

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
 Data File : BG060212.D
 Acq On : 3 Jan 2024 3:57
 Operator : MA/JU
 Sample : 05900-02
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 GHL-SS-55

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: BG060212.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	411611	435754	3.61%	0.591%
2	5.038	325	332	338	rBV2	104572	173449	1.44%	0.235%
3	5.509	405	412	434	rBV	3850996	6288437	52.13%	8.535%
4	7.101	675	683	697	rBV	3623965	6351733	52.65%	8.620%
5	7.935	816	825	835	rBV	768527	1370506	11.36%	1.860%
6	9.098	1016	1023	1037	rBV	2154850	3847914	31.90%	5.222%
7	10.738	1295	1302	1315	rBV	1131877	2076032	17.21%	2.818%
8	13.199	1713	1721	1732	rBV	5778075	9352944	77.53%	12.694%
9	14.574	1947	1955	1962	rBV	2364668	3511552	29.11%	4.766%
10	16.061	2201	2208	2220	rBV	4807406	7549538	62.58%	10.246%
11	17.324	2416	2423	2435	rBV	3025982	4618440	38.28%	6.268%
12	18.211	2570	2574	2581	rBV2	342844	527583	4.37%	0.716%
13	19.945	2863	2869	2882	rBV	8834775	12063708	100.00%	16.373%
14	20.744	2998	3005	3008	rBV2	104824	145577	1.21%	0.198%
15	21.231	3084	3088	3097	rBV	724861	1139786	9.45%	1.547%
16	21.590	3142	3149	3159	rBV	2759925	4620366	38.30%	6.271%
17	21.778	3177	3181	3186	rVB3	106824	155512	1.29%	0.211%
18	22.019	3218	3222	3227	rVB5	90581	132178	1.10%	0.179%
19	22.383	3279	3284	3296	rVB2	234911	523249	4.34%	0.710%
20	23.059	3395	3399	3407	rVB3	77314	129704	1.08%	0.176%
21	23.411	3452	3459	3468	rVB	311133	605465	5.02%	0.822%
22	23.858	3528	3535	3541	rBV2	226876	505140	4.19%	0.686%
23	23.916	3541	3545	3556	rVB9	87203	227649	1.89%	0.309%
24	24.762	3680	3689	3701	rBV	1674532	4675040	38.75%	6.345%
25	25.309	3773	3782	3794	rBV4	418932	1167201	9.68%	1.584%
26	25.902	3876	3883	3893	rVB5	142005	415407	3.44%	0.564%
27	26.032	3897	3905	3913	rVV4	92827	302775	2.51%	0.411%
28	28.017	4236	4243	4244	rBV5	126833	219222	1.82%	0.298%
29	28.670	4346	4354	4366	rVB9	133408	550265	4.56%	0.747%

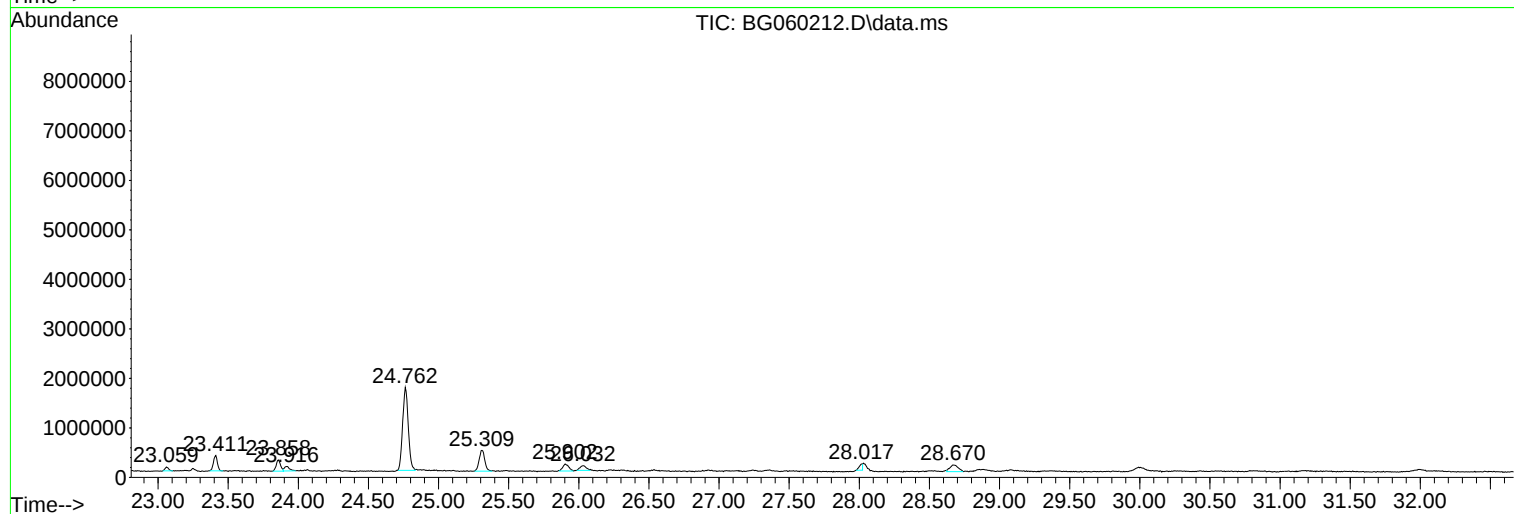
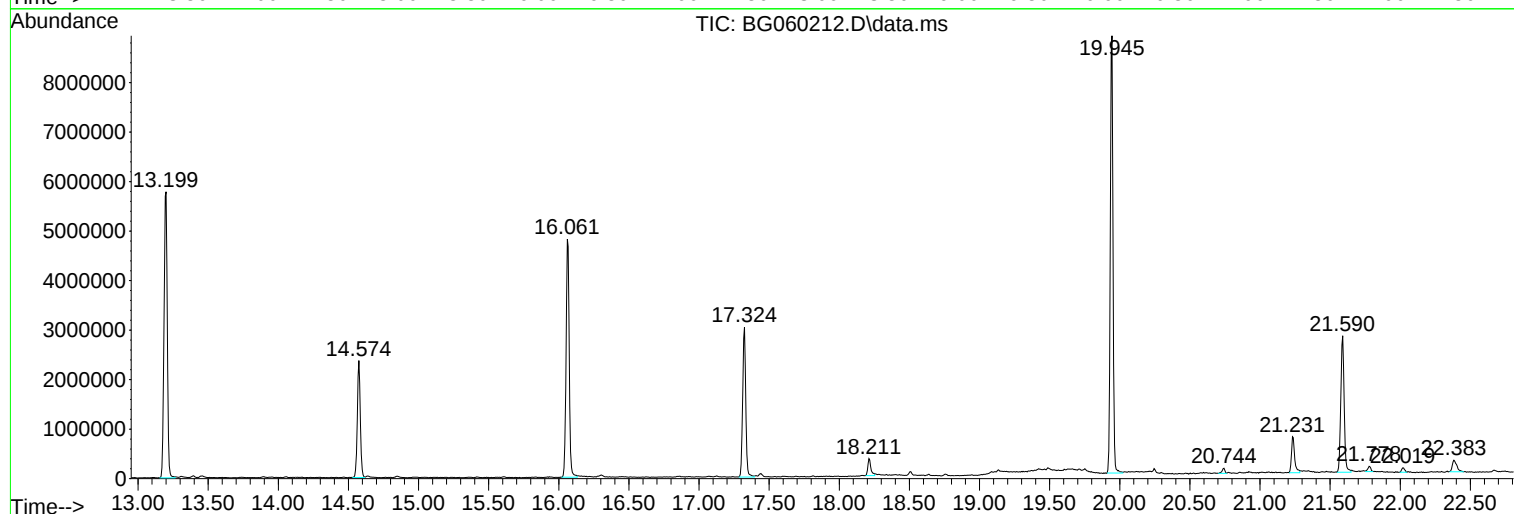
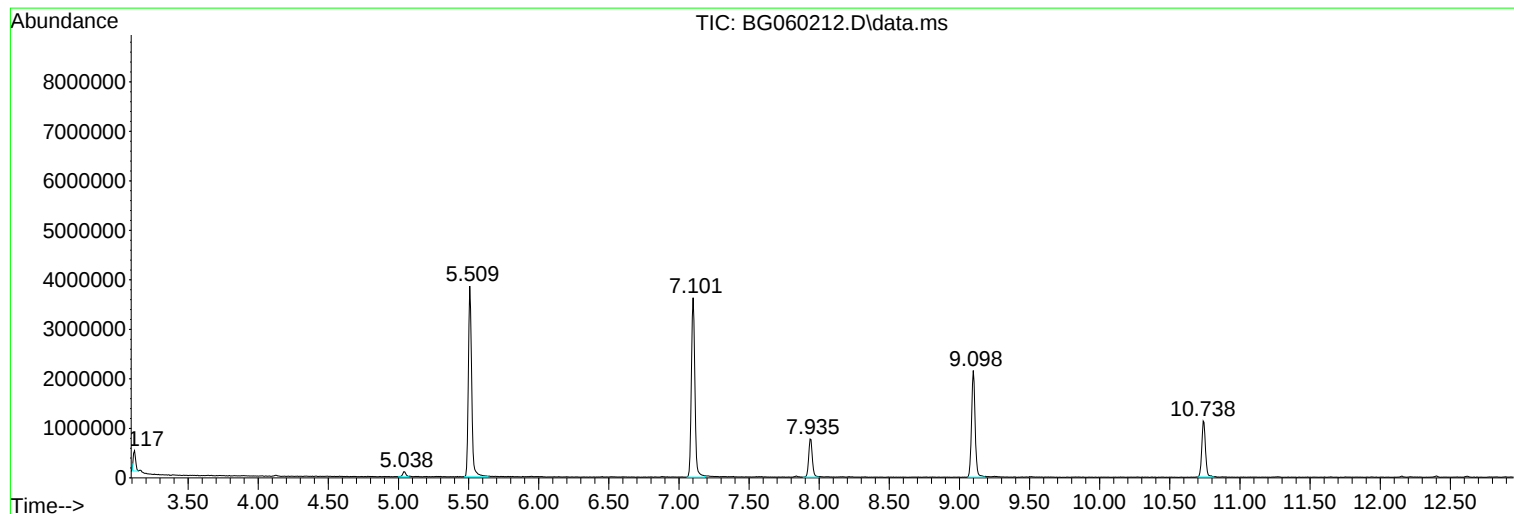
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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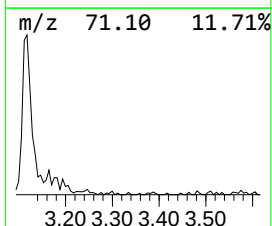
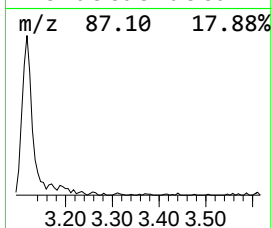
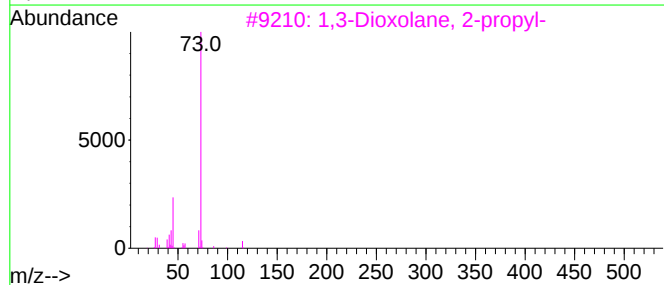
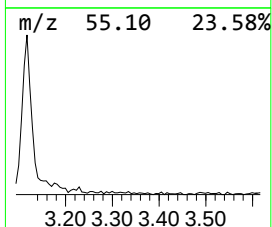
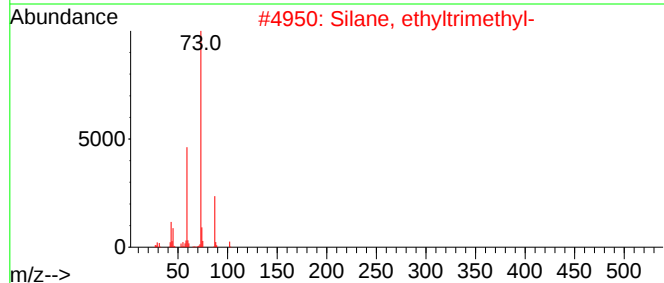
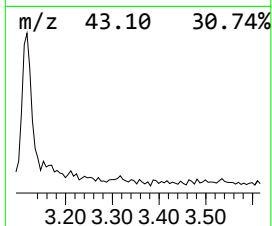
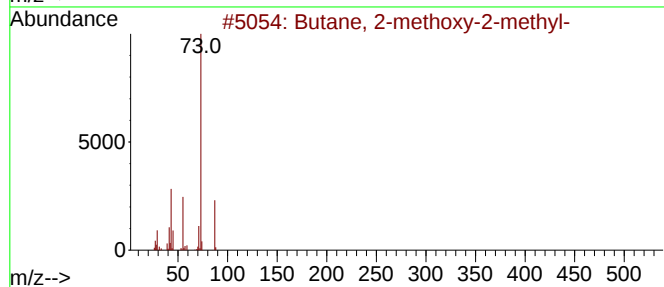
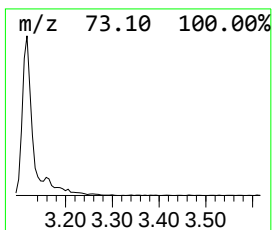
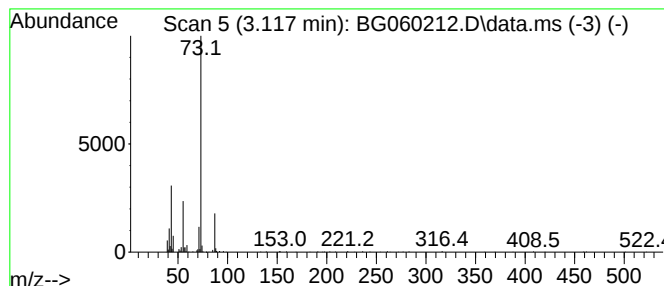
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.117	6.36 ng	435754	1,4-Dichlorobenzene-d4	7.941

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	59
2			Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	28
3			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
4			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	12
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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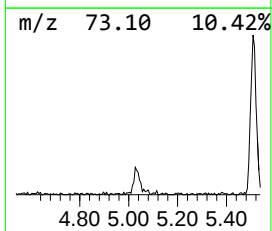
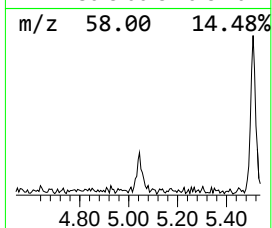
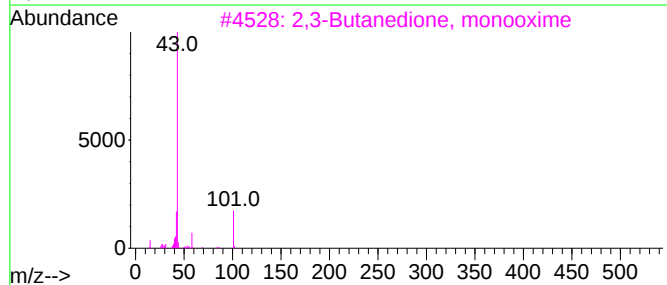
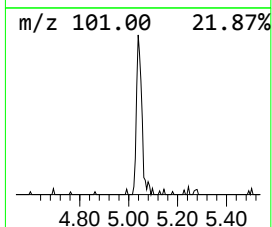
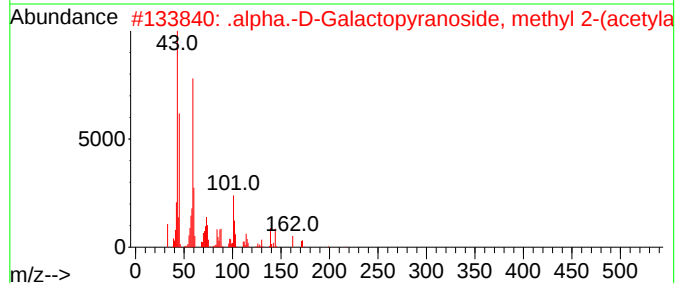
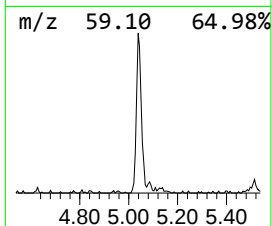
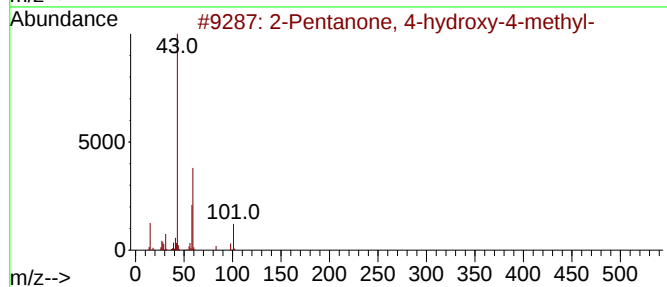
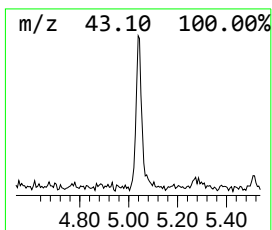
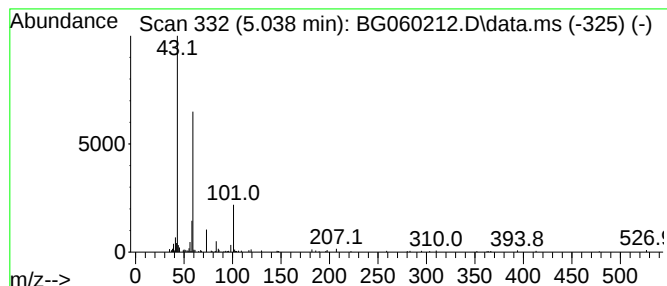
Instrument :
BNA_G
ClientSampleId :
GHL-SS-55

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 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.038	2.53 ng	173449	1,4-Dichlorobenzene-d4	7.941	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	.alpha.-D-Galactopyranoside, met...	249	C10H19NO6	017296-07-0	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4	Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	35
5	5-Hydroxypentanehydroxylamine, N...	245	C11H19NO5	104556-13-0	12



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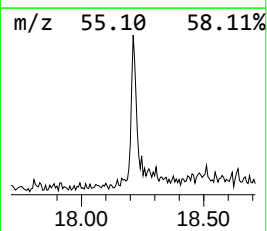
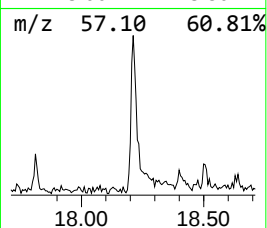
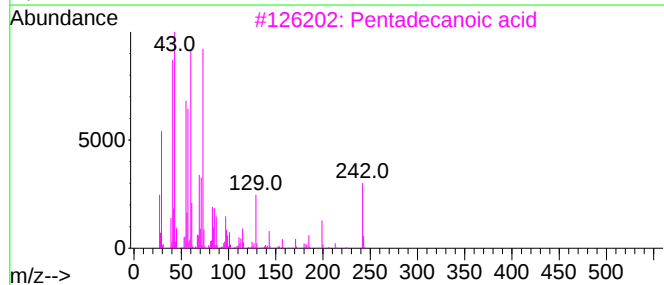
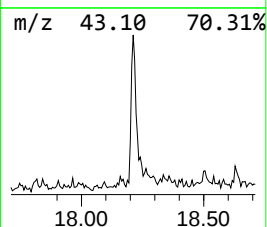
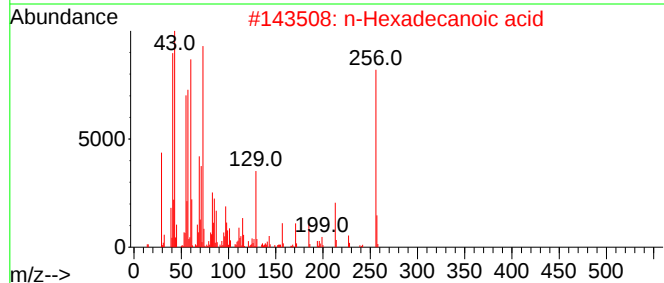
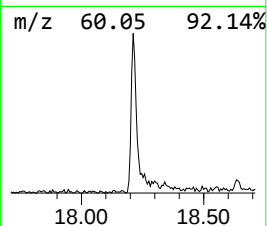
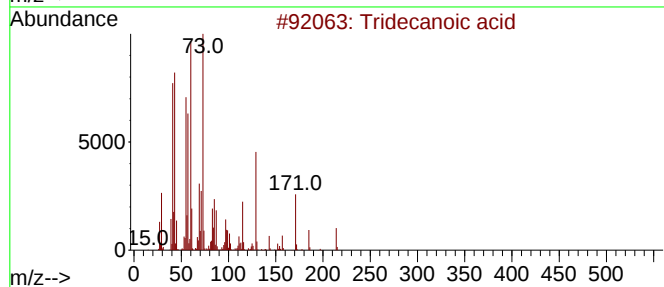
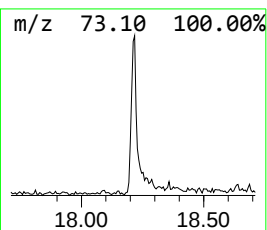
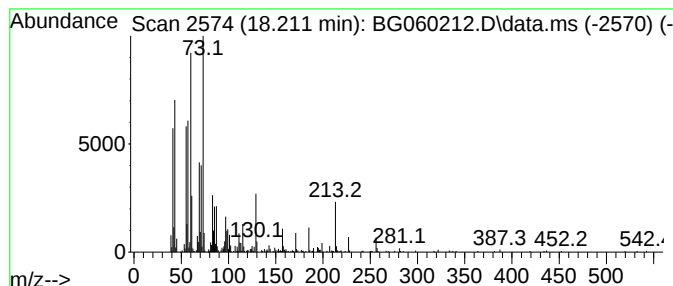
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Tridecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.211	2.28 ng	527583	Phenanthrene-d10	17.324

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	92
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Octadecanoic acid	284	C18H36O2	000057-11-4	87
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



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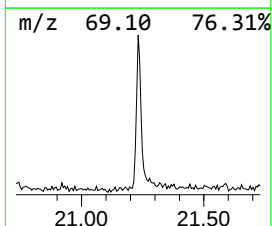
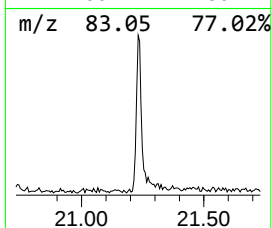
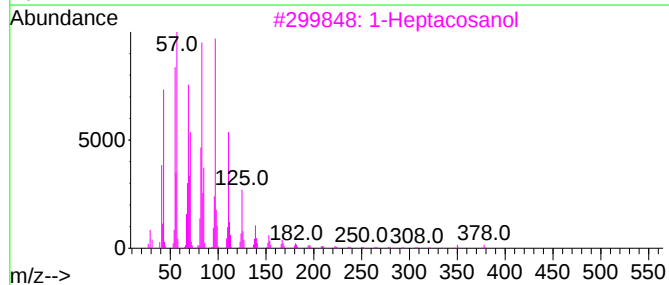
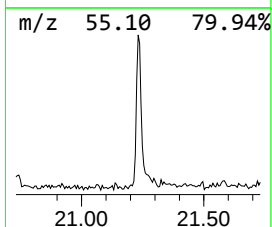
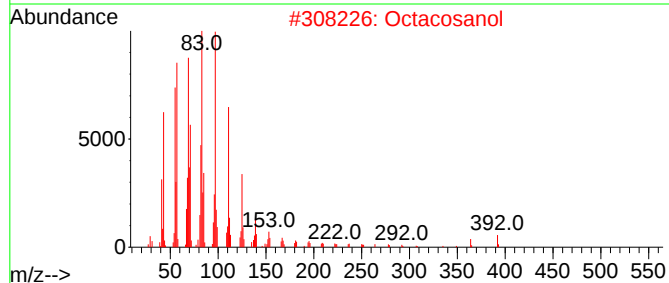
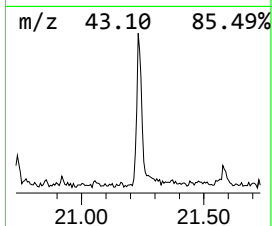
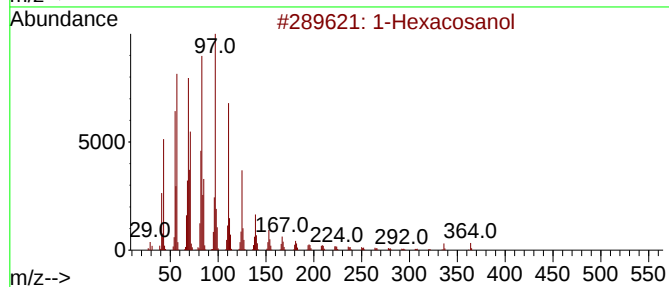
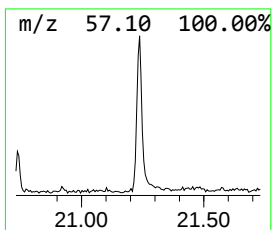
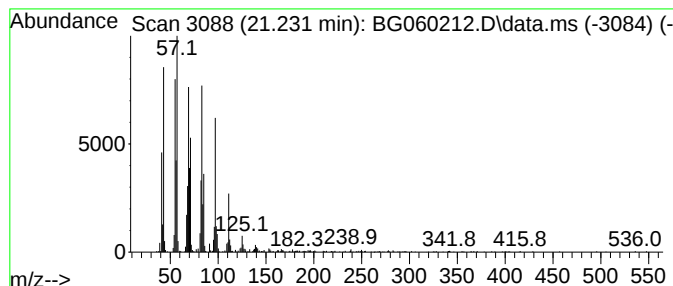
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Peak Number 4 1-Hexacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.231	4.93 ng	1139790	Chrysene-d12	21.590

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexacosanol	382	C26H54O	000506-52-5	91
2			Octacosanol	410	C28H58O	000557-61-9	91
3			1-Heptacosanol	396	C27H56O	002004-39-9	91
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5			n-Nonadecanol-1	284	C19H40O	001454-84-8	90



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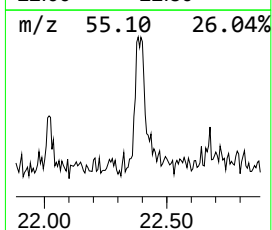
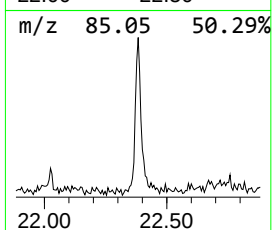
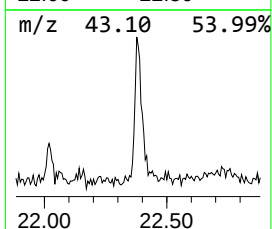
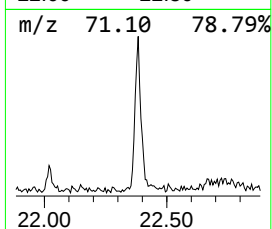
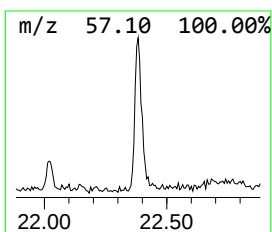
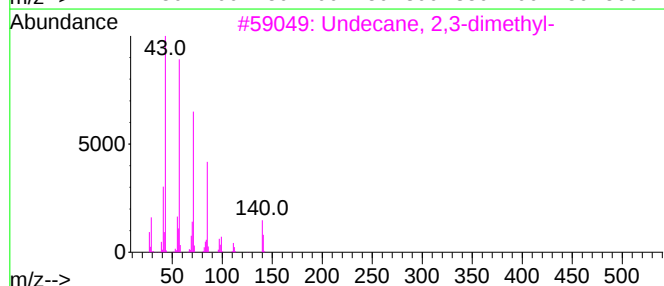
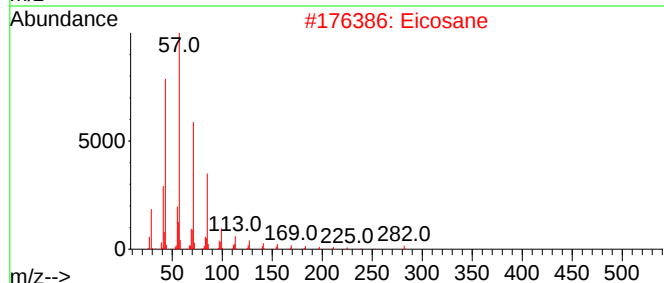
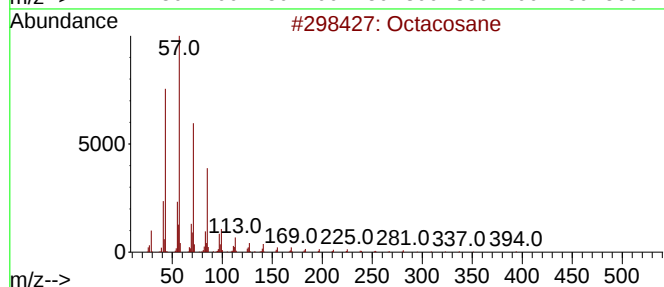
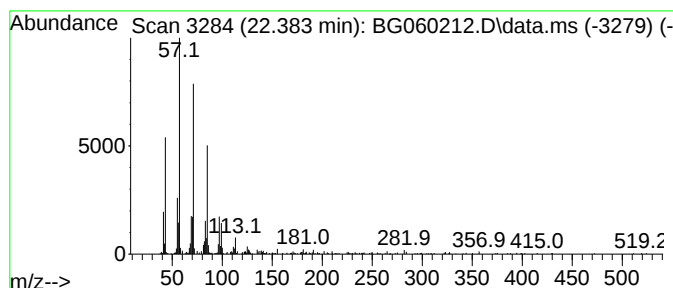
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.383	2.26 ng	523249	Chrysene-d12	21.590

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	93
2			Eicosane	282	C20H42	000112-95-8	87
3			Undecane, 2,3-dimethyl-	184	C13H28	017312-77-5	78
4			Heptadecane	240	C17H36	000629-78-7	72
5			Undecane, 6-ethyl-	184	C13H28	017312-60-6	68



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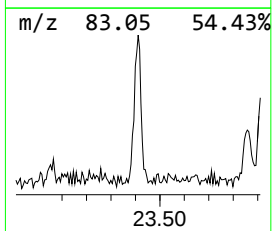
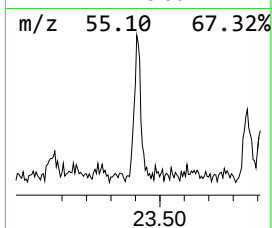
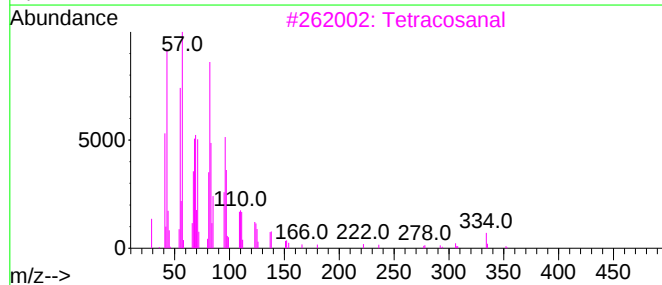
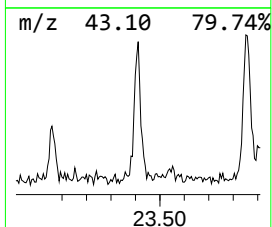
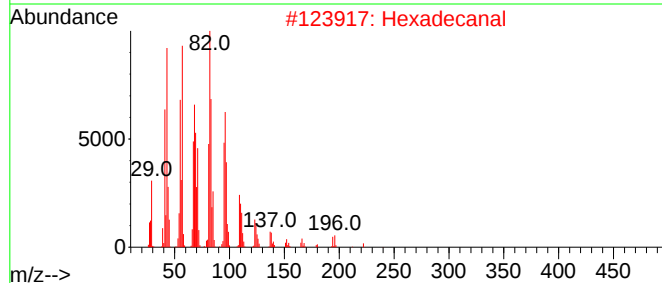
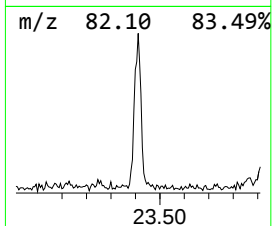
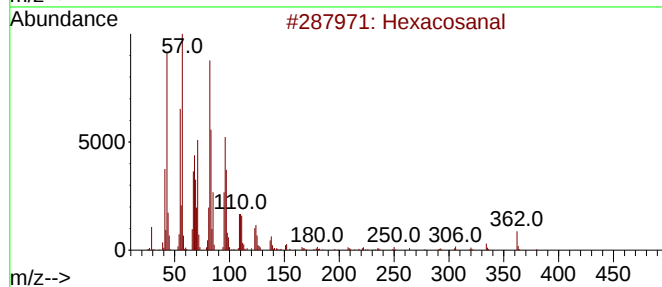
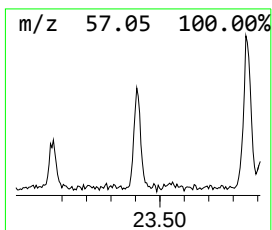
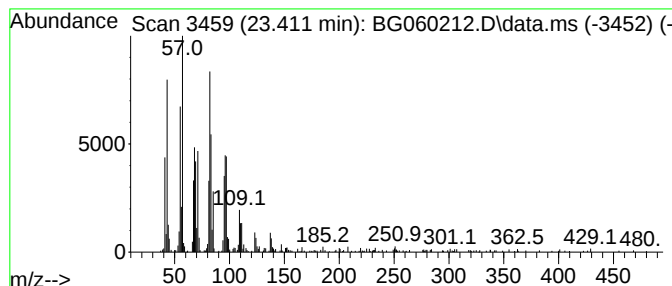
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexacosanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.411	2.59 ng	605465	Perylene-d12	24.762

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosanal	380	C26H52O	026627-85-0	90
2			Hexadecanal	240	C16H32O	000629-80-1	87
3			Tetracosanal	352	C24H48O	057866-08-7	83
4			Octadecanal	268	C18H36O	000638-66-4	80
5			1,19-Eicosadiene	278	C20H38	014811-95-1	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060212.D
Acq On : 3 Jan 2024 3:57
Operator : MA/JU
Sample : 05900-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-55

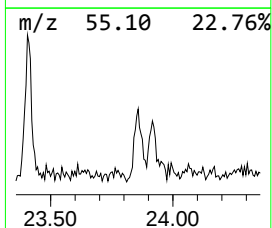
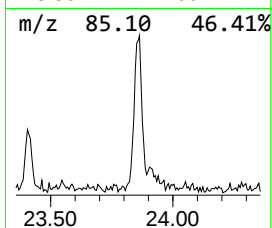
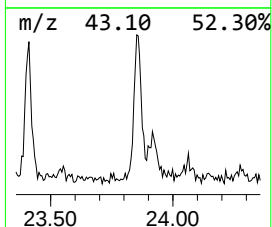
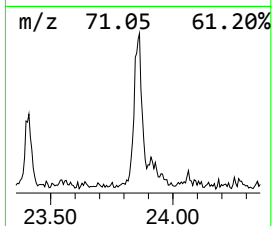
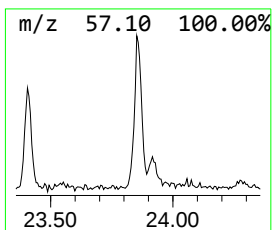
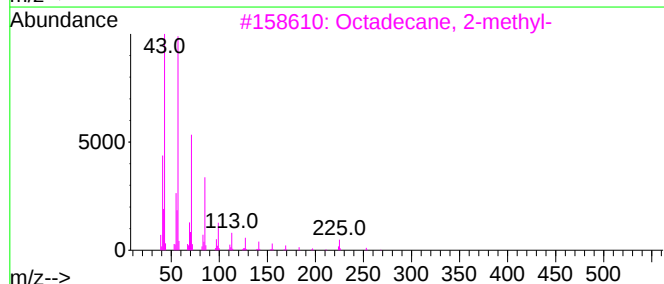
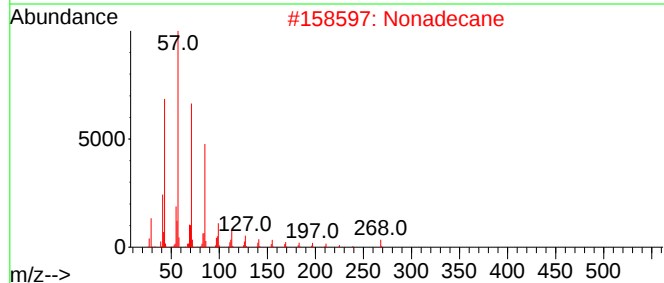
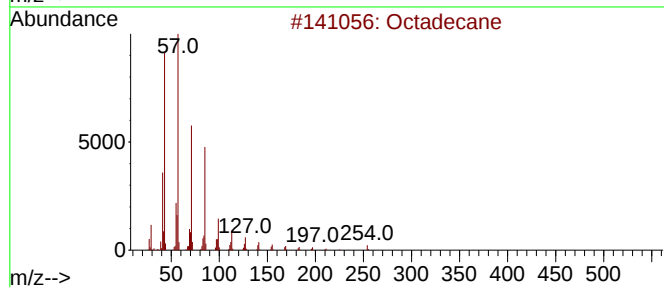
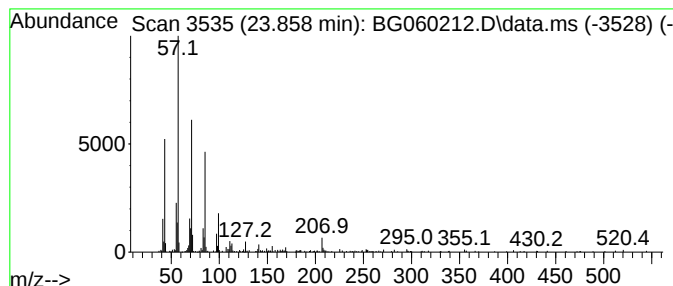
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.858	2.16 ng	505140	Perylene-d12	24.762

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	87
2			Nonadecane	268	C19H40	000629-92-5	83
3			Octadecane, 2-methyl-	268	C19H40	001560-88-9	83
4			Heptacosane	380	C27H56	000593-49-7	83
5			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060212.D
Acq On : 3 Jan 2024 3:57
Operator : MA/JU
Sample : 05900-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-55

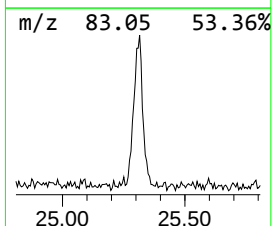
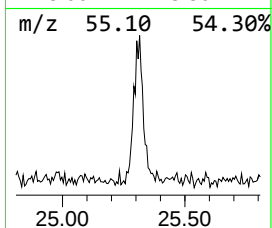
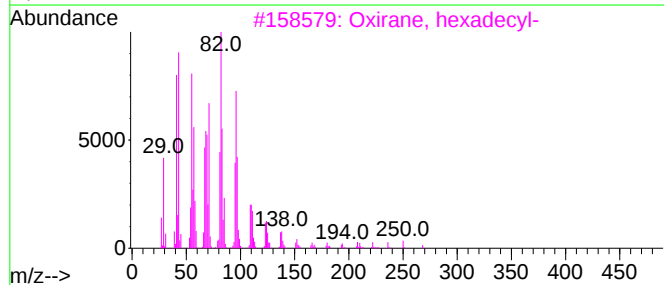
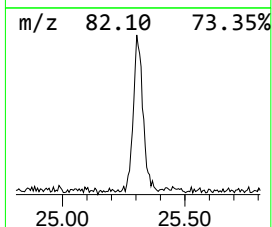
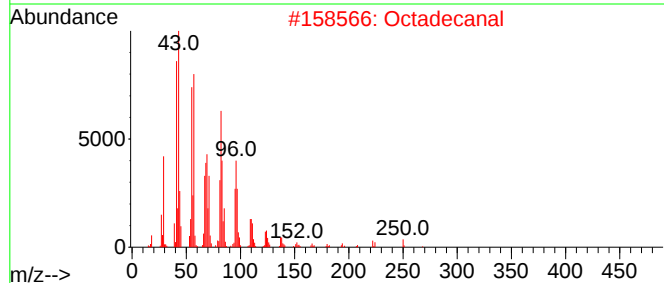
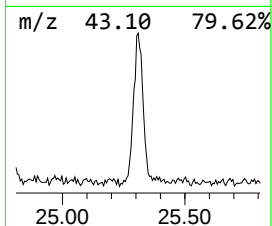
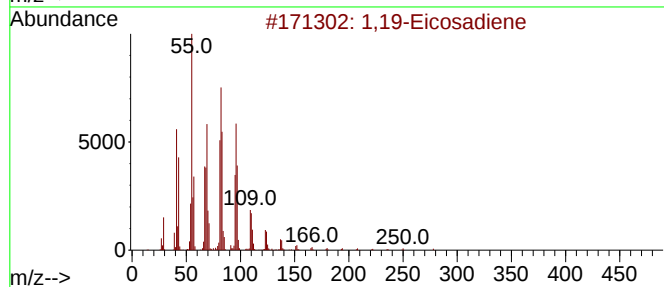
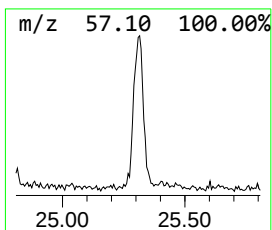
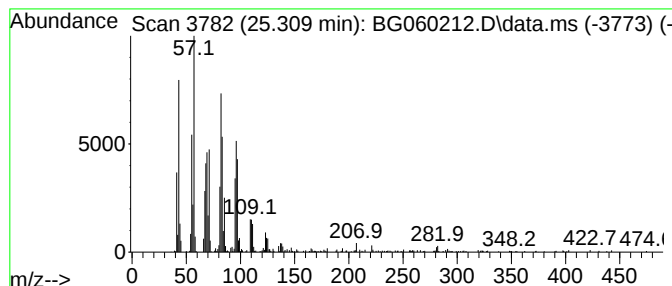
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1,19-Eicosadiene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.309	4.99 ng	1167200	Perylene-d12	24.762

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,19-Eicosadiene	278	C20H38	014811-95-1	95
2			Octadecanal	268	C18H36O	000638-66-4	93
3			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
4			Eicosanal-	296	C20H40O	002400-66-0	90
5			Pentadecanal-	226	C15H30O	002765-11-9	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060212.D
Acq On : 3 Jan 2024 3:57
Operator : MA/JU
Sample : 05900-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

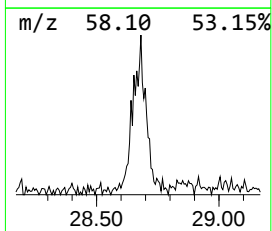
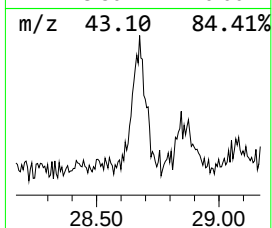
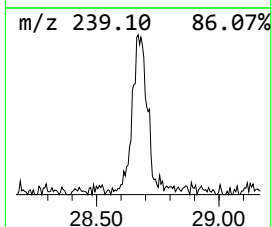
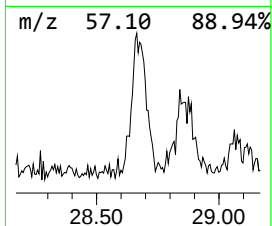
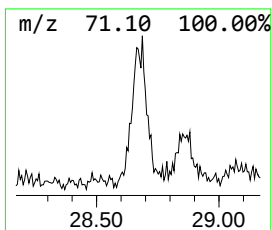
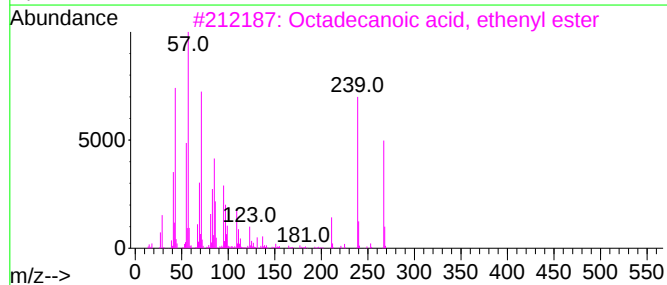
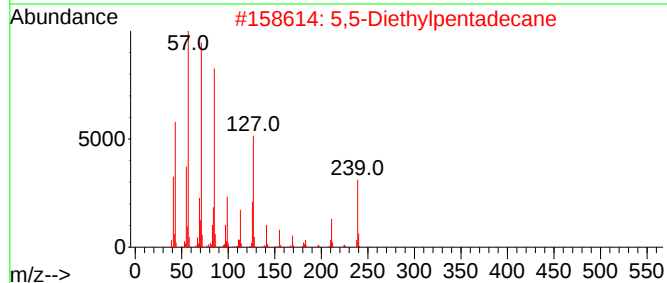
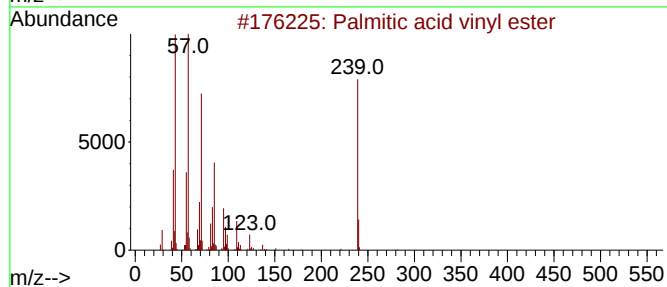
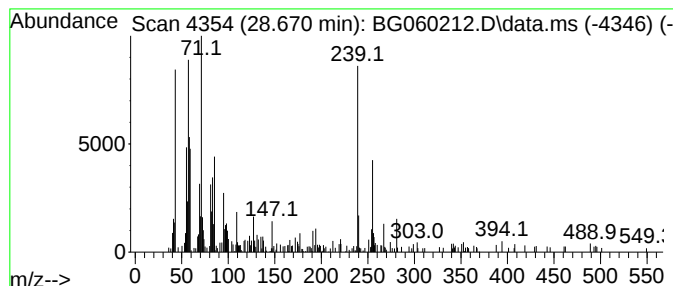
Instrument :
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ClientSampleId :
GHL-SS-55

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 unknown28.670 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
28.670	2.35 ng	550265	Perylene-d12	24.762	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Palmitic acid vinyl ester	282	C18H34O2	000693-38-9	43
2	5,5-Diethylpentadecane	268	C19H40	1000360-41-0	32
3	Octadecanoic acid, ethenyl ester	310	C20H38O2	000111-63-7	32
4	Hexadecanoic acid, 4-nitrophenyl...	377	C22H35NO4	001492-30-4	16
5	1-Heptadecanamine	255	C17H37N	004200-95-7	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060212.D
Acq On : 3 Jan 2024 3:57
Operator : MA/JU
Sample : 05900-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-55

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	6.4	ng	435754	1	7.941	1370510	20.0
2-Pentanone, 4-...	5.038	2.5	ng	173449	1	7.941	1370510	20.0
Tridecanoic acid	18.211	2.3	ng	527583	4	17.324	4618440	20.0
1-Hexacosanol	21.231	4.9	ng	1139790	5	21.590	4620370	20.0
Octacosane	22.383	2.3	ng	523249	5	21.590	4620370	20.0
Hexacosanal	23.411	2.6	ng	605465	6	24.762	4675040	20.0
Octadecane	23.858	2.2	ng	505140	6	24.762	4675040	20.0
1,19-Eicosadiene	25.309	5.0	ng	1167200	6	24.762	4675040	20.0
unknown28.670	28.670	2.4	ng	550265	6	24.762	4675040	20.0