

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112917\
 Data File : BF101009.D
 Acq On : 30 Nov 2017 6:36
 Operator : SJ/JU
 Sample : I6579-11
 Misc :
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HAR-2-E(7-8)

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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	5.087	507	510	525	rBB	71667	102704	6.74%	0.830%
2	5.481	572	577	580	rBV	1528769	1473725	96.75%	11.912%
3	6.492	743	749	762	rVB	1391701	1523300	100.00%	12.312%
4	6.628	767	772	775	rBV	1680225	1508891	99.05%	12.196%
5	6.851	807	810	814	rBV	391255	327487	21.50%	2.647%
6	7.010	833	837	840	rBV	1209578	1002038	65.78%	8.099%
7	7.422	901	907	910	rBV	899948	861348	56.54%	6.962%
8	8.133	1025	1028	1031	rBV	484141	401821	26.38%	3.248%
9	8.692	1119	1123	1126	rBV	85346	74515	4.89%	0.602%
10	9.210	1206	1211	1214	rBV	1526131	1212647	79.61%	9.801%
11	9.598	1274	1277	1281	rBV	70201	58252	3.82%	0.471%
12	9.892	1323	1327	1330	rBV	431153	370432	24.32%	2.994%
13	10.604	1444	1448	1451	rBV	371869	293227	19.25%	2.370%
14	10.680	1457	1461	1465	rBV	811264	714902	46.93%	5.778%
15	11.380	1576	1580	1582	rBV	366044	313176	20.56%	2.531%
16	11.404	1582	1584	1587	rVB	79357	62626	4.11%	0.506%
17	12.592	1783	1786	1789	rBV	110125	87206	5.72%	0.705%
18	12.821	1820	1825	1829	rBV	87589	91889	6.03%	0.743%
19	12.963	1845	1849	1852	rBV	1009443	828551	54.39%	6.697%
20	13.151	1872	1881	1884	rBV	24328	32719	2.15%	0.264%
21	13.216	1890	1892	1895	rBV	21643	17417	1.14%	0.141%
22	13.851	1998	2000	2007	rVB3	24967	26274	1.72%	0.212%
23	14.021	2024	2029	2032	rBV	417170	406188	26.67%	3.283%
24	14.045	2032	2033	2038	rVB	56825	39756	2.61%	0.321%
25	15.062	2202	2206	2213	rBV	42793	81563	5.35%	0.659%
26	15.368	2254	2258	2262	rBV	24423	34135	2.24%	0.276%
27	15.427	2265	2268	2274	rVB	37846	49080	3.22%	0.397%
28	15.492	2275	2279	2283	rBV	238863	292488	19.20%	2.364%
29	15.927	2350	2353	2359	rVB7	11388	17738	1.16%	0.143%
30	16.439	2435	2440	2443	rVB5	11479	17646	1.16%	0.143%
31	16.968	2527	2530	2538	rVB4	15330	26544	1.74%	0.215%
32	17.415	2602	2606	2610	rBV5	11842	21961	1.44%	0.178%

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ALS Vial : 36 Sample Multiplier: 1

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ClientSampleId :
HAR-2-E(7-8)

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-BF110817.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

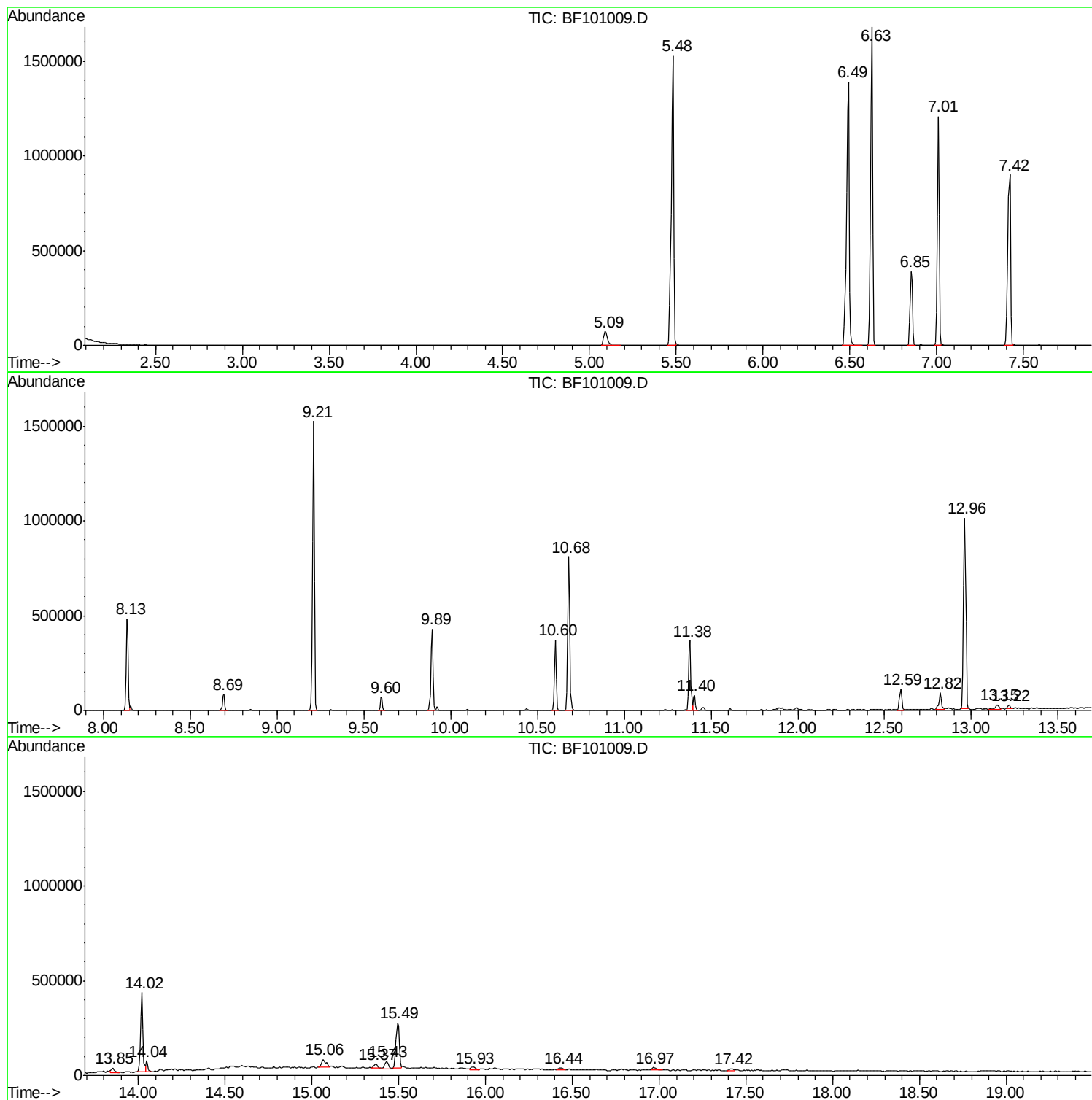
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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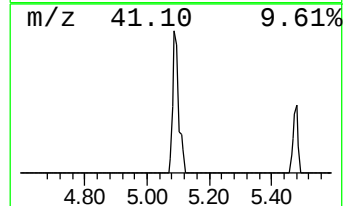
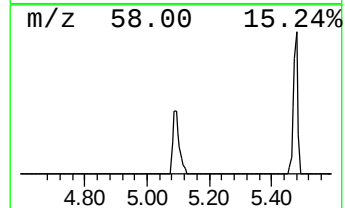
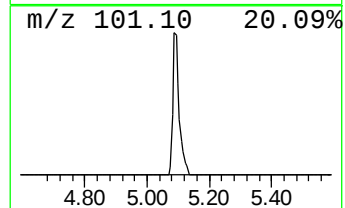
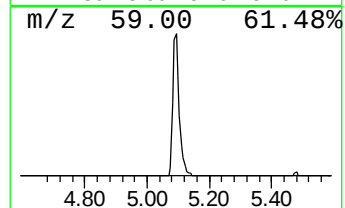
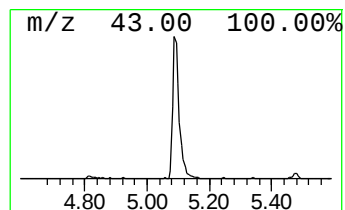
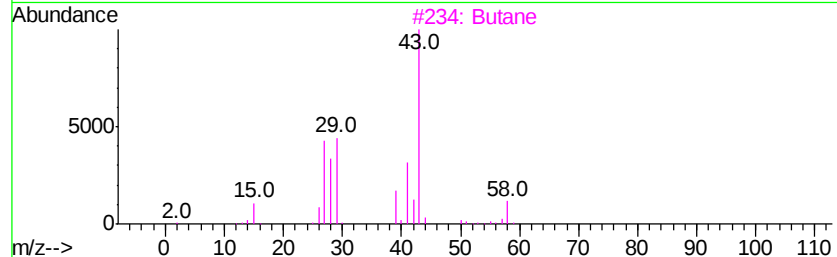
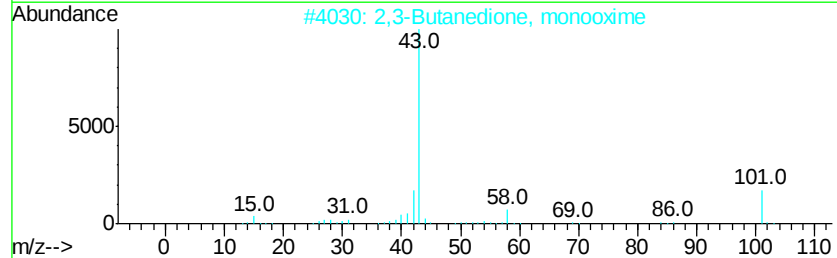
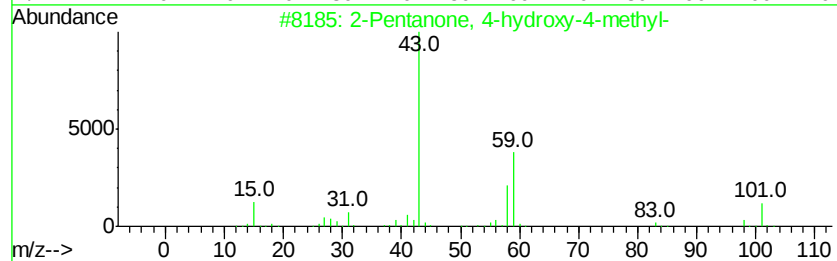
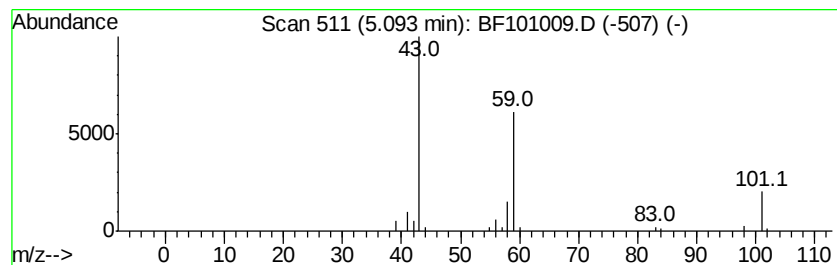
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	6.27 ng	102704	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Butane	58	C4H10	000106-97-8	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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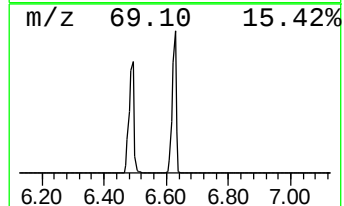
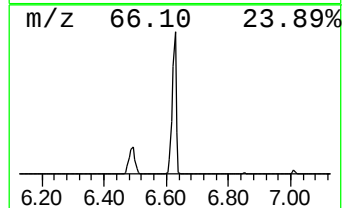
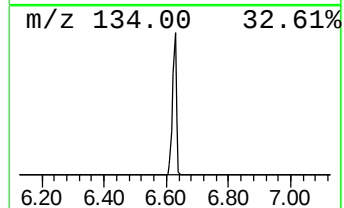
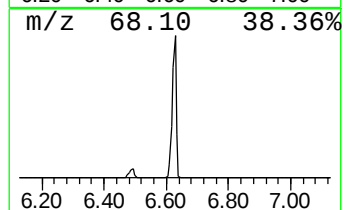
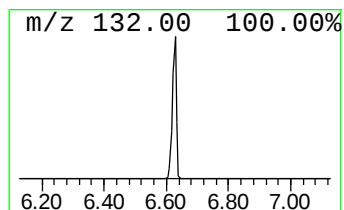
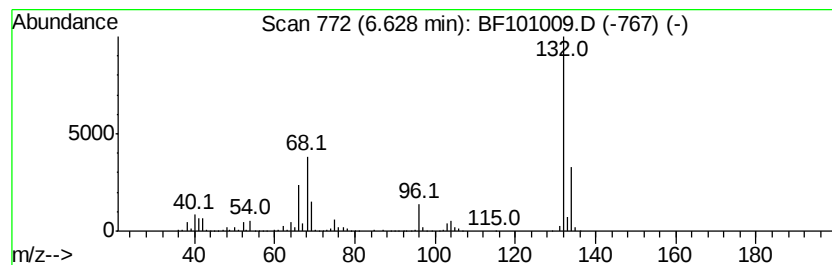
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	92.15 ng	1508890	1,4-Dichlorobenzene-d4	6.85

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		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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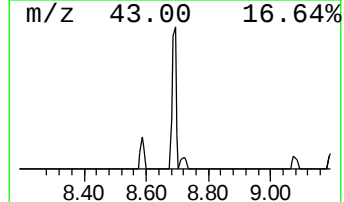
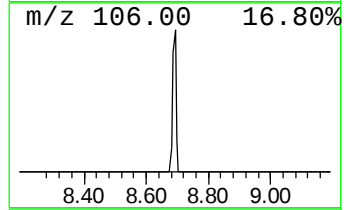
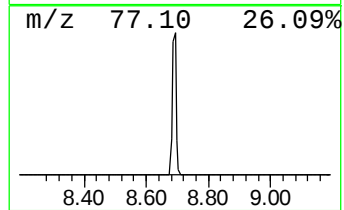
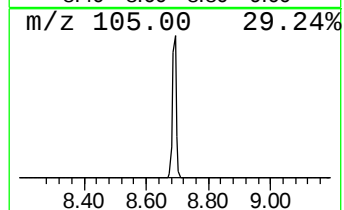
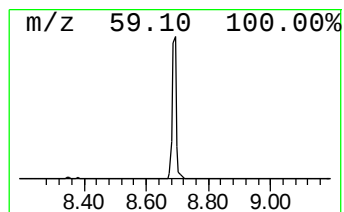
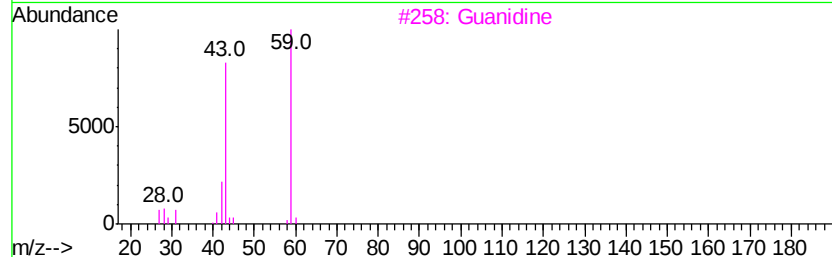
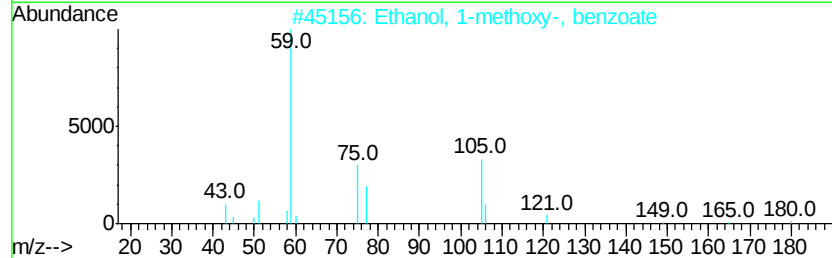
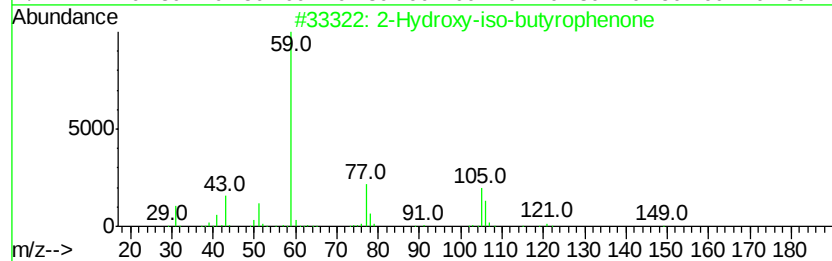
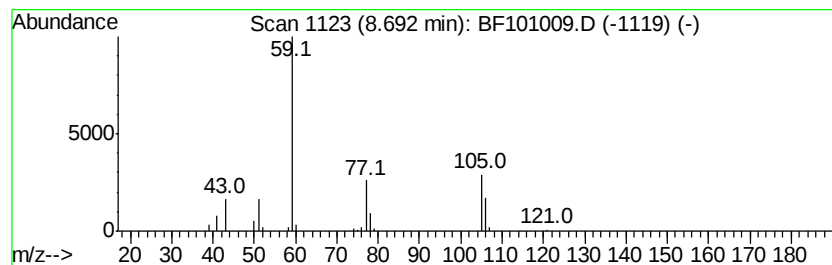
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.69	3.71 ng	74515	Napthalene-d8	8.13

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	59
3		Guanidine	59	CH5N3	000113-00-8	7
4		Acetamide	59	C2H5NO	000060-35-5	5
5		Propane, 2-methoxy-	74	C4H10O	000598-53-8	4



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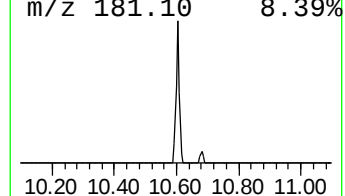
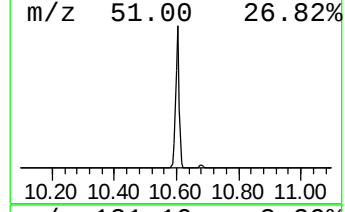
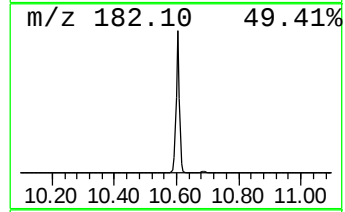
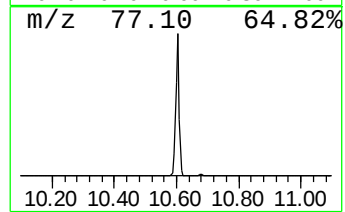
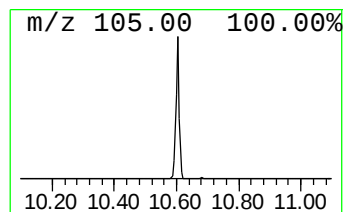
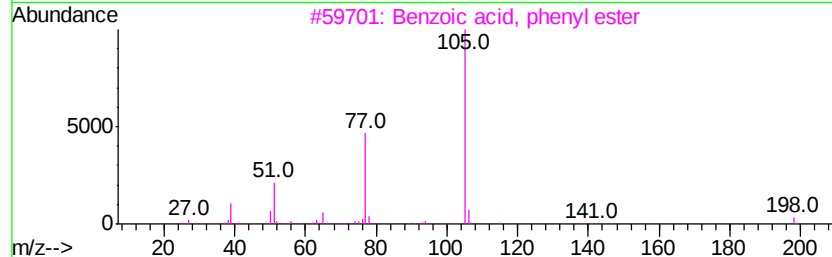
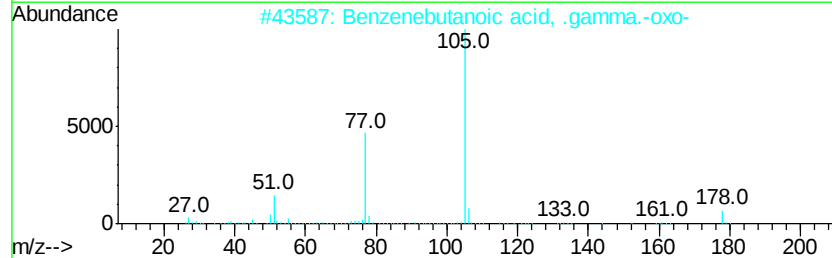
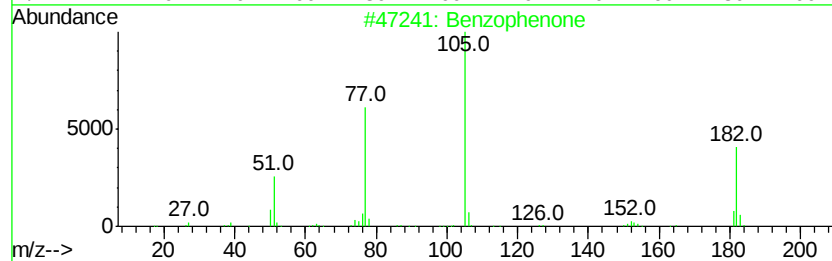
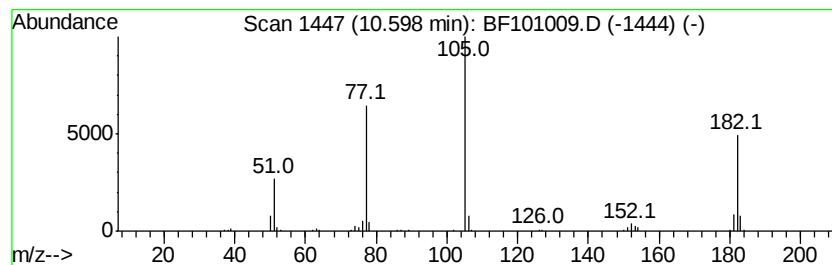
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	15.83 ng	293227	Acenaphthene-d10	9.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzophenone	182	C13H10O	000119-61-9	97
2		Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
3		Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	47
4		Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	47
5		1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47



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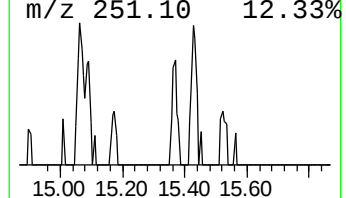
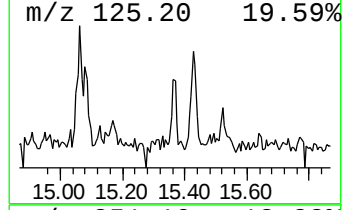
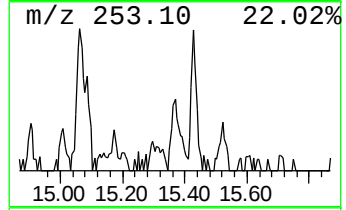
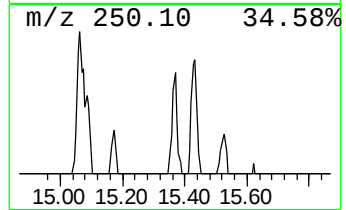
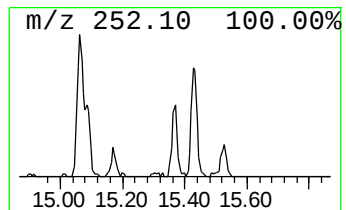
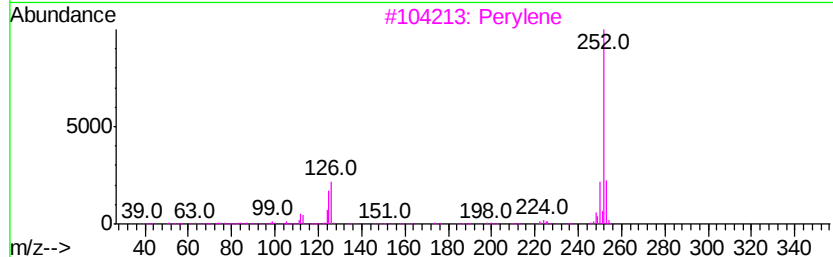
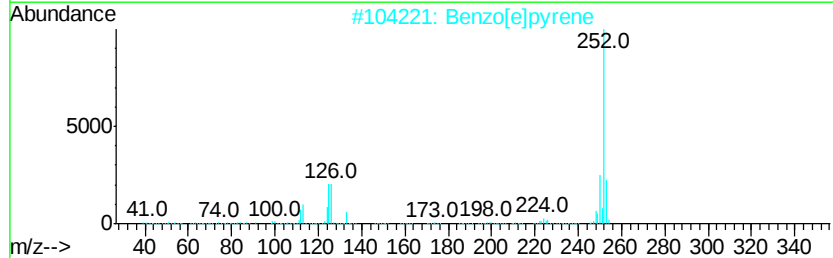
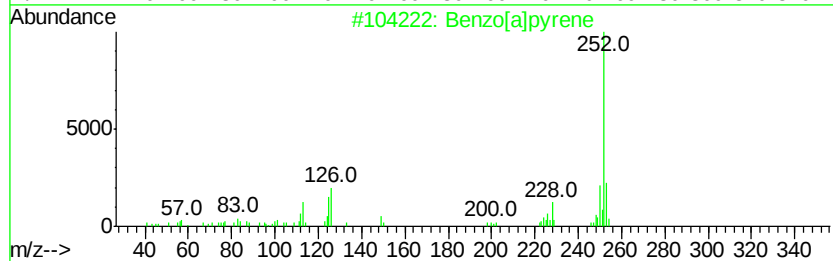
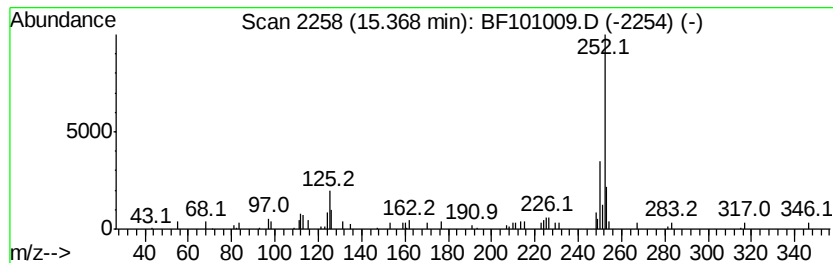
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzo[a]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.37	2.33 ng	34135	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[a]pyrene	252	C20H12	000050-32-8	90
2		Benzo[e]pyrene	252	C20H12	000192-97-2	81
3		Perylene	252	C20H12	000198-55-0	81
4		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	81
5		Benzo[j]fluoranthene	252	C20H12	000205-82-3	76



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.09	6.3	ng	102704	1	6.85	327487	20.0
unknown6.63	6.63	92.2	ng	1508890	1	6.85	327487	20.0
2-Hydroxy-iso-but...	8.69	3.7	ng	74515	2	8.13	401821	20.0
Benzophenone	10.60	15.8	ng	293227	3	9.89	370432	20.0
Benzo[a]pyrene	15.37	2.3	ng	34135	6	15.49	292488	20.0