

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082316\
 Data File : BF089849.D
 Acq On : 23 Aug 2016 23:49
 Operator : UM/SJ
 Sample : PB93042BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB93042BL

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-BF081916.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	1.656	4	6	14	rVV	495935	818076	6.69%	0.840%
2	1.770	14	16	22	rVV	2532854	4094268	33.50%	4.204%
3	1.850	22	23	44	rVB	385618	942752	7.71%	0.968%
4	4.799	278	281	291	rVB	1377118	2550730	20.87%	2.619%
5	5.244	317	320	323	rBV	7032847	8903408	72.85%	9.142%
6	6.307	410	413	415	rBV	8292330	9097344	74.44%	9.341%
7	6.433	421	424	426	rBV	9621709	9699515	79.36%	9.960%
8	6.662	442	444	447	rBV	2352631	2264431	18.53%	2.325%
9	6.822	455	458	460	rBV	8509561	7390721	60.47%	7.589%
10	7.233	491	494	496	rBV	6003455	6062125	49.60%	6.225%
11	7.953	554	557	559	rBV	3734478	3310551	27.09%	3.399%
12	9.039	648	652	654	rBV	11003875	12221631	100.00%	12.549%
13	9.702	707	710	713	rBV	4116565	3606716	29.51%	3.703%
14	10.491	776	779	781	rBV	6099143	6338782	51.87%	6.509%
15	11.176	837	839	842	rBV	3381094	3376359	27.63%	3.467%
16	12.777	976	979	981	rBV	10181214	10893521	89.13%	11.186%
17	13.840	1069	1072	1074	rBV	2773005	3318029	27.15%	3.407%
18	15.303	1197	1200	1203	rBV	2153477	2499190	20.45%	2.566%

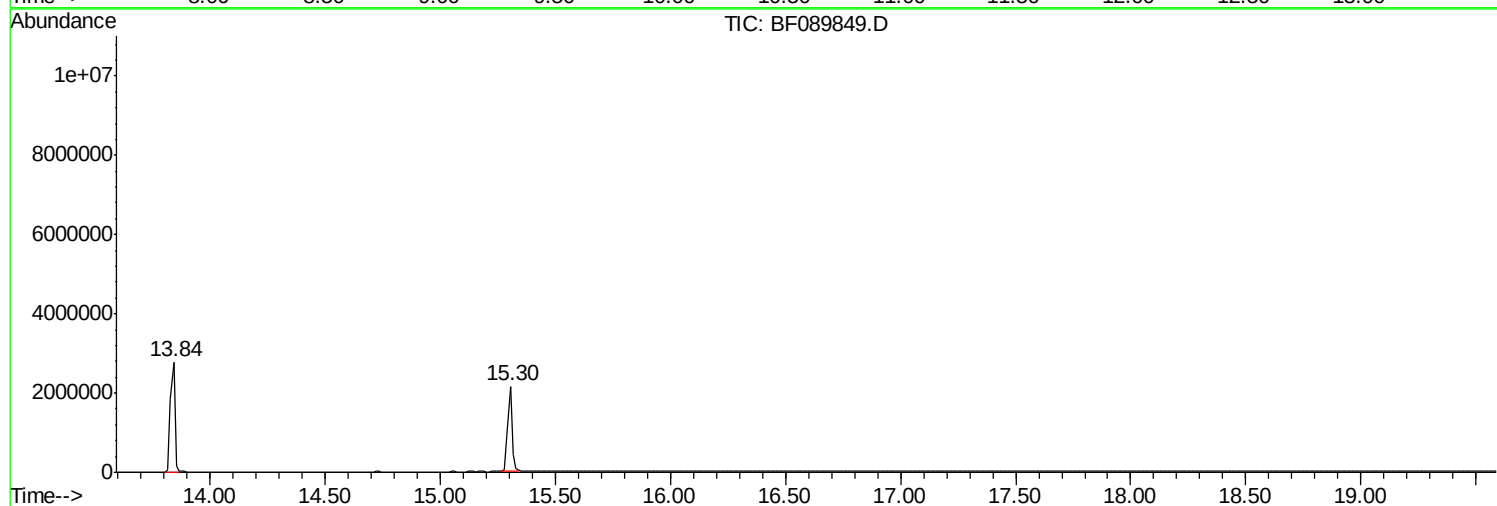
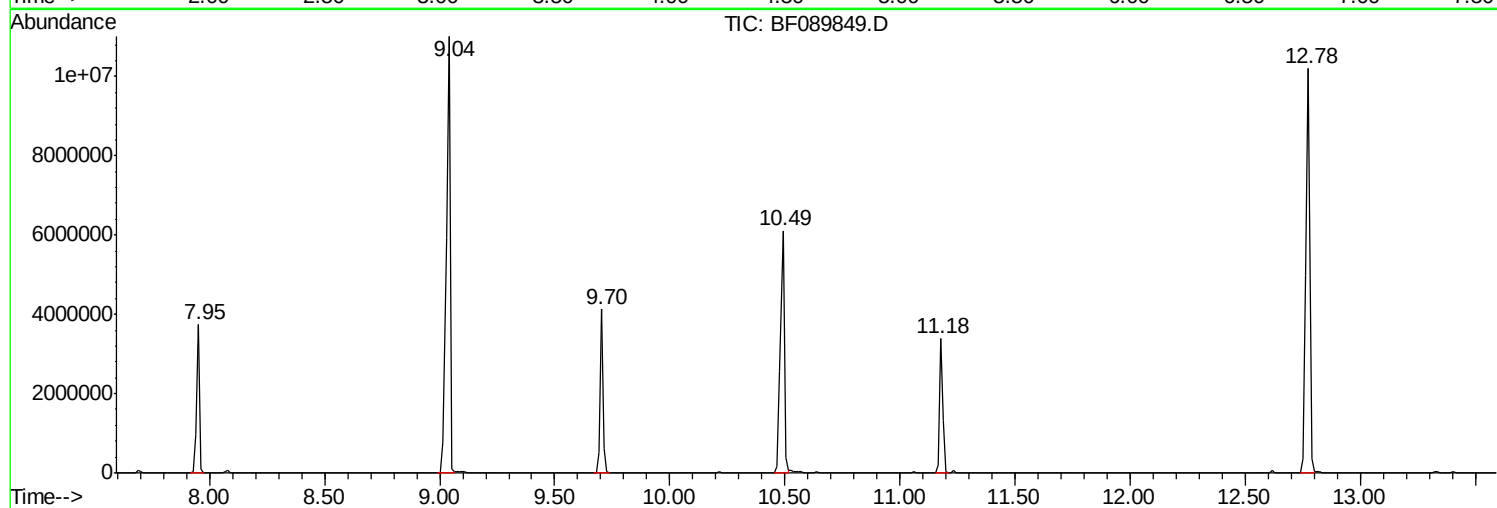
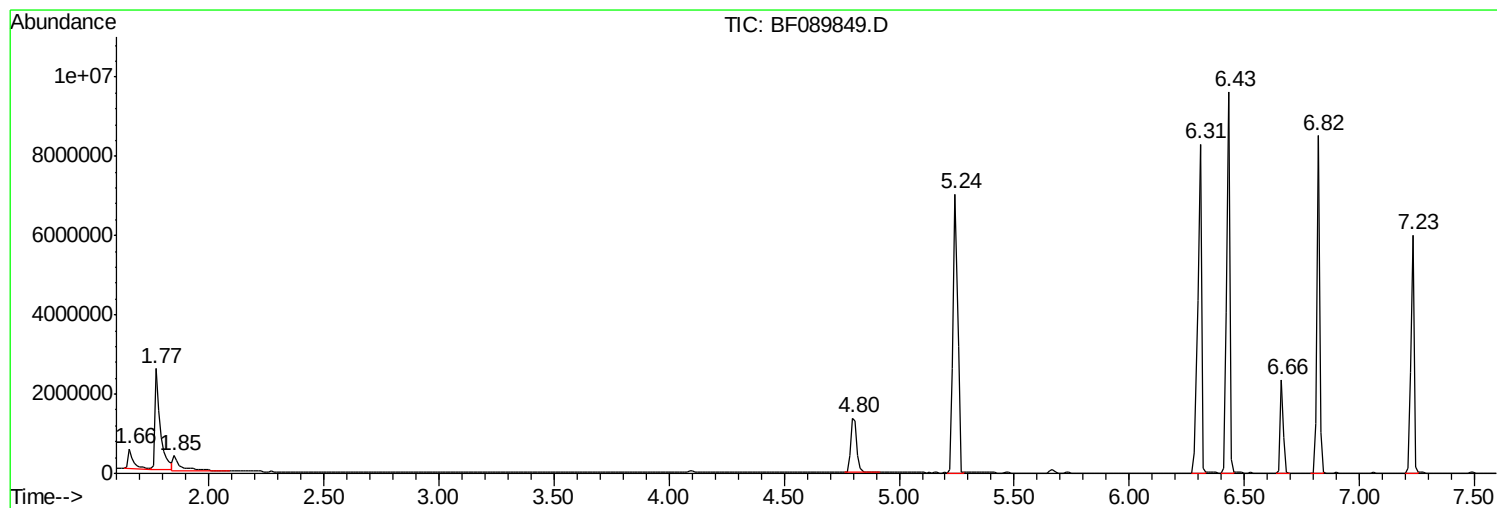
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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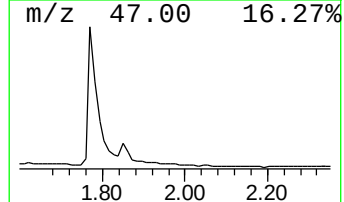
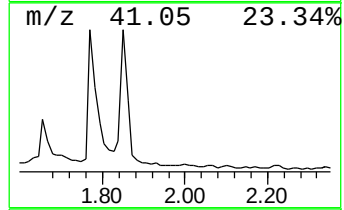
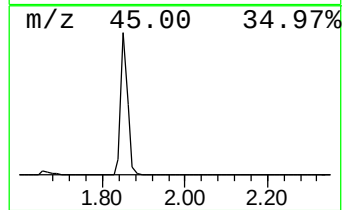
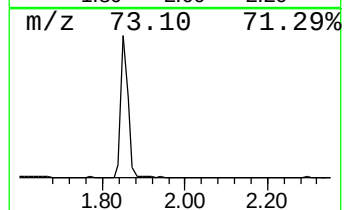
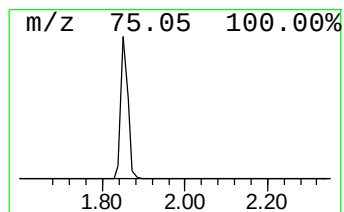
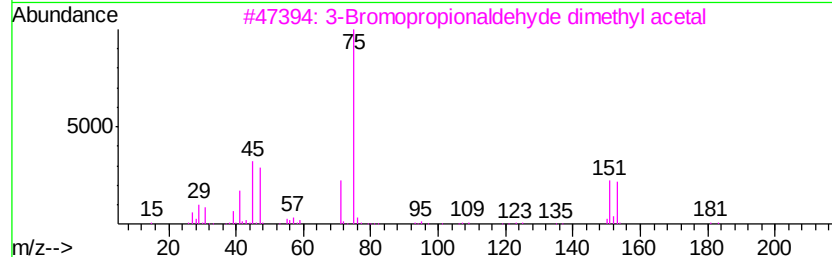
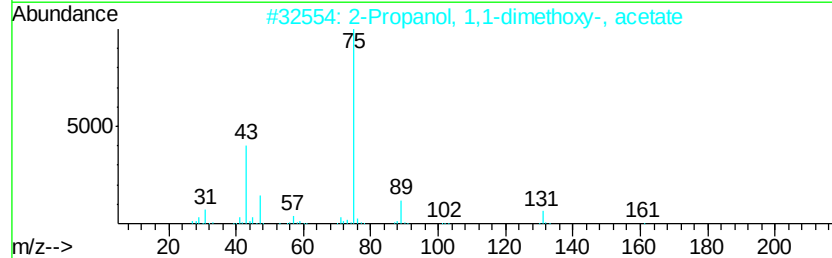
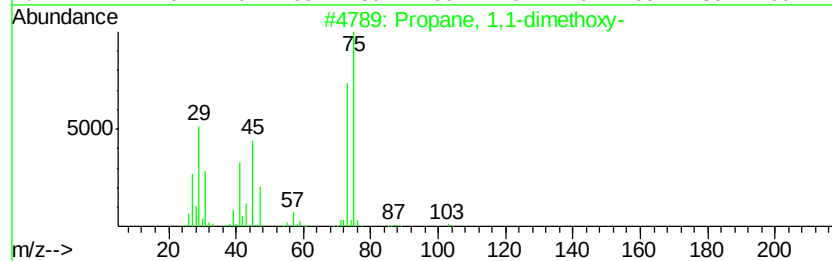
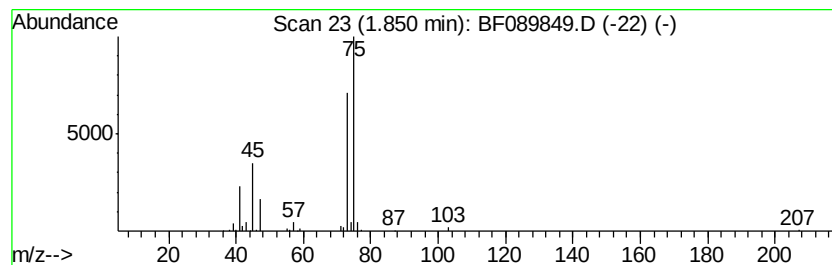
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.85	8.33 ng	942752	1,4-Dichlorobenzene-d4	6.66	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2	2-Propanol, 1,1-dimethoxy-, acetate	162	C7H14O4	074495-37-7	38
3	3-Bromopropionaldehyde dimethyl ...	182	C5H11BrO2	036255-44-4	38
4	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	14
5	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	14



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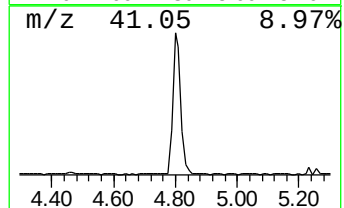
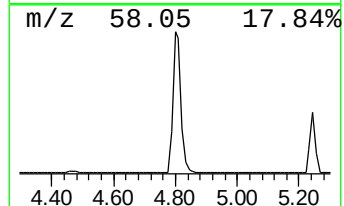
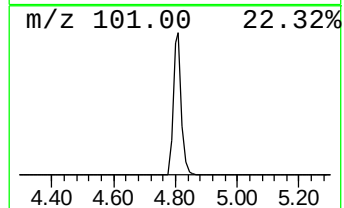
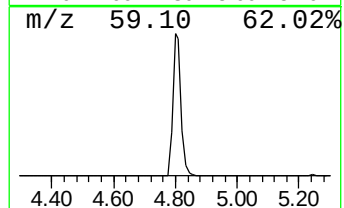
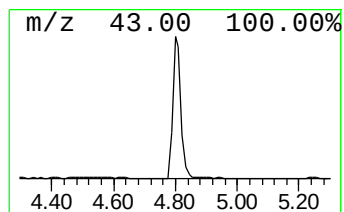
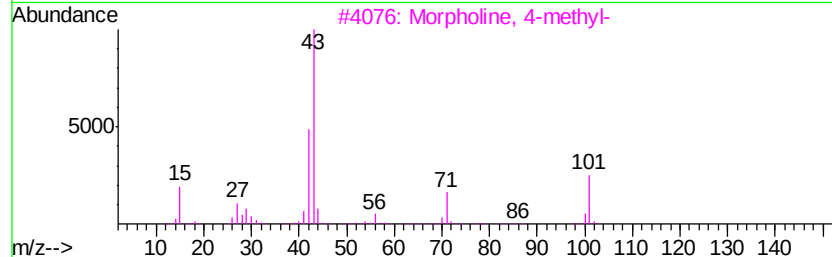
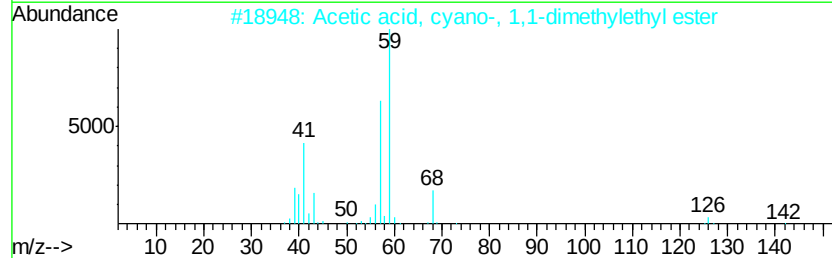
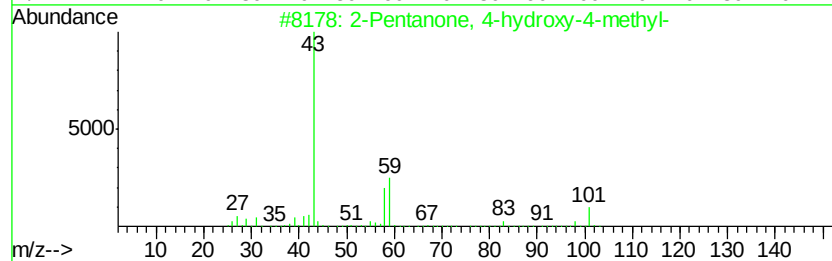
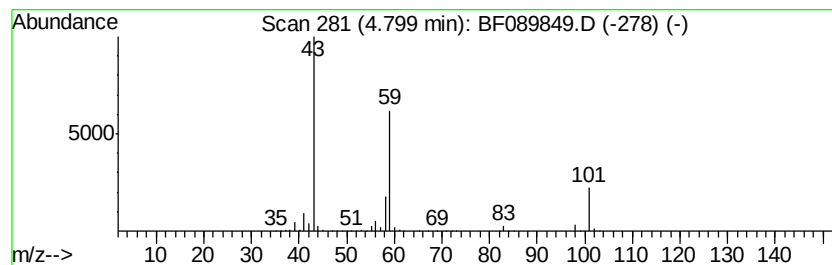
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	22.53 ng	2550730	1,4-Dichlorobenzene-d4	6.66

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	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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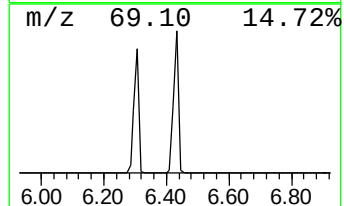
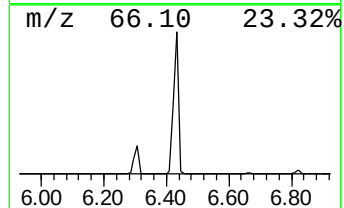
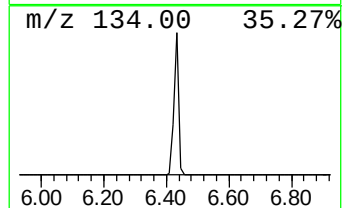
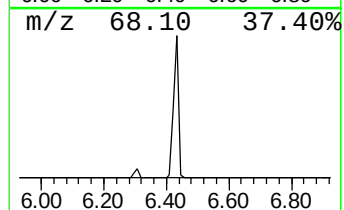
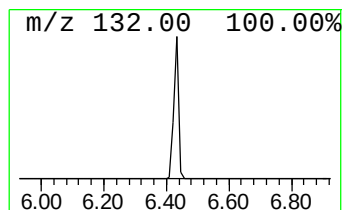
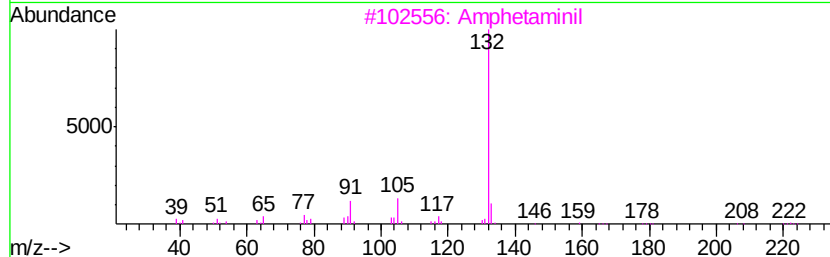
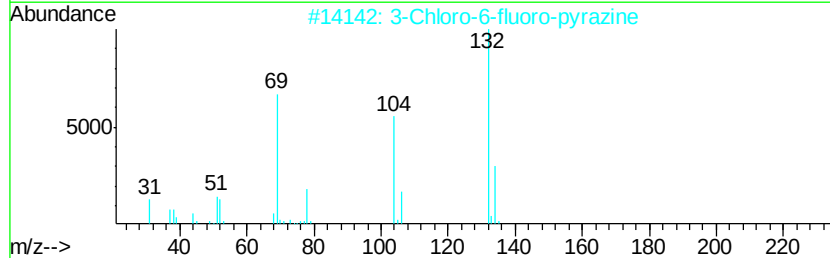
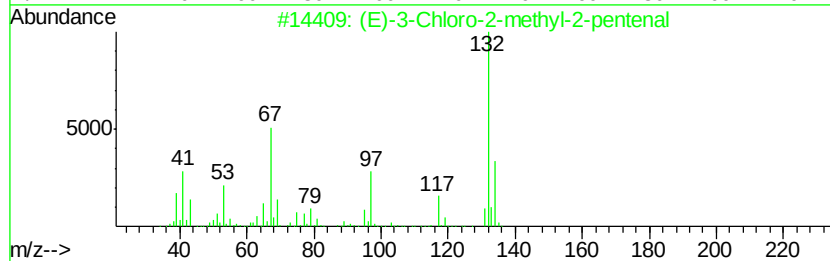
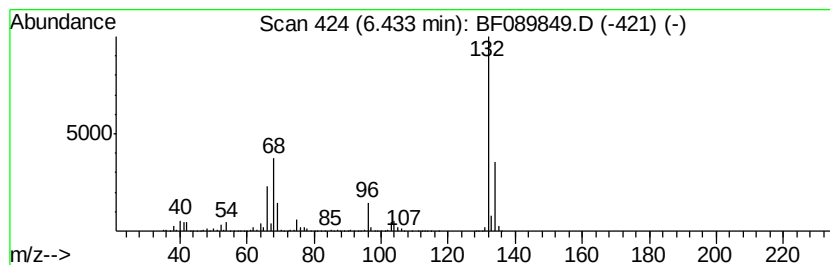
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Peak Number 5 unknown6.43 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.43	85.67 ng	9699520	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3		Amphetaminil	250	C17H18N2	017590-01-1	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	1.85	8.3	ng	942752	1	6.66	2264430	20.0
2-Pentanone, 4-hy...	4.80	22.5	ng	2550730	1	6.66	2264430	20.0
unknown6.43	6.43	85.7	ng	9699520	1	6.66	2264430	20.0