LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081022\
Data File : BG054593.D
Acq On : 10 Aug 2022 18:10
Operator : CG/JU
Sample : N3972-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-4

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: BG054593.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.094	12	18	31	rVB	239588	458335	27.57%	6.931%
2	4.410	236	242	254	rVB	69653	120053	7.22%	1.816%
3	5.056	346	352	362	rBV	22590	40598	2.44%	0.614%
4	5.562	432	438	451	rBV	128147	227304	13.67%	3.437%
5	6.607	610	616	626	rVB	25758	42778	2.57%	0.647%
6	7.177	707	713	726	rBV	79466	149101	8.97%	2.255%
7	7.976	842	849	855	rBV	59577	105042	6.32%	1.589%
8	8.035	855	859	867	rVB2	9855	16968	1.02%	0.257%
9	9.140	1040	1047	1061	rBV	183984	343948	20.69%	5.201%
10	9.704	1137	1143	1150	rBB	10532	19454	1.17%	0.294%
11	10.785	1318	1327	1334	rBV	81948	145274	8.74%	2.197%
12	11.713	1478	1485	1497	rVB2	32789	76252	4.59%	1.153%
13	13.235	1735	1744	1755	rBV	567677	919867	55.33%	13.911%
14	13.470	1777	1784	1796	rBB	154763	245428	14.76%	3.712%
15	14.616	1972	1979	1985	rBV	141139	220951	13.29%	3.341%
16	16.114	2227	2234	2249	rBV	505956	790522	47.55%	11.955%
17	17.365	2437	2447	2456	rBV	178174	285456	17.17%	4.317%
18	18.018	2553	2558	2561	rBV2	16713	20433	1.23%	0.309%
19	19.974	2884	2891	2897	rBV	1225643	1662369	100.00%	25.139%
20	21.631	3167	3173	3182	rVB2	211986	360001	21.66%	5.444%
21	24.839	3711	3719	3729	rVB2	124283	362448	21.80%	5.481%

Sum of corrected areas: 6612582

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Misc :
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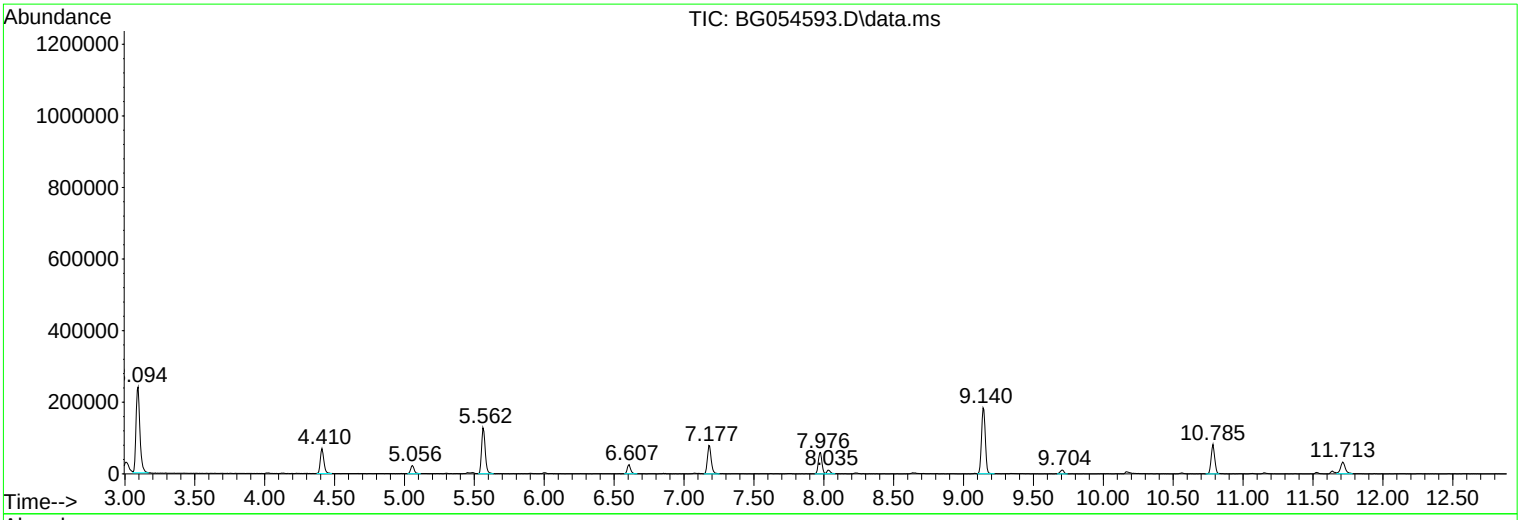
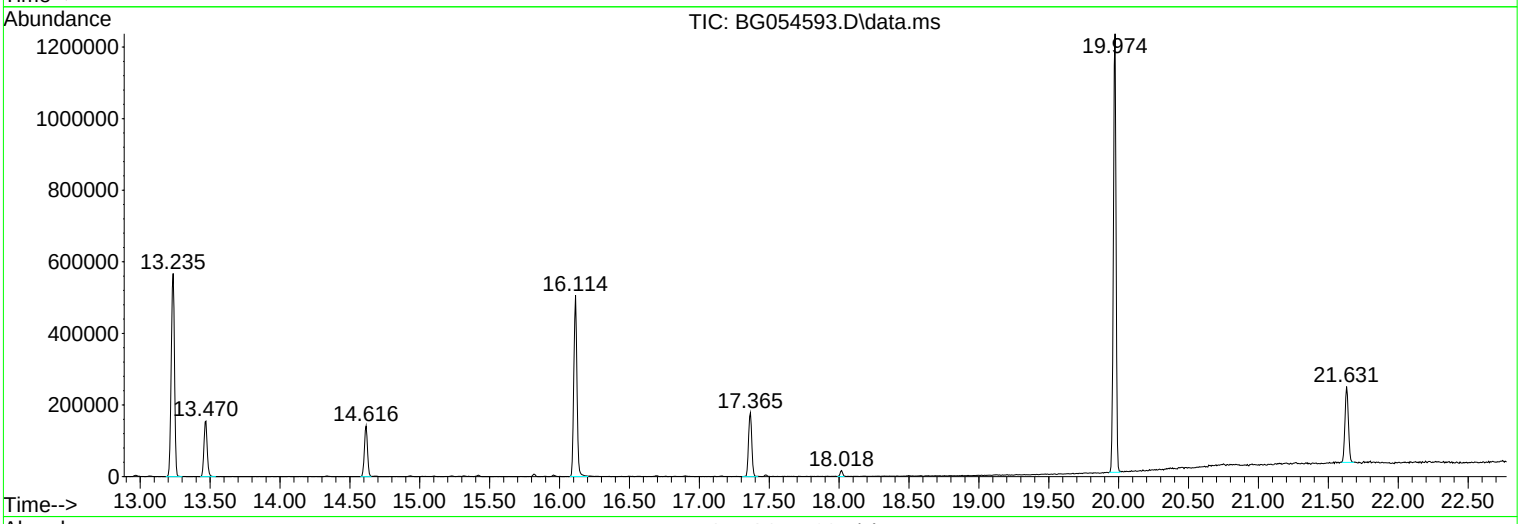
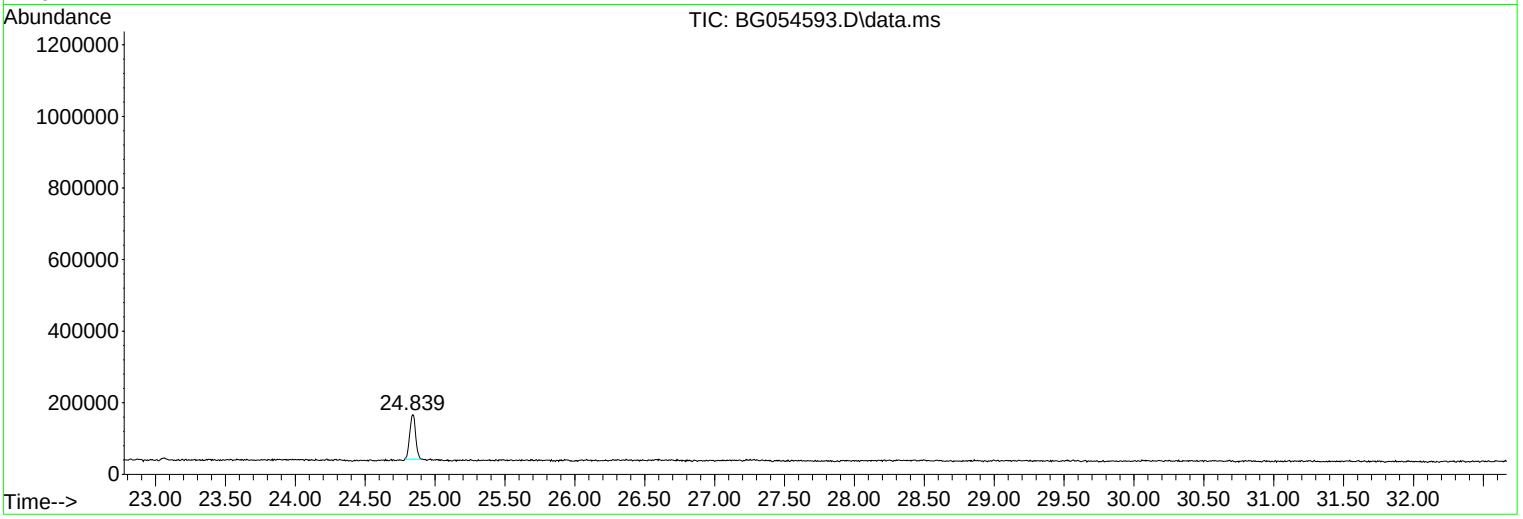
Instrument :
BNA_G
ClientSampleId :
SPN-4

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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Data File : BG054593.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

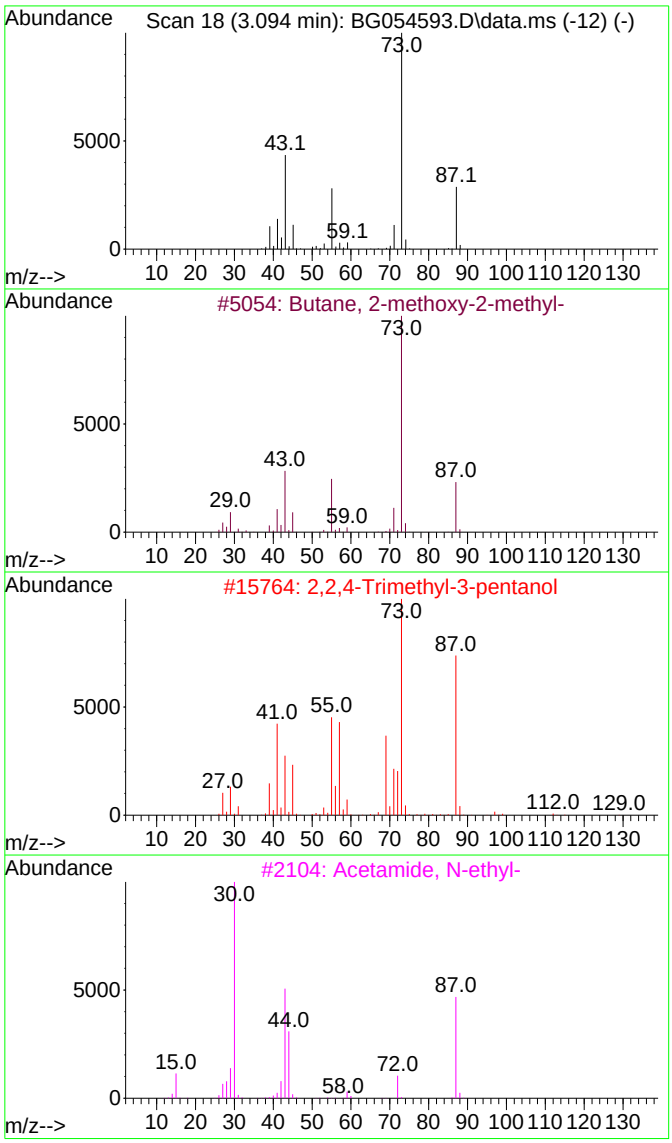
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

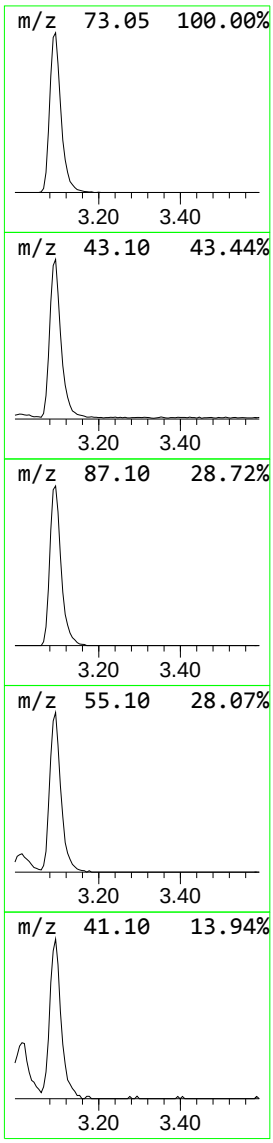
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.094	87.27 ng	458335	1,4-Dichlorobenzene-d4	7.976

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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Data File : BG054593.D
Acq On : 10 Aug 2022 18:10
Operator : CG/JU
Sample : N3972-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-4

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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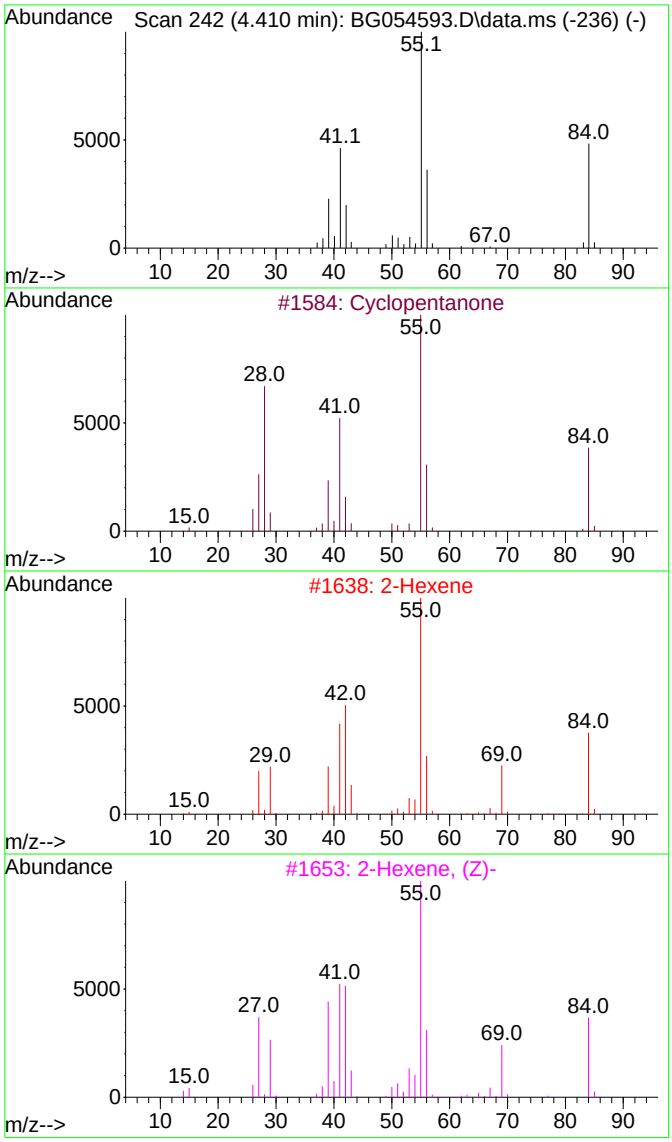
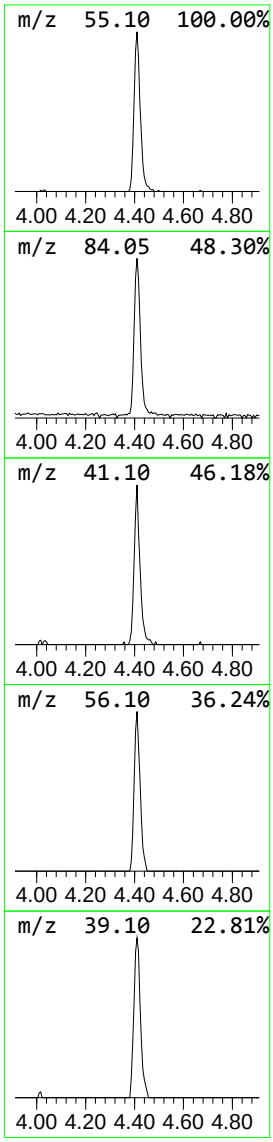
Peak Number 2 Cyclopentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.410	22.86 ng	120053	1,4-Dichlorobenzene-d4	7.976

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, (Z)-	84	C6H12	007688-21-3	53
4	2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	50
5	3-Hexene, (E)-	84	C6H12	013269-52-8	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081022\
Data File : BG054593.D
Acq On : 10 Aug 2022 18:10
Operator : CG/JU
Sample : N3972-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-4

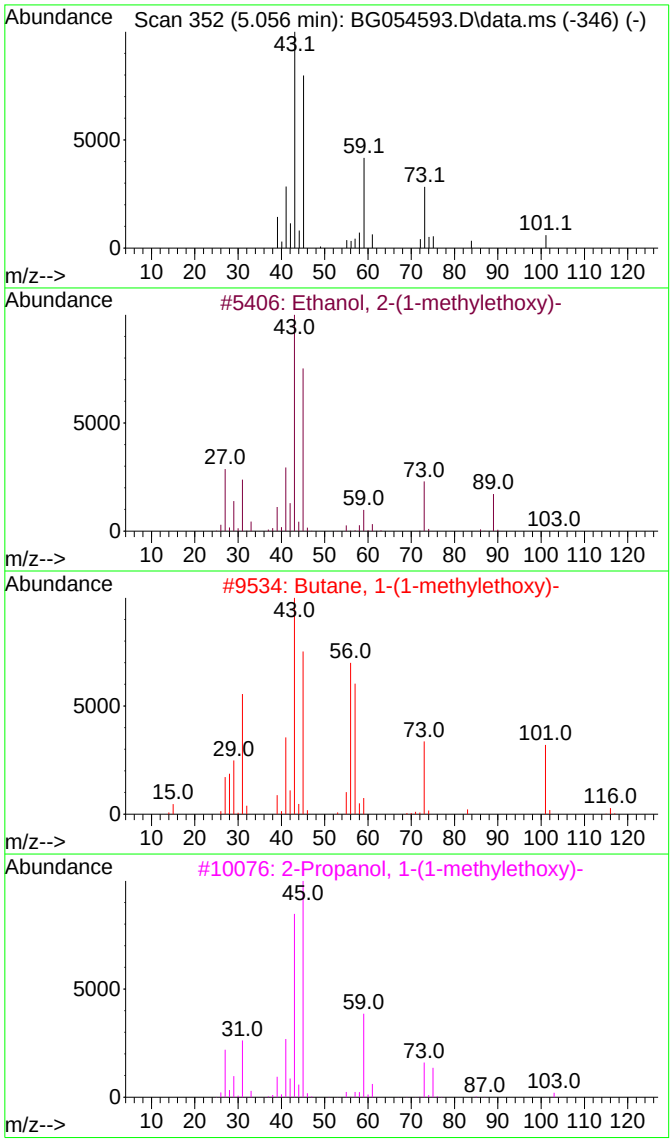
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

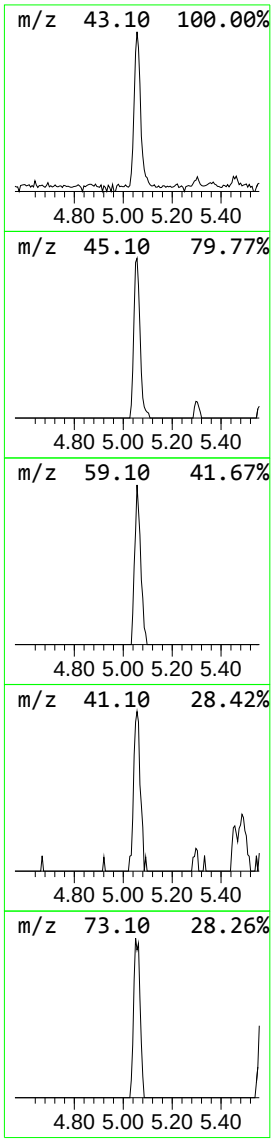
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol, 2-(1-methylethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.056	7.73 ng	40598	1,4-Dichlorobenzene-d4	7.976

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	59
2	Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	42
3	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	39
4	Diacetamide	101	C4H7NO2	000625-77-4	38
5	2-O-Mesyl arabinose	228	C6H12O7S	1000130-06-0	36





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Operator : CG/JU
Sample : N3972-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-4

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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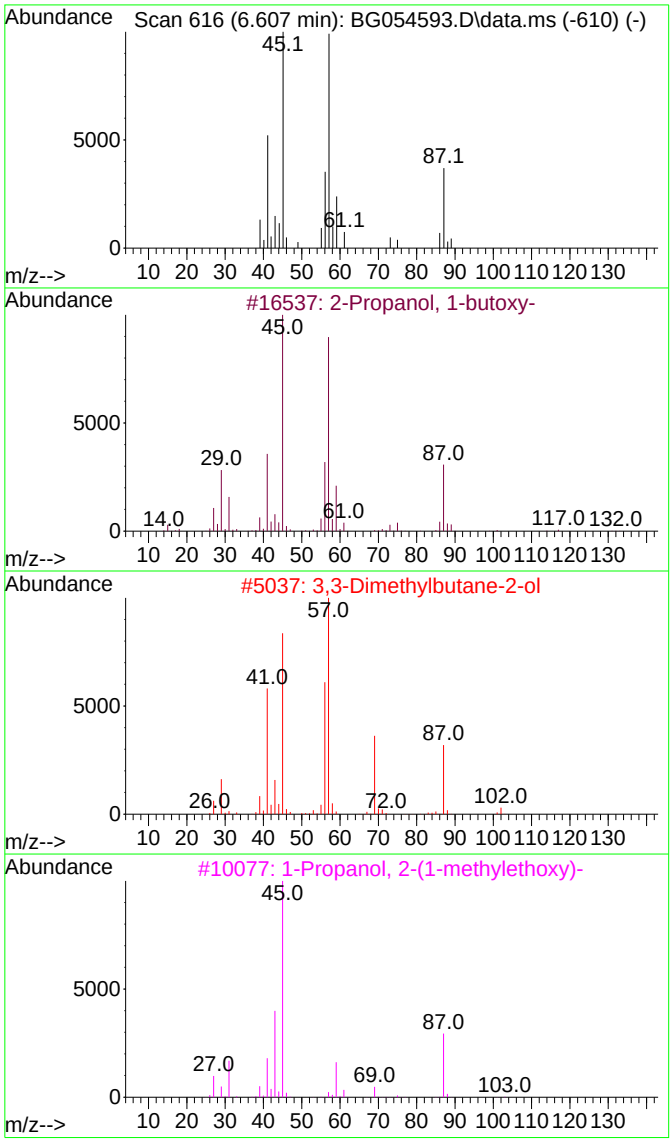
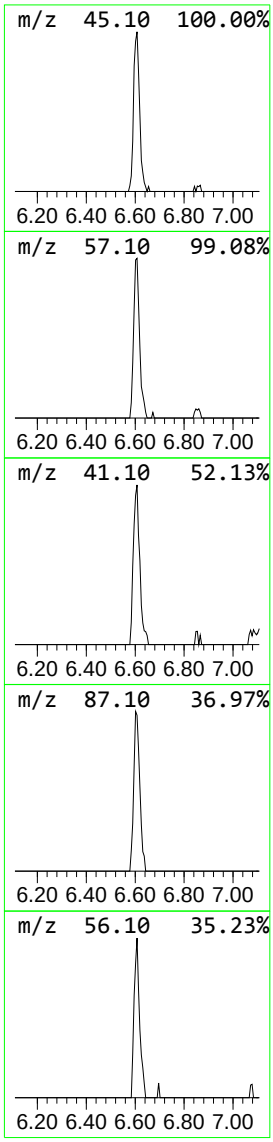
Peak Number 4 2-Propanol, 1-butoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.607	8.14 ng	42778	1,4-Dichlorobenzene-d4	7.976

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	83
2	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50
3	1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	42
4	Formic acid, 1-methylpropyl ester	102	C5H10O2	000589-40-2	38
5	2-Butanol	74	C4H10O	000078-92-2	37





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Sample : N3972-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-4

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

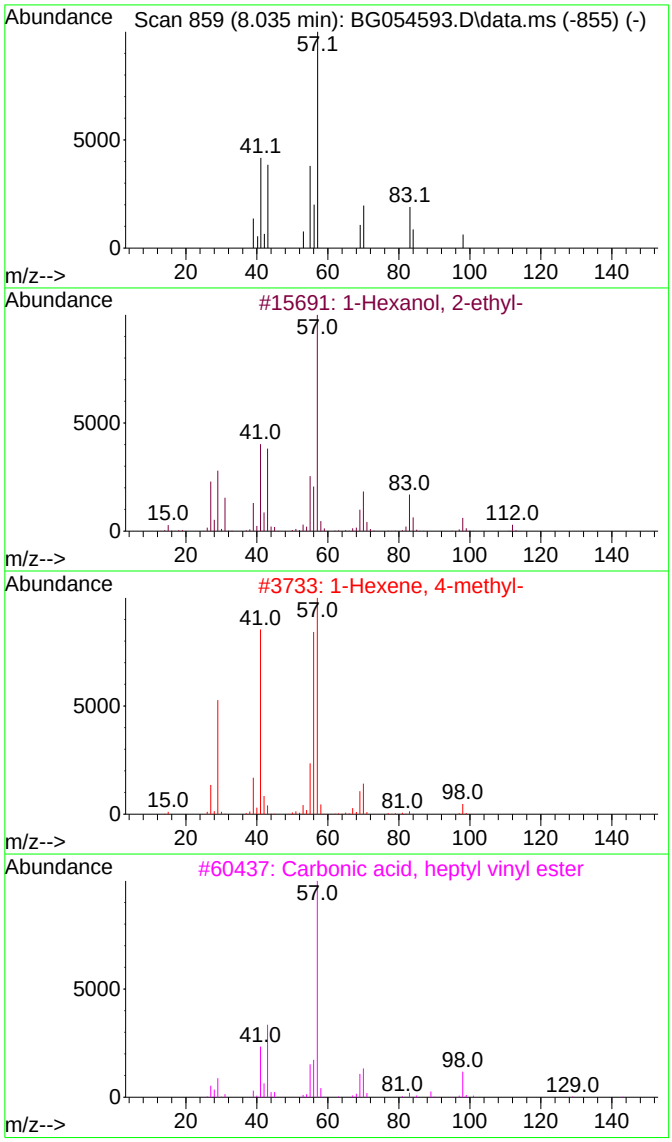
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

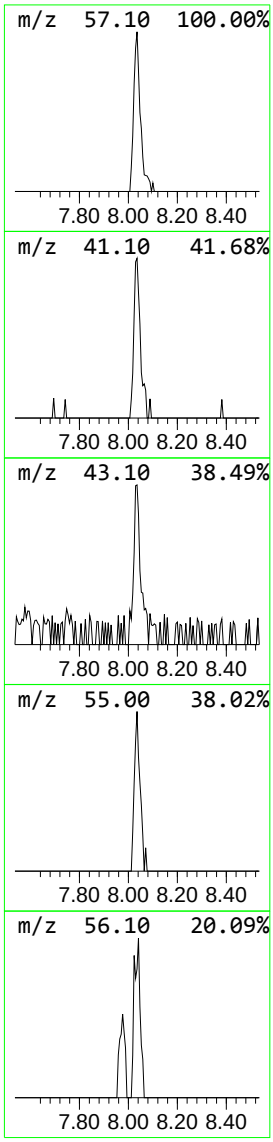
****

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.035	3.23 ng	16968	1,4-Dichlorobenzene-d4	7.976

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	38
3	Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	36
4	Acetic acid, cyano-, 2-ethylhexy...	197	C11H19NO2	013361-34-7	36
5	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	33





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-4

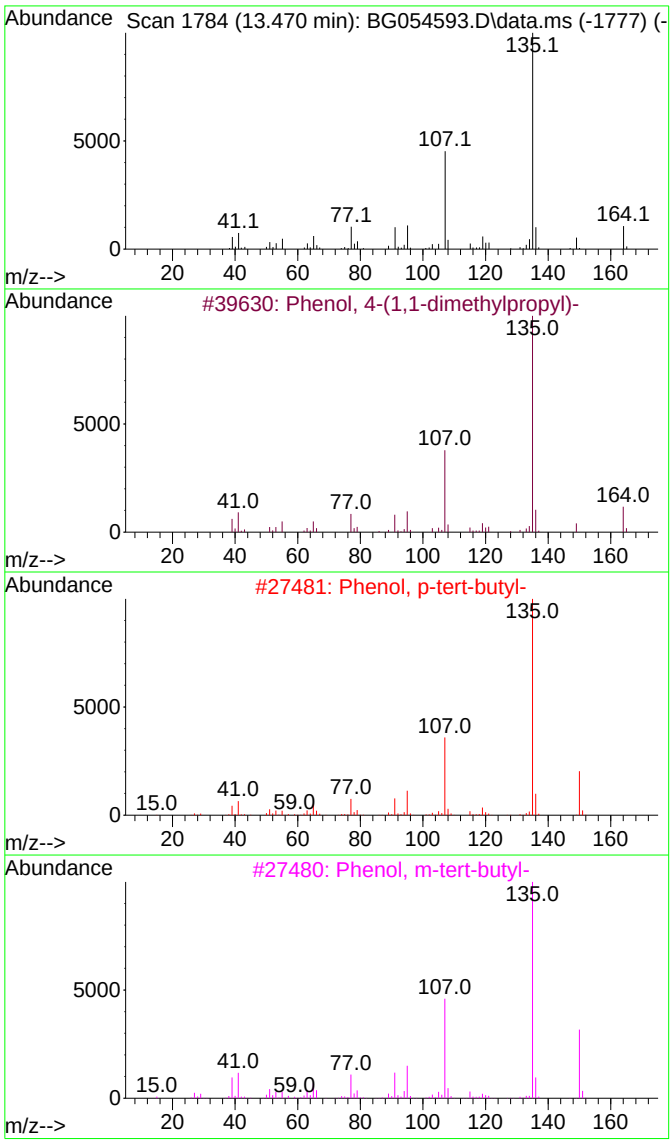
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

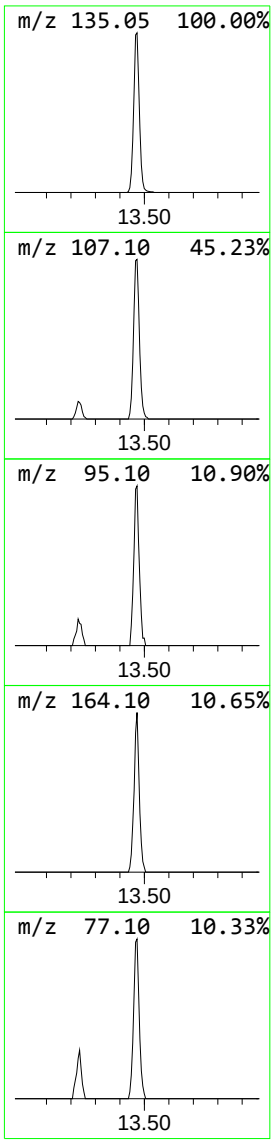
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Phenol, 4-(1,1-dimethylprop... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.470	22.22 ng	245428	Acenaphthene-d10	14.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	97
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	86
3	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	72
4	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	64
5	Hexestrol, O-trifluoroacetyl-	366	C20H21F3O3	1000365-31-7	64





Tentatively Identified Compound (LSC) summary

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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...	3.094	87.3	ng	458335	1	7.976	105042	20.0
Cyclopentanone	4.410	22.9	ng	120053	1	7.976	105042	20.0
Ethanol, 2-(1-m...	5.056	7.7	ng	40598	1	7.976	105042	20.0
2-Propanol, 1-b...	6.607	8.1	ng	42778	1	7.976	105042	20.0
1-Hexanol, 2-et...	8.035	3.2	ng	16968	1	7.976	105042	20.0
Phenol, 4-(1,1-...	13.470	22.2	ng	245428	3	14.616	220951	20.0