

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010524\
 Data File : BG060278.D
 Acq On : 5 Jan 2024 19:59
 Operator : MA/JU
 Sample : P1040-02
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 COMP-2

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: BG060278.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.040	325	332	343	rBV	1153493	1823332	12.86%	2.765%
2	5.505	403	411	429	rBV	2698031	4646181	32.78%	7.045%
3	7.097	672	682	698	rBV	3010274	5392660	38.04%	8.177%
4	7.931	817	824	832	rBV	683520	1240923	8.75%	1.882%
5	9.094	1014	1022	1039	rBV	1953917	3531725	24.91%	5.355%
6	10.734	1293	1301	1310	rBV	893120	1651368	11.65%	2.504%
7	13.190	1712	1719	1733	rBV	5585129	8720466	61.52%	13.223%
8	14.570	1946	1954	1962	rBV	1645403	2536621	17.89%	3.846%
9	16.057	2200	2207	2224	rBV	3130807	4712569	33.25%	7.146%
10	17.320	2415	2422	2427	rBV	2197913	3425030	24.16%	5.193%
11	18.207	2568	2573	2577	rBV3	119830	199411	1.41%	0.302%
12	19.371	2766	2771	2779	rVB	196622	288782	2.04%	0.438%
13	19.735	2830	2833	2840	rVB	167670	251625	1.78%	0.382%
14	19.941	2861	2868	2881	rBV	10241244	14175132	100.00%	21.494%
15	21.227	3082	3087	3098	rBV2	505502	823631	5.81%	1.249%
16	21.404	3109	3117	3120	rBV7	68014	189066	1.33%	0.287%
17	21.580	3140	3147	3154	rBV	2540948	4240280	29.91%	6.430%
18	21.774	3176	3180	3185	rVB2	135114	185330	1.31%	0.281%
19	22.320	3267	3273	3278	rBV3	143692	265763	1.87%	0.403%
20	22.367	3278	3281	3288	rVB3	124135	207354	1.46%	0.314%
21	23.037	3388	3395	3406	rBV4	287239	729862	5.15%	1.107%
22	23.172	3413	3418	3425	rBV	170876	336696	2.38%	0.511%
23	24.200	3586	3593	3601	rVB3	228956	574614	4.05%	0.871%
24	24.753	3677	3687	3701	rBV2	1533305	4483989	31.63%	6.799%
25	25.458	3798	3807	3816	rBV5	214646	696863	4.92%	1.057%
26	27.015	4064	4072	4084	rVB5	168564	619537	4.37%	0.939%

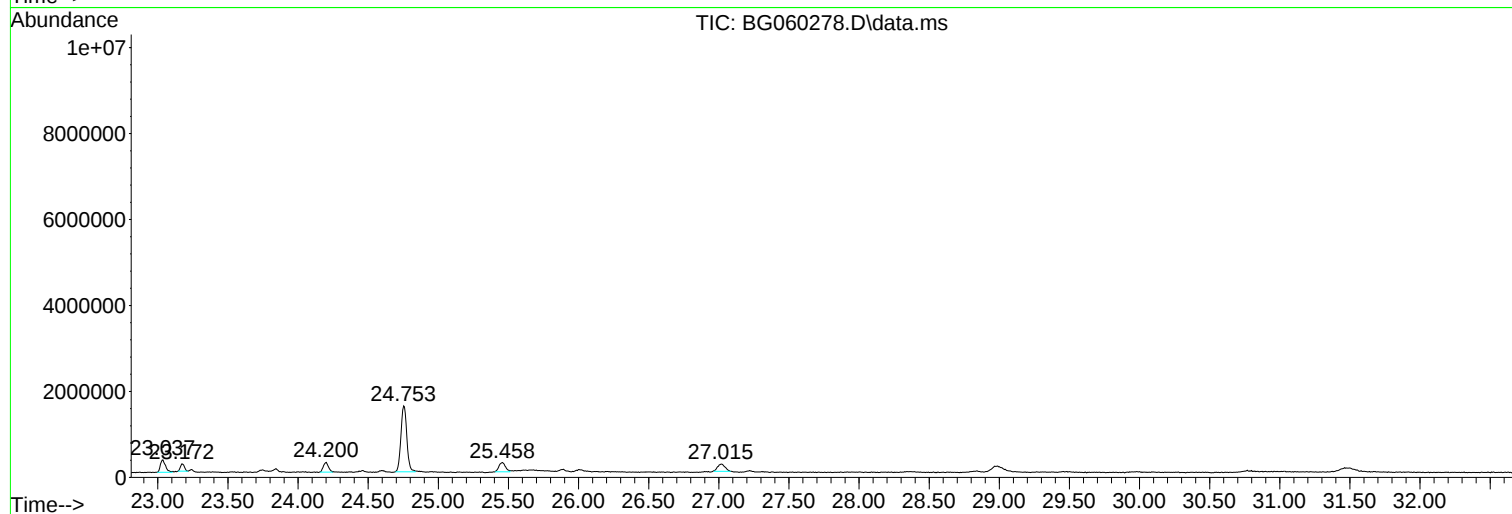
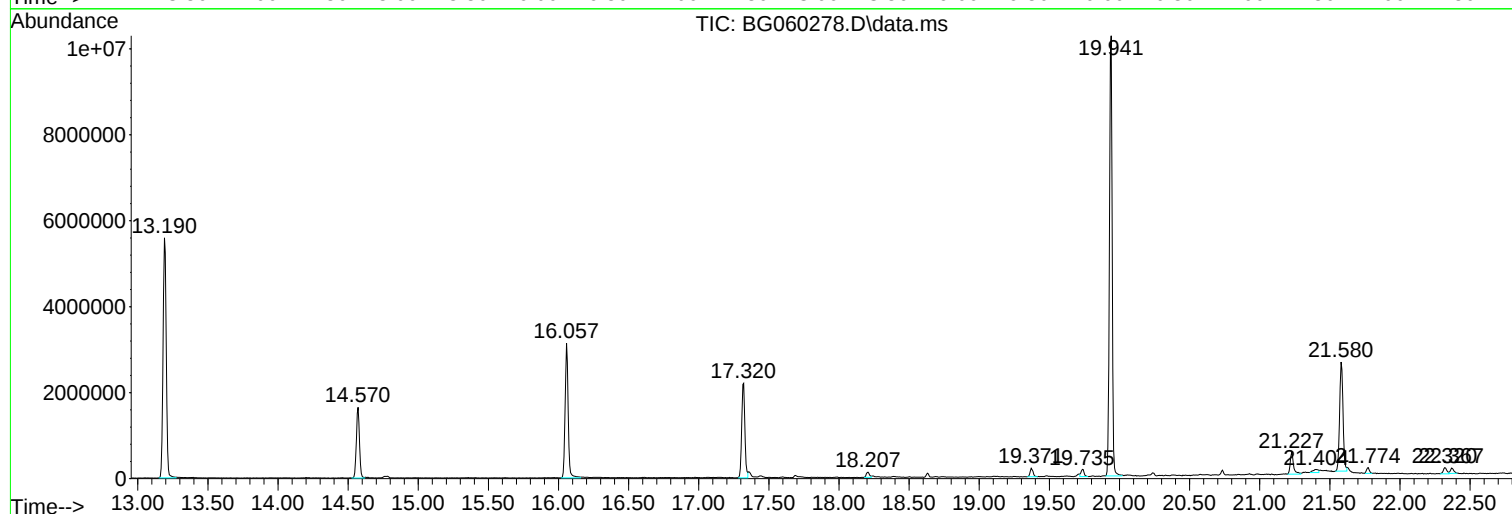
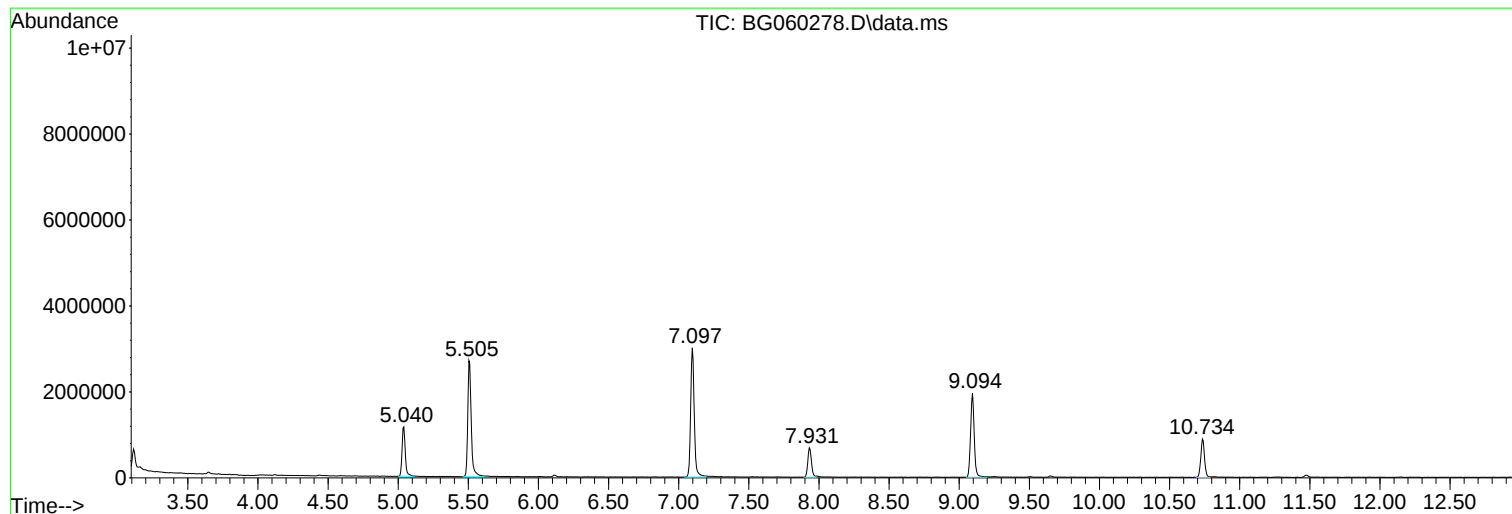
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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-2

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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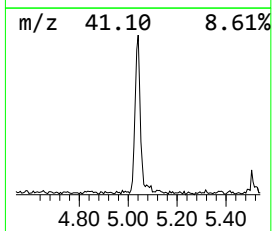
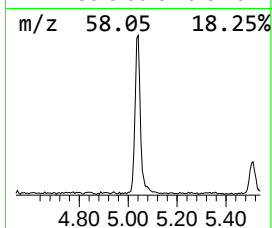
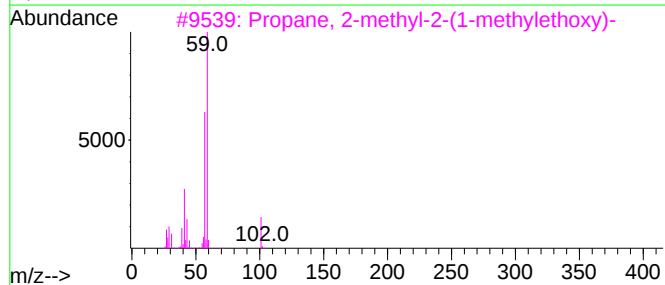
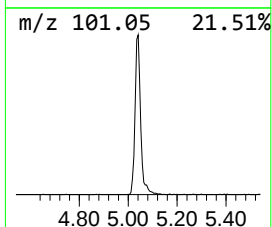
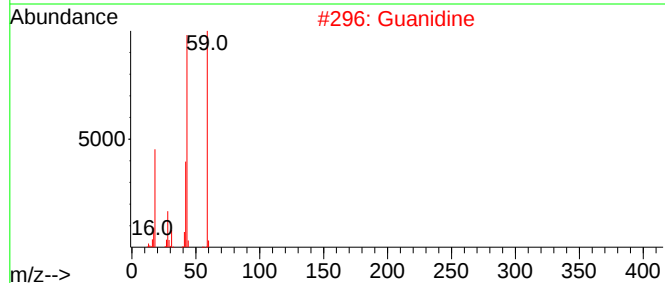
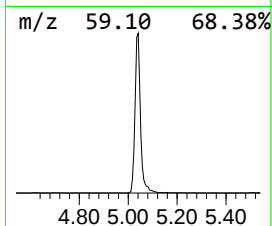
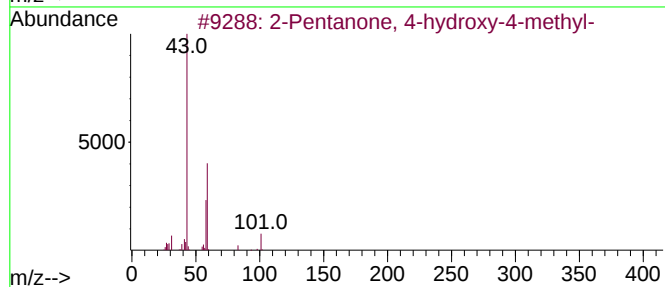
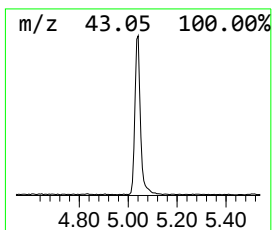
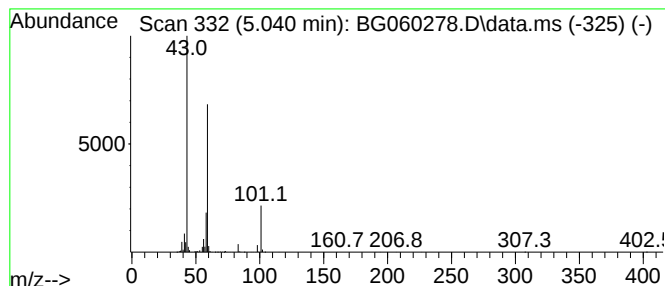
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.040	29.39 ng	1823330	1,4-Dichlorobenzene-d4	7.931

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Guanidine	59	CH5N3	000113-00-8	43		
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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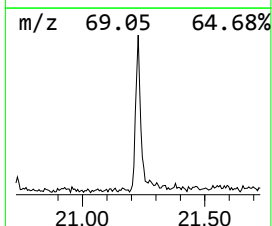
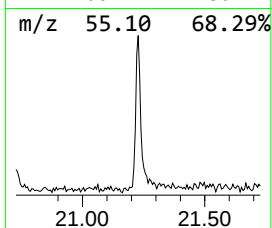
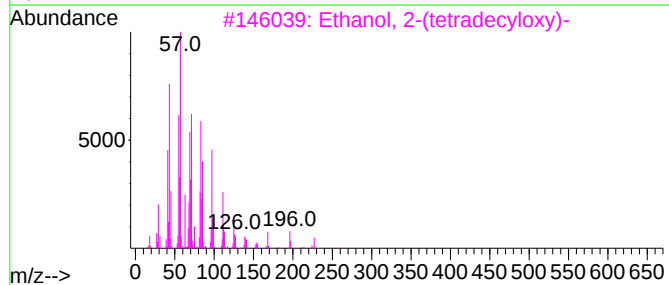
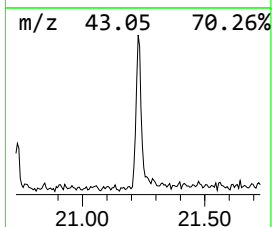
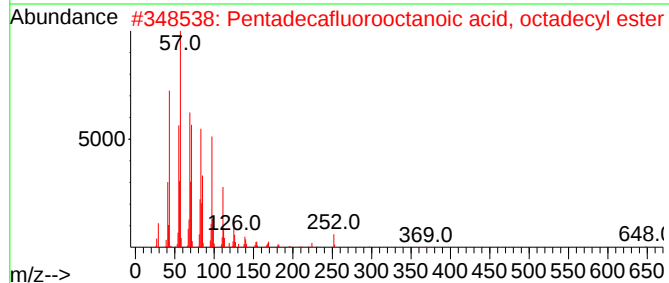
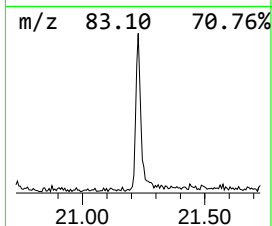
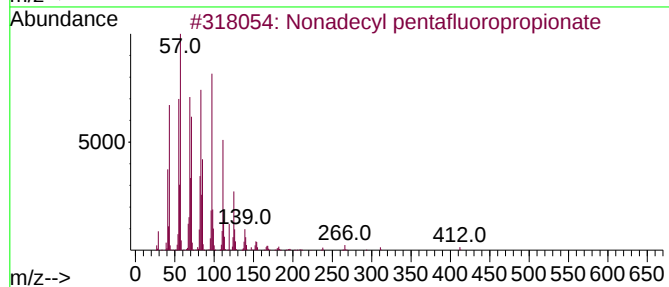
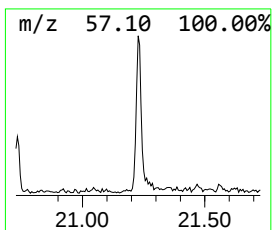
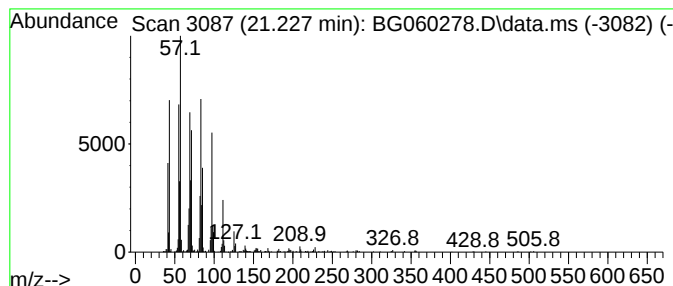
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Nonadecyl pentafluoropropio... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.227	3.88 ng	823631	Chrysene-d12	21.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	87
3			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
4			Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	87
5			17-Pentatriacontene	491	C35H70	006971-40-0	83



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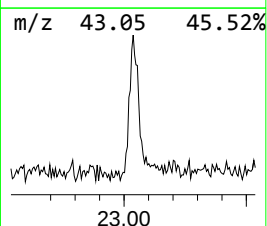
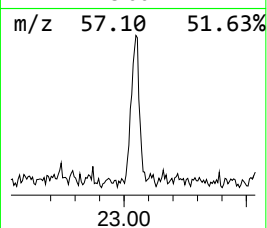
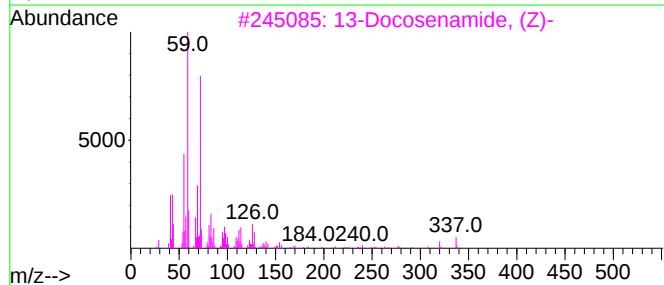
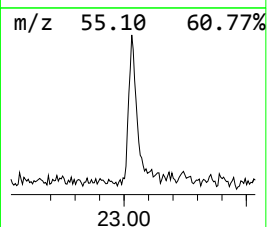
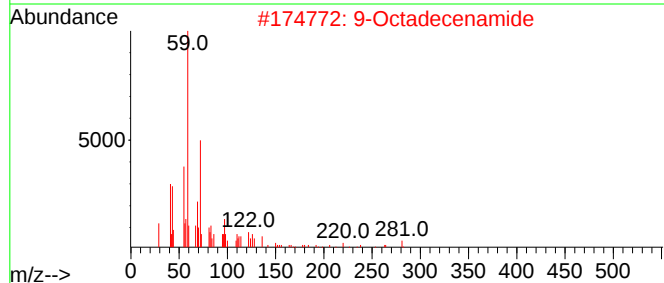
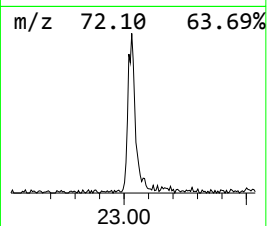
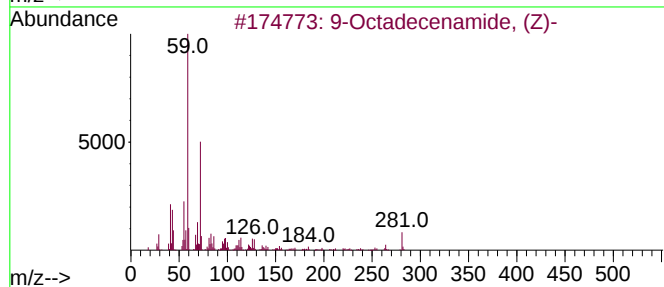
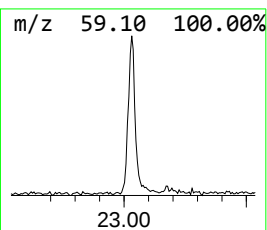
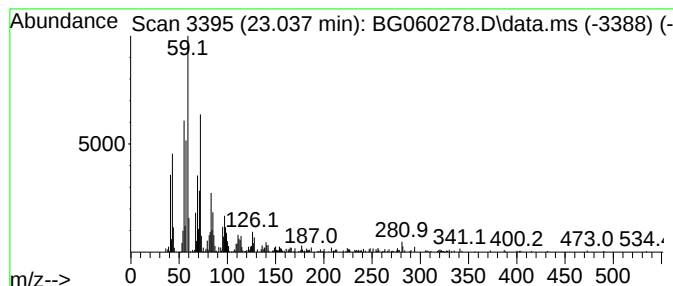
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.037	3.44 ng	729862	Chrysene-d12	21.580

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		9-Octadecenamide	281	C18H35NO	003322-62-1	81
3		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	68
4		Palmitoleamide	253	C16H31NO	106010-22-4	59
5		Allyldimethylsilane	100	C5H12Si	003937-30-2	43



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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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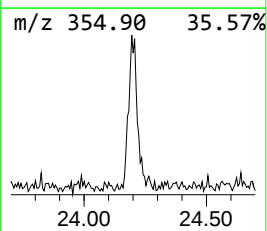
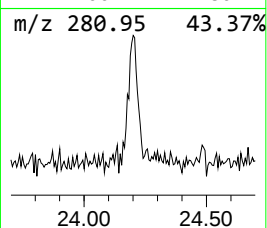
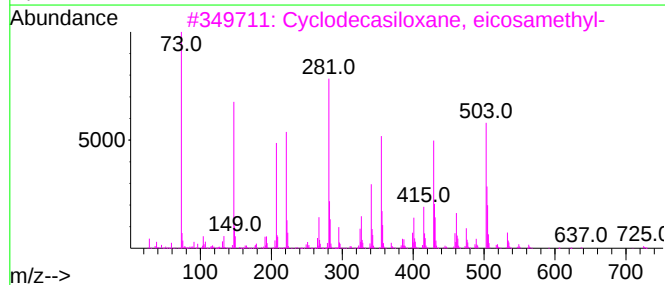
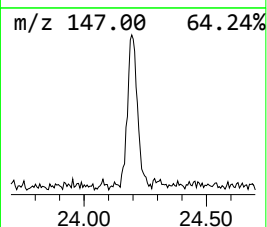
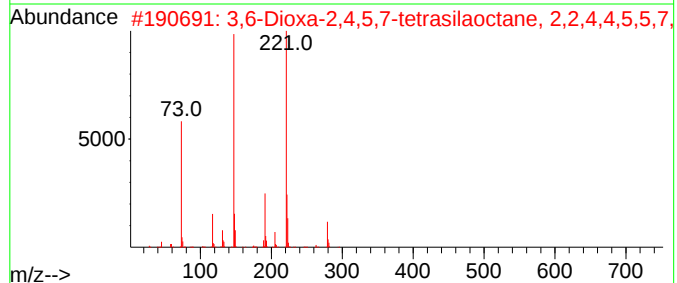
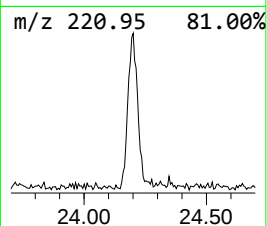
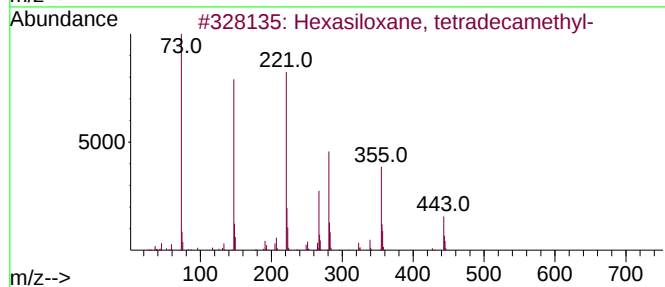
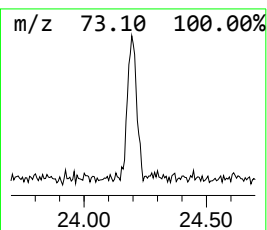
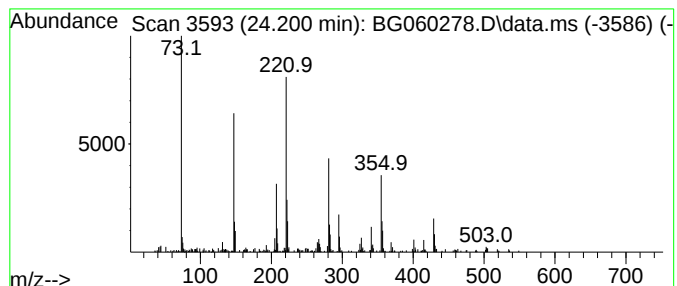
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Hexasiloxane, tetradecamethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.200	2.56 ng	574614	Perylene-d12	24.753

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	83
2			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	47
3			Cyclodecasiloxane, eicosamethyl-	740	C20H60O10Si10	018772-36-6	46
4			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	42
5			1,2-Dibenzoyl-3-phenylcyclopropane	326	C23H18O2	029128-64-1	38



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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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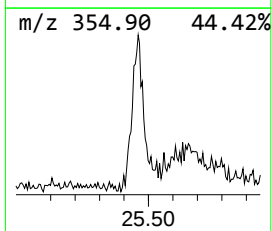
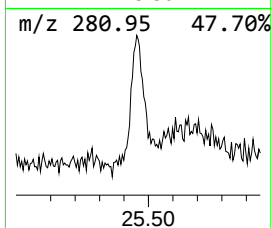
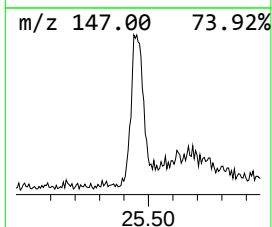
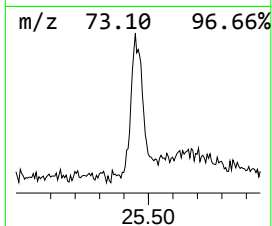
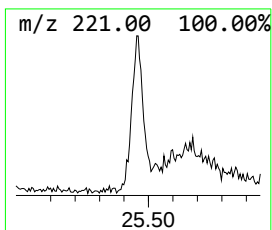
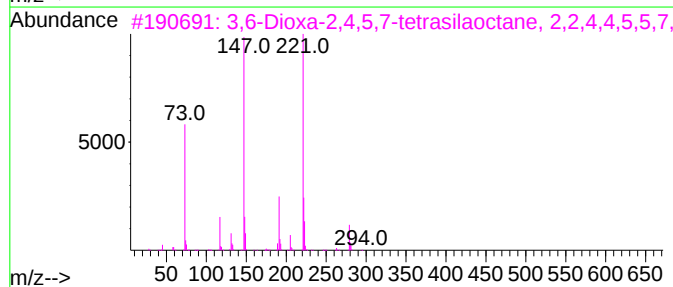
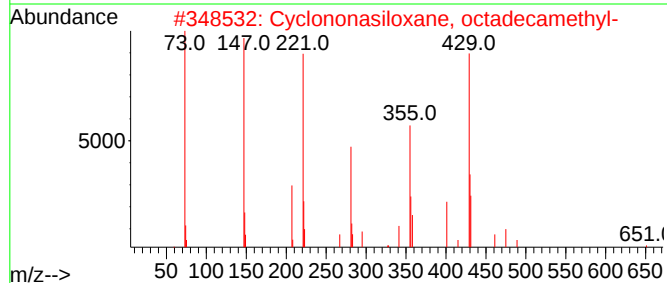
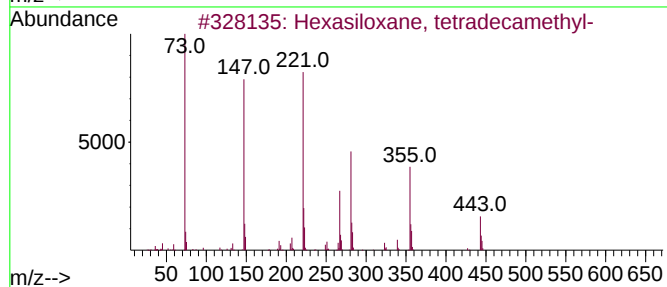
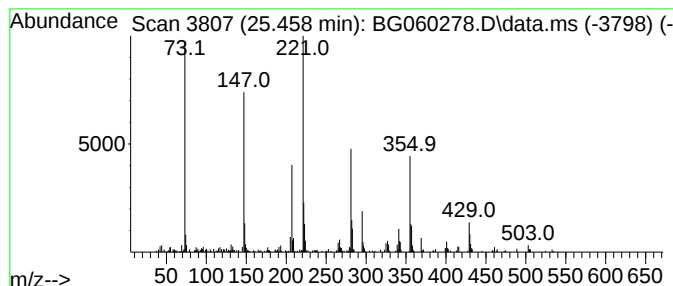
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown25.458 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.458	3.11 ng	696863	Perylene-d12	24.753

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	64
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	38
3			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37
4			Thioglycolic acid, S-(tert-butyl...	320	C14H32O2SSi2	082112-29-6	27
5			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	27



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ALS Vial : 14 Sample Multiplier: 1

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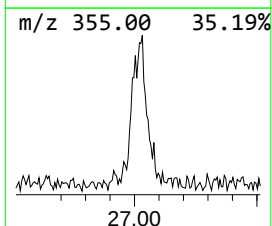
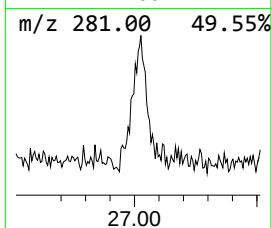
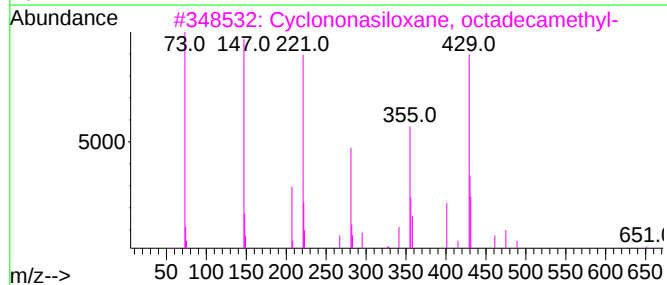
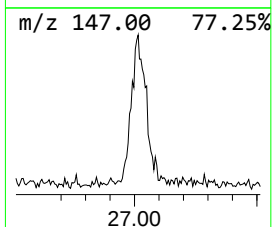
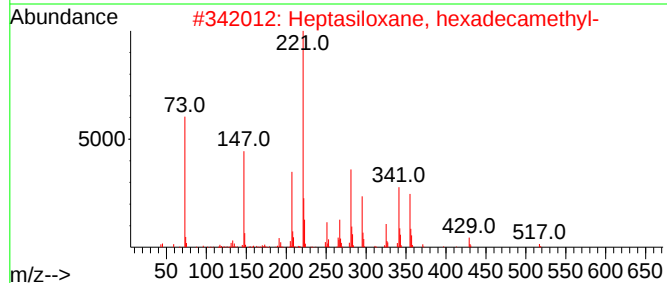
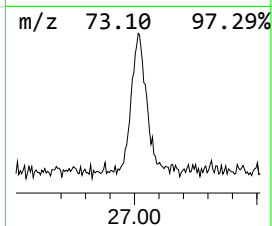
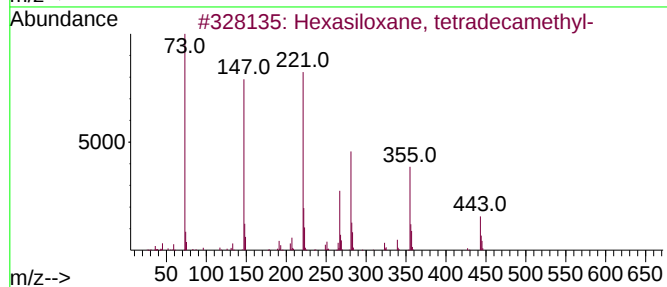
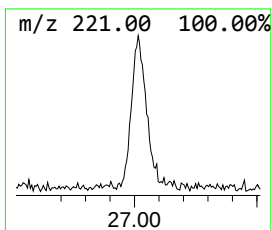
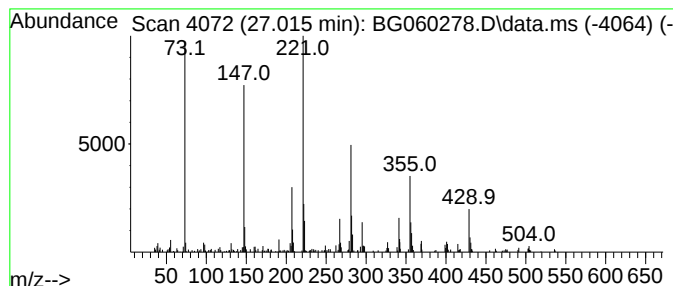
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptasiloxane, hexadecamethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.015	2.76 ng	619537	Perylene-d12	24.753

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	72
2			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	59
3			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	40
4			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	40
5			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	754	C22H66O9Si10	000556-70-7	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010524\
Data File : BG060278.D
Acq On : 5 Jan 2024 19:59
Operator : MA/JU
Sample : P1040-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.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-...	5.040	29.4	ng	1823330	1	7.931	1240920	20.0
Nonadecyl penta...	21.227	3.9	ng	823631	5	21.580	4240280	20.0
9-Octadecenamid...	23.037	3.4	ng	729862	5	21.580	4240280	20.0
Hexasiloxane, t...	24.200	2.6	ng	574614	6	24.753	4483990	20.0
unknown25.458	25.458	3.1	ng	696863	6	24.753	4483990	20.0
Heptasiloxane, ...	27.015	2.8	ng	619537	6	24.753	4483990	20.0