

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052216\
 Data File : BF087283.D
 Acq On : 22 May 2016 11:29
 Operator : UM/SJ
 Sample : PB90787BL
 Misc :
 ALS Vial : 51 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB90787BL

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-BF051716.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	1.701	8	10	44	rVB	1275658	2579245	55.02%	6.852%
2	4.719	271	274	286	rBV	81642	203305	4.34%	0.540%
3	5.153	310	312	329	rBV	2779188	4178037	89.13%	11.099%
4	6.227	403	406	413	rBV	3441054	3698073	78.89%	9.824%
5	6.330	413	415	418	rBV	4288842	4106956	87.61%	10.910%
6	6.559	432	435	441	rVB	723001	851497	18.16%	2.262%
7	6.707	446	448	451	rBV	3101911	2908062	62.04%	7.725%
8	7.130	483	485	488	rBV	2134049	2420054	51.63%	6.429%
9	7.839	546	547	562	rBV	819859	1167382	24.90%	3.101%
10	8.925	639	642	644	rBV	4562904	4687719	100.00%	12.453%
11	9.588	698	700	703	rBV	1376975	1253202	26.73%	3.329%
12	10.376	767	769	772	rBV	2191988	2227559	47.52%	5.918%
13	11.062	827	829	835	rBV	973445	1161327	24.77%	3.085%
14	12.479	951	953	956	rBV	414112	335912	7.17%	0.892%
15	12.559	959	960	962	rVB	70714	50950	1.09%	0.135%
16	12.651	965	968	970	rBV	3980177	3919025	83.60%	10.411%
17	13.177	1012	1014	1016	rBV	140838	165975	3.54%	0.441%
18	13.222	1016	1018	1020	rBV	58527	59991	1.28%	0.159%
19	13.691	1057	1059	1069	rBV	727535	837046	17.86%	2.224%
20	13.862	1072	1074	1076	rVB	56922	59701	1.27%	0.159%
21	14.468	1124	1127	1129	rBV	36912	52794	1.13%	0.140%
22	15.051	1176	1178	1186	rBV	453978	719451	15.35%	1.911%

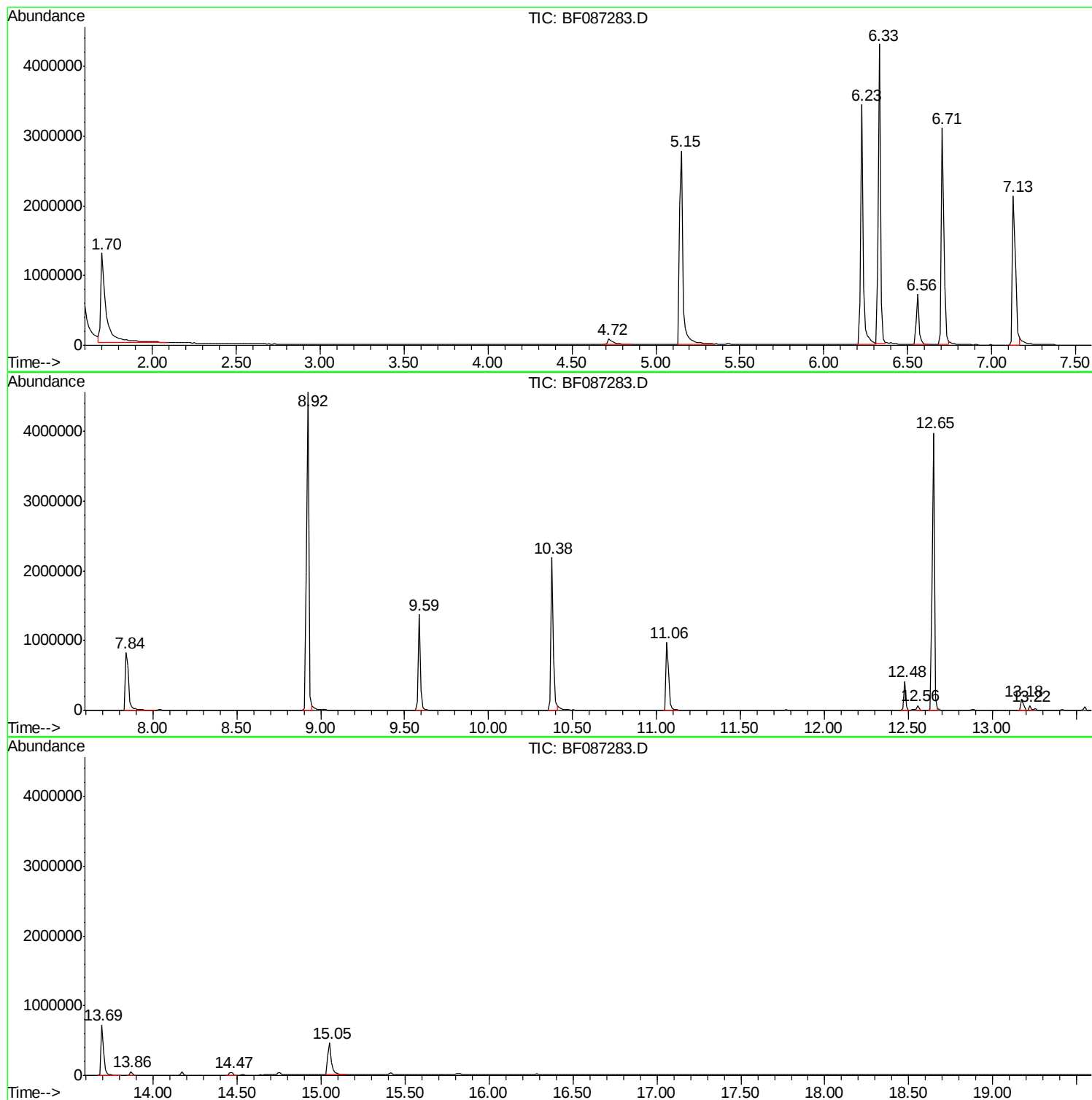
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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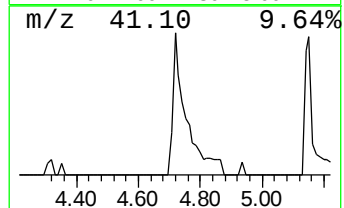
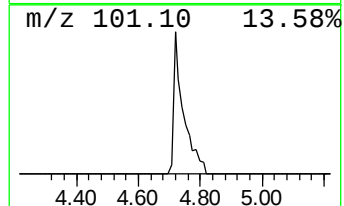
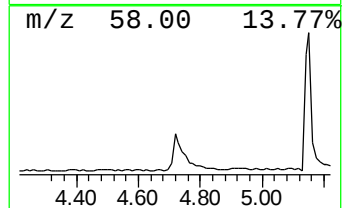
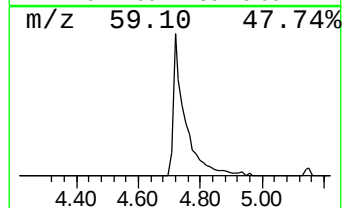
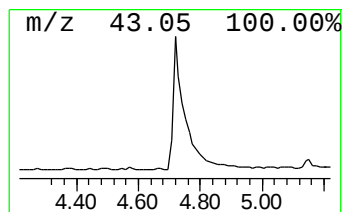
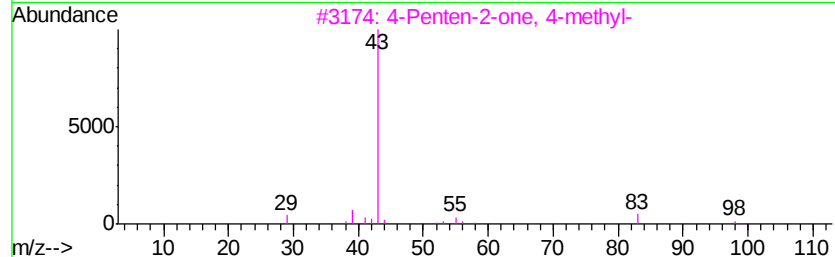
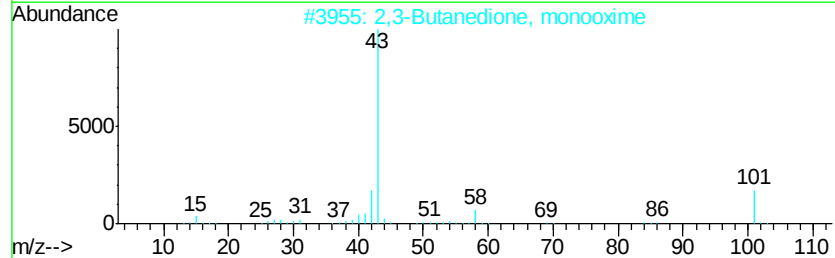
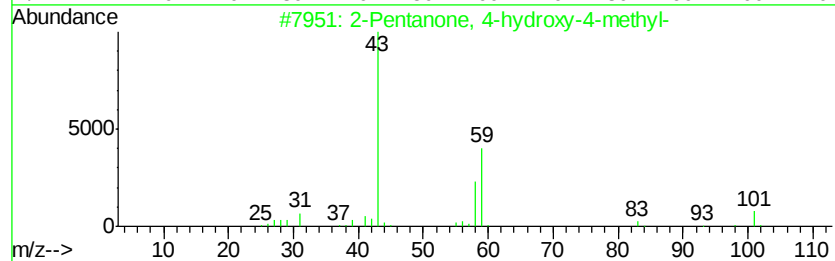
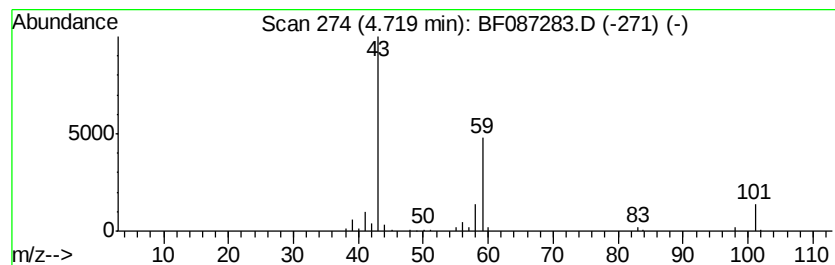
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.72	4.78 ng	203305	1,4-Dichlorobenzene-d4	6.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
4		Diacetamide	101	C4H7NO2	000625-77-4	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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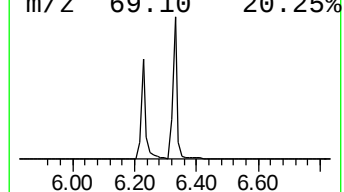
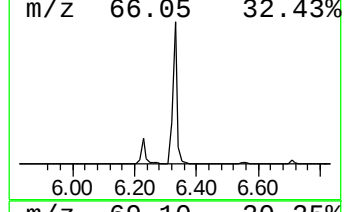
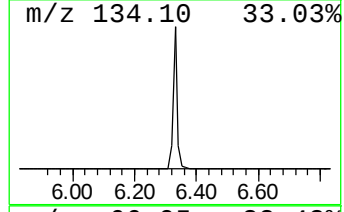
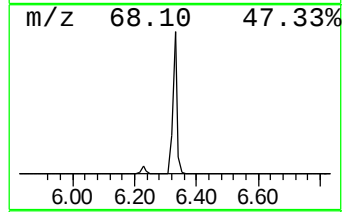
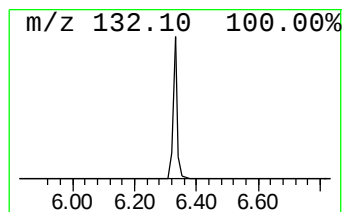
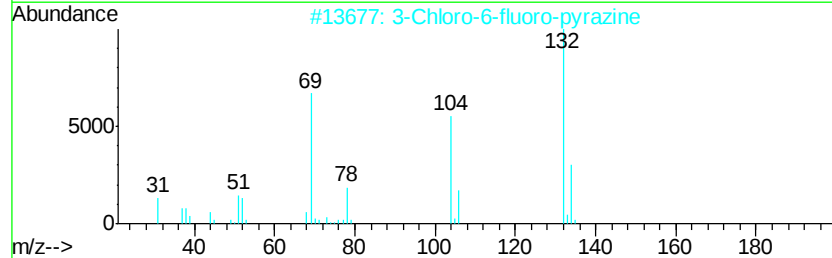
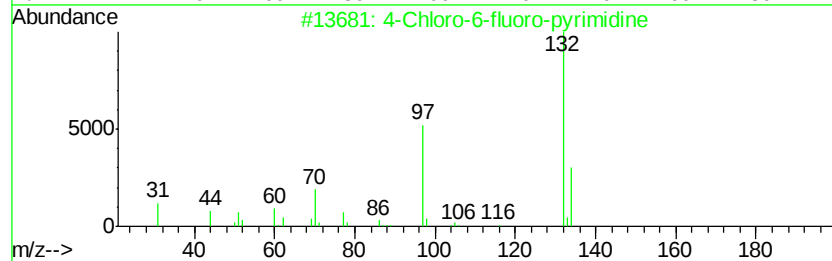
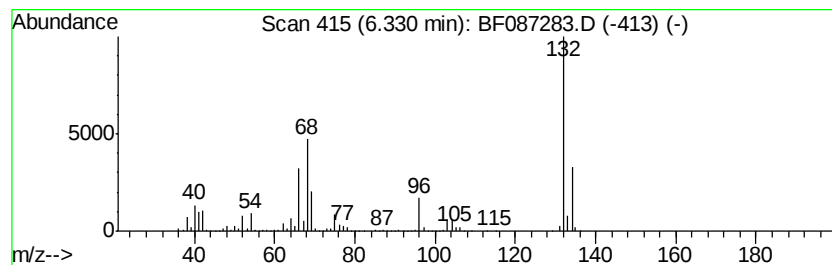
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Peak Number 3 unknown6.33 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.33	96.46 ng	4106960	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27	
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
3	Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	22	
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22	
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12	



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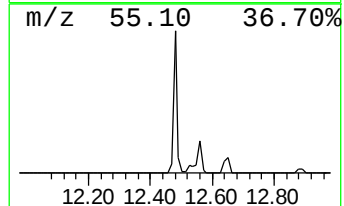
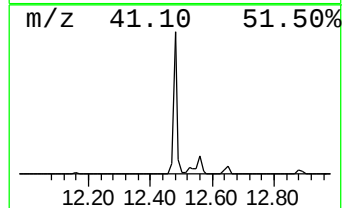
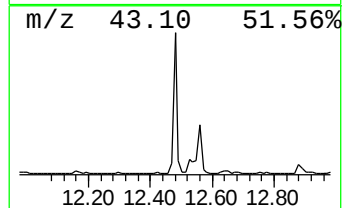
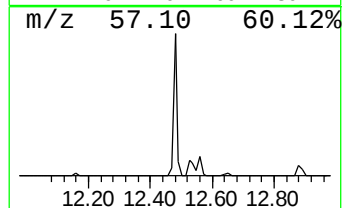
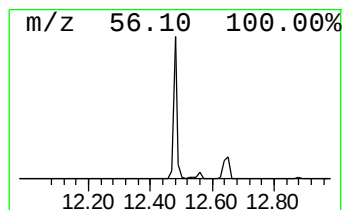
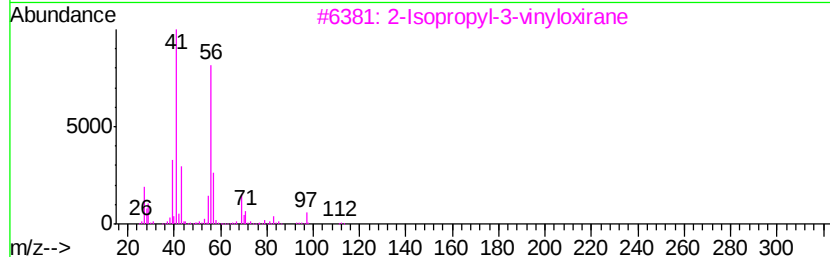
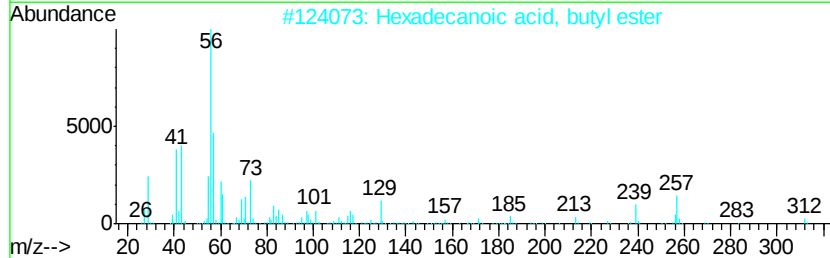
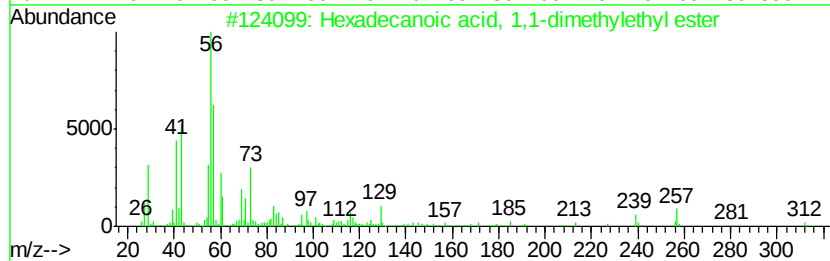
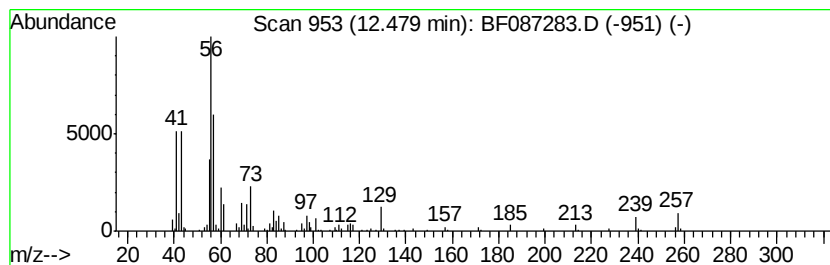
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Peak Number 5 Hexadecanoic acid, 1,1-dime... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	8.03 ng	335912	Chrysene-d12	13.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	76
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	53
3		2-Isopropyl-3-vinylloxirane	112	C7H12O	070777-23-0	38
4		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	37
5		1-Hexene, 2-methyl-	98	C7H14	006094-02-6	35



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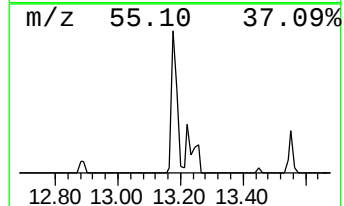
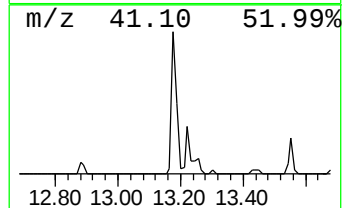
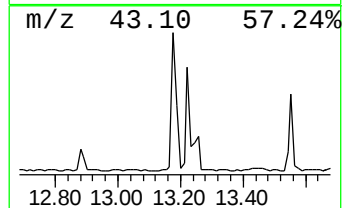
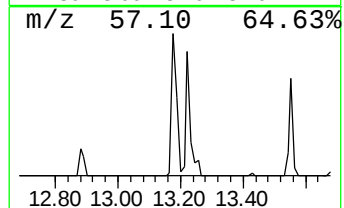
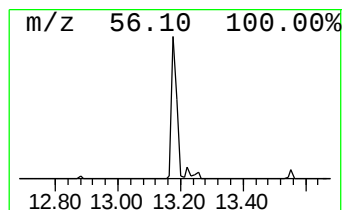
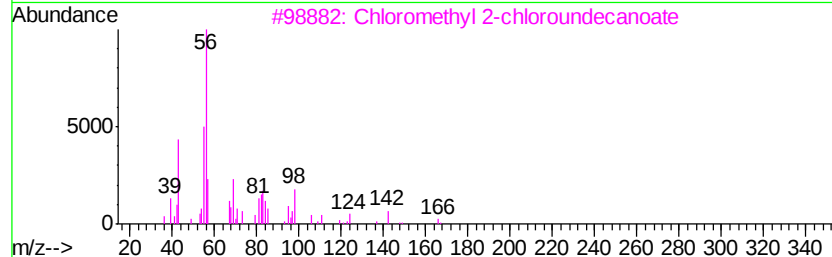
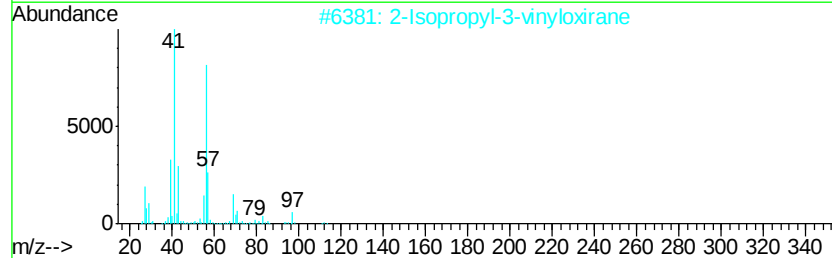
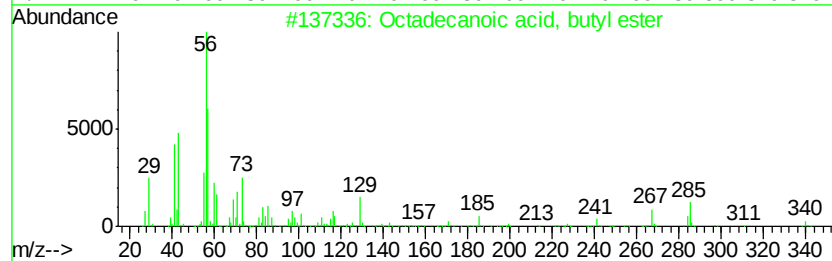
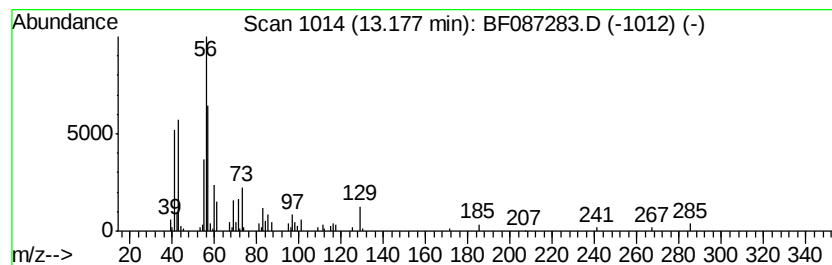
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Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.18	3.97 ng	165975	Chrysene-d12	13.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	86
2		2-Isopropyl-3-vinylloxirane	112	C7H12O	070777-23-0	38
3		Chloromethyl 2-chloroundecanoate	268	C12H22Cl2O2	080418-88-8	37
4		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	35
5		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.72	4.8	ng	203305	1	6.56	851497	20.0
unknown6.33	6.33	96.5	ng	4106960	1	6.56	851497	20.0
Hexadecanoic acid...	12.48	8.0	ng	335912	5	13.69	837046	20.0
Octadecanoic acid...	13.18	4.0	ng	165975	5	13.69	837046	20.0