

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101221\
 Data File : BG050561.D
 Acq On : 12 Oct 2021 20:34
 Operator : CG/JU
 Sample : M4169-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 P287-DITCH

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-BG100621.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG050561.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.327	306	313	322	rVB	249816	413301	13.28%	2.961%
2	5.797	386	393	402	rBV	296960	490629	15.77%	3.516%
3	7.401	659	666	677	rBV	215696	384585	12.36%	2.756%
4	8.259	804	812	823	rVB	188935	328874	10.57%	2.356%
5	9.428	1002	1011	1021	rBV	645977	1196082	38.44%	8.570%
6	10.826	1241	1249	1260	rBV	323751	535040	17.20%	3.834%
7	11.085	1285	1293	1300	rBV	274958	505260	16.24%	3.620%
8	13.500	1696	1704	1718	rVB	1529705	2421354	77.82%	17.350%
9	13.747	1738	1746	1755	rVB	50359	84025	2.70%	0.602%
10	14.875	1930	1938	1949	rBV	448327	711139	22.86%	5.096%
11	16.355	2184	2190	2199	rBV	554986	856817	27.54%	6.139%
12	16.537	2215	2221	2228	rBV2	29798	57738	1.86%	0.414%
13	17.619	2398	2405	2411	rBV	532012	806114	25.91%	5.776%
14	18.253	2508	2513	2520	rBV	74537	92912	2.99%	0.666%
15	19.411	2707	2710	2715	rVB	168570	192063	6.17%	1.376%
16	19.546	2728	2733	2737	rVB	45512	53679	1.73%	0.385%
17	20.204	2839	2845	2851	rBV	2246099	3111442	100.00%	22.294%
18	21.514	3063	3068	3075	rBV	80400	133197	4.28%	0.954%
19	21.913	3130	3136	3145	rVB	437959	798969	25.68%	5.725%
20	25.327	3708	3717	3730	rVB3	248381	782899	25.16%	5.610%

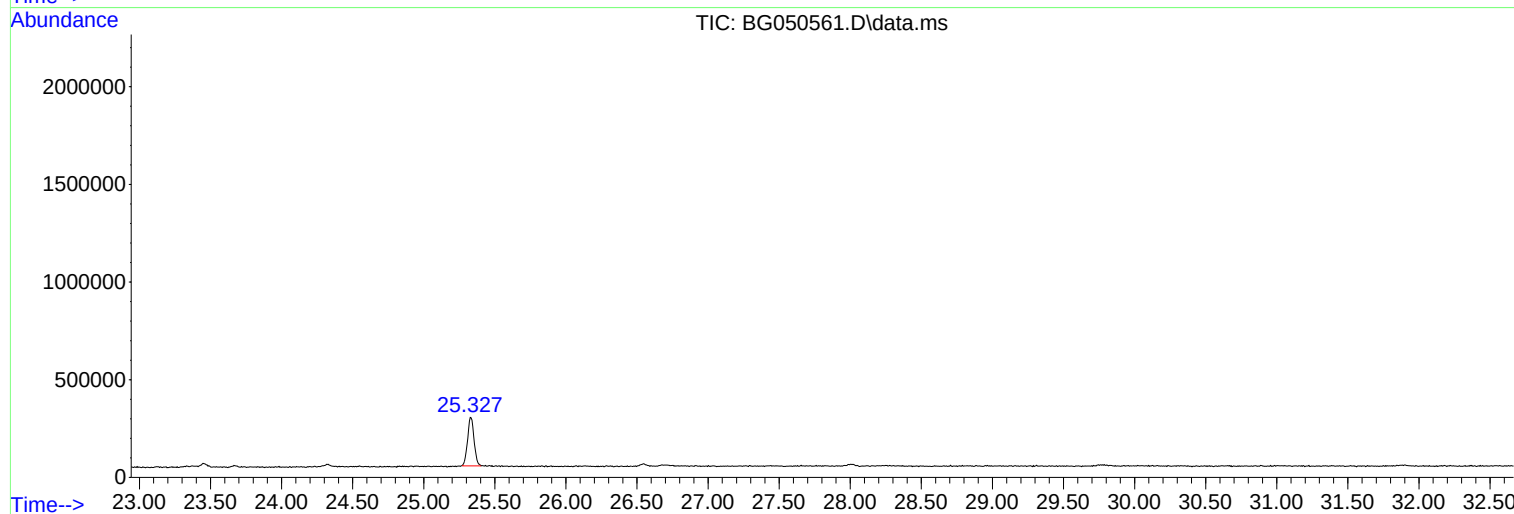
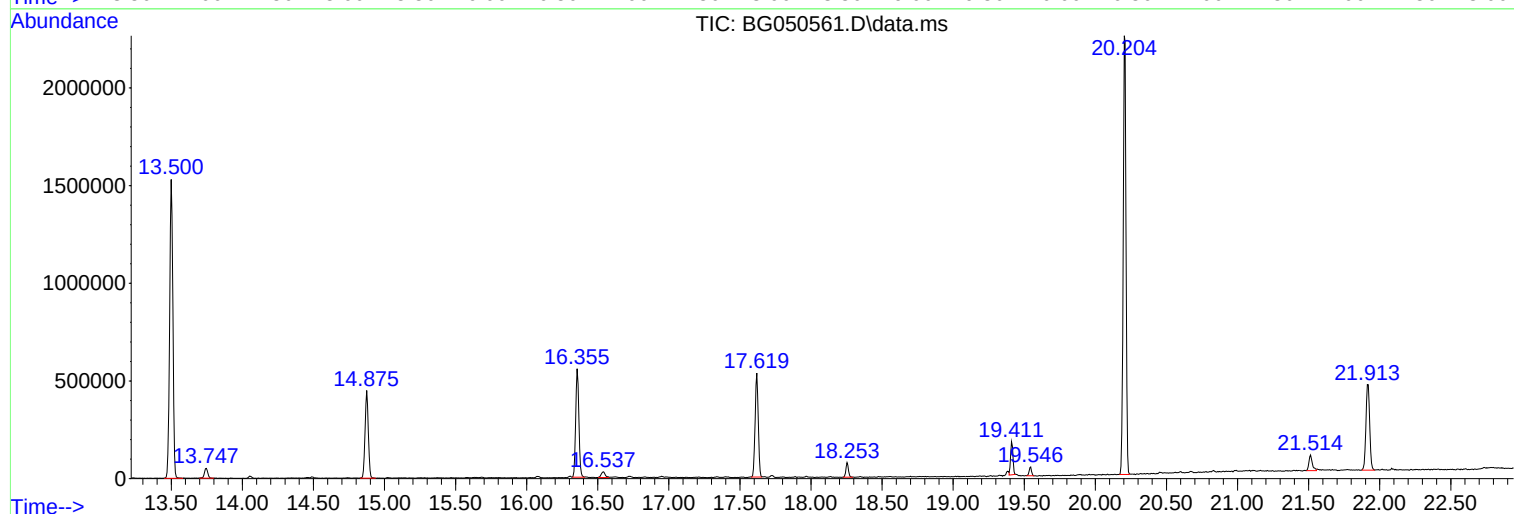
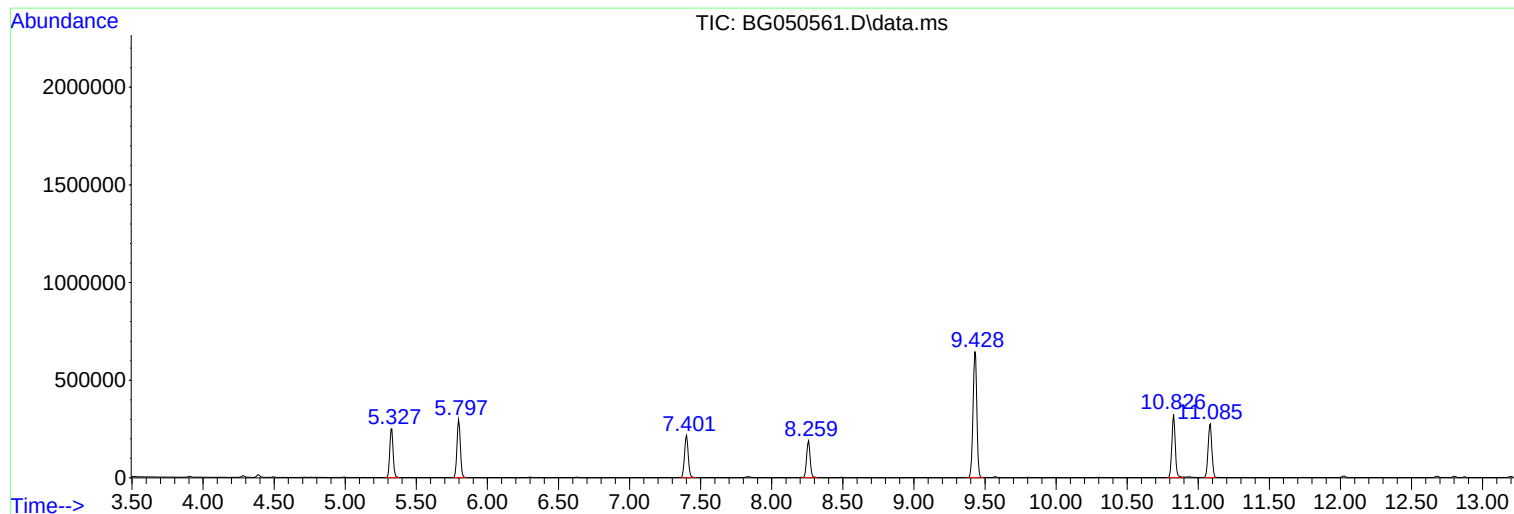
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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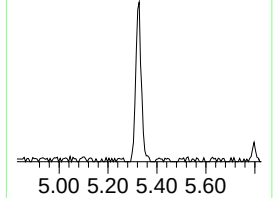
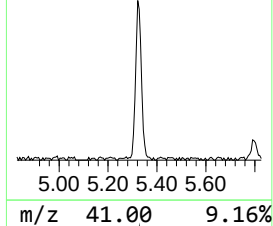
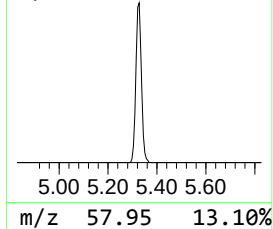
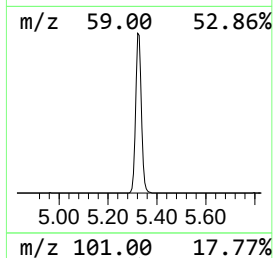
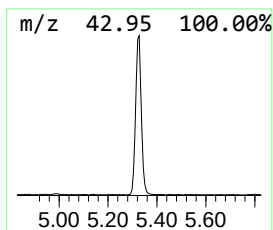
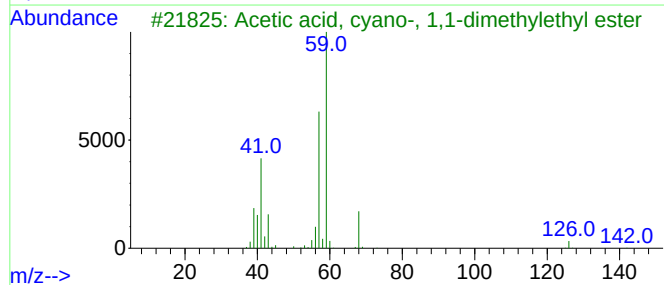
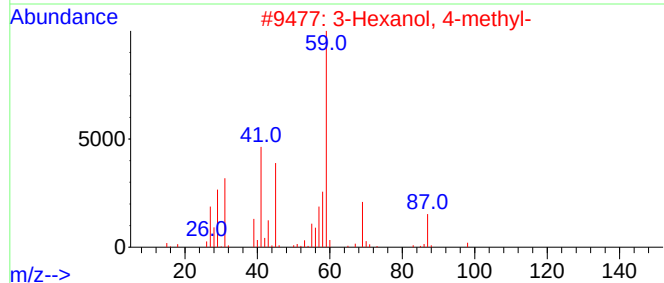
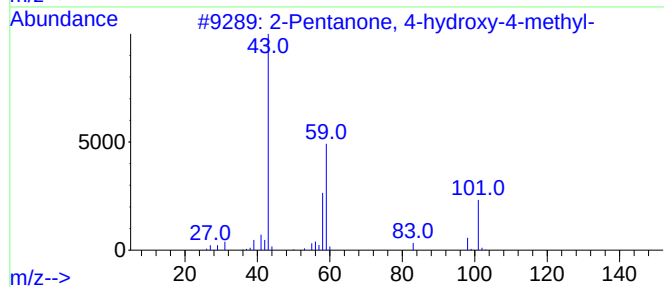
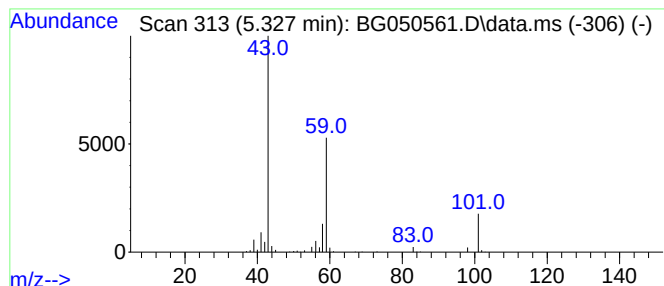
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.327	25.13 ng	413301	1,4-Dichlorobenzene-d4	8.259

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		



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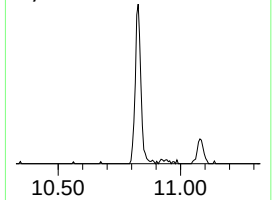
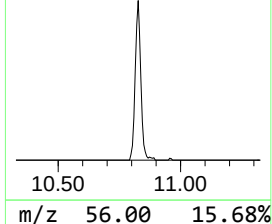
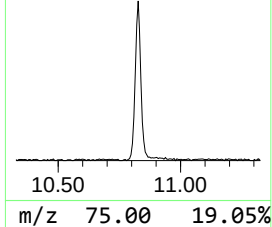
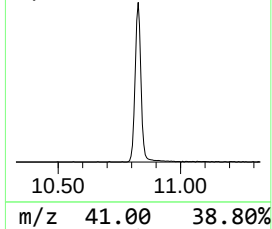
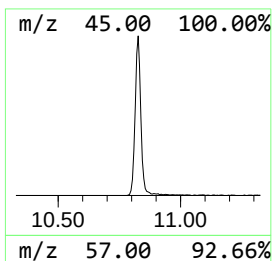
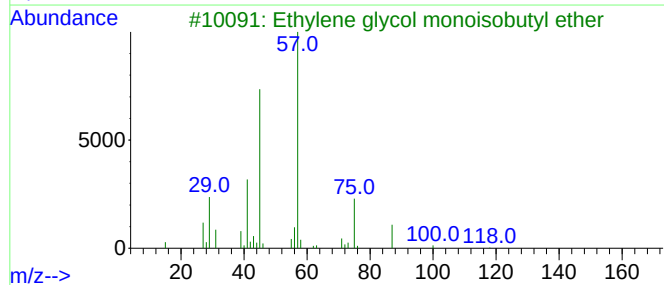
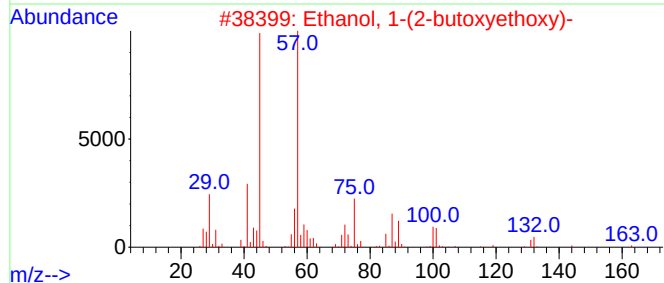
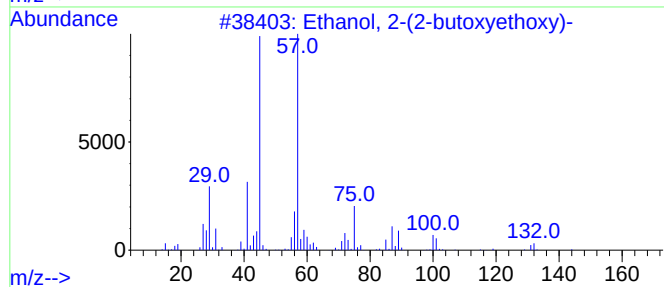
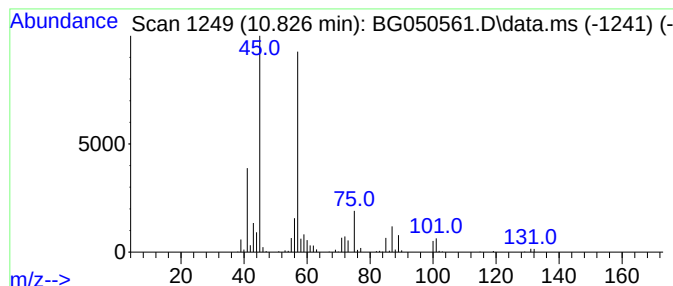
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.826	21.18 ng	535040	Naphthalene-d8	11.085

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	56
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	53



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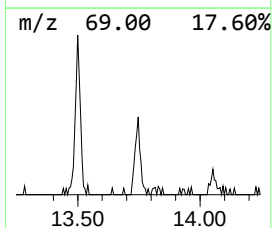
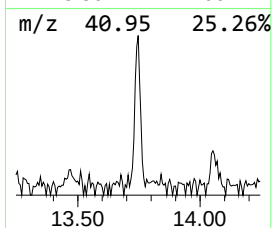
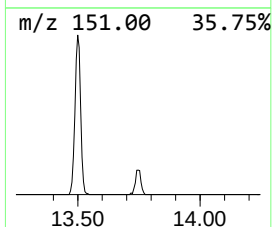
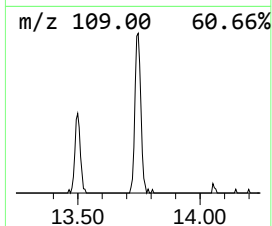
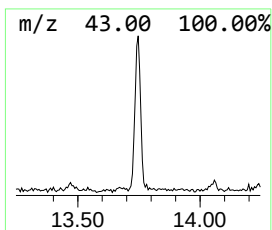
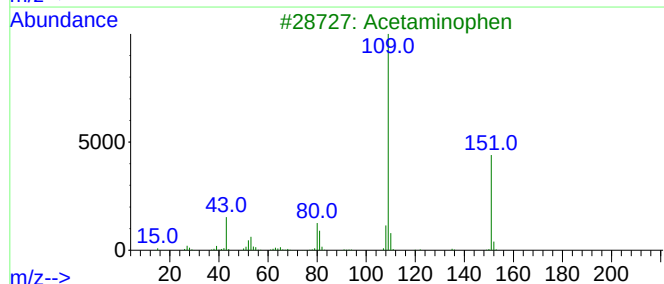
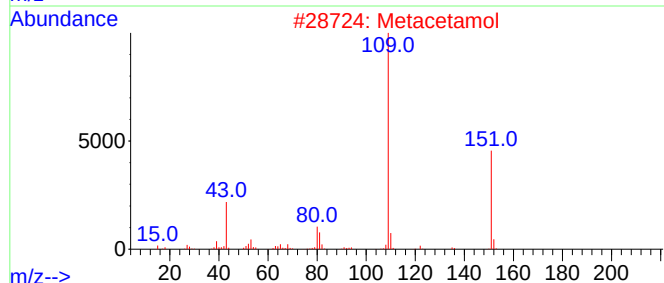
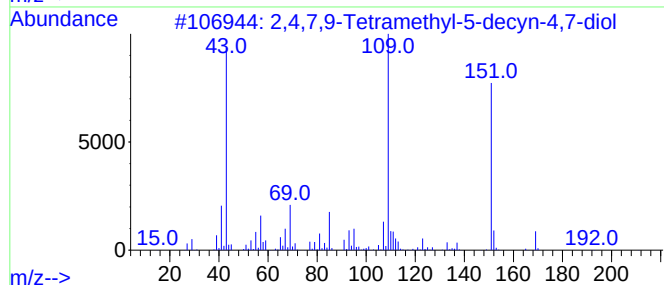
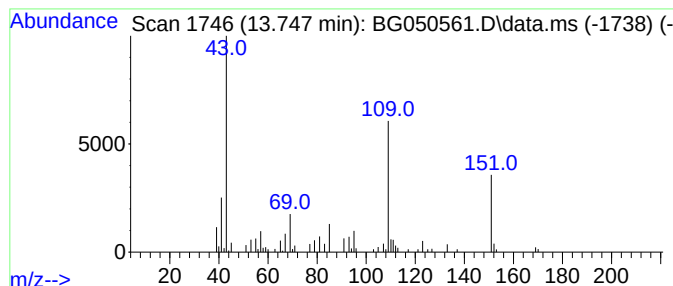
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Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.747	2.36 ng	84025	Acenaphthene-d10	14.875

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2		000126-86-3	56
2	Metacetamol	151	C8H9NO2		000621-42-1	52
3	Acetaminophen	151	C8H9NO2		000103-90-2	50
4	Pyridine, 3-butyl-, 1-oxide	151	C9H13NO		031396-33-5	40
5	4-Pyridinemethanol, acetate (ester)	151	C8H9NO2		001007-48-3	40



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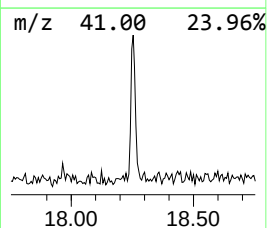
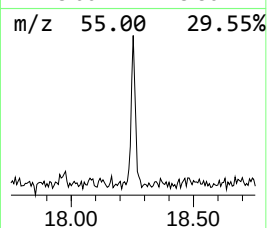
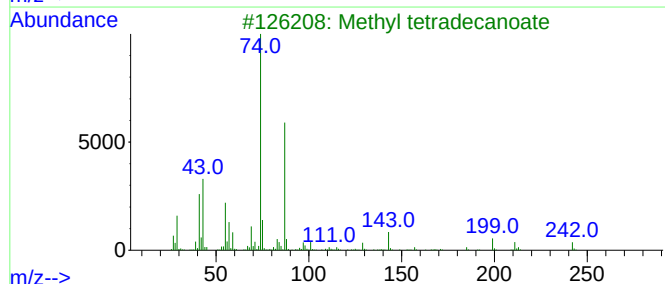
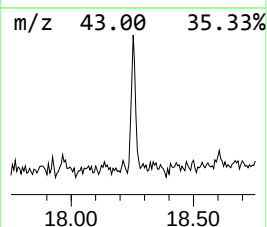
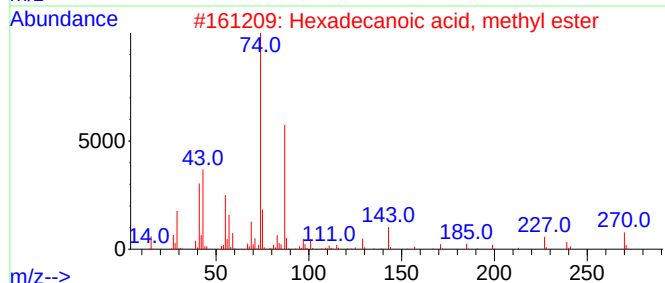
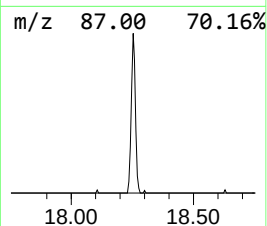
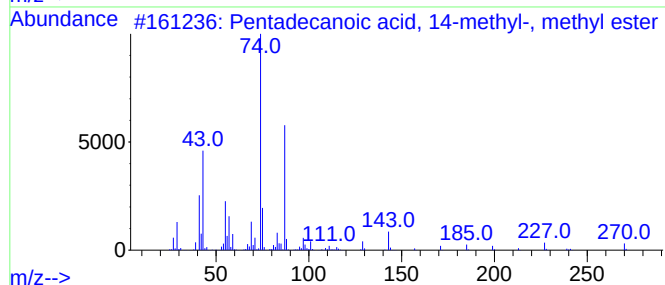
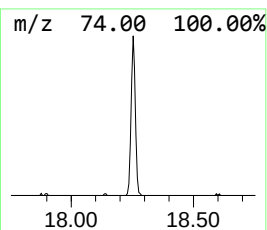
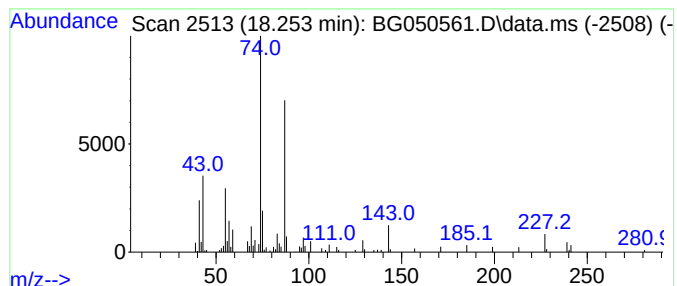
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Peak Number 4 Pentadecanoic acid, 14-meth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.253	2.31 ng	92912	Phenanthrene-d10	17.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
2			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	91
3			Methyl tetradecanoate	242	C15H30O2	000124-10-7	86
4			Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	86
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86



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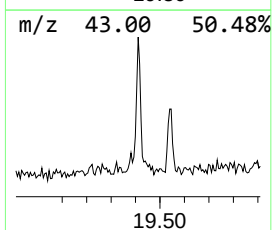
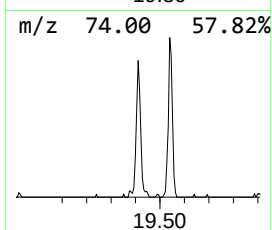
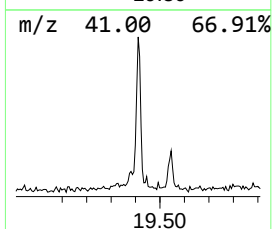
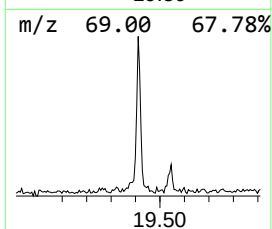
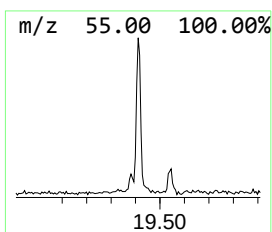
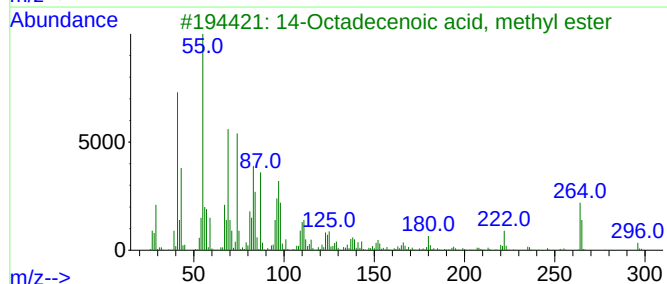
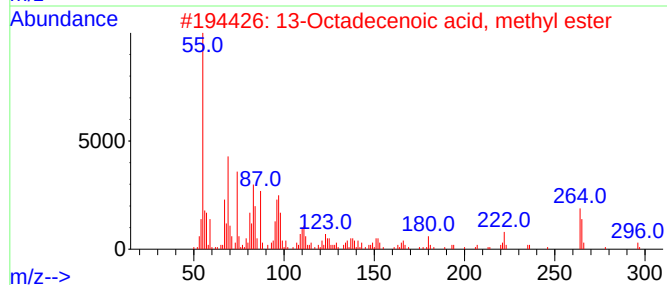
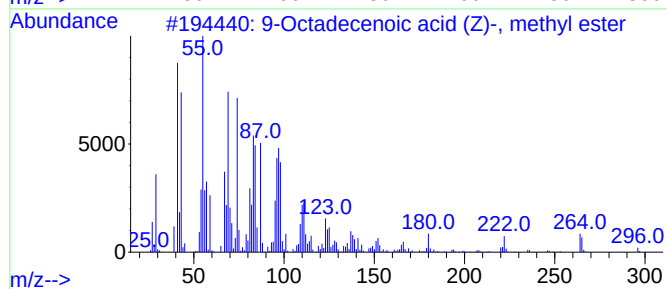
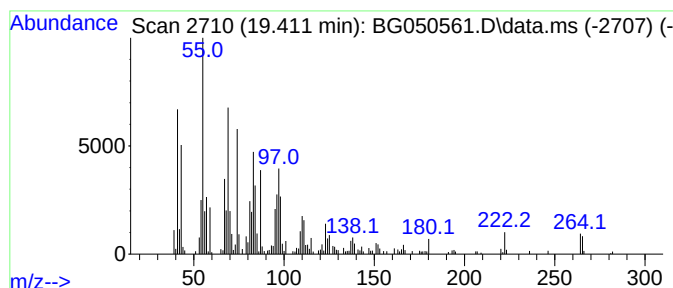
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Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.411	4.77 ng	192063	Phenanthrene-d10	17.619	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
3	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
4	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
5	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	91



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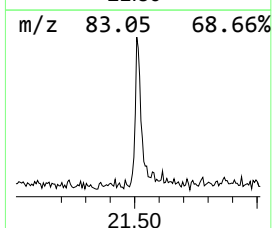
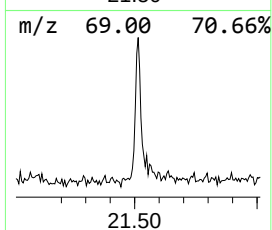
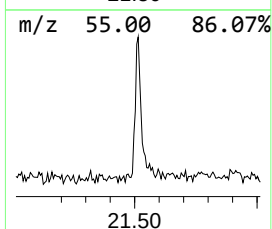
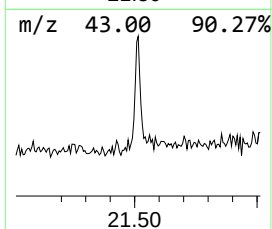
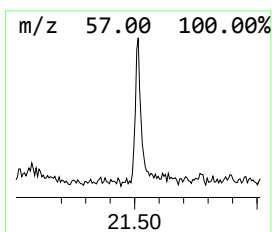
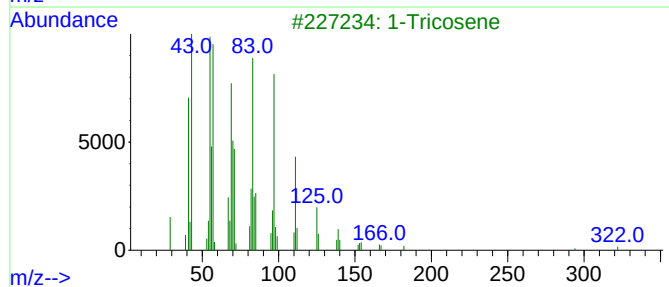
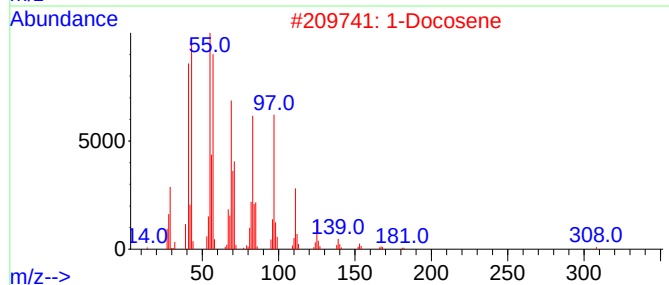
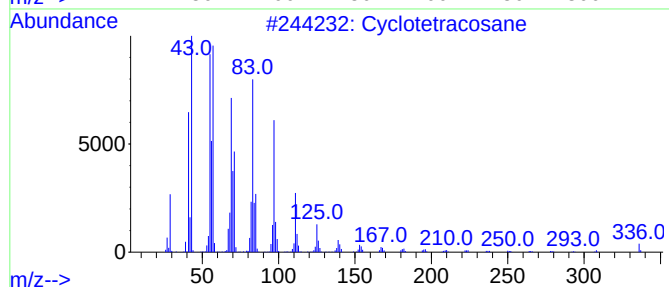
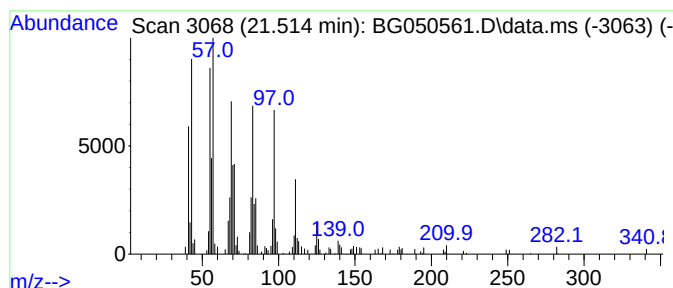
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclotetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.514	3.33 ng	133197	Chrysene-d12	21.919

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclotetracosane	336	C24H48	000297-03-0	94
2		1-Docosene	308	C22H44	001599-67-3	94
3		1-Tricosene	322	C23H46	018835-32-0	93
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5		1-Hexacosene	364	C26H52	018835-33-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101221\
Data File : BG050561.D
Acq On : 12 Oct 2021 20:34
Operator : CG/JU
Sample : M4169-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P287-DITCH

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.327	25.1	ng	413301	1	8.259	328874	20.0
Ethanol, 2-(2-b...	10.826	21.2	ng	535040	2	11.085	505260	20.0
2,4,7,9-Tetrame...	13.747	2.4	ng	84025	3	14.875	711139	20.0
Pentadecanoic a...	18.253	2.3	ng	92912	4	17.619	806114	20.0
9-Octadecenoic ...	19.411	4.8	ng	192063	4	17.619	806114	20.0
Cyclotetracosane	21.514	3.3	ng	133197	5	21.919	798969	20.0