

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
 Data File : BF089253.D
 Acq On : 24 Jul 2016 1:31
 Operator : UM/SJ
 Sample : H4154-04
 Misc :
 ALS Vial : 51 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GCF-WW-1

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-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	9	11	48	rVB	443500	924751	60.78%	7.451%
2	4.707	271	273	279	rBV	37692	67179	4.42%	0.541%
3	5.164	311	313	330	rBV	1072435	1360994	89.45%	10.966%
4	6.239	404	407	414	rBV	1135674	1422970	93.52%	11.465%
5	6.353	414	417	419	rBV	887844	1296928	85.24%	10.450%
6	6.582	435	437	448	rBV	206269	261407	17.18%	2.106%
7	6.730	448	450	453	rBV	968668	993202	65.28%	8.002%
8	7.153	484	487	496	rBV	663468	885466	58.19%	7.134%
9	7.279	496	498	503	rVB	12267	22578	1.48%	0.182%
10	7.862	547	549	560	rBV	389711	396212	26.04%	3.192%
11	8.948	641	644	646	rBV	1306258	1521550	100.00%	12.259%
12	9.348	676	679	681	rBV	249064	339631	22.32%	2.736%
13	9.611	699	702	704	rBV	393073	394705	25.94%	3.180%
14	10.399	768	771	773	rBV	515717	706417	46.43%	5.692%
15	10.525	781	782	786	rBV	10226	16718	1.10%	0.135%
16	11.085	828	831	833	rBV	287361	320679	21.08%	2.584%
17	12.502	954	955	957	rBB	52727	50231	3.30%	0.405%
18	12.662	967	969	972	rBV	913005	895367	58.85%	7.214%
19	13.211	1015	1017	1018	rBB	32453	32425	2.13%	0.261%
20	13.577	1046	1049	1057	rBV	26181	42086	2.77%	0.339%
21	13.702	1057	1060	1068	rBV	215853	231855	15.24%	1.868%
22	15.040	1175	1177	1180	rBV	154853	227850	14.97%	1.836%

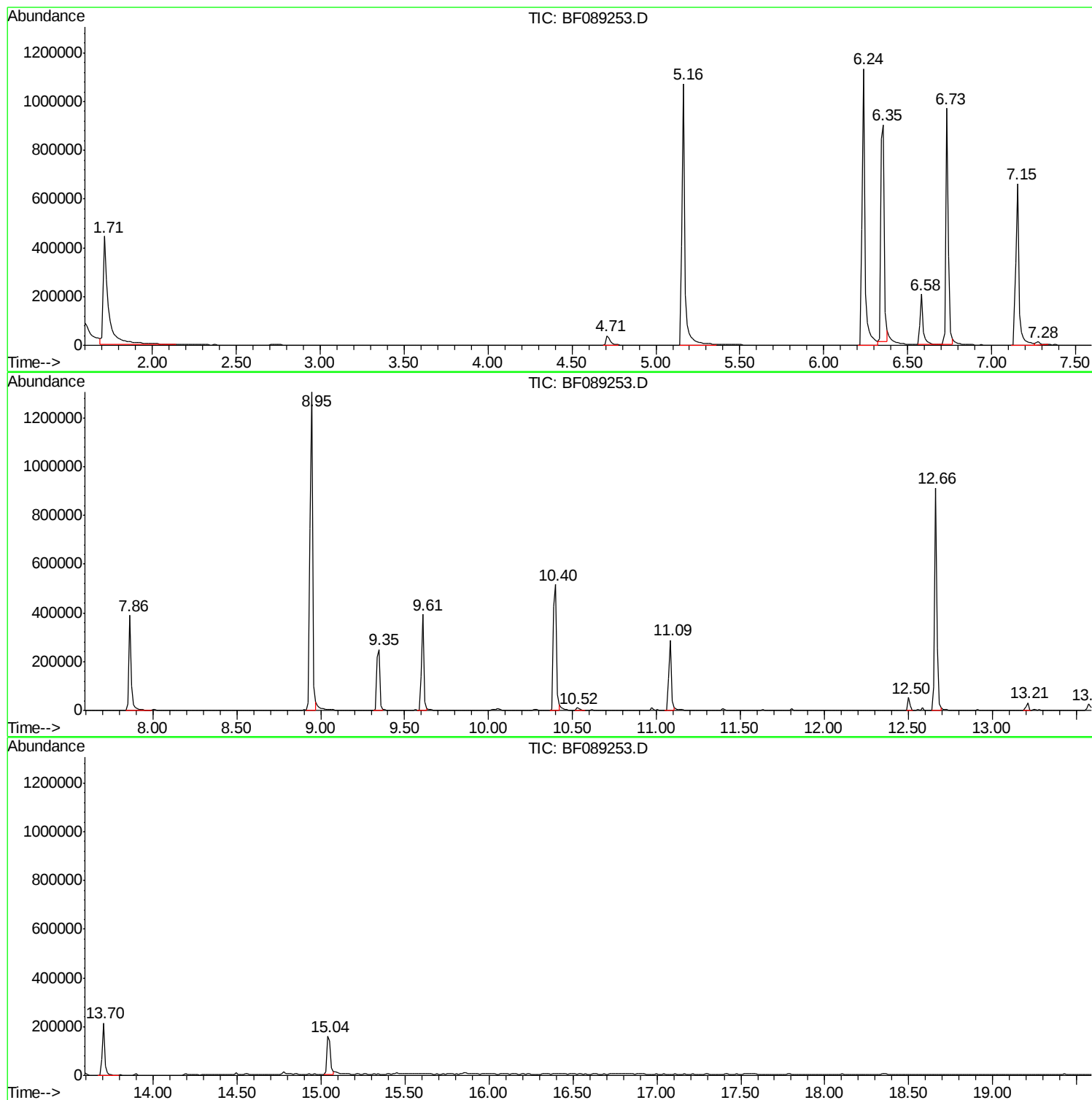
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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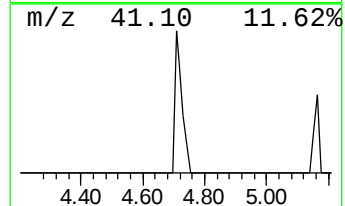
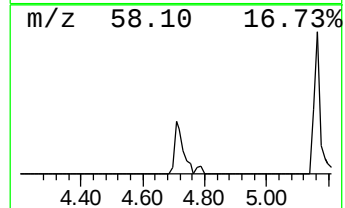
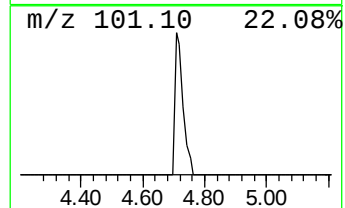
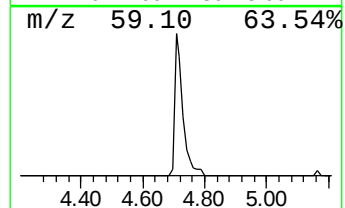
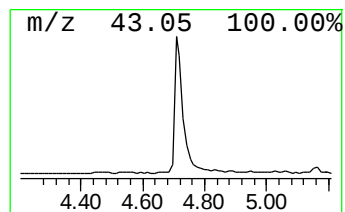
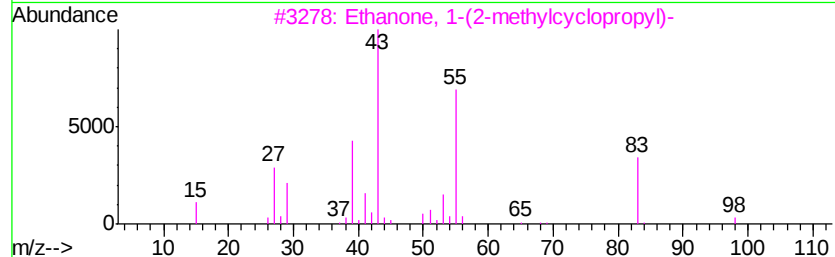
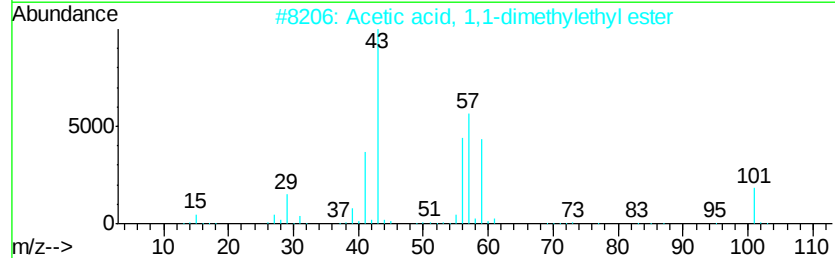
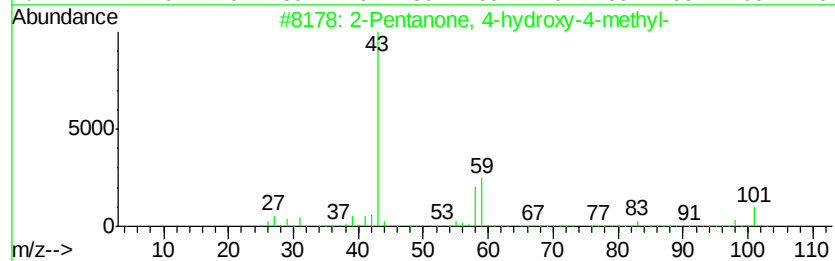
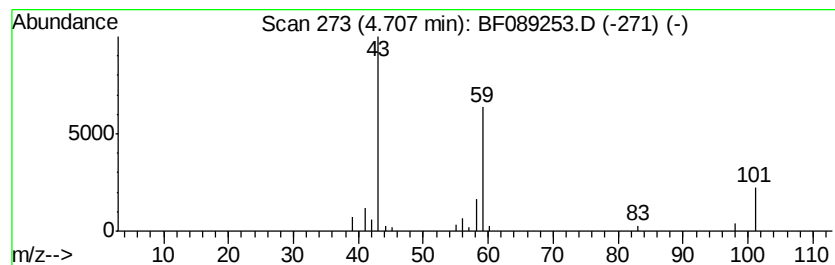
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.71	5.14 ng	67179	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	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9



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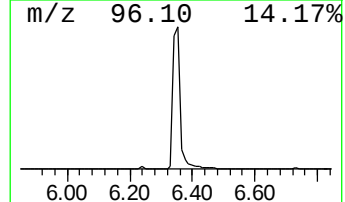
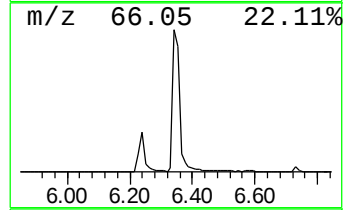
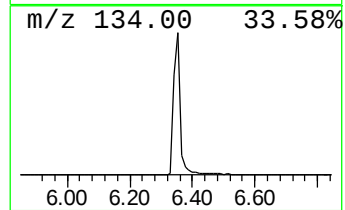
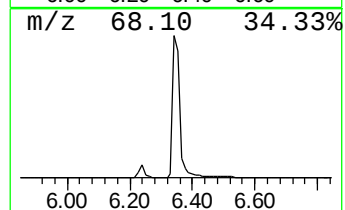
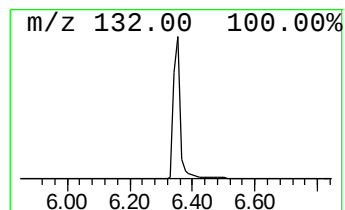
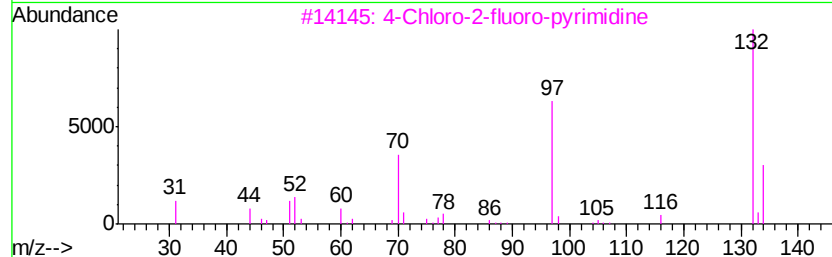
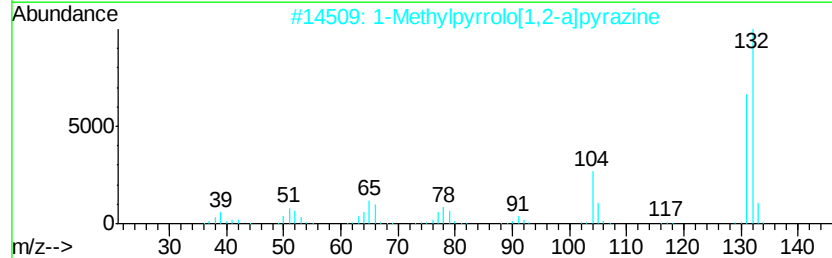
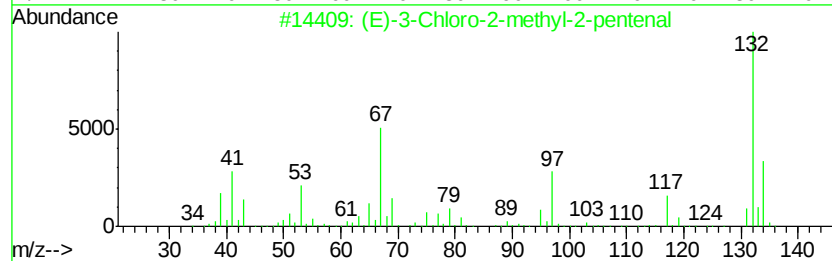
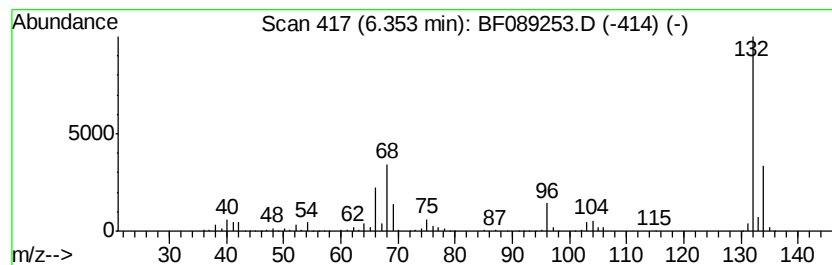
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Peak Number 3 unknown6.35 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	99.23 ng	1296930	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	25
2		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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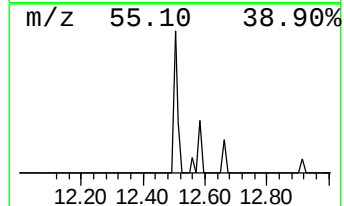
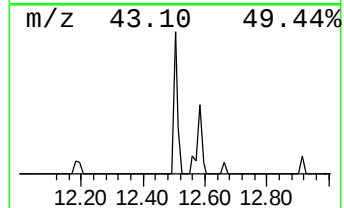
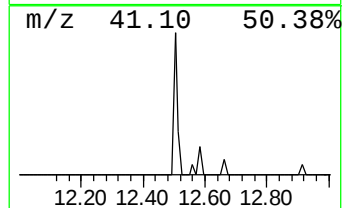
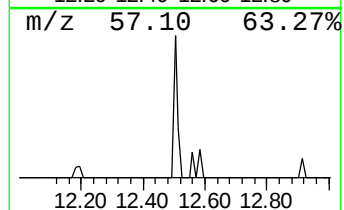
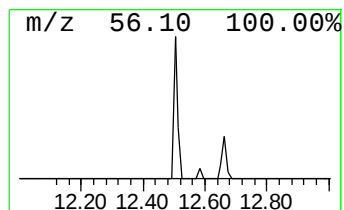
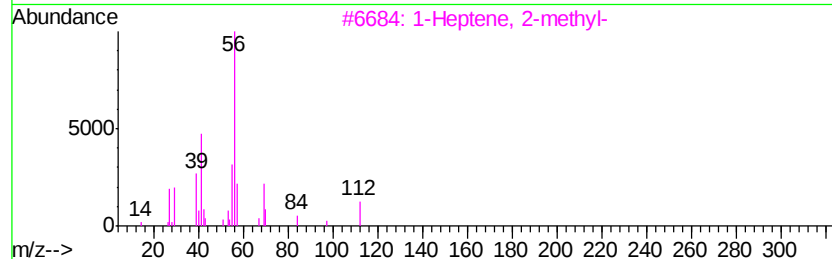
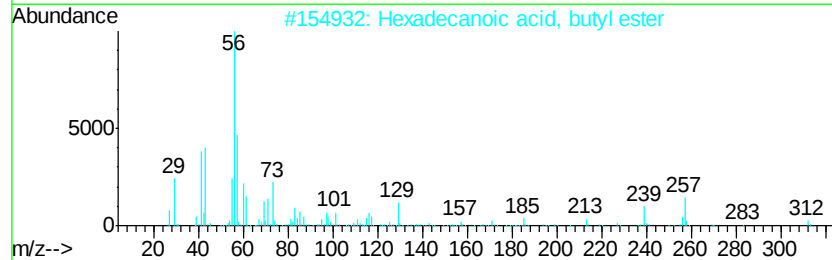
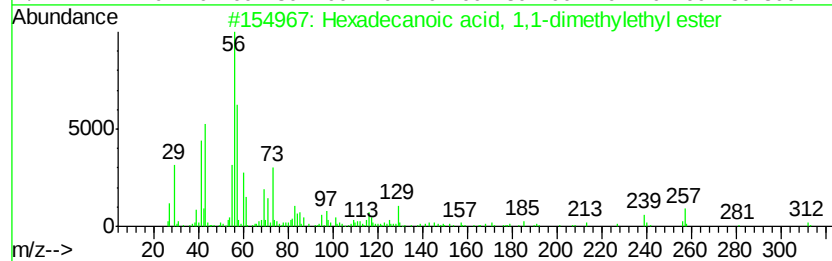
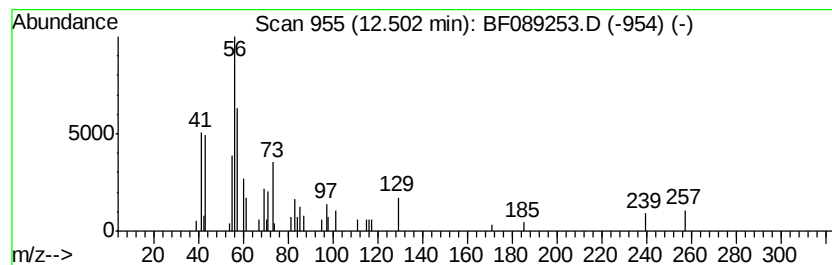
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Peak Number 5 Hexadecanoic acid, 1,1-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.50	4.33 ng	50231	Chrysene-d12	13.70

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	87
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	72
3		1-Heptene, 2-methyl-	112	C8H16	015870-10-7	27
4		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27
5		1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27



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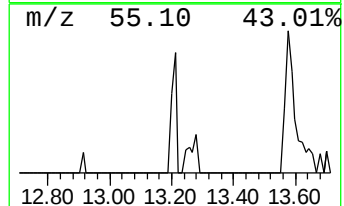
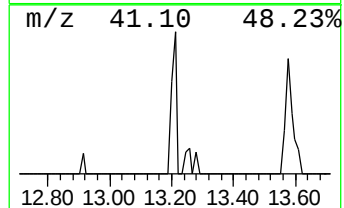
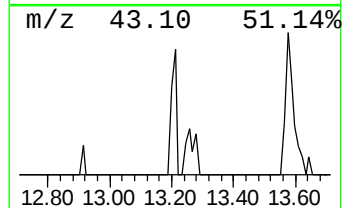
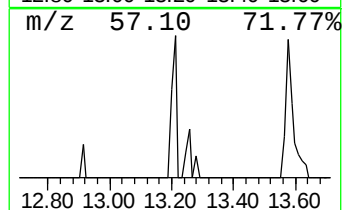
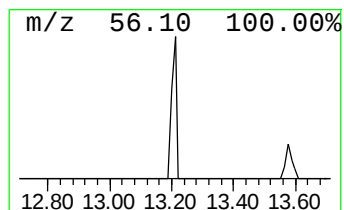
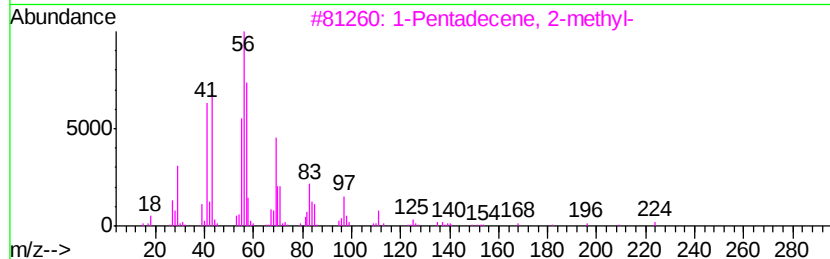
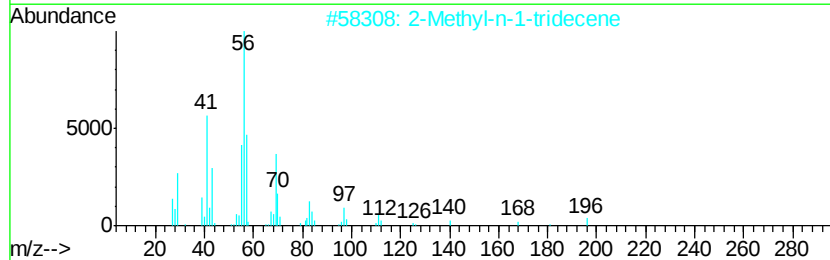
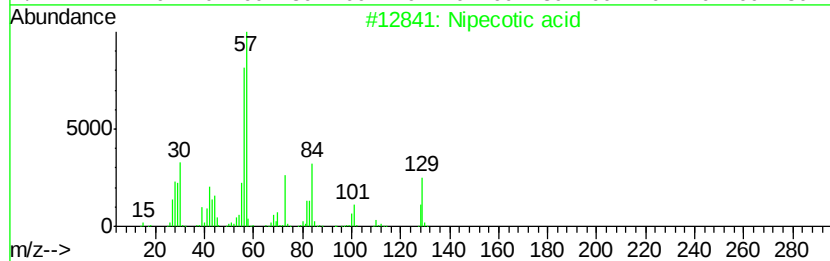
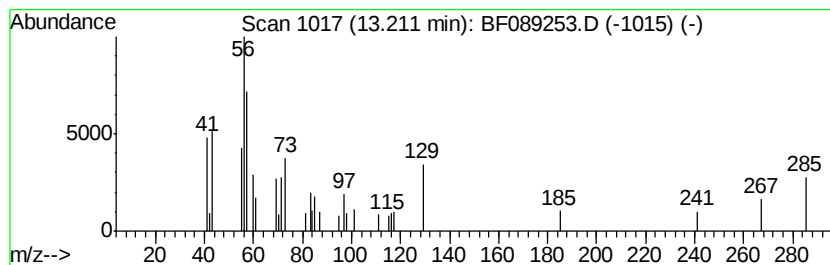
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Peak Number 6 unknown13.21 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.21	2.80 ng	32425	Chrysene-d12	13.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nipecotic acid	129	C6H11NO2	000498-95-3	37
2		2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35
3		1-Pentadecene, 2-methyl-	224	C16H32	029833-69-0	25
4		2-Methyl-1-octadecene	266	C19H38	061868-20-0	25
5		Cyclohexane, (1,1-dimethylethyl)-	140	C10H20	003178-22-1	22



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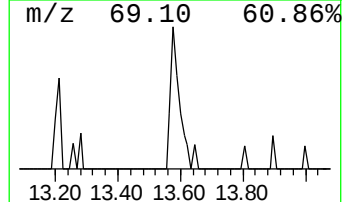
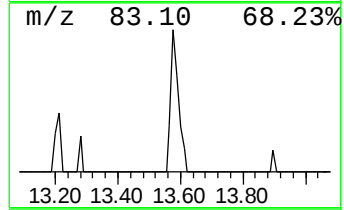
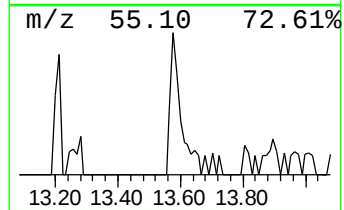
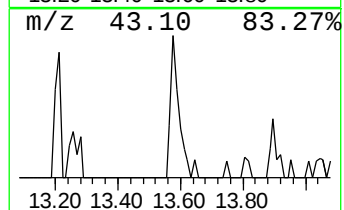
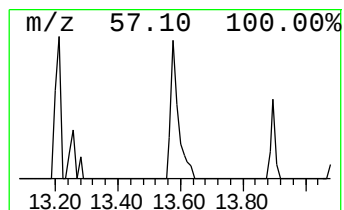
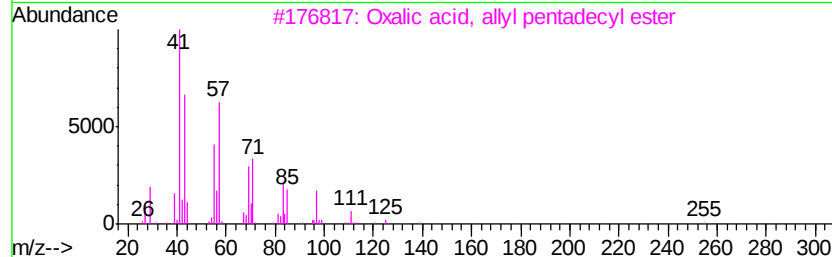
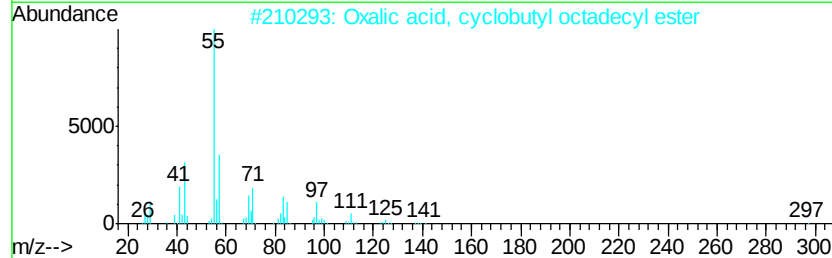
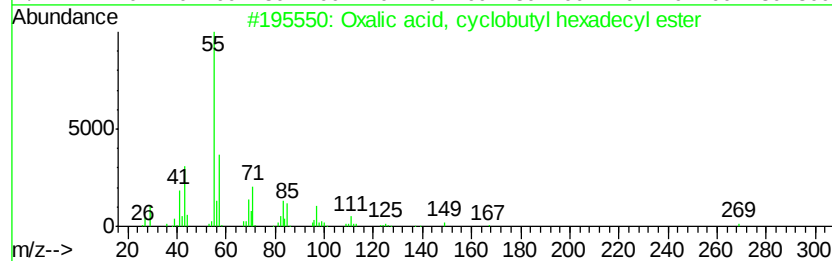
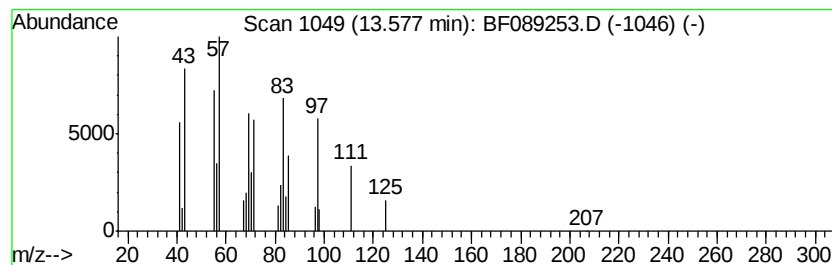
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Peak Number 7 Oxalic acid, cyclobutyl hex... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.58	3.63 ng	42086	Chrysene-d12	13.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxalic acid, cyclobutyl hexadecy...	368	C22H40O4	1000309-70-6	83
2		Oxalic acid, cyclobutyl octadecy...	396	C24H44O4	1000309-70-8	83
3		Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	78
4		Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	78
5		Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	78



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.71	5.1	ng	67179	1	6.58	261407	20.0
unknown6.35	6.35	99.2	ng	1296930	1	6.58	261407	20.0
Hexadecanoic acid...	12.50	4.3	ng	50231	5	13.70	231855	20.0
unknown13.21	13.21	2.8	ng	32425	5	13.70	231855	20.0
Oxalic acid, cycl...	13.58	3.6	ng	42086	5	13.70	231855	20.0