

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061818\
 Data File : BF106528.D
 Acq On : 18 Jun 2018 10:29
 Operator : JU/SJ
 Sample : J3509-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MWHR3-8-061318

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	5.196	482	486	492	rBV	104444	109425	2.87%	0.421%
2	5.613	553	557	565	rBV	1380834	1414537	37.10%	5.440%
3	6.607	722	726	734	rBV	1003408	925886	24.28%	3.560%
4	6.743	745	749	753	rBV	2572184	2429159	63.71%	9.341%
5	6.966	783	787	790	rBV	918576	730828	19.17%	2.810%
6	7.125	809	814	817	rBV	2556152	2386388	62.59%	9.177%
7	7.531	877	883	886	rBV	2069600	2108878	55.31%	8.110%
8	8.248	1001	1005	1008	rBV	1113261	921117	24.16%	3.542%
9	8.801	1095	1099	1102	rBV	127672	109552	2.87%	0.421%
10	9.325	1183	1188	1191	rBV	3457907	3553048	93.19%	13.663%
11	9.713	1250	1254	1257	rBV	360843	285494	7.49%	1.098%
12	10.007	1300	1304	1311	rVB2	1225706	1069486	28.05%	4.113%
13	10.719	1421	1425	1429	rBV	453620	360109	9.44%	1.385%
14	10.801	1434	1439	1443	rBV	2219906	2288750	60.03%	8.801%
15	11.430	1543	1546	1550	rBV	42635	38246	1.00%	0.147%
16	11.501	1553	1558	1561	rBV	1284382	1175240	30.82%	4.519%
17	11.695	1587	1591	1594	rBV	51310	41978	1.10%	0.161%
18	11.866	1618	1620	1623	rBV	116926	98591	2.59%	0.379%
19	11.907	1623	1627	1630	rVB3	31933	40789	1.07%	0.157%
20	12.289	1688	1692	1698	rBV	137740	123796	3.25%	0.476%
21	13.089	1823	1828	1831	rBV	3570798	3812838	100.00%	14.662%
22	13.971	1975	1978	1981	rBV	45900	48407	1.27%	0.186%
23	14.154	2005	2009	2013	rBV	1047160	1001205	26.26%	3.850%
24	14.313	2033	2036	2041	rVB5	30252	40684	1.07%	0.156%
25	14.548	2072	2076	2081	rBV6	23166	39338	1.03%	0.151%
26	14.671	2094	2097	2101	rBV3	31947	44514	1.17%	0.171%
27	15.707	2267	2273	2281	rBV	626453	806532	21.15%	3.101%

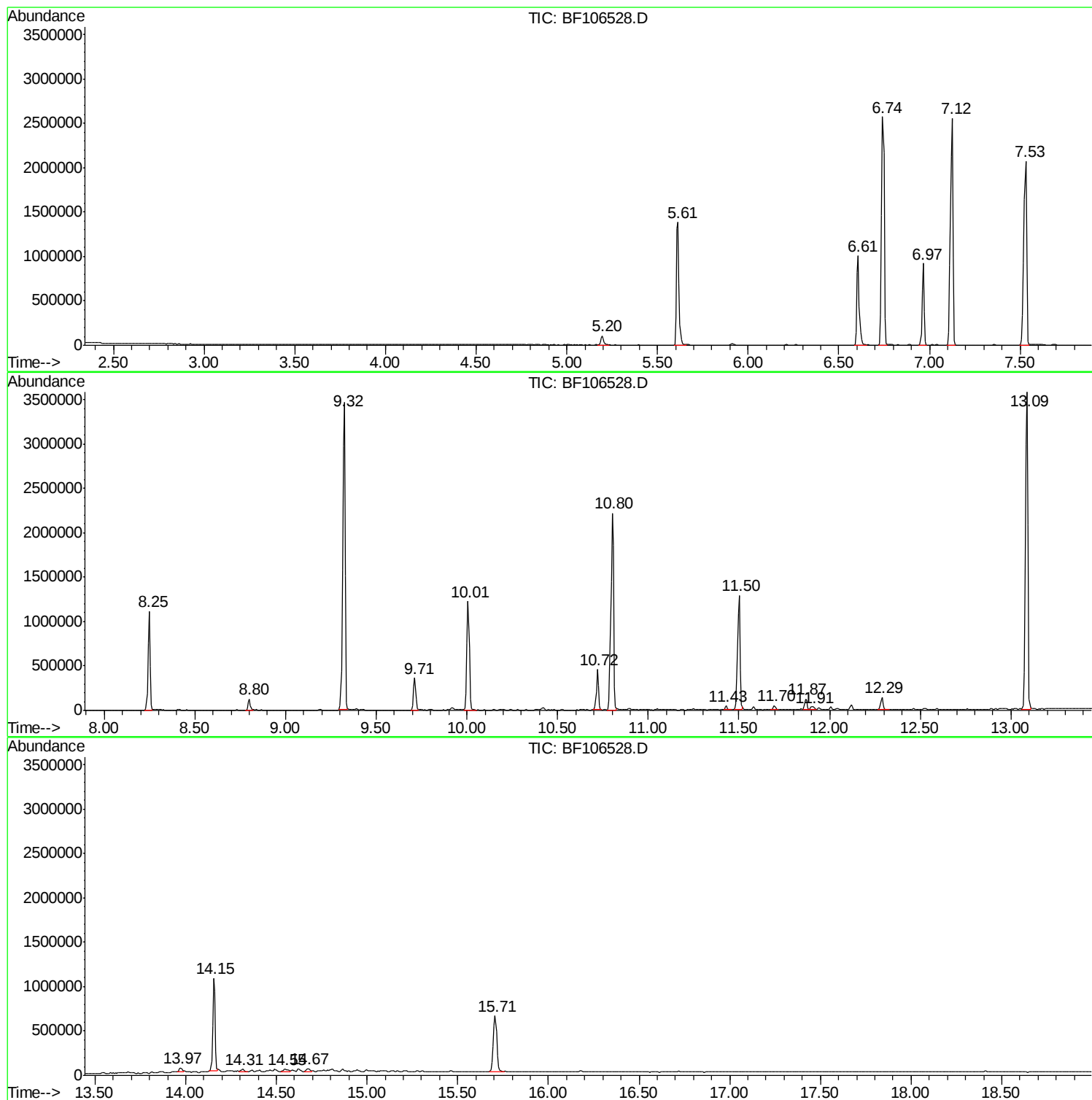
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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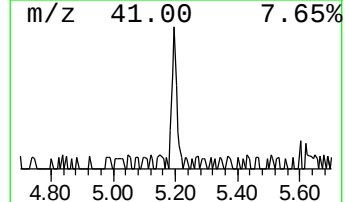
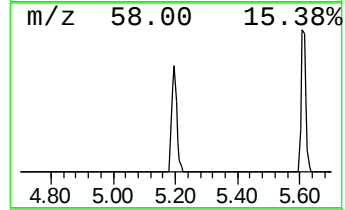
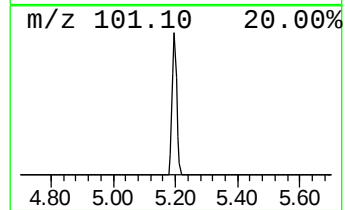
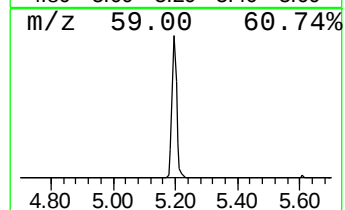
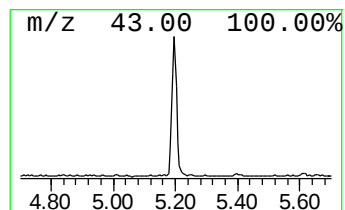
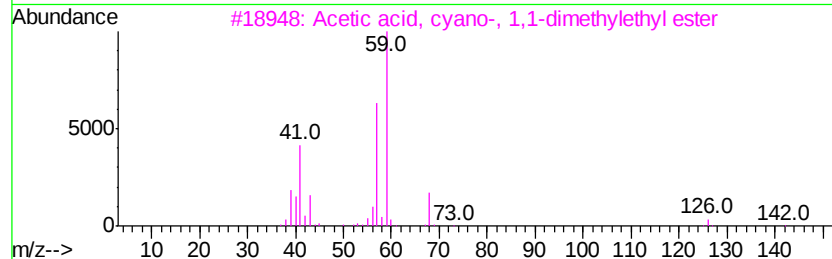
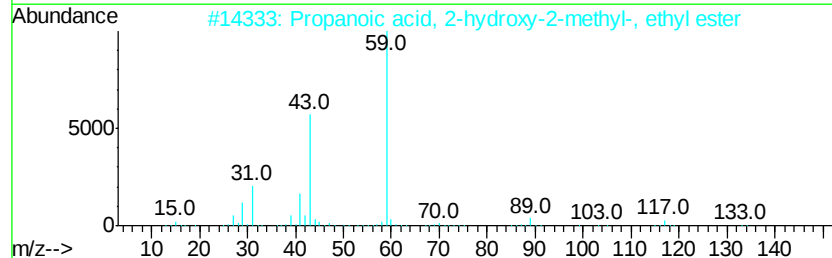
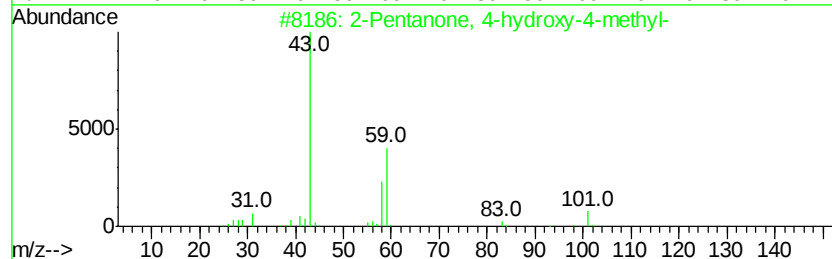
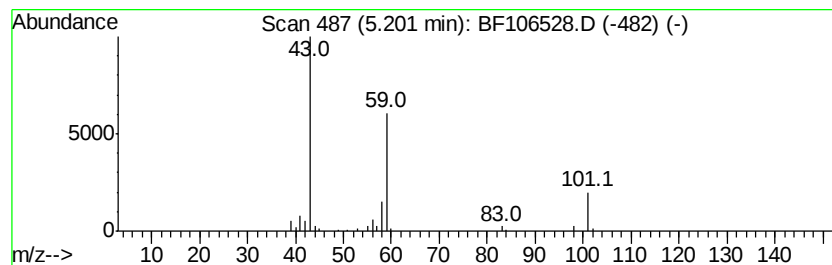
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.20	2.99 ng	109425	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	45
2	Propanoic acid, 2-hydroxy-2-meth...	132	C6H12O3	000080-55-7	25
3	Acetic acid, cyano-, 1,1-dimethv...	141	C7H11NO2	001116-98-9	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9



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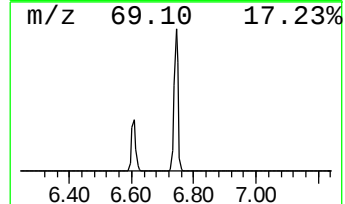
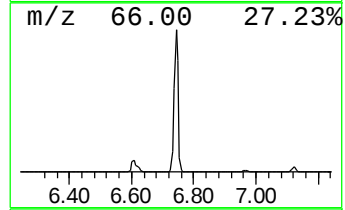
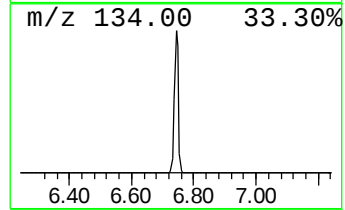
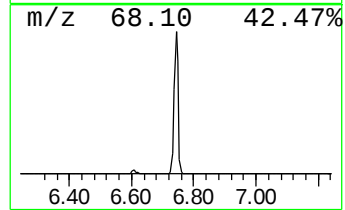
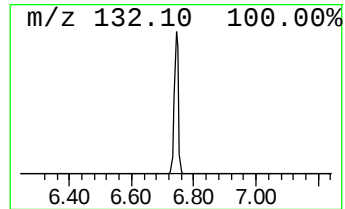
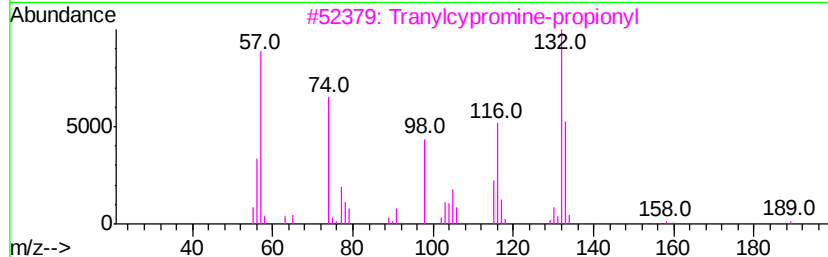
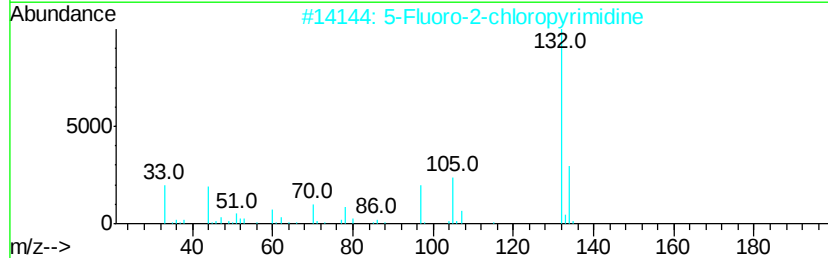
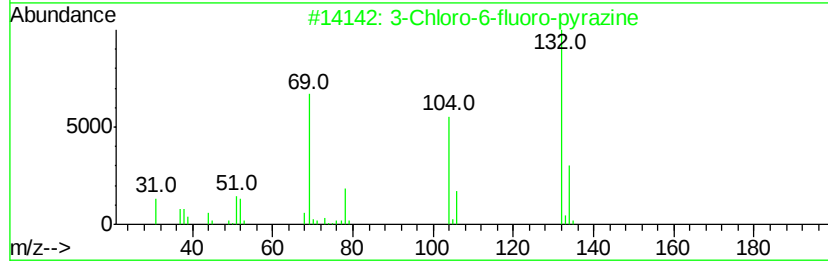
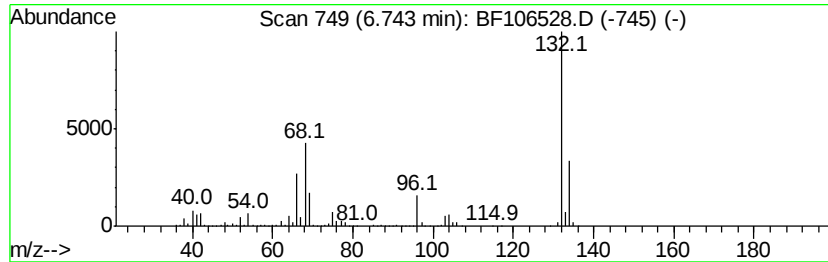
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Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	66.48 ng	2429160	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		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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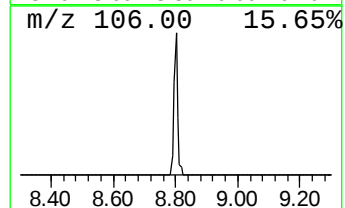
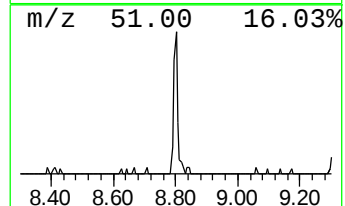
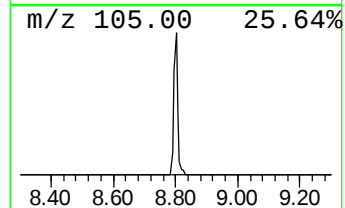
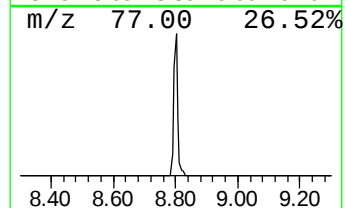
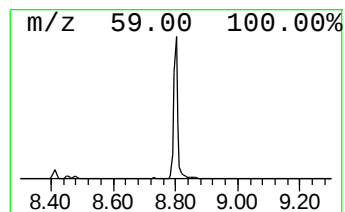
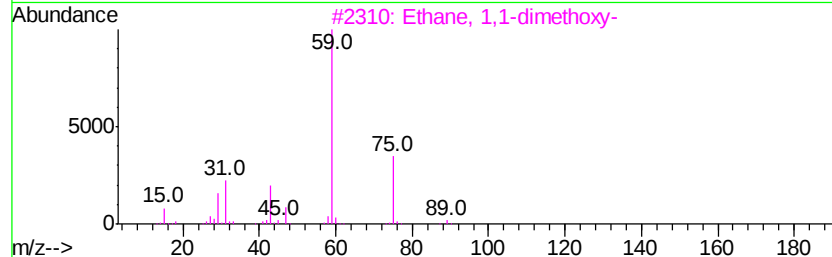
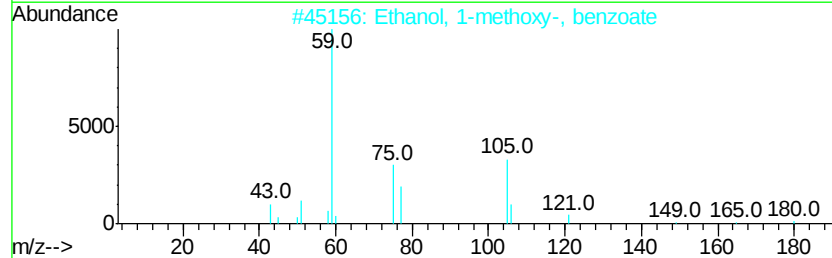
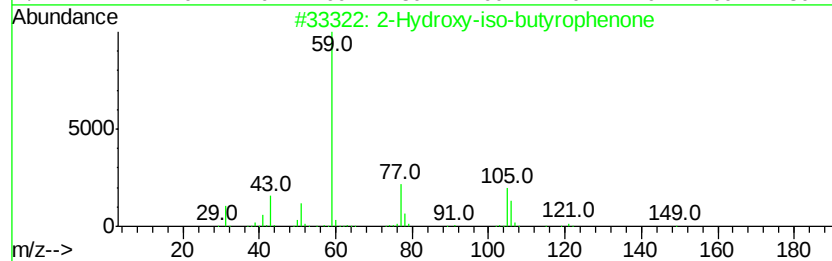
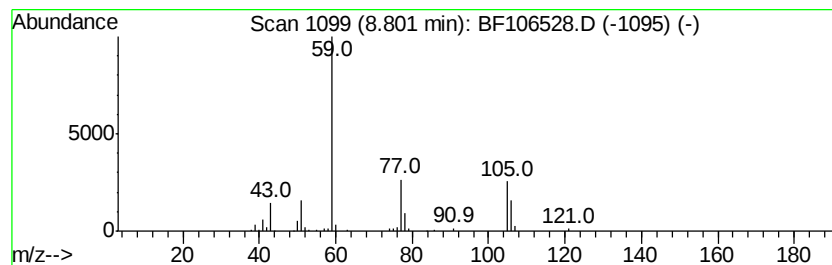
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.80	2.38 ng	109552	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	59
3		Ethane, 1,1-dimethoxy-	90	C4H10O2	000534-15-6	9
4		Acetic acid, chloro-, methyl ester	108	C3H5ClO2	000096-34-4	9
5		Propionic acid, 2-isopropoxy-, m...	146	C7H14O3	1000151-15-1	9



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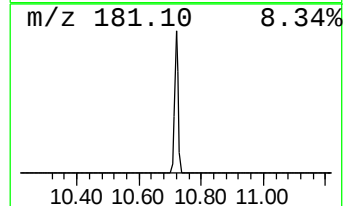
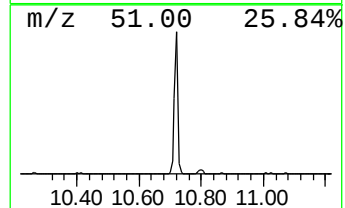
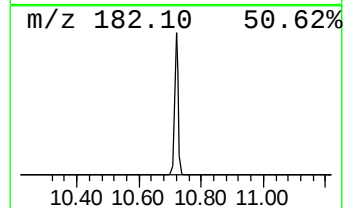
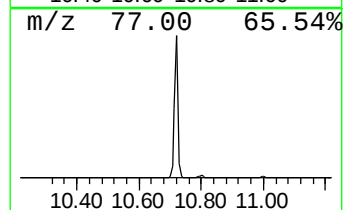
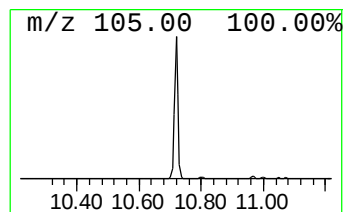
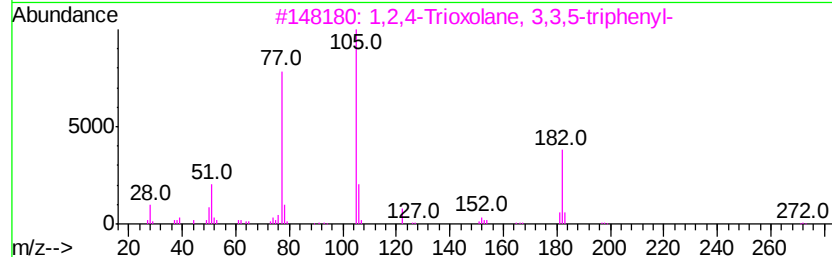
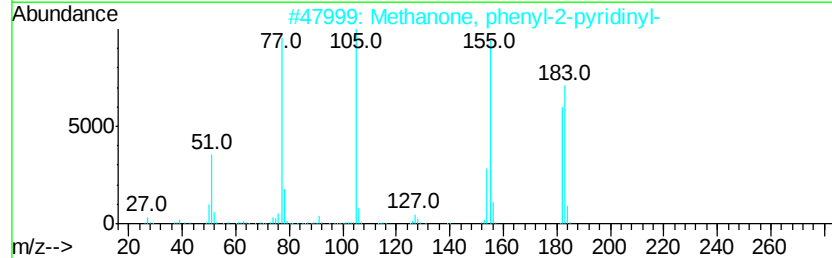
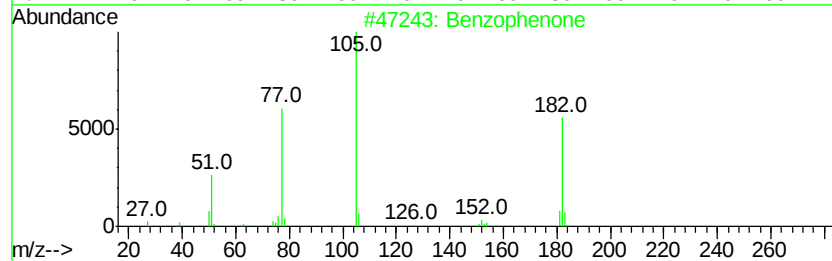
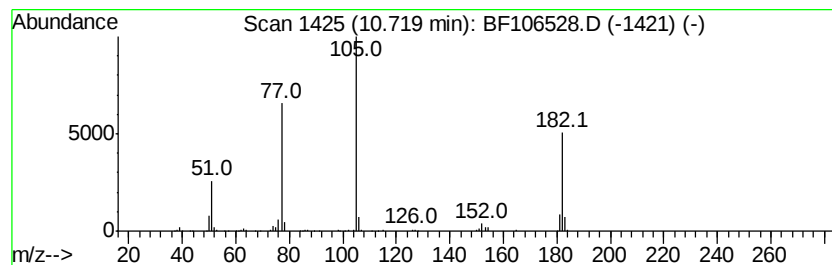
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Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	6.73 ng	360109	Acenaphthene-d10	10.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzophenone	182	C13H10O	000119-61-9	96
2		Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	72
3		1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	72
4		Benzilamide	227	C14H13NO2	004746-87-6	50
5		Vinyl benzoate	148	C9H8O2	000769-78-8	47



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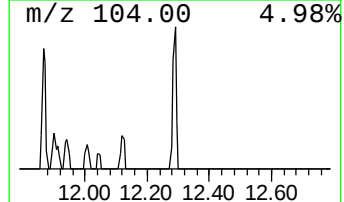
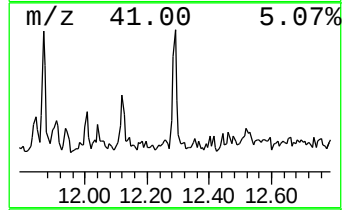
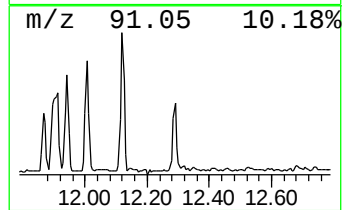
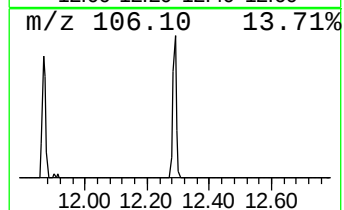
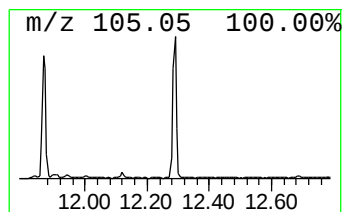
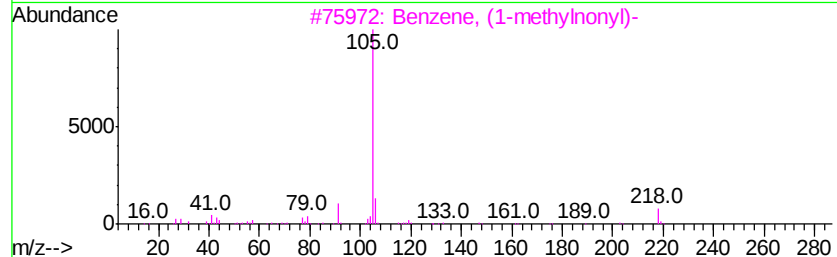
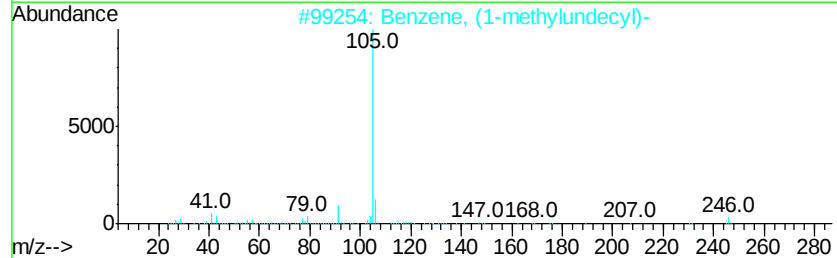
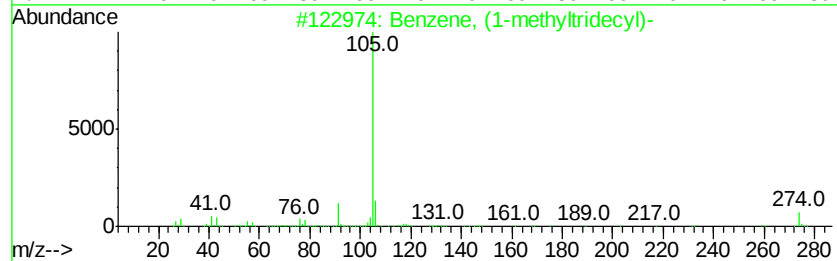
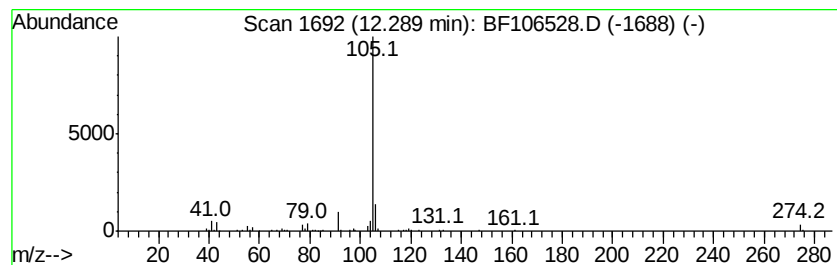
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Benzene, (1-methyltridecyl)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	2.11 ng	123796	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, (1-methyltridecyl)-	274	C20H34	004534-59-2	72
2		Benzene, (1-methylundecyl)-	246	C18H30	002719-61-1	72
3		Benzene, (1-methylnonyl)-	218	C16H26	004537-13-7	64
4		Benzene, (1-methyldodecyl)-	260	C19H32	004534-53-6	64
5		Benzene, (1-methyldecyl)-	232	C17H28	004536-88-3	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.20	3.0	ng	109425	1	6.97	730828	20.0
unknown6.74	6.74	66.5	ng	2429160	1	6.97	730828	20.0
2-Hydroxy-iso-but...	8.80	2.4	ng	109552	2	8.25	921117	20.0
Benzophenone	10.72	6.7	ng	360109	3	10.01	1069490	20.0
Benzene, (1-methy...	12.29	2.1	ng	123796	4	11.50	1175240	20.0