene-d4	6.80	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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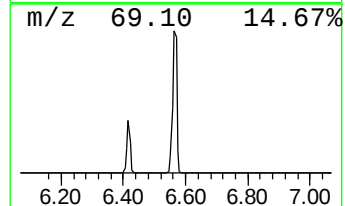
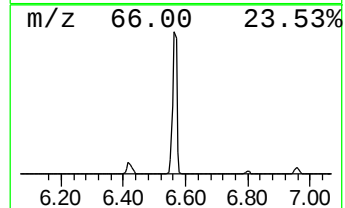
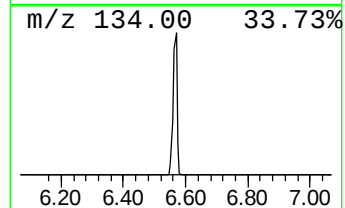
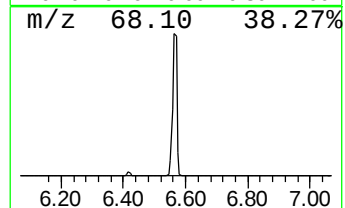
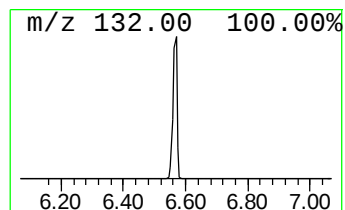
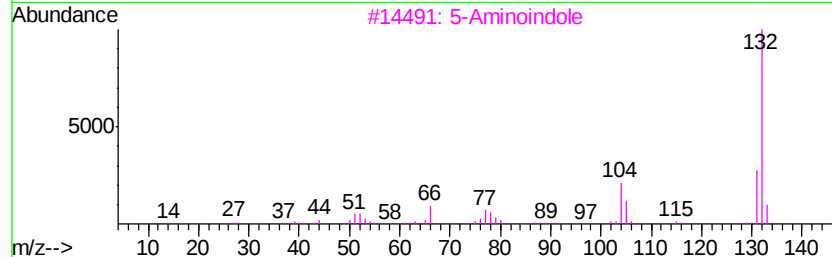
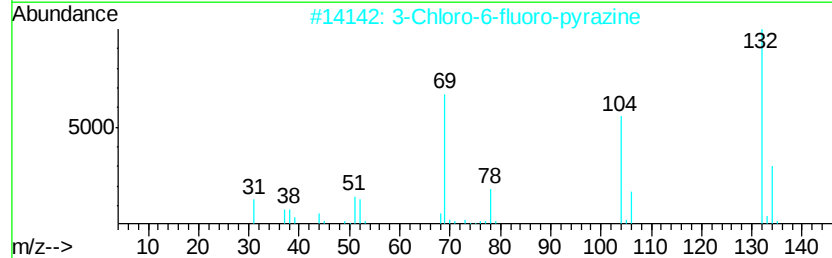
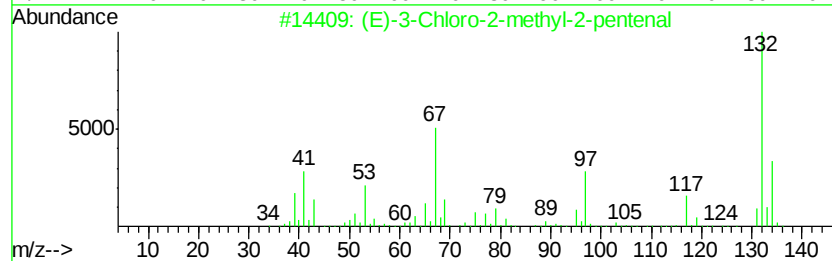
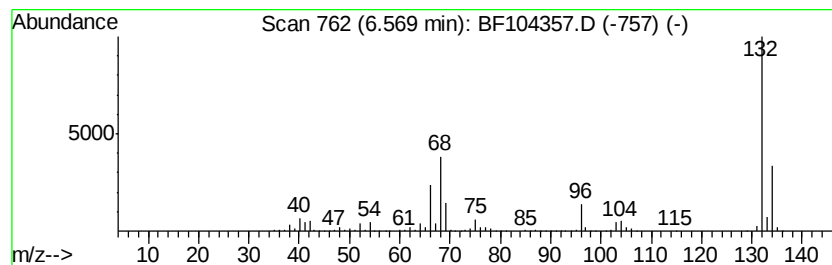
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	49.28 ng	2039910	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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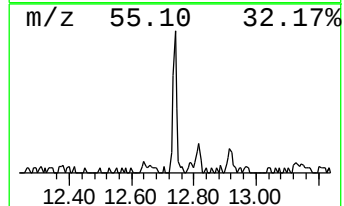
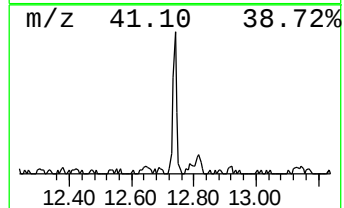
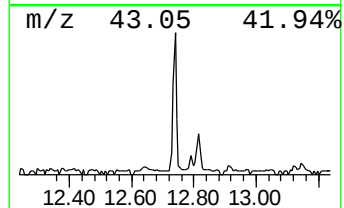
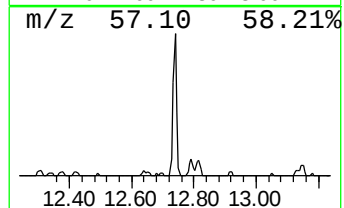
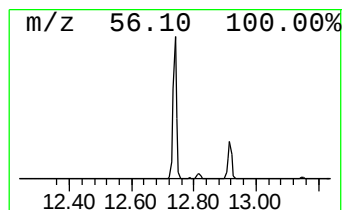
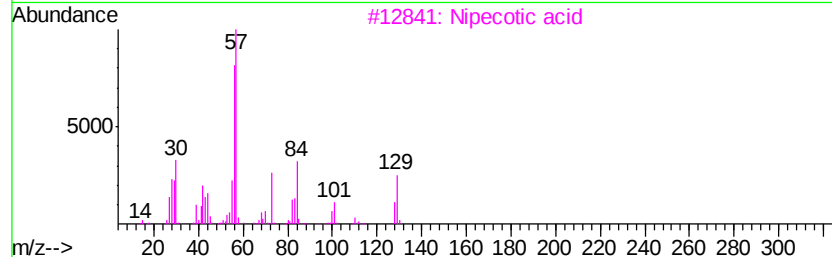
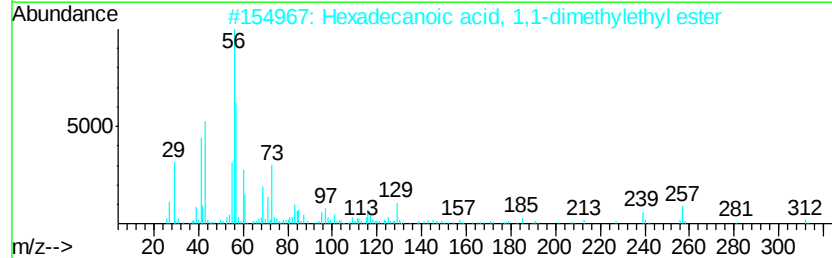
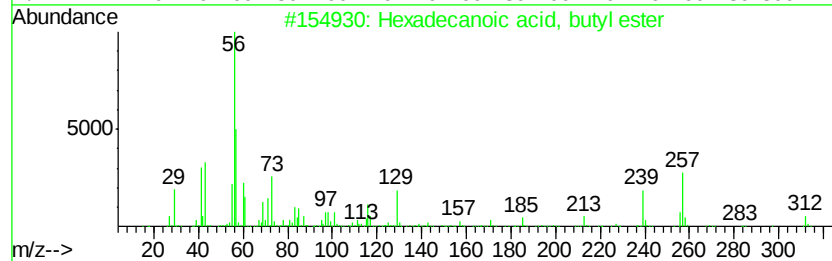
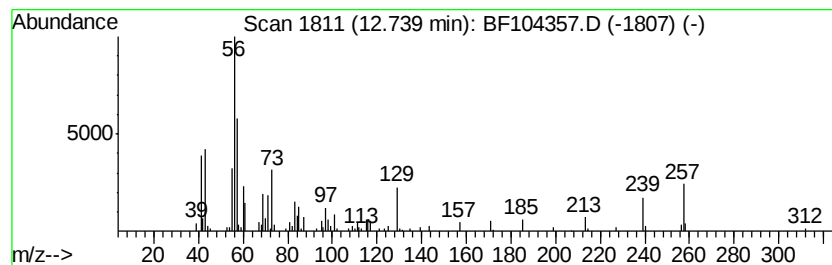
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	3.99 ng	152180	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	64
3		Nipecotic acid	129	C6H11NO2	000498-95-3	37
4		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5		Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	32



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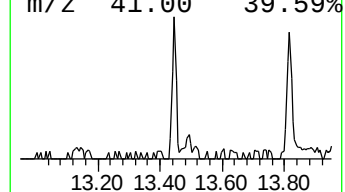
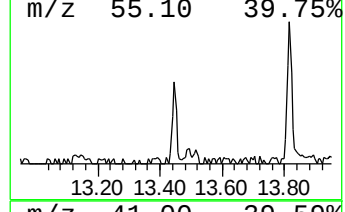
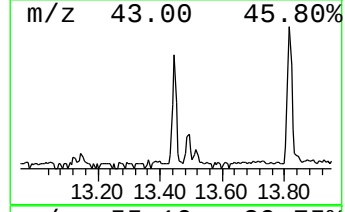
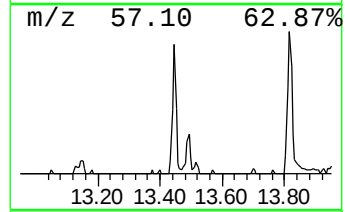
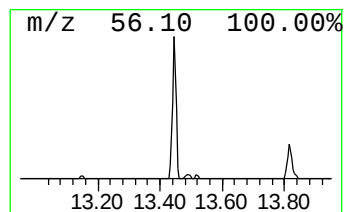
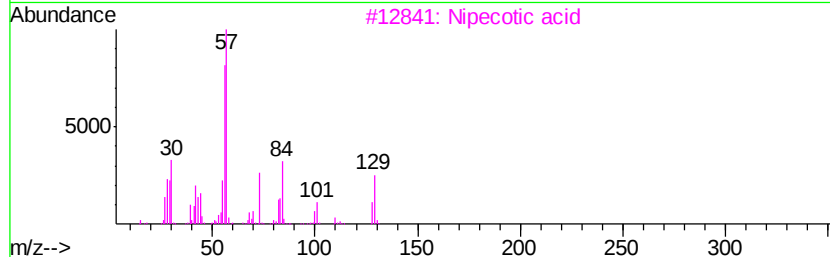
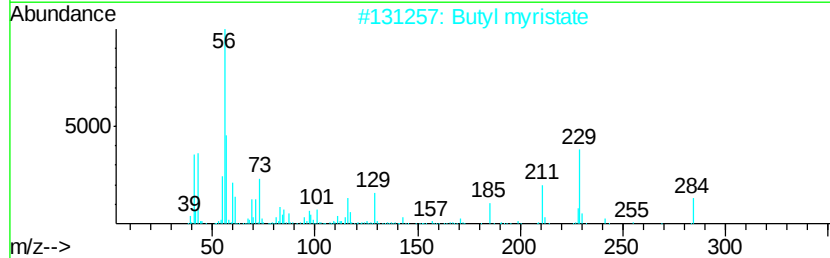
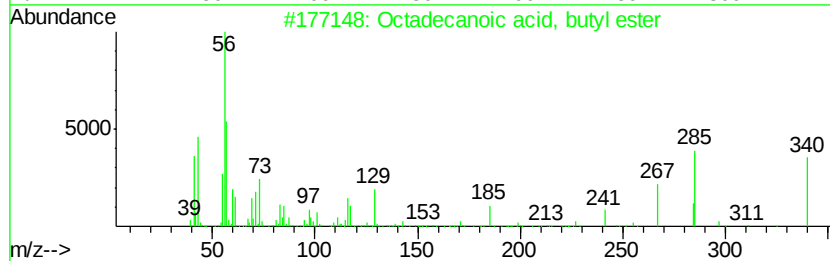
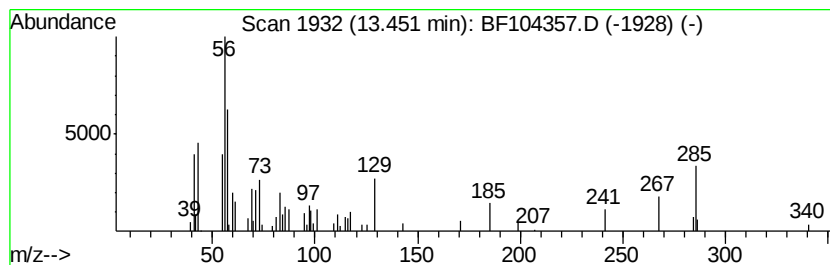
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Peak Number 5 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	2.49 ng	94928	Chrysene-d12	13.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	94
2		Butyl myristate	284	C18H36O2	000110-36-1	80
3		Nipecotic acid	129	C6H11NO2	000498-95-3	50
4		Octadecanoic acid, 2-methylpropyl...	340	C22H44O2	000646-13-9	43
5		Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32



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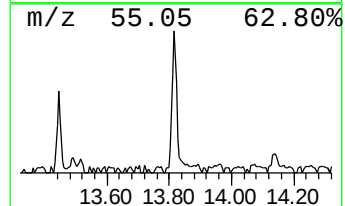
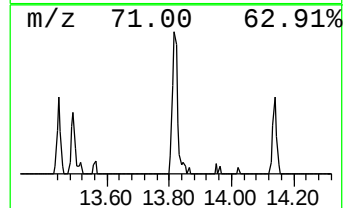
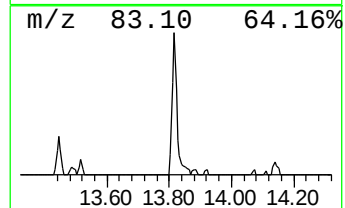
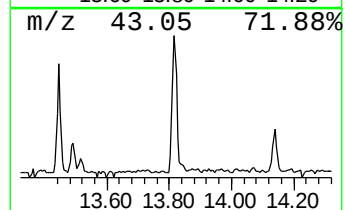
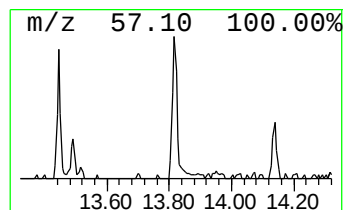
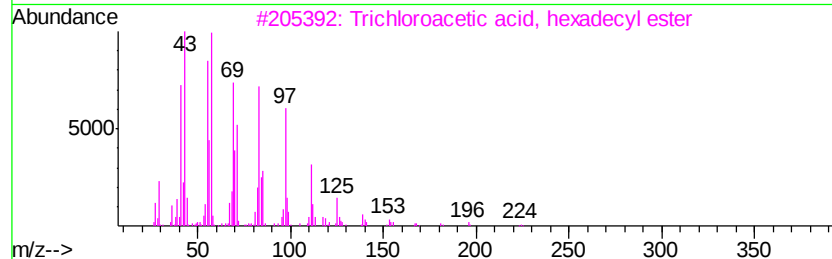
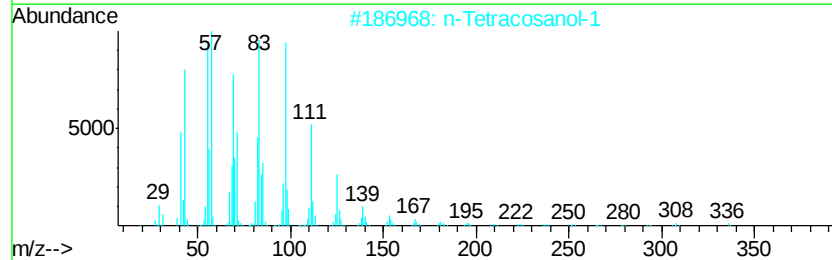
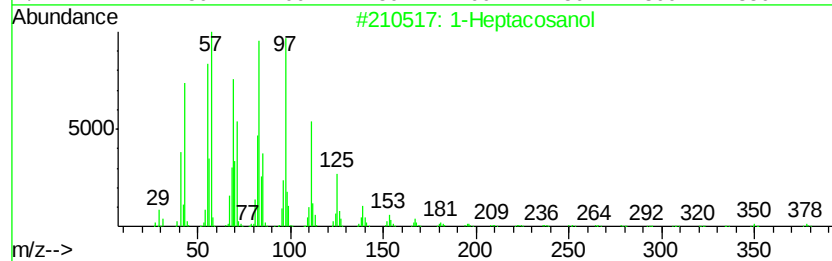
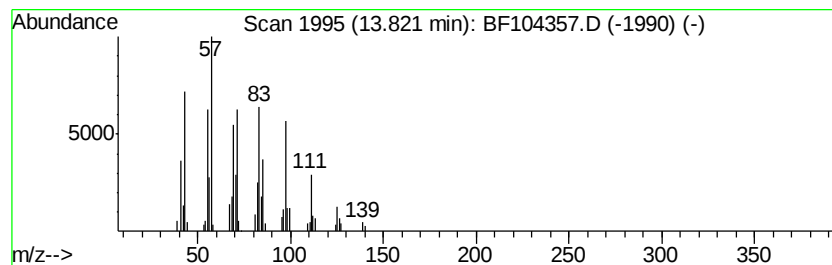
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Peak Number 6 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.82	3.49 ng	132894	Chrysene-d12	13.97	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5	Behenic alcohol	326	C22H46O	000661-19-8	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.00	3.5	ng	145740	1	6.80	827852	20.0
unknown6.57	6.57	49.3	ng	2039910	1	6.80	827852	20.0
Hexadecanoic acid...	12.74	4.0	ng	152180	5	13.97	762059	20.0
Octadecanoic acid...	13.45	2.5	ng	94928	5	13.97	762059	20.0
1-Heptacosanol	13.82	3.5	ng	132894	5	13.97	762059	20.0