

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090217\
 Data File : BF098261.D
 Acq On : 2 Sep 2017 22:24
 Operator : SJ/JU
 Sample : I5055-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RT3992-20-41-RT3451-1550

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-BF081517.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	3.075	165	168	177	rBV	18744	47665	1.65%	0.191%
2	4.245	363	367	376	rBV	44406	59180	2.05%	0.237%
3	4.904	476	479	490	rVB	184742	253679	8.80%	1.017%
4	5.322	545	550	554	rBV	2463841	2736035	94.94%	10.966%
5	6.357	721	726	743	rBV	2422651	2881928	100.00%	11.551%
6	6.486	743	748	751	rBV	2626191	2653539	92.08%	10.635%
7	6.710	783	786	790	rBV	872519	675904	23.45%	2.709%
8	6.869	809	813	816	rBV	2397560	2099470	72.85%	8.415%
9	7.281	878	883	886	rBV	1799212	1686053	58.50%	6.758%
10	7.992	1000	1004	1008	rBV	958434	834174	28.94%	3.343%
11	9.075	1182	1188	1191	rBV	2765985	2729115	94.70%	10.938%
12	9.145	1196	1200	1203	rVV2	46668	54611	1.89%	0.219%
13	9.463	1250	1254	1257	rBV2	304550	389702	13.52%	1.562%
14	9.510	1259	1262	1266	rVV3	75337	98467	3.42%	0.395%
15	9.610	1276	1279	1282	rBV3	218918	285032	9.89%	1.142%
16	9.657	1284	1287	1290	rVB	408980	348812	12.10%	1.398%
17	9.698	1290	1294	1296	rBV3	123213	183786	6.38%	0.737%
18	9.745	1299	1302	1306	rVB	901246	834500	28.96%	3.345%
19	9.786	1306	1309	1313	rBV3	143653	255121	8.85%	1.023%
20	10.116	1362	1365	1368	rBV3	219581	272985	9.47%	1.094%
21	10.151	1368	1371	1374	rVV2	516783	482085	16.73%	1.932%
22	10.539	1433	1437	1440	rBV	1122686	1161460	40.30%	4.655%
23	11.233	1553	1555	1559	rVB	614156	561306	19.48%	2.250%
24	12.821	1821	1825	1832	rVB	1984082	1974840	68.52%	7.915%
25	13.868	1999	2003	2006	rVB	801874	719383	24.96%	2.883%
26	15.280	2239	2243	2252	rVB	528495	671373	23.30%	2.691%

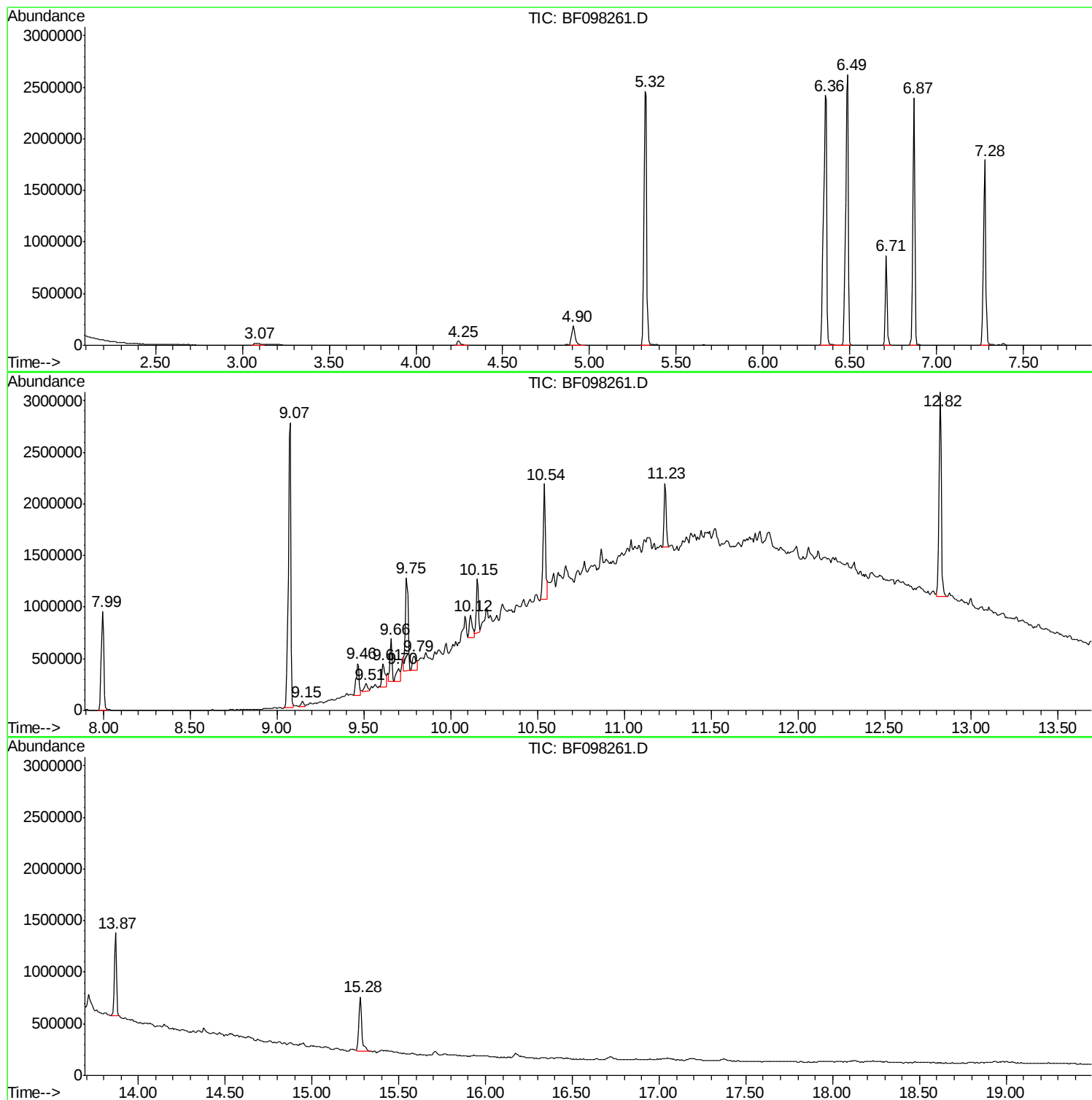
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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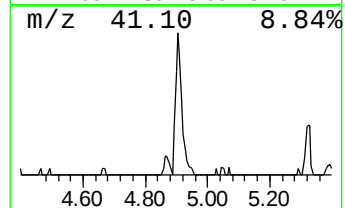
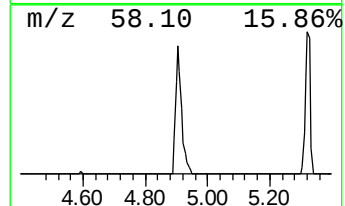
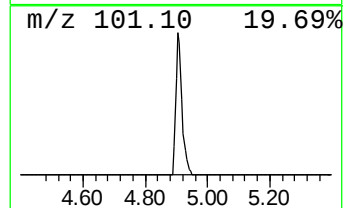
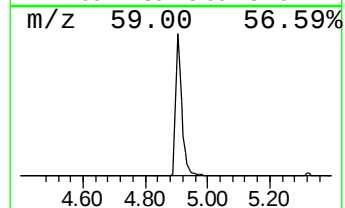
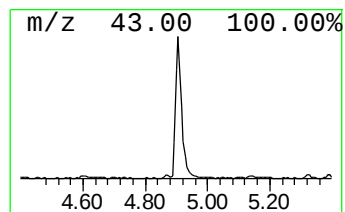
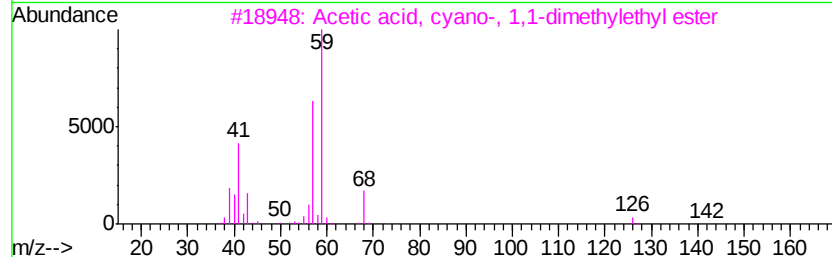
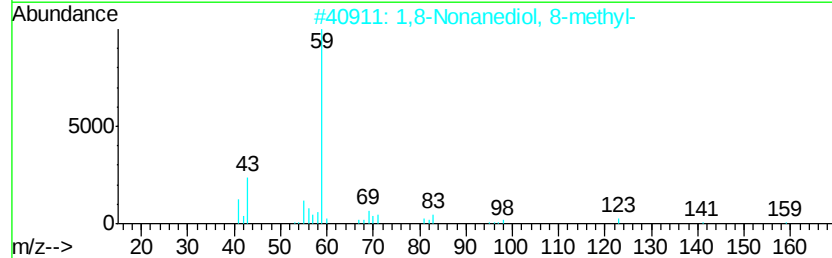
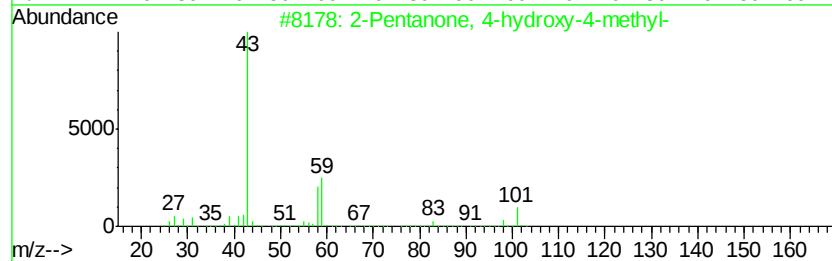
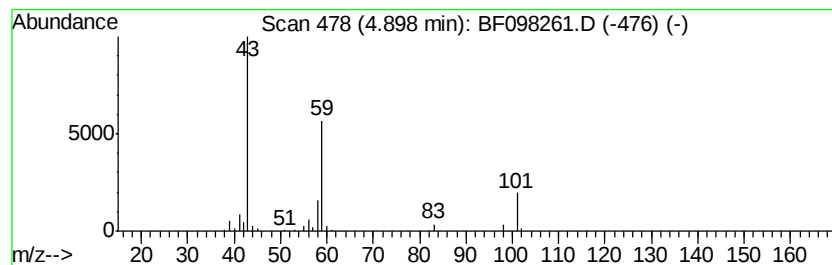
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	7.51 ng	253679	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			Acetone	58	C3H6O	000067-64-1	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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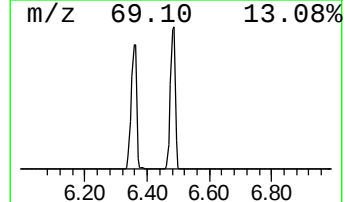
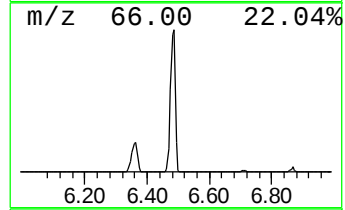
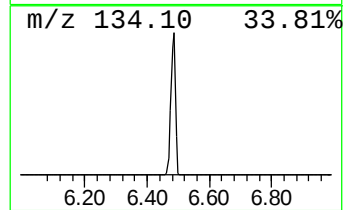
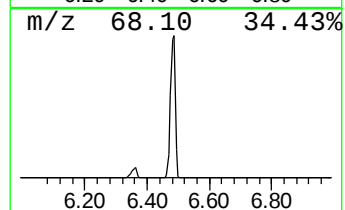
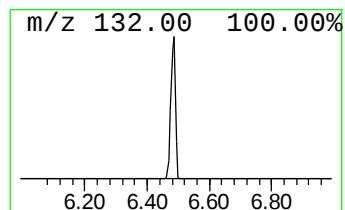
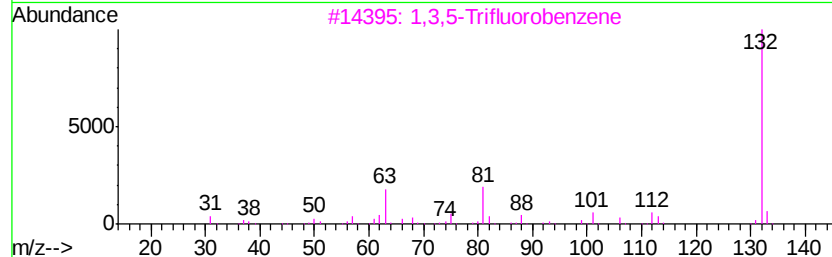
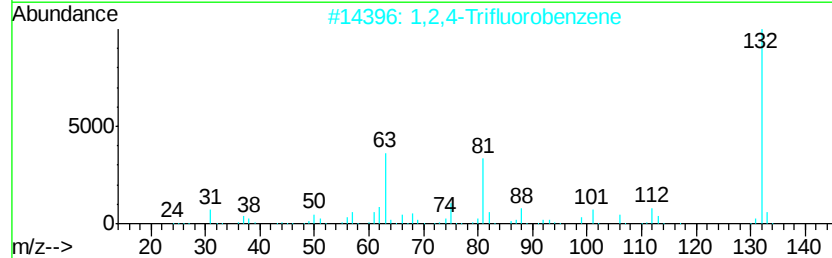
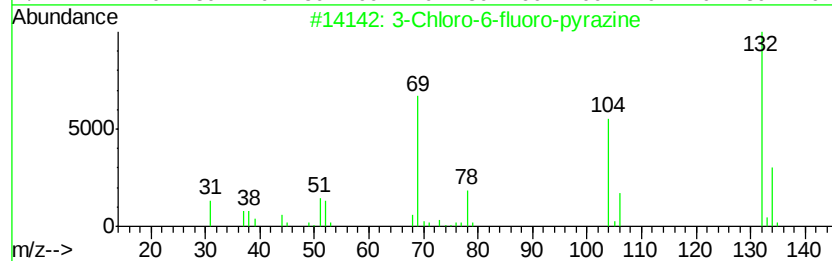
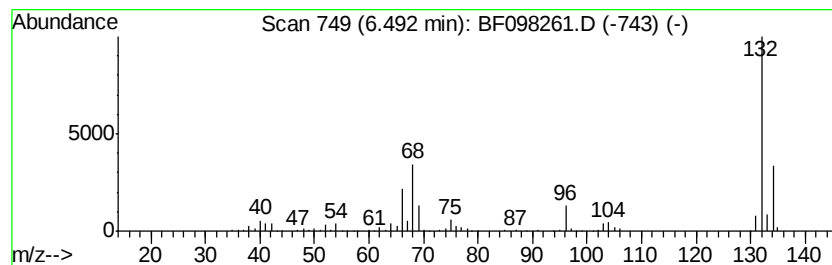
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	78.52 ng	2653540	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		Xenon	132	Xe	007440-63-3	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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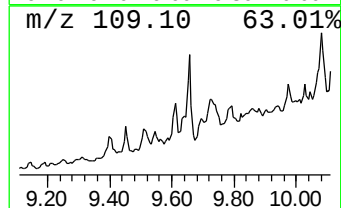
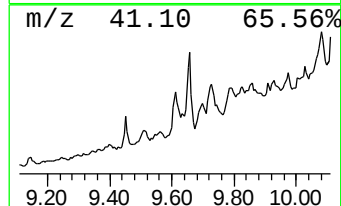
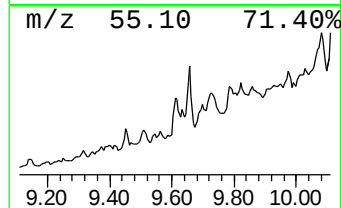
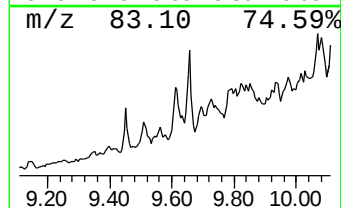
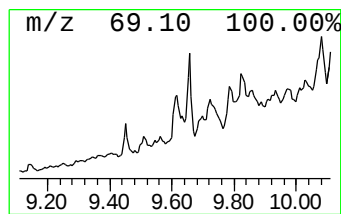
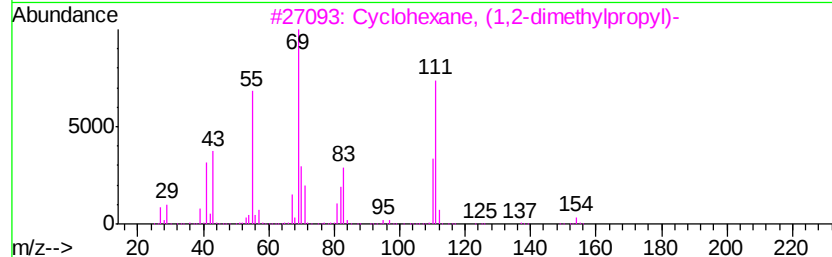
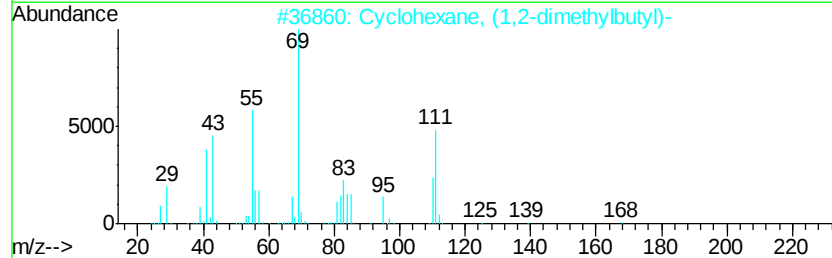
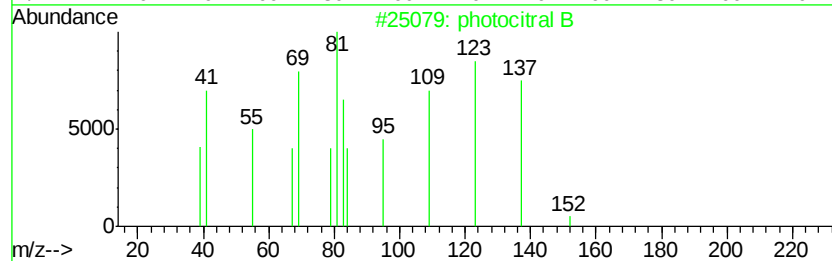
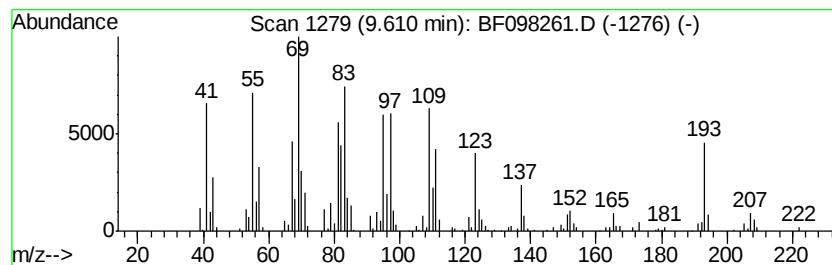
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TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown9.61 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.61	6.83 ng	285032	Acenaphthene-d10	9.75
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		photocitral B	152 C10H16O	006040-45-5 38
2		Cyclohexane, (1,2-dimethylbutyl)-	168 C12H24	061142-37-8 22
3		Cyclohexane, (1,2-dimethylpropyl)-	154 C11H22	051284-29-8 22
4		Cyclopropane carboxamide, 2-cycl...	207 C13H21NO	331416-19-4 18
5		2(1H)-Naphthalenone, octahydro-4...	208 C14H24O	054594-42-2 18



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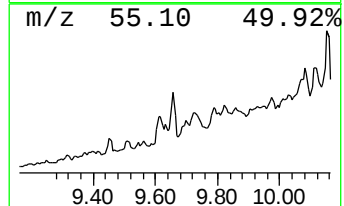
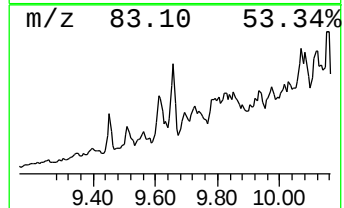
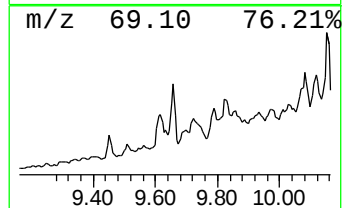
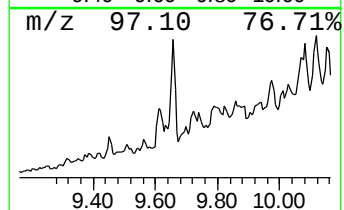
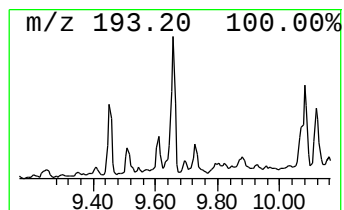
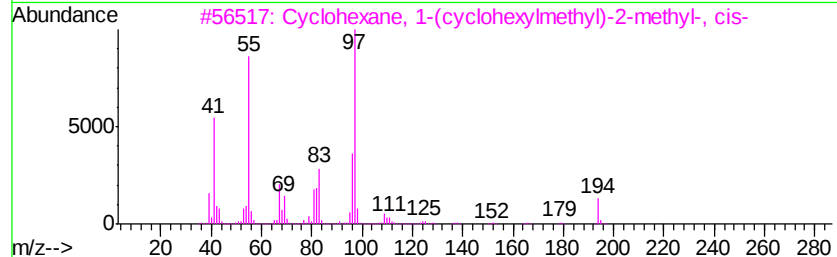
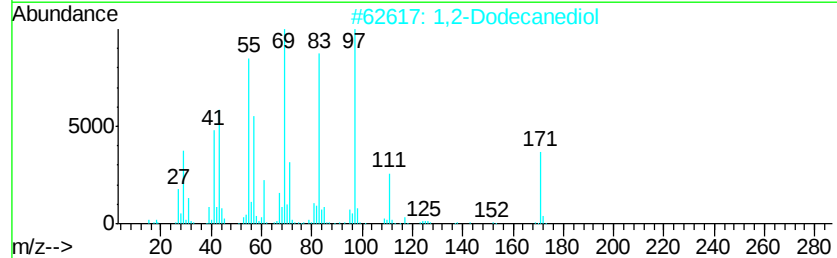
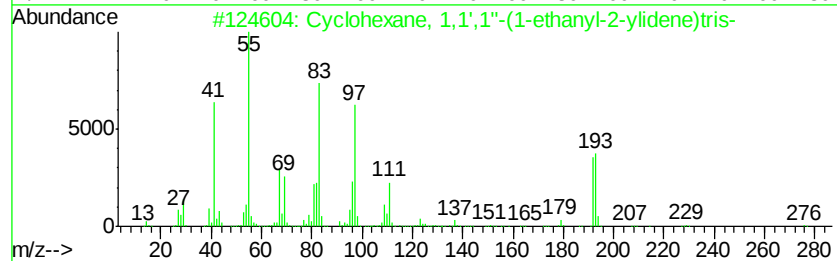
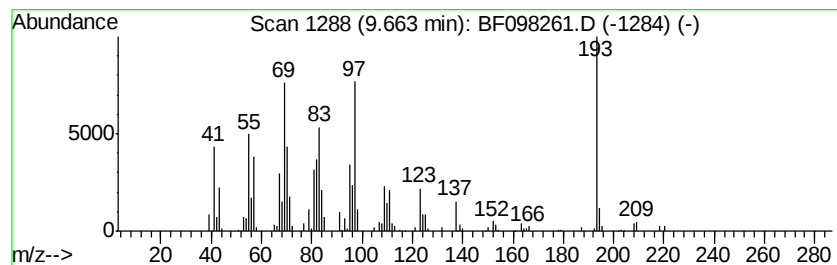
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Peak Number 5 unknown9.66 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.66	8.36 ng	348812	Acenaphthene-d10	9.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,1',1''-(1-ethanyl...	276	C20H36	055682-86-5	35
2		1,2-Dodecanediol	202	C12H26O2	001119-87-5	27
3		Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054824-04-3	18
4		Oxiranecarboxaldehyde, 3-methyl-...	168	C10H16O2	016996-12-6	18
5		Cyclohexanemethanol, 4-methyl-, ...	128	C8H16O	003937-49-3	14



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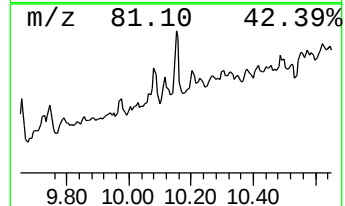
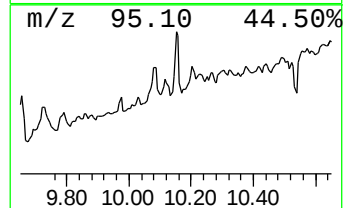
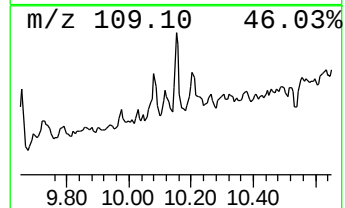
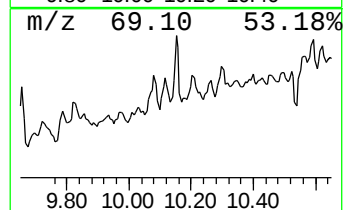
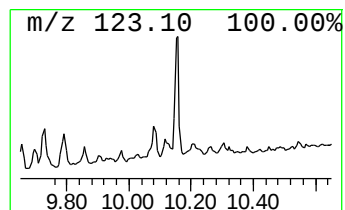
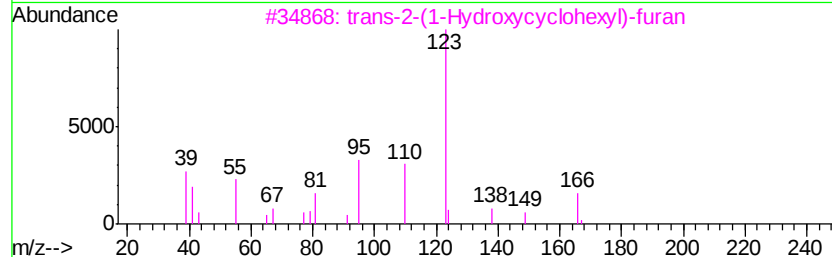
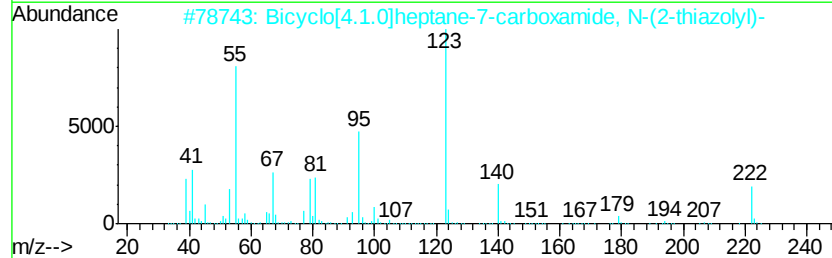
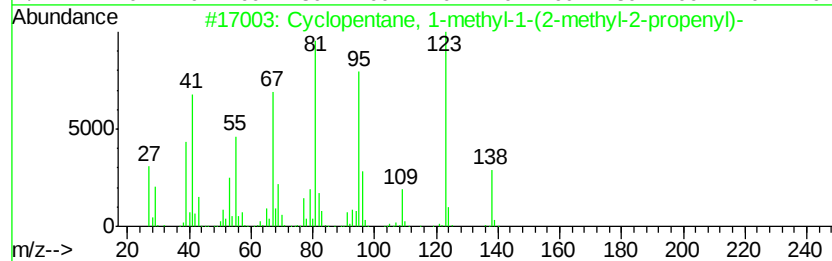
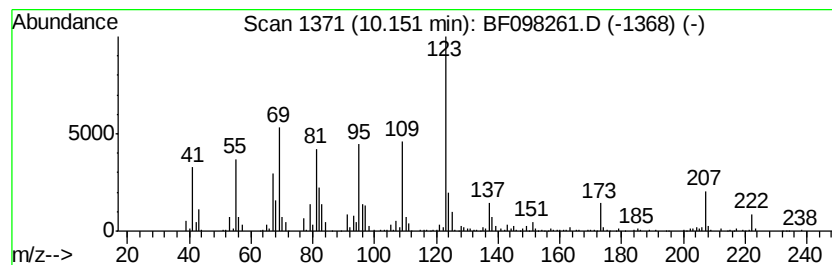
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Peak Number 7 unknown10.15 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.15	11.55 ng	482085	Acenaphthene-d10	9.75
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclopentane, 1-methyl-1-(2-meth...	138 C10H18	074764-47-9 43
2		Bicyclo[4.1.0]heptane-7-carboxam...	222 C11H14N2OS	329912-72-3 38
3		trans-2-(1-Hydroxycyclohexyl)-furan	166 C10H14O2	115754-87-5 38
4		4-Fluorobenzoic acid, 5-pentadec...	350 C22H35FO2	1000280-68-6 35
5		3-Fluorobenzoic acid, 2-ethylcyc...	250 C15H19FO2	1000279-04-9 32



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	7.5	ng	253679	1	6.71	675904	20.0
unknown6.49	6.49	78.5	ng	2653540	1	6.71	675904	20.0
unknown9.61	9.61	6.8	ng	285032	3	9.75	834500	20.0
unknown9.66	9.66	8.4	ng	348812	3	9.75	834500	20.0
unknown10.15	10.15	11.6	ng	482085	3	9.75	834500	20.0