

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013017\
 Data File : BF092647.D
 Acq On : 30 Jan 2017 21:32
 Operator : SJ/MA
 Sample : I1569-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ELT-GW-01

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-BF013017.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	4.499	209	211	215	rBV	59791	92869	1.68%	0.247%
2	5.139	265	267	270	rBV	721032	883764	16.02%	2.347%
3	5.573	302	305	307	rBV	2053448	2544252	46.11%	6.756%
4	6.590	392	394	397	rVB	1495862	1486086	26.93%	3.946%
5	6.727	403	406	409	rBV	3566088	3624950	65.69%	9.625%
6	6.956	424	426	429	rBV	1170791	992260	17.98%	2.635%
7	7.116	437	440	443	rBV	3612189	3450602	62.53%	9.162%
8	7.310	452	457	461	rBV	63631	121015	2.19%	0.321%
9	7.527	473	476	478	rBV	2837121	2981567	54.03%	7.917%
10	7.973	510	515	519	rBV3	51792	130229	2.36%	0.346%
11	8.248	536	539	542	rBV	1453468	1316562	23.86%	3.496%
12	8.910	592	597	600	rVB4	25555	61141	1.11%	0.162%
13	9.322	630	633	636	rBV	3782743	5518087	100.00%	14.652%
14	9.928	678	686	690	rVV	162781	395371	7.17%	1.050%
15	10.008	690	693	695	rVB	1688727	1774972	32.17%	4.713%
16	10.431	727	730	732	rVB3	38326	60105	1.09%	0.160%
17	10.796	759	762	765	rBV	2714257	3081255	55.84%	8.181%
18	11.494	820	823	825	rBV	1850013	1675278	30.36%	4.448%
19	13.082	959	962	964	rBV	4675718	4928431	89.31%	13.086%
20	14.134	1051	1054	1056	rVB	1205237	1430346	25.92%	3.798%
21	14.980	1124	1128	1130	rBV	31094	56055	1.02%	0.149%
22	15.597	1179	1182	1189	rVB	784000	1056052	19.14%	2.804%

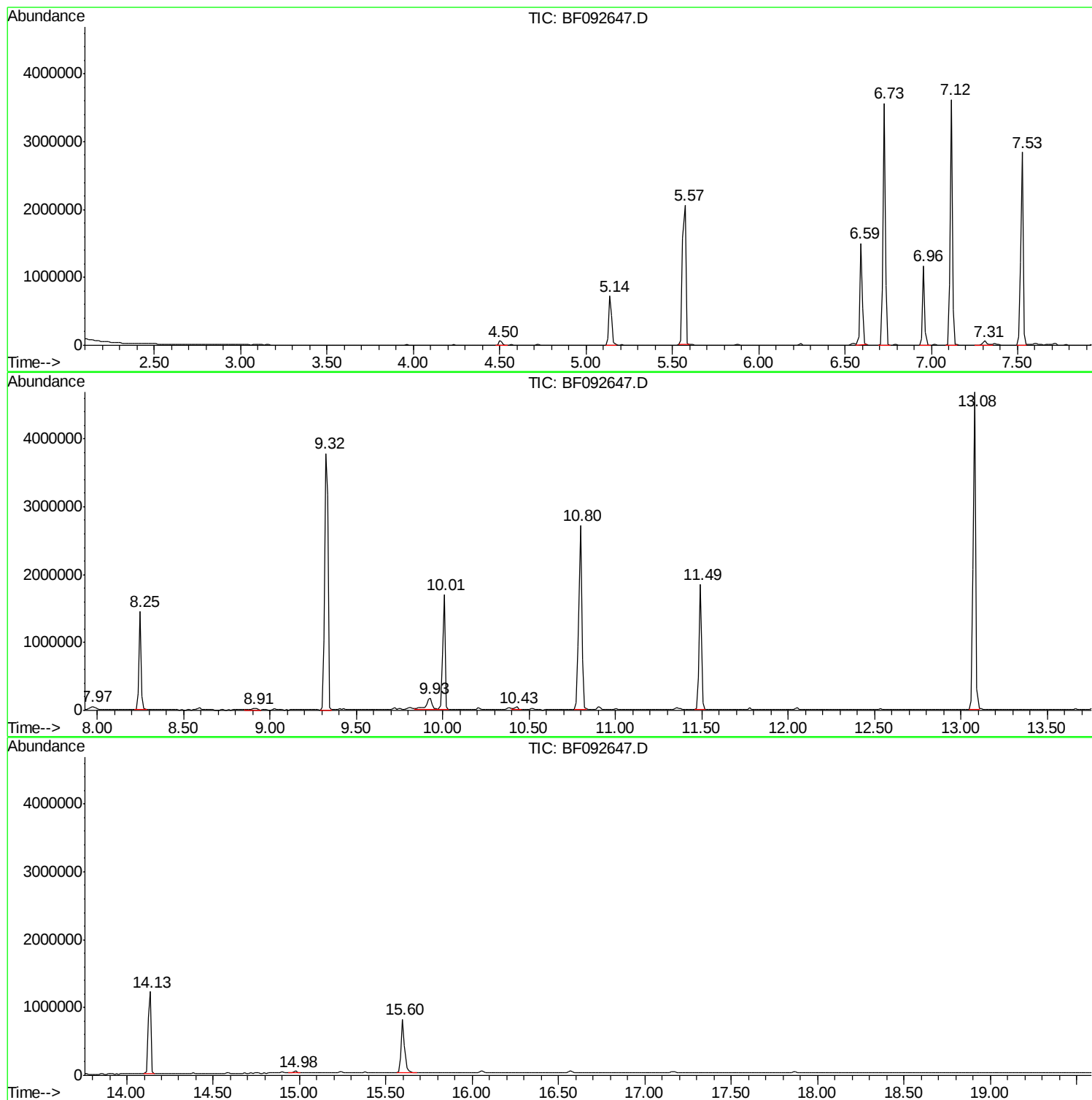
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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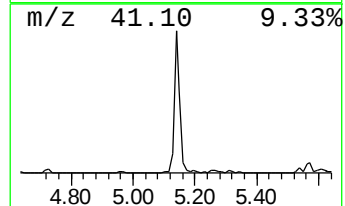
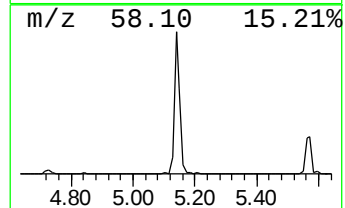
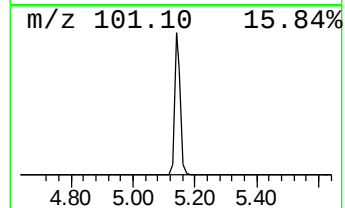
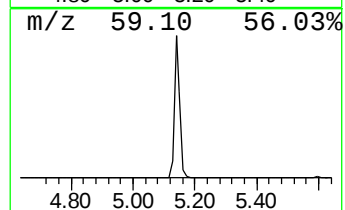
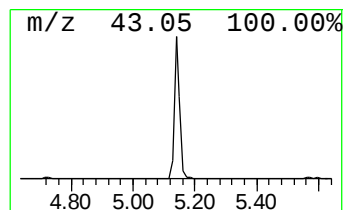
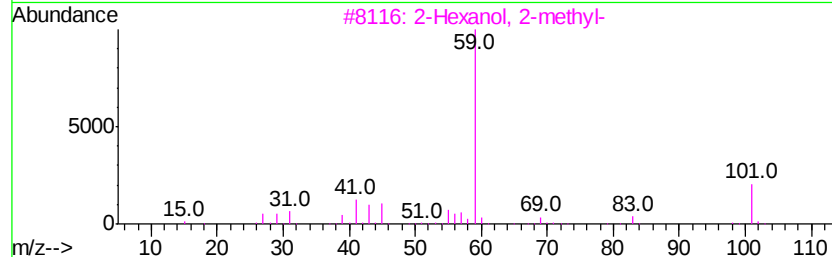
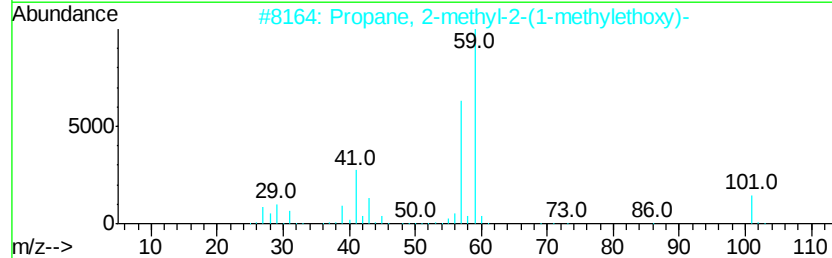
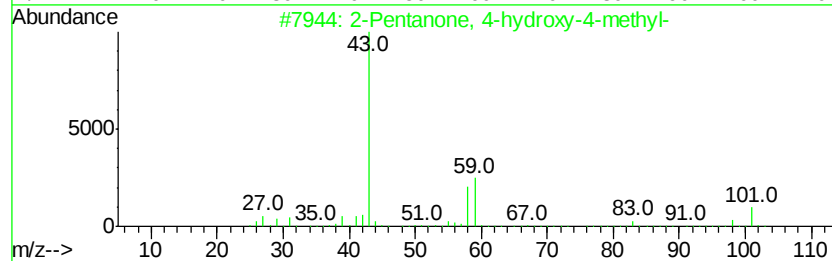
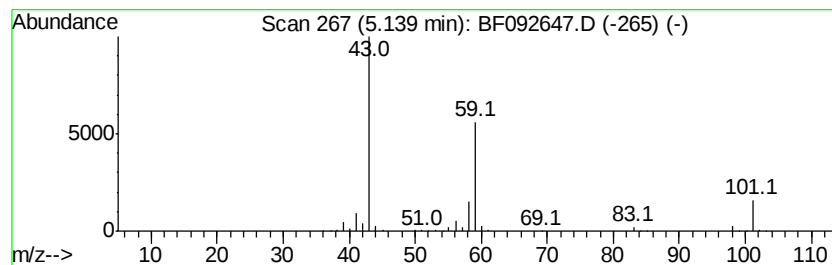
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.14	17.81 ng	883764	1,4-Dichlorobenzene-d4	6.96

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	25



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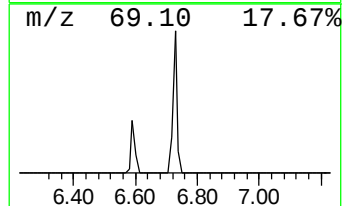
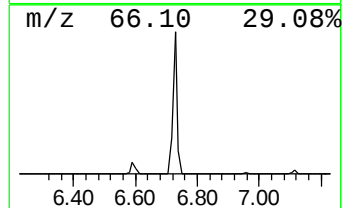
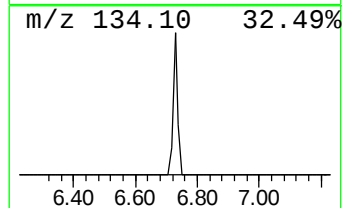
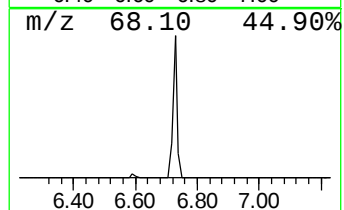
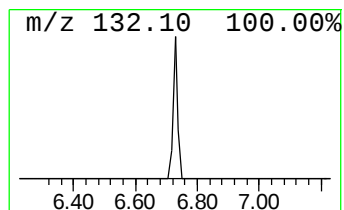
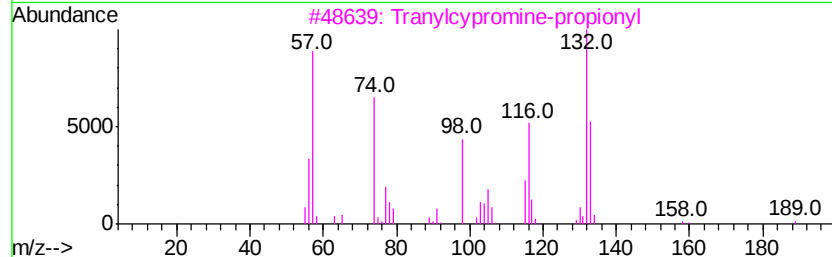
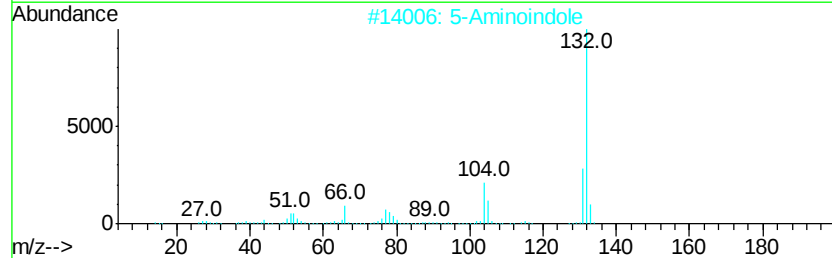
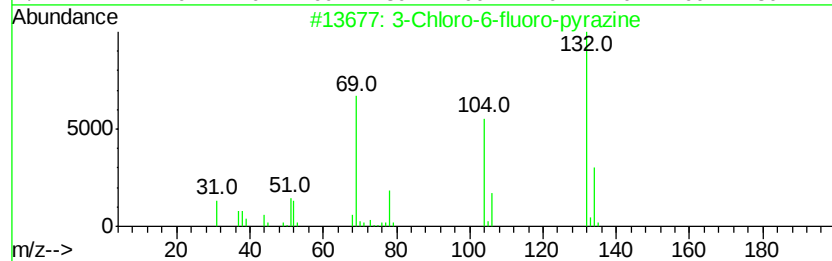
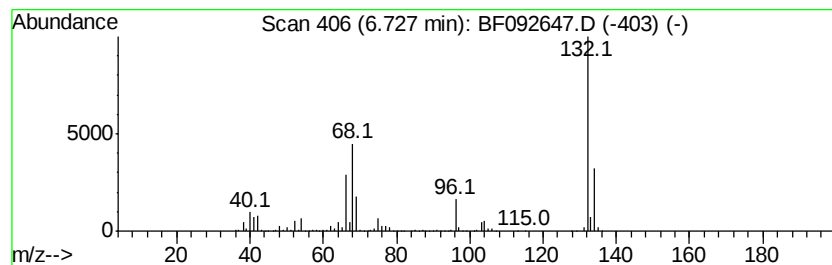
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Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	73.06 ng	3624950	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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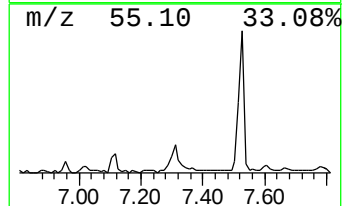
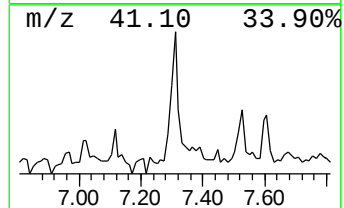
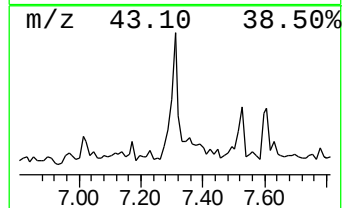
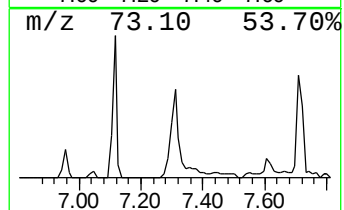
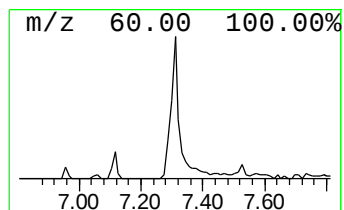
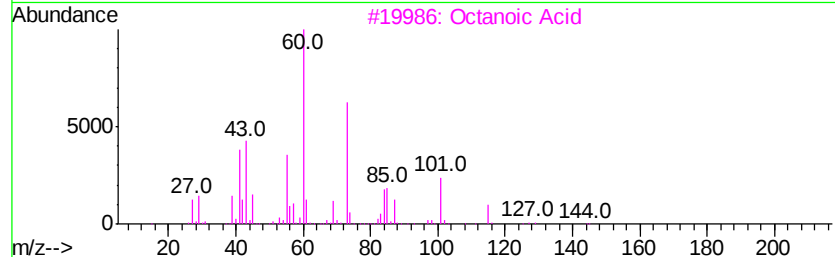
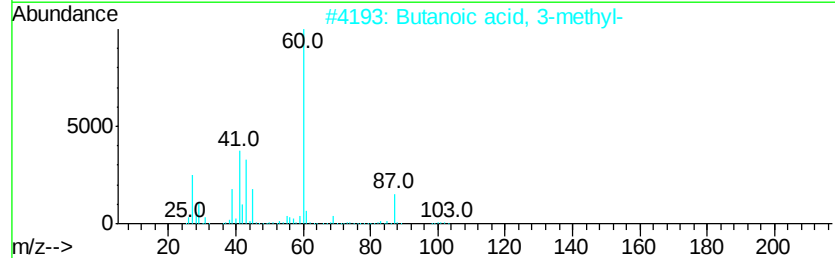
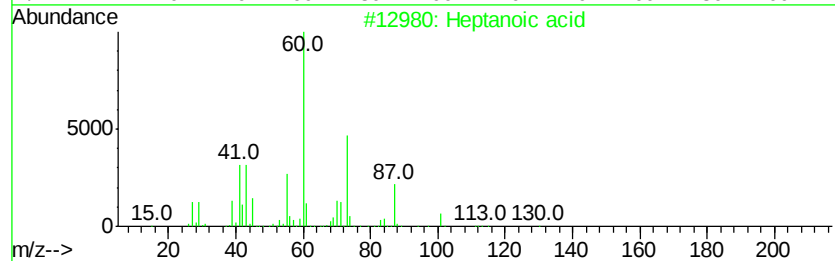
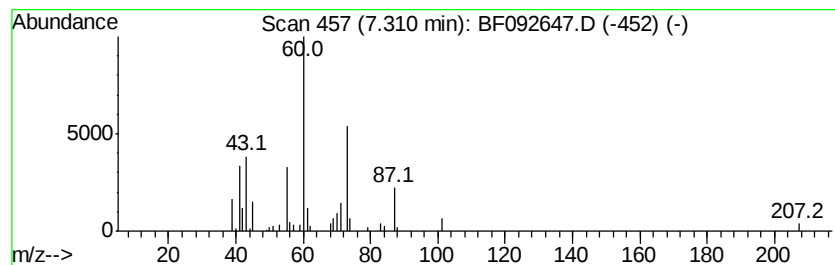
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Peak Number 4 Heptanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.31	2.44 ng	121015	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptanoic acid	130	C7H14O2	000111-14-8	90
2		Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	53
3		Octanoic Acid	144	C8H16O2	000124-07-2	45
4		Hexanoic acid	116	C6H12O2	000142-62-1	45
5		Pentanoic acid	102	C5H10O2	000109-52-4	40



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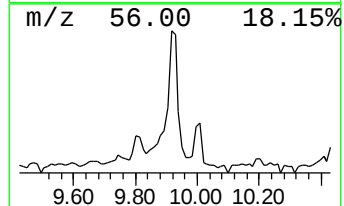
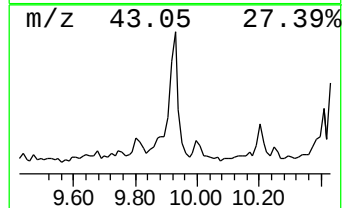
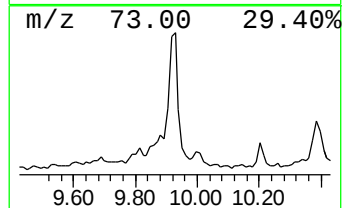
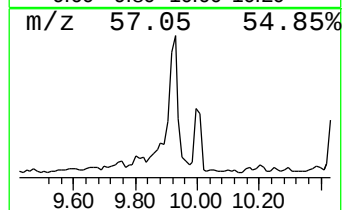
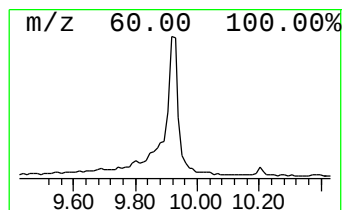
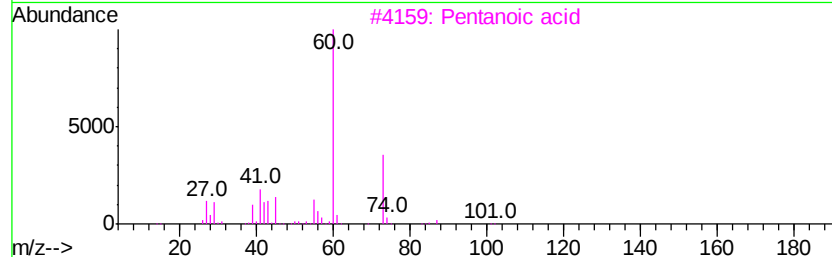
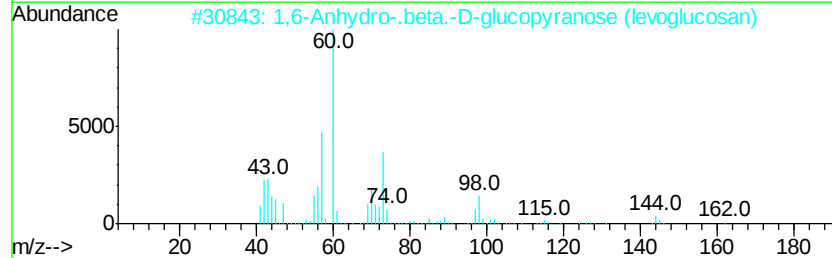
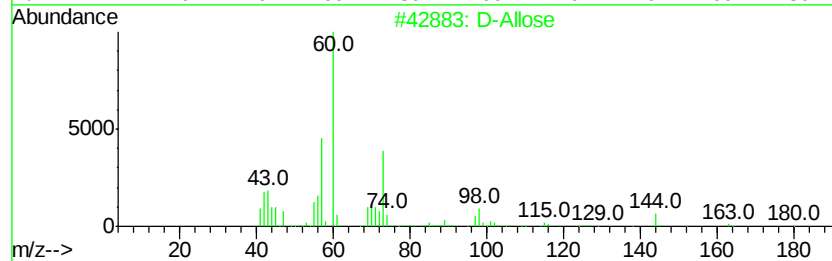
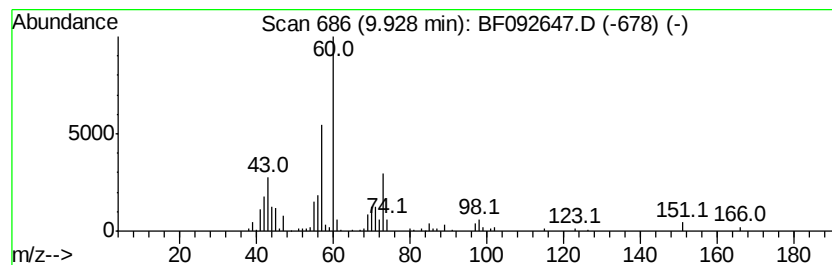
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Peak Number 5 D-Allose Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.93	4.45 ng	395371	Acenaphthene-d10	10.01

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Allose		180	C6H12O6	002595-97-3	78
2	1,6-Anhydro-.beta.-D-glucopyrano...		162	C6H10O5	000498-07-7	78
3	Pentanoic acid		102	C5H10O2	000109-52-4	50
4	Heptanoic acid		130	C7H14O2	000111-14-8	50
5	.beta.-D-Ribopyranoside, methyl		164	C6H12O5	017289-61-1	42



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.14	17.8	ng	883764	1	6.96	992260	20.0
unknown6.73	6.73	73.1	ng	3624950	1	6.96	992260	20.0
Heptanoic acid	7.31	2.4	ng	121015	1	6.96	992260	20.0
D-Allose	9.93	4.5	ng	395371	3	10.01	1774970	20.0