LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081022\
Data File : BG054592.D
Acq On : 10 Aug 2022 17:29
Operator : CG/JU
Sample : N3972-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SPN-8

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: BG054592.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	12	17	40	rVB	250629	497472	30.31%	7.159%
2	4.410	236	242	256	rVB2	61014	113048	6.89%	1.627%
3	5.056	344	352	359	rBV	17901	30406	1.85%	0.438%
4	5.461	416	421	432	rVB4	8330	17441	1.06%	0.251%
5	5.561	432	438	455	rVB	136349	253068	15.42%	3.642%
6	6.607	608	616	626	rBV	20946	36903	2.25%	0.531%
7	6.942	667	673	681	rVB2	17687	29847	1.82%	0.429%
8	7.183	707	714	727	rVB	87921	166091	10.12%	2.390%
9	7.359	738	744	752	rVB	33111	53648	3.27%	0.772%
10	7.976	842	849	855	rBV	64218	111899	6.82%	1.610%
11	8.088	863	868	874	rVB	24244	42561	2.59%	0.612%
12	8.346	906	912	918	rBV2	11122	17604	1.07%	0.253%
13	9.081	1031	1037	1041	rBV2	12318	17783	1.08%	0.256%
14	9.139	1041	1047	1059	rVB	193618	365527	22.27%	5.260%
15	9.709	1136	1144	1150	rBB2	10674	20559	1.25%	0.296%
16	10.179	1217	1224	1230	rBV5	13942	29450	1.79%	0.424%
17	10.785	1320	1327	1333	rBV	83660	153584	9.36%	2.210%
18	11.719	1480	1486	1494	rVB3	13949	31640	1.93%	0.455%
19	13.235	1736	1744	1759	rBV	605065	958144	58.37%	13.787%
20	13.470	1777	1784	1795	rVB	147060	240011	14.62%	3.454%
21	14.615	1972	1979	1986	rBV2	148353	233595	14.23%	3.361%
22	16.114	2227	2234	2247	rBV	502024	805561	49.07%	11.592%
23	17.365	2440	2447	2461	rVB	191928	297058	18.10%	4.275%
24	18.017	2553	2558	2566	rVB2	14109	18344	1.12%	0.264%
25	19.974	2884	2891	2897	rBV	1235415	1641539	100.00%	23.621%
26	21.631	3168	3173	3181	rVB	221502	368102	22.42%	5.297%
27	24.845	3710	3720	3730	rVB2	133339	398497	24.28%	5.734%

Sum of corrected areas: 6949382

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081022\
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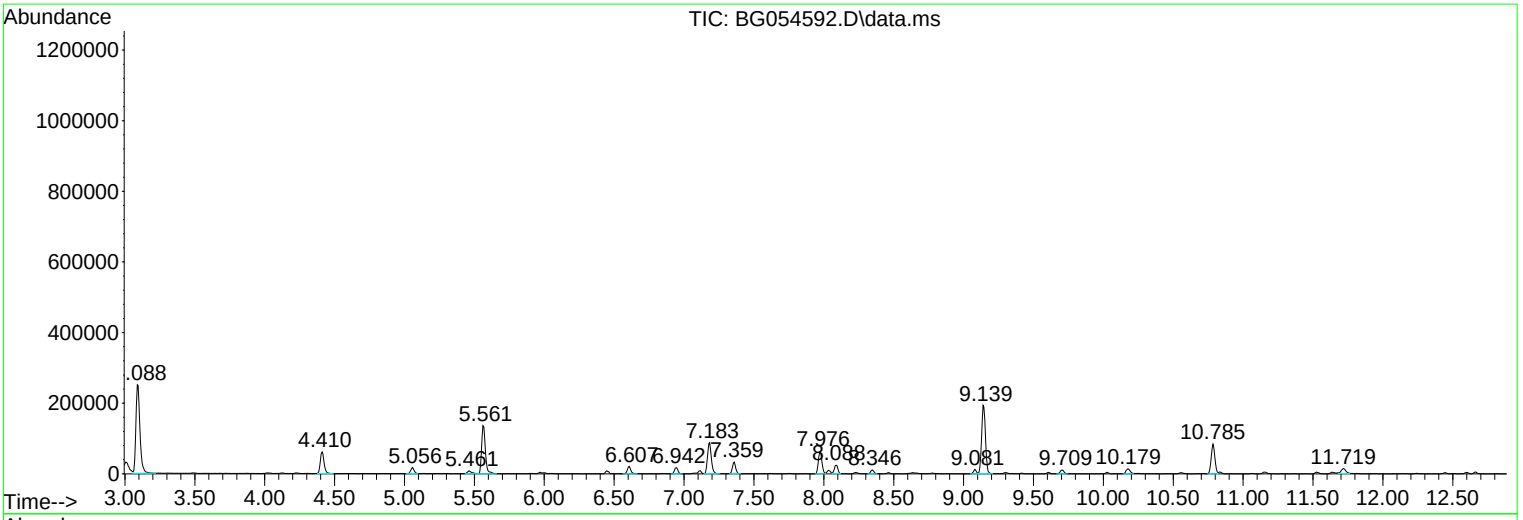
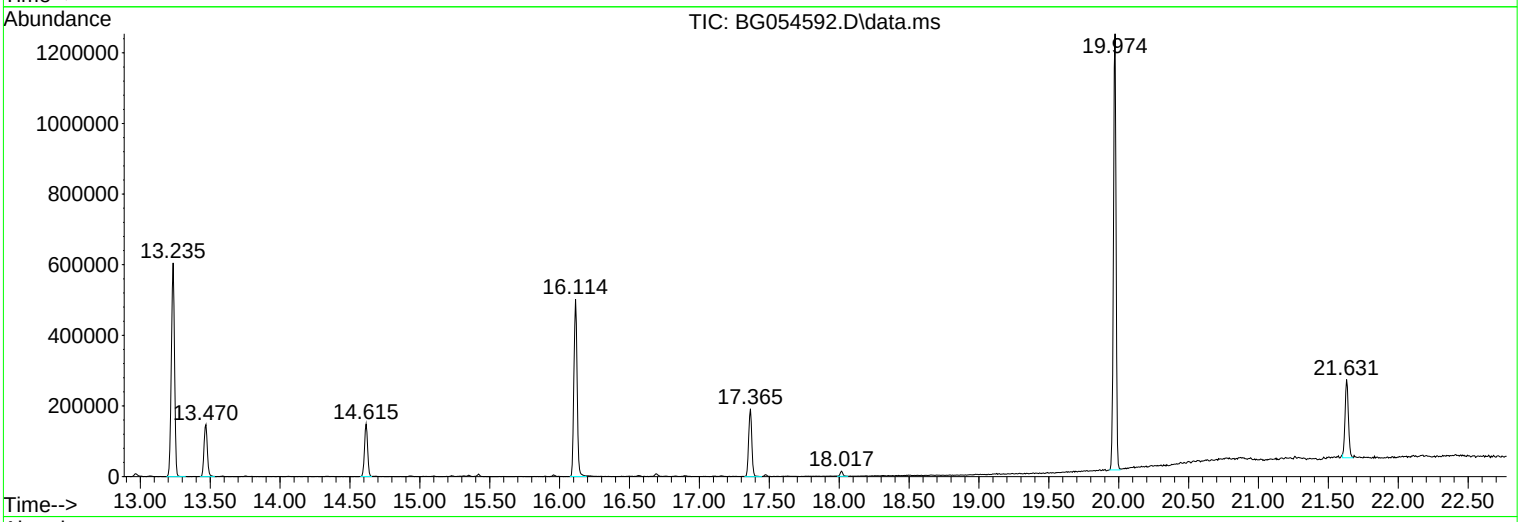
Sample : N3972-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

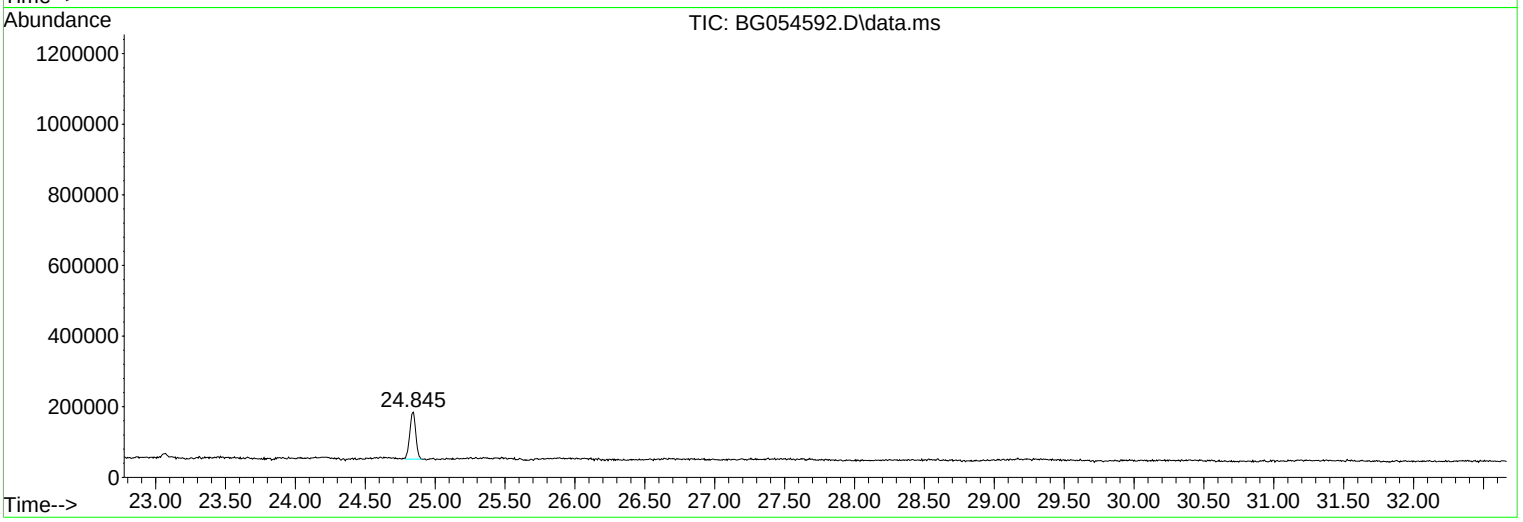
Instrument :
BNA_G
ClientSampleId :
SPN-8

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

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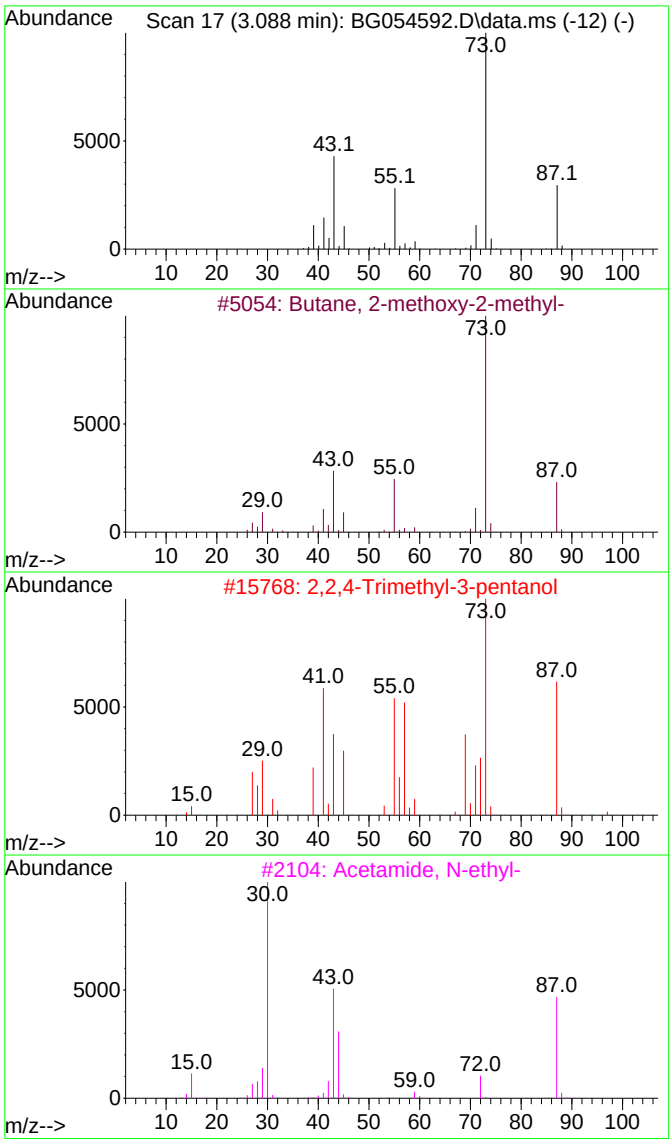
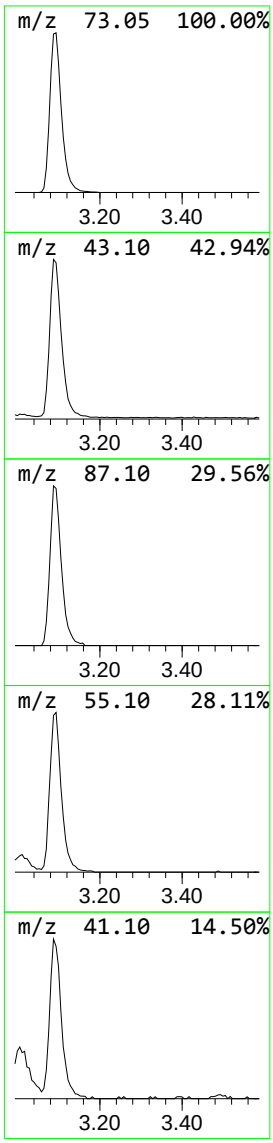
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.088	88.91 ng	497472	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	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Data File : BG054592.D
Acq On : 10 Aug 2022 17:29
Operator : CG/JU
Sample : N3972-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-8

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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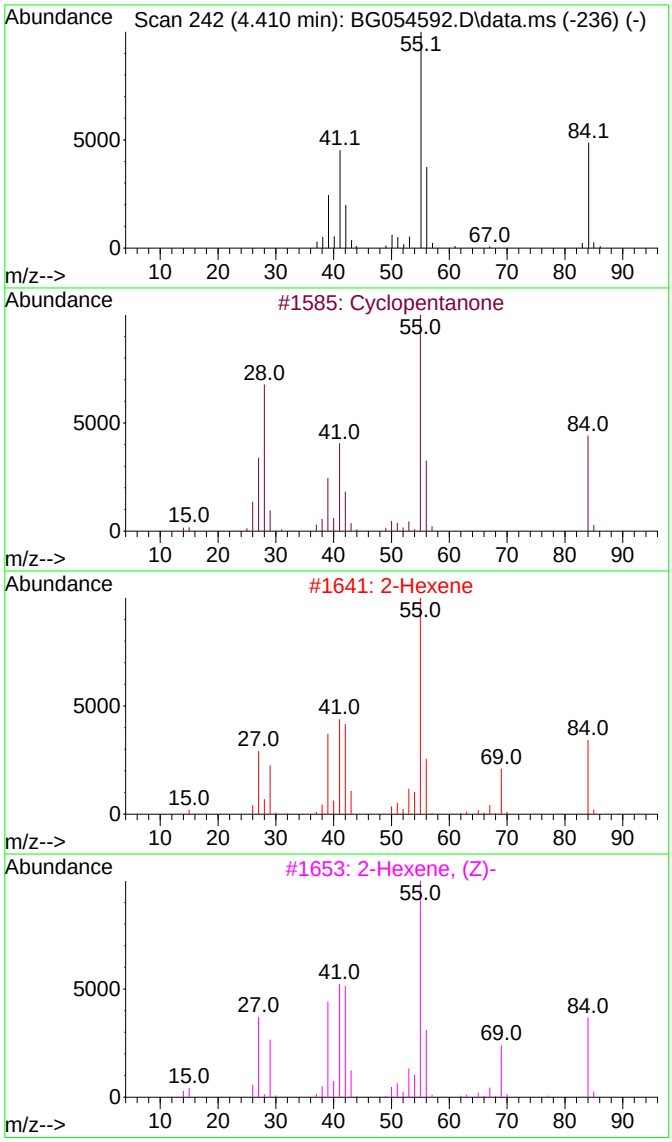
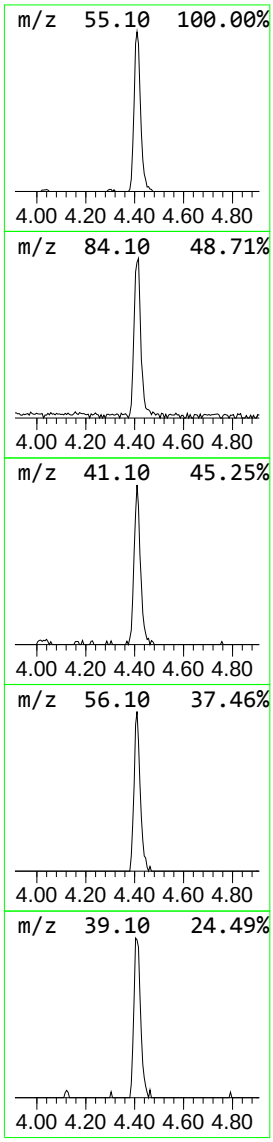
Peak Number 2 Cyclopentanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.410	20.21 ng	113048	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	64
3	2-Hexene, (Z)-	84	C6H12	007688-21-3	53
4	3-Hexene, (E)-	84	C6H12	013269-52-8	50
5	3-Hexene, (Z)-	84	C6H12	007642-09-3	50





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Acq On : 10 Aug 2022 17:29
Operator : CG/JU
Sample : N3972-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-8

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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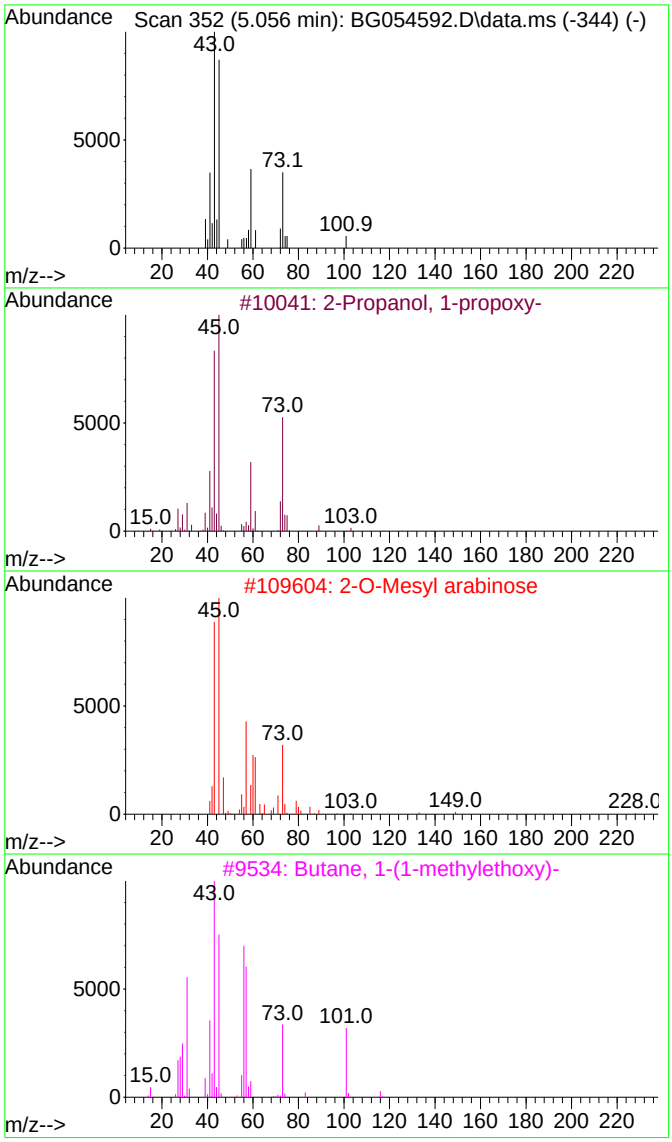
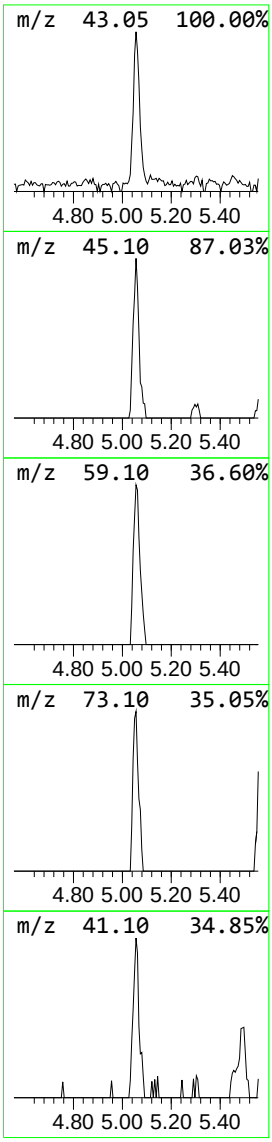
Peak Number 3 2-Propanol, 1-propoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.056	5.43 ng	30406	1,4-Dichlorobenzene-d4	7.976

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	64
2	2-O-Mesyl arabinose	228	C6H12O7S	1000130-06-0	39
3	Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	38
4	Boronic acid, ethyl-, diethyl ester	130	C6H15BO2	053907-92-9	38
5	Diacetamide	101	C4H7NO2	000625-77-4	17





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Data File : BG054592.D
Acq On : 10 Aug 2022 17:29
Operator : CG/JU
Sample : N3972-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
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TIC Library : C:\Database\NIST20.L
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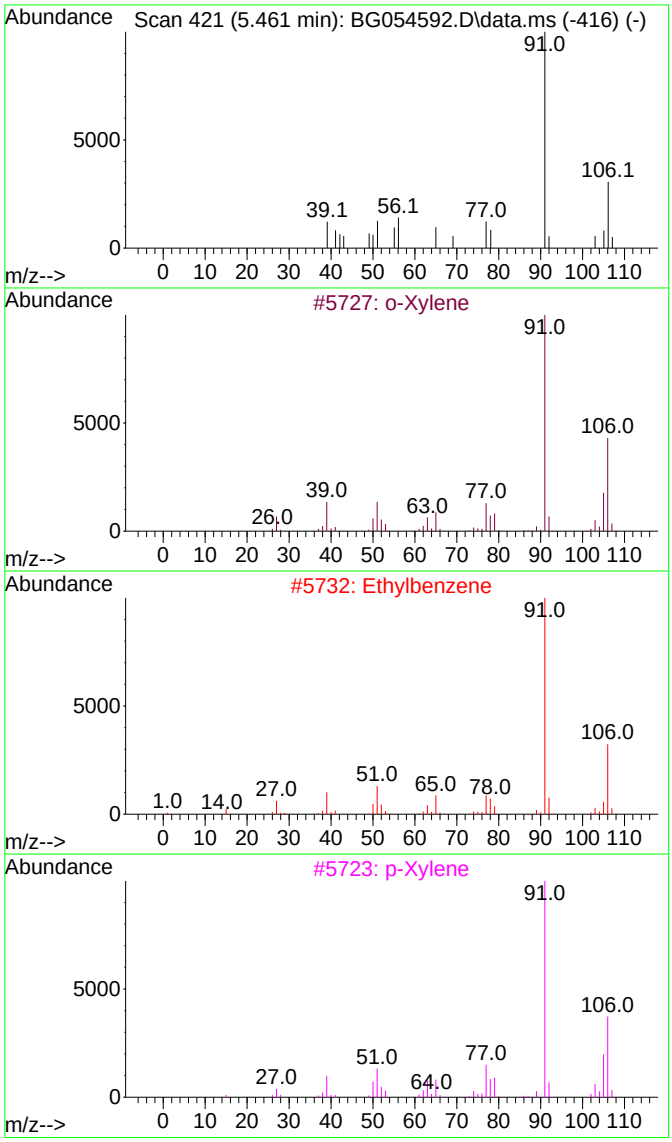
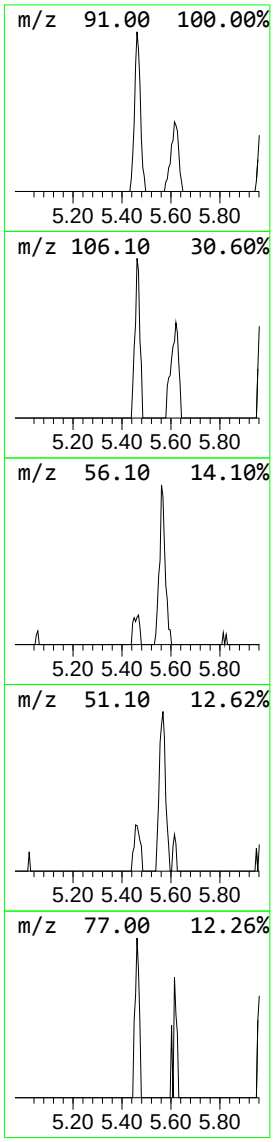
Peak Number 4 o-Xylene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.461	3.12 ng	17441	1,4-Dichlorobenzene-d4	7.976

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Xylene	106	C8H10	000095-47-6	80
2	Ethylbenzene	106	C8H10	000100-41-4	72
3	p-Xylene	106	C8H10	000106-42-3	72
4	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	59
5	1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081022\
Data File : BG054592.D
Acq On : 10 Aug 2022 17:29
Operator : CG/JU
Sample : N3972-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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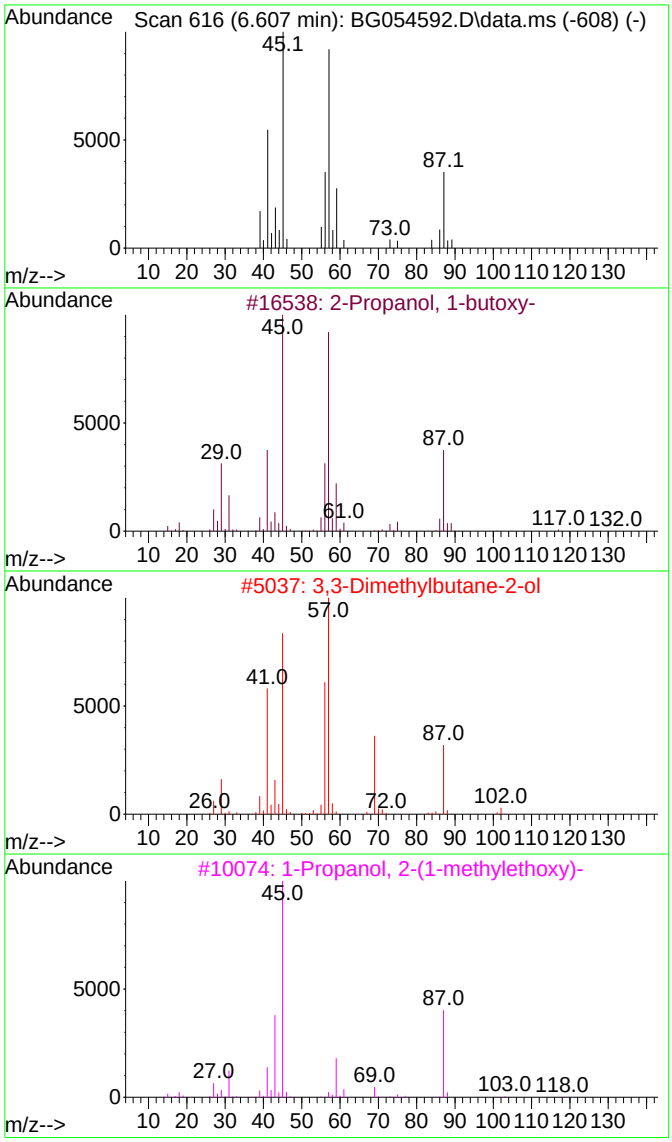
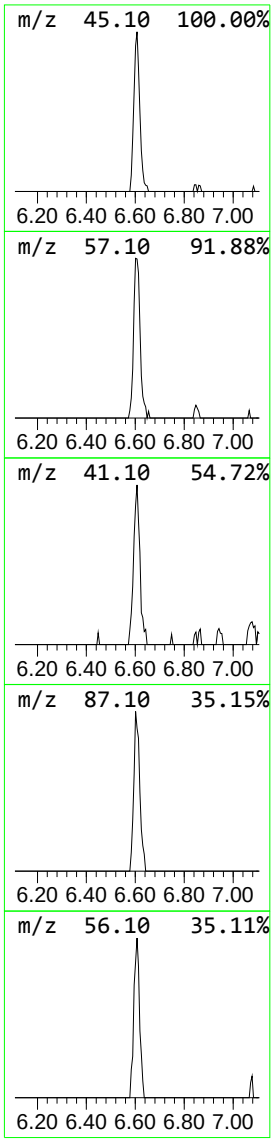
Peak Number 5 2-Propanol, 1-butoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.607	6.60 ng	36903	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	90
2	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
3	1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	53
4	Formic acid, 1-methylpropyl ester	102	C5H10O2	000589-40-2	38
5	2-Hydroxy-3-pentanone	102	C5H10O2	005704-20-1	36





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Data File : BG054592.D
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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
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TIC Library : C:\Database\NIST20.L
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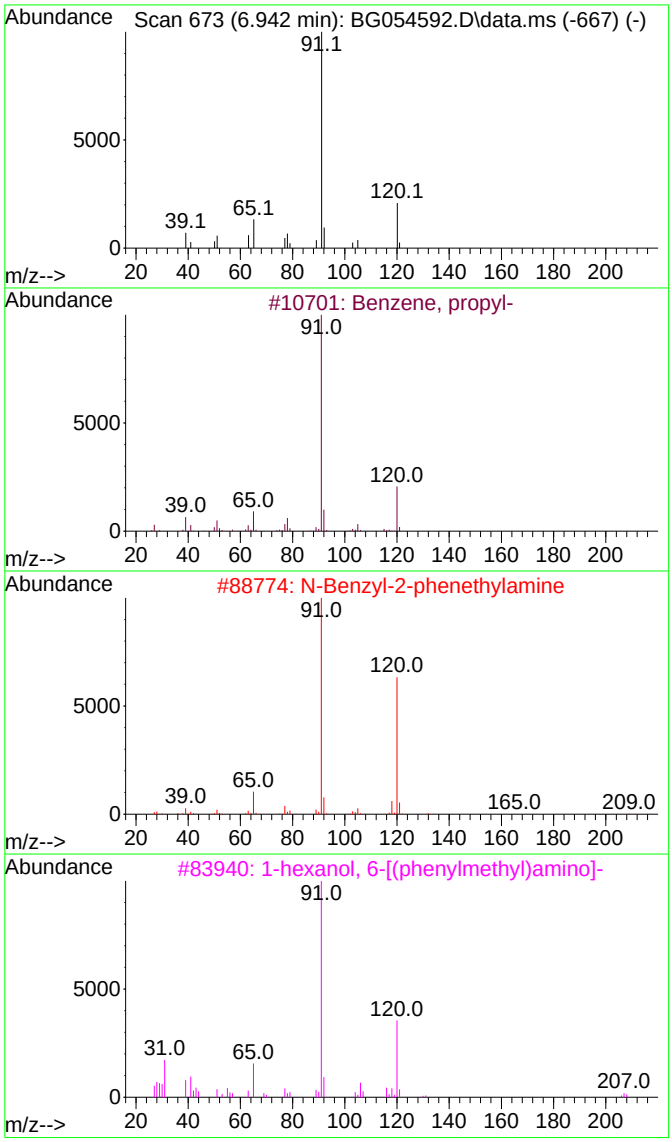
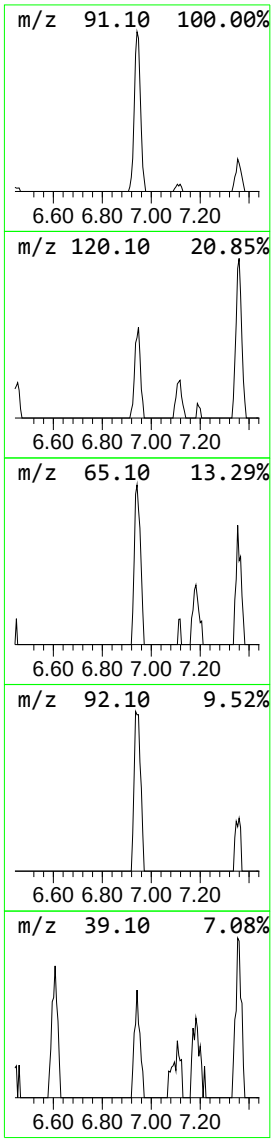
Peak Number 6 Benzene, propyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.942	5.33 ng	29847	1,4-Dichlorobenzene-d4	7.976

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, propyl-	120	C9H12	000103-65-1	91
2	N-Benzyl-2-phenethylamine	211	C15H17N	003647-71-0	83
3	1-hexanol, 6-[(phenylmethyl)amino]-	207	C13H21NO	1000400-55-6	72
4	Ethanol, 2-[(phenylmethyl)amino]-	151	C9H13NO	000104-63-2	72
5	Benzyl(2-chloroethyl)amine	169	C9H12ClN	042074-16-8	72





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Data File : BG054592.D
Acq On : 10 Aug 2022 17:29
Operator : CG/JU
Sample : N3972-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-8

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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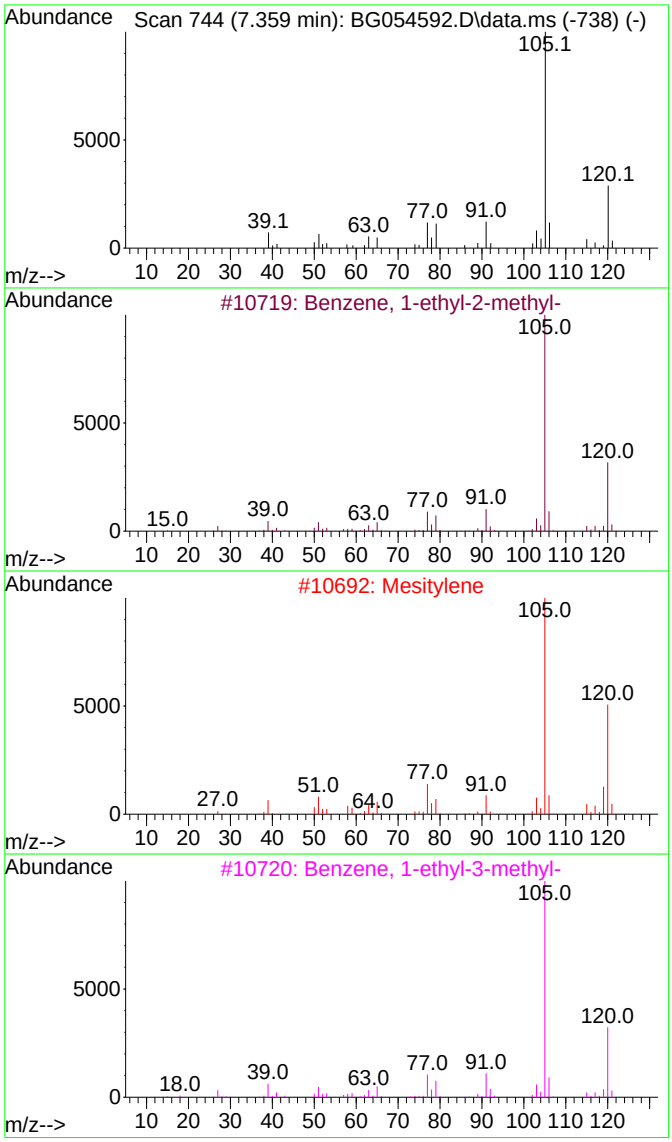
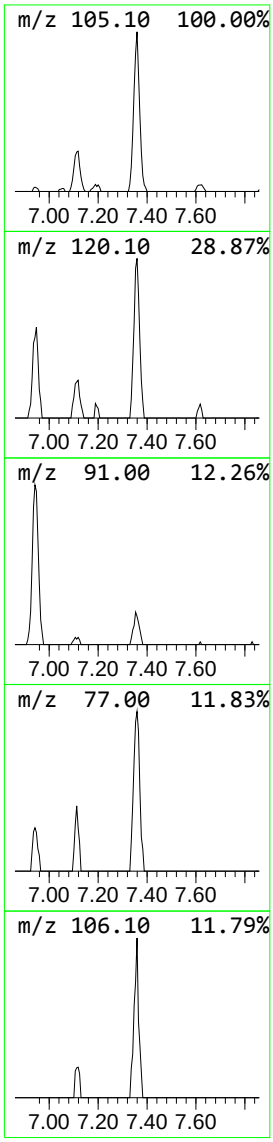
Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.359	9.59 ng	53648	1,4-Dichlorobenzene-d4	7.976

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Mesitylene	120	C9H12	000108-67-8	91
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





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

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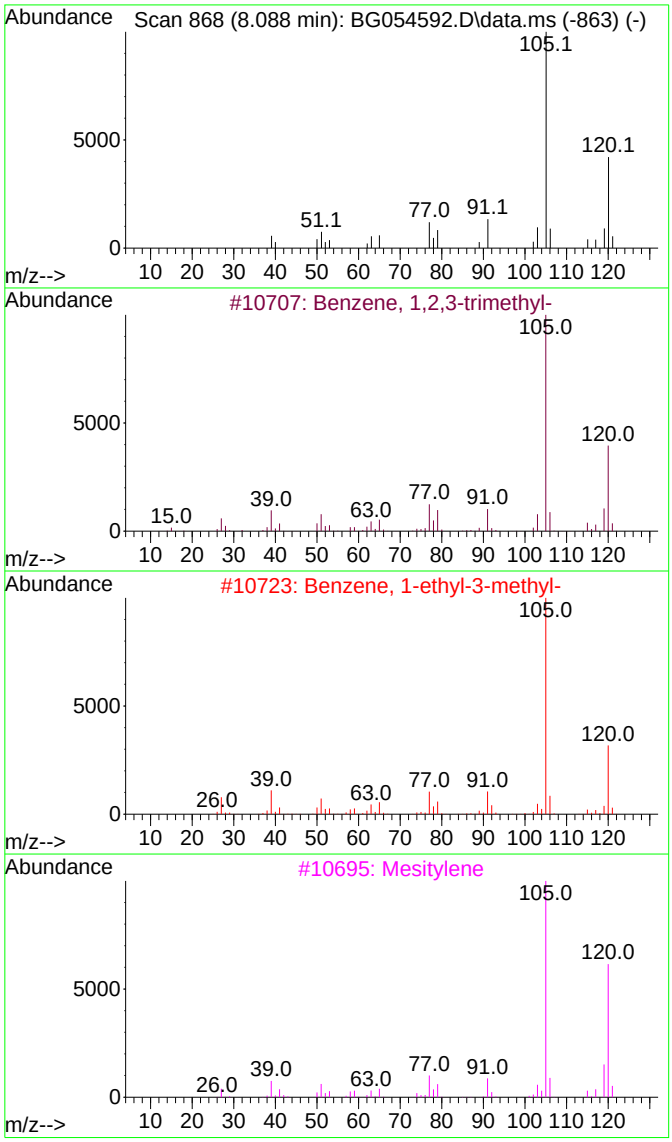
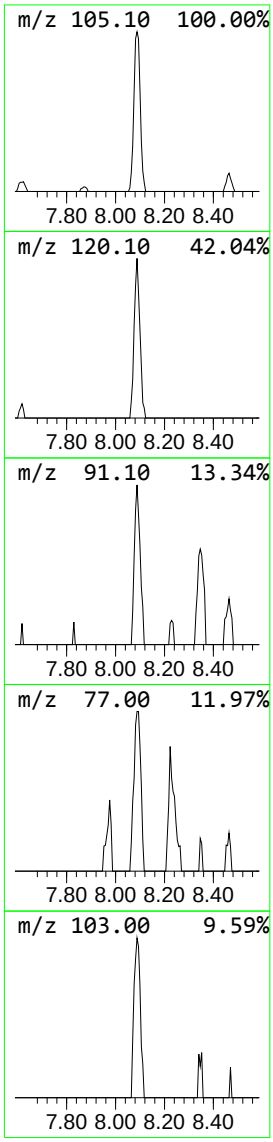
Peak Number 8 Benzene, 1,2,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.088	7.61 ng	42561	1,4-Dichlorobenzene-d4	7.976

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	94
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91





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Data File : BG054592.D
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Operator : CG/JU
Sample : N3972-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-8

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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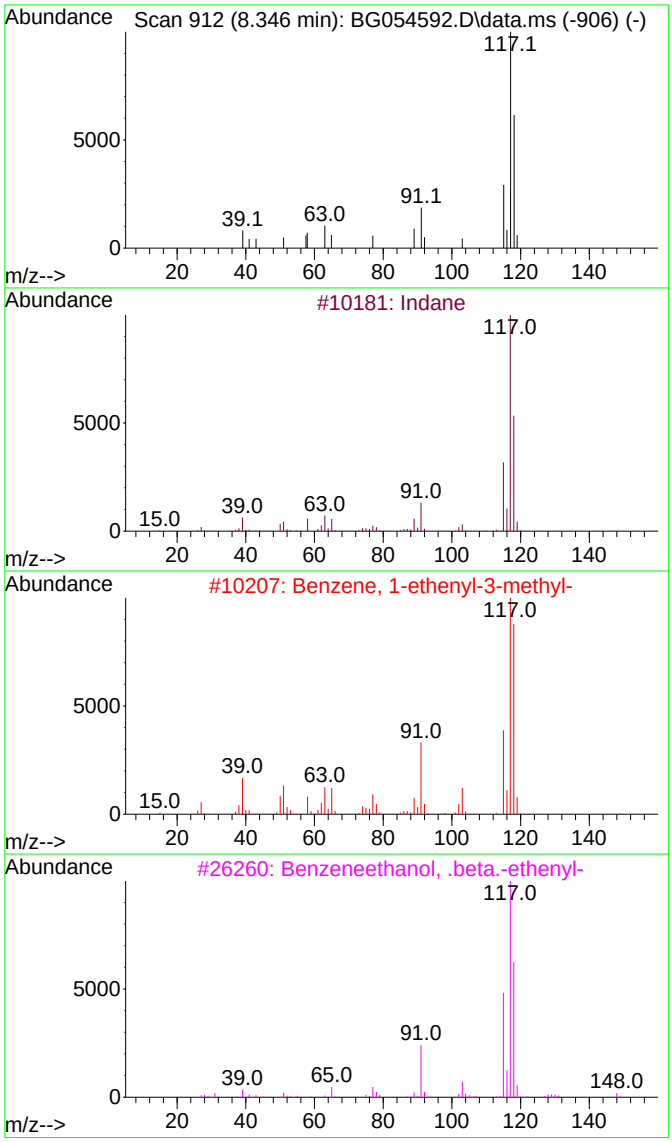
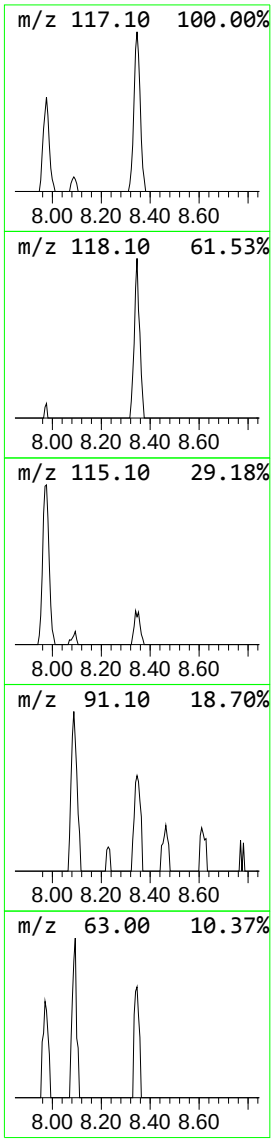
Peak Number 9 Indane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.346	3.15 ng	17604	1,4-Dichlorobenzene-d4	7.976

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	83
2	Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	80
3	Benzeneethanol, .beta.-ethenyl-	148	C10H12O	006052-63-7	78
4	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	72
5	Benzene, 2-propenyl-	118	C9H10	000300-57-2	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081022\
Data File : BG054592.D
Acq On : 10 Aug 2022 17:29
Operator : CG/JU
Sample : N3972-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-8

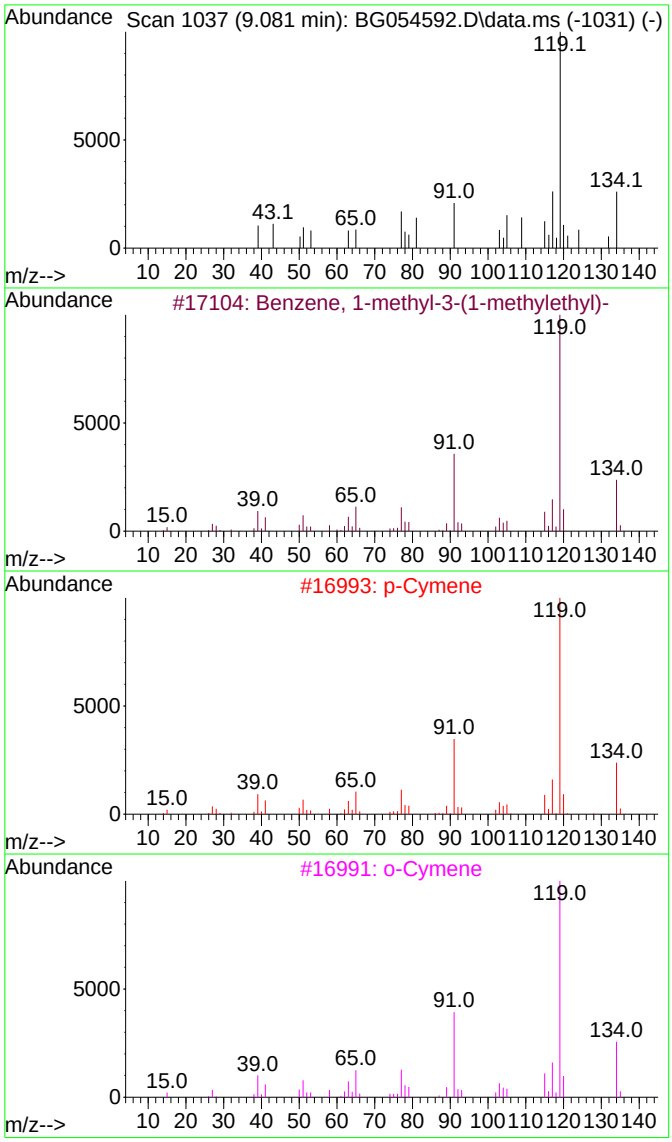
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

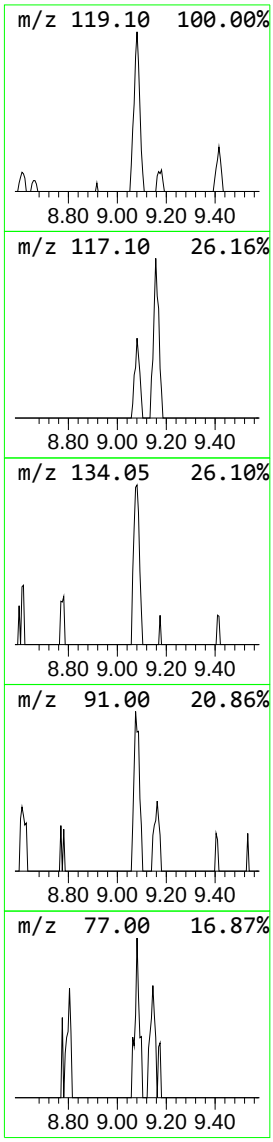
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 1-methyl-3-(1-meth... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.081	3.18 ng	17783	1,4-Dichlorobenzene-d4	7.976

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	64
2	p-Cymene	134	C10H14	000099-87-6	64
3	o-Cymene	134	C10H14	000527-84-4	64
4	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	64
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081022\
Data File : BG054592.D
Acq On : 10 Aug 2022 17:29
Operator : CG/JU
Sample : N3972-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-8

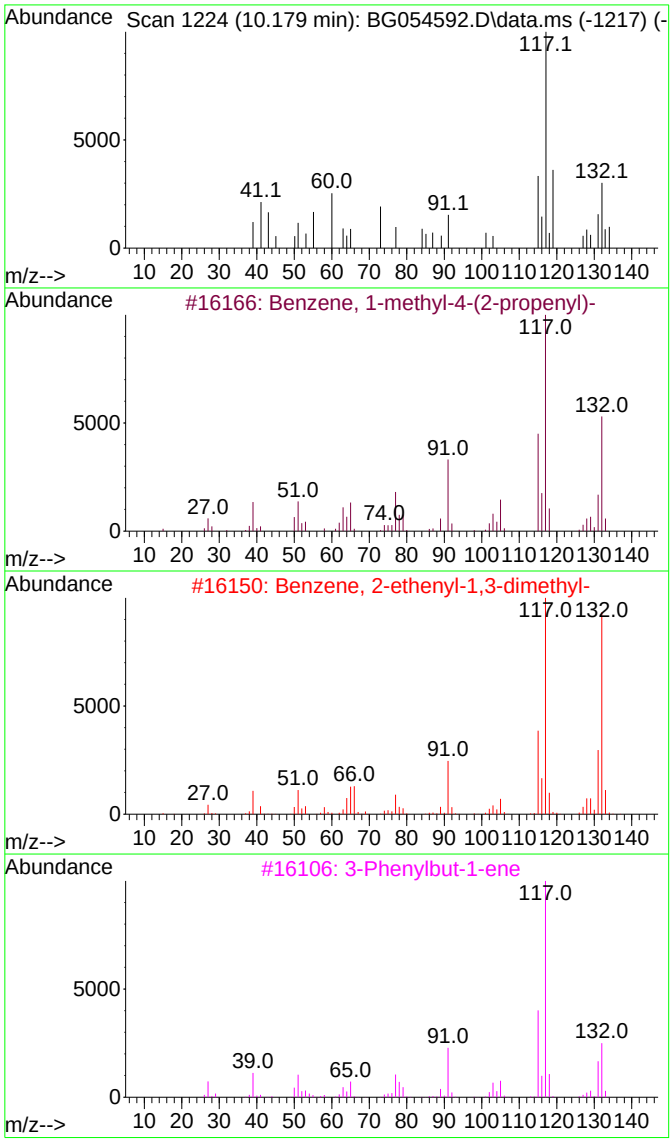
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

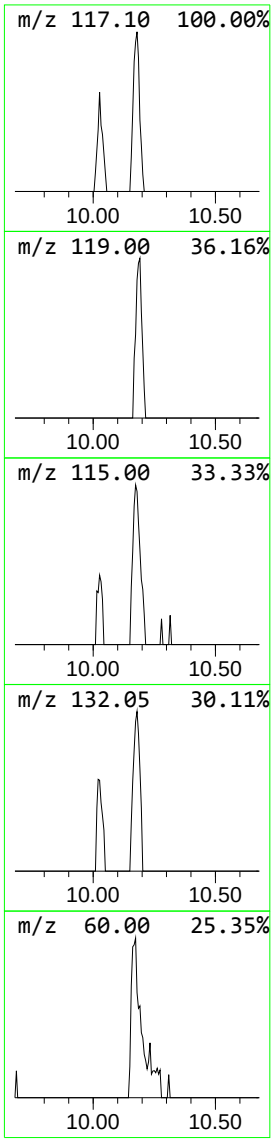
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Benzene, 1-methyl-4-(2-prop... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.179	3.84 ng	29450	Naphthalene-d8	10.785

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	64
2	Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	64
3	3-Phenylbut-1-ene	132	C10H12	000934-10-1	64
4	1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	53
5	1-Phenyl-1-butene	132	C10H12	000824-90-8	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081022\
Data File : BG054592.D
Acq On : 10 Aug 2022 17:29
Operator : CG/JU
Sample : N3972-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-8

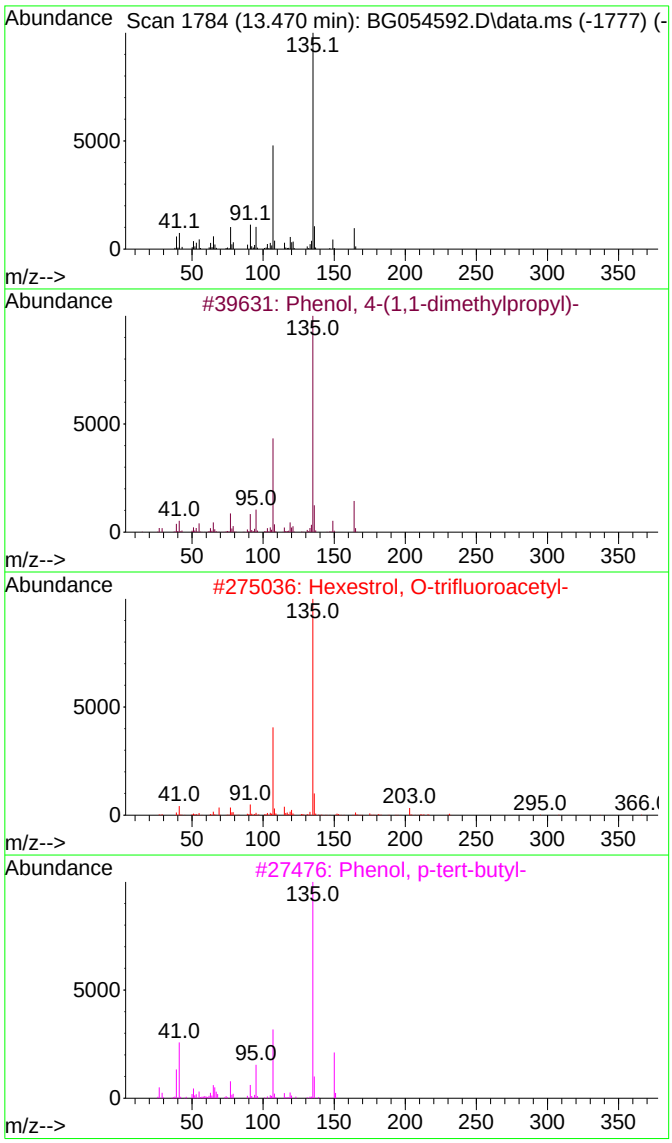
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

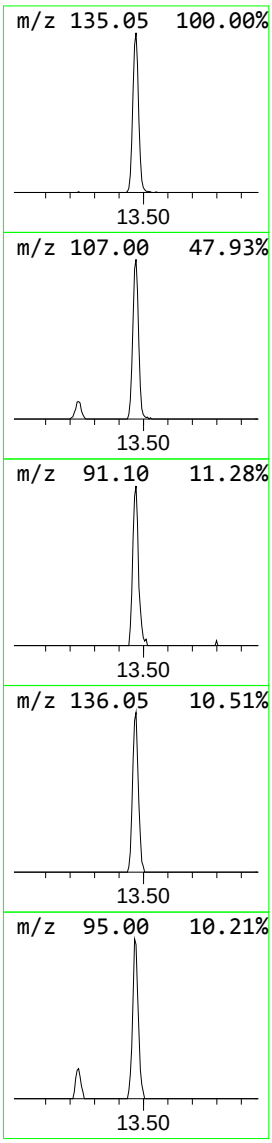
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Phenol, 4-(1,1-dimethylprop... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.470	20.55 ng	240011	Acenaphthene-d10	14.615

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	95
2	Hexestrol, O-trifluoroacetyl-	366	C20H21F3O3	1000365-31-7	64
3	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	64
4	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	59
5	Phenol, 2-(1,1,3,3-tetramethylbu...	206	C14H22O	003884-95-5	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081022\
Data File : BG054592.D
Acq On : 10 Aug 2022 17:29
Operator : CG/JU
Sample : N3972-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-8

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	88.9	ng	497472	1	7.976	111899	20.0
Cyclopentanone	4.410	20.2	ng	113048	1	7.976	111899	20.0
2-Propanol, 1-p...	5.056	5.4	ng	30406	1	7.976	111899	20.0
o-Xylene	5.461	3.1	ng	17441	1	7.976	111899	20.0
2-Propanol, 1-b...	6.607	6.6	ng	36903	1	7.976	111899	20.0
Benzene, propyl-	6.942	5.3	ng	29847	1	7.976	111899	20.0
Benzene, 1-ethy...	7.359	9.6	ng	53648	1	7.976	111899	20.0
Benzene, 1,2,3-...	8.088	7.6	ng	42561	1	7.976	111899	20.0
Indane	8.346	3.1	ng	17604	1	7.976	111899	20.0
Benzene, 1-meth...	9.081	3.2	ng	17783	1	7.976	111899	20.0
Benzene, 1-meth...	10.179	3.8	ng	29450	2	10.785	153584	20.0
Phenol, 4-(1,1-...	13.470	20.6	ng	240011	3	14.615	233595	20.0