

Data Path : Z:\HPCHEM1\BNA G\DATA\BG112117\
 Data File : BG031172.D
 Acq On : 22 Nov 2017 4:06
 Operator : SJ/JU
 Sample : PB104448BL
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB104448BL

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_G\METHODS\8270-BG111017.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	4.602	218	223	232	rBV2	46838	72024	1.52%	0.383%
2	5.213	320	327	337	rBV	340562	527970	11.15%	2.807%
3	5.700	402	410	423	rBV	524922	913747	19.31%	4.858%
4	7.304	674	683	695	rBV	542126	973045	20.56%	5.173%
5	7.669	738	745	755	rBV	551600	984816	20.81%	5.235%
6	8.133	817	824	834	rBV	171434	302036	6.38%	1.606%
7	8.462	872	880	891	rBV	650367	1164827	24.61%	6.192%
8	9.302	1015	1023	1037	rBV	448225	874683	18.48%	4.650%
9	10.953	1296	1304	1321	rBV	213332	441745	9.33%	2.348%
10	13.380	1710	1717	1730	rBV	1586481	2510698	53.05%	13.347%
11	14.760	1944	1952	1966	rBV2	368638	679049	14.35%	3.610%
12	16.241	2198	2204	2220	rBV	716191	1262619	26.68%	6.712%
13	17.498	2411	2418	2433	rBV2	561079	946407	20.00%	5.031%
14	20.089	2852	2859	2870	rBV	3586917	4733109	100.00%	25.162%
15	21.770	3138	3145	3158	rBV2	714294	1291289	27.28%	6.865%
16	25.072	3696	3707	3724	rBV2	373520	1132499	23.93%	6.021%

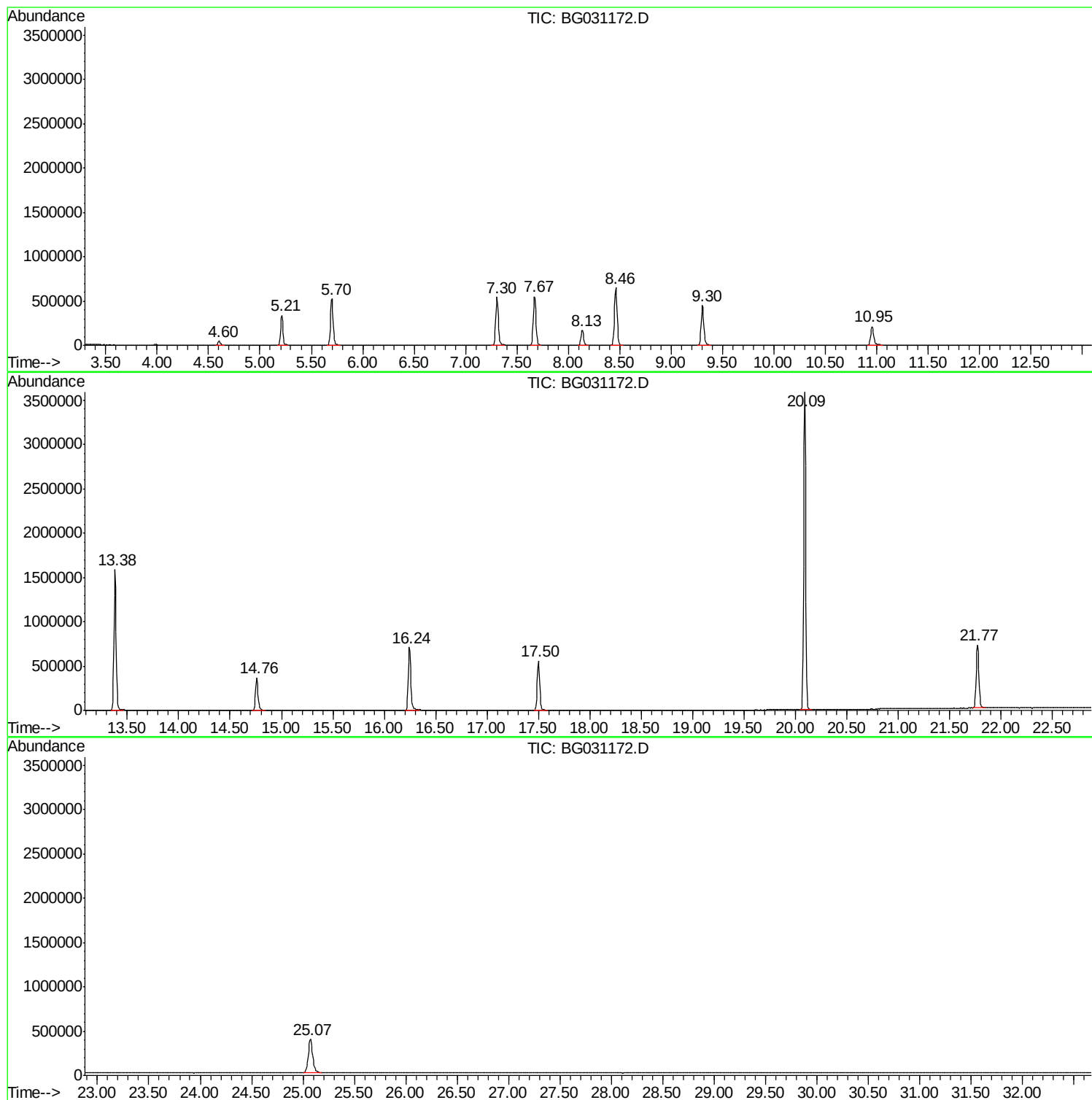
Sum of corrected areas: 18810563

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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG111017.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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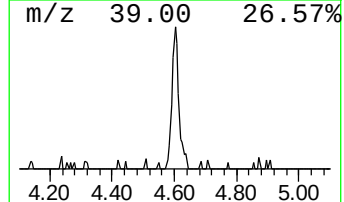
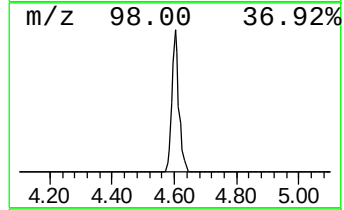
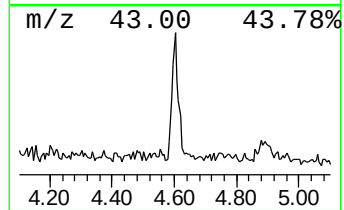
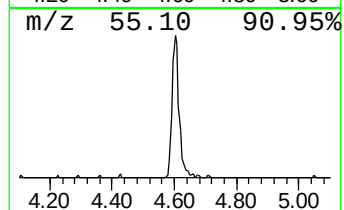
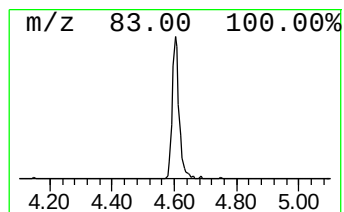
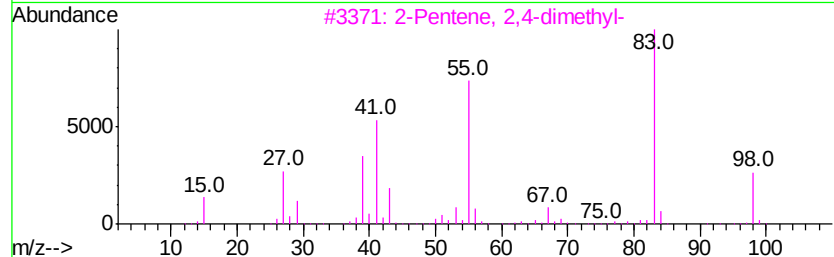
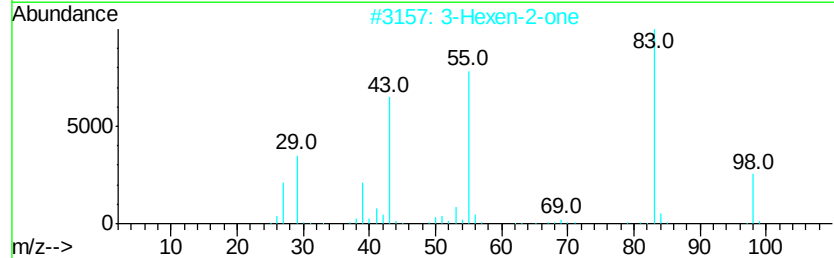
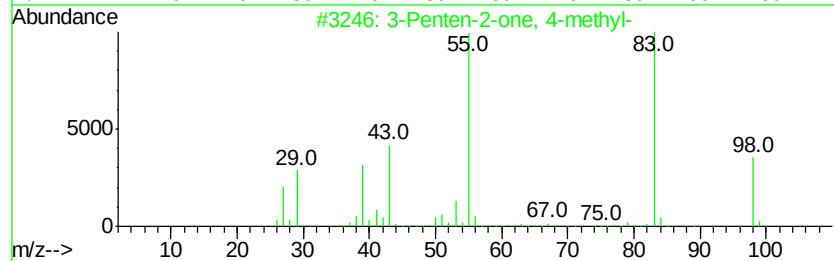
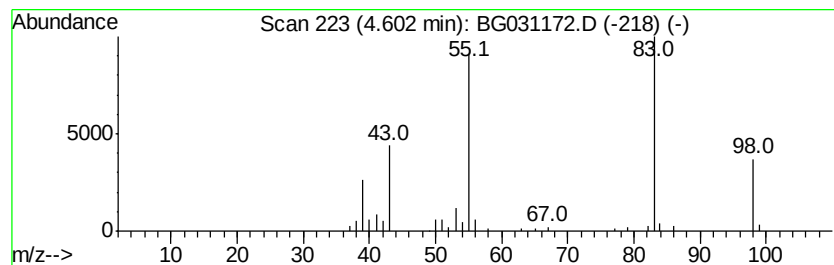
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.60	4.77 ng	72024	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2		3-Hexen-2-one	98	C6H10O	000763-93-9	86
3		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	80
5		2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	80



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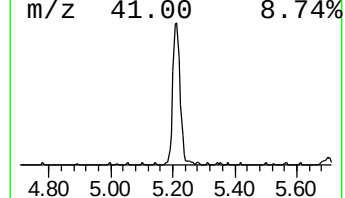
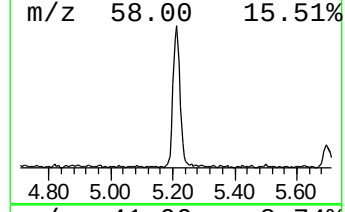
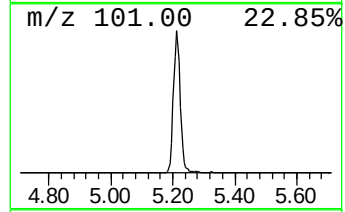
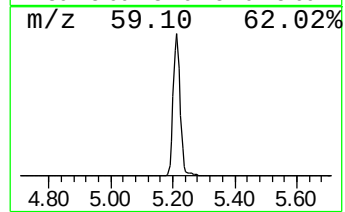
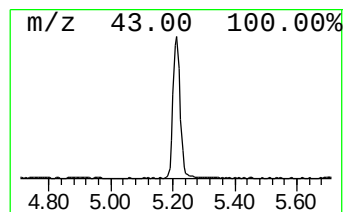
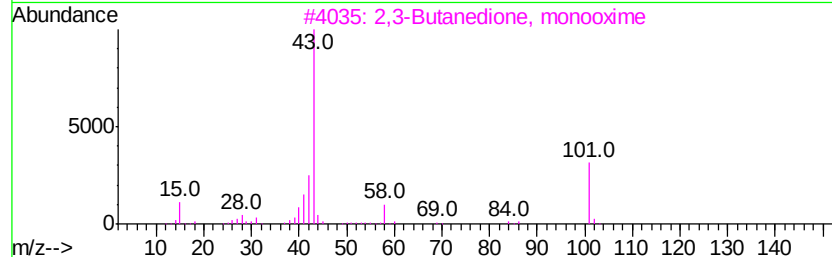
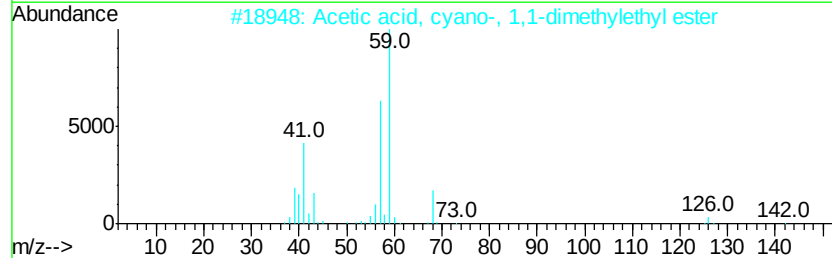
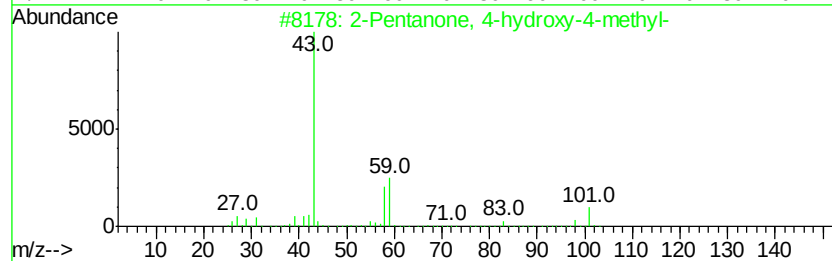
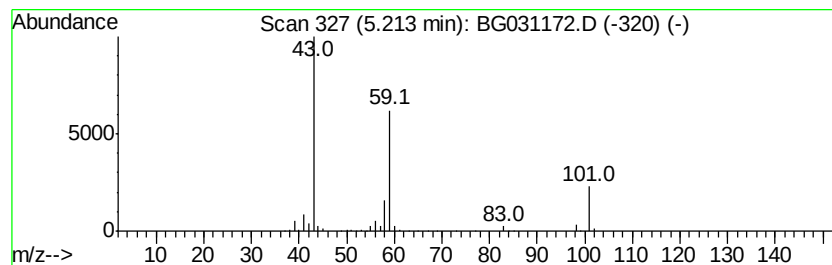
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	34.96 ng	527970	1,4-Dichlorobenzene-d4	8.13

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-dimethyl...	141	C7H11NO2	001116-98-9	17
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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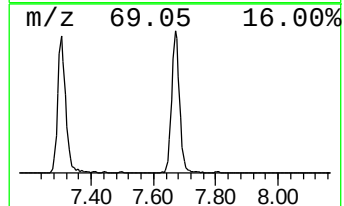
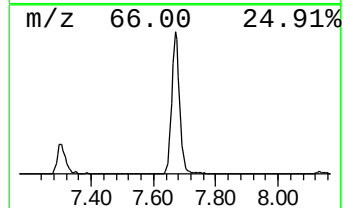
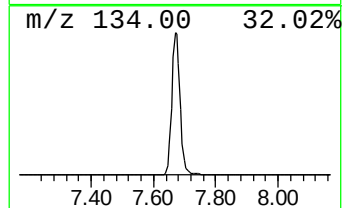
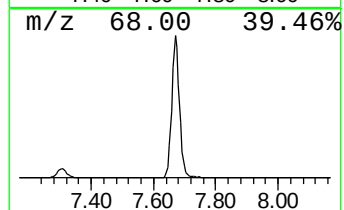
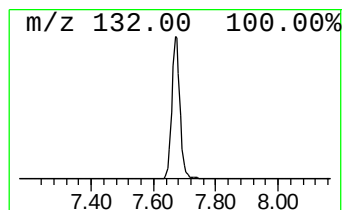
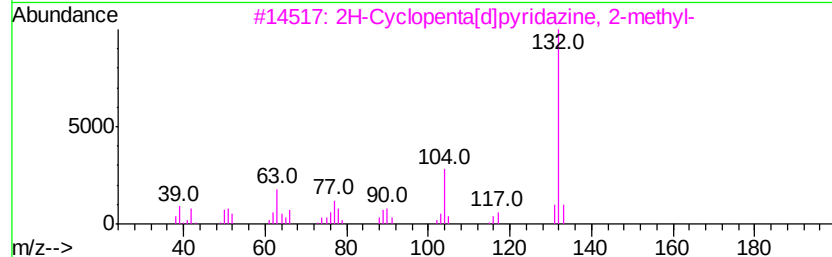
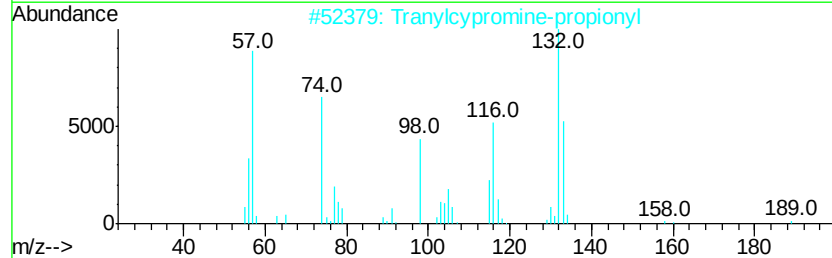
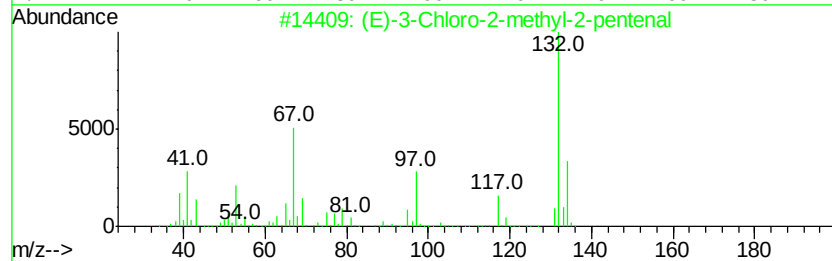
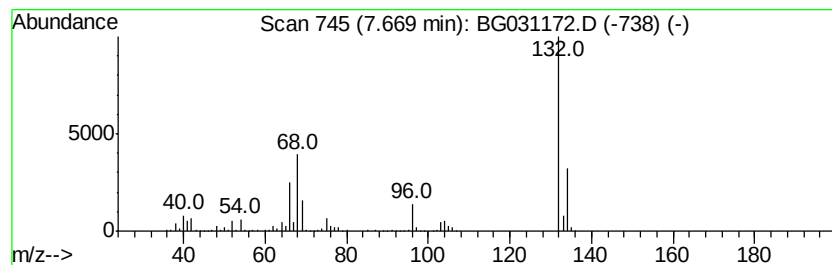
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Peak Number 3 unknown7.67 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.67	65.21 ng	984816	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.60	4.8	ng	72024	1	8.13	302036	20.0
2-Pentanone, 4-hy...	5.21	35.0	ng	527970	1	8.13	302036	20.0
unknown7.67	7.67	65.2	ng	984816	1	8.13	302036	20.0