

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032318\
 Data File : BF103907.D
 Acq On : 24 Mar 2018 3:59
 Operator : JU/SJ
 Sample : J2014-05
 Misc :
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 032018-JETT-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-BF031518.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	2.299	30	36	46	rVB	337495	441784	12.95%	2.130%
2	5.198	526	529	539	rVB	98842	96569	2.83%	0.466%
3	5.593	592	596	615	rVB	1204729	1061444	31.10%	5.117%
4	6.587	761	765	768	rBV	857593	703429	20.61%	3.391%
5	6.616	768	770	778	rVB	100619	89708	2.63%	0.433%
6	6.740	787	791	795	rBV	2148878	1880179	55.09%	9.065%
7	6.975	827	831	834	rBV	870626	700535	20.53%	3.377%
8	7.134	853	858	861	rBV	2921173	2630025	77.07%	12.680%
9	7.540	921	927	930	rBV	2060188	1957993	57.37%	9.440%
10	8.257	1045	1049	1052	rBV	1058366	843070	24.70%	4.065%
11	9.328	1227	1231	1235	rBV	3416625	3412671	100.00%	16.453%
12	9.716	1292	1297	1303	rBV	68416	71753	2.10%	0.346%
13	9.928	1330	1333	1336	rBV	64228	45665	1.34%	0.220%
14	9.986	1341	1343	1345	rVV	49753	38577	1.13%	0.186%
15	10.016	1345	1348	1360	rVB	935513	827656	24.25%	3.990%
16	10.428	1416	1418	1422	rVB	71970	53836	1.58%	0.260%
17	10.804	1479	1482	1492	rBV	1149428	1101716	32.28%	5.312%
18	10.904	1496	1499	1505	rVB	54199	54774	1.61%	0.264%
19	11.510	1598	1602	1610	rBV	813865	690706	20.24%	3.330%
20	13.098	1867	1872	1875	rBV	2883955	2643843	77.47%	12.747%
21	13.974	2018	2021	2031	rBV	144175	158684	4.65%	0.765%
22	14.163	2049	2053	2058	rBV	786396	701700	20.56%	3.383%
23	15.704	2310	2315	2323	rBV2	391378	535397	15.69%	2.581%

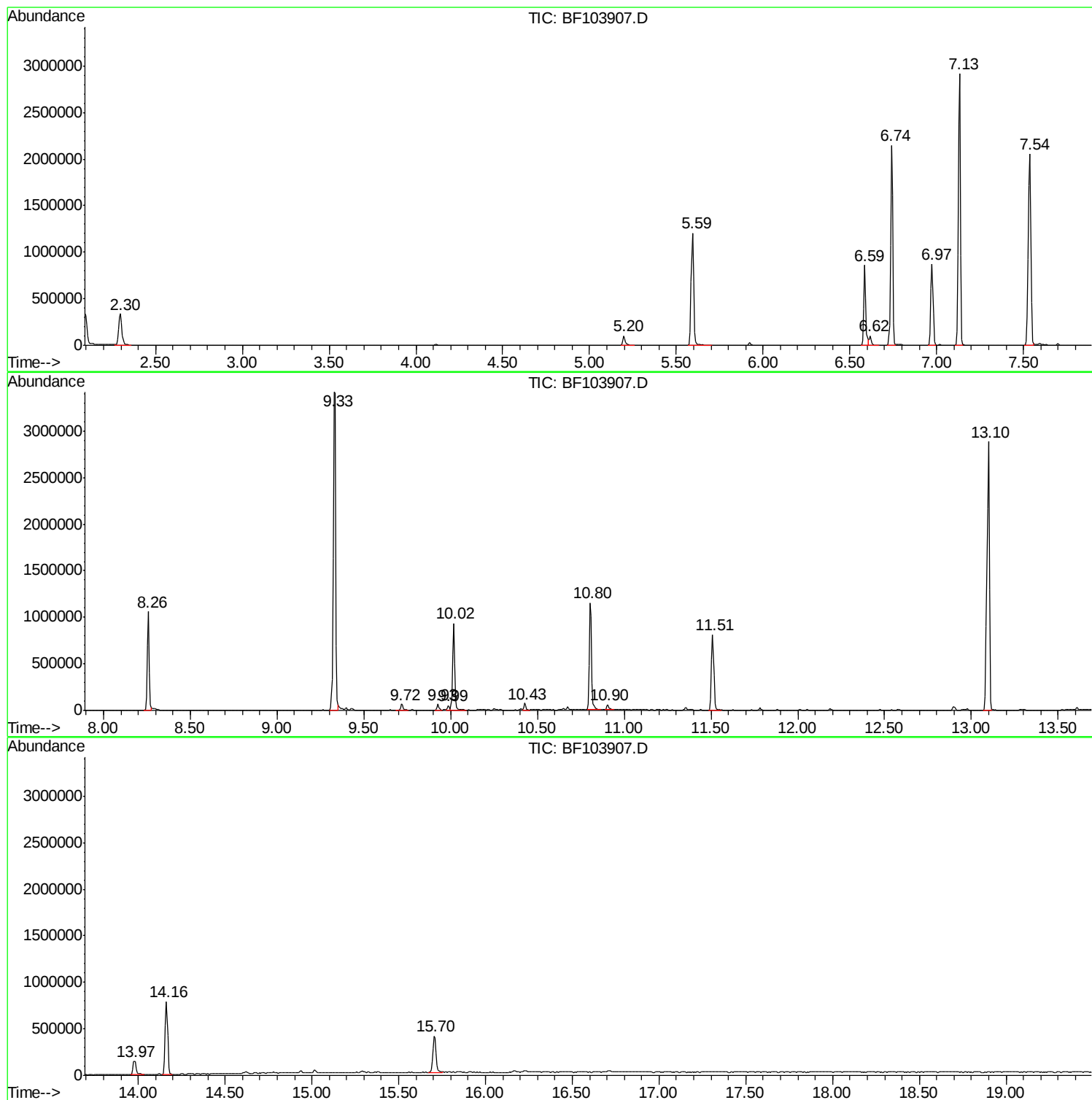
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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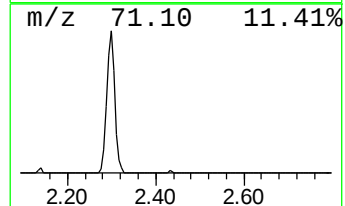
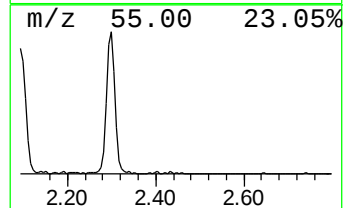
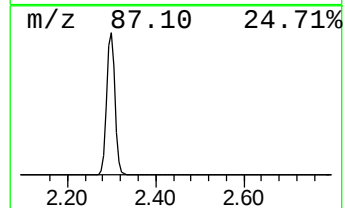
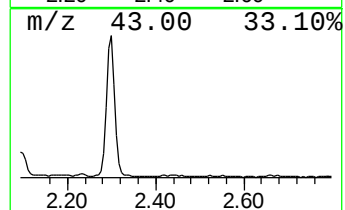
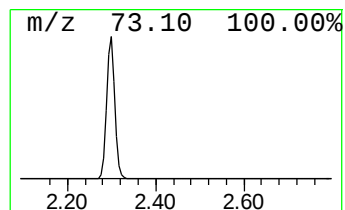
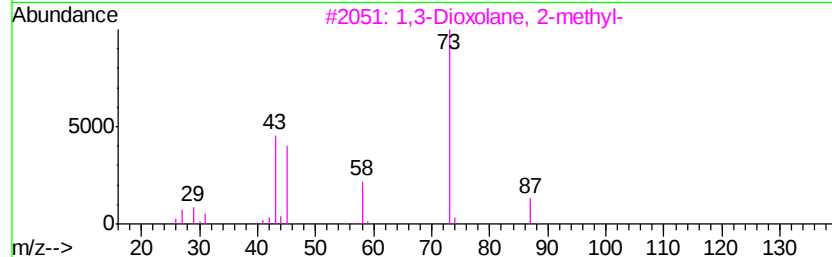
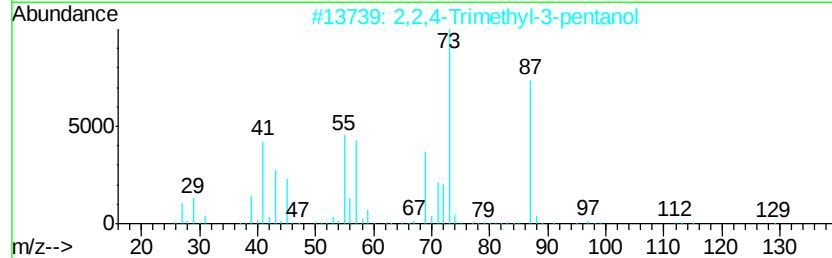
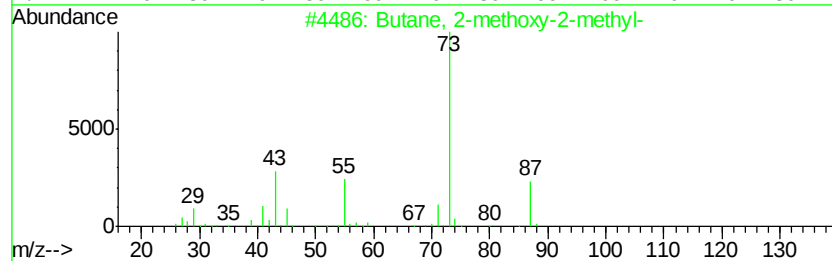
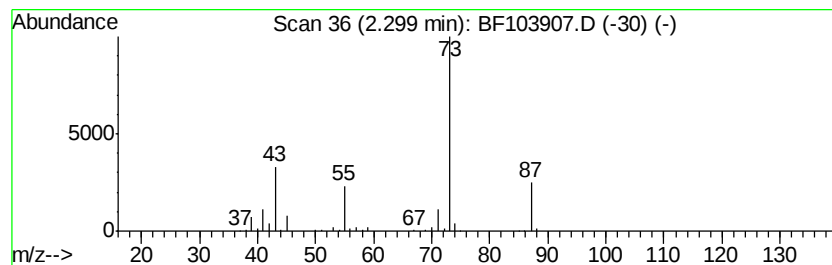
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.30	12.61 ng	441784	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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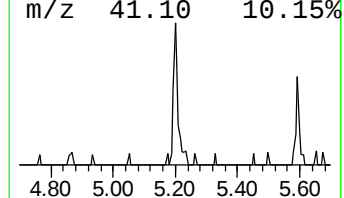
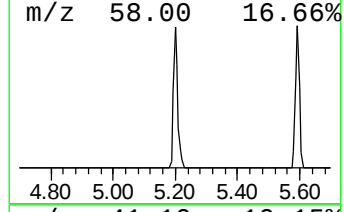
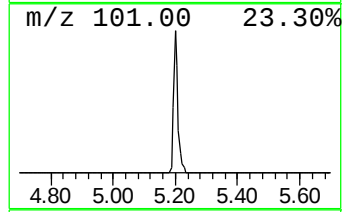
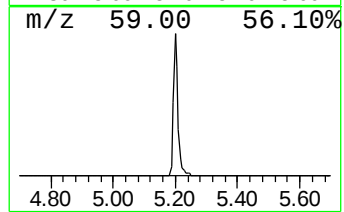
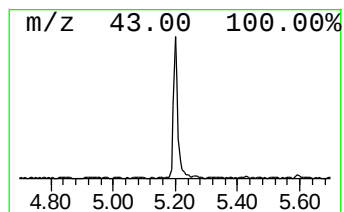
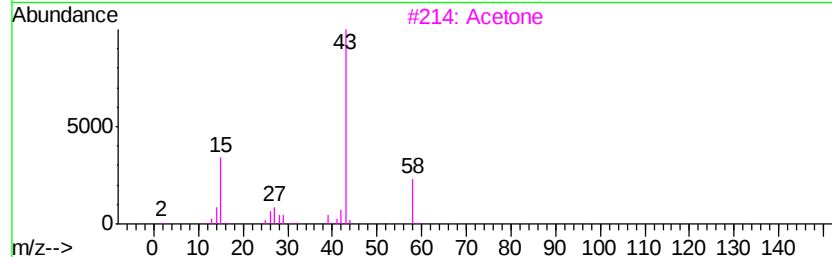
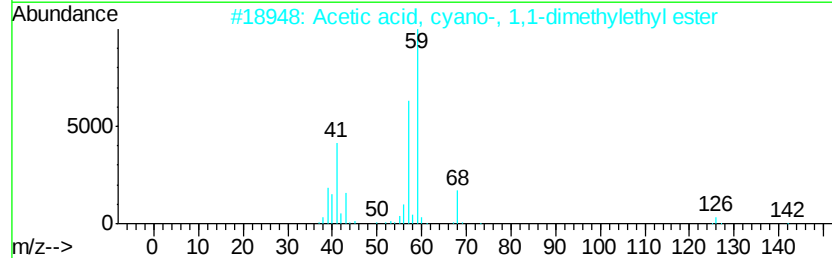
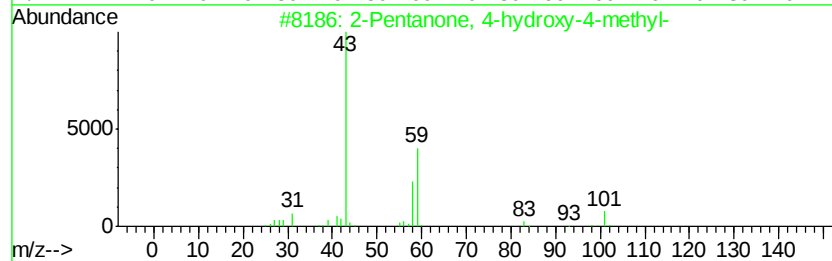
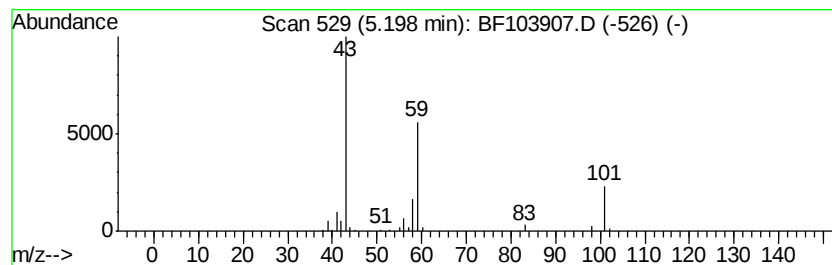
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	2.76 ng	96569	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		Acetone	58	C3H6O	000067-64-1	10
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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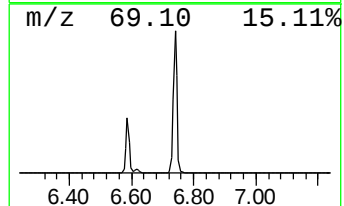
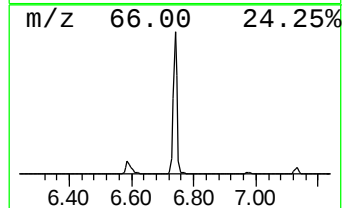
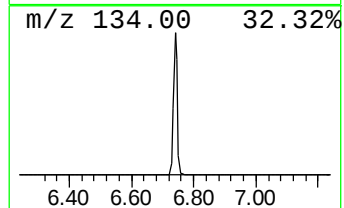
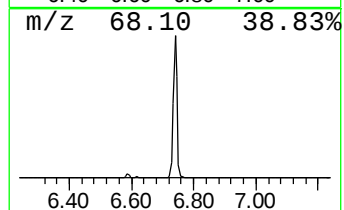
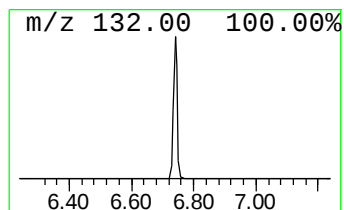
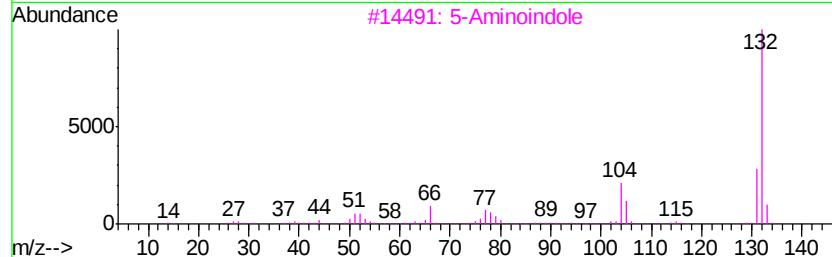
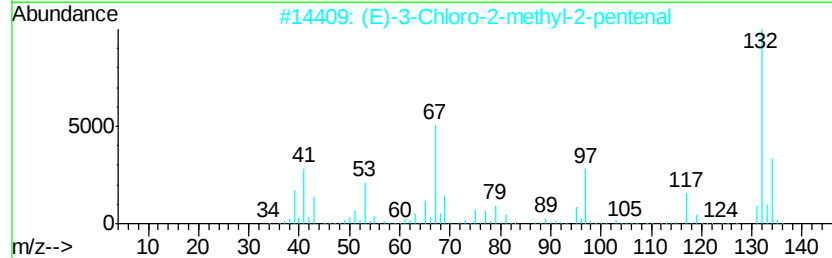
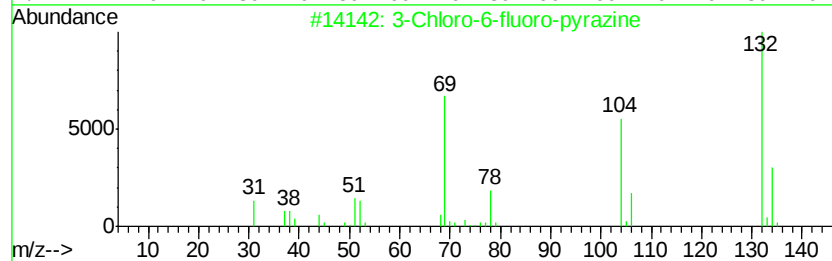
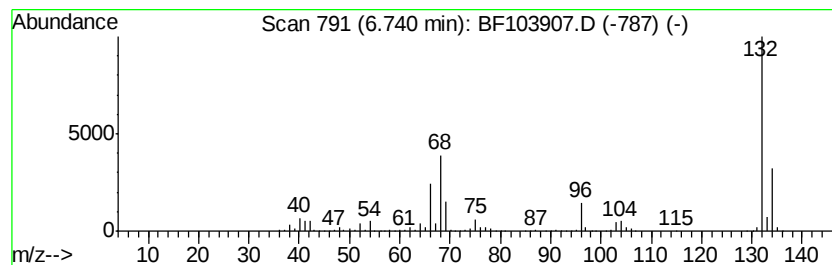
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Peak Number 3 unknown6.74 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	53.68 ng	1880180	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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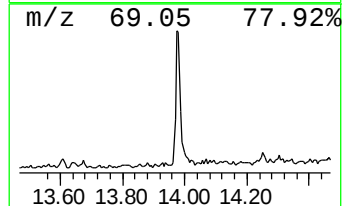
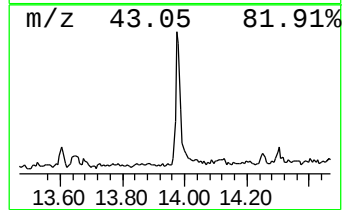
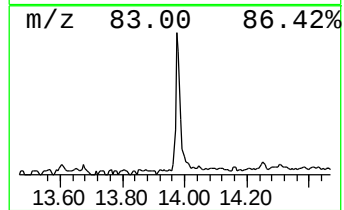
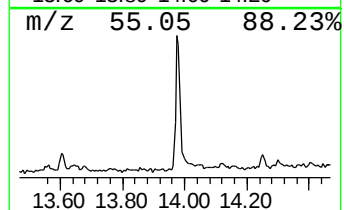
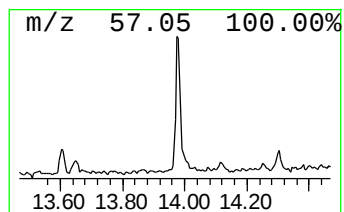
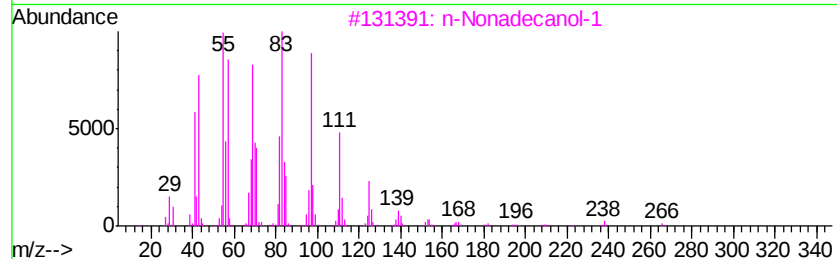
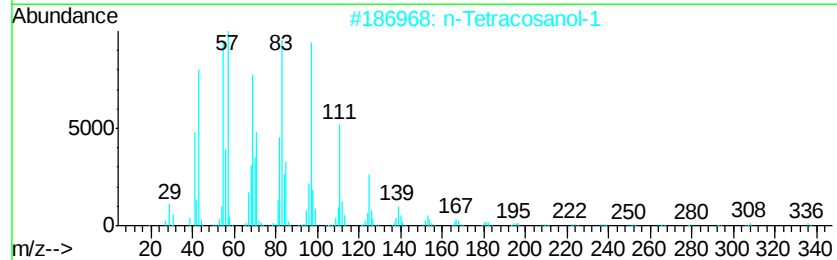
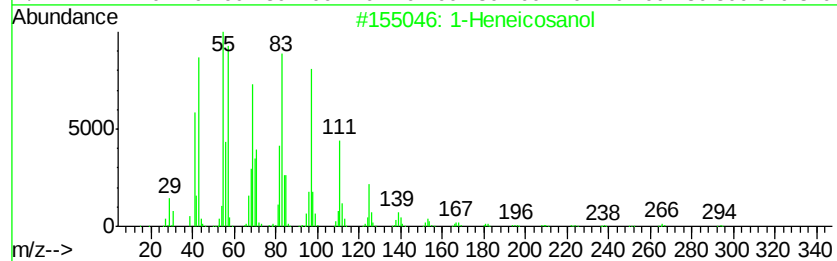
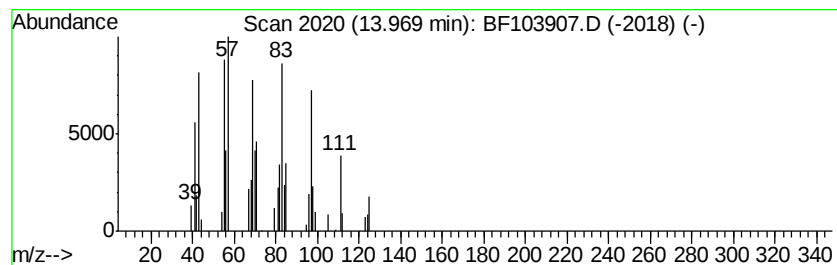
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Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	4.52 ng	158684	Chrysene-d12	14.16

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	95
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.30	12.6	ng	441784	1	6.97	700535	20.0
2-Pentanone, 4-hy...	5.20	2.8	ng	96569	1	6.97	700535	20.0
unknown6.74	6.74	53.7	ng	1880180	1	6.97	700535	20.0
1-Heneicosanol	13.97	4.5	ng	158684	5	14.16	701700	20.0