

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092617\
 Data File : BF098843.D
 Acq On : 26 Sep 2017 20:19
 Operator : SJ/JU
 Sample : I5426-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 092517-TIDO-F-D-M

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-BF092317.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	2.204	16	20	38	rVB	340871	544931	10.85%	1.666%
2	5.134	514	518	528	rVB	280009	294590	5.86%	0.901%
3	5.528	581	585	588	rBV	1971645	1682121	33.49%	5.143%
4	6.528	751	755	758	rBV	1264853	1079962	21.50%	3.302%
5	6.681	776	781	784	rBV	3042643	2792658	55.60%	8.539%
6	6.916	817	821	824	rBV	1056599	937179	18.66%	2.866%
7	7.075	843	848	851	rBV	3505070	3400570	67.70%	10.398%
8	7.481	911	917	920	rBV	2705381	2861298	56.96%	8.749%
9	8.198	1034	1039	1042	rBV	1398760	1283663	25.56%	3.925%
10	9.274	1216	1222	1225	rBV	4915163	5023113	100.00%	15.359%
11	9.657	1284	1287	1290	rBV	74198	52691	1.05%	0.161%
12	9.927	1330	1333	1334	rBV	184982	145370	2.89%	0.444%
13	9.951	1334	1337	1341	rVB2	1659731	1384033	27.55%	4.232%
14	10.621	1446	1451	1454	rBV	2685478	2421958	48.22%	7.405%
15	10.739	1466	1471	1474	rBV	2020815	1816795	36.17%	5.555%
16	11.439	1586	1590	1593	rBV	1516135	1265371	25.19%	3.869%
17	13.027	1854	1860	1863	rBV	3908595	3922613	78.09%	11.994%
18	14.074	2034	2038	2042	rBV	1035793	894421	17.81%	2.735%
19	15.568	2286	2292	2301	rBV	703188	901833	17.95%	2.757%

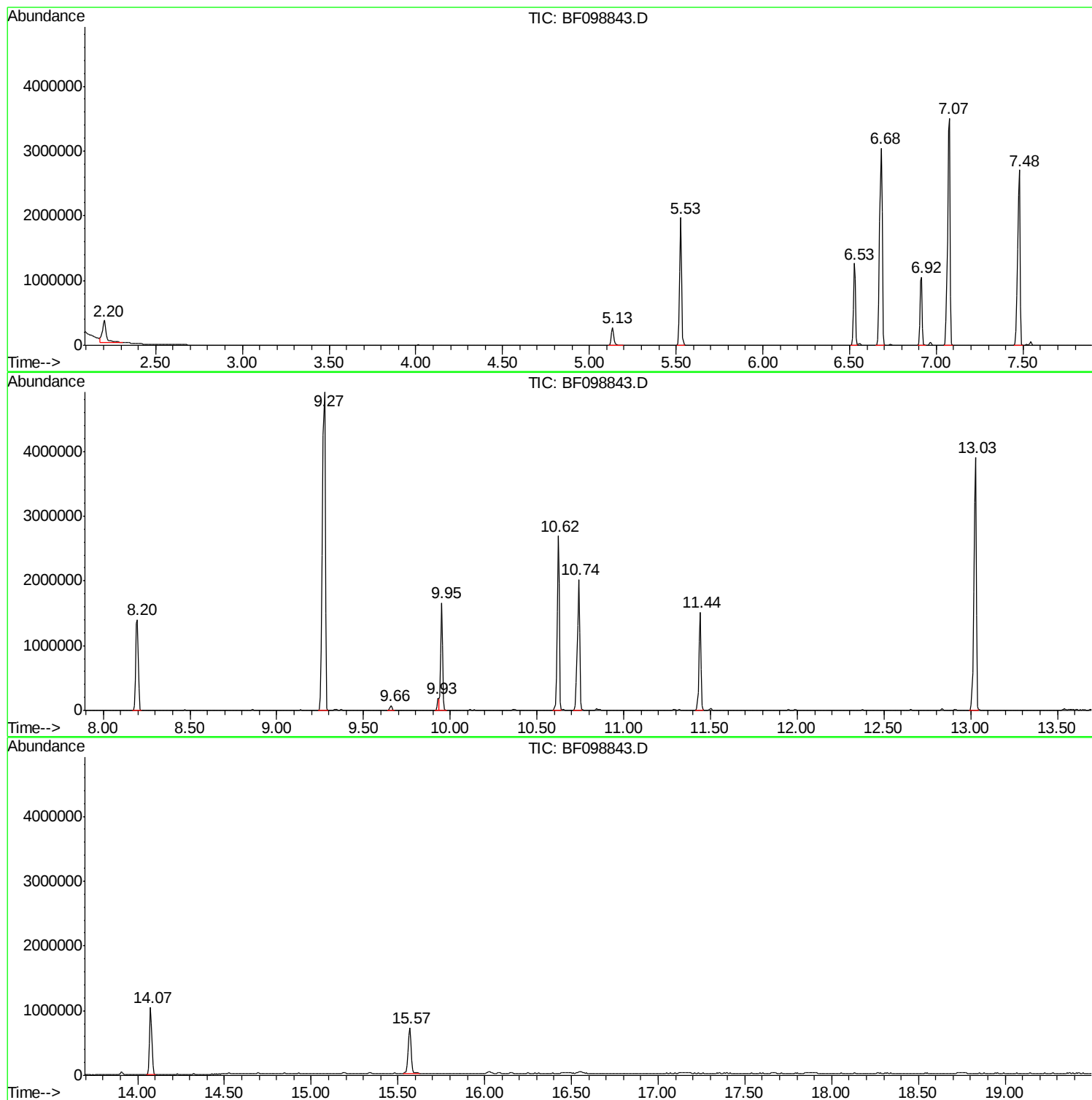
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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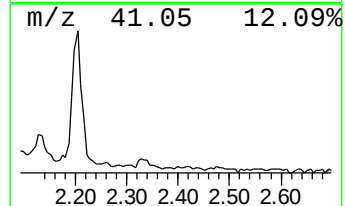
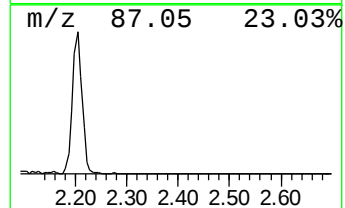
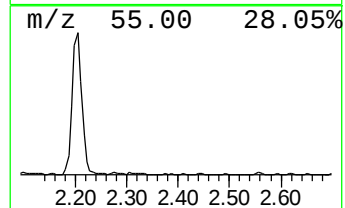
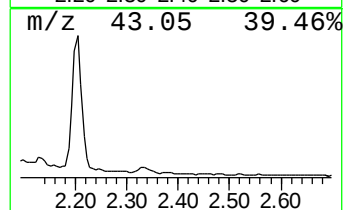
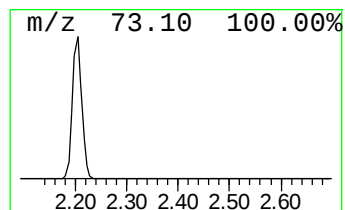
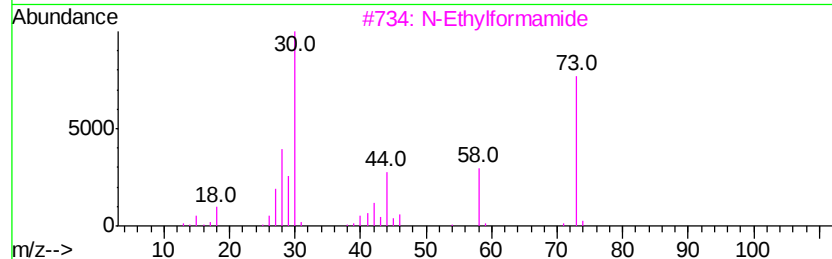
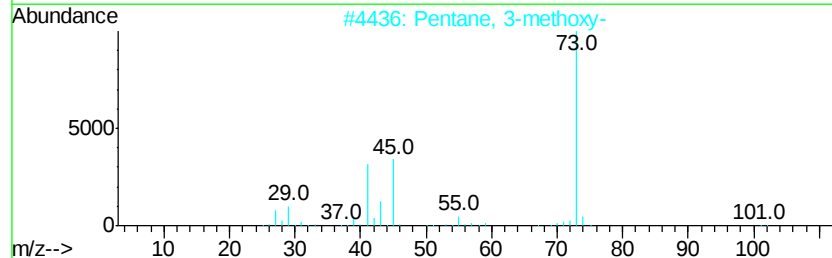
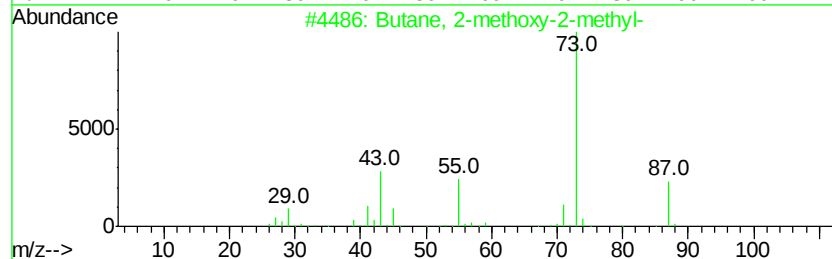
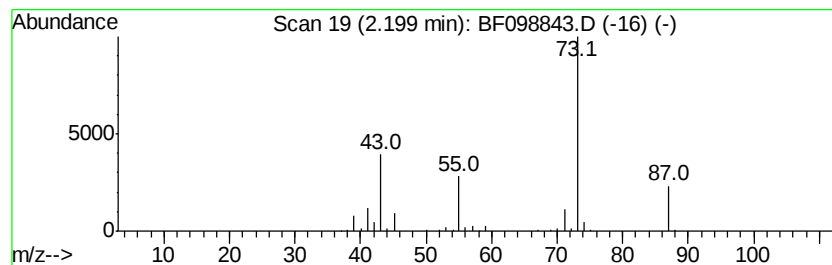
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.20	11.63 ng	544931	1,4-Dichlorobenzene-d4	6.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
3			N-Ethylformamide	73	C3H7NO	000627-45-2	9
4			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9



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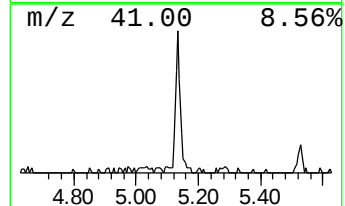
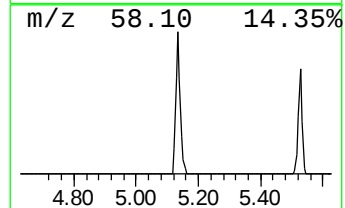
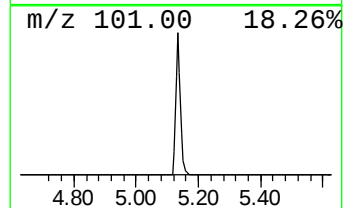
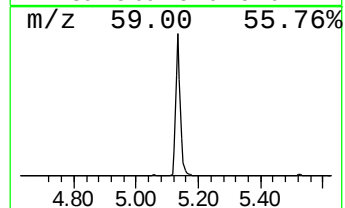
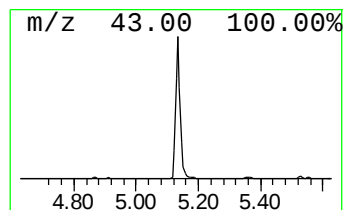
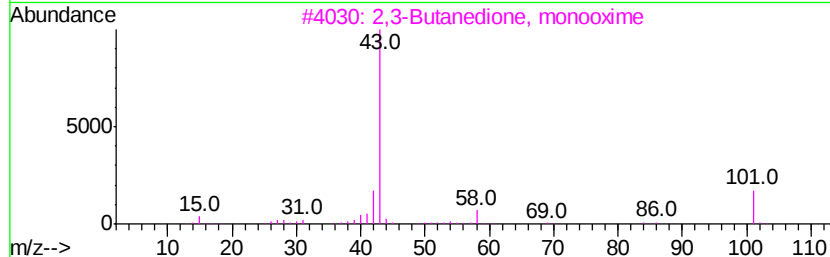
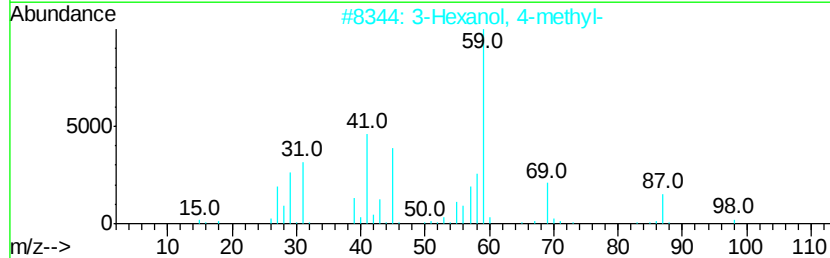
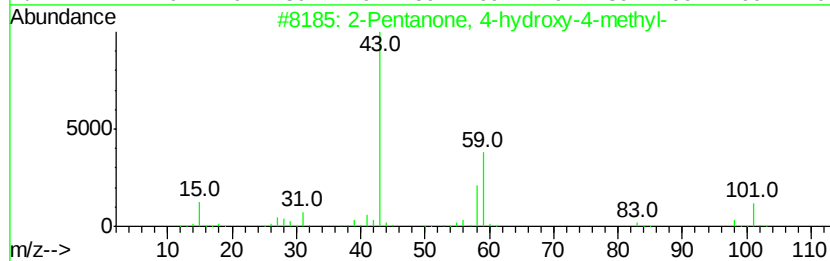
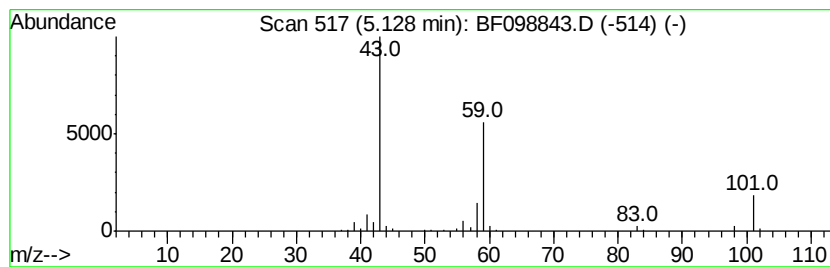
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	6.29 ng	294590	1,4-Dichlorobenzene-d4	6.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9



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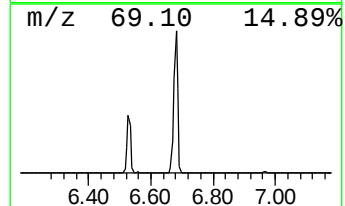
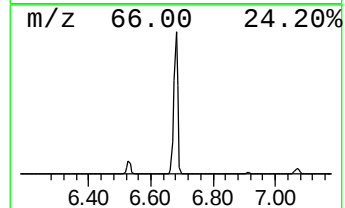
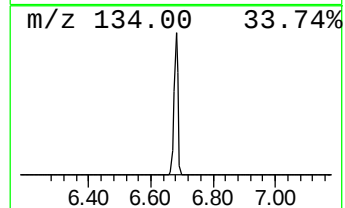
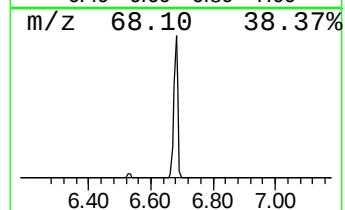
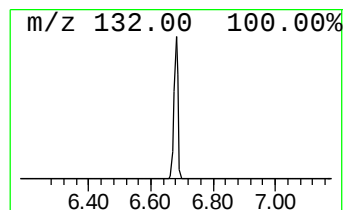
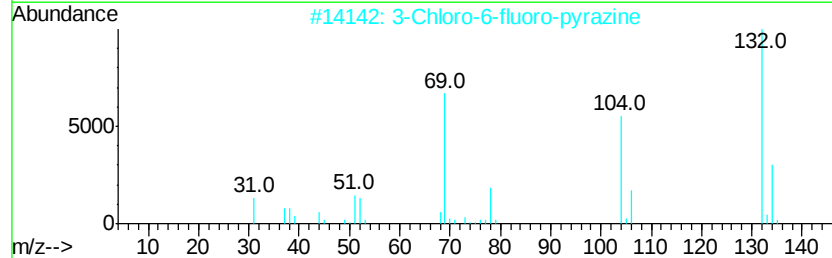
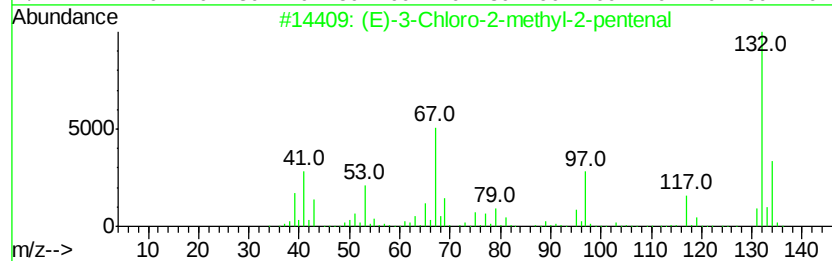
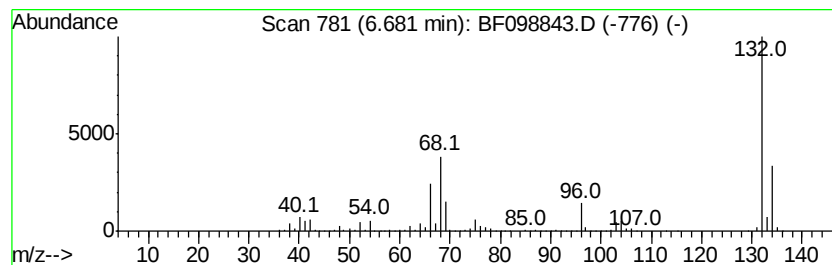
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Peak Number 3 unknown6.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	59.60 ng	2792660	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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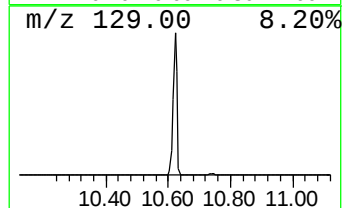
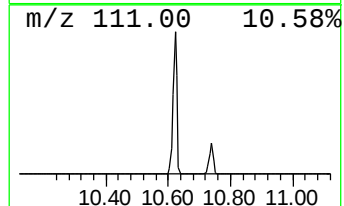
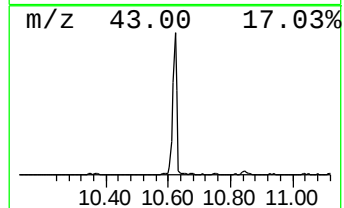
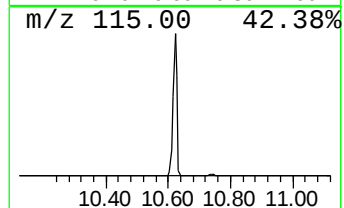
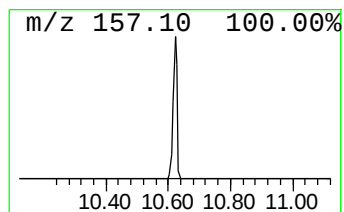
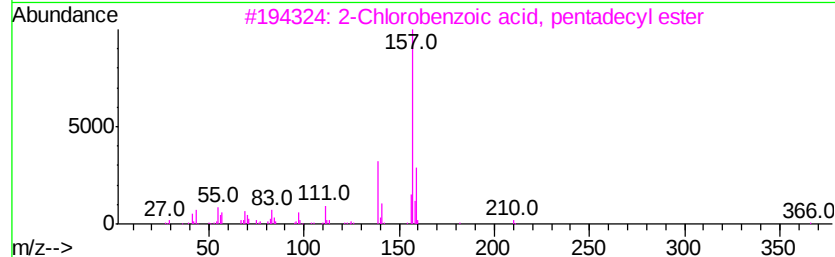
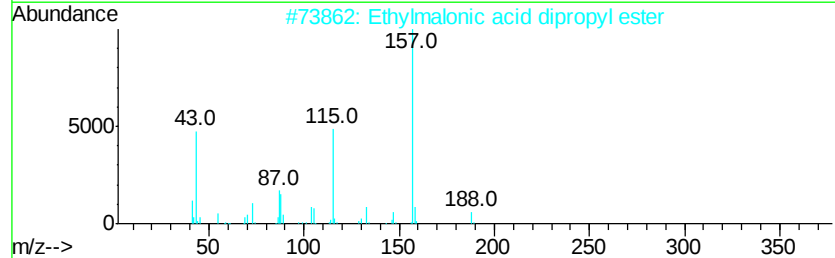
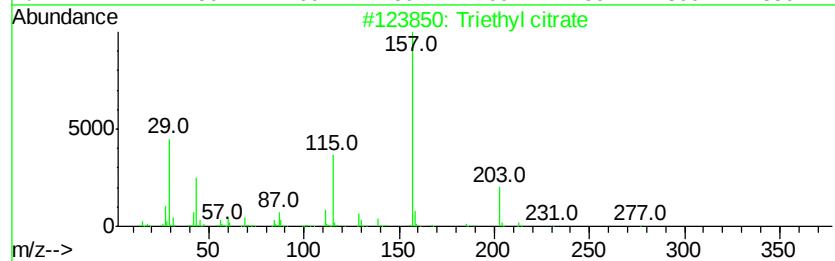
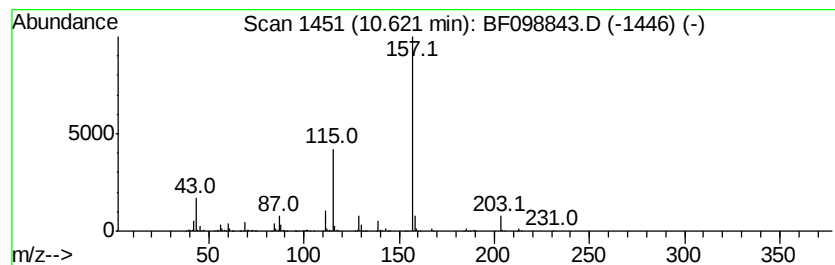
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Peak Number 5 Triethyl citrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.62	35.00 ng	2421960	Acenaphthene-d10	9.95	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	91
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	64
3	2-Chlorobenzoic acid, pentadecyl...	366	C22H35ClO2	1000292-43-0	38
4	N-(5-[3-(2-Oxo-benzooxazol-3-yl)]...	318	C14H14N4O3S	1000300-11-5	38
5	1-Amino-2-methylnaphthalene	157	C11H11N	002246-44-8	37



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.20	11.6	ng	544931	1	6.92	937179	20.0
2-Pentanone, 4-hy...	5.13	6.3	ng	294590	1	6.92	937179	20.0
unknown6.68	6.68	59.6	ng	2792660	1	6.92	937179	20.0
Triethyl citrate	10.62	35.0	ng	2421960	3	9.95	1384030	20.0