LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081122\
Data File : BG054605.D
Acq On : 11 Aug 2022 15:07
Operator : CG/JU
Sample : N3972-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-1

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-BG071522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054605.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.088	11	17	32	rVB	242750	405486	23.93%	6.865%
2	4.404	236	241	249	rVB	11651	19223	1.13%	0.325%
3	5.556	431	437	447	rBV	93553	163743	9.66%	2.772%
4	7.172	705	712	726	rVB	57690	115188	6.80%	1.950%
5	7.501	763	768	773	rBV	12652	19951	1.18%	0.338%
6	7.554	773	777	785	rVB2	12124	20140	1.19%	0.341%
7	7.742	803	809	817	rBV	18553	32673	1.93%	0.553%
8	7.971	841	848	854	rBV	43920	74696	4.41%	1.265%
9	9.140	1040	1047	1059	rVB	134435	253232	14.95%	4.287%
10	9.293	1068	1073	1079	rBV	18221	34421	2.03%	0.583%
11	10.544	1281	1286	1295	rBV2	13953	27038	1.60%	0.458%
12	10.779	1319	1326	1339	rBB	55759	102088	6.03%	1.728%
13	11.144	1382	1388	1403	rBV2	15808	33646	1.99%	0.570%
14	12.965	1692	1698	1711	rBV	34357	60500	3.57%	1.024%
15	13.229	1733	1743	1753	rBV	465427	784482	46.30%	13.281%
16	13.464	1774	1783	1794	rBB	44223	70846	4.18%	1.199%
17	14.610	1972	1978	1985	rBV	114014	175700	10.37%	2.975%
18	15.345	2099	2103	2109	rVB	33491	46522	2.75%	0.788%
19	15.415	2109	2115	2121	rVB	23467	33984	2.01%	0.575%
20	16.108	2227	2233	2249	rBV	447856	711022	41.96%	12.038%
21	17.360	2439	2446	2456	rBV	179138	266689	15.74%	4.515%
22	18.012	2553	2557	2562	rBV2	24664	32105	1.89%	0.544%
23	19.969	2884	2890	2897	rBV	1285776	1694378	100.00%	28.686%
24	21.625	3166	3172	3180	rBV	223876	363861	21.47%	6.160%
25	24.833	3708	3718	3730	rVB2	123094	365014	21.54%	6.180%

Sum of corrected areas: 5906628

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Misc :
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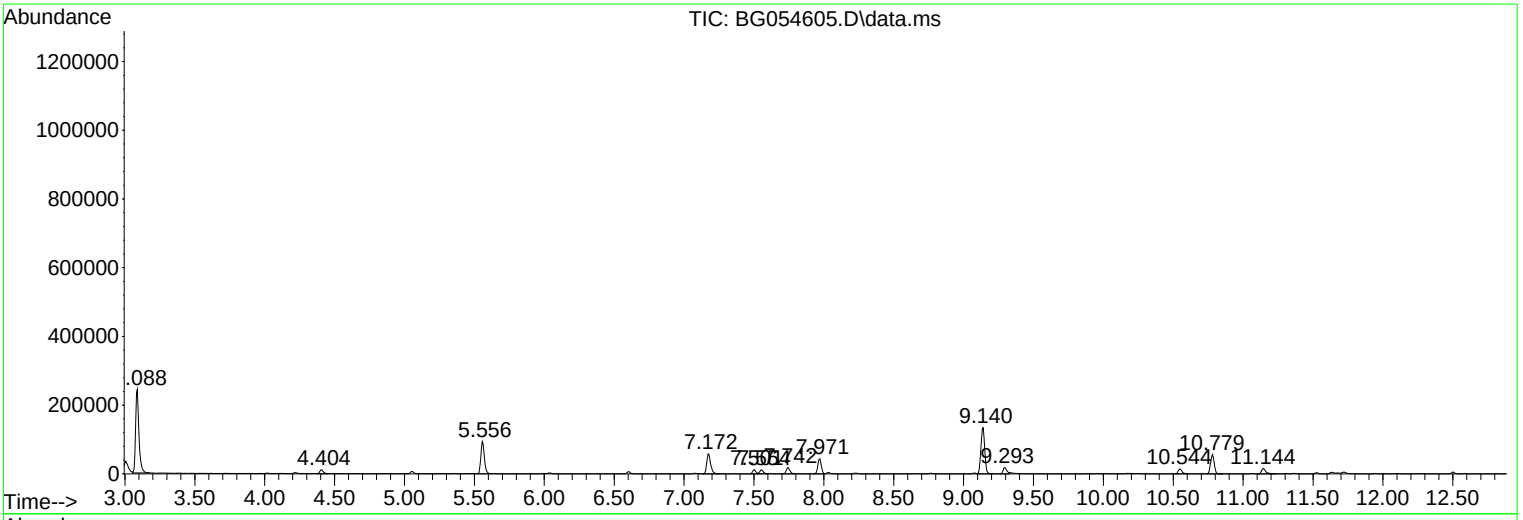
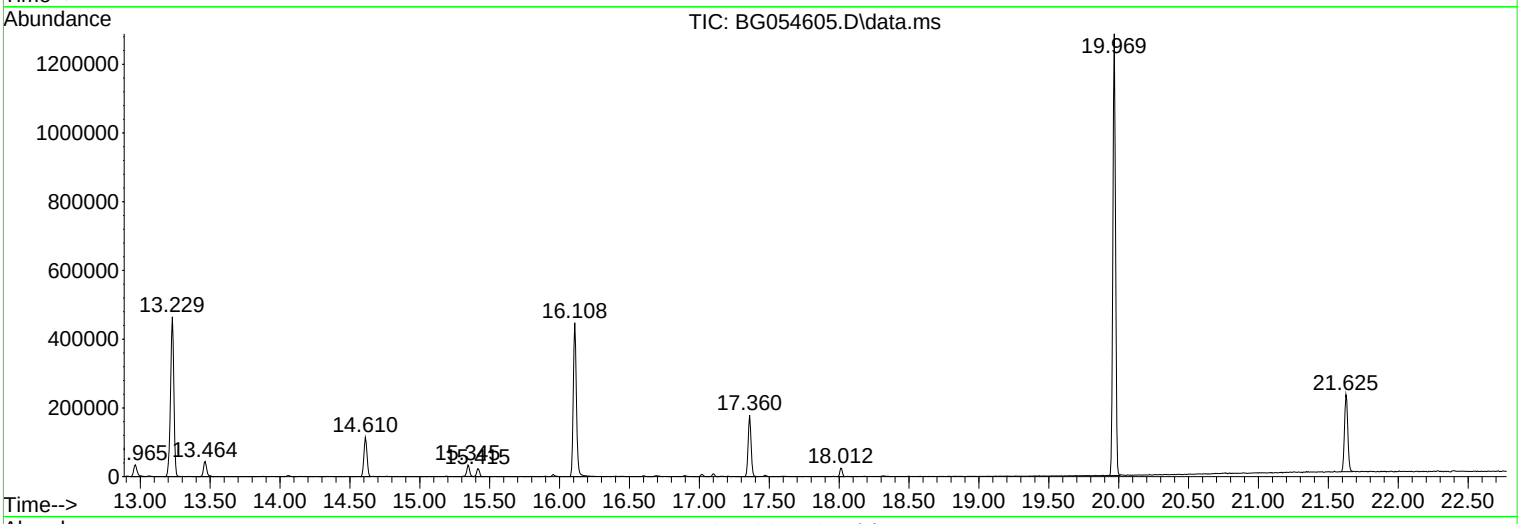
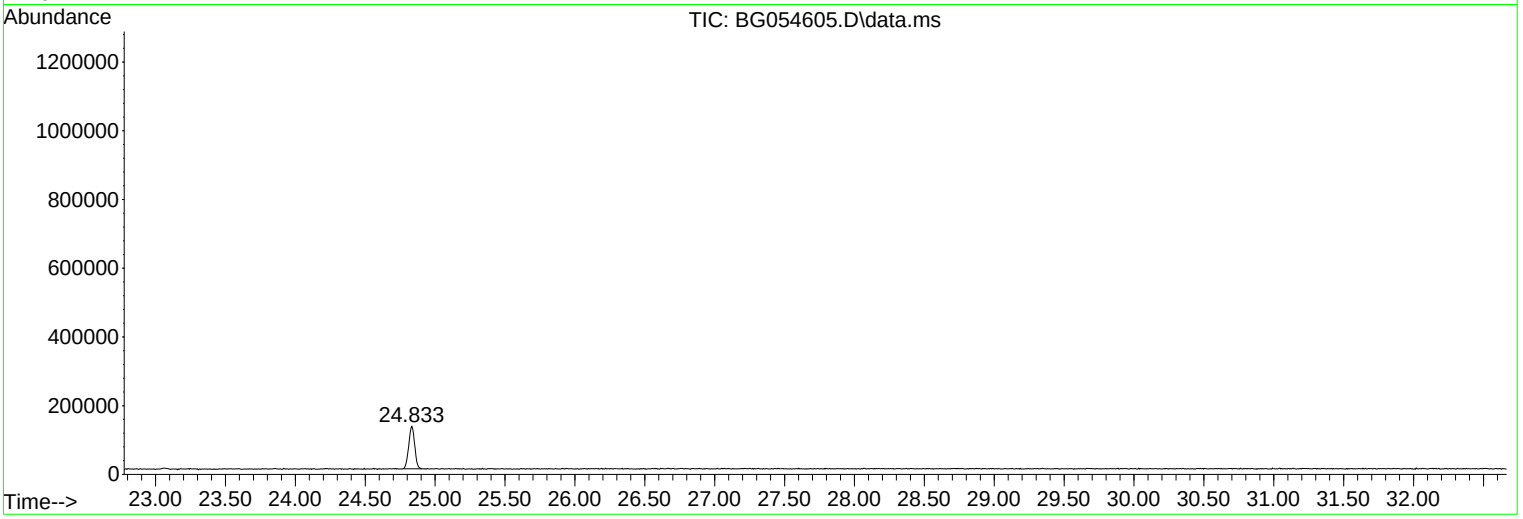
Instrument :
BNA_G
ClientSampleId :
SPN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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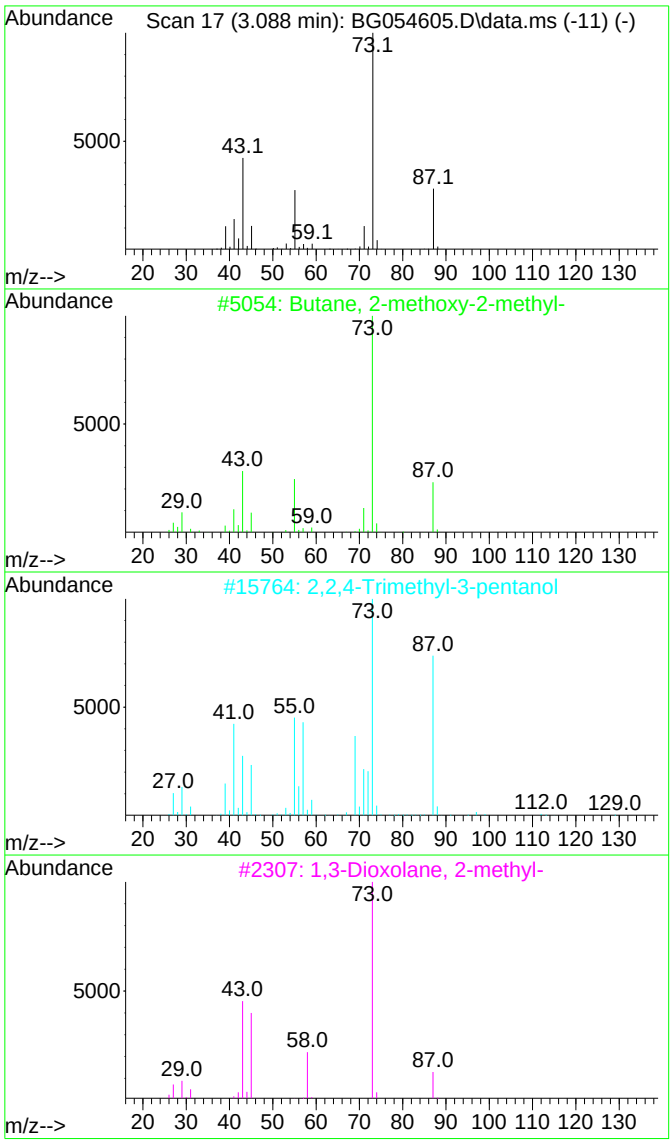
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

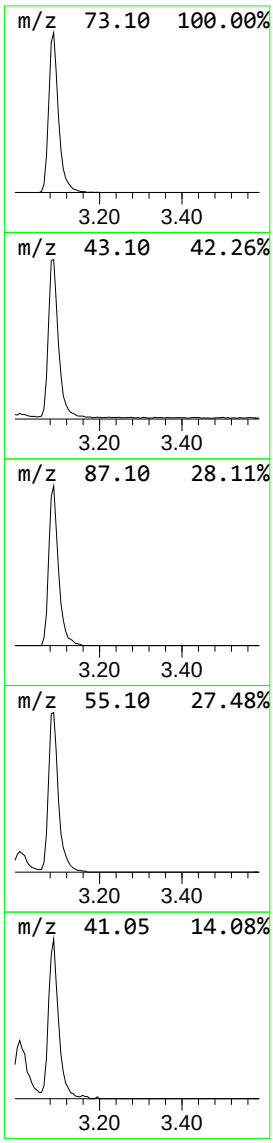
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.088	108.57 ng	405486	1,4-Dichlorobenzene-d4	7.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	16





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Data File : BG054605.D
Acq On : 11 Aug 2022 15:07
Operator : CG/JU
Sample : N3972-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

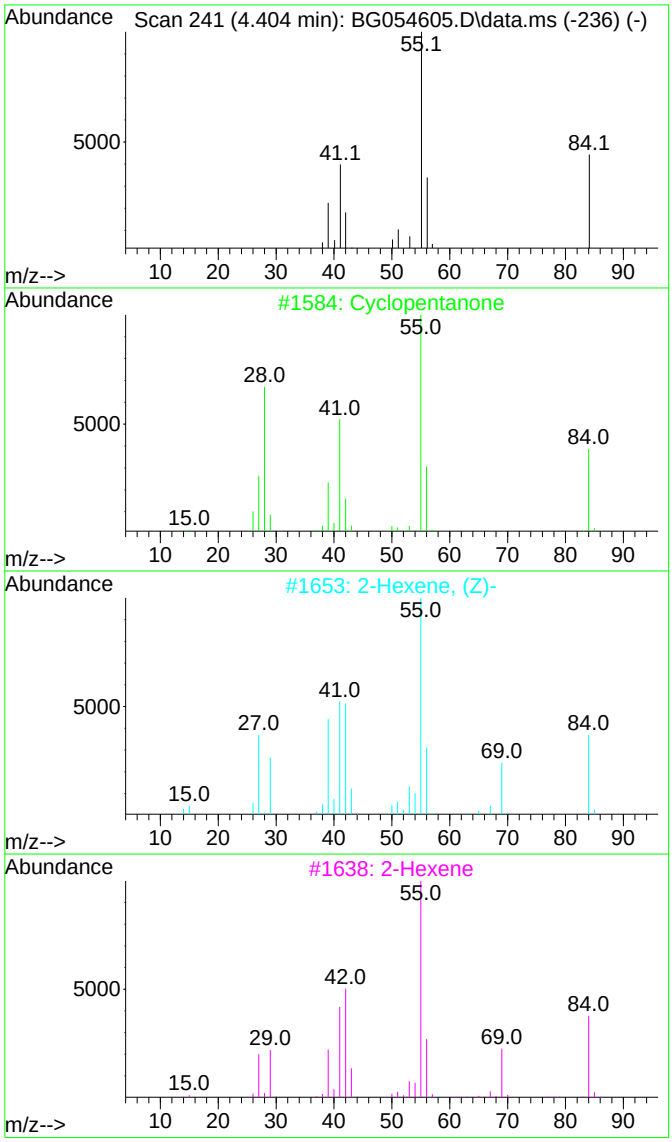
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

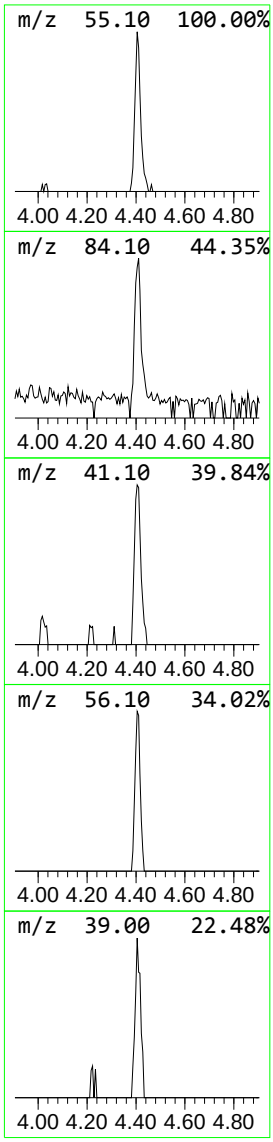
****

Peak Number 2 Cyclopentanone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.404	5.15 ng	19223	1,4-Dichlorobenzene-d4	7.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	86
2	2-Hexene, (Z)-	84	C6H12	007688-21-3	64
3	2-Hexene	84	C6H12	000592-43-8	64
4	3-Hexene, (E)-	84	C6H12	013269-52-8	64
5	3-Hexene, (Z)-	84	C6H12	007642-09-3	64





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Operator : CG/JU
Sample : N3972-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-1

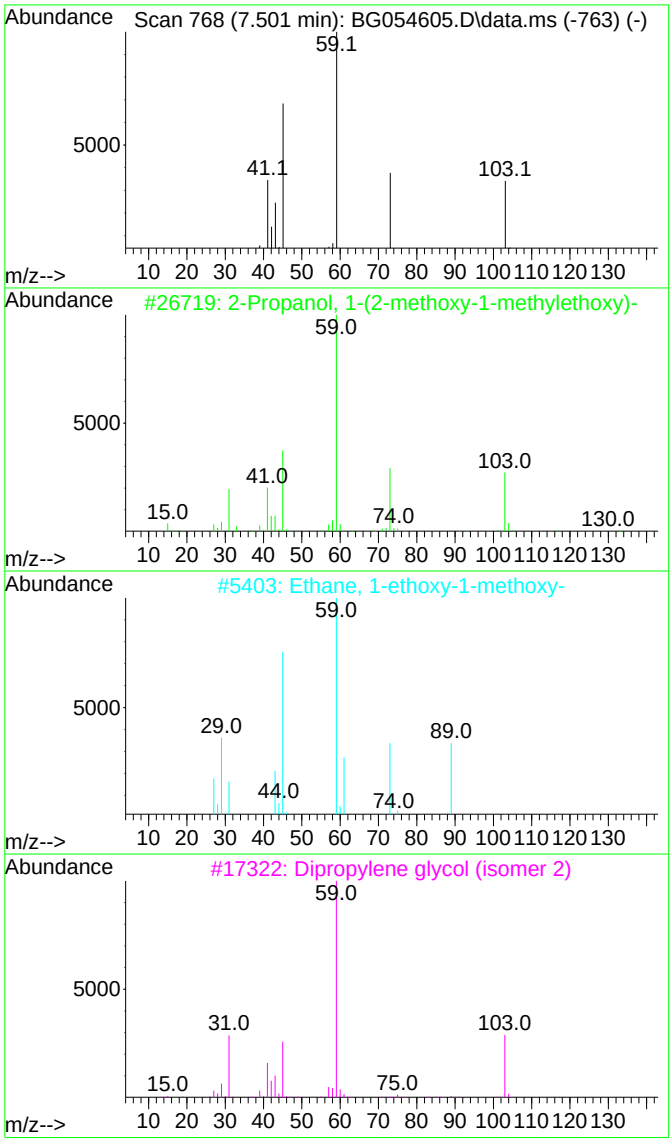
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

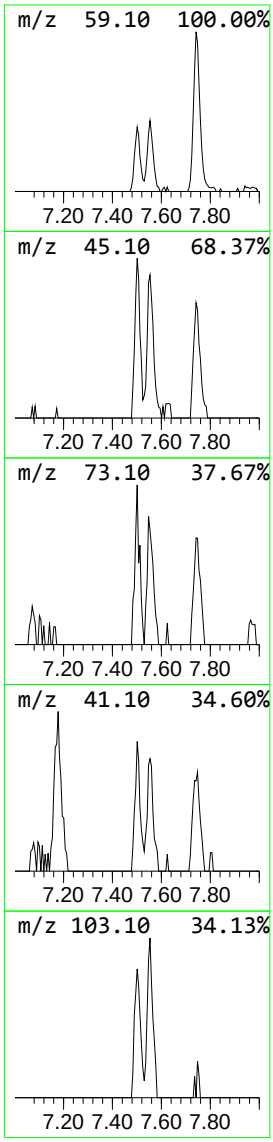
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.501	5.34 ng	19951	1,4-Dichlorobenzene-d4	7.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	78
2	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	50
3	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	45
4	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	45
5	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	45





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Acq On : 11 Aug 2022 15:07
Operator : CG/JU
Sample : N3972-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

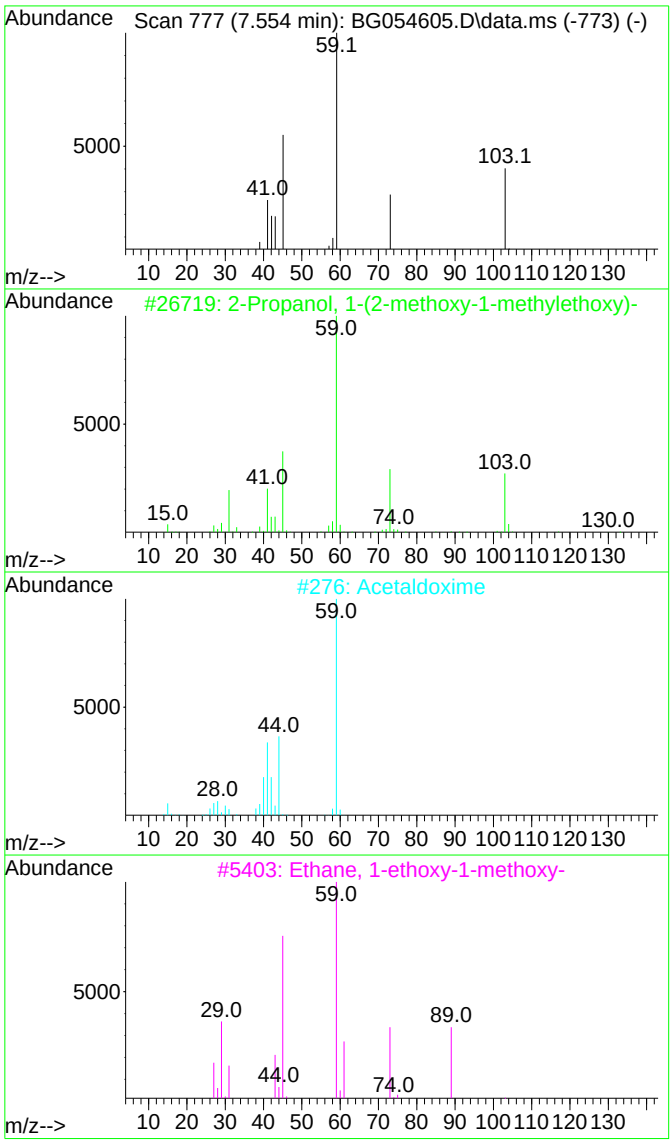
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

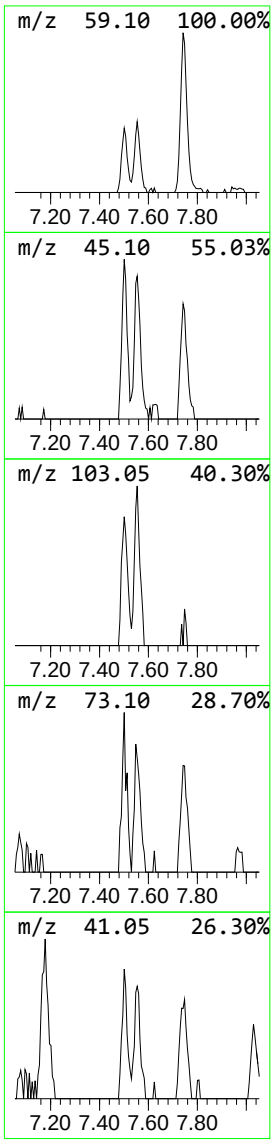
****

Peak Number 4 unknown7.554 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.554	5.39 ng	20140	1,4-Dichlorobenzene-d4	7.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	39
2	Acetaldoxime	59	C2H5NO	000107-29-9	9
3	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	9
4	Silane, dimethyl-	60	C2H8Si	001111-74-6	9
5	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081122\
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Operator : CG/JU
Sample : N3972-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-1

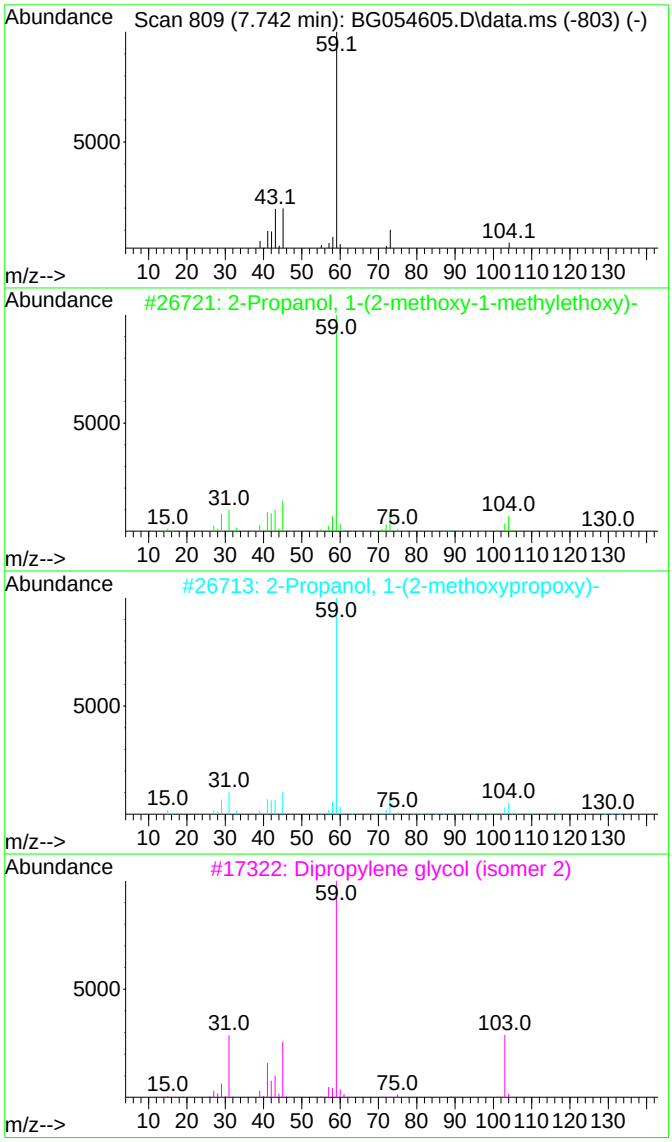
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

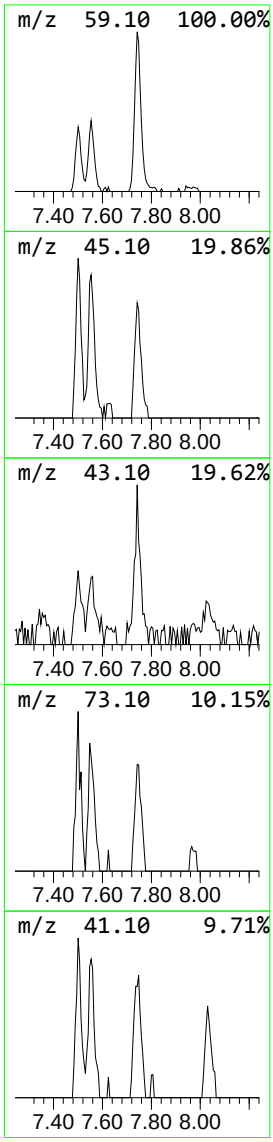
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Propanol, 1-(2-methoxypro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.742	8.75 ng	32673	1,4-Dichlorobenzene-d4	7.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	78
2	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	72
3	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	56
4	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	56
5	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	43





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TIC Library : C:\Database\NIST20.L
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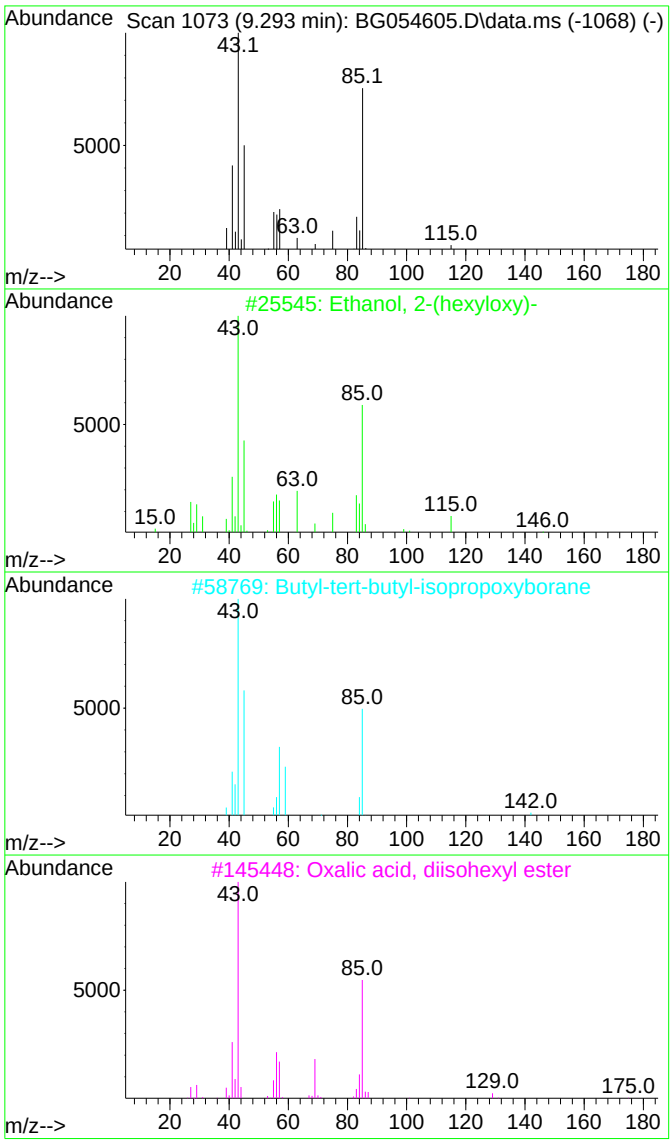
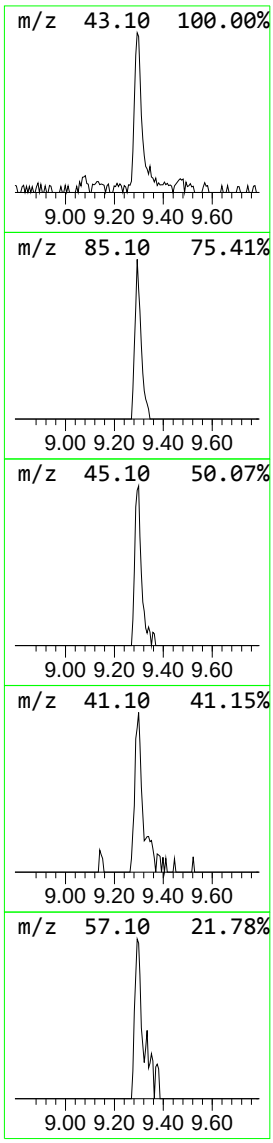
****

Peak Number 6 Ethanol, 2-(hexyloxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.293	9.22 ng	34421	1,4-Dichlorobenzene-d4	7.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(hexyloxy)-	146	C8H18O2	000112-25-4	78
2	Butyl-tert-butyl-isopropoxyborane	184	C11H25BO	097782-82-6	64
3	Oxalic acid, diisohexyl ester	258	C14H26O4	1010309-32-9	53
4	Sulfurous acid, isohexyl hexyl e...	250	C12H26O3S	1000309-12-8	50
5	Heptane, 4,4-dimethyl-	128	C9H20	001068-19-5	43





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BNA_G
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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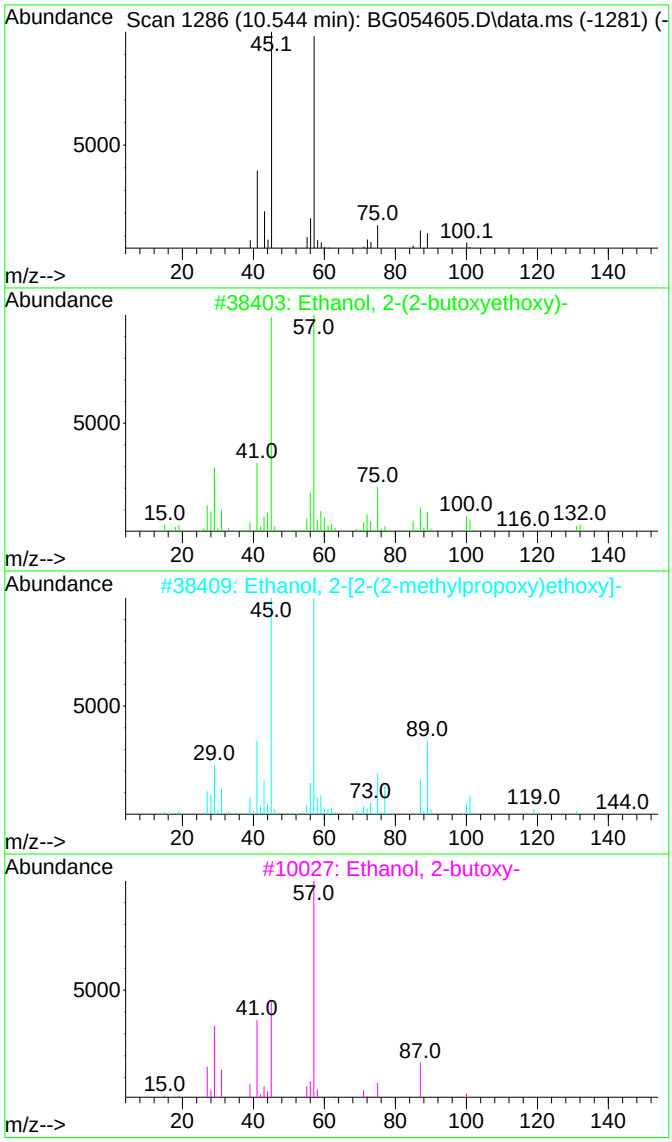
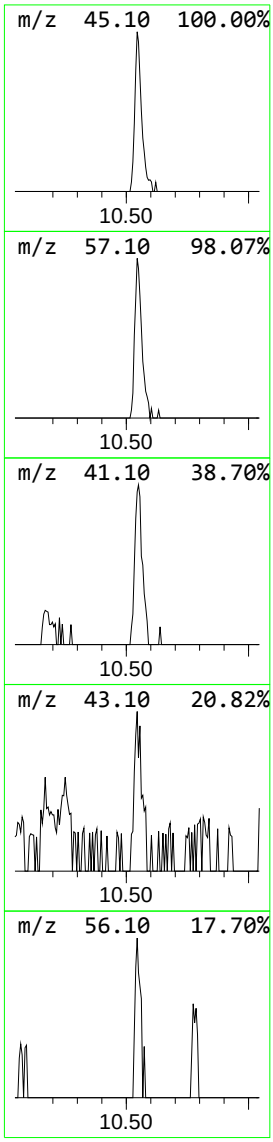
****

Peak Number 7 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.544	5.30 ng	27038	Naphthalene-d8	10.779

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	50
4	Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	50
5	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	43





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TIC Library : C:\Database\NIST20.L
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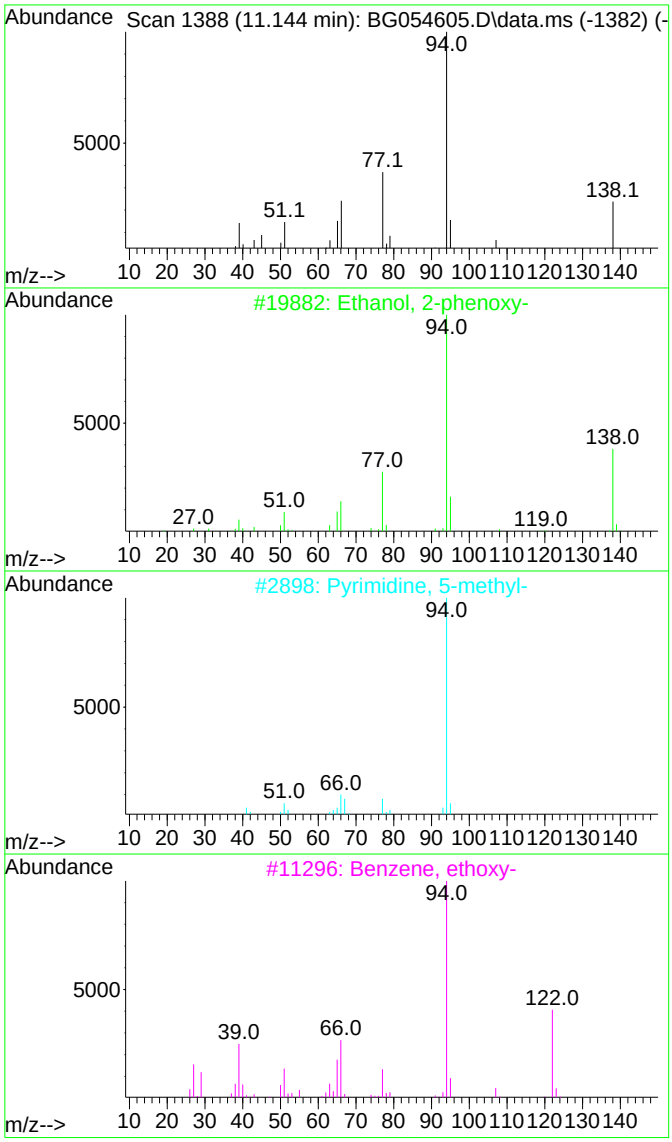
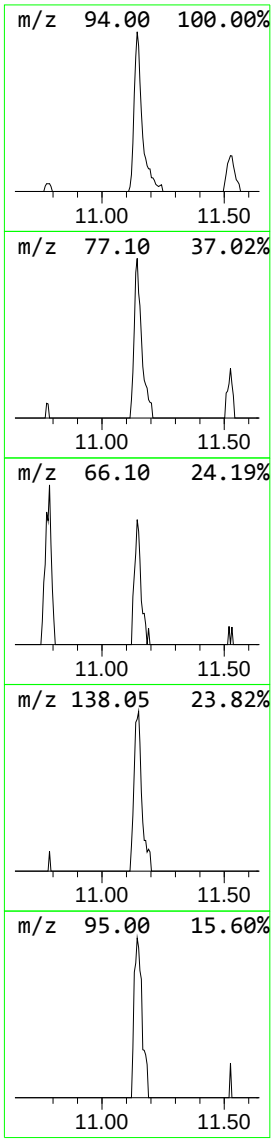
****

Peak Number 8 Ethanol, 2-phenoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.144	6.59 ng	33646	Naphthalene-d8	10.779

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	91
2	Pyrimidine, 5-methyl-	94	C5H6N2	002036-41-1	64
3	Benzene, ethoxy-	122	C8H10O	000103-73-1	64
4	Acetic acid, phenyl ester	136	C8H8O2	000122-79-2	59
5	Carbamic acid, phenyl ester	137	C7H7NO2	000622-46-8	59





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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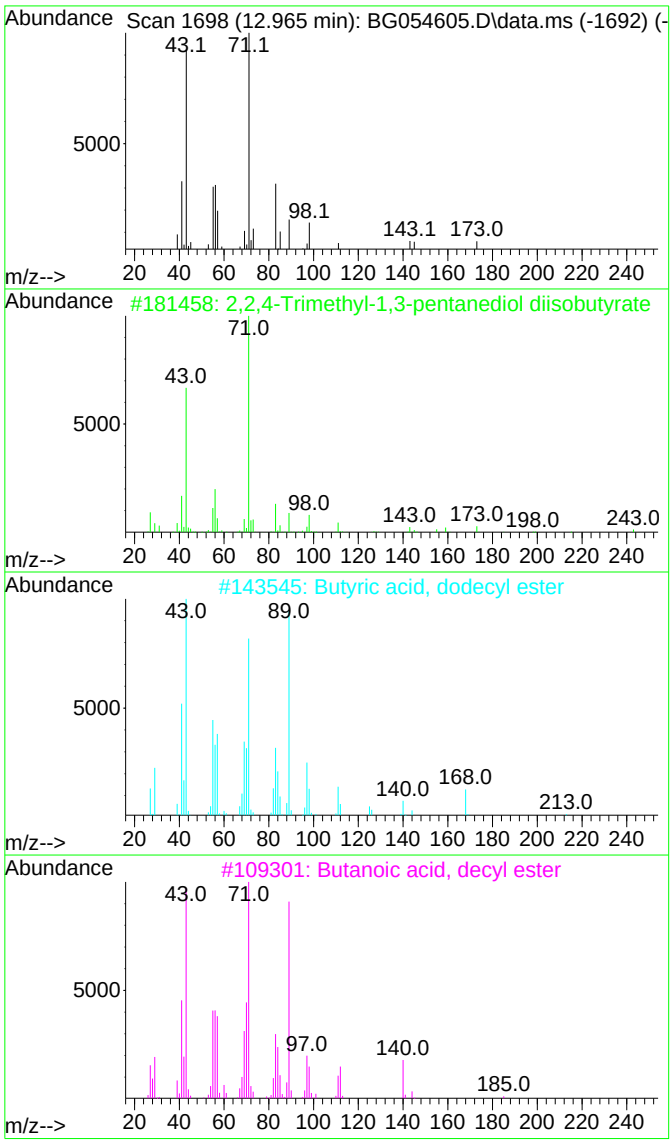
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

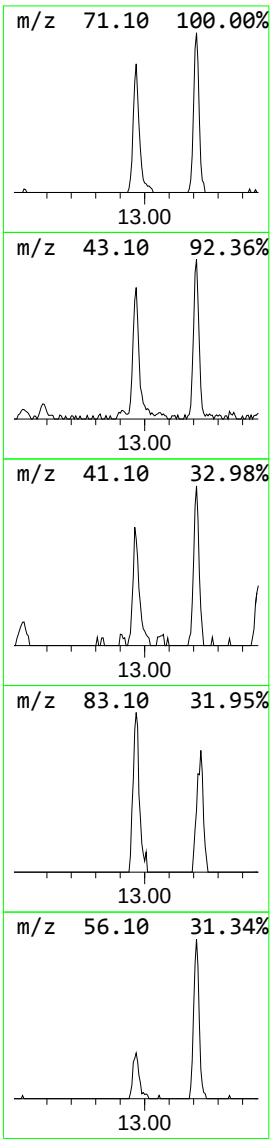
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.965	6.89 ng	60500	Acenaphthene-d10	14.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	72
2	Butyric acid, dodecyl ester	256	C16H32O2	003724-61-6	50
3	Butanoic acid, decyl ester	228	C14H28O2	005454-09-1	50
4	Carbonic acid, decyl nonyl ester	328	C20H40O3	1000383-15-8	45
5	Sulfurous acid, octyl 2-pentyl e...	264	C13H28O3S	1000309-15-7	43





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Data File : BG054605.D
Acq On : 11 Aug 2022 15:07
Operator : CG/JU
Sample : N3972-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-1

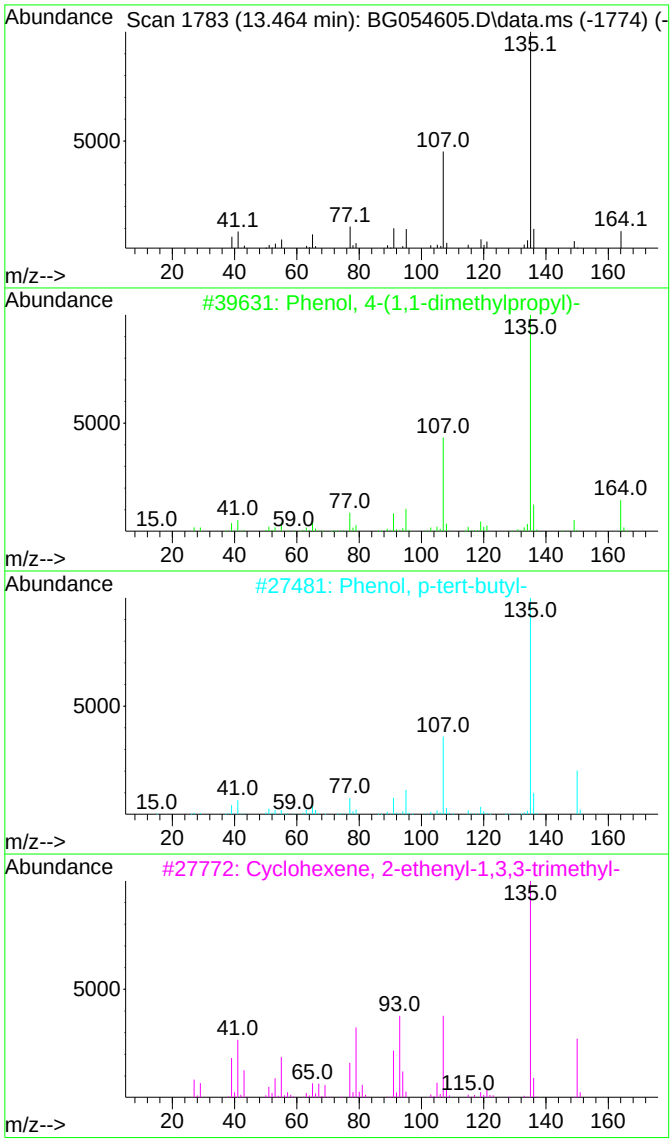
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

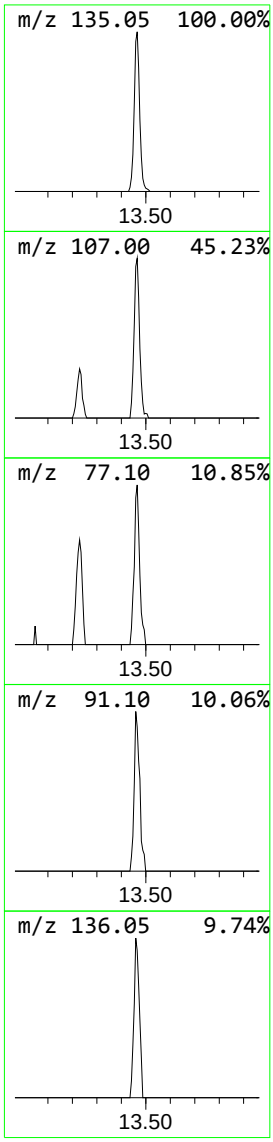
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Phenol, 4-(1,1-dimethylprop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.464	8.06 ng	70846	Acenaphthene-d10	14.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	91
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	78
3	Cyclohexene, 2-ethenyl-1,3,3-tri...	150	C11H18	005293-90-3	72
4	4,4'-(1,2-diethylethylene)diphenol	270	C18H22O2	005635-50-7	64
5	Imidazo[1,2-c]pyrimidin-5-ol	135	C6H5N3O	055662-66-3	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081122\
Data File : BG054605.D
Acq On : 11 Aug 2022 15:07
Operator : CG/JU
Sample : N3972-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

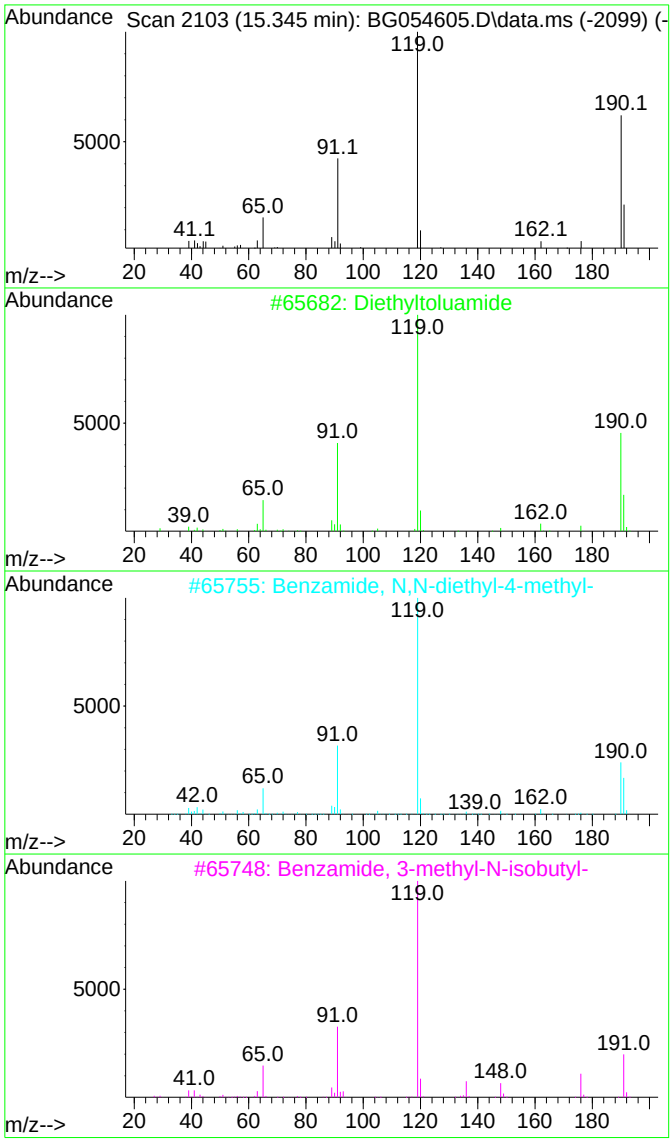
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

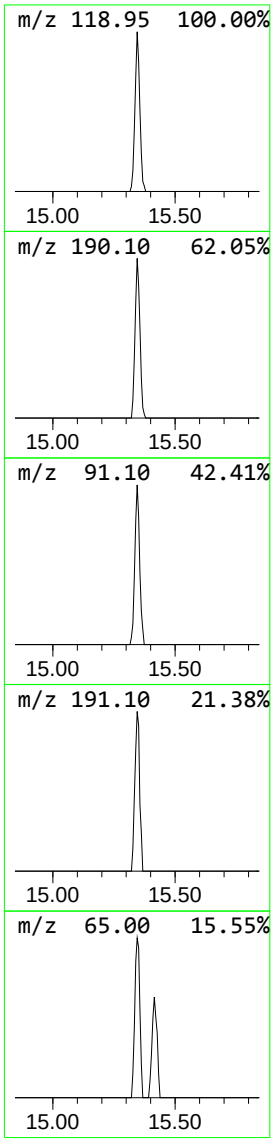
****

Peak Number 11 Diethyltoluamide Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.345	5.30 ng	46522	Acenaphthene-d10	14.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyltoluamide	191	C12H17NO	000134-62-3	94
2	Benzamide, N,N-diethyl-4-methyl-	191	C12H17NO	002728-05-4	80
3	Benzamide, 3-methyl-N-isobutyl-	191	C12H17NO	1000407-41-0	58
4	1-Propanone, 2-methyl-1-(4-methy...	162	C11H14O	050390-51-7	53
5	Benzamide, 2-methyl-N-propyl-	177	C11H15NO	1000407-39-2	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081122\
Data File : BG054605.D
Acq On : 11 Aug 2022 15:07
Operator : CG/JU
Sample : N3972-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-1

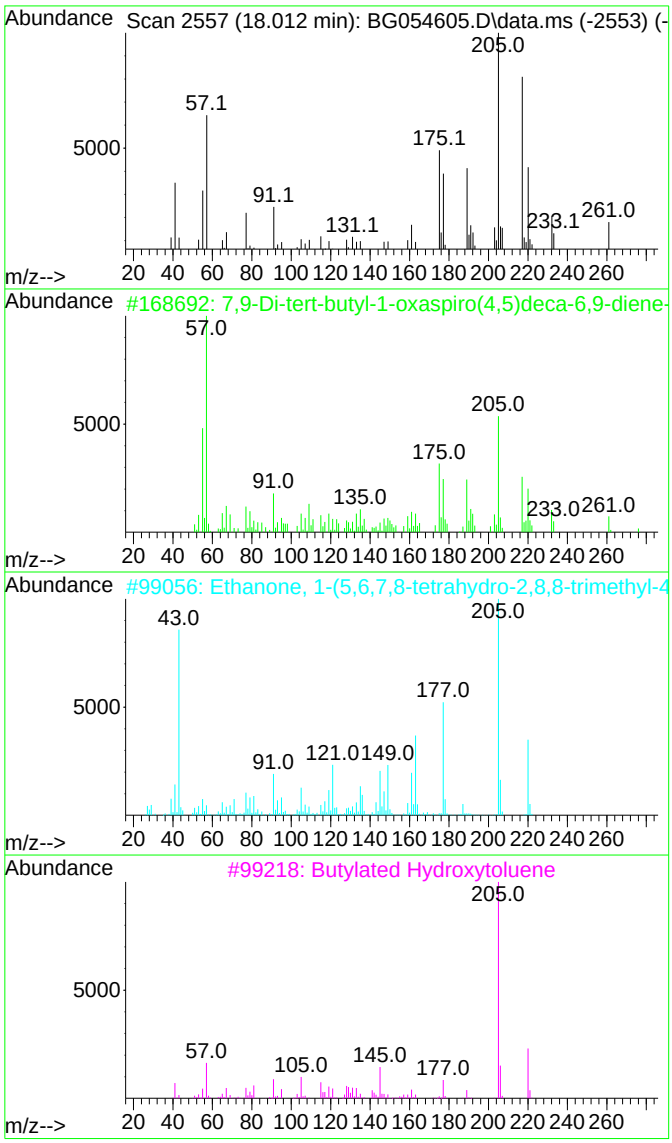
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

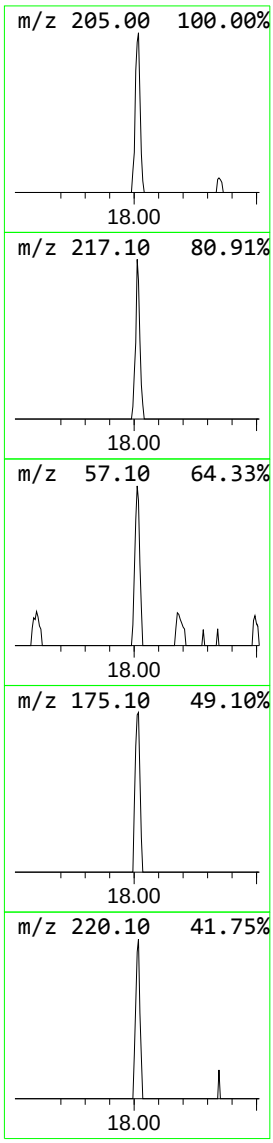
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.012	2.41 ng	32105	Phenanthrene-d10	17.360

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	90
2	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	41
3	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	38
4	1-Ethyl-2-methylphenanthrene	220	C17H16	061983-53-7	38
5	2,3-Quinoxalinedione, 6-amino-1,...	205	C10H11N3O2	1010338-06-6	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081122\
Data File : BG054605.D
Acq On : 11 Aug 2022 15:07
Operator : CG/JU
Sample : N3972-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.088	108.6	ng	405486	1	7.971	74696	20.0
Cyclopentanone	4.404	5.2	ng	19223	1	7.971	74696	20.0
2-Propanol, 1-(...	7.501	5.3	ng	19951	1	7.971	74696	20.0
unknown7.554	7.554	5.4	ng	20140	1	7.971	74696	20.0
2-Propanol, 1-(...	7.742	8.8	ng	32673	1	7.971	74696	20.0
Ethanol, 2-(hex...	9.293	9.2	ng	34421	1	7.971	74696	20.0
Ethanol, 2-(2-b...	10.544	5.3	ng	27038	2	10.779	102088	20.0
Ethanol, 2-phen...	11.144	6.6	ng	33646	2	10.779	102088	20.0
2,2,4-Trimethyl...	12.965	6.9	ng	60500	3	14.610	175700	20.0
Phenol, 4-(1,1-...	13.464	8.1	ng	70846	3	14.610	175700	20.0
Diethyltoluamide	15.345	5.3	ng	46522	3	14.610	175700	20.0
7,9-Di-tert-but...	18.012	2.4	ng	32105	4	17.360	266689	20.0