

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
 Data File : BG060195.D
 Acq On : 2 Jan 2024 15:10
 Operator : MA/JU
 Sample : 05909-15
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 GHL-SS-53

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-BG122923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060195.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.114	3	4	13	rVB	425975	432071	3.36%	0.681%
2	5.511	405	412	426	rBV	2909292	4778404	37.11%	7.536%
3	7.097	675	682	700	rBV	2772394	4933853	38.32%	7.781%
4	7.938	817	825	832	rBV	619058	1075717	8.36%	1.696%
5	9.101	1015	1023	1036	rBV	1487031	2736702	21.26%	4.316%
6	10.740	1294	1302	1313	rBV	946300	1679519	13.05%	2.649%
7	13.196	1713	1720	1732	rBV	5078452	7785875	60.47%	12.279%
8	14.577	1948	1955	1963	rBV	1805111	2854152	22.17%	4.501%
9	16.063	2199	2208	2222	rBV	4081184	6279697	48.78%	9.903%
10	17.321	2416	2422	2430	rBV	2675010	4004860	31.11%	6.316%
11	18.214	2569	2574	2583	rBV2	120156	208885	1.62%	0.329%
12	19.941	2862	2868	2881	rBV	9490490	12874647	100.00%	20.304%
13	21.234	3083	3088	3100	rBV	427568	697704	5.42%	1.100%
14	21.586	3141	3148	3164	rBV2	2652209	4539982	35.26%	7.160%
15	22.338	3270	3276	3280	rBV2	178697	314948	2.45%	0.497%
16	22.385	3281	3284	3293	rVB6	66337	148487	1.15%	0.234%
17	23.196	3415	3422	3428	rBV2	256651	570484	4.43%	0.900%
18	23.854	3531	3534	3541	rVB2	94117	166644	1.29%	0.263%
19	24.230	3587	3598	3611	rBV2	292260	858546	6.67%	1.354%
20	24.765	3678	3689	3704	rBV	1564599	4486165	34.84%	7.075%
21	25.499	3803	3814	3827	rBV3	238148	840967	6.53%	1.326%
22	27.062	4071	4080	4082	rBV4	174147	410604	3.19%	0.648%
23	29.060	4406	4420	4434	rBV7	126490	730468	5.67%	1.152%

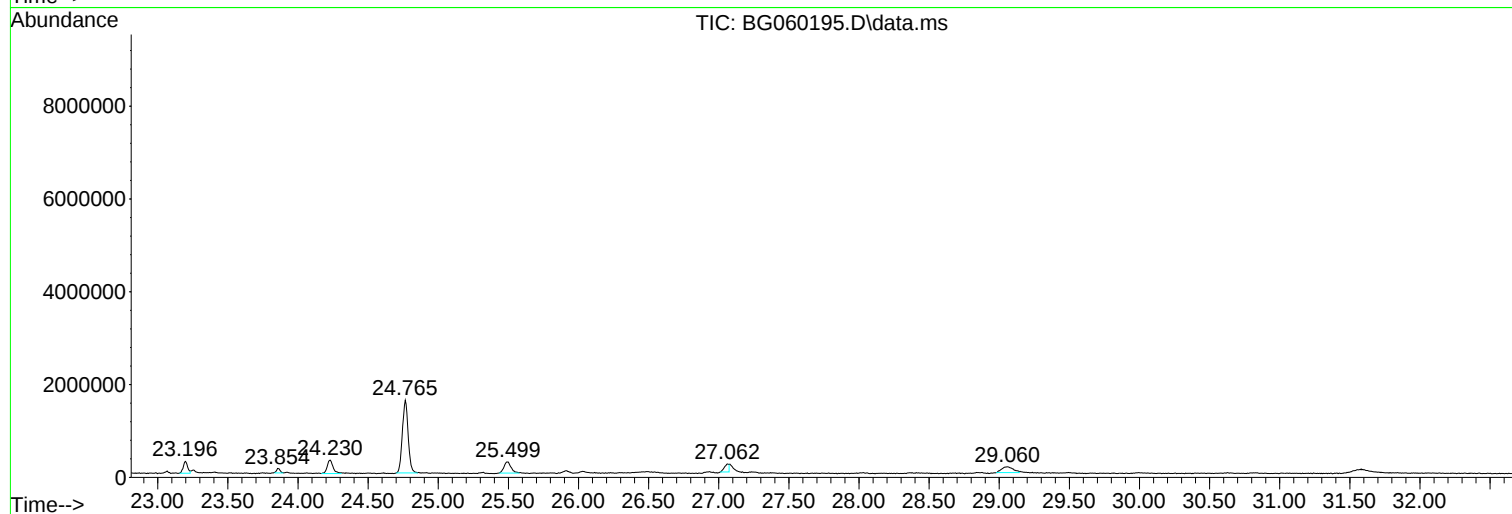
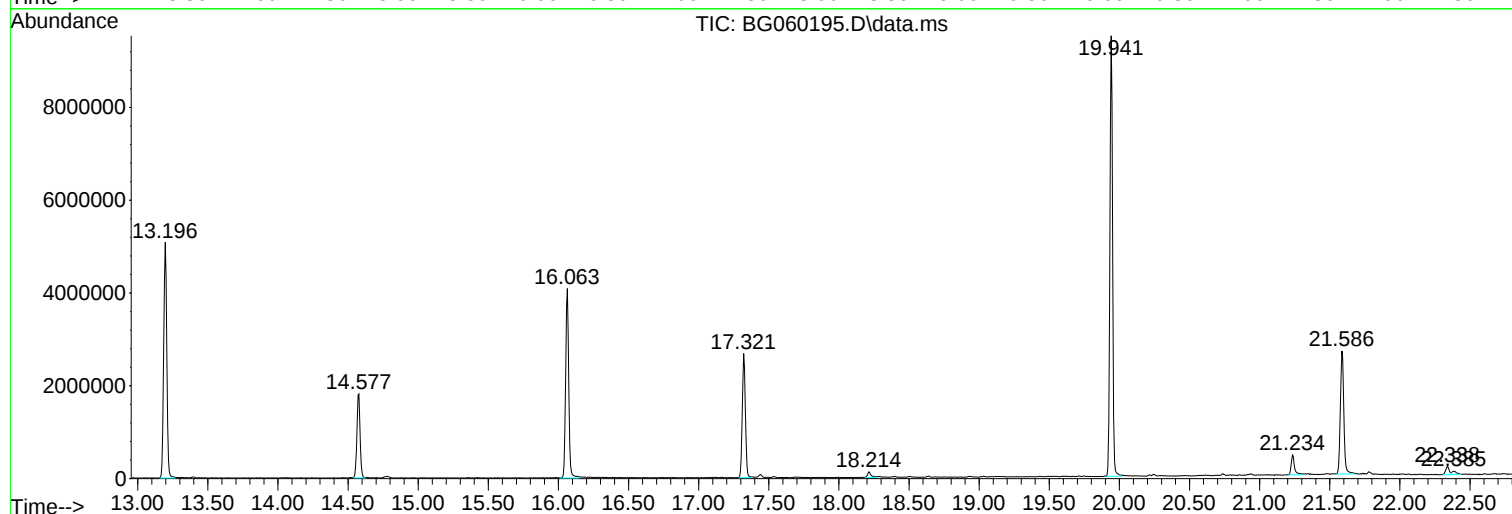
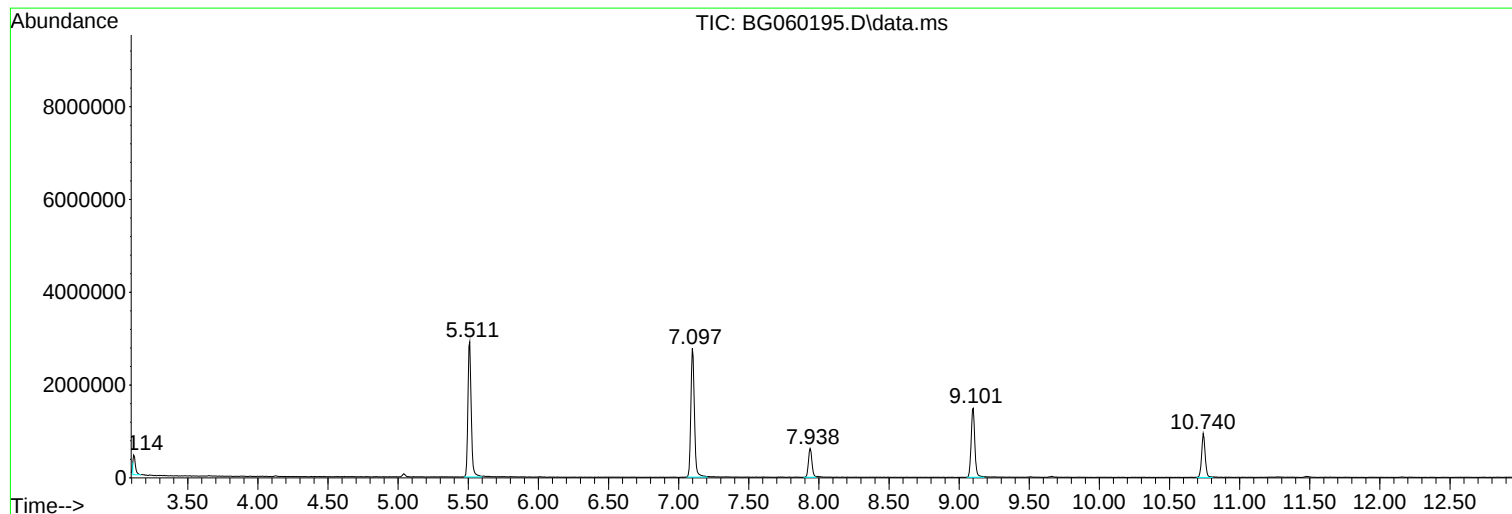
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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
GHL-SS-53

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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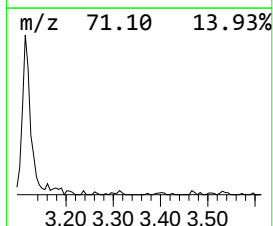
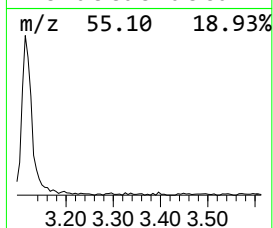
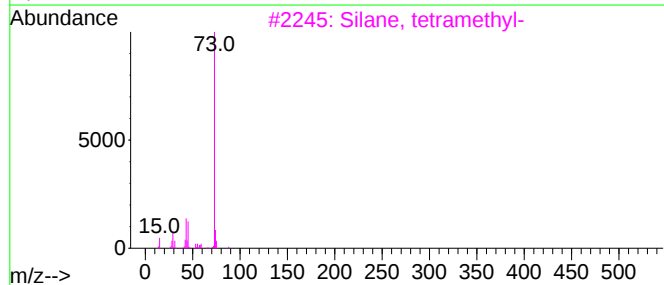
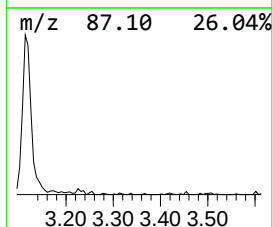
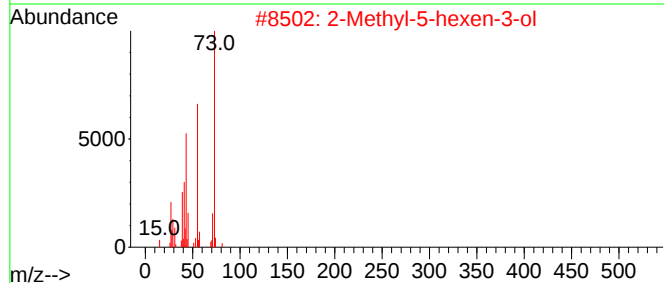
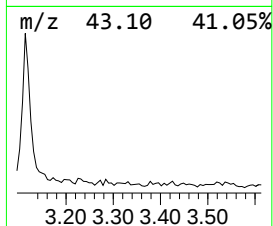
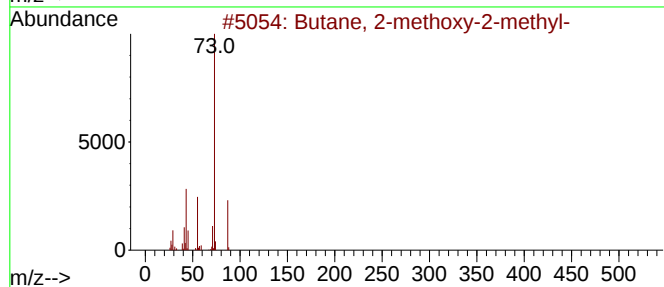
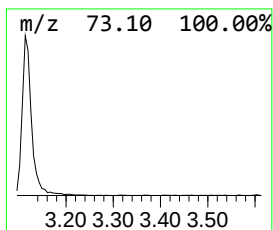
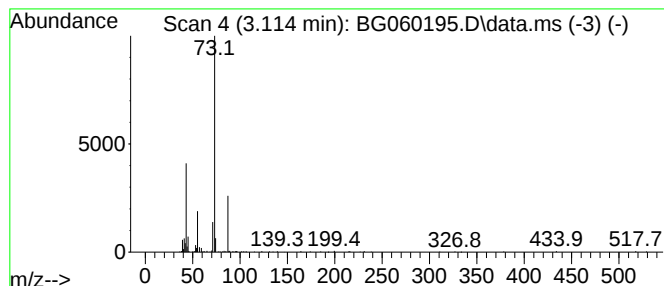
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.114 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.114	8.03 ng	432071	1,4-Dichlorobenzene-d4	7.938

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	45
2			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	22
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			Butane, 2,3-dimethoxy-2-methyl-	132	C7H16O2	074421-00-4	9



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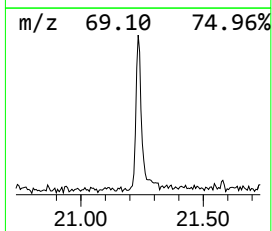
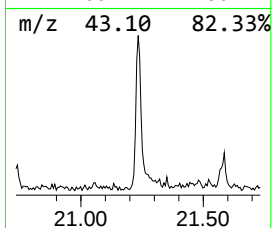
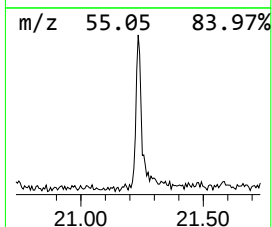
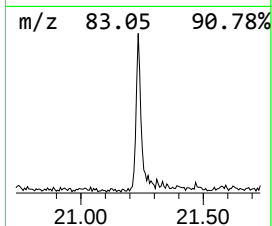
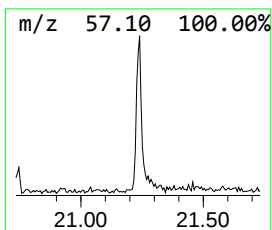
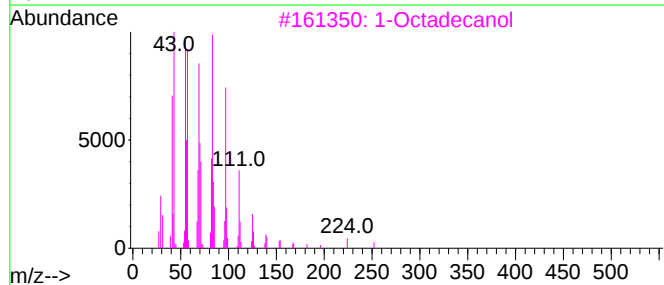
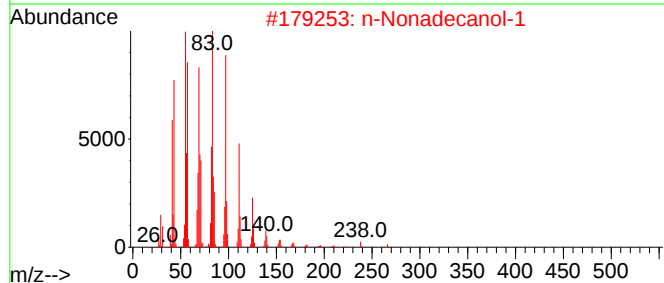
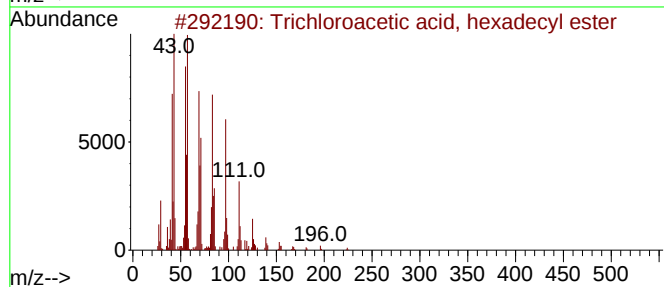
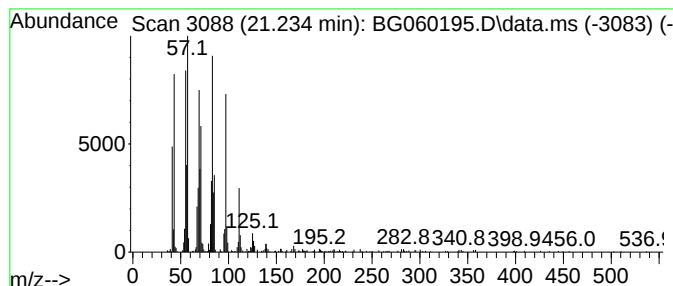
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.234	3.07 ng	697704	Chrysene-d12	21.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	87
3			1-Octadecanol	270	C18H38O	000112-92-5	86
4			1-Hexacosanol	382	C26H54O	000506-52-5	76
5			1-Hexadecanol	242	C16H34O	036653-82-4	74



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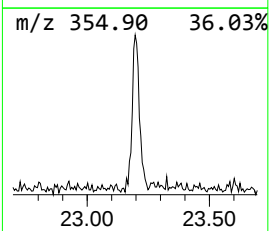
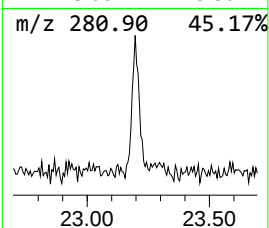
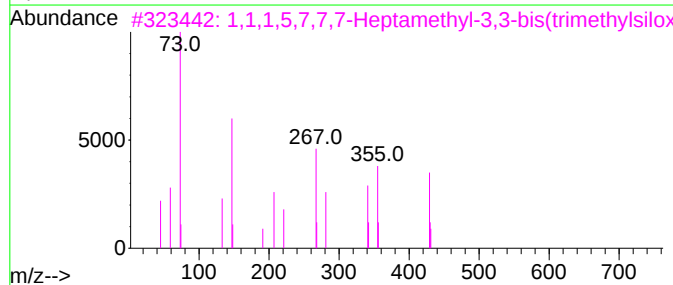
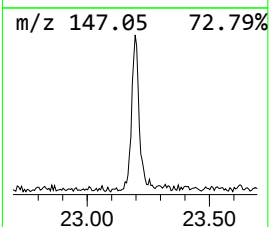
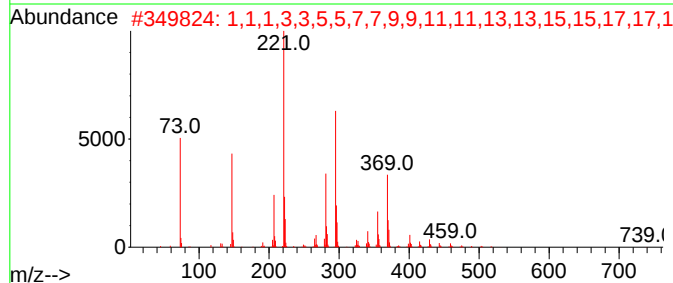
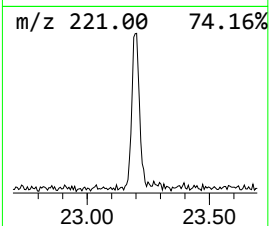
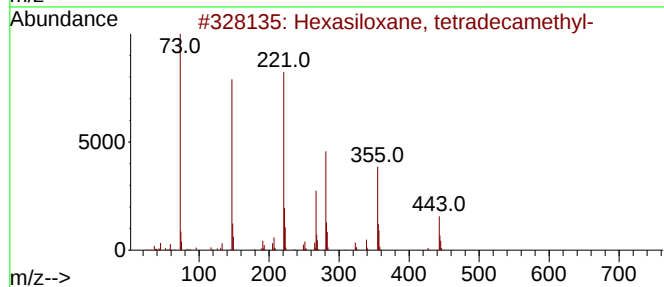
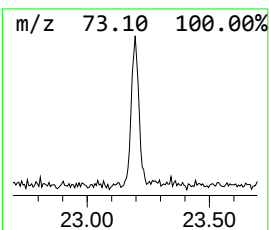
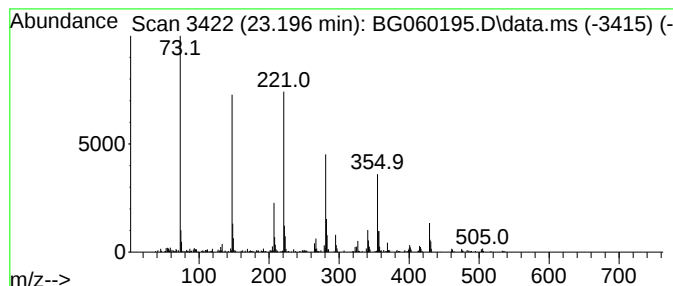
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexasiloxane, tetradecamethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.196	2.54 ng	570484	Perylene-d12	24.765

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	72
2			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	754	C22H66O9Si10	000556-70-7	37
3			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	35
4			1H-Indole-2-carboxylic acid, 6-(...	369	C22H27NO4	1000316-17-3	35
5			Thioglycolic acid, S-(tert-butyl...	320	C14H32O2SSi2	082112-29-6	27



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ClientSampleId :
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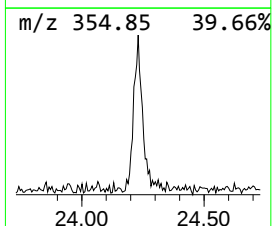
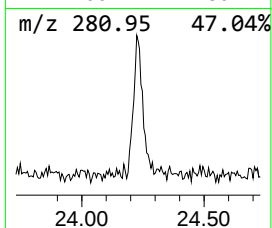
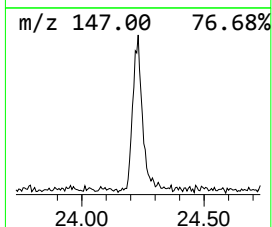
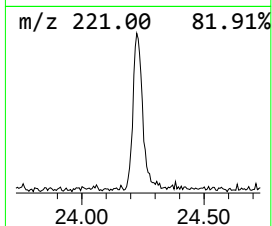
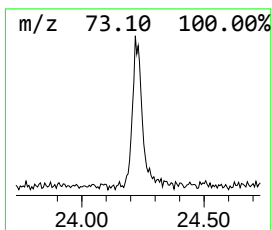
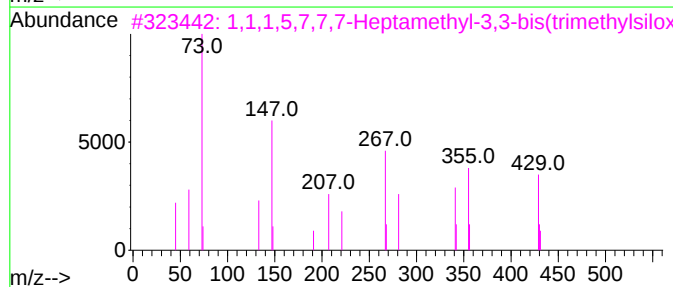
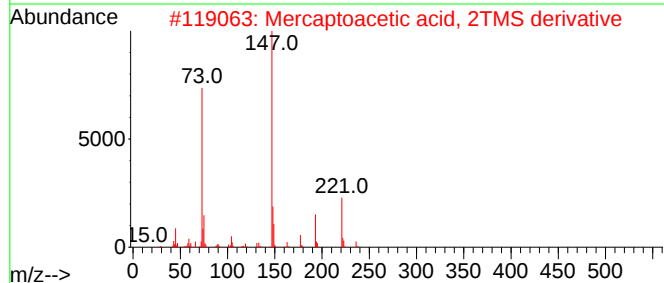
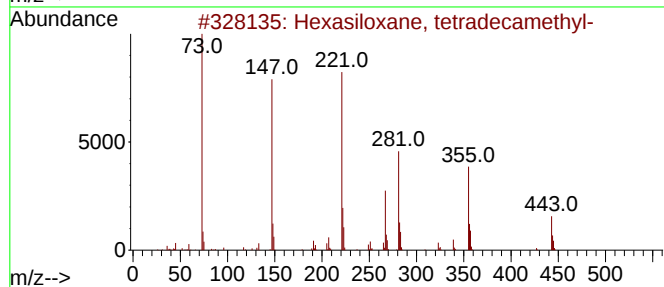
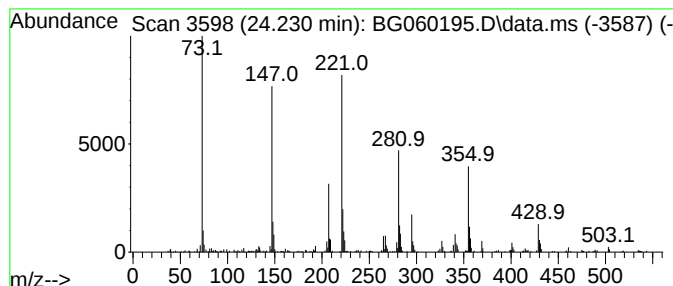
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Peak Number 4 unknown24.230 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.230	3.83 ng	858546	Perylene-d12	24.765

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	87
2			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	47
3			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	38
4			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	32
5			Pyrazophos	373	C14H20N3O5PS	013457-18-6	22



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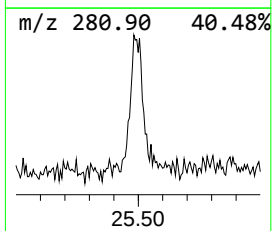
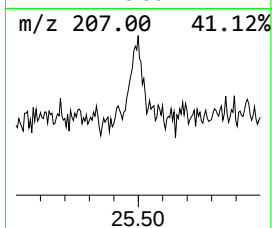
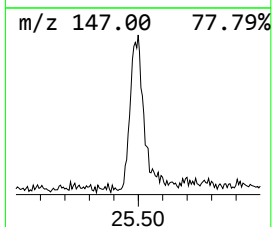
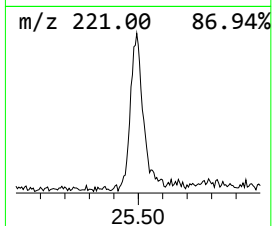
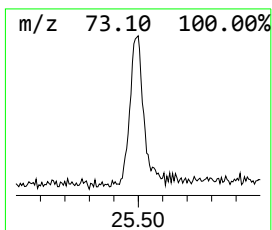
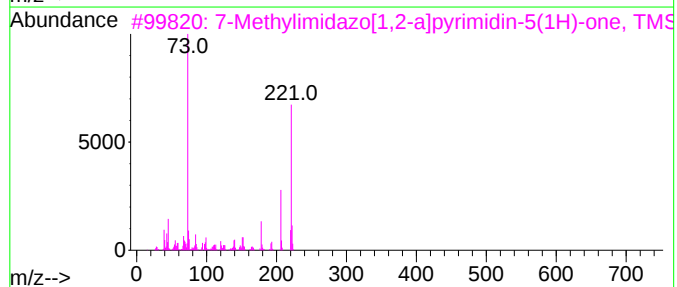
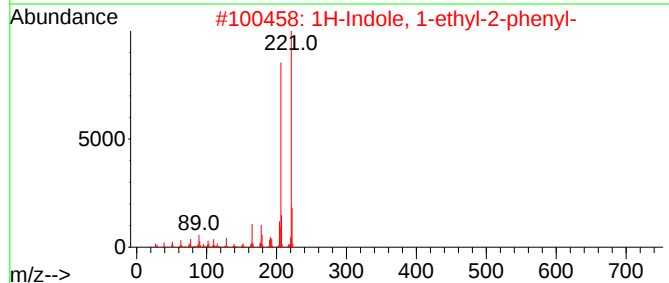
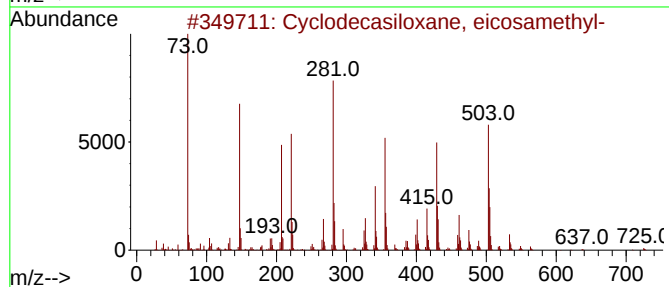
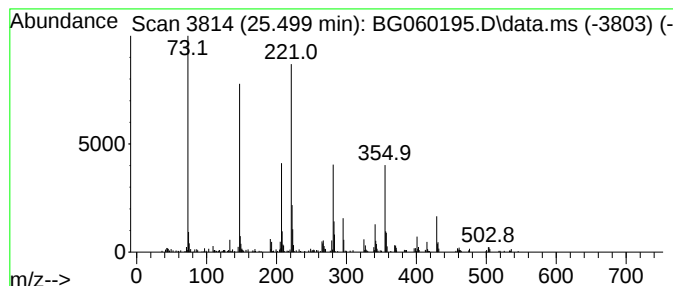
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown25.499 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.499	3.75 ng	840967	Perylene-d12	24.765

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclodecasiloxane, eicosamethyl-	740	C20H60O10Si10	018772-36-6	25
2			1H-Indole, 1-ethyl-2-phenyl-	221	C16H15N	013228-39-2	22
3			7-Methylimidazo[1,2-a]pyrimidin-...	221	C10H15N3OSi	1010468-48-3	18
4			Hexasiloxane, 1,1,3,3,5,5,7,7,9,...	430	C12H38O5Si6	000995-82-4	14
5			Bis(4-tert-butyltrimethylsiloxy)b...	458	C26H42O3Si2	1000431-17-0	14



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GHL-SS-53

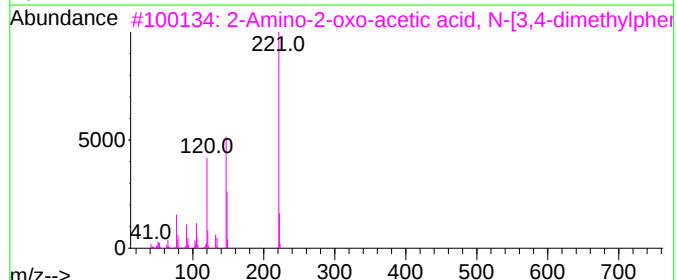
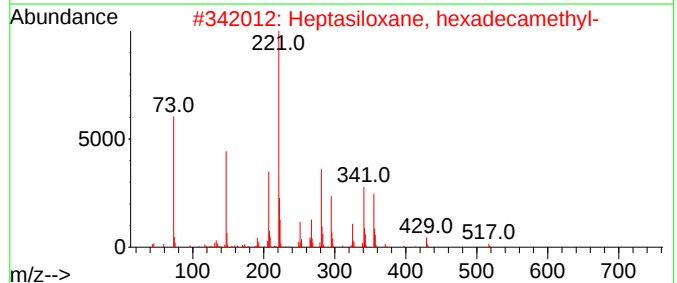
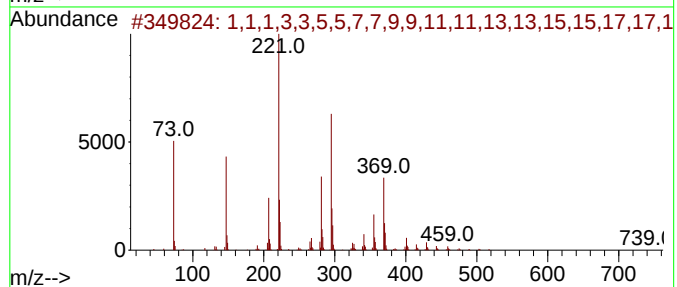
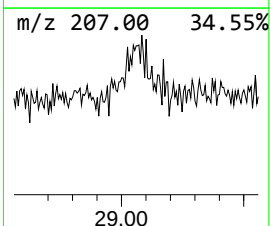
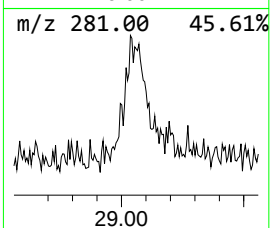
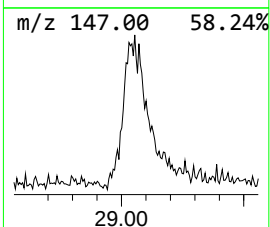
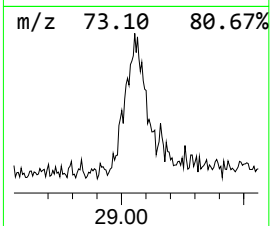
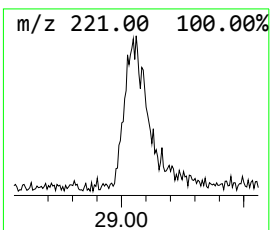
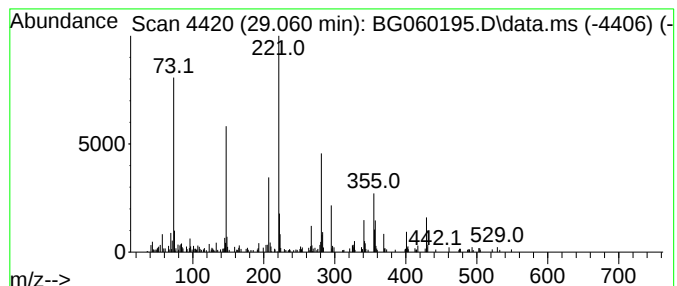
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown29.060 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.060	3.26 ng	730468	Perylene-d12	24.765

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	754	C22H66O9Si10	000556-70-7	38		
2	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	35		
3	2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	32		
4	1H-Benzimidazol-2-yl 3-nitrobenz...	357	C17H19N3O2SSi	1000486-73-3	25		
5	7-Methylimidazo[1,2-a]pyrimidin-...	221	C10H15N3OSi	1010468-48-3	25		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060195.D
Acq On : 2 Jan 2024 15:10
Operator : MA/JU
Sample : 05909-15
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-53

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.114	3.114	8.0	ng	432071	1	7.938	1075720	20.0
Trichloroacetic...	21.234	3.1	ng	697704	5	21.586	4539980	20.0
Hexasiloxane, t...	23.196	2.5	ng	570484	6	24.765	4486170	20.0
unknown24.230	24.230	3.8	ng	858546	6	24.765	4486170	20.0
unknown25.499	25.499	3.8	ng	840967	6	24.765	4486170	20.0
unknown29.060	29.060	3.3	ng	730468	6	24.765	4486170	20.0