

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_G\DATA\BG062417\
 Data File : BG027658.D
 Acq On : 24 Jun 2017 14:11
 Operator : SJ/JU
 Sample : I3743-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 FNDFL-ESTN-061417-COMP

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-BG062117.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	5.641	292	298	307	rVB	56211	90079	6.14%	1.153%
2	6.088	367	374	383	rBV	321252	548598	37.40%	7.022%
3	7.645	630	639	653	rBV	348909	644387	43.93%	8.248%
4	8.038	698	706	718	rBB	333812	605556	41.28%	7.751%
5	8.502	778	785	794	rBB2	69956	124480	8.49%	1.593%
6	8.831	833	841	850	rBV	230640	417816	28.48%	5.348%
7	9.666	975	983	993	rBV	201414	380896	25.97%	4.875%
8	11.323	1257	1265	1274	rVB	102661	192154	13.10%	2.460%
9	13.708	1664	1671	1680	rBV	561365	894422	60.97%	11.448%
10	14.519	1802	1809	1815	rBV	75498	113750	7.75%	1.456%
11	15.089	1897	1906	1913	rVB2	164219	280031	19.09%	3.584%
12	16.569	2151	2158	2168	rBV	378494	587828	40.07%	7.524%
13	16.746	2180	2188	2196	rBV2	8787	14891	1.02%	0.191%
14	17.839	2366	2374	2384	rVB	239052	386796	26.37%	4.951%
15	18.673	2512	2516	2524	rBV3	21824	36442	2.48%	0.466%
16	20.412	2806	2812	2822	rVB	1113405	1466933	100.00%	18.776%
17	22.204	3109	3117	3125	rVB	259051	489529	33.37%	6.266%
18	23.814	3385	3391	3402	rBV3	41906	87002	5.93%	1.114%
19	25.841	3725	3736	3750	rVB3	136607	451092	30.75%	5.774%

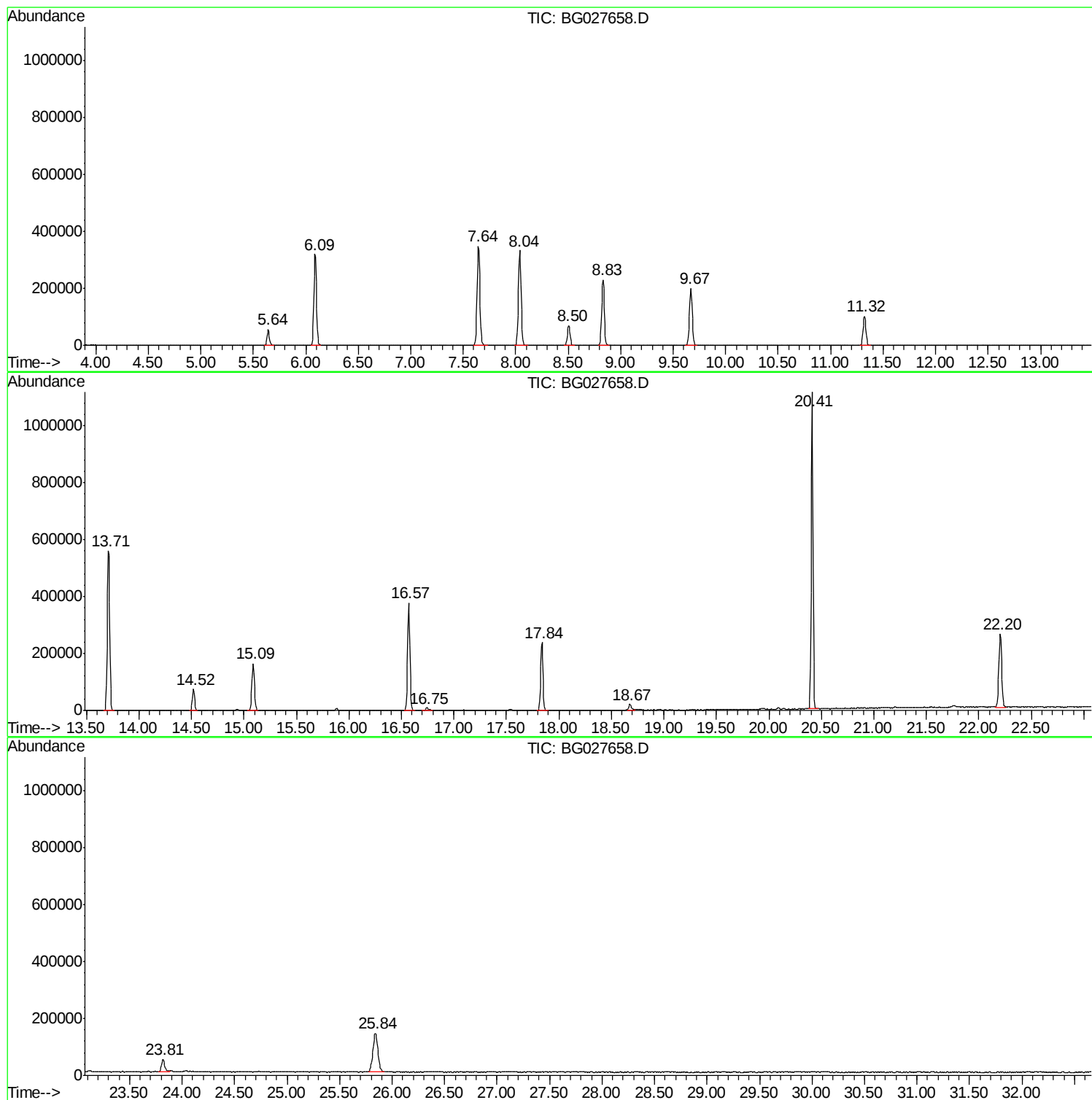
Sum of corrected areas: 7812682

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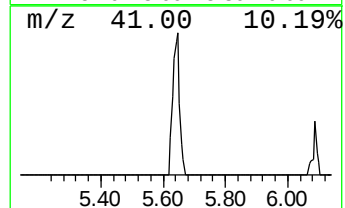
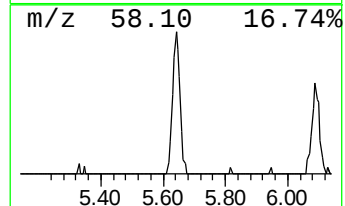
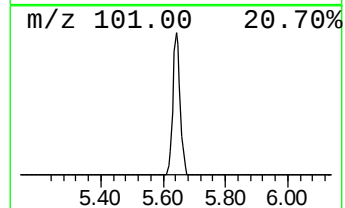
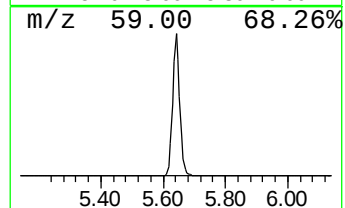
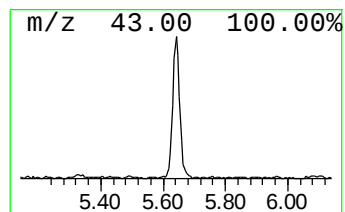
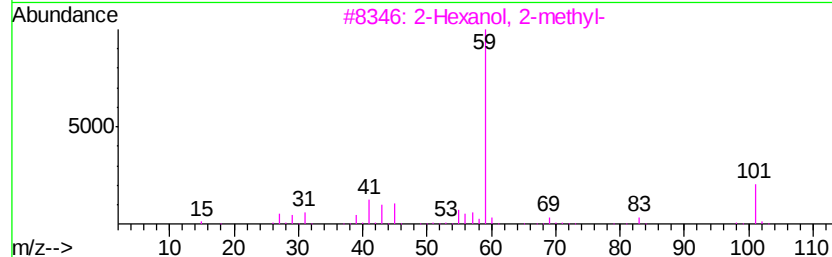
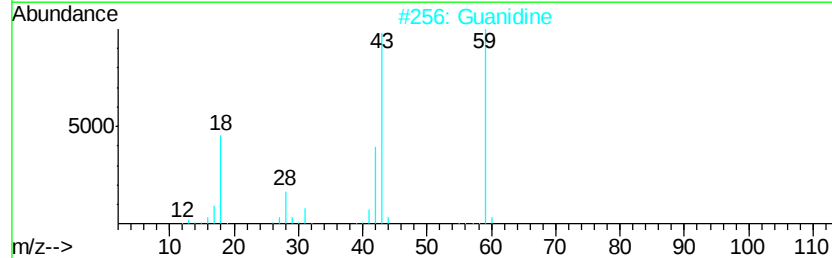
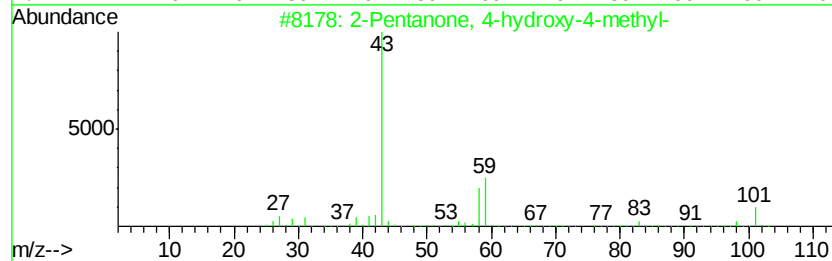
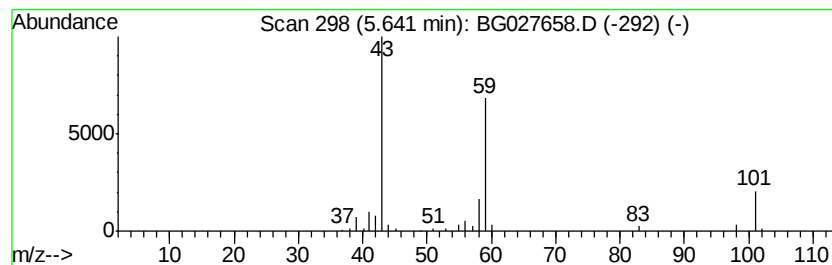
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.64	14.47 ng	90079	1,4-Dichlorobenzene-d4	8.51

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Guanidine	59	CH5N3	000113-00-8	43
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
4			2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	28
5			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25



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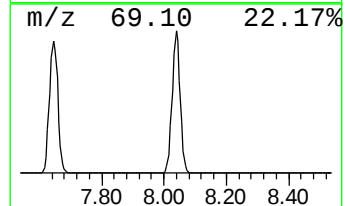
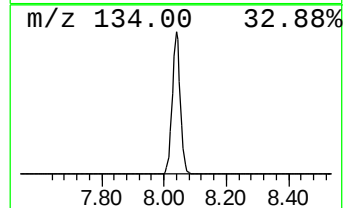
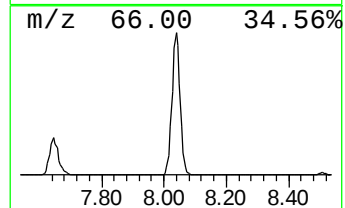
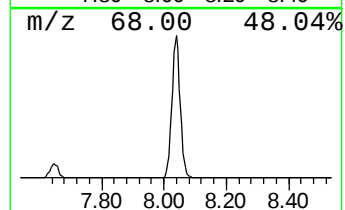
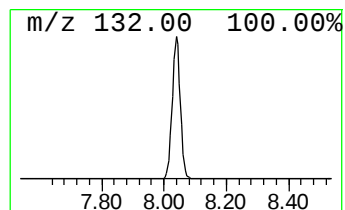
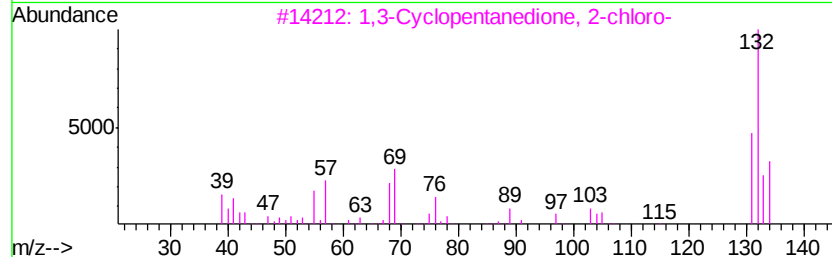
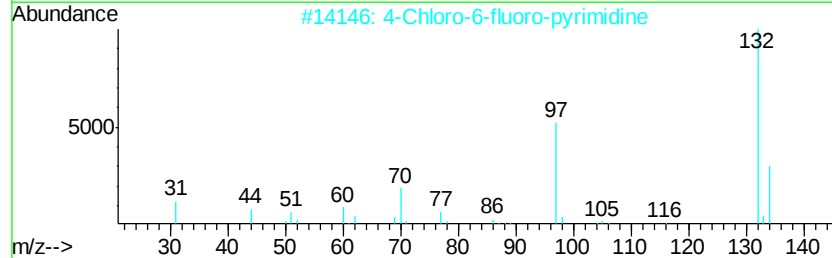
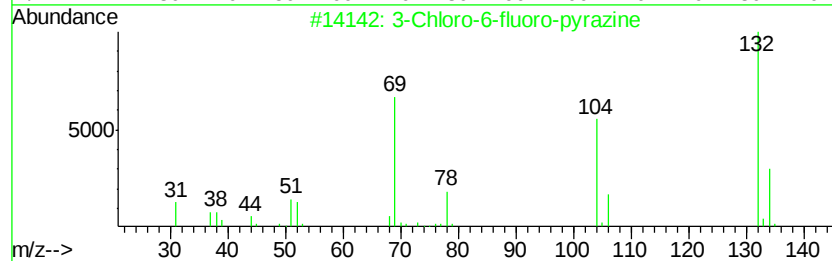
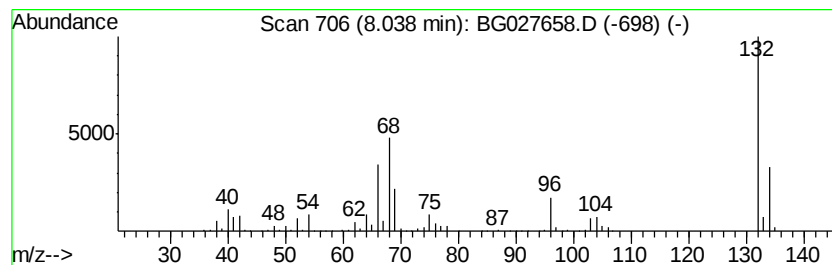
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Peak Number 2 unknown8.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.04	97.29 ng	605556	1,4-Dichlorobenzene-d4	8.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
4		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	12
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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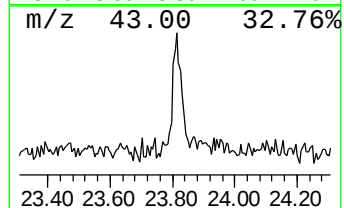
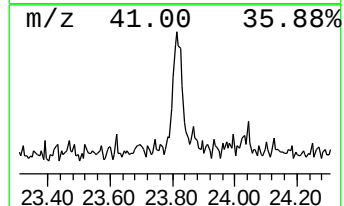
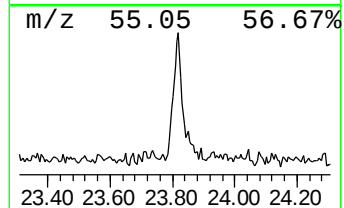
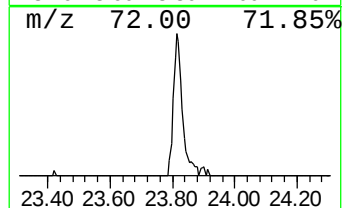
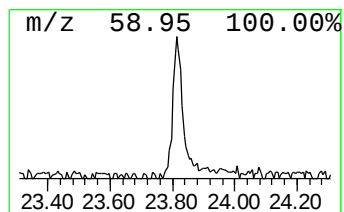
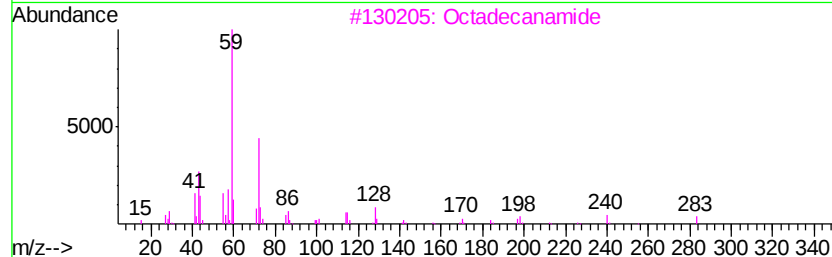
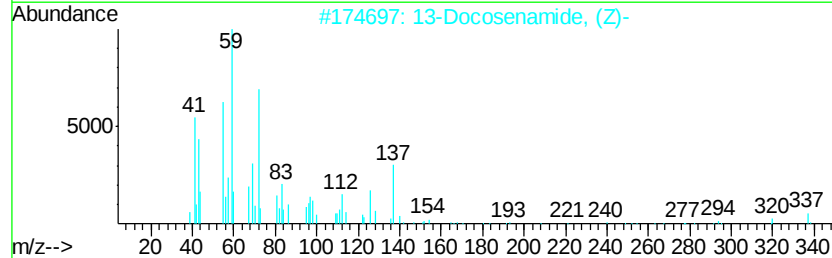
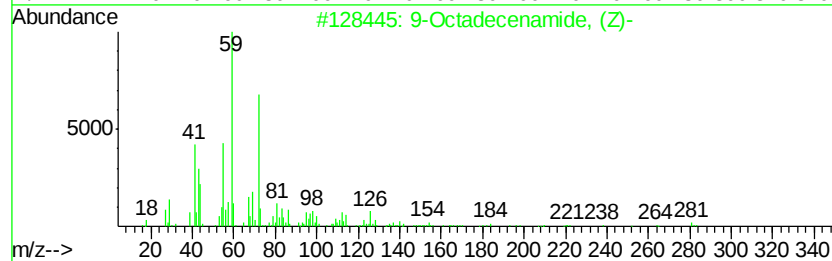
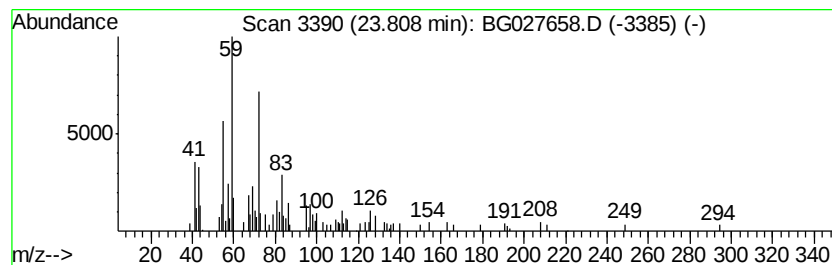
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Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.81	3.55 ng	87002	Chrysene-d12	22.20	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	96
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	78
3	Octadecanamide	283	C18H37NO	000124-26-5	60
4	d-Glucosamine	179	C6H13NO5	000090-77-7	53
5	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	53



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.64	14.5	ng	90079	1	8.51	124480	20.0
unknown8.04	8.04	97.3	ng	605556	1	8.51	124480	20.0
9-Octadecenamide, ...	23.81	3.5	ng	87002	5	22.20	489529	20.0