

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
 Data File : BG059869.D
 Acq On : 24 Nov 2023 22:24
 Operator : MA/JU
 Sample : 05408-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 710-NEW-YORK-AVE

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: BG059869.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.808	406	412	420	rBV	379859	622936	23.02%	4.648%
2	7.441	681	690	698	rBV2	364888	631518	23.34%	4.712%
3	8.317	832	839	846	rBV2	150042	260026	9.61%	1.940%
4	9.521	1035	1044	1051	rBV	358179	663218	24.51%	4.948%
5	11.160	1317	1323	1330	rBV2	161887	304003	11.23%	2.268%
6	13.569	1726	1733	1740	rBV	1117352	1683940	62.23%	12.564%
7	14.950	1960	1968	1975	rBV	416168	632766	23.38%	4.721%
8	16.431	2214	2220	2227	rBV	960820	1506831	55.69%	11.243%
9	17.700	2426	2436	2441	rBV	505919	794725	29.37%	5.929%
10	18.511	2567	2574	2581	rBV3	120953	193312	7.14%	1.442%
11	18.605	2588	2590	2596	rVB7	18524	30344	1.12%	0.226%
12	19.733	2777	2782	2786	rBV2	50623	82811	3.06%	0.618%
13	19.768	2786	2788	2792	rVB5	36496	45937	1.70%	0.343%
14	20.097	2840	2844	2849	rVB3	40845	62795	2.32%	0.469%
15	20.273	2868	2874	2880	rBV	2199432	2705988	100.00%	20.189%
16	21.078	3008	3011	3014	rVB5	22550	30462	1.13%	0.227%
17	21.554	3088	3092	3100	rVB10	58460	110960	4.10%	0.828%
18	21.760	3123	3127	3132	rVB2	68132	100563	3.72%	0.750%
19	22.018	3165	3171	3177	rBV	375234	638946	23.61%	4.767%
20	22.529	3252	3258	3262	rBV3	90194	171078	6.32%	1.276%
21	23.152	3361	3364	3368	rVB6	25212	36361	1.34%	0.271%
22	23.411	3401	3408	3413	rBV3	135116	273970	10.12%	2.044%
23	24.480	3583	3590	3600	rVB5	159611	452258	16.71%	3.374%
24	25.585	3771	3778	3788	rVB3	197634	570614	21.09%	4.257%
25	25.796	3800	3814	3823	rBV6	136267	479743	17.73%	3.579%
26	27.406	4078	4088	4089	rBV10	102102	196693	7.27%	1.468%
27	29.410	4425	4429	4431	rBV5	22078	36531	1.35%	0.273%
28	29.457	4431	4437	4438	rBV6	44670	83637	3.09%	0.624%

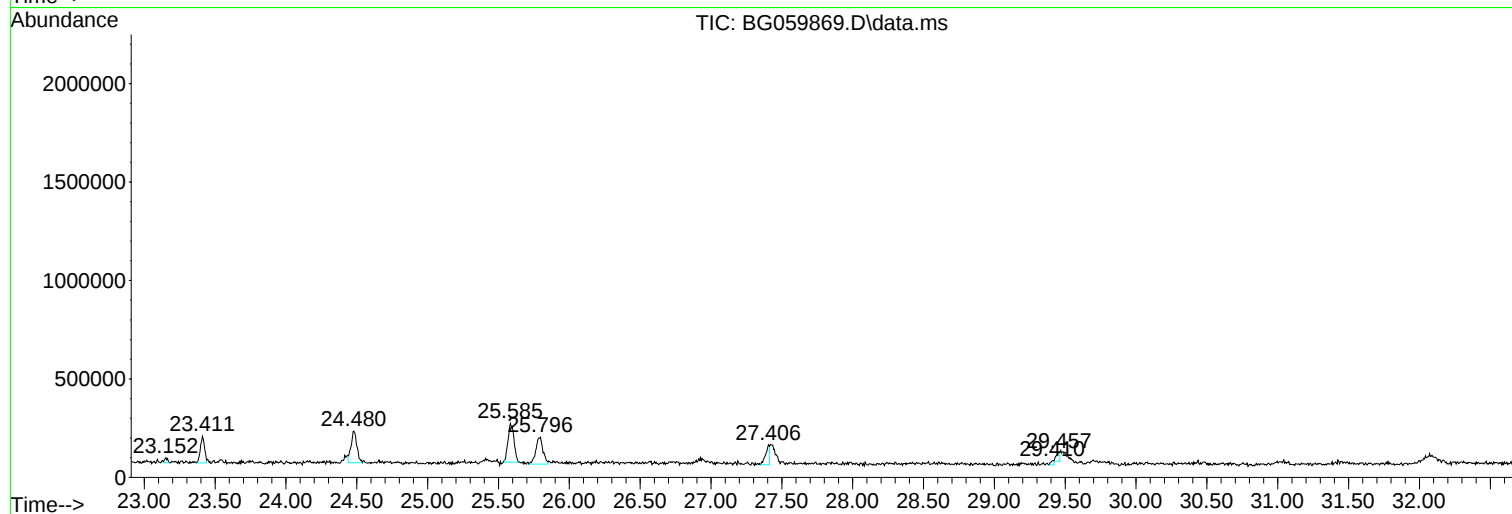
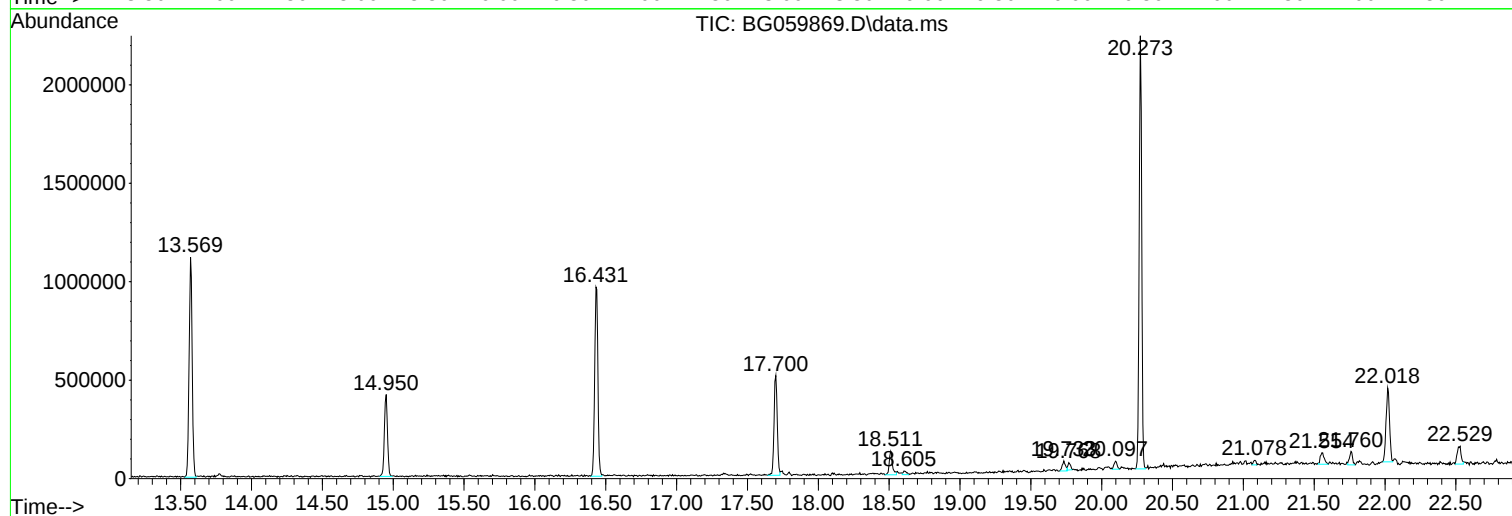
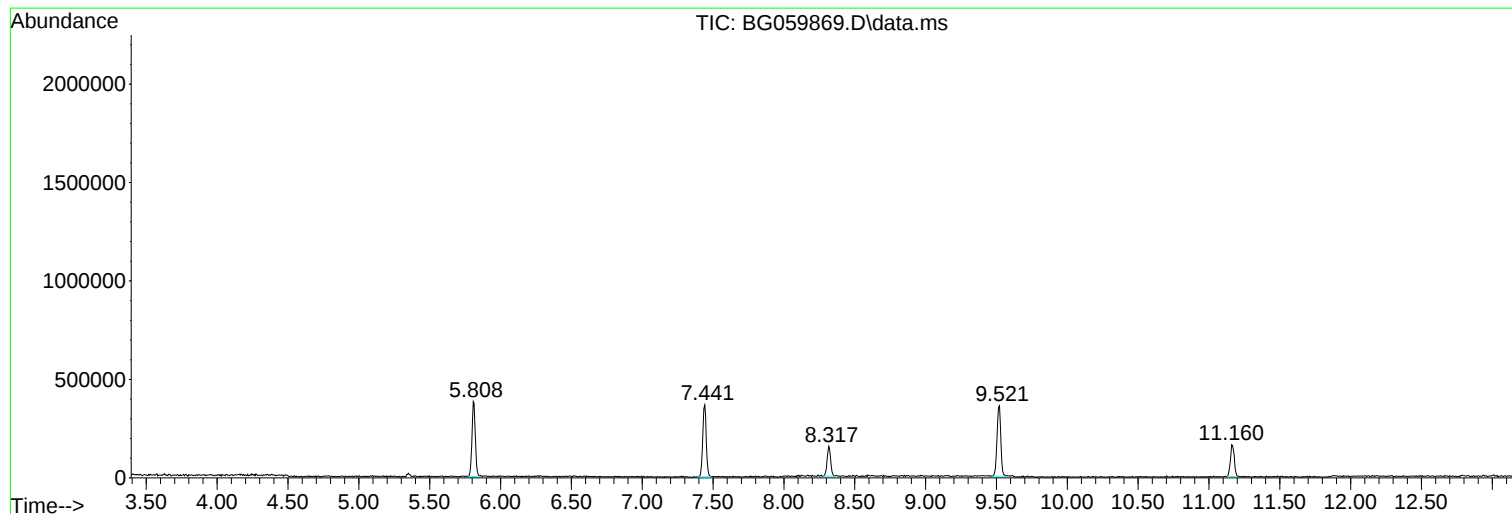
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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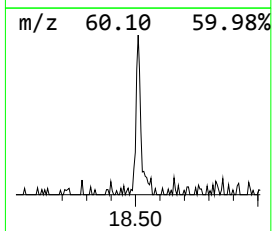
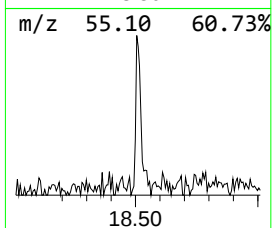
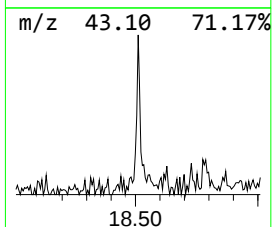
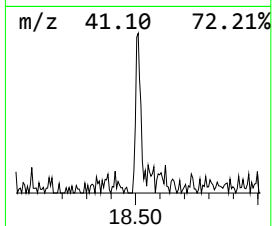
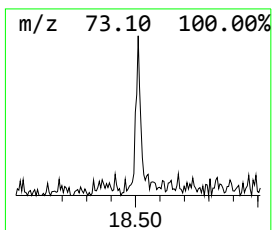
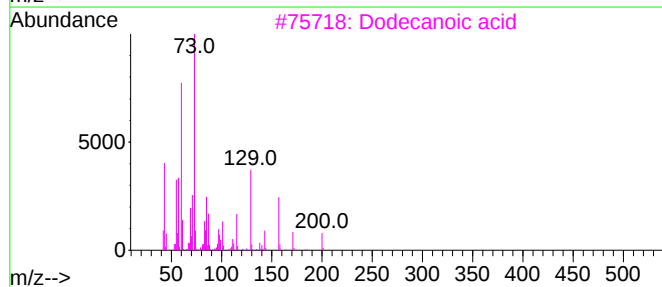
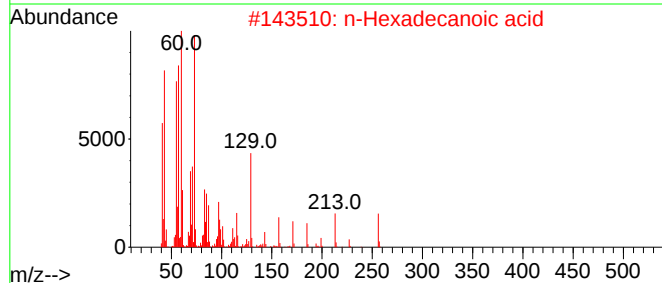
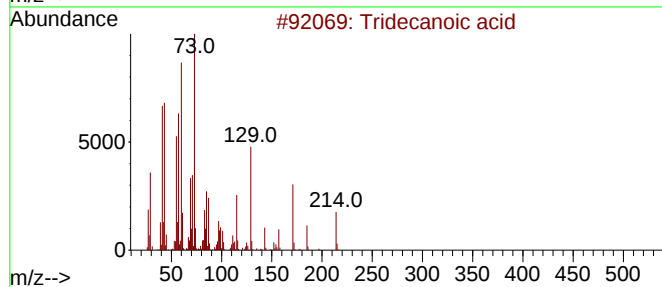
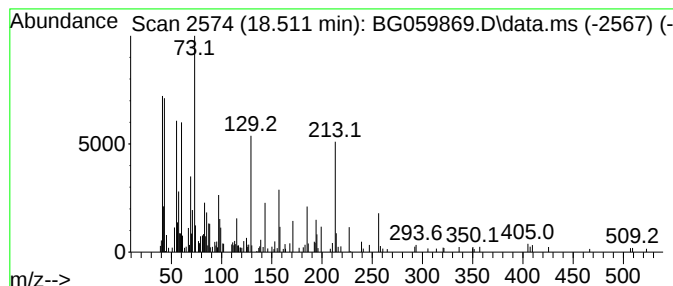
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown18.511 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.511	4.86 ng	193312	Phenanthrene-d10	17.700

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	25
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	25
3			Dodecanoic acid	200	C12H24O2	000143-07-7	22
4			Hexanoic acid, morpholide	185	C10H19NO2	1000307-28-4	14
5			n-Decanoic acid	172	C10H20O2	000334-48-5	14



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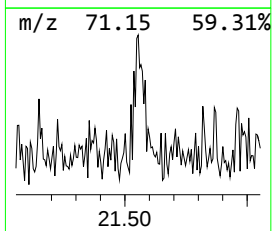
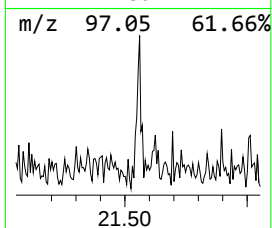
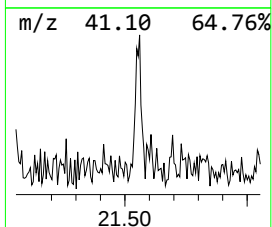
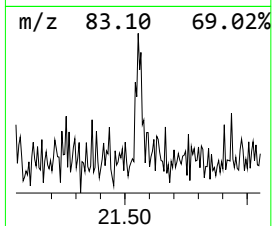
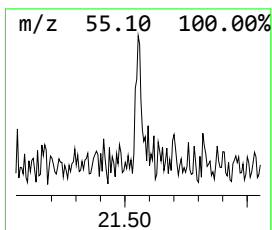
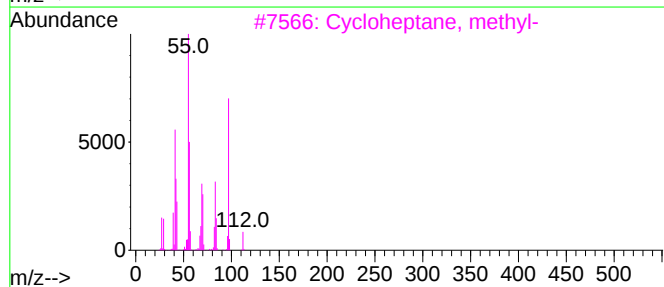
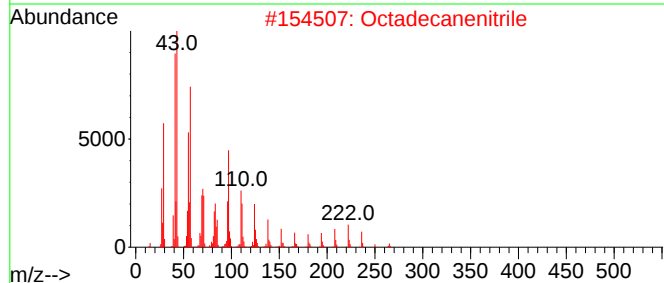
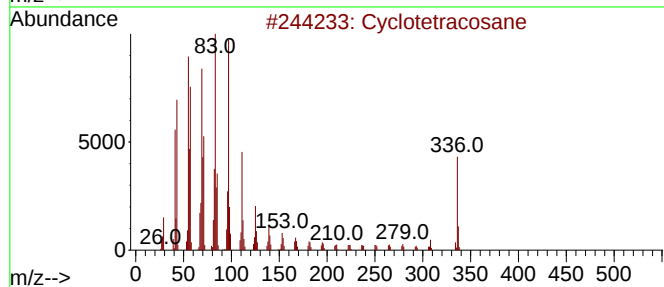
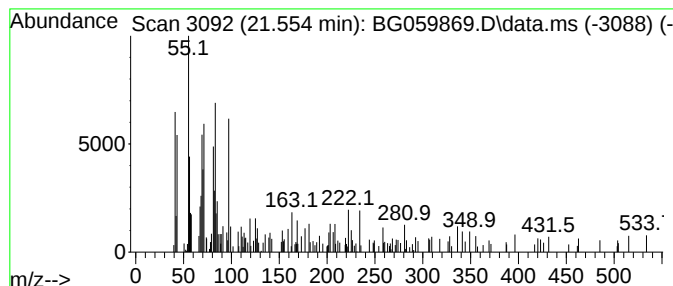
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown21.554 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.554	3.47 ng	110960	Chrysene-d12	22.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetracosane	336	C24H48	000297-03-0	47
2			Octadecanenitrile	265	C18H35N	000638-65-3	43
3			Cycloheptane, methyl-	112	C8H16	004126-78-7	20
4			4-Undecene, 4-methyl-, (Z)-	168	C12H24	074630-57-2	18
5			1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	18



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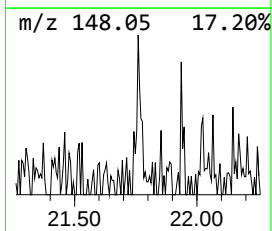
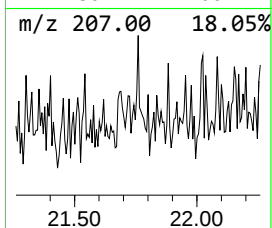
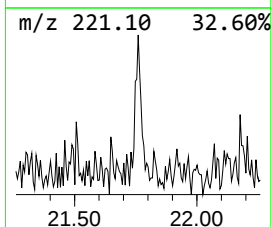
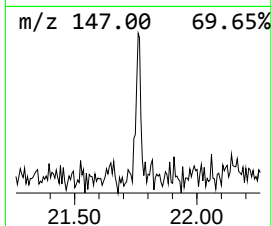
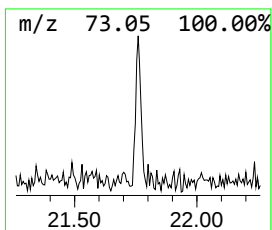
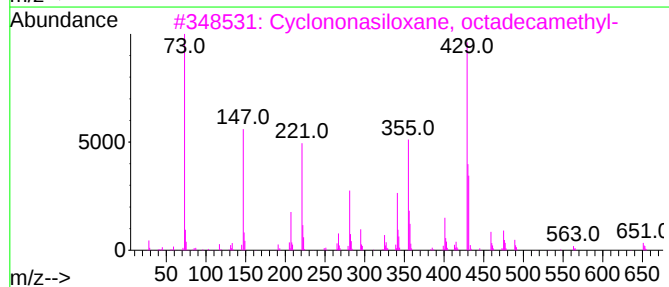
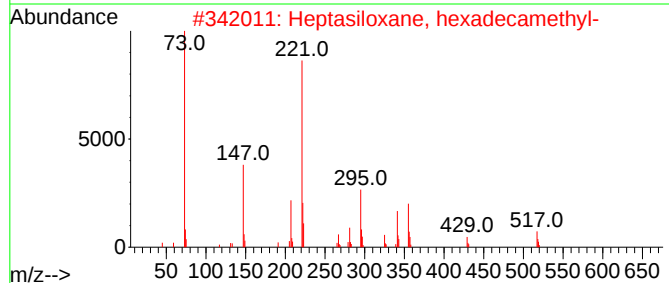
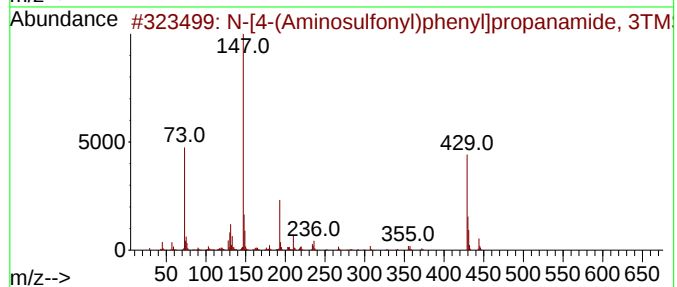
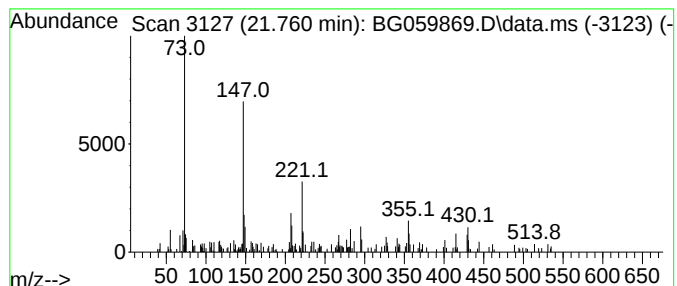
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 N-[4-(Aminosulfonyl)phenyl]... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.760	3.15 ng	100563	Chrysene-d12	22.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-[4-(Aminosulfonyl)phenyl]propa...	444	C18H36N2O3SSi3	1000500-82-8	52
2			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	43
3			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	40
4			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	40
5			Benzyloxyamine, 2TMS derivative	267	C13H25NOSi2	079208-41-6	38



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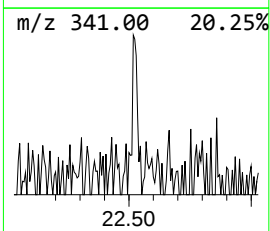
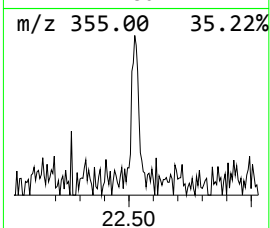
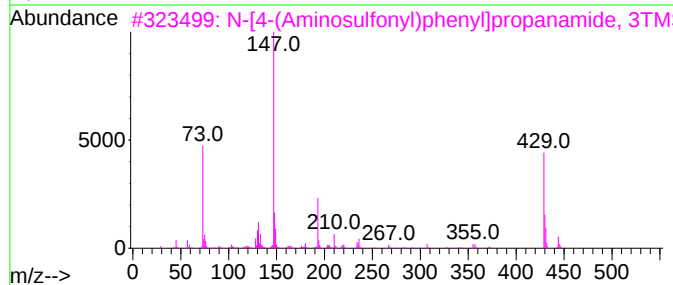
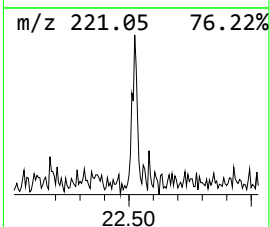
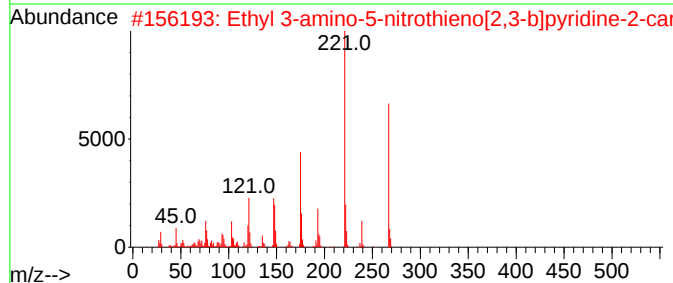
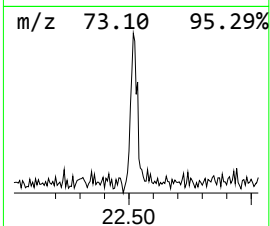
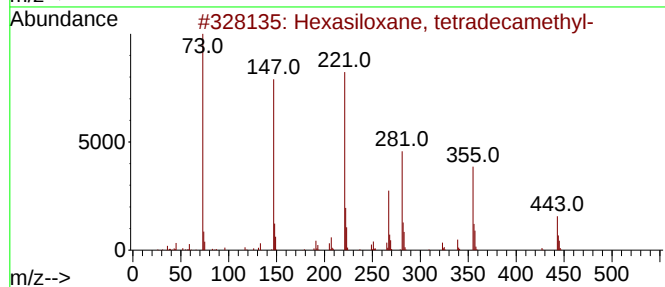
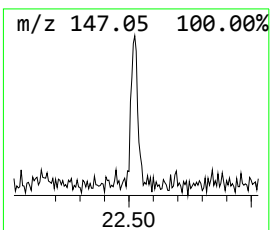
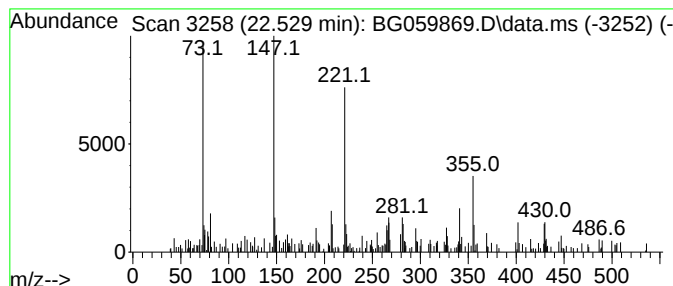
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Peak Number 5 unknown22.529 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.529	5.36 ng	171078	Chrysene-d12	22.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	43
2			Ethyl 3-amino-5-nitrothieno[2,3-...	267	C10H9N3O4S	052505-43-8	42
3			N-[4-(Aminosulfonyl)phenyl]propa...	444	C18H36N2O3SSi3	1000500-82-8	35
4			2-[2-(Methoxycarbonyl)anilino]c...	371	C19H21NO5Si	1000475-02-2	30
5			Thioglycolic acid, S-(tert-butyl...	320	C14H32O2SSi2	082112-29-6	27



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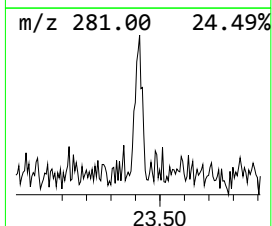
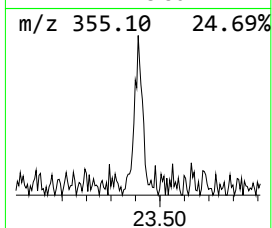
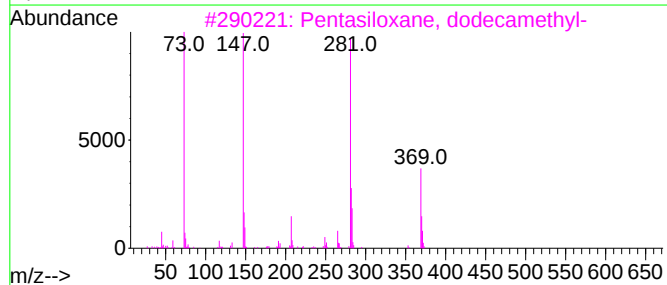
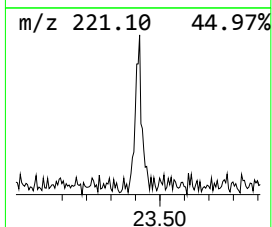
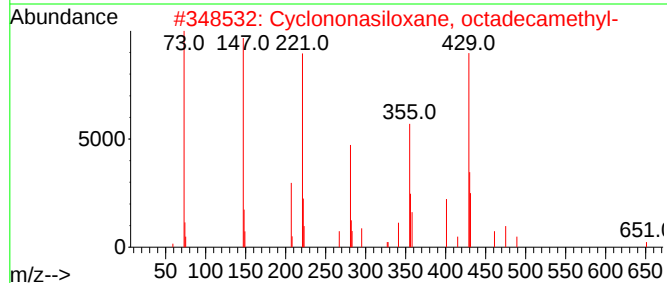
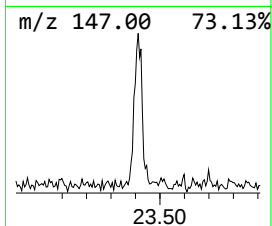
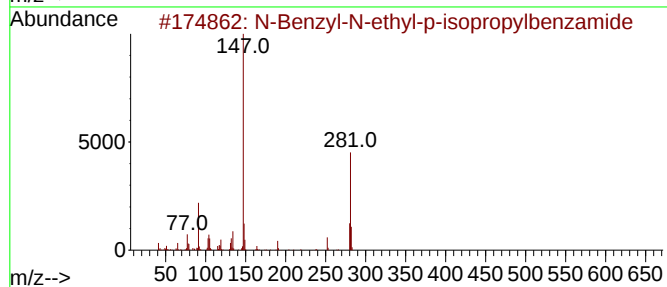
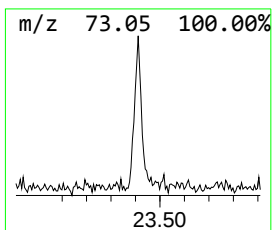
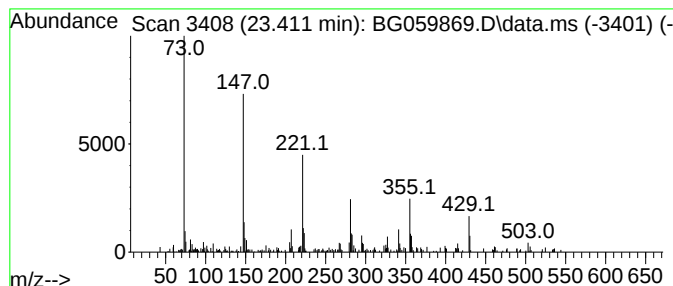
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Peak Number 6 unknown23.411 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.411	8.58 ng	273970	Chrysene-d12	22.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	43
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	43
3			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	43
4			2-(2',4',4',6',6',8',8'-Heptamet...	652	C16H48O10Si9	145344-72-5	38
5			4-(3-Aminophenoxy)phthalic acid,...	489	C23H35NO5Si3	1000468-77-9	27



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710-NEW-YORK-AVE

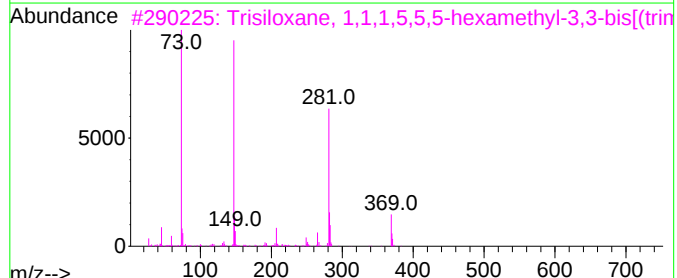
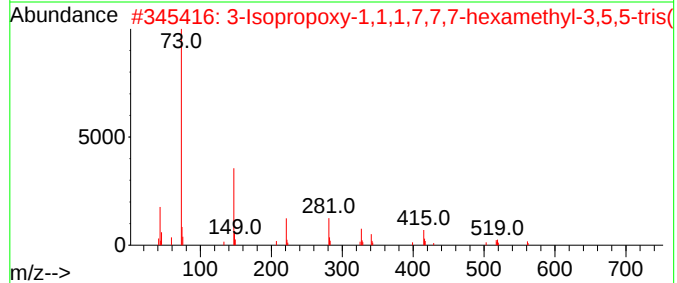
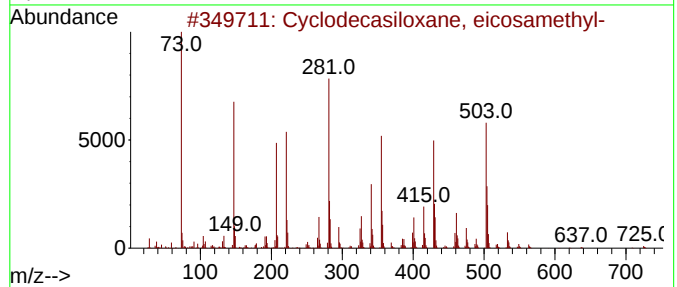
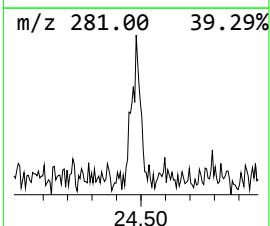
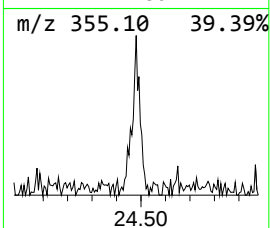
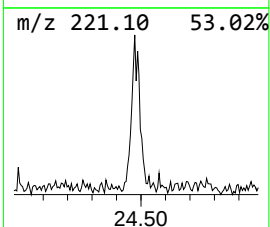
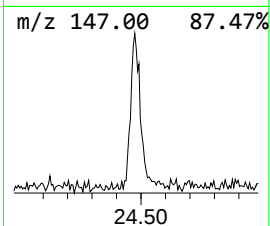
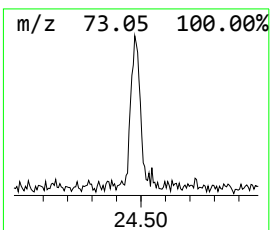
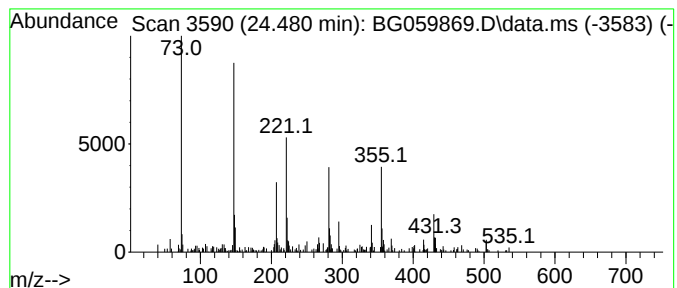
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown24.480 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.480	15.85 ng	452258	Perylene-d12	25.585

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclodecasiloxane, eicosamethyl-	740	C20H60O10Si10	018772-36-6	42
2			3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	37
3			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	35
4			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	35
5			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059869.D
Acq On : 24 Nov 2023 22:24
Operator : MA/JU
Sample : 05408-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
710-NEW-YORK-AVE

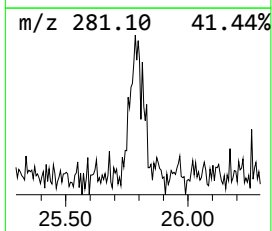
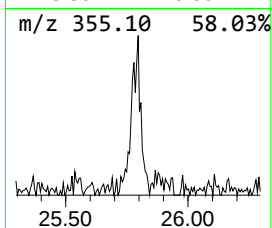
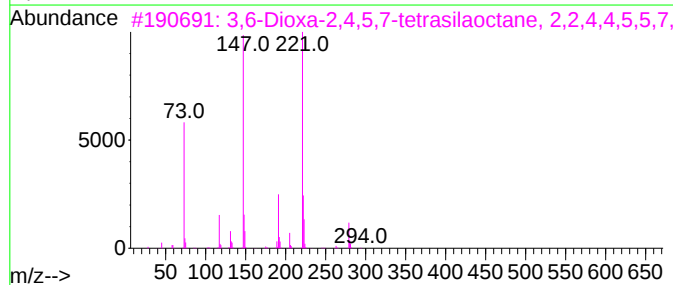
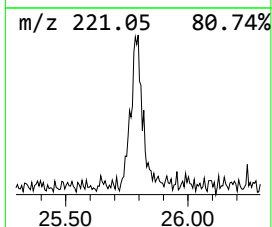
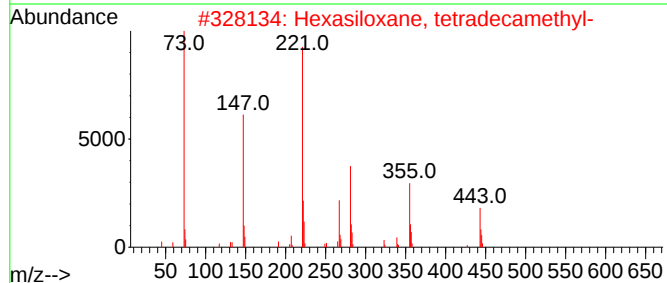
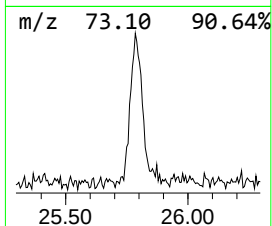
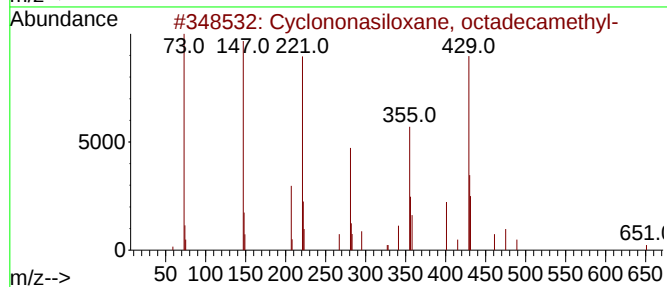
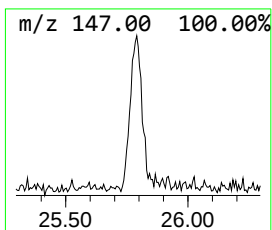
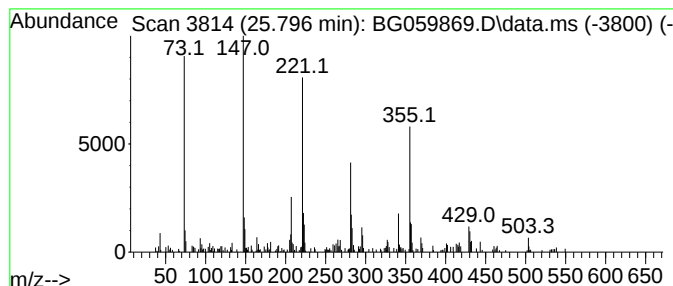
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclononasiloxane, octadeca... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.796	16.82 ng	479743	Perylene-d12	25.585

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	72
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	52
3			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	47
4			1,1,1,3,5,7,7,7-Octamethyl-3,5-b...	458	C14H42O5Si6	002003-92-1	37
5			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059869.D
Acq On : 24 Nov 2023 22:24
Operator : MA/JU
Sample : 05408-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
710-NEW-YORK-AVE

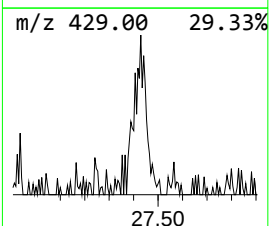
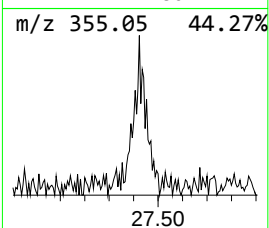
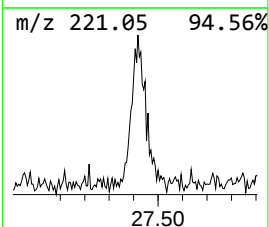
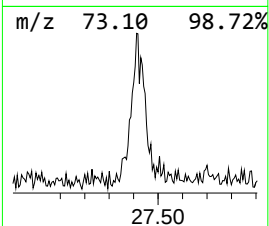
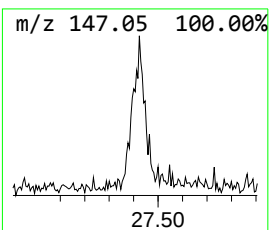
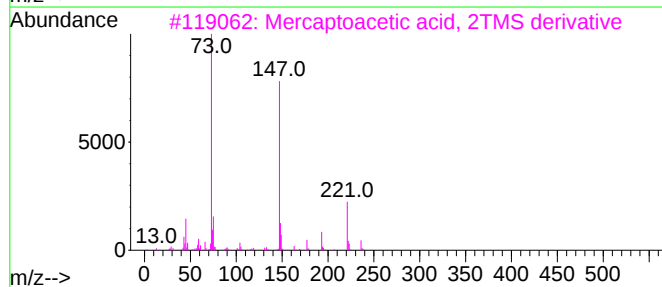
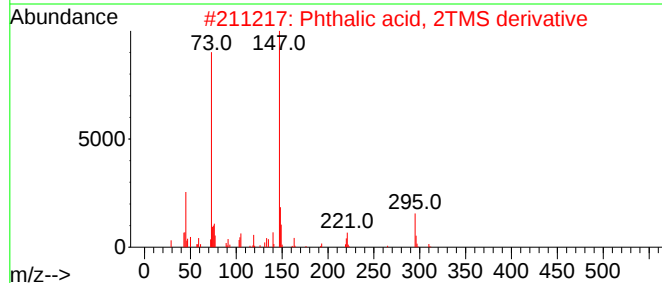
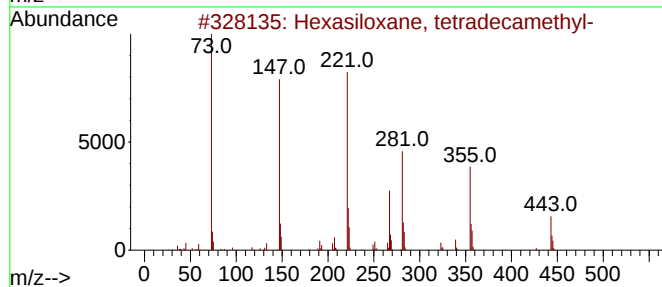
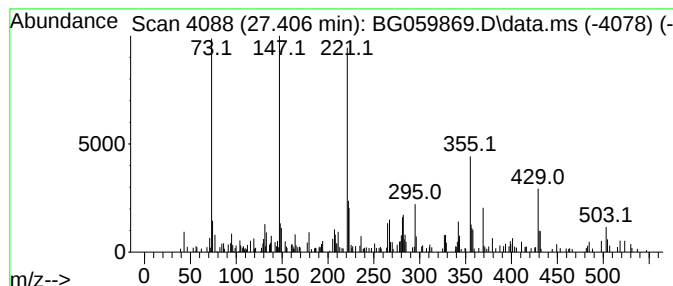
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexasiloxane, tetradecamethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.406	6.89 ng	196693	Perylene-d12	25.585

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	59
2			Phthalic acid, 2TMS derivative	310	C14H22O4Si2	002078-22-0	35
3			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	30
4			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	27
5			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059869.D
Acq On : 24 Nov 2023 22:24
Operator : MA/JU
Sample : 05408-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
710-NEW-YORK-AVE

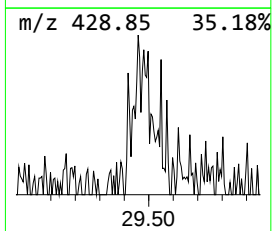
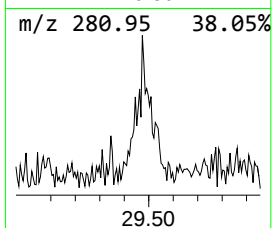
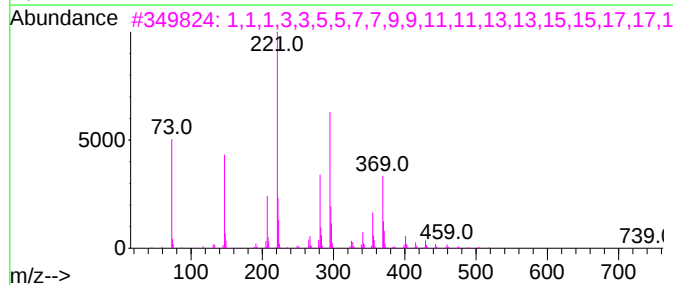
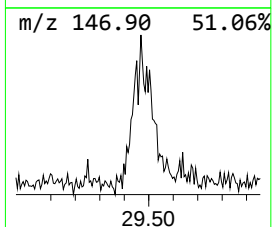
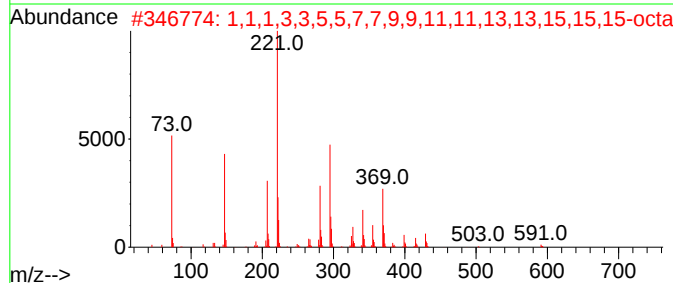
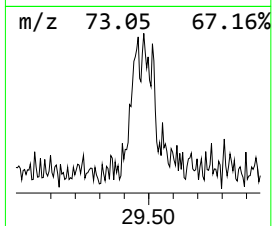
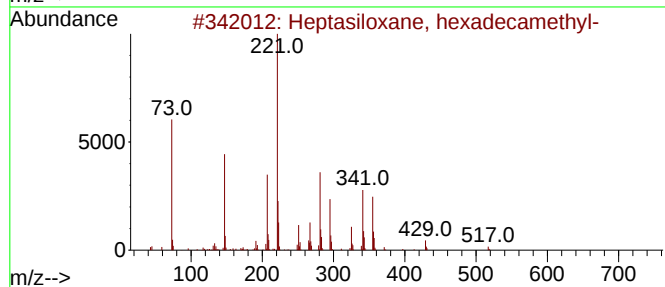
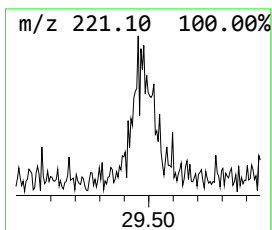
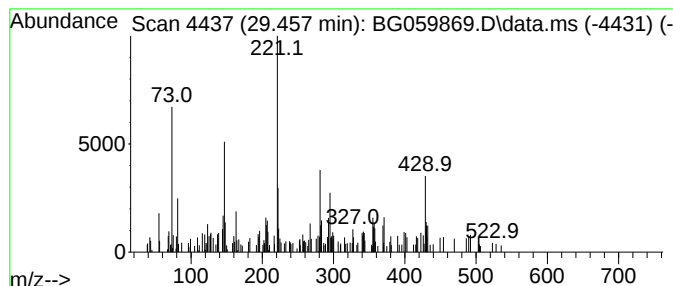
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptasiloxane, hexadecamethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.456	2.93 ng	83637	Perylene-d12	25.585

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	50
2			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	606	C18H54O7Si8	000556-69-4	50
3			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	754	C22H66O9Si10	000556-70-7	50
4			Tetrahydropyran-4-carboxamide, 4...	369	C22H27N04	1010310-01-9	38
5			Stemphol, dimethyl ether	264	C17H28O2	126838-67-3	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059869.D
Acq On : 24 Nov 2023 22:24
Operator : MA/JU
Sample : 05408-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
710-NEW-YORK-AVE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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N-[4-(Aminosulf...	21.760	3.1	ng	100563	5	22.024	638946	20.0
unknown22.529	22.529	5.4	ng	171078	5	22.024	638946	20.0
unknown23.411	23.411	8.6	ng	273970	5	22.024	638946	20.0
unknown24.480	24.480	15.9	ng	452258	6	25.585	570614	20.0
Cyclononasiloxa...	25.796	16.8	ng	479743	6	25.585	570614	20.0
Hexasiloxane, t...	27.406	6.9	ng	196693	6	25.585	570614	20.0
Heptasiloxane, ...	29.456	2.9	ng	83637	6	25.585	570614	20.0