

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102416\
 Data File : BF090790.D
 Acq On : 24 Oct 2016 16:32
 Operator : UM/SJ
 Sample : PB94262BL
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB94262BL

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-BF102116.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	5.023	233	235	247	rBV	576727	902165	16.04%	2.085%
2	5.446	269	272	274	rBV	3733903	3863022	68.68%	8.929%
3	6.474	359	362	364	rBV	3307782	4081072	72.55%	9.432%
4	6.600	371	373	376	rBV	3962575	4003941	71.18%	9.254%
5	6.829	391	393	404	rBV	1049415	1264580	22.48%	2.923%
6	6.989	404	407	409	rBV	3451075	3389741	60.26%	7.835%
7	7.400	440	443	445	rBV	1811953	2368264	42.10%	5.474%
8	8.120	503	506	508	rBV	1494520	1715485	30.50%	3.965%
9	9.195	597	600	603	rBV	4360489	4970133	88.36%	11.487%
10	9.869	656	659	662	rBV	1931025	2022959	35.96%	4.676%
11	10.658	725	728	731	rBV2	2152367	3157743	56.14%	7.298%
12	11.355	787	789	792	rBV	1877794	1901758	33.81%	4.395%
13	11.515	801	803	810	rVB	140948	142375	2.53%	0.329%
14	12.772	911	913	915	rBV	436203	356024	6.33%	0.823%
15	12.852	915	920	922	rVB2	57268	75550	1.34%	0.175%
16	12.944	926	928	931	rBV	4261395	5625026	100.00%	13.001%
17	13.481	973	975	977	rBV	221930	221464	3.94%	0.512%
18	13.995	1018	1020	1033	rBV	1851893	1871188	33.27%	4.325%
19	15.424	1142	1145	1148	rBV	1084043	1333639	23.71%	3.082%

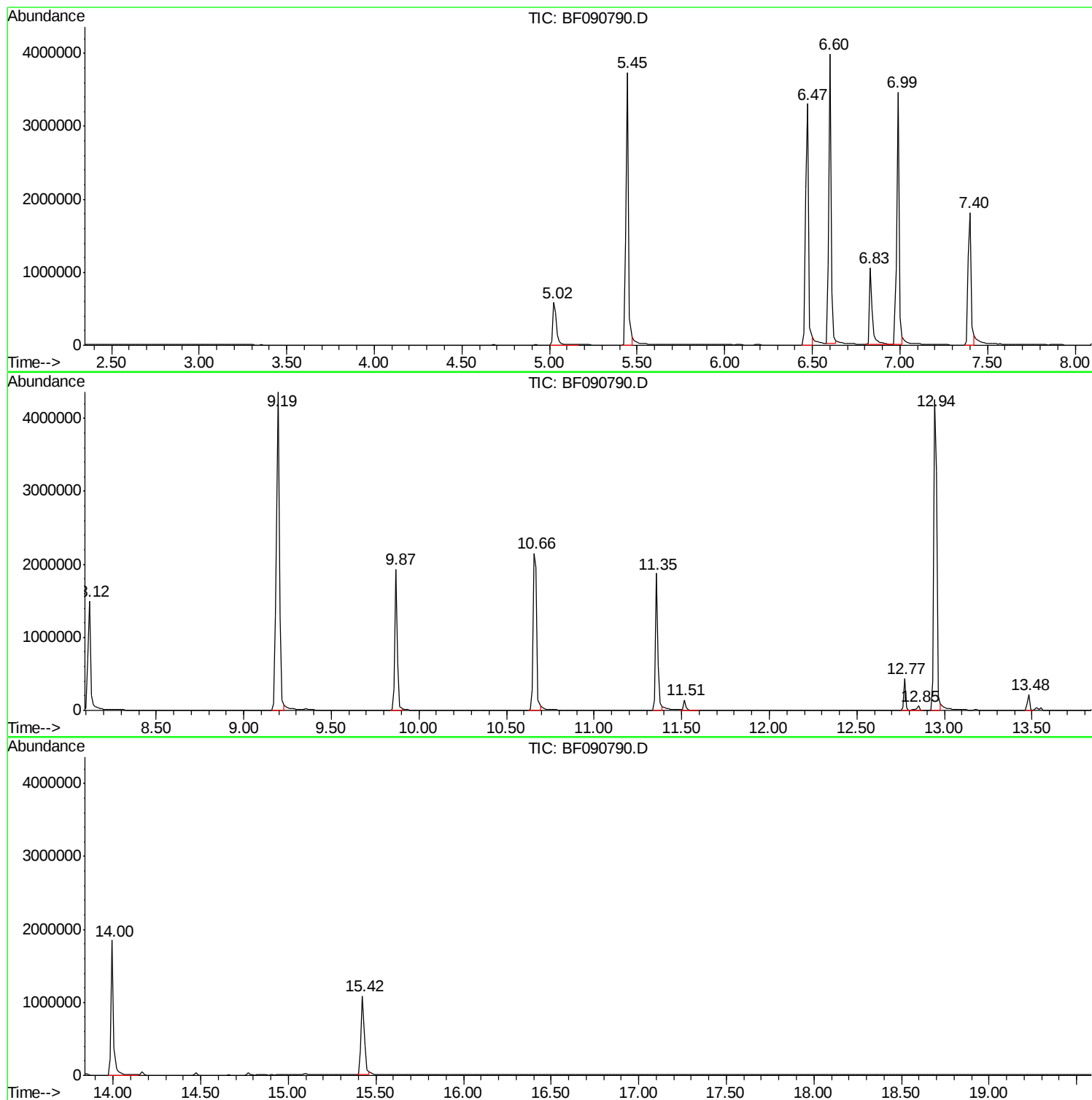
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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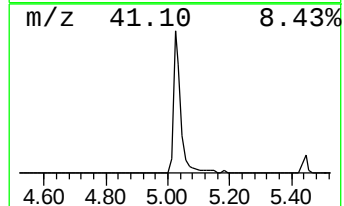
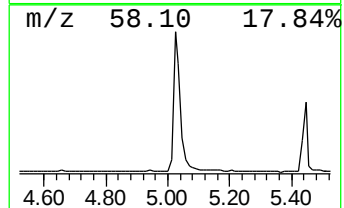
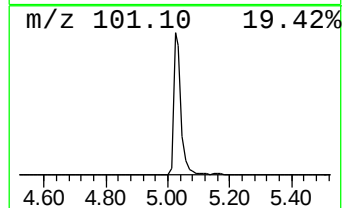
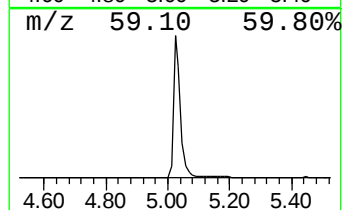
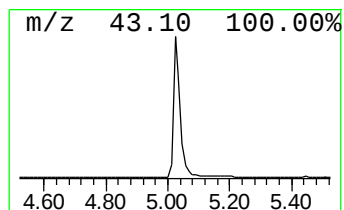
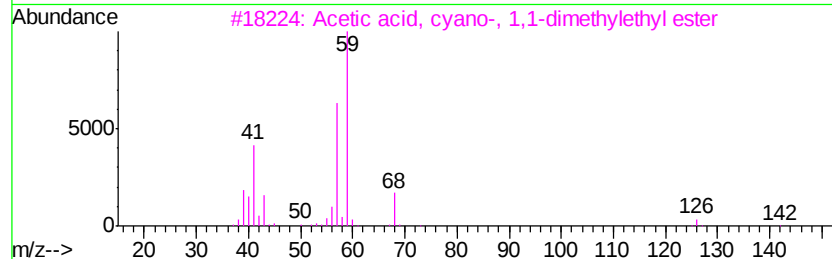
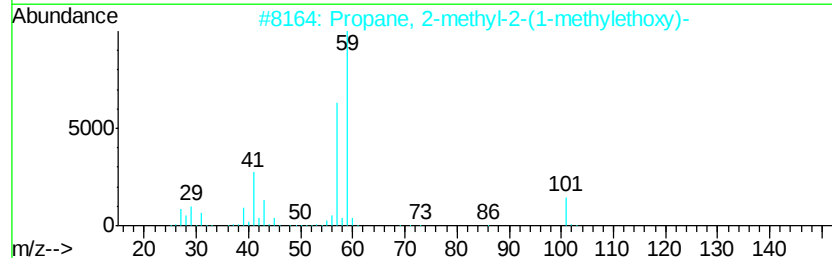
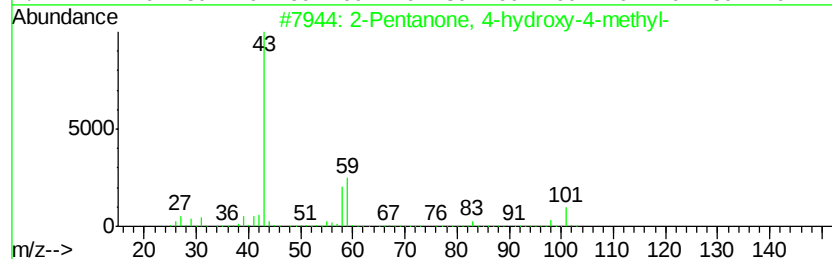
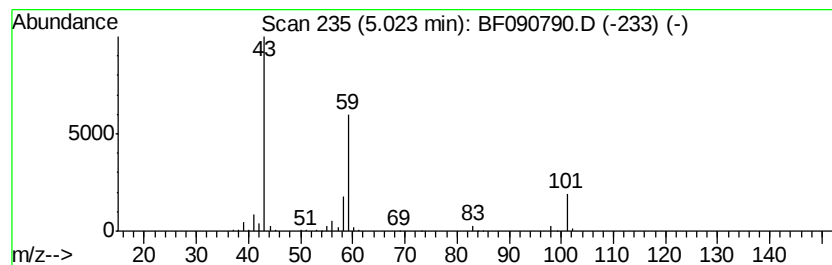
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	14.27 ng	902165	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	28
3		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	23
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Acetone	58	C3H6O	000067-64-1	9



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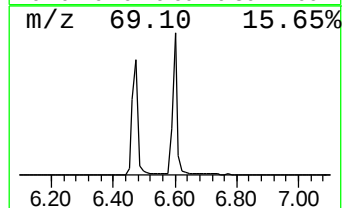
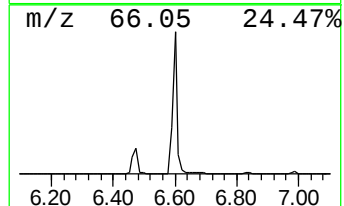
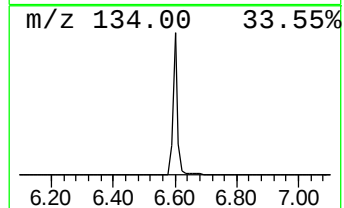
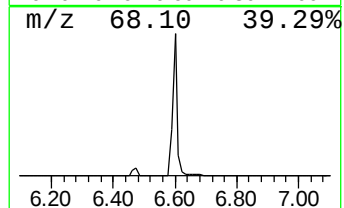
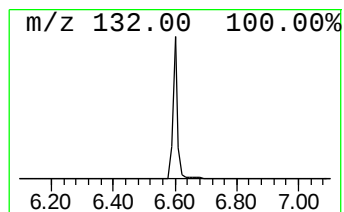
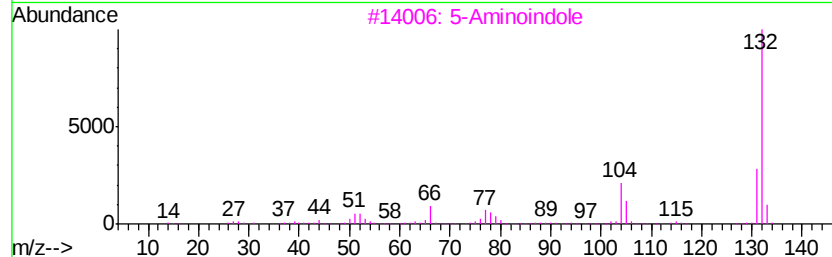
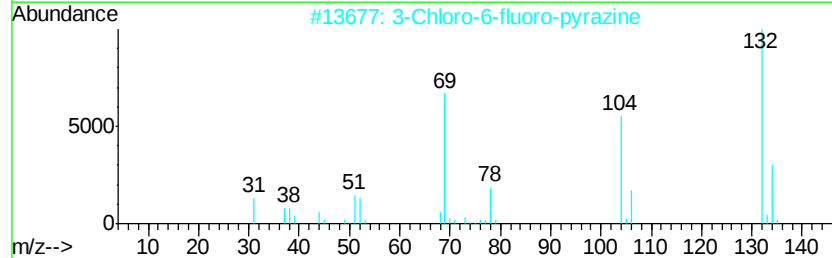
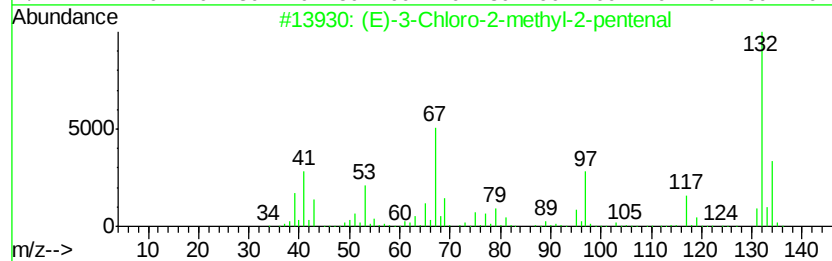
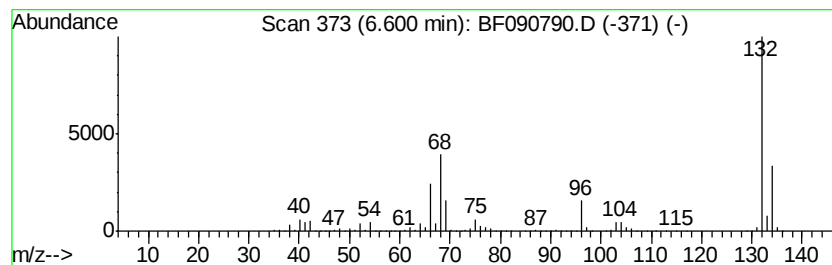
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Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	63.32 ng	4003940	1,4-Dichlorobenzene-d4	6.83

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



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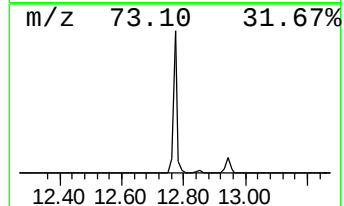
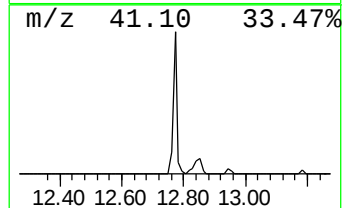
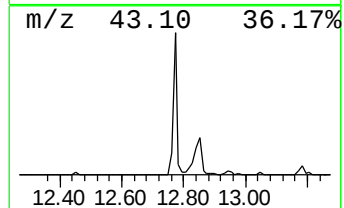
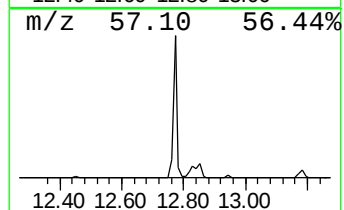
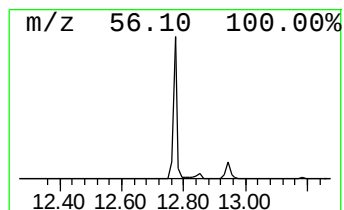
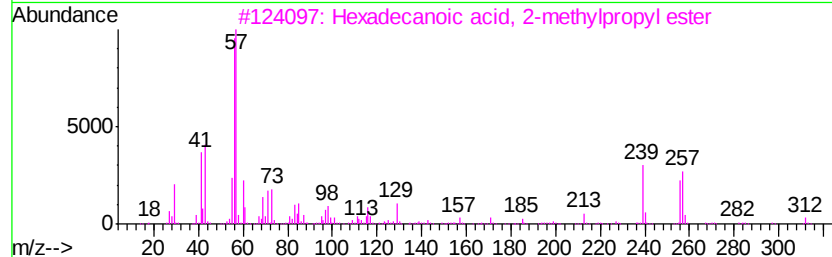
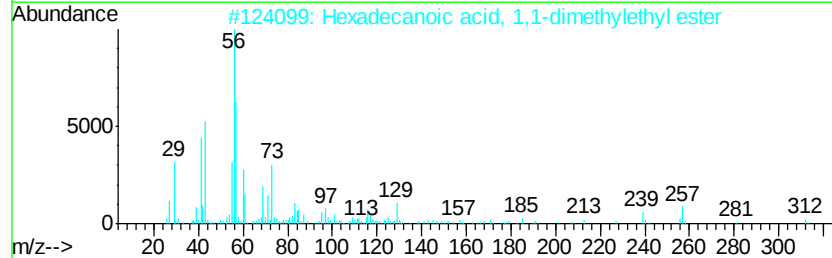
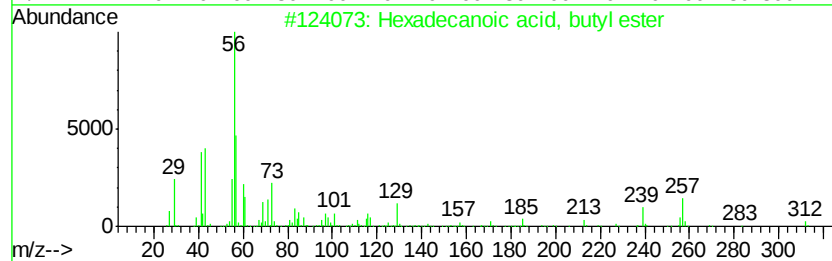
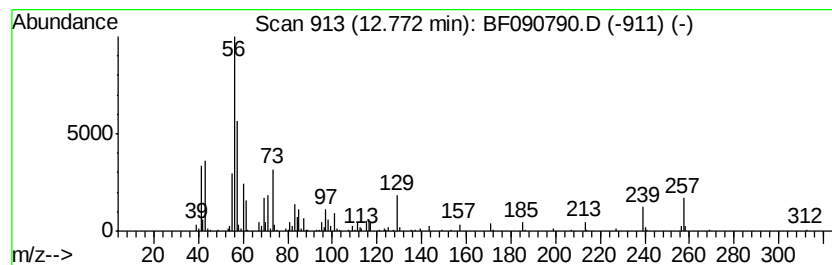
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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	3.81 ng	356024	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	95
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	87
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	35
4		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5		Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32



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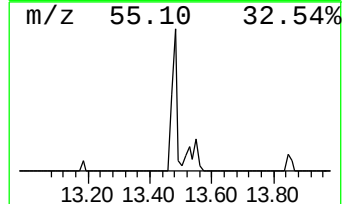
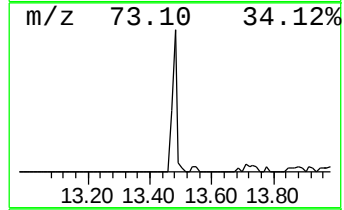
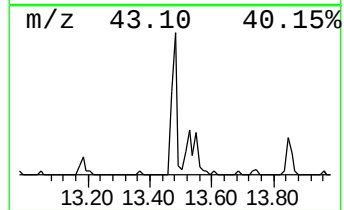
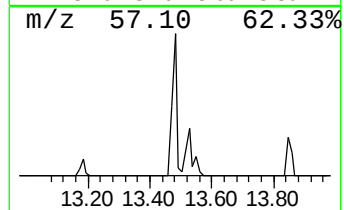
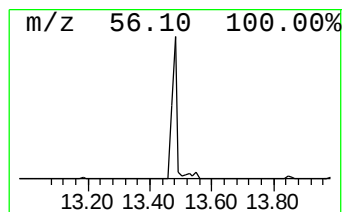
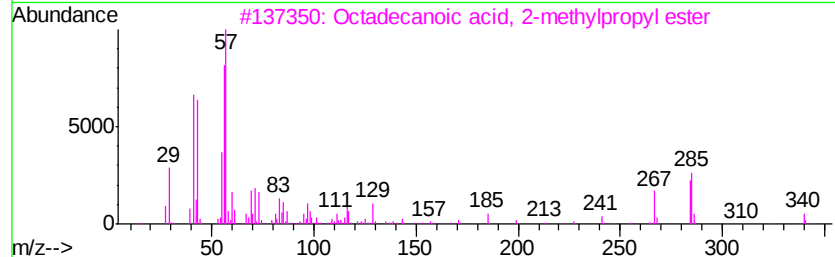
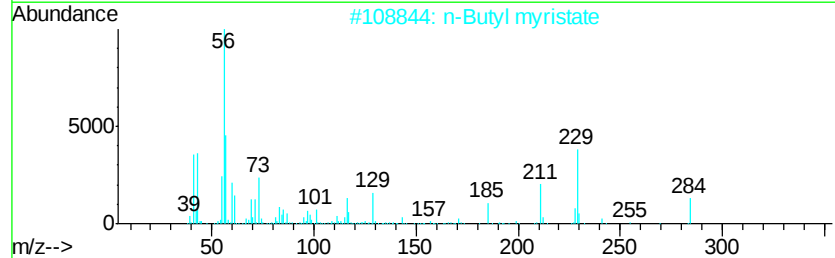
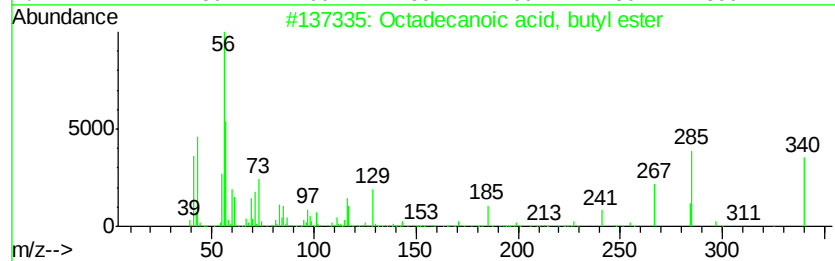
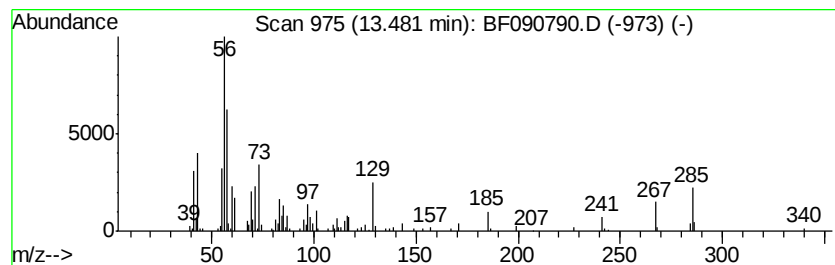
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Peak Number 5 Octadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	2.37 ng	221464	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	94
2		n-Butyl myristate	284	C18H36O2	000110-36-1	64
3		Octadecanoic acid, 2-methylpropyl ester	340	C22H44O2	000646-13-9	58
4		Nipecotic acid	129	C6H11NO2	000498-95-3	50
5		Cyclohexane, (1,1-dimethylethyl)-	140	C10H20	003178-22-1	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.02	14.3	ng	902165	1	6.83	1264580	20.0
unknown6.60	6.60	63.3	ng	4003940	1	6.83	1264580	20.0
Hexadecanoic acid...	12.77	3.8	ng	356024	5	14.00	1871190	20.0
Octadecanoic acid...	13.48	2.4	ng	221464	5	14.00	1871190	20.0