

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
 Data File : BG060213.D
 Acq On : 3 Jan 2024 4:37
 Operator : MA/JU
 Sample : 05900-24
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 GHL-SS-66a

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: BG060213.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.117	3	5	10	rVB	352687	358032	2.16%	0.403%
2	5.038	327	332	339	rBV	193982	286943	1.73%	0.323%
3	5.508	405	412	422	rBV	4707911	7423268	44.84%	8.354%
4	7.100	674	683	700	rBV	4503487	7721540	46.64%	8.690%
5	7.935	818	825	834	rBV	738186	1276342	7.71%	1.436%
6	9.098	1014	1023	1039	rBV	2604938	4704007	28.41%	5.294%
7	10.743	1293	1303	1310	rBV	1082145	2038879	12.32%	2.295%
8	13.199	1711	1721	1730	rBV	7895480	12528436	75.67%	14.099%
9	14.574	1944	1955	1962	rBV	2248006	3493529	21.10%	3.932%
10	16.066	2200	2209	2229	rBV	6417833	10141359	61.26%	11.413%
11	17.324	2416	2423	2434	rBV	3026742	4545427	27.46%	5.115%
12	18.211	2569	2574	2585	rBV	389121	640007	3.87%	0.720%
13	19.944	2863	2869	2883	rBV	12283760	16555756	100.00%	18.632%
14	21.237	3084	3089	3099	rBV	996655	1566155	9.46%	1.763%
15	21.589	3142	3149	3161	rBV2	2607969	4373700	26.42%	4.922%
16	22.400	3279	3287	3298	rBV4	545095	1350650	8.16%	1.520%
17	23.405	3454	3458	3467	rVB5	150354	301721	1.82%	0.340%
18	23.857	3529	3535	3539	rBV	177364	352398	2.13%	0.397%
19	23.916	3539	3545	3563	rVB2	543362	1288410	7.78%	1.450%
20	24.762	3679	3689	3703	rBV	1592614	4616097	27.88%	5.195%
21	25.308	3774	3782	3793	rVB6	174954	491656	2.97%	0.553%
22	25.908	3877	3884	3894	rVB4	167602	481425	2.91%	0.542%
23	26.031	3895	3905	3915	rBV5	263775	879363	5.31%	0.990%
24	26.225	3932	3938	3946	rBV7	64751	180401	1.09%	0.203%
25	28.023	4235	4244	4256	rVB9	105864	357412	2.16%	0.402%
26	29.997	4567	4580	4596	rBV9	172066	905313	5.47%	1.019%

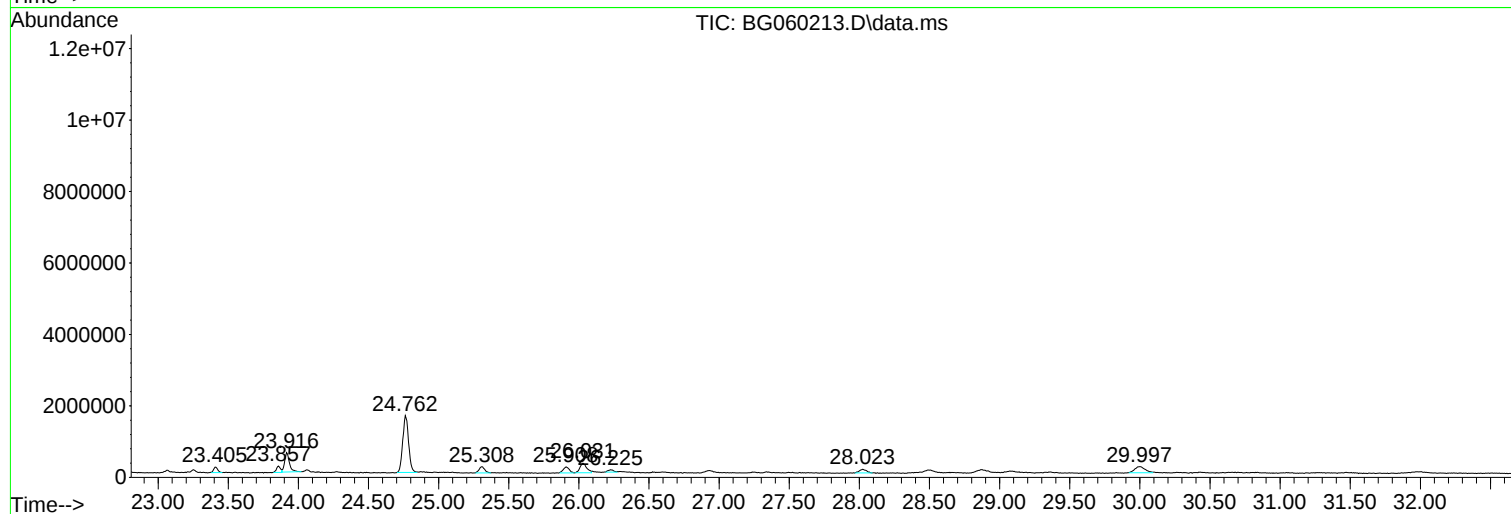
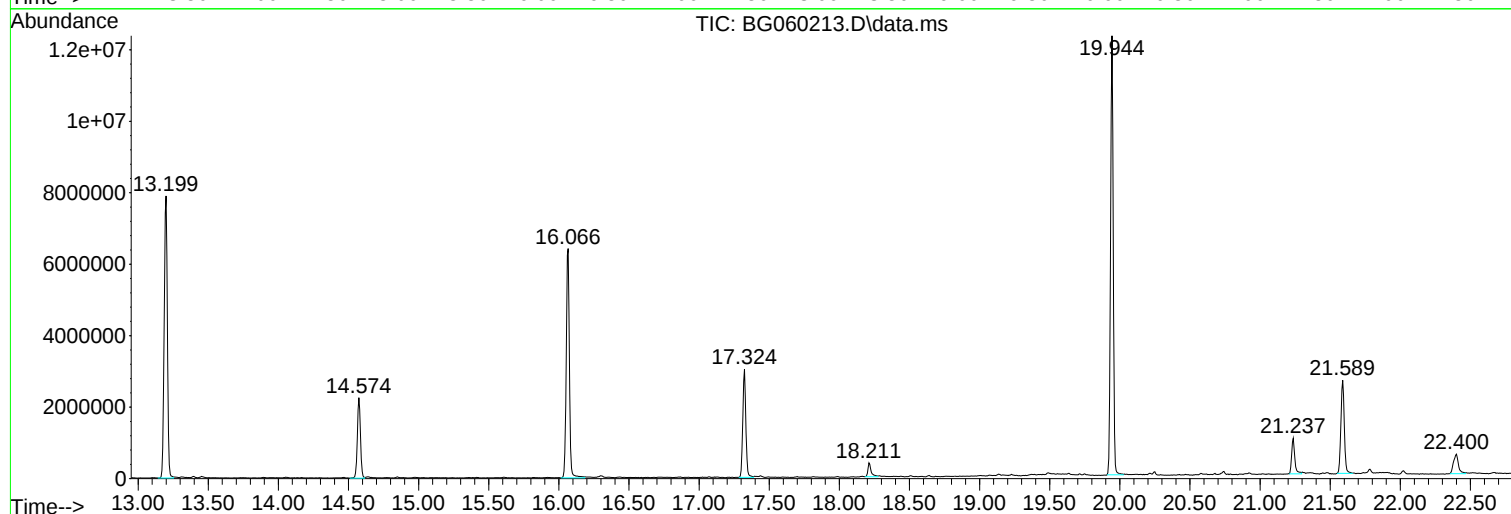
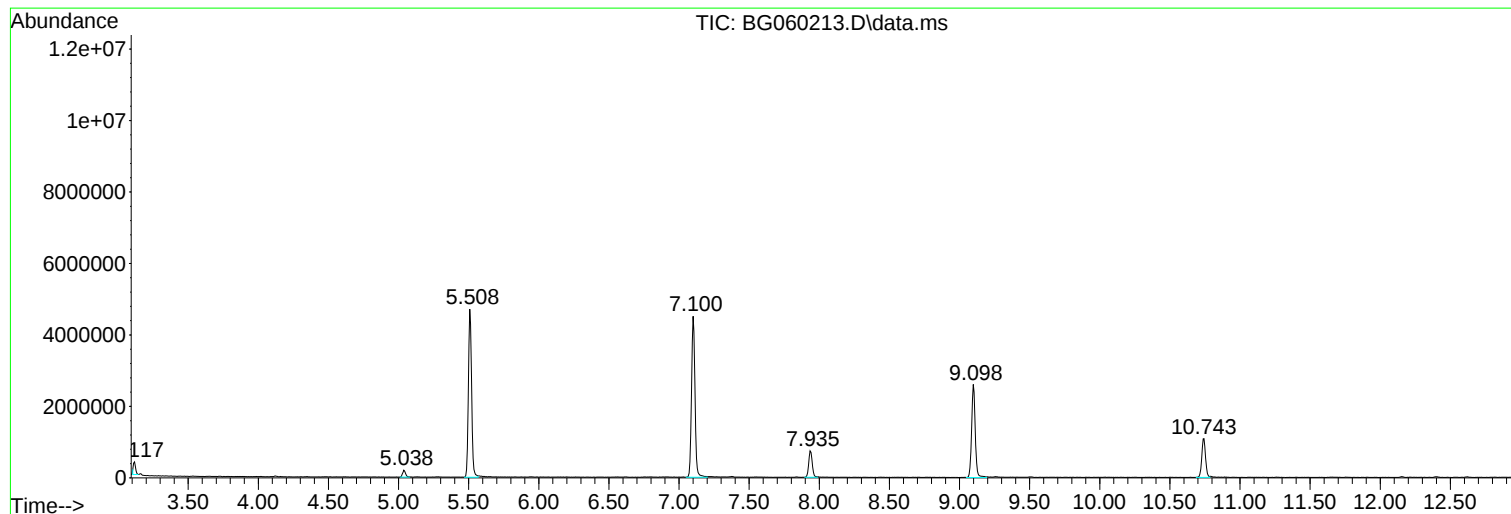
Sum of corrected areas: 88858226

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060213.D
Acq On : 3 Jan 2024 4:37
Operator : MA/JU
Sample : 05900-24
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-66a

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060213.D
Acq On : 3 Jan 2024 4:37
Operator : MA/JU
Sample : 05900-24
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-66a

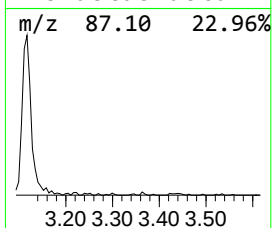
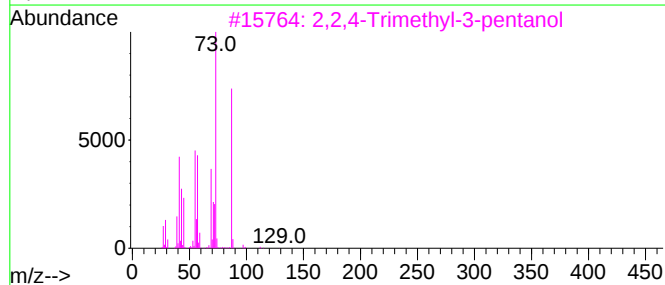
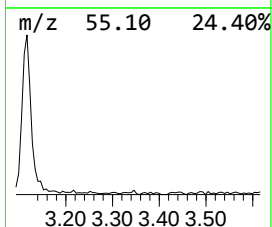
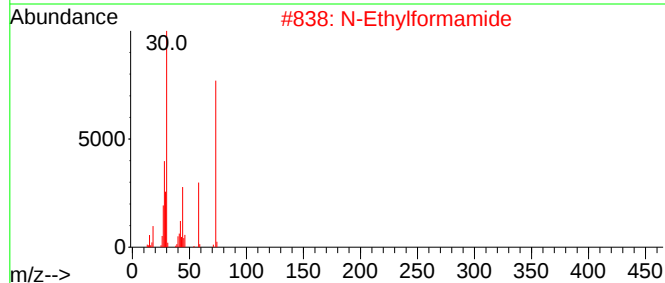
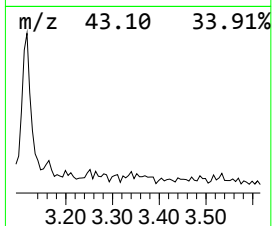
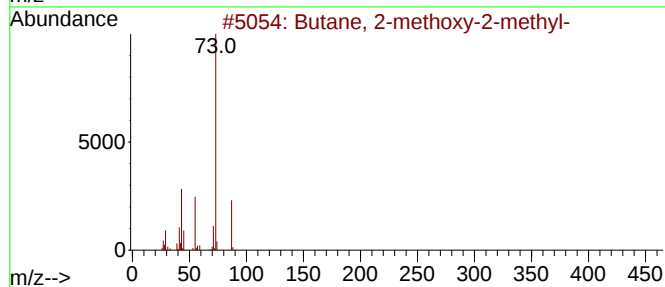
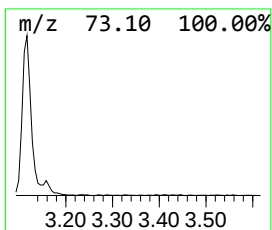
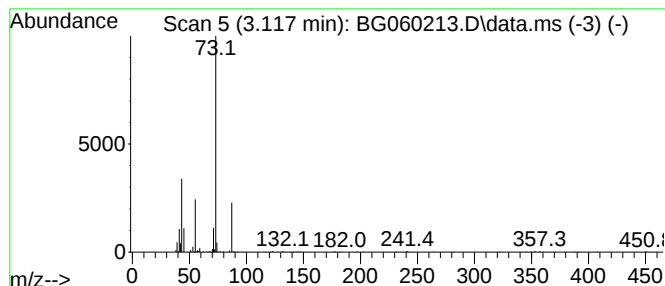
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.117	5.61 ng	358032	1,4-Dichlorobenzene-d4	7.935

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2		N-Ethylformamide	73	C3H7NO	000627-45-2	9
3		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9
4		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060213.D
Acq On : 3 Jan 2024 4:37
Operator : MA/JU
Sample : 05900-24
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-66a

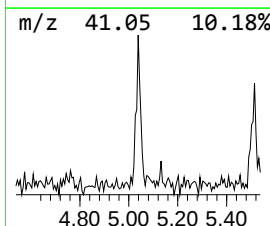
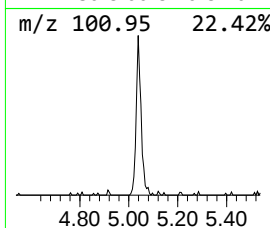
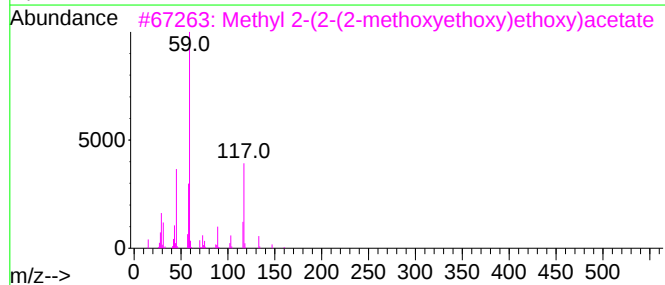
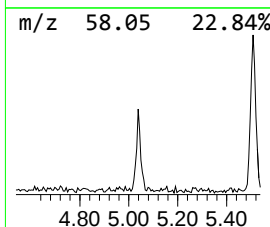
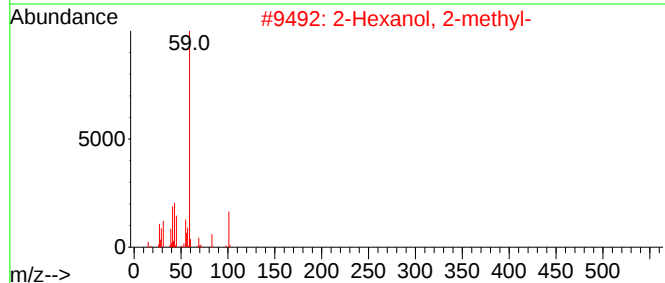
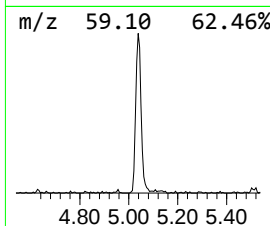
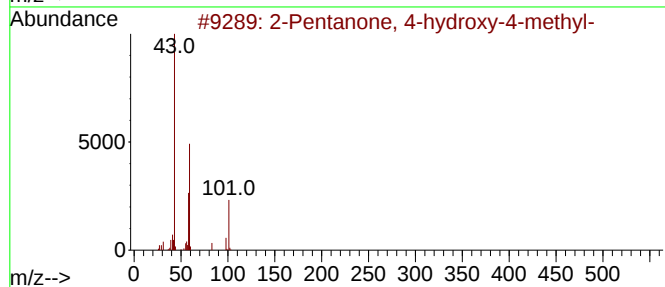
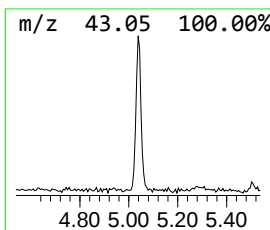
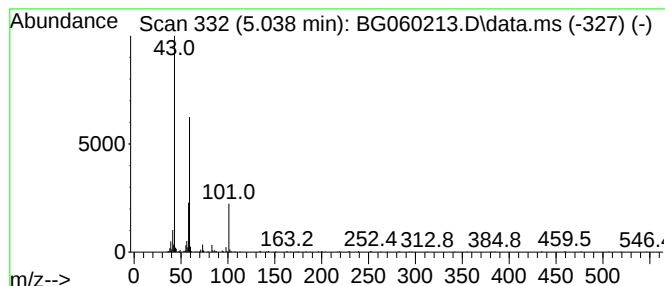
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown5.038 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.038	4.50 ng	286943	1,4-Dichlorobenzene-d4	7.935

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	47
3		Methyl 2-(2-(2-methoxyethoxy)ethoxy)acetate	192	C8H16O5	1000366-88-2	33
4		Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	33
5		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060213.D
Acq On : 3 Jan 2024 4:37
Operator : MA/JU
Sample : 05900-24
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-66a

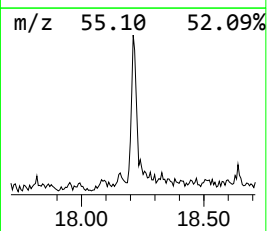
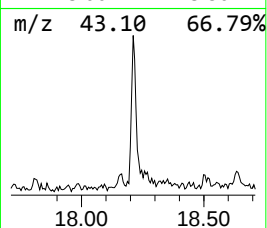
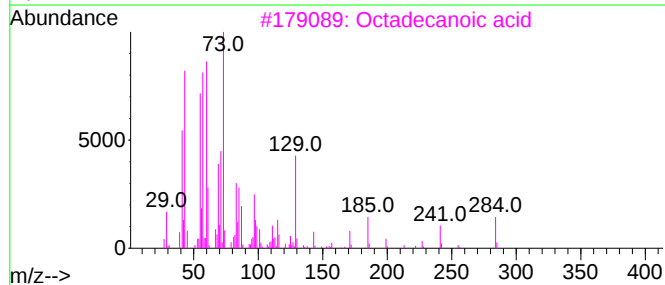
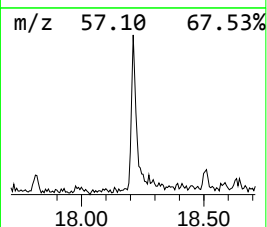
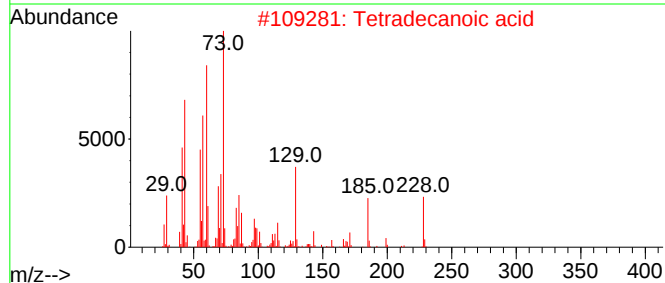
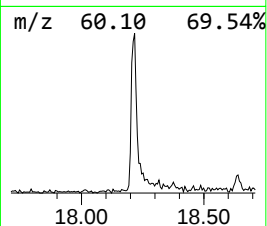
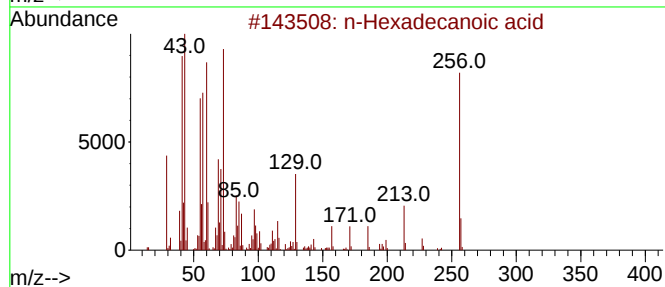
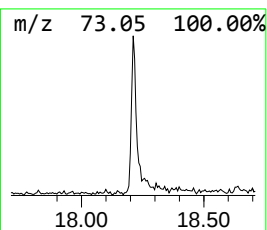
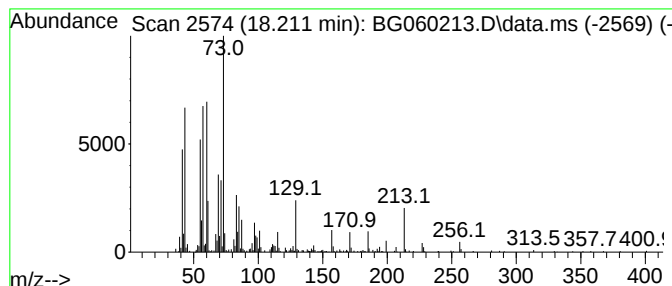
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.211	2.82 ng	640007	Phenanthrene-d10	17.324

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3			Octadecanoic acid	284	C18H36O2	000057-11-4	53
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	52
5			Tridecanoic acid	214	C13H26O2	000638-53-9	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060213.D
Acq On : 3 Jan 2024 4:37
Operator : MA/JU
Sample : 05900-24
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-66a

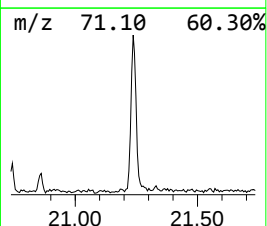
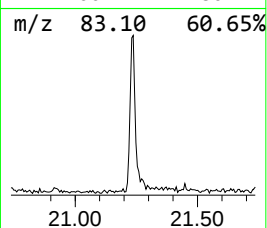
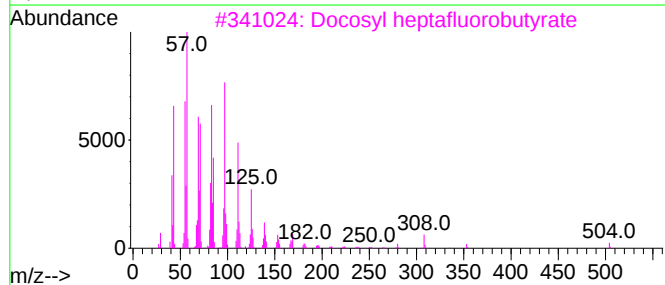
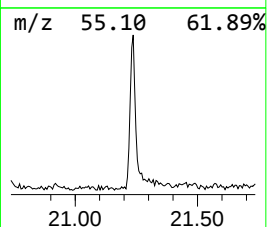
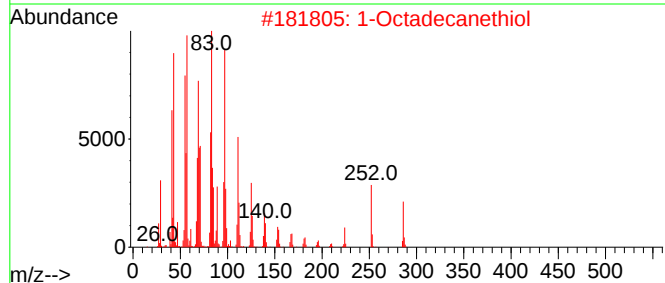
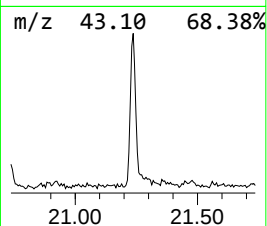
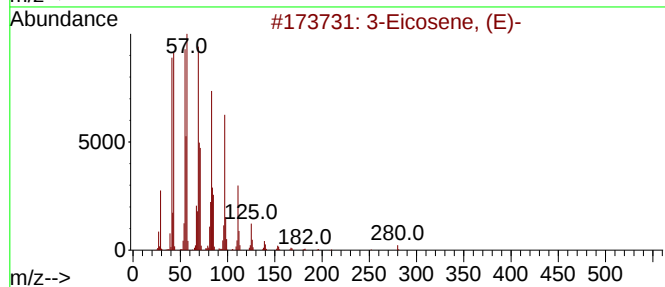
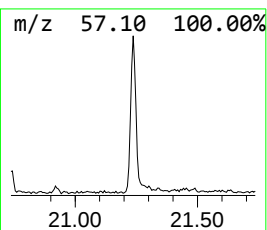
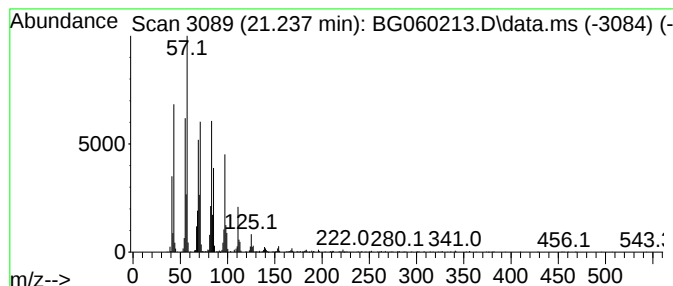
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 3-Eicosene, (E)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.237	7.16 ng	1566160	Chrysene-d12	21.589

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Eicosene, (E)-	280	C20H40	074685-33-9	96
2			1-Octadecanethiol	286	C18H38S	002885-00-9	94
3			Docosyl heptafluorobutyrate	522	C26H45F7O2	1000351-83-1	91
4			Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1010351-81-4	91
5			Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060213.D
Acq On : 3 Jan 2024 4:37
Operator : MA/JU
Sample : 05900-24
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-66a

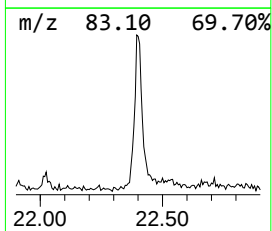
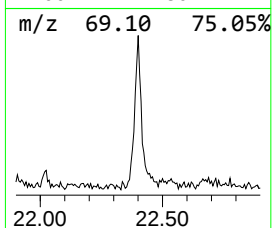
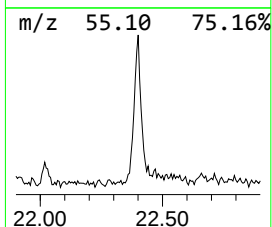
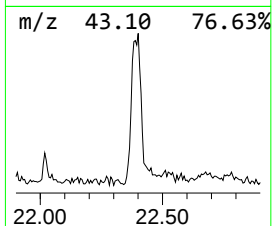
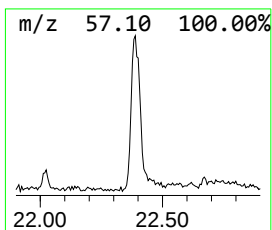
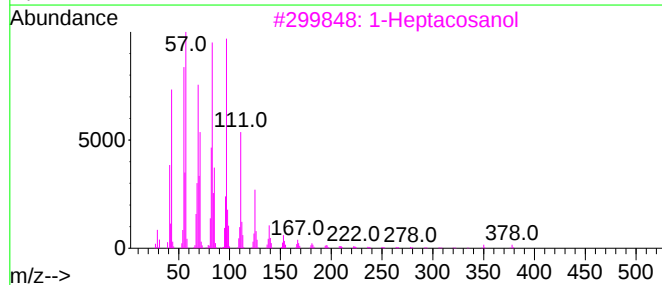
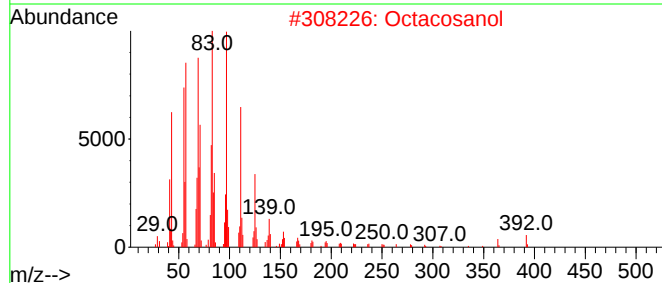
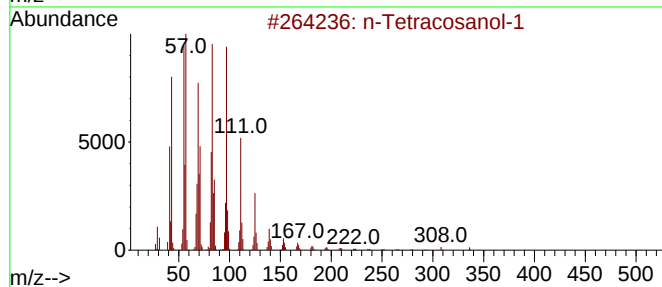
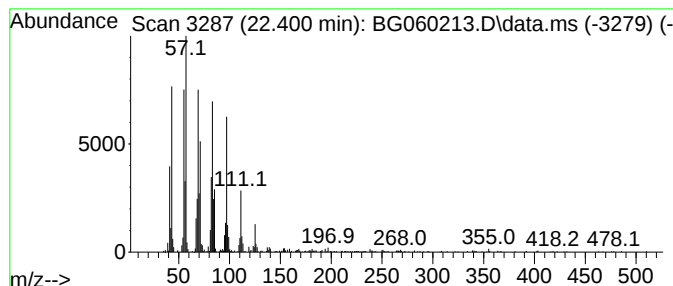
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Tetracosanol-1 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.400	6.18 ng	1350650	Chrysene-d12	21.589

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2			Octacosanol	410	C28H58O	000557-61-9	91
3			1-Heptacosanol	396	C27H56O	002004-39-9	91
4			Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	91
5			Nonacos-1-ene	406	C29H58	018835-35-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060213.D
Acq On : 3 Jan 2024 4:37
Operator : MA/JU
Sample : 05900-24
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-66a

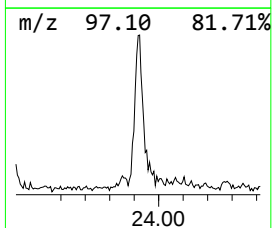
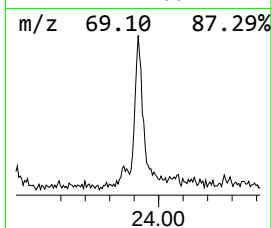
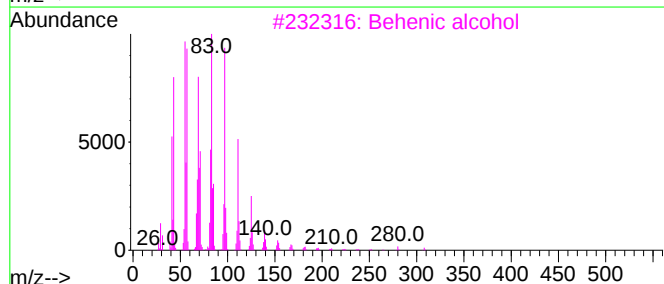
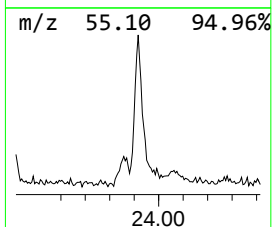
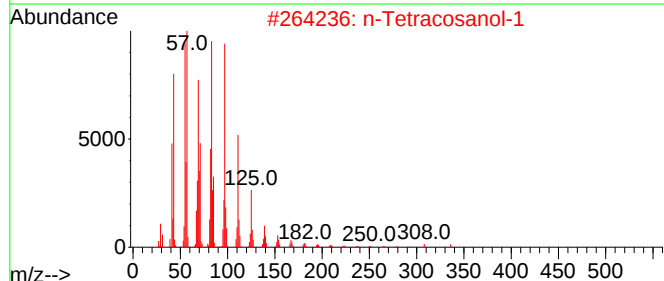
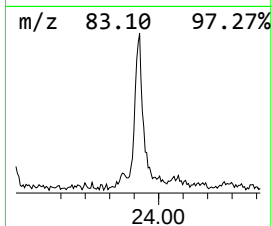
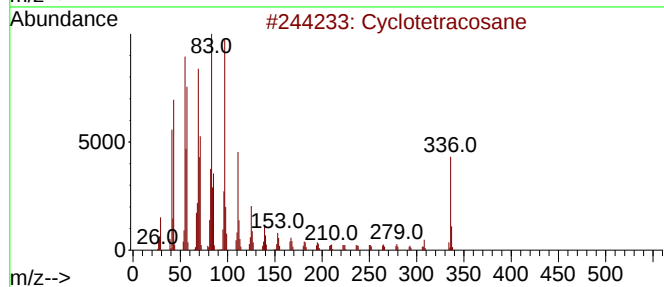
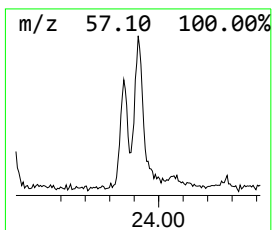
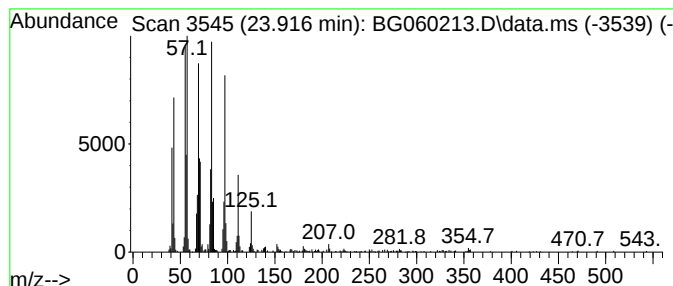
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclotetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.916	5.58 ng	1288410	Perylene-d12	24.762

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclotetracosane	336	C24H48	000297-03-0	96
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	90
3		Behenic alcohol	326	C22H46O	000661-19-8	90
4		1-Heneicosanol	312	C21H44O	015594-90-8	87
5		Cyclohexadecane	224	C16H32	000295-65-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060213.D
Acq On : 3 Jan 2024 4:37
Operator : MA/JU
Sample : 05900-24
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-66a

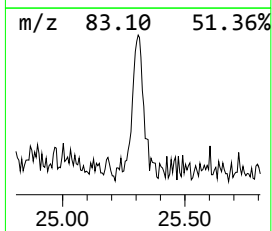
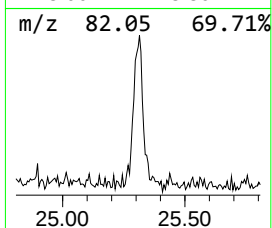
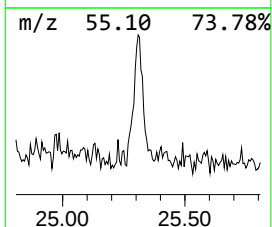
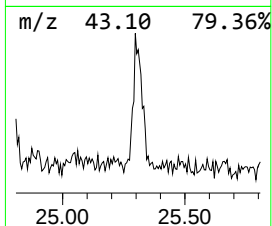
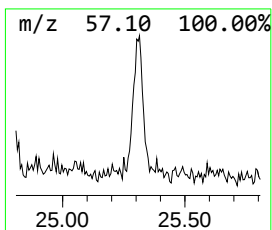
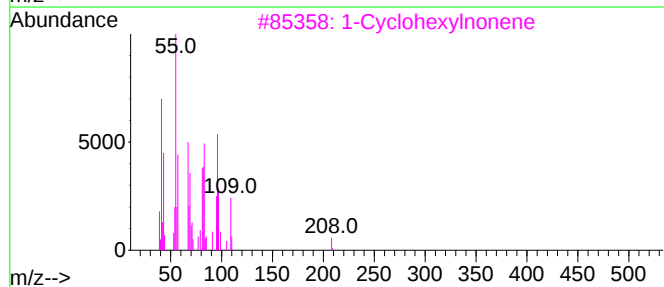
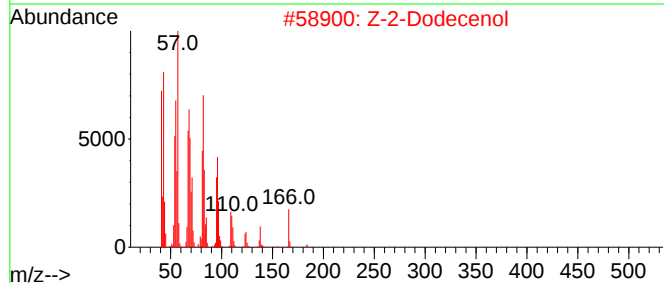
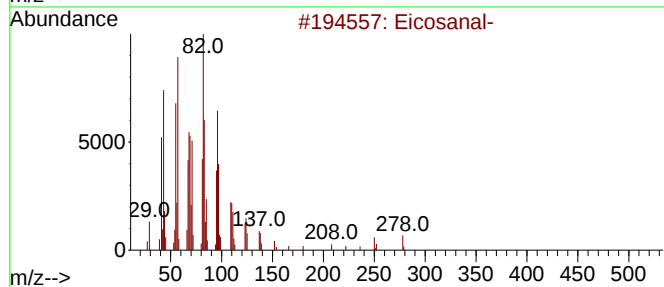
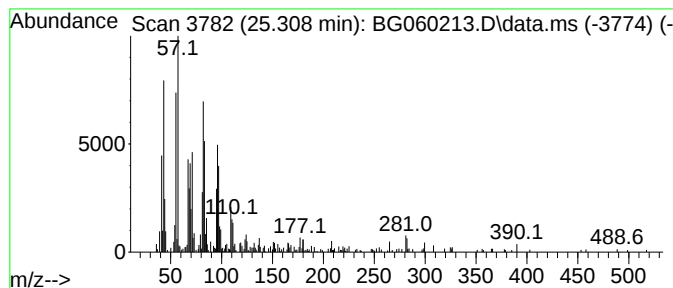
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosanal- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.308	2.13 ng	491656	Perylene-d12	24.762

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosanal-	296	C20H40O	002400-66-0	80
2			Z-2-Dodecenol	184	C12H24O	069064-36-4	55
3			1-Cyclohexylnonene	208	C15H28	114614-84-5	55
4			Pentadecanal-	226	C15H30O	002765-11-9	52
5			1,16-Hexadecanediol	258	C16H34O2	007735-42-4	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060213.D
Acq On : 3 Jan 2024 4:37
Operator : MA/JU
Sample : 05900-24
Misc :
ALS Vial : 26 Sample Multiplier: 1

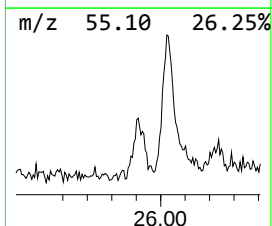
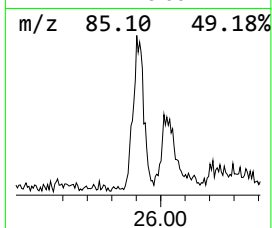
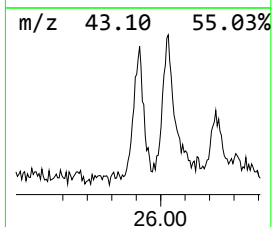
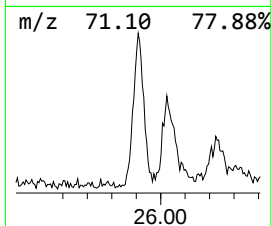
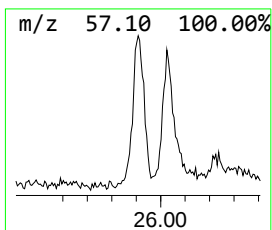
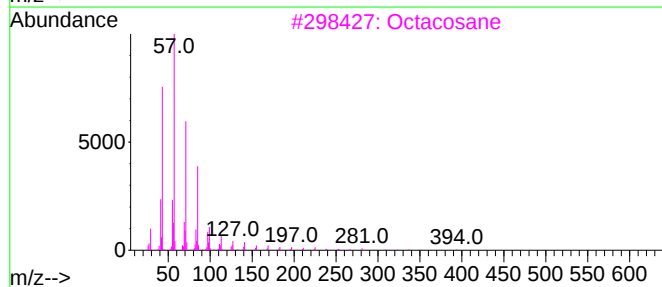
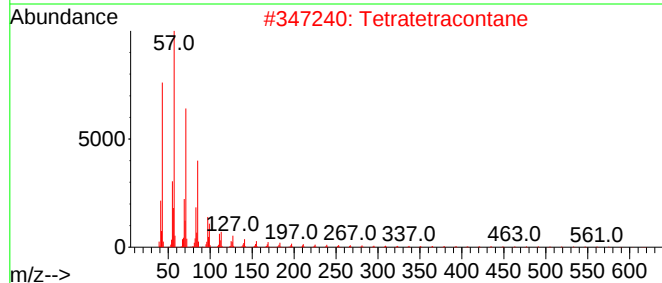
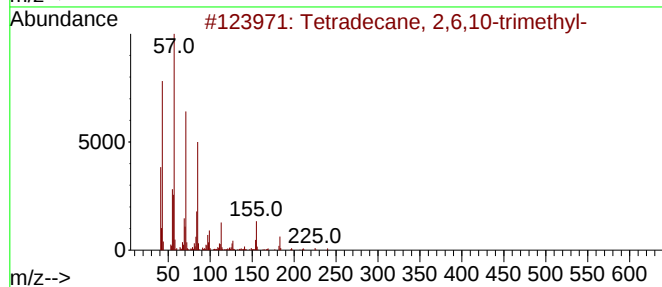
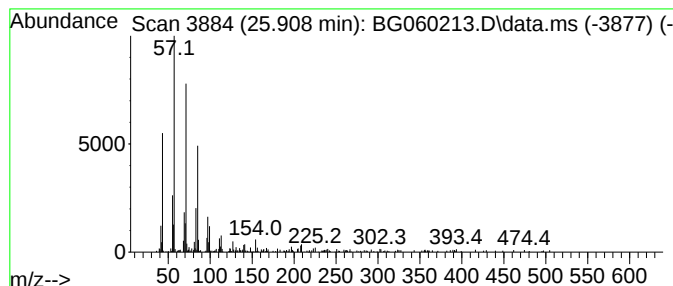
Instrument :
BNA_G
ClientSampleId :
GHL-SS-66a

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 8 Tetradecane, 2,6,10-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
25.908	2.09 ng	481425	Perylene-d12	24.762	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	90
2	Tetratetracontane	619	C44H90	007098-22-8	90
3	Octacosane	394	C28H58	000630-02-4	87
4	Nonadecane	268	C19H40	000629-92-5	72
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060213.D
Acq On : 3 Jan 2024 4:37
Operator : MA/JU
Sample : 05900-24
Misc :
ALS Vial : 26 Sample Multiplier: 1

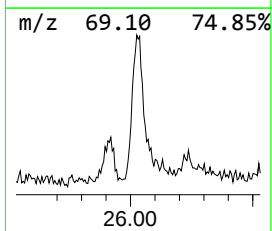
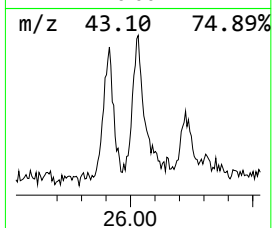
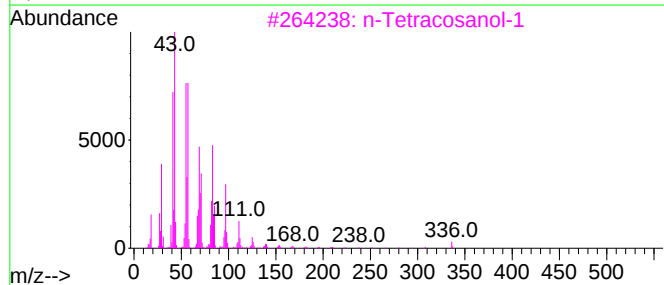
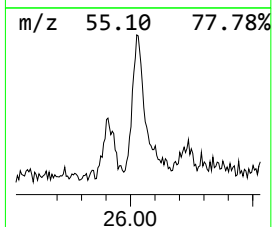
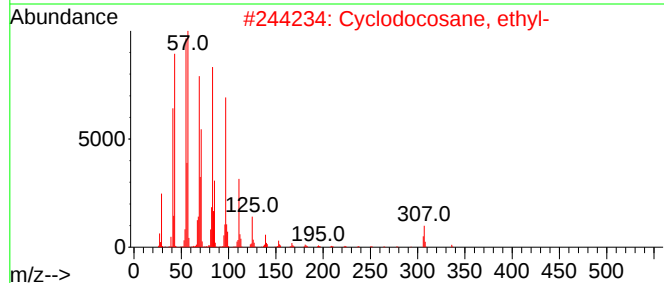
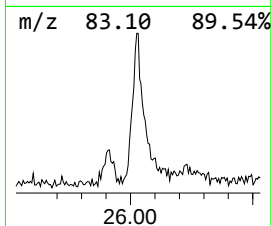
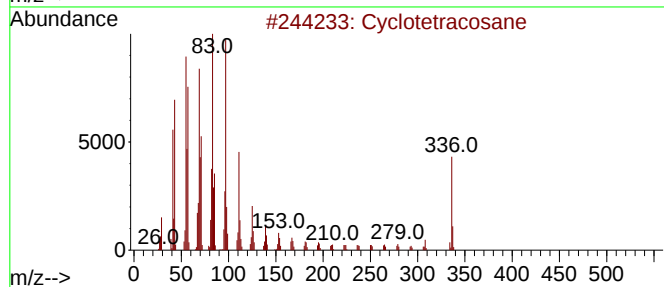
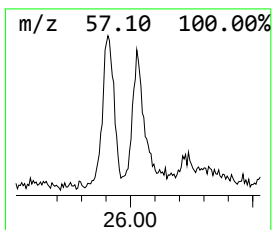
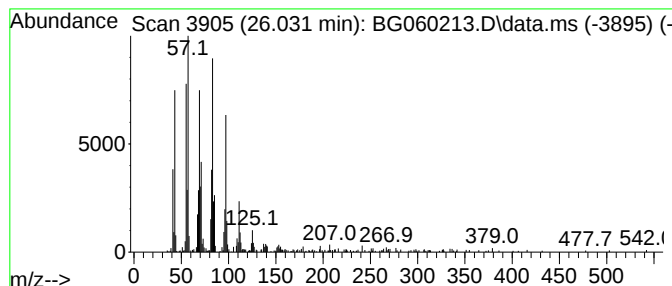
Instrument :
BNA_G
ClientSampleId :
GHL-SS-66a

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 9 Cyclodocosane, ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
26.031	3.81 ng	879363	Perylene-d12	24.762	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	94
2	Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	93
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	1-Heptacosanol	396	C27H56O	002004-39-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060213.D
Acq On : 3 Jan 2024 4:37
Operator : MA/JU
Sample : 05900-24
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-66a

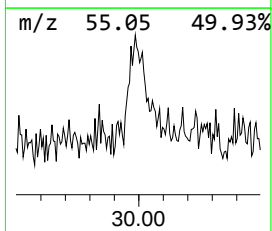
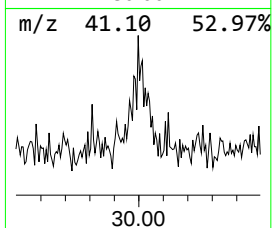
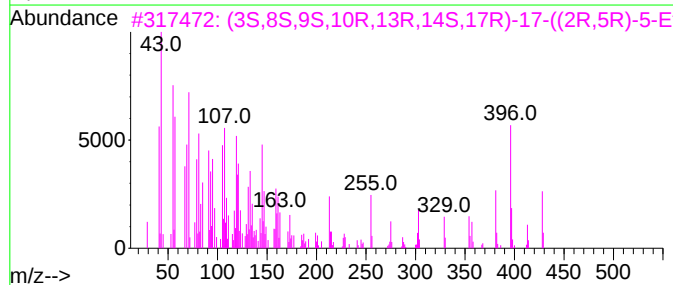
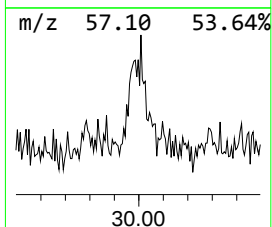
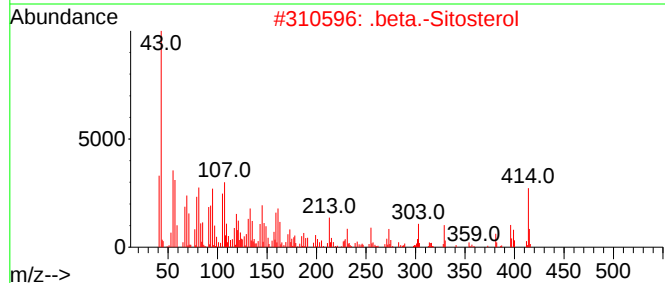
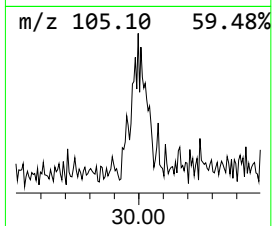
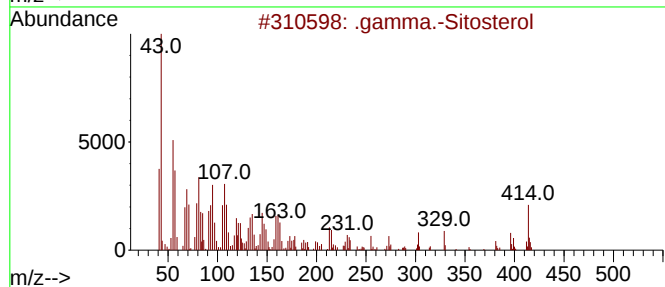
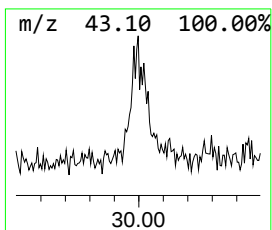
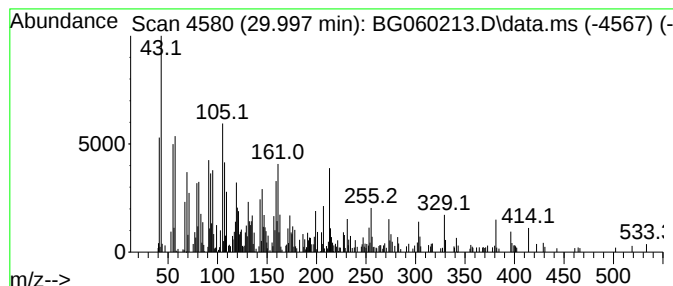
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 .gamma.-Sitosterol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.997	3.92 ng	905313	Perylene-d12	24.762

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.gamma.-Sitosterol	414	C29H50O	000083-47-6	64
2		.beta.-Sitosterol	414	C29H50O	000083-46-5	62
3		(3S,8S,9S,10R,13R,14S,17R)-17-((... 428	C30H52O		020194-50-7	38
4		Cyclohexanemethanol, 4-ethenyl-.... 264	C17H28O2		060031-93-8	25
5		Cholest-5-ene, 3-ethoxy-, (3.bet... 414	C29H50O		000986-19-6	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060213.D
Acq On : 3 Jan 2024 4:37
Operator : MA/JU
Sample : 05900-24
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-66a

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
Butane, 2-metho...	3.117	5.6	ng	358032	1	7.935	1276340	20.0
unknown5.038	5.038	4.5	ng	286943	1	7.935	1276340	20.0
n-Hexadecanoic ...	18.211	2.8	ng	640007	4	17.324	4545430	20.0
3-Eicosene, (E)-	21.237	7.2	ng	1566160	5	21.589	4373700	20.0
n-Tetracosanol-1	22.400	6.2	ng	1350650	5	21.589	4373700	20.0
Cyclotetracosane	23.916	5.6	ng	1288410	6	24.762	4616100	20.0
Eicosanal-	25.308	2.1	ng	491656	6	24.762	4616100	20.0
Tetradecane, 2,...	25.908	2.1	ng	481425	6	24.762	4616100	20.0
Cyclodocosane, ...	26.031	3.8	ng	879363	6	24.762	4616100	20.0
.gamma.-Sitosterol	29.997	3.9	ng	905313	6	24.762	4616100	20.0