

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
 Data File : BF093623.D
 Acq On : 13 Mar 2017 22:28
 Operator : SJ/MA
 Sample : I2137-06
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 38D-9-11

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-BF030717.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	4.847	256	259	275	rBV	298446	620652	10.90%	1.541%
2	5.304	297	299	309	rBV	1249612	2300181	40.40%	5.712%
3	5.442	309	311	320	rVB	49340	130323	2.29%	0.324%
4	5.704	332	334	343	rVB	66449	108097	1.90%	0.268%
5	6.367	391	392	400	rBV2	939583	1708235	30.00%	4.242%
6	6.482	400	402	417	rVV	2877421	4422192	77.67%	10.981%
7	6.710	420	422	433	rVV	807198	1159697	20.37%	2.880%
8	6.859	433	435	444	rVB	3757954	3747252	65.82%	9.305%
9	7.282	470	472	486	rBV	3069935	3429576	60.24%	8.516%
10	8.002	533	535	546	rBV2	1350909	1918259	33.69%	4.763%
11	8.722	596	598	602	rVV	180851	193660	3.40%	0.481%
12	8.825	604	607	612	rVB	101646	136252	2.39%	0.338%
13	9.088	627	630	632	rBV	3922689	5693390	100.00%	14.137%
14	9.190	637	639	645	rVB	35208	61556	1.08%	0.153%
15	9.431	658	660	661	rVV	52839	77080	1.35%	0.191%
16	9.488	664	665	668	rVV	154439	148769	2.61%	0.369%
17	9.636	674	678	682	rBV3	24254	66246	1.16%	0.164%
18	9.762	686	689	690	rBV	1224421	1620870	28.47%	4.025%
19	9.785	690	691	698	rVB	244902	376479	6.61%	0.935%
20	9.979	705	708	710	rBV	93281	134963	2.37%	0.335%
21	10.185	725	726	728	rVB	54127	59970	1.05%	0.149%
22	10.311	736	737	740	rVB	176751	188666	3.31%	0.468%
23	10.551	756	758	761	rBV2	2240810	2998326	52.66%	7.445%
24	10.665	766	768	771	rVB	70538	90243	1.59%	0.224%
25	11.111	805	807	808	rBV	84327	63616	1.12%	0.158%
26	11.248	817	819	827	rBV2	1768569	1999945	35.13%	4.966%
27	11.534	842	844	846	rBV	55157	71085	1.25%	0.177%
28	12.711	943	947	951	rVB2	32998	65576	1.15%	0.163%
29	12.837	955	958	961	rBV	4296730	4423889	77.70%	10.985%
30	13.900	1049	1051	1056	rBV	934664	1311160	23.03%	3.256%
31	15.305	1171	1174	1187	rBV	589664	945923	16.61%	2.349%

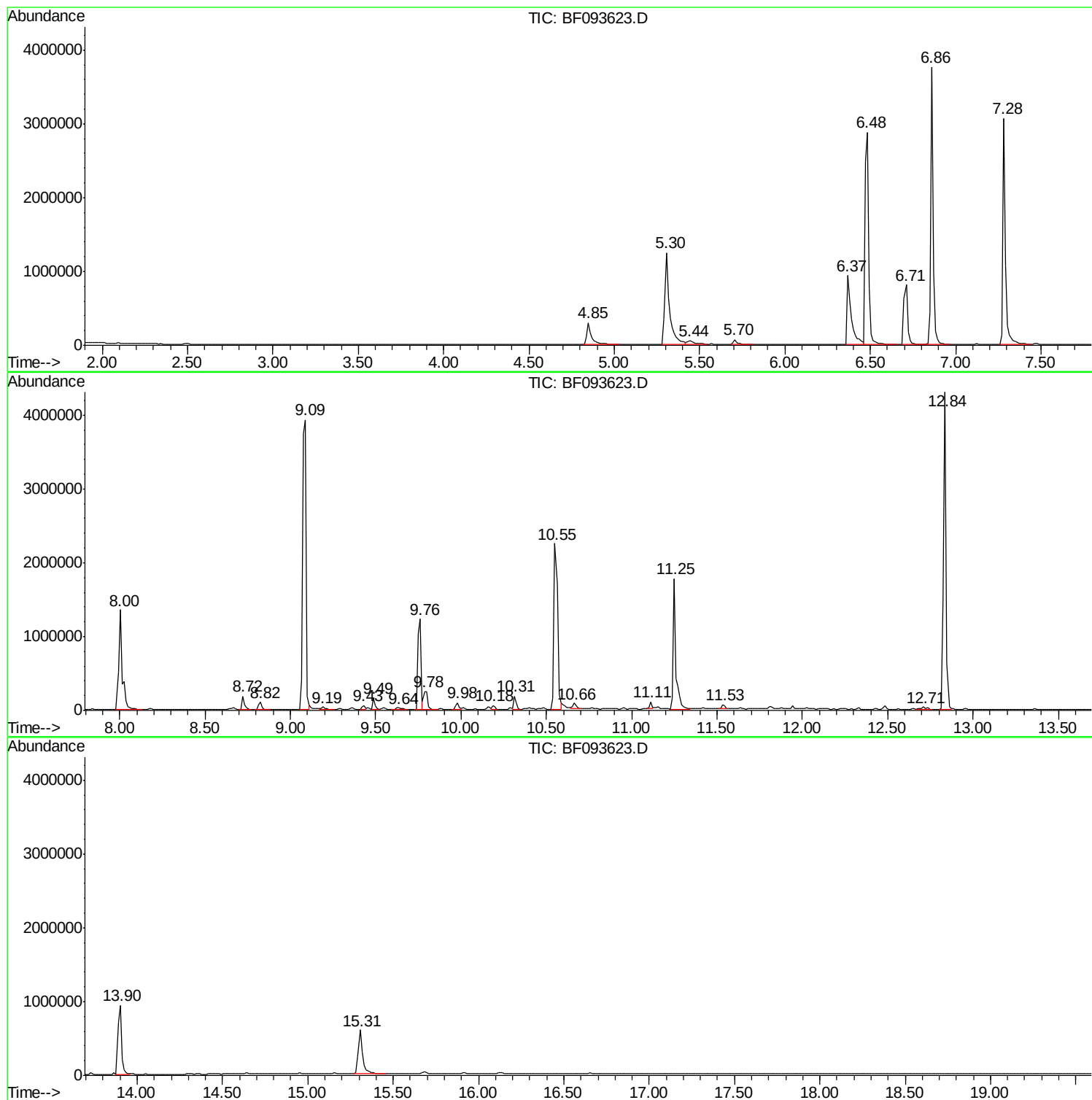
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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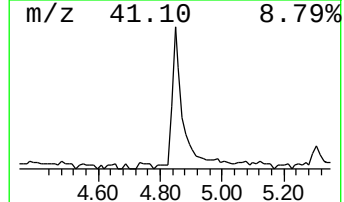
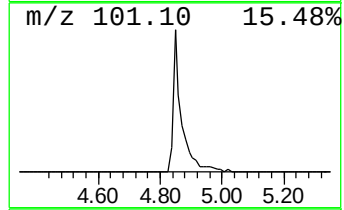
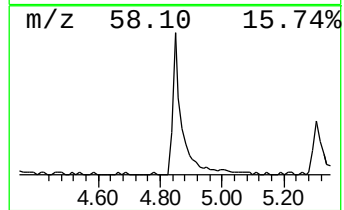
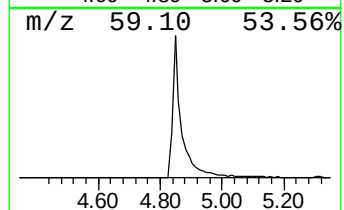
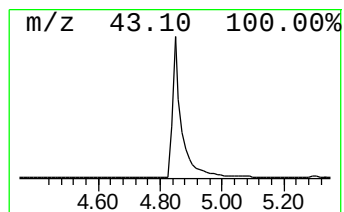
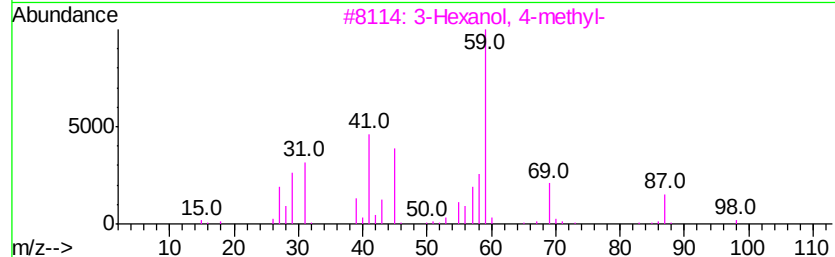
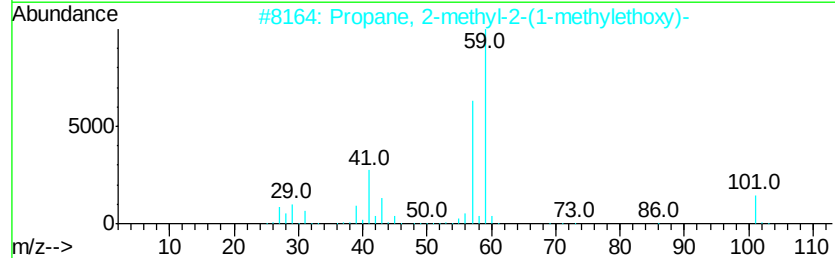
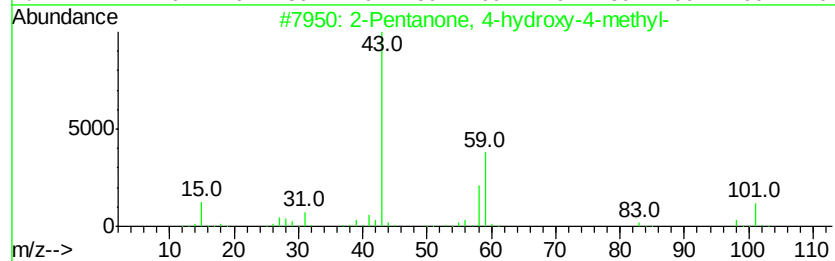
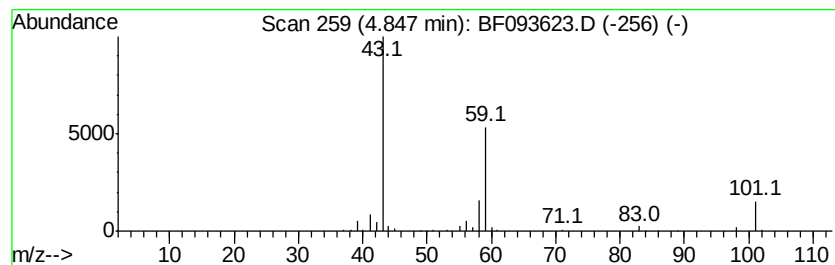
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	10.70 ng	620652	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25



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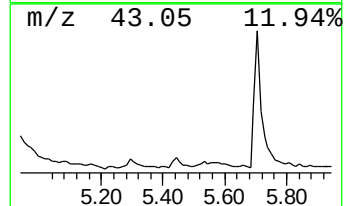
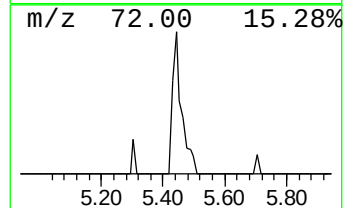
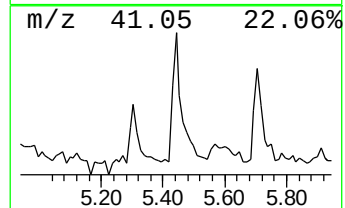
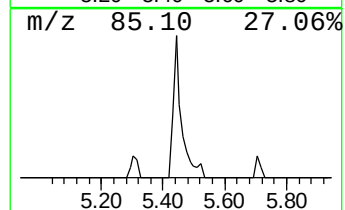
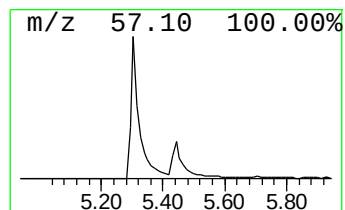
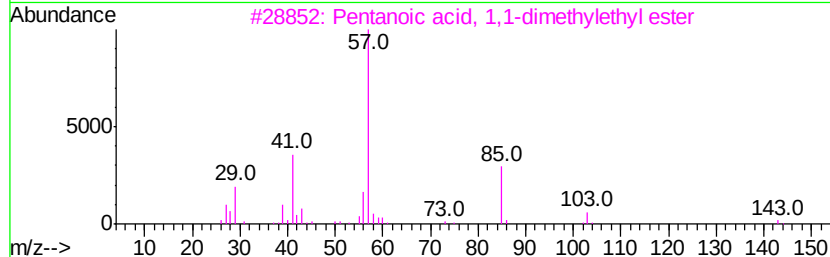
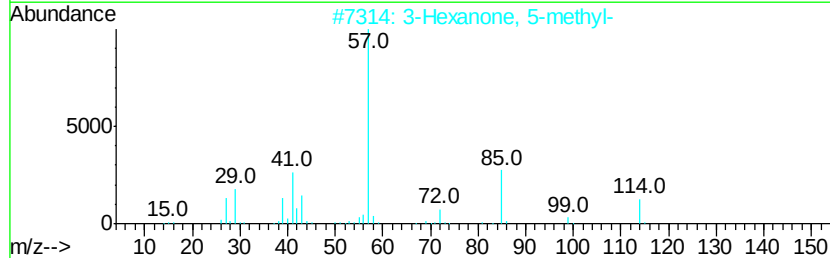
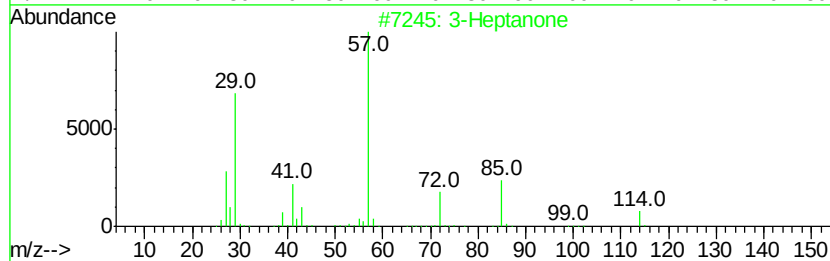
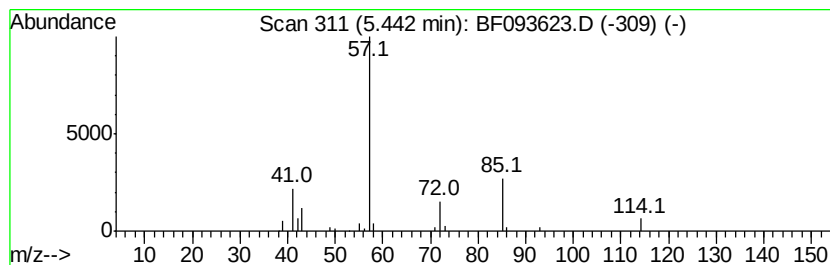
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Peak Number 2 3-Heptanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.44	2.25 ng	130323	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Heptanone	114	C7H14O	000106-35-4	86
2			3-Hexanone, 5-methyl-	114	C7H14O	000623-56-3	86
3			Pentanoic acid, 1,1-dimethylethyl...	158	C9H18O2	023361-78-6	42
4			Hexane, 1-(hexyloxy)-5-methyl-	200	C13H28O	074421-19-5	36
5			1-Penten-3-ol	86	C5H10O	000616-25-1	25



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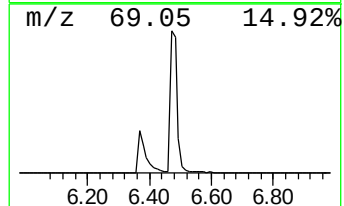
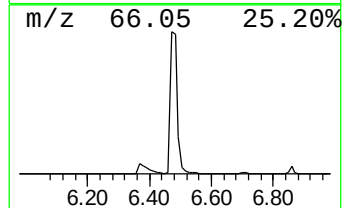
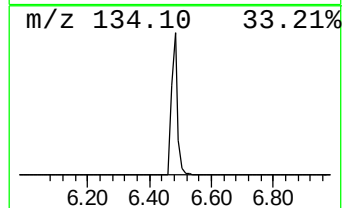
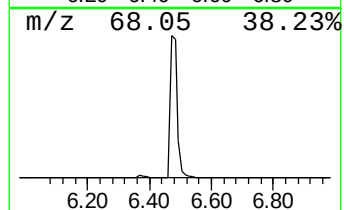
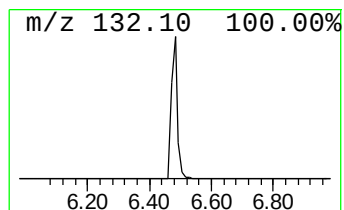
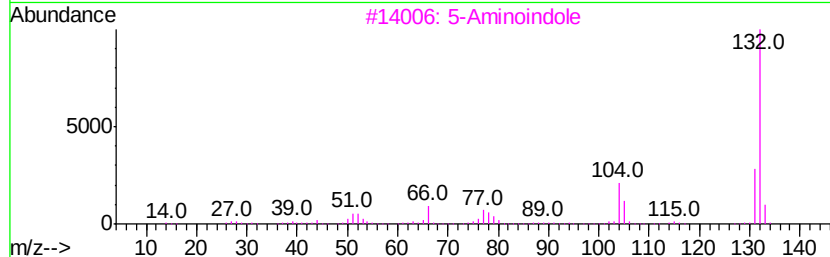
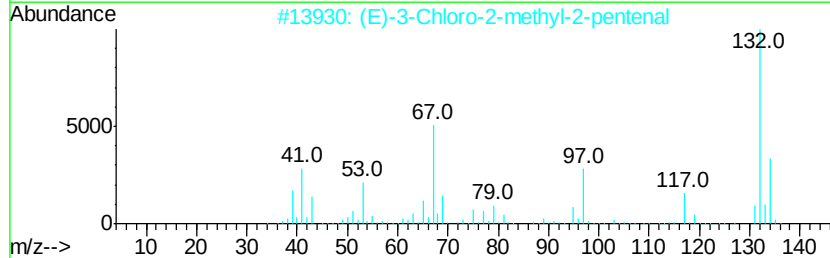
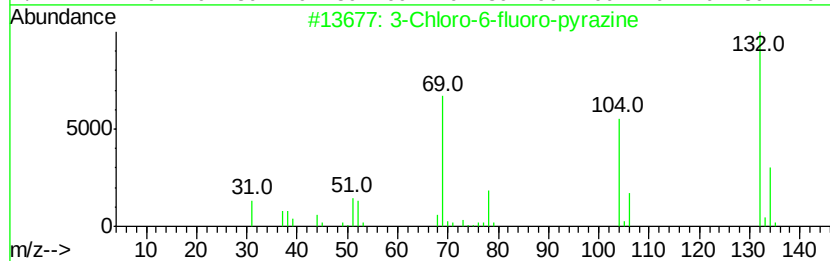
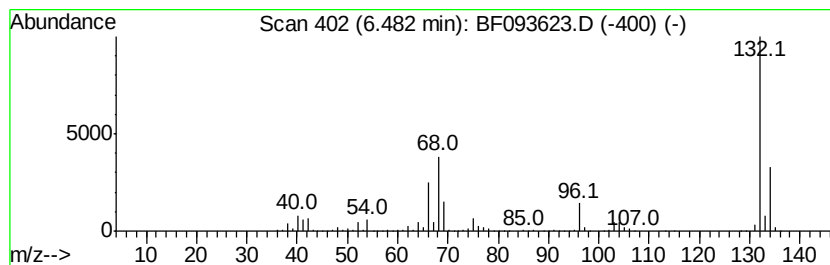
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Peak Number 3 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	76.26 ng	4422190	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		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.85	10.7	ng	620652	1	6.71	1159700	20.0
3-Heptanone	5.44	2.3	ng	130323	1	6.71	1159700	20.0
unknown6.48	6.48	76.3	ng	4422190	1	6.71	1159700	20.0