

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051416\
 Data File : BF087031.D
 Acq On : 14 May 2016 20:38
 Operator : UM/SJ
 Sample : PB90490BL
 Misc :
 ALS Vial : 53 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB90490BL

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-BF050916.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	1.735	11	13	45	rVB	1753464	3323869	75.70%	8.661%
2	4.764	276	278	289	rBV	113654	246939	5.62%	0.643%
3	5.210	314	317	336	rBV	3653474	3928376	89.47%	10.236%
4	6.273	408	410	413	rBV	2656017	3852142	87.73%	10.037%
5	6.387	417	420	422	rBV	3661964	4028604	91.75%	10.497%
6	6.604	437	439	442	rBV	738413	937271	21.35%	2.442%
7	6.764	450	453	456	rBV	3180659	2899410	66.03%	7.555%
8	7.187	487	490	492	rBV	2294374	2692480	61.32%	7.016%
9	7.896	550	552	565	rBV	1232815	1241707	28.28%	3.235%
10	8.982	643	647	649	rBV	3643502	4390957	100.00%	11.441%
11	9.645	702	705	708	rBV	1416198	1345918	30.65%	3.507%
12	10.433	771	774	777	rBV	2387367	2386737	54.36%	6.219%
13	11.119	832	834	837	rBV	1182545	1280860	29.17%	3.337%
14	12.548	956	959	961	rBV	135156	161018	3.67%	0.420%
15	12.708	970	973	976	rBV	3671622	3741410	85.21%	9.749%
16	13.245	1018	1020	1022	rBV	125438	103425	2.36%	0.269%
17	13.748	1062	1064	1073	rBV	1029141	983589	22.40%	2.563%
18	15.108	1180	1183	1194	rBV	650363	833204	18.98%	2.171%

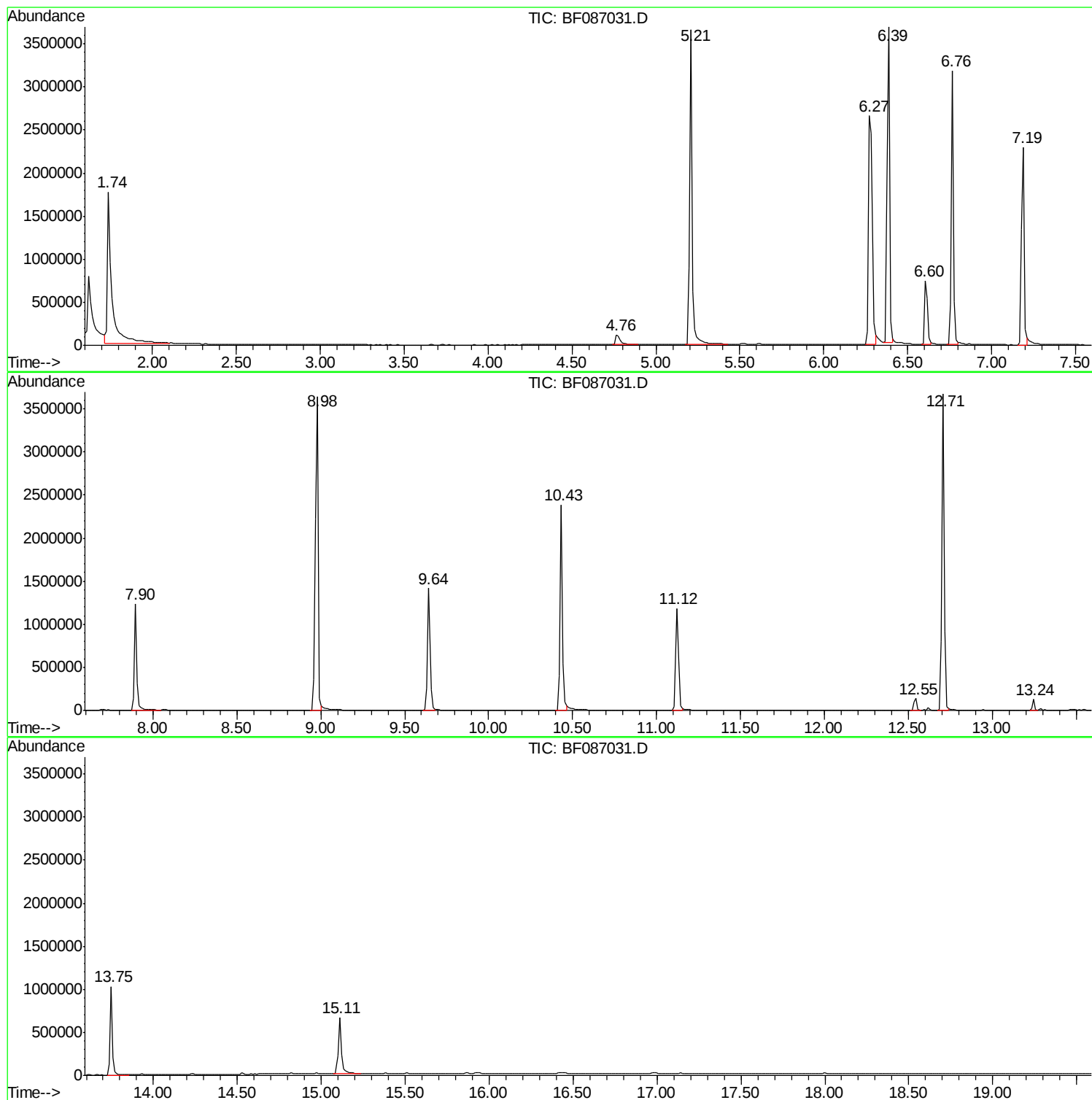
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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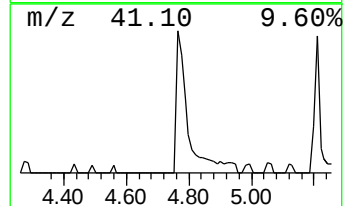
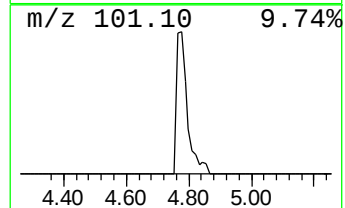
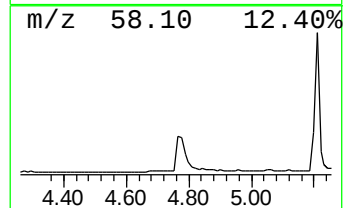
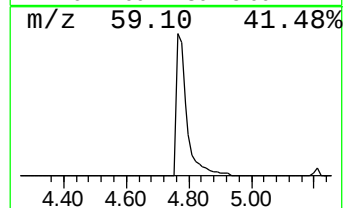
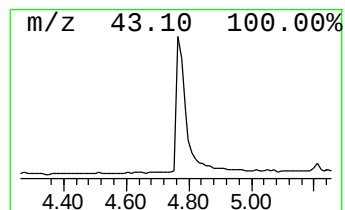
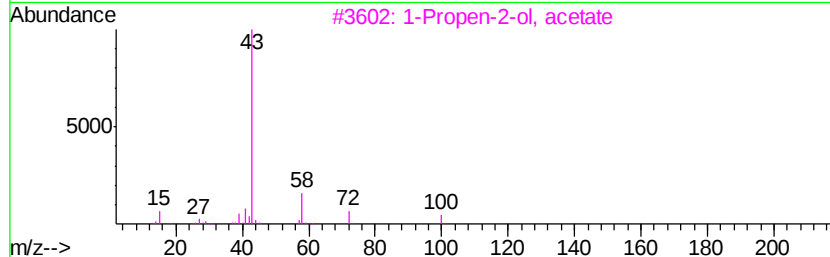
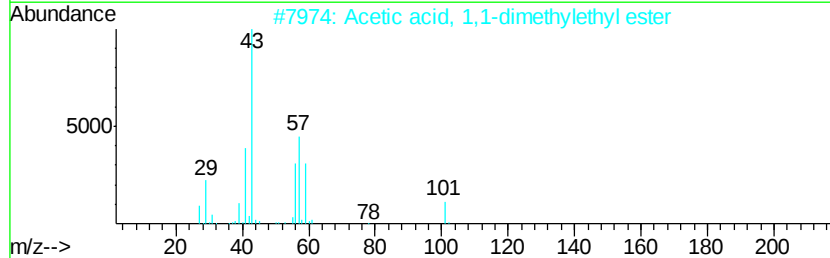
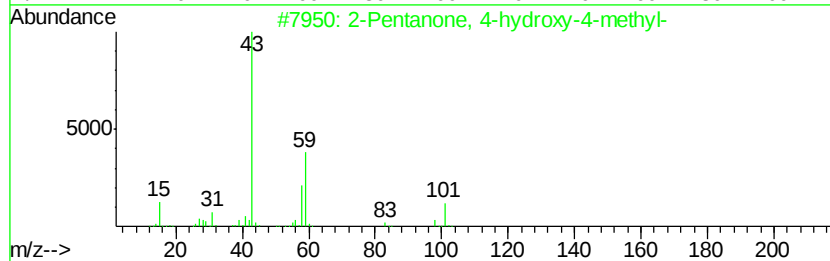
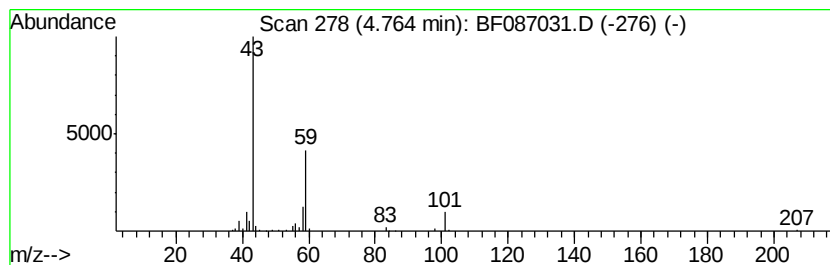
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.76	5.27 ng	246939	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		Diacetamide	101	C4H7NO2	000625-77-4	9
5		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9



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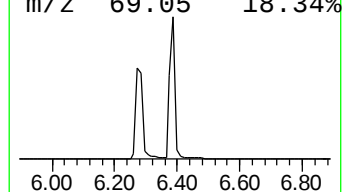
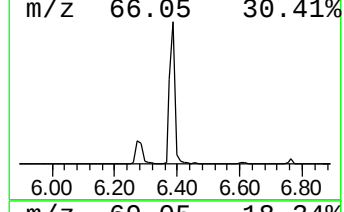
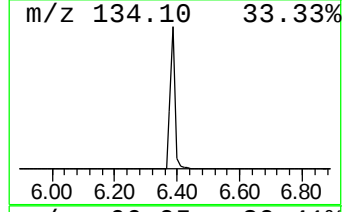
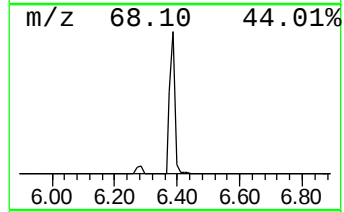
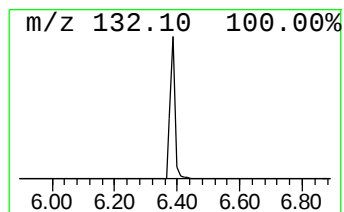
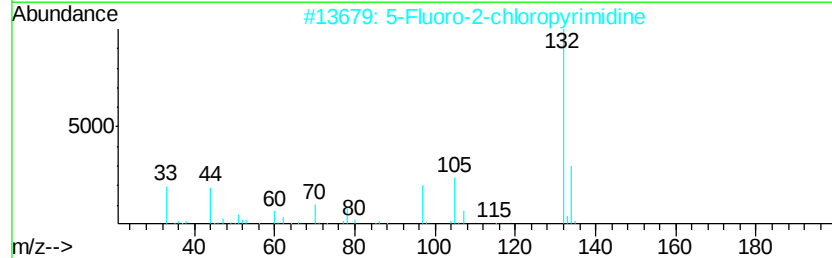
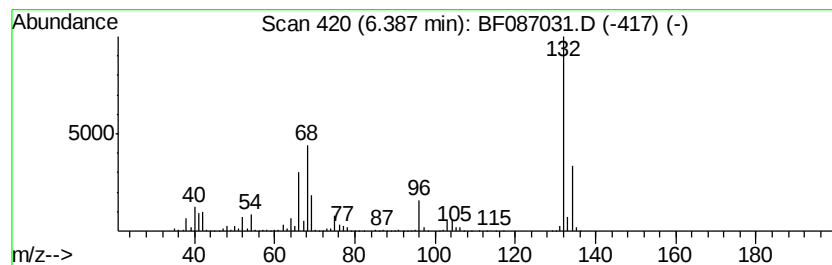
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.39 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.39	85.96 ng	4028600	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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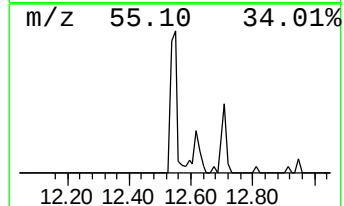
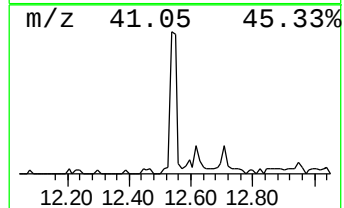
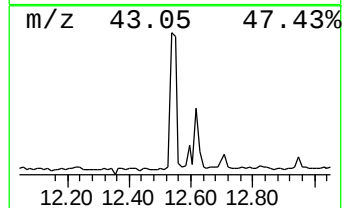
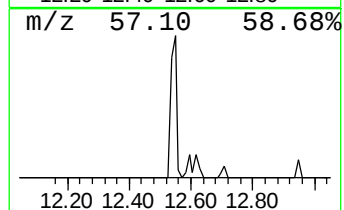
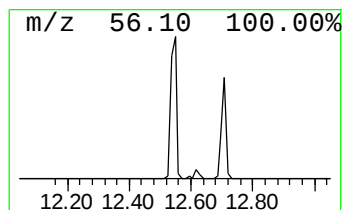
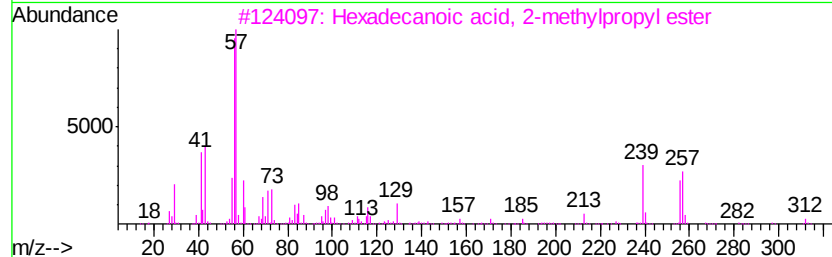
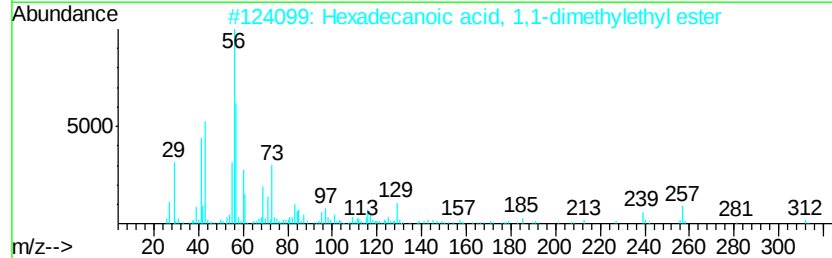
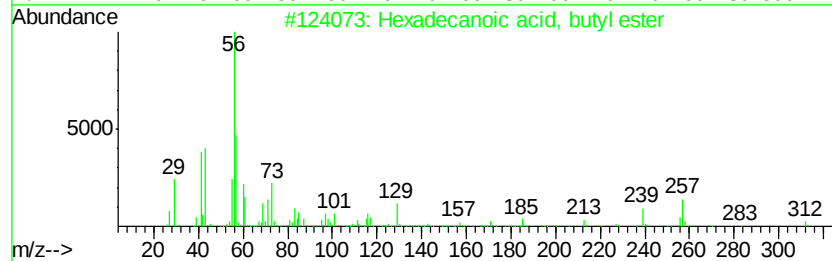
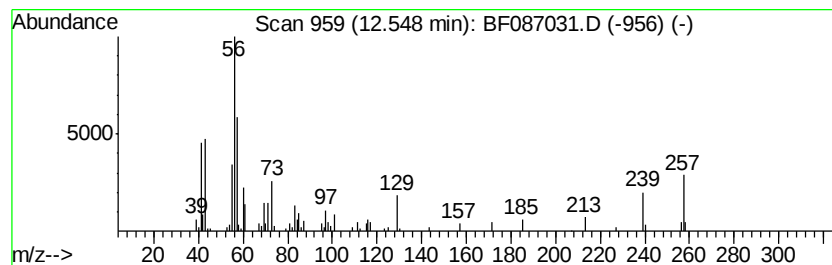
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.55	3.27 ng	161018	Chrysene-d12	13.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	83
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	74
3		Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	72
4		2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	37
5		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27



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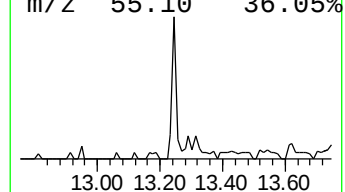
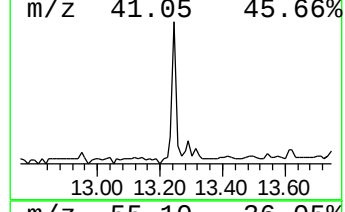
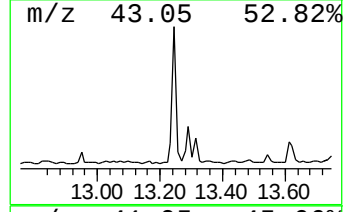
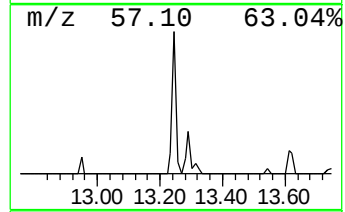
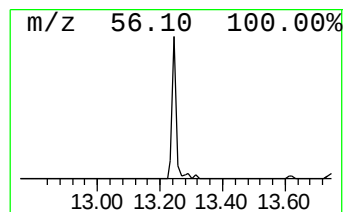
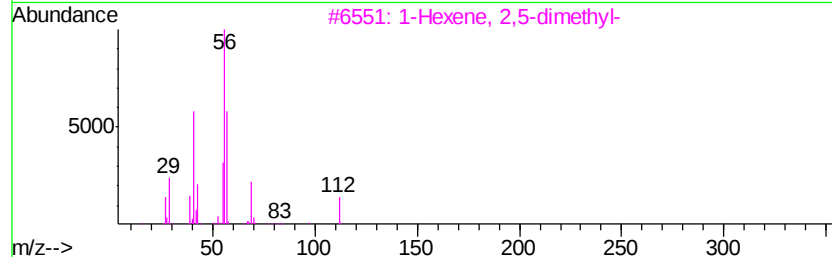
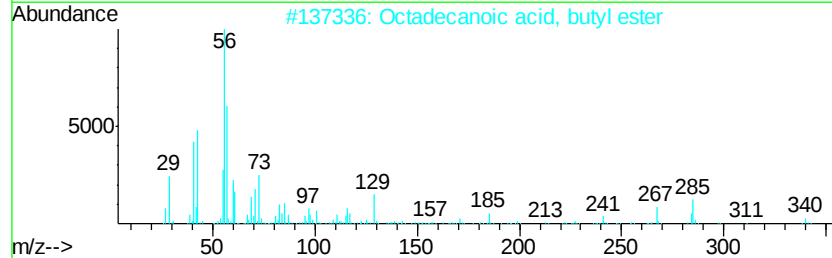
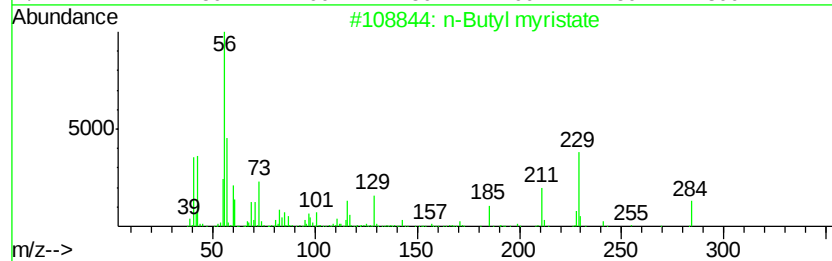
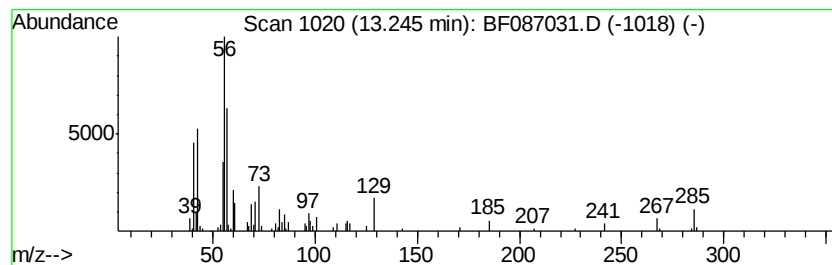
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Peak Number 6 n-Butyl myristate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.25	2.10 ng	103425	Chrysene-d12	13.75		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Butyl myristate	284	C18H36O2	000110-36-1	86	
2	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	76	
3	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35	
4	Octadecanoic acid	284	C18H36O2	000057-11-4	35	
5	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	35	



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.76	5.3	ng	246939	1	6.60	937271	20.0
unknown6.39	6.39	86.0	ng	4028600	1	6.60	937271	20.0
Hexadecanoic acid...	12.55	3.3	ng	161018	5	13.75	983589	20.0
n-Butyl myristate	13.25	2.1	ng	103425	5	13.75	983589	20.0