LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049847.D
Acq On : 16 Aug 2021 12:32
Operator : CG/JU
Sample : M3408-14
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 34N

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-BG080321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049847.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.139	12	17	23	rBV	97983	160081	11.36%	1.772%
2	5.107	346	352	362	rVB2	35651	57753	4.10%	0.639%
3	5.583	426	433	446	rVB	365256	617970	43.84%	6.840%
4	7.192	700	707	718	rBV	382744	680891	48.31%	7.537%
5	8.026	840	849	856	rVB2	99355	177493	12.59%	1.965%
6	9.201	1039	1049	1057	rBV	238657	448674	31.83%	4.966%
7	10.611	1282	1289	1296	rBV4	28690	58072	4.12%	0.643%
8	10.852	1322	1330	1338	rVB	129194	247368	17.55%	2.738%
9	13.302	1739	1747	1754	rBV	606193	968894	68.74%	10.725%
10	14.682	1975	1982	1990	rVB2	206786	328651	23.32%	3.638%
11	16.174	2230	2236	2245	rBV	543186	847886	60.16%	9.385%
12	17.437	2444	2451	2457	rBV	249012	415857	29.50%	4.603%
13	18.083	2559	2561	2568	rVB7	12399	20649	1.47%	0.229%
14	19.440	2784	2792	2806	rVB4	81291	266727	18.92%	2.952%
15	19.752	2837	2845	2856	rVB3	83084	245533	17.42%	2.718%
16	20.045	2889	2895	2900	rVB	1120579	1409488	100.00%	15.602%
17	20.556	2975	2982	2993	rVB2	117921	294270	20.88%	3.257%
18	21.344	3113	3116	3125	rBV8	29975	57724	4.10%	0.639%
19	21.555	3145	3152	3161	rVB2	108649	286823	20.35%	3.175%
20	21.714	3173	3179	3186	rBV2	236346	393335	27.91%	4.354%
21	22.701	3338	3347	3362	rBV3	88342	310800	22.05%	3.440%
22	23.400	3463	3466	3472	rVB6	18668	33296	2.36%	0.369%
23	24.992	3728	3737	3746	rVB2	148544	416763	29.57%	4.613%
24	25.761	3855	3868	3872	rBV9	48550	186679	13.24%	2.066%
25	26.989	4068	4077	4079	rBV10	38931	102382	7.26%	1.133%

Sum of corrected areas: 9034059

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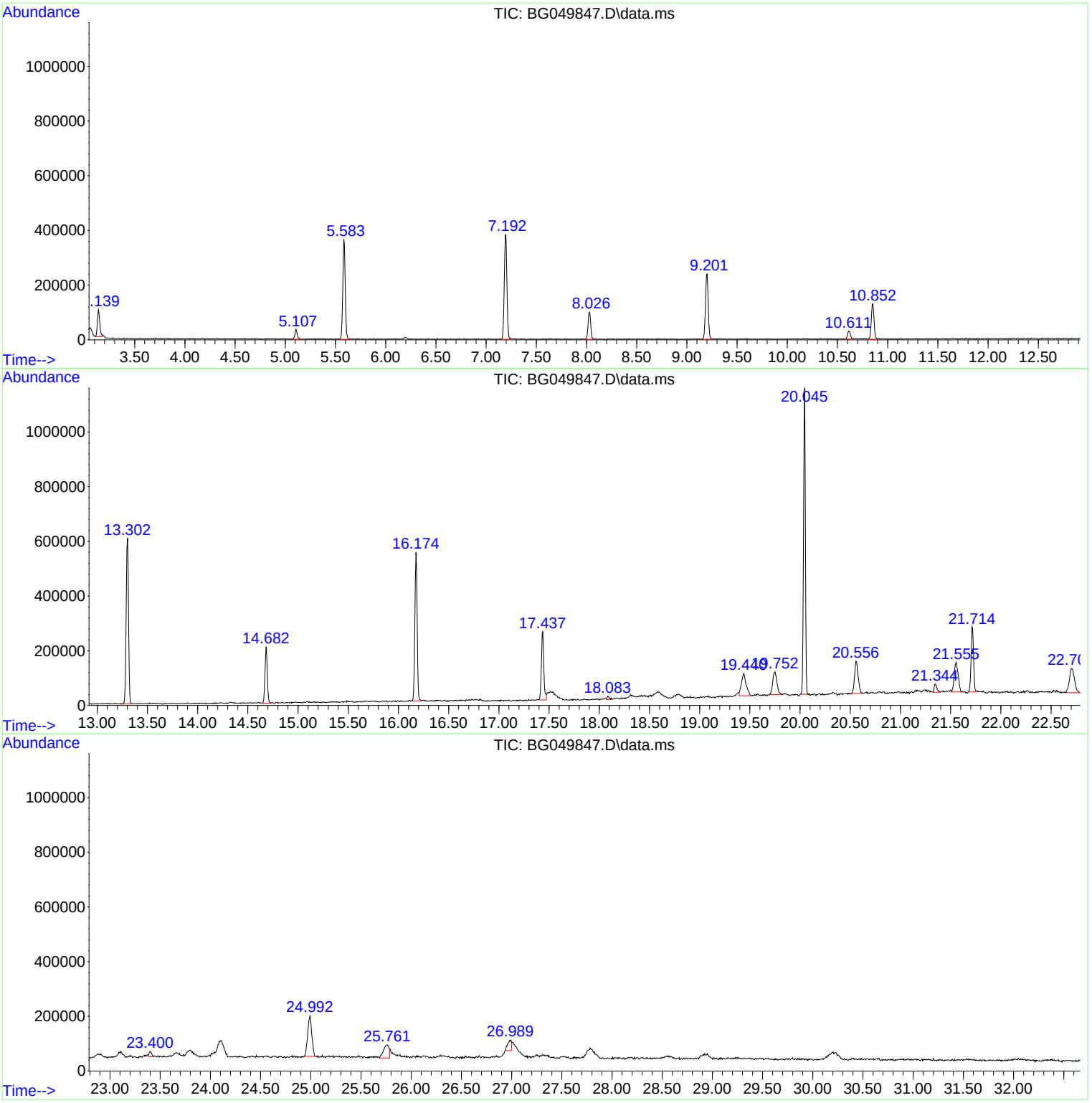
Instrument :
BNA_G
ClientSampleId :
34N

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.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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Data File : BG049847.D
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Operator : CG/JU
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Misc :
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Instrument : BNA_G
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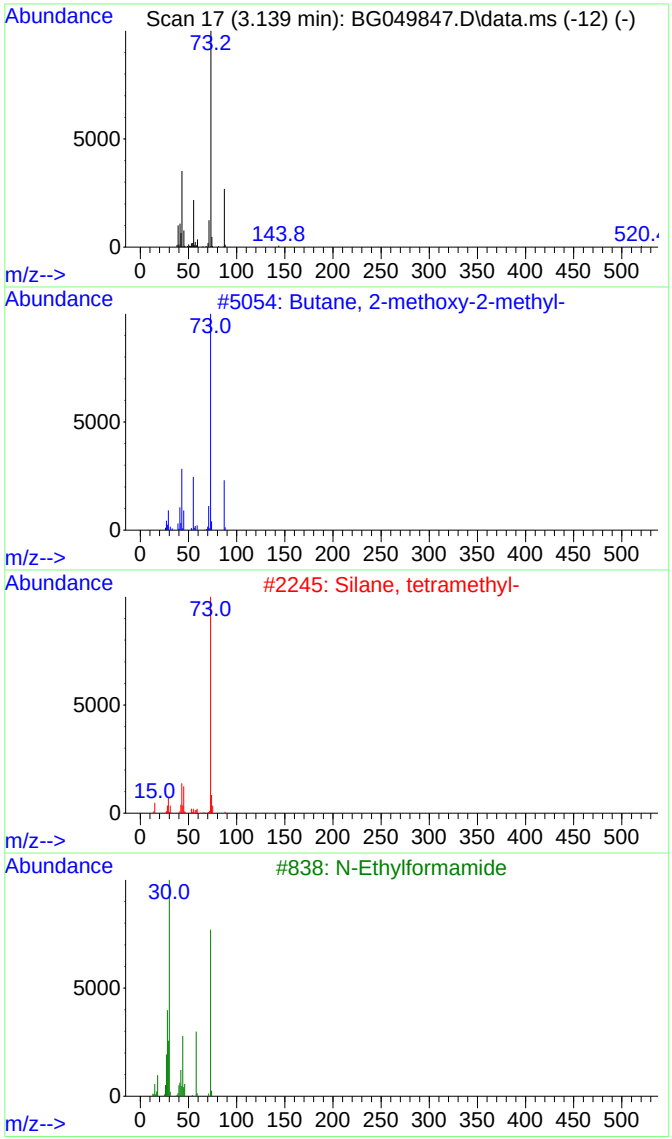
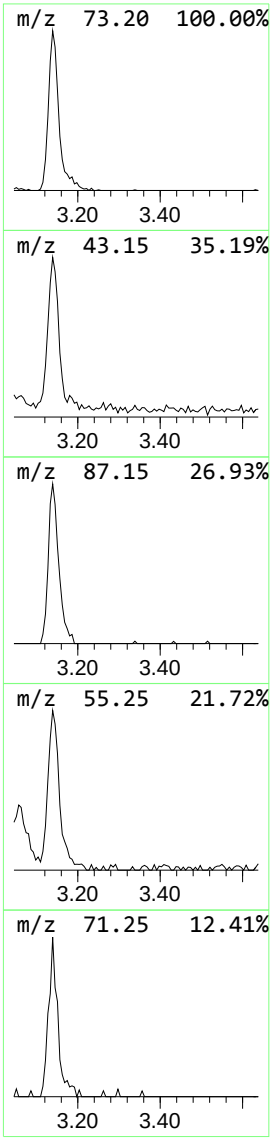
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.139	18.04 ng	160081	1,4-Dichlorobenzene-d4	8.026

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	9





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Operator : CG/JU
Sample : M3408-14
Misc :
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Instrument : BNA_G
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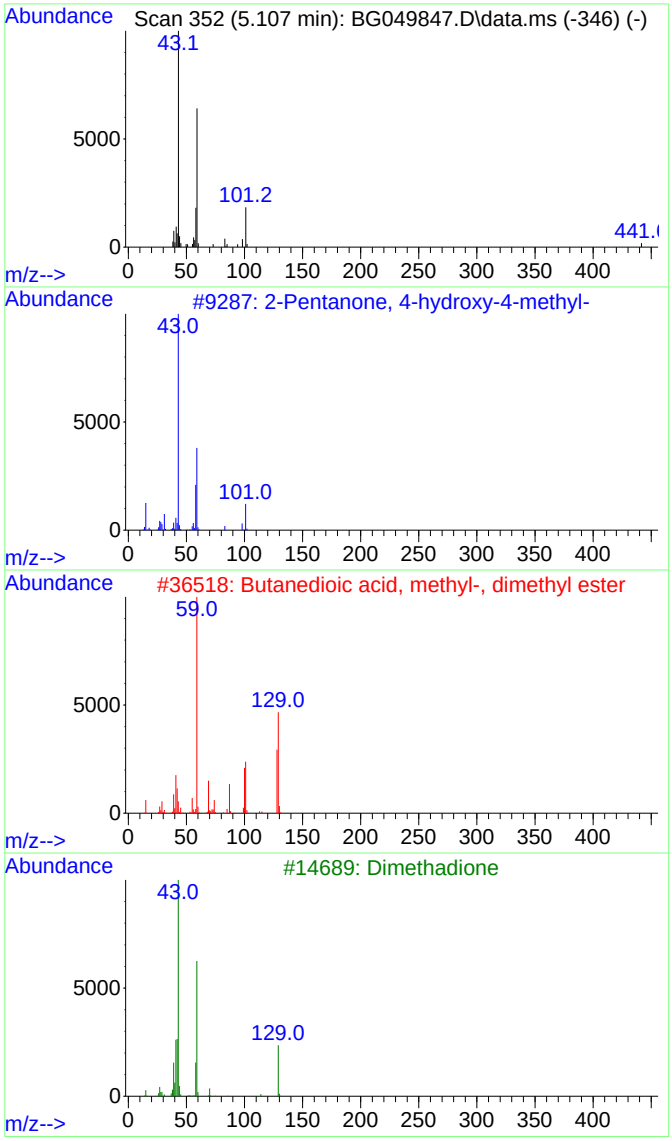
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

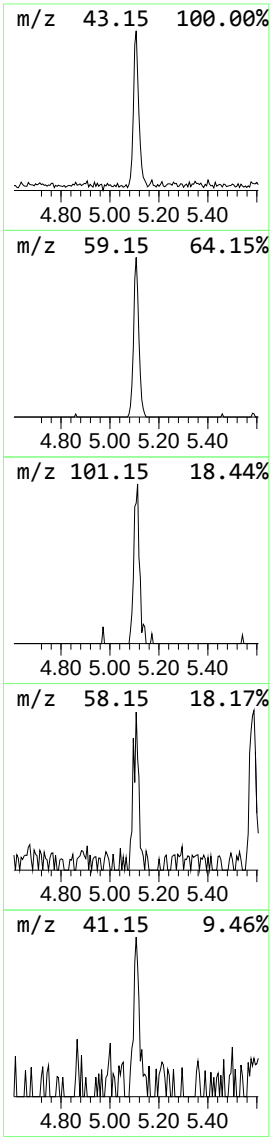
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.107	6.51 ng	57753	1,4-Dichlorobenzene-d4	8.026

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	37
3	Dimethadione	129	C5H7NO3	000695-53-4	36
4	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	25
5	Propanoic acid, 3-nitro-, methyl...	133	C4H7NO4	020497-95-4	17





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Misc :
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Instrument : BNA_G
ClientSampleId : 34N

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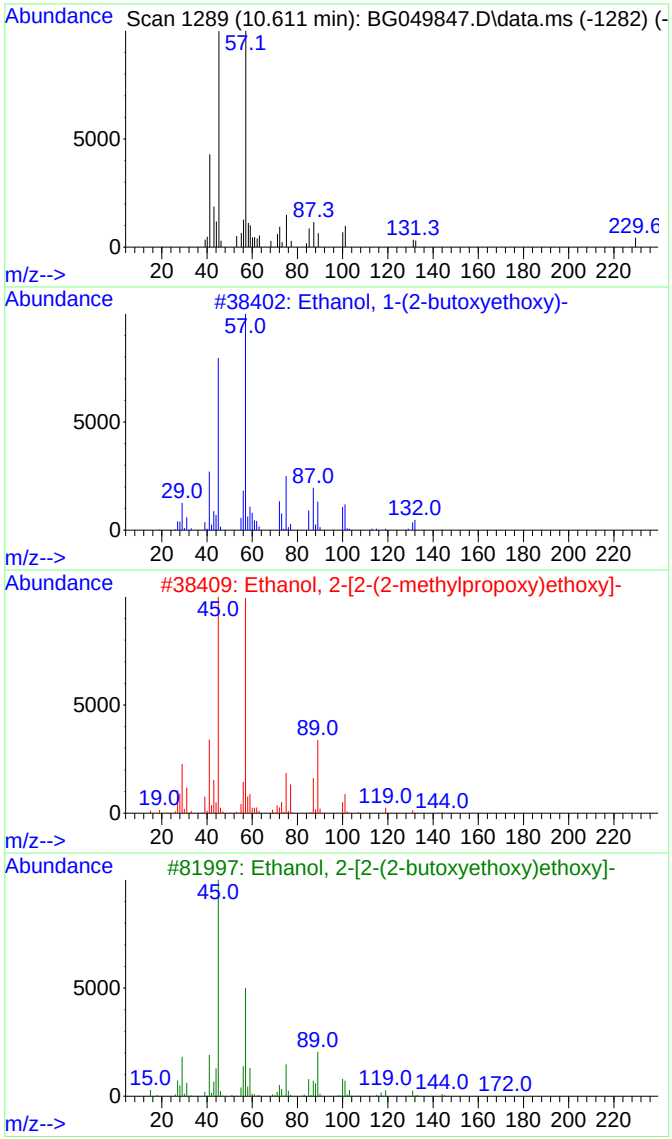
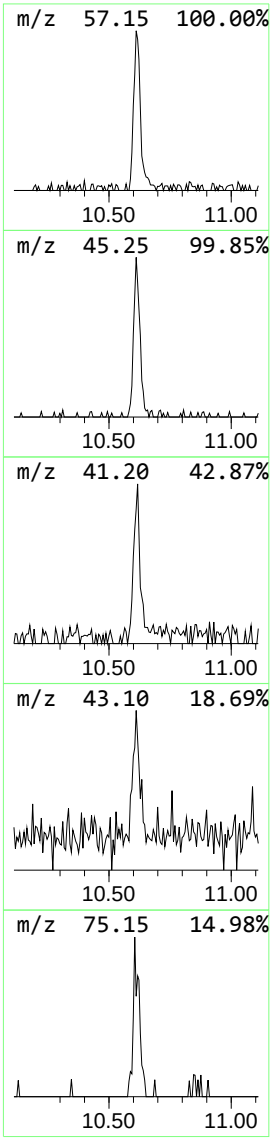
Peak Number 3 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.611	4.70 ng	58072	Naphthalene-d8	10.846

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	74
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
3	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	72
4	3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	64
5	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	64





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Operator : CG/JU
Sample : M3408-14
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 34N

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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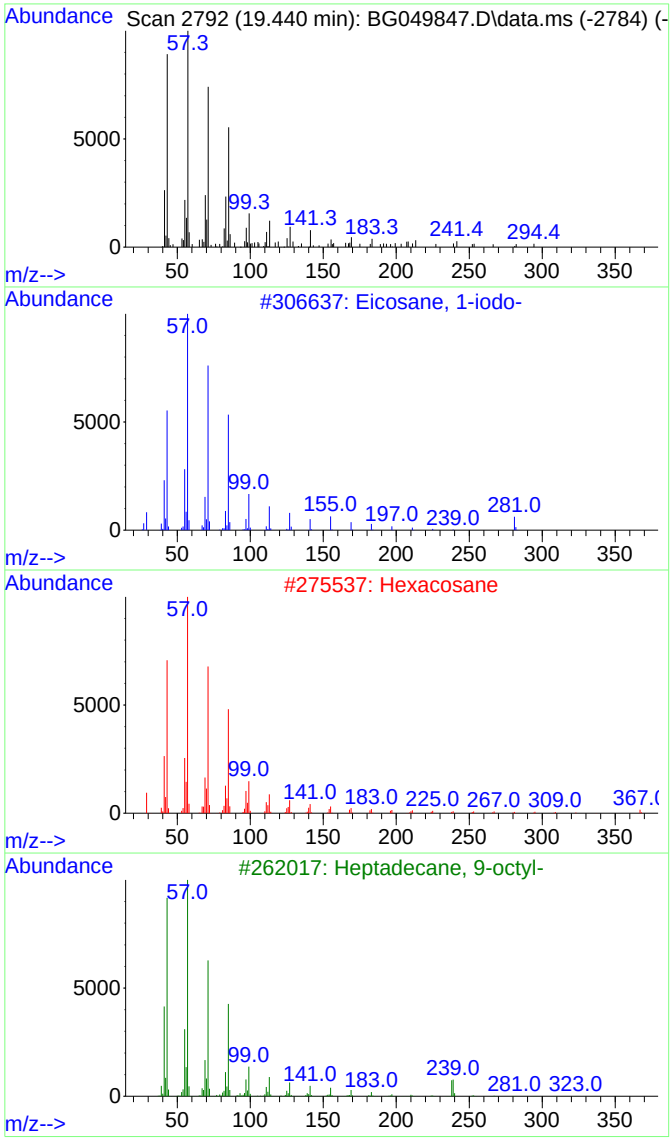
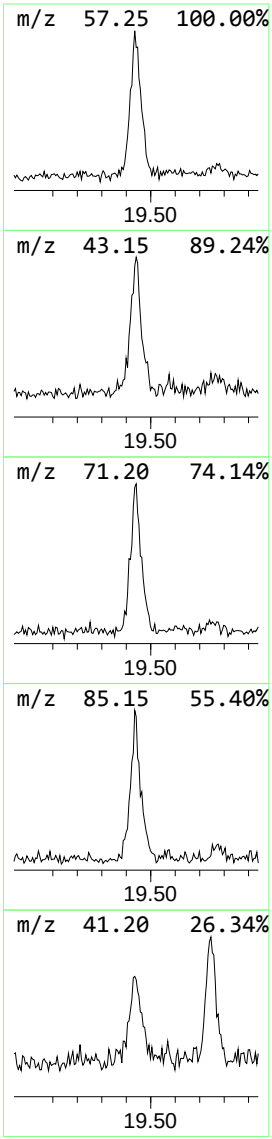
Peak Number 4 Eicosane, 1-iodo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.440	12.83 ng	266727	Phenanthrene-d10	17.431

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	87
2	Hexacosane	366	C26H54	000630-01-3	86
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
4	Eicosane	282	C20H42	000112-95-8	86
5	Tetratetracontane	619	C44H90	007098-22-8	80





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Operator : CG/JU
Sample : M3408-14
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 34N

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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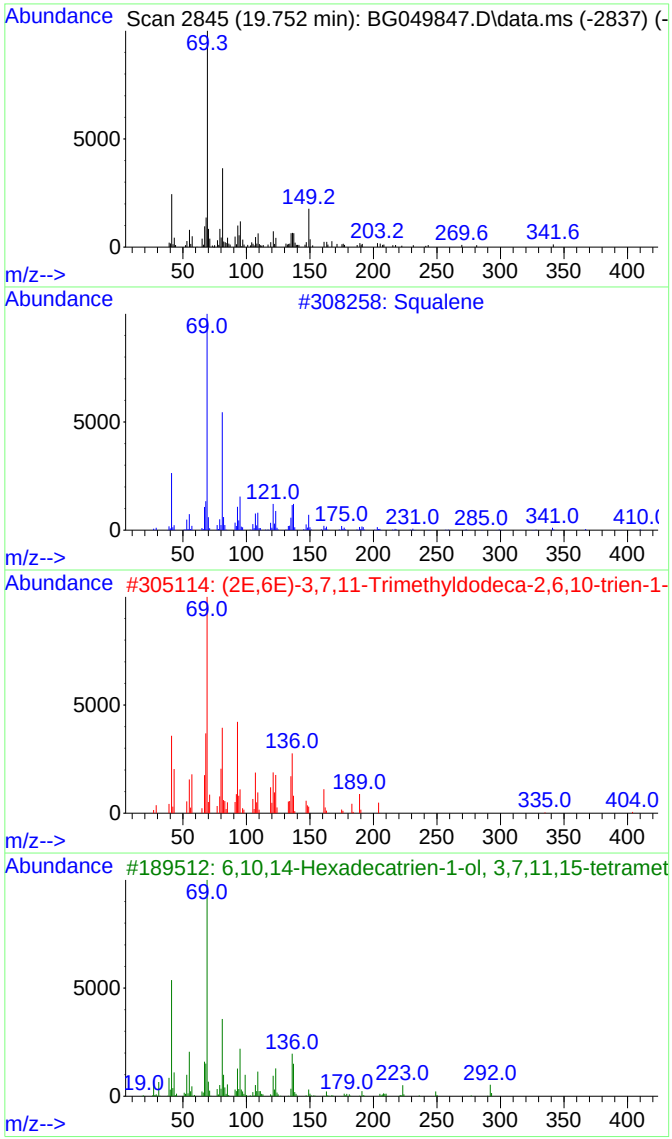
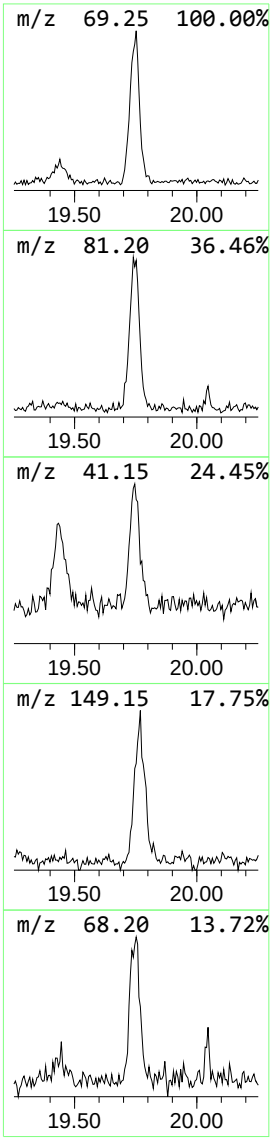
Peak Number 5 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.752	12.48 ng	245533	Chrysene-d12	21.714

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	72
2	(2E,6E)-3,7,11-Trimethyldodeca-2...	404	C27H48O2	078368-58-8	64
3	6,10,14-Hexadecatrien-1-ol, 3,7,...	292	C20H36O	036237-66-8	64
4	trans-Farnesol	222	C15H26O	000106-28-5	59
5	4-Aza-5-thiatricyclo[5.2.1.0(3,7...	283	C14H21NO3S	1000156-44-2	53





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Misc :
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Instrument : BNA_G
ClientSampleId : 34N

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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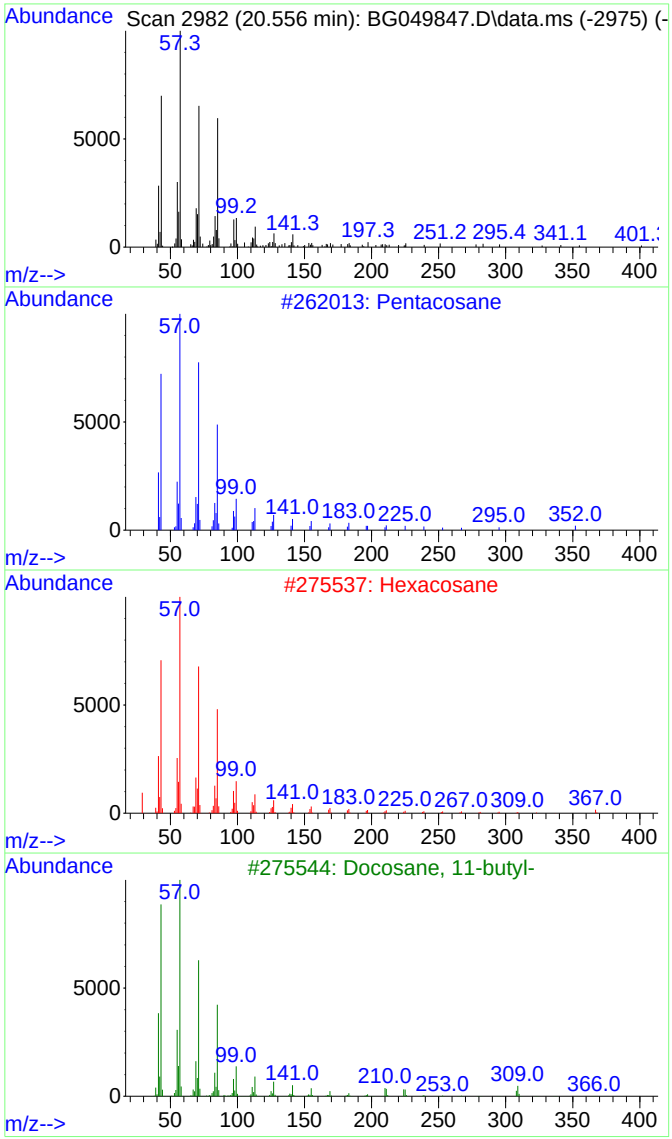
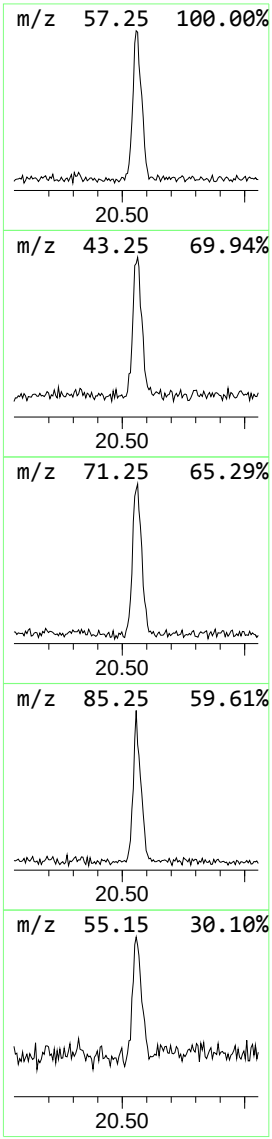
Peak Number 6 Pentacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.557	14.96 ng	294270	Chrysene-d12	21.714

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	91
2	Hexacosane	366	C26H54	000630-01-3	90
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	87
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	87
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87





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Sample : M3408-14
Misc :
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Instrument : BNA_G
ClientSampleId : 34N

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.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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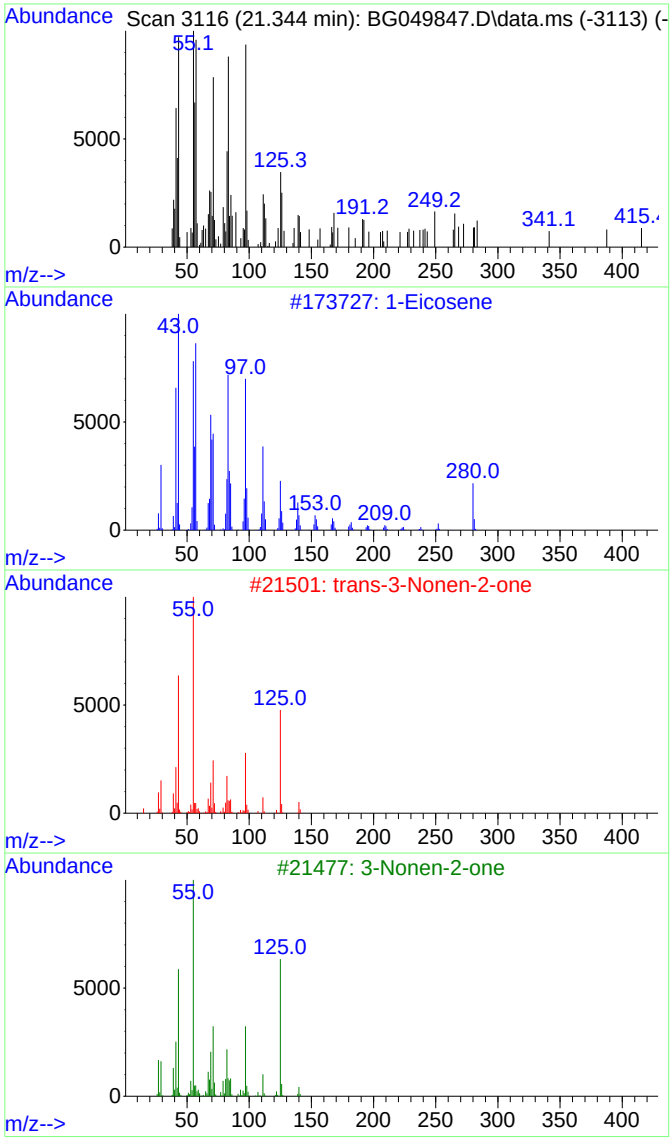
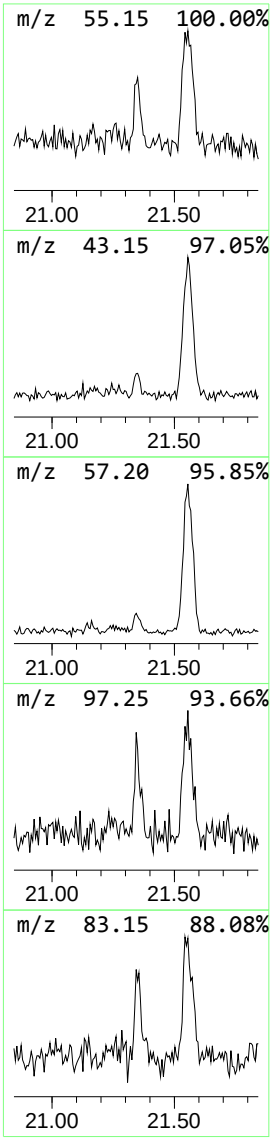
Peak Number 7 1-Eicosene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.344	2.94 ng	57724	Chrysene-d12	21.714

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosene	280	C20H40	003452-07-1	70
2	trans-3-Nonen-2-one	140	C9H16O	018402-83-0	43
3	3-Nonen-2-one	140	C9H16O	014309-57-0	43
4	Cycloeicosane	280	C20H40	000296-56-0	38
5	1-Tetradecene	196	C14H28	001120-36-1	38





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

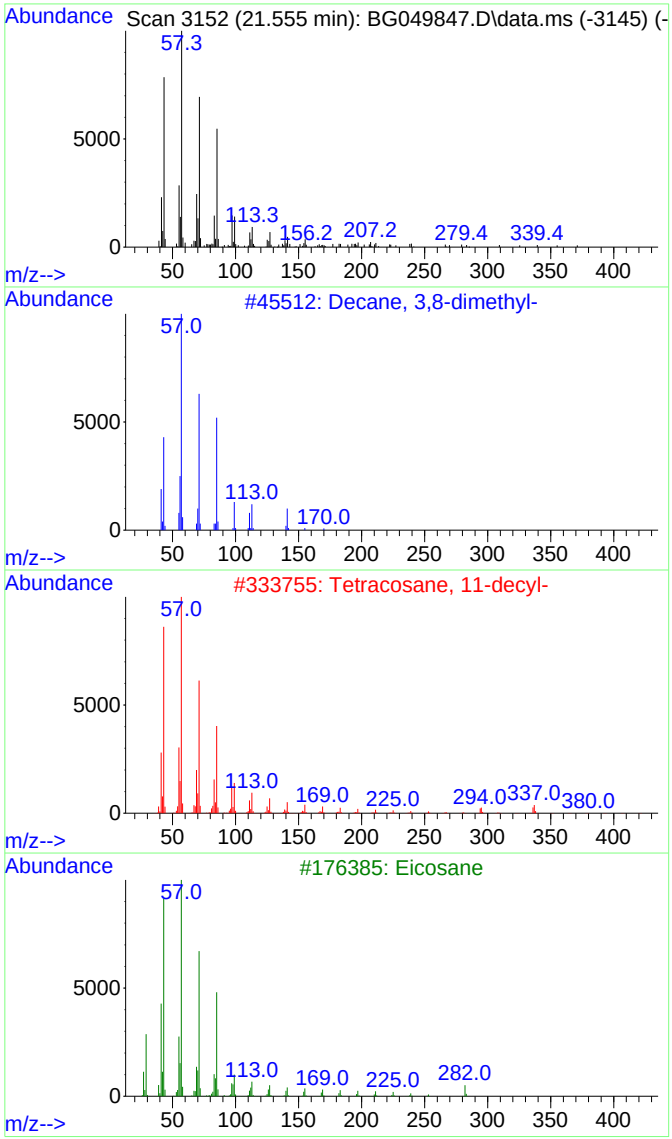
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

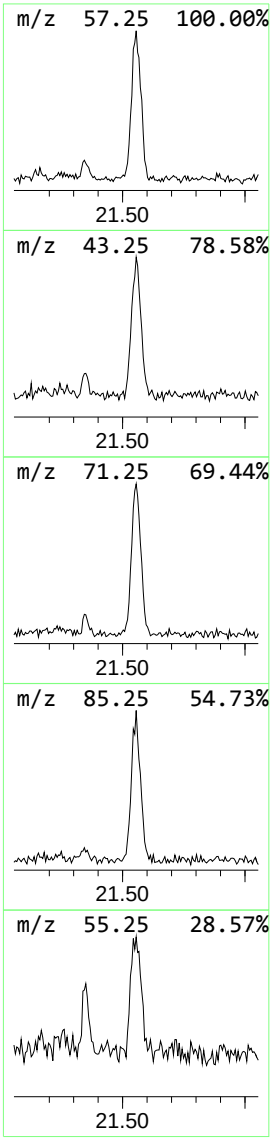
****

Peak Number 8 Decane, 3,8-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.555	14.58 ng	286823	Chrysene-d12	21.714

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	91
2	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	90
3	Eicosane	282	C20H42	000112-95-8	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	87





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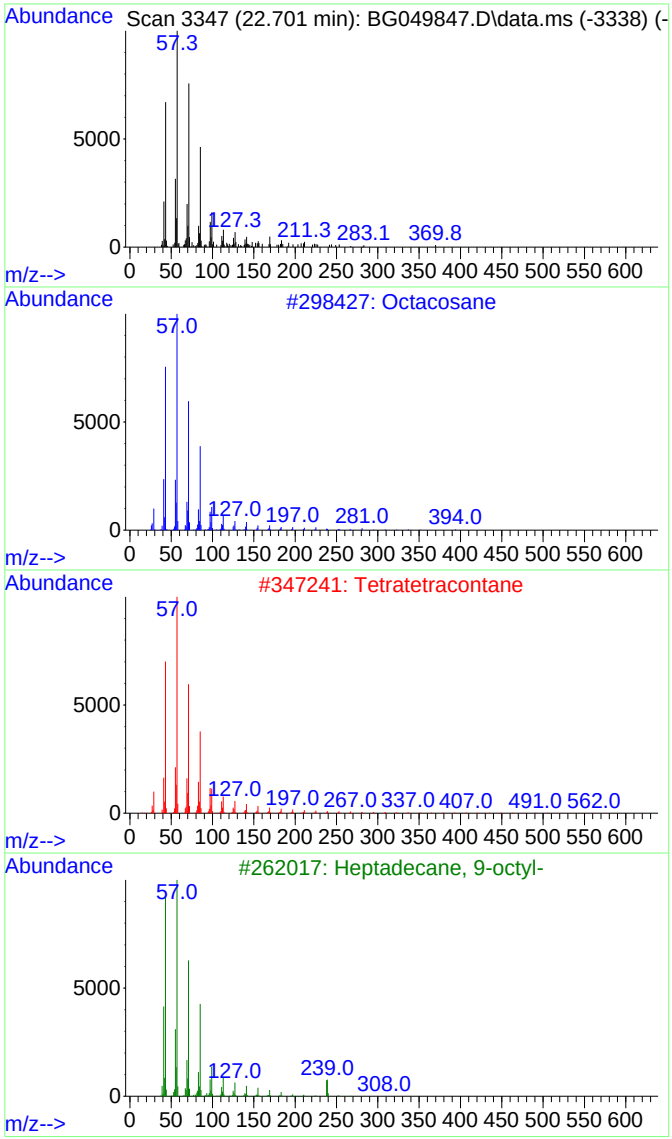
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

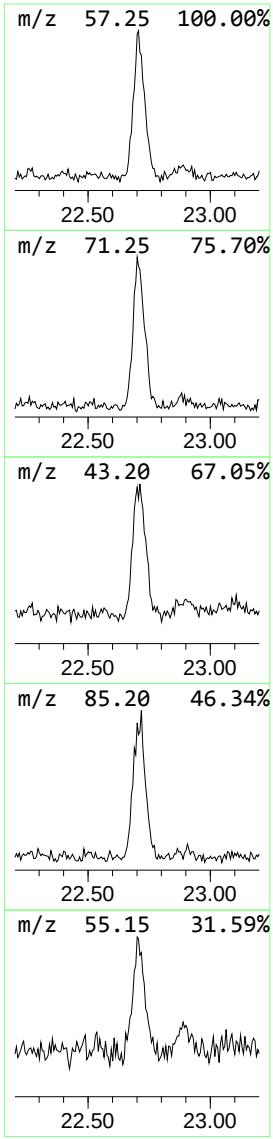
****

Peak Number 9 Octacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.701	15.80 ng	310800	Chrysene-d12	21.714

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Tetratetracontane	619	C44H90	007098-22-8	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Heneicosane	296	C21H44	000629-94-7	90
5	Hexacosane	366	C26H54	000630-01-3	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
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Acq On : 16 Aug 2021 12:32
Operator : CG/JU
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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
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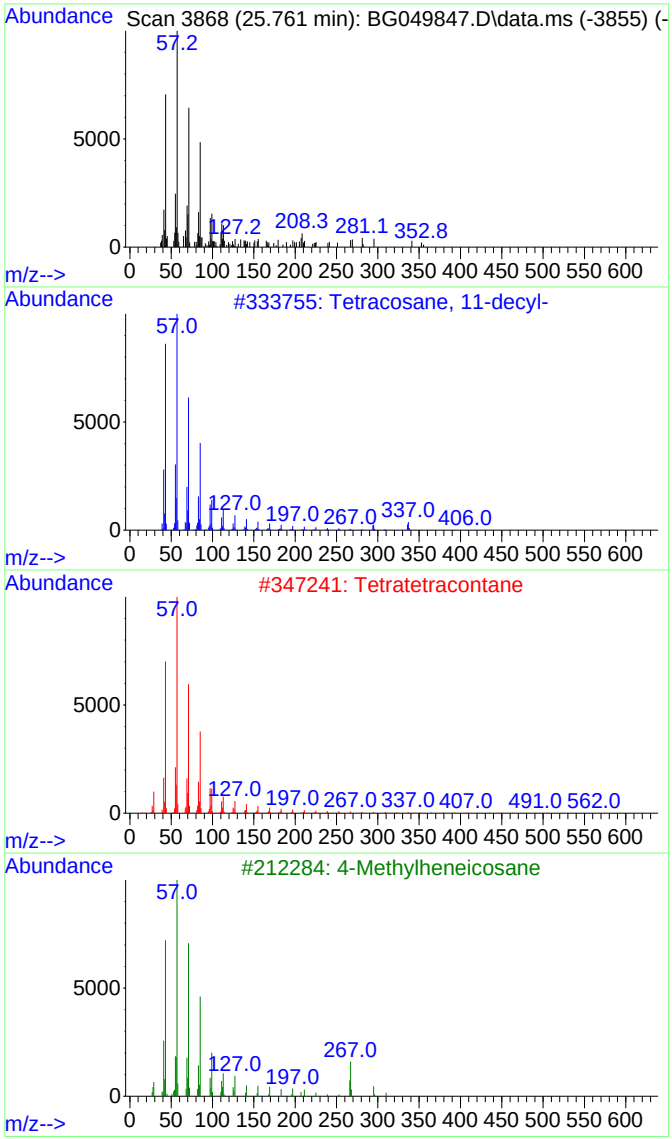
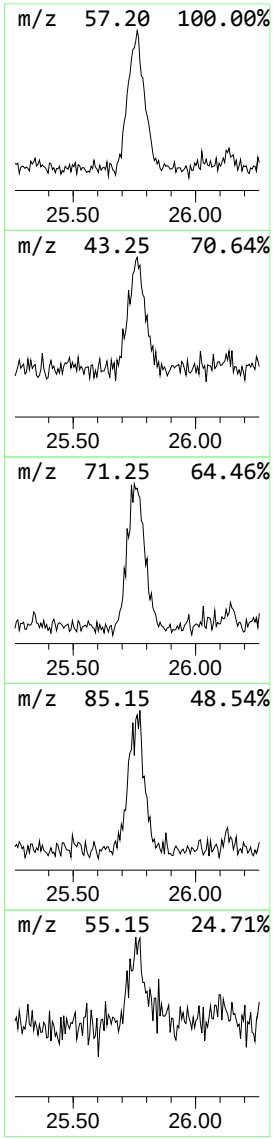
****

Peak Number 10 Tetracosane, 11-decyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.761	8.96 ng	186679	Perylene-d12	24.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	87
2	Tetratetracontane	619	C44H90	007098-22-8	87
3	4-Methylheneicosane	310	C22H46	025117-29-7	87
4	Triacontane	422	C30H62	000638-68-6	80
5	Hentriacontane	437	C31H64	000630-04-6	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049847.D
Acq On : 16 Aug 2021 12:32
Operator : CG/JU
Sample : M3408-14
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 34N

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

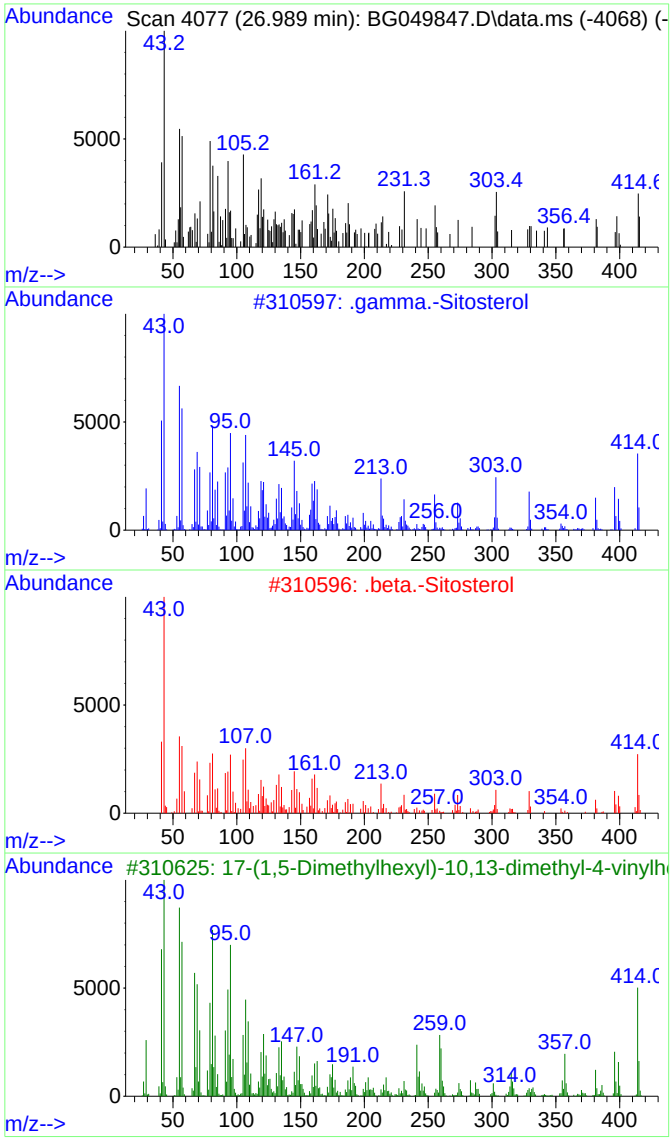
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

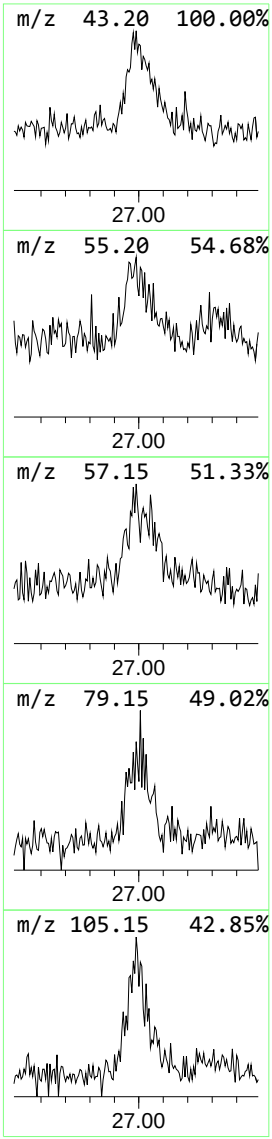
****

Peak Number 11 unknown26.989 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.989	4.91 ng	102382	Perylene-d12	24.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	38
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	38
3	17-(1,5-Dimethylhexyl)-10,13-dim...	414	C29H50O	1000210-86-9	14
4	Dihydrosarsasapogenin-5,17(20)-dien	414	C27H42O3	096974-10-6	11
5	Cholic acid, triacetate	534	C30H46O8	052840-09-2	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049847.D
Acq On : 16 Aug 2021 12:32
Operator : CG/JU
Sample : M3408-14
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 34N

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.139	18.0	ng	160081	1	8.026	177493	20.0
2-Pentanone, 4-...	5.107	6.5	ng	57753	1	8.026	177493	20.0
Ethanol, 1-(2-b...	10.611	4.7	ng	58072	2	10.846	247368	20.0
Eicosane, 1-iodo-	19.440	12.8	ng	266727	4	17.431	415857	20.0
Squalene	19.752	12.5	ng	245533	5	21.714	393335	20.0
Pentacosane	20.557	15.0	ng	294270	5	21.714	393335	20.0
1-Eicosene	21.344	2.9	ng	57724	5	21.714	393335	20.0
Decane, 3,8-dim...	21.555	14.6	ng	286823	5	21.714	393335	20.0
Octacosane	22.701	15.8	ng	310800	5	21.714	393335	20.0
Tetracosane, 11...	25.761	9.0	ng	186679	6	24.992	416763	20.0
unknown26.989	26.989	4.9	ng	102382	6	24.992	416763	20.0