

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100622\
 Data File : BG055084.D
 Acq On : 6 Oct 2022 16:08
 Operator : CG/JU
 Sample : N5002-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 5486-3

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-BG100322.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055084.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.381	10	16	41	rVB	901759	1624908	44.19%	7.861%
2	5.385	351	357	368	rVB	64940	104598	2.84%	0.506%
3	5.855	430	437	451	rVB	273426	454898	12.37%	2.201%
4	7.465	704	711	718	rBV	167350	287957	7.83%	1.393%
5	8.340	853	860	867	rBV	121969	206654	5.62%	1.000%
6	9.509	1051	1059	1068	rBV	403504	716043	19.47%	3.464%
7	11.166	1334	1341	1349	rBV	158558	283440	7.71%	1.371%
8	13.575	1744	1751	1760	rVB	1033608	1554817	42.29%	7.522%
9	14.944	1977	1984	1994	rVB	249091	405882	11.04%	1.964%
10	16.419	2228	2235	2241	rBV	887596	1364815	37.12%	6.603%
11	17.153	2344	2360	2381	rVB4	77832	445088	12.11%	2.153%
12	17.676	2443	2449	2455	rVB	322217	486864	13.24%	2.355%
13	18.528	2591	2594	2602	rVB3	40013	68923	1.87%	0.333%
14	18.616	2603	2609	2615	rVB	2717225	3676812	100.00%	17.788%
15	19.116	2685	2694	2711	rVB	183387	647986	17.62%	3.135%
16	19.774	2799	2806	2822	rVB4	211837	674478	18.34%	3.263%
17	20.256	2881	2888	2892	rBV	2070269	2821073	76.73%	13.648%
18	20.514	2925	2932	2941	rVB2	154665	329693	8.97%	1.595%
19	21.237	3044	3055	3065	rBV	270777	679463	18.48%	3.287%
20	21.965	3172	3179	3186	rBV2	343730	614938	16.72%	2.975%
21	22.300	3227	3236	3246	rVB2	175082	489530	13.31%	2.368%
22	23.546	3438	3448	3461	rVB	140225	470126	12.79%	2.274%
23	23.916	3501	3511	3521	rBV7	47015	171925	4.68%	0.832%
24	24.621	3623	3631	3648	rVB7	41789	176572	4.80%	0.854%
25	25.056	3694	3705	3717	rVB3	79983	309874	8.43%	1.499%
26	25.420	3756	3767	3783	rBV2	203145	659458	17.94%	3.190%
27	26.865	4004	4013	4031	rVB4	60432	280623	7.63%	1.358%
28	28.064	4202	4217	4236	rBV6	122350	662801	18.03%	3.207%

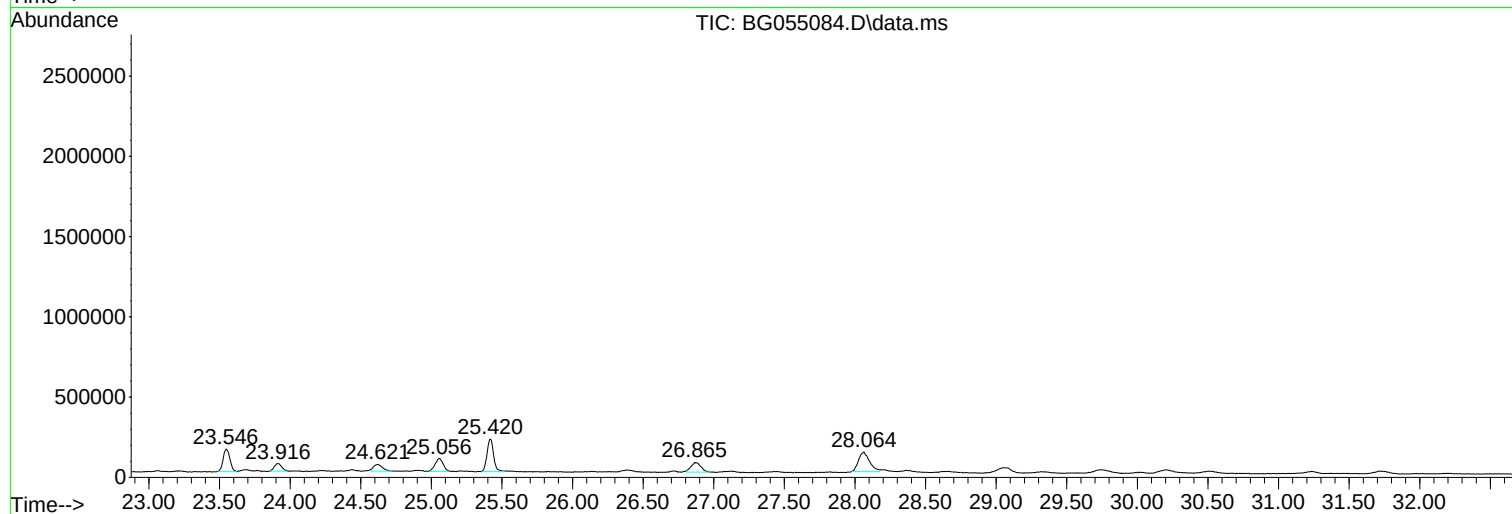
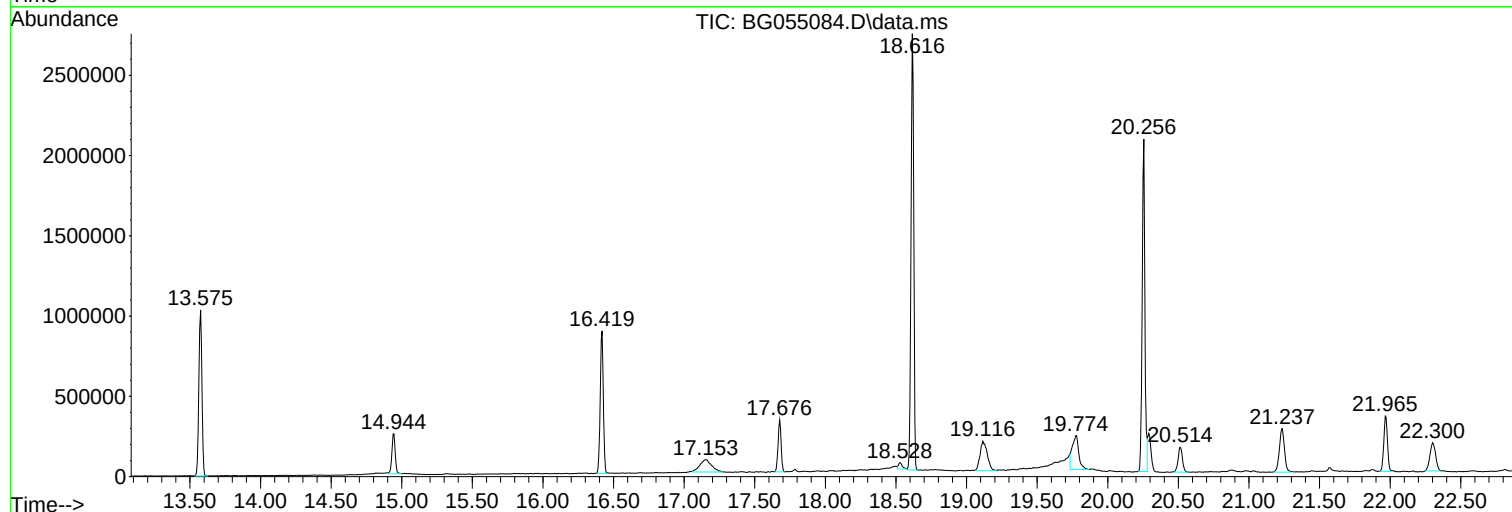
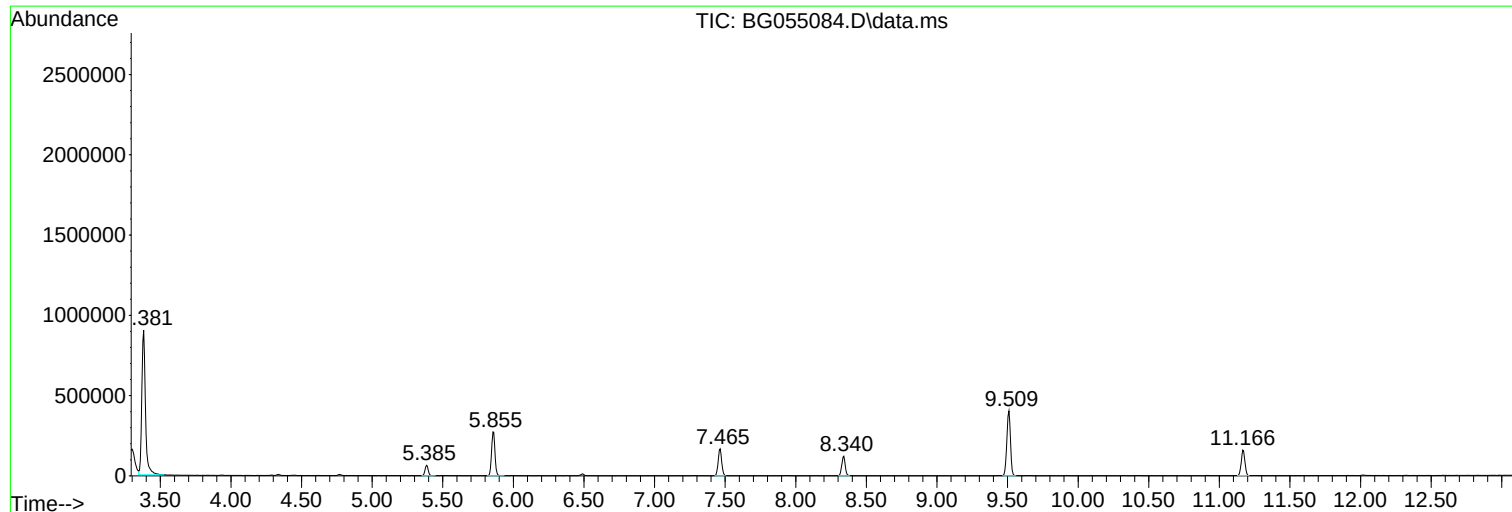
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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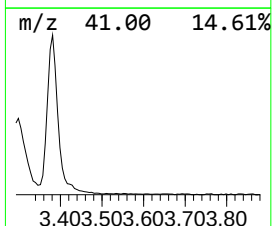
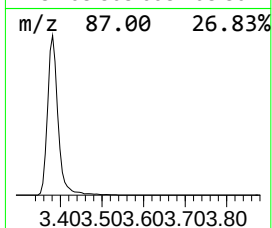
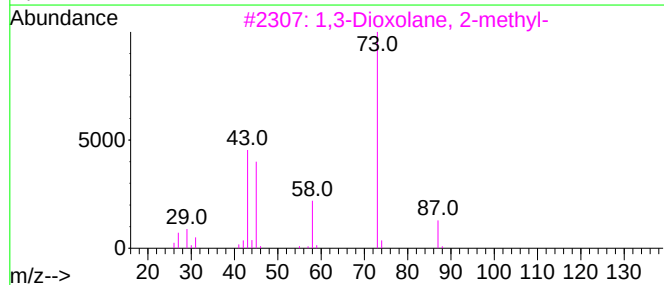
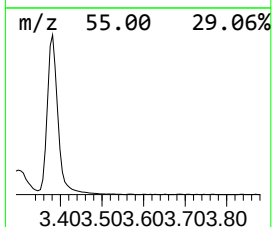
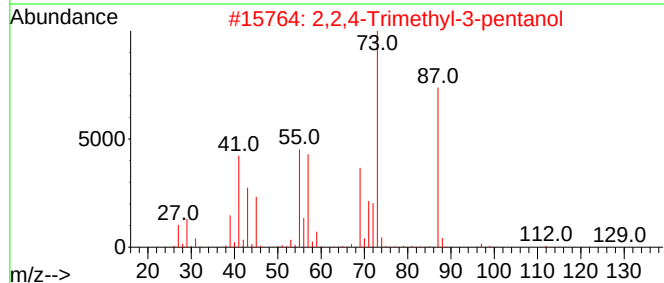
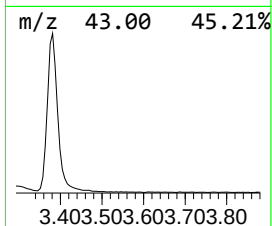
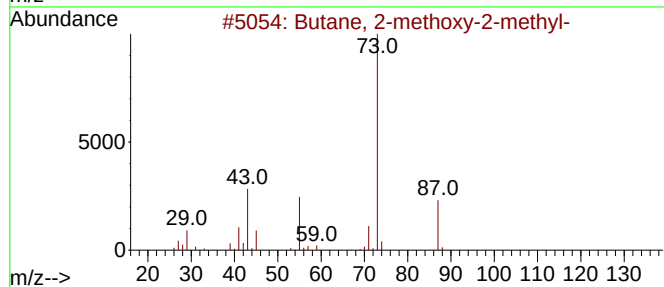
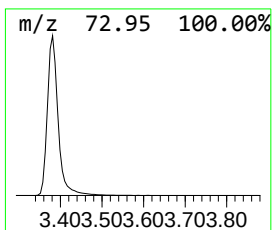
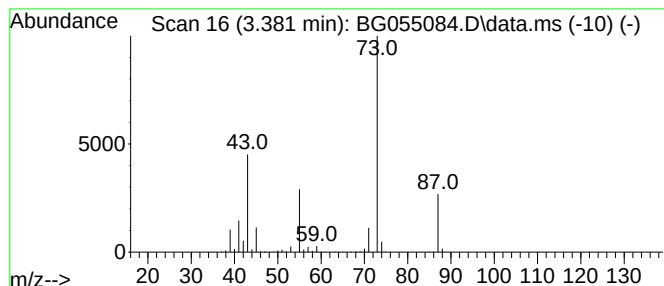
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.381	157.26 ng	1624910	1,4-Dichlorobenzene-d4	8.340

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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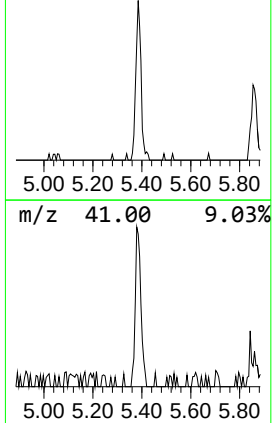
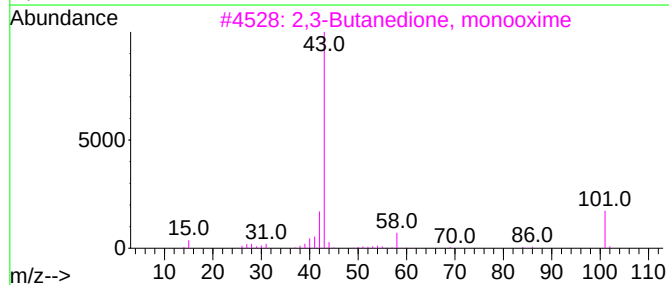
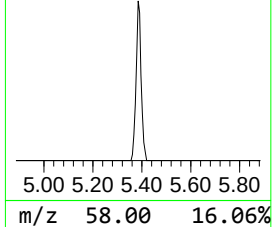
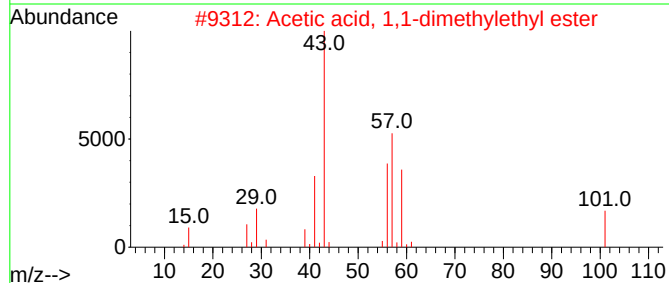
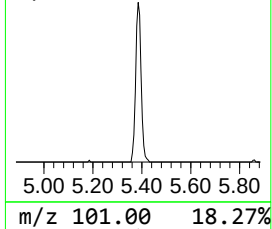
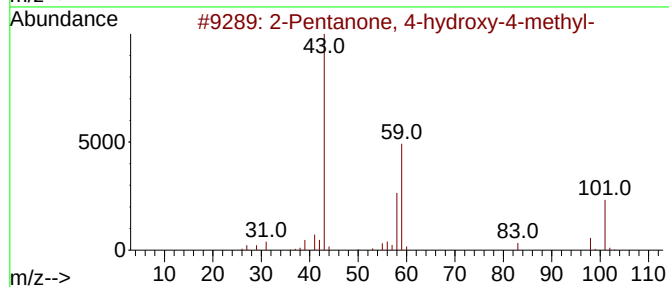
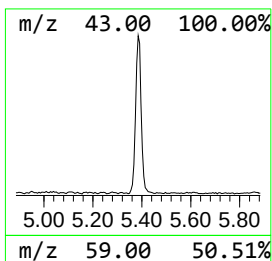
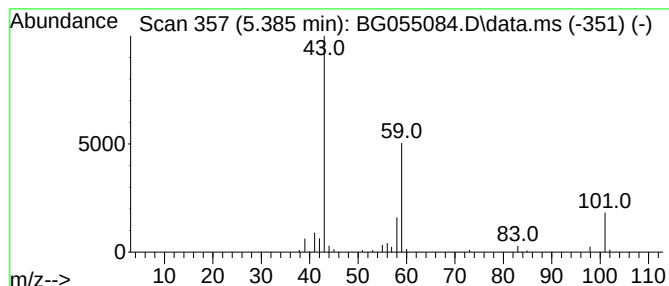
Instrument :
BNA_G
ClientSampleId :
5486-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.385	10.12 ng	104598	1,4-Dichlorobenzene-d4			8.340
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...		116	C6H12O2	000540-88-5	38
3	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	27
4	Butyl aldoxime, 3-methyl-, syn-		101	C5H11NO	005780-40-5	23
5	1-Butene, 4-ethoxy-		100	C6H12O	044611-46-3	23



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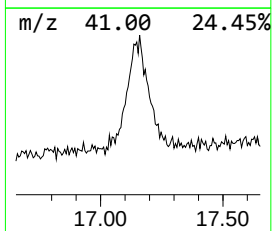
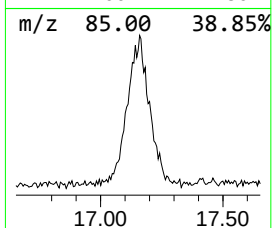
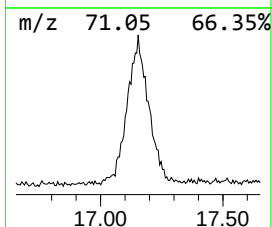
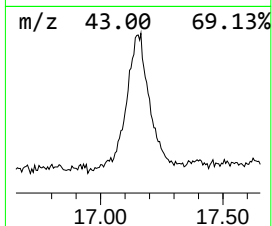
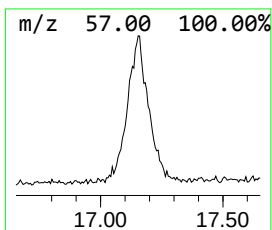
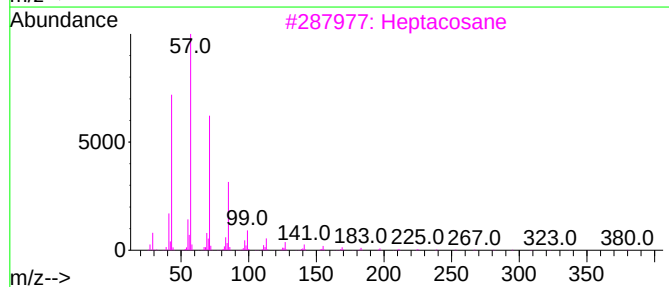
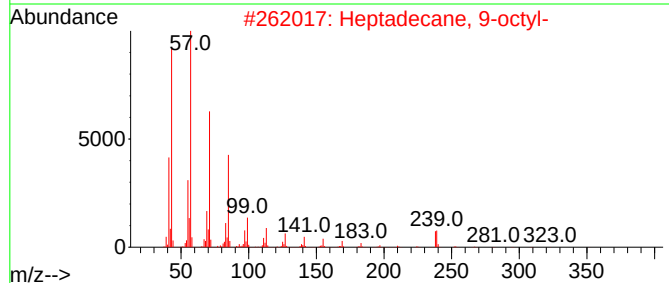
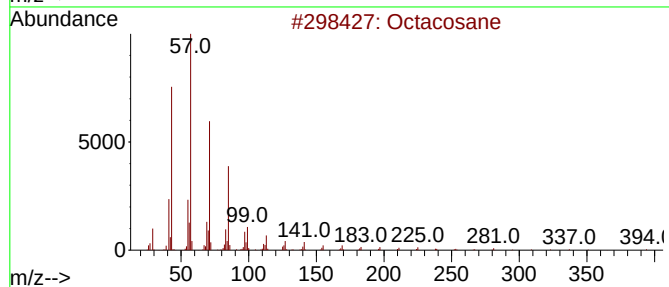
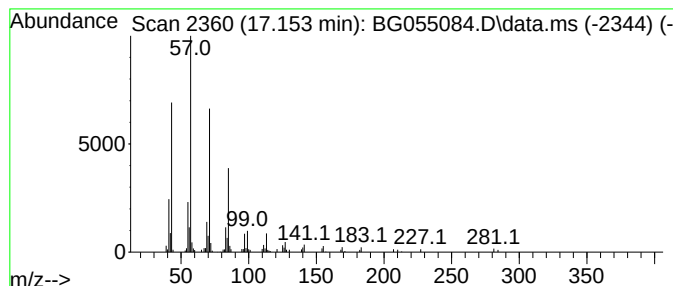
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.153	18.28 ng	445088	Phenanthrene-d10	17.676

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	90
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
3			Heptacosane	380	C27H56	000593-49-7	90
4			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87
5			Hexacosane	366	C26H54	000630-01-3	87



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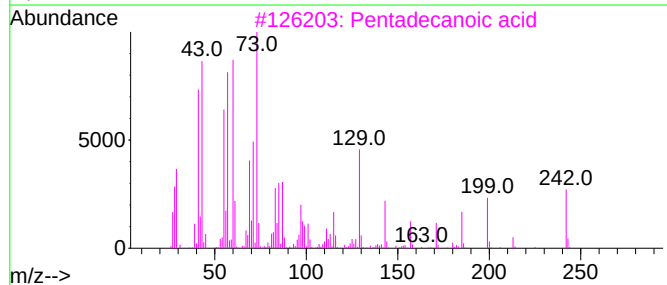
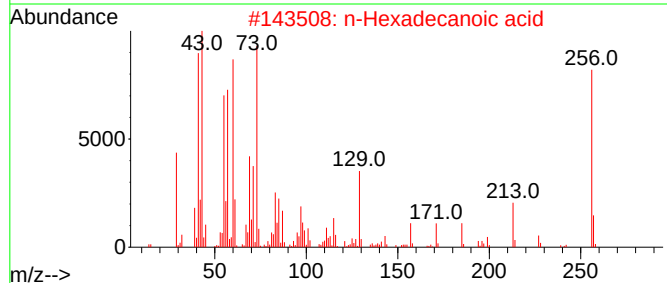
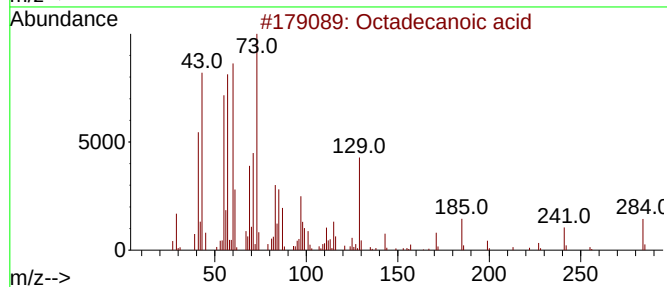
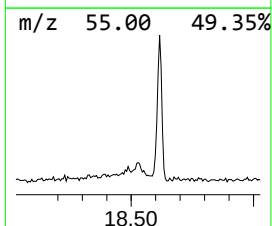
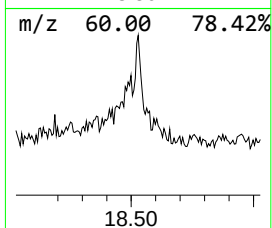
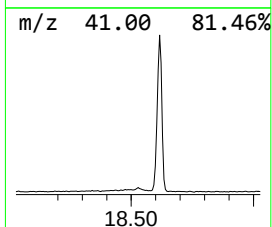
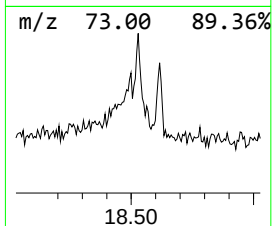
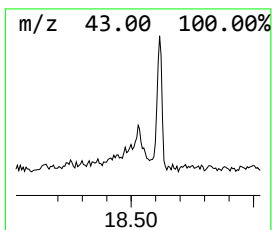
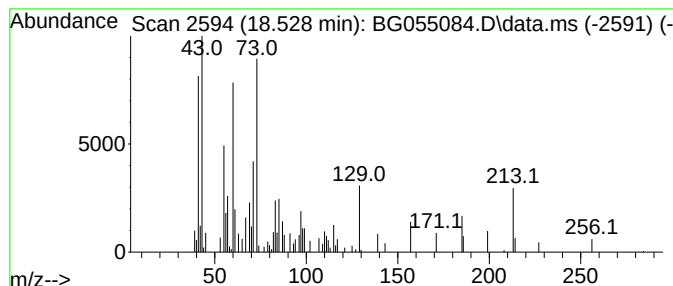
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.528	2.83 ng	68923	Phenanthrene-d10	17.676

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	87
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tridecanoic acid	214	C13H26O2	000638-53-9	80
5			Dodecanoic acid	200	C12H24O2	000143-07-7	53



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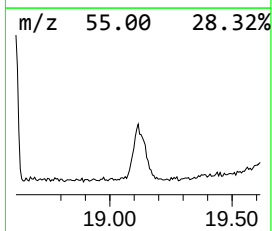
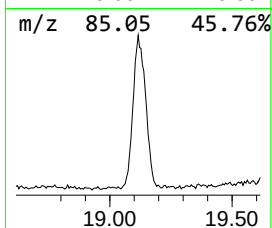
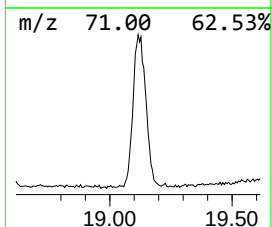
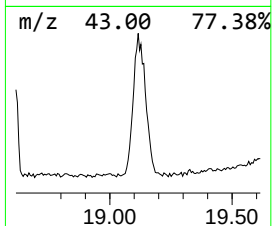
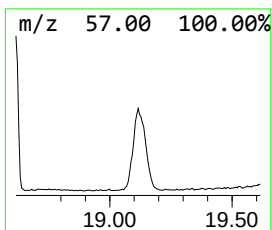
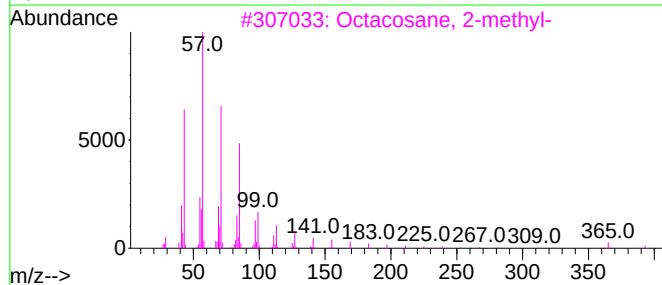
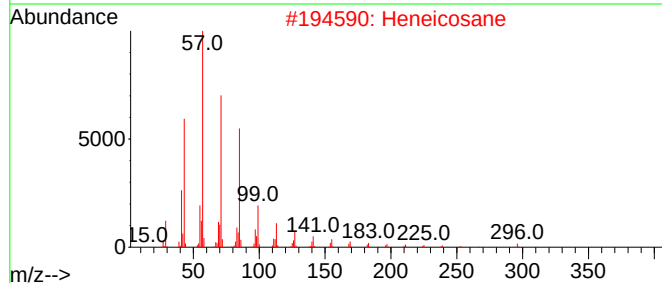
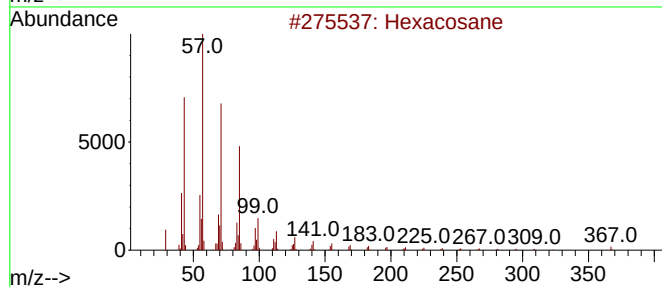
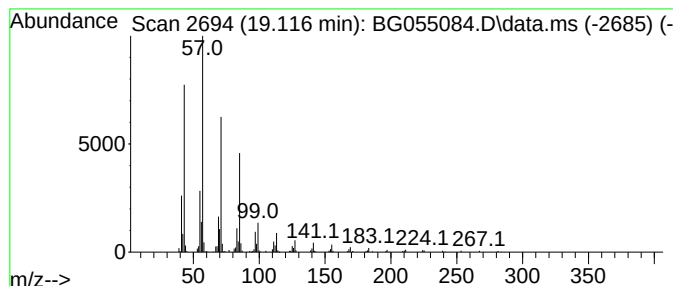
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.116	26.62 ng	647986	Phenanthrene-d10		17.676	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	91
2	Heneicosane		296	C21H44	000629-94-7	91
3	Octacosane, 2-methyl-		408	C29H60	001560-98-1	91
4	Pentacosane		352	C25H52	000629-99-2	91
5	Eicosane, 7-hexyl-		366	C26H54	055333-99-8	91



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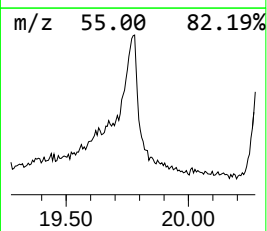
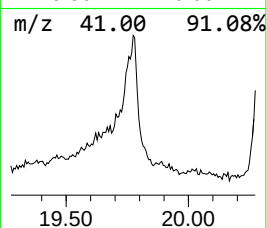
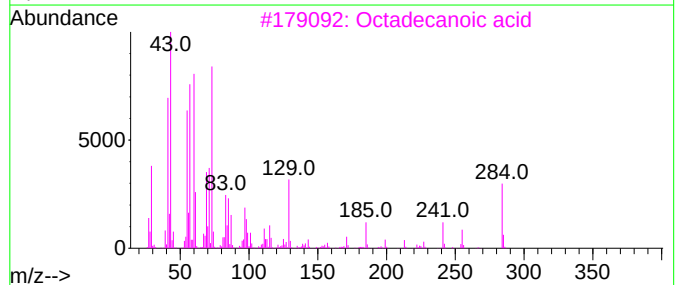
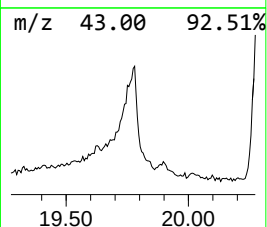
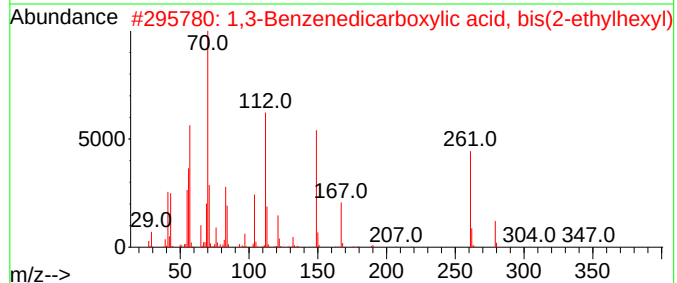
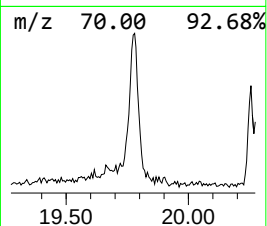
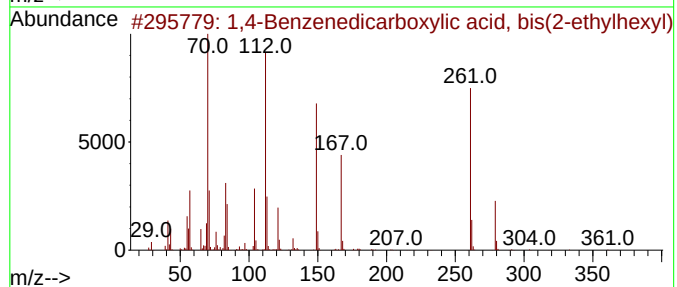
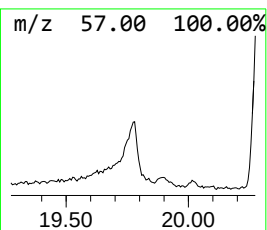
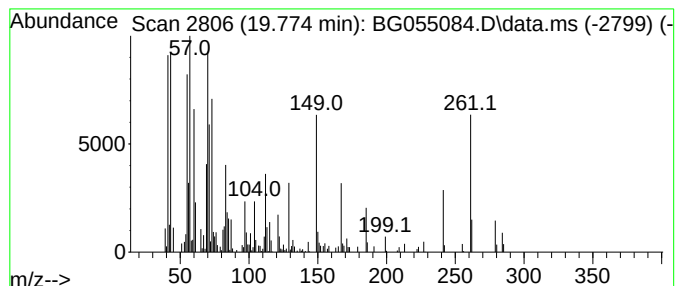
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,4-Benzenedicarboxylic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.774	27.71 ng	674478	Phenanthrene-d10	17.676	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	52
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	49
3	Octadecanoic acid	284	C18H36O2	000057-11-4	25
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	25
5	(1S,2S)-1,2-Dihydroxy-3,14-dioxo...	262	C10H18N2O6	1000111-03-0	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100622\
Data File : BG055084.D
Acq On : 6 Oct 2022 16:08
Operator : CG/JU
Sample : N5002-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

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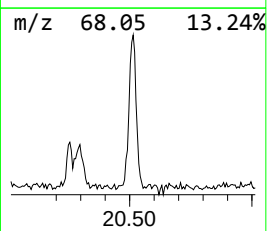
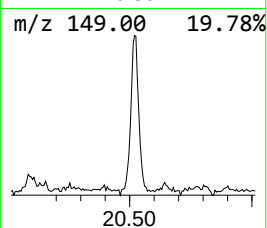
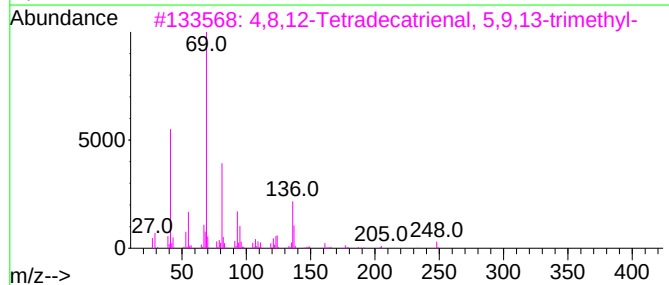
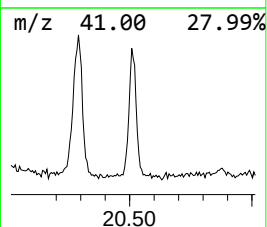
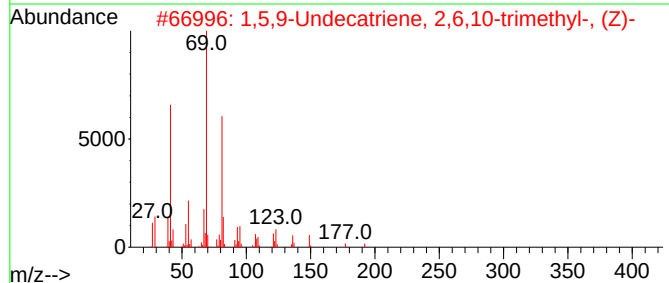
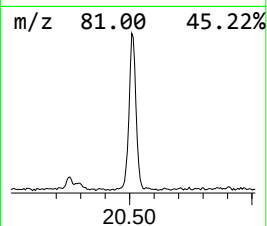
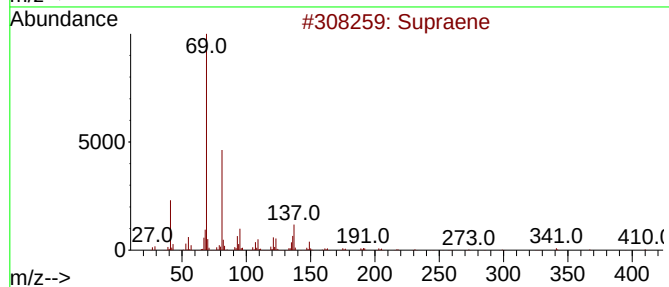
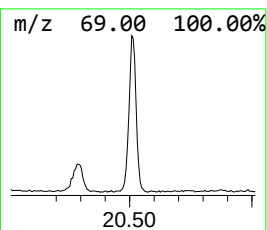
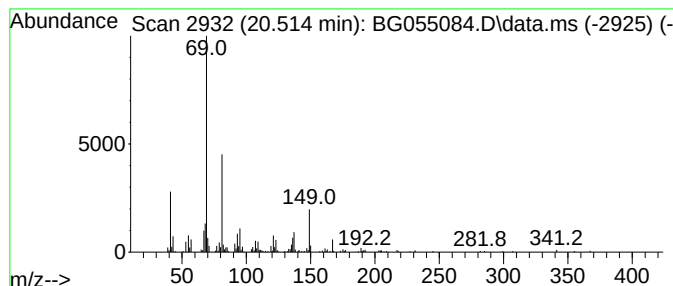
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Supraene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.514	10.72 ng	329693	Chrysene-d12	21.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	68
2			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64
3			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	59
4			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59
5			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100622\
Data File : BG055084.D
Acq On : 6 Oct 2022 16:08
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ALS Vial : 6 Sample Multiplier: 1

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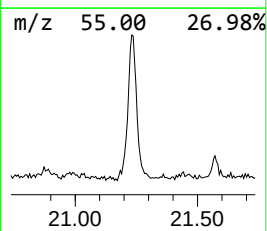
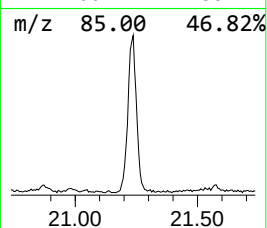
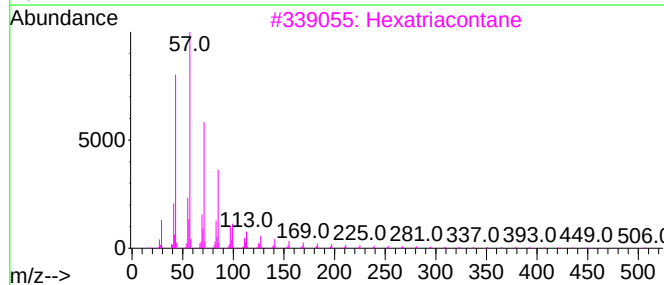
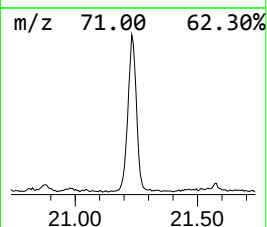
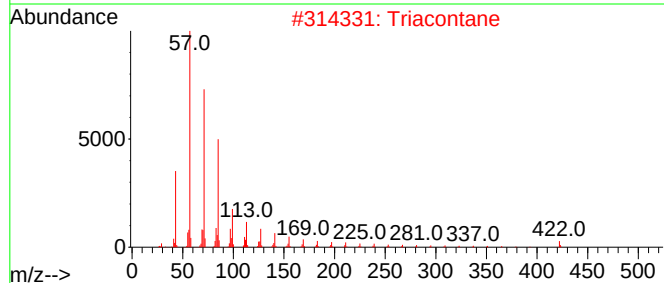
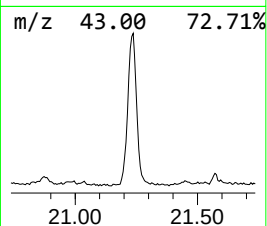
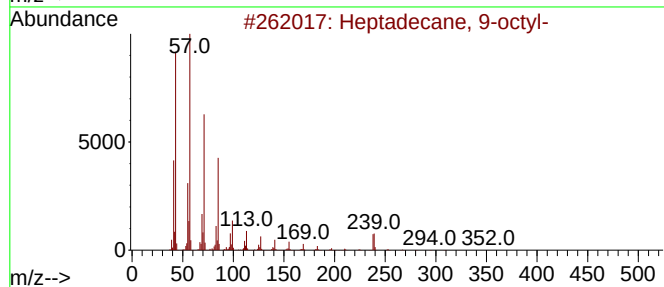
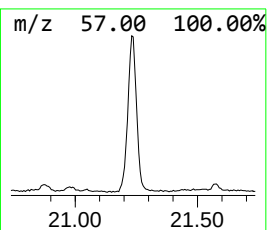
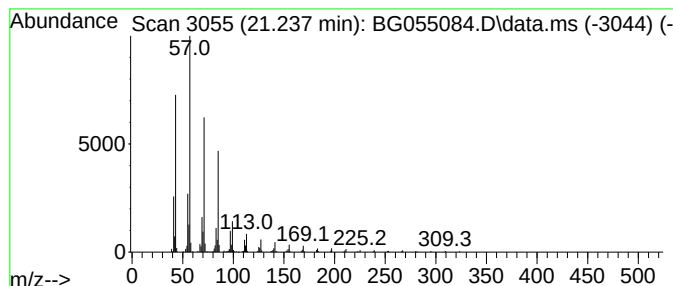
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane, 9-octyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.237	22.10 ng	679463	Chrysene-d12	21.965

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2		Triacontane	422	C30H62	000638-68-6	91
3		Hexatriacontane	507	C36H74	000630-06-8	91
4		Octacosane	394	C28H58	000630-02-4	91
5		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100622\
Data File : BG055084.D
Acq On : 6 Oct 2022 16:08
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ClientSampleId :
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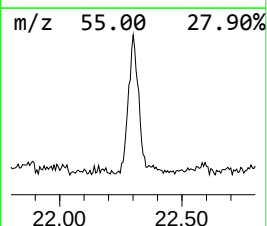
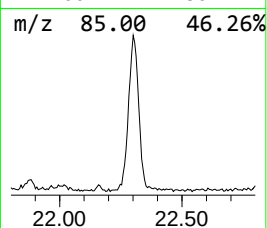
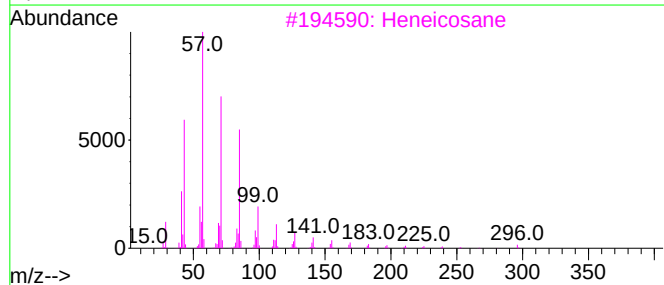
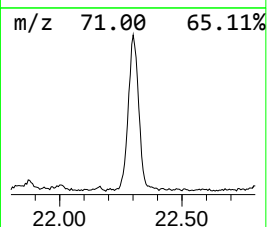
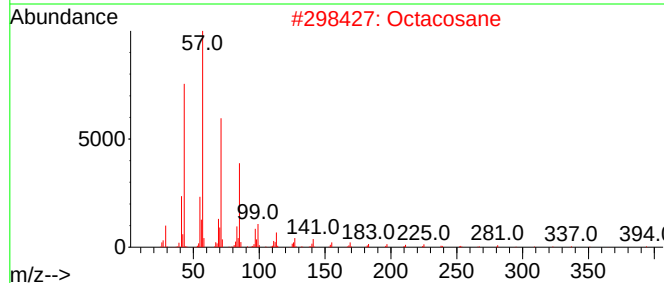
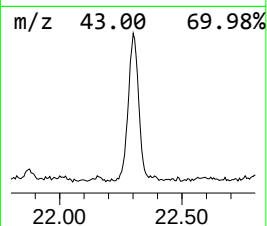
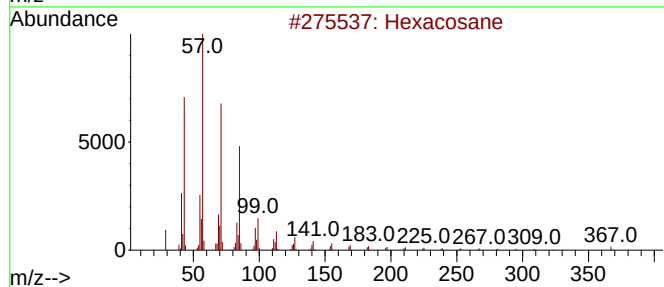
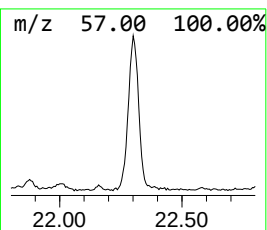
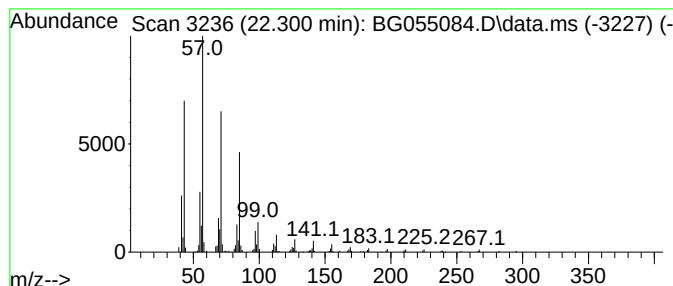
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.300	15.92 ng	489530	Chrysene-d12	21.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	94
2			Octacosane	394	C28H58	000630-02-4	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Heptacosane	380	C27H56	000593-49-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100622\
Data File : BG055084.D
Acq On : 6 Oct 2022 16:08
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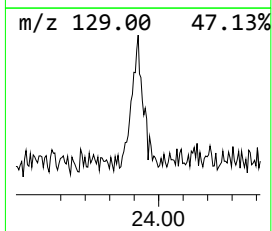
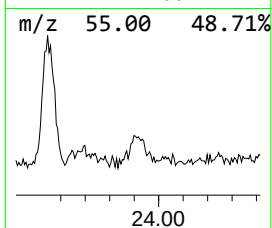
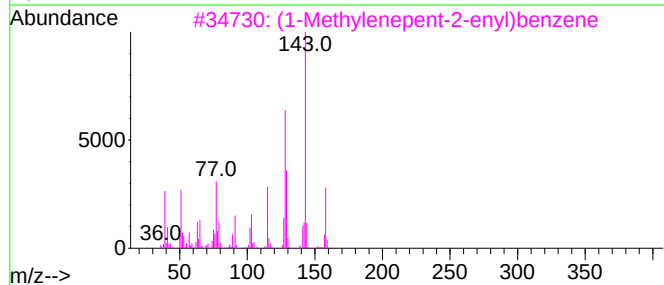
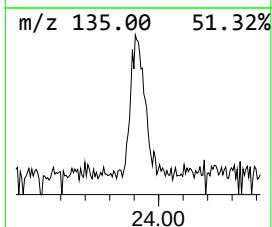
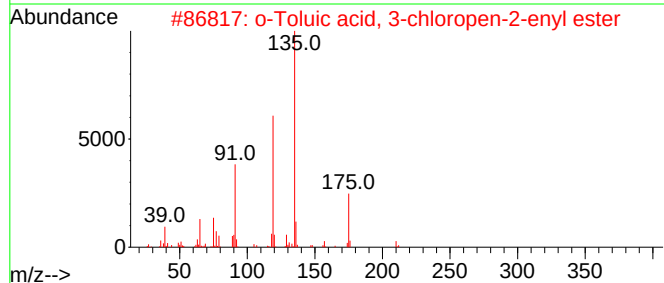
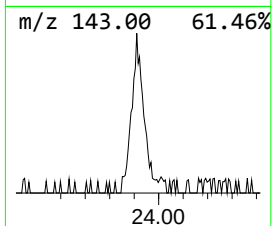
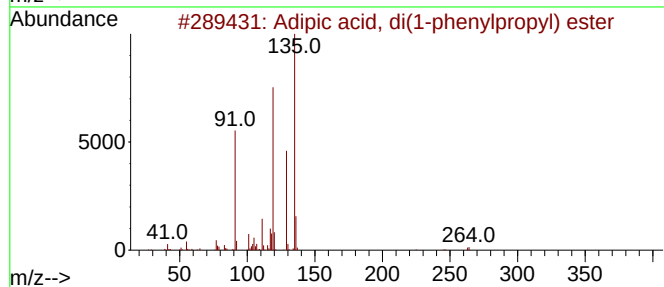
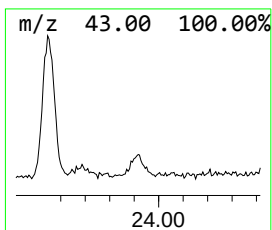
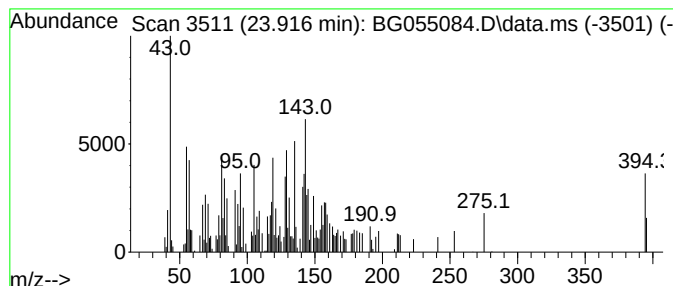
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown23.916 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.916	5.21 ng	171925	Perylene-d12	25.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Adipic acid, di(1-phenylpropyl) ...	382	C24H30O4	1000324-71-2	16
2			o-Toluic acid, 3-chloropen-2-enyl...	210	C11H11ClO2	1000292-51-8	14
3			(1-Methylenepent-2-enyl)benzene	158	C12H14	084313-24-6	14
4			Succinic acid, tridec-2-yn-1-yl ...	414	C26H38O4	1000389-93-7	14
5			Glutaric acid, di(1-phenylpropyl)...	368	C23H28O4	1000358-96-3	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100622\
Data File : BG055084.D
Acq On : 6 Oct 2022 16:08
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Misc :
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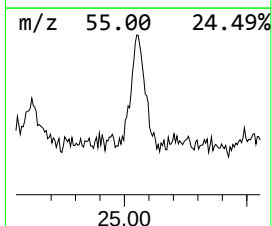
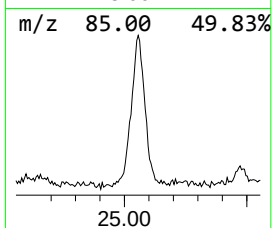
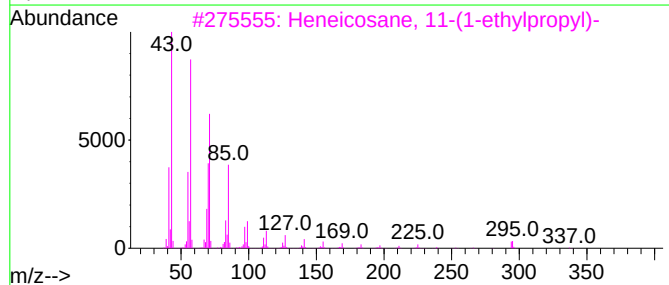
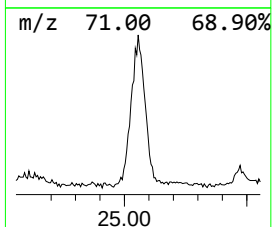
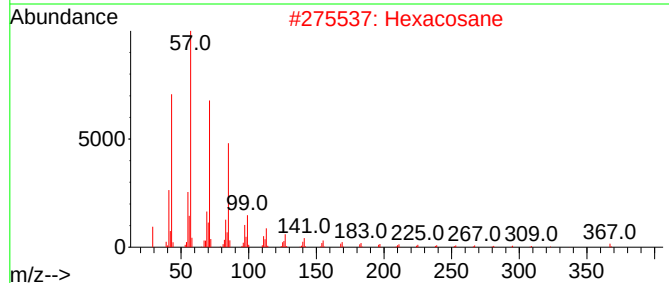
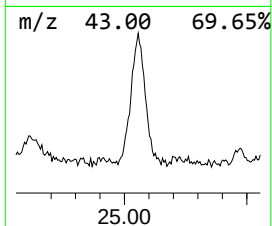
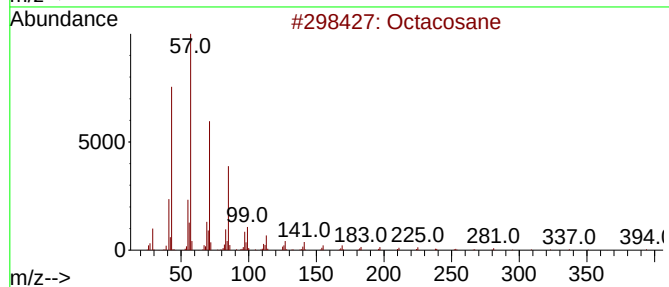
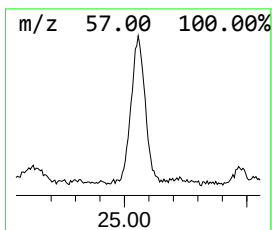
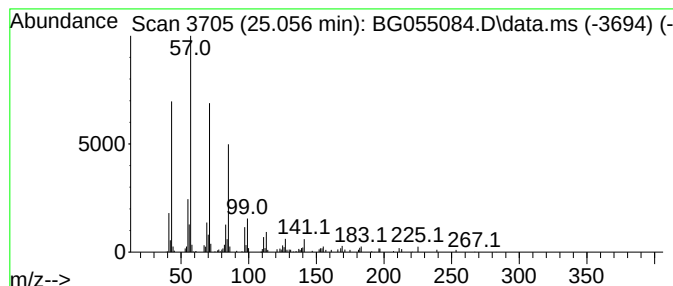
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Heneicosane, 11-(1-ethylpro... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.056	9.40 ng	309874	Perylene-d12	25.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Hexacosane	366	C26H54	000630-01-3	91
3			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Tetracosane	338	C24H50	000646-31-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100622\
Data File : BG055084.D
Acq On : 6 Oct 2022 16:08
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Misc :
ALS Vial : 6 Sample Multiplier: 1

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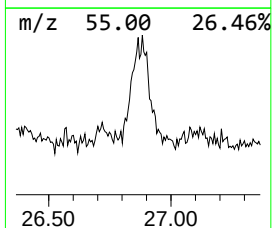
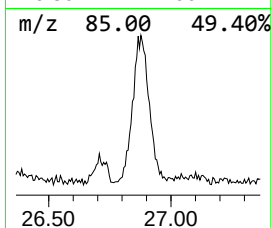
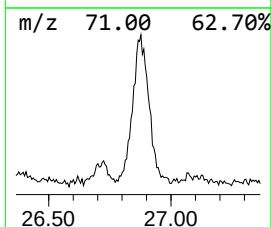
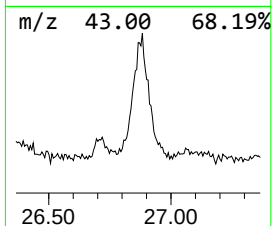
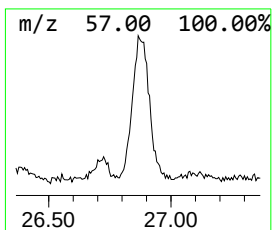
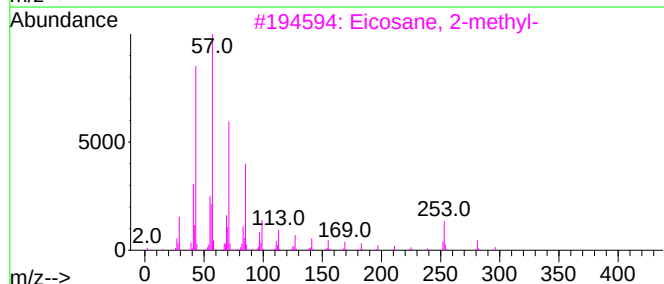
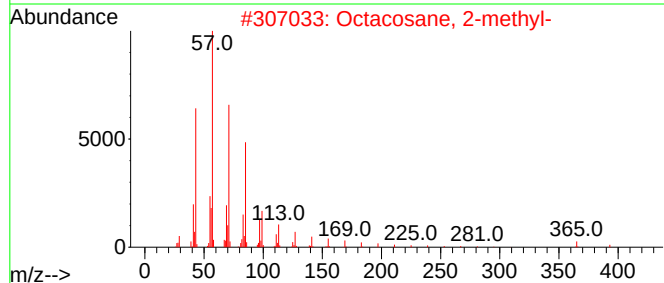
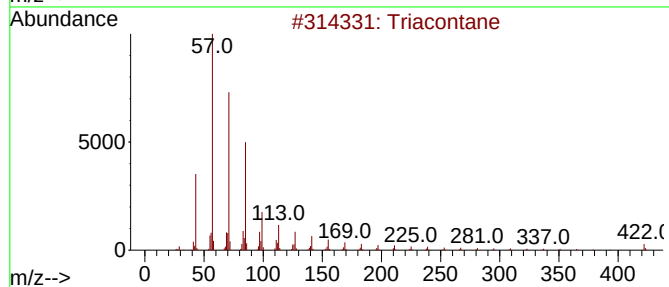
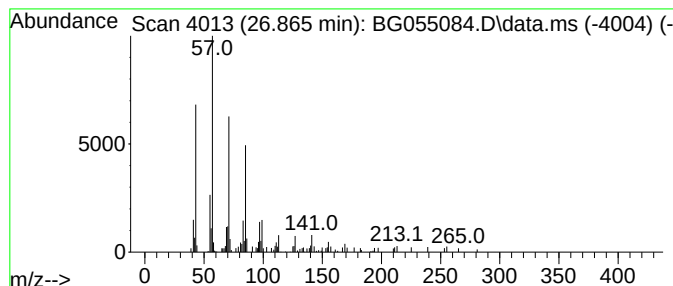
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Octacosane, 2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.866	8.51 ng	280623	Perylene-d12	25.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacontane	422	C30H62	000638-68-6	90
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
3			Eicosane, 2-methyl-	296	C21H44	001560-84-5	87
4			Heptacosane	380	C27H56	000593-49-7	86
5			Octacosane	394	C28H58	000630-02-4	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100622\
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Acq On : 6 Oct 2022 16:08
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Misc :
ALS Vial : 6 Sample Multiplier: 1

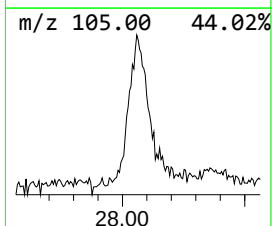
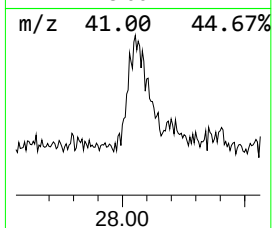
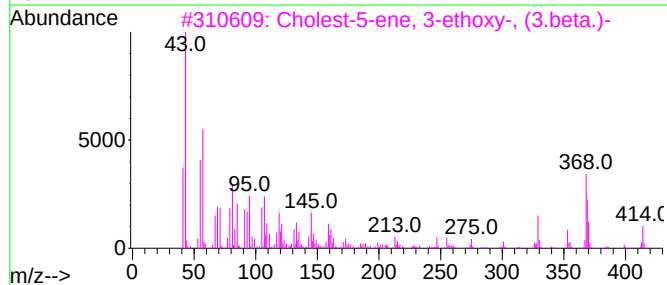
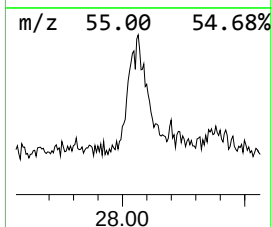
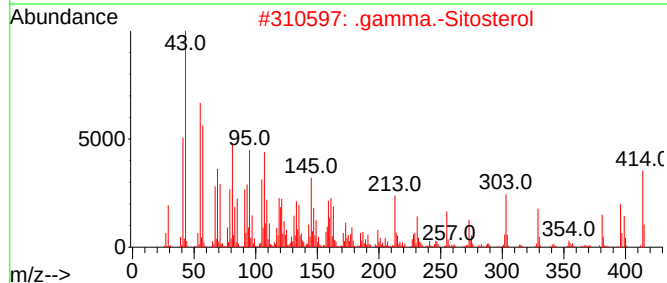
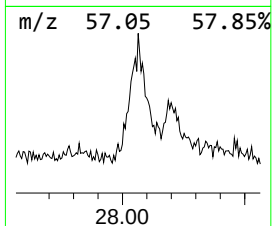
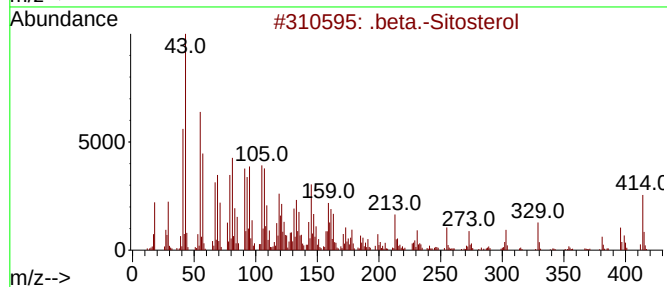
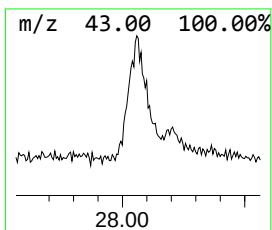
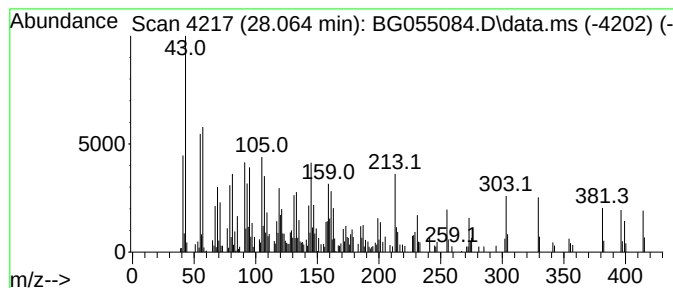
Instrument :
BNA_G
ClientSampleId :
5486-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 .beta.-Sitosterol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
28.064	20.10 ng	662801	Perylene-d12		25.420	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol		414	C29H50O	000083-46-5	97
2	.gamma.-Sitosterol		414	C29H50O	000083-47-6	93
3	Cholest-5-ene, 3-ethoxy-, (3.beta.-)		414	C29H50O	000986-19-6	64
4	Stigmasta-3,5-diene		396	C29H48	004970-37-0	38
5	Ergost-7-en-3-ol		400	C28H48O	116179-22-7	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100622\
 Data File : BG055084.D
 Acq On : 6 Oct 2022 16:08
 Operator : CG/JU
 Sample : N5002-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 5486-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.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
Butane, 2-metho...	3.381	157.3	ng	1624910	1	8.340	206654	20.0
2-Pentanone, 4-...	5.385	10.1	ng	104598	1	8.340	206654	20.0
Octacosane	17.153	18.3	ng	445088	4	17.676	486864	20.0
Octadecanoic acid	18.528	2.8	ng	68923	4	17.676	486864	20.0
Hexacosane	19.116	26.6	ng	647986	4	17.676	486864	20.0
1,4-Benzenedica...	19.774	27.7	ng	674478	4	17.676	486864	20.0
Supraene	20.514	10.7	ng	329693	5	21.965	614938	20.0
Heptadecane, 9-...	21.237	22.1	ng	679463	5	21.965	614938	20.0
Heneicosane	22.300	15.9	ng	489530	5	21.965	614938	20.0
Triacontane	23.546	15.3	ng	470126	5	21.965	614938	20.0
unknown23.916	23.916	5.2	ng	171925	6	25.420	659458	20.0
26-Nor-5-choles...	24.621	5.4	ng	176572	6	25.420	659458	20.0
Heneicosane, 11...	25.056	9.4	ng	309874	6	25.420	659458	20.0
Octacosane, 2-m...	26.866	8.5	ng	280623	6	25.420	659458	20.0
.beta.-Sitosterol	28.064	20.1	ng	662801	6	25.420	659458	20.0