

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013017\
 Data File : BF092642.D
 Acq On : 30 Jan 2017 19:16
 Operator : SJ/MA
 Sample : PB96532BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB96532BL

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	4.521	210	213	216	rVB	55274	79121	1.58%	0.188%
2	5.161	265	269	278	rVB	1494212	2107222	42.18%	5.013%
3	5.584	302	306	308	rBV	3214391	4448675	89.04%	10.583%
4	6.601	392	395	397	rBV	3648232	3894035	77.94%	9.263%
5	6.727	403	406	409	rBV	3295242	4065560	81.37%	9.671%
6	6.956	424	426	429	rVB	1057552	956419	19.14%	2.275%
7	7.116	437	440	443	rBV	3346786	3154245	63.13%	7.503%
8	7.527	473	476	478	rBV	2534596	2732484	54.69%	6.500%
9	8.247	537	539	542	rBV	1117920	1248360	24.99%	2.970%
10	9.333	630	634	636	rBV	4147363	4996171	100.00%	11.885%
11	9.928	678	686	690	rVV	113994	292667	5.86%	0.696%
12	10.008	690	693	695	rVB	1579304	1510914	30.24%	3.594%
13	10.796	759	762	765	rBV	2462317	2751202	55.07%	6.545%
14	11.493	820	823	825	rBV	1683075	1559225	31.21%	3.709%
15	12.568	911	917	924	rBV6	13325	54154	1.08%	0.129%
16	13.082	959	962	964	rBV	4545951	4866293	97.40%	11.576%
17	14.134	1051	1054	1056	rBV	1394127	1567720	31.38%	3.729%
18	14.979	1123	1128	1130	rBV	258662	411058	8.23%	0.978%
19	15.597	1179	1182	1185	rBV	862738	1341780	26.86%	3.192%

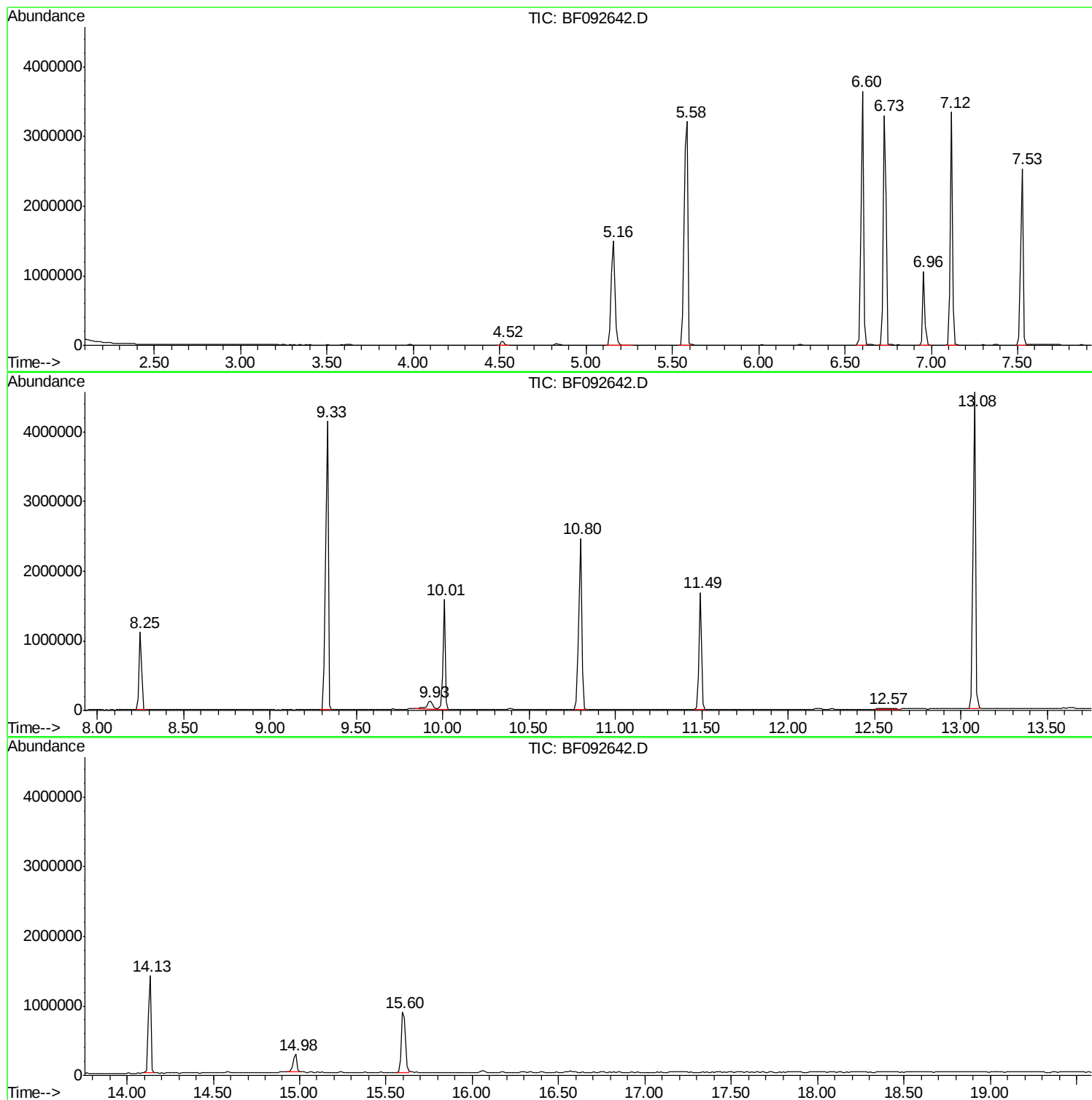
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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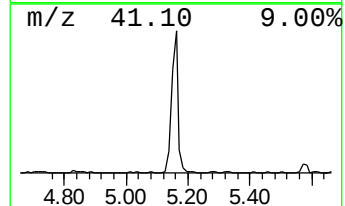
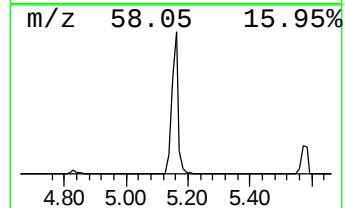
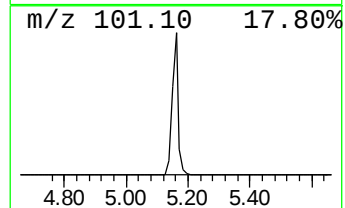
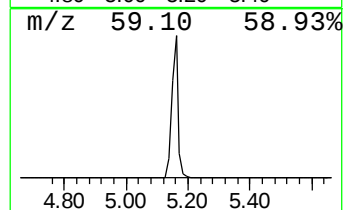
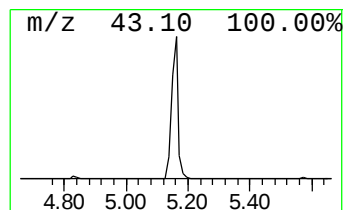
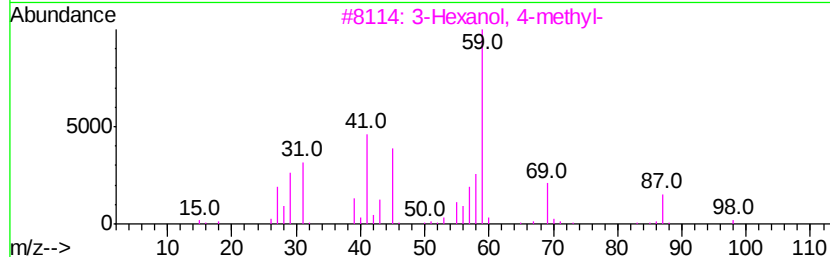
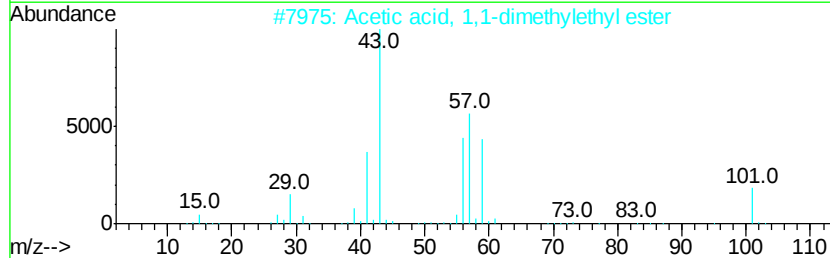
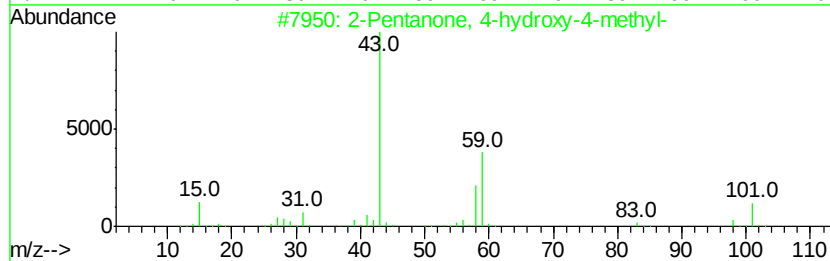
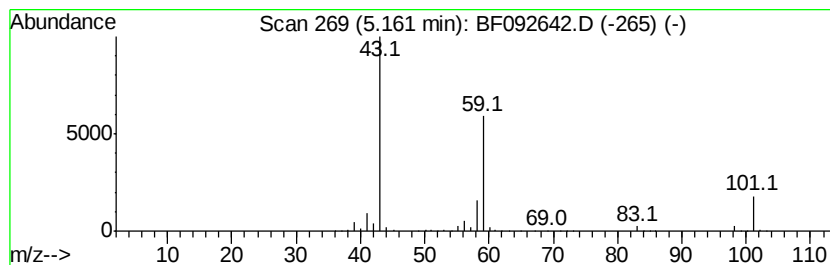
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	44.06 ng	2107220	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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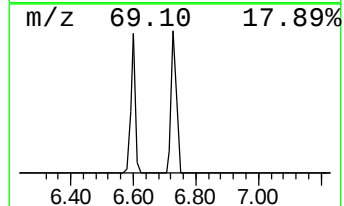
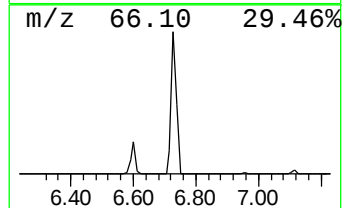
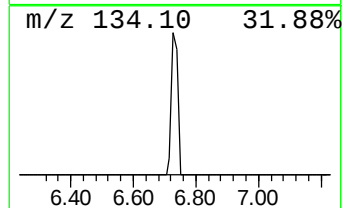
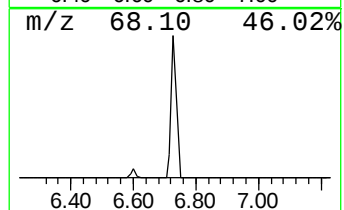
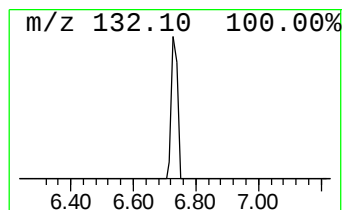
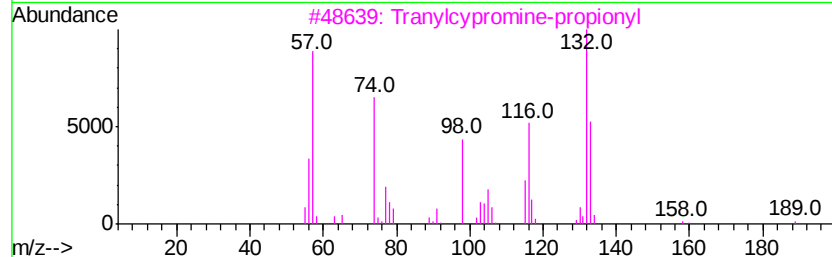
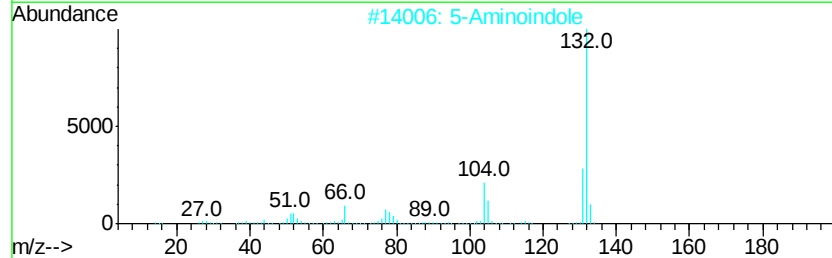
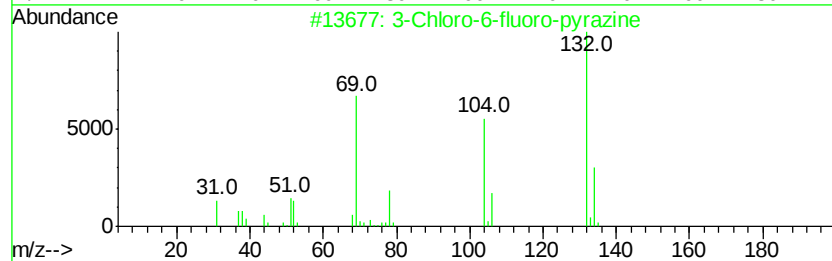
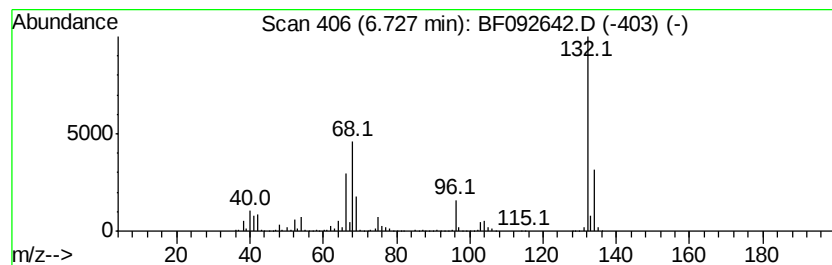
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Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	85.02 ng	4065560	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		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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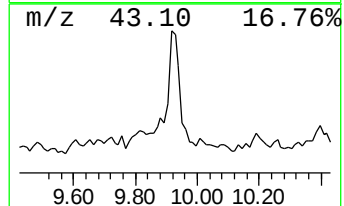
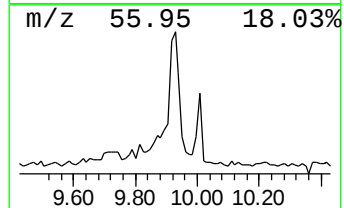
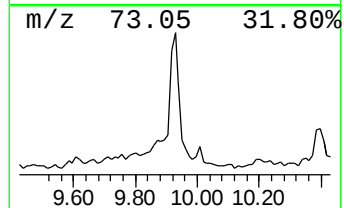
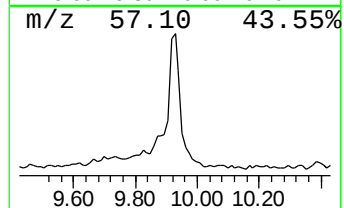
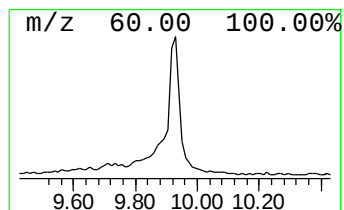
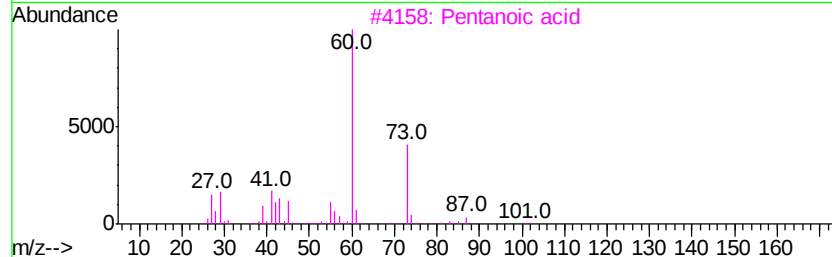
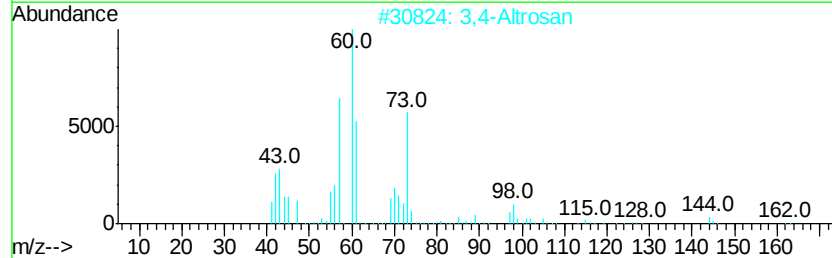
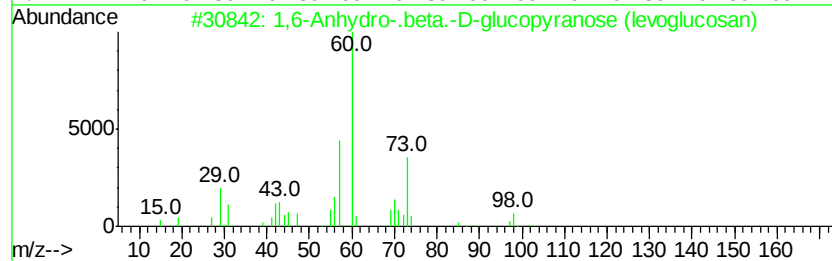
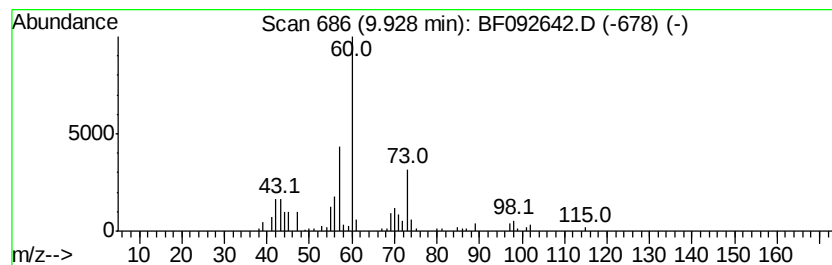
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Peak Number 4 1,6-Anhydro-.beta.-D-glucop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.93	3.87 ng	292667	Acenaphthene-d10	10.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	72
2		3,4-Altrosan	162	C6H10O5	1000129-76-4	53
3		Pentanoic acid	102	C5H10O2	000109-52-4	50
4		Heptanoic acid	130	C7H14O2	000111-14-8	42
5		L-Mannose, 6-deoxy-	164	C6H12O5	003615-41-6	42



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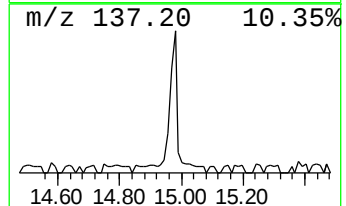
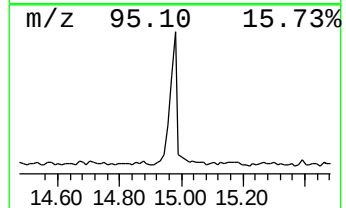
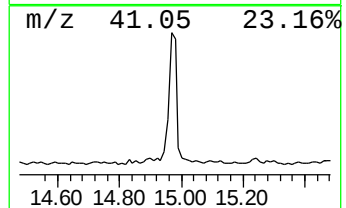
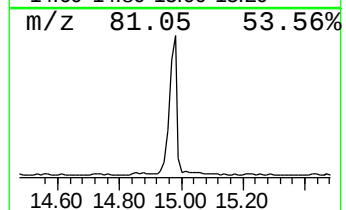
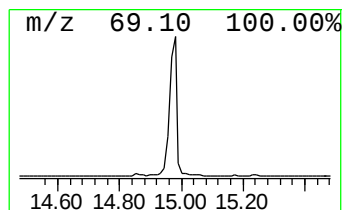
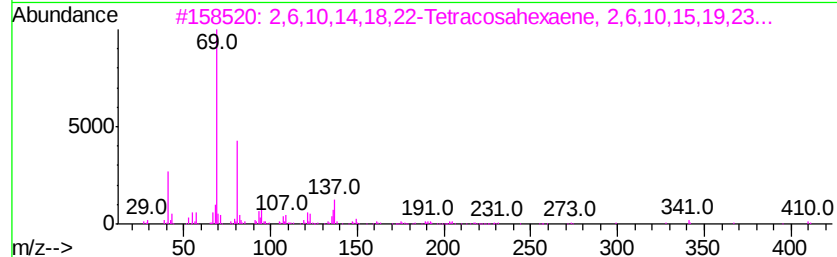
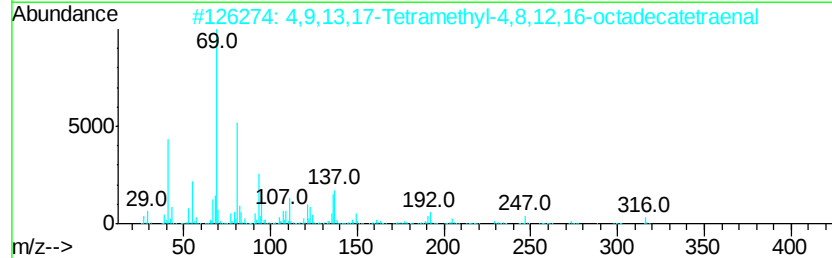
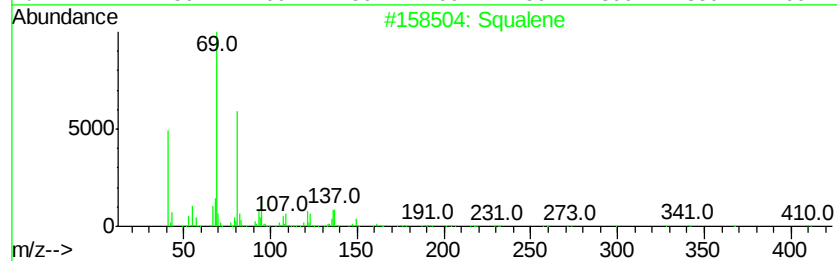
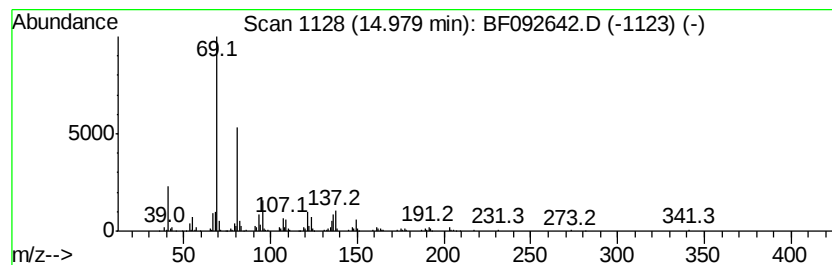
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Peak Number 5 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	6.13 ng	411058	Perylene-d12	15.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	91
2		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
3		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	78
4		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72
5		Trideca-1,7,11-triene-1,1-dicarb...	270	C18H26N2	1000161-46-0	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.16	44.1	ng	2107220	1	6.96	956419	20.0
unknown6.73	6.73	85.0	ng	4065560	1	6.96	956419	20.0
1,6-Anhydro-.beta...	9.93	3.9	ng	292667	3	10.01	1510910	20.0
Squalene	14.98	6.1	ng	411058	6	15.61	1341780	20.0