

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062321\
 Data File : BG049063.D
 Acq On : 23 Jun 2021 16:06
 Operator : CG/JU
 Sample : M2748-07
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-8A

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049063.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.157	13	20	29	rBV2	53485	124289	6.01%	1.455%
2	3.234	29	33	39	rVB4	15379	30535	1.48%	0.357%
3	5.190	359	366	375	rBV	33979	58571	2.83%	0.686%
4	5.660	437	446	455	rBV	388800	649488	31.39%	7.602%
5	7.258	710	718	728	rBV	405056	696051	33.64%	8.147%
6	8.104	856	862	870	rBV	100618	171084	8.27%	2.002%
7	9.274	1054	1061	1068	rBV	244700	443820	21.45%	5.195%
8	10.930	1330	1343	1350	rBV	124903	230706	11.15%	2.700%
9	13.369	1751	1758	1766	rBV	613780	962813	46.54%	11.269%
10	14.744	1986	1992	2000	rBV	193011	317841	15.36%	3.720%
11	15.537	2122	2127	2133	rBV	48739	66876	3.23%	0.783%
12	16.236	2239	2246	2257	rBV	540572	875463	42.32%	10.247%
13	17.499	2454	2461	2469	rBV	269924	435693	21.06%	5.099%
14	18.375	2603	2610	2616	rBV6	18456	31755	1.53%	0.372%
15	20.102	2898	2904	2913	rVB	1555386	2068817	100.00%	24.214%
16	21.412	3123	3127	3139	rVB6	45650	106953	5.17%	1.252%
17	21.782	3184	3190	3198	rBV2	322367	563667	27.25%	6.597%
18	22.828	3362	3368	3369	rBV5	13161	23358	1.13%	0.273%
19	22.999	3392	3397	3402	rBV4	35390	77785	3.76%	0.910%
20	25.108	3744	3756	3769	rBV2	189873	608330	29.40%	7.120%

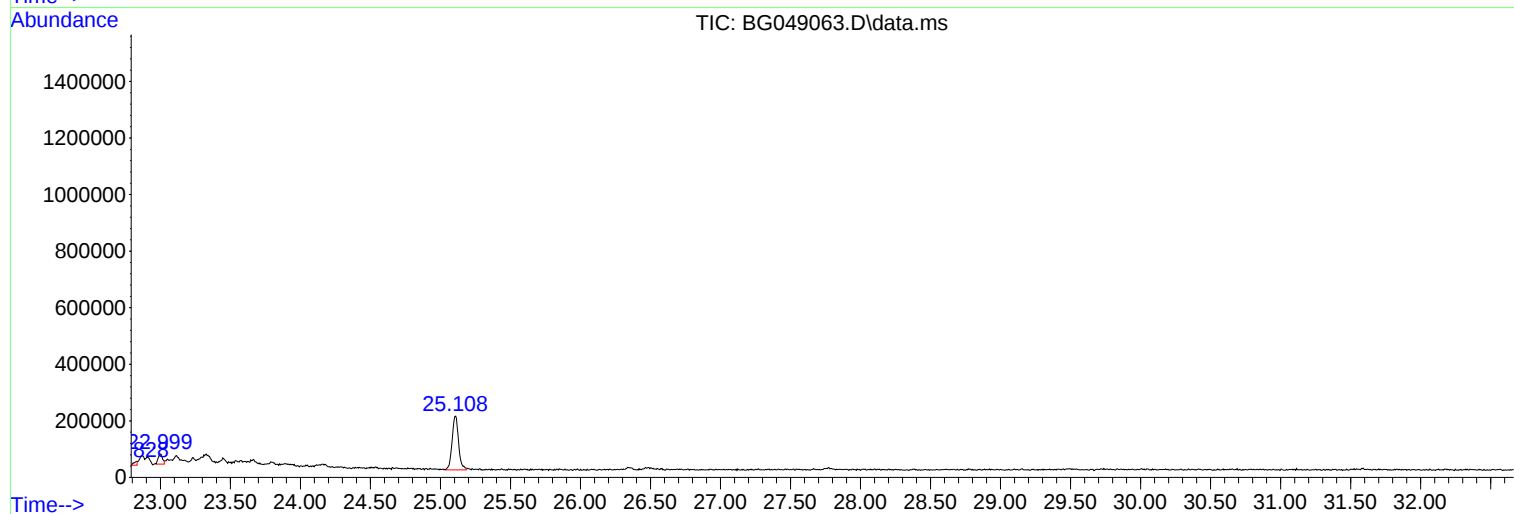
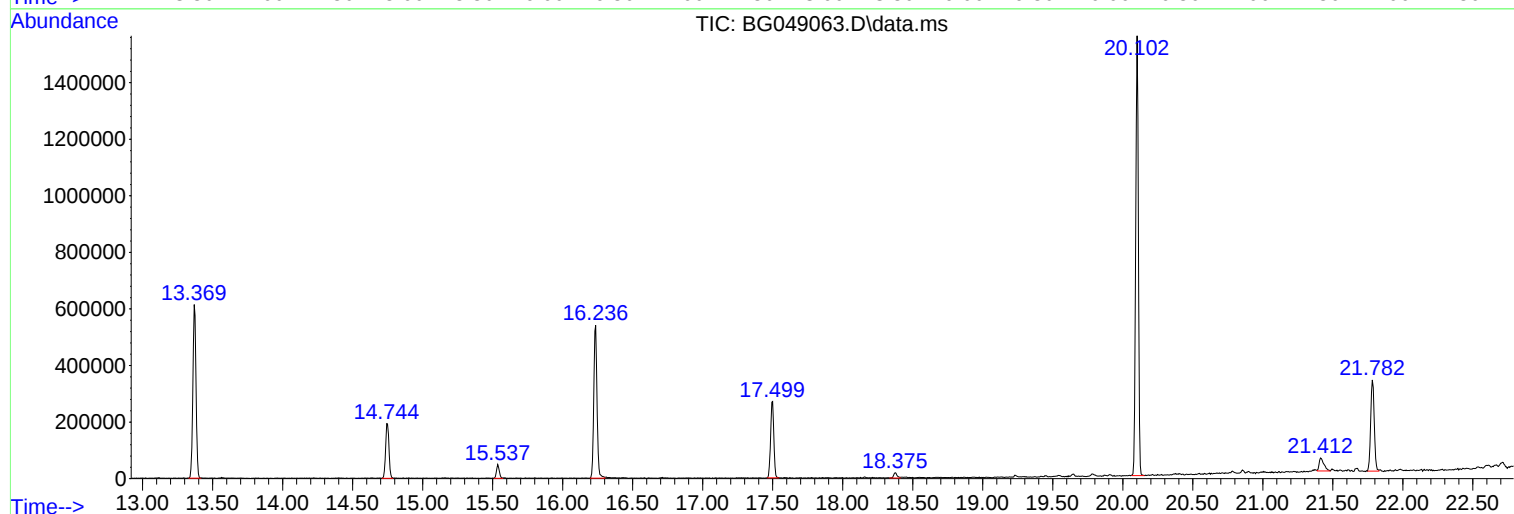
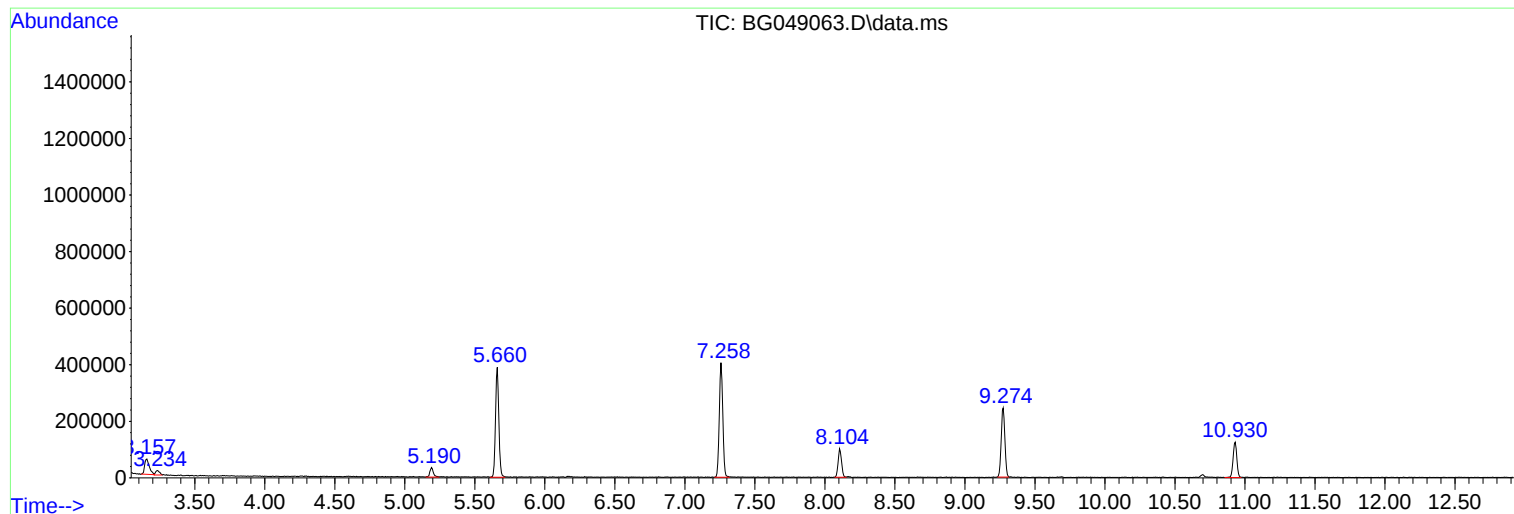
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Acq On : 23 Jun 2021 16:06
Operator : CG/JU
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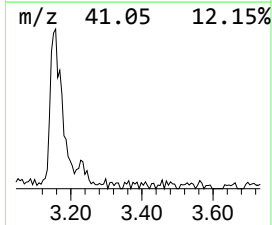
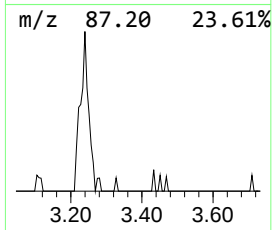
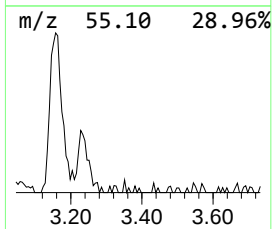
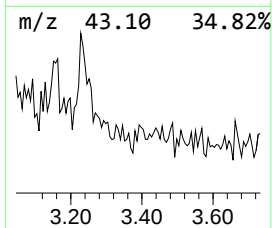
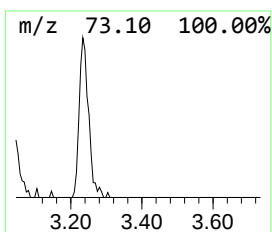
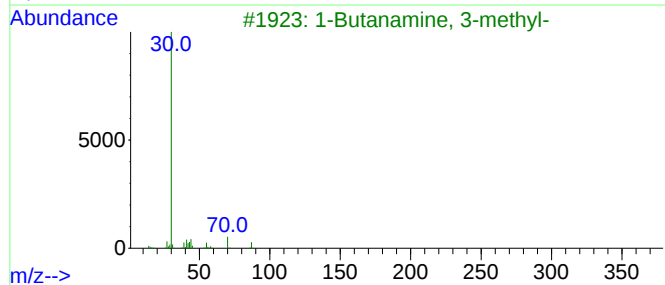
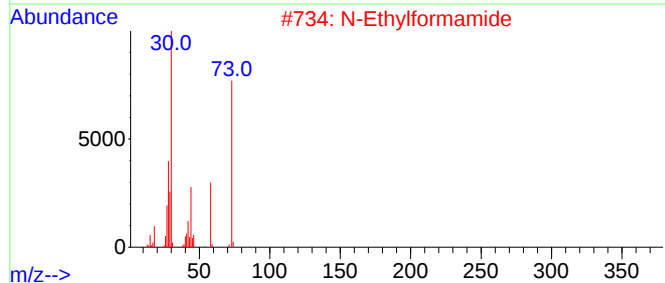
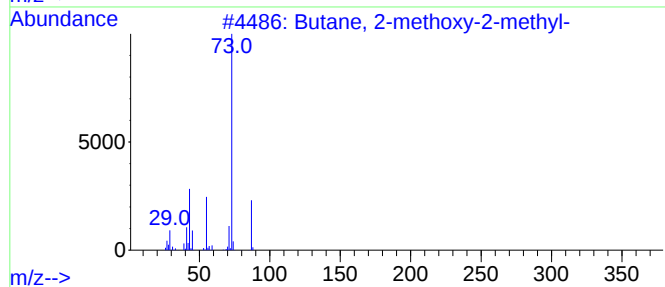
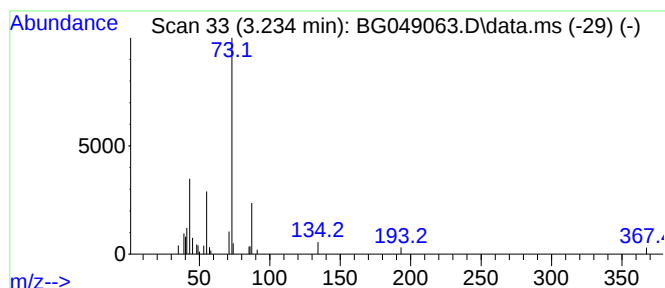
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown3.234 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.234	3.57 ng	30535	1,4-Dichlorobenzene-d4	8.104

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	47
2		N-Ethylformamide	73	C3H7NO	000627-45-2	5
3		1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	4
4		1-Pentanamine	87	C5H13N	000110-58-7	4
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	4



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

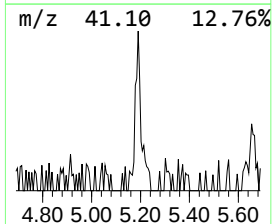
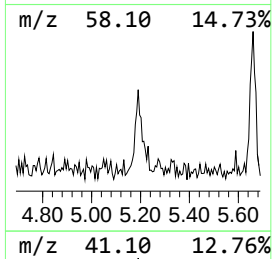
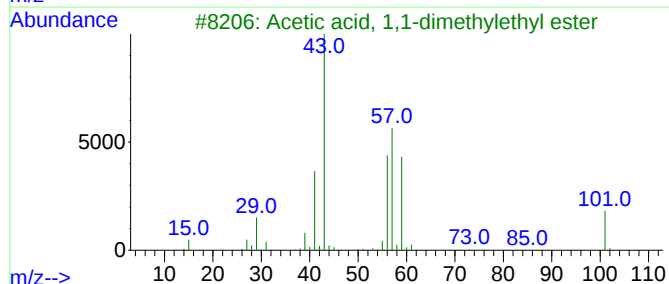
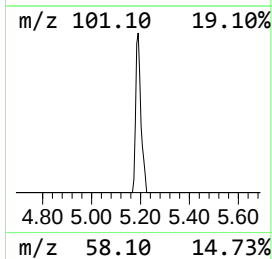
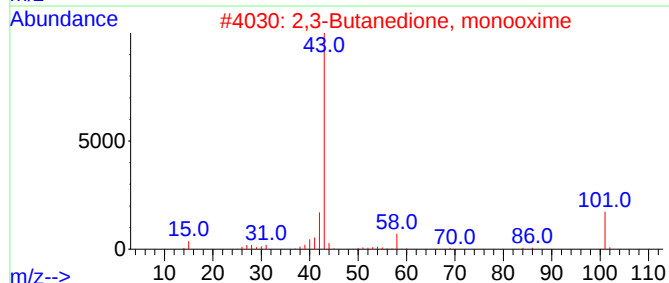
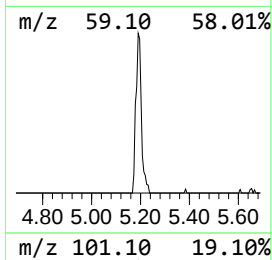
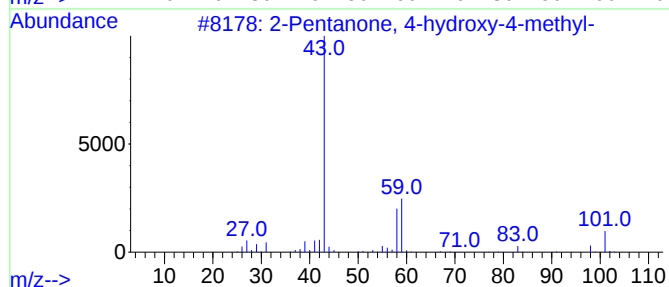
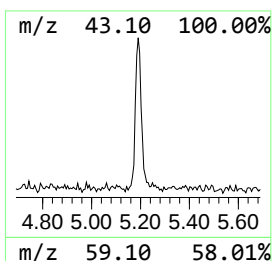
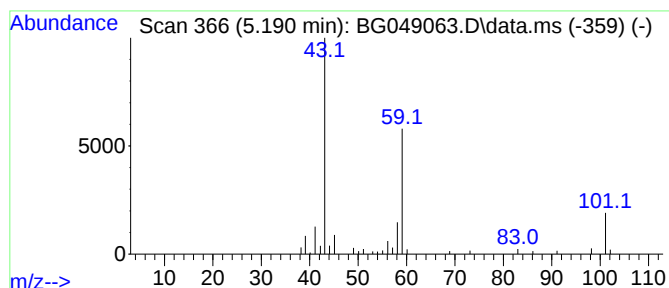
TIC Library : C:\Database\NIST11.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.190	6.85 ng	58571	1,4-Dichlorobenzene-d4	8.104

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	43
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4		3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	38
5		3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	38



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ClientSampled :
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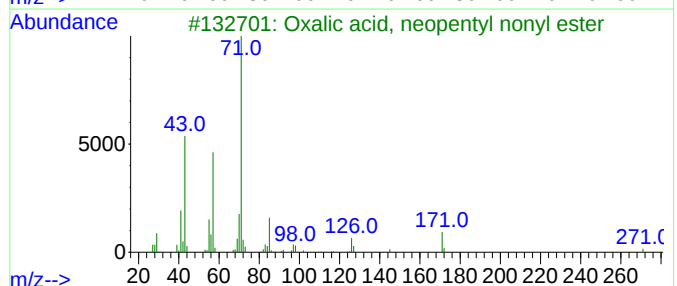
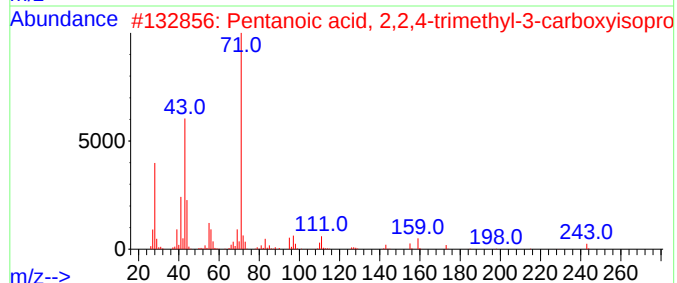
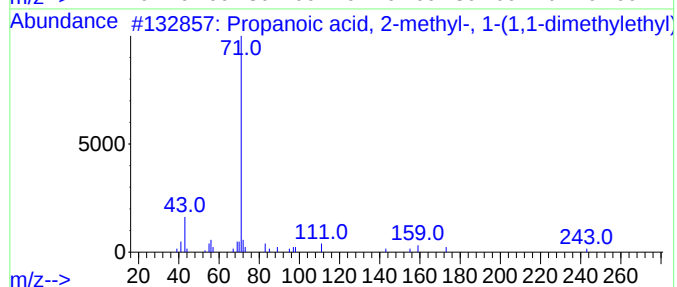
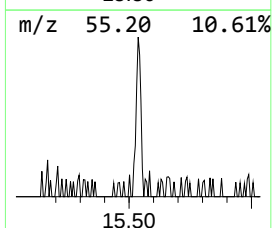
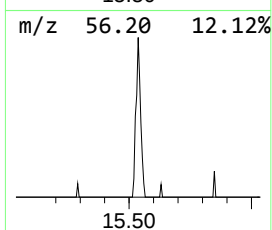
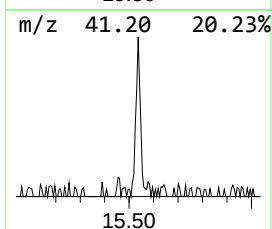
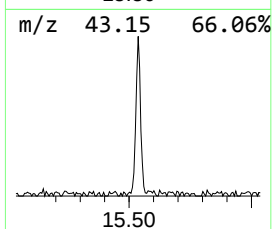
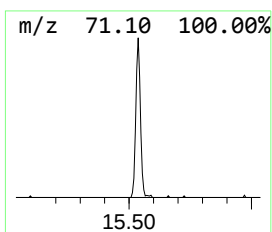
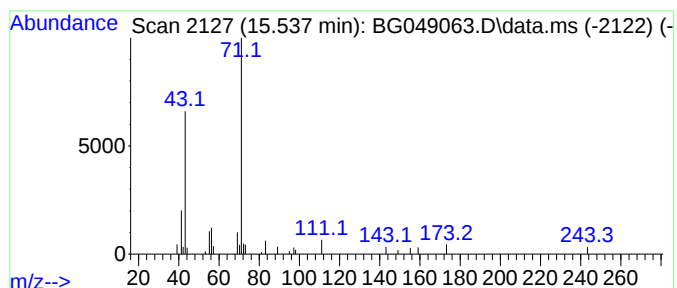
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.537	4.21 ng	66876	Acenaphthene-d10	14.749

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 1-(1,...	286	C16H30O4	074381-40-1	72
2			Pentanoic acid, 2,2,4-trimethyl-...	286	C16H30O4	1000140-77-5	64
3			Oxalic acid, neopentyl nonyl ester	286	C16H30O4	1000309-73-3	50
4			Sulfurous acid, decyl 2-pentyl e...	292	C15H32O3S	1000309-15-9	50
5			Sulfurous acid, dipentyl ester	222	C10H22O3S	1000309-13-9	45



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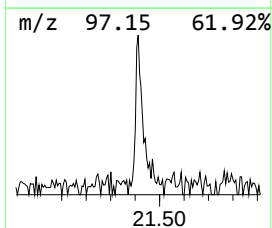
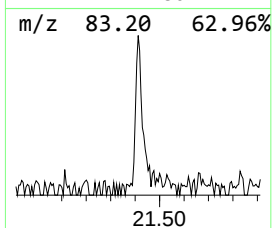
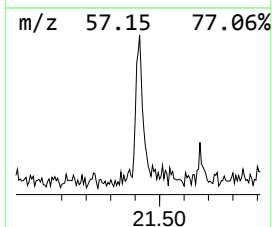
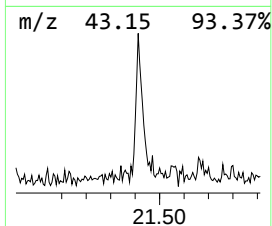
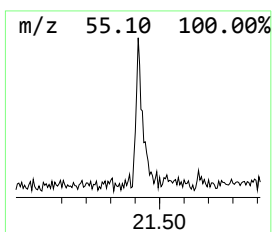
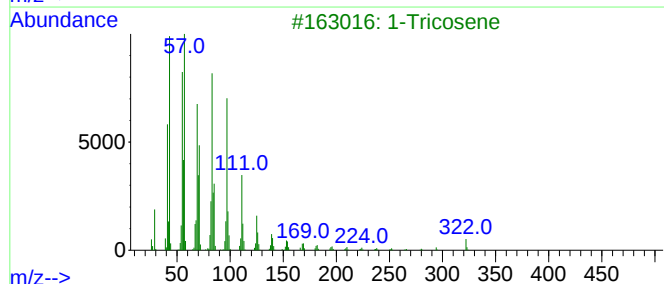
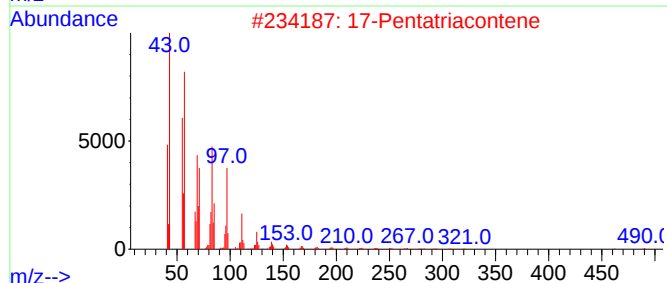
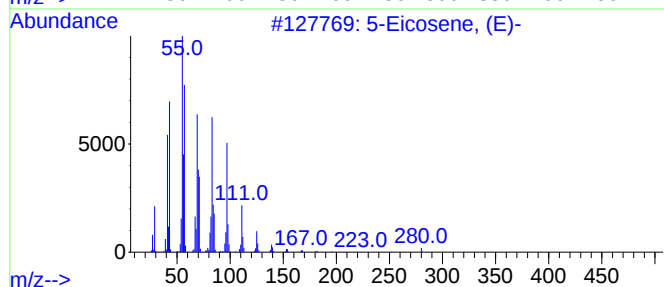
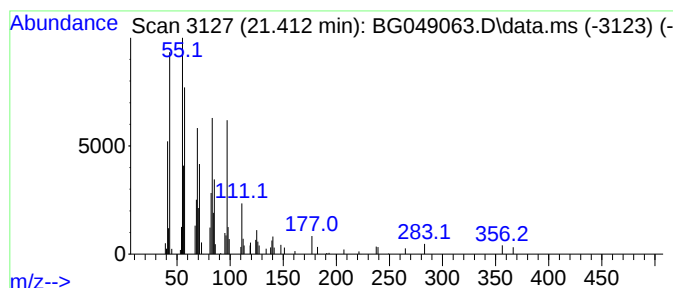
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Peak Number 5 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.412	3.79 ng	106953	Chrysene-d12	21.782

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Eicosene, (E)-	280	C20H40	074685-30-6	90
2			17-Pentatriacontene	491	C35H70	006971-40-0	81
3			1-Tricosene	322	C23H46	018835-32-0	72
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	72
5			3-Octadecene, (E)-	252	C18H36	007206-19-1	68



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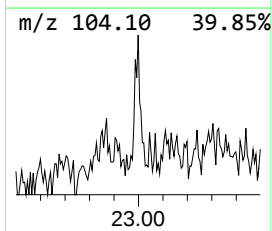
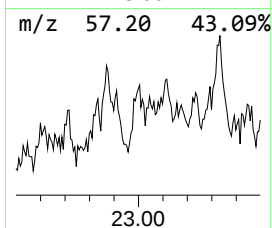
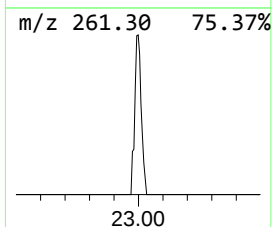
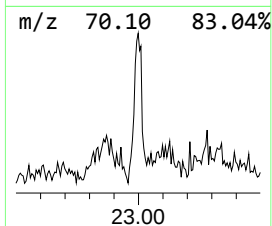
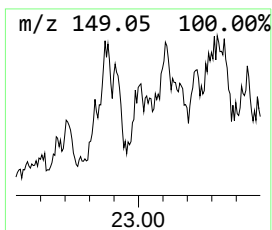
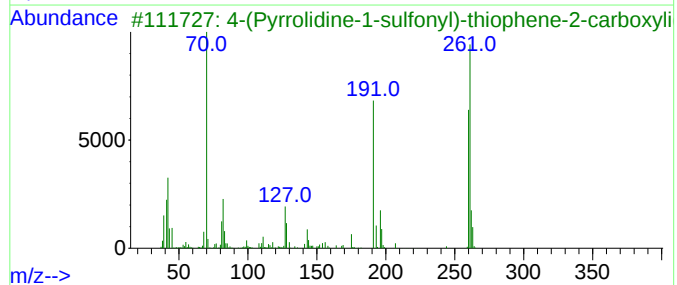
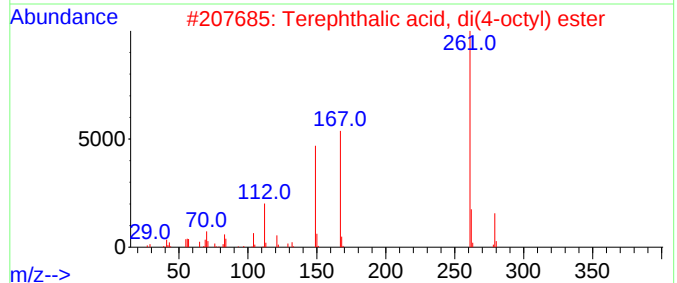
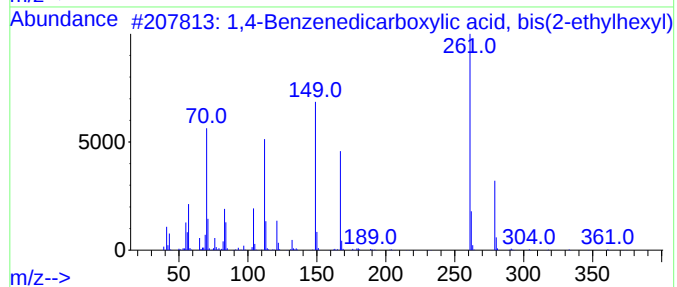
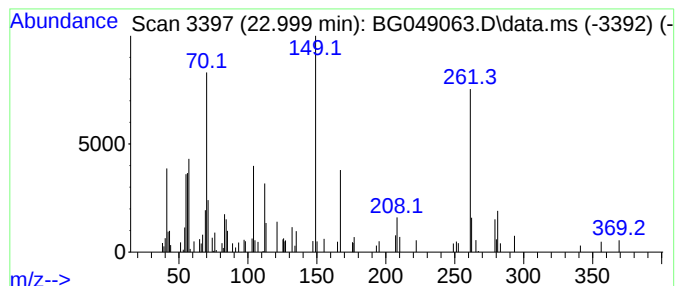
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown22.999 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.999	2.76 ng	77785	Chrysene-d12	21.782

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H3804	006422-86-2	27
2			Terephthalic acid, di(4-octyl) e...	390	C24H3804	1000323-74-2	27
3			4-(Pyrrolidine-1-sulfonyl)-thiop...	261	C9H11N04S2	1000300-36-7	25
4			1,3-Benzenedicarboxylic acid, bi...	390	C24H3804	000137-89-3	22
5			Diisooctyl phthalate	390	C24H3804	000131-20-4	16



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TIC Library : C:\Database\NIST11.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.234	3.234	3.6	ng	30535	1	8.104	171084	20.0
2-Pentanone, 4-...	5.190	6.8	ng	58571	1	8.104	171084	20.0
Propanoic acid,...	15.537	4.2	ng	66876	3	14.749	317841	20.0
5-Eicosene, (E)-	21.412	3.8	ng	106953	5	21.782	563667	20.0
unknown22.999	22.999	2.8	ng	77785	5	21.782	563667	20.0