

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
 Data File : BF089266.D
 Acq On : 24 Jul 2016 8:05
 Operator : UM/SJ
 Sample : H4152-11
 Misc :
 ALS Vial : 64 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-16-14.0-15.0

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-BF072016.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	1.713	10	11	37	rVB	430538	826349	47.13%	6.125%
2	4.707	271	273	282	rVB	43137	79912	4.56%	0.592%
3	5.164	310	313	337	rBV	1102648	1534144	87.50%	11.370%
4	6.239	405	407	414	rBV	1208649	1534817	87.54%	11.375%
5	6.353	414	417	419	rBV	1117757	1495790	85.31%	11.086%
6	6.582	435	437	448	rBV	196966	246169	14.04%	1.824%
7	6.730	448	450	453	rBV	1038008	1080457	61.62%	8.008%
8	7.153	484	487	503	rBV	836608	1044894	59.60%	7.744%
9	7.862	547	549	560	rBV	378298	376274	21.46%	2.789%
10	8.948	641	644	646	rBV	1568581	1753279	100.00%	12.994%
11	9.336	676	678	681	rBV	220952	317743	18.12%	2.355%
12	9.610	700	702	704	rBV	373928	376658	21.48%	2.792%
13	10.399	768	771	773	rBV	625418	832506	47.48%	6.170%
14	10.525	781	782	788	rVB	15465	20675	1.18%	0.153%
15	11.085	829	831	835	rBV	248368	329210	18.78%	2.440%
16	12.502	954	955	958	rBV	54836	59141	3.37%	0.438%
17	12.662	967	969	972	rBV	974195	1009408	57.57%	7.481%
18	13.211	1015	1017	1018	rBV	28312	29354	1.67%	0.218%
19	13.577	1045	1049	1055	rBV	24905	41999	2.40%	0.311%
20	13.702	1057	1060	1067	rBV	240627	257809	14.70%	1.911%
21	15.051	1175	1178	1181	rBV	144629	227668	12.99%	1.687%
22	16.903	1335	1340	1346	rBV5	5019	18251	1.04%	0.135%

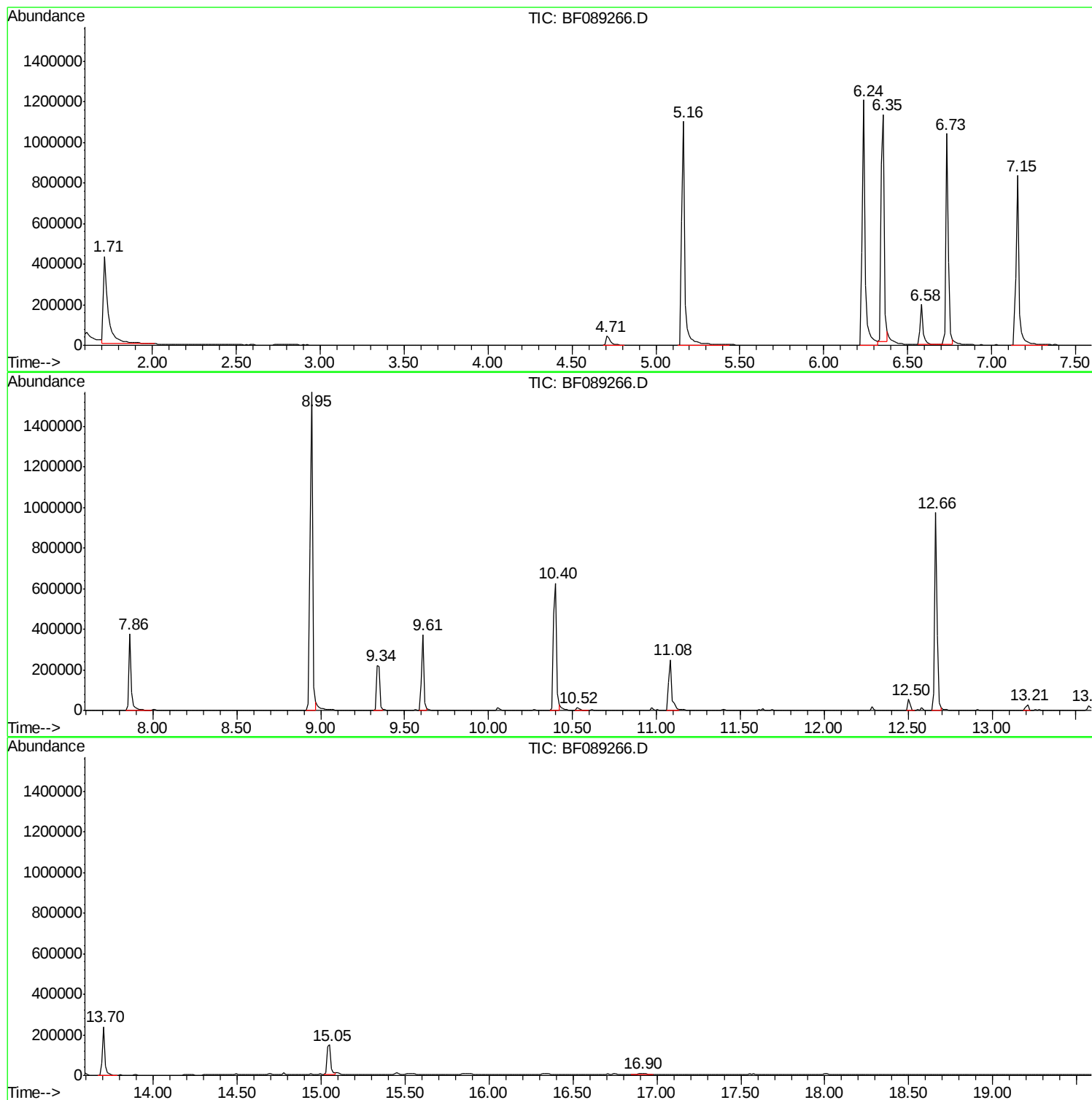
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SB-16-14.0-15.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.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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Instrument :
BNA_F
ClientSampled :
SB-16-14.0-15.0

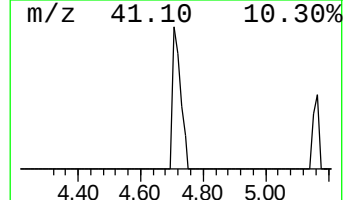
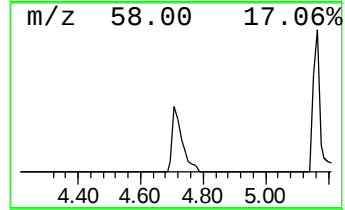
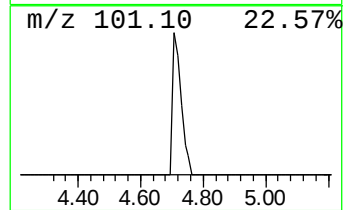
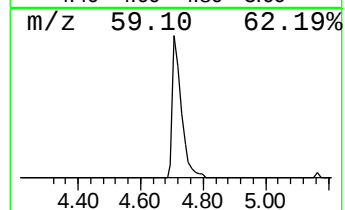
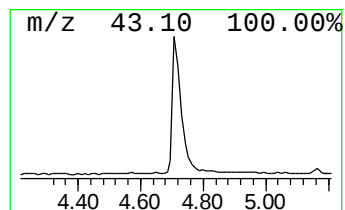
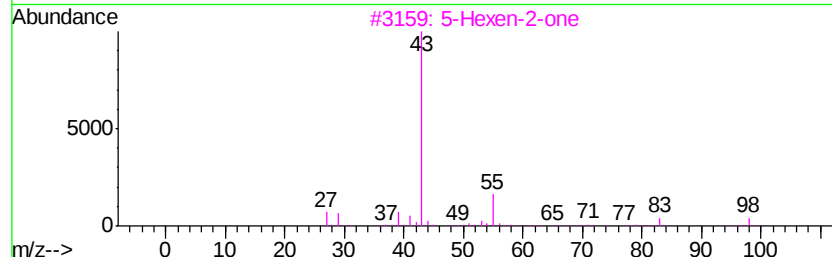
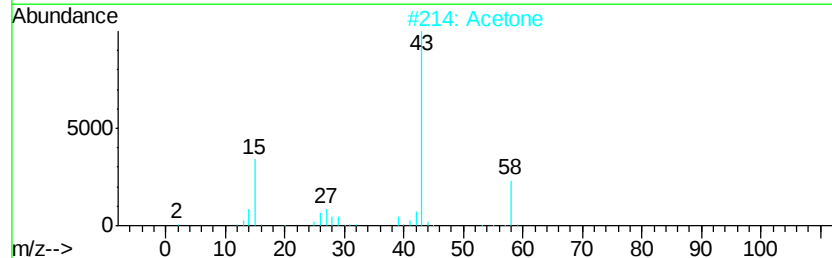
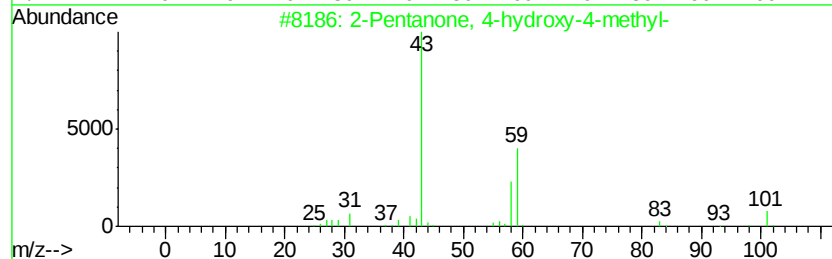
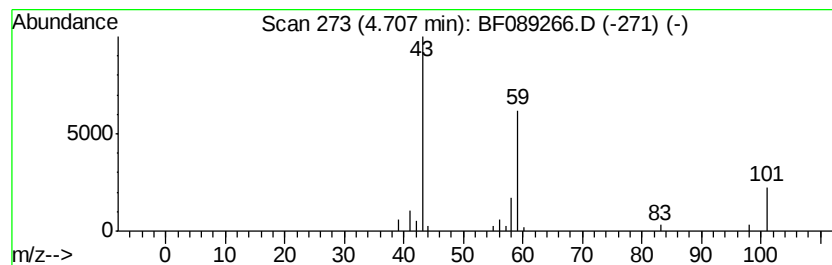
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.71	6.49 ng	79912	1,4-Dichlorobenzene-d4	6.58

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetone	58	C3H6O	000067-64-1	9
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



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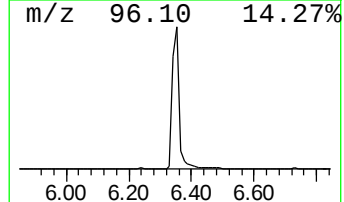
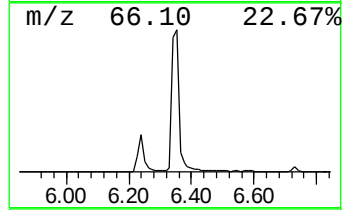
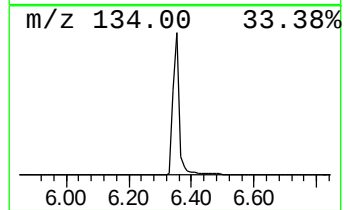
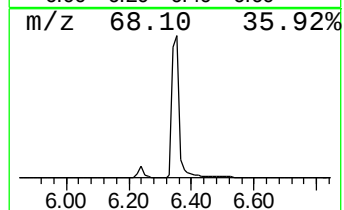
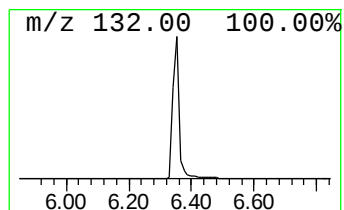
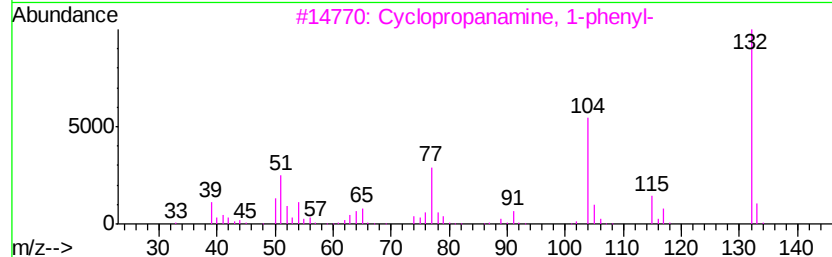
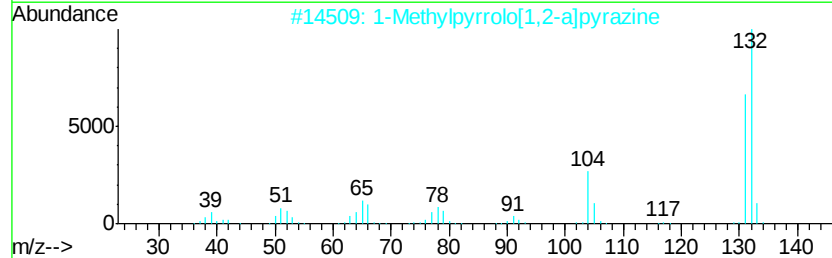
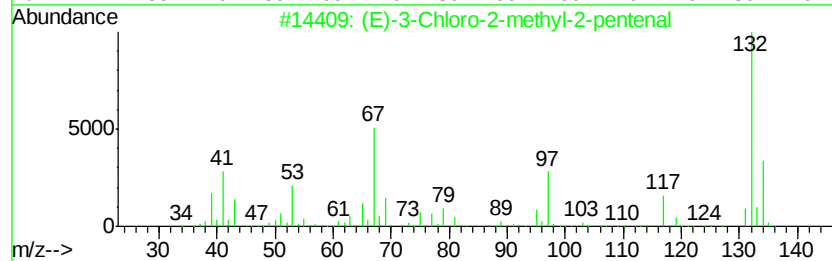
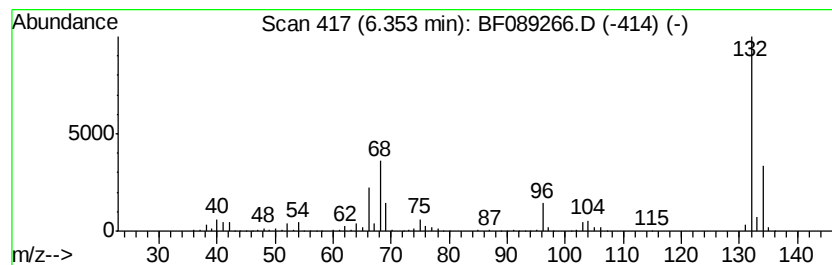
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TIC Library : C:\Database\NIST11.L
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Peak Number 3 unknown6.35 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	121.53 ng	1495790	1,4-Dichlorobenzene-d4	6.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
3		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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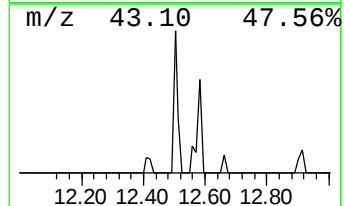
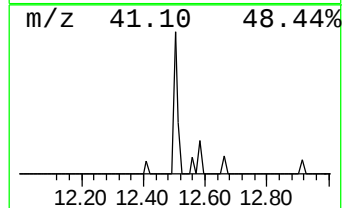
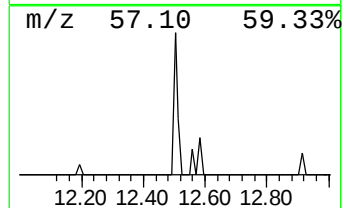
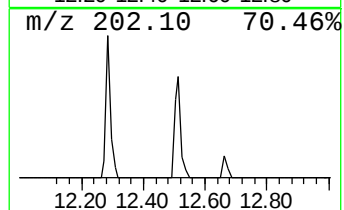
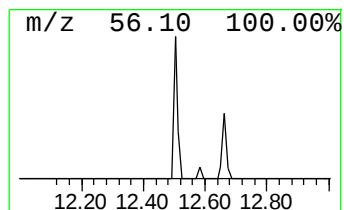
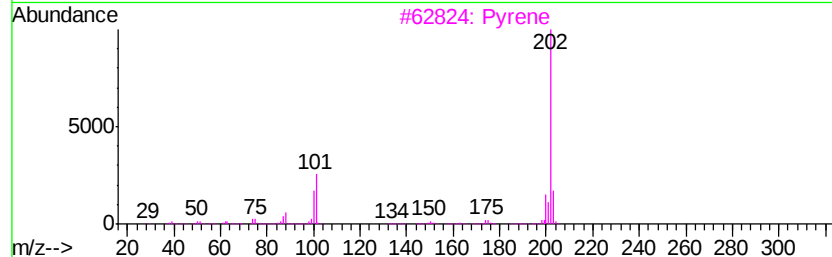
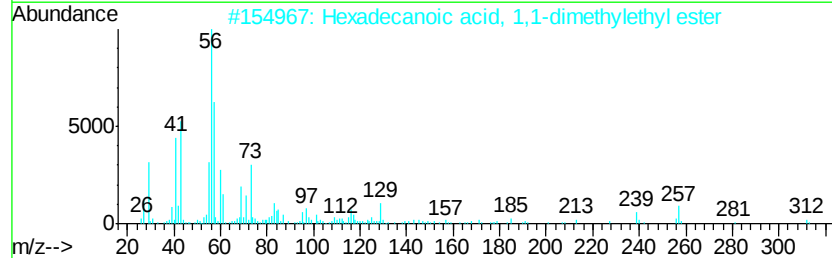
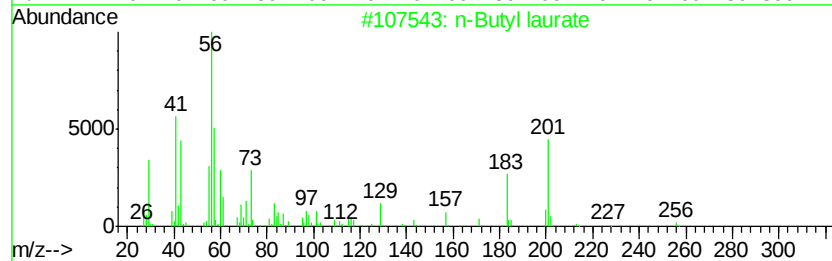
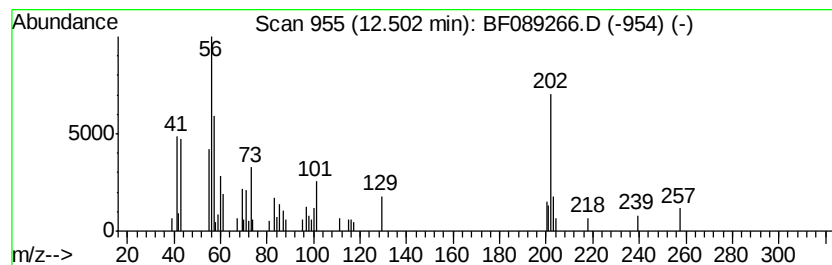
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Peak Number 5 n-Butyl laurate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.50	4.59 ng	59141	Chrysene-d12	13.70
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	n-Butyl laurate	256 C16H32O2	000106-18-3	50
2	Hexadecanoic acid, 1,1-dimethyle...	312 C20H40O2	031158-91-5	49
3	Pyrene	202 C16H10	000129-00-0	18
4	1-Pentene, 2,4-dimethyl-	98 C7H14	002213-32-3	14
5	Benzene, 1,1'-(1,3-butadiyne-1,4...	202 C16H10	000886-66-8	14



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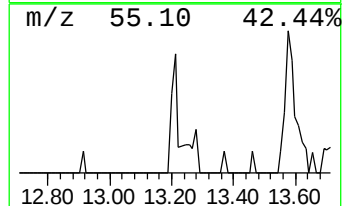
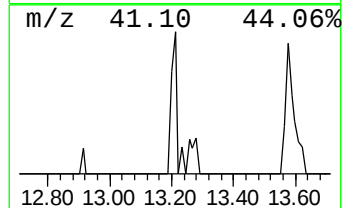
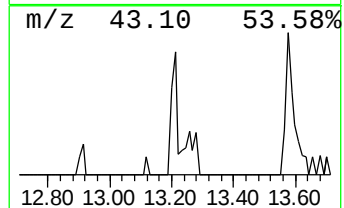
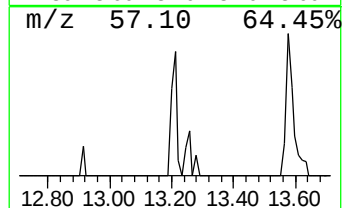
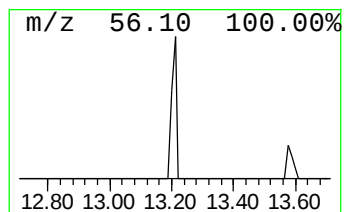
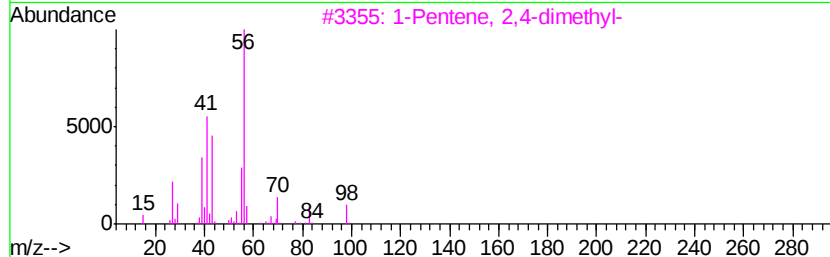
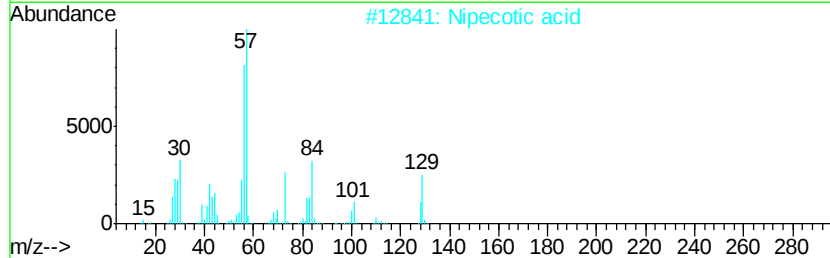
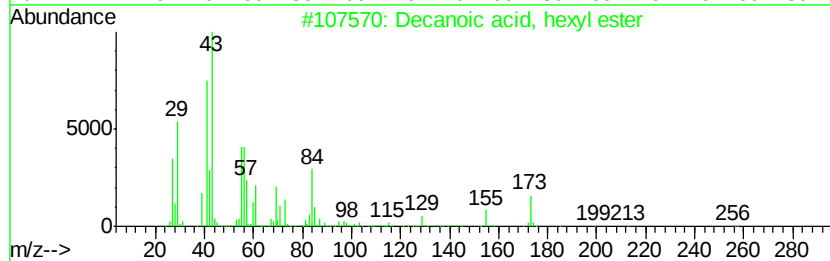
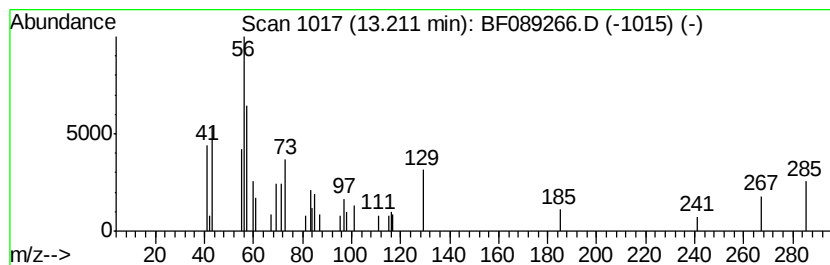
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Peak Number 6 unknown13.21 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.21	2.28 ng	29354	Chrysene-d12	13.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decanoic acid, hexyl ester	256	C16H32O2	010448-26-7	38
2		Nipecotic acid	129	C6H11NO2	000498-95-3	38
3		1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27
4		2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	27
5		5-Methyl-2-hexanol, chlorodifluo...	228	C9H15ClF2O2	1000376-27-1	27



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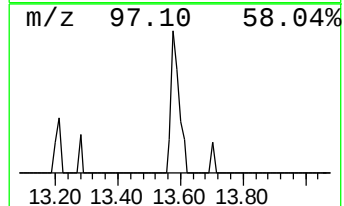
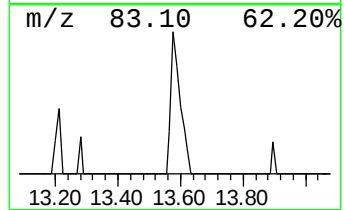
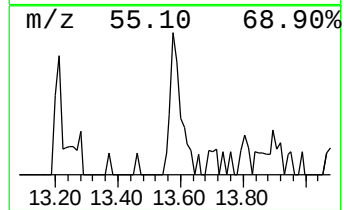
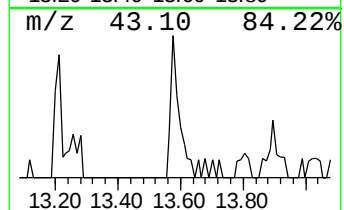
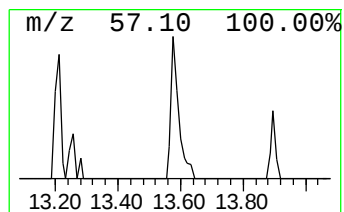
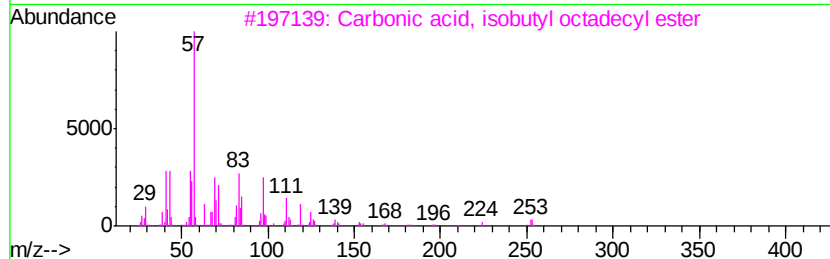
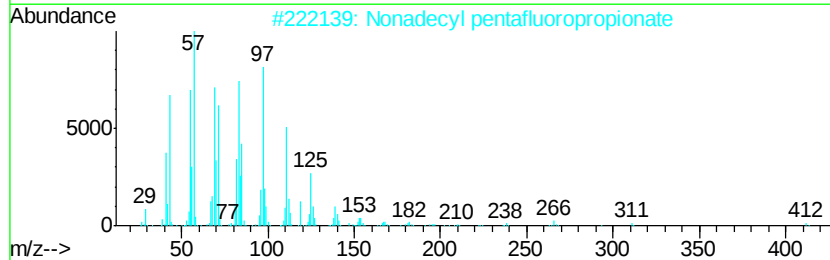
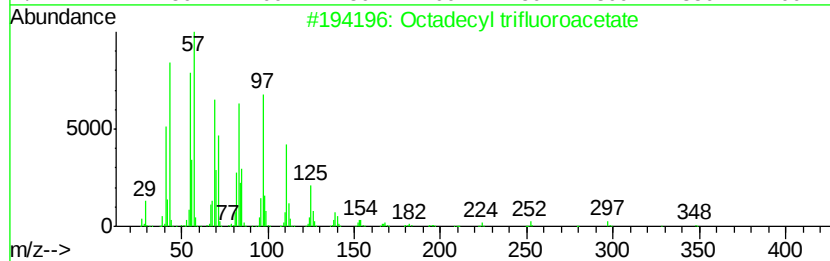
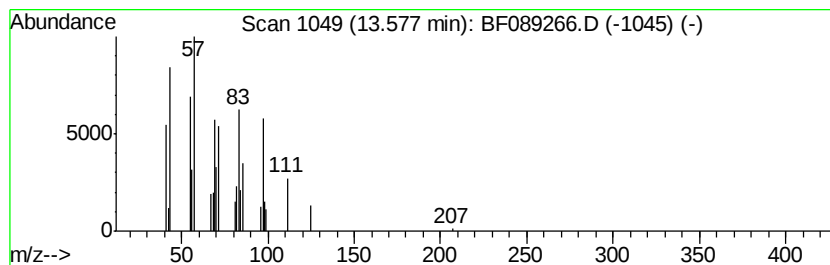
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Peak Number 7 Octadecyl trifluoroacetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.58	3.26 ng	41999	Chrysene-d12	13.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
2		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	90
3		Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	90
4		17-Pentatriacontene	491	C35H70	006971-40-0	87
5		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.71	6.5	ng	79912	1	6.58	246169	20.0
unknown6.35	6.35	121.5	ng	1495790	1	6.58	246169	20.0
n-Butyl laurate	12.50	4.6	ng	59141	5	13.70	257809	20.0
unknown13.21	13.21	2.3	ng	29354	5	13.70	257809	20.0
Octadecyl trifluo...	13.58	3.3	ng	41999	5	13.70	257809	20.0