

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_G\DATA\BG011718\
 Data File : BG032113.D
 Acq On : 17 Jan 2018 22:58
 Operator : SJ/JU
 Sample : J1166-02
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 18A-11

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-BG011218.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	5.661	396	404	413	rBV	56479	97001	2.41%	0.479%
2	6.172	483	491	501	rBV	714400	1239170	30.81%	6.123%
3	7.853	767	777	789	rBV	717305	1413972	35.16%	6.986%
4	8.252	837	845	860	rVB	767162	1422359	35.37%	7.028%
5	8.740	921	928	938	rBV	140859	261218	6.50%	1.291%
6	9.081	976	986	997	rVB	589954	1099868	27.35%	5.434%
7	9.938	1122	1132	1141	rBV	451097	836682	20.81%	4.134%
8	11.625	1411	1419	1433	rVB	192913	372743	9.27%	1.842%
9	12.882	1626	1633	1641	rBV2	35523	60948	1.52%	0.301%
10	14.004	1817	1824	1835	rVB	1336284	2192354	54.52%	10.832%
11	14.803	1954	1960	1967	rVB	161712	244626	6.08%	1.209%
12	15.379	2051	2058	2068	rVB2	358167	602153	14.97%	2.975%
13	16.713	2278	2285	2294	rVB	249324	386309	9.61%	1.909%
14	16.854	2302	2309	2317	rBV	1550370	2468708	61.39%	12.198%
15	18.111	2516	2523	2537	rVB2	558360	872219	21.69%	4.310%
16	18.928	2657	2662	2670	rBV2	71762	115845	2.88%	0.572%
17	20.168	2867	2873	2878	rBV5	45689	68492	1.70%	0.338%
18	20.649	2949	2955	2962	rBV	3021493	4021431	100.00%	19.870%
19	21.989	3177	3183	3190	rBV9	38833	73387	1.82%	0.363%
20	22.447	3253	3261	3275	rVB2	628320	1183504	29.43%	5.848%
21	26.149	3880	3891	3904	rVB2	371955	1206070	29.99%	5.959%

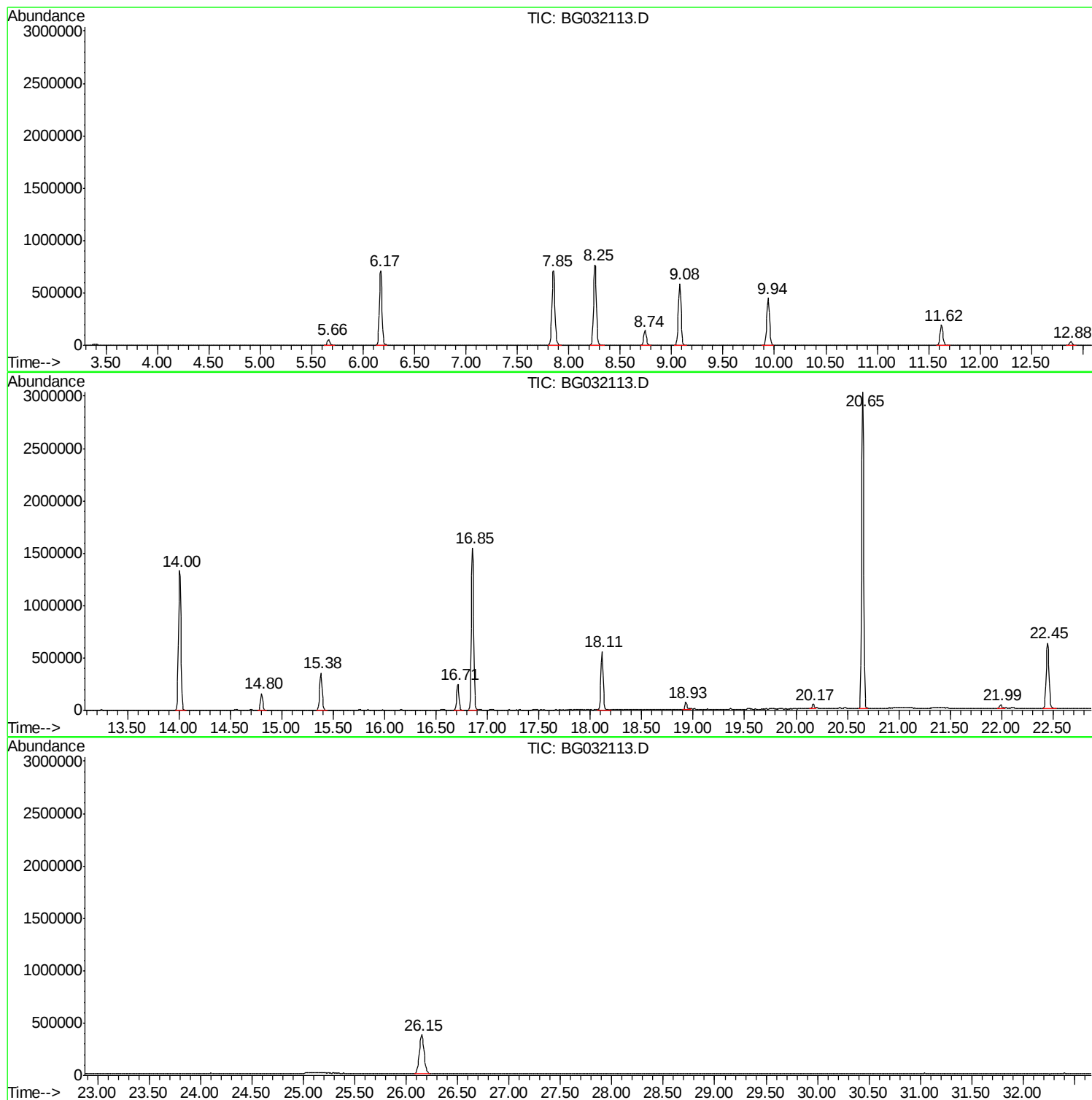
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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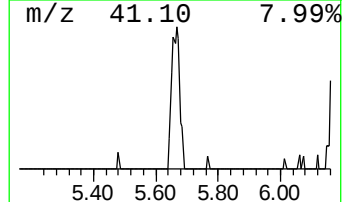
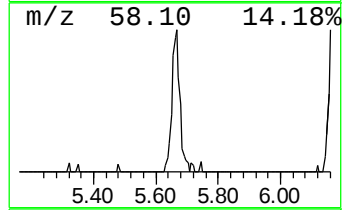
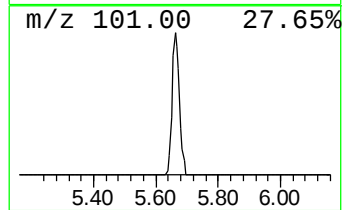
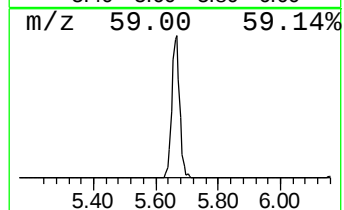
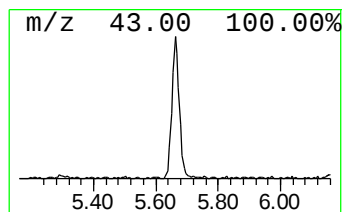
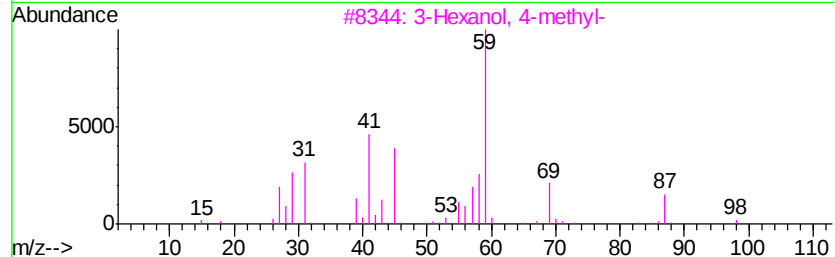
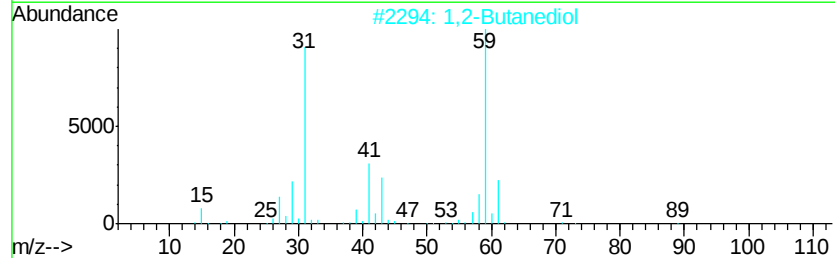
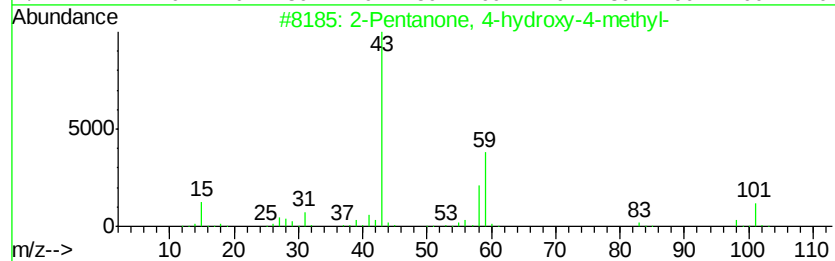
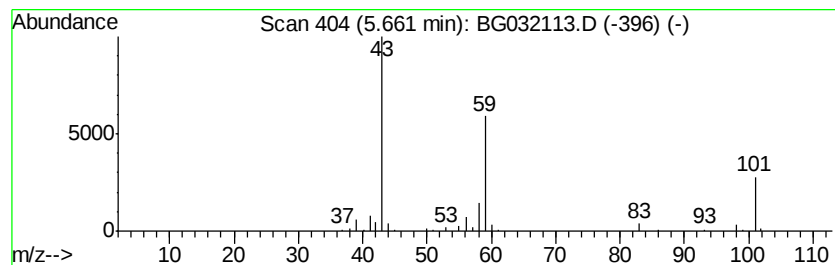
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.66	7.43 ng	97001	1,4-Dichlorobenzene-d4	8.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			1,2-Butanediol	90	C4H10O2	000584-03-2	23
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	23
4			5-Hexen-2-one	98	C6H10O	000109-49-9	14
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	12



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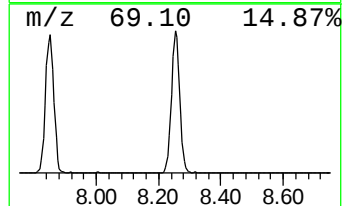
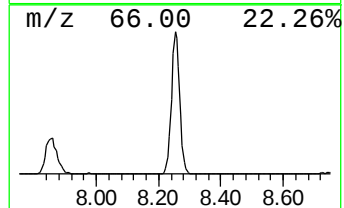
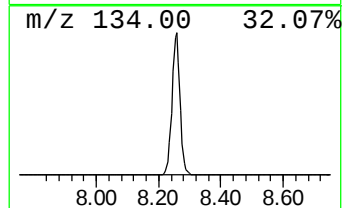
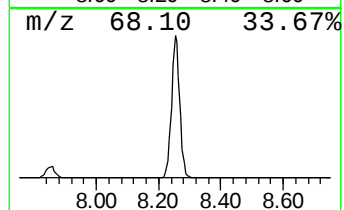
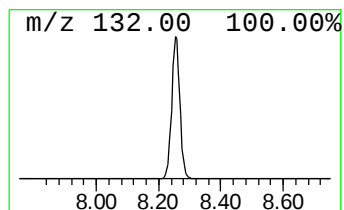
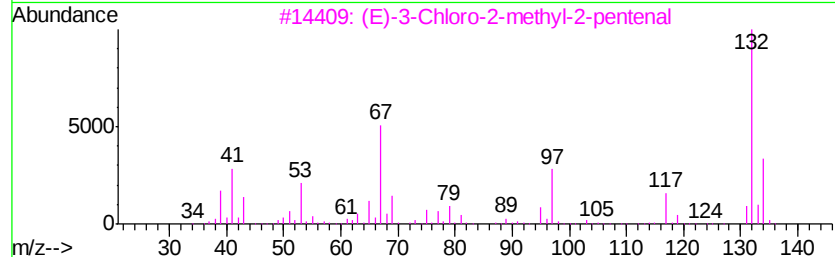
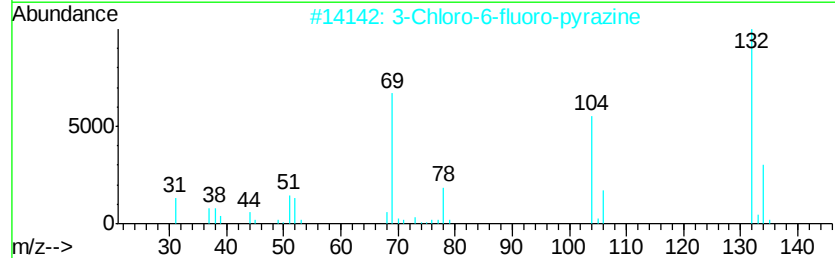
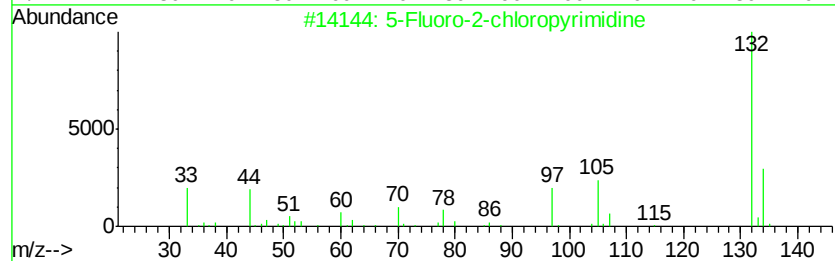
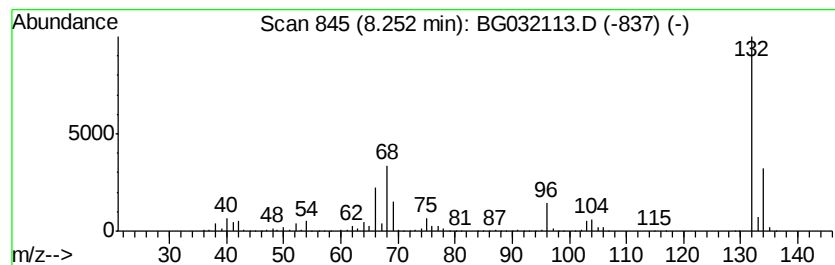
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Peak Number 2 unknown8.25 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.25	108.90 ng	1422360	1,4-Dichlorobenzene-d4	8.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	25
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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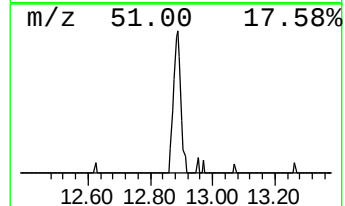
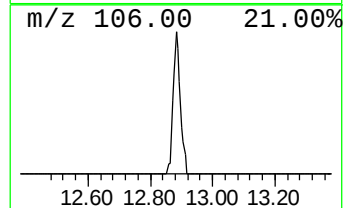
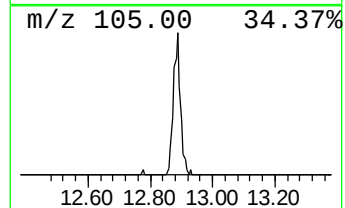
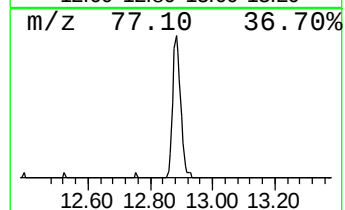
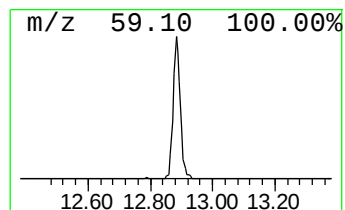
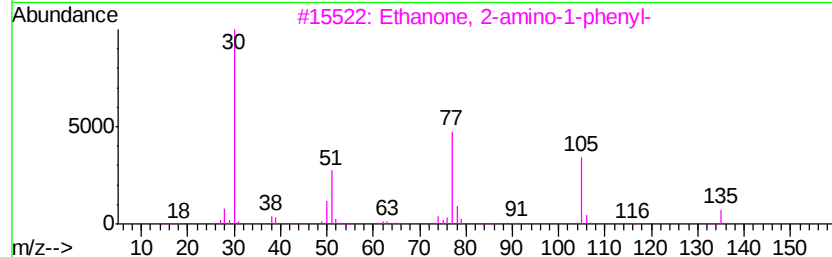
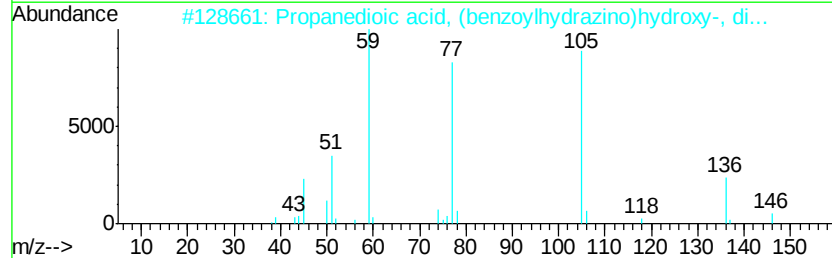
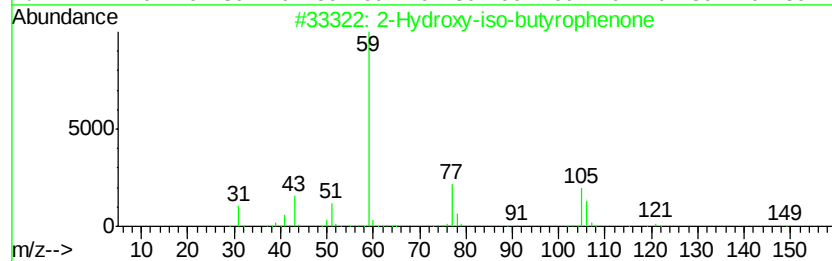
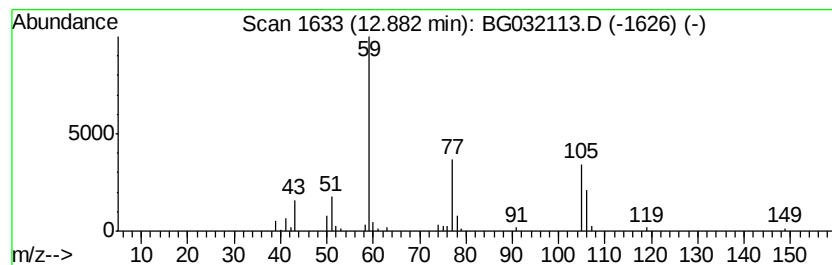
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Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.88	3.27 ng	60948	Napthalene-d8	11.62		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	78
2		Propanedioic acid, (benzoylhydra...	282	C12H14N2O6	1000142-99-9	33
3		Ethanone, 2-amino-1-phenyl-	135	C8H9NO	000613-89-8	22
4		1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	9
5		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	9



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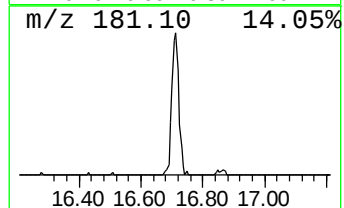
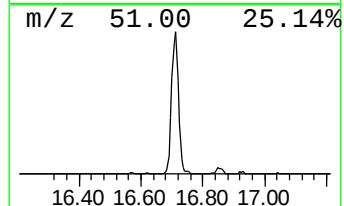
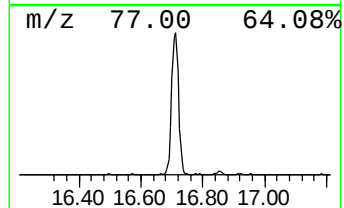
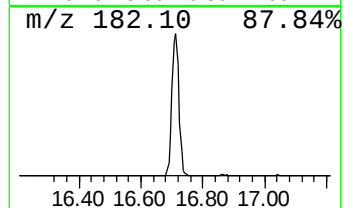
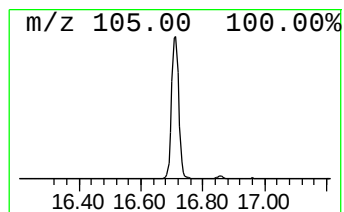
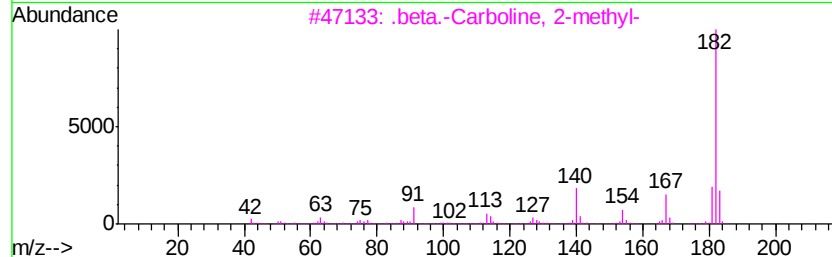
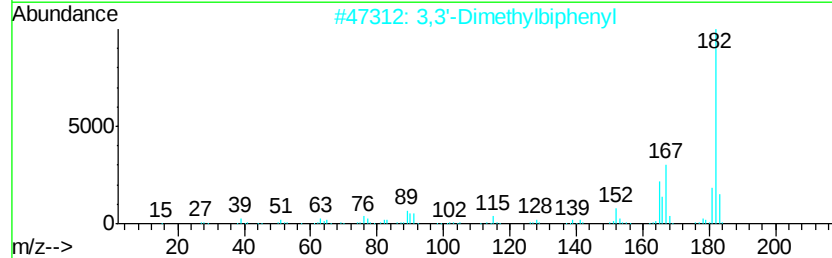
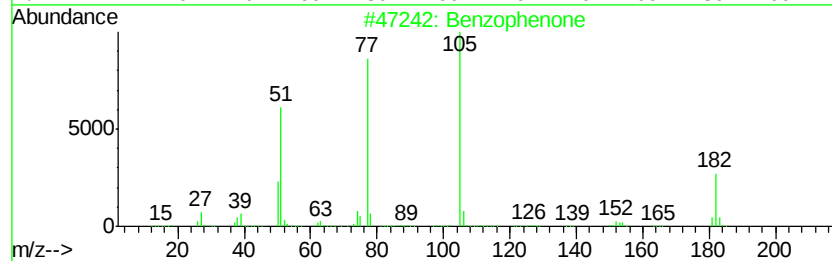
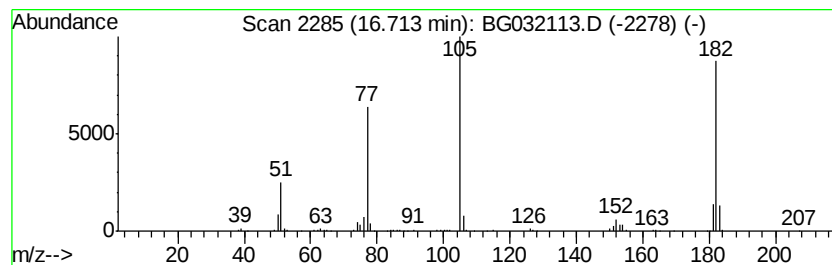
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Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.71	12.83 ng	386309	Acenaphthene-d10	15.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzophenone	182	C13H10O	000119-61-9	97
2		3,3'-Dimethylbiphenyl	182	C14H14	000612-75-9	43
3		.beta.-Carboline, 2-methyl-	182	C12H10N2	013099-99-5	43
4		Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	38
5		Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	35



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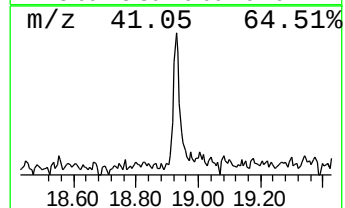
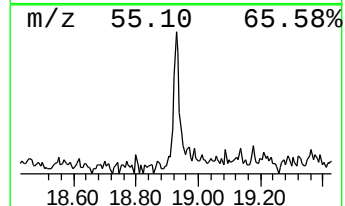
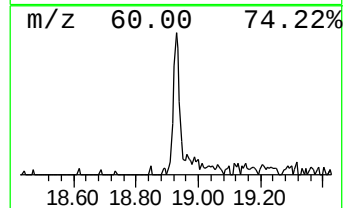
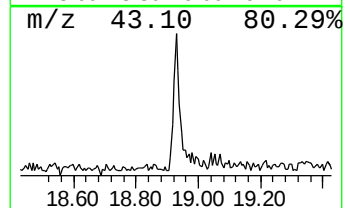
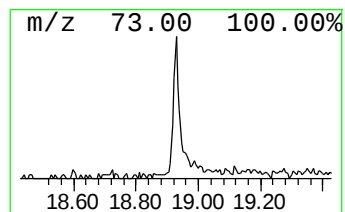
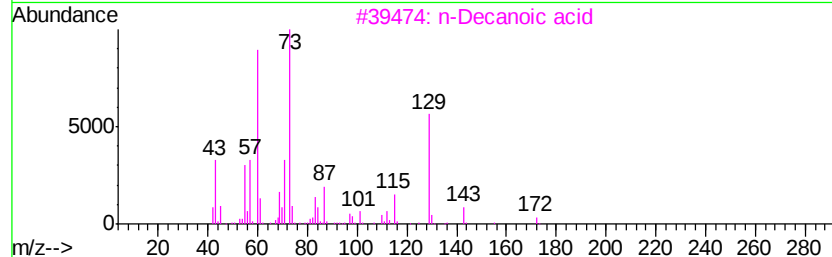
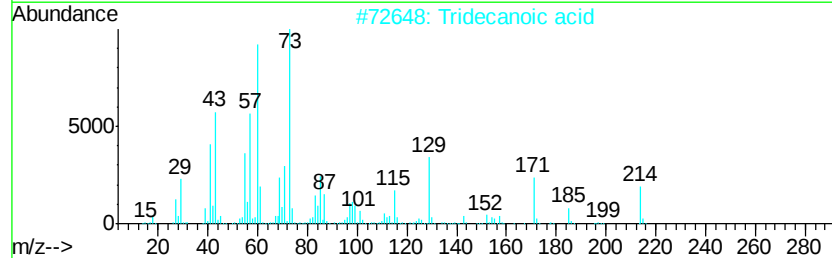
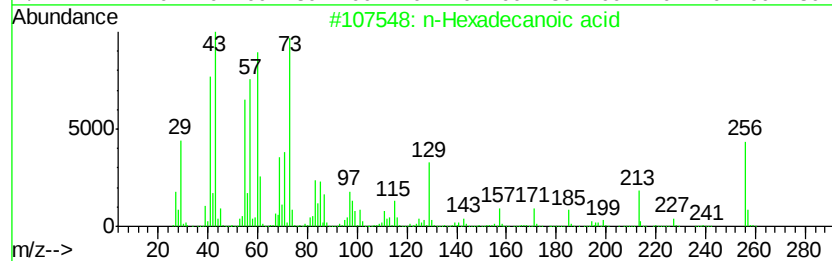
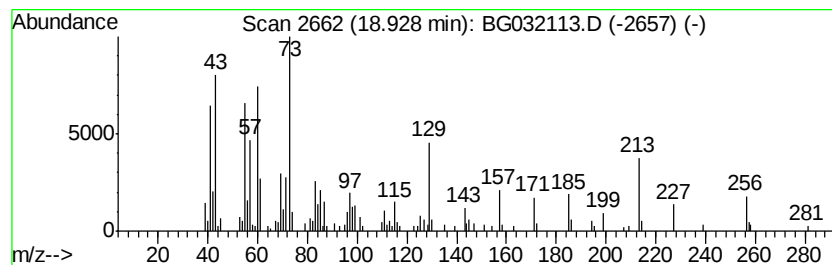
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.93	2.66 ng	115845	Phenanthrene-d10		18.11	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		n-Decanoic acid	172	C10H20O2	000334-48-5	78
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.66	7.4	ng	97001	1	8.75	261218	20.0
unknown8.25	8.25	108.9	ng	1422360	1	8.75	261218	20.0
2-Hydroxy-iso-but...	12.88	3.3	ng	60948	2	11.62	372743	20.0
Benzophenone	16.71	12.8	ng	386309	3	15.38	602153	20.0
n-Hexadecanoic acid	18.93	2.7	ng	115845	4	18.11	872219	20.0