

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101717\
 Data File : BF099587.D
 Acq On : 17 Oct 2017 18:05
 Operator : SJ/JU
 Sample : I5794-07
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ENV-105-4(0-5)

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_F\METHODS\8270-BF092317.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	5.057	501	505	521	rBV	213357	297100	13.47%	1.581%
2	5.451	568	572	593	rBV	1837813	1812943	82.19%	9.646%
3	6.463	740	744	757	rBV	1804518	1964534	89.06%	10.453%
4	6.598	763	767	770	rBV	2122220	1904067	86.32%	10.131%
5	6.828	802	806	814	rBV	612443	568793	25.79%	3.026%
6	6.981	828	832	836	rBV	1726003	1516198	68.74%	8.068%
7	7.392	897	902	905	rBV	1225839	1118873	50.72%	5.953%
8	8.104	1019	1023	1027	rBV	870340	790125	35.82%	4.204%
9	8.563	1098	1101	1106	rBV	31783	26097	1.18%	0.139%
10	8.663	1114	1118	1128	rBB	171933	140117	6.35%	0.746%
11	9.180	1201	1206	1209	rBV	2491862	2205835	100.00%	11.737%
12	9.575	1269	1273	1276	rBV	590917	442108	20.04%	2.352%
13	9.863	1317	1322	1326	rBV	966695	882648	40.01%	4.696%
14	10.574	1439	1443	1446	rBV	836748	680836	30.87%	3.623%
15	10.651	1452	1456	1465	rBV	915117	808085	36.63%	4.300%
16	11.351	1571	1575	1578	rBV	942747	823511	37.33%	4.382%
17	12.927	1839	1843	1847	rBV	1744852	1598418	72.46%	8.505%
18	13.810	1990	1993	2002	rBV2	85951	105830	4.80%	0.563%
19	13.986	2020	2023	2027	rBV	557391	523651	23.74%	2.786%
20	14.721	2145	2148	2154	rBV3	31381	37299	1.69%	0.198%
21	15.451	2267	2272	2277	rBV	426581	518332	23.50%	2.758%
22	16.356	2421	2426	2429	rBV4	17205	28489	1.29%	0.152%

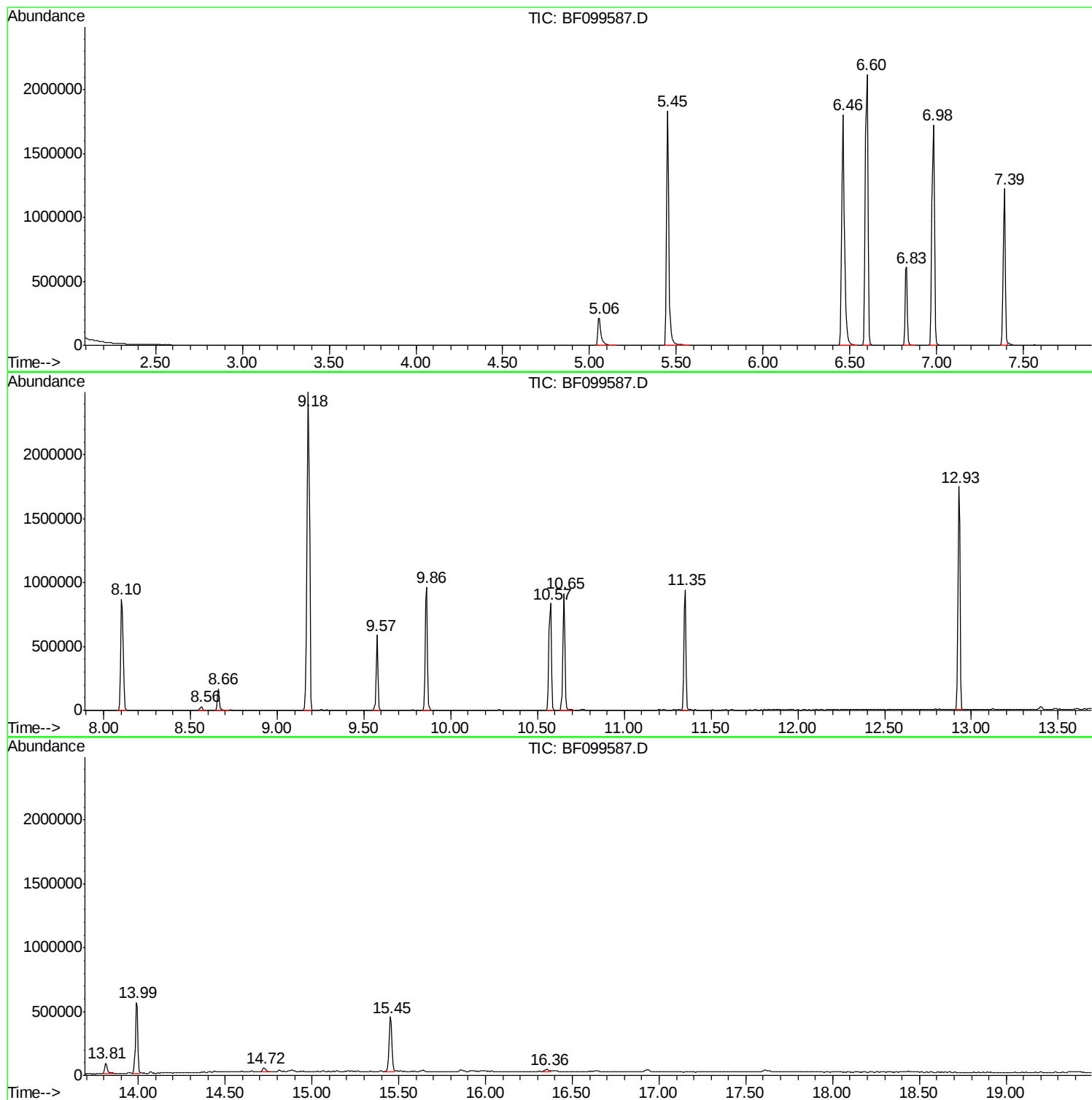
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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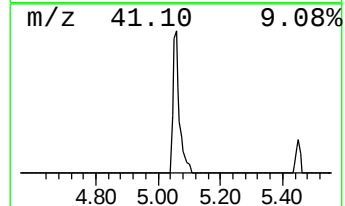
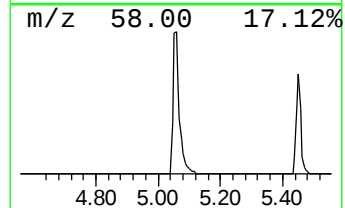
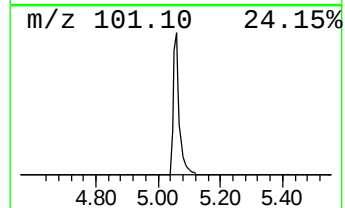
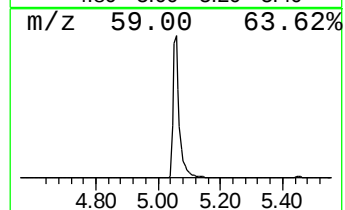
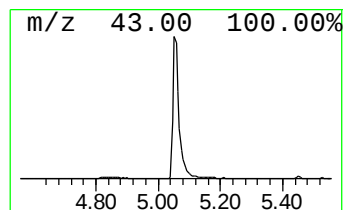
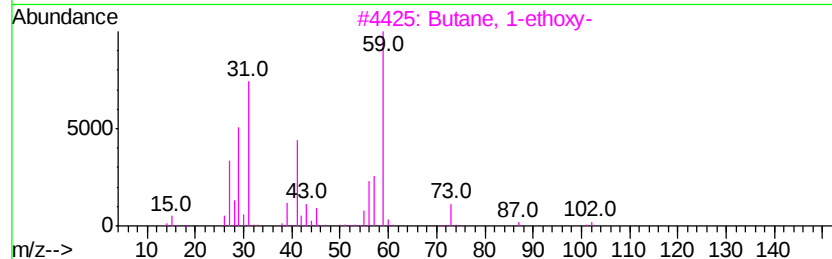
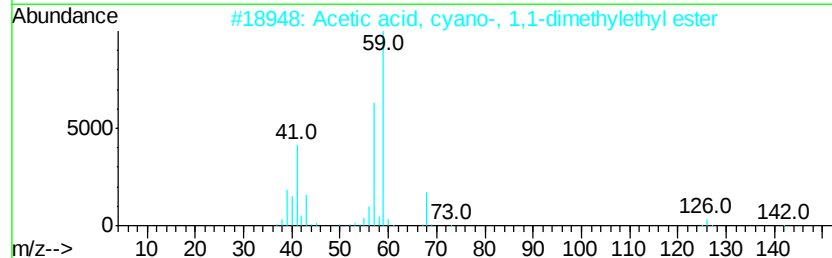
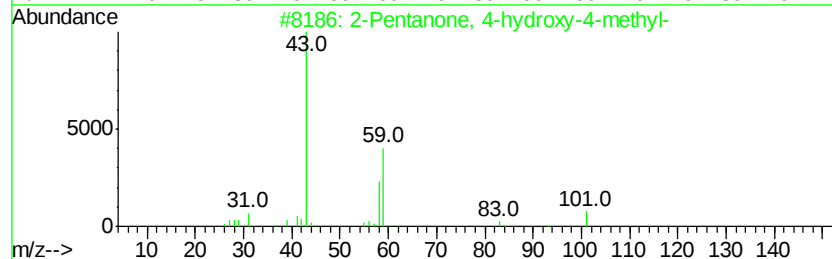
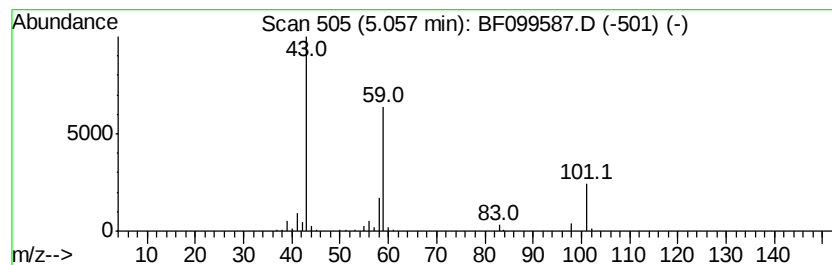
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.06	10.45 ng	297100	1,4-Dichlorobenzene-d4	6.83

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	17
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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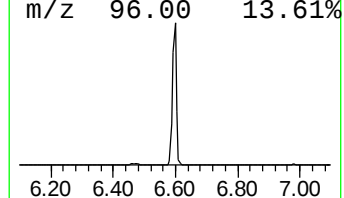
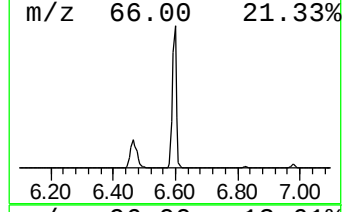
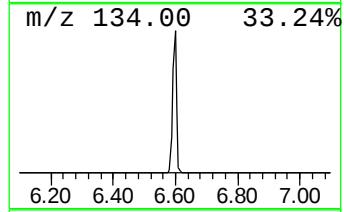
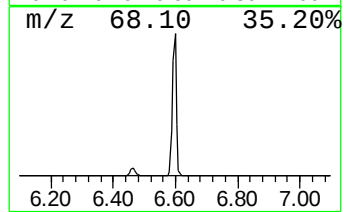
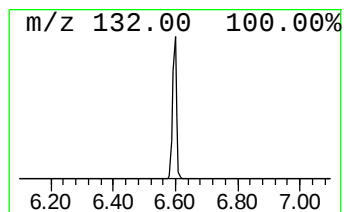
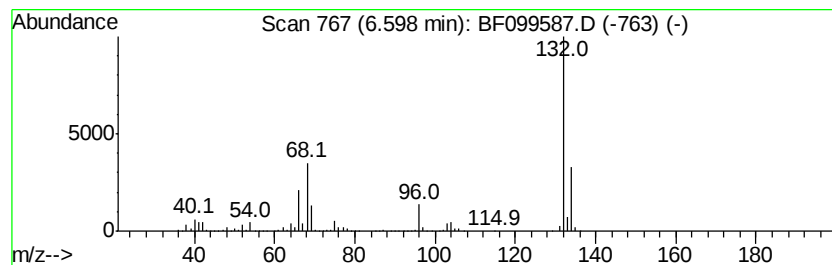
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	66.95 ng	1904070	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		Xenon	132	Xe	007440-63-3	9



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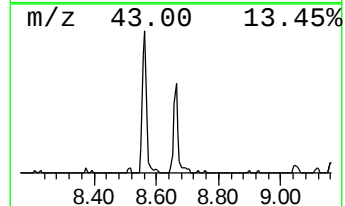
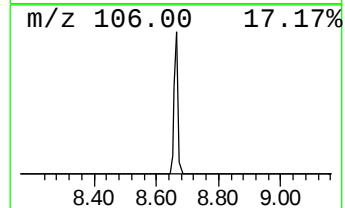
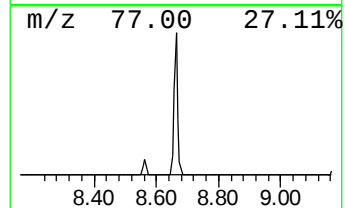
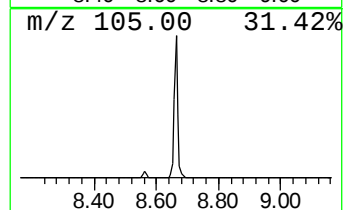
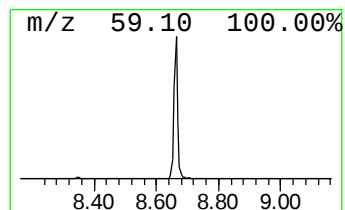
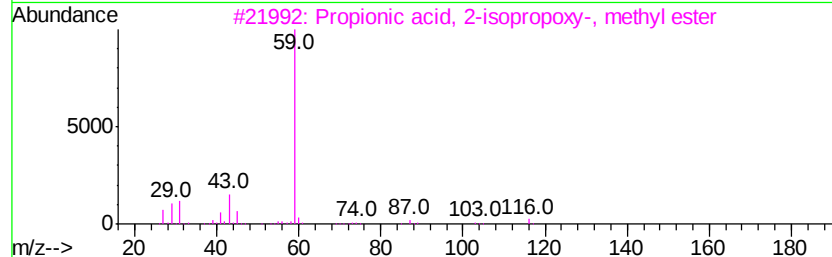
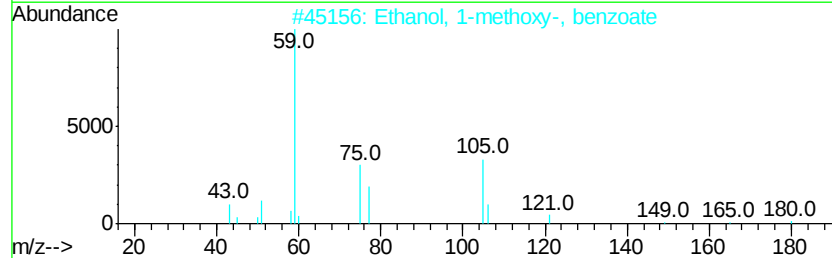
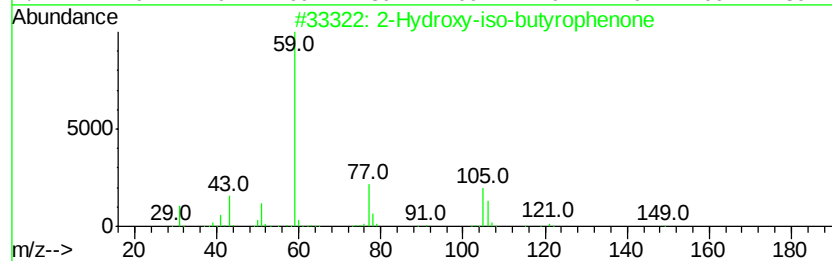
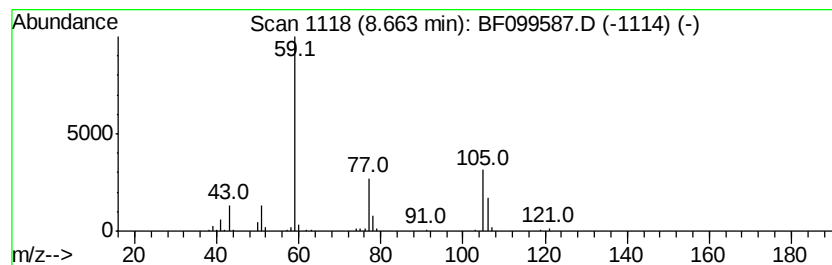
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Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.66	3.55 ng	140117	Napthalene-d8	8.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2		Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	72
3		Propionic acid, 2-isopropoxy-, m...	146	C7H14O3	1000151-15-1	9
4		.alpha.-(Methylthio)acetamide	105	C3H7NOS	022551-24-2	7
5		Guanidine	59	CH5N3	000113-00-8	7



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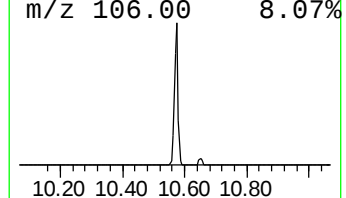
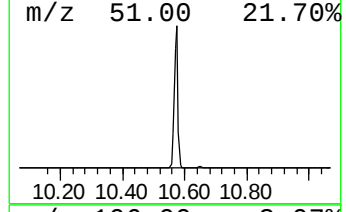
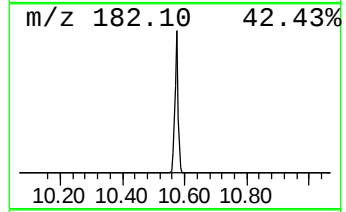
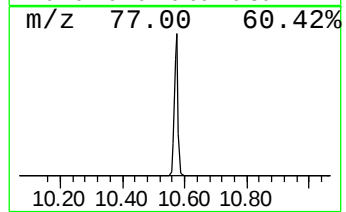
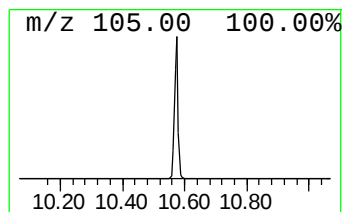
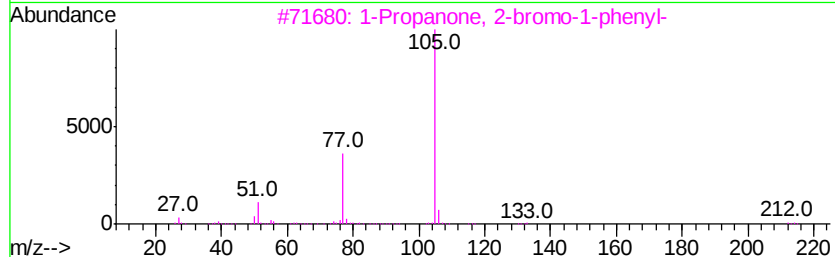
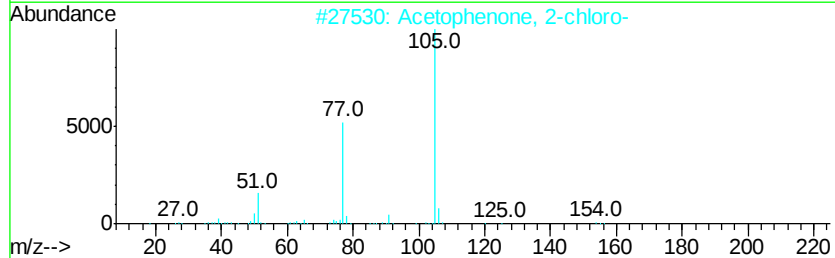
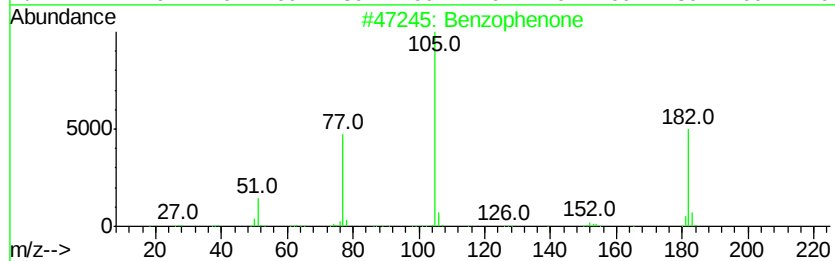
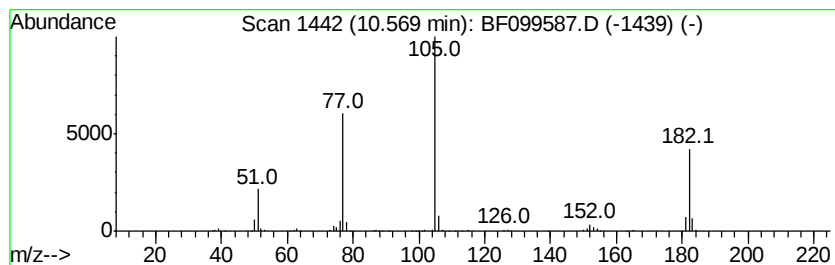
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Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.57	15.43 ng	680836	Acenaphthene-d10	9.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzophenone	182	C13H10O	000119-61-9	97
2		Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3		1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4		Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47
5		Ethanone, 2-hydroxy-1-phenyl-	136	C8H8O2	000582-24-1	47



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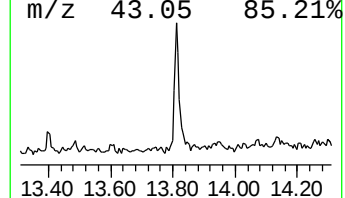
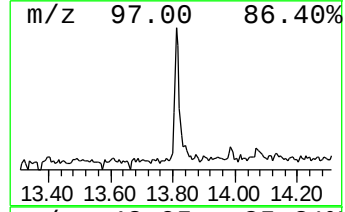
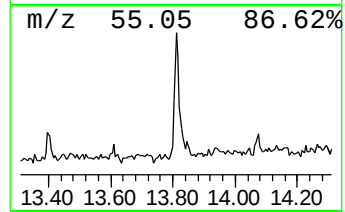
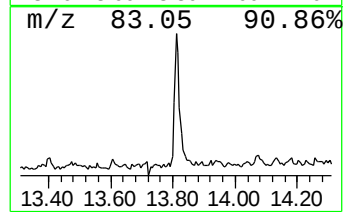
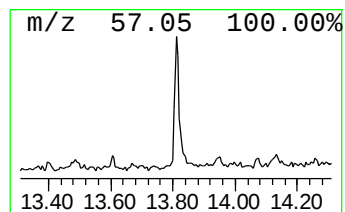
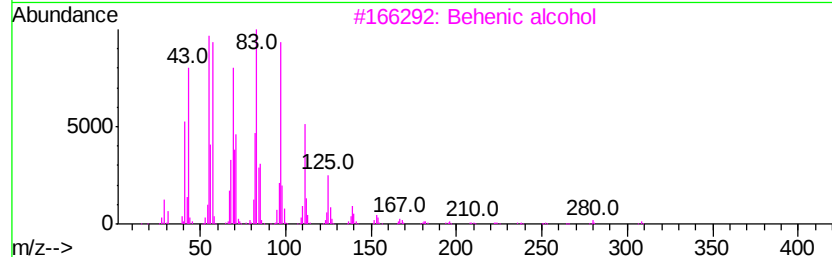
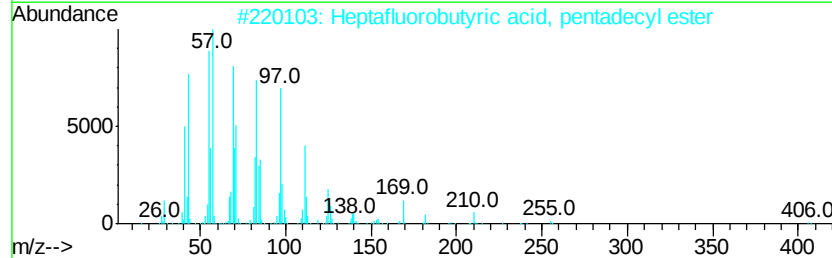
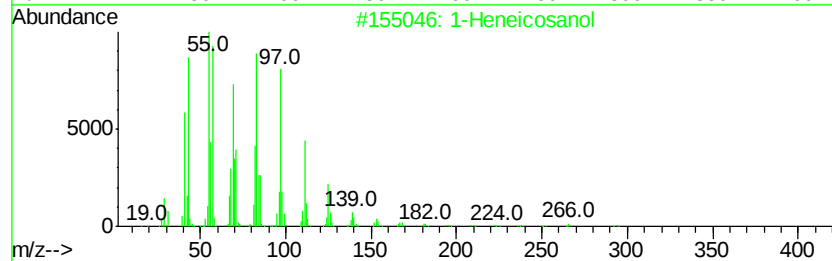
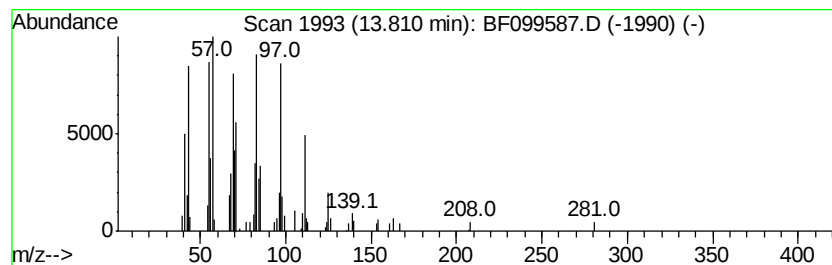
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Peak Number 6 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	4.04 ng	105830	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	94
2		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3		Behenic alcohol	326	C22H46O	000661-19-8	94
4		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



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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...	5.06	10.4	ng	297100	1	6.83	568793	20.0
unknown6.60	6.60	67.0	ng	1904070	1	6.83	568793	20.0
2-Hydroxy-iso-but...	8.66	3.5	ng	140117	2	8.10	790125	20.0
Benzophenone	10.57	15.4	ng	680836	3	9.86	882648	20.0
1-Heneicosanol	13.81	4.0	ng	105830	5	13.99	523651	20.0