LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048955.D
Acq On : 14 Jun 2021 18:52
Operator : CG/JU
Sample : M2678-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0239-AMND-COMP-D(CL-01A)

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: BG048955.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.170	16	22	34	rVB	227206	394222	5.74%	2.513%
2	3.287	38	42	51	rVB	101889	153955	2.24%	0.981%
3	5.226	361	372	383	rBV	3357595	6869504	100.00%	43.786%
4	5.743	454	460	472	rVB	31247	72402	1.05%	0.461%
5	7.283	714	722	729	rBV2	92381	171222	2.49%	1.091%
6	8.123	857	865	871	rBV	151985	262490	3.82%	1.673%
7	9.286	1056	1063	1071	rVB	458257	822913	11.98%	5.245%
8	10.708	1297	1305	1312	rBV	384116	656612	9.56%	4.185%
9	10.943	1337	1345	1354	rVB	198897	373920	5.44%	2.383%
10	13.387	1753	1761	1769	rBV	669375	1050762	15.30%	6.698%
11	14.762	1988	1995	2002	rBV	316243	517355	7.53%	3.298%
12	16.160	2228	2233	2239	rBV2	72712	108737	1.58%	0.693%
13	17.512	2456	2463	2468	rBV	395710	635561	9.25%	4.051%
14	18.176	2571	2576	2581	rVB2	60741	82388	1.20%	0.525%
15	19.556	2807	2811	2818	rVB	97595	148051	2.16%	0.944%
16	19.921	2870	2873	2881	rVB	90448	132304	1.93%	0.843%
17	20.120	2900	2907	2918	rVB	1232830	1678744	24.44%	10.700%
18	21.695	3171	3175	3180	rVB	69166	97641	1.42%	0.622%
19	21.801	3186	3193	3199	rBV3	372307	732439	10.66%	4.669%
20	24.086	3576	3582	3588	rBV2	28615	79819	1.16%	0.509%
21	25.138	3752	3761	3771	rBV3	216484	647786	9.43%	4.129%

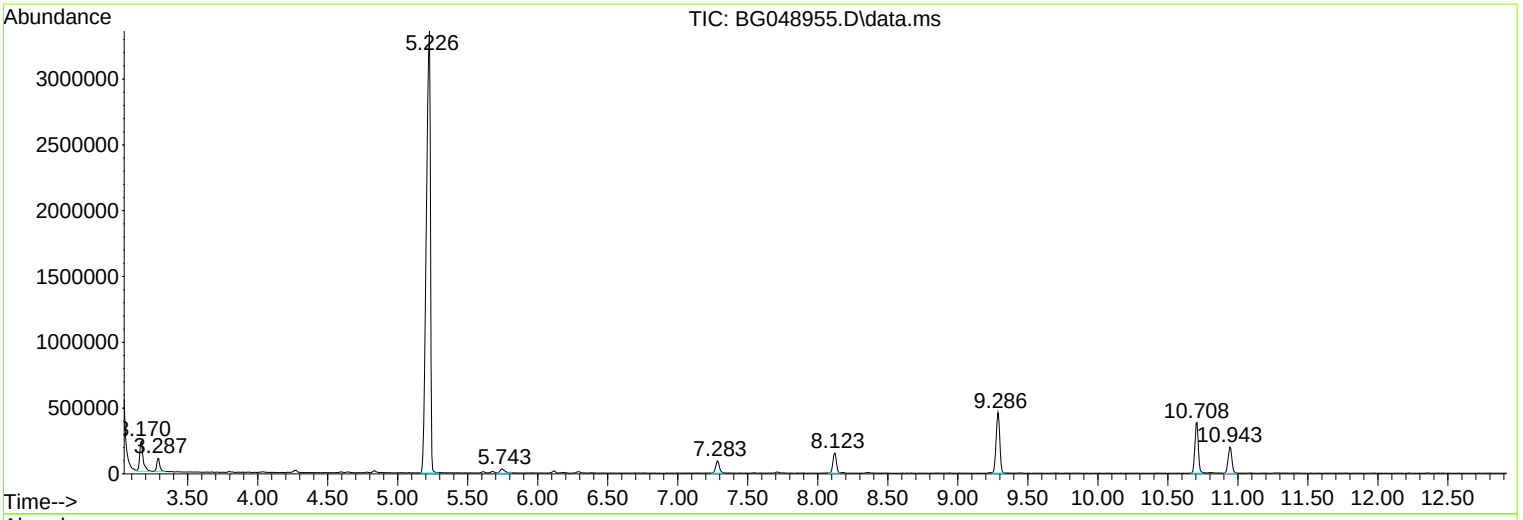
Sum of corrected areas: 15688827

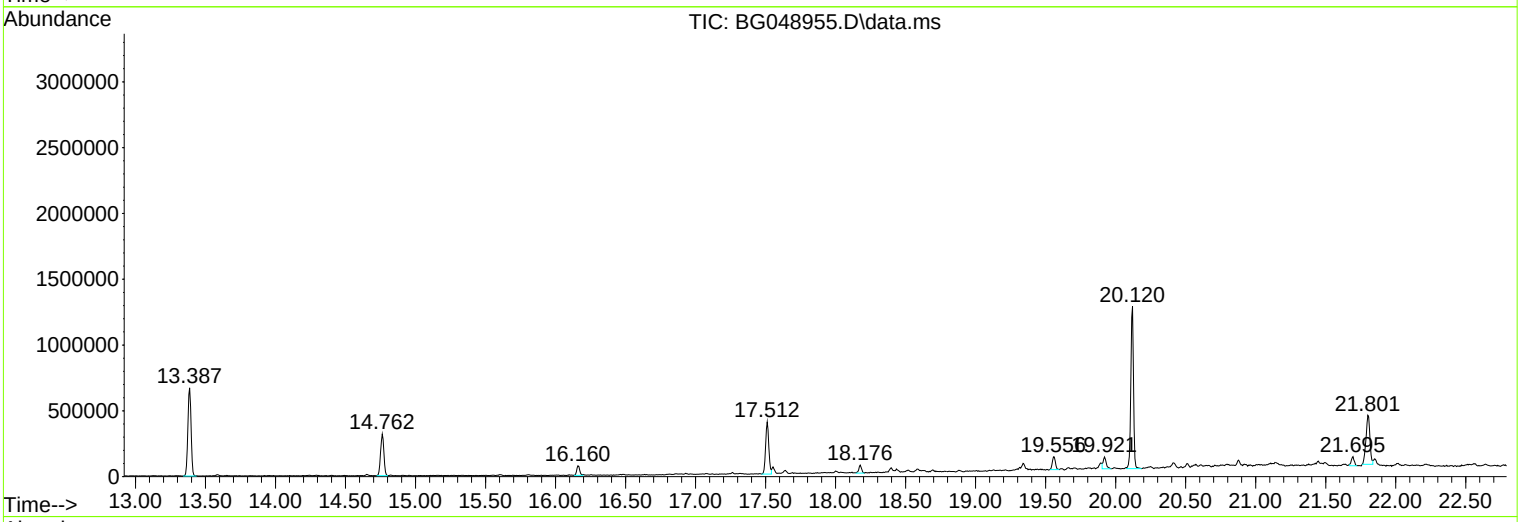
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048955.D
Acq On : 14 Jun 2021 18:52
Operator : CG/JU
Sample : M2678-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

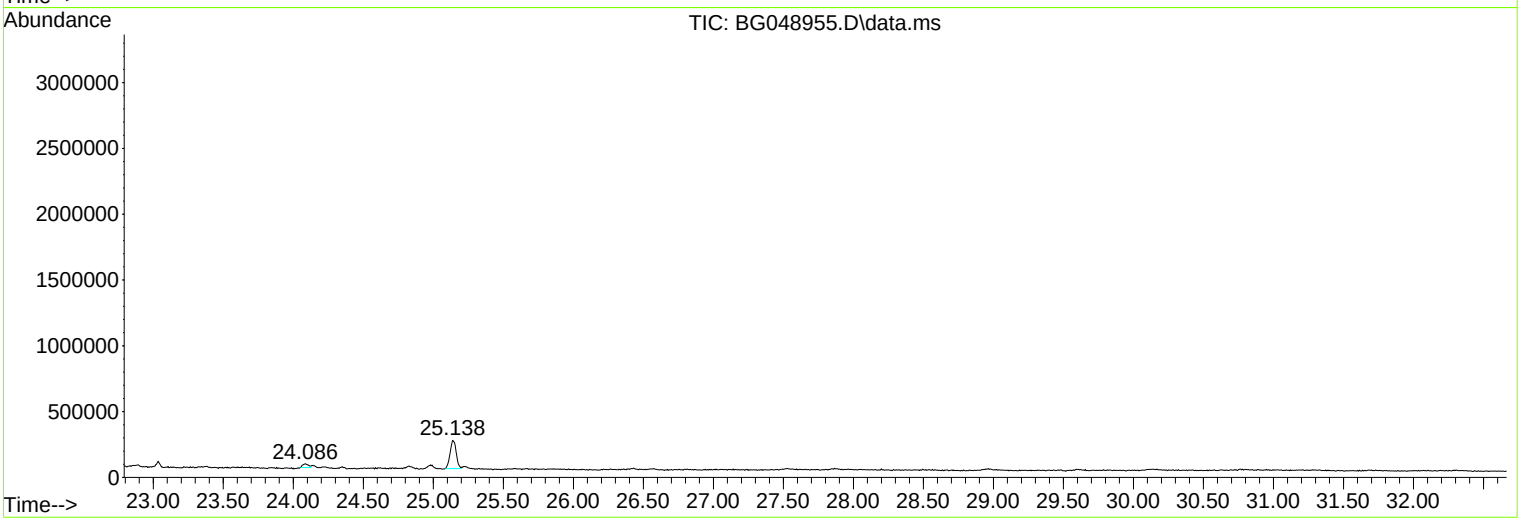
Instrument :
BNA_G
ClientSampleId :
0239-AMND-COMP-D(CL-01A)

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 : BG048955.D
Acq On : 14 Jun 2021 18:52
Operator : CG/JU
Sample : M2678-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0239-AMND-COMP-D(CL-01A)

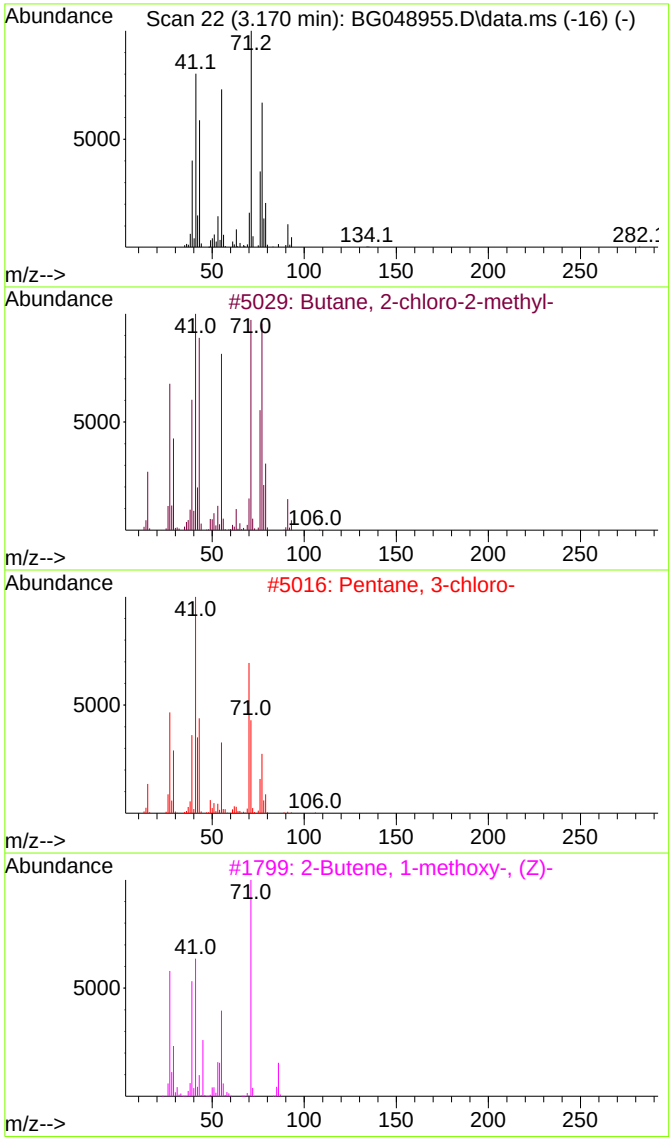
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

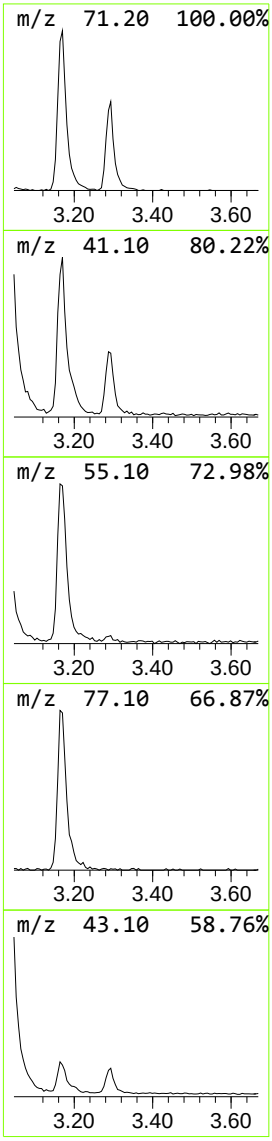
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-chloro-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.170	30.04 ng	394222	1,4-Dichlorobenzene-d4	8.117

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	45
3	2-Butene, 1-methoxy-, (Z)-	86	C5H10O	010034-16-9	32
4	2-Penten-1-ol, 2-methyl-, (E)-	100	C6H12O	016958-19-3	32
5	Butanoyl chloride	106	C4H7ClO	000141-75-3	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048955.D
Acq On : 14 Jun 2021 18:52
Operator : CG/JU
Sample : M2678-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0239-AMND-COMP-D(CL-01A)

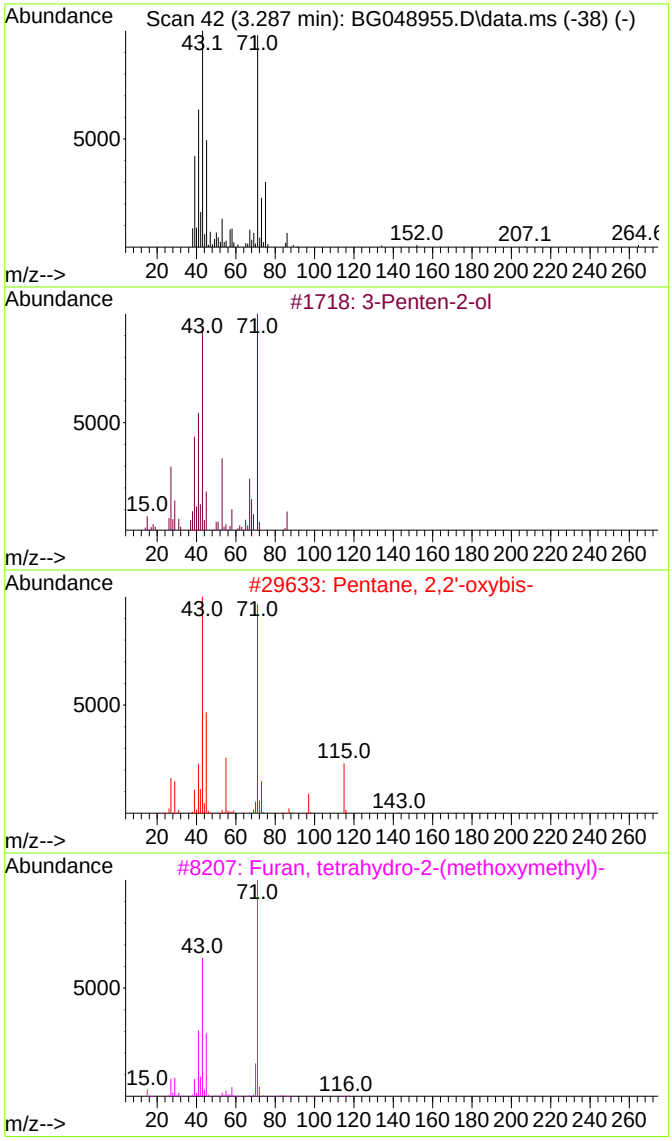
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

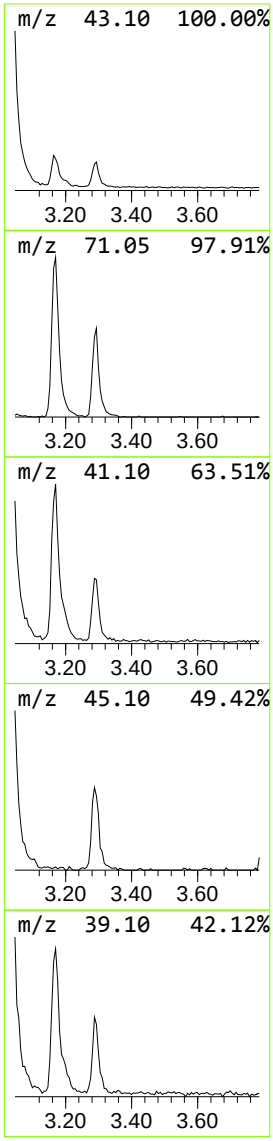
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 unknown3.287 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.287	11.73 ng	153955	1,4-Dichlorobenzene-d4	8.117

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-ol	86	C5H10O	001569-50-2	47
2	Pentane, 2,2'-oxybis-	158	C10H22O	056762-00-6	47
3	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	43
4	1,6-Heptadien-4-ol	112	C7H12O	002883-45-6	43
5	2-Butene, 1-methoxy-, (Z)-	86	C5H10O	010034-16-9	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048955.D
Acq On : 14 Jun 2021 18:52
Operator : CG/JU
Sample : M2678-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0239-AMND-COMP-D(CL-01A)

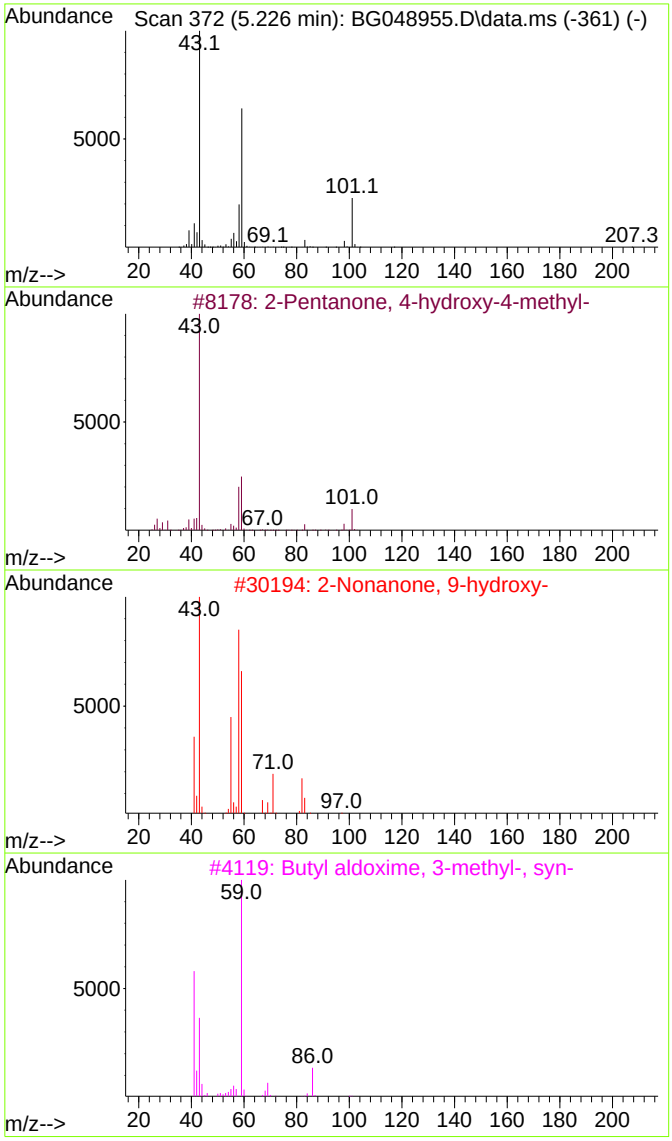
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

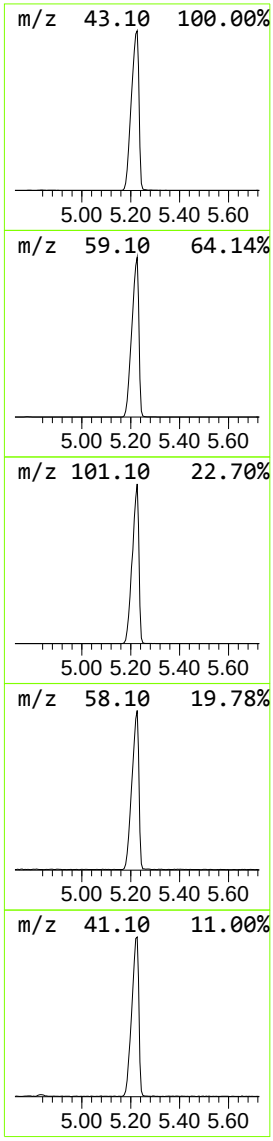
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.226	523.41 ng	6869500	1,4-Dichlorobenzene-d4	8.117

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	25
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	16
5	Acetone	58	C3H6O	000067-64-1	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048955.D
Acq On : 14 Jun 2021 18:52
Operator : CG/JU
Sample : M2678-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0239-AMND-COMP-D(CL-01A)

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

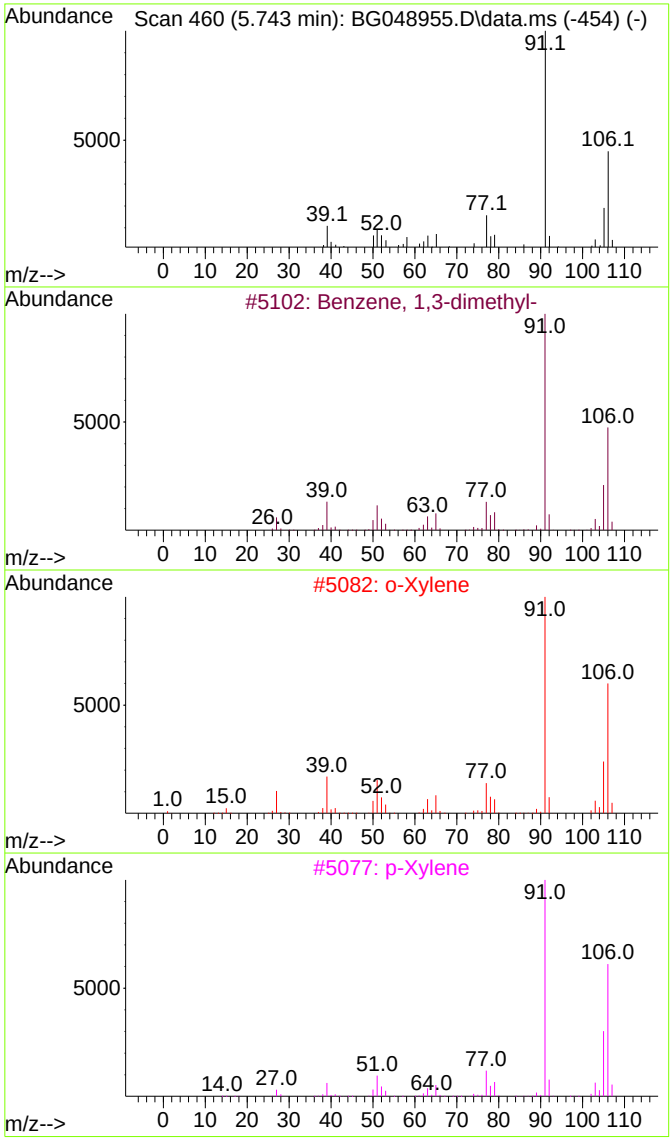
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

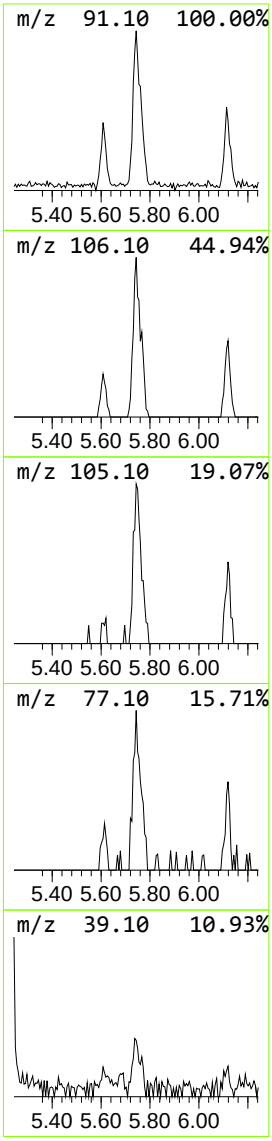
****

Peak Number 4 Benzene, 1,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.743	5.52 ng	72402	1,4-Dichlorobenzene-d4	8.117

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	95
2	o-Xylene	106	C8H10	000095-47-6	91
3	p-Xylene	106	C8H10	000106-42-3	91
4	Cyclopentene, 1-ethenyl-3-methyl...	106	C8H10	061142-07-2	83
5	1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048955.D
Acq On : 14 Jun 2021 18:52
Operator : CG/JU
Sample : M2678-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0239-AMND-COMP-D(CL-01A)

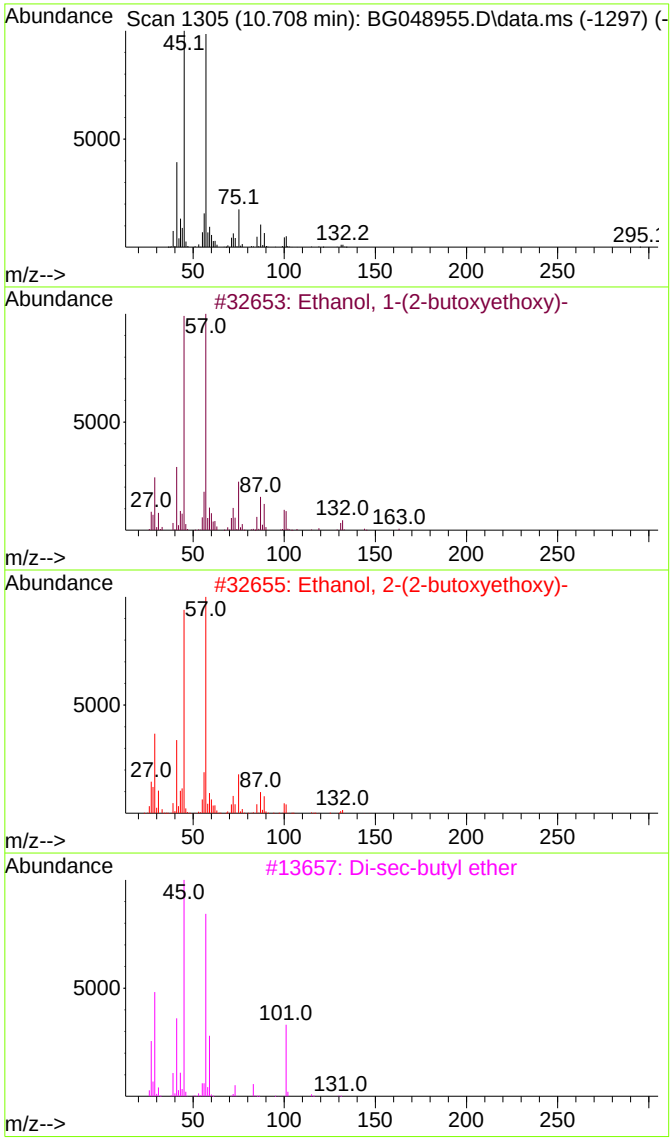
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

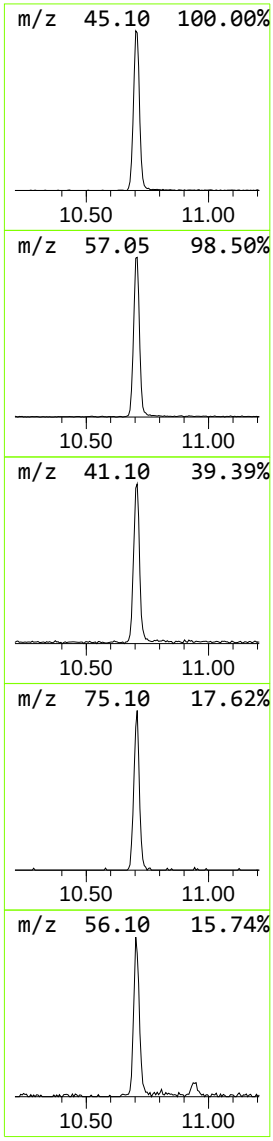
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.708	35.12 ng	656612	Naphthalene-d8	10.943

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3	Di-sec-butyl ether	130	C8H18O	006863-58-7	53
4	2-Heptanol, 3-methyl-	130	C8H18O	031367-46-1	50
5	Propanoic acid, 2-hydroxy-, buty...	146	C7H14O3	000138-22-7	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048955.D
Acq On : 14 Jun 2021 18:52
Operator : CG/JU
Sample : M2678-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0239-AMND-COMP-D(CL-01A)

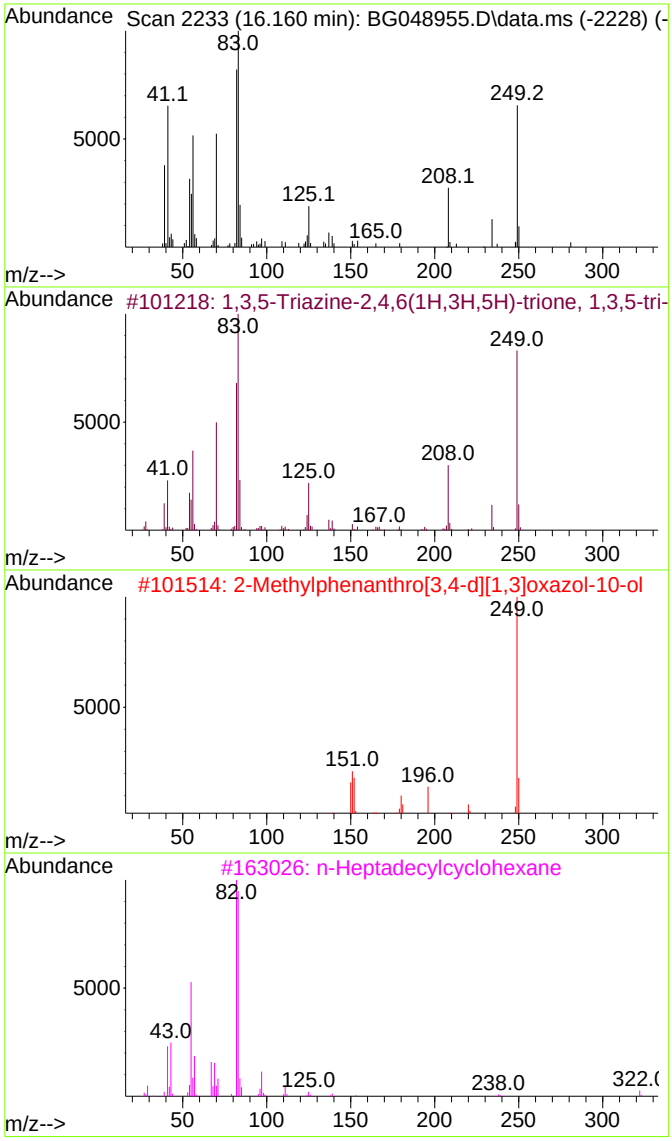
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

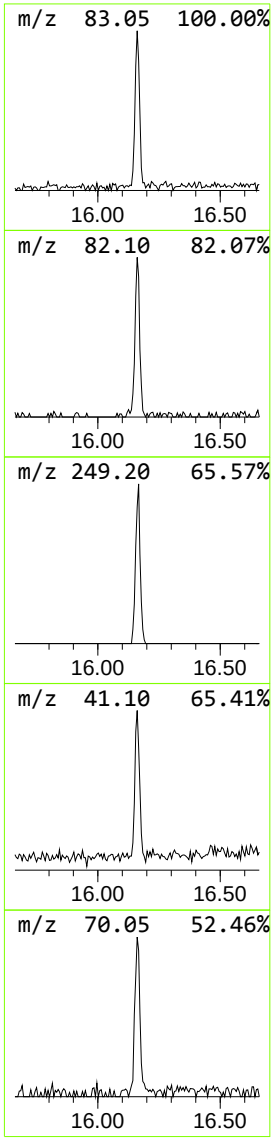
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.160	3.42 ng	108737	Phenanthrene-d10	17.512

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	2-Methylphenanthro[3,4-d][1,3]ox...	249	C16H11NO2	098033-24-0	40
3	n-Heptadecylcyclohexane	322	C23H46	019781-73-8	32
4	1H-Pyrrole, 2,3-dihydro-1-methyl-	83	C5H9N	033838-11-8	25
5	Cyclohexane, hexyl-	168	C12H24	004292-75-5	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048955.D
Acq On : 14 Jun 2021 18:52
Operator : CG/JU
Sample : M2678-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0239-AMND-COMP-D(CL-01A)

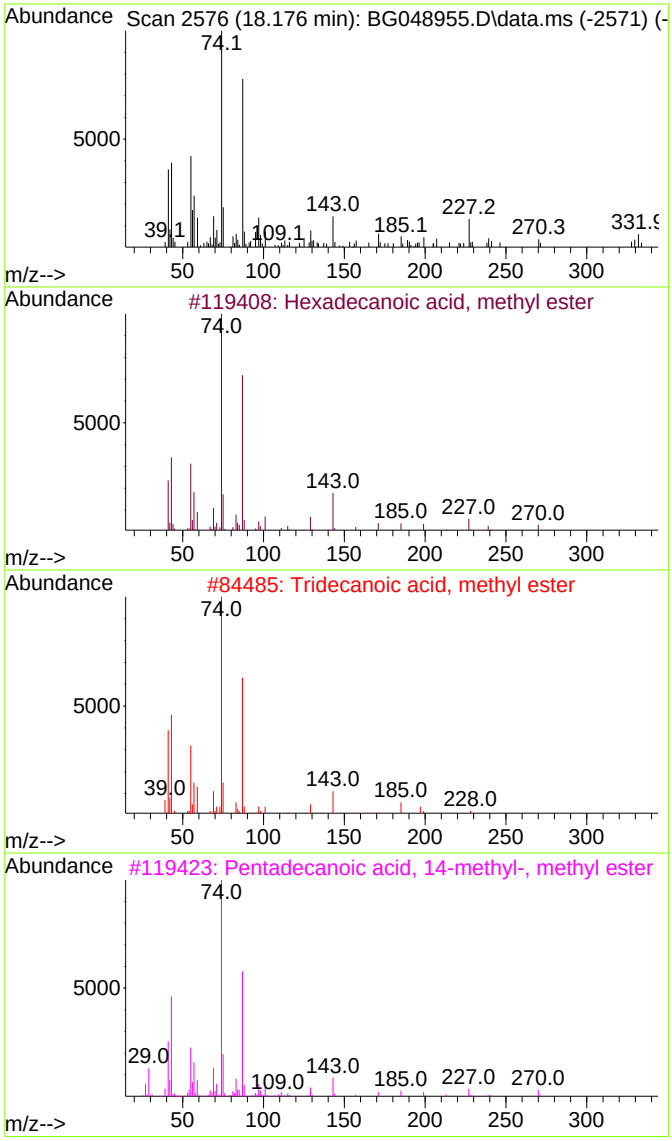
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

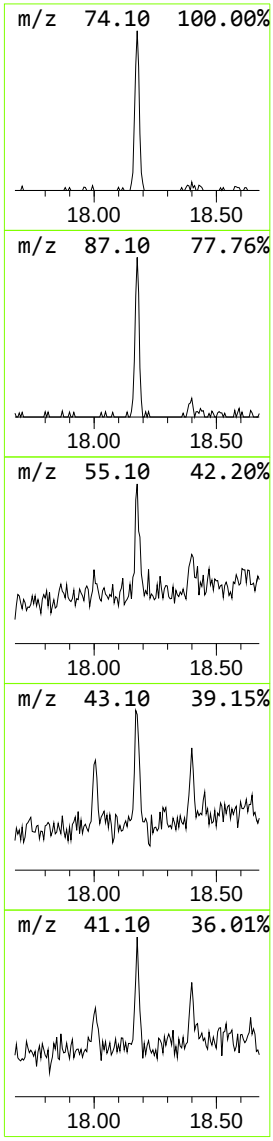
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Hexadecanoic acid, methyl e... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.176	2.59 ng	82388	Phenanthrene-d10	17.512

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	96
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	87
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87
4	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	81
5	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048955.D
Acq On : 14 Jun 2021 18:52
Operator : CG/JU
Sample : M2678-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0239-AMND-COMP-D(CL-01A)

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...	3.170	30.0	ng	394222	1	8.117	262490	20.0
unknown3.287	3.287	11.7	ng	153955	1	8.117	262490	20.0
2-Pentanone, 4-...	5.226	523.4	ng	6869500	1	8.117	262490	20.0
Benzene, 1,3-di...	5.743	5.5	ng	72402	1	8.117	262490	20.0
Ethanol, 1-(2-b...	10.708	35.1	ng	656612	2	10.943	373920	20.0
1,3,5-Triazine-...	16.160	3.4	ng	108737	4	17.512	635561	20.0
Hexadecanoic ac...	18.176	2.6	ng	82388	4	17.512	635561	20.0