LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048989.D
Acq On : 15 Jun 2021 22:47
Operator : CG/JU
Sample : M2672-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(56-60)

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: BG048989.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	16	21	33	rVB	93286	164578	5.85%	1.219%
2	3.285	37	42	50	rVB2	73783	110559	3.93%	0.819%
3	5.200	362	368	374	rBV	16082	28920	1.03%	0.214%
4	5.664	440	447	455	rBV	686479	1127643	40.10%	8.352%
5	5.735	455	459	471	rVB2	27858	63500	2.26%	0.470%
6	7.268	710	720	728	rBV	711598	1262755	44.90%	9.353%
7	8.114	856	864	871	rBV	111594	201124	7.15%	1.490%
8	9.278	1055	1062	1072	rVB	432741	787144	27.99%	5.830%
9	10.699	1298	1304	1311	rBV2	25402	46557	1.66%	0.345%
10	10.934	1337	1344	1352	rBV	149909	270057	9.60%	2.000%
11	13.379	1752	1760	1768	rBV	1049857	1663729	59.16%	12.323%
12	14.753	1988	1994	2002	rVB	248227	399010	14.19%	2.955%
13	16.152	2228	2232	2238	rVB	66825	88065	3.13%	0.652%
14	16.246	2240	2248	2260	rBV	986888	1579627	56.17%	11.700%
15	17.503	2455	2462	2469	rBV	348580	542047	19.27%	4.015%
16	17.621	2477	2482	2487	rVB3	53821	76743	2.73%	0.568%
17	18.161	2570	2574	2579	rVB4	28250	43401	1.54%	0.321%
18	18.390	2608	2613	2619	rBV	159828	233816	8.31%	1.732%
19	19.313	2766	2770	2778	rBV4	19478	39074	1.39%	0.289%
20	19.654	2824	2828	2836	rBV	141471	178559	6.35%	1.323%
21	20.112	2900	2906	2912	rVB	2161939	2812327	100.00%	20.831%
22	20.793	3015	3022	3031	rBV	82671	124958	4.44%	0.926%
23	20.870	3031	3035	3038	rBV2	37334	46763	1.66%	0.346%
24	21.428	3125	3130	3136	rBV2	98250	156804	5.58%	1.161%
25	21.681	3169	3173	3182	rVB2	67155	108757	3.87%	0.806%
26	21.798	3186	3193	3202	rVV	348043	620590	22.07%	4.597%
27	22.503	3311	3313	3319	rVB7	20311	31063	1.10%	0.230%
28	23.020	3396	3401	3407	rVB5	42563	77865	2.77%	0.577%
29	25.135	3750	3761	3773	rBV2	197081	614782	21.86%	4.554%

Sum of corrected areas: 13500817

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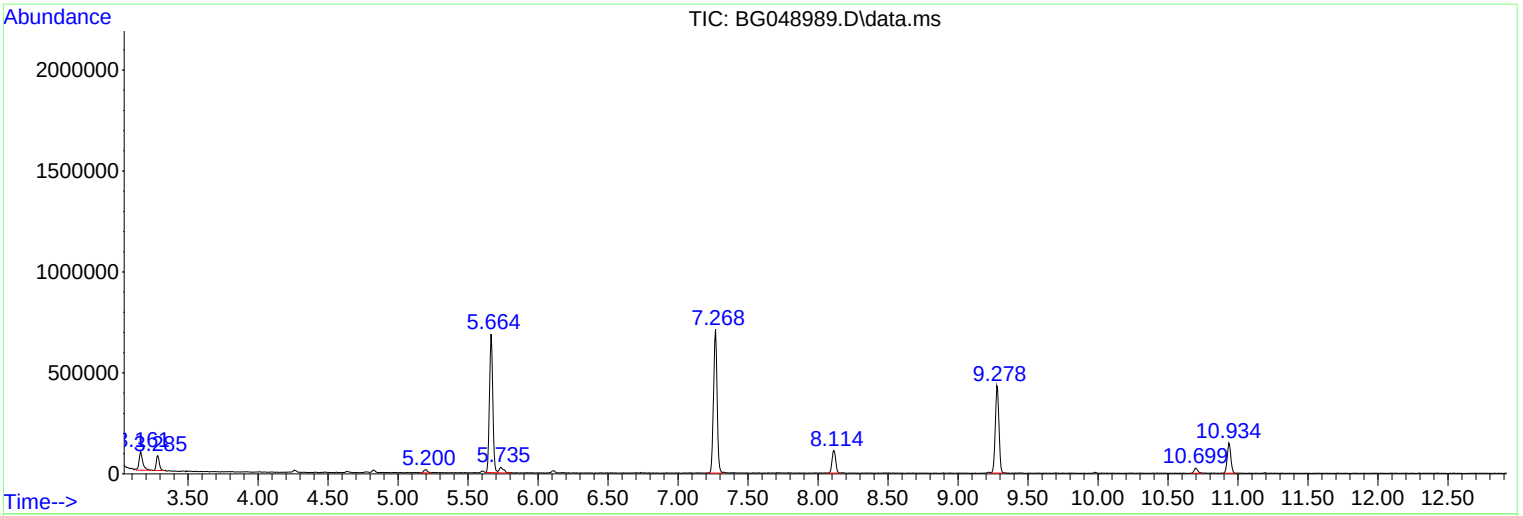
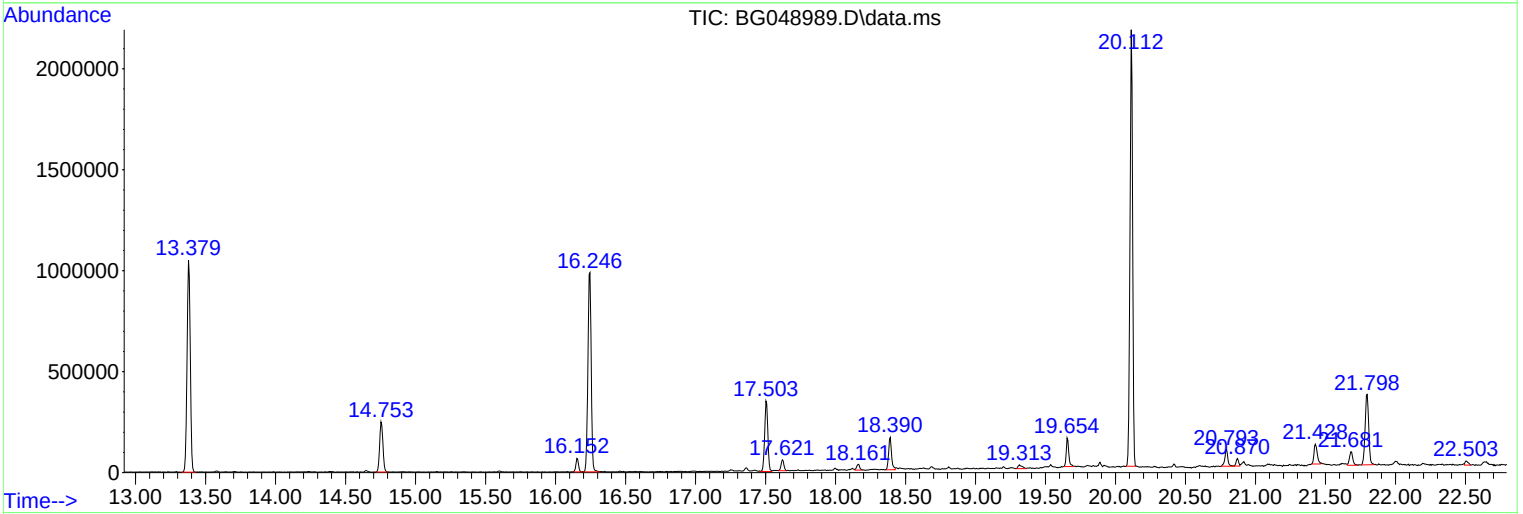
Misc :
ALS Vial : 17 Sample Multiplier: 1

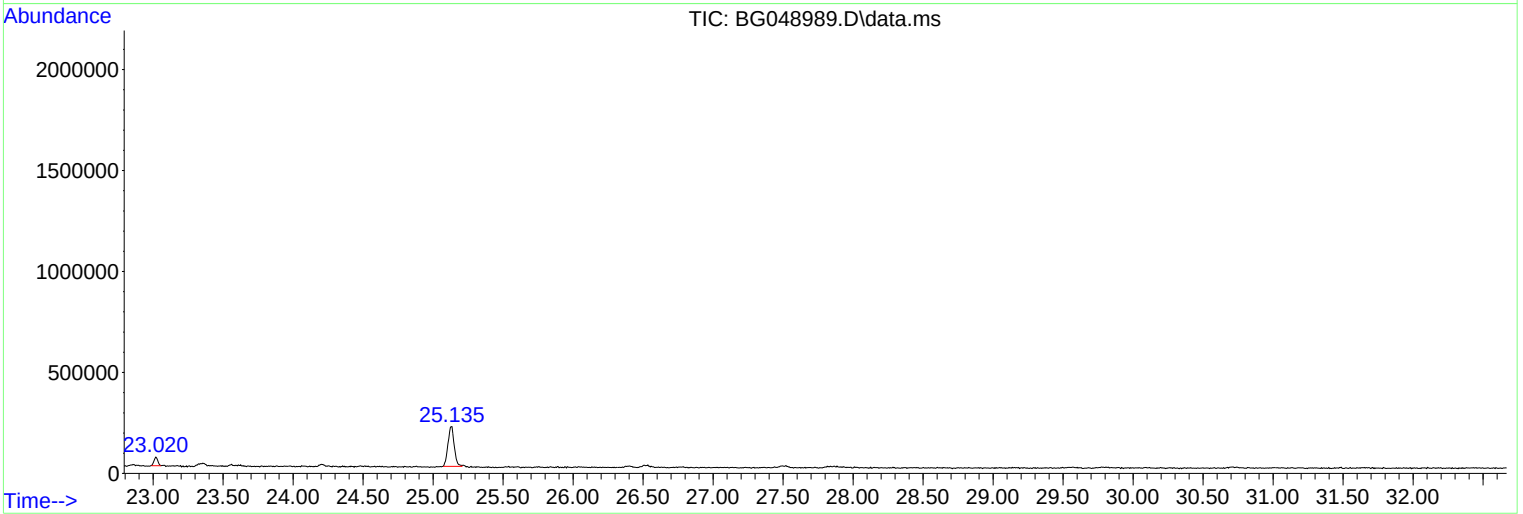
Instrument :
BNA_G
ClientSampleId :
17-B6(56-60)

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 : BG048989.D
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Operator : CG/JU
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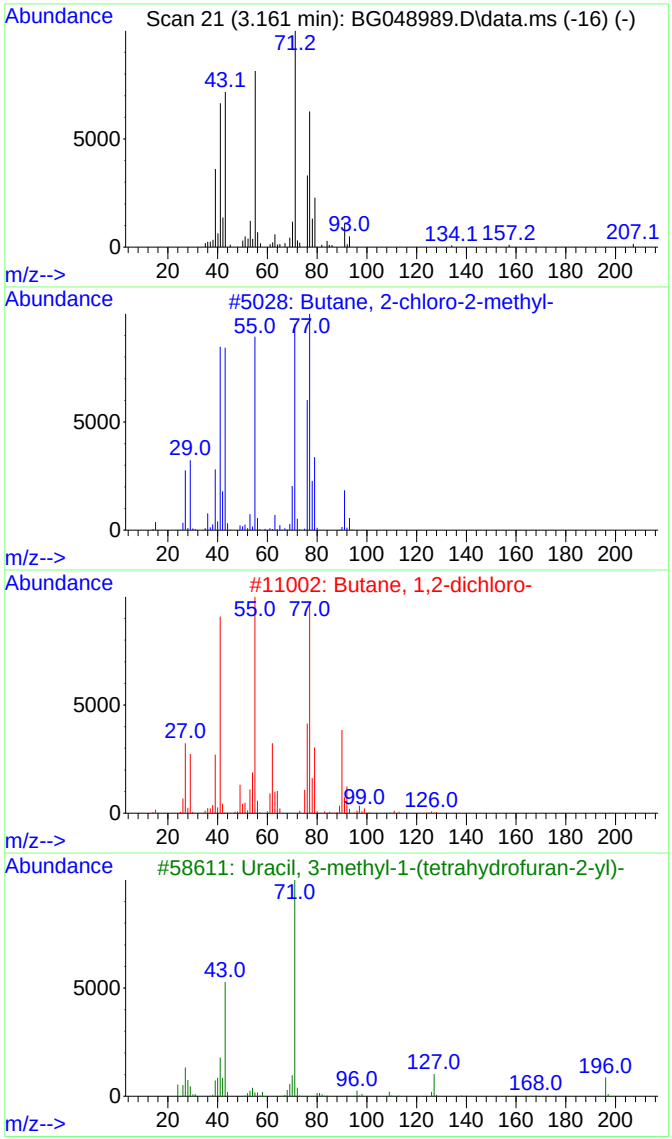
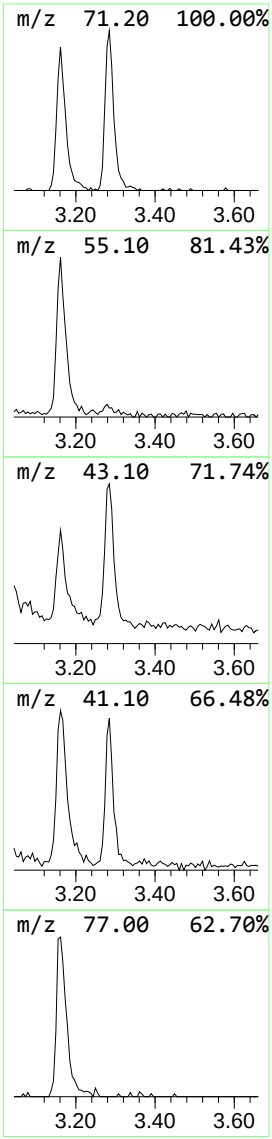
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.161	16.37 ng	164578	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	53
2	Butane, 1,2-dichloro-	126	C4H8Cl2	000616-21-7	17
3	Uracil, 3-methyl-1-(tetrahydrofu...	196	C9H12N2O3	1000151-99-4	16
4	2-Butene, 1-methoxy-, (Z)-	86	C5H10O	010034-16-9	16
5	Butanoyl chloride	106	C4H7ClO	000141-75-3	16





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Data File : BG048989.D
Acq On : 15 Jun 2021 22:47
Operator : CG/JU
Sample : M2672-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(56-60)

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

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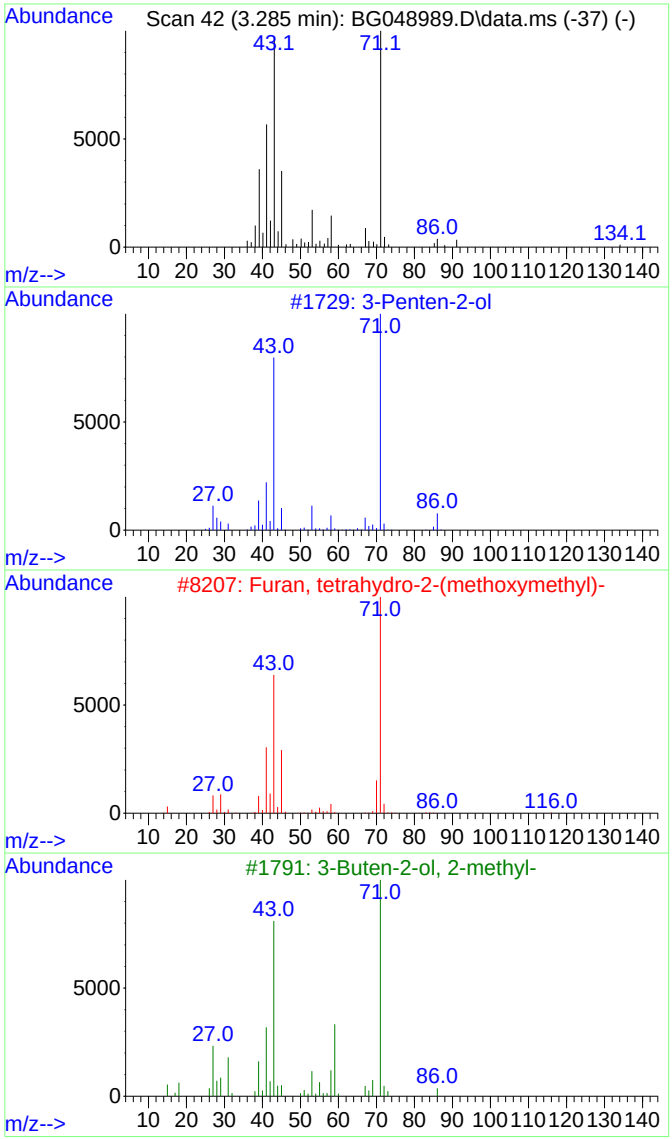
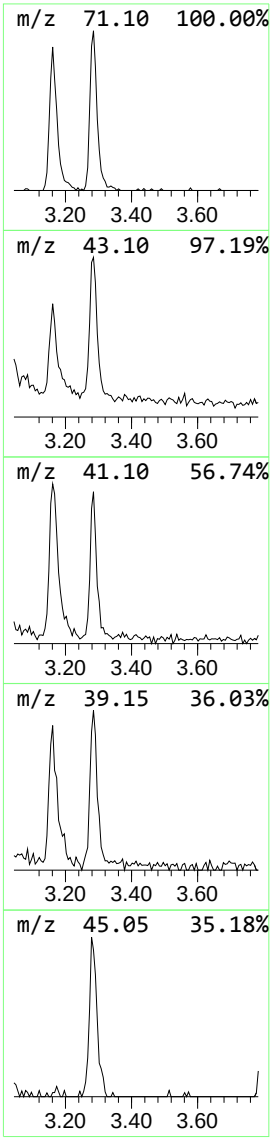
****

Peak Number 2 3-Penten-2-ol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.285	10.99 ng	110559	1,4-Dichlorobenzene-d4	8.114

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-ol	86	C5H10O	001569-50-2	72
2	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	72
3	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	64
4	Pentane, 2,2'-oxybis-	158	C10H22O	056762-00-6	50
5	Butanoyl chloride	106	C4H7ClO	000141-75-3	50





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Acq On : 15 Jun 2021 22:47
Operator : CG/JU
Sample : M2672-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(56-60)

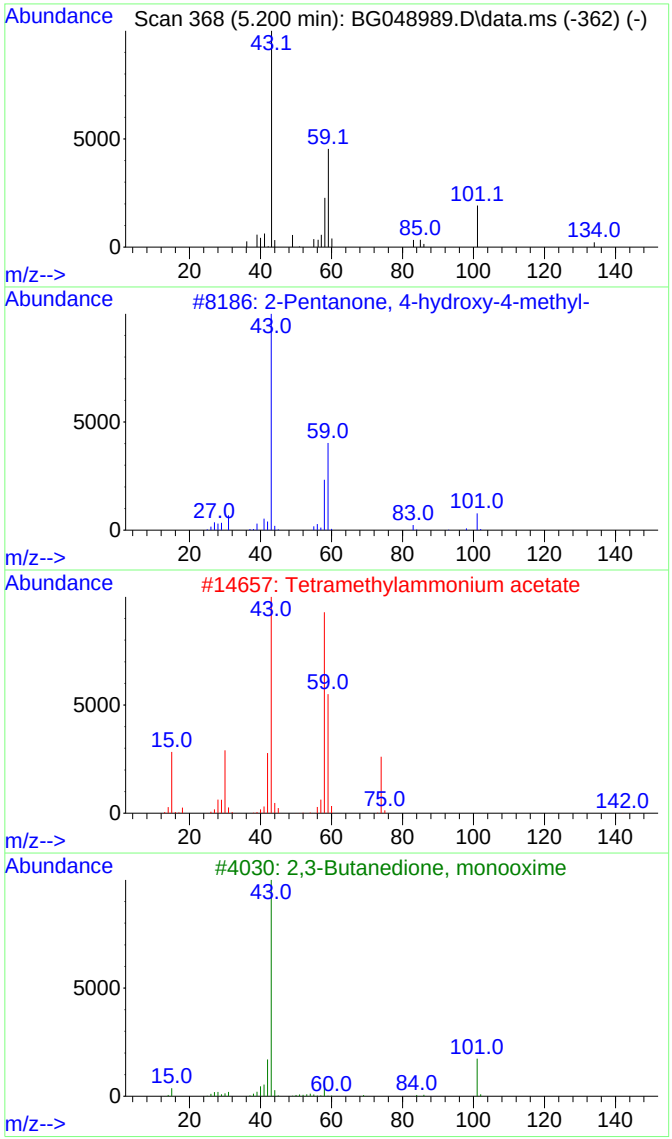
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

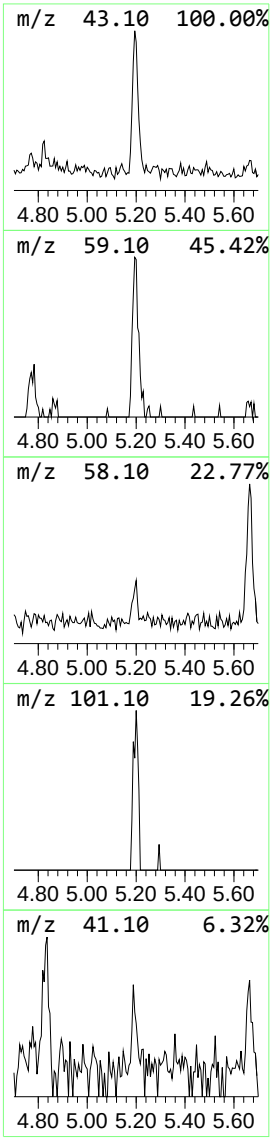
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.200	2.88 ng	28920	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	64
2	Tetramethylammonium acetate	133	C6H15NO2	010581-12-1	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	(2,3,3-Trimethyloxiranyl)methanol	116	C6H12O2	1000306-64-7	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
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Acq On : 15 Jun 2021 22:47
Operator : CG/JU
Sample : M2672-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(56-60)

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

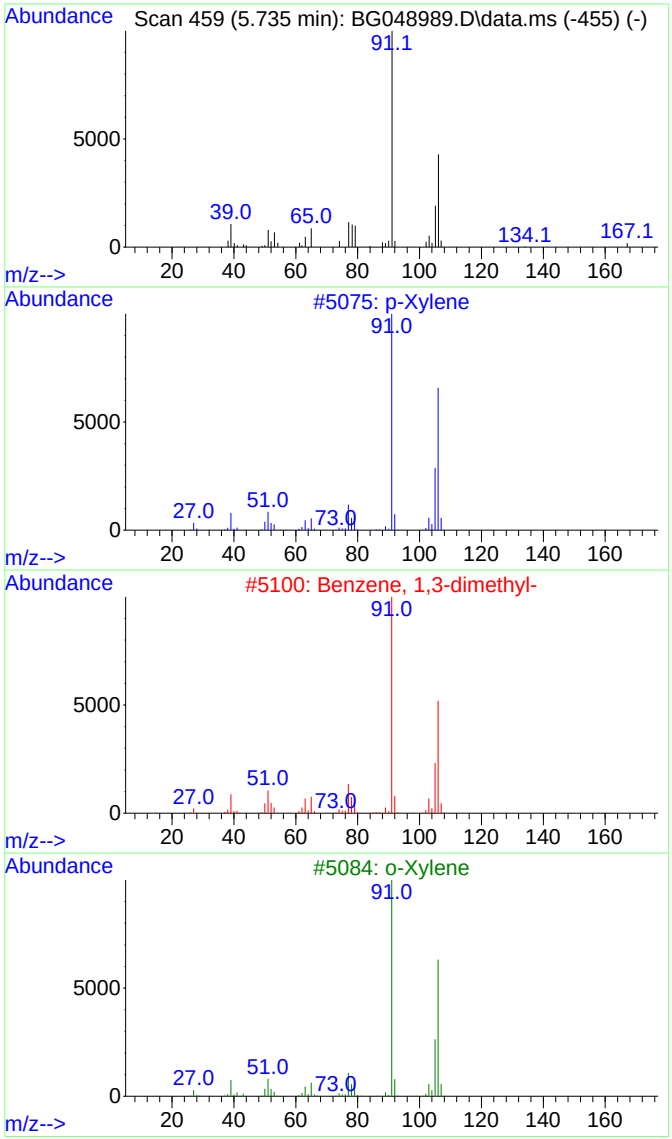
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

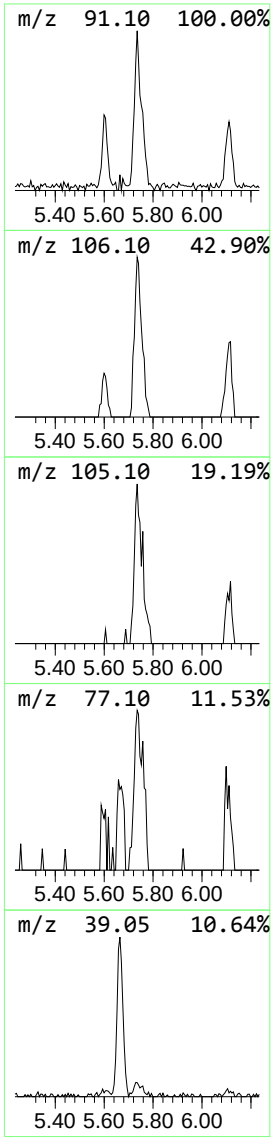
****

Peak Number 4 p-Xylene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.735	6.31 ng	63500	1,4-Dichlorobenzene-d4	8.114

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Xylene	106	C8H10	000106-42-3	91
2	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	91
3	o-Xylene	106	C8H10	000095-47-6	91
4	1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	91
5	Ethylbenzene	106	C8H10	000100-41-4	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048989.D
Acq On : 15 Jun 2021 22:47
Operator : CG/JU
Sample : M2672-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(56-60)

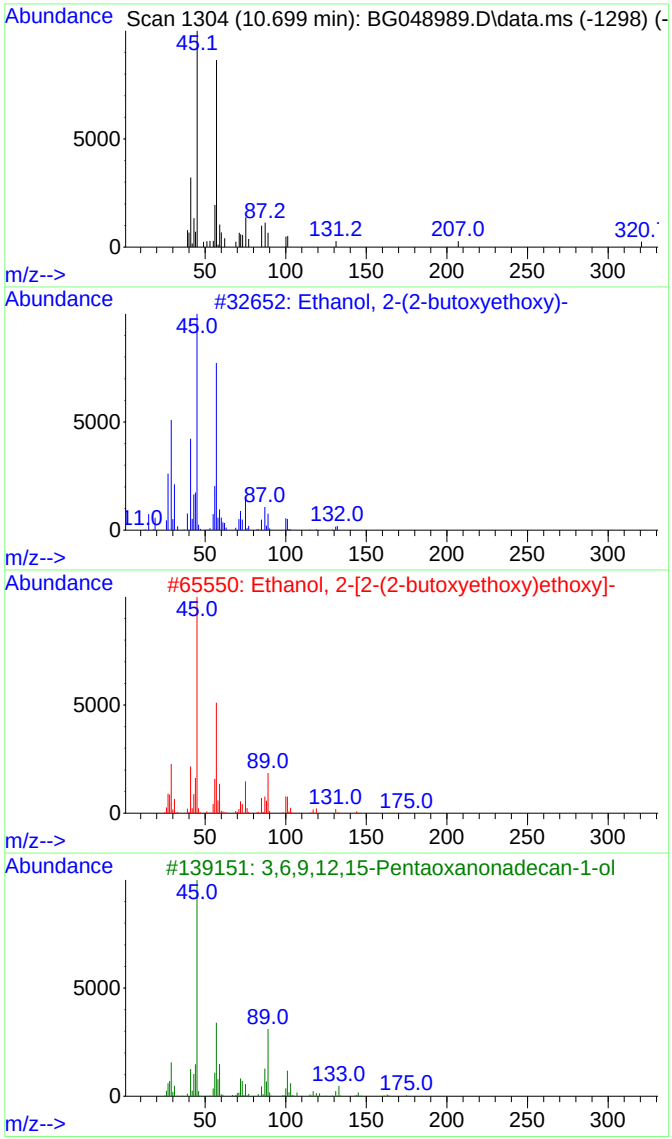
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

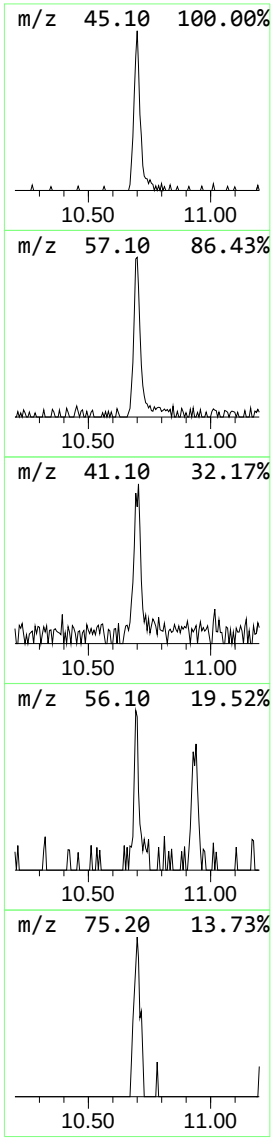
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.699	3.45 ng	46557	Naphthalene-d8	10.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	45
3	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	40
4	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	38
5	Heptaethylene glycol	326	C14H30O8	005617-32-3	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048989.D
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Sample : M2672-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(56-60)

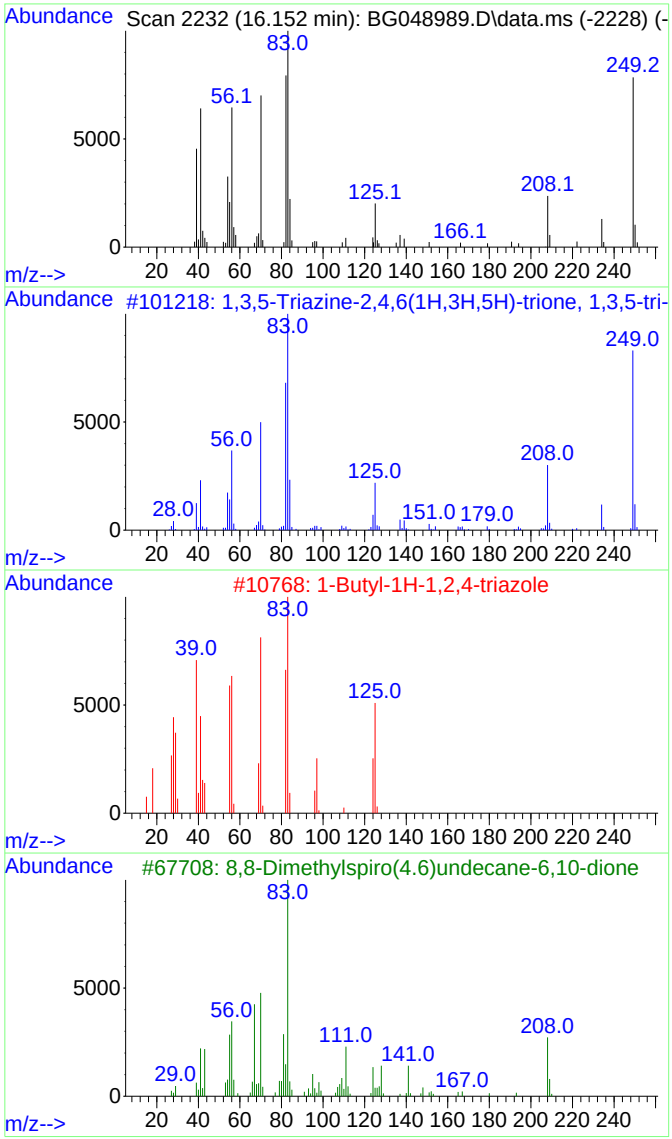
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

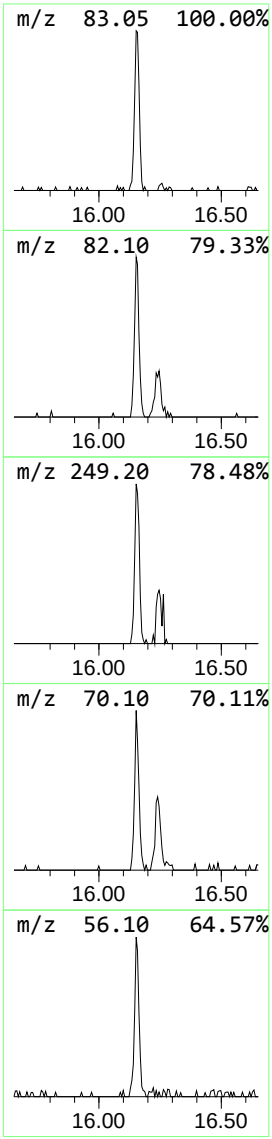
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1,3,5-Triazine-2,4,6(1H,3H,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.152	3.25 ng	88065	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	98
2	1-Butyl-1H-1,2,4-triazole	125	C6H11N3	006086-22-2	40
3	8,8-Dimethylspiro(4.6)undecane-6...	208	C13H20O2	068181-81-7	25
4	Cyclohexane, 1,1'-(1,3-propanedi...	208	C15H28	003178-24-3	25
5	16-Octadecenal	266	C18H34O	056554-87-1	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
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Acq On : 15 Jun 2021 22:47
Operator : CG/JU
Sample : M2672-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(56-60)

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

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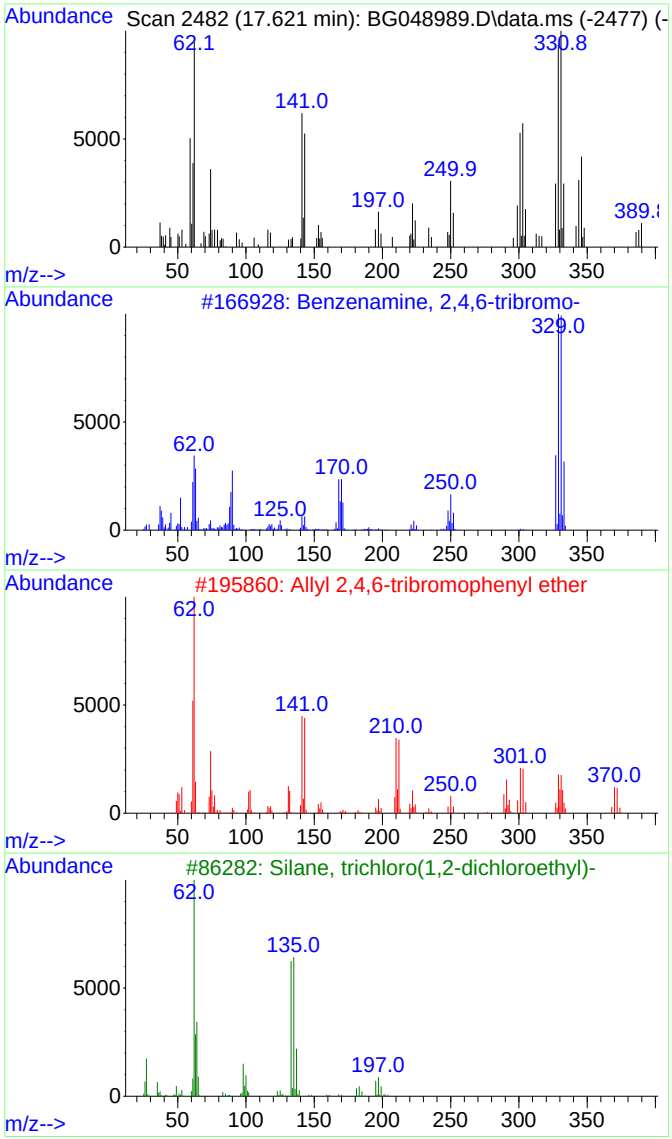
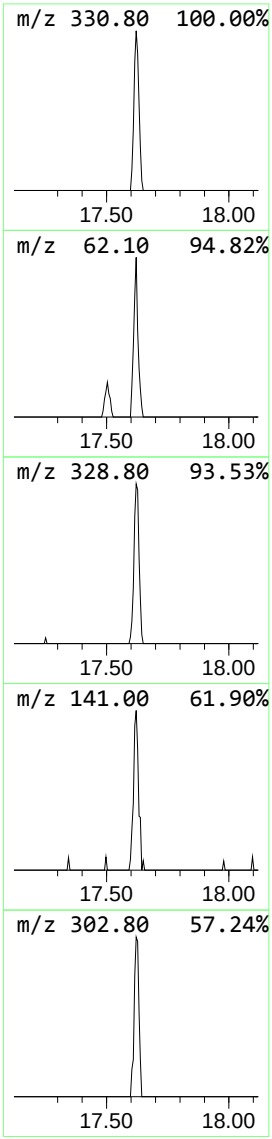
****

Peak Number 7 Benzenamine, 2,4,6-tribromo- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.621	2.83 ng	76743	Phenanthrene-d10	17.503

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	25
3	Silane, trichloro(1,2-dichloroet...	230	C2H3Cl5Si	000684-00-4	17
4	Tetrachlorvinphos	364	C10H9Cl4O4P	022248-79-9	10
5	Estra-1,3,5(10)-trien-17-one, 2-...	329	C20H27NO3	074299-30-2	9





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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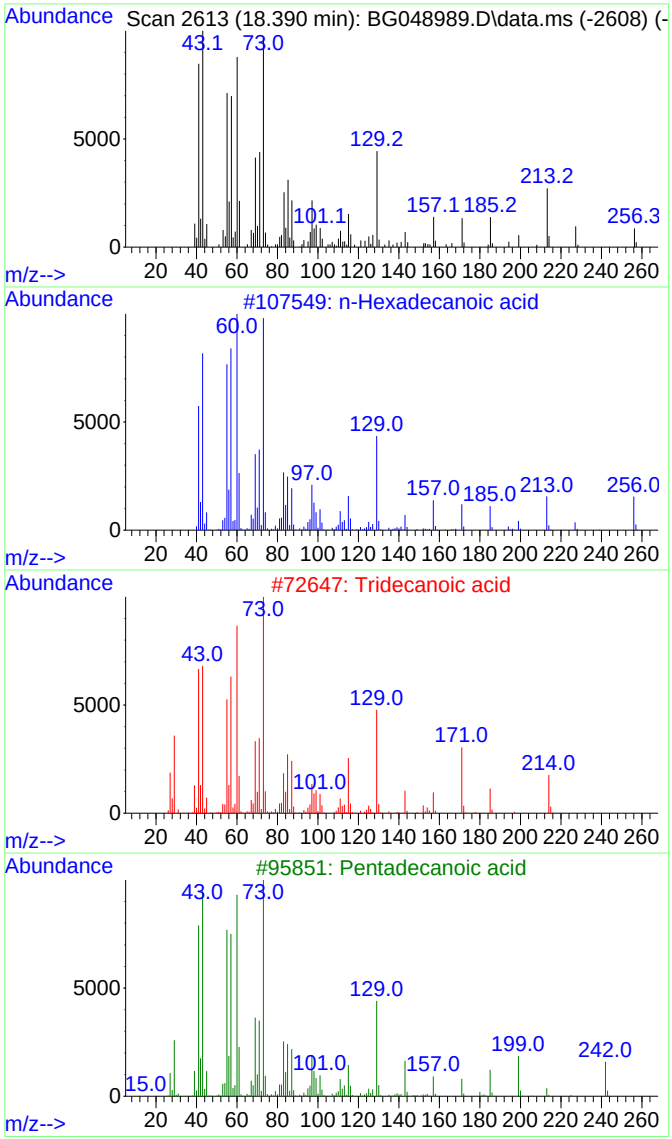
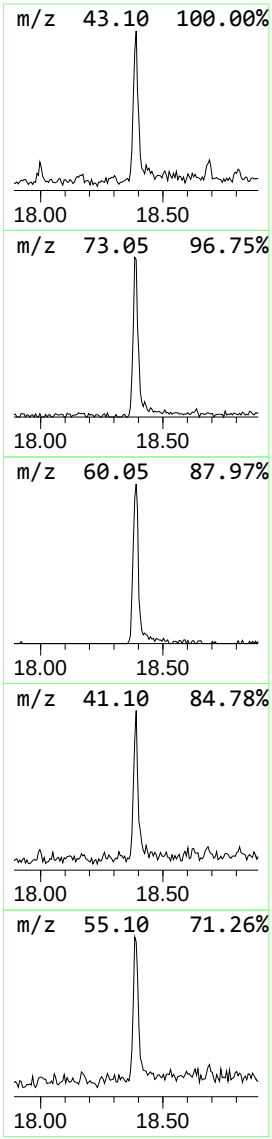
Peak Number 8 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.390	8.63 ng	233816	Phenanthrene-d10	17.503

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048989.D
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Operator : CG/JU
Sample : M2672-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(56-60)

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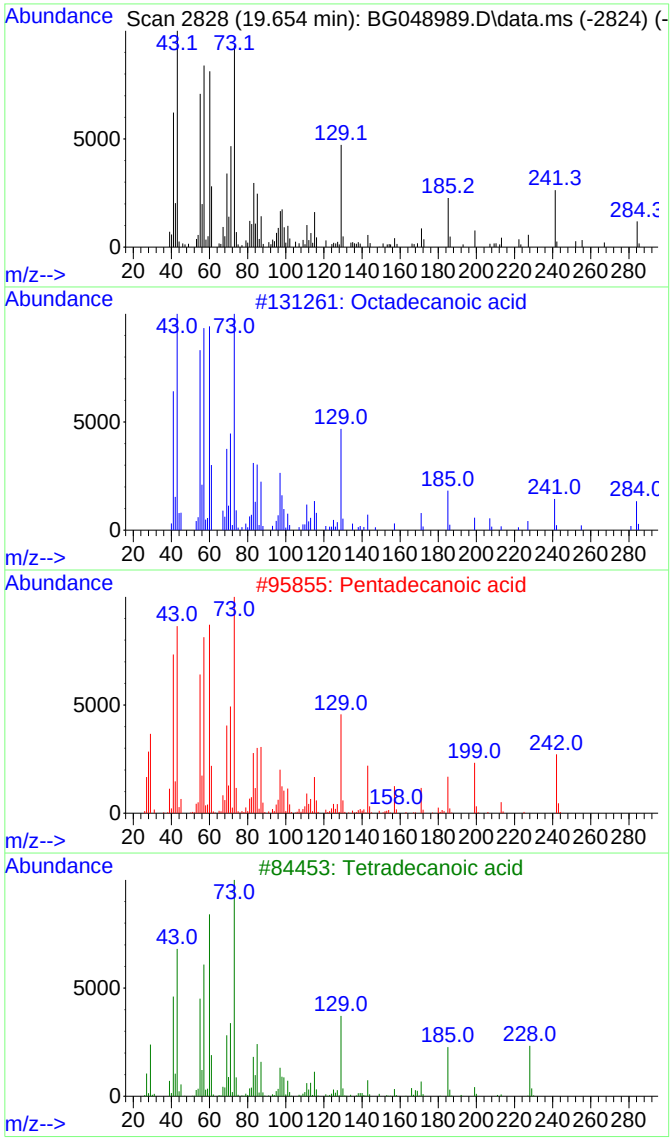
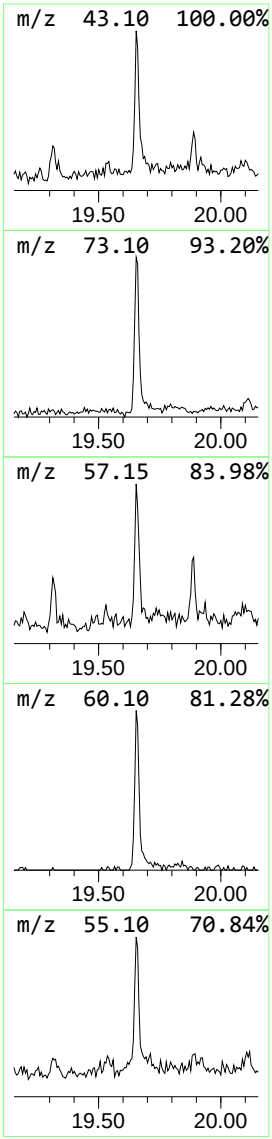
****

Peak Number 9 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.654	5.75 ng	178559	Chrysene-d12	21.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	n-Decanoic acid	172	C10H20O2	000334-48-5	53
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	52





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Data File : BG048989.D
Acq On : 15 Jun 2021 22:47
Operator : CG/JU
Sample : M2672-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(56-60)

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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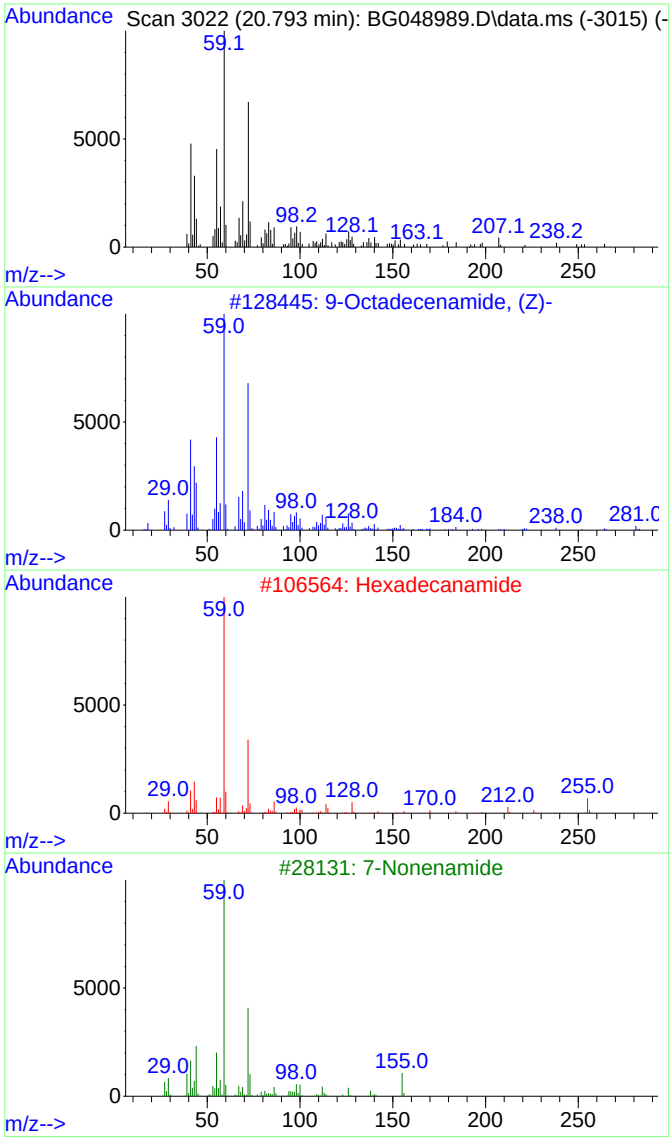
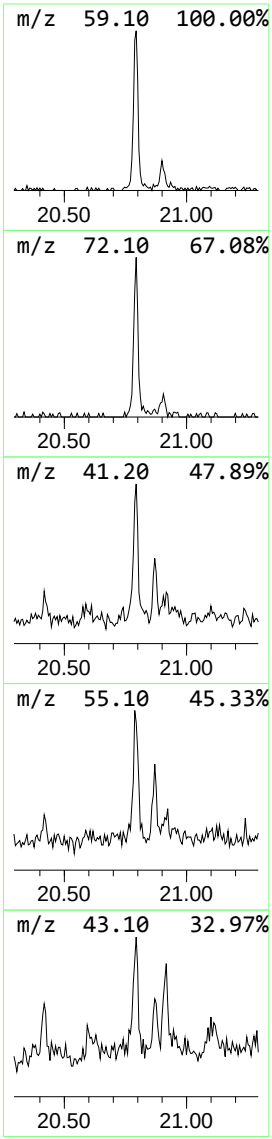
Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.794	4.03 ng	124958	Chrysene-d12	21.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2	Hexadecanamide	255	C16H33NO	000629-54-9	72
3	7-Nonenamide	155	C9H17NO	090949-53-4	72
4	Tetradecanamide	227	C14H29NO	000638-58-4	64
5	Dodecanamide	199	C12H25NO	001120-16-7	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048989.D
Acq On : 15 Jun 2021 22:47
Operator : CG/JU
Sample : M2672-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(56-60)

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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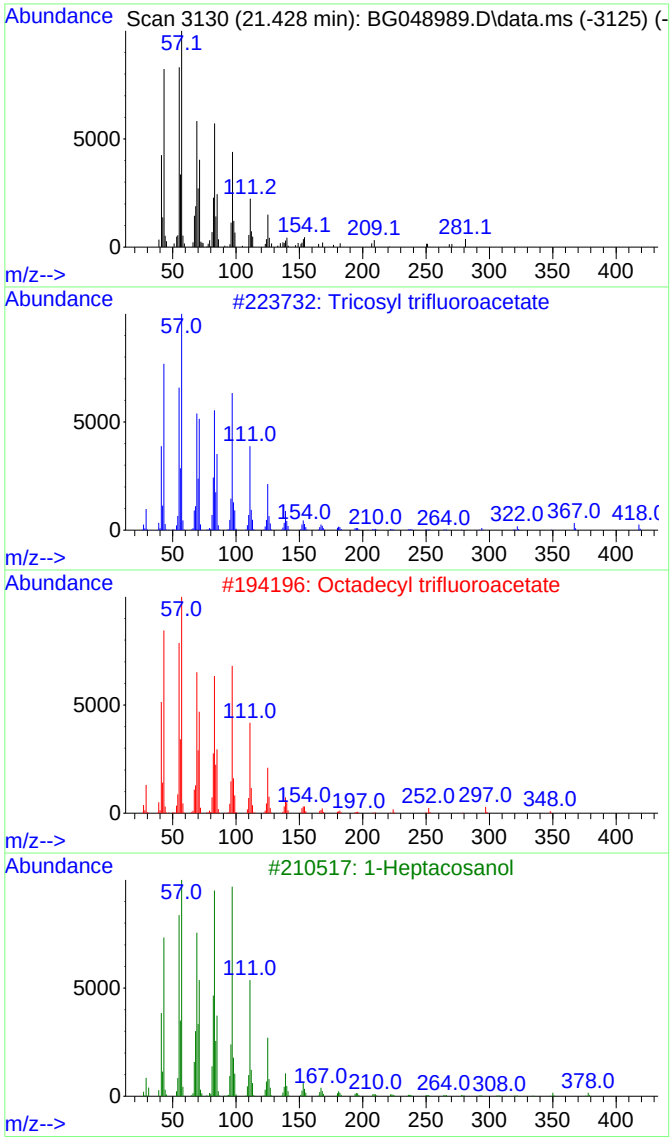
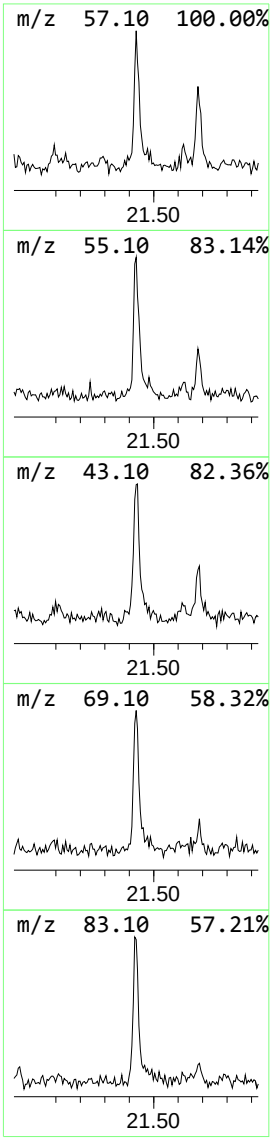
Peak Number 11 Tricosyl trifluoroacetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.428	5.05 ng	156804	Chrysene-d12	21.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
2	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
3	1-Heptacosanol	396	C27H56O	002004-39-9	91
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048989.D
Acq On : 15 Jun 2021 22:47
Operator : CG/JU
Sample : M2672-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(56-60)

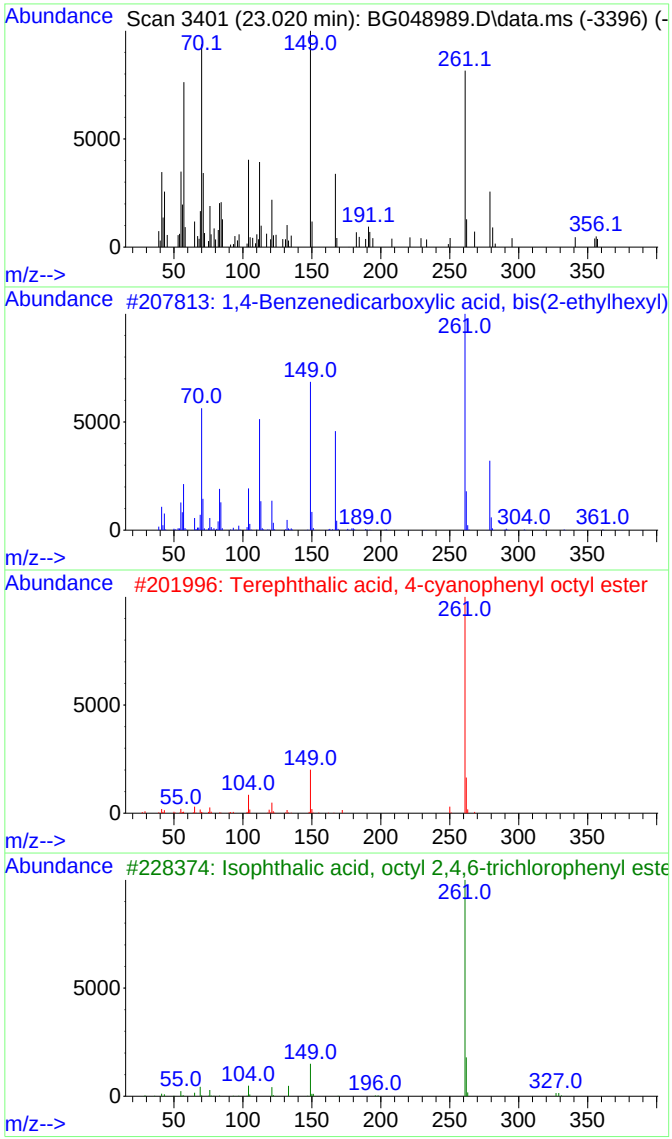
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

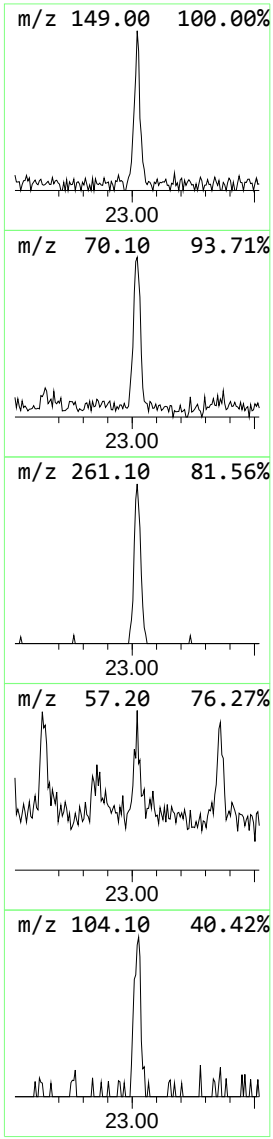
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 1,4-Benzenedicarboxylic aci... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.020	2.51 ng	77865	Chrysene-d12	21.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	52
2	Terephthalic acid, 4-cyanophenyl...	379	C23H25NO4	1000323-66-6	38
3	Isophthalic acid, octyl 2,4,6-tr...	456	C22H23Cl3O4	1000344-57-2	38
4	Phthalic acid, 3,5-difluoropheny...	348	C19H18F2O4	1000315-54-1	35
5	Isophthalic acid, 2,4-dichloroph...	422	C22H24Cl2O4	1000344-41-2	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048989.D
Acq On : 15 Jun 2021 22:47
Operator : CG/JU
Sample : M2672-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(56-60)

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	16.4	ng	164578	1	8.114	201124	20.0
3-Penten-2-ol	3.285	11.0	ng	110559	1	8.114	201124	20.0
2-Pentanone, 4-...	5.200	2.9	ng	28920	1	8.114	201124	20.0
p-Xylene	5.735	6.3	ng	63500	1	8.114	201124	20.0
Ethanol, 2-(2-b...	10.699	3.5	ng	46557	2	10.934	270057	20.0
1,3,5-Triazine-...	16.152	3.3	ng	88065	4	17.503	542047	20.0
Benzenamine, 2,...	17.621	2.8	ng	76743	4	17.503	542047	20.0
n-Hexadecanoic ...	18.390	8.6	ng	233816	4	17.503	542047	20.0
Octadecanoic acid	19.654	5.8	ng	178559	5	21.798	620590	20.0
9-Octadecenamid...	20.794	4.0	ng	124958	5	21.798	620590	20.0
Tricosyl triflu...	21.428	5.0	ng	156804	5	21.798	620590	20.0
1,4-Benzenedica...	23.020	2.5	ng	77865	5	21.798	620590	20.0