LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048986.D
Acq On : 15 Jun 2021 20:45
Operator : CG/JU
Sample : M2672-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(44-48)

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: BG048986.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.157	15	20	35	rVB	185052	302787	10.53%	2.268%
2	3.281	37	41	49	rVB	74240	104506	3.64%	0.783%
3	5.666	440	447	454	rBV	697491	1140654	39.68%	8.545%
4	5.731	454	458	469	rVB2	24128	59506	2.07%	0.446%
5	7.270	711	720	728	rBV	672709	1220990	42.48%	9.147%
6	8.111	857	863	870	rVB	113378	201271	7.00%	1.508%
7	9.280	1053	1062	1075	rVB	425198	768908	26.75%	5.760%
8	10.702	1298	1304	1312	rBV4	16034	34434	1.20%	0.258%
9	10.937	1334	1344	1351	rBV2	141898	269574	9.38%	2.019%
10	13.381	1752	1760	1769	rBV	986439	1558922	54.23%	11.678%
11	14.756	1988	1994	2002	rBV	250426	388706	13.52%	2.912%
12	16.154	2227	2232	2240	rVB2	53147	71633	2.49%	0.537%
13	16.242	2240	2247	2263	rBV	995202	1512870	52.63%	11.333%
14	17.505	2455	2462	2468	rBV	354687	551264	19.18%	4.130%
15	17.623	2477	2482	2490	rVB3	63039	90985	3.17%	0.682%
16	18.163	2569	2574	2579	rVB3	45071	68683	2.39%	0.515%
17	18.387	2607	2612	2623	rBV2	139766	210494	7.32%	1.577%
18	19.656	2823	2828	2838	rBV2	133093	188139	6.54%	1.409%
19	20.114	2899	2906	2917	rVB	2255811	2874602	100.00%	21.534%
20	20.790	3015	3021	3028	rBV	48013	74981	2.61%	0.562%
21	20.872	3031	3035	3039	rVV2	31510	33652	1.17%	0.252%
22	21.430	3125	3130	3139	rBV2	74816	132333	4.60%	0.991%
23	21.683	3169	3173	3181	rVB	58841	95678	3.33%	0.717%
24	21.794	3186	3192	3203	rVB2	387109	668049	23.24%	5.004%
25	23.022	3396	3401	3409	rVB7	36324	69187	2.41%	0.518%
26	25.132	3750	3760	3771	rBV2	212119	656312	22.83%	4.917%

Sum of corrected areas: 13349120

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Instrument :
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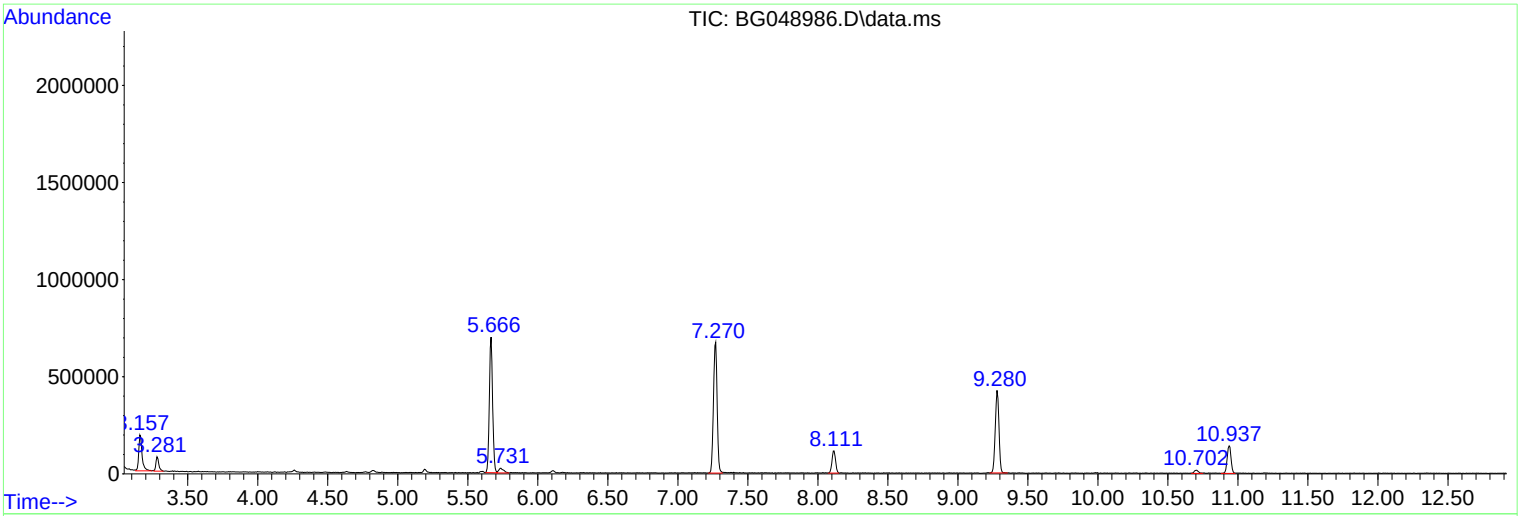
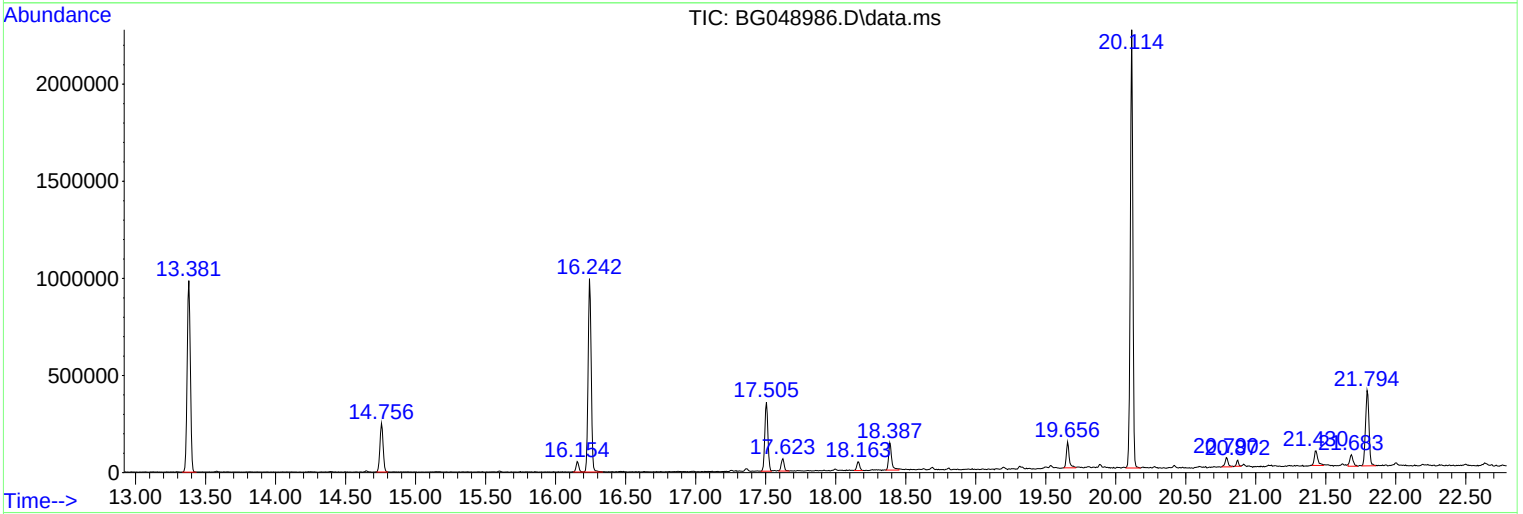
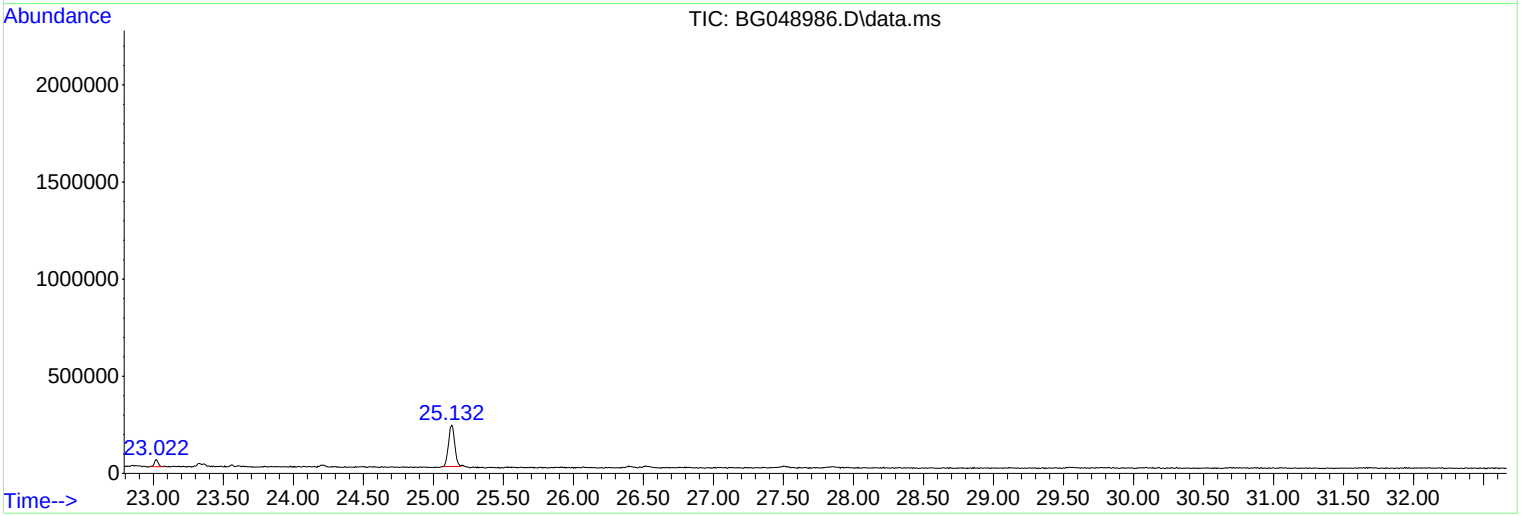
ClientSampleId :
17-B6(44-48)

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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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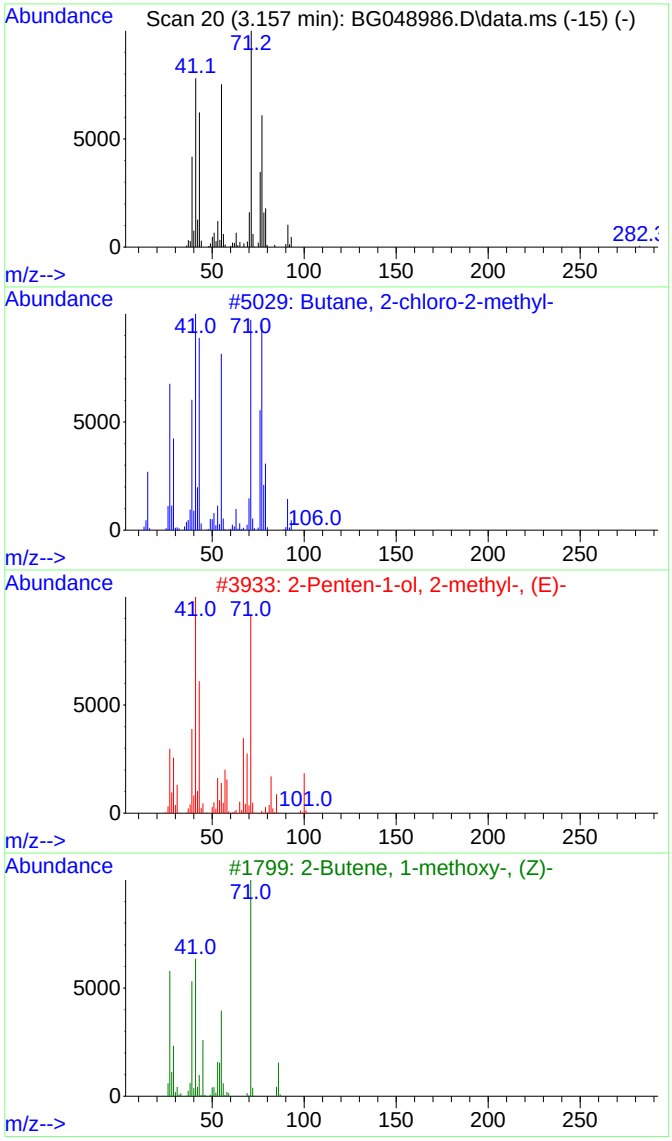
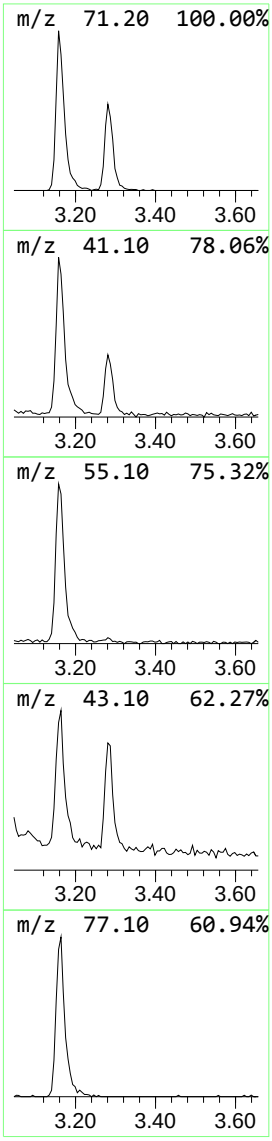
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.157	30.09 ng	302787	1,4-Dichlorobenzene-d4	8.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-chloro-2-methyl-	106	C5H11Cl	000594-36-5	78
2	2-Penten-1-ol, 2-methyl-, (E)-	100	C6H12O	016958-19-3	32
3	2-Butene, 1-methoxy-, (Z)-	86	C5H10O	010034-16-9	32
4	Butane, 2-bromo-2-methyl-	150	C5H11Br	000507-36-8	27
5	Tetrahydrofuran, 2-propyl-	114	C7H14O	003208-22-8	27





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Data File : BG048986.D
Acq On : 15 Jun 2021 20:45
Operator : CG/JU
Sample : M2672-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(44-48)

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
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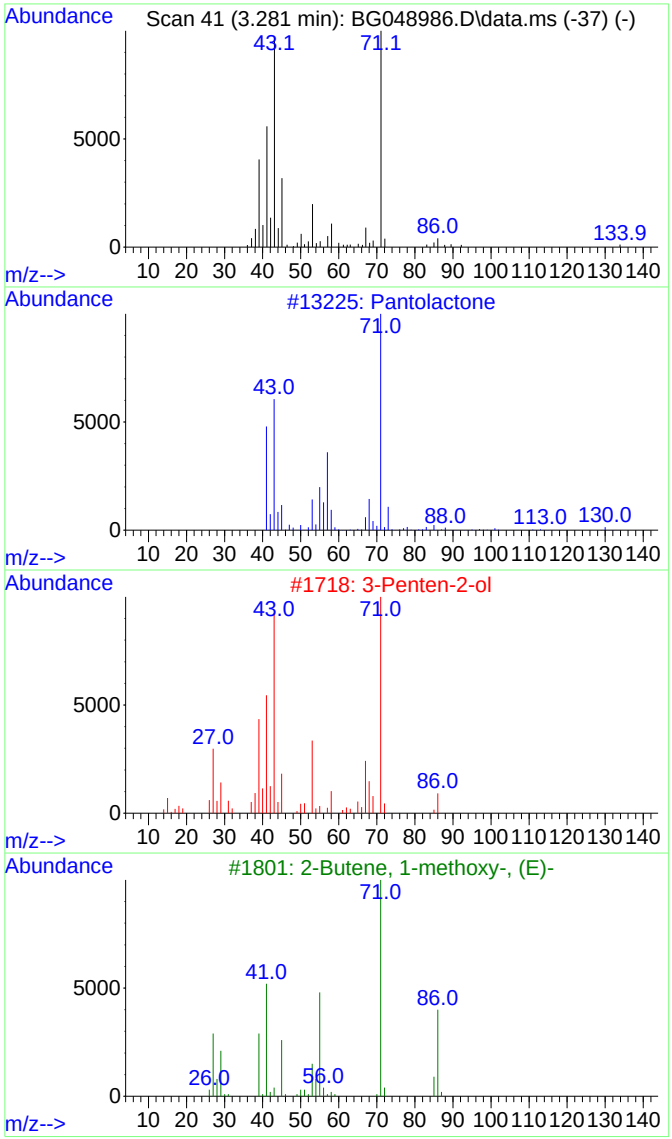
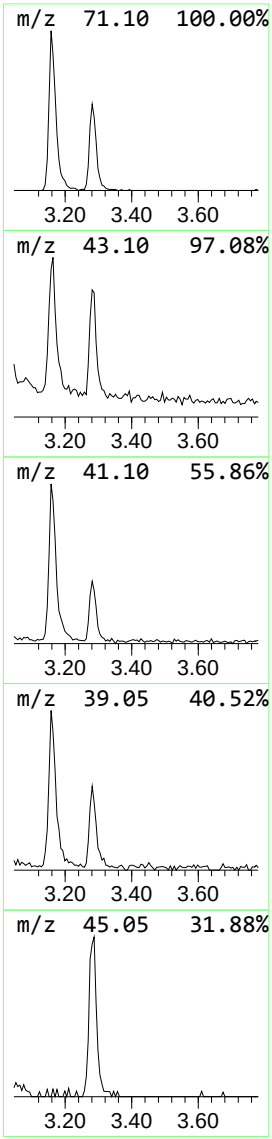
Peak Number 2 Pantolactone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.281	10.38 ng	104506	1,4-Dichlorobenzene-d4	8.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pantolactone	130	C6H10O3	000599-04-2	64
2	3-Penten-2-ol	86	C5H10O	001569-50-2	59
3	2-Butene, 1-methoxy-, (E)-	86	C5H10O	010034-14-7	50
4	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	47
5	3-Chloro-2-buten-1-ol	106	C4H7ClO	040605-42-3	45





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Data File : BG048986.D
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Operator : CG/JU
Sample : M2672-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(44-48)

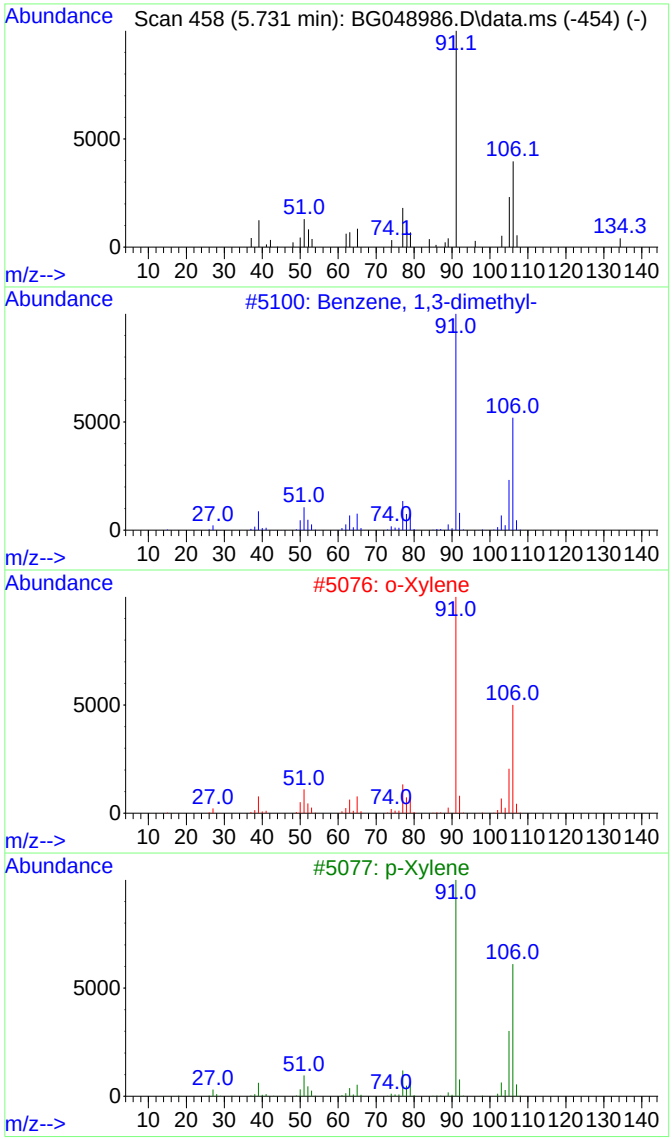
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

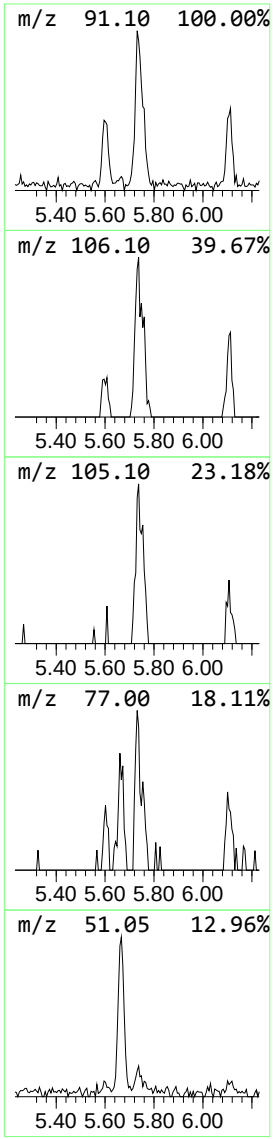
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, 1,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.731	5.91 ng	59506	1,4-Dichlorobenzene-d4	8.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	90
2	o-Xylene	106	C8H10	000095-47-6	87
3	p-Xylene	106	C8H10	000106-42-3	87
4	Ethylbenzene	106	C8H10	000100-41-4	64
5	1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	64





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Sample : M2672-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(44-48)

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

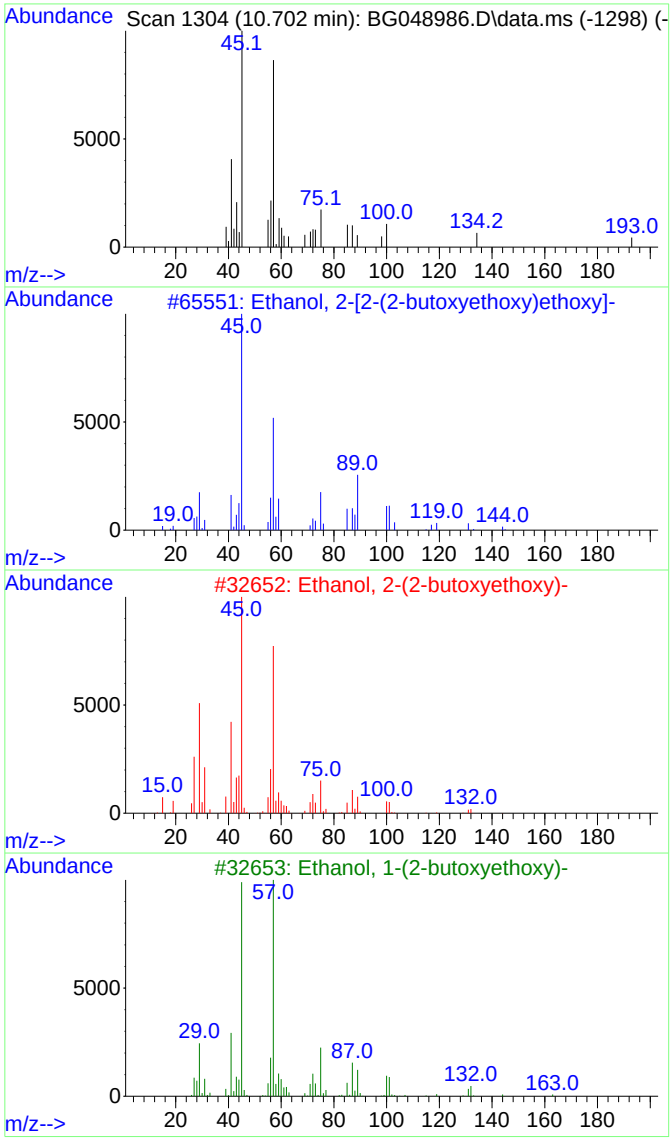
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

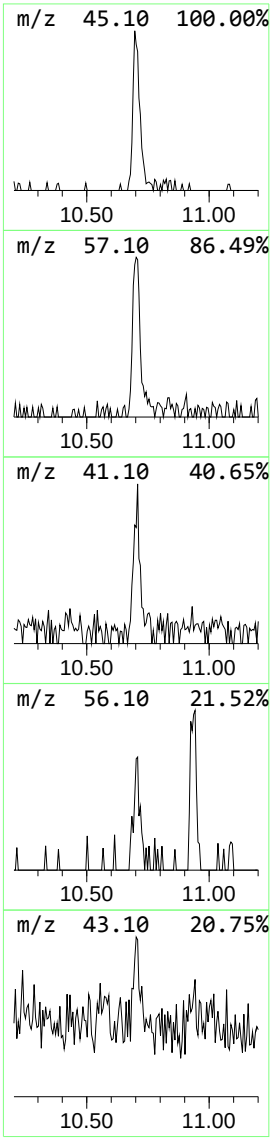
****

Peak Number 4 Ethanol, 2-[2-(2-butoxyetho... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.702	2.55 ng	34434	Naphthalene-d8	10.937

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	64
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	56
3	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	45
4	Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	40
5	3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	38





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Instrument : BNA_G
ClientSampleId : 17-B6(44-48)

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

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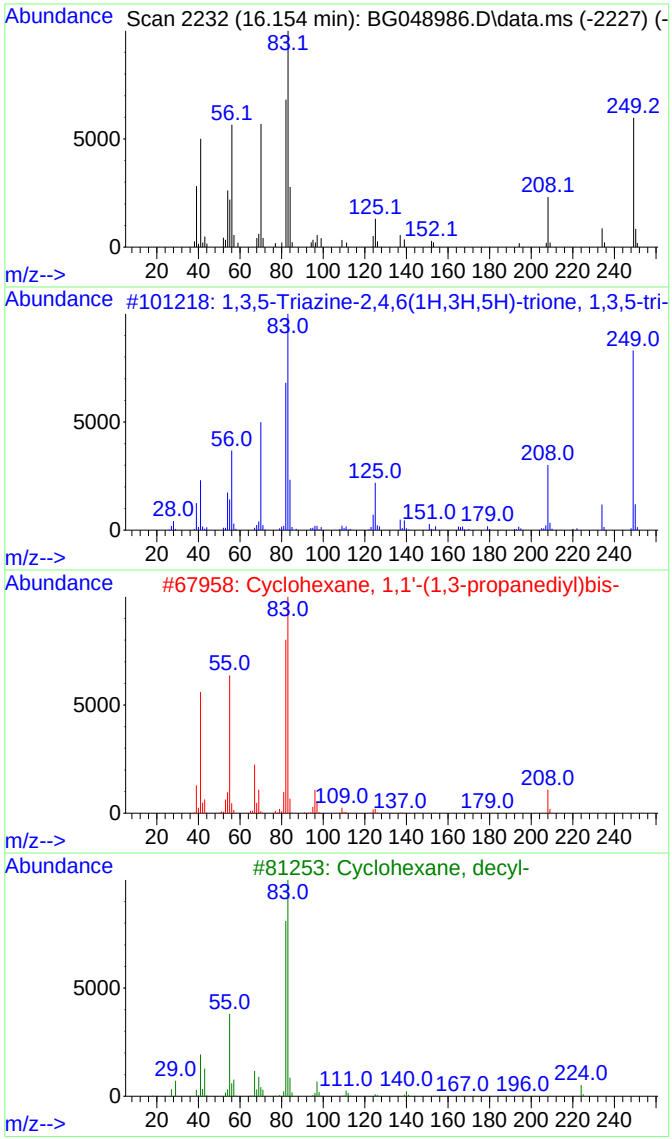
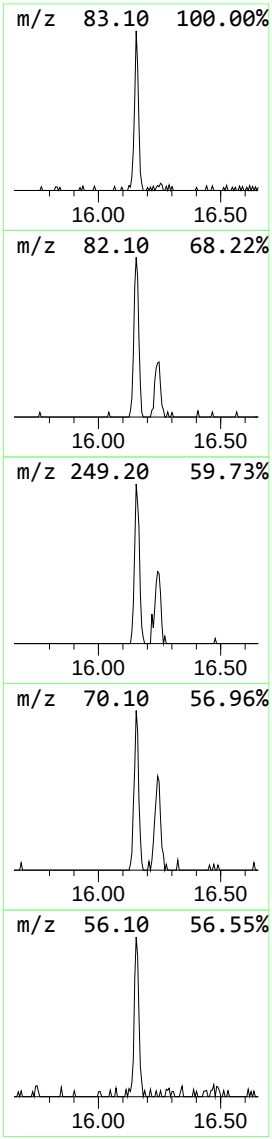
****

Peak Number 5 1,3,5-Triazine-2,4,6(1H,3H,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.154	2.60 ng	71633	Phenanthrene-d10	17.505

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	96
2	Cyclohexane, 1,1'-(1,3-propanedi...	208	C15H28	003178-24-3	38
3	Cyclohexane, decyl-	224	C16H32	001795-16-0	35
4	Cyclohexane, (4-methylpentyl)-	168	C12H24	061142-20-9	35
5	Hexane, 1,6-dicyclohexyl-	250	C18H34	001610-23-7	35





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

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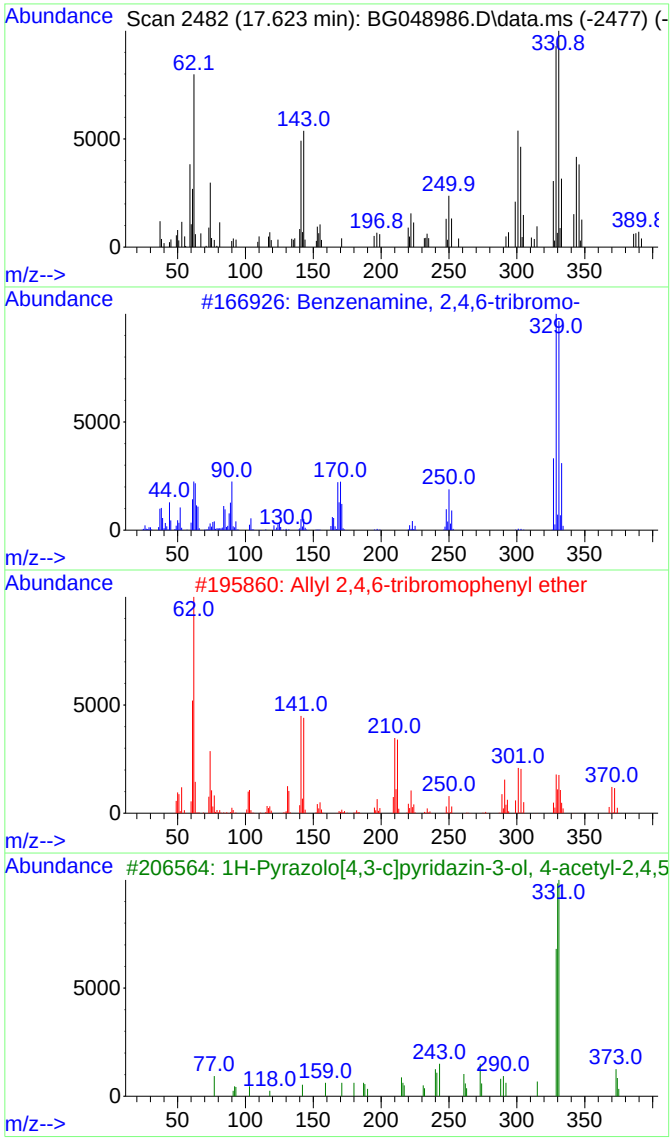
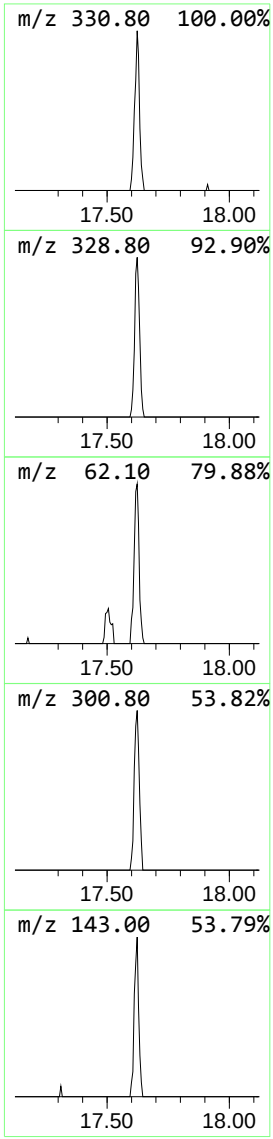
****

Peak Number 6 Benzenamine, 2,4,6-tribromo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.623	3.30 ng	90985	Phenanthrene-d10	17.505

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 2,4,6-tribromo-	327	C6H4Br3N	000147-82-0	80
2	Allyl 2,4,6-tribromophenyl ether	368	C9H7Br3O	003278-89-5	32
3	1H-Pyrazolo[4,3-c]pyridazin-3-ol...	388	C22H20N4O3	035426-81-4	12
4	6-Chloro-4-phenyl-2-(p-tolyl)qui...	329	C22H16ClN	021923-41-1	9
5	Silylamine, 1,1,1-trimethyl-N-[4...	329	C18H27NOSi2	031396-30-2	9





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Sample : M2672-10
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ClientSampleId :
17-B6(44-48)

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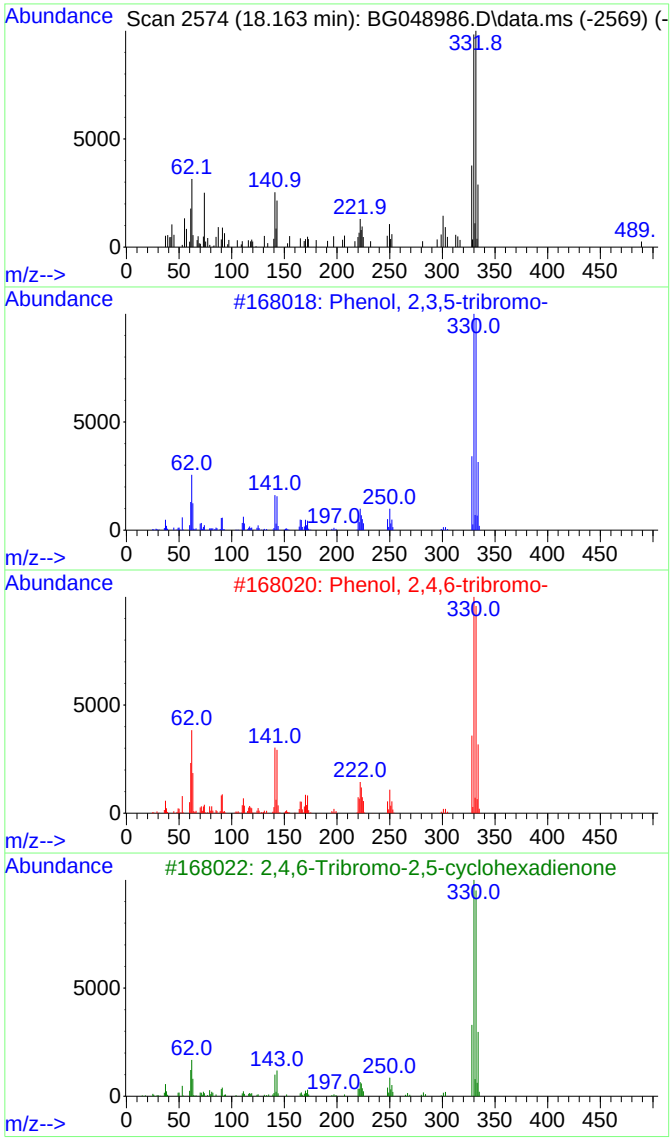
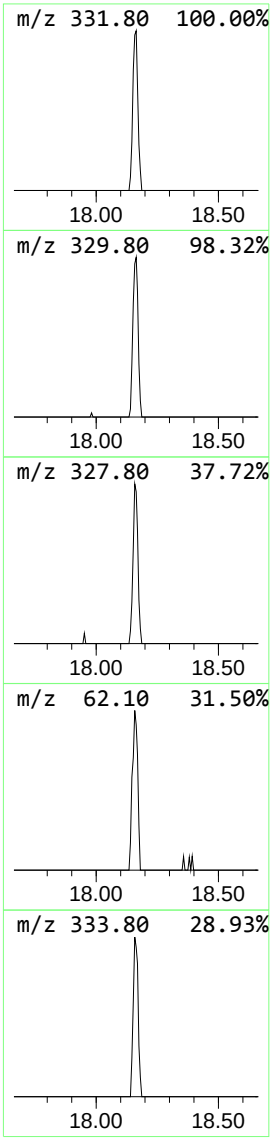
****
Peak Number 7 Phenol, 2,3,5-tribromo- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.163	2.49 ng	68683	Phenanthrene-d10	17.505

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,3,5-tribromo-	328	C6H3Br3O	057383-81-0	96
2	Phenol, 2,4,6-tribromo-	328	C6H3Br3O	000118-79-6	94
3	2,4,6-Tribromo-2,5-cyclohexadienone	328	C6H3Br3O	020244-61-5	90
4	2,4,6-Tribromophenyl-.beta.,d-xy...	460	C11H11Br3O5	1000129-97-6	72
5	2-Bromo-4-chloro-5,8-dimethoxy-3...	330	C13H12BrClO3	104506-11-8	25





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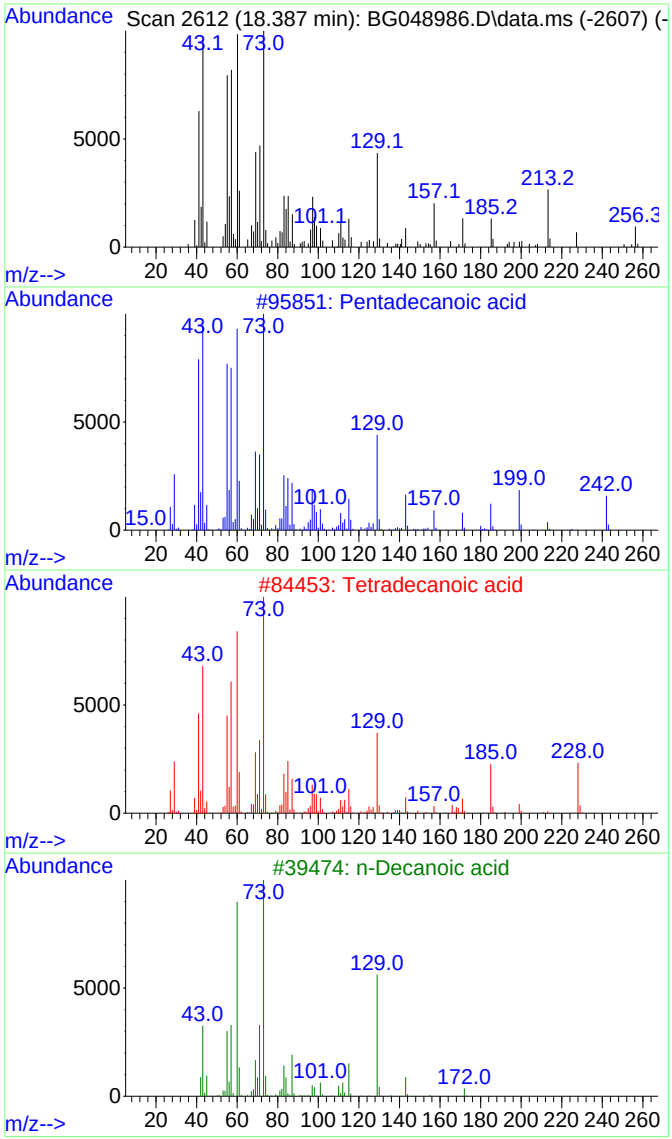
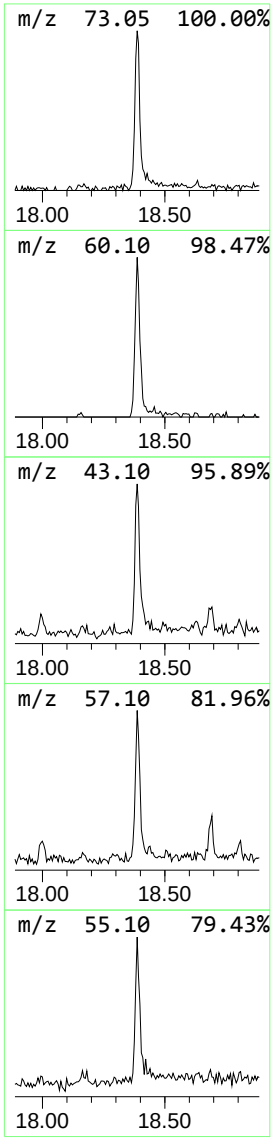
Peak Number 8 Pentadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.387	7.64 ng	210494	Phenanthrene-d10	17.505

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	n-Decanoic acid	172	C10H20O2	000334-48-5	60
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	60
5	Tridecanoic acid	214	C13H26O2	000638-53-9	58





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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(44-48)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
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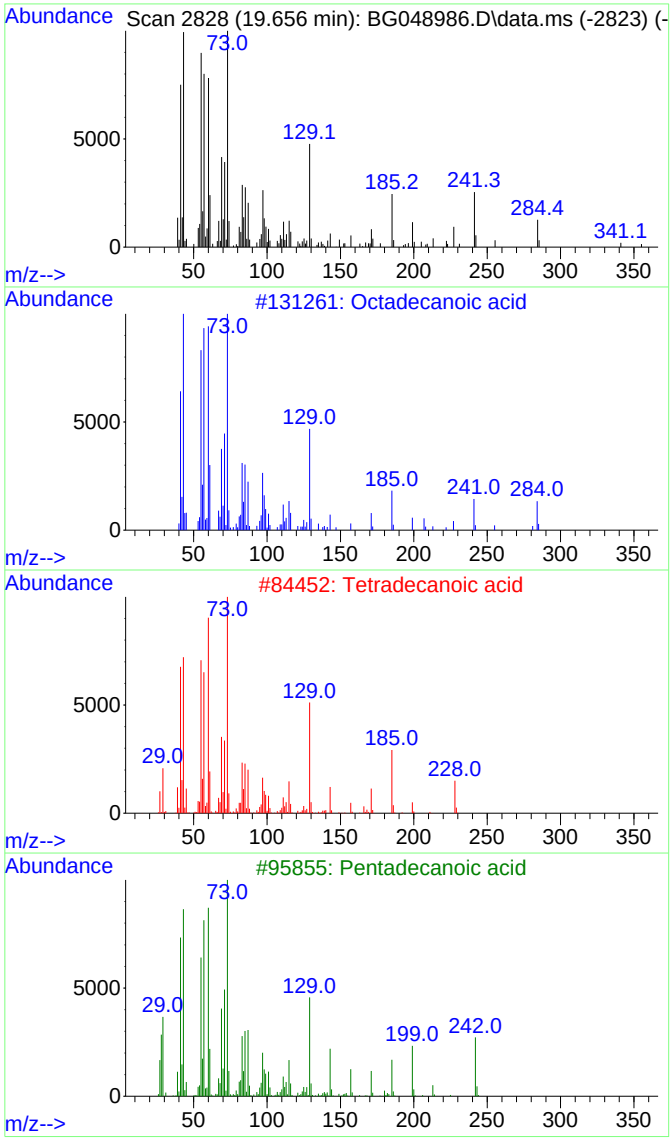
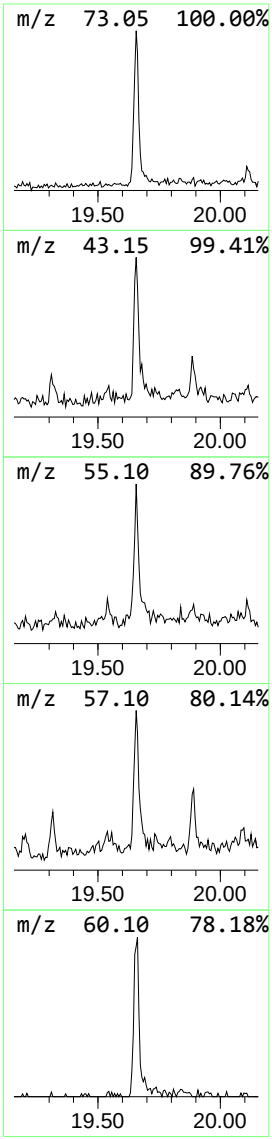
Peak Number 9 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.656	5.63 ng	188139	Chrysene-d12	21.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048986.D
Acq On : 15 Jun 2021 20:45
Operator : CG/JU
Sample : M2672-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(44-48)

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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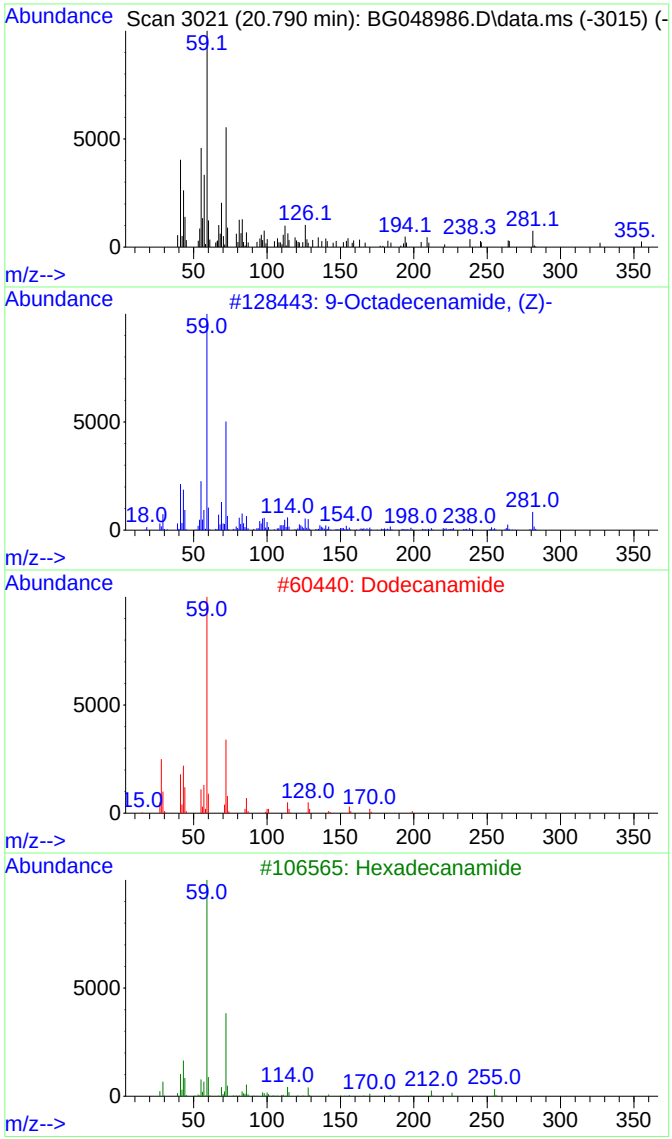
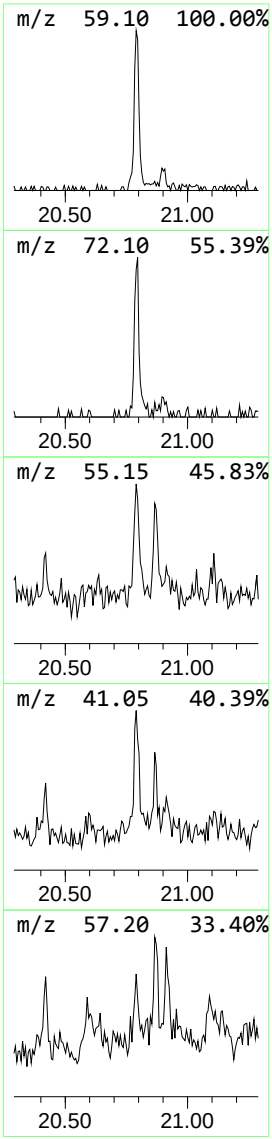
Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.790	2.24 ng	74981	Chrysene-d12	21.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2	Dodecanamide	199	C12H25NO	001120-16-7	64
3	Hexadecanamide	255	C16H33NO	000629-54-9	64
4	Octadecanamide	283	C18H37NO	000124-26-5	64
5	7-Nonenamide	155	C9H17NO	090949-53-4	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048986.D
Acq On : 15 Jun 2021 20:45
Operator : CG/JU
Sample : M2672-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(44-48)

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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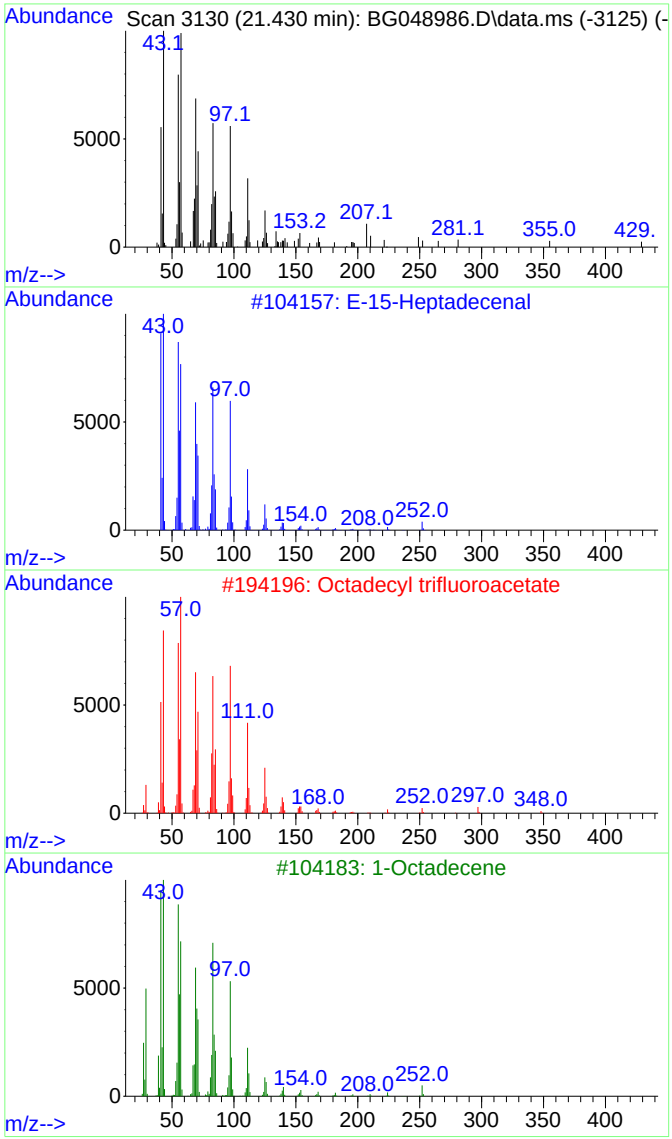
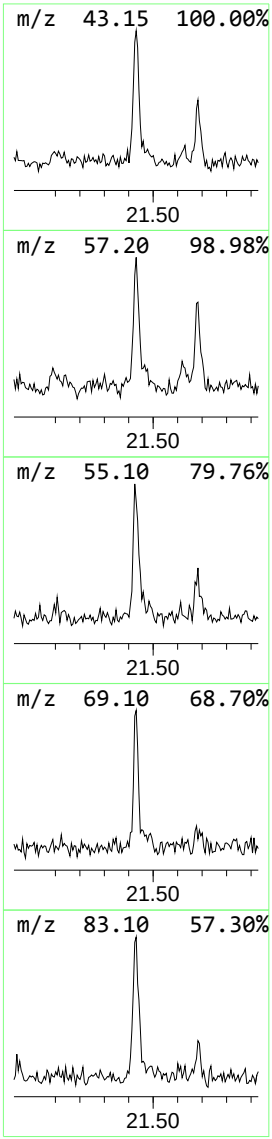
Peak Number 11 E-15-Heptadecenal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.430	3.96 ng	132333	Chrysene-d12	21.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	93
2	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	93
3	1-Octadecene	252	C18H36	000112-88-9	92
4	1-Tricosanol	340	C23H48O	003133-01-5	90
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048986.D
Acq On : 15 Jun 2021 20:45
Operator : CG/JU
Sample : M2672-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(44-48)

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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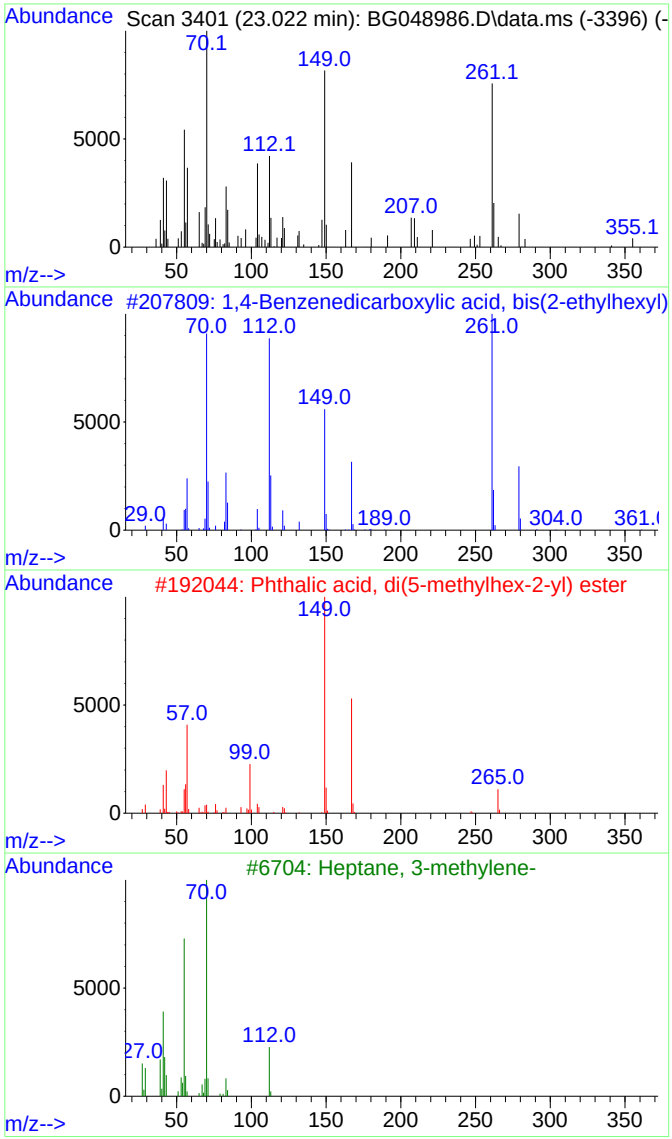
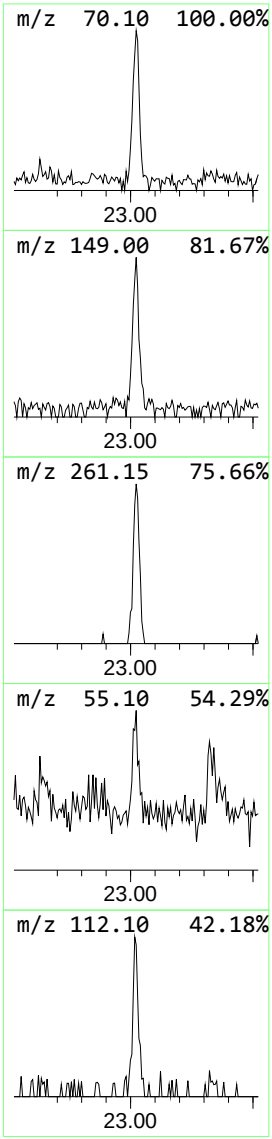
Peak Number 12 unknown23.022 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.022	2.07 ng	69187	Chrysene-d12	21.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	43
2	Phthalic acid, di(5-methylhex-2-...	362	C22H34O4	1000371-09-4	14
3	Heptane, 3-methylene-	112	C8H16	001632-16-2	14
4	2-Octene	112	C8H16	000111-67-1	14
5	Cyclopentane, 1,2,4-trimethyl-, ...	112	C8H16	016883-48-0	14





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048986.D
Acq On : 15 Jun 2021 20:45
Operator : CG/JU
Sample : M2672-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(44-48)

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...	3.157	30.1	ng	302787	1	8.116	201271	20.0
Pantolactone	3.281	10.4	ng	104506	1	8.116	201271	20.0
Benzene, 1,3-di...	5.731	5.9	ng	59506	1	8.116	201271	20.0
Ethanol, 2-[2-(...	10.702	2.5	ng	34434	2	10.937	269574	20.0
1,3,5-Triazine-...	16.154	2.6	ng	71633	4	17.505	551264	20.0
Benzenamine, 2,...	17.623	3.3	ng	90985	4	17.505	551264	20.0
Phenol, 2,3,5-t...	18.163	2.5	ng	68683	4	17.505	551264	20.0
Pentadecanoic acid	18.387	7.6	ng	210494	4	17.505	551264	20.0
Octadecanoic acid	19.656	5.6	ng	188139	5	21.794	668049	20.0
9-Octadecenamid...	20.790	2.2	ng	74981	5	21.794	668049	20.0
E-15-Heptadecenal	21.430	4.0	ng	132333	5	21.794	668049	20.0
unknown23.022	23.022	2.1	ng	69187	5	21.794	668049	20.0