

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030817\
 Data File : BF093434.D
 Acq On : 8 Mar 2017 17:56
 Operator : SJ/MA
 Sample : PB97426BL
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB97426BL

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	4.253	205	207	219	rBV	82756	219521	4.19%	0.486%
2	4.916	263	265	277	rBV	1153508	1895299	36.14%	4.199%
3	5.362	301	304	327	rBV	4333713	5000729	95.36%	11.079%
4	5.762	336	339	343	rBV	55907	64130	1.22%	0.142%
5	6.413	393	396	404	rBV	4133959	4520734	86.21%	10.016%
6	6.527	404	406	409	rBV	3529223	4492209	85.67%	9.953%
7	6.756	424	426	429	rBV	875024	1108727	21.14%	2.456%
8	6.916	438	440	443	rBV	3686734	3464286	66.06%	7.675%
9	7.339	474	477	479	rBV	3121363	3304439	63.02%	7.321%
10	8.047	537	539	542	rBV	1121151	1424549	27.17%	3.156%
11	9.133	631	634	636	rBV	4260286	5243882	100.00%	11.618%
12	9.751	681	688	690	rBV	167118	374391	7.14%	0.829%
13	9.808	690	693	695	rVB	1168053	1594923	30.41%	3.534%
14	10.231	724	730	737	rBV4	13975	58360	1.11%	0.129%
15	10.596	759	762	775	rBV	2653241	2985652	56.94%	6.615%
16	11.282	820	822	825	rBV	1248010	1602905	30.57%	3.551%
17	12.871	958	961	964	rBV	4155057	4688336	89.41%	10.387%
18	13.922	1051	1053	1056	rBV	1302219	1645234	31.37%	3.645%
19	15.340	1174	1177	1188	rBV	1081543	1447218	27.60%	3.206%

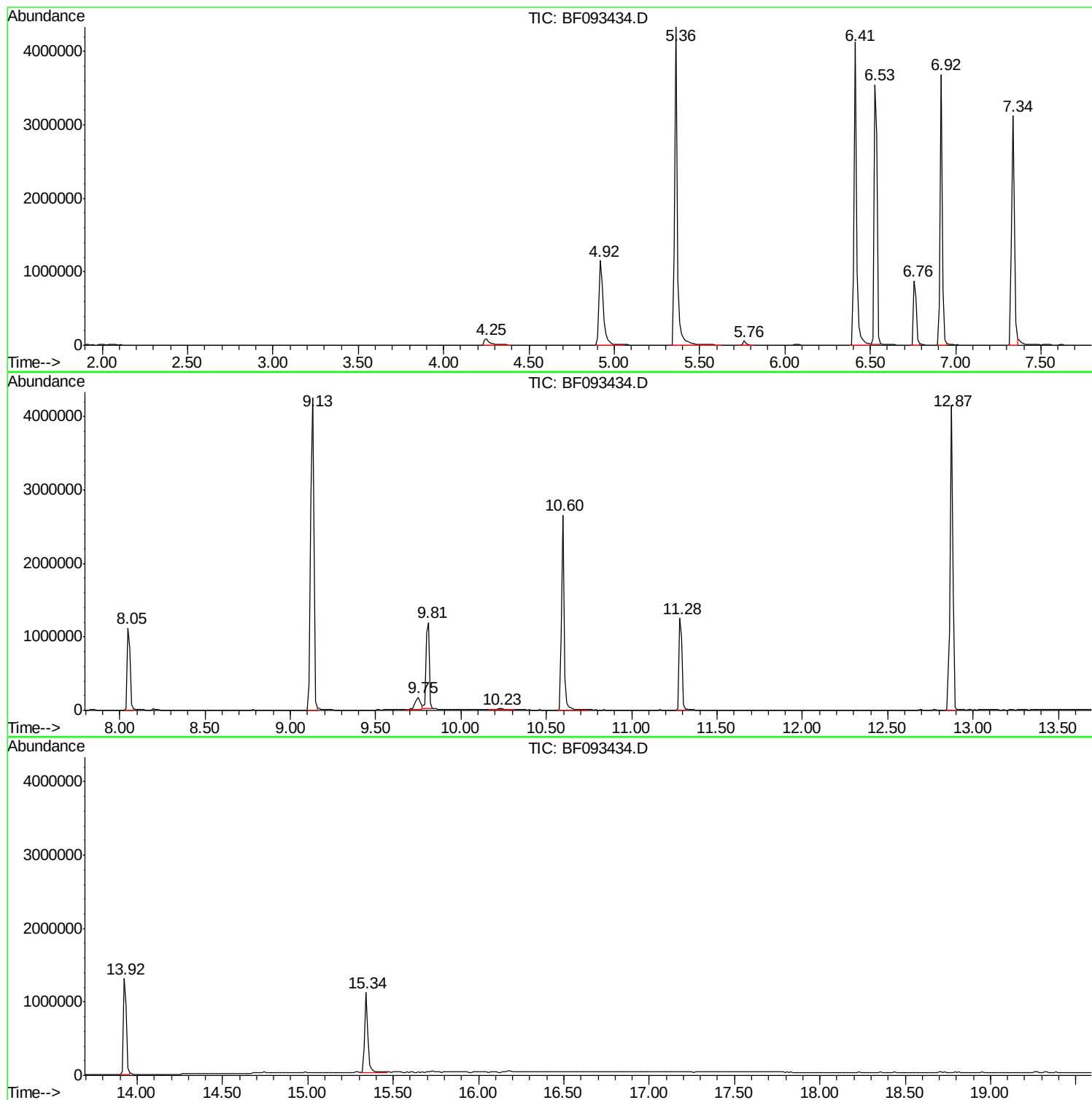
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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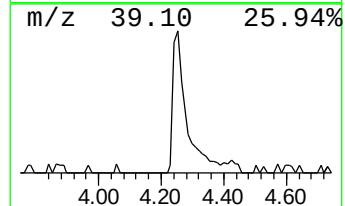
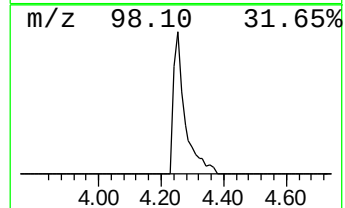
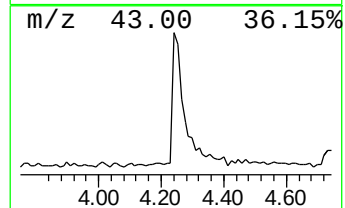
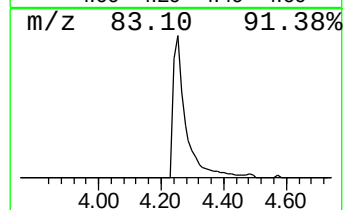
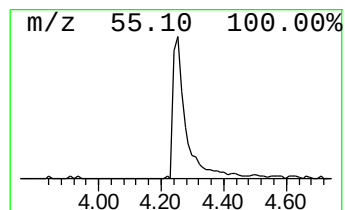
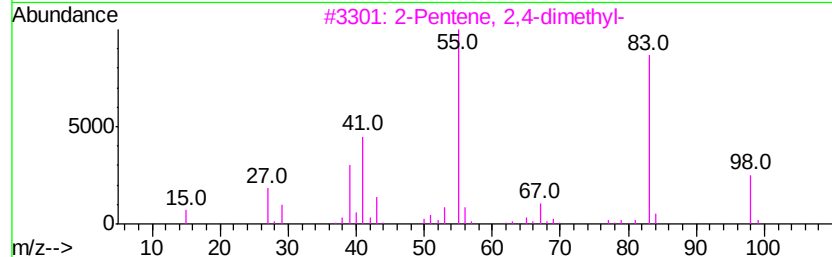
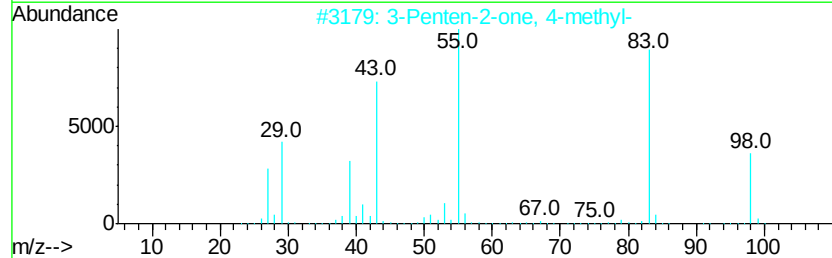
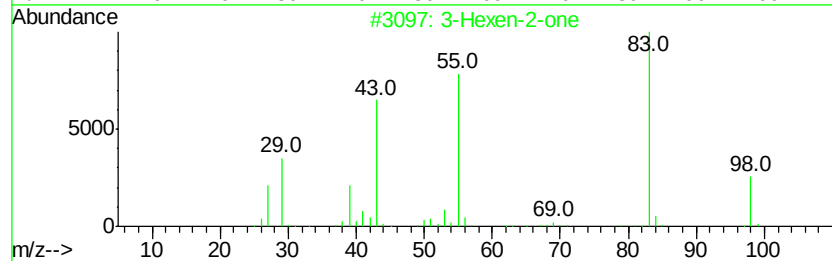
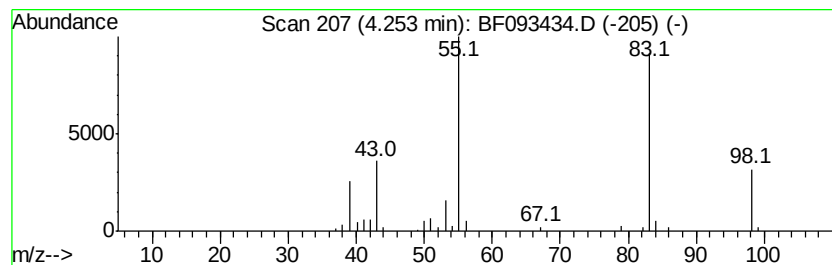
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Hexen-2-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.25	3.96 ng	219521	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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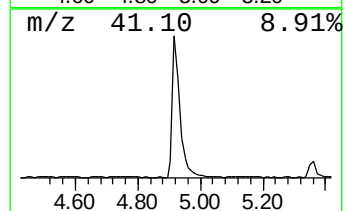
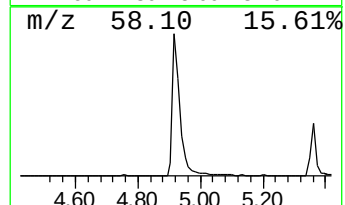
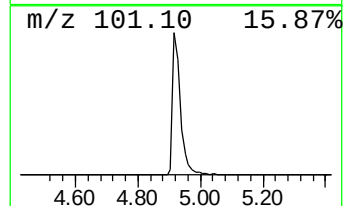
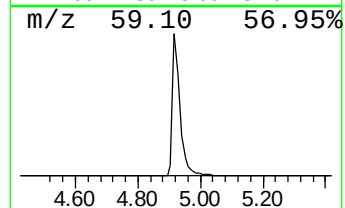
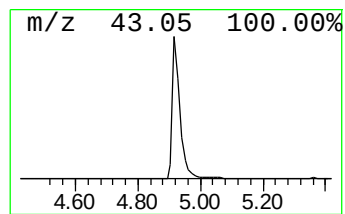
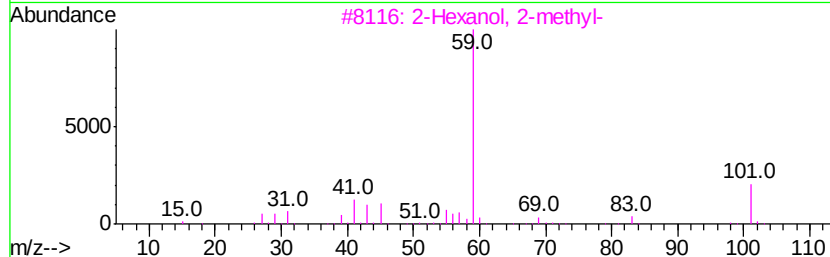
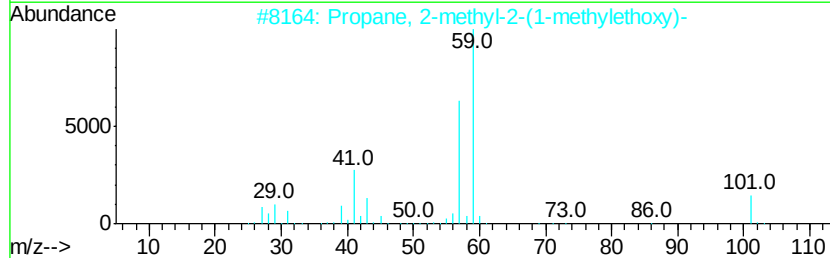
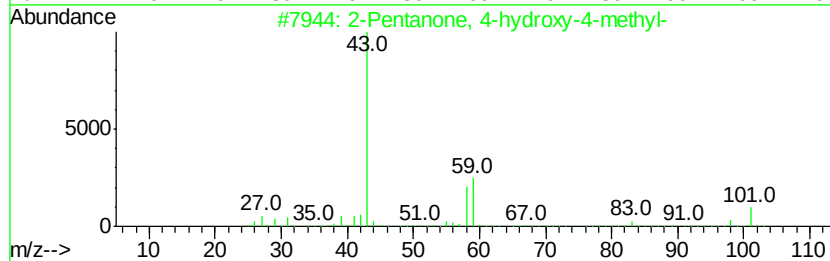
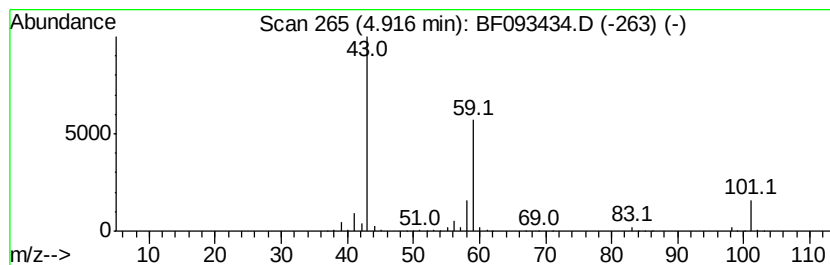
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TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	34.19 ng	1895300	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	42
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	23



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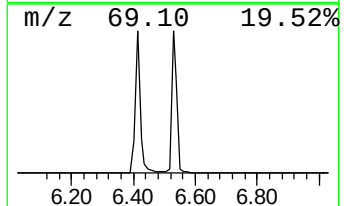
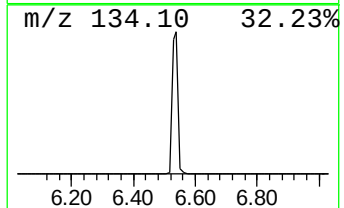
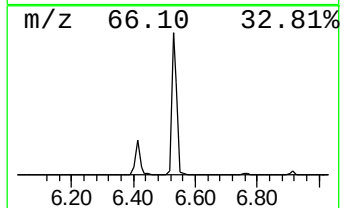
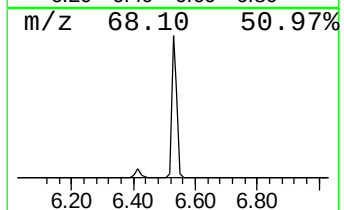
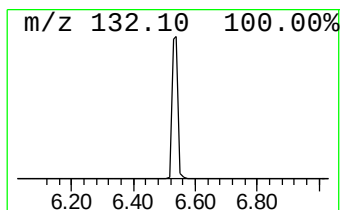
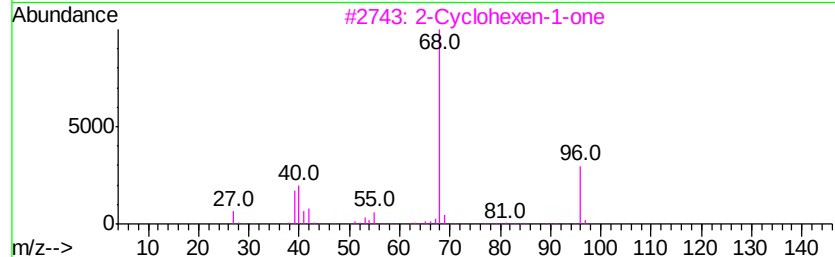
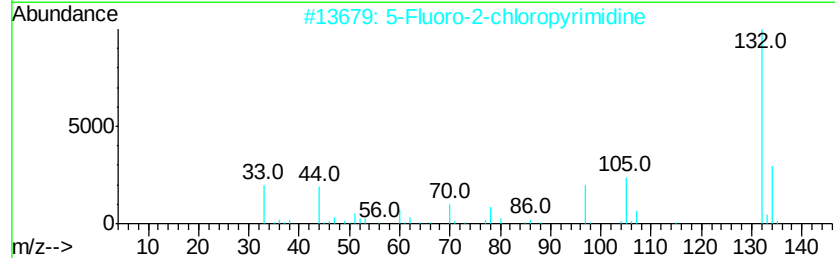
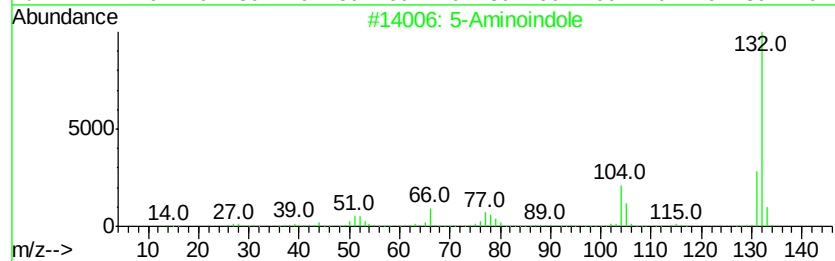
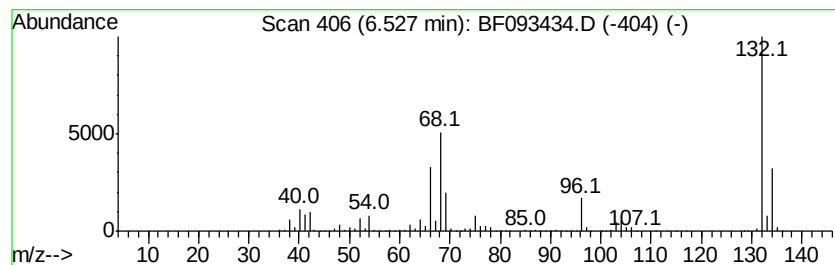
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Peak Number 3 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	81.03 ng	4492210	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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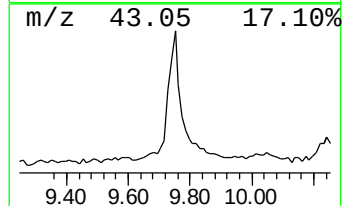
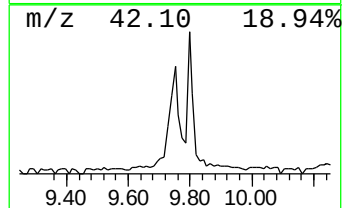
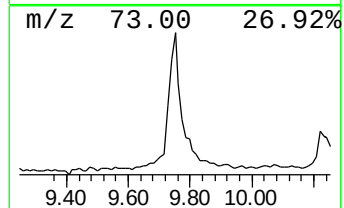
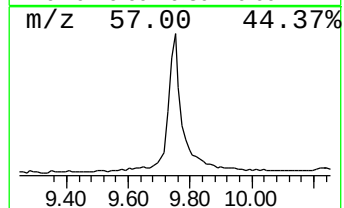
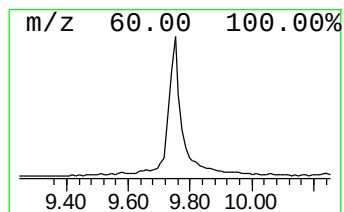
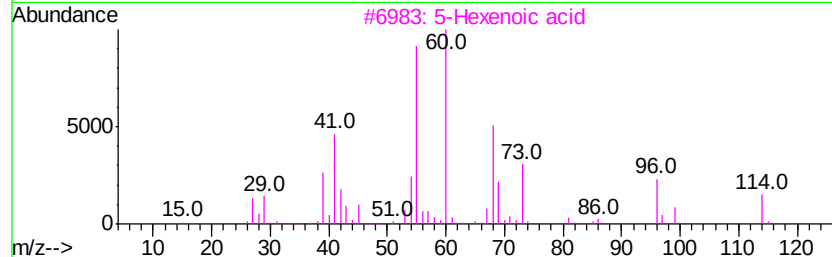
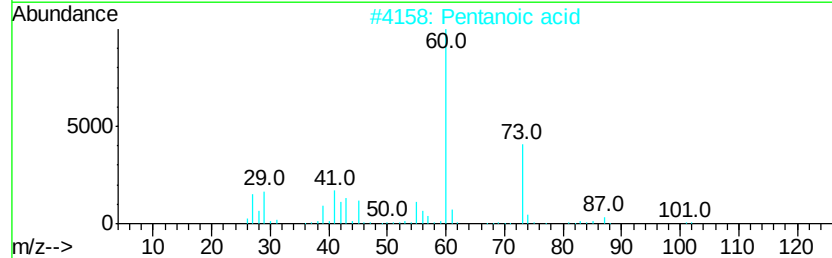
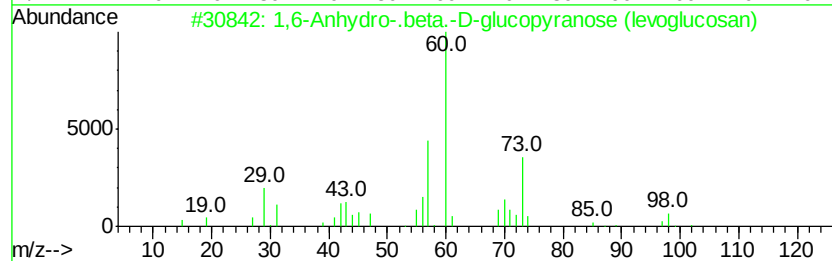
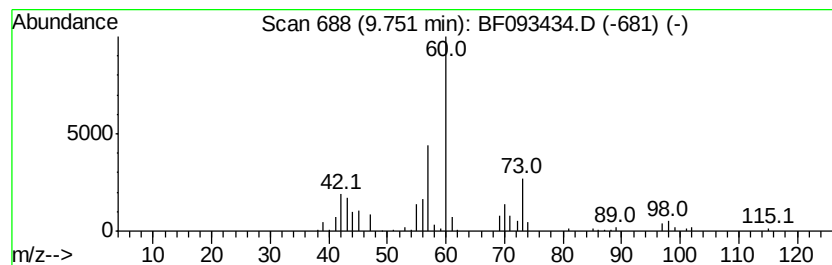
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Peak Number 5 1,6-Anhydro-.beta.-D-glucop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.75	4.69 ng	374391	Acenaphthene-d10	9.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	64
2		Pentanoic acid	102	C5H10O2	000109-52-4	59
3		5-Hexenoic acid	114	C6H10O2	001577-22-6	42
4		3,4-Altrosan	162	C6H10O5	1000129-76-4	40
5		.beta.-D-Ribopyranoside, methyl	164	C6H12O5	017289-61-1	36



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Hexen-2-one	4.25	4.0	ng	219521	1	6.76	1108730	20.0
2-Pentanone, 4-hy...	4.92	34.2	ng	1895300	1	6.76	1108730	20.0
unknown6.53	6.53	81.0	ng	4492210	1	6.76	1108730	20.0
1,6-Anhydro-.beta...	9.75	4.7	ng	374391	3	9.81	1594920	20.0