LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081122\
Data File : BG054601.D
Acq On : 11 Aug 2022 12:23
Operator : CG/JU
Sample : N3971-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-8R

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: BG054601.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	34	rVB	249089	428456	22.66%	6.494%
2	4.404	235	241	255	rVB	58116	98057	5.19%	1.486%
3	5.051	345	351	360	rBV2	16535	27945	1.48%	0.424%
4	5.556	431	437	448	rBV	112575	198594	10.50%	3.010%
5	6.602	609	615	622	rBV	17462	28291	1.50%	0.429%
6	7.172	705	712	724	rBV	69743	131005	6.93%	1.985%
7	7.971	842	848	854	rBV	48855	84107	4.45%	1.275%
8	8.030	854	858	868	rVB	35672	59415	3.14%	0.900%
9	9.140	1040	1047	1060	rVB	157234	300527	15.89%	4.555%
10	10.779	1318	1326	1333	rBV	61208	112649	5.96%	1.707%
11	11.713	1479	1485	1496	rVB3	16482	37170	1.97%	0.563%
12	13.229	1735	1743	1755	rBV	536193	845152	44.69%	12.809%
13	13.464	1776	1783	1795	rBB	183227	291523	15.42%	4.418%
14	14.610	1972	1978	1986	rBV	120405	188827	9.99%	2.862%
15	16.108	2226	2233	2247	rBV	489397	774639	40.96%	11.740%
16	16.690	2327	2332	2339	rVB	12455	19998	1.06%	0.303%
17	17.360	2438	2446	2455	rBV	176162	267492	14.14%	4.054%
18	18.012	2551	2557	2562	rBV2	22720	28589	1.51%	0.433%
19	19.969	2884	2890	2896	rBV	1445328	1891089	100.00%	28.661%
20	21.625	3166	3172	3181	rBV	217787	370649	19.60%	5.617%
21	23.059	3410	3416	3425	rVB4	16926	33776	1.79%	0.512%
22	24.833	3708	3718	3729	rVB	129741	380206	20.11%	5.762%

Sum of corrected areas: 6598156

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081122\
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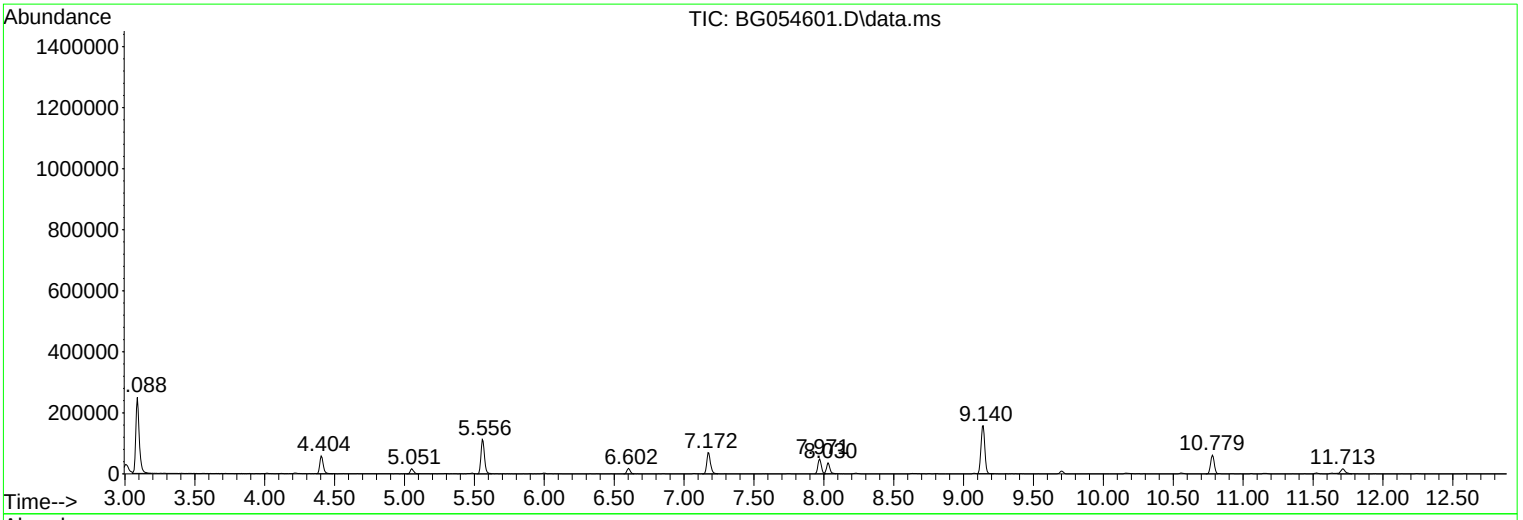
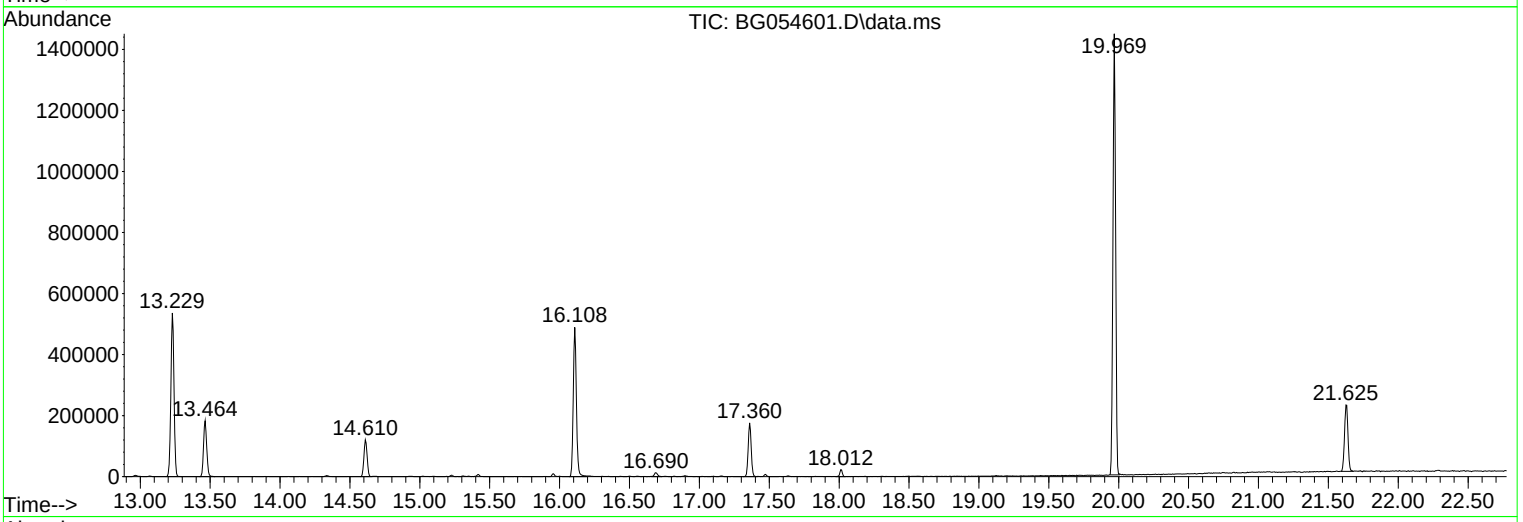
Sample : N3971-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

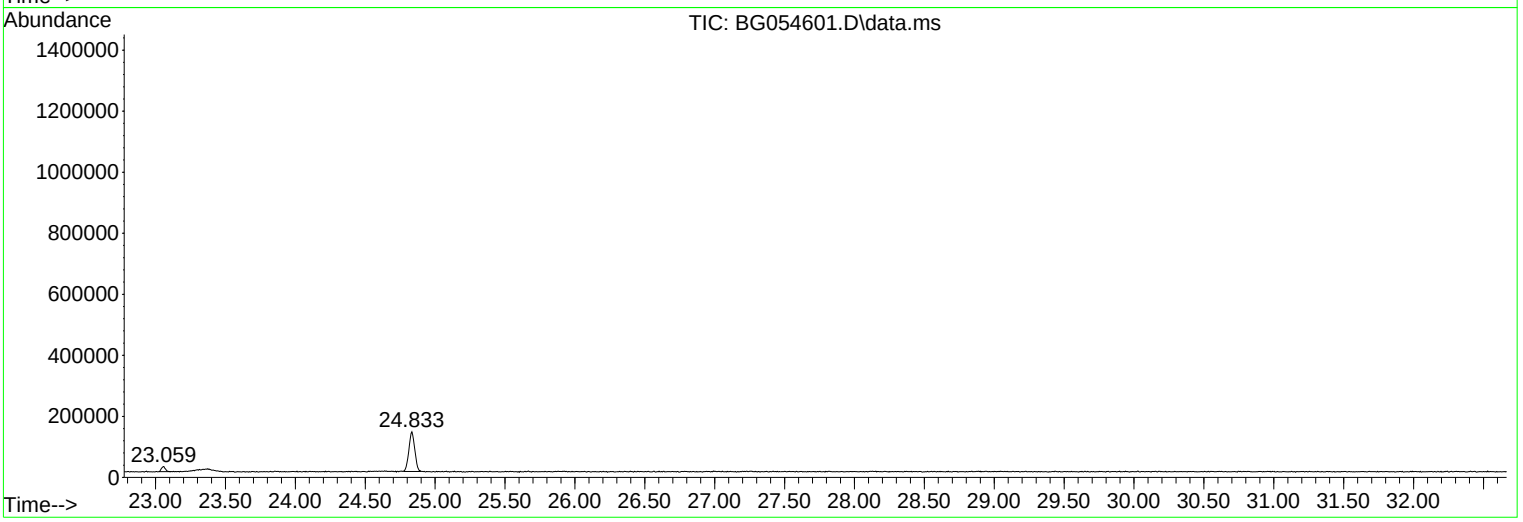
Instrument :
BNA_G
ClientSampleId :
MW-8R

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081122\
Data File : BG054601.D
Acq On : 11 Aug 2022 12:23
Operator : CG/JU
Sample : N3971-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-8R

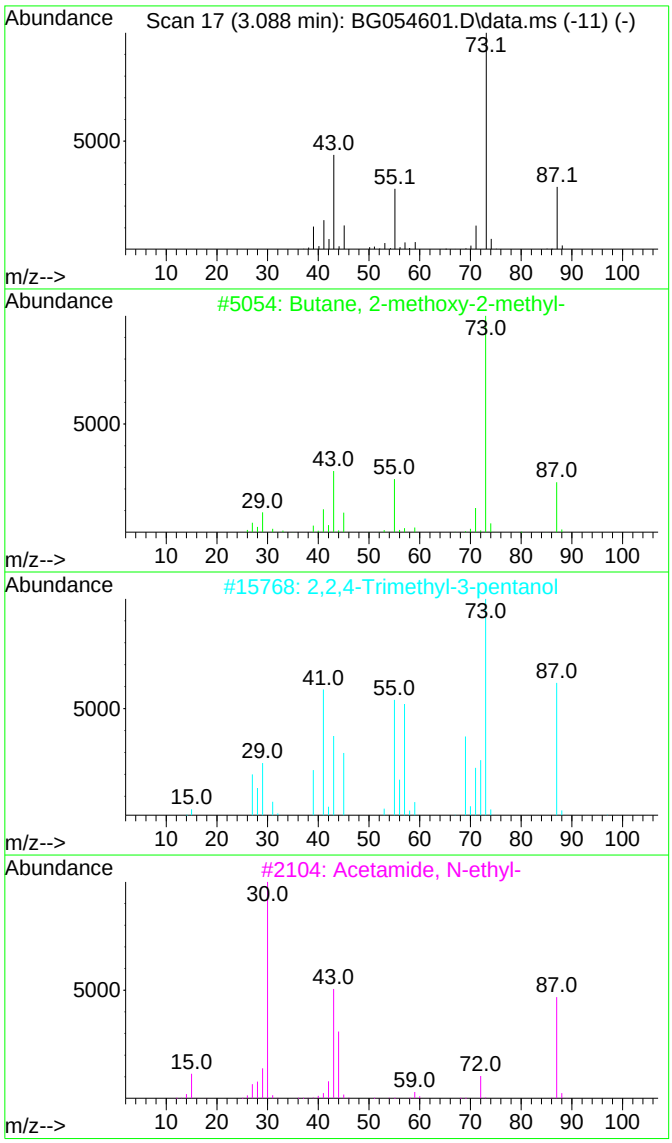
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

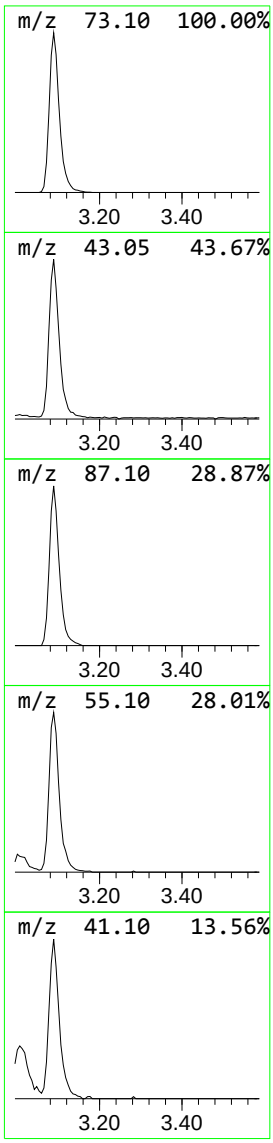
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.088	101.88 ng	428456	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	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	35
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Data File : BG054601.D
Acq On : 11 Aug 2022 12:23
Operator : CG/JU
Sample : N3971-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-8R

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

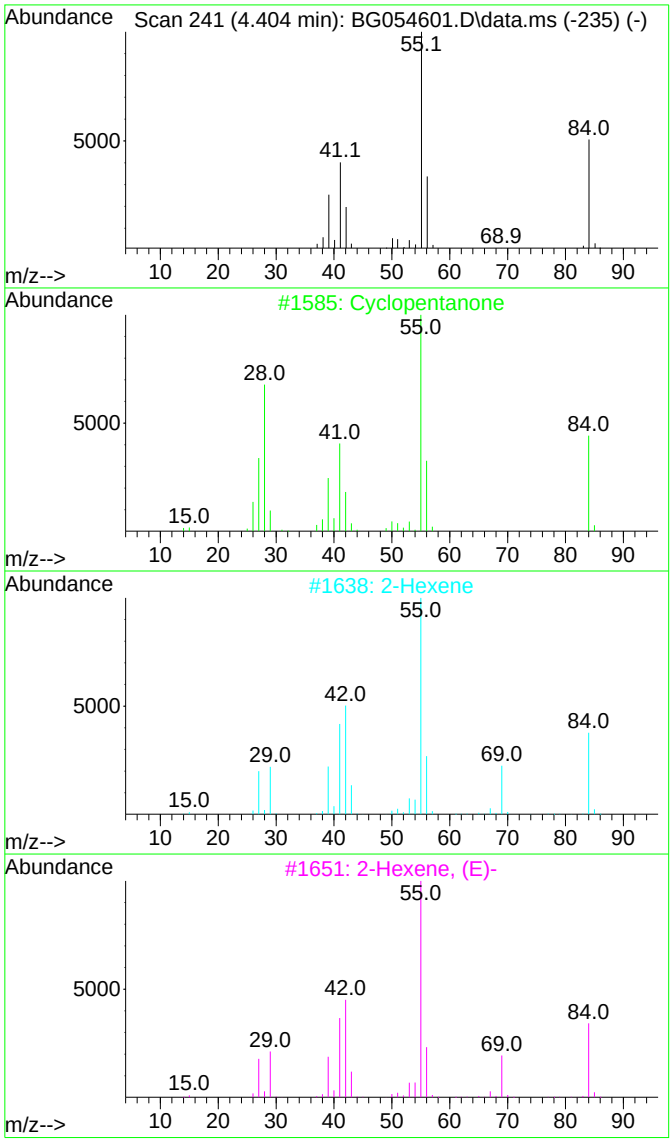
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

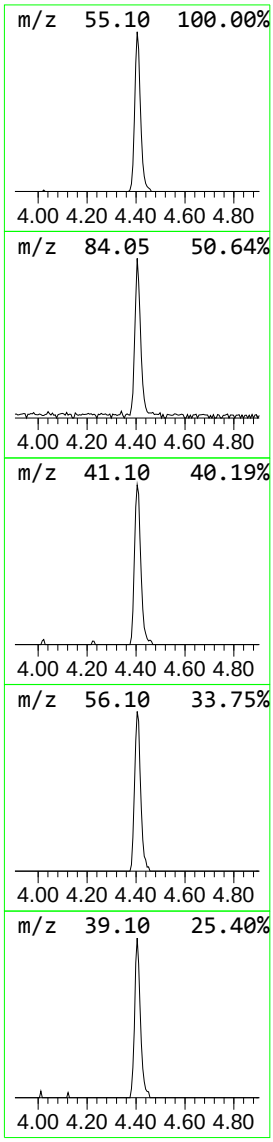
****

Peak Number 2 Cyclopentanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.404	23.32 ng	98057	1,4-Dichlorobenzene-d4	7.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	91
2	2-Hexene	84	C6H12	000592-43-8	59
3	2-Hexene, (E)-	84	C6H12	004050-45-7	59
4	2-Hexene, (Z)-	84	C6H12	007688-21-3	59
5	Furan, 2,3-dihydro-4-methyl-	84	C5H8O	034314-83-5	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081122\
Data File : BG054601.D
Acq On : 11 Aug 2022 12:23
Operator : CG/JU
Sample : N3971-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-8R

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

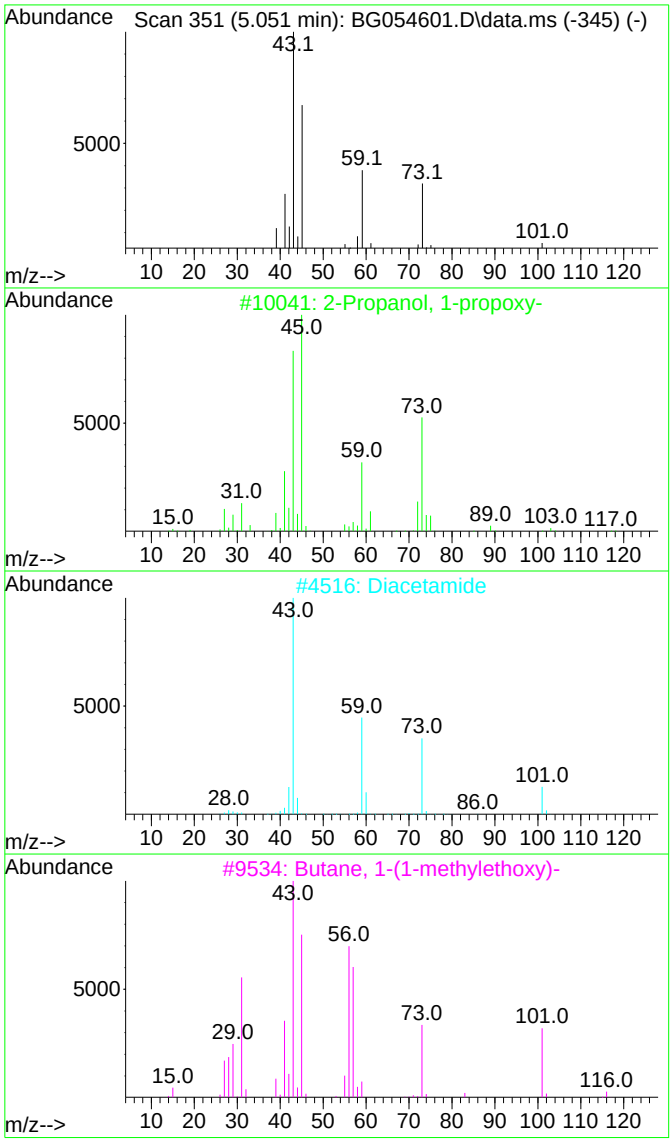
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

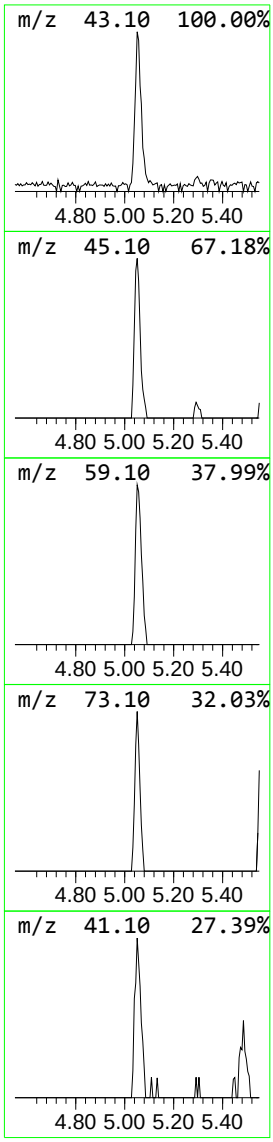
****

Peak Number 3 unknown5.051 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.051	6.65 ng	27945	1,4-Dichlorobenzene-d4	7.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	38
2	Diacetamide	101	C4H7NO2	000625-77-4	37
3	Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	36
4	2-Methyoxirane-2-carboxylic acid...	116	C5H8O3	1010306-64-8	33
5	Ethanol, 2-propoxy-	104	C5H12O2	002807-30-9	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081122\
Data File : BG054601.D
Acq On : 11 Aug 2022 12:23
Operator : CG/JU
Sample : N3971-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-8R

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

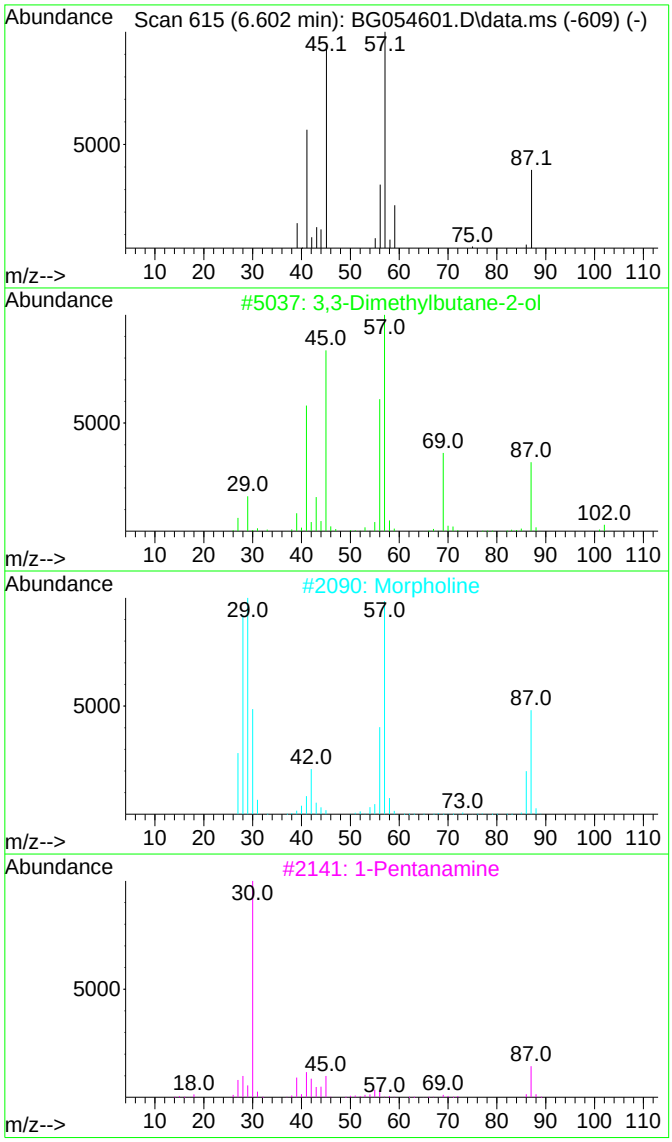
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

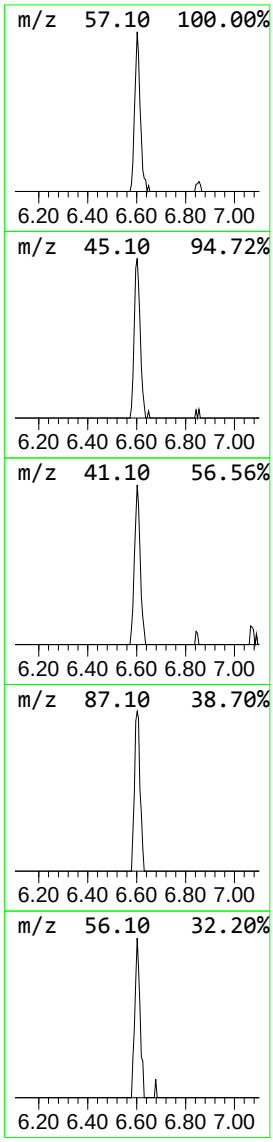
****

Peak Number 4 unknown6.602 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.602	6.73 ng	28291	1,4-Dichlorobenzene-d4	7.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	38
2	Morpholine	87	C4H9NO	000110-91-8	17
3	1-Pentanamine	87	C5H13N	000110-58-7	9
4	Butane, 1-chloro-2-methyl-, (S)-	106	C5H11Cl	040560-29-0	9
5	di-t-Butylhydrazodicarboxylate	232	C10H20N2O4	016466-61-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081122\
Data File : BG054601.D
Acq On : 11 Aug 2022 12:23
Operator : CG/JU
Sample : N3971-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-8R

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

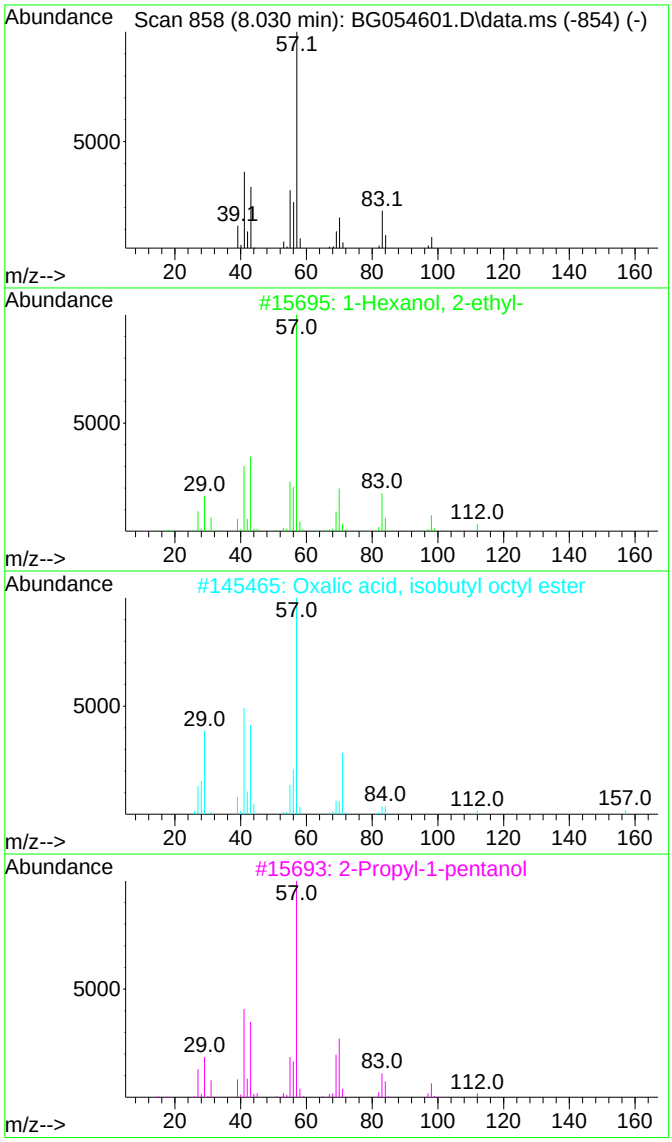
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

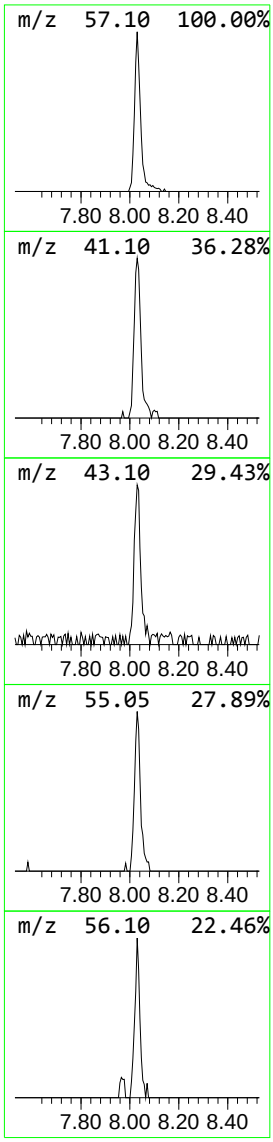
****

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.030	14.13 ng	59415	1,4-Dichlorobenzene-d4	7.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2	Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	64
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	45
4	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	43
5	Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	42





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Data File : BG054601.D
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-8R

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

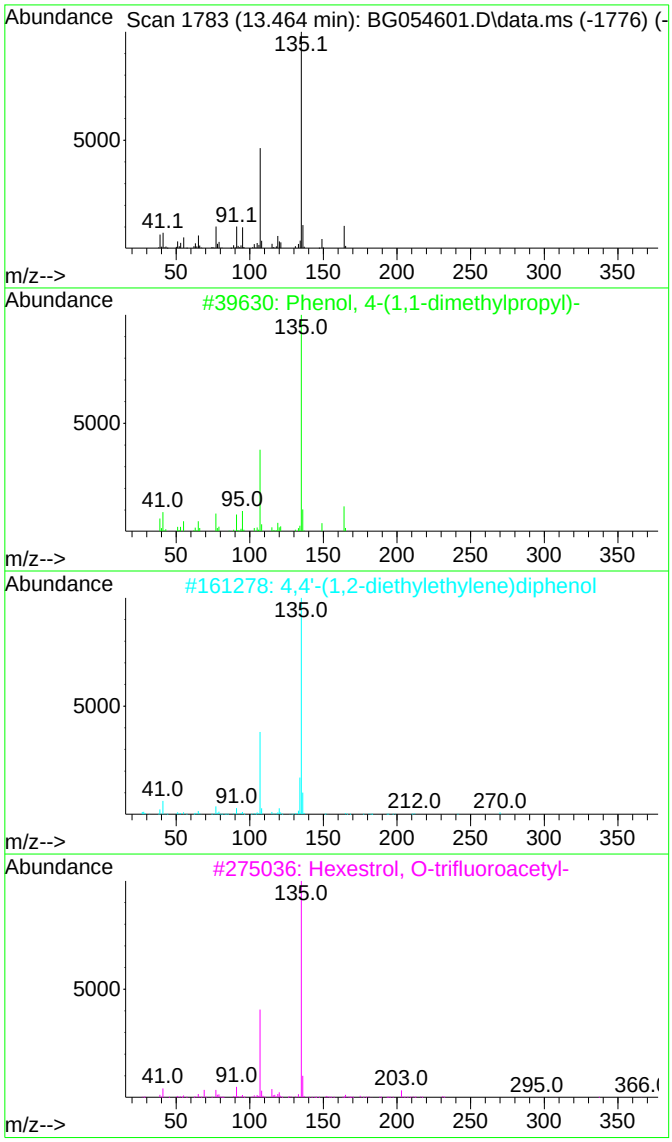
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

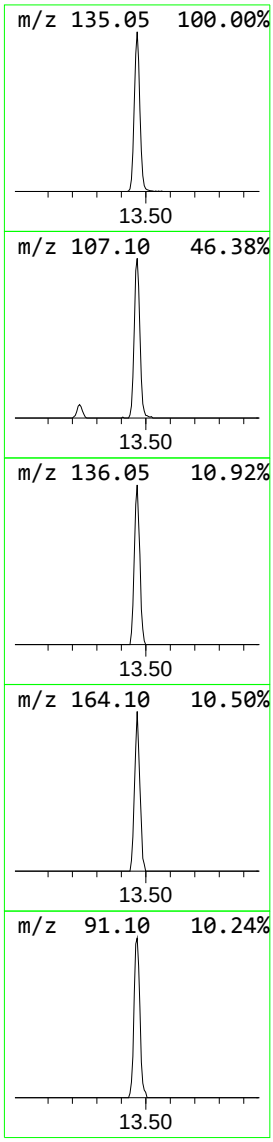
****

Peak Number 6 Phenol, 4-(1,1-dimethylprop... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.464	30.88 ng	291523	Acenaphthene-d10	14.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	97
2	4,4'-(1,2-diethylethylene)diphenol	270	C18H22O2	005635-50-7	64
3	Hexestrol, O-trifluoroacetyl-	366	C20H21F3O3	1000365-31-7	64
4	4-Hydroxy-2-methylacetophenone	150	C9H10O2	000875-59-2	59
5	1,5,6,7-Tetrahydro-4-indolone	135	C8H9NO	013754-86-4	59





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Operator : CG/JU
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ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-8R

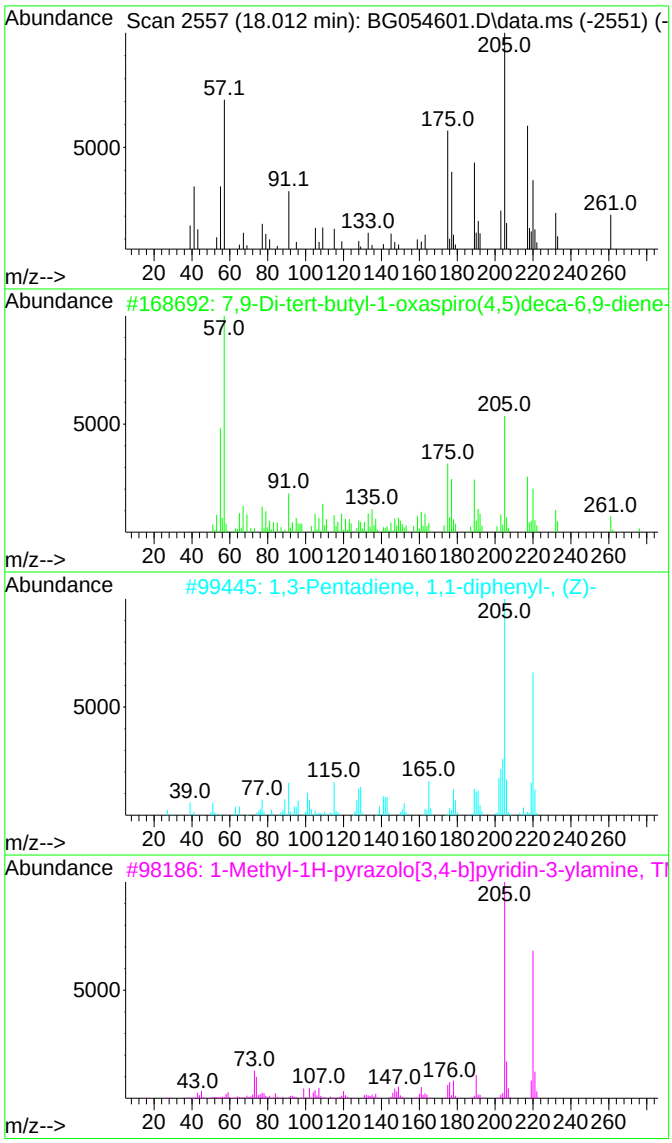
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

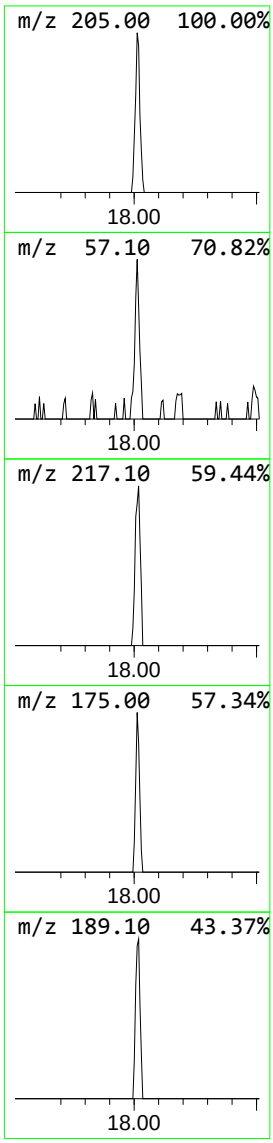
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.012	2.14 ng	28589	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	87
2	1,3-Pentadiene, 1,1-diphenyl-, (Z)-	220	C17H16	015295-31-5	38
3	1-Methyl-1H-pyrazolo[3,4-b]pyrid...	220	C10H16N4Si	1000468-34-6	38
4	Glutaric acid, 2,3-dichloropheny...	366	C18H16Cl2O4	1000391-81-6	35
5	2,3-Quinoxalinedione, 6-amino-1,...	205	C10H11N3O2	1010338-06-6	30





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.088	101.9	ng	428456	1	7.971	84107	20.0
Cyclopentanone	4.404	23.3	ng	98057	1	7.971	84107	20.0
unknown5.051	5.051	6.7	ng	27945	1	7.971	84107	20.0
unknown6.602	6.602	6.7	ng	28291	1	7.971	84107	20.0
1-Hexanol, 2-et...	8.030	14.1	ng	59415	1	7.971	84107	20.0
Phenol, 4-(1,1-...	13.464	30.9	ng	291523	3	14.610	188827	20.0
7,9-Di-tert-but...	18.012	2.1	ng	28589	4	17.360	267492	20.0