

Data Path : Z:\HPCHEM1\BNA G\DATA\BG103117\
 Data File : BG030615.D
 Acq On : 31 Oct 2017 16:50
 Operator : SJ/JU
 Sample : I6133-02
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SW-02(18-20)

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	5.244	327	333	342	rVB	130088	203581	5.99%	1.017%
2	5.720	407	414	424	rBV	644105	1066379	31.39%	5.327%
3	7.318	677	686	699	rBV	735755	1313633	38.67%	6.562%
4	7.694	742	750	760	rBV	704032	1206440	35.52%	6.026%
5	8.164	822	830	837	rBV	234001	409461	12.05%	2.045%
6	8.487	876	885	893	rBV	481431	845944	24.90%	4.226%
7	9.322	1019	1027	1036	rBV	420474	765103	22.52%	3.822%
8	10.973	1300	1308	1317	rBV	362665	667573	19.65%	3.335%
9	12.271	1523	1529	1536	rBV2	21636	38684	1.14%	0.193%
10	13.399	1714	1721	1731	rBV	1434921	2257364	66.45%	11.276%
11	14.216	1854	1860	1869	rBV	163406	249361	7.34%	1.246%
12	14.774	1948	1955	1966	rVB2	628811	1041576	30.66%	5.203%
13	16.120	2177	2184	2190	rBV	87555	132578	3.90%	0.662%
14	16.261	2200	2208	2218	rBV	1023970	1655400	48.73%	8.269%
15	17.512	2415	2421	2431	rBV2	789541	1224306	36.04%	6.116%
16	20.103	2856	2862	2870	rBV	2584467	3396903	100.00%	16.968%
17	20.773	2969	2976	2986	rBV	464337	657987	19.37%	3.287%
18	21.789	3142	3149	3156	rVB2	857599	1431616	42.14%	7.151%
19	25.097	3701	3712	3724	rBV2	485429	1455714	42.85%	7.271%

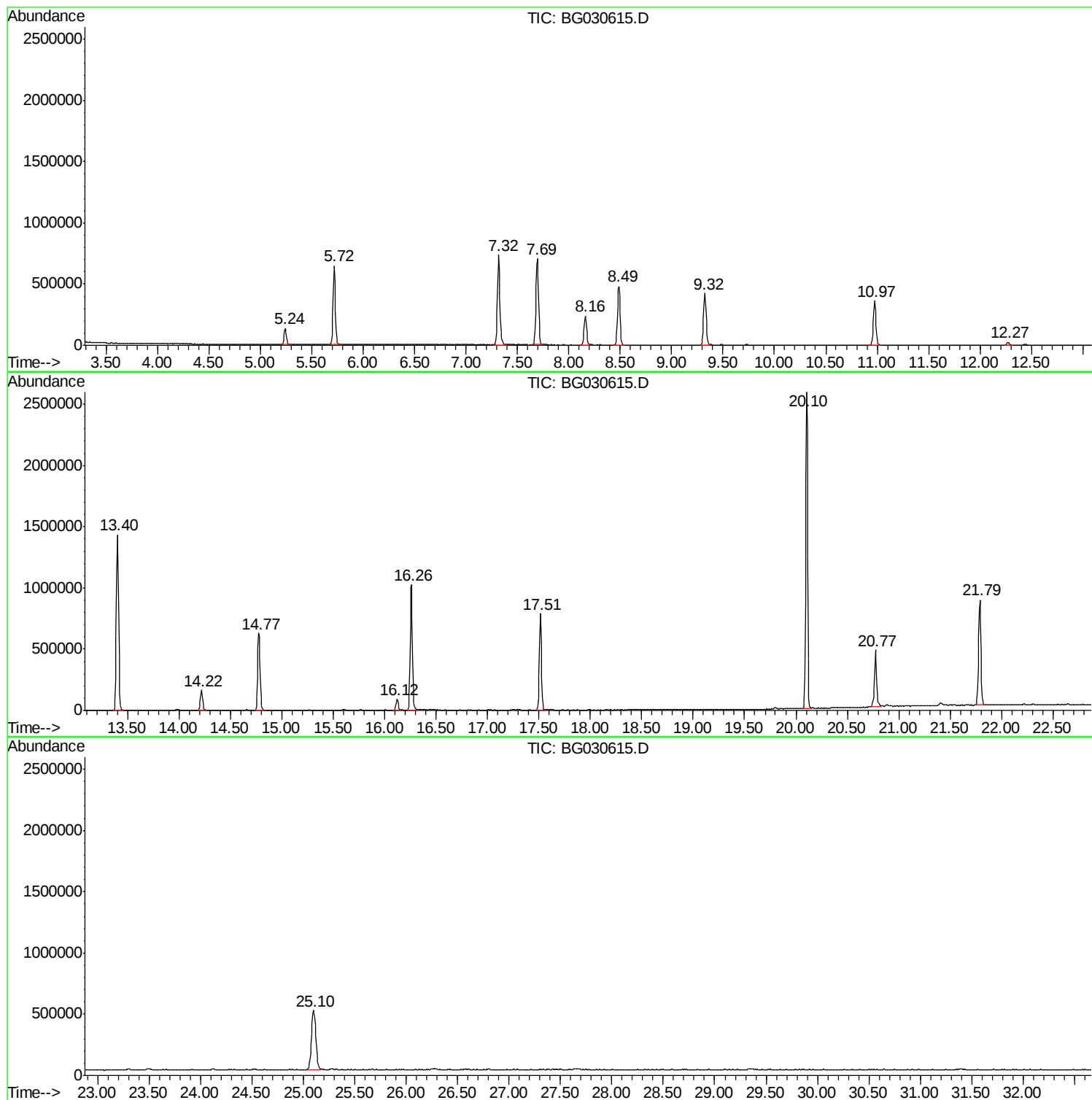
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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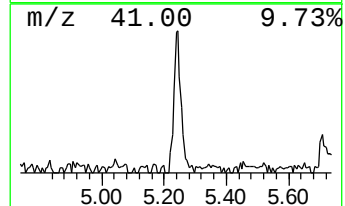
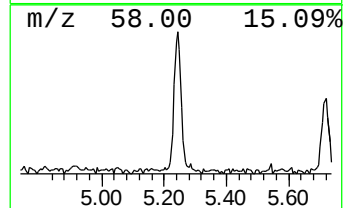
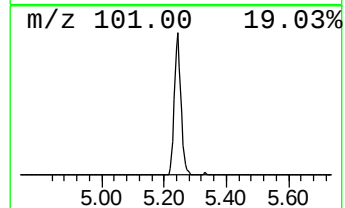
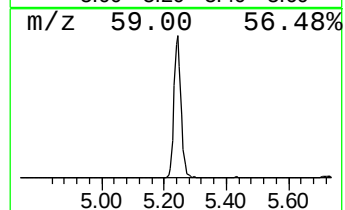
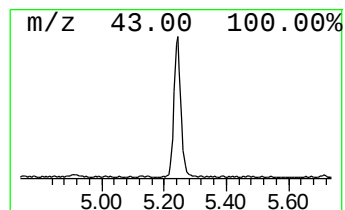
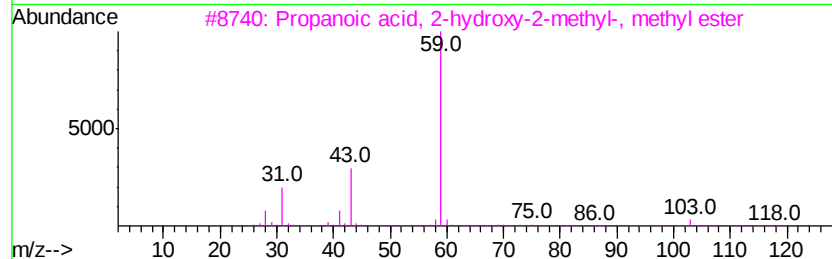
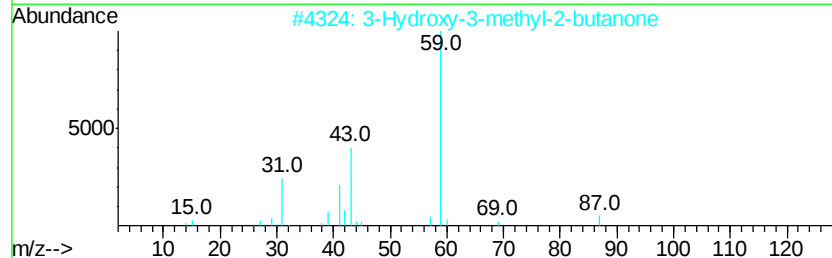
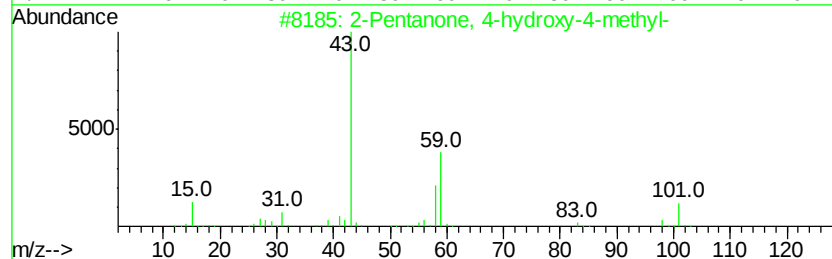
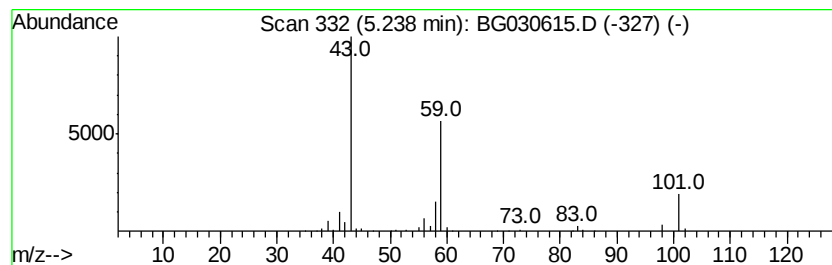
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown5.24 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	9.94 ng	203581	1,4-Dichlorobenzene-d4	8.16

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40		
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17		
3	Propanoic acid, 2-hydroxy-2-meth...	118	C5H10O3	002110-78-3	12		
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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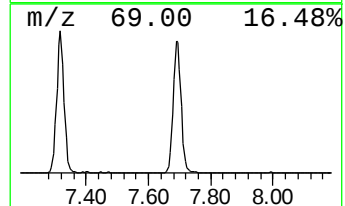
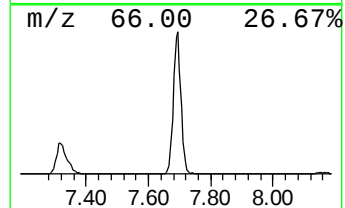
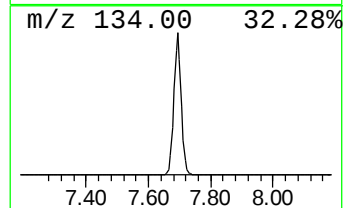
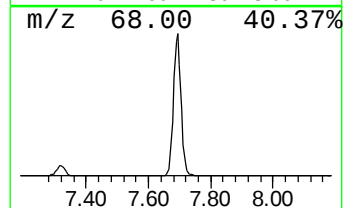
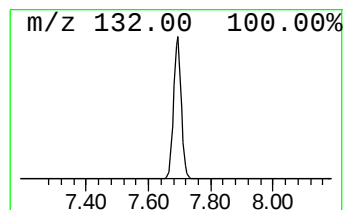
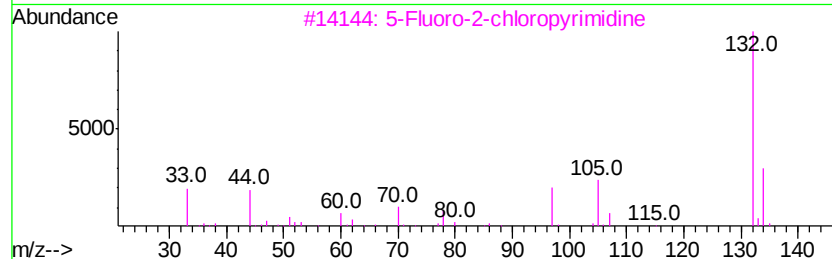
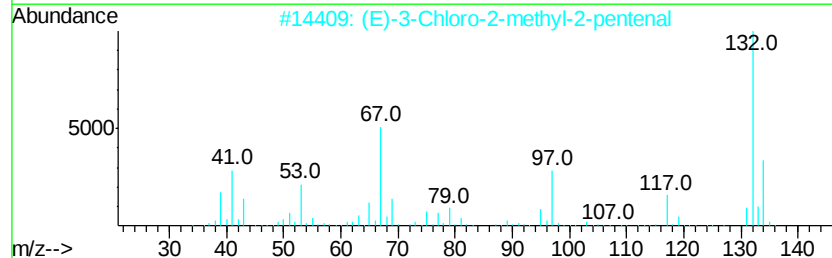
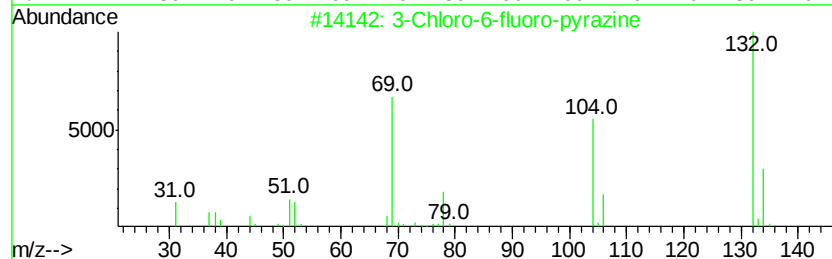
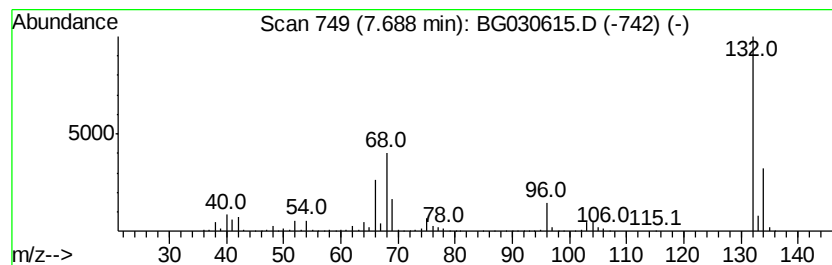
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Peak Number 2 unknown7.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.69	58.93 ng	1206440	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		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9



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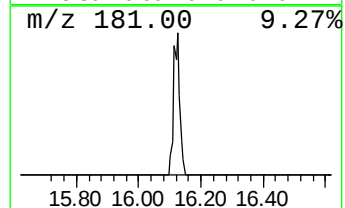
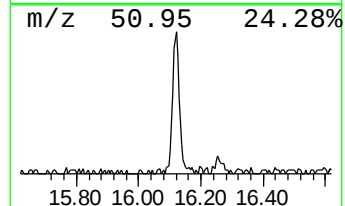
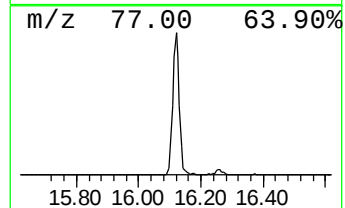
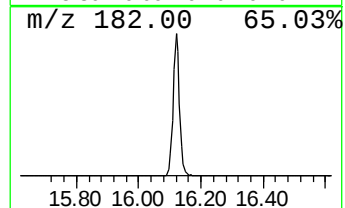
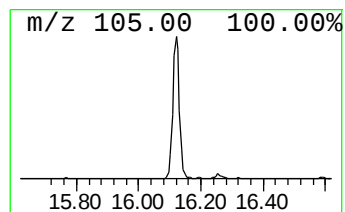
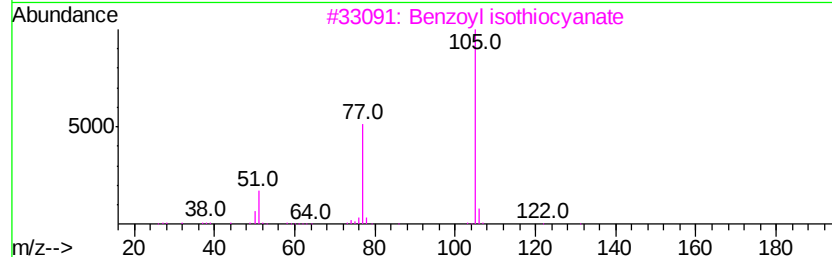
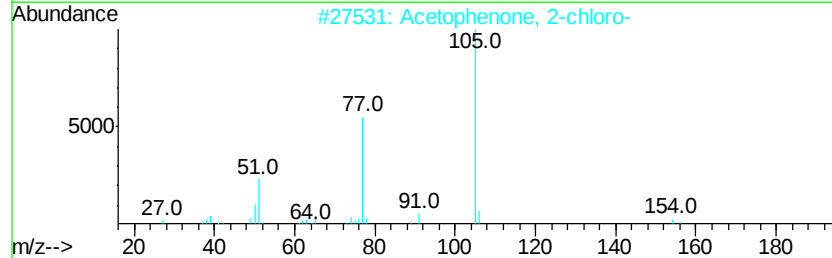
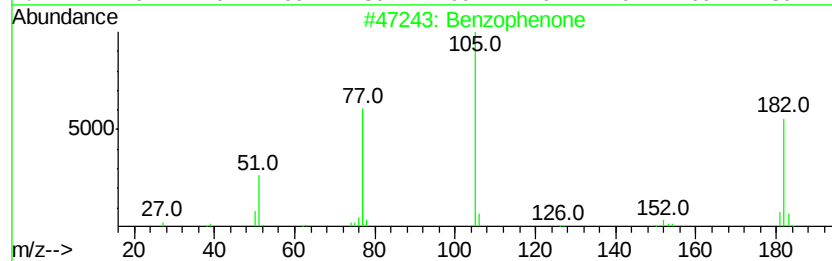
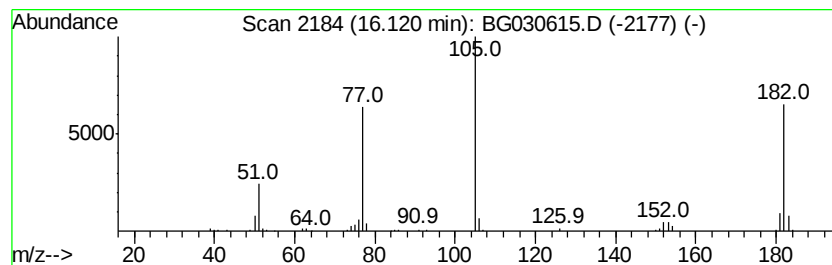
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Peak Number 4 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.12	2.55 ng	132578	Acenaphthene-d10	14.77

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzophenone	182	C13H10O	000119-61-9	96
2		Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
3		Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	43
4		Pentanediamide, N,N'-di-benzoyloxv-	370	C19H18N2O6	1000253-26-3	43
5		2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	43



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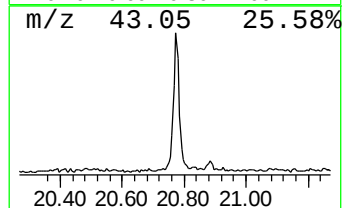
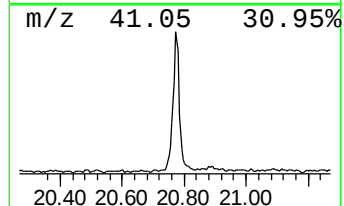
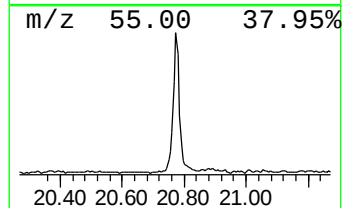
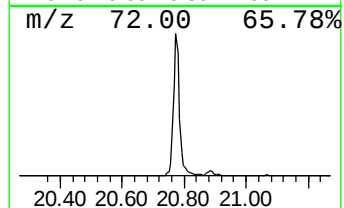
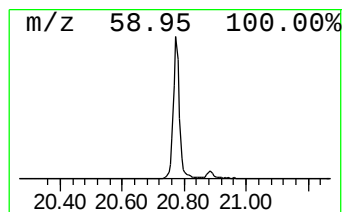
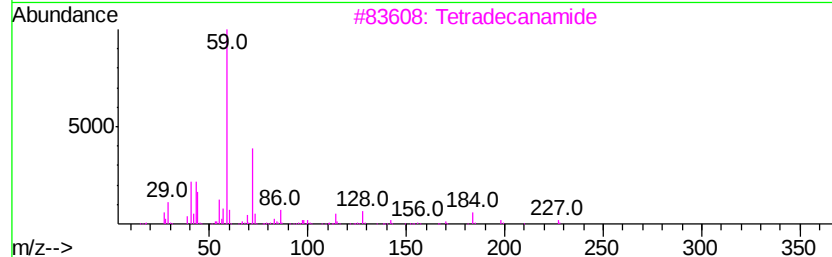
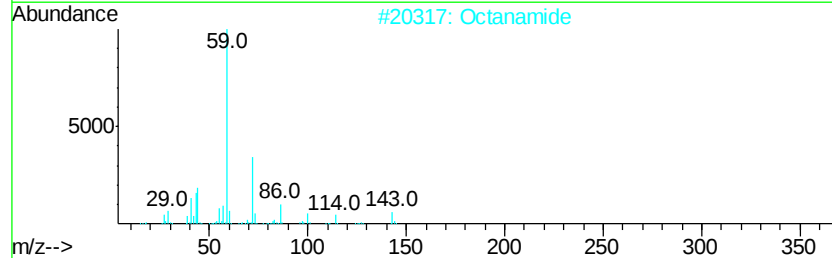
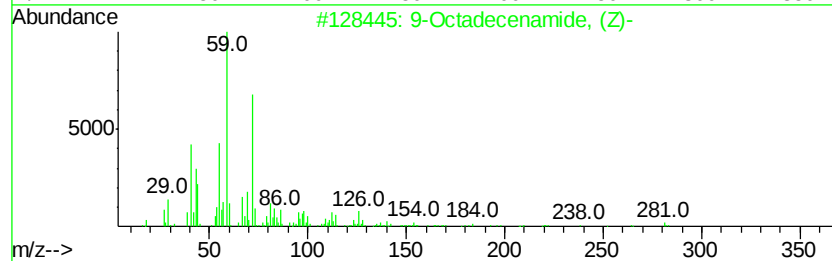
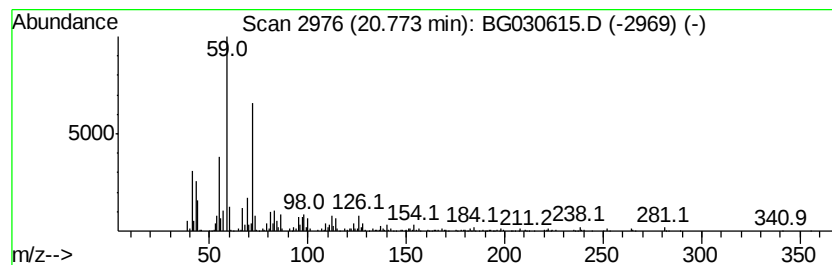
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.77	9.19 ng	657987	Chrysene-d12	21.79

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2		Octanamide	143	C8H17NO	000629-01-6	78
3		Tetradecanamide	227	C14H29NO	000638-58-4	59
4		Hexadecanamide	255	C16H33NO	000629-54-9	56
5		Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown5.24	5.24	9.9	ng	203581	1	8.16	409461	20.0
unknown7.69	7.69	58.9	ng	1206440	1	8.16	409461	20.0
Benzophenone	16.12	2.5	ng	132578	3	14.77	1041580	20.0
9-Octadecenamide,...	20.77	9.2	ng	657987	5	21.79	1431620	20.0