

Data Path : Z:\HPCHEM1\BNA F\Data\BF031617\
 Data File : BF093713.D
 Acq On : 16 Mar 2017 18:29
 Operator : SJ/MA
 Sample : I2261-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TRAP-ROCK-FINES

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-BF030717.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	4.196	200	202	210	rBV4	12183	51684	1.09%	0.121%
2	4.836	256	258	276	rBV	1721009	2878819	60.79%	6.723%
3	5.293	296	298	318	rBV	3416550	4670825	98.63%	10.909%
4	5.693	331	333	341	rVB	120937	173175	3.66%	0.404%
5	6.356	389	391	399	rBV	3965315	4735483	100.00%	11.060%
6	6.470	399	401	404	rVB	3700315	4533683	95.74%	10.588%
7	6.699	418	421	428	rBV	687012	1066474	22.52%	2.491%
8	6.847	432	434	448	rVB	3394995	3426965	72.37%	8.004%
9	7.270	469	471	485	rBV	2669294	2934684	61.97%	6.854%
10	7.979	531	533	546	rBV	942813	1445619	30.53%	3.376%
11	9.065	625	628	630	rBV	3870612	4550478	96.09%	10.628%
12	9.465	661	663	671	rVB	423167	382857	8.08%	0.894%
13	9.728	684	686	689	rBV	962695	1354840	28.61%	3.164%
14	10.162	723	724	726	rVB	61600	51215	1.08%	0.120%
15	10.528	754	756	764	rBV	2299454	2378051	50.22%	5.554%
16	10.631	764	765	770	rVB	73975	106112	2.24%	0.248%
17	11.076	803	804	806	rBV	44694	66428	1.40%	0.155%
18	11.214	814	816	819	rBV2	1121669	1382340	29.19%	3.228%
19	11.751	861	863	869	rBV3	98927	192949	4.07%	0.451%
20	12.539	929	932	937	rBV3	27357	56278	1.19%	0.131%
21	12.802	952	955	957	rBV	3854447	3922910	82.84%	9.162%
22	13.854	1045	1047	1050	rBV	1088173	1239809	26.18%	2.896%
23	13.911	1051	1052	1054	rVB	71178	50946	1.08%	0.119%
24	14.665	1116	1118	1120	rBV	107532	113499	2.40%	0.265%
25	15.248	1167	1169	1180	rVB	578467	992577	20.96%	2.318%
26	16.265	1255	1258	1263	rBV4	28498	59193	1.25%	0.138%

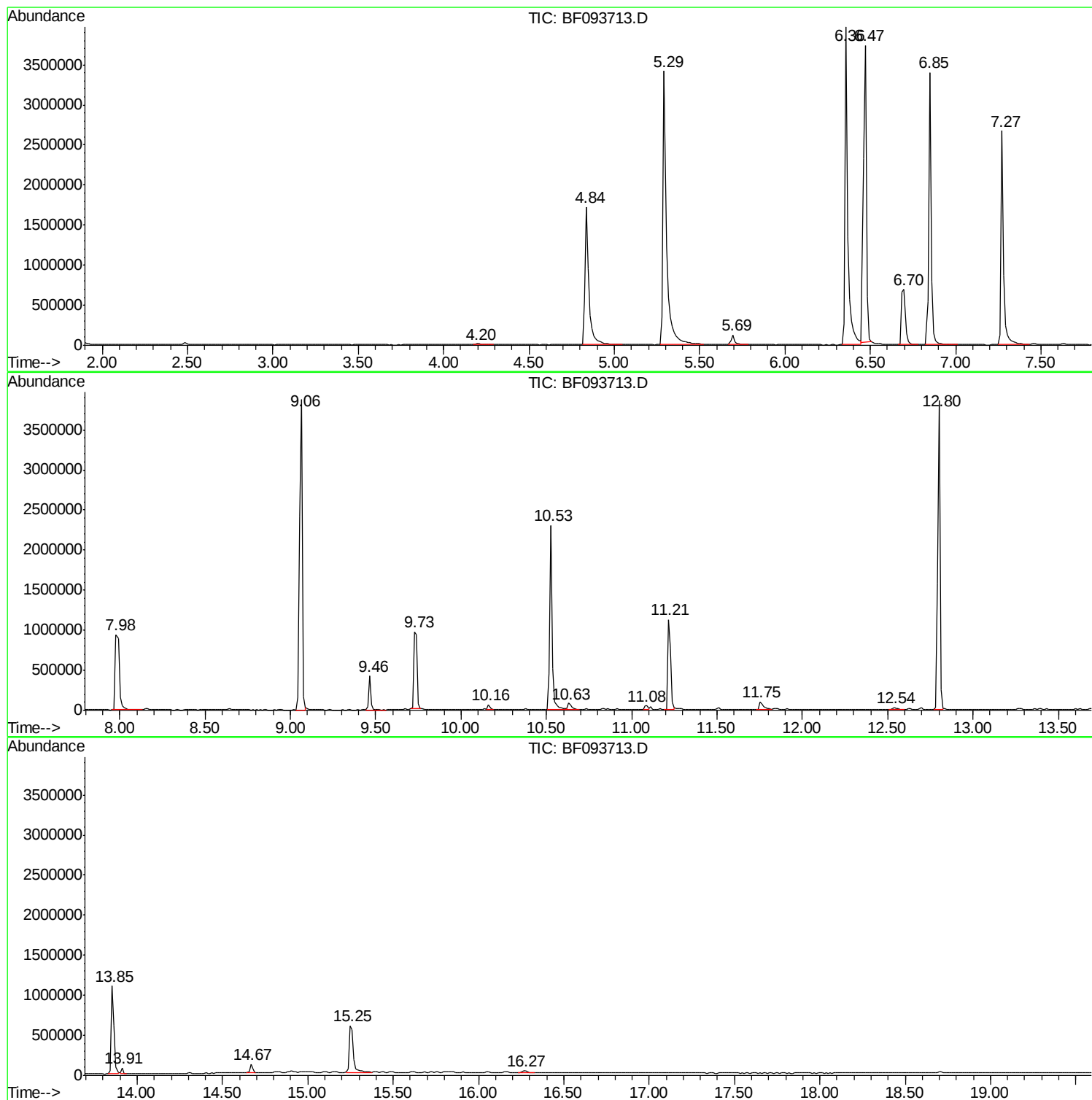
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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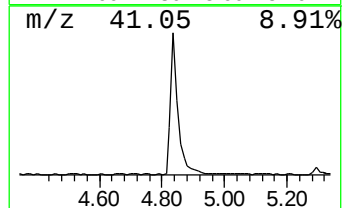
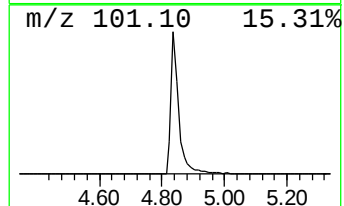
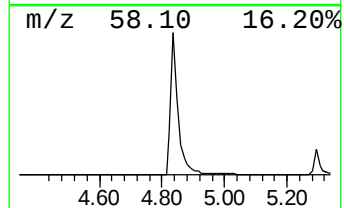
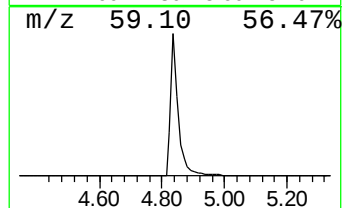
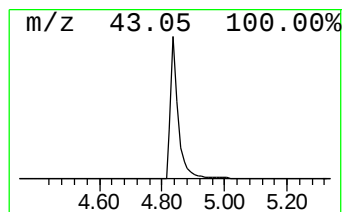
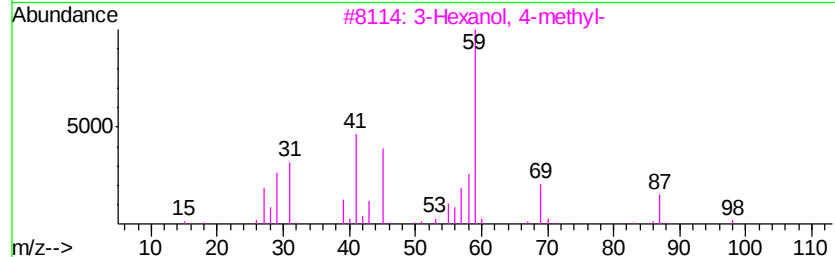
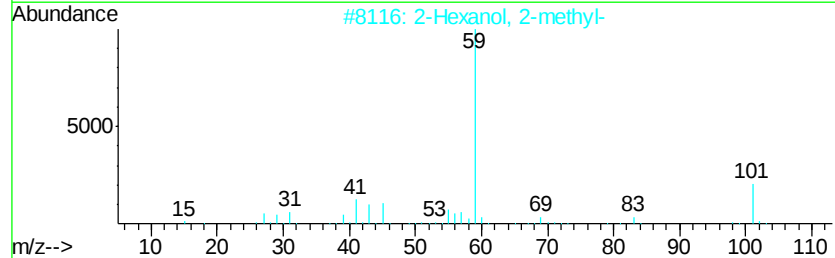
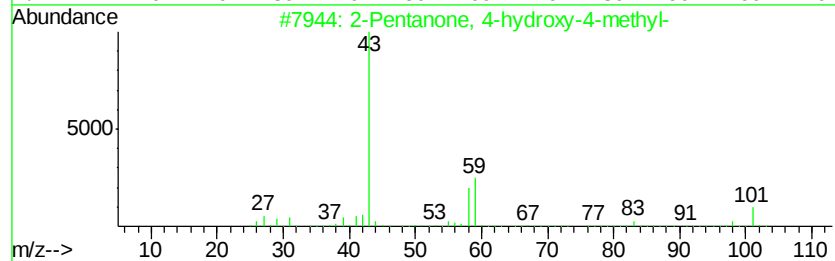
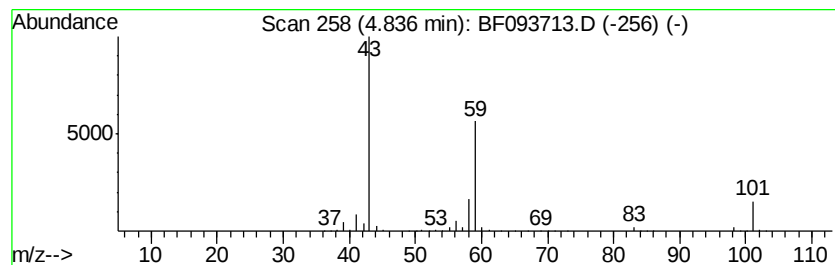
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.84	53.99 ng	2878820	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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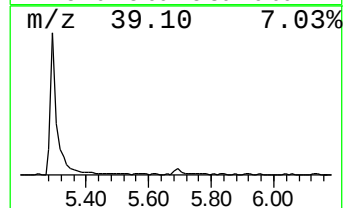
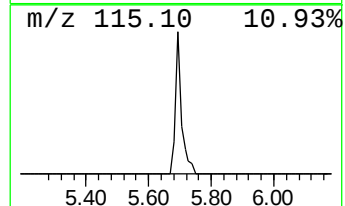
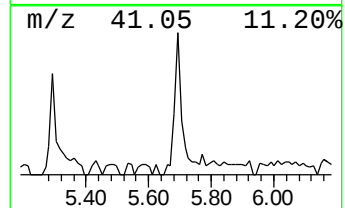
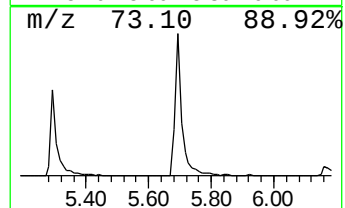
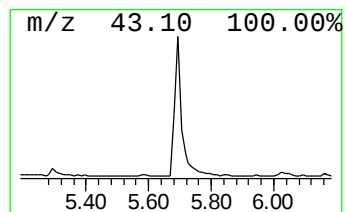
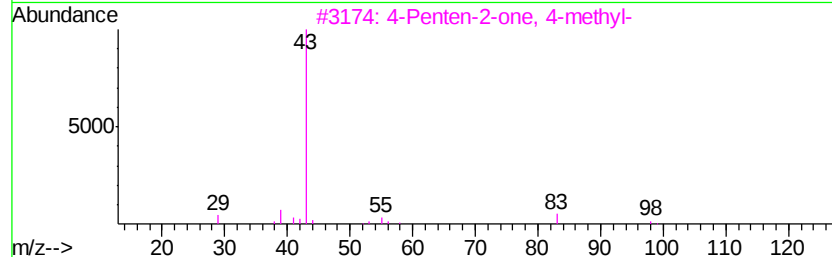
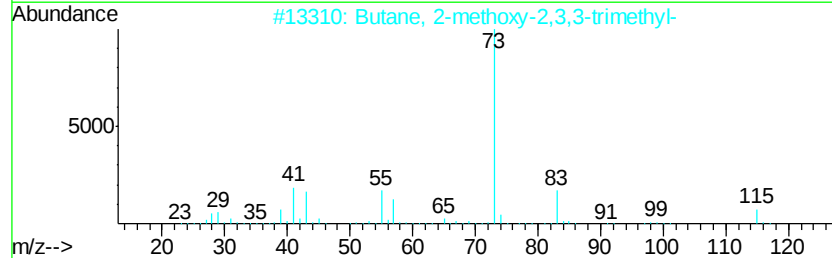
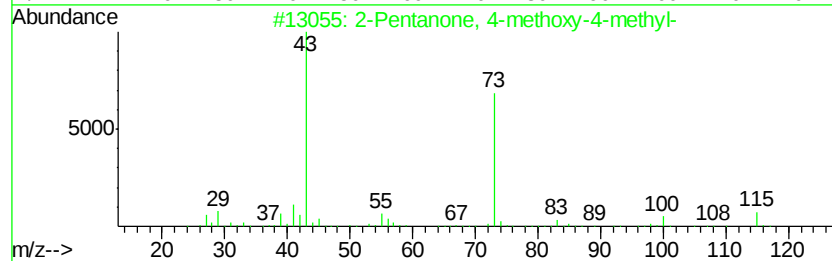
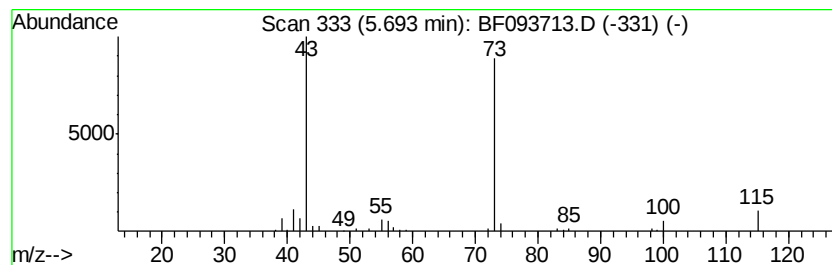
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Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.69	3.25 ng	173175	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	25
3		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	10
4		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9
5		Guanidine, methyl-	73	C2H7N3	000471-29-4	9



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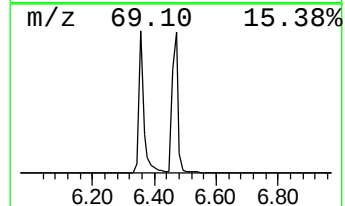
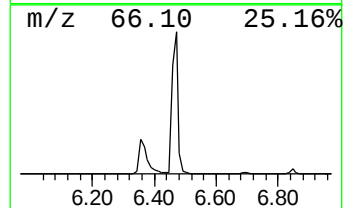
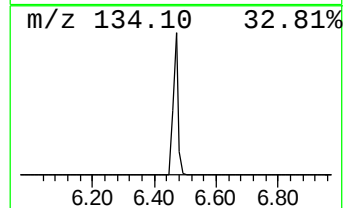
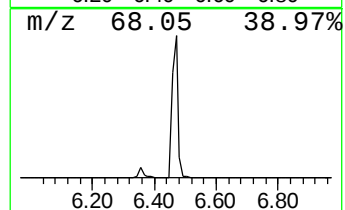
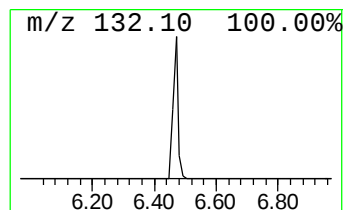
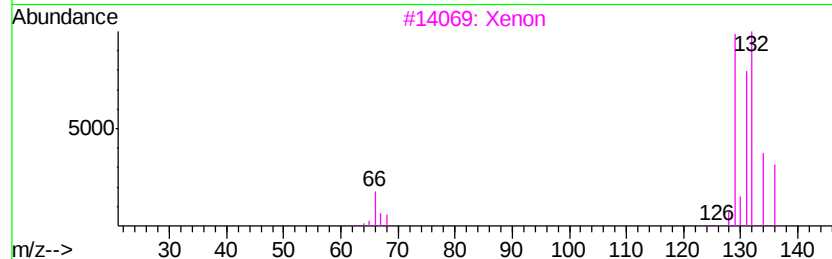
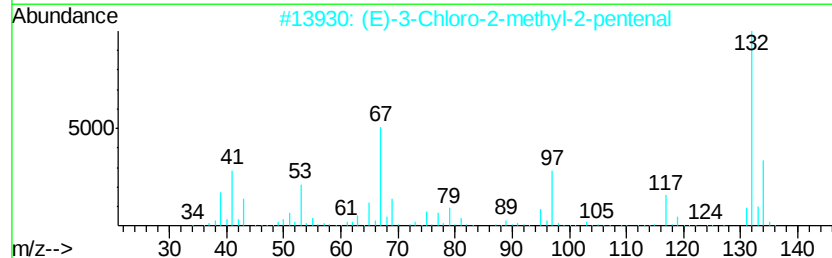
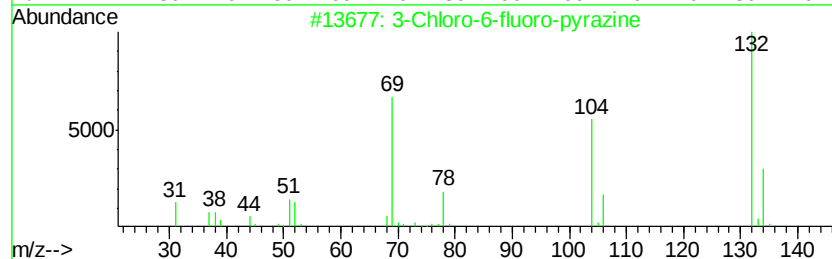
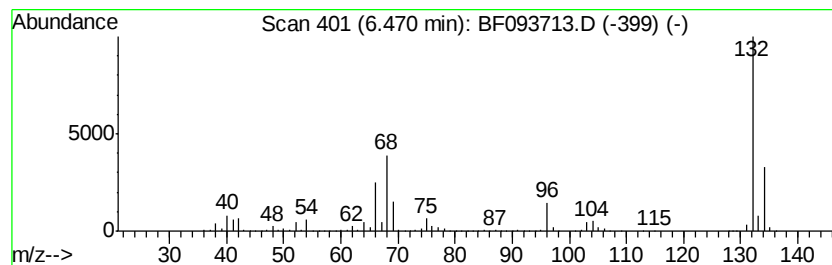
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	85.02 ng	4533680	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27		
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16		
3	Xenon	132	Xe	007440-63-3	9		
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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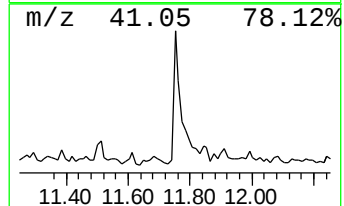
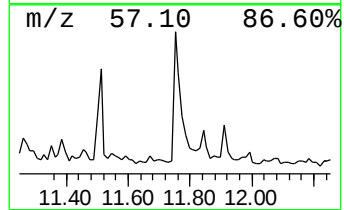
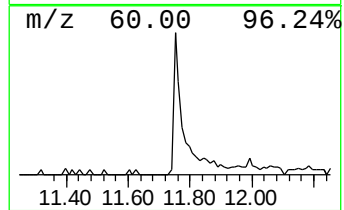
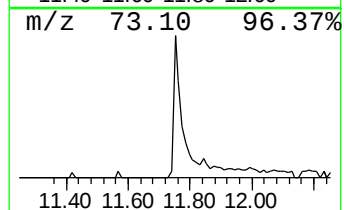
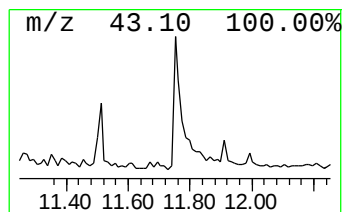
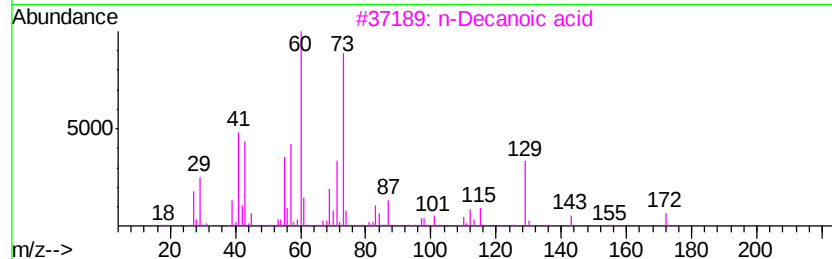
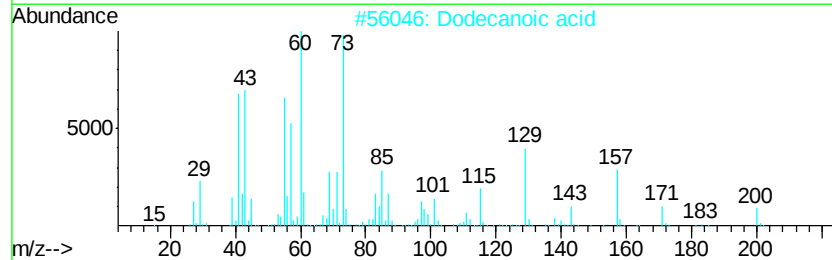
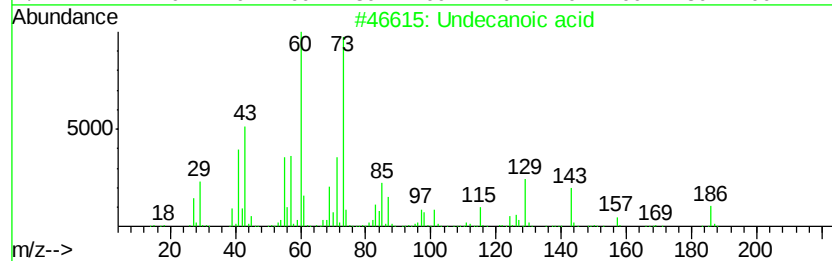
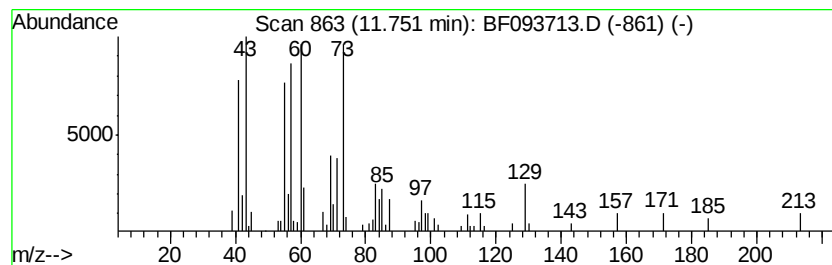
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Peak Number 5 Undecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.75	2.79 ng	192949	Phenanthrene-d10		11.21

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecanoic acid	186	C11H22O2	000112-37-8	64
2			Dodecanoic acid	200	C12H24O2	000143-07-7	53
3			n-Decanoic acid	172	C10H20O2	000334-48-5	47
4			d-Glucohexodialdose	178	C6H10O6	1000149-19-1	47
5			Octanoic Acid	144	C8H16O2	000124-07-2	47



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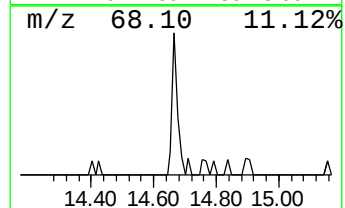
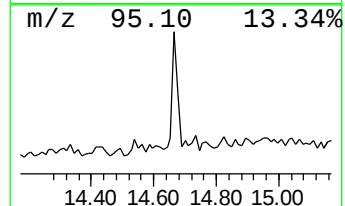
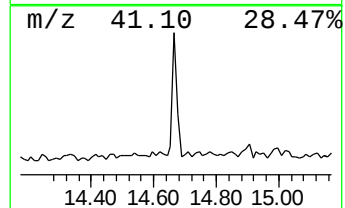
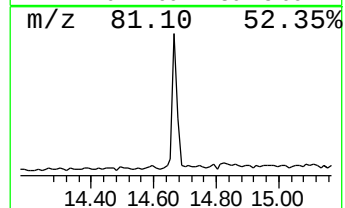
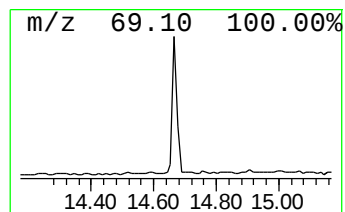
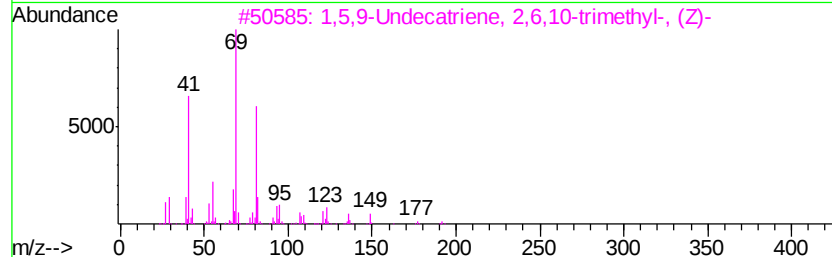
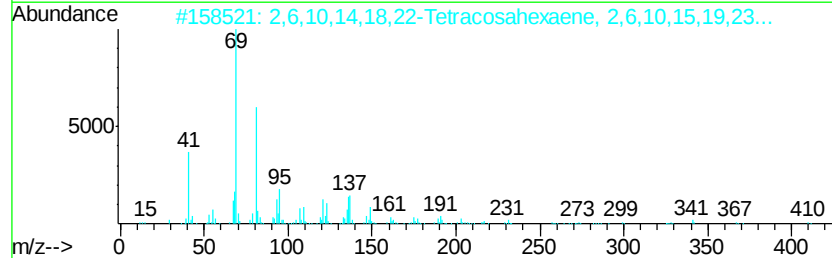
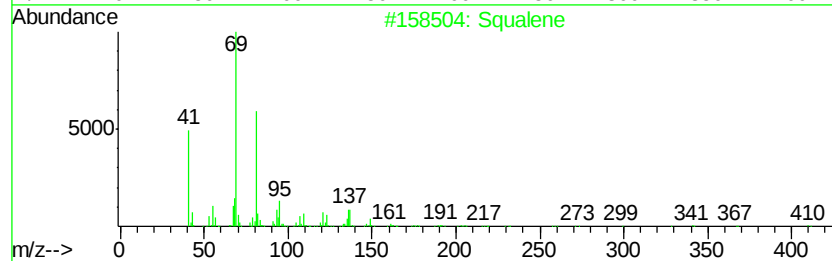
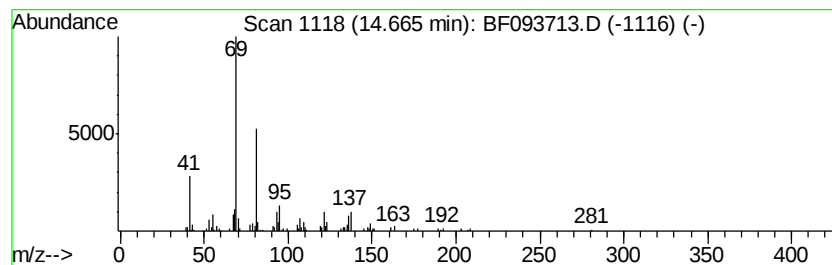
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	2.29 ng	113499	Perylene-d12	15.26
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	007683-64-9	91
2	2,6,10,14,18,22-Tetracosahexaene...	410 C30H50	000111-02-4	90
3	1,5,9-Undecatriene, 2,6,10-trime...	192 C14H24	062951-96-6	72
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222 C15H26O	004602-84-0	64
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222 C15H26O	000106-28-5	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.84	54.0	ng	2878820	1	6.70	1066470	20.0
2-Pentanone, 4-me...	5.69	3.3	ng	173175	1	6.70	1066470	20.0
unknown6.47	6.47	85.0	ng	4533680	1	6.70	1066470	20.0
Undecanoic acid	11.75	2.8	ng	192949	4	11.21	1382340	20.0
Squalene	14.67	2.3	ng	113499	6	15.26	992577	20.0