

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112217\
 Data File : BF100868.D
 Acq On : 23 Nov 2017 11:59
 Operator : SJ/JU
 Sample : I6541-10
 Misc :
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 111717-SIDI-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	2.140	7	9	27	rVB3	59375	142631	5.77%	1.041%
2	5.075	504	508	515	rBV	133012	148807	6.02%	1.086%
3	5.475	572	576	579	rBV	688950	635907	25.71%	4.640%
4	6.481	743	747	757	rBB	472974	421402	17.04%	3.075%
5	6.628	767	772	775	rBV	1304279	1182387	47.81%	8.627%
6	6.857	807	811	814	rBV	556897	431774	17.46%	3.150%
7	7.016	833	838	841	rBV	1879979	1648119	66.64%	12.025%
8	7.422	902	907	910	rBV	1233740	1354596	54.77%	9.883%
9	8.139	1025	1029	1032	rBV	688564	555835	22.47%	4.055%
10	9.216	1206	1212	1215	rBV	2589265	2473248	100.00%	18.045%
11	9.604	1275	1278	1281	rBV	38227	29507	1.19%	0.215%
12	9.892	1322	1327	1331	rBV	672245	621039	25.11%	4.531%
13	10.316	1391	1399	1402	rBV2	27514	25214	1.02%	0.184%
14	10.680	1457	1461	1465	rBV	919234	878337	35.51%	6.408%
15	10.786	1476	1479	1484	rBV2	31225	30296	1.22%	0.221%
16	11.380	1576	1580	1584	rBV	674697	550259	22.25%	4.015%
17	12.968	1845	1850	1853	rBV	1909944	1776417	71.83%	12.961%
18	14.021	2025	2029	2032	rBV	434163	380020	15.37%	2.773%
19	15.492	2273	2279	2289	rBV	332009	420153	16.99%	3.065%

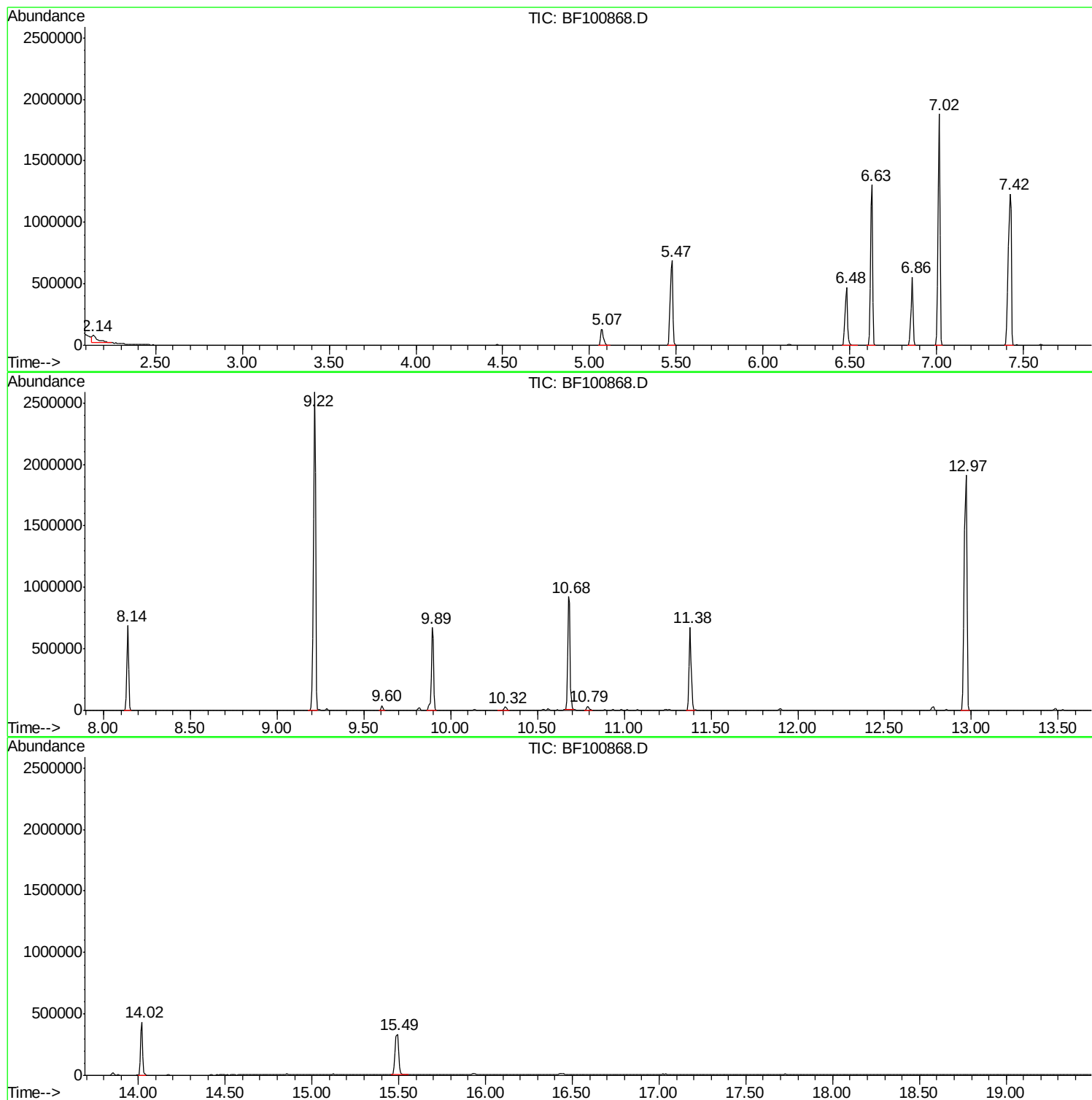
Sum of corrected areas: 13705948

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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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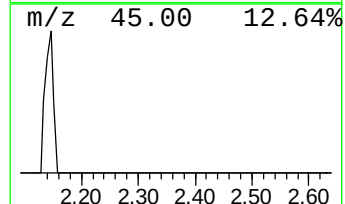
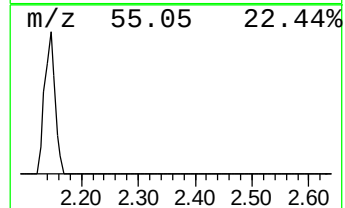
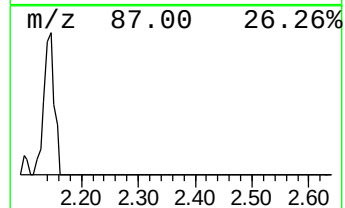
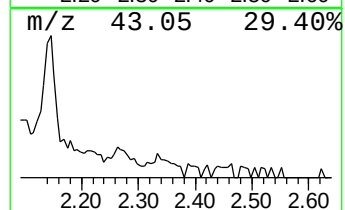
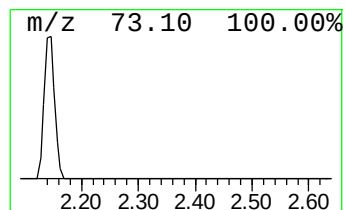
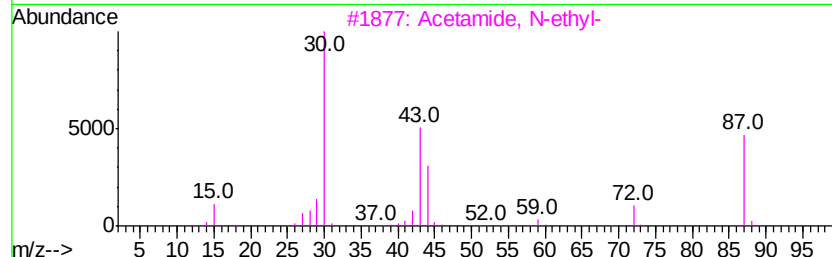
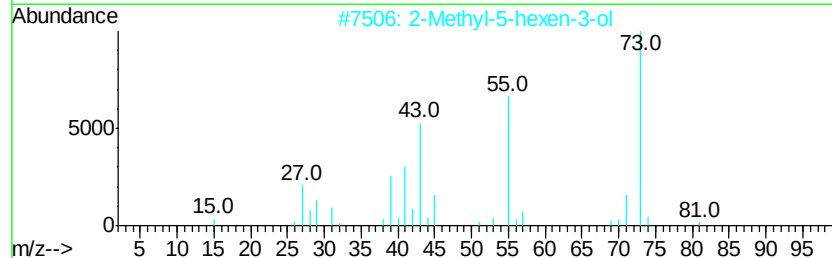
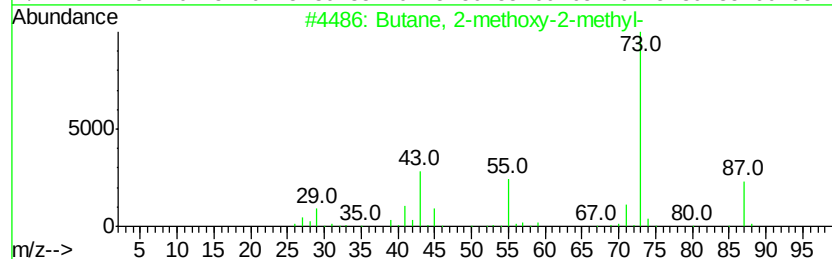
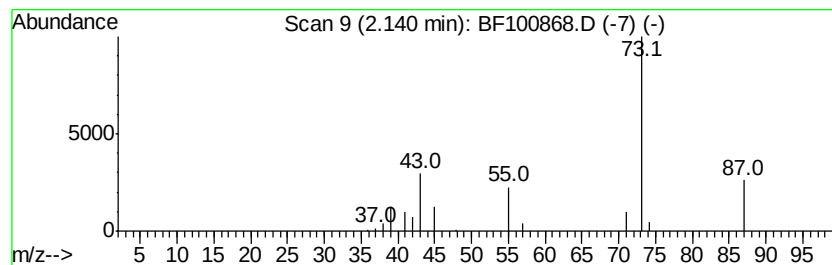
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.14	6.61 ng	142631	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	5
4			N-Ethylformamide	73	C3H7NO	000627-45-2	5
5			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	5



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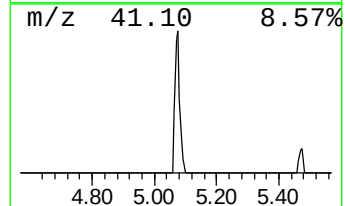
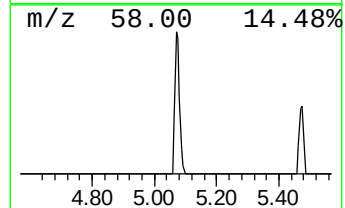
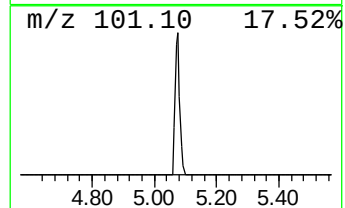
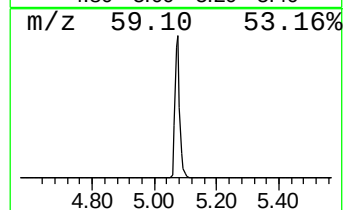
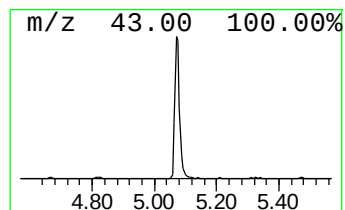
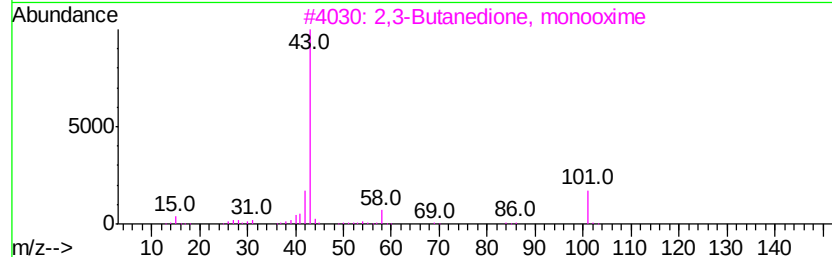
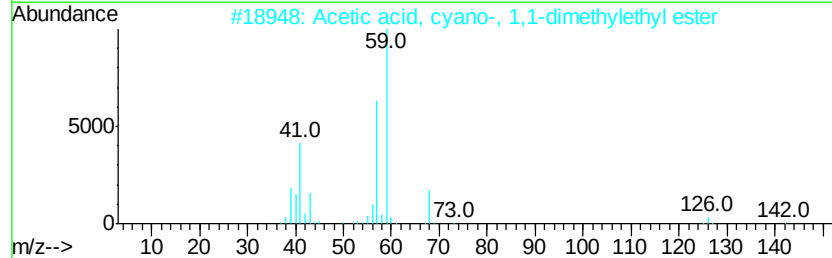
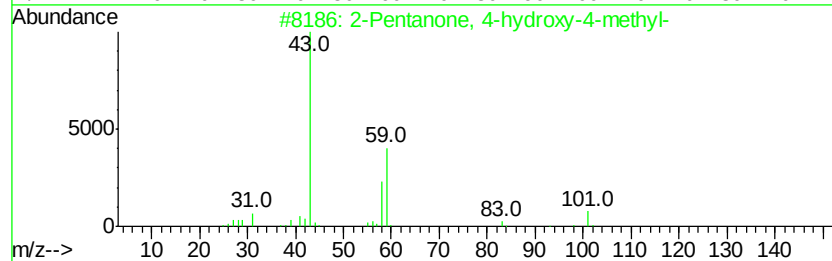
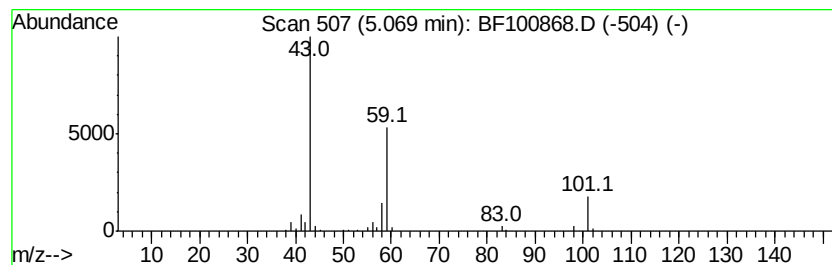
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	6.89 ng	148807	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			1,2-Butanediol	90	C4H10O2	000584-03-2	9
5			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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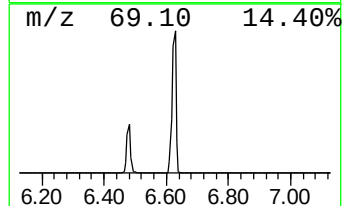
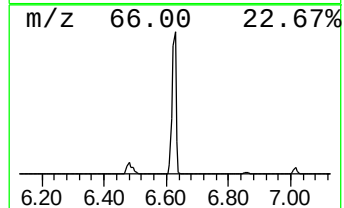
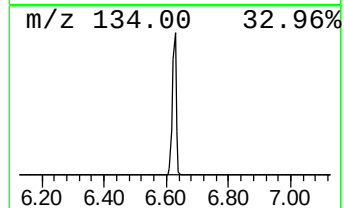
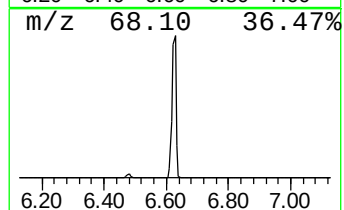
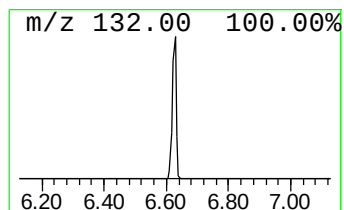
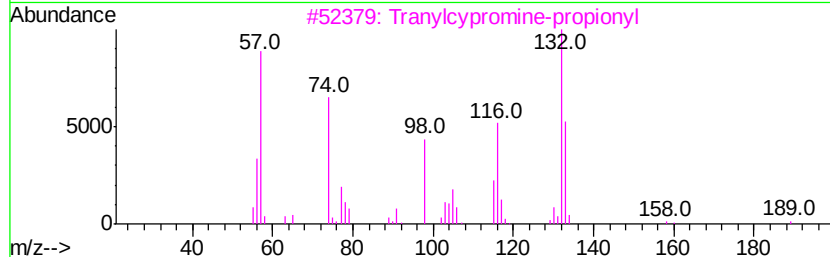
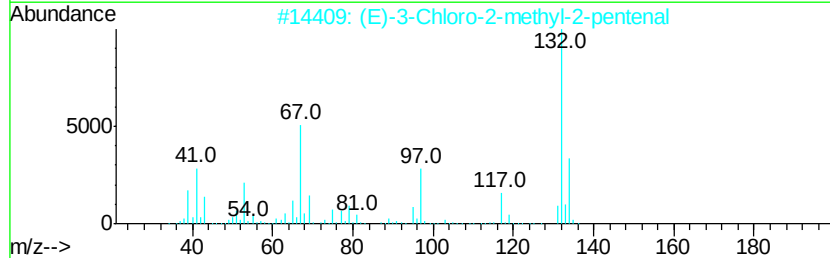
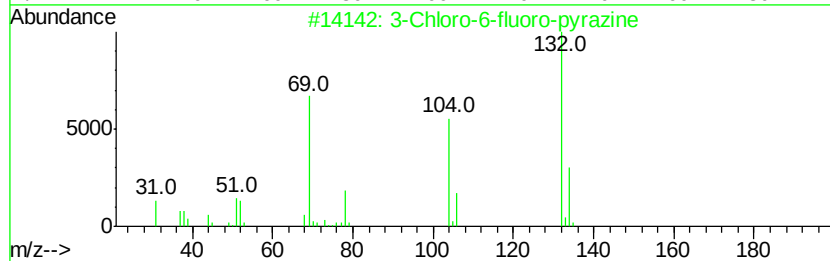
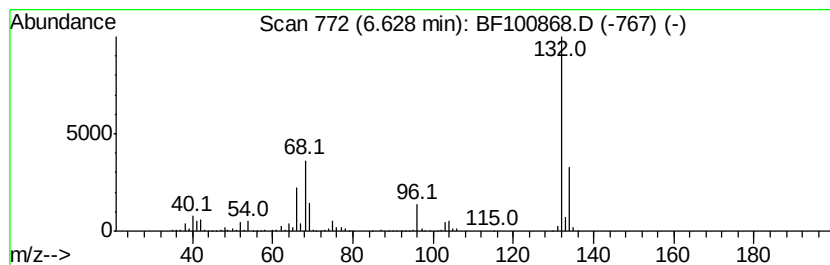
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Peak Number 3 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	54.77 ng	1182390	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	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	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...	2.14	6.6	ng	142631	1	6.86	431774	20.0
2-Pentanone, 4-hy...	5.07	6.9	ng	148807	1	6.86	431774	20.0
unknown6.63	6.63	54.8	ng	1182390	1	6.86	431774	20.0