

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051517\
 Data File : BF095135.D
 Acq On : 15 May 2017 20:19
 Operator : SJ/MA
 Sample : I3147-02
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-1COMP

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-BF050217.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	1.966	3	5	16	rVB2	50674	72299	2.30%	0.325%
2	5.137	540	544	567	rBV	264017	562280	17.92%	2.531%
3	5.748	644	648	681	rBV	1369789	2519203	80.27%	11.340%
4	6.325	742	746	755	rBV2	19153	34532	1.10%	0.155%
5	7.319	911	915	932	rBV	1394086	2153601	68.62%	9.695%
6	7.442	932	936	947	rVB	1782989	2477138	78.93%	11.151%
7	7.784	990	994	1004	rBV	388383	489933	15.61%	2.205%
8	8.019	1029	1034	1050	rVB	1823564	2156717	68.72%	9.709%
9	8.678	1141	1146	1177	rBV	1072742	1472755	46.93%	6.630%
10	9.795	1332	1336	1360	rBV	482706	672637	21.43%	3.028%
11	11.566	1632	1637	1661	rBV	2439948	3138442	100.00%	14.128%
12	12.260	1750	1755	1770	rBV	172875	289205	9.21%	1.302%
13	12.624	1812	1817	1836	rBV2	462322	655204	20.88%	2.949%
14	13.919	2032	2037	2058	rBV	964198	1535342	48.92%	6.911%
15	14.230	2087	2090	2094	rBV	24914	31750	1.01%	0.143%
16	15.030	2221	2226	2239	rBV	431192	609443	19.42%	2.743%
17	15.989	2384	2389	2398	rBV5	15806	36751	1.17%	0.165%
18	17.124	2578	2582	2591	rVB	24514	35013	1.12%	0.158%
19	17.348	2615	2620	2633	rBV	1925103	2171097	69.18%	9.773%
20	18.042	2734	2738	2747	rBV2	22253	33875	1.08%	0.152%
21	18.695	2845	2849	2866	rVB	334569	513223	16.35%	2.310%
22	19.977	3064	3067	3070	rBV	26200	36487	1.16%	0.164%
23	20.371	3130	3134	3146	rBV	354281	517642	16.49%	2.330%

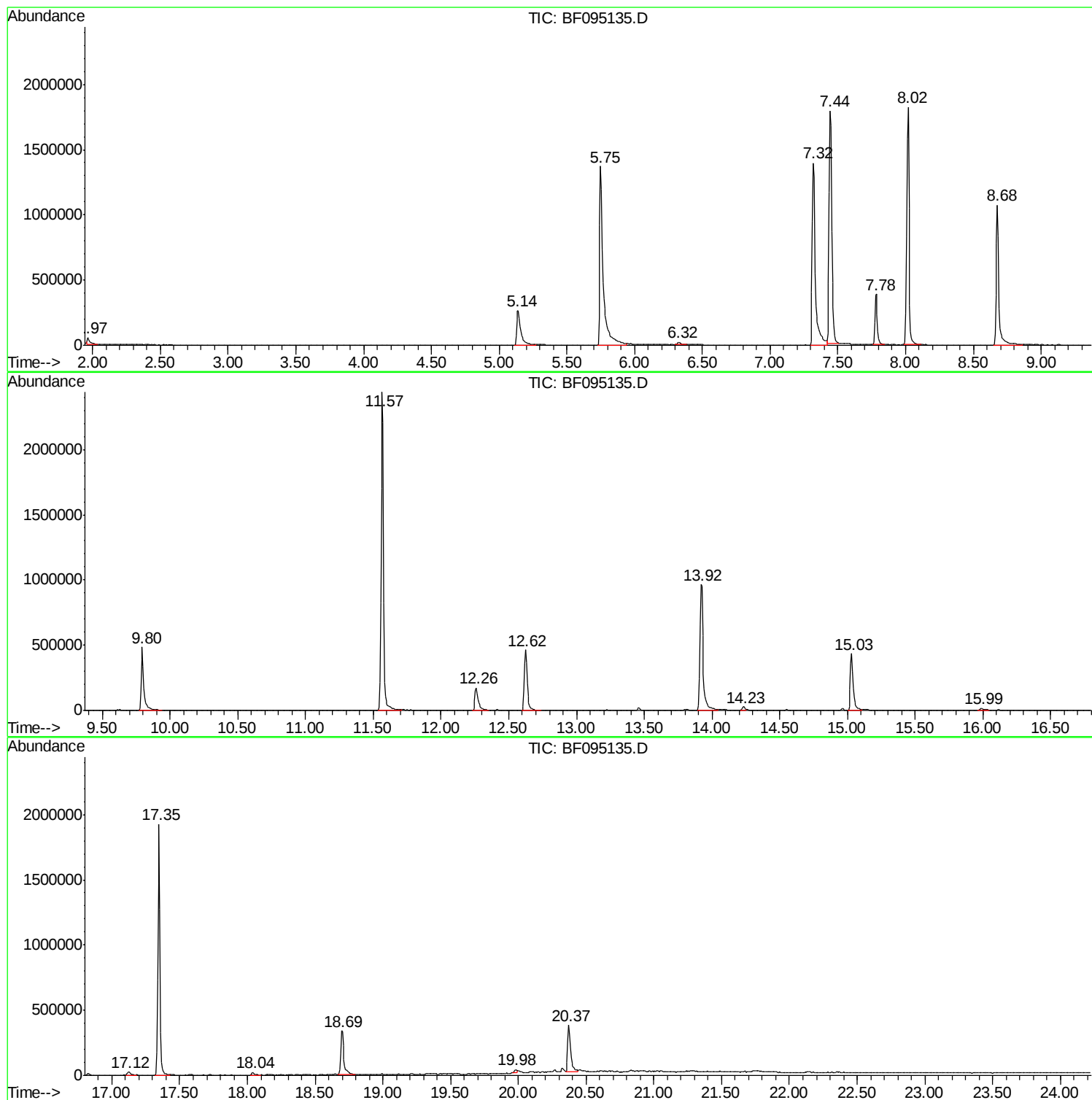
Sum of corrected areas: 22214569

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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Acq On : 15 May 2017 20:19
Operator : SJ/MA
Sample : I3147-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
TP-1COMP

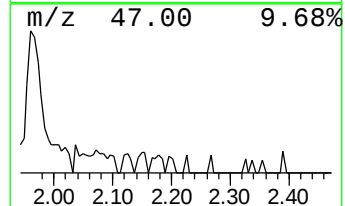
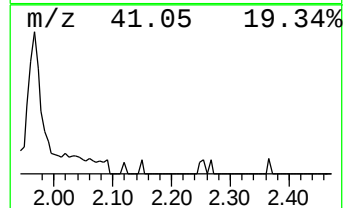
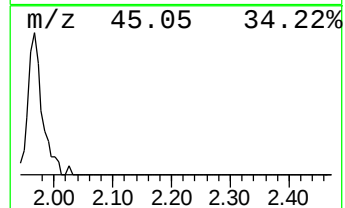
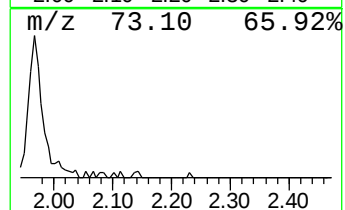
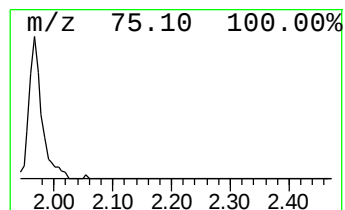
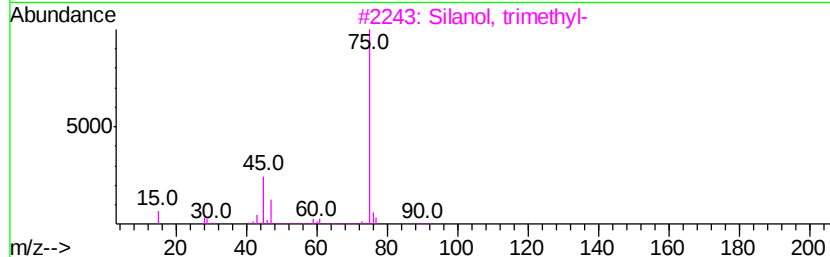
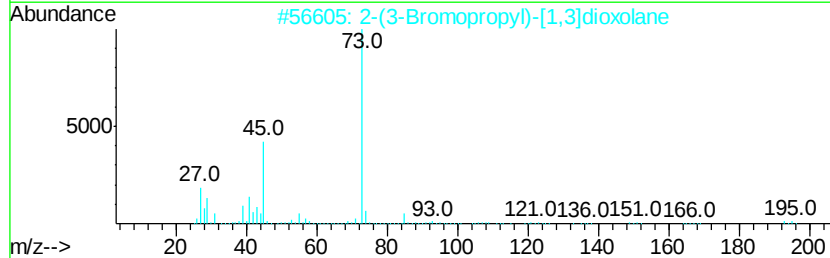
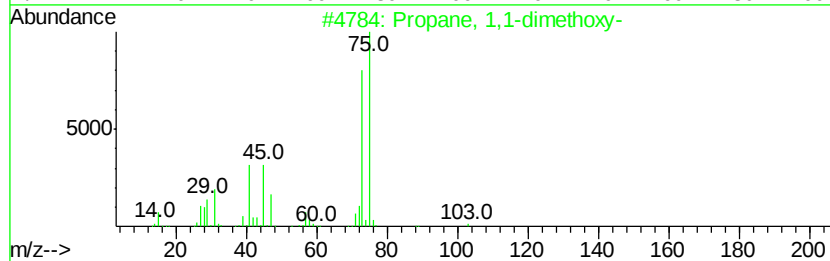
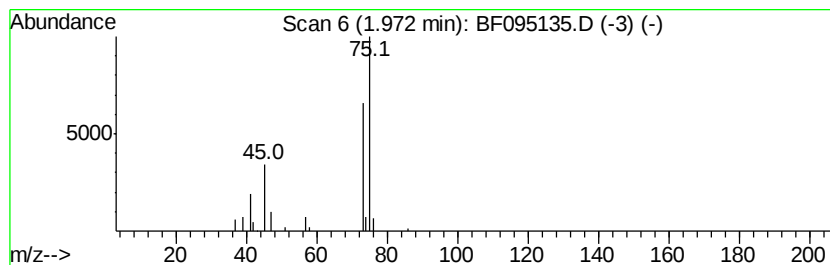
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown1.97 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.97	2.95 ng	72299	1,4-Dichlorobenzene-d4	7.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	39
2		2-(3-Bromopropyl)-[1,3]dioxolane	194	C6H11BrO2	062563-07-9	9
3		Silanol, trimethyl-	90	C3H10OSi	001066-40-6	9
4		Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	7
5		Glycine	75	C2H5NO2	000056-40-6	5



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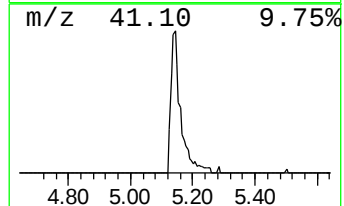
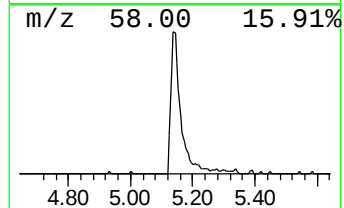
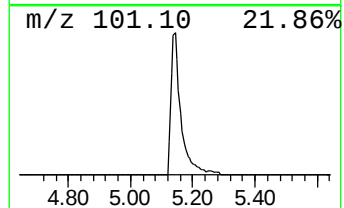
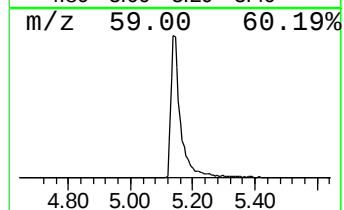
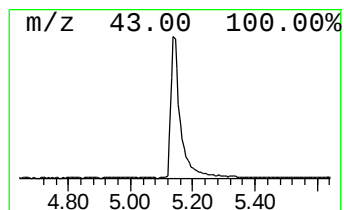
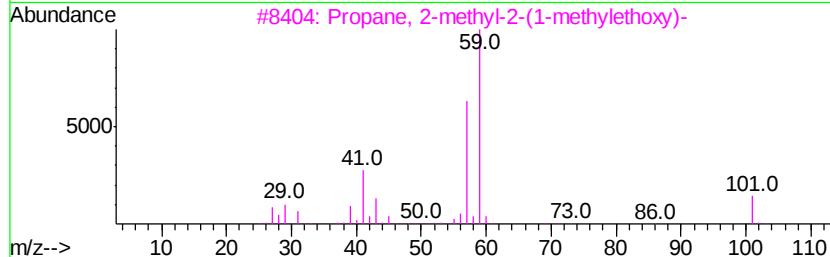
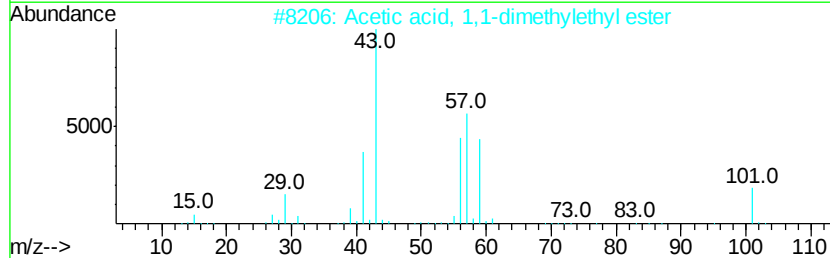
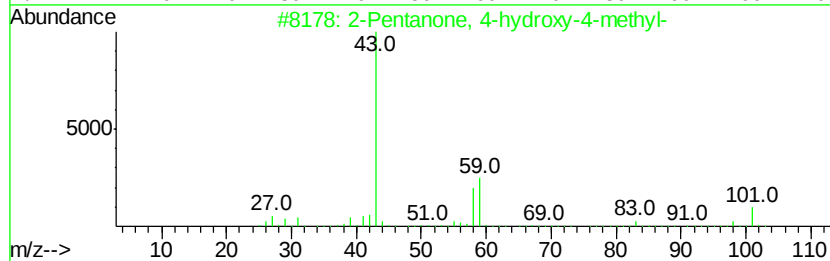
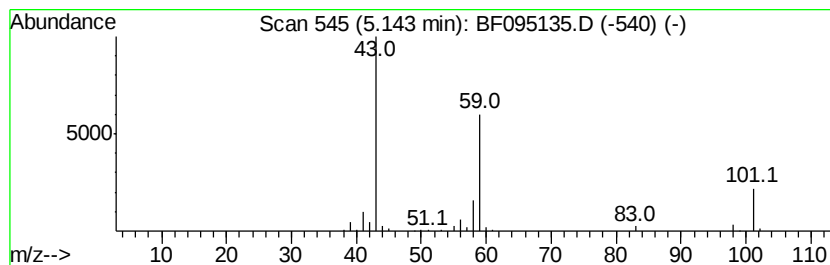
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	22.95 ng	562280	1,4-Dichlorobenzene-d4	7.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
4		3-Hexanol	102	C6H14O	000623-37-0	28
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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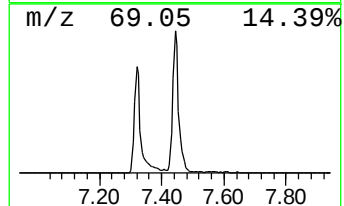
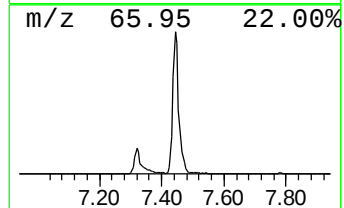
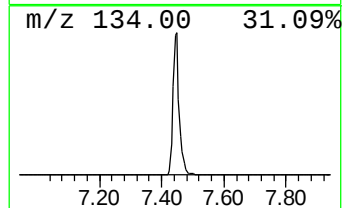
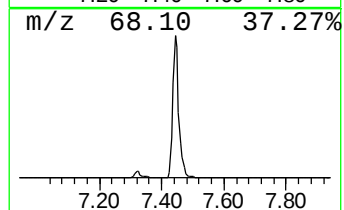
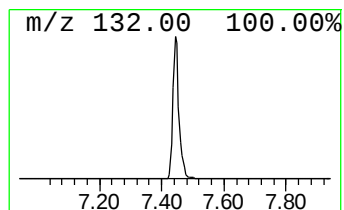
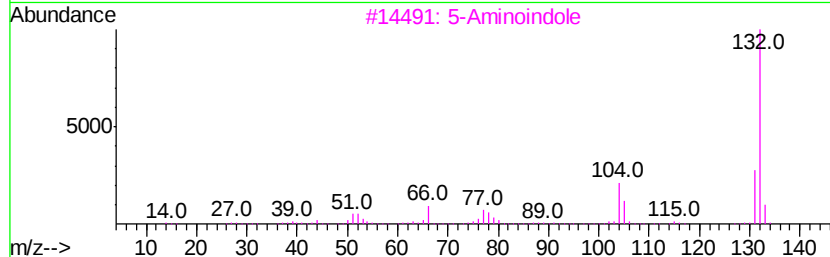
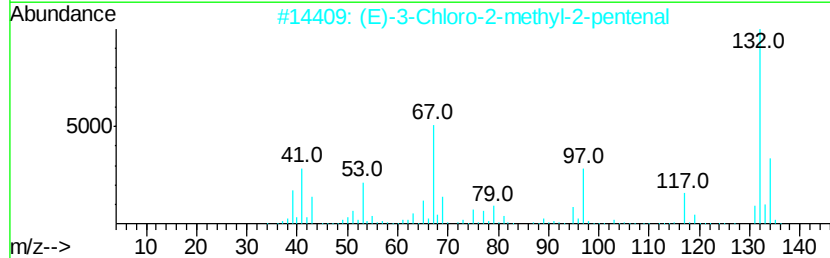
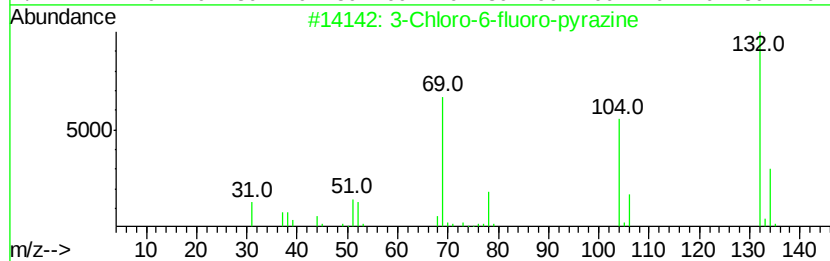
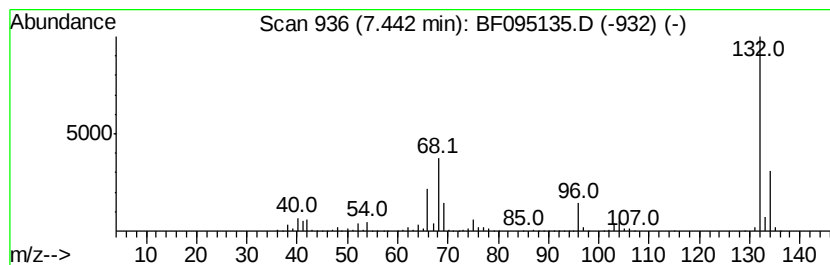
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Peak Number 3 unknown7.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.44	101.12 ng	2477140	1,4-Dichlorobenzene-d4	7.78

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	25
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.97	1.97	3.0	ng	72299	1	7.78	489933	20.0
2-Pentanone, 4-hy...	5.14	22.9	ng	562280	1	7.78	489933	20.0
unknown7.44	7.44	101.1	ng	2477140	1	7.78	489933	20.0