

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061818\
 Data File : BF106534.D
 Acq On : 18 Jun 2018 13:18
 Operator : JU/SJ
 Sample : J3509-05
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MWHR2-6-061318

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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	5.195	482	486	496	rVB	115852	123789	3.45%	0.501%
2	5.607	553	556	568	rVB	1445866	1372482	38.29%	5.555%
3	6.601	722	725	732	rBV	902731	860738	24.01%	3.484%
4	6.742	745	749	752	rBV	2612829	2421832	67.57%	9.802%
5	6.966	783	787	790	rVB	894904	720568	20.10%	2.916%
6	7.125	809	814	817	rBV	2575388	2435081	67.94%	9.855%
7	7.531	877	883	886	rBV	2057157	2134584	59.55%	8.639%
8	8.248	1001	1005	1008	rBV	1090189	895037	24.97%	3.622%
9	8.801	1095	1099	1107	rVB	117546	100618	2.81%	0.407%
10	9.325	1183	1188	1191	rBV	3490354	3534368	98.60%	14.304%
11	9.713	1250	1254	1259	rBV	244910	205985	5.75%	0.834%
12	10.007	1300	1304	1308	rBV	1153383	1006741	28.09%	4.075%
13	10.377	1363	1367	1371	rBV	127098	104748	2.92%	0.424%
14	10.719	1421	1425	1429	rBV	432357	334127	9.32%	1.352%
15	10.801	1434	1439	1442	rBV	2246733	2215439	61.81%	8.966%
16	11.501	1554	1558	1561	rBV	1160475	1040751	29.04%	4.212%
17	13.089	1823	1828	1831	rBV	3408886	3584384	100.00%	14.507%
18	13.971	1975	1978	1983	rBV	58141	67652	1.89%	0.274%
19	14.154	2005	2009	2013	rBV	1026584	867664	24.21%	3.512%
20	15.707	2267	2273	2283	rVB	508599	681515	19.01%	2.758%

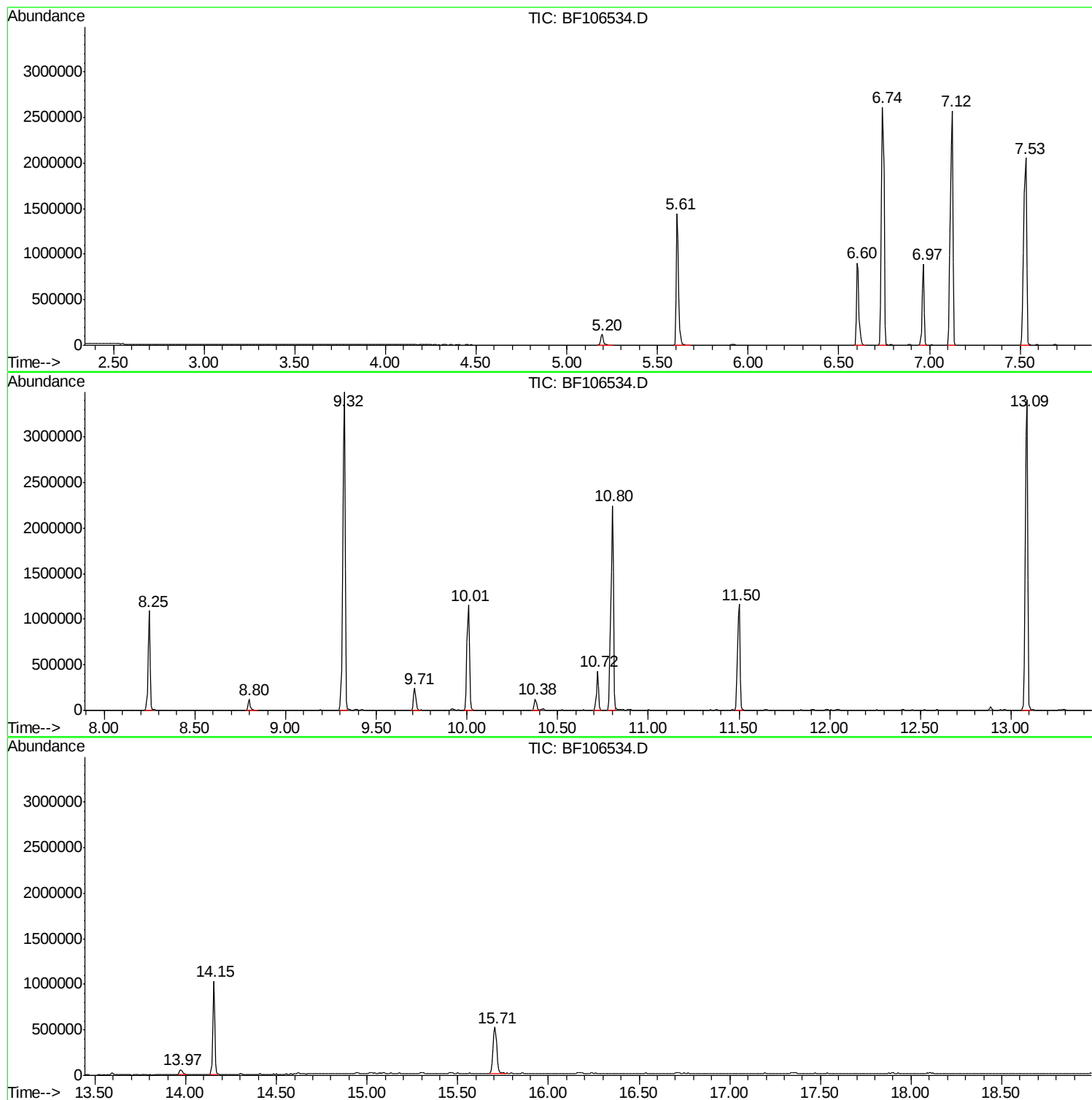
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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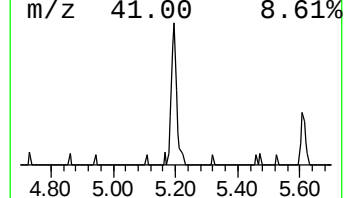
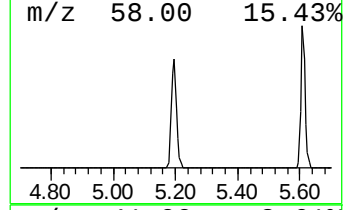
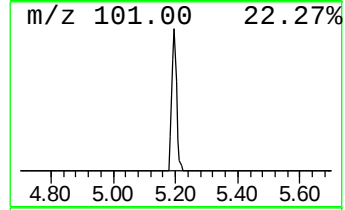
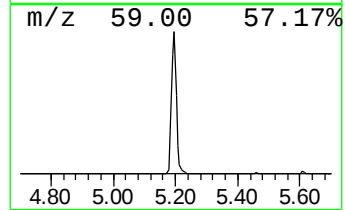
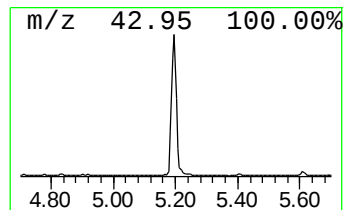
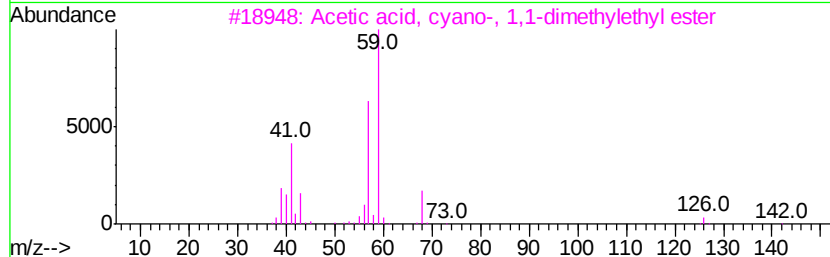
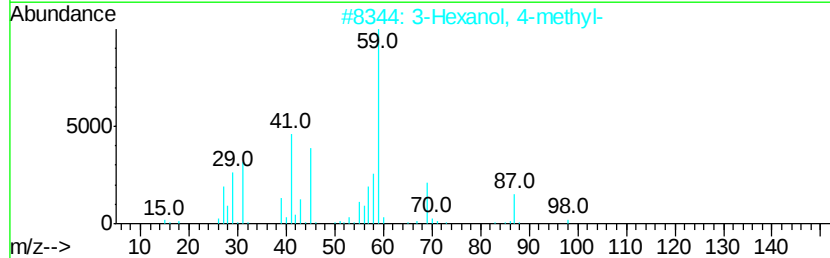
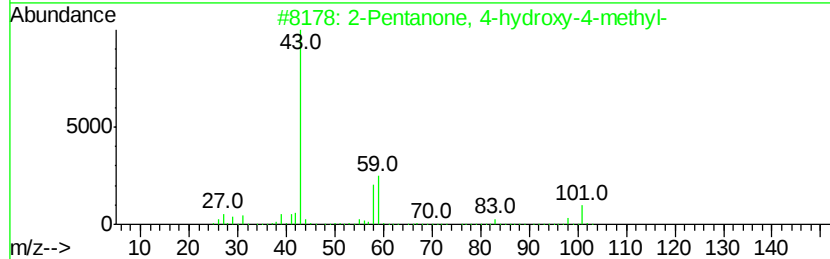
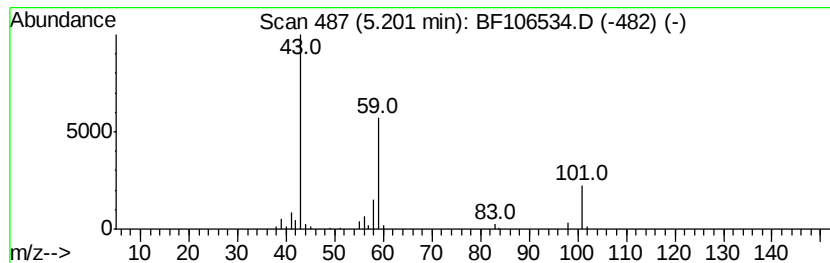
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.20	3.44 ng	123789	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
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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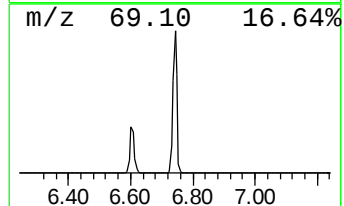
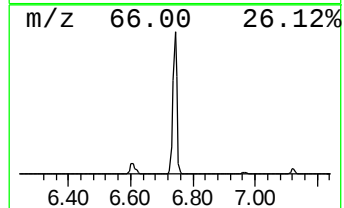
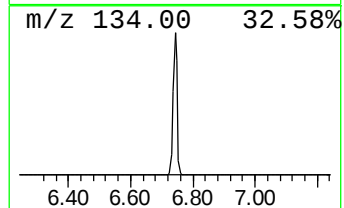
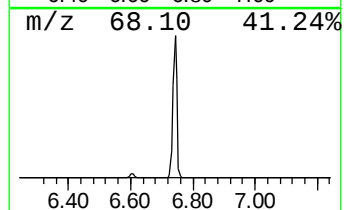
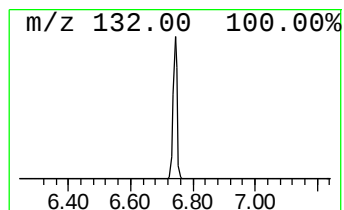
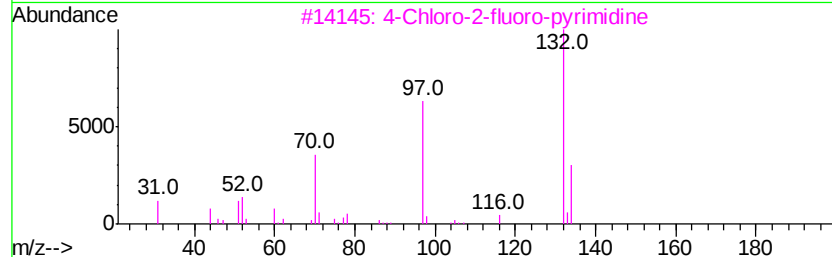
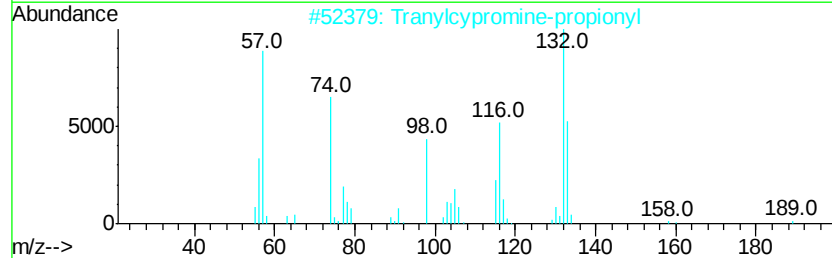
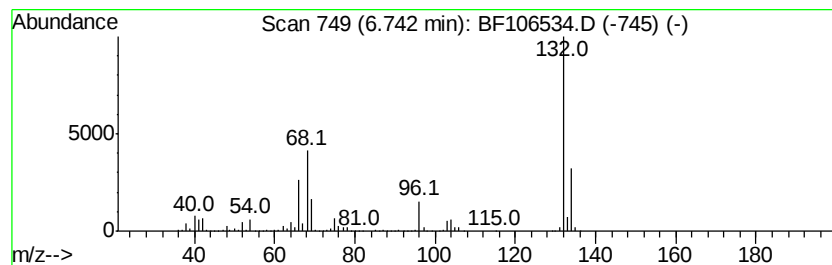
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.74 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	67.22 ng	2421830	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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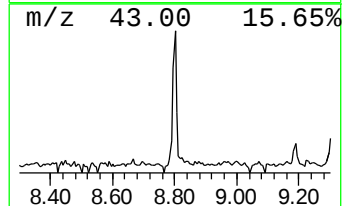
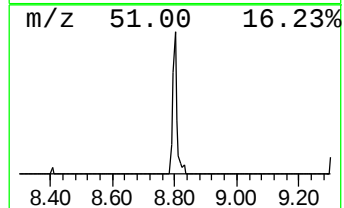
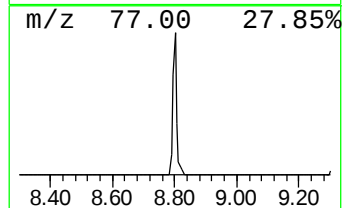
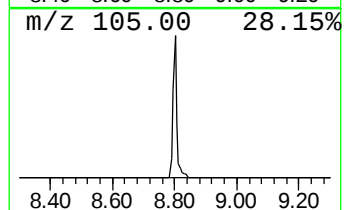
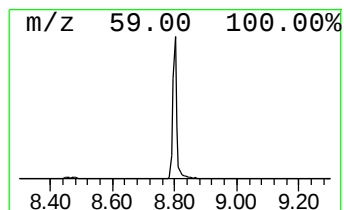
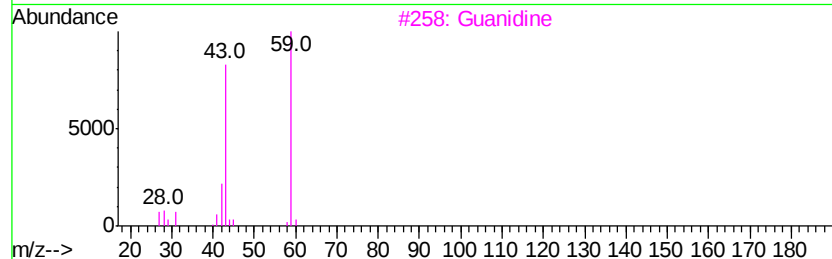
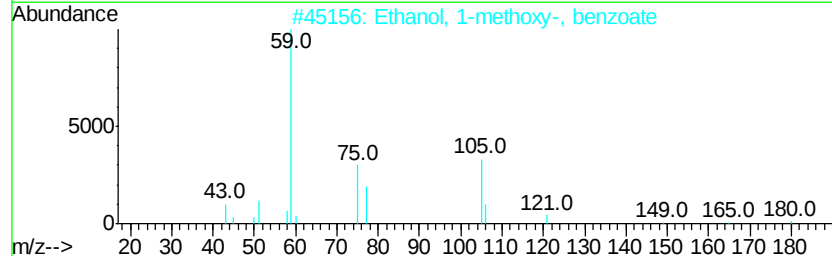
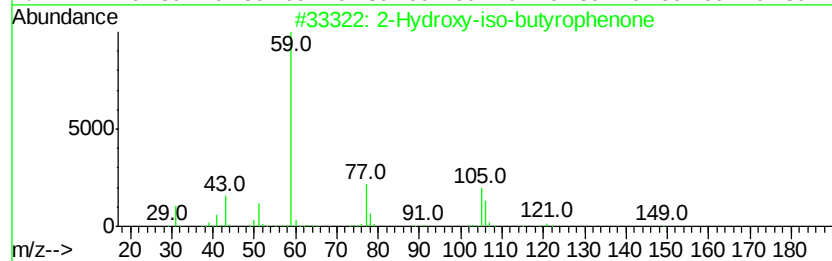
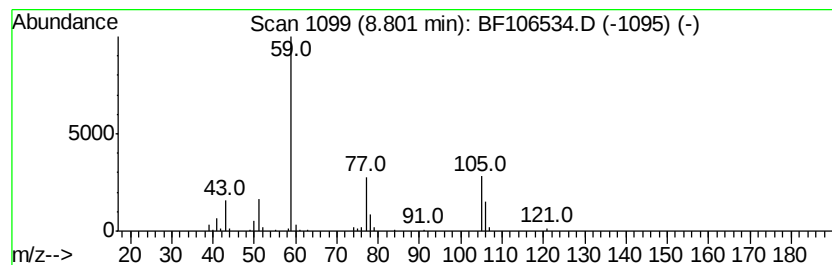
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Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.80	2.25 ng	100618	Napthalene-d8	8.25

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	56
3		Guanidine	59	CH5N3	000113-00-8	9
4		Propane, 2-methoxy-	74	C4H10O	000598-53-8	9
5		Acetic acid, chloro-, methyl ester	108	C3H5ClO2	000096-34-4	9



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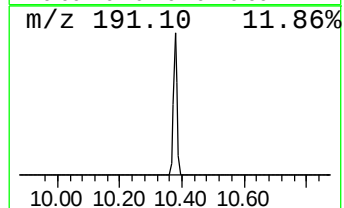
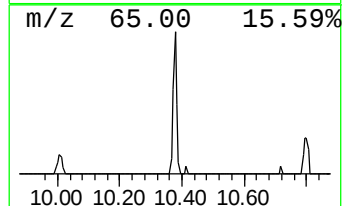
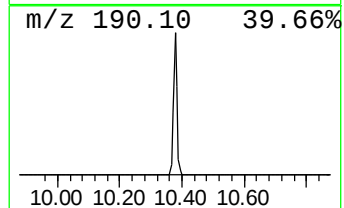
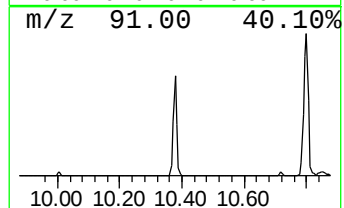
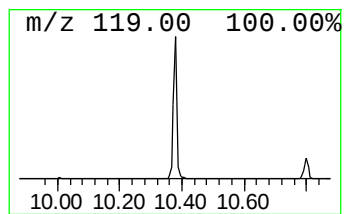
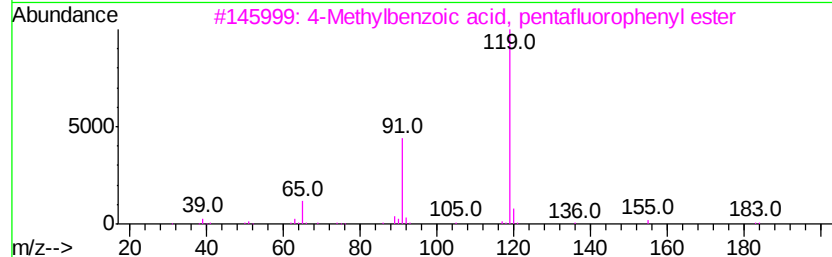
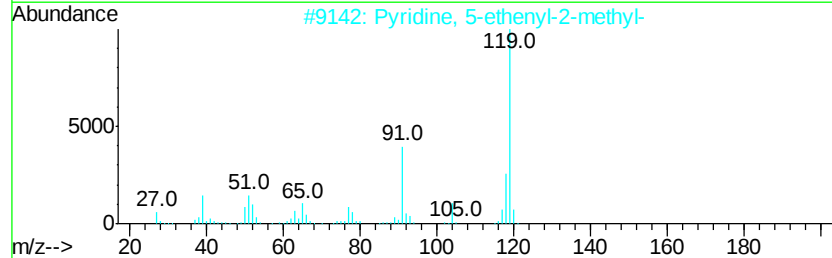
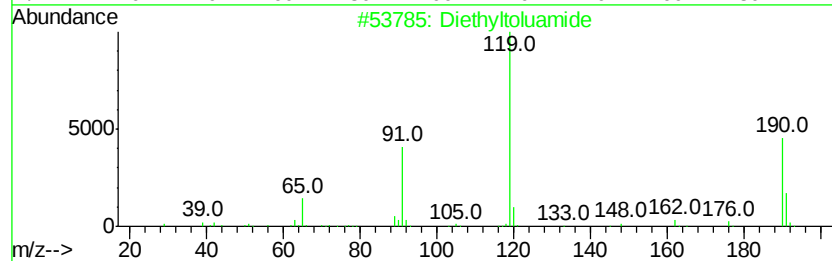
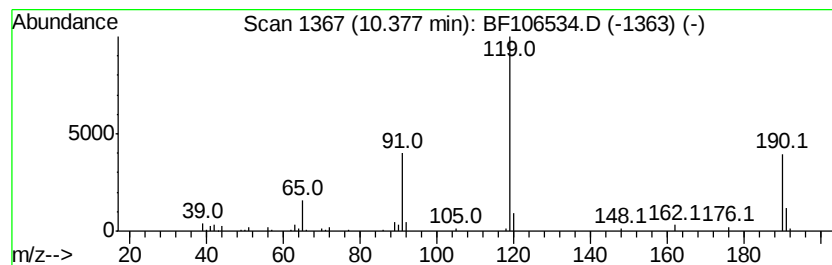
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Peak Number 5 Diethyltoluamide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.38	2.08 ng	104748	Acenaphthene-d10	10.01
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Diethyltoluamide	191 C12H17NO	000134-62-3 97
2		Pyridine, 5-ethenyl-2-methyl-	119 C8H9N	000140-76-1 52
3		4-Methylbenzoic acid, pentafluor...	302 C14H7F5O2	1000354-15-1 52
4		Benzoic acid, 4-methyl-, 1-methy...	192 C12H16O2	100556-51-2 50
5		Benzhydrazide, 4-methyl-N2-[1-me...	303 C12H13N7O3	324021-25-2 50



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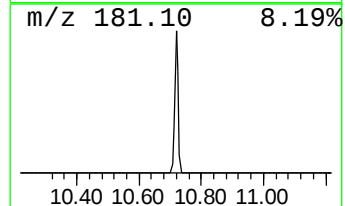
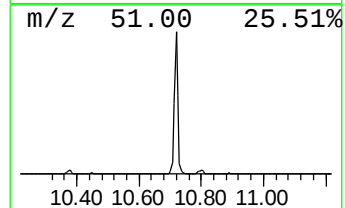
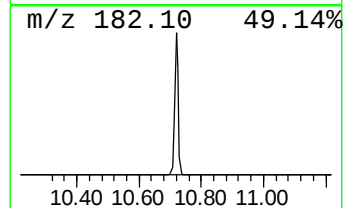
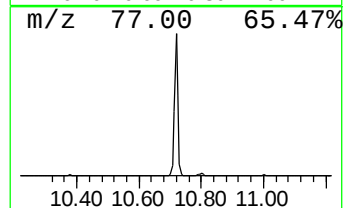
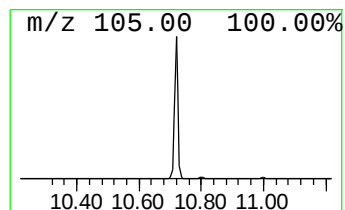
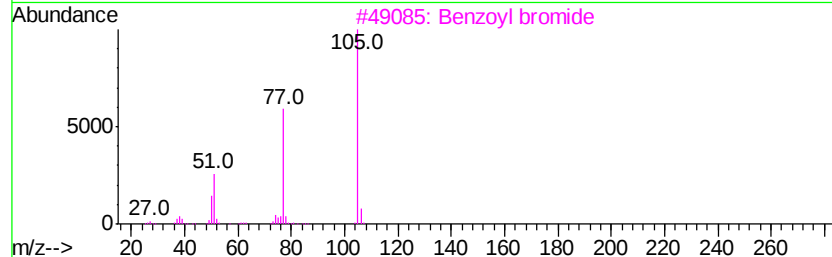
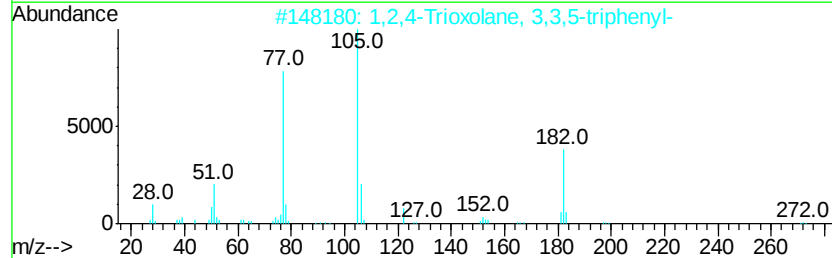
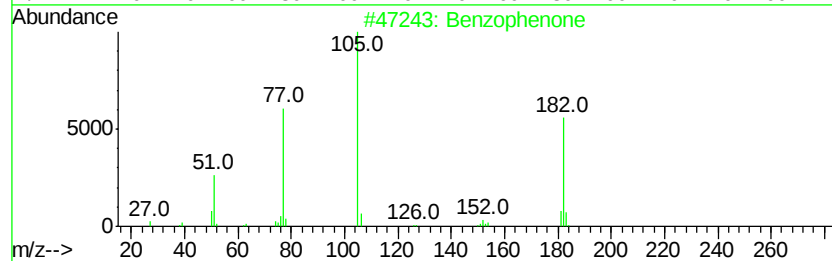
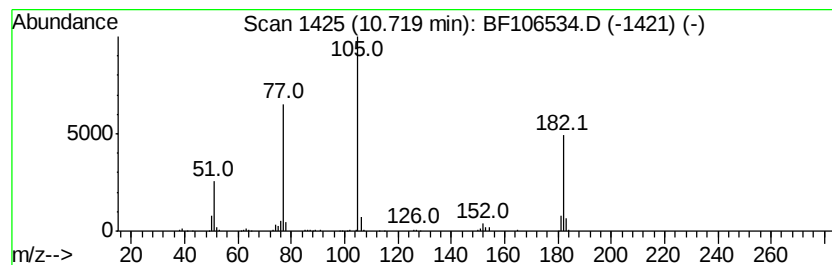
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	6.64 ng	334127	Acenaphthene-d10	10.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzophenone	182	C13H10O	000119-61-9	96
2		1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	72
3		Benzoyl bromide	184	C7H5BrO	000618-32-6	47
4		Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
5		1-Butanone, 1-phenyl-	148	C10H12O	000495-40-9	47



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.20	3.4	ng	123789	1	6.97	720568	20.0
unknown6.74	6.74	67.2	ng	2421830	1	6.97	720568	20.0
2-Hydroxy-iso-but...	8.80	2.3	ng	100618	2	8.25	895037	20.0
Diethyltoluamide	10.38	2.1	ng	104748	3	10.01	1006740	20.0
Benzophenone	10.72	6.6	ng	334127	3	10.01	1006740	20.0