

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112217\
 Data File : BF100862.D
 Acq On : 23 Nov 2017 9:20
 Operator : SJ/JU
 Sample : I6541-04
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 111717-JETT-F-U-S

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	2.134	5	8	14	rVB2	30661	49249	2.27%	0.420%
2	5.069	504	507	513	rBV	98614	96946	4.47%	0.827%
3	5.469	572	575	579	rBV	588276	525166	24.24%	4.482%
4	6.481	743	747	755	rBB	408177	361242	16.67%	3.083%
5	6.628	767	772	775	rBV	1083585	982797	45.36%	8.388%
6	6.857	807	811	814	rBV	491846	383688	17.71%	3.275%
7	7.016	833	838	841	rBV	1572273	1392884	64.29%	11.888%
8	7.422	902	907	910	rBV	1120688	1121609	51.77%	9.573%
9	8.139	1025	1029	1032	rBV	632950	492786	22.74%	4.206%
10	9.216	1206	1212	1215	rBV	2355829	2166670	100.00%	18.492%
11	9.604	1274	1278	1281	rBV	35656	28171	1.30%	0.240%
12	9.898	1322	1328	1331	rBV	575690	550927	25.43%	4.702%
13	10.680	1458	1461	1465	rBV	826900	767639	35.43%	6.552%
14	10.786	1477	1479	1486	rBV	25894	25919	1.20%	0.221%
15	11.380	1576	1580	1584	rBV	574838	478418	22.08%	4.083%
16	12.969	1845	1850	1853	rBV	1700947	1524654	70.37%	13.013%
17	13.851	1997	2000	2004	rBV	29253	31531	1.46%	0.269%
18	14.021	2025	2029	2032	rBV	372057	317712	14.66%	2.712%
19	15.492	2274	2279	2288	rBV	297414	369386	17.05%	3.153%
20	16.445	2436	2441	2445	rVB4	15318	25262	1.17%	0.216%
21	17.033	2535	2541	2550	rBV5	12542	24178	1.12%	0.206%

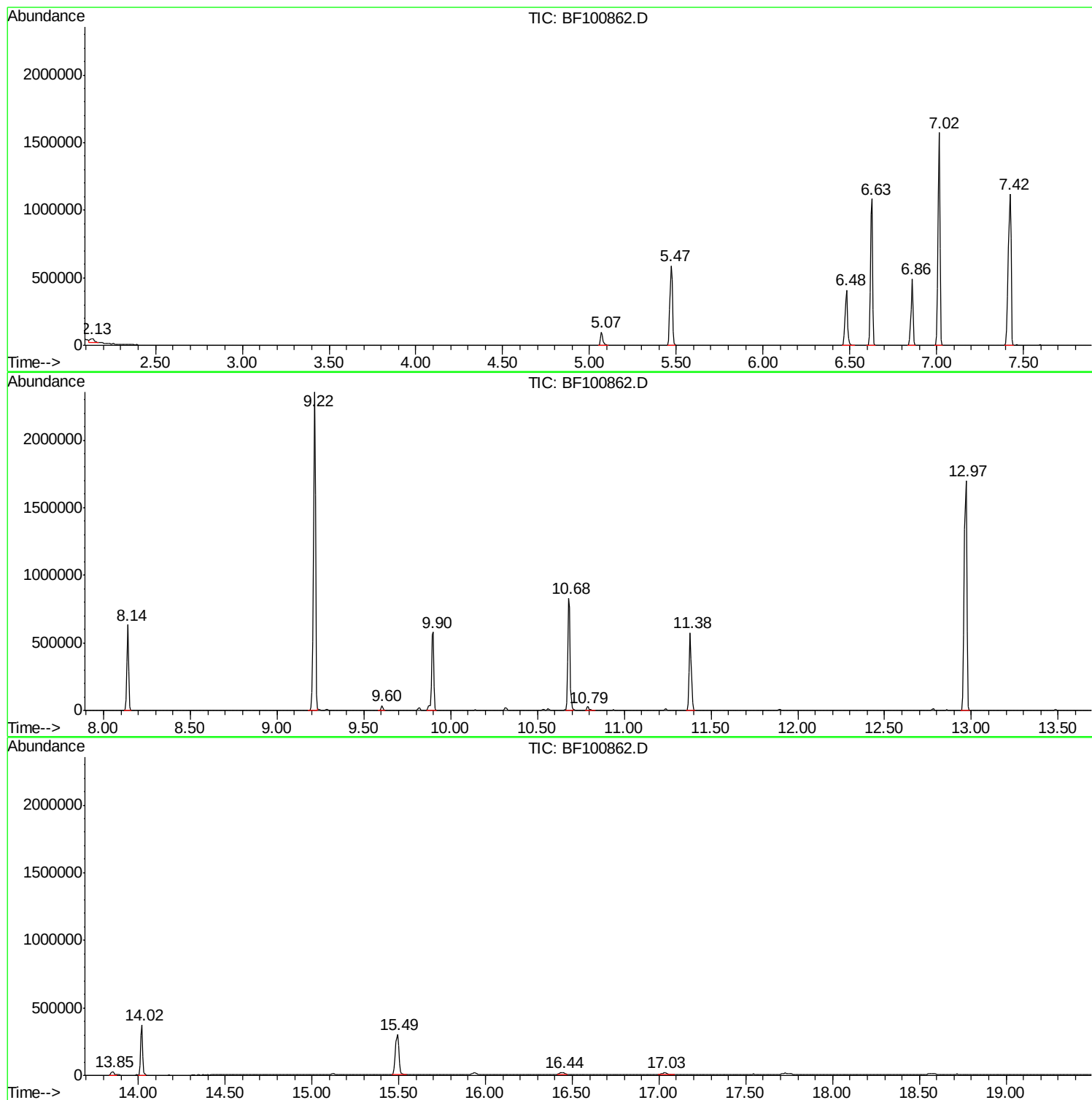
Sum of corrected areas: 11716834

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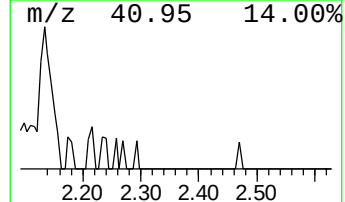
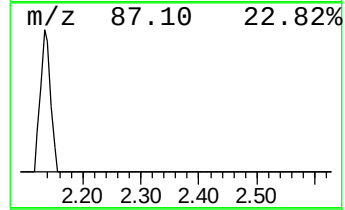
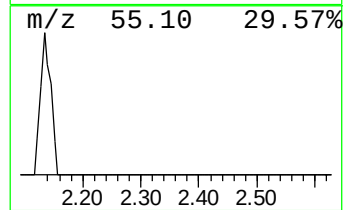
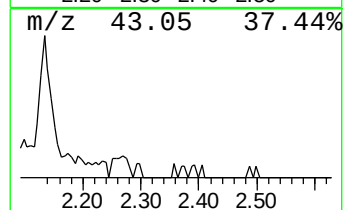
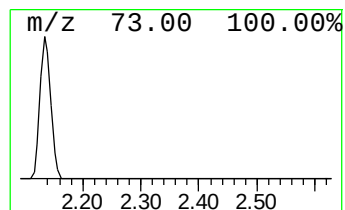
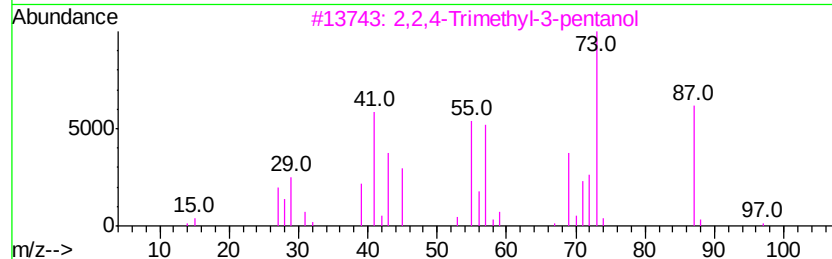
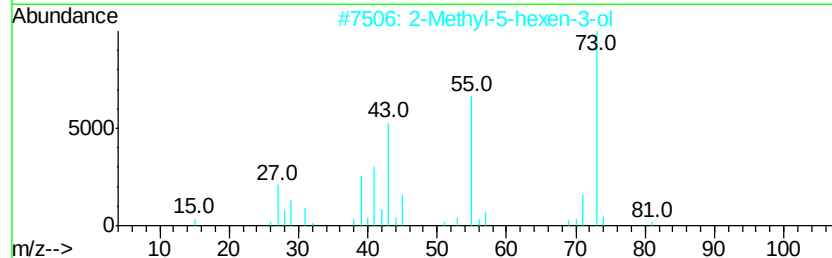
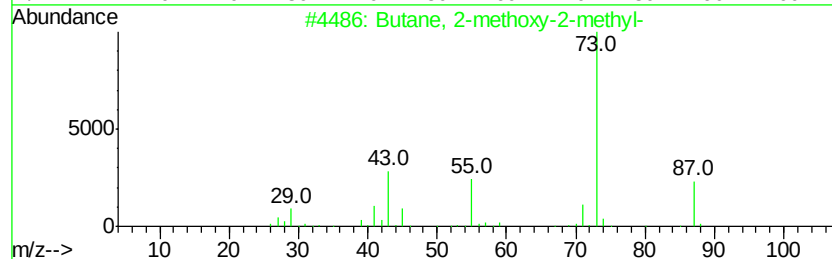
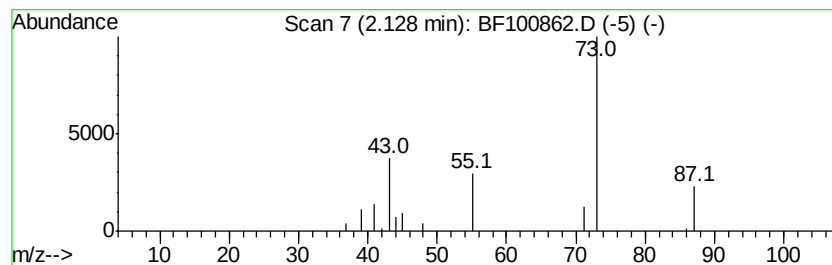
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	2.57 ng	49249	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	56
2		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9
3		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9
4		3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	9
5		Acetic acid, 3-[1,3]dioxolan-2-y...	174	C8H14O4	1000186-02-3	9



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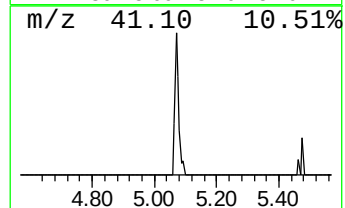
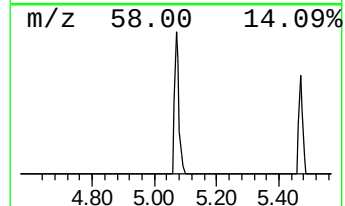
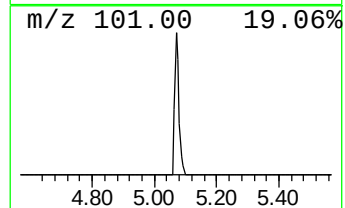
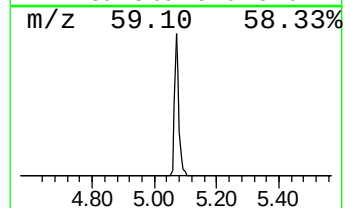
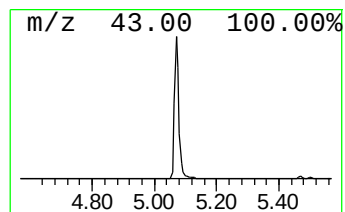
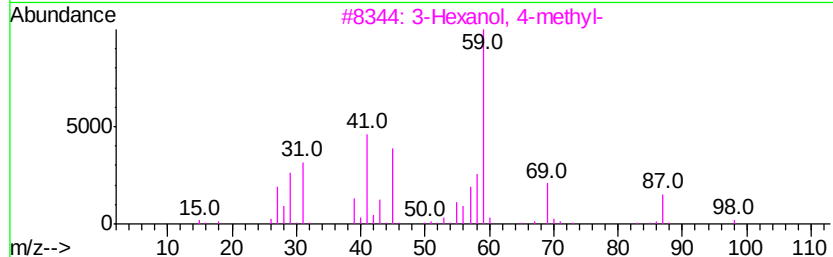
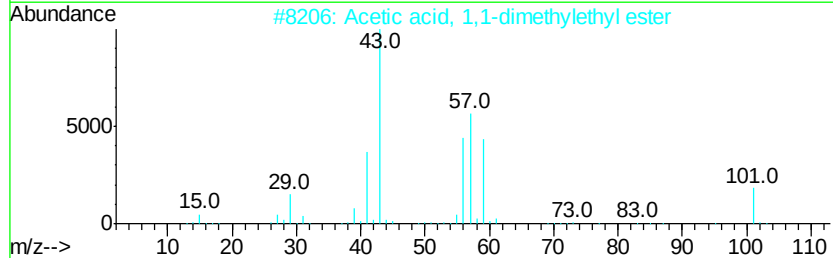
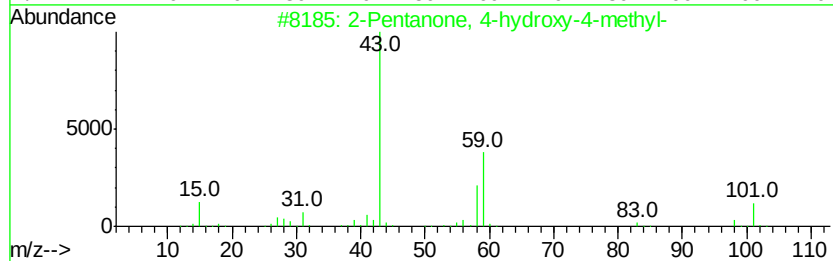
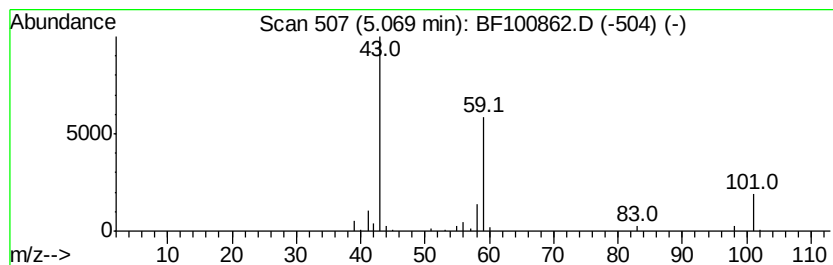
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	5.05 ng	96946	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	56
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9



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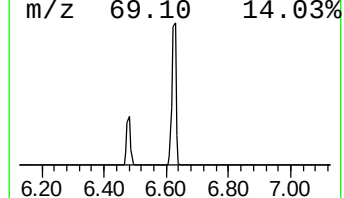
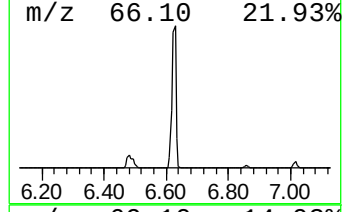
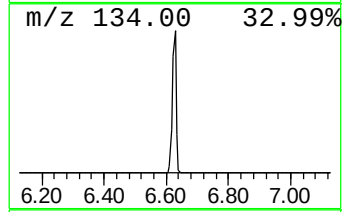
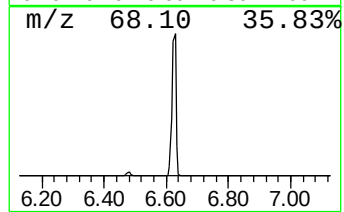
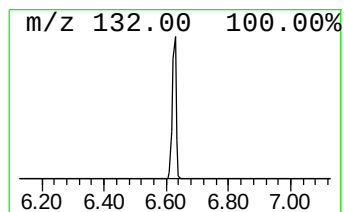
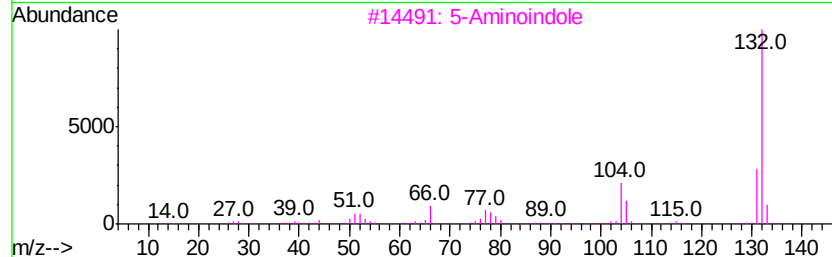
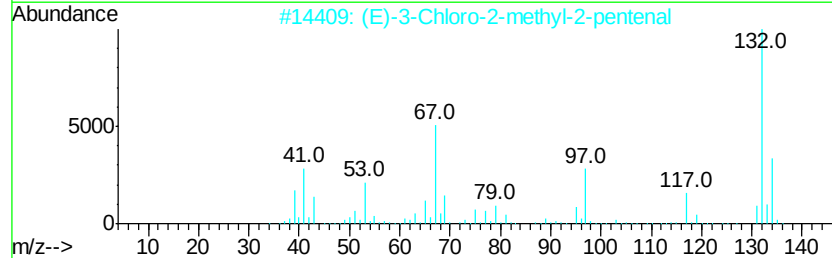
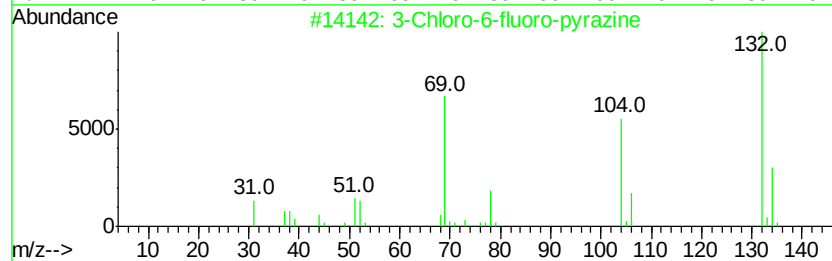
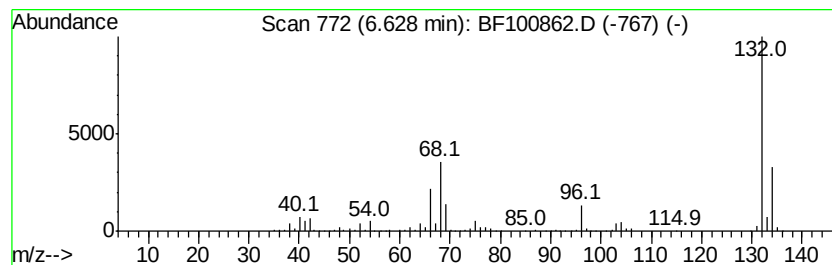
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Peak Number 3 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	51.23 ng	982797	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	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.13	2.6	ng	49249	1	6.86	383688	20.0
2-Pentanone, 4-hy...	5.07	5.0	ng	96946	1	6.86	383688	20.0
unknown6.63	6.63	51.2	ng	982797	1	6.86	383688	20.0