

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100817\
 Data File : BF099256.D
 Acq On : 9 Oct 2017 3:03
 Operator : SJ/JU
 Sample : I5645-03
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 100317-TIDO-F-U-B

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-BF092317.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	2.163	8	13	23	rVB	625160	804707	20.36%	3.343%
2	5.087	507	510	519	rBV	183542	201492	5.10%	0.837%
3	5.487	574	578	590	rBV	1406110	1263837	31.98%	5.251%
4	6.492	745	749	762	rVB	996310	807384	20.43%	3.354%
5	6.634	769	773	776	rBV	2384293	2106743	53.30%	8.753%
6	6.863	808	812	816	rBV	917431	701633	17.75%	2.915%
7	7.022	834	839	842	rBV	2963205	2745127	69.45%	11.405%
8	7.434	903	909	912	rBV	2170416	2247252	56.86%	9.337%
9	8.145	1026	1030	1038	rBV	1157573	970457	24.55%	4.032%
10	9.222	1207	1213	1216	rBV	3854735	3952475	100.00%	16.422%
11	9.610	1276	1279	1288	rBV	130453	104336	2.64%	0.433%
12	9.898	1324	1328	1332	rBV	1122585	1051657	26.61%	4.369%
13	10.316	1393	1399	1402	rVB2	40894	40769	1.03%	0.169%
14	10.692	1459	1463	1471	rBV	1472544	1415306	35.81%	5.880%
15	10.792	1477	1480	1489	rVB	40681	42797	1.08%	0.178%
16	11.386	1577	1581	1585	rBV	1184961	1011127	25.58%	4.201%
17	12.780	1815	1818	1821	rBV	60131	43748	1.11%	0.182%
18	12.974	1846	1851	1854	rBV	3188712	3206723	81.13%	13.323%
19	13.851	1997	2000	2008	rBV	36538	43452	1.10%	0.181%
20	14.027	2026	2030	2039	rVB	763407	675570	17.09%	2.807%
21	15.504	2275	2281	2288	rBV	472891	632218	16.00%	2.627%

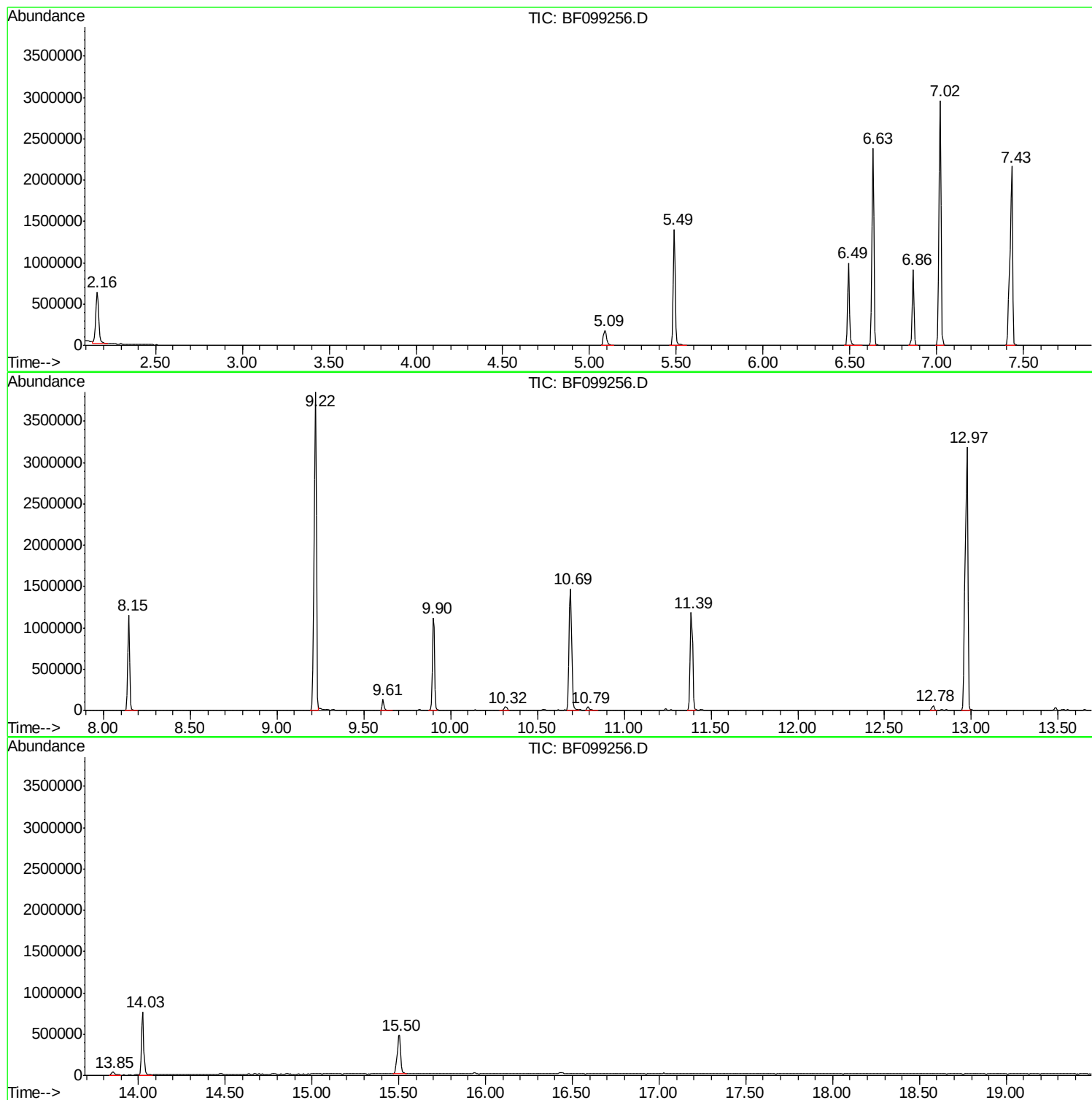
Sum of corrected areas: 24068810

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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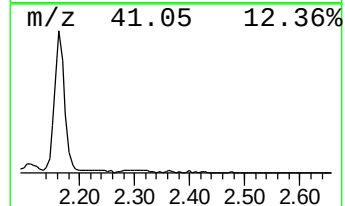
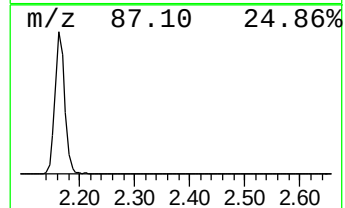
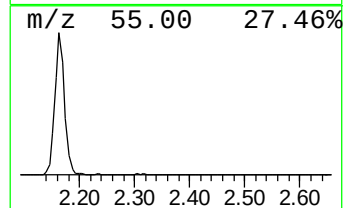
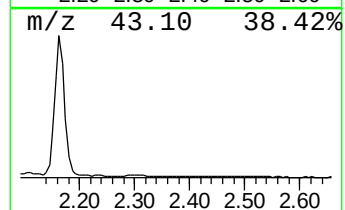
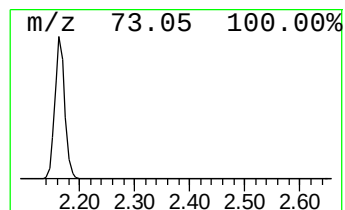
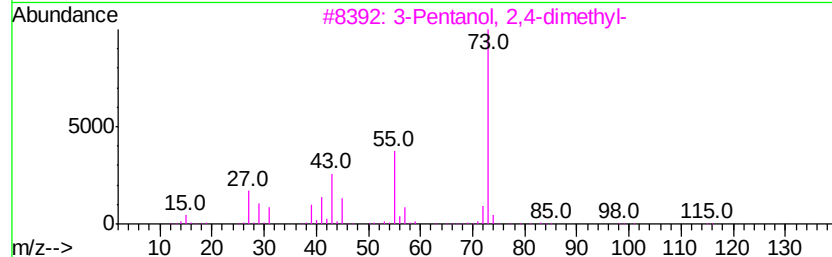
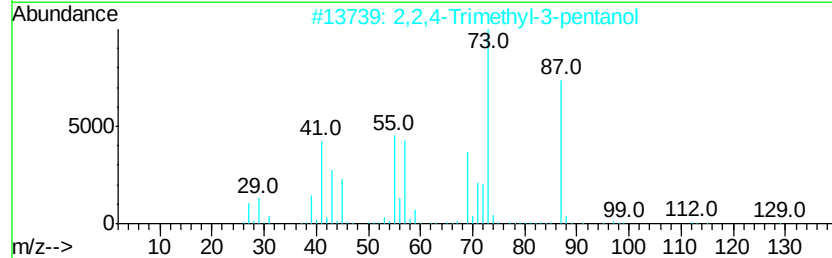
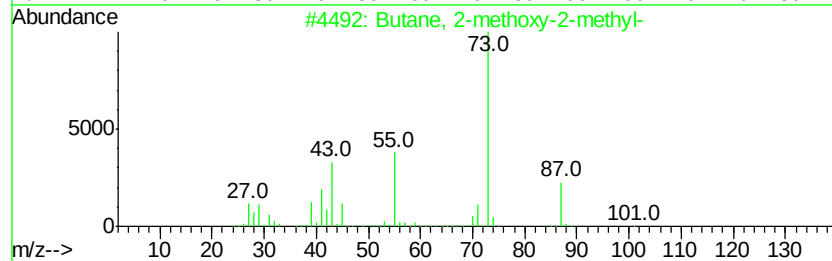
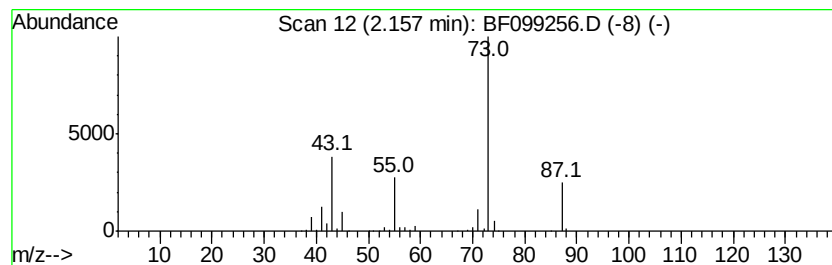
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	22.94 ng	804707	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	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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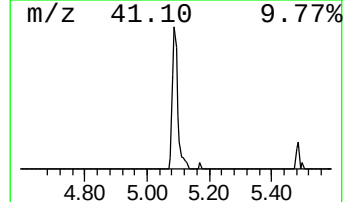
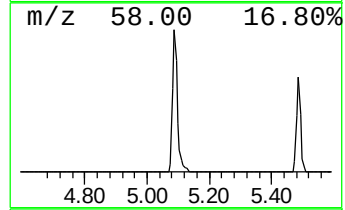
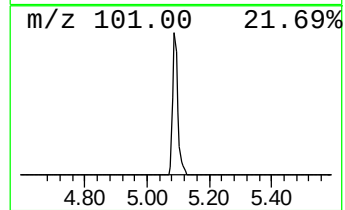
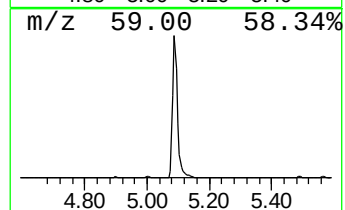
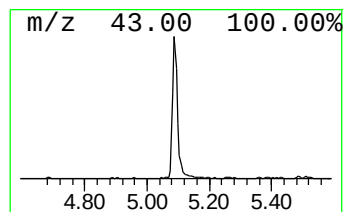
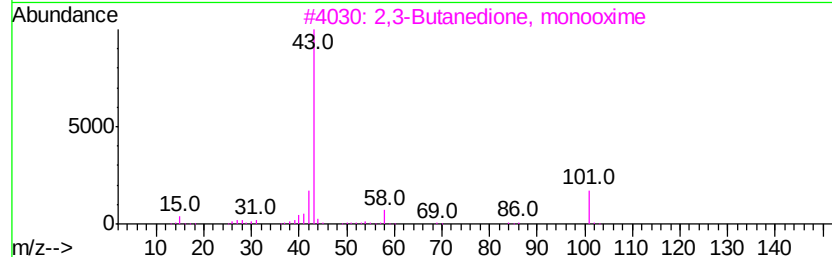
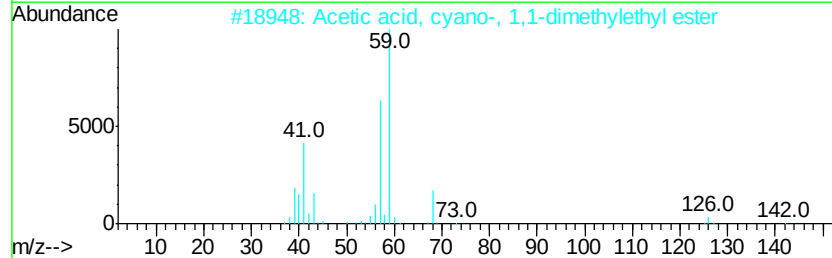
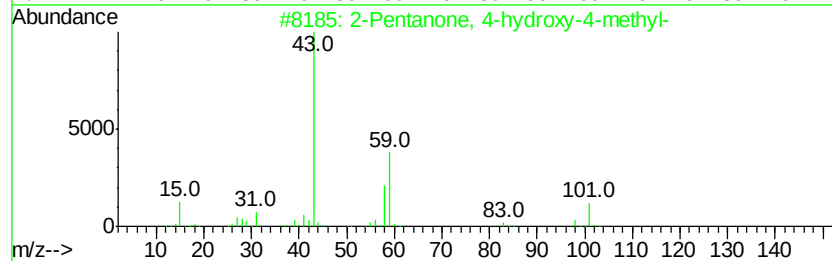
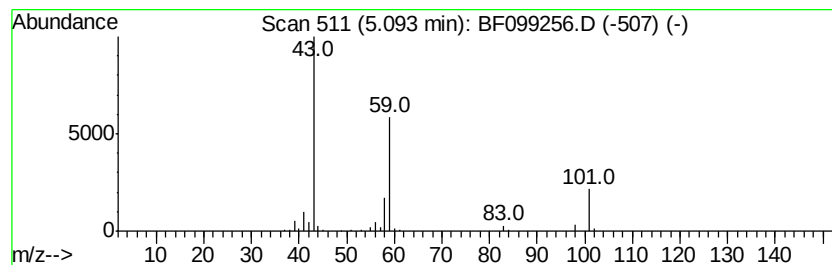
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	5.74 ng	201492	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	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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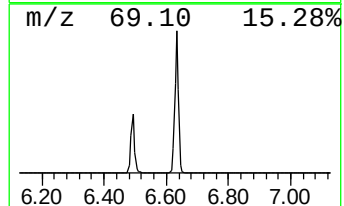
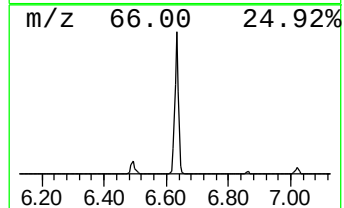
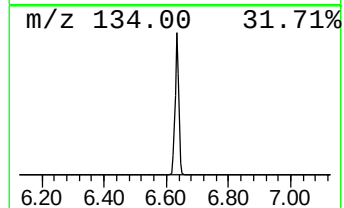
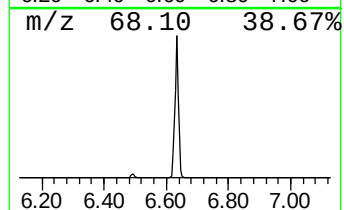
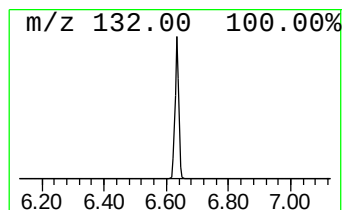
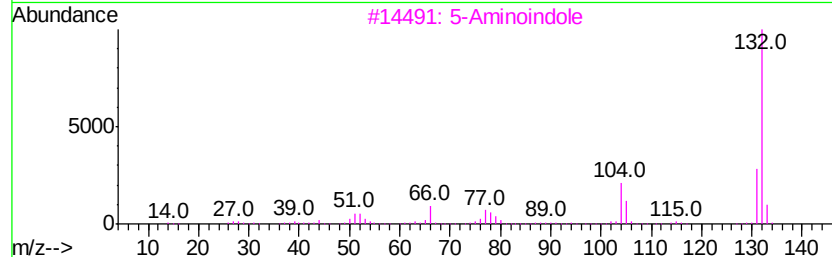
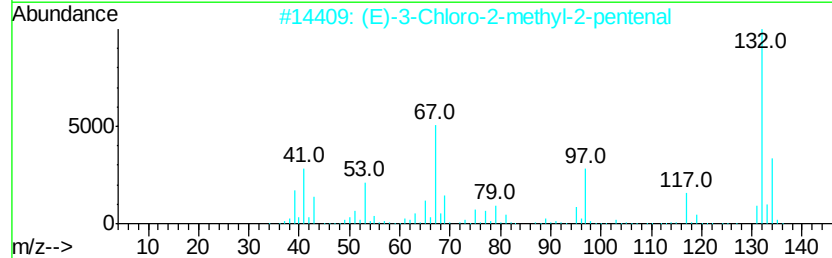
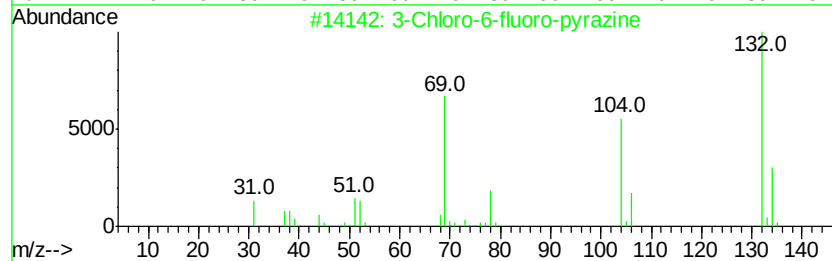
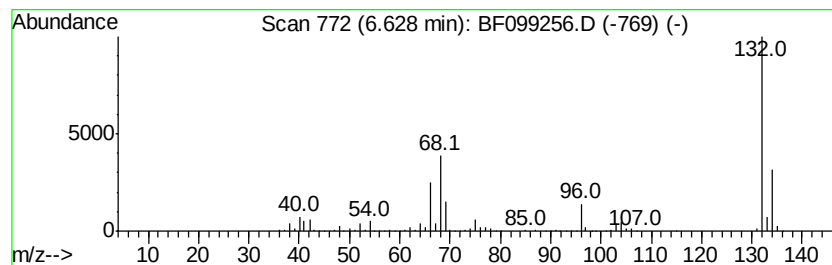
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Peak Number 3 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	60.05 ng	2106740	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	35
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...	2.16	22.9	ng	804707	1	6.86	701633	20.0
2-Pentanone, 4-hy...	5.09	5.7	ng	201492	1	6.86	701633	20.0
unknown6.63	6.63	60.0	ng	2106740	1	6.86	701633	20.0