

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010524\
 Data File : BG060277.D
 Acq On : 5 Jan 2024 19:18
 Operator : MA/JU
 Sample : 05967-10
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 COMA1

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: BG060277.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.116	3	5	17	rVB	974003	1299820	7.55%	1.890%
2	5.507	402	412	425	rBV	1455324	2457116	14.26%	3.573%
3	7.094	675	682	695	rBV	820206	1452646	8.43%	2.113%
4	7.934	818	825	835	rBV	687294	1194429	6.93%	1.737%
5	9.092	1014	1022	1039	rBV	2223432	4077138	23.67%	5.929%
6	10.737	1295	1302	1310	rBV	910666	1604064	9.31%	2.333%
7	13.193	1712	1720	1734	rBV	6196068	9733523	56.50%	14.155%
8	14.567	1948	1954	1963	rBV	1595795	2486399	14.43%	3.616%
9	16.060	2200	2208	2216	rBV	5387736	8172387	47.44%	11.885%
10	17.317	2415	2422	2432	rBV	2381835	3511794	20.39%	5.107%
11	18.204	2568	2573	2581	rBV3	158639	241188	1.40%	0.351%
12	19.938	2862	2868	2881	rBV	12351601	17227221	100.00%	25.053%
13	21.583	3141	3148	3155	rBV	2743866	4422709	25.67%	6.432%
14	22.323	3268	3274	3280	rBV	232685	433475	2.52%	0.630%
15	23.175	3413	3419	3426	rBV2	380397	744492	4.32%	1.083%
16	24.197	3585	3593	3604	rVB5	429250	1108444	6.43%	1.612%
17	24.750	3677	3687	3702	rBV	1614188	4672748	27.12%	6.795%
18	25.455	3798	3807	3821	rVB4	429468	1352801	7.85%	1.967%
19	27.018	4062	4073	4086	rVB5	330889	1328623	7.71%	1.932%
20	28.980	4395	4407	4424	rVB9	252056	1242188	7.21%	1.806%

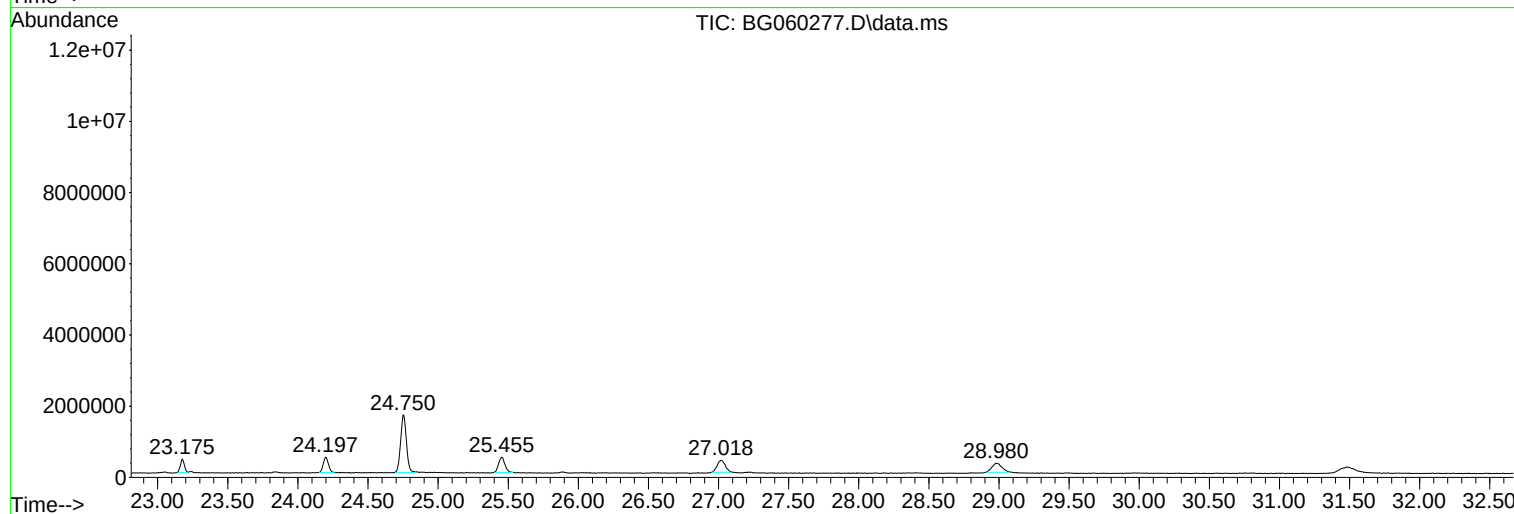
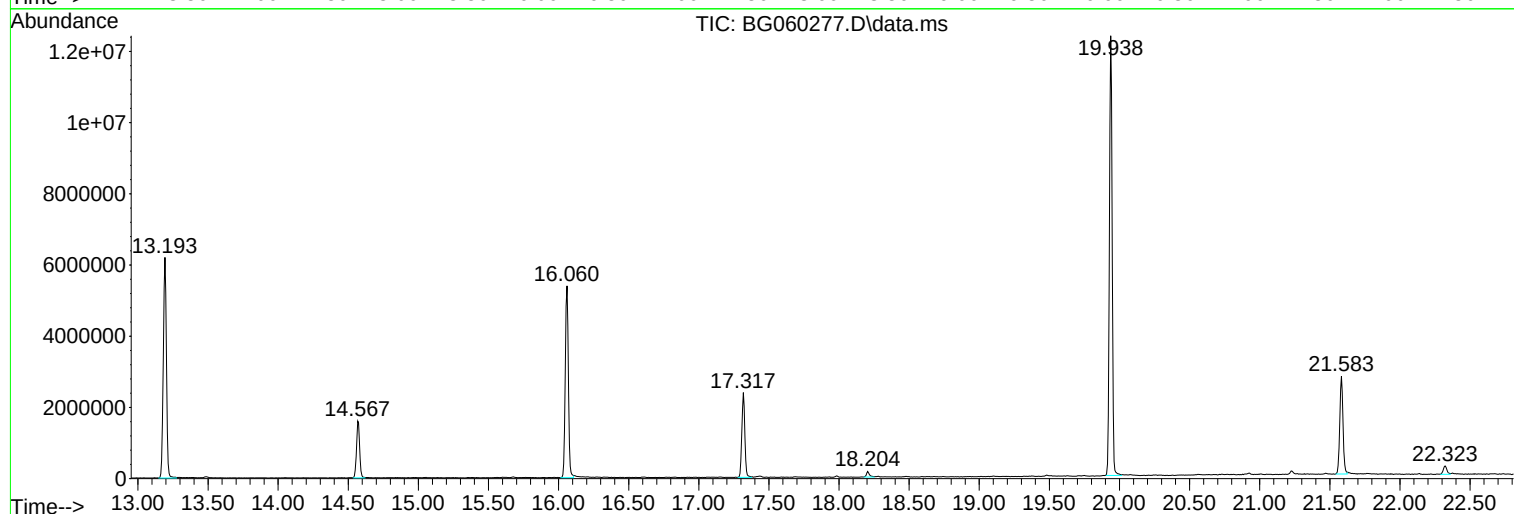
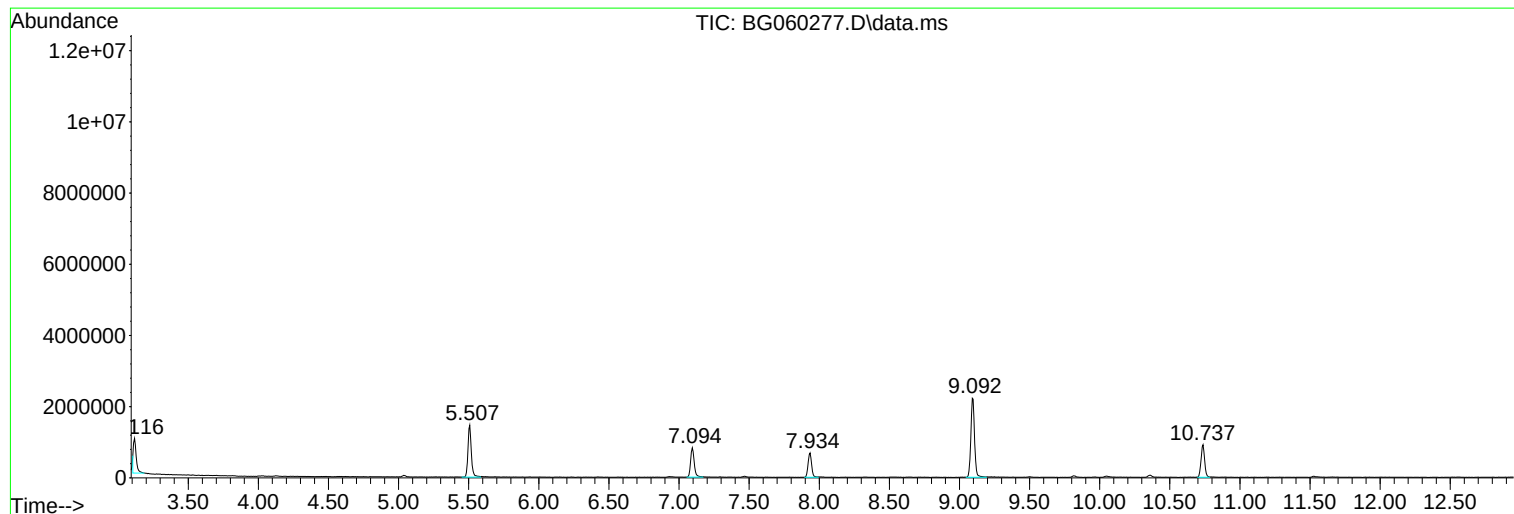
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BNA_G
ClientSampleId :
C0MA1

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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Operator : MA/JU
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Instrument :
BNA_G
ClientSampleId :
COMA1

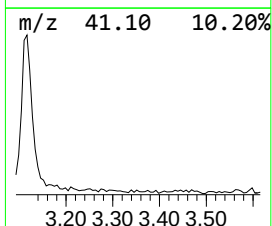
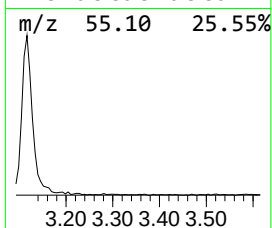
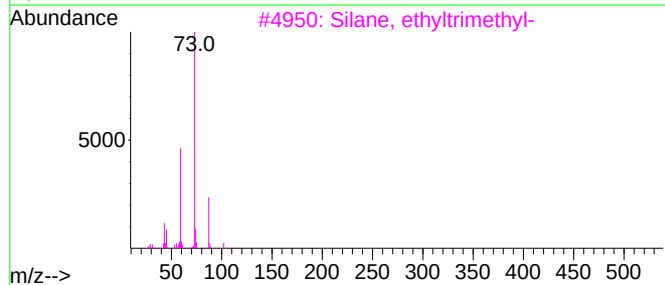
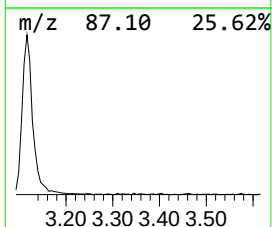
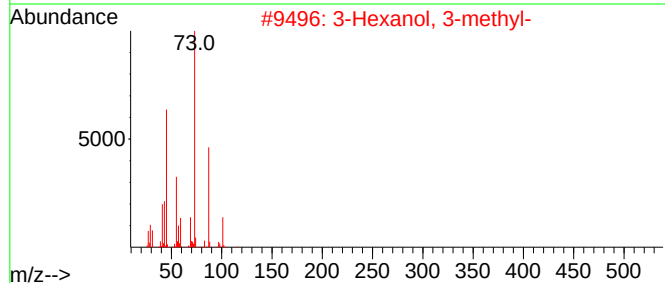
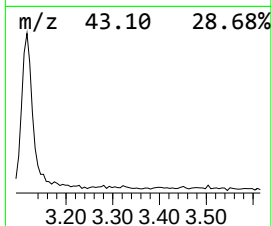
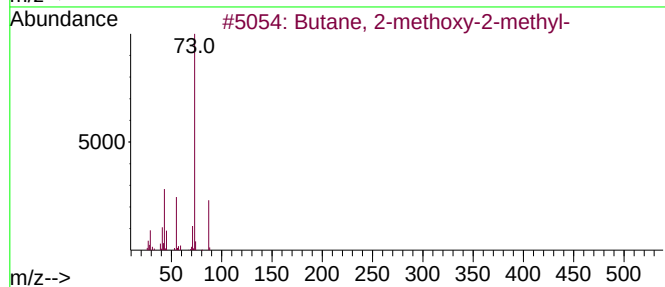
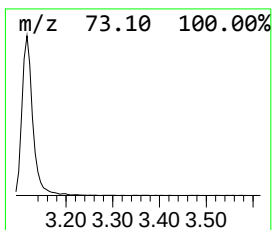
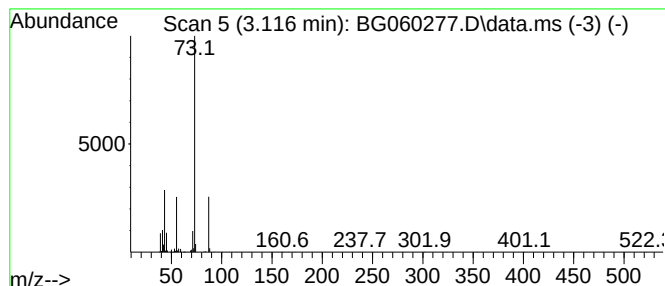
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.116	21.76 ng	1299820	1,4-Dichlorobenzene-d4	7.934

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			3-Hexanol, 3-methyl-	116	C7H16O	000597-96-6	64
3			Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
4			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
5			1-Propene-1-thiol	74	C3H6S	000925-89-3	9



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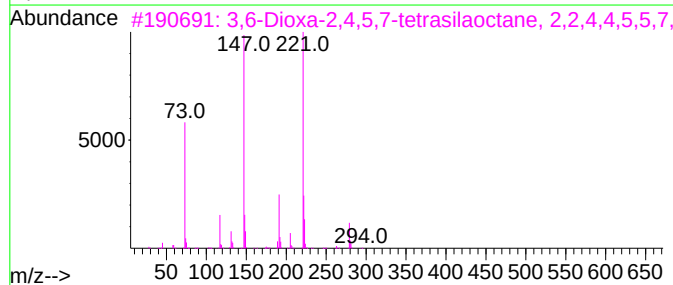
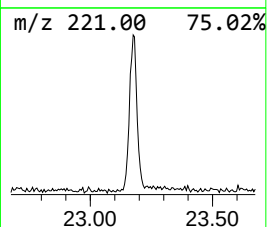
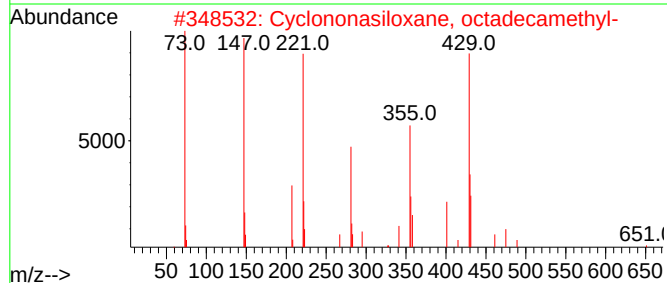
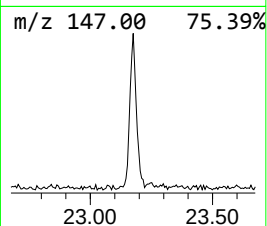
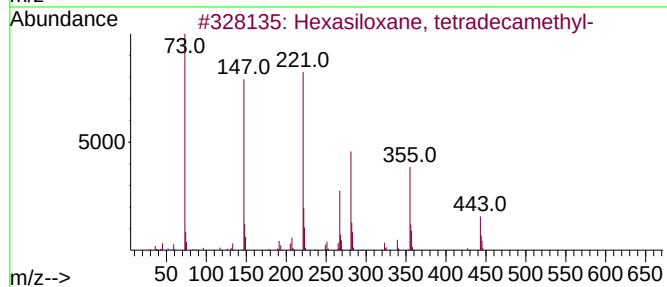
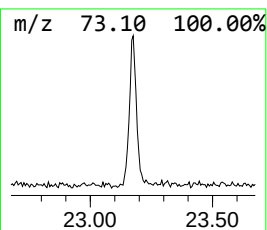
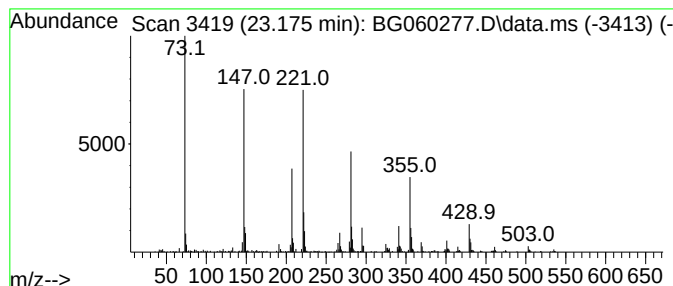
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Hexasiloxane, tetradecamethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.175	3.19 ng	744492	Perylene-d12	24.756

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	76
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	72
3			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	55
4			Cyclodecasiloxane, eicosamethyl-	740	C20H60O10Si10	018772-36-6	53
5			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	754	C22H66O9Si10	000556-70-7	38



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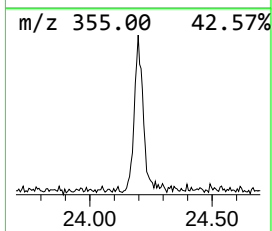
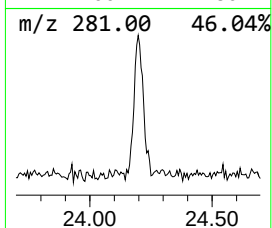
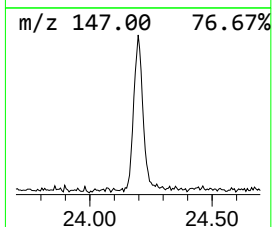
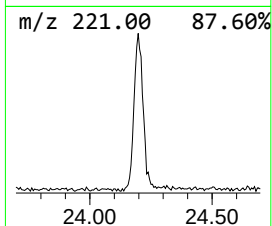
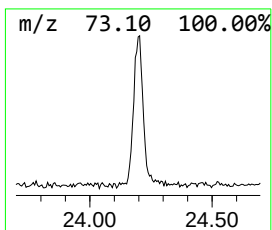
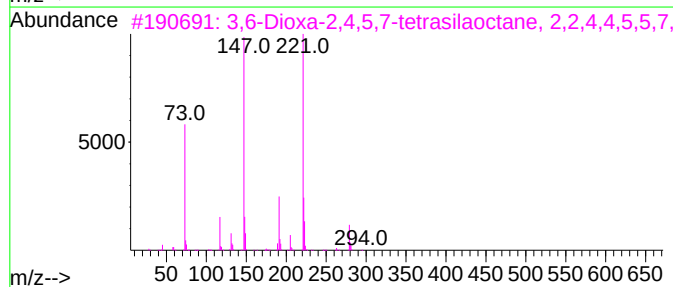
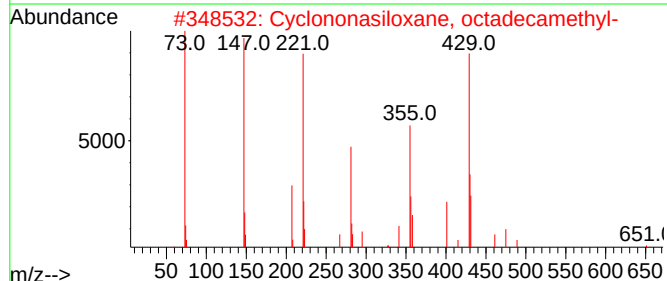
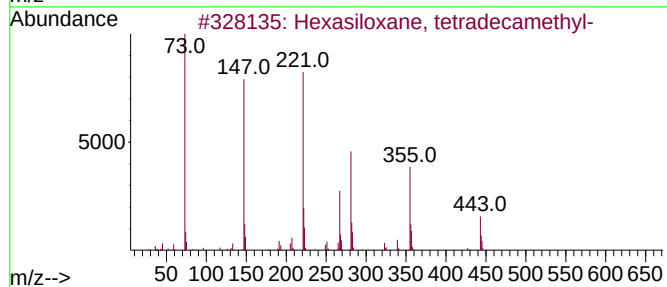
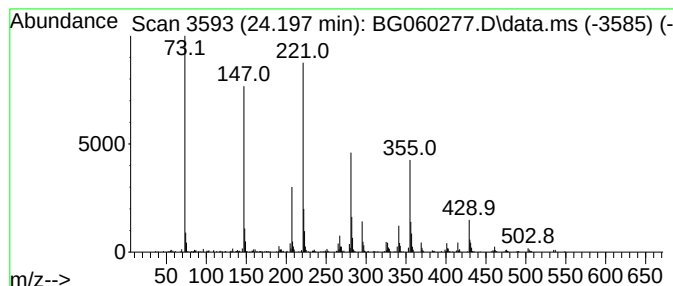
Instrument :
BNA_G
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Cyclononasiloxane, octadeca... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
24.197	4.74 ng	1108440	Perylene-d12	24.756	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	90
2	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	50
3	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	40
4	2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	40
5	N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	27



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Misc :
ALS Vial : 13 Sample Multiplier: 1

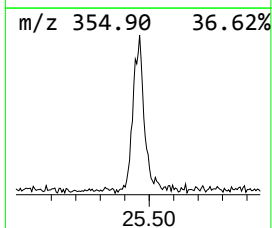
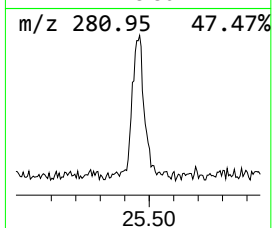
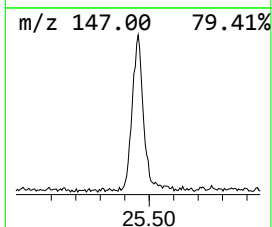
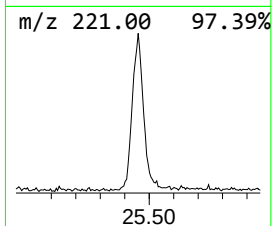
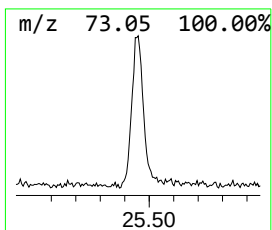
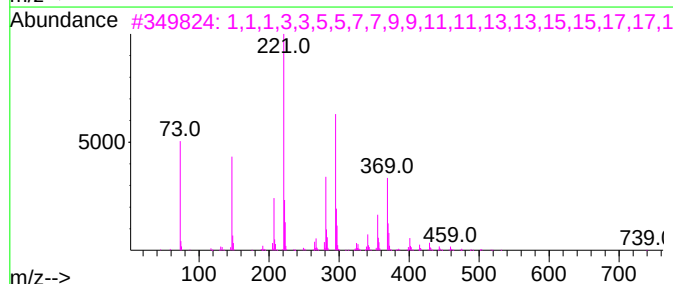
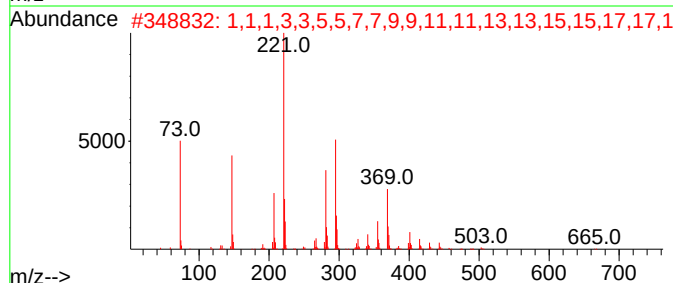
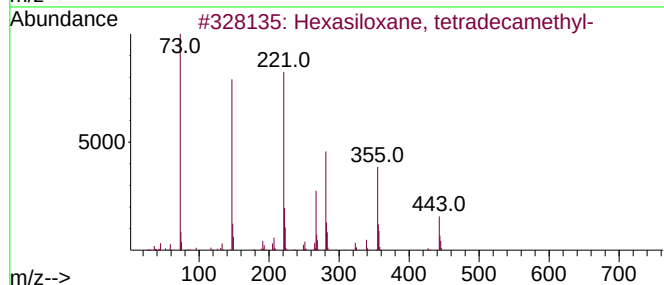
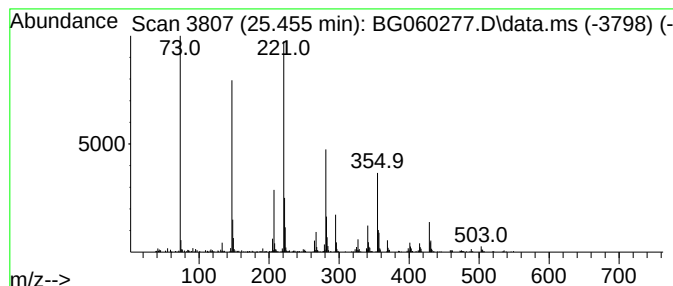
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown25.455 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
25.455	5.79 ng	1352800	Perylene-d12	24.756	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	86
2	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	680	C20H60O8Si9	002652-13-3	46
3	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	754	C22H66O9Si10	000556-70-7	45
4	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	42
5	Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	38



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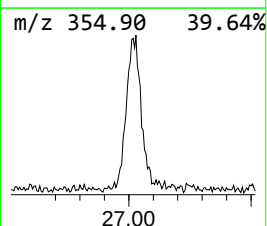
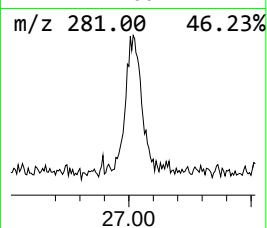
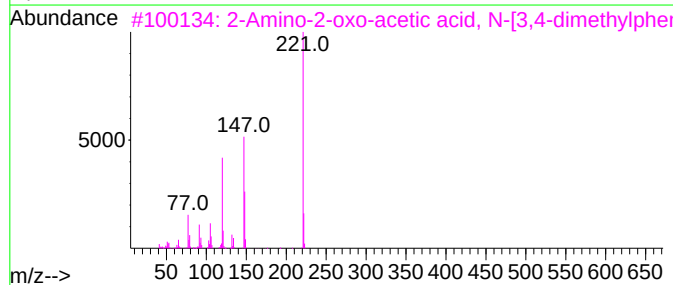
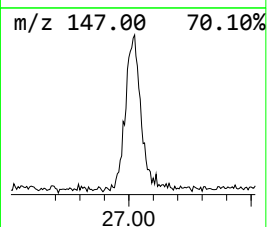
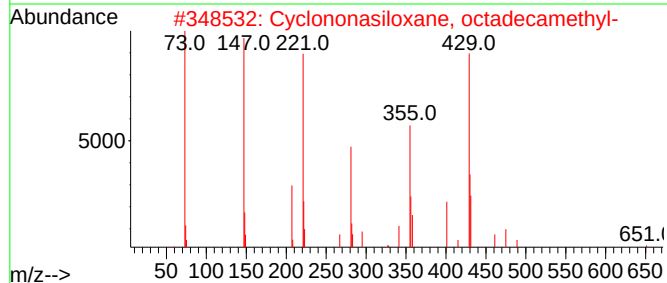
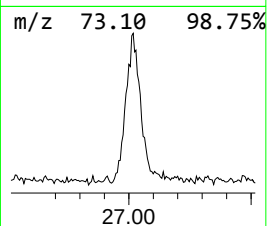
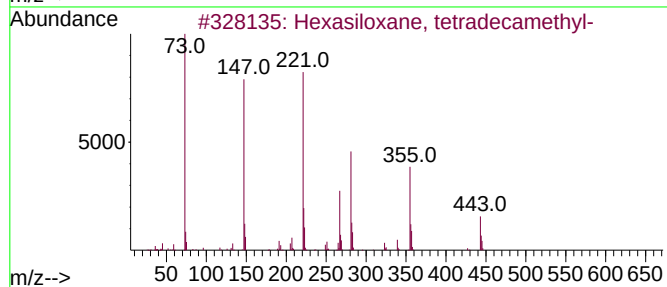
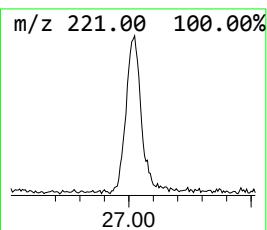
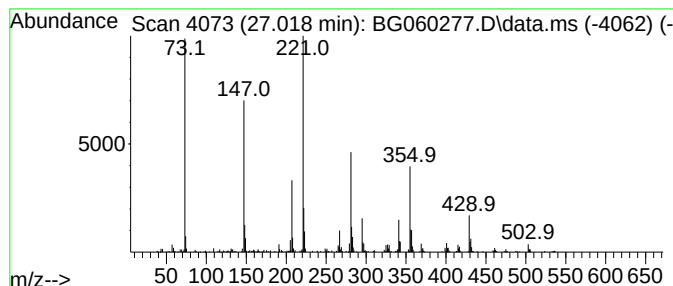
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown27.018 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.018	5.69 ng	1328620	Perylene-d12	24.756

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	86
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	68
3			2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	37
4			2-Methyl-6-tert-butylphenol, TBD...	278	C17H30O5Si	1000467-05-0	35
5			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	32



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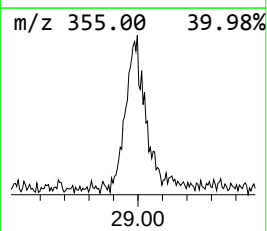
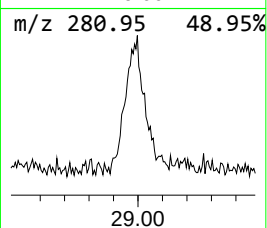
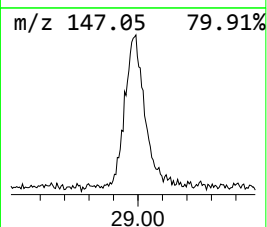
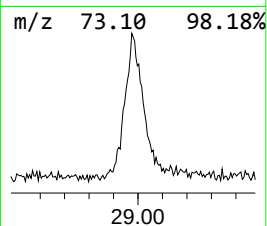
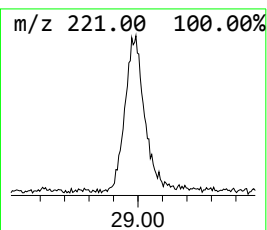
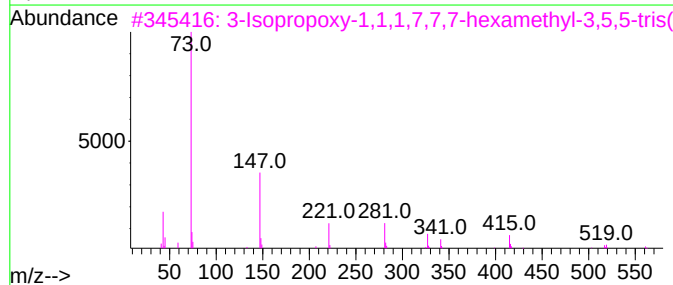
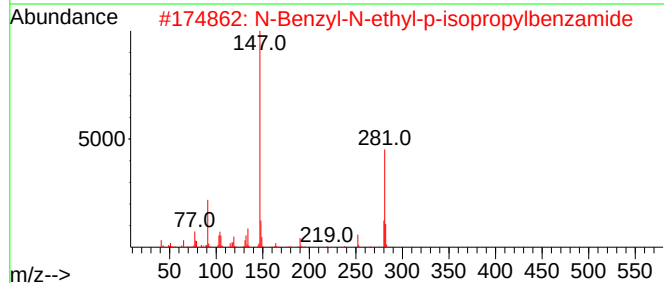
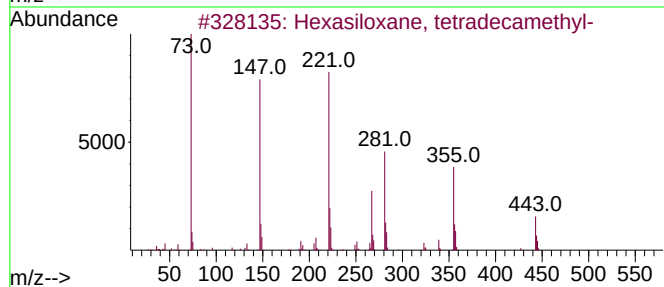
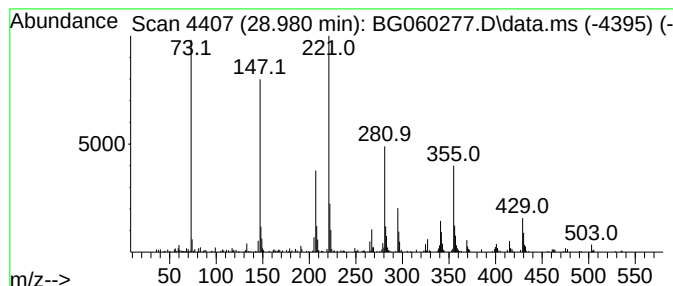
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown28.980 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.980	5.32 ng	1242190	Perylene-d12	24.756

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	87
2			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	27
3			3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	25
4			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	25
5			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010524\
Data File : BG060277.D
Acq On : 5 Jan 2024 19:18
Operator : MA/JU
Sample : 05967-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0MA1

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
Butane, 2-metho...	3.116	21.8	ng	1299820	1	7.934	1194430	20.0
Hexasiloxane, t...	23.175	3.2	ng	744492	6	24.756	4672750	20.0
Cyclononasiloxa...	24.197	4.7	ng	1108440	6	24.756	4672750	20.0
unknown25.455	25.455	5.8	ng	1352800	6	24.756	4672750	20.0
unknown27.018	27.018	5.7	ng	1328620	6	24.756	4672750	20.0
unknown28.980	28.980	5.3	ng	1242190	6	24.756	4672750	20.0