

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102817\
 Data File : BF099942.D
 Acq On : 29 Oct 2017 4:40
 Operator : SJ/JU
 Sample : I6059-01
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 101817-TIDO-F-D-B

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-BF102317.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	4.998	493	495	518	rBV	87082	124486	4.31%	0.722%
2	5.410	562	565	586	rBV	649969	809761	28.02%	4.696%
3	6.428	736	738	757	rBV	493778	644723	22.31%	3.739%
4	6.557	757	760	776	rVB	1625726	1504372	52.06%	8.724%
5	6.787	796	799	809	rBV	618567	577307	19.98%	3.348%
6	6.940	821	825	841	rBV	2147391	2093481	72.45%	12.140%
7	7.357	892	896	915	rBV	1479412	1574572	54.49%	9.131%
8	8.069	1013	1017	1028	rBV	868406	768823	26.61%	4.458%
9	8.628	1109	1112	1121	rBV	116791	98951	3.42%	0.574%
10	9.145	1195	1200	1203	rBV	2969548	2889515	100.00%	16.756%
11	9.539	1264	1267	1275	rVB	163231	129409	4.48%	0.750%
12	9.822	1306	1315	1318	rBV	904711	777458	26.91%	4.508%
13	9.857	1318	1321	1327	rVB	126686	121405	4.20%	0.704%
14	10.033	1348	1351	1359	rVB	60288	56374	1.95%	0.327%
15	10.375	1406	1409	1413	rBV	85742	73698	2.55%	0.427%
16	10.492	1426	1429	1433	rBV	58108	46389	1.61%	0.269%
17	10.533	1433	1436	1440	rBV	455126	358172	12.40%	2.077%
18	10.616	1447	1450	1460	rBV	826944	746026	25.82%	4.326%
19	11.310	1565	1568	1571	rBV	649896	605813	20.97%	3.513%
20	11.339	1571	1573	1578	rVB	164515	143131	4.95%	0.830%
21	12.533	1772	1776	1783	rVB	68082	62540	2.16%	0.363%
22	12.698	1801	1804	1808	rVB	80830	70311	2.43%	0.408%
23	12.763	1808	1815	1821	rVB	44969	62063	2.15%	0.360%
24	12.898	1833	1838	1841	rBV	1948405	1855649	64.22%	10.761%
25	13.404	1921	1924	1928	rVB	54741	43505	1.51%	0.252%
26	13.774	1984	1987	1995	rBV3	29855	36386	1.26%	0.211%
27	13.963	2015	2019	2027	rBV	566870	499580	17.29%	2.897%
28	15.421	2263	2267	2277	rVB	377260	470931	16.30%	2.731%

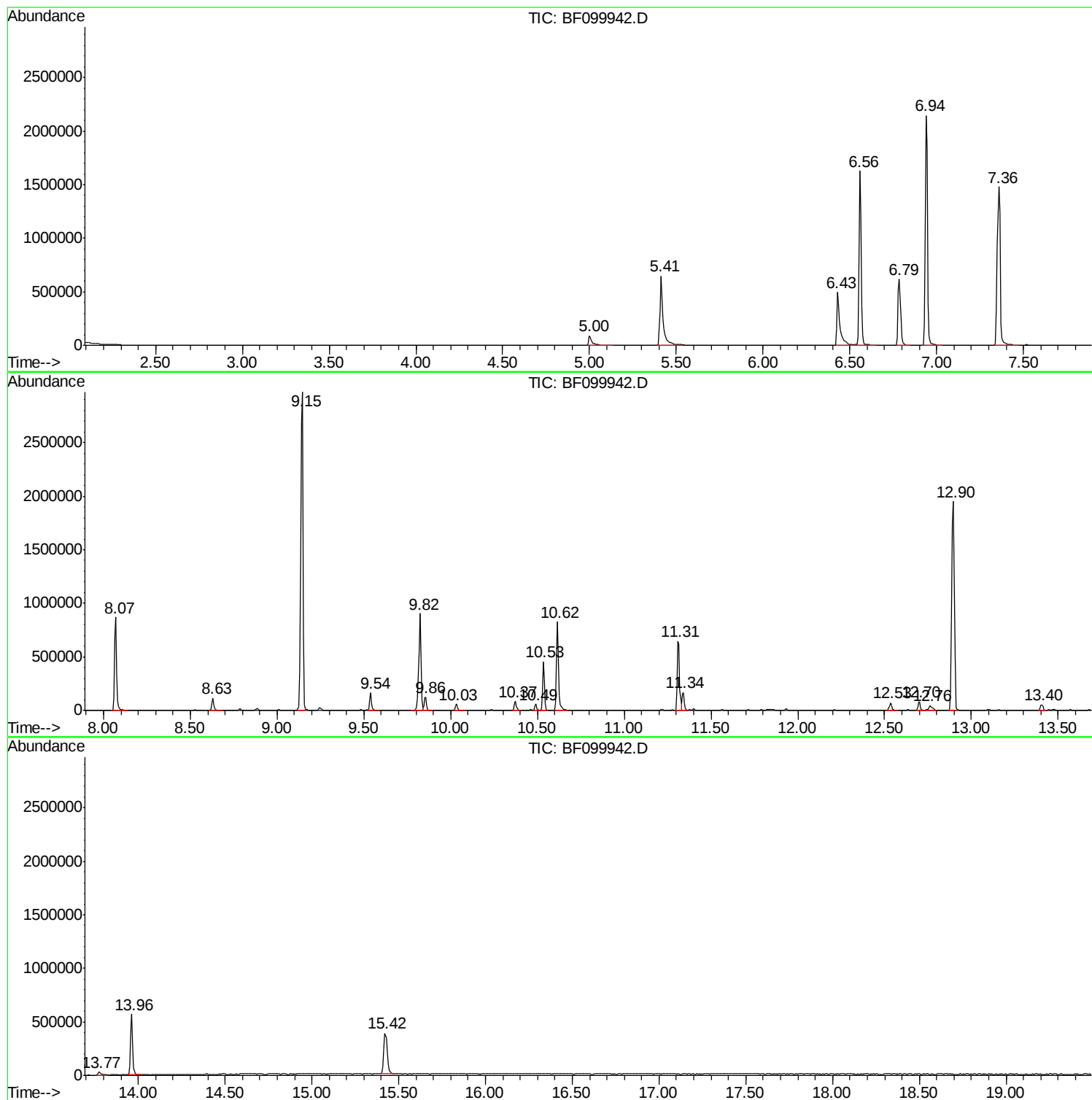
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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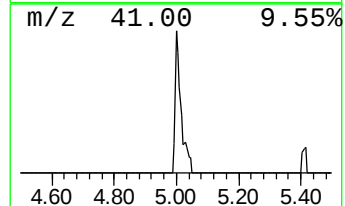
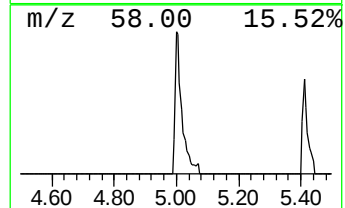
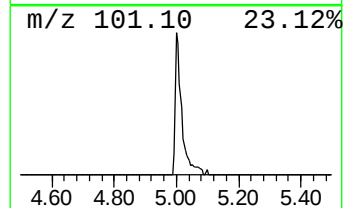
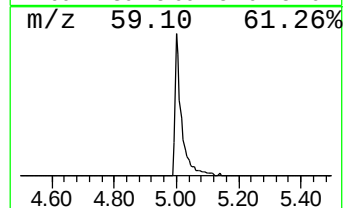
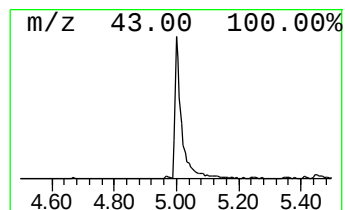
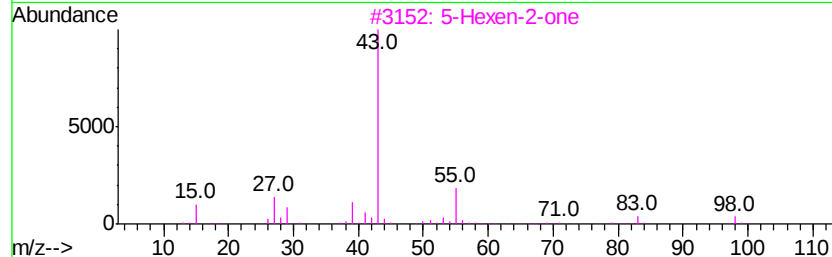
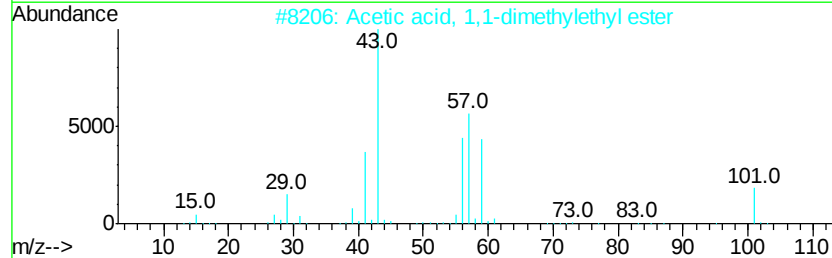
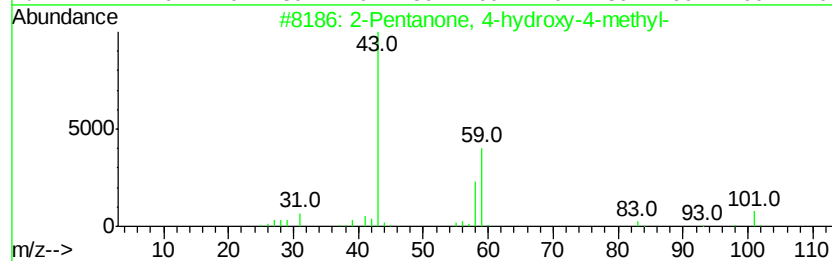
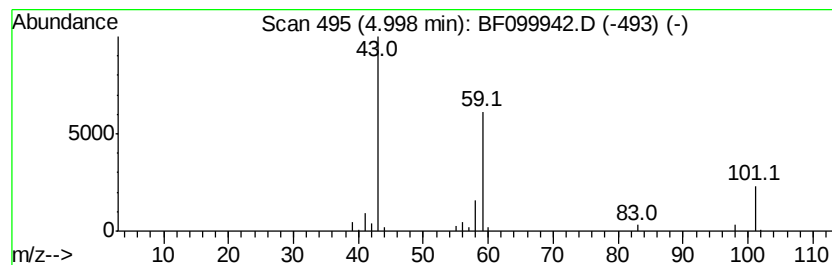
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.00	4.31 ng	124486	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



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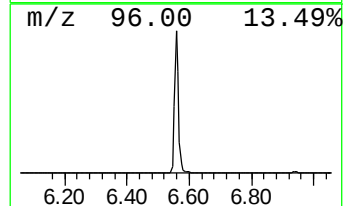
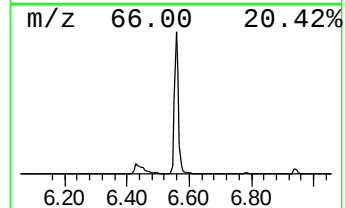
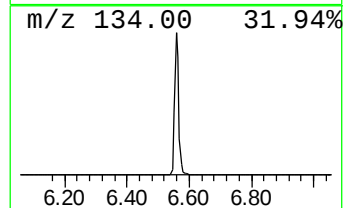
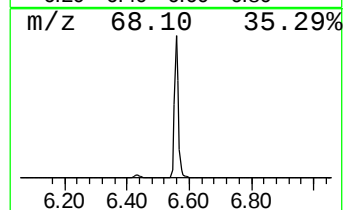
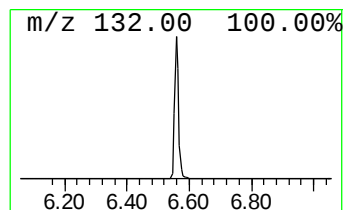
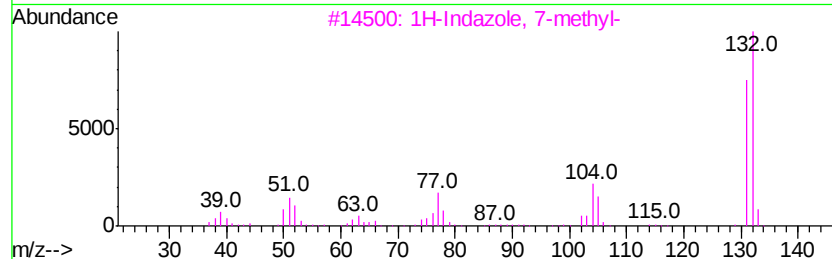
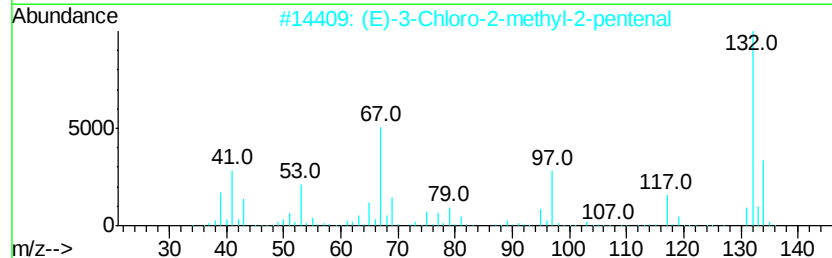
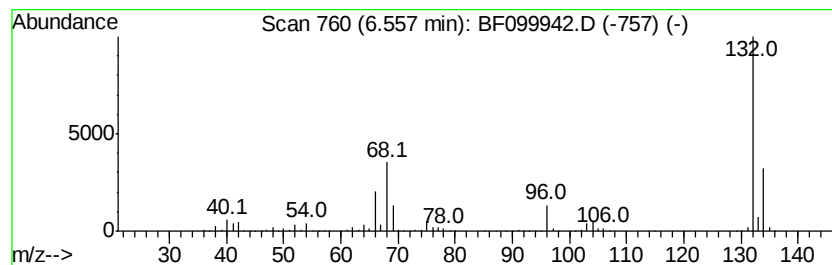
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	52.12 ng	1504370	1,4-Dichlorobenzene-d4	6.79

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	35
3		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
4		1-Aminoindan	133	C9H11N	034698-41-4	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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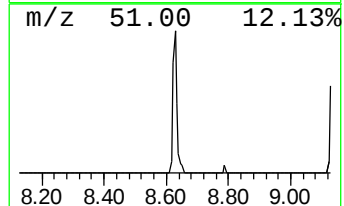
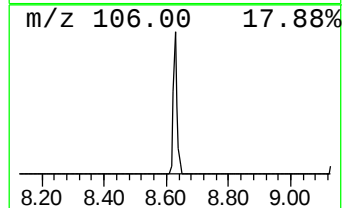
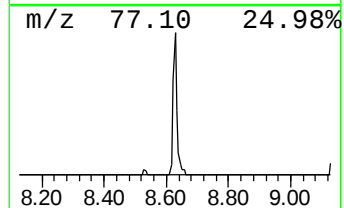
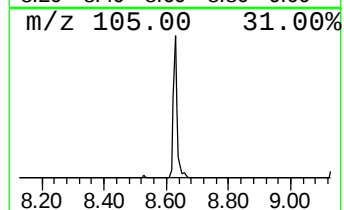
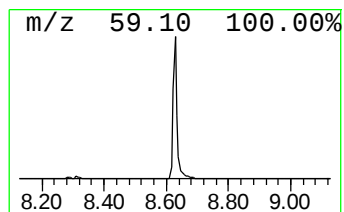
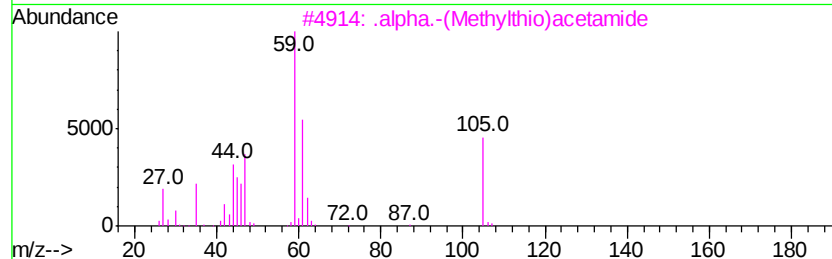
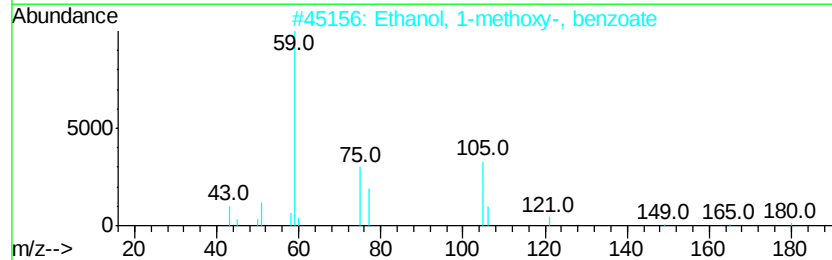
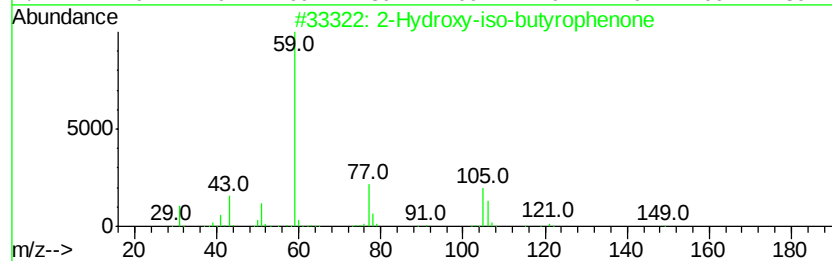
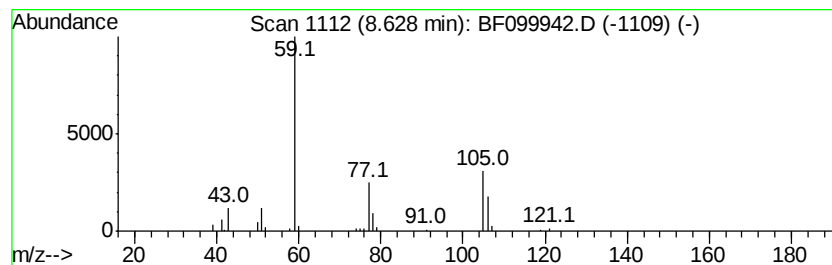
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Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.63	2.57 ng	98951	Napthalene-d8	8.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	83
2		Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	50
3		.alpha.-(Methylthio)acetamide	105	C3H7NOS	022551-24-2	7
4		Guanidine	59	CH5N3	000113-00-8	5
5		Acetamide	59	C2H5NO	000060-35-5	5



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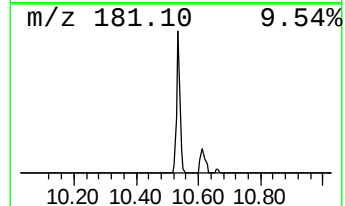
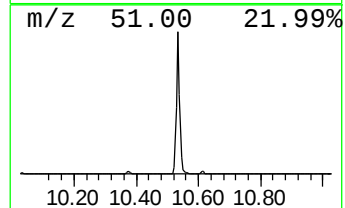
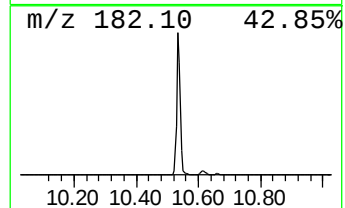
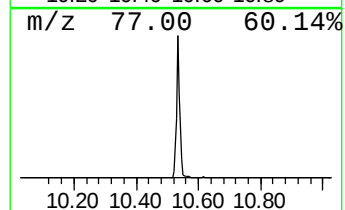
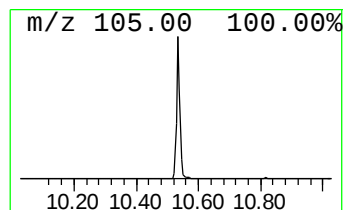
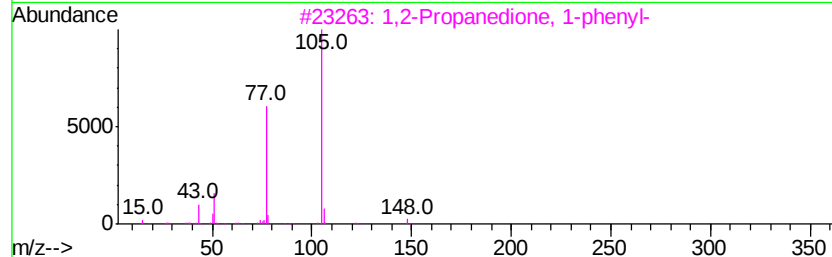
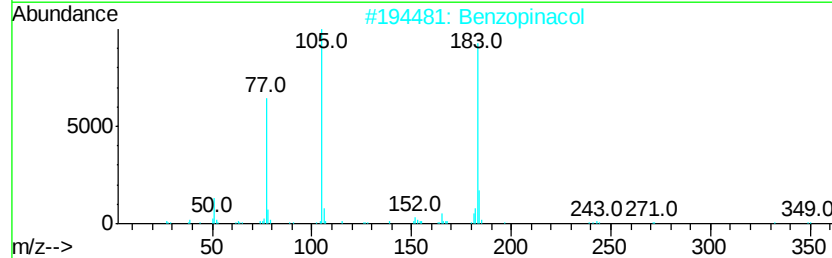
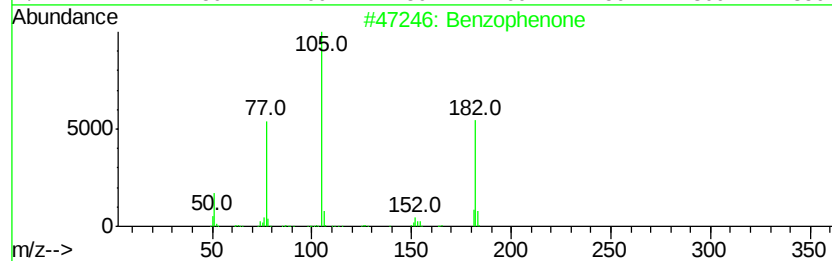
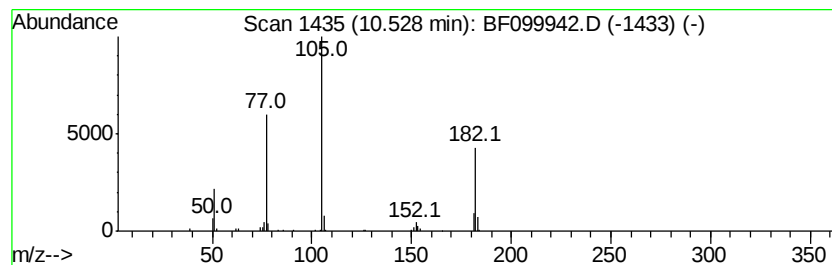
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.53	9.21 ng	358172	Acenaphthene-d10	9.82

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzophenone	182	C13H10O	000119-61-9	96
2		Benzopinacol	366	C26H22O2	000464-72-2	50
3		1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	43
4		Vinyl benzoate	148	C9H8O2	000769-78-8	43
5		Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	43



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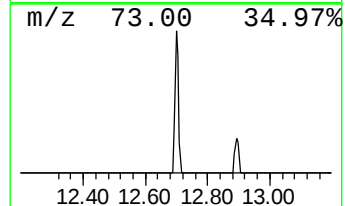
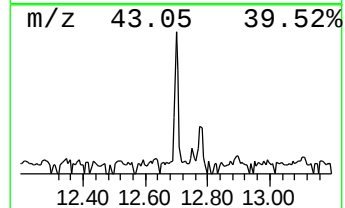
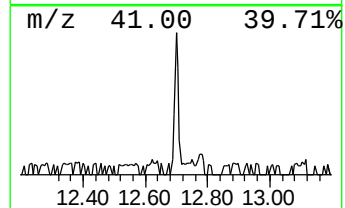
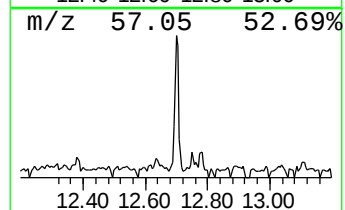
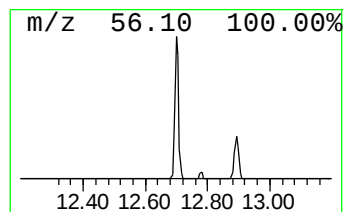
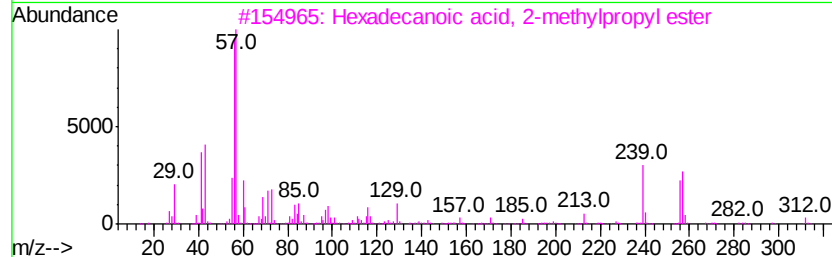
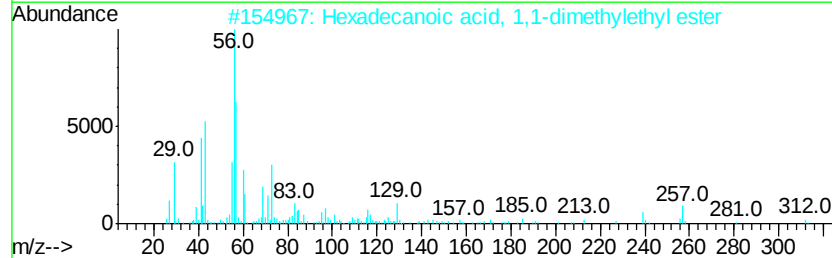
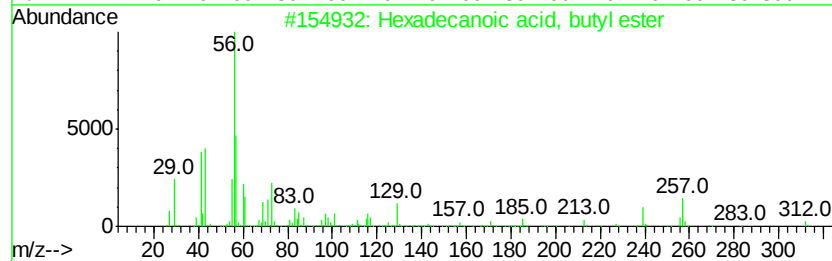
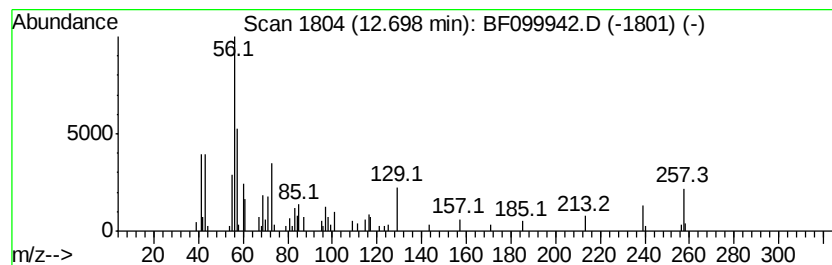
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Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	2.81 ng	70311	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	74
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	45
4		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5		1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.00	4.3	ng	124486	1	6.79	577307	20.0
unknown6.56	6.56	52.1	ng	1504370	1	6.79	577307	20.0
2-Hydroxy-iso-but...	8.63	2.6	ng	98951	2	8.07	768823	20.0
Benzophenone	10.53	9.2	ng	358172	3	9.82	777458	20.0
Hexadecanoic acid...	12.70	2.8	ng	70311	5	13.96	499580	20.0