

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032117\
Data File : BF093817.D
Acq On : 22 Mar 2017 5:29
Operator : SJ/MA
Sample : PB97716BL
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB97716BL

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-BF032017.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	4.356	213	216	221	rVB	200939	232286	4.34%	0.586%
2	5.007	270	273	276	rBV	1734373	2817163	52.59%	7.101%
3	5.430	307	310	313	rBV	3177161	3174238	59.25%	8.001%
4	6.459	397	400	402	rBV	3429907	3724271	69.52%	9.388%
5	6.596	409	412	414	rBV	3170108	3717923	69.40%	9.372%
6	6.824	430	432	434	rVB	1460103	1209394	22.57%	3.049%
7	6.984	443	446	448	rBV	4057548	3816469	71.24%	9.620%
8	7.384	478	481	484	rBV	2736741	2909574	54.31%	7.334%
9	8.105	542	544	547	rBV	1224578	1624170	30.32%	4.094%
10	9.190	635	639	641	rBV	5215579	5357299	100.00%	13.504%
11	9.865	695	698	700	rBV	1767079	1752758	32.72%	4.418%
12	10.642	763	766	769	rBV	1856543	1811655	33.82%	4.567%
13	11.339	824	827	829	rBV	1824612	1539666	28.74%	3.881%
14	12.928	963	966	968	rBV	3804762	4000882	74.68%	10.085%
15	13.968	1054	1057	1059	rBV	973708	1024980	19.13%	2.584%
16	15.374	1177	1180	1183	rBV	754961	958329	17.89%	2.416%

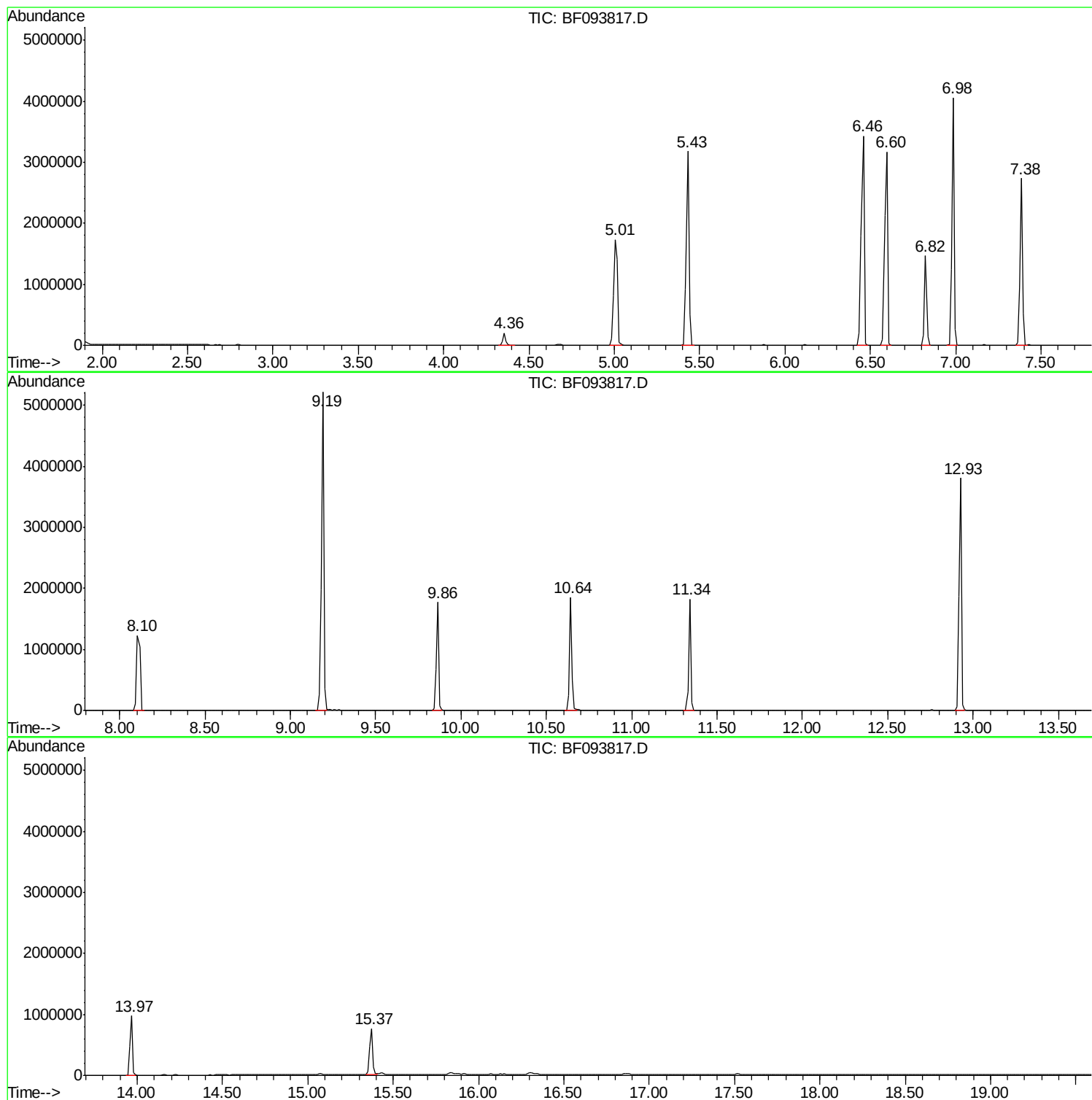
Sum of corrected areas: 39671057

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.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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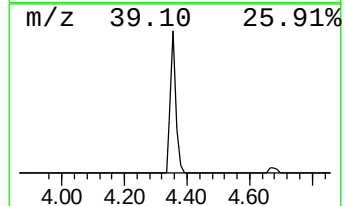
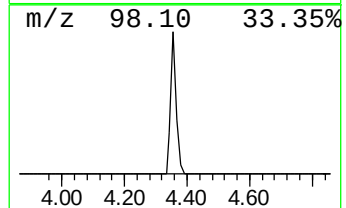
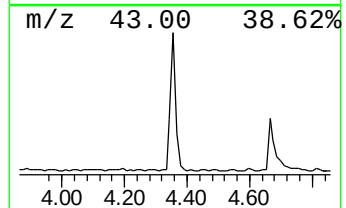
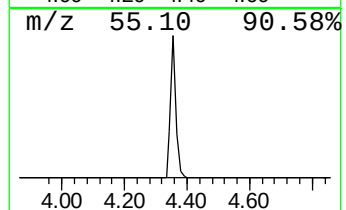
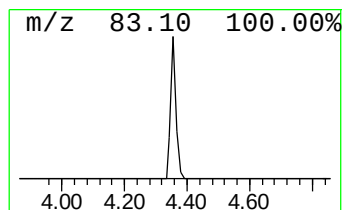
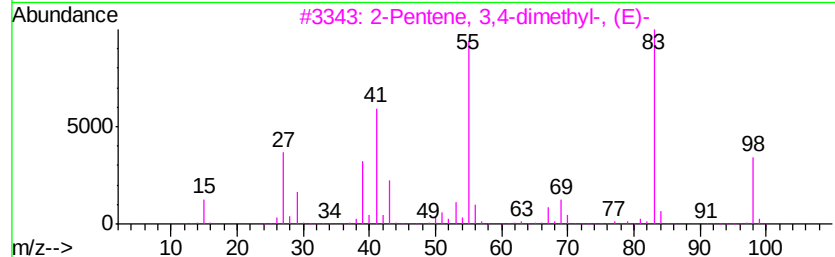
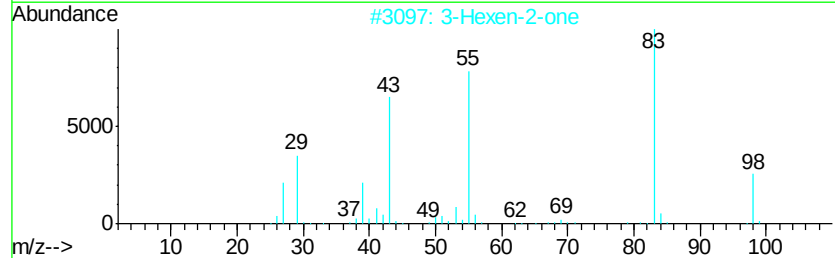
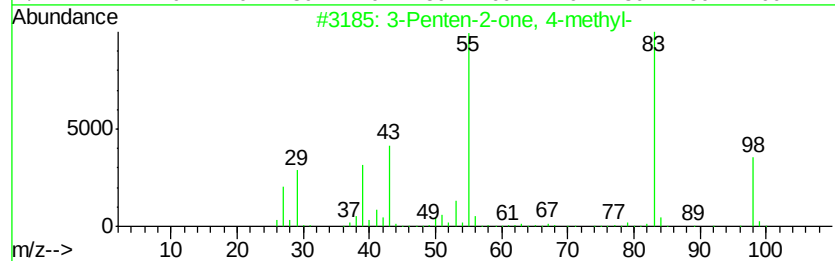
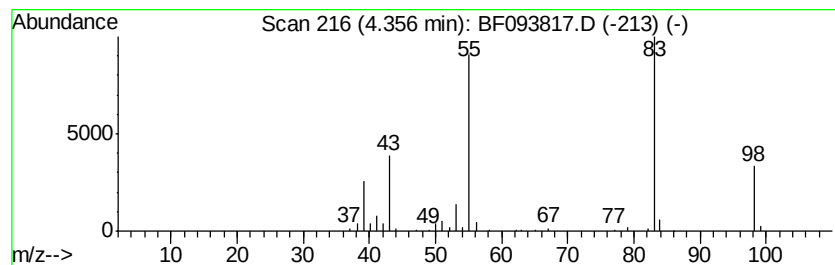
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.36	3.84 ng	232286	1,4-Dichlorobenzene-d4	6.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86



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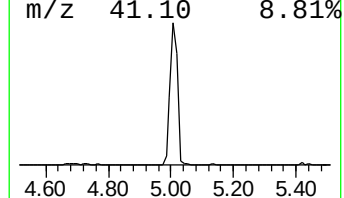
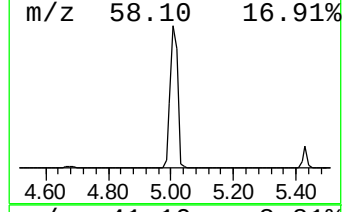
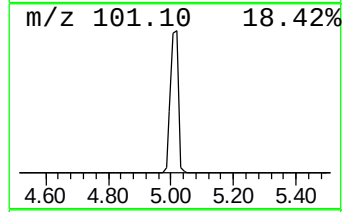
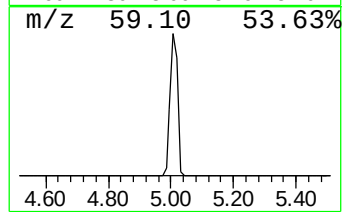
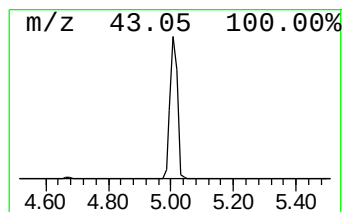
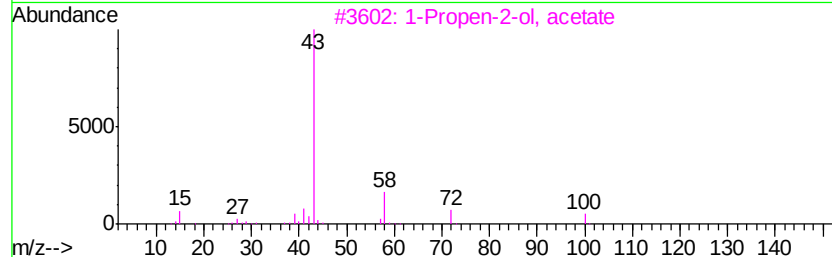
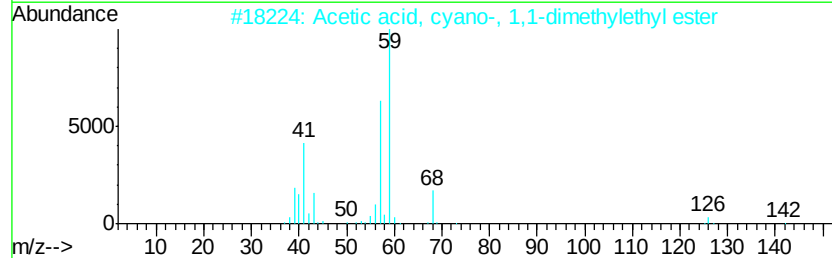
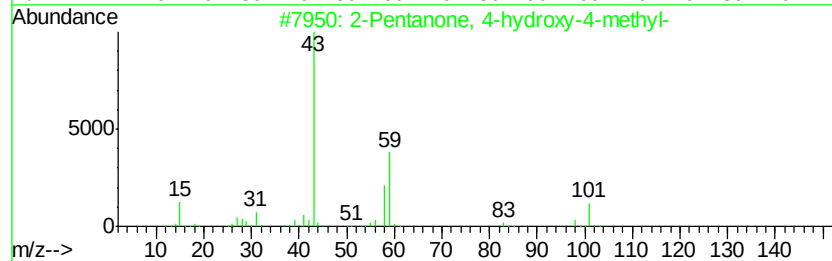
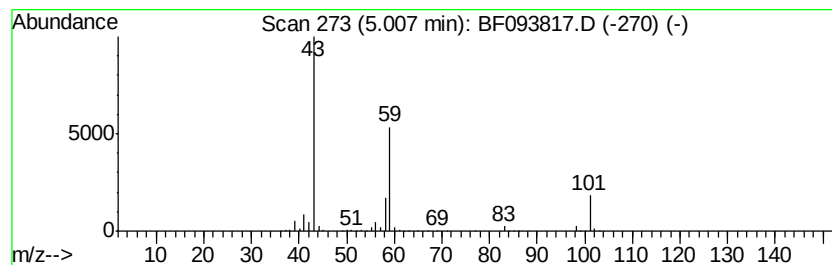
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	46.59 ng	2817160	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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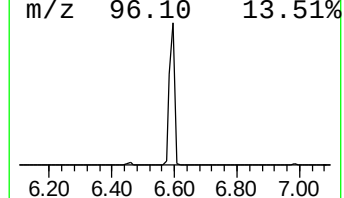
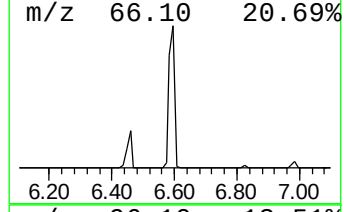
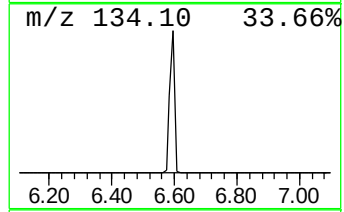
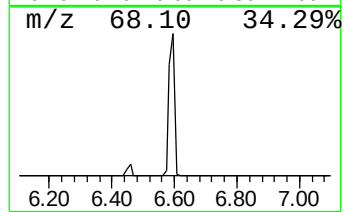
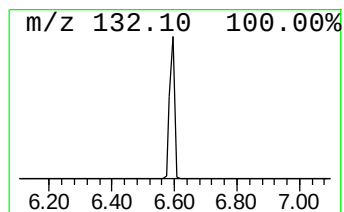
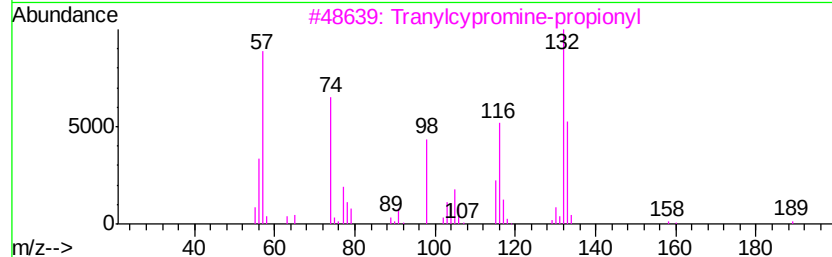
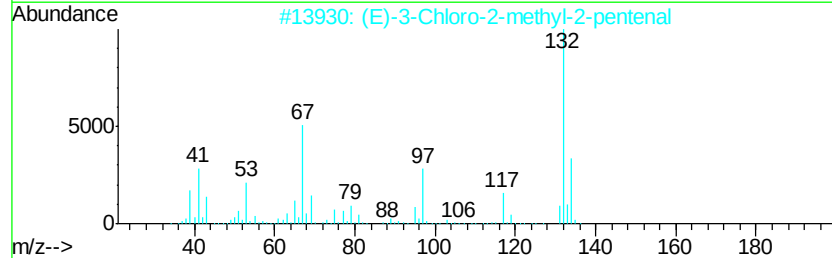
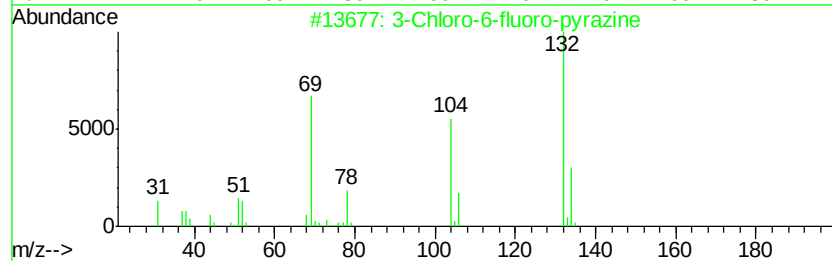
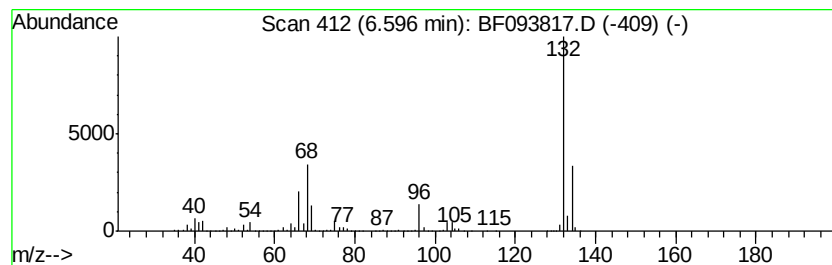
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Peak Number 3 unknown6.60 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	61.48 ng	3717920	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.36	3.8	ng	232286	1	6.82	1209390	20.0
2-Pentanone, 4-hy...	5.01	46.6	ng	2817160	1	6.82	1209390	20.0
unknown6.60	6.60	61.5	ng	3717920	1	6.82	1209390	20.0