

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080116\
 Data File : BF089520.D
 Acq On : 1 Aug 2016 19:56
 Operator : UM/SJ
 Sample : H4251-02
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-05

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-BF072716.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	62	rVB	669419	1709798	100.00%	16.962%
2	4.559	258	260	268	rBV	53297	90834	5.31%	0.901%
3	5.039	301	302	325	rBV5	319254	496859	29.06%	4.929%
4	6.136	396	398	405	rBV	237049	303378	17.74%	3.010%
5	6.239	405	407	423	rVB	708178	937416	54.83%	9.300%
6	6.479	426	428	439	rBV	175358	200734	11.74%	1.991%
7	6.627	439	441	444	rBV	761762	847093	49.54%	8.404%
8	7.050	476	478	504	rBV	598469	729062	42.64%	7.233%
9	7.759	538	540	552	rBV	218811	299776	17.53%	2.974%
10	8.159	573	575	583	rBB	34824	51671	3.02%	0.513%
11	8.719	622	624	632	rBB	31368	37140	2.17%	0.368%
12	8.845	632	635	637	rBV	1567233	1439410	84.19%	14.280%
13	9.245	668	670	675	rVB	50213	43754	2.56%	0.434%
14	9.508	691	693	695	rBV	352066	337793	19.76%	3.351%
15	10.296	759	762	764	rBV	607448	752049	43.98%	7.461%
16	10.982	819	822	824	rBV	214871	299715	17.53%	2.973%
17	11.531	869	870	875	rBB	12059	17984	1.05%	0.178%
18	12.559	958	960	963	rBV	1128568	1091118	63.82%	10.825%
19	13.600	1048	1051	1060	rBV	140563	211877	12.39%	2.102%
20	14.925	1165	1167	1174	rBV	141456	182459	10.67%	1.810%

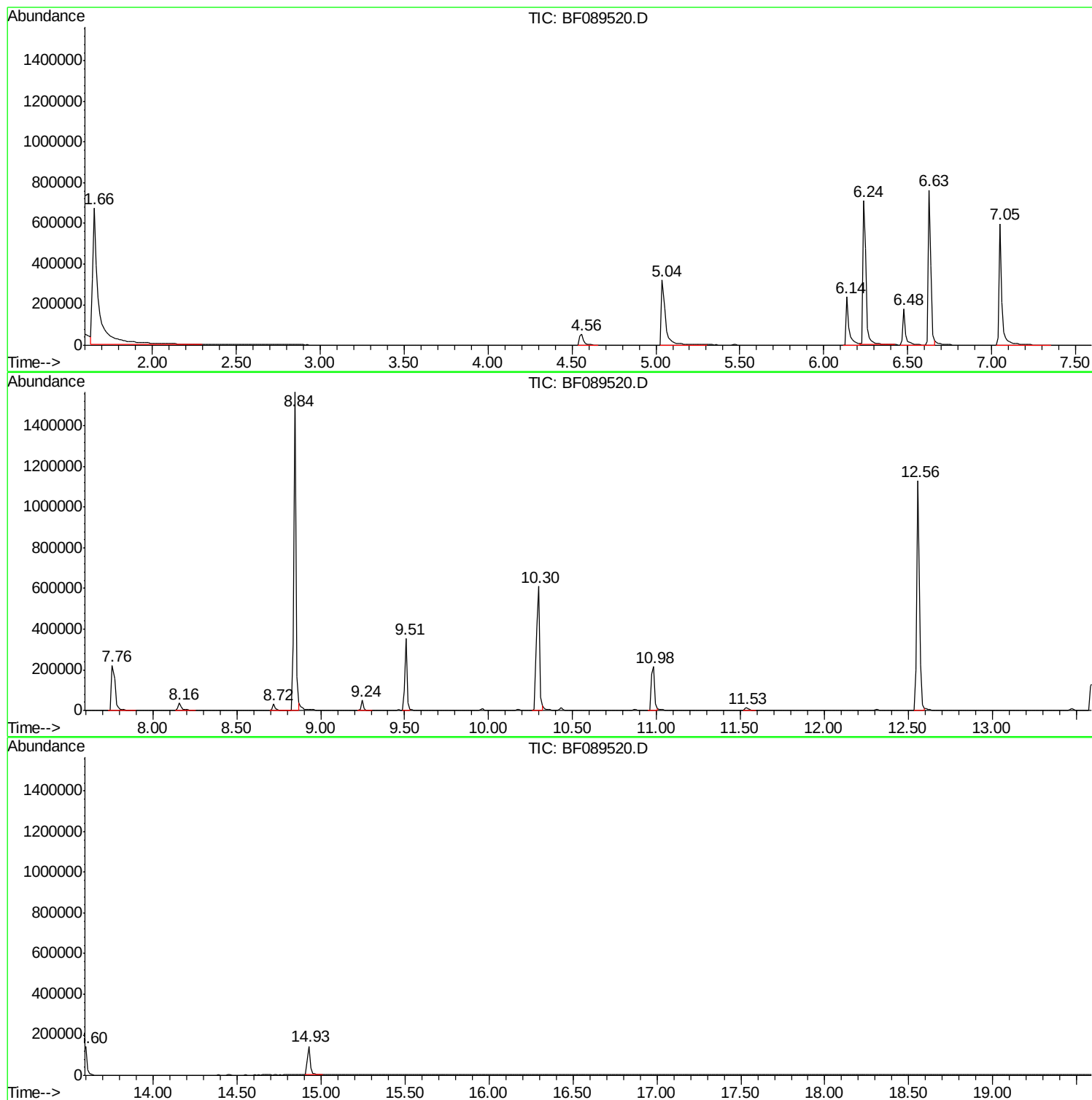
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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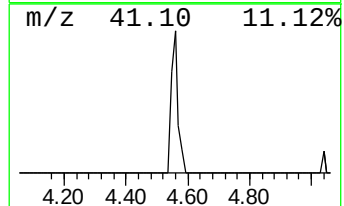
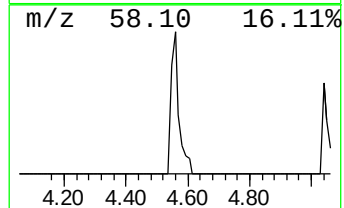
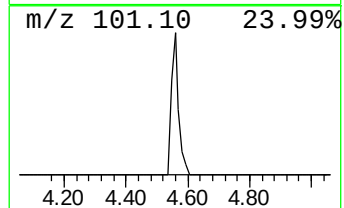
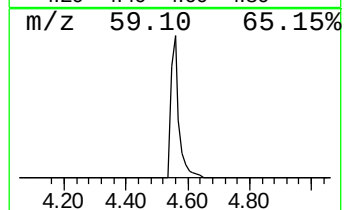
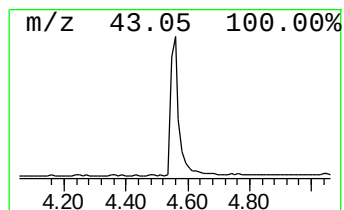
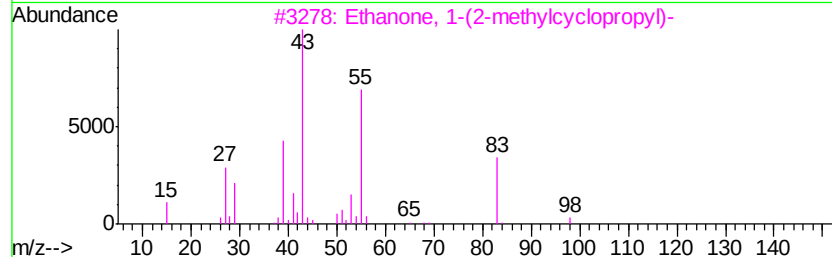
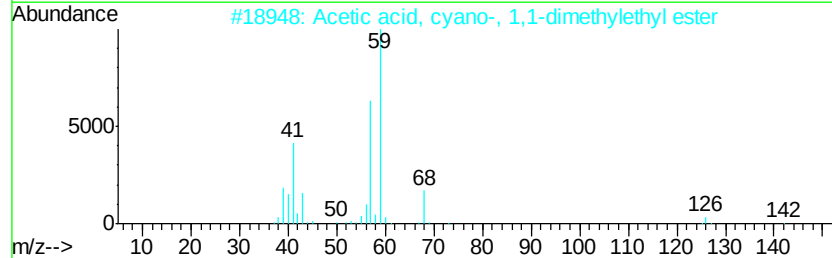
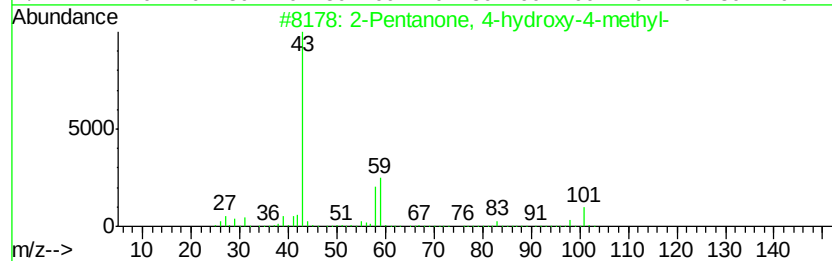
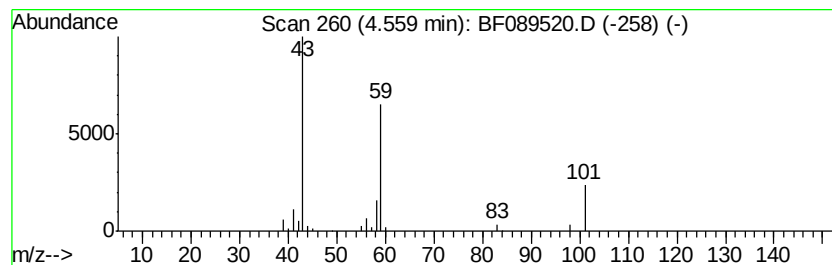
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.56	9.05 ng	90834	1,4-Dichlorobenzene-d4	6.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Acetone	58	C3H6O	000067-64-1	9



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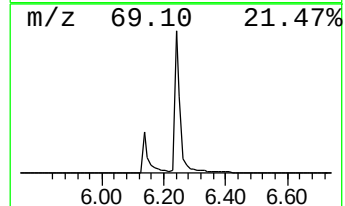
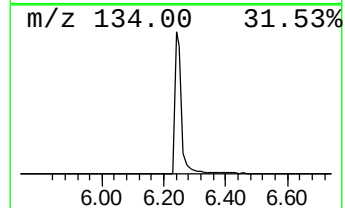
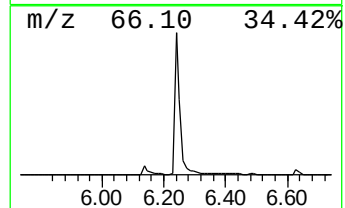
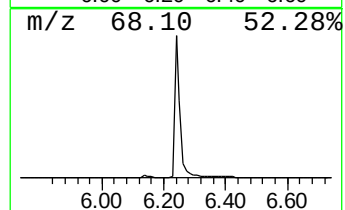
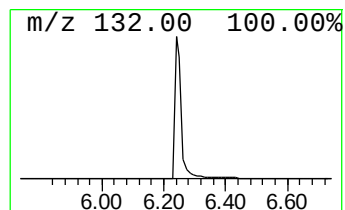
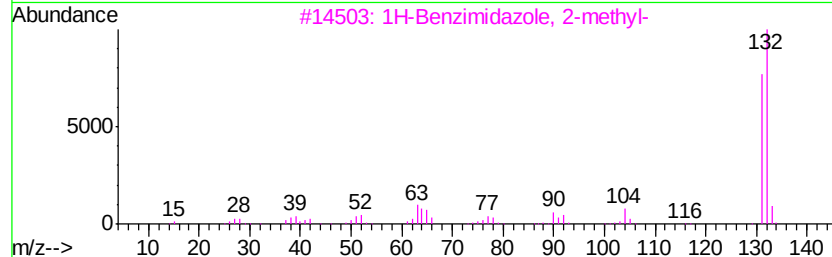
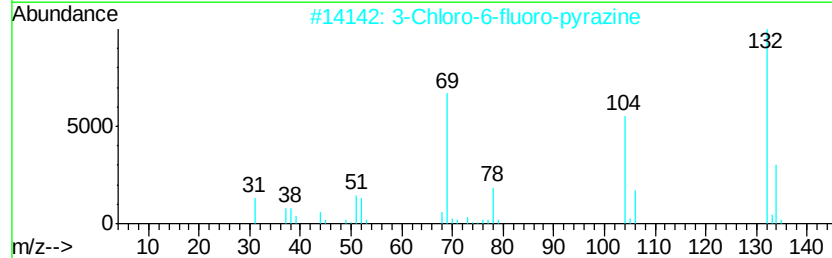
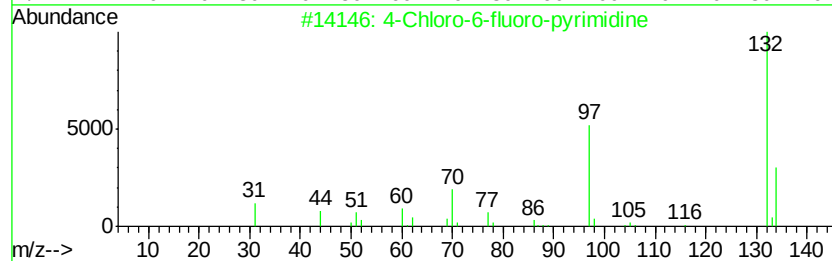
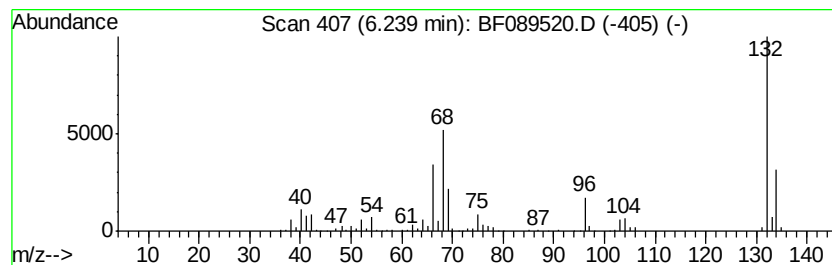
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Peak Number 3 unknown6.24 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.24	93.40 ng	937416	1,4-Dichlorobenzene-d4	6.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10



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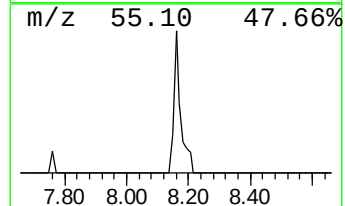
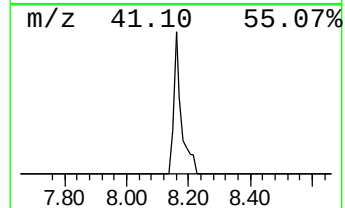
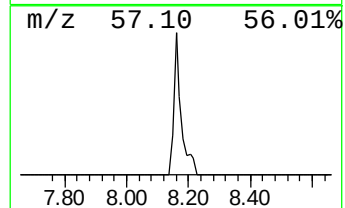
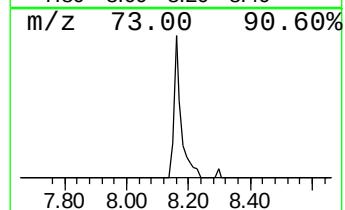
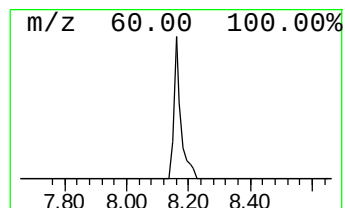
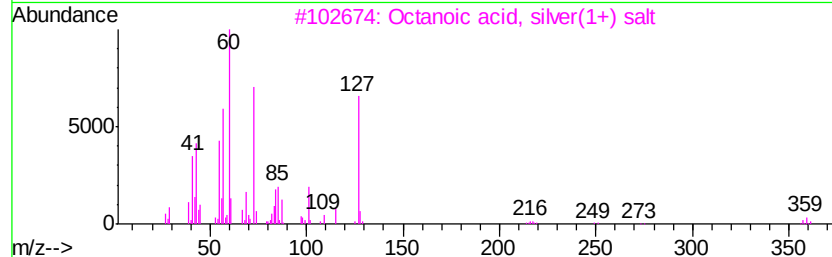
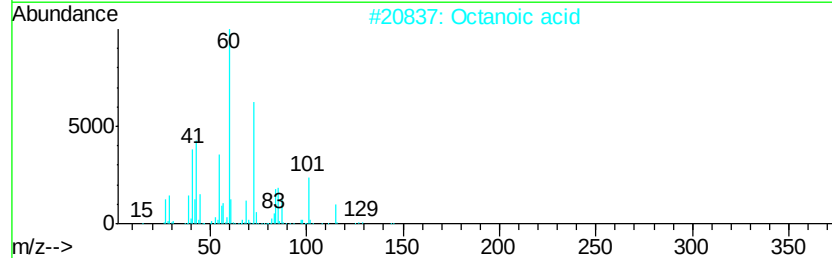
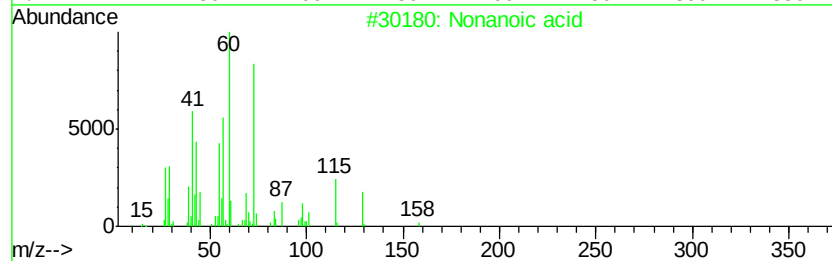
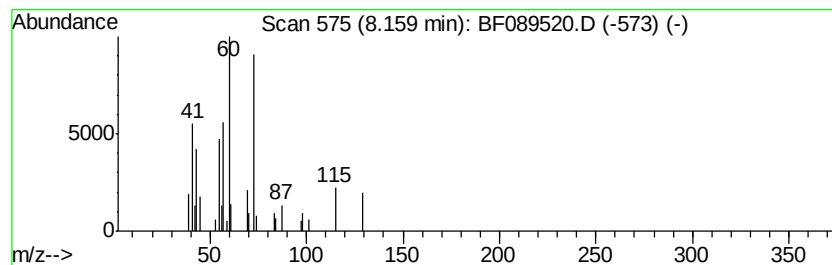
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Peak Number 5 Nonanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.16	3.45 ng	51671	Naphthalene-d8	7.76

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid		158	C9H18O2	000112-05-0	90
2	Octanoic acid		144	C8H16O2	000124-07-2	53
3	Octanoic acid, silver(1+) salt		250	C8H15AgO2	024927-67-1	50
4	Hexanoic acid		116	C6H12O2	000142-62-1	50
5	Pentanoic acid, 3-methyl-		116	C6H12O2	000105-43-1	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.56	9.1	ng	90834	1	6.48	200734	20.0
unknown6.24	6.24	93.4	ng	937416	1	6.48	200734	20.0
Nonanoic acid	8.16	3.5	ng	51671	2	7.76	299776	20.0