

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111623\
 Data File : BG059721.D
 Acq On : 16 Nov 2023 16:48
 Operator : MA/JU
 Sample : PB157140BL
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB157140BL

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-BG111623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG059721.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.371	332	337	342	rVB3	37172	55507	1.58%	0.328%
2	5.829	408	415	423	rBV	518959	817141	23.29%	4.822%
3	7.457	683	692	701	rBV	578537	955592	27.23%	5.639%
4	8.338	836	842	849	rBV3	103580	182828	5.21%	1.079%
5	9.537	1037	1046	1053	rBV	345432	624482	17.80%	3.685%
6	11.188	1319	1327	1333	rBV	126018	232424	6.62%	1.372%
7	13.591	1728	1736	1742	rBV	1062216	1618244	46.12%	9.550%
8	14.966	1964	1970	1977	rBV3	218075	335816	9.57%	1.982%
9	16.452	2216	2223	2229	rBV	958700	1398632	39.86%	8.254%
10	17.715	2431	2438	2452	rVB	315045	478016	13.62%	2.821%
11	18.632	2586	2594	2597	rBV	24461	37345	1.06%	0.220%
12	20.295	2870	2877	2882	rBV	2859928	3508885	100.00%	20.707%
13	20.970	2989	2992	2995	rBV4	27809	37207	1.06%	0.220%
14	21.000	2995	2997	3003	rVB2	37603	46282	1.32%	0.273%
15	21.117	3013	3017	3021	rVB2	55689	74740	2.13%	0.441%
16	21.805	3129	3134	3139	rBV2	175471	285484	8.14%	1.685%
17	21.846	3139	3141	3147	rVB4	41158	74361	2.12%	0.439%
18	22.040	3167	3174	3180	rVV	273992	519986	14.82%	3.069%
19	22.580	3259	3266	3273	rBV3	262367	500019	14.25%	2.951%
20	23.479	3412	3419	3430	rBV2	323416	730929	20.83%	4.313%
21	24.472	3580	3588	3589	rBV5	27760	56046	1.60%	0.331%
22	24.572	3594	3605	3620	rVV	382847	1062459	30.28%	6.270%
23	25.630	3775	3785	3797	rVB2	231518	720552	20.54%	4.252%
24	25.906	3819	3832	3845	rBV5	332303	1150052	32.78%	6.787%
25	27.580	4102	4117	4129	rBV7	211493	910231	25.94%	5.372%
26	29.678	4458	4474	4476	rBV8	132749	447266	12.75%	2.639%
27	32.334	4919	4926	4928	rBV6	39147	84636	2.41%	0.499%

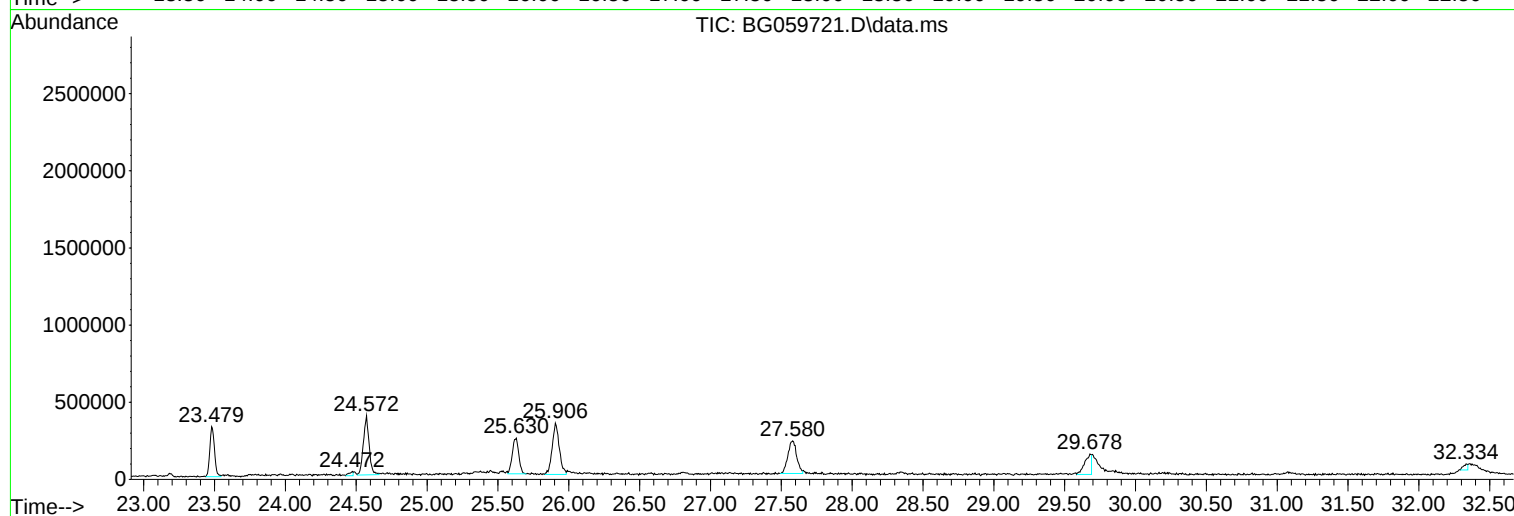
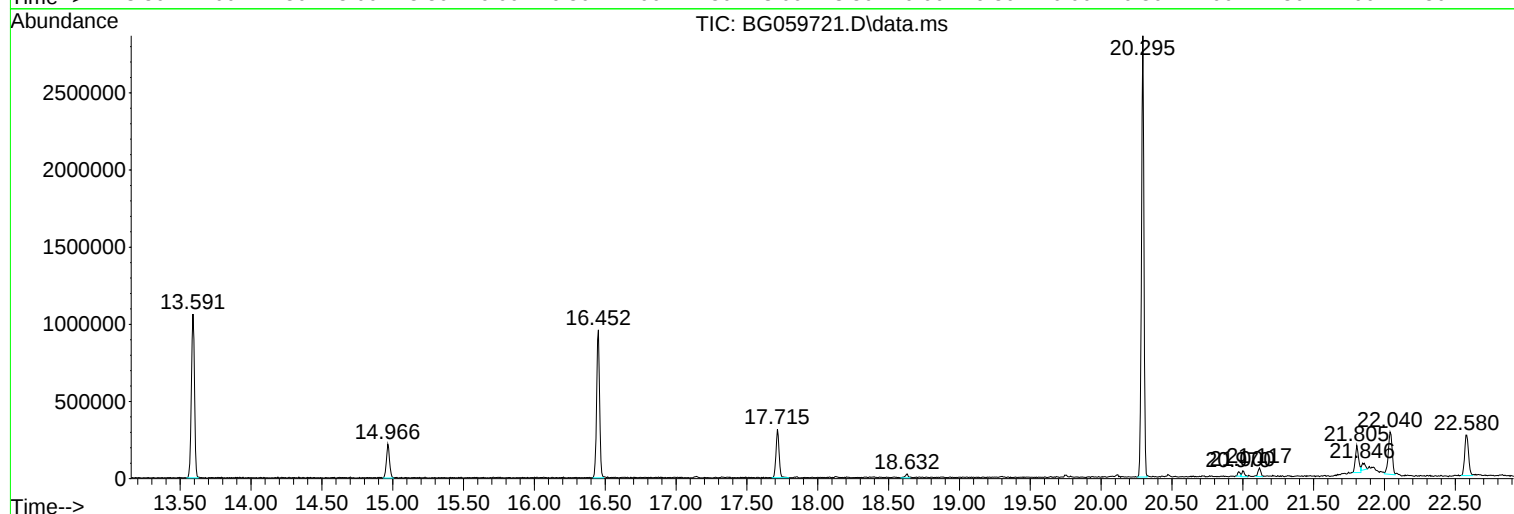
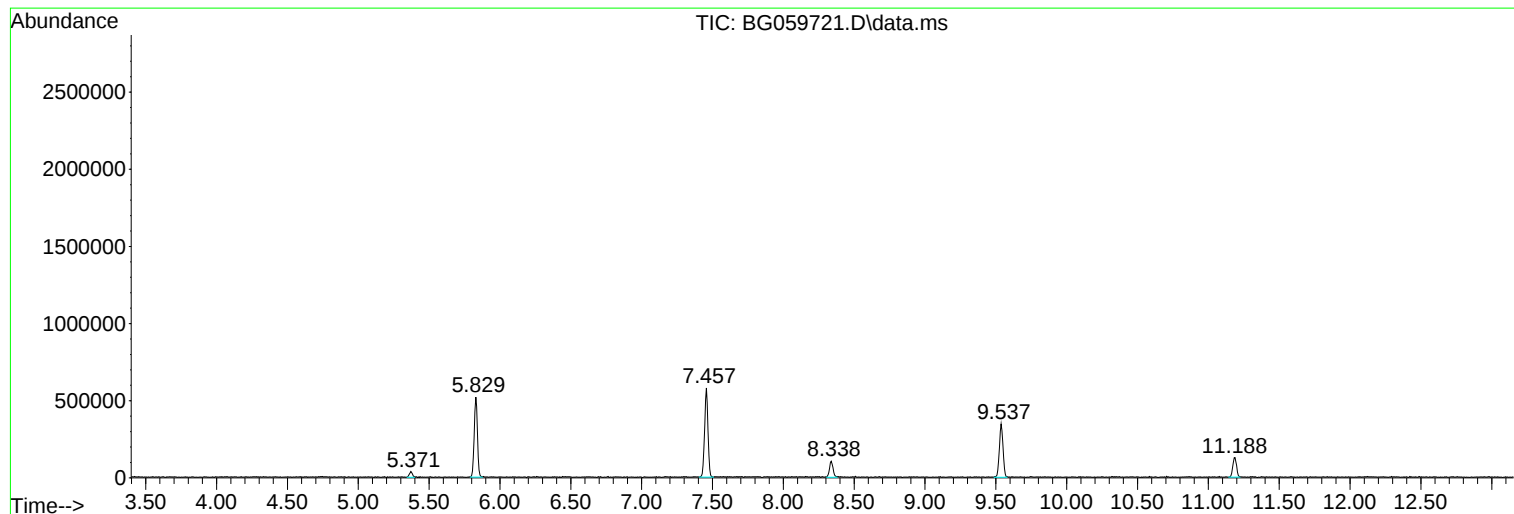
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.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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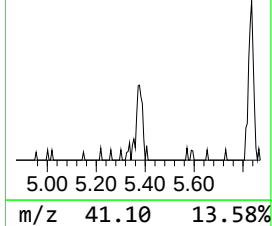
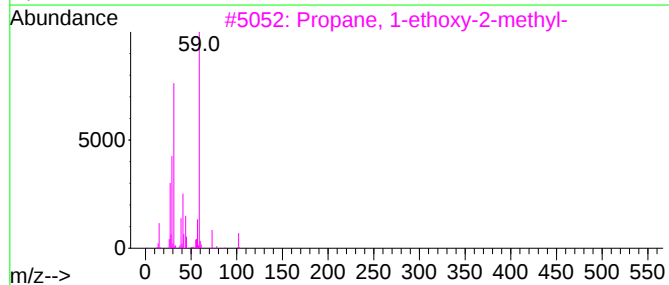
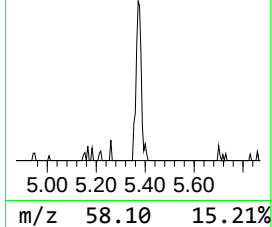
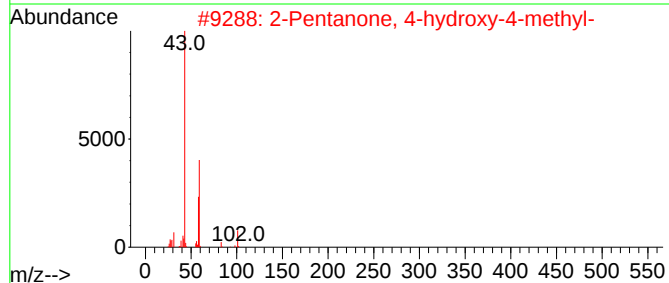
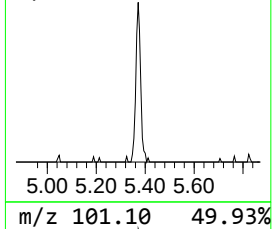
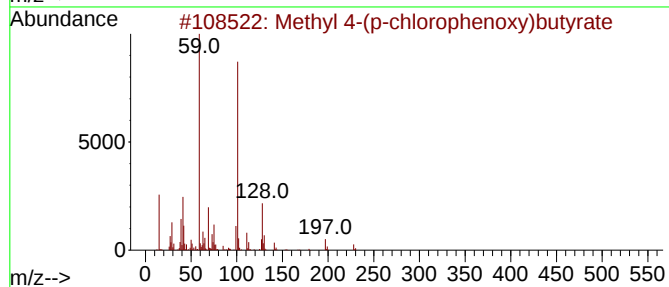
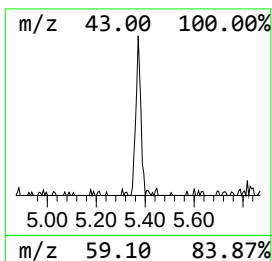
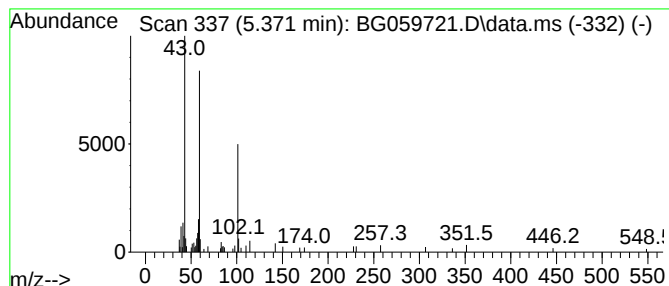
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Methyl 4-(p-chlorophenoxy)b... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.371	6.07 ng	55507	1,4-Dichlorobenzene-d4	8.344

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 4-(p-chlorophenoxy)butyrate	228	C11H13ClO3	209052-80-2	72
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
3			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	46
4			2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	43
5			2,3-Dimethyloxirane-2-carboxylic...	130	C6H10O3	1000306-64-4	37



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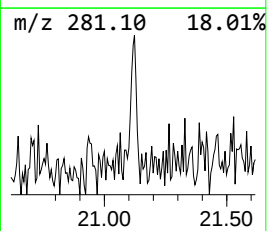
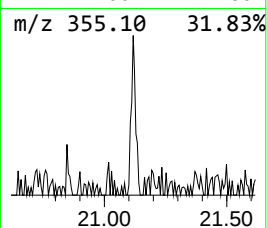
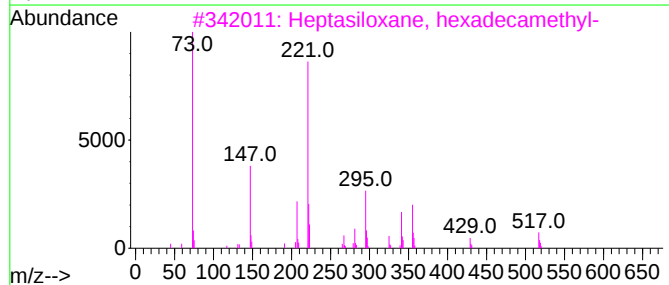
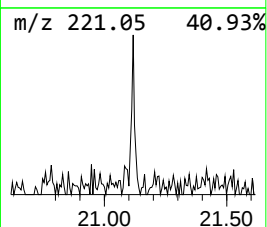
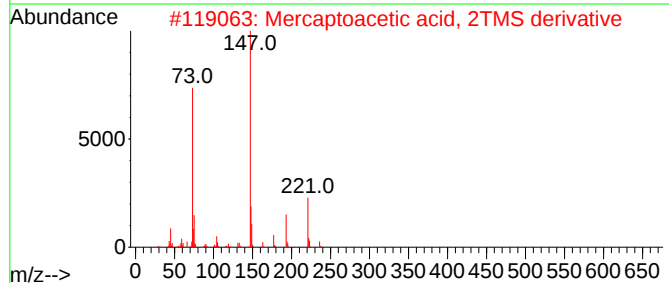
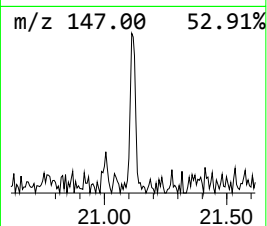
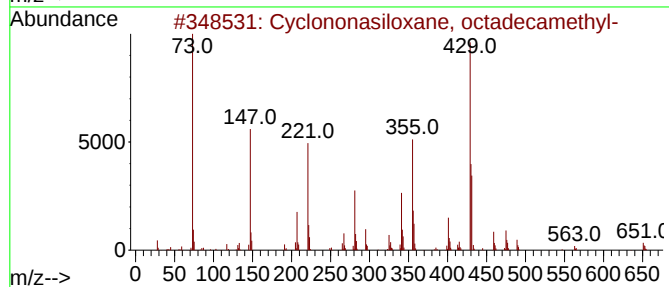
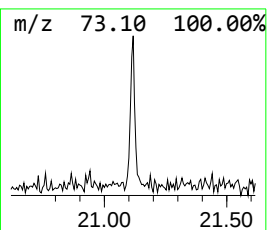
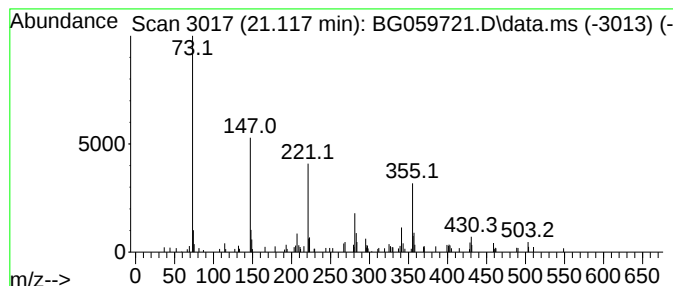
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Peak Number 2 unknown21.117 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.117	2.87 ng	74740	Chrysene-d12	22.040

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	42
2			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	38
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	38
4			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	37
5			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	32



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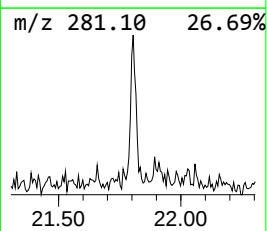
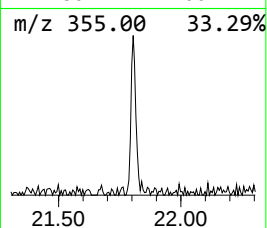
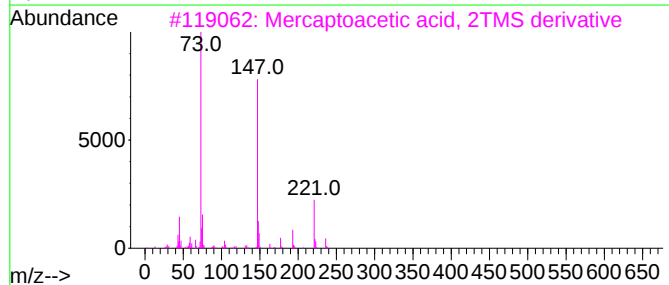
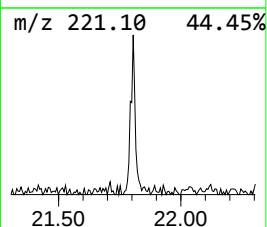
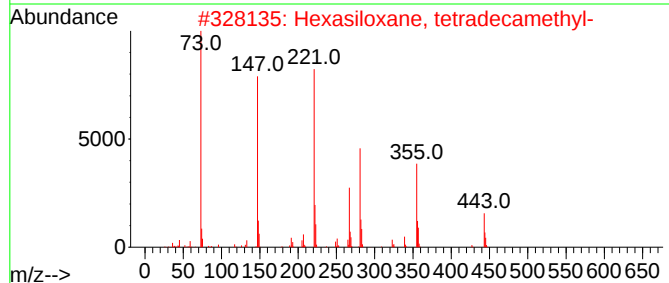
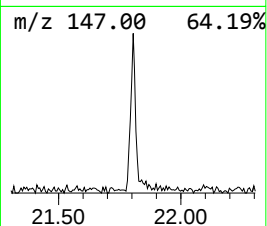
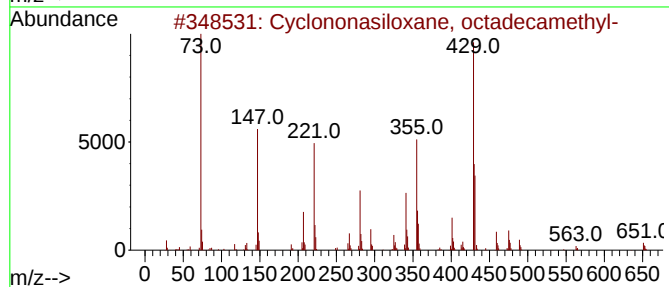
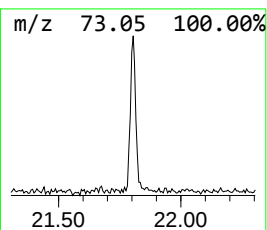
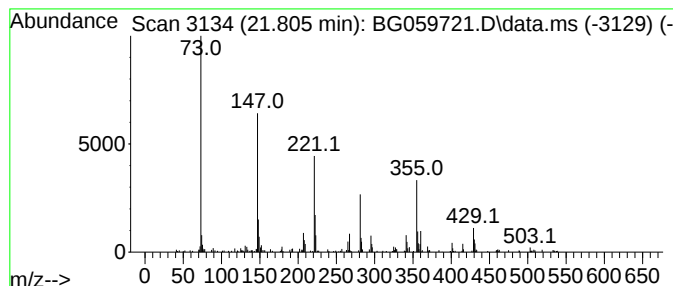
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Cyclononasiloxane, octadeca... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.805	10.98 ng	285484	Chrysene-d12	22.040

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	64
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	45
3			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	43
4			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	30
5			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	25



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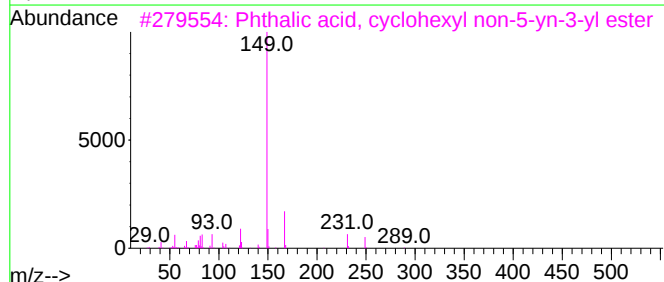
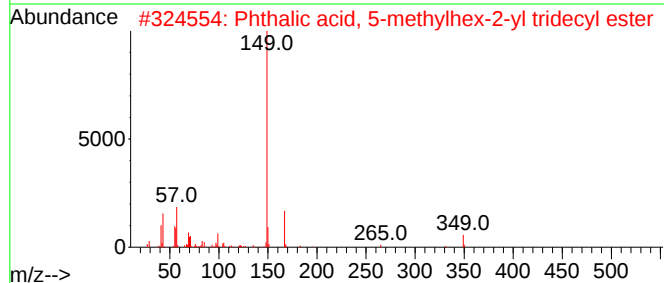
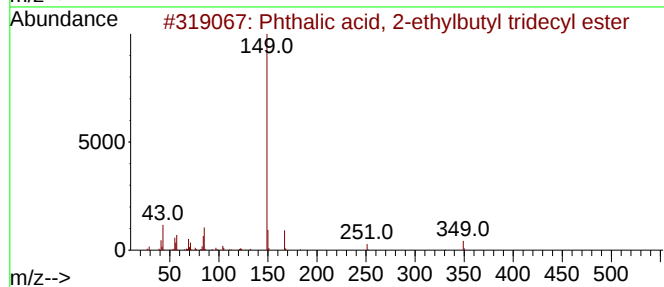
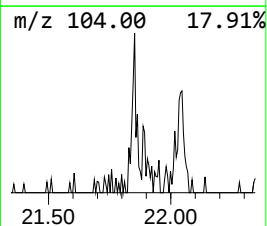
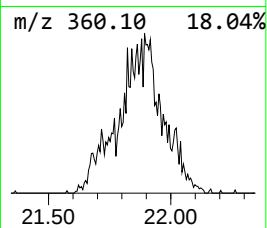
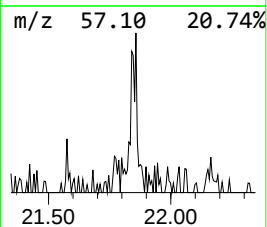
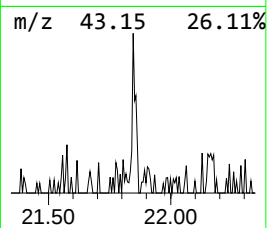
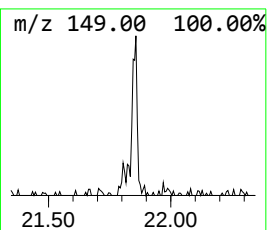
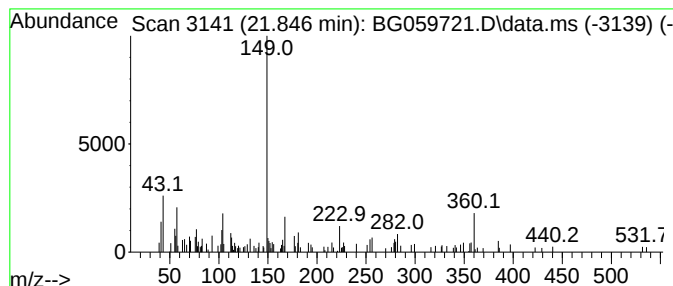
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Peak Number 4 Phthalic acid, 2-ethylbutyl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.846	2.86 ng	74361	Chrysene-d12	22.040

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic acid, 2-ethylbutyl trid...	432	C27H44O4	1000356-89-8	53
2			Phthalic acid, 5-methylhex-2-yl ...	446	C28H46O4	1000371-08-1	53
3			Phthalic acid, cyclohexyl non-5-...	370	C23H30O4	1000315-75-1	50
4			Succinic acid, 2-(3-nitrophenyl)...	379	C20H29NO6	1000380-99-7	50
5			Phthalic acid, undec-2-en-1-yl u...	472	C30H48O4	1000315-42-2	50



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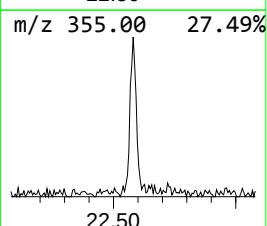
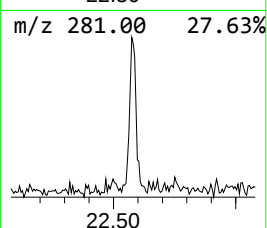
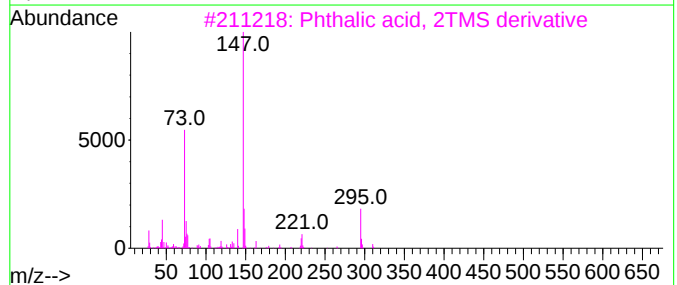
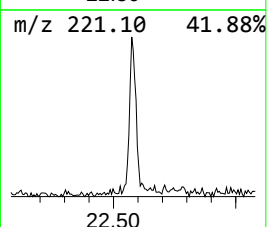
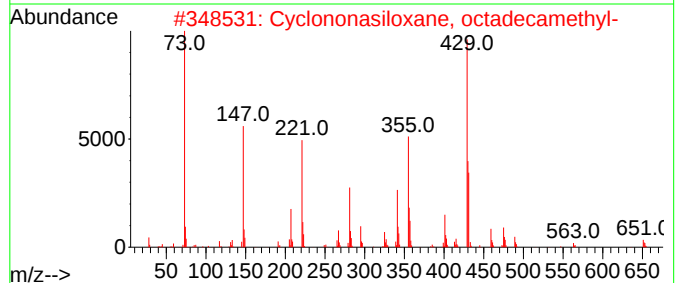
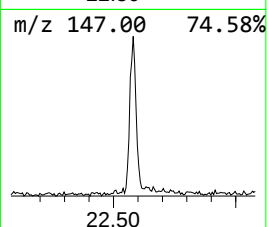
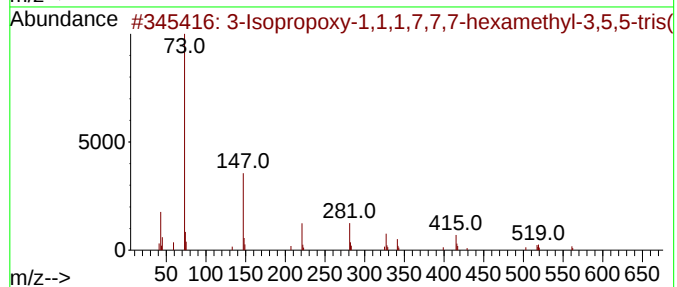
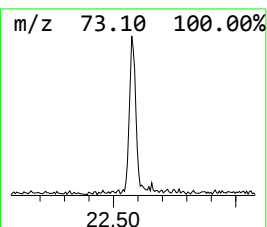
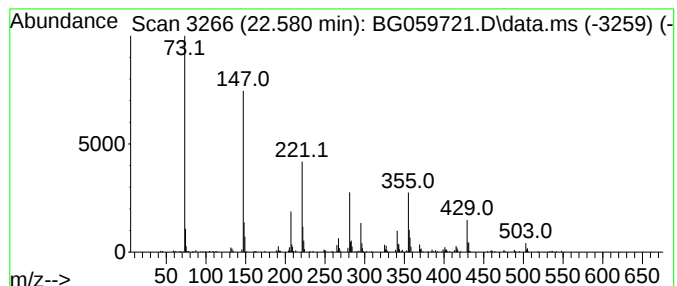
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown22.580 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.580	19.23 ng	500019	Chrysene-d12	22.040

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	38		
2	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	38		
3	Phthalic acid, 2TMS derivative	310	C14H22O4Si2	002078-22-0	35		
4	Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	32		
5	Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	32		



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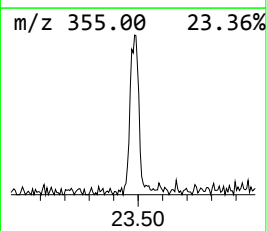
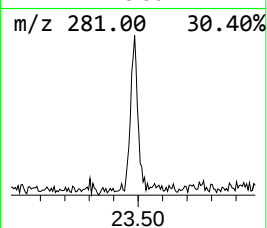
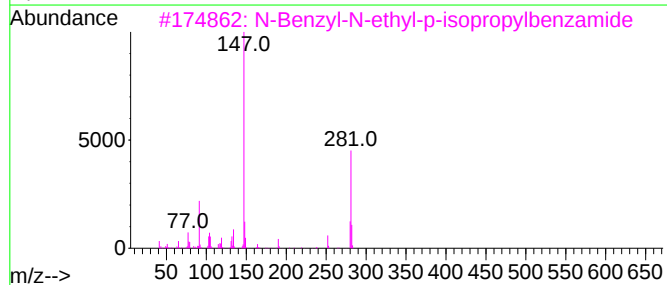
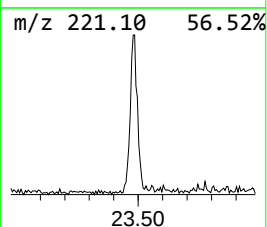
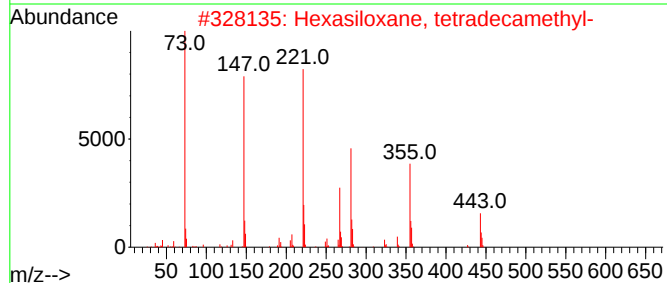
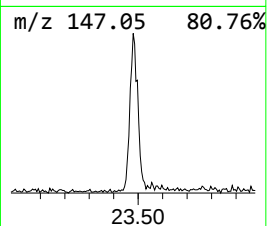
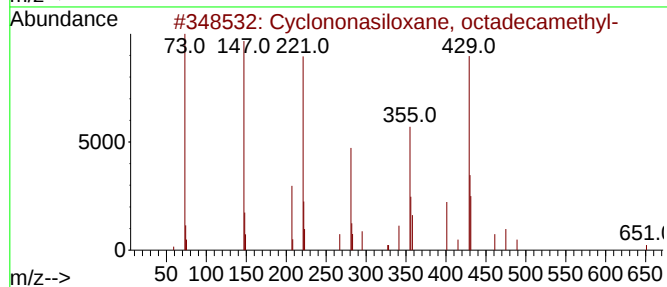
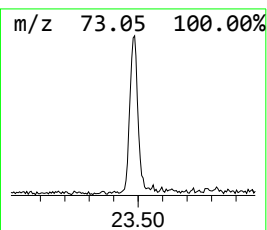
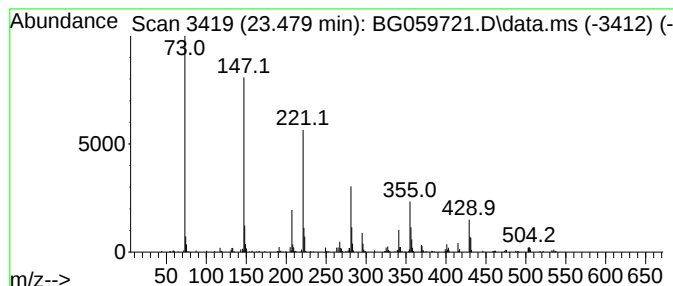
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown23.479 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.479	28.11 ng	730929	Chrysene-d12	22.040

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	86
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	49
3			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	43
4			benzoic acid, 2,4,5-trimethyl-, ...	236	C13H20O2Si	1000396-43-7	28
5			2-Phenyl-N-(4-sulfamoylphenyl)ac...	506	C23H38N2O3SSi3	1000514-11-6	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111623\
Data File : BG059721.D
Acq On : 16 Nov 2023 16:48
Operator : MA/JU
Sample : PB157140BL
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB157140BL

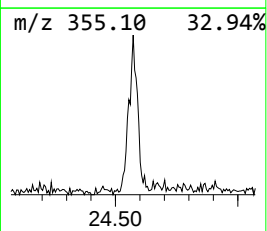
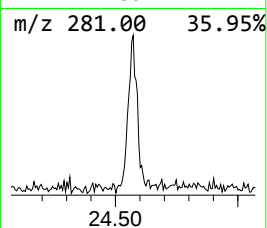
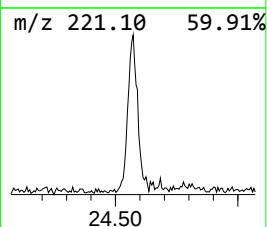
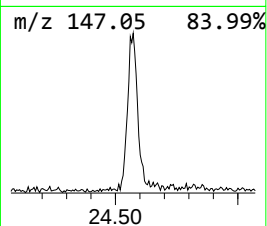
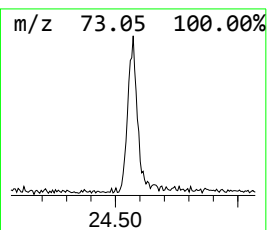
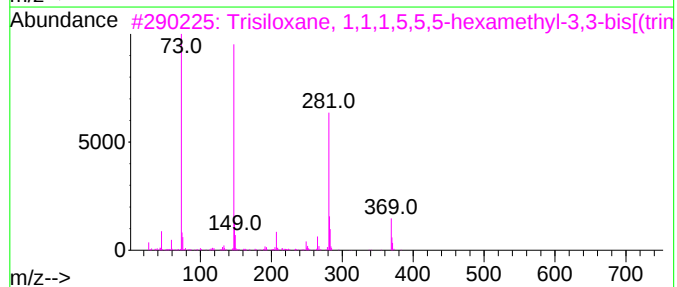
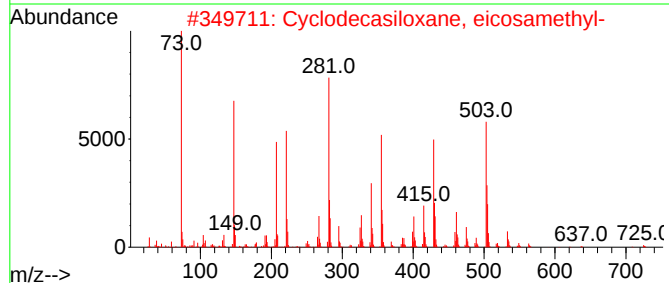
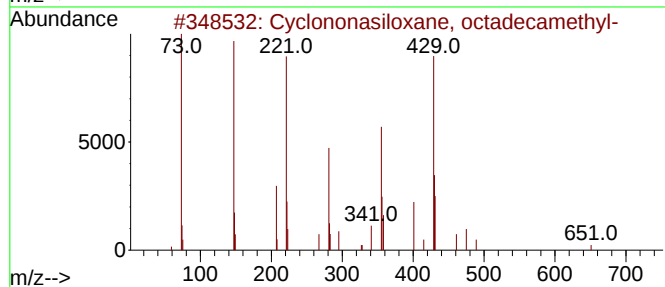
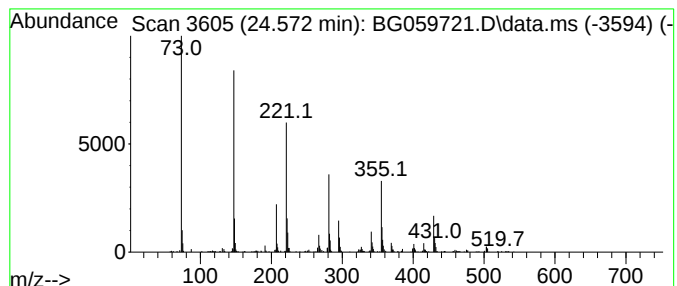
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown24.572 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.572	29.49 ng	1062460	Perylene-d12	25.630

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	91
2			Cyclodecasiloxane, eicosamethyl-	740	C20H60O10Si10	018772-36-6	45
3			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	38
4			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	38
5			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	754	C22H66O9Si10	000556-70-7	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111623\
Data File : BG059721.D
Acq On : 16 Nov 2023 16:48
Operator : MA/JU
Sample : PB157140BL
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB157140BL

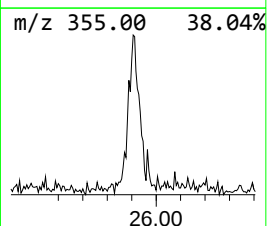
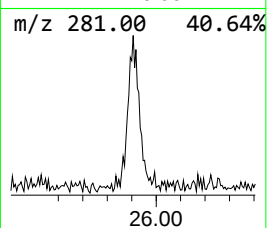
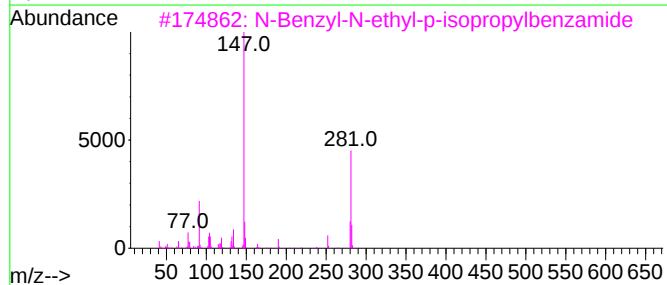
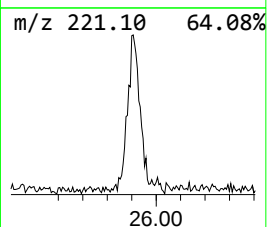
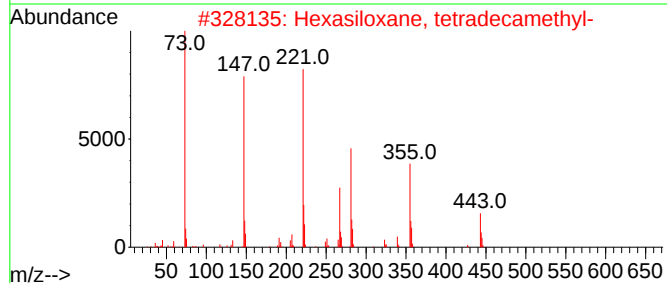
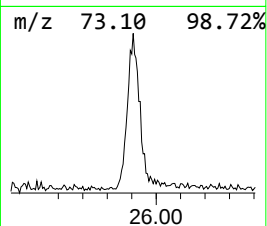
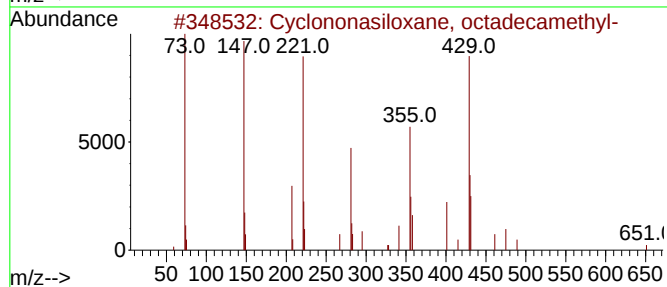
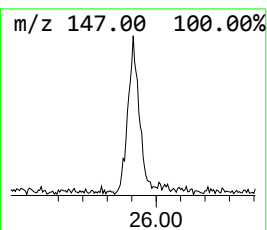
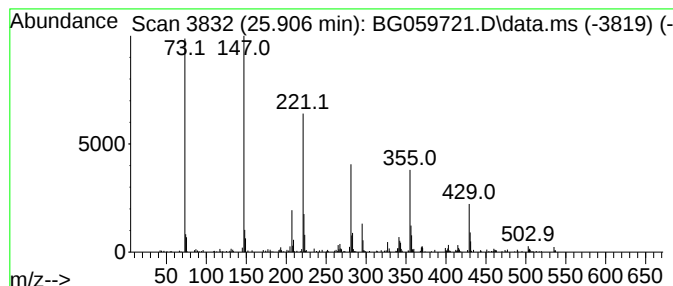
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown25.906 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.906	31.92 ng	1150050	Perylene-d12	25.630

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	49
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	47
3			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	38
4			benzoic acid, 2,4,5-trimethyl-, ...	236	C13H20O2Si	1000396-43-7	32
5			L-Ribulose, tetrakis(trimethylsi...	633	C24H44F5NO5Si4	1000394-62-4	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111623\
Data File : BG059721.D
Acq On : 16 Nov 2023 16:48
Operator : MA/JU
Sample : PB157140BL
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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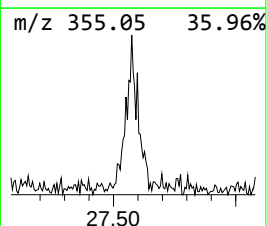
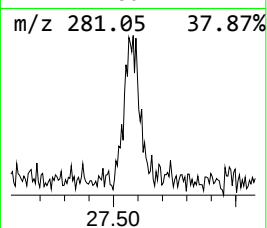
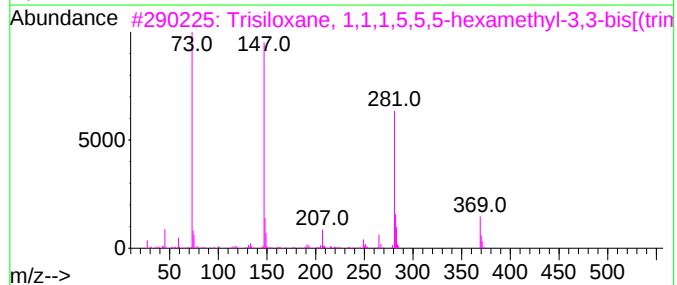
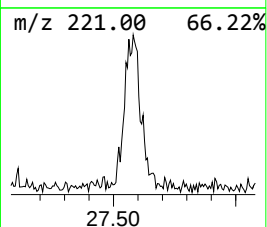
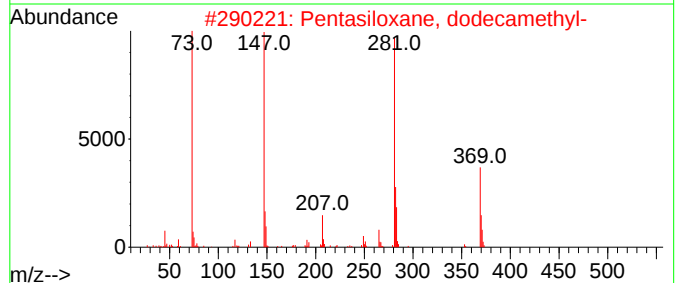
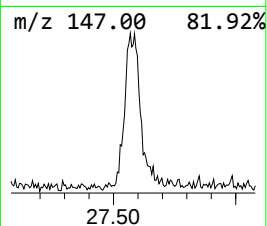
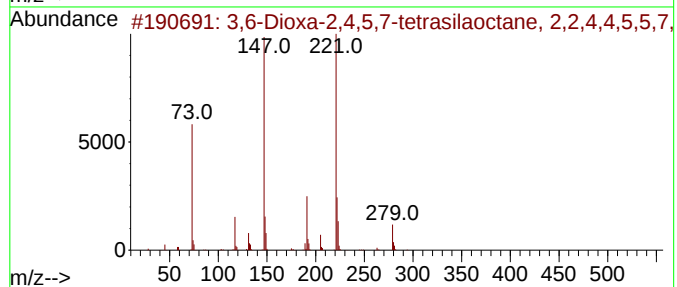
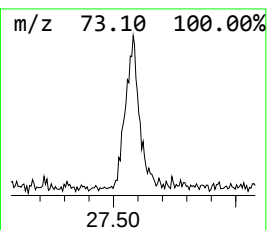
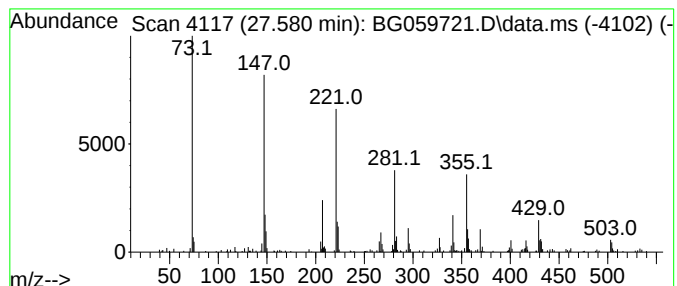
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown27.580 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.580	25.26 ng	910231	Perylene-d12	25.630

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	40
2			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	38
3			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	38
4			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	38
5			8-Azaxanthin, 3TMS derivative	369	C13H27N5O2Si3	1000478-52-4	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111623\
Data File : BG059721.D
Acq On : 16 Nov 2023 16:48
Operator : MA/JU
Sample : PB157140BL
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB157140BL

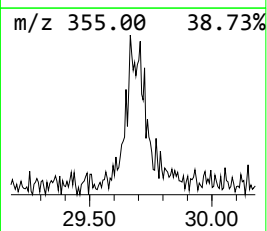
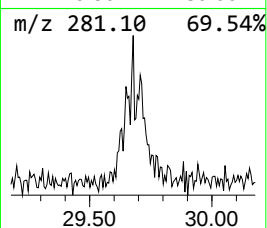
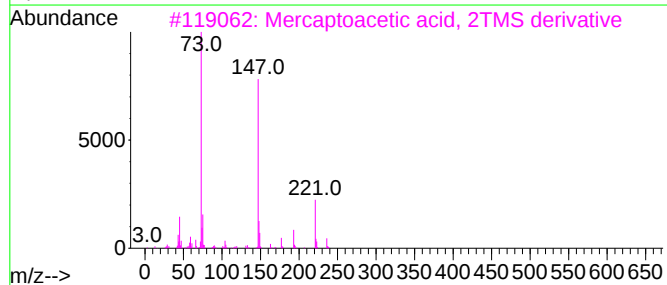
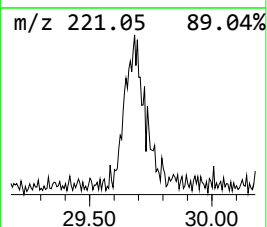
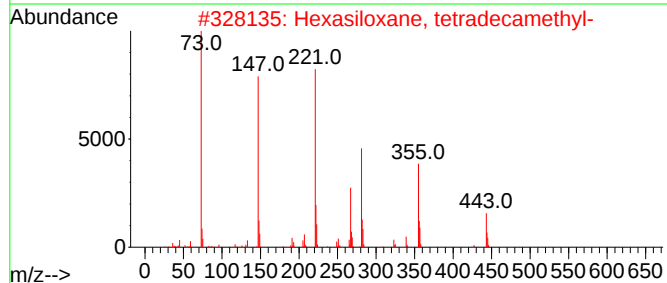
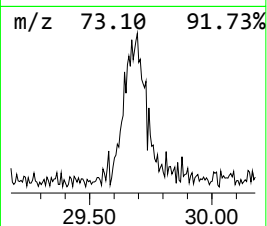
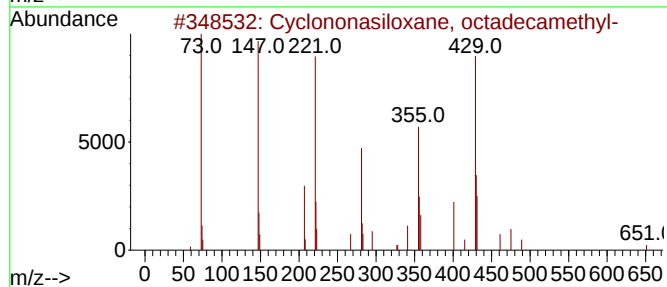
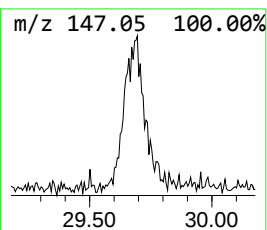
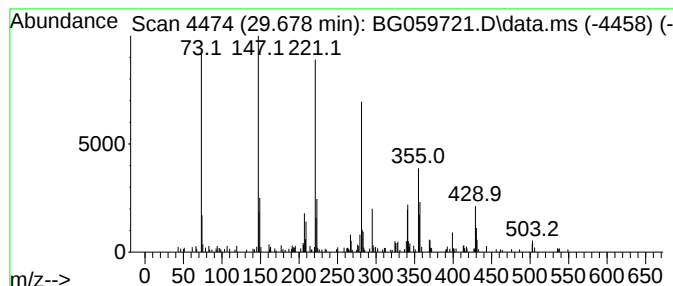
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown29.678 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.678	12.41 ng	447266	Perylene-d12	25.630

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	45
2		Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	32
3		Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	25
4		3,6-Dioxo-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	12
5		Boron, diethyl(5-ethyl-4,6-nonan...	250	C15H31BN2	136705-03-8	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111623\
Data File : BG059721.D
Acq On : 16 Nov 2023 16:48
Operator : MA/JU
Sample : PB157140BL
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB157140BL

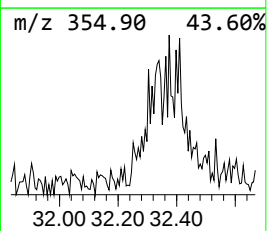
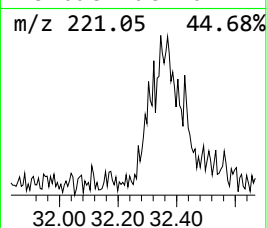
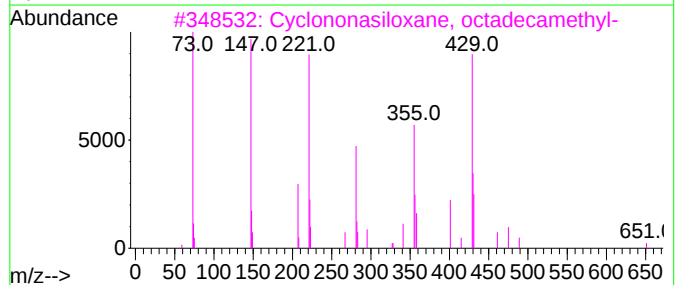
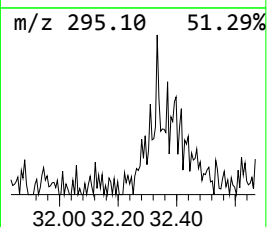
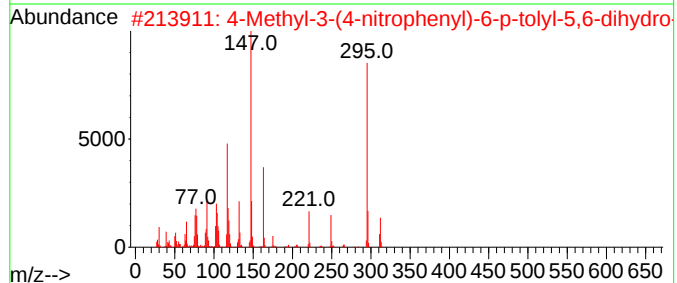
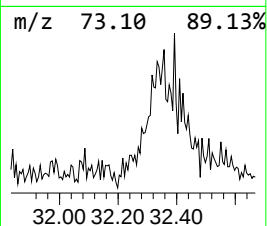
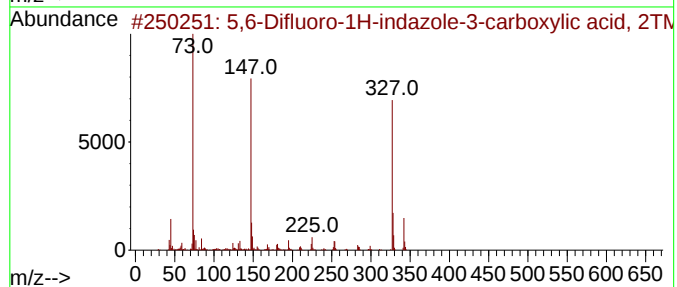
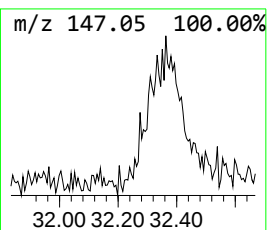
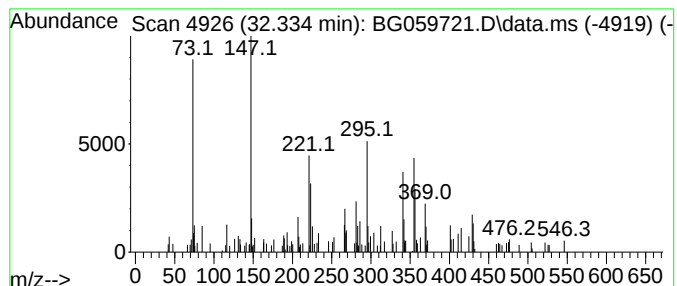
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown32.334 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
32.334	2.35 ng	84636	Perylene-d12	25.630

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5,6-Difluoro-1H-indazole-3-carbo...	342	C14H20F2N2O2Si2	1000500-32-0	25
2			4-Methyl-3-(4-nitrophenyl)-6-p-t...	312	C16H16N4O3	1000210-54-0	22
3			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	14
4			Paracetamol, 2TMS derivative	295	C14H25N02Si2	055530-61-5	11
5			Nickel, bis(N,N,N'-trimethyl-o-p...	356	C18H26N4Ni	1000153-51-1	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111623\
Data File : BG059721.D
Acq On : 16 Nov 2023 16:48
Operator : MA/JU
Sample : PB157140BL
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB157140BL

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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					#	RT	Resp	Conc
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unknown21.117	21.117	2.9	ng	74740	5	22.040	519986	20.0
Cyclononasiloxa...	21.805	11.0	ng	285484	5	22.040	519986	20.0
Phthalic acid, ...	21.846	2.9	ng	74361	5	22.040	519986	20.0
unknown22.580	22.580	19.2	ng	500019	5	22.040	519986	20.0
unknown23.479	23.479	28.1	ng	730929	5	22.040	519986	20.0
unknown24.572	24.572	29.5	ng	1062460	6	25.630	720552	20.0
unknown25.906	25.906	31.9	ng	1150050	6	25.630	720552	20.0
unknown27.580	27.580	25.3	ng	910231	6	25.630	720552	20.0
unknown29.678	29.678	12.4	ng	447266	6	25.630	720552	20.0
unknown32.334	32.334	2.4	ng	84636	6	25.630	720552	20.0