

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061416\
 Data File : BF088026.D
 Acq On : 15 Jun 2016 4:48
 Operator : UM/SJ
 Sample : H3425-04
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP16-LF2MW6

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-BF060716.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	1.724	11	12	21	rVB	178883	281188	9.07%	1.390%
2	1.850	21	23	75	rVB	1481925	3098854	100.00%	15.318%
3	4.936	291	293	300	rVB	54449	66887	2.16%	0.331%
4	5.370	329	331	334	rBV	1238769	1107017	35.72%	5.472%
5	6.410	420	422	425	rBV	572241	657196	21.21%	3.249%
6	6.547	431	434	437	rBV	1979334	1819540	58.72%	8.994%
7	6.776	452	454	457	rBV	443317	515993	16.65%	2.551%
8	6.936	466	468	471	rVB	1802499	1760002	56.80%	8.700%
9	7.347	501	504	507	rBV	1347075	1392179	44.93%	6.882%
10	8.067	565	567	570	rBV	841397	696604	22.48%	3.443%
11	9.153	659	662	664	rBV	2718368	2758877	89.03%	13.637%
12	9.828	718	721	723	rBB	564016	664511	21.44%	3.285%
13	10.605	787	789	792	rBV2	861504	1144199	36.92%	5.656%
14	11.302	848	850	853	rBV	671529	560469	18.09%	2.770%
15	12.719	972	974	976	rBV	299691	241338	7.79%	1.193%
16	12.799	976	981	982	rVB	24131	32636	1.05%	0.161%
17	12.891	986	989	992	rBV	2045442	1951239	62.97%	9.645%
18	13.428	1033	1036	1038	rBV	164833	175950	5.68%	0.870%
19	13.474	1038	1040	1043	rVB	20364	33283	1.07%	0.165%
20	13.931	1078	1080	1083	rBV	477195	613884	19.81%	3.034%
21	14.114	1094	1096	1098	rBV	40544	34739	1.12%	0.172%
22	14.708	1146	1148	1151	rBV	32108	41131	1.33%	0.203%
23	15.028	1174	1176	1178	rBV	34311	33991	1.10%	0.168%
24	15.348	1201	1204	1206	rBV	377244	474246	15.30%	2.344%
25	15.382	1206	1207	1211	rVB	34682	36991	1.19%	0.183%
26	15.783	1239	1242	1251	rVB	21265	37603	1.21%	0.186%

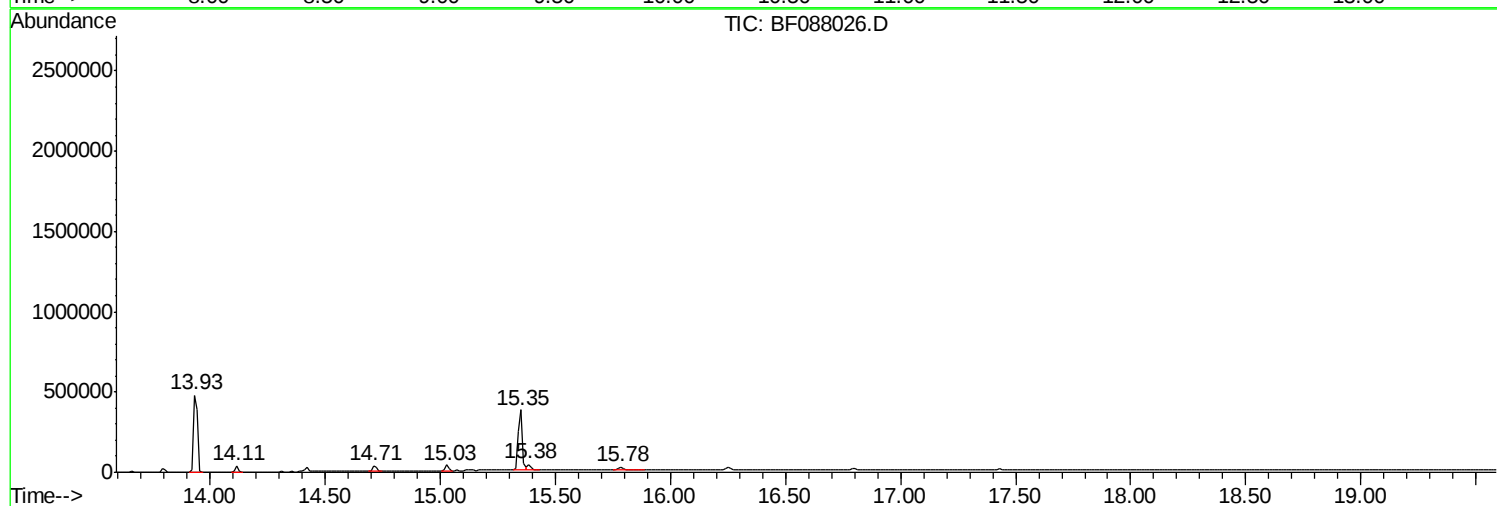
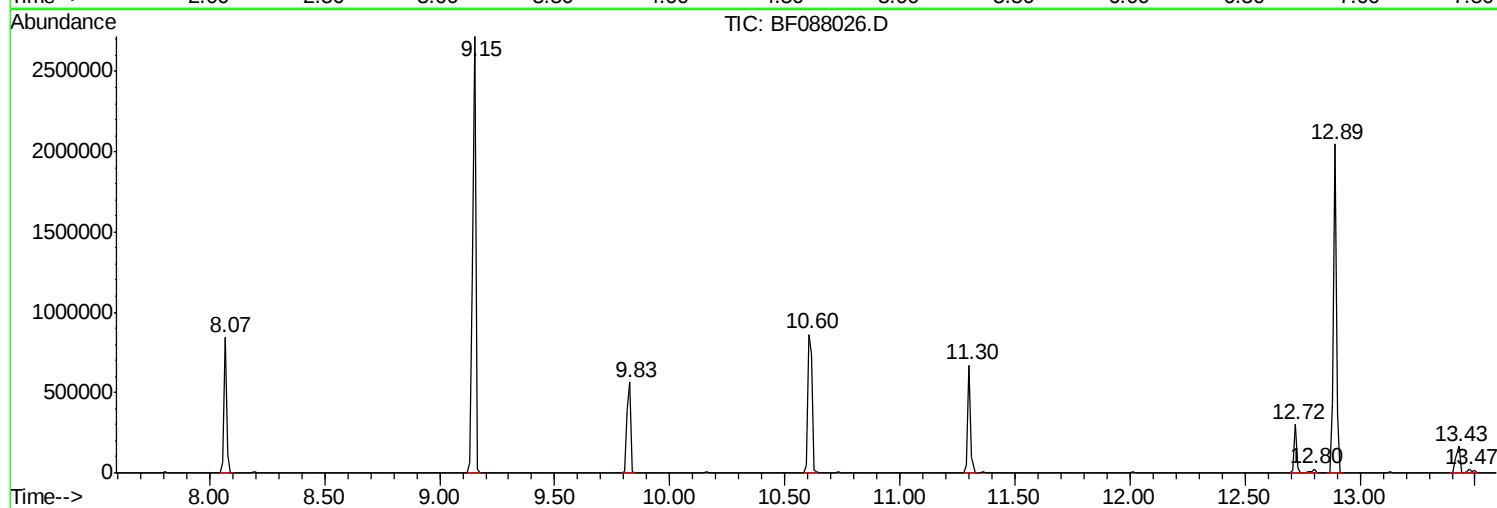
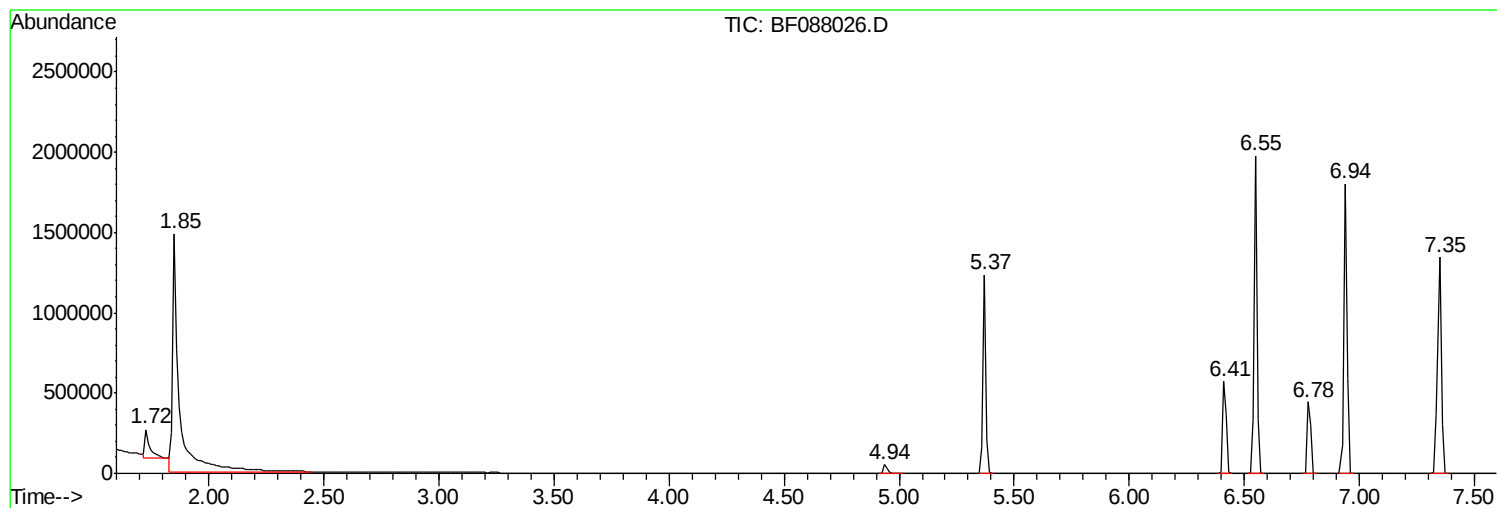
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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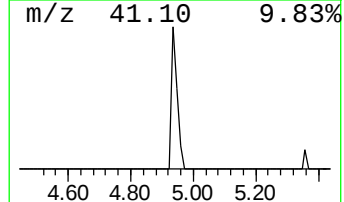
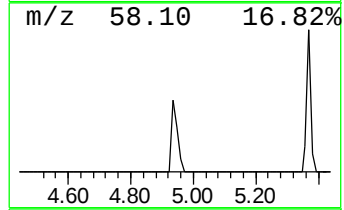
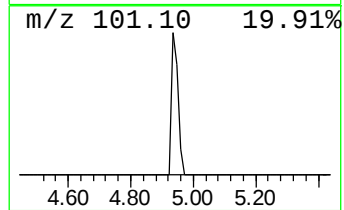
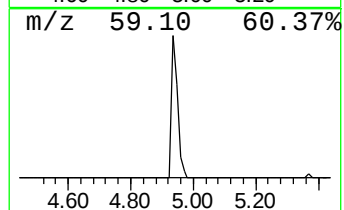
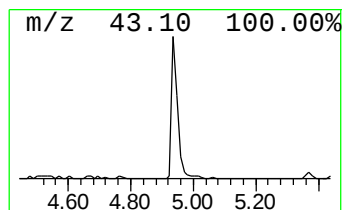
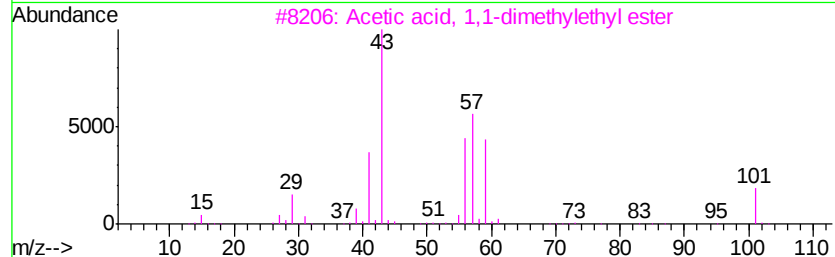
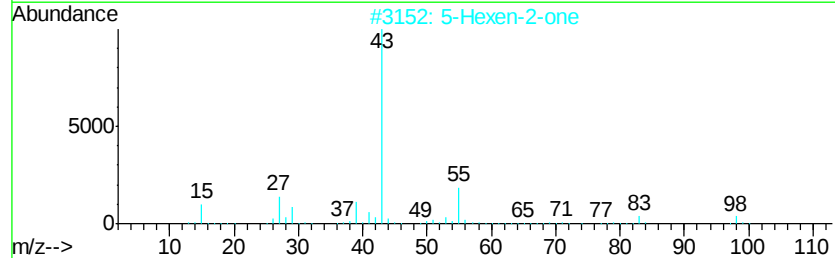
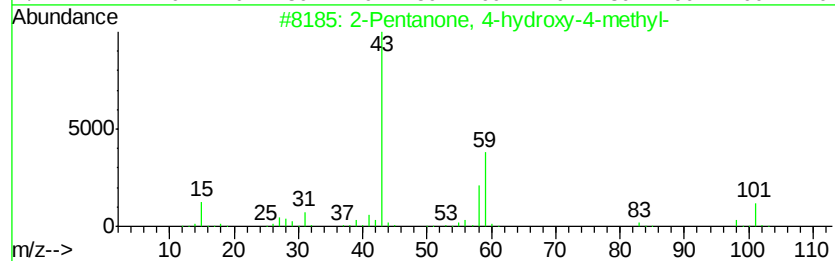
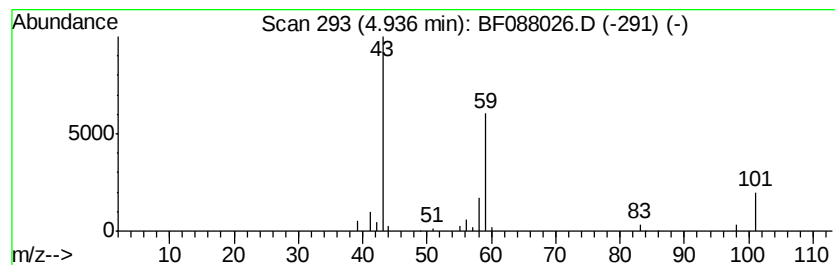
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TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	2.59 ng	66887	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2		5-Hexen-2-one	98	C6H10O	000109-49-9	10
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9



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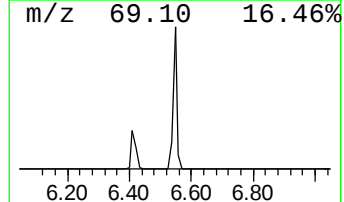
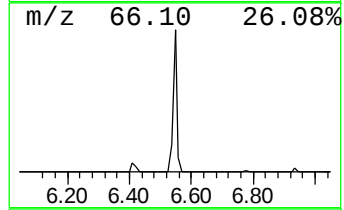
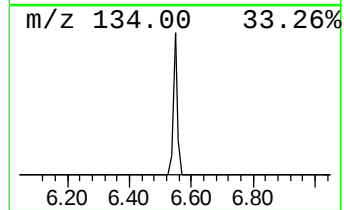
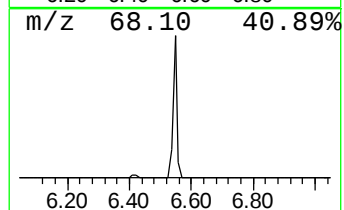
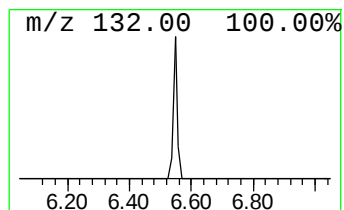
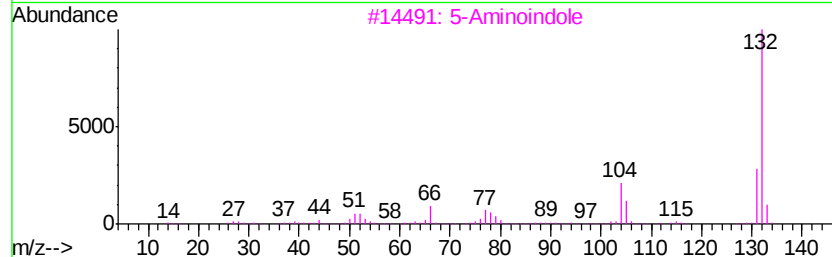
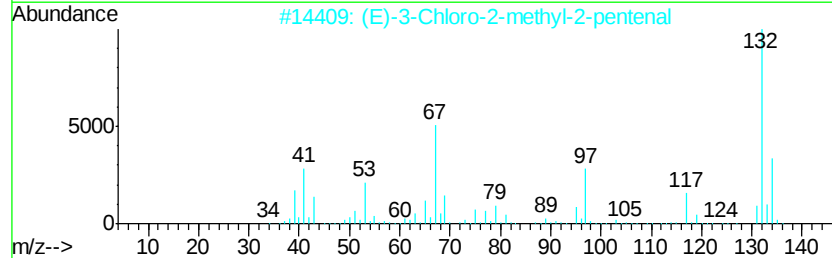
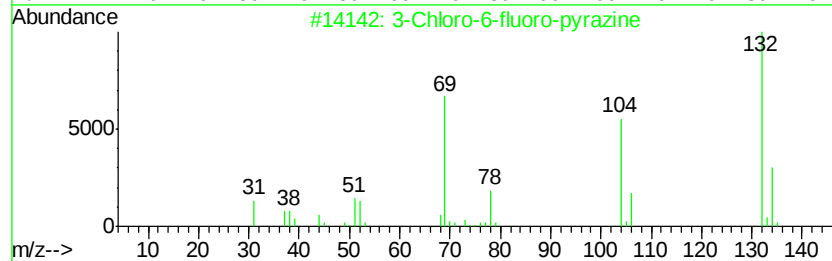
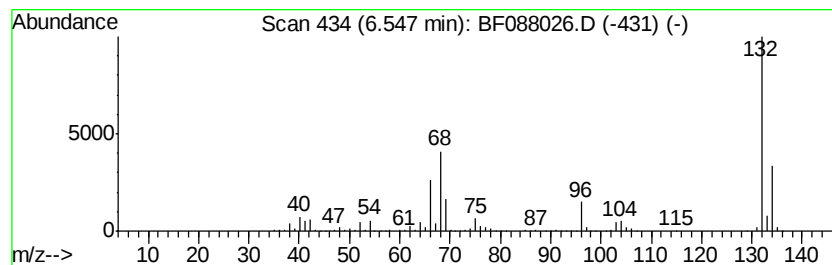
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Peak Number 4 unknown6.55 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	70.53 ng	1819540	1,4-Dichlorobenzene-d4	6.78

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		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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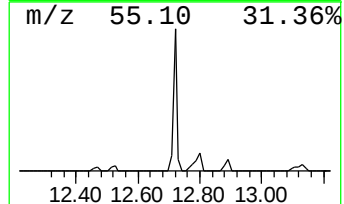
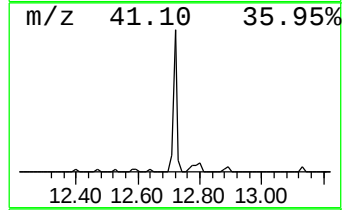
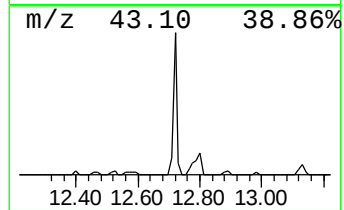
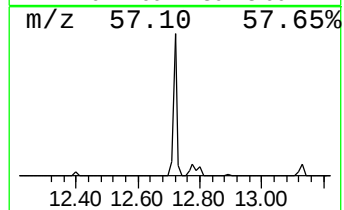
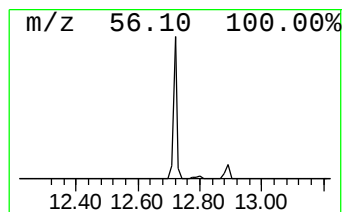
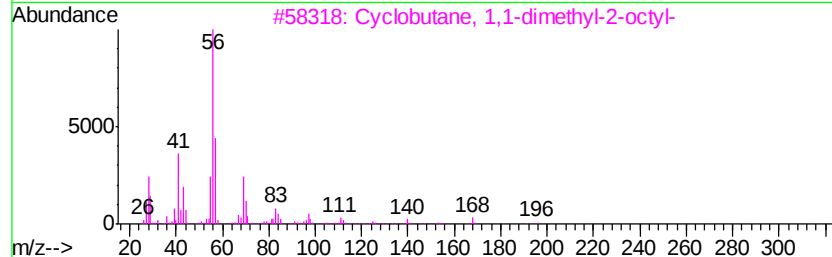
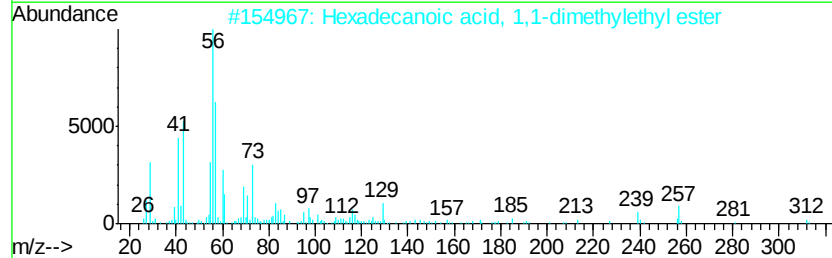
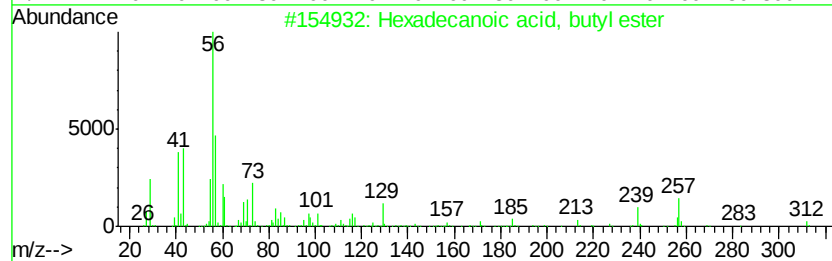
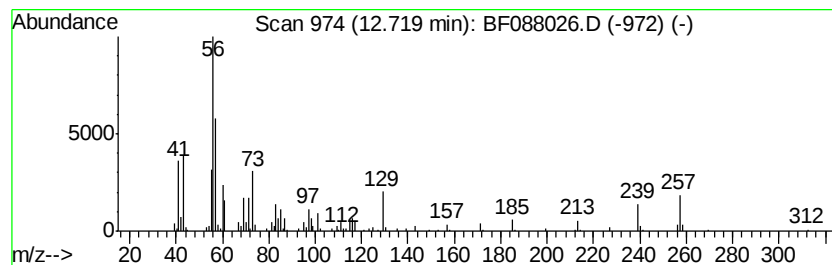
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Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	7.86 ng	241338	Chrysene-d12	13.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	92
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	83
3		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
4		Trifluoroacetic acid, 4-methylpe...	198	C8H13F3O2	000327-71-9	32
5		Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32



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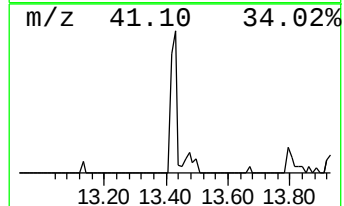
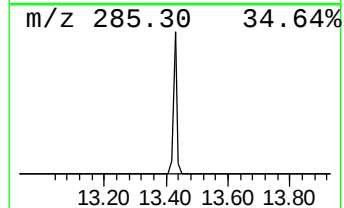
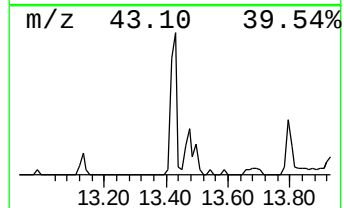
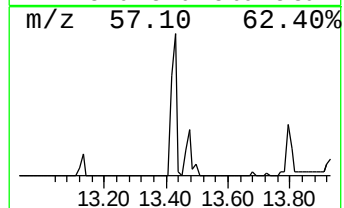
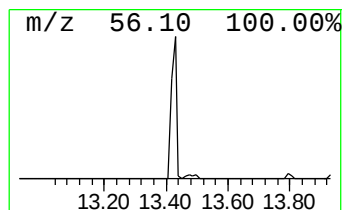
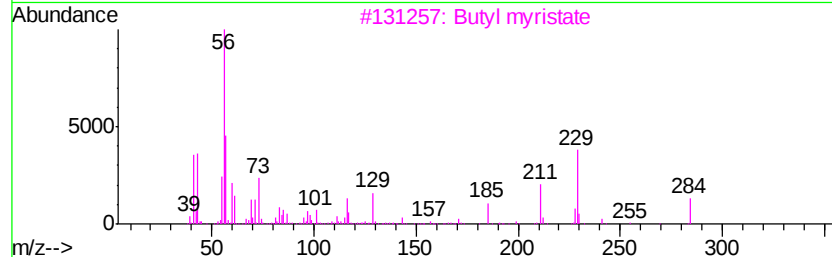
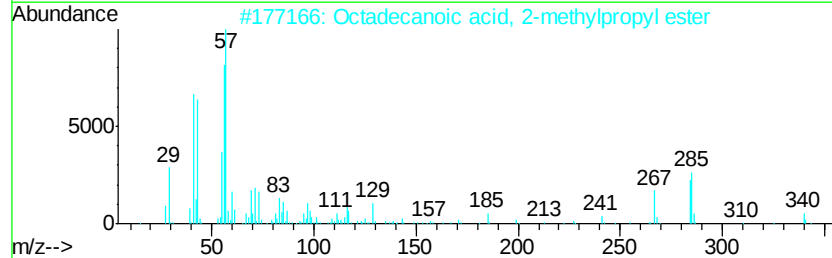
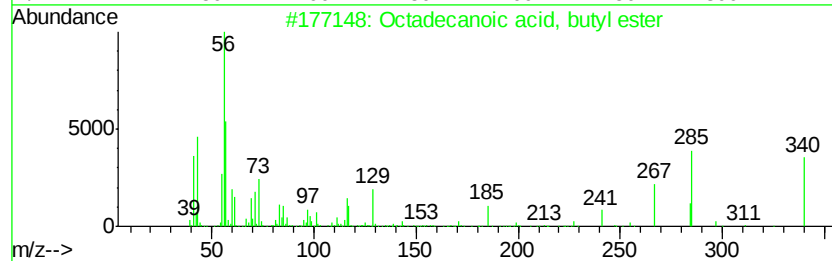
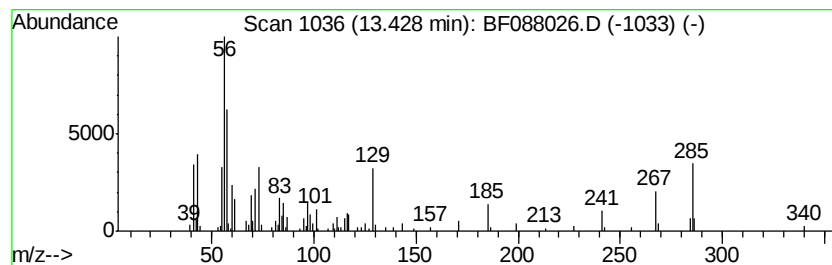
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Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.43	5.73 ng	175950	Chrysene-d12	13.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	93
2		Octadecanoic acid, 2-methylpropyl...	340	C22H44O2	000646-13-9	83
3		Butyl myristate	284	C18H36O2	000110-36-1	47
4		Nipecotic acid	129	C6H11NO2	000498-95-3	43
5		1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.94	2.6	ng	66887	1	6.78	515993	20.0
unknown6.55	6.55	70.5	ng	1819540	1	6.78	515993	20.0
Hexadecanoic acid...	12.72	7.9	ng	241338	5	13.94	613884	20.0
Octadecanoic acid...	13.43	5.7	ng	175950	5	13.94	613884	20.0