

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112217\
 Data File : BF100863.D
 Acq On : 23 Nov 2017 9:47
 Operator : SJ/JU
 Sample : I6541-05
 Misc :
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 111717-SIDI-F-D-B

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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	2.151	8	11	23	rVB2	39361	64647	2.55%	0.470%
2	5.075	505	508	517	rBB	131429	137801	5.43%	1.002%
3	5.475	572	576	579	rBV	802698	686261	27.04%	4.992%
4	6.481	743	747	757	rBB	582429	473137	18.65%	3.442%
5	6.628	767	772	775	rBV	1402847	1226018	48.32%	8.919%
6	6.857	807	811	814	rBV	573909	436855	17.22%	3.178%
7	7.016	833	838	841	rBV	1872137	1696559	66.86%	12.342%
8	7.428	901	908	910	rBV	1234108	1385028	54.58%	10.075%
9	8.139	1025	1029	1032	rBV	709759	556997	21.95%	4.052%
10	9.216	1206	1212	1215	rBV	2606902	2537545	100.00%	18.459%
11	9.892	1322	1327	1331	rBV	612739	609399	24.02%	4.433%
12	10.686	1457	1462	1465	rBV	931991	877175	34.57%	6.381%
13	11.380	1576	1580	1584	rBV	644203	517859	20.41%	3.767%
14	12.968	1845	1850	1853	rBV	1906717	1736259	68.42%	12.630%
15	13.851	1995	2000	2004	rBV	34037	36088	1.42%	0.263%
16	14.021	2025	2029	2033	rBV	402751	358366	14.12%	2.607%
17	15.492	2273	2279	2286	rBV	319848	410661	16.18%	2.987%

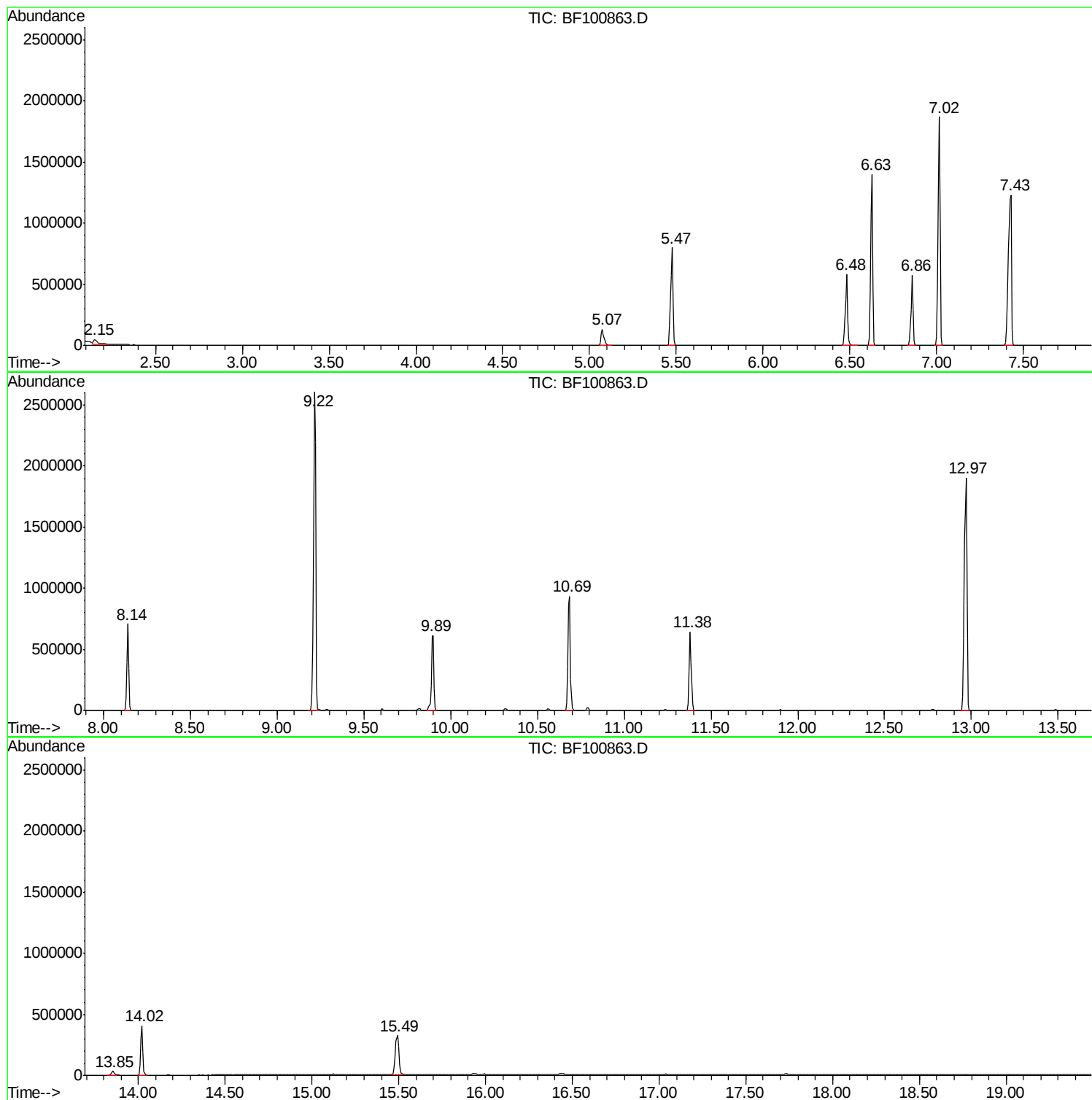
Sum of corrected areas: 13746655

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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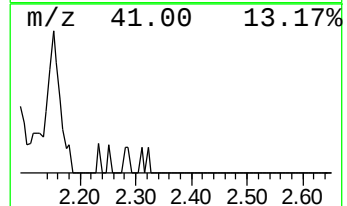
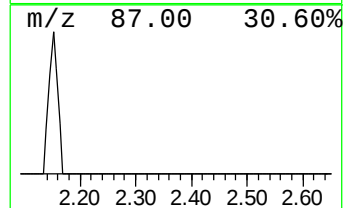
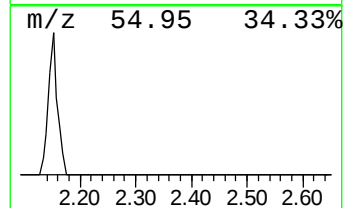
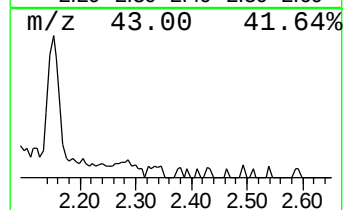
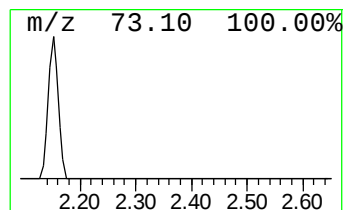
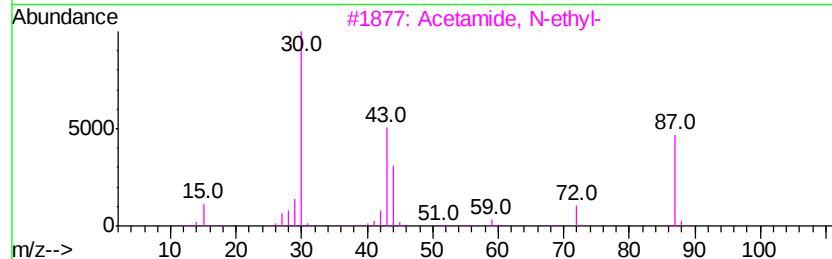
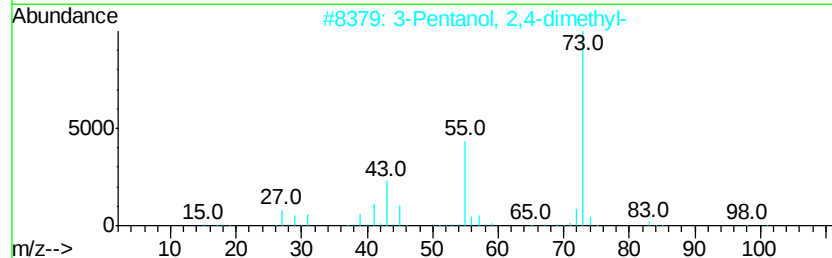
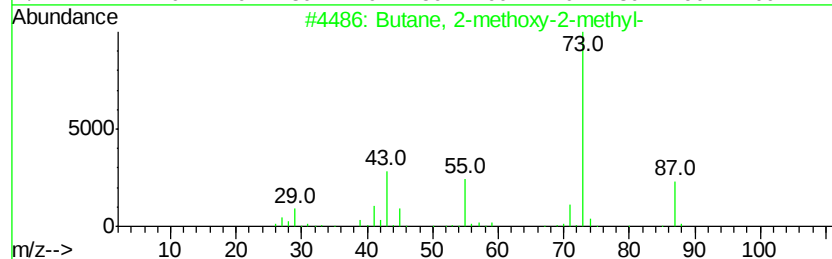
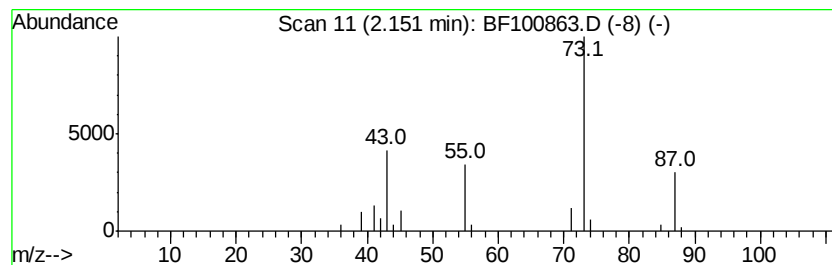
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	2.96 ng	64647	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	74
2		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4		2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	9
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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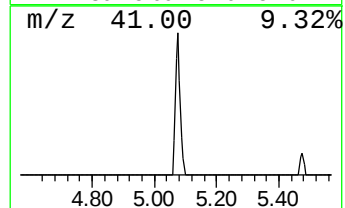
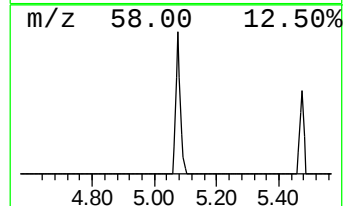
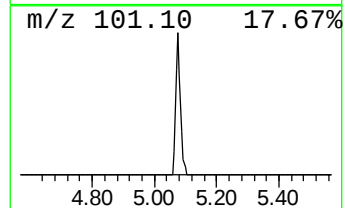
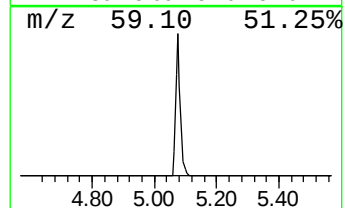
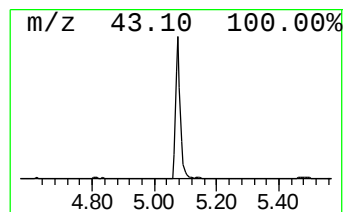
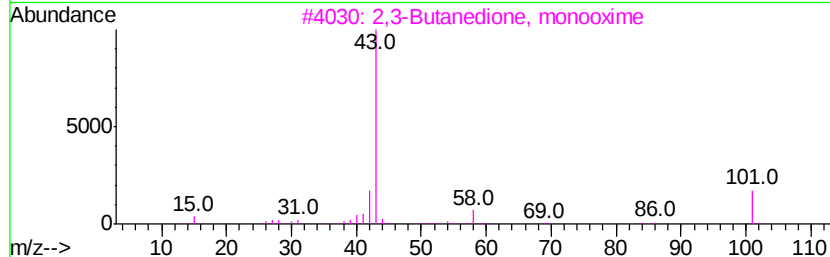
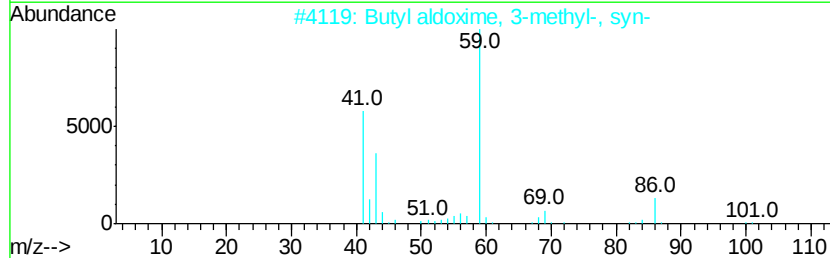
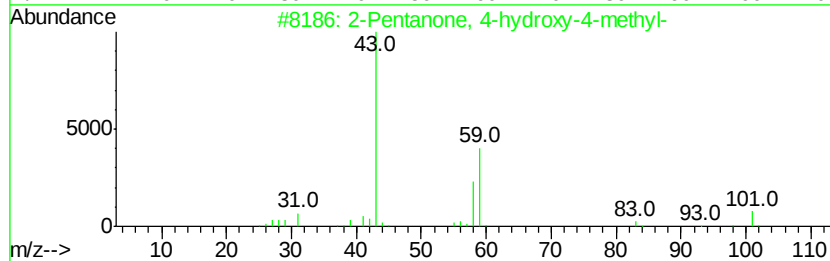
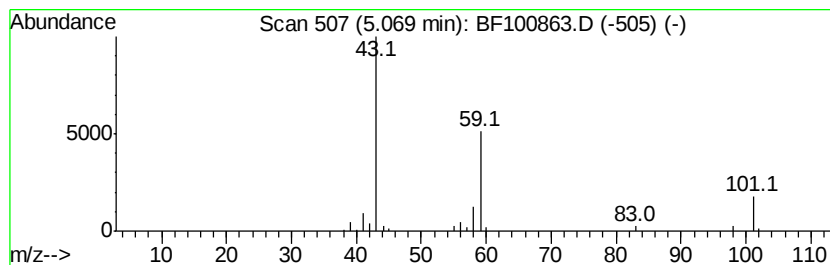
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	6.31 ng	137801	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		5-Aminovaleric acid	117	C5H11NO2	000660-88-8	9



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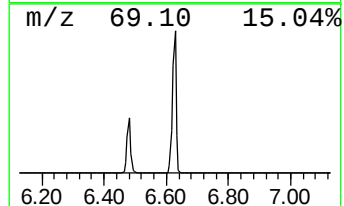
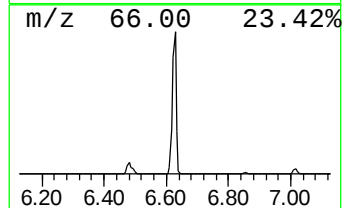
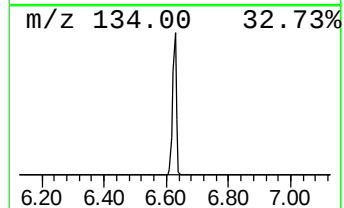
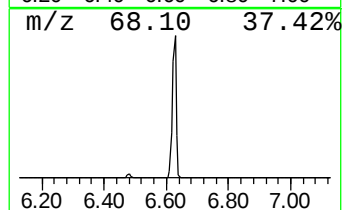
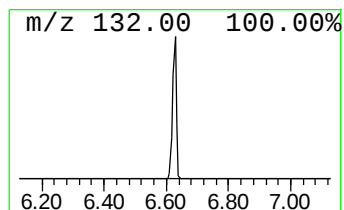
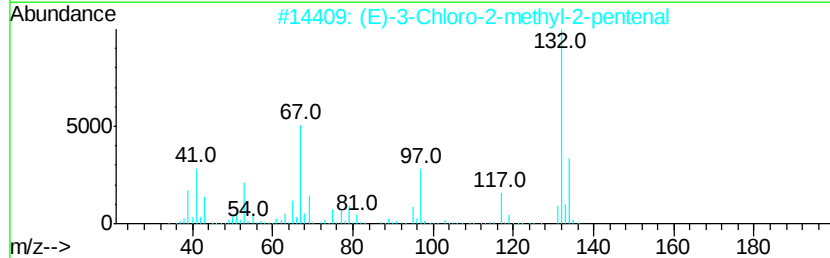
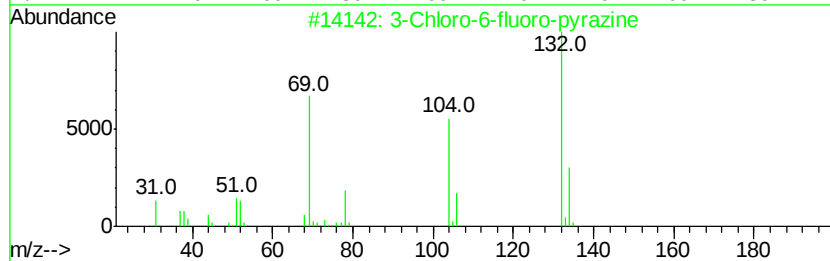
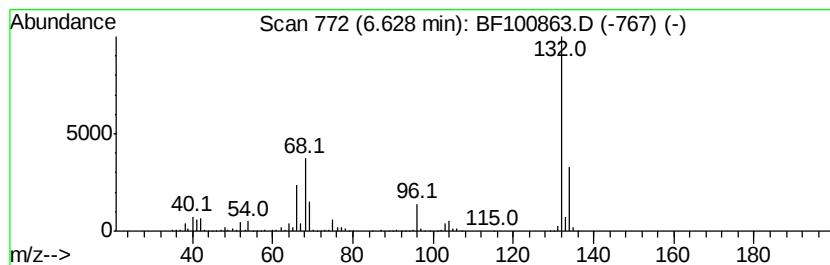
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Peak Number 3 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	56.13 ng	1226020	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	12
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



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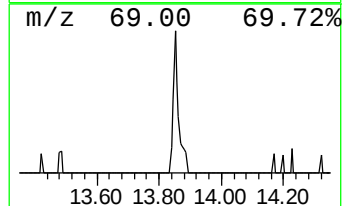
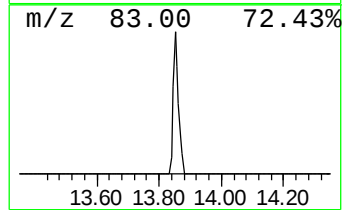
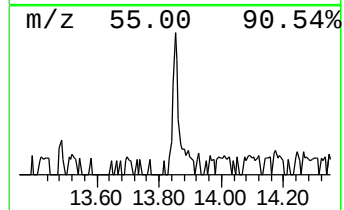
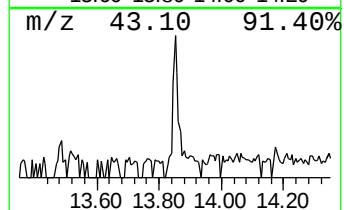
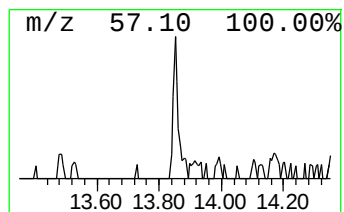
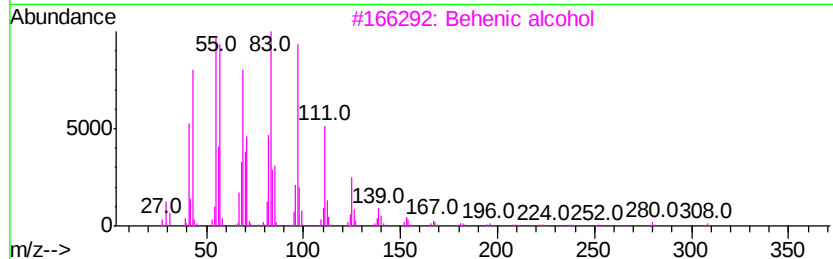
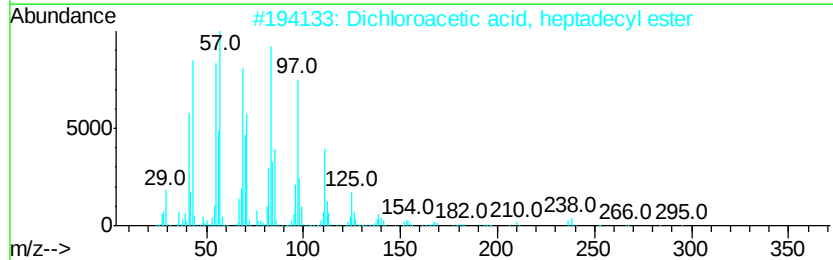
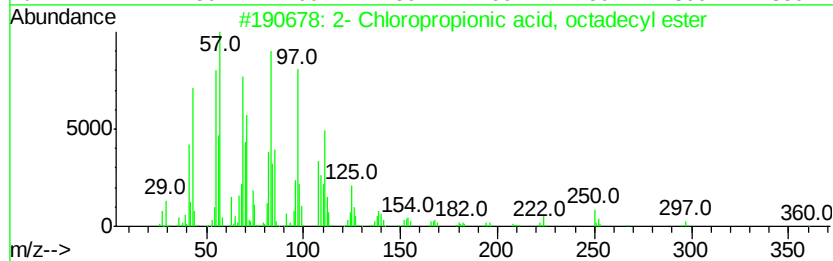
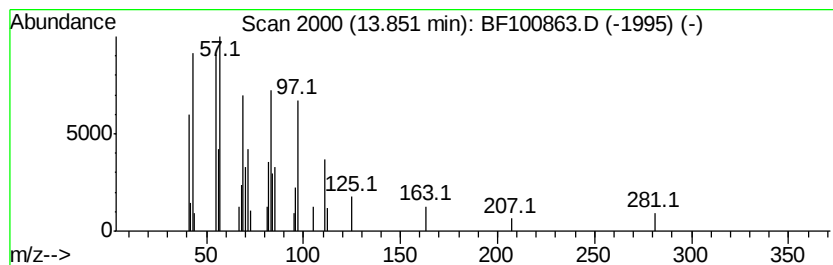
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Peak Number 5 2- Chloropropionic acid, oc... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	2.01 ng	36088	Chrysene-d12	14.02

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-		Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	90
2			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90
3			Behenic alcohol	326	C22H46O	000661-19-8	90
4			n-Nonadecanol-1	284	C19H40O	001454-84-8	87
5			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.15	3.0	ng	64647	1	6.86	436855	20.0
2-Pentanone, 4-hy...	5.07	6.3	ng	137801	1	6.86	436855	20.0
unknown6.63	6.63	56.1	ng	1226020	1	6.86	436855	20.0
2- Chloropropioni...	13.85	2.0	ng	36088	5	14.02	358366	20.0