LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048985.D
Acq On : 15 Jun 2021 20:03
Operator : CG/JU
Sample : M2672-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(40-44)

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-BG061121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048985.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.161	15	21	30	rVB	189826	286021	9.49%	2.053%
2	3.285	37	42	47	rBV	66443	91828	3.05%	0.659%
3	5.194	360	367	373	rBV3	18055	30657	1.02%	0.220%
4	5.664	441	447	454	rBV	699746	1159812	38.48%	8.326%
5	5.741	454	460	468	rVB3	21335	51053	1.69%	0.366%
6	7.268	712	720	731	rBV	712646	1249843	41.46%	8.972%
7	8.114	857	864	871	rBV	122986	211394	7.01%	1.518%
8	9.278	1054	1062	1072	rBV	432971	792488	26.29%	5.689%
9	10.700	1300	1304	1310	rBV4	17753	30958	1.03%	0.222%
10	10.935	1338	1344	1352	rVB	153023	287876	9.55%	2.067%
11	13.379	1753	1760	1768	rVB	1019390	1602708	53.17%	11.505%
12	14.754	1988	1994	2002	rVB	251662	425338	14.11%	3.053%
13	16.158	2227	2233	2238	rVB	51282	70849	2.35%	0.509%
14	16.240	2240	2247	2259	rBV	953851	1548667	51.38%	11.118%
15	17.503	2456	2462	2471	rBV	379519	584122	19.38%	4.193%
16	17.621	2478	2482	2487	rVB2	68654	91894	3.05%	0.660%
17	18.161	2568	2574	2580	rBV3	45655	68767	2.28%	0.494%
18	18.385	2607	2612	2618	rBV3	99747	142843	4.74%	1.025%
19	19.654	2824	2828	2835	rBV2	86087	119509	3.96%	0.858%
20	20.112	2900	2906	2914	rVB	2291584	3014353	100.00%	21.639%
21	20.794	3014	3022	3026	rBV	177653	260224	8.63%	1.868%
22	20.870	3031	3035	3039	rBV	33340	36629	1.22%	0.263%
23	21.428	3125	3130	3137	rBV3	78705	133488	4.43%	0.958%
24	21.681	3168	3173	3179	rVB	54960	85929	2.85%	0.617%
25	21.798	3186	3193	3204	rVB	400386	704874	23.38%	5.060%
26	23.020	3397	3401	3408	rVB6	35984	67691	2.25%	0.486%
27	23.326	3448	3453	3464	rBV9	28567	68038	2.26%	0.488%
28	25.136	3749	3761	3772	rBV3	216093	712109	23.62%	5.112%

Sum of corrected areas: 13929962

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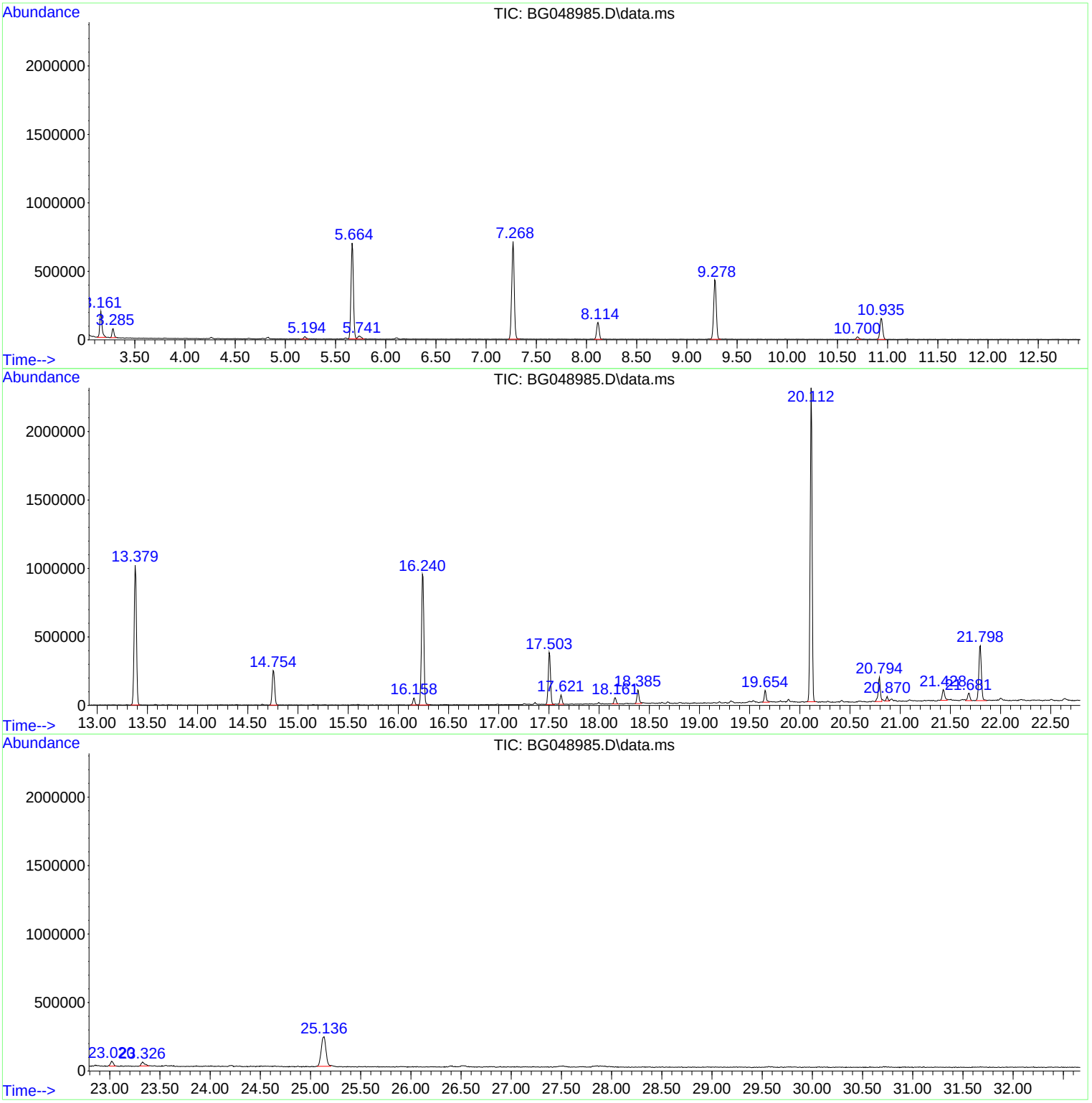
Instrument :
BNA_G
ClientSampleId :
17-B6(40-44)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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Data File : BG048985.D
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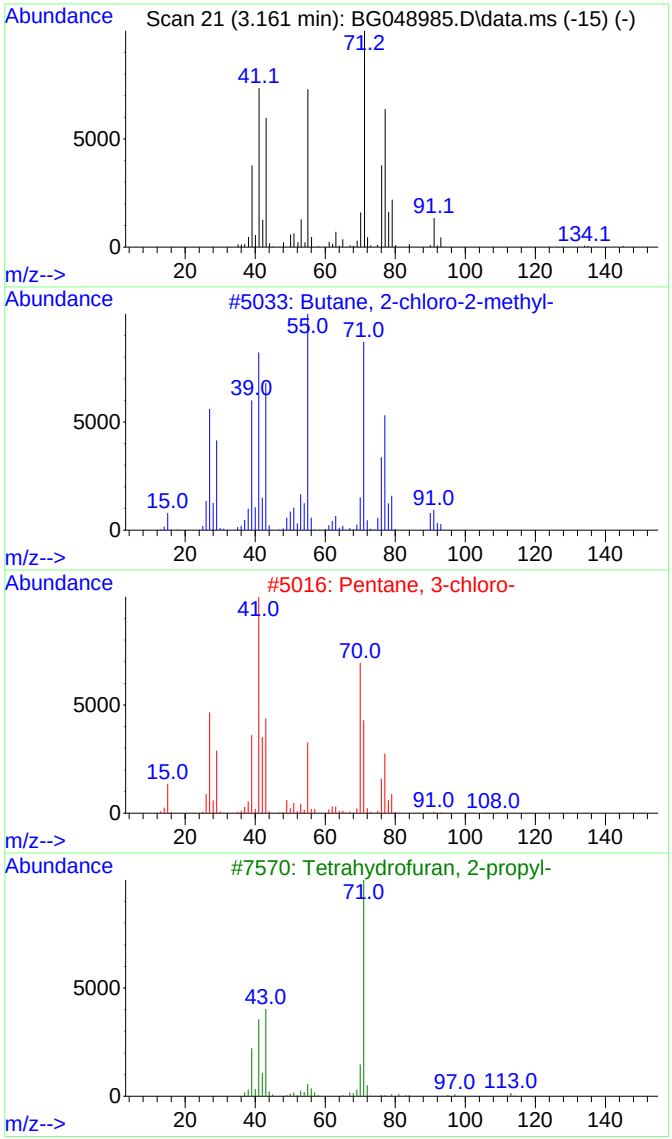
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

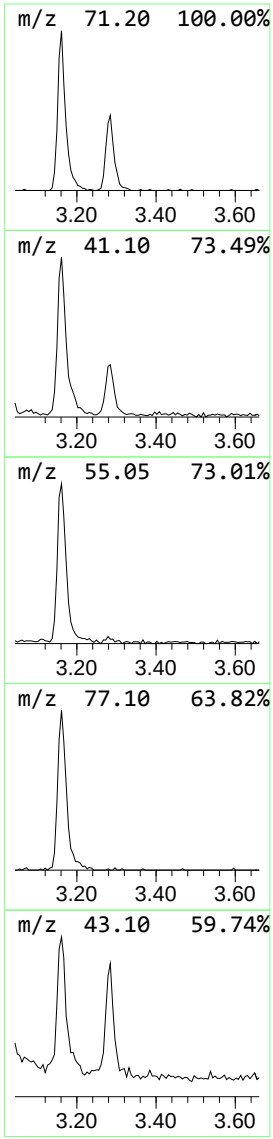
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.161	27.06 ng	286021	1,4-Dichlorobenzene-d4	8.114

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-chloro-2-methyl-	106	C5H11Cl	000594-36-5	74
2	Pentane, 3-chloro-	106	C5H11Cl	000616-20-6	56
3	Tetrahydrofuran, 2-propyl-	114	C7H14O	003208-22-8	35
4	Furan-2-carbonyl chloride, tetra...	134	C5H7ClO2	052449-98-6	35
5	Butanoyl chloride	106	C4H7ClO	000141-75-3	32





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Data File : BG048985.D
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Operator : CG/JU
Sample : M2672-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(40-44)

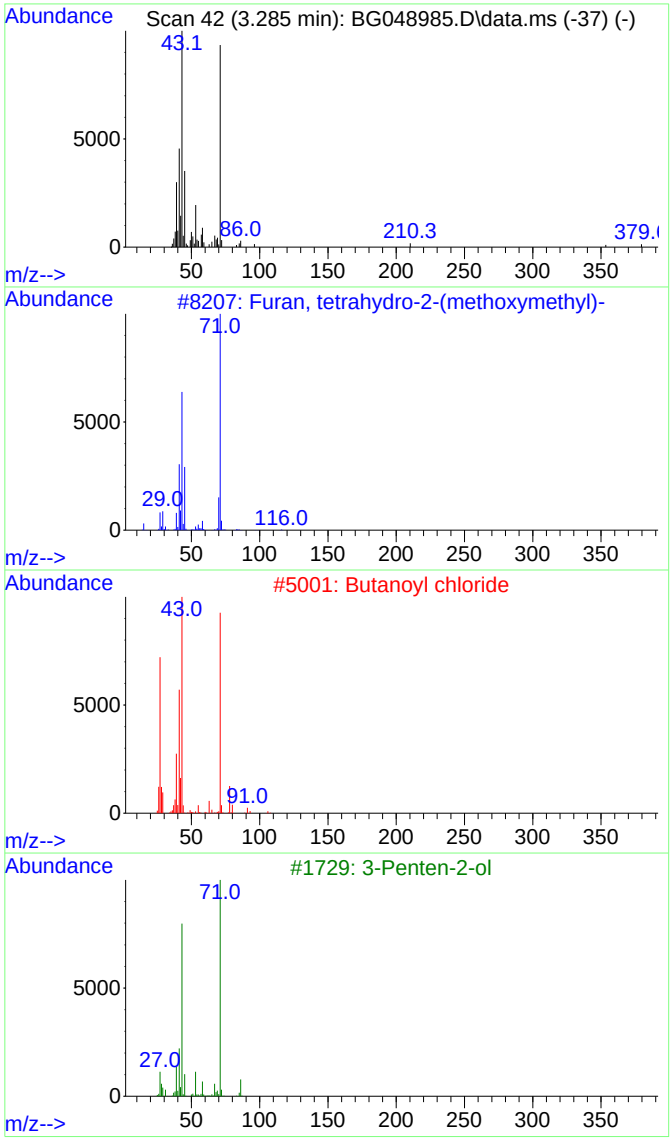
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

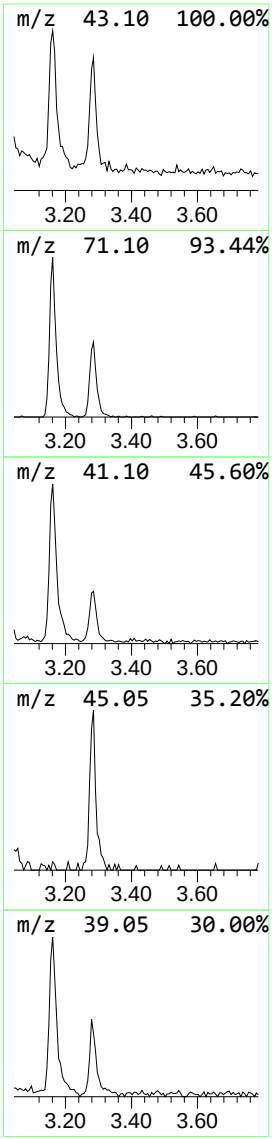
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Furan, tetrahydro-2-(methox... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.285	8.69 ng	91828	1,4-Dichlorobenzene-d4	8.114

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	72
2	Butanoyl chloride	106	C4H7ClO	000141-75-3	53
3	3-Penten-2-ol	86	C5H10O	001569-50-2	50
4	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	47
5	3-Chloro-2-buten-1-ol	106	C4H7ClO	040605-42-3	42





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Instrument :
BNA_G
ClientSampleId :
17-B6(40-44)

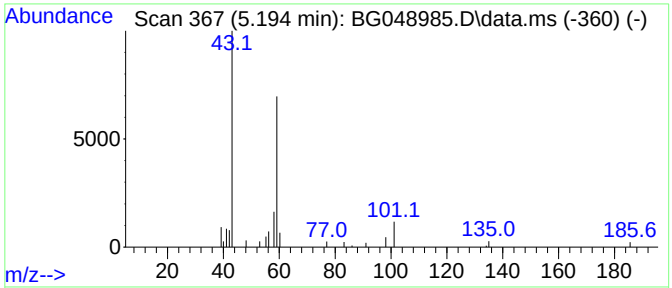
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

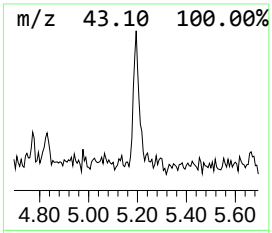
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

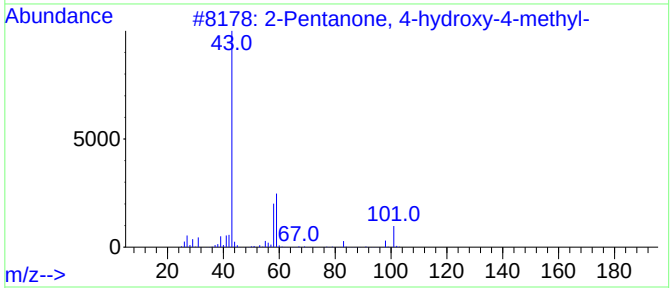
****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

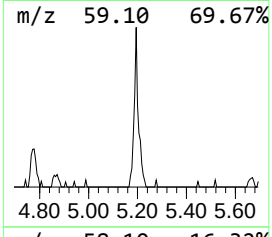
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.194	2.90 ng	30657	1,4-Dichlorobenzene-d4	8.114

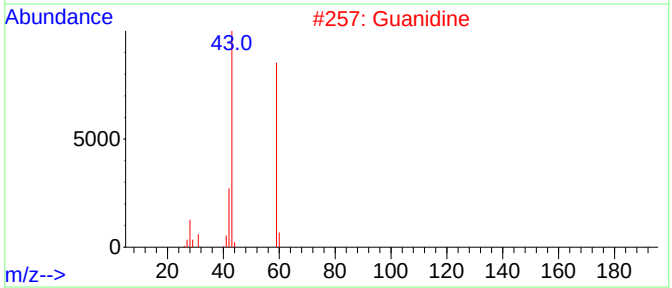
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	Guanidine	59	CH5N3	000113-00-8	9
3	Formamide, N-butyl-	101	C5H11NO	000871-71-6	9
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9
5	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	9

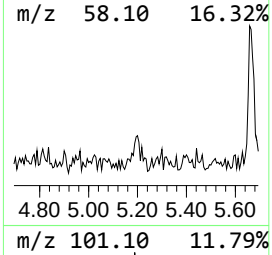


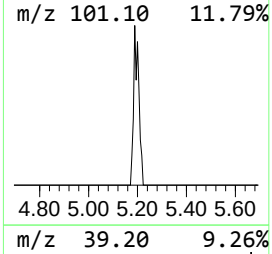


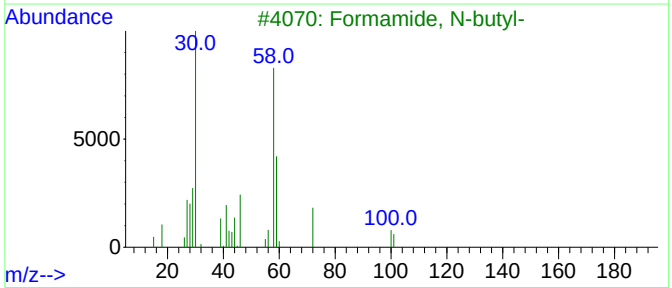


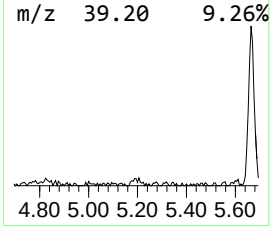












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ClientSampleId :
17-B6(40-44)

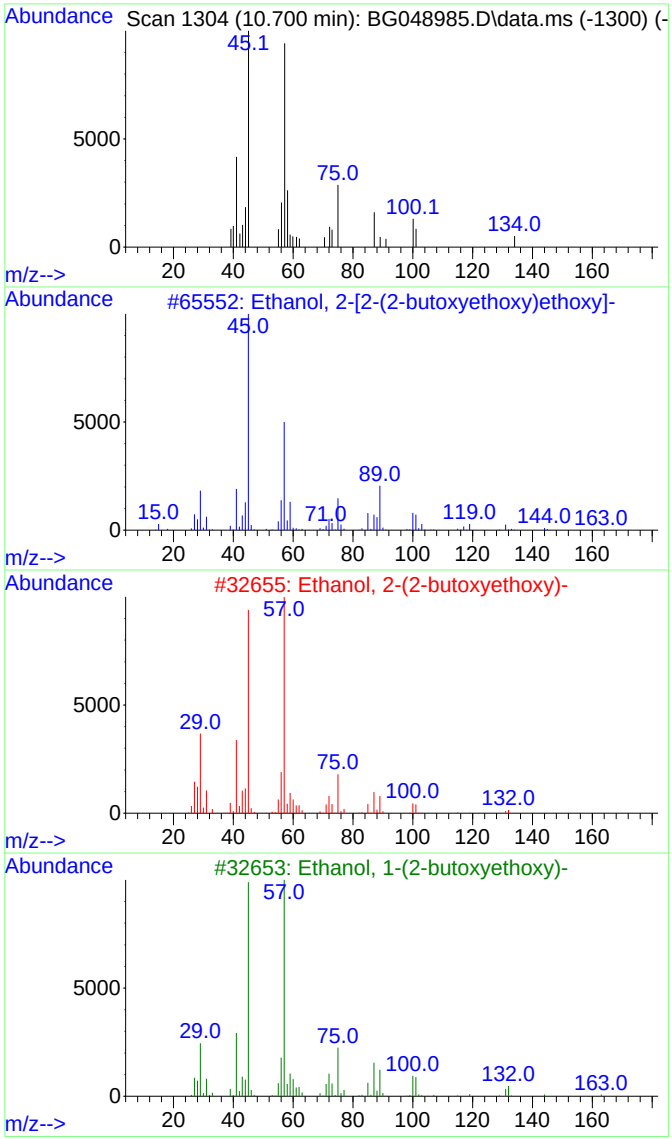
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

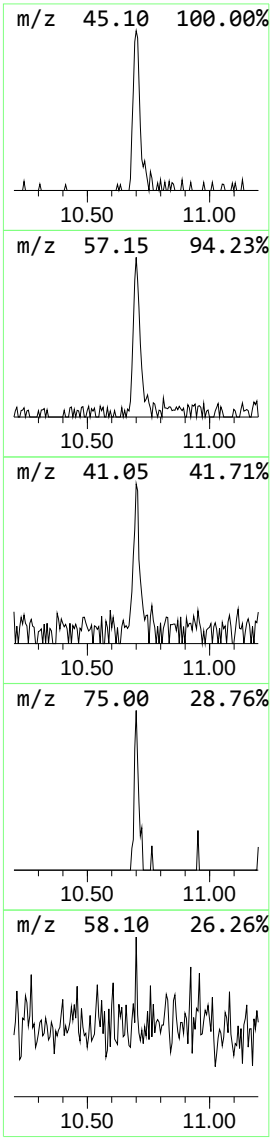
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Ethanol, 2-[2-(2-butoxyetho... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.700	2.15 ng	30958	Naphthalene-d8	10.935

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	45
3	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	45
4	Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	42
5	Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	37





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Instrument :
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ClientSampleId :
17-B6(40-44)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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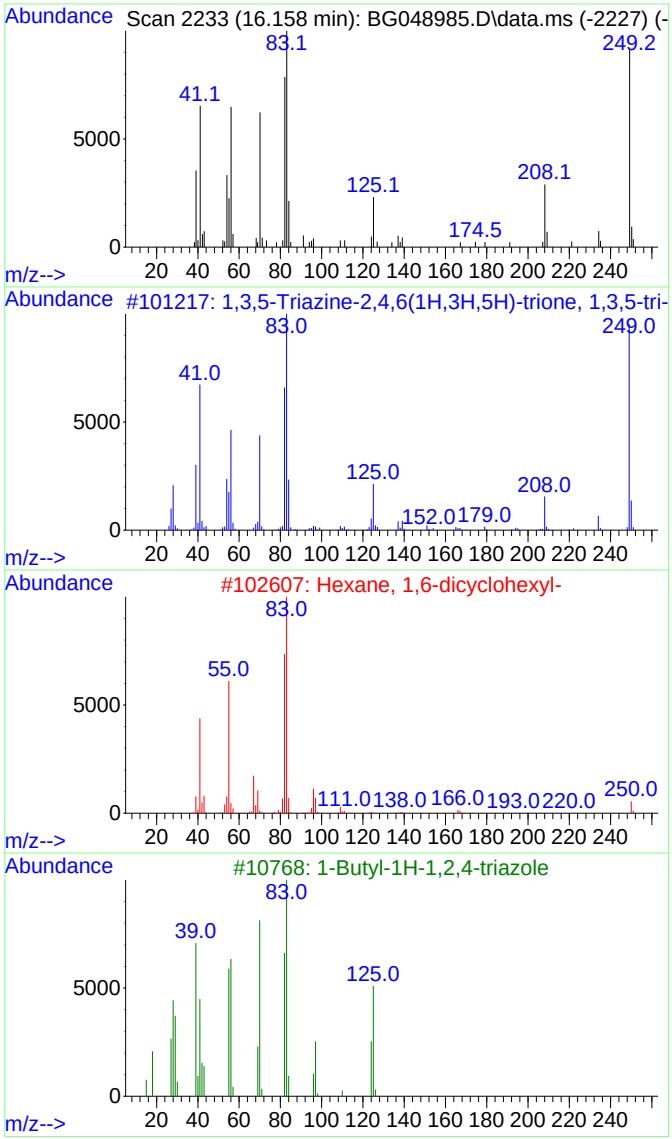
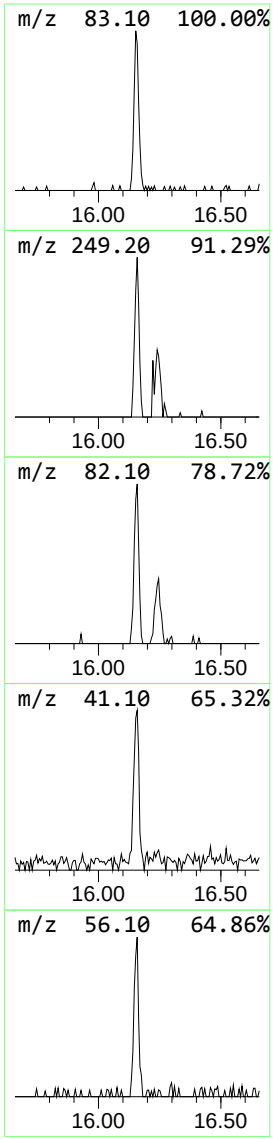
****
Peak Number 6 1,3,5-Triazine-2,4,6(1H,3H,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.158	2.43 ng	70849	Phenanthrene-d10	17.503

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4,6(1H,3H,5H)-t...	249	C12H15N3O3	001025-15-6	91
2	Hexane, 1,6-dicyclohexyl-	250	C18H34	001610-23-7	38
3	1-Butyl-1H-1,2,4-triazole	125	C6H11N3	006086-22-2	37
4	Triallyl cyanurate	249	C12H15N3O3	000101-37-1	25
5	Cyclohexane, undecyl-	238	C17H34	054105-66-7	25





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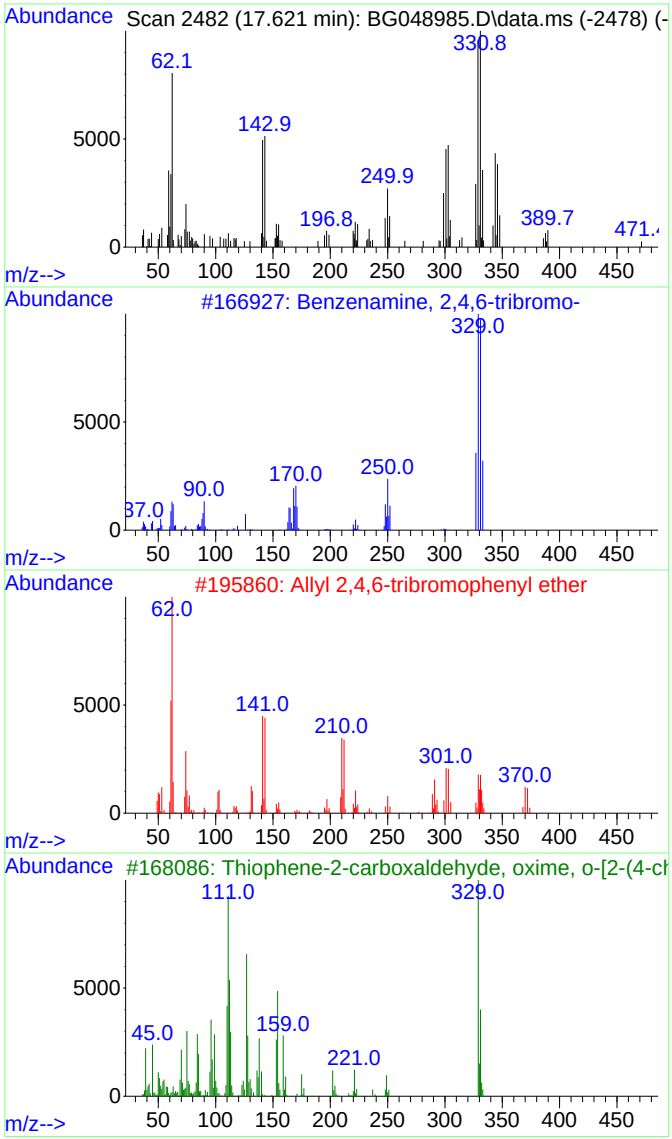
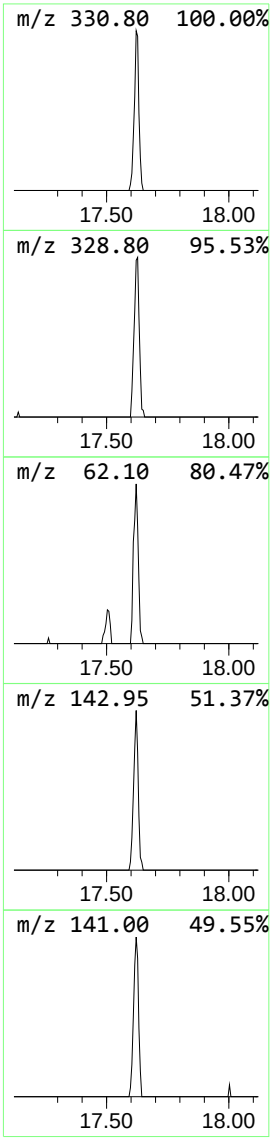
****

Peak Number 7 unknown17.621 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.621	3.15 ng	91894	Phenanthrene-d10	17.503

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 2,4,6-tribromo-	327	C6H4Br3N	000147-82-0	25
2	Allyl 2,4,6-tribromophenyl ether	368	C9H7Br3O	003278-89-5	23
3	Thiophene-2-carboxaldehyde, oxim...	329	C13H12ClNO3S2	1000264-79-9	11
4	Tetrachlorvinphos	364	C10H9Cl4O4P	022248-79-9	10
5	1,3,4-Oxadiazol-2-amine, 5-(2-br...	329	C11H12BrN3O4	1000350-74-8	10





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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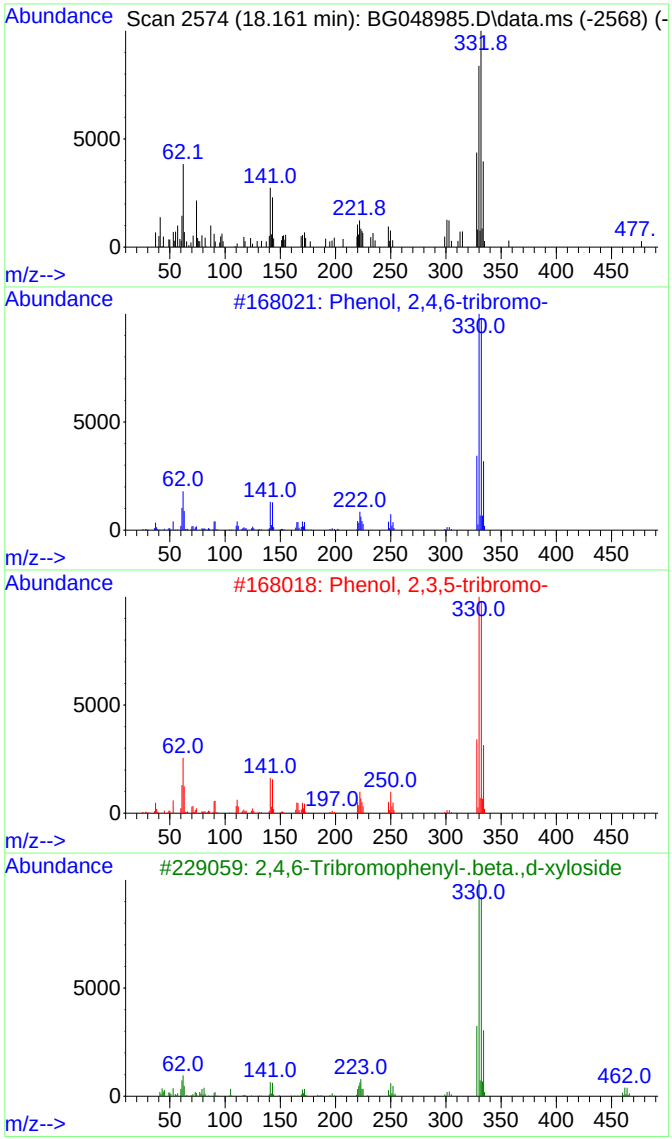
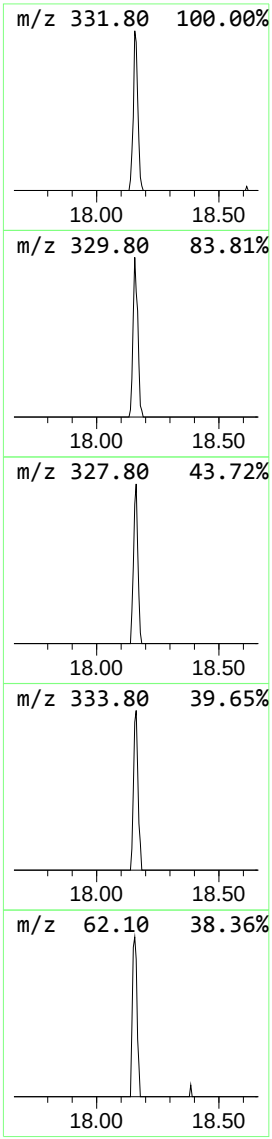
****

Peak Number 8 Phenol, 2,3,5-tribromo- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.161	2.35 ng	68767	Phenanthrene-d10	17.503

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,4,6-tribromo-	328	C6H3Br3O	000118-79-6	95
2	Phenol, 2,3,5-tribromo-	328	C6H3Br3O	057383-81-0	91
3	2,4,6-Tribromophenyl-.beta.,d-xy...	460	C11H11Br3O5	1000129-97-6	38
4	2,4,6-Tribromo-2,5-cyclohexadienone	328	C6H3Br3O	020244-61-5	35
5	Bis-(3,4-dichloro-phenyl)-carbod...	330	C13H6Cl4N2	063875-68-3	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
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Operator : CG/JU
Sample : M2672-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(40-44)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
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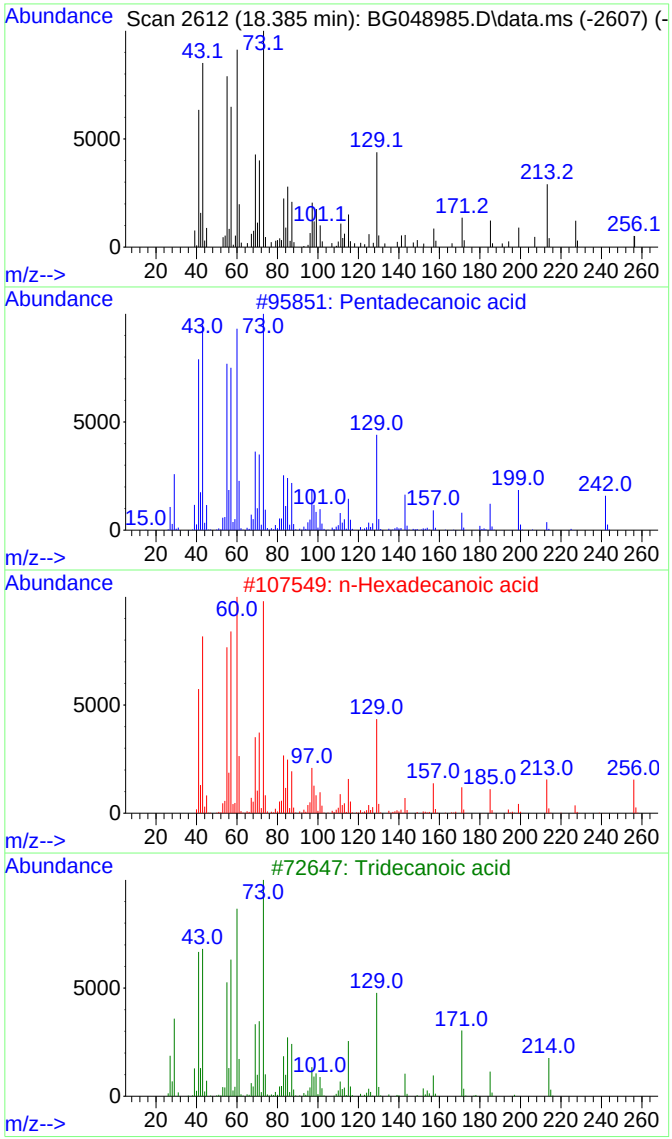
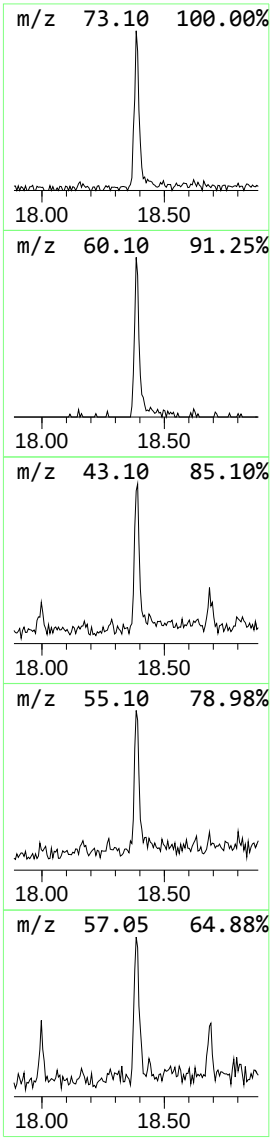
****

Peak Number 9 Pentadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.385	4.89 ng	142843	Phenanthrene-d10	17.503

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





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Data File : BG048985.D
Acq On : 15 Jun 2021 20:03
Operator : CG/JU
Sample : M2672-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(40-44)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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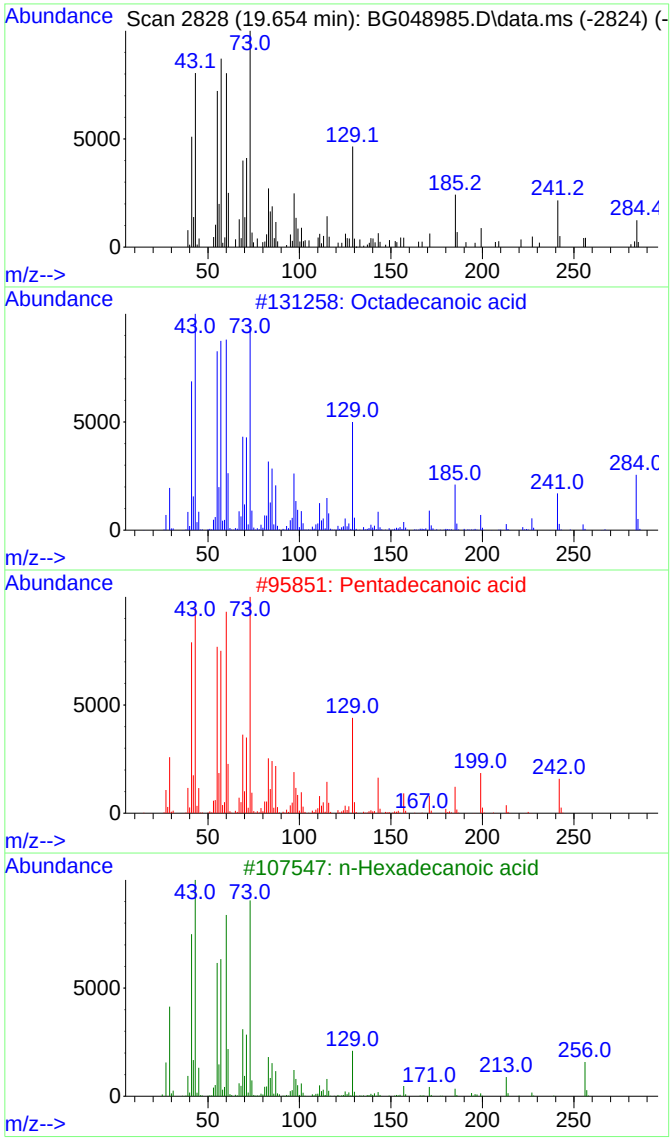
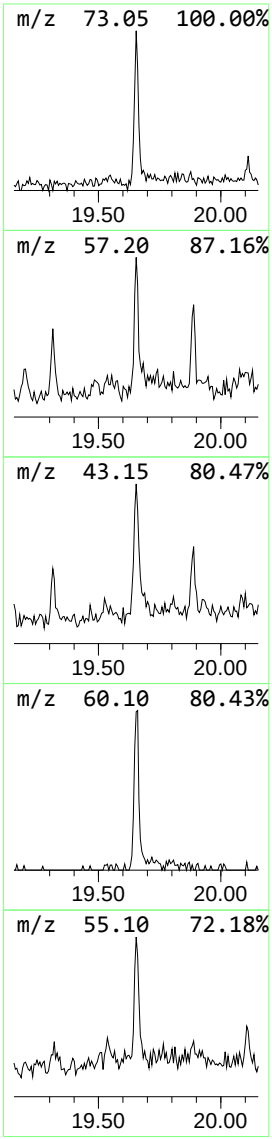
Peak Number 10 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.654	3.39 ng	119509	Chrysene-d12	21.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	60
4	n-Decanoic acid	172	C10H20O2	000334-48-5	47
5	Undecanoic acid	186	C11H22O2	000112-37-8	43





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Data File : BG048985.D
Acq On : 15 Jun 2021 20:03
Operator : CG/JU
Sample : M2672-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(40-44)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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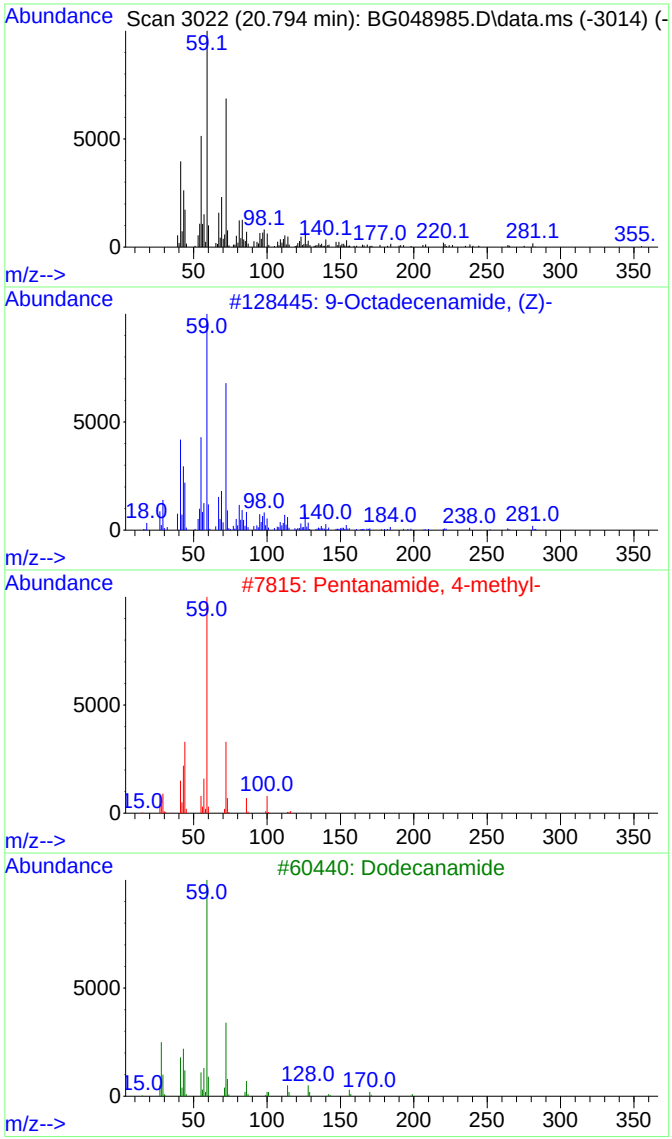
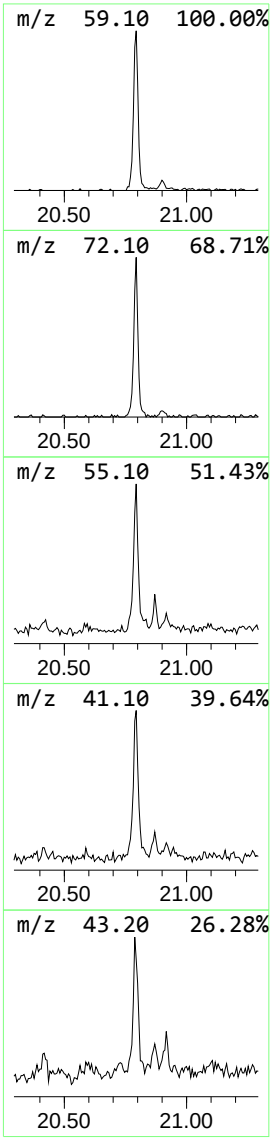
Peak Number 11 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.794	7.38 ng	260224	Chrysene-d12	21.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	64
3	Dodecanamide	199	C12H25NO	001120-16-7	59
4	Nonanamide	157	C9H19NO	001120-07-6	59
5	Pentanamide	101	C5H11NO	000626-97-1	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048985.D
Acq On : 15 Jun 2021 20:03
Operator : CG/JU
Sample : M2672-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(40-44)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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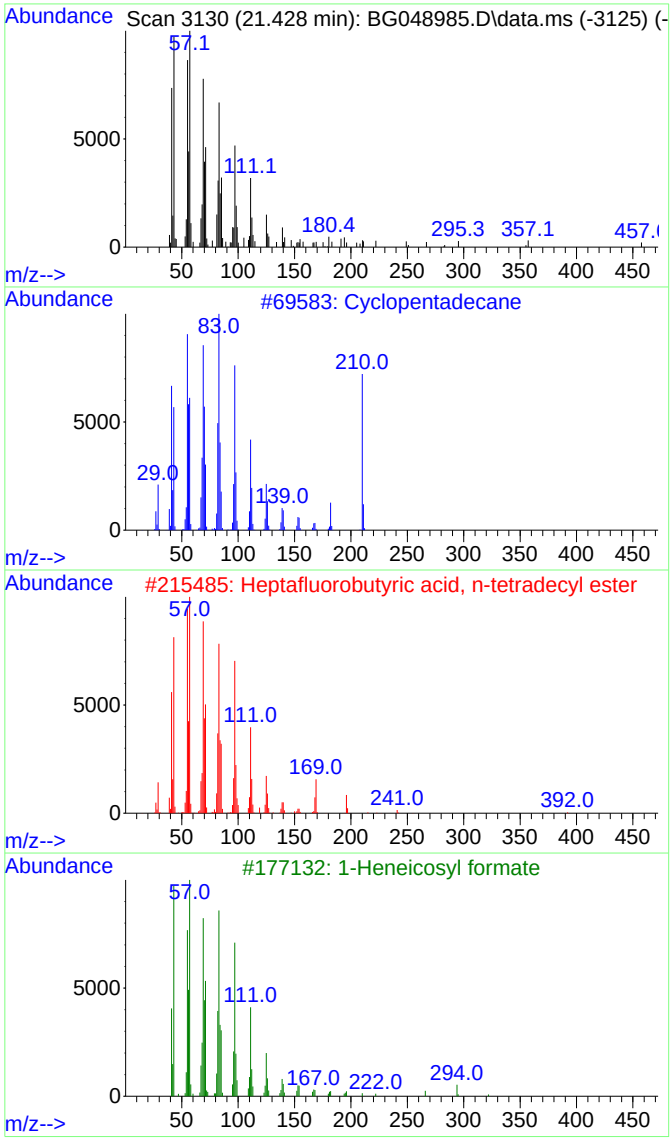
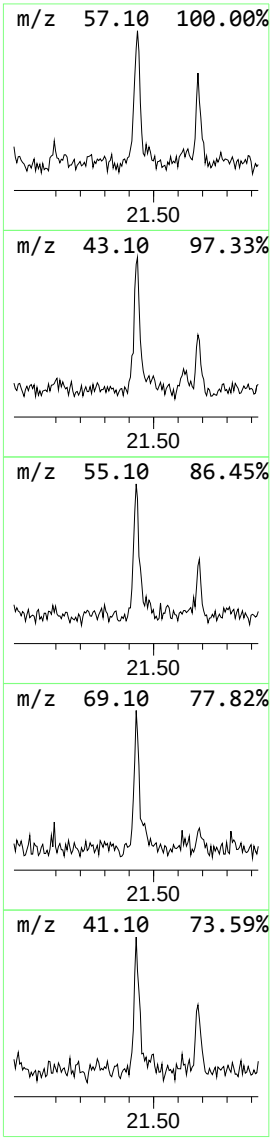
Peak Number 12 Cyclopentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.428	3.79 ng	133488	Chrysene-d12	21.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	93
2	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
4	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91
5	4-Trifluoroacetoxyhexadecane	338	C18H33F3O2	1000215-97-5	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048985.D
Acq On : 15 Jun 2021 20:03
Operator : CG/JU
Sample : M2672-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(40-44)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-chlor...	3.161	27.1	ng	286021	1	8.114	211394	20.0
Furan, tetrahyd...	3.285	8.7	ng	91828	1	8.114	211394	20.0
2-Pentanone, 4-...	5.194	2.9	ng	30657	1	8.114	211394	20.0
Ethanol, 2-[2-(...	10.700	2.1	ng	30958	2	10.935	287876	20.0
1,3,5-Triazine-...	16.158	2.4	ng	70849	4	17.503	584122	20.0
unknown17.621	17.621	3.1	ng	91894	4	17.503	584122	20.0
Phenol, 2,3,5-t...	18.161	2.4	ng	68767	4	17.503	584122	20.0
Pentadecanoic acid	18.385	4.9	ng	142843	4	17.503	584122	20.0
Octadecanoic acid	19.654	3.4	ng	119509	5	21.798	704874	20.0
9-Octadecenamid...	20.794	7.4	ng	260224	5	21.798	704874	20.0
Cyclopentadecane	21.428	3.8	ng	133488	5	21.798	704874	20.0