LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048947.D
Acq On : 14 Jun 2021 13:21
Operator : CG/JU
Sample : M2678-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0231-COMPOSITE-H

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: BG048947.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.167	17	22	31	rVB	211875	336397	12.72%	2.446%
2	3.291	37	43	52	rVB	88679	134815	5.10%	0.980%
3	5.200	361	368	376	rBV2	71692	115664	4.37%	0.841%
4	5.664	441	447	456	rVV	744582	1213297	45.87%	8.822%
5	5.741	456	460	468	rVB2	26356	58050	2.19%	0.422%
6	7.262	711	719	729	rBV	781576	1387351	52.45%	10.088%
7	8.120	857	865	872	rBV	134593	241729	9.14%	1.758%
8	9.284	1056	1063	1074	rVB	472903	865761	32.73%	6.295%
9	10.705	1299	1305	1312	rBV2	68769	120480	4.55%	0.876%
10	10.941	1338	1345	1355	rVB	184808	337690	12.77%	2.455%
11	13.385	1754	1761	1768	rVB	1111544	1739000	65.74%	12.644%
12	14.760	1985	1995	2003	rBV	290827	486977	18.41%	3.541%
13	16.164	2228	2234	2240	rBV2	61095	87946	3.32%	0.639%
14	16.246	2241	2248	2263	rVB	909717	1416280	53.54%	10.298%
15	17.509	2457	2463	2470	rBV	397028	604577	22.86%	4.396%
16	17.627	2478	2483	2488	rVB2	60073	90598	3.43%	0.659%
17	18.167	2570	2575	2579	rVB2	47022	65516	2.48%	0.476%
18	18.391	2608	2613	2620	rBV3	41566	64708	2.45%	0.470%
19	19.319	2768	2771	2777	rBV4	15875	30142	1.14%	0.219%
20	19.660	2826	2829	2833	rBV6	19888	30785	1.16%	0.224%
21	20.118	2901	2907	2913	rVB	1959293	2645090	100.00%	19.233%
22	20.876	3032	3036	3042	rBV3	36358	48108	1.82%	0.350%
23	21.440	3127	3132	3137	rBV3	59747	107134	4.05%	0.779%
24	21.693	3171	3175	3185	rVB	68857	111771	4.23%	0.813%
25	21.804	3185	3194	3202	rBV	381223	682234	25.79%	4.961%
26	23.032	3398	3403	3412	rVB4	38836	73514	2.78%	0.535%
27	25.142	3751	3762	3772	rBV2	216130	657494	24.86%	4.781%

Sum of corrected areas: 13753108

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
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Acq On : 14 Jun 2021 13:21
Operator : CG/JU
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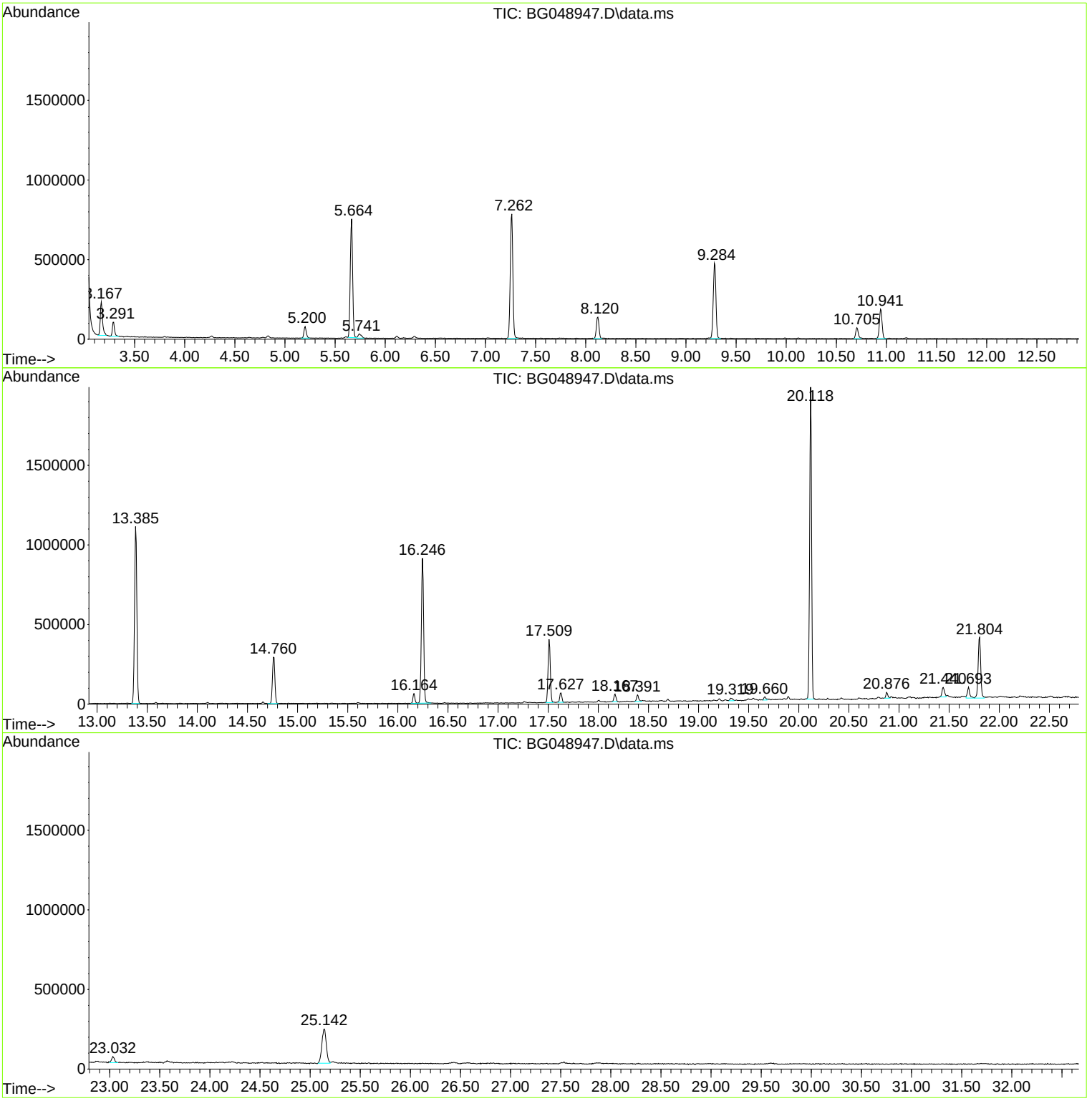
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0231-COMPOSITE-H

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048947.D
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Operator : CG/JU
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ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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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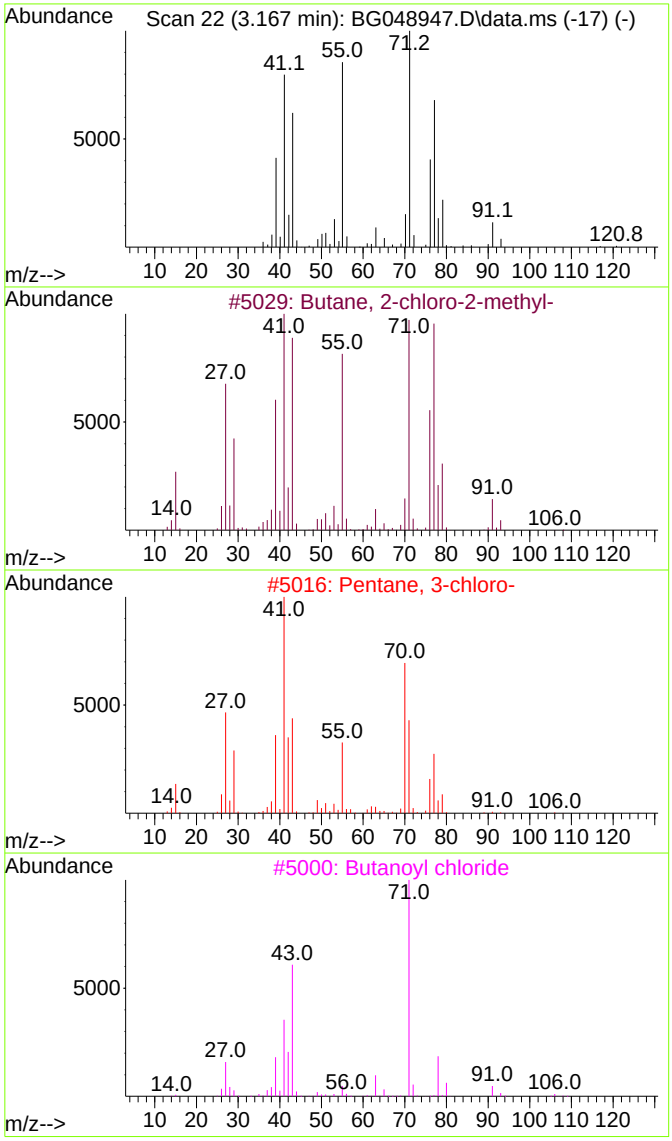
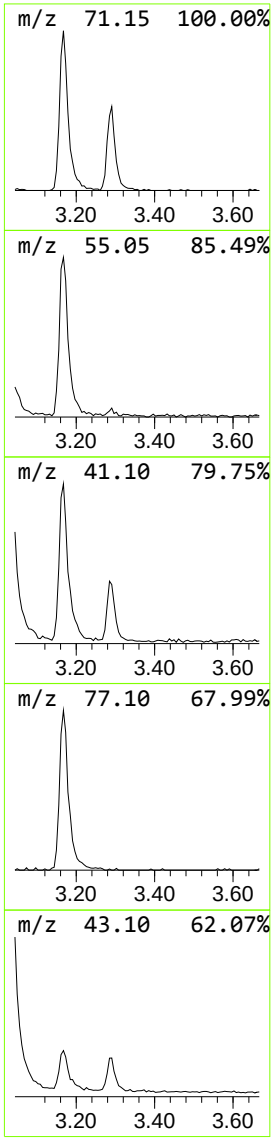
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.167	27.83 ng	336397	1,4-Dichlorobenzene-d4	8.120

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-chloro-2-methyl-	106	C5H11Cl	000594-36-5	72
2	Pentane, 3-chloro-	106	C5H11Cl	000616-20-6	53
3	Butanoyl chloride	106	C4H7ClO	000141-75-3	27
4	2-Penten-1-ol, 2-methyl-, (E)-	100	C6H12O	016958-19-3	25
5	2-Butene, 1-methoxy-, (Z)-	86	C5H10O	010034-16-9	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048947.D
Acq On : 14 Jun 2021 13:21
Operator : CG/JU
Sample : M2678-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0231-COMPOSITE-H

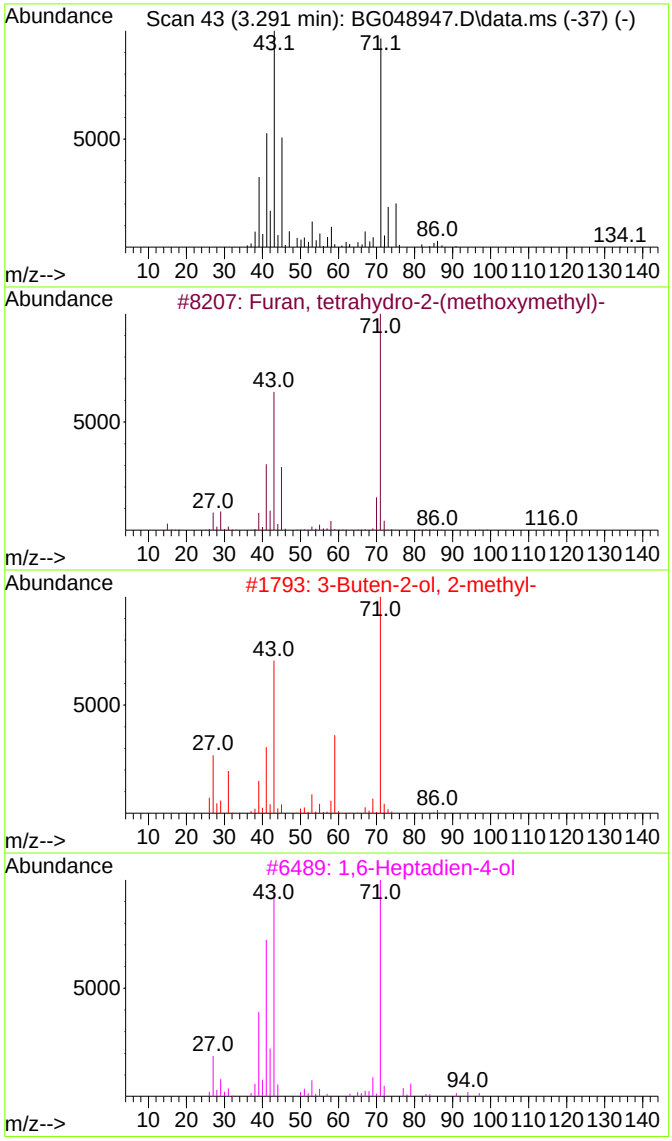
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

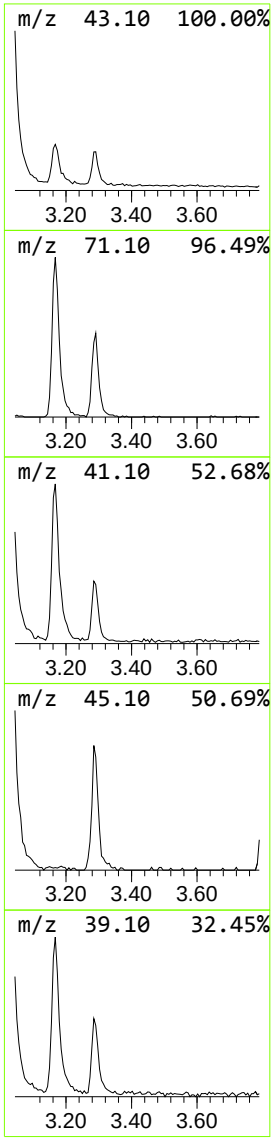
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.291	11.15 ng	134815	1,4-Dichlorobenzene-d4	8.120

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	64
2	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	43
3	1,6-Heptadien-4-ol	112	C7H12O	002883-45-6	38
4	Butane, 2-bromo-2-methyl-	150	C5H11Br	000507-36-8	38
5	3-Penten-2-ol	86	C5H10O	001569-50-2	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048947.D
Acq On : 14 Jun 2021 13:21
Operator : CG/JU
Sample : M2678-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0231-COMPOSITE-H

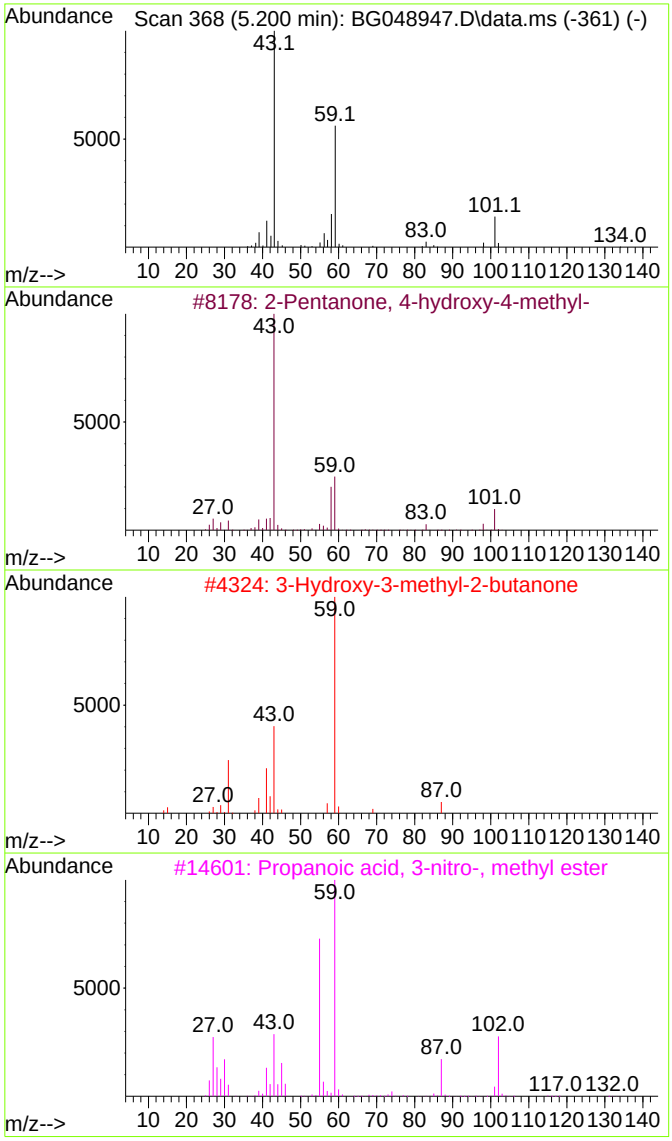
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

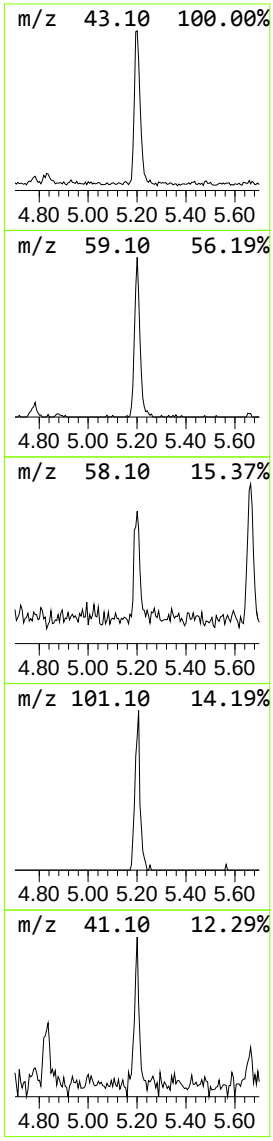
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.200	9.57 ng	115664	1,4-Dichlorobenzene-d4	8.120

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23
3	Propanoic acid, 3-nitro-, methyl...	133	C4H7NO4	020497-95-4	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048947.D
Acq On : 14 Jun 2021 13:21
Operator : CG/JU
Sample : M2678-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0231-COMPOSITE-H

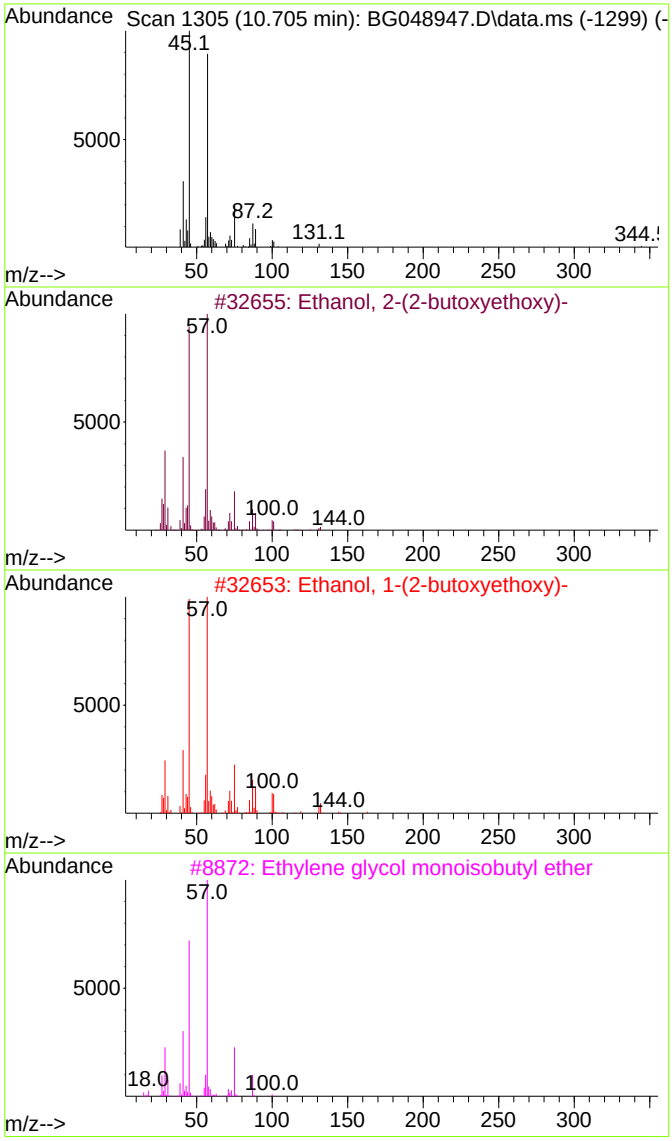
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

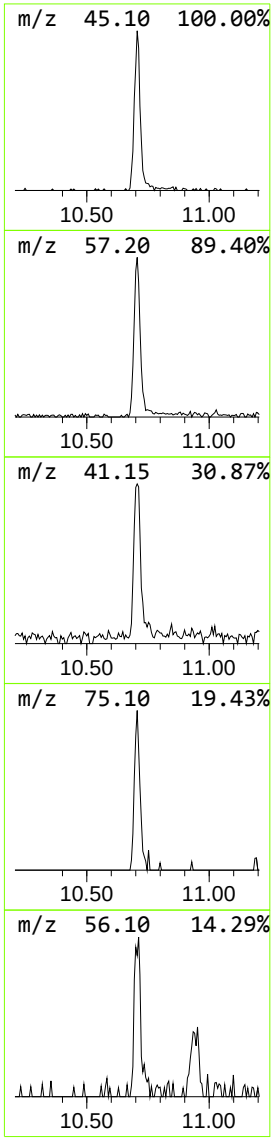
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.706	7.14 ng	120480	Naphthalene-d8	10.941

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	78
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	72
4	Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	47
5	1-Butene, 4-methoxy	86	C5H10O	004696-30-4	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048947.D
Acq On : 14 Jun 2021 13:21
Operator : CG/JU
Sample : M2678-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0231-COMPOSITE-H

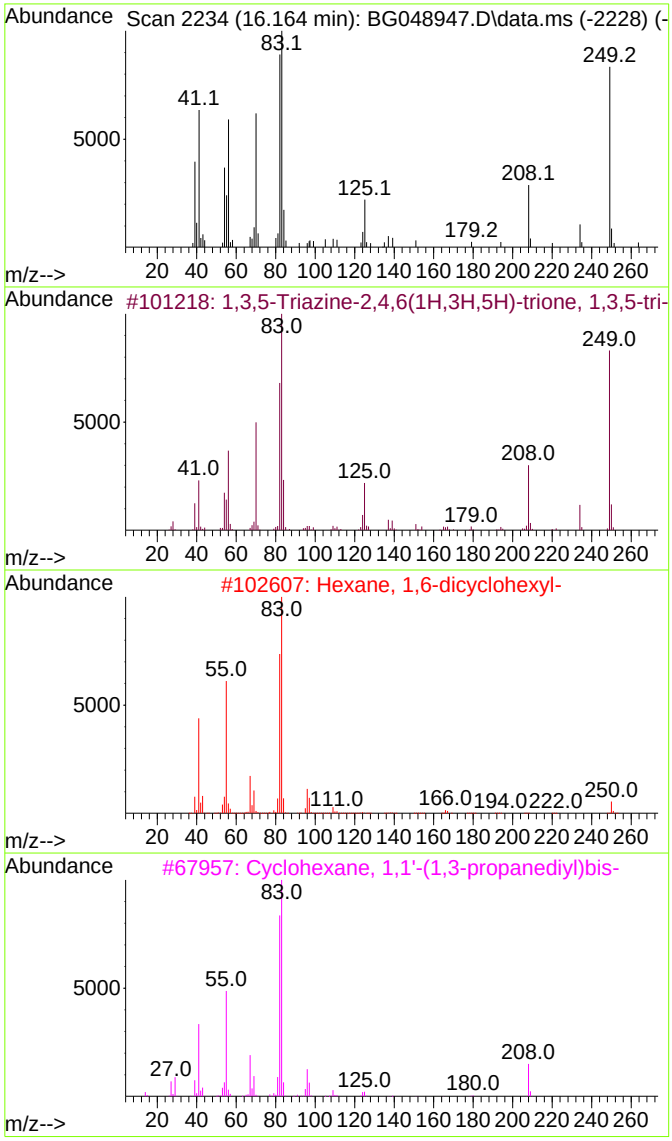
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

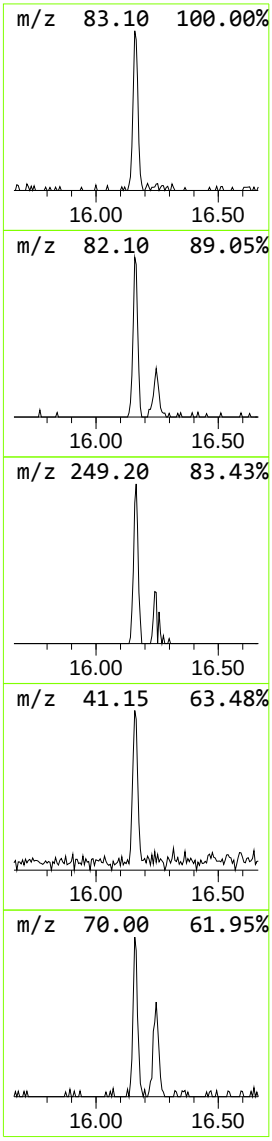
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.164	2.91 ng	87946	Phenanthrene-d10	17.509

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	95
2	Hexane, 1,6-dicyclohexyl-	250	C18H34	001610-23-7	38
3	Cyclohexane, 1,1'-(1,3-propanedi...	208	C15H28	003178-24-3	35
4	Cyclohexane, decyl-	224	C16H32	001795-16-0	35
5	Cyclohexane, octyl-	196	C14H28	001795-15-9	35





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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0231-COMPOSITE-H

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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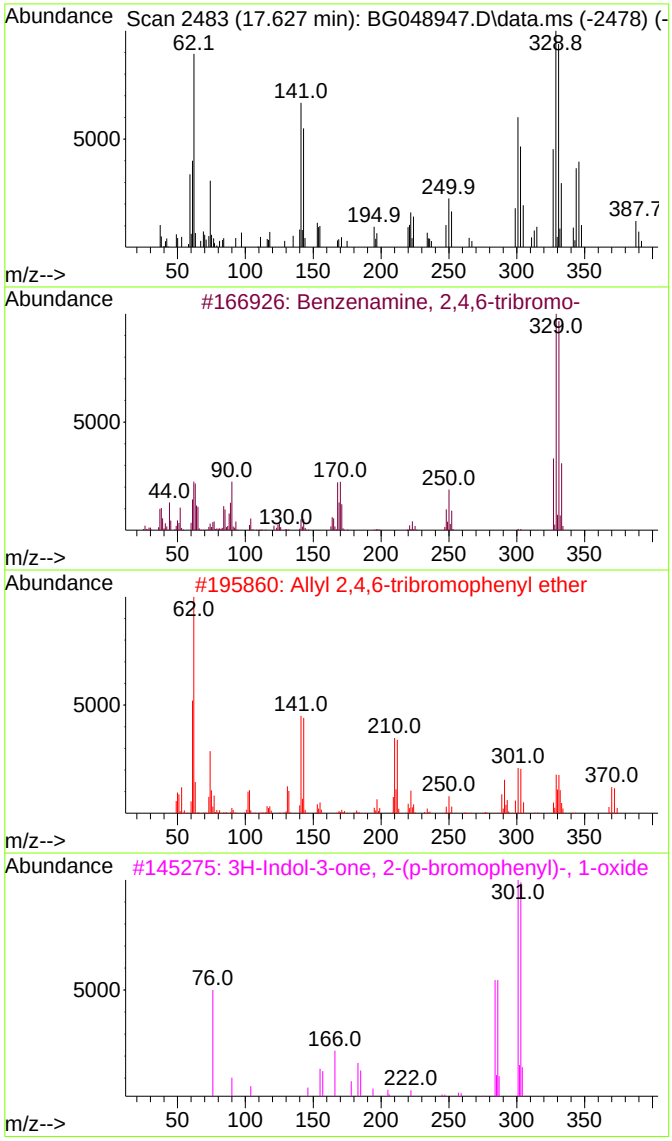
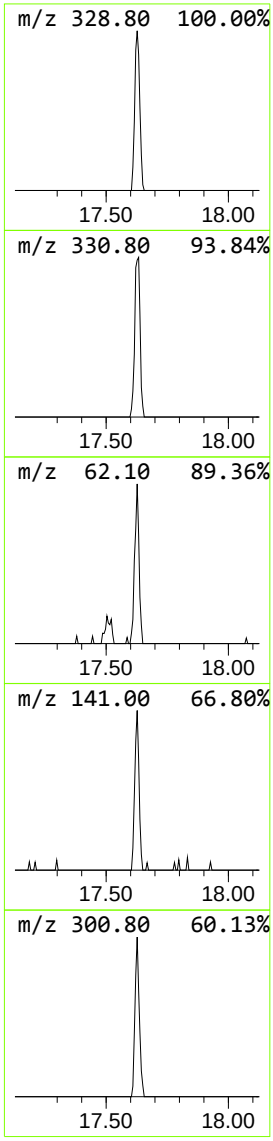
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.627	3.00 ng	90598	Phenanthrene-d10	17.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 2,4,6-tribromo-	327	C6H4Br3N	000147-82-0	56
2	Allyl 2,4,6-tribromophenyl ether	368	C9H7Br3O	003278-89-5	23
3	3H-Indol-3-one, 2-(p-bromophenyl...	301	C14H8BrNO2	027820-27-5	9
4	4H-3,1-Benzoxazin-4-one, 2-(4-br...	301	C14H8BrNO2	018600-53-8	9
5	Bromophos	364	C8H8BrCl2O3PS	002104-96-3	9





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Data File : BG048947.D
Acq On : 14 Jun 2021 13:21
Operator : CG/JU
Sample : M2678-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0231-COMPOSITE-H

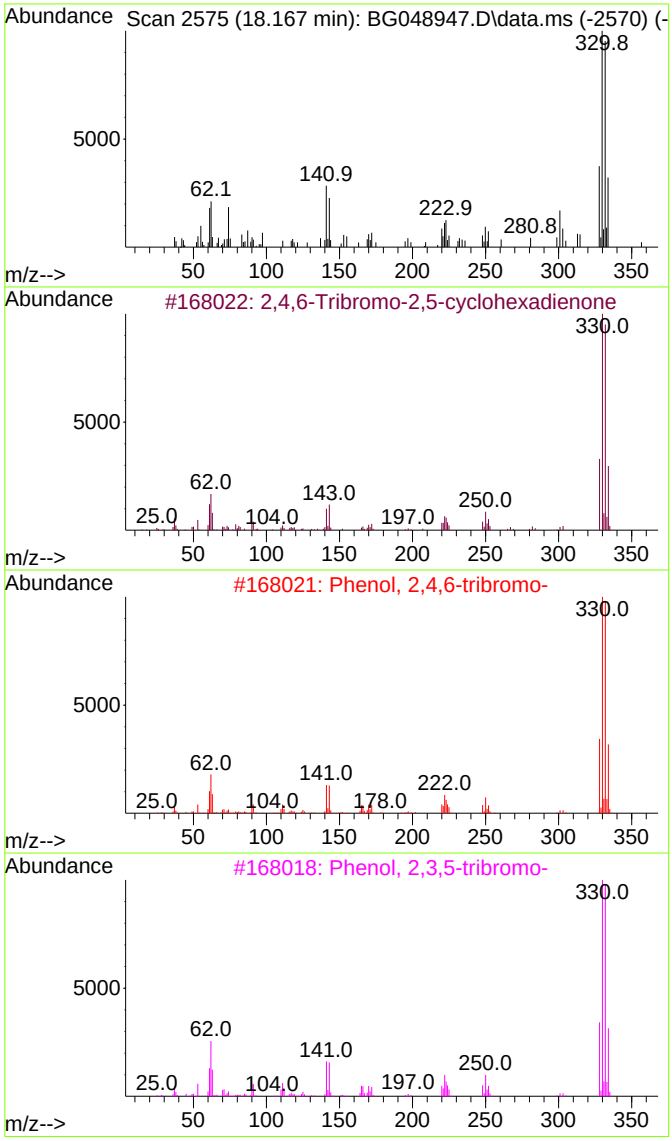
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

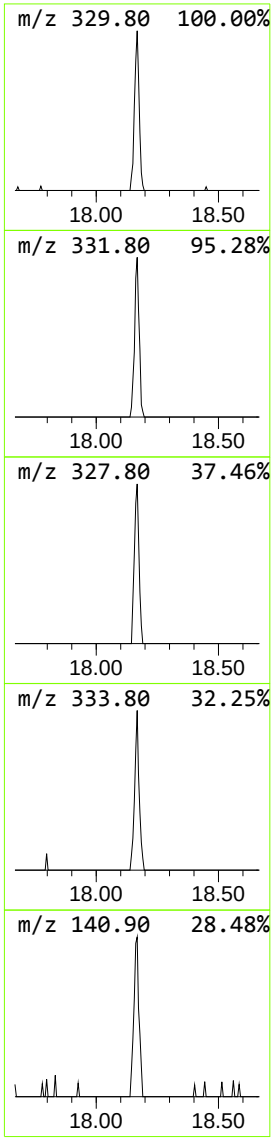
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2,4,6-Tribromo-2,5-cyclohex... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.167	2.17 ng	65516	Phenanthrene-d10	17.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,6-Tribromo-2,5-cyclohexadienone	328	C6H3Br3O	020244-61-5	98
2	Phenol, 2,4,6-tribromo-	328	C6H3Br3O	000118-79-6	97
3	Phenol, 2,3,5-tribromo-	328	C6H3Br3O	057383-81-0	96
4	2-Bromo-4-chloro-5,8-dimethoxy-3...	330	C13H12BrClO3	104506-11-8	27
5	4-[p-Chlorophenoxy]-6-methoxy-8-...	330	C16H11ClN2O4	063456-77-9	17





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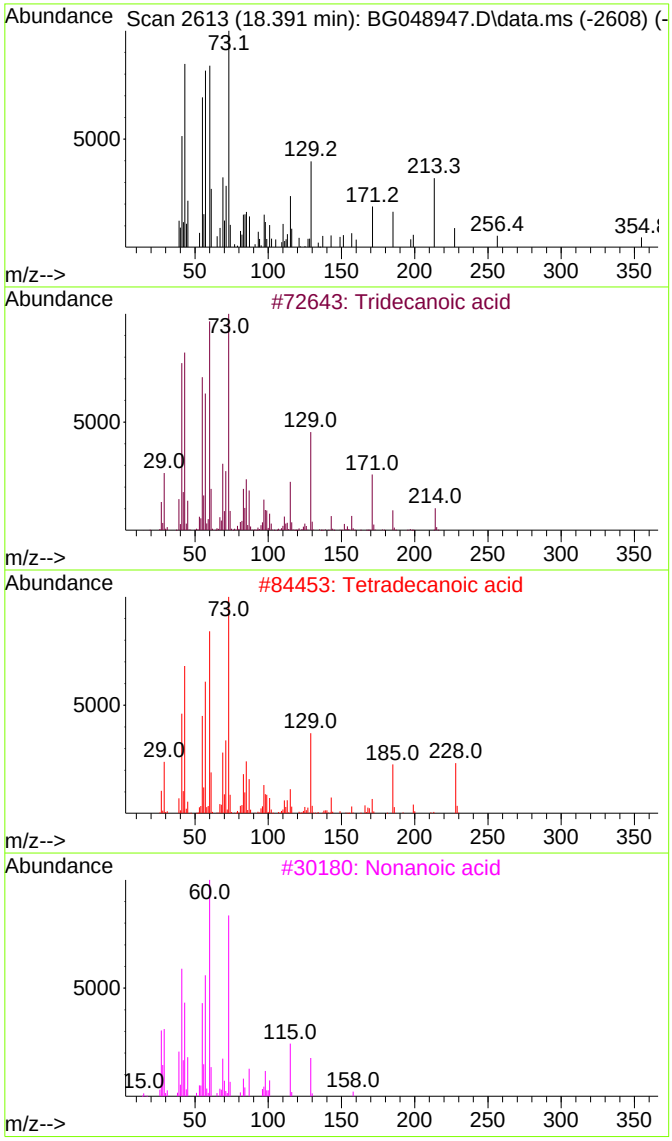
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

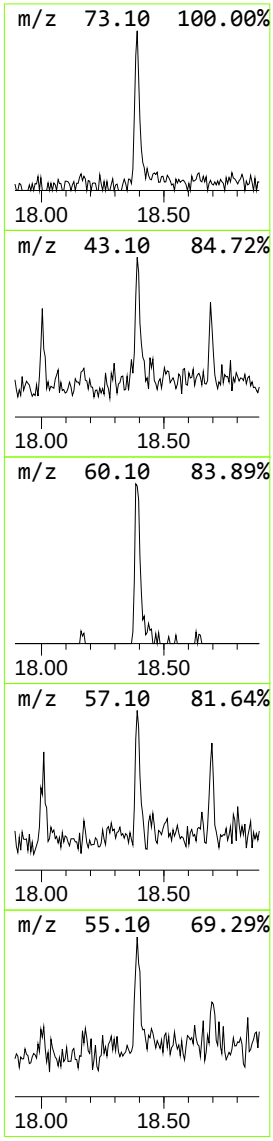
****

Peak Number 9 Tridecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.391	2.14 ng	64708	Phenanthrene-d10	17.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	64
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	47
3	Nonanoic acid	158	C9H18O2	000112-05-0	43
4	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	43
5	Undecanoic acid	186	C11H22O2	000112-37-8	43





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Data File : BG048947.D
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Operator : CG/JU
Sample : M2678-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0231-COMPOSITE-H

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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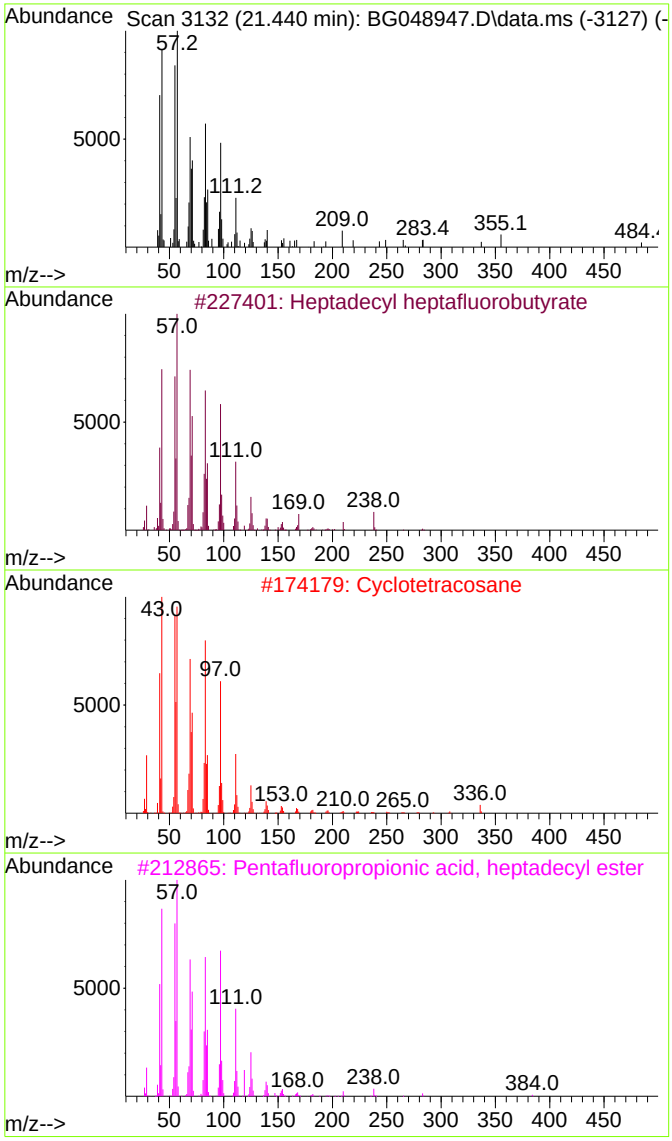
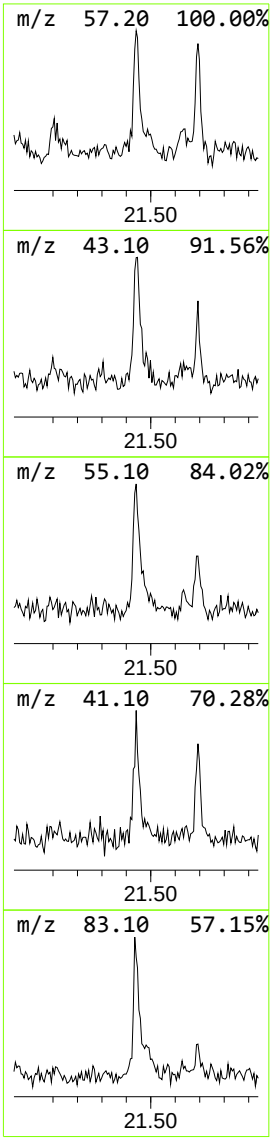
****

Peak Number 10 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.440	3.14 ng	107134	Chrysene-d12	21.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
2	Cyclotetracosane	336	C24H48	000297-03-0	90
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	87
4	1-Tricosene	322	C23H46	018835-32-0	86
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048947.D
Acq On : 14 Jun 2021 13:21
Operator : CG/JU
Sample : M2678-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0231-COMPOSITE-H

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

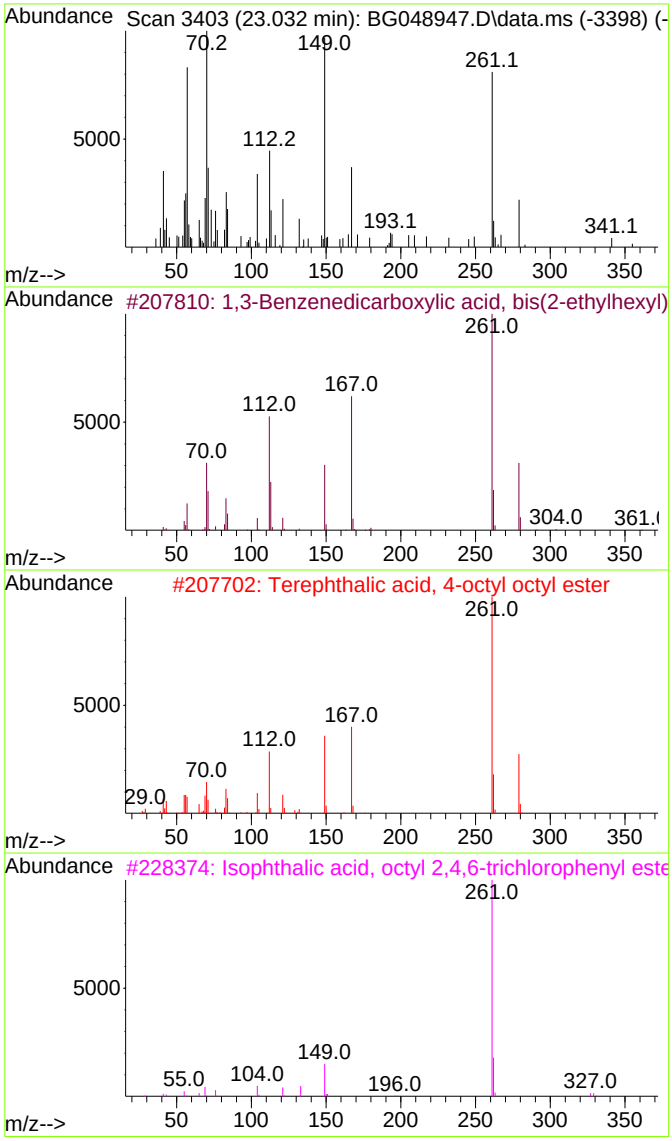
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

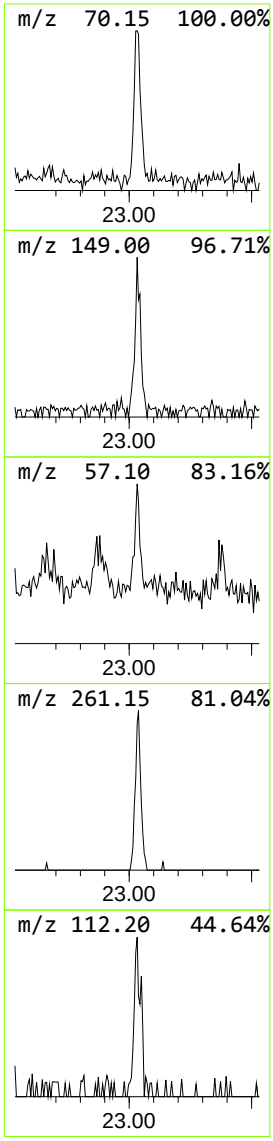
****

Peak Number 11 unknown23.032 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.032	2.16 ng	73514	Chrysene-d12	21.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	43
2	Terephthalic acid, 4-octyl octyl...	390	C24H38O4	1000323-73-7	38
3	Isophthalic acid, octyl 2,4,6-tr...	456	C22H23Cl3O4	1000344-57-2	27
4	Di-n-octyl phthalate	390	C24H38O4	000117-84-0	16
5	Terephthalic acid, 2-heptyl octy...	376	C23H36O4	1000356-29-2	16





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048947.D
Acq On : 14 Jun 2021 13:21
Operator : CG/JU
Sample : M2678-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0231-COMPOSITE-H

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...	3.167	27.8	ng	336397	1	8.120	241729	20.0
Furan, tetrahyd...	3.291	11.2	ng	134815	1	8.120	241729	20.0
2-Pentanone, 4-...	5.200	9.6	ng	115664	1	8.120	241729	20.0
Ethanol, 2-(2-b...	10.706	7.1	ng	120480	2	10.941	337690	20.0
1,3,5-Triazine-...	16.164	2.9	ng	87946	4	17.509	604577	20.0
Benzenamine, 2,...	17.627	3.0	ng	90598	4	17.509	604577	20.0
2,4,6-Tribromo-...	18.167	2.2	ng	65516	4	17.509	604577	20.0
Tridecanoic acid	18.391	2.1	ng	64708	4	17.509	604577	20.0
Heptadecyl hept...	21.440	3.1	ng	107134	5	21.804	682234	20.0
unknown23.032	23.032	2.2	ng	73514	5	21.804	682234	20.0