

Data Path : Z:\HPCHEM1\BNA G\DATA\BG103117\
 Data File : BG030614.D
 Acq On : 31 Oct 2017 16:12
 Operator : SJ/JU
 Sample : I6133-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SW-01(17.5-19.5)

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-BG101617.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	5.241	326	332	341	rBV	166368	260173	5.97%	1.015%
2	5.717	406	413	428	rVB	918714	1491212	34.23%	5.817%
3	7.321	677	686	701	rBV	981233	1795852	41.22%	7.005%
4	7.691	741	749	758	rBV	954180	1669811	38.33%	6.513%
5	8.161	821	829	836	rBV	253093	443273	10.18%	1.729%
6	8.484	877	884	893	rBV	712189	1253124	28.77%	4.888%
7	9.324	1018	1027	1036	rBV	582853	1054400	24.20%	4.113%
8	10.975	1298	1308	1318	rBV	396665	719012	16.50%	2.805%
9	12.268	1519	1528	1541	rVB	47448	87232	2.00%	0.340%
10	13.402	1714	1721	1729	rBV	2034241	3085234	70.82%	12.034%
11	14.218	1853	1860	1867	rBV	202821	296443	6.80%	1.156%
12	14.777	1948	1955	1964	rVB2	717932	1134744	26.05%	4.426%
13	16.122	2177	2184	2189	rBV	230454	334466	7.68%	1.305%
14	16.257	2197	2207	2223	rBV	1482902	2293789	52.65%	8.947%
15	17.515	2414	2421	2430	rBV2	894700	1341131	30.79%	5.231%
16	20.106	2856	2862	2868	rBV	3291093	4356377	100.00%	16.993%
17	20.775	2968	2976	2986	rBV	573506	807720	18.54%	3.151%
18	21.404	3079	3083	3092	rBV	22123	55512	1.27%	0.217%
19	21.786	3141	3148	3157	rBV	934555	1559203	35.79%	6.082%
20	23.490	3435	3438	3445	rVB2	28598	48035	1.10%	0.187%
21	25.100	3700	3712	3725	rBV2	514312	1550098	35.58%	6.046%

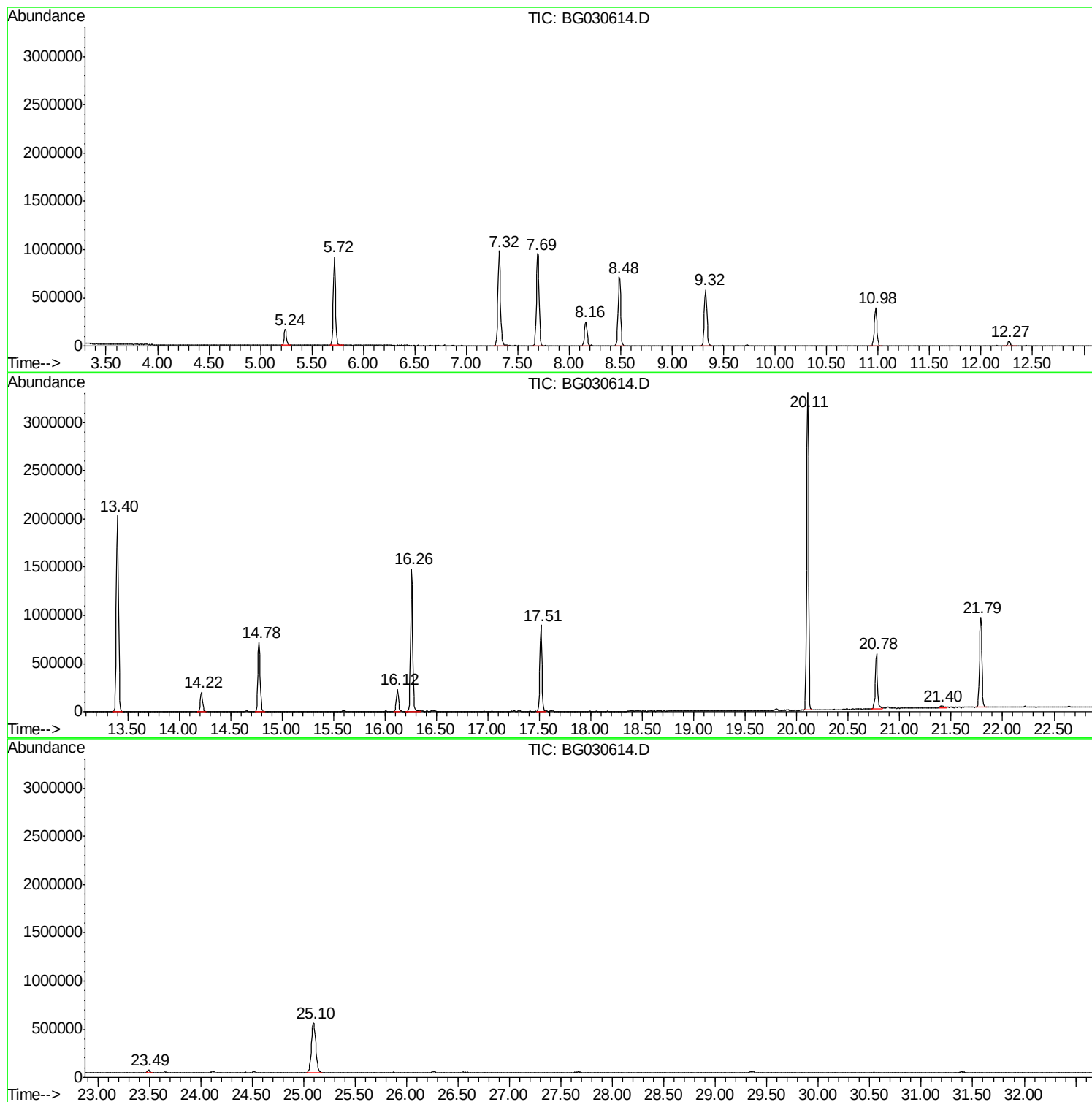
Sum of corrected areas: 25636841

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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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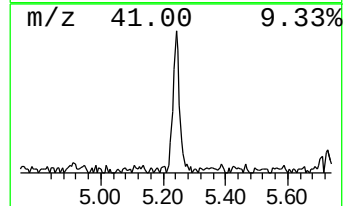
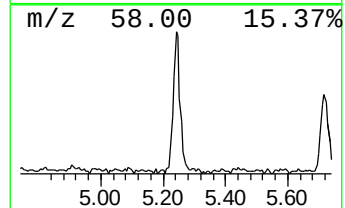
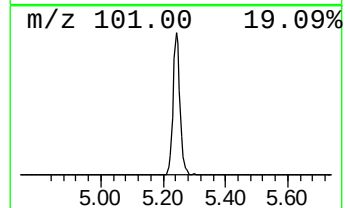
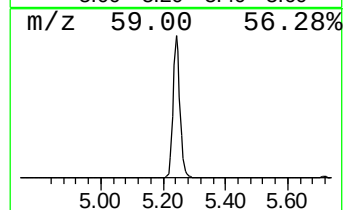
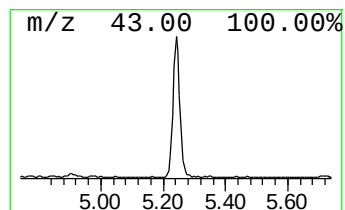
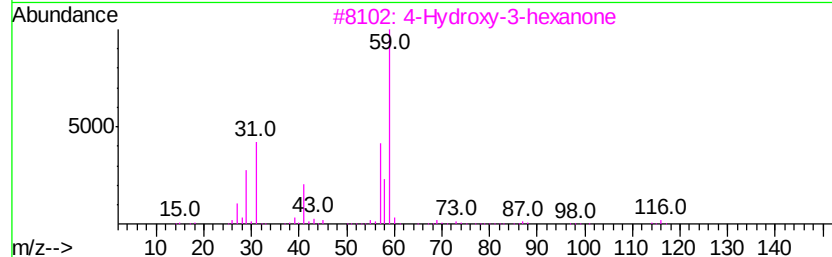
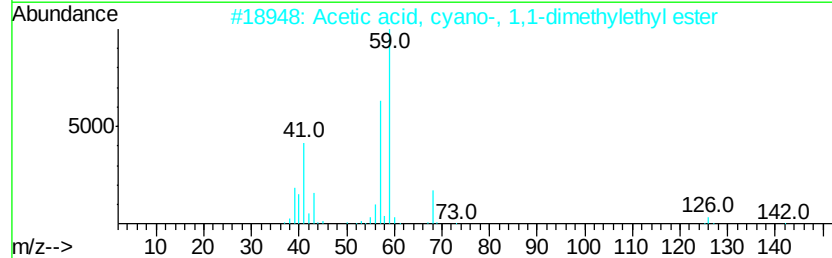
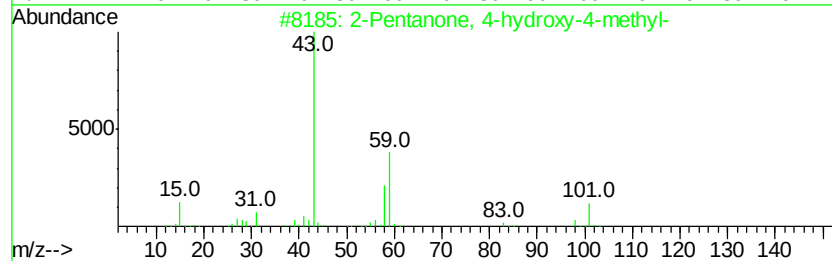
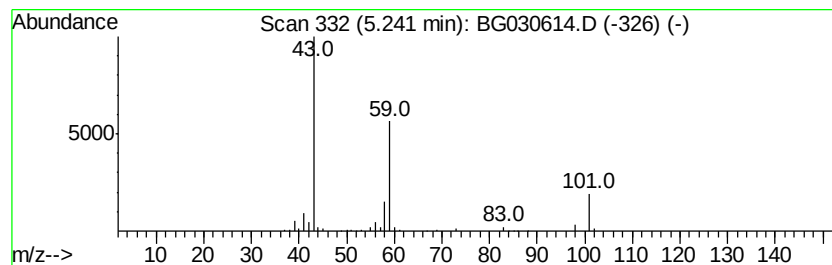
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	11.74 ng	260173	1,4-Dichlorobenzene-d4	8.16

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		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	17
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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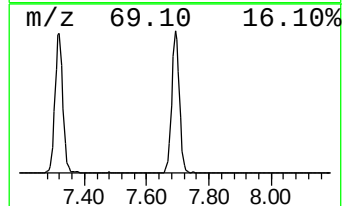
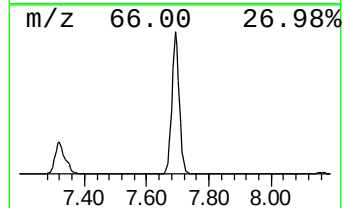
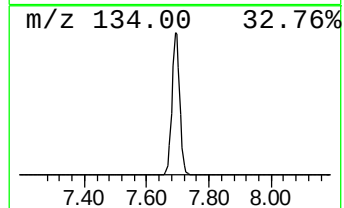
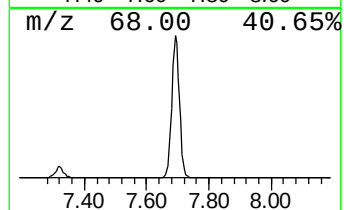
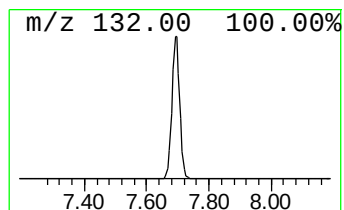
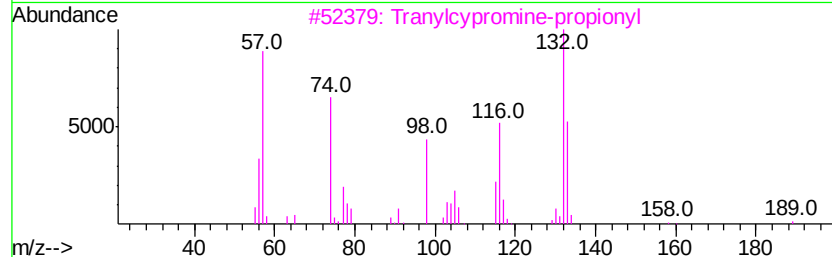
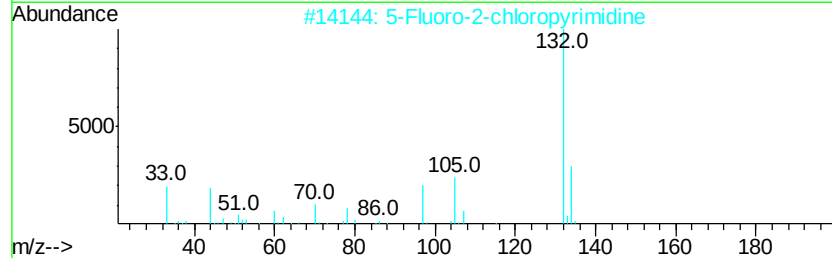
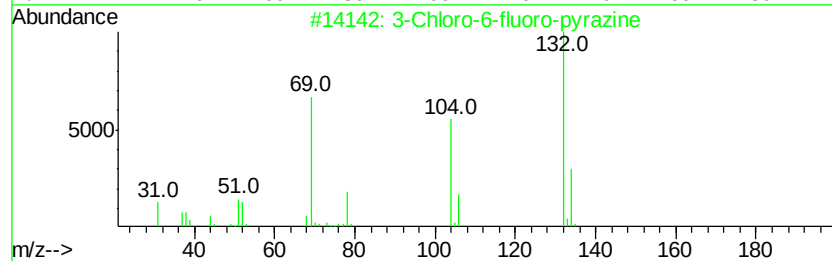
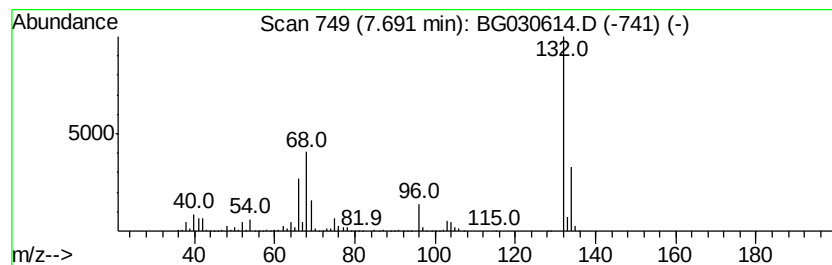
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Peak Number 2 unknown7.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.69	75.34 ng	1669810	1,4-Dichlorobenzene-d4	8.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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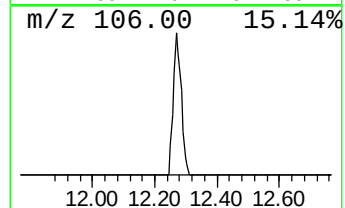
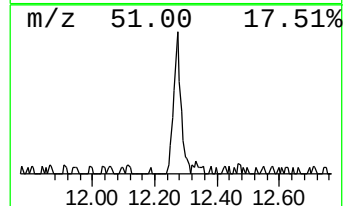
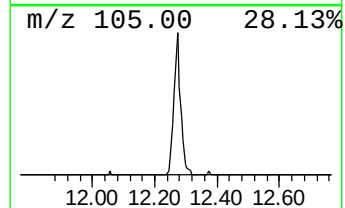
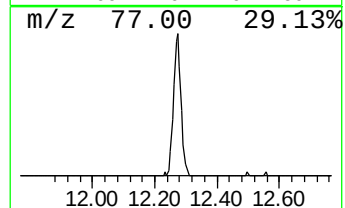
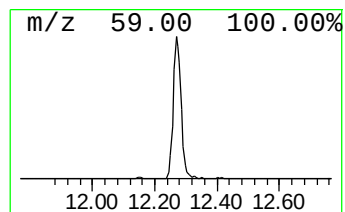
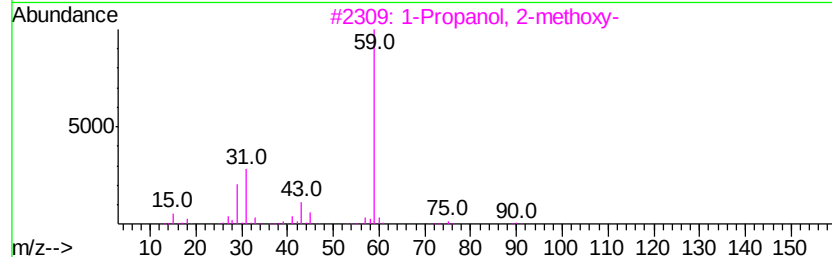
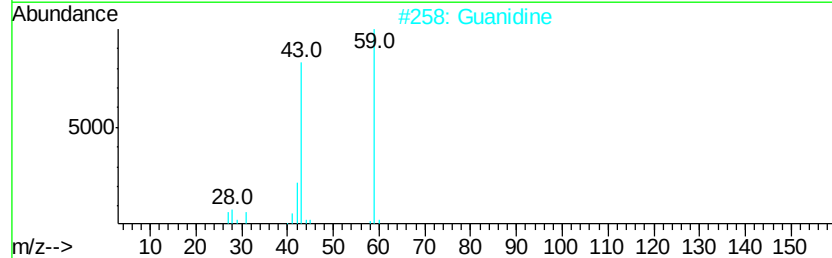
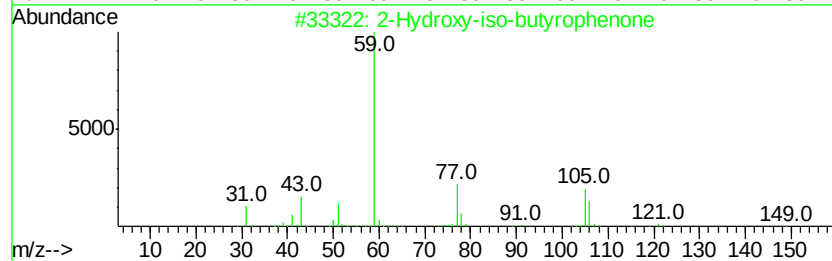
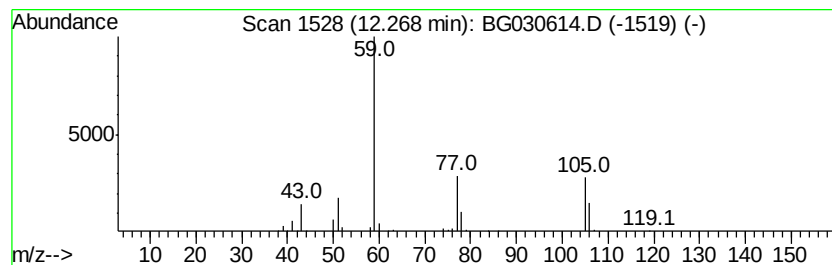
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Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.27	2.43 ng	87232	Napthalene-d8	10.98
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Hydroxy-iso-butyrophenone	164 C10H12O2	007473-98-5	83
2	Guanidine	59 CH5N3	000113-00-8	9
3	1-Propanol, 2-methoxy-	90 C4H10O2	001589-47-5	9
4	Formamide, N-methyl-	59 C2H5NO	000123-39-7	5
5	Acetamide	59 C2H5NO	000060-35-5	5



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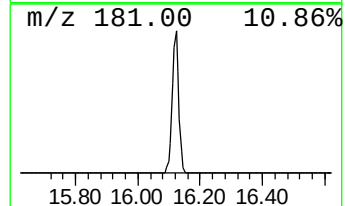
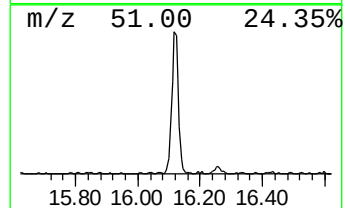
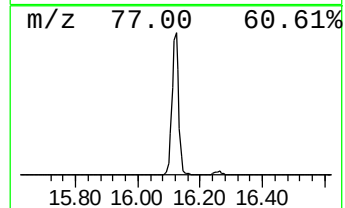
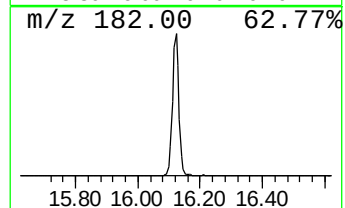
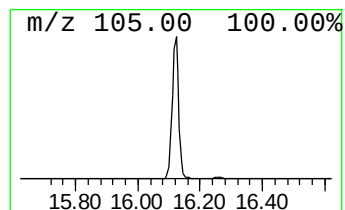
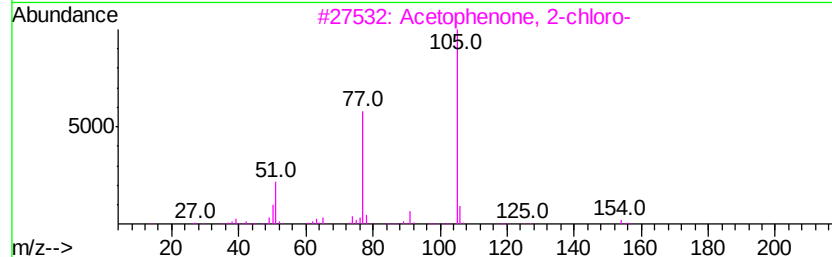
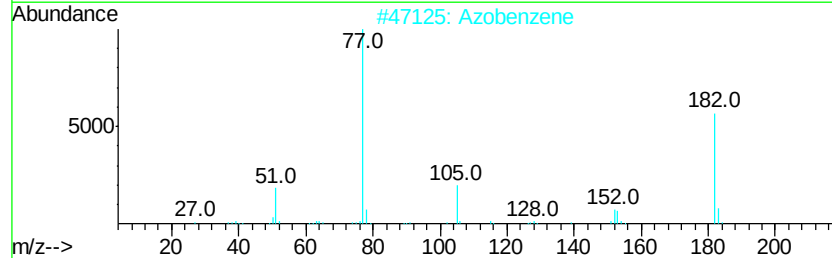
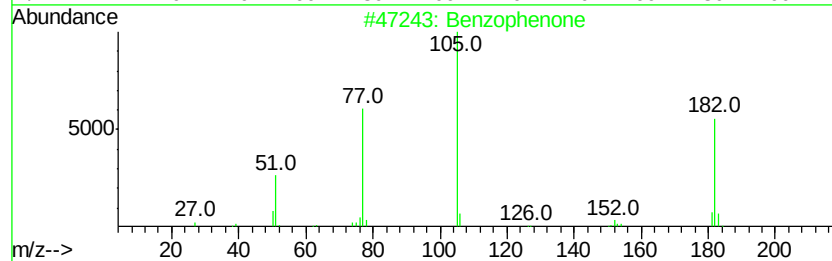
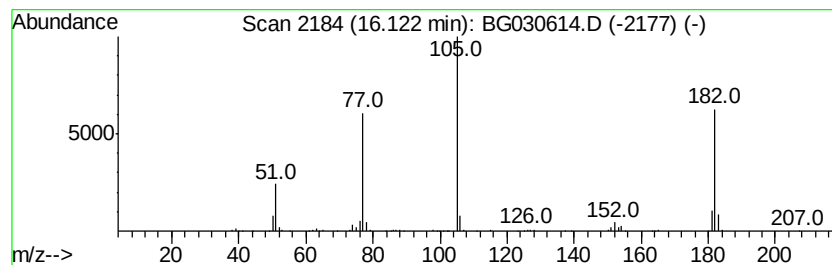
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Peak Number 5 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.12	5.90 ng	334466	Acenaphthene-d10	14.78
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzophenone	182 C13H10O	000119-61-9 96
2		Azobenzene	182 C12H10N2	000103-33-3 59
3		Acetophenone, 2-chloro-	154 C8H7ClO	000532-27-4 49
4		Benzenebutanoic acid, .gamma.-oxo-	178 C10H10O3	002051-95-8 47
5		2-Pyrazoline-3-carbonitrile, 1-b...	199 C11H9N3O	067872-68-8 47



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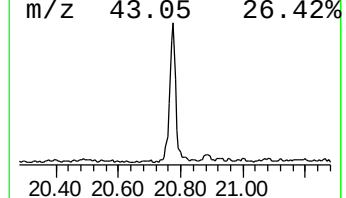
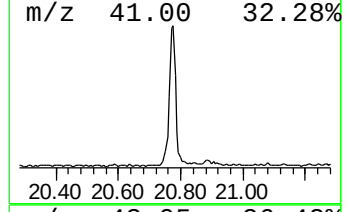
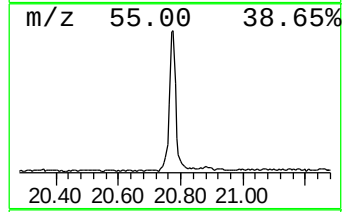
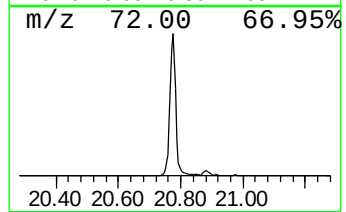
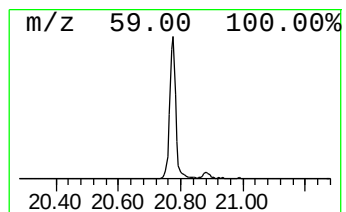
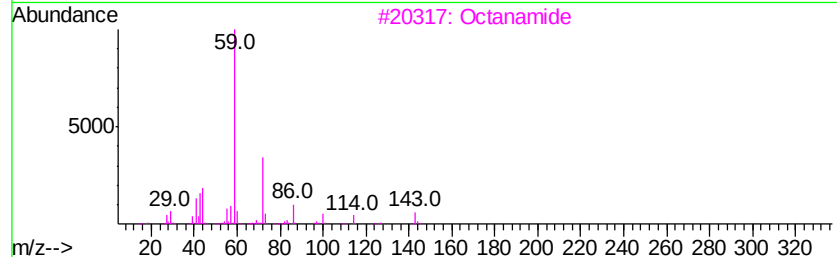
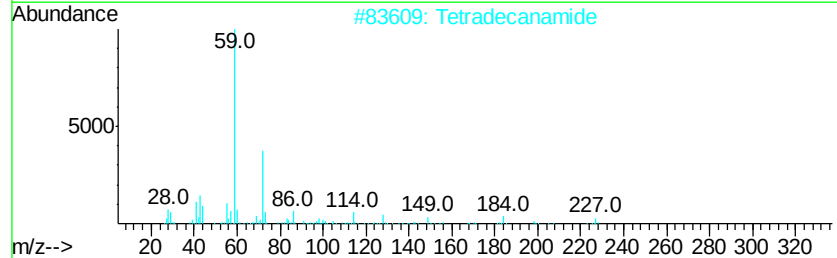
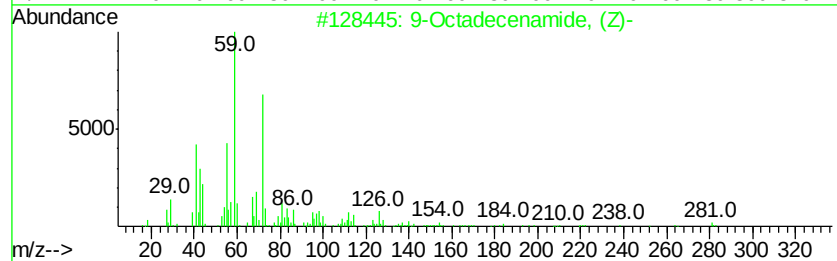
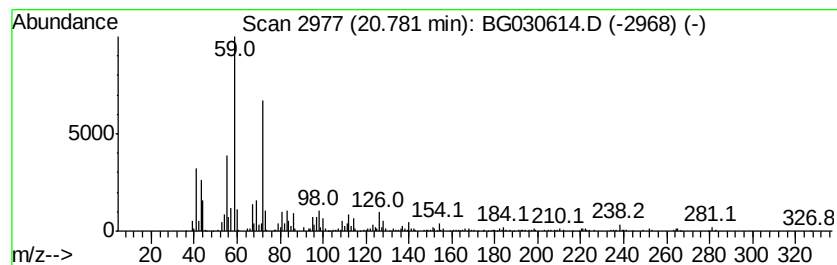
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Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.78	10.36 ng	807720	Chrysene-d12	21.79
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	9-Octadecenamide, (Z)-	281 C18H35NO	000301-02-0	99
2	Tetradecanamide	227 C14H29NO	000638-58-4	72
3	Octanamide	143 C8H17NO	000629-01-6	64
4	Nonanamide	157 C9H19NO	001120-07-6	59
5	Pentadecanamide, 15-bromo-	319 C15H30BrNO	1000163-86-1	56



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.24	11.7	ng	260173	1	8.16	443273	20.0
unknown7.69	7.69	75.3	ng	1669810	1	8.16	443273	20.0
2-Hydroxy-iso-but...	12.27	2.4	ng	87232	2	10.98	719012	20.0
Benzophenone	16.12	5.9	ng	334466	3	14.78	1134740	20.0
9-Octadecenamide,...	20.78	10.4	ng	807720	5	21.79	1559200	20.0