LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
Data File : BG053337.D
Acq On : 27 Apr 2022 2:00
Operator : CG/JU
Sample : N2482-18
Misc :
ALS Vial : 18 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-BG040822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053337.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.548	191	197	210	rVB	28759	50837	1.87%	0.598%
2	5.605	370	377	382	rBV	50629	82493	3.03%	0.971%
3	5.670	382	388	395	rVV	163490	280187	10.28%	3.297%
4	5.735	395	399	408	rVB2	34845	70527	2.59%	0.830%
5	7.262	653	659	676	rBV	101829	197526	7.25%	2.324%
6	7.491	693	698	707	rVB2	18249	30106	1.10%	0.354%
7	7.632	716	722	727	rBV2	17332	28214	1.04%	0.332%
8	7.685	727	731	737	rVV	17395	28953	1.06%	0.341%
9	7.750	737	742	749	rVB	34799	55420	2.03%	0.652%
10	7.873	756	763	771	rBV	26094	47529	1.74%	0.559%
11	8.102	797	802	807	rBV	58206	103613	3.80%	1.219%
12	8.161	807	812	818	rVV2	24669	40215	1.48%	0.473%
13	9.265	993	1000	1012	rVB	233326	429349	15.75%	5.052%
14	10.916	1274	1281	1287	rBV	82492	141796	5.20%	1.668%
15	13.089	1645	1651	1658	rBV	36881	62682	2.30%	0.738%
16	13.348	1686	1695	1704	rBV	610557	1083674	39.76%	12.750%
17	13.571	1726	1733	1748	rVB	152492	245786	9.02%	2.892%
18	14.728	1923	1930	1936	rBV	147142	232562	8.53%	2.736%
19	15.527	2060	2066	2072	rVB	35491	49627	1.82%	0.584%
20	16.068	2152	2158	2162	rBV	30134	41940	1.54%	0.493%
21	16.215	2176	2183	2196	rBV	662347	1029212	37.76%	12.110%
22	17.472	2390	2397	2404	rBV	251943	365716	13.42%	4.303%
23	18.130	2503	2509	2513	rBV2	39422	49952	1.83%	0.588%
24	20.074	2834	2840	2846	rBV	1936267	2725666	100.00%	32.070%
25	21.754	3119	3126	3136	rBV2	302527	517850	19.00%	6.093%
26	25.050	3676	3687	3698	rBV	169881	507690	18.63%	5.973%

Sum of corrected areas: 8499122

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
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Operator : CG/JU
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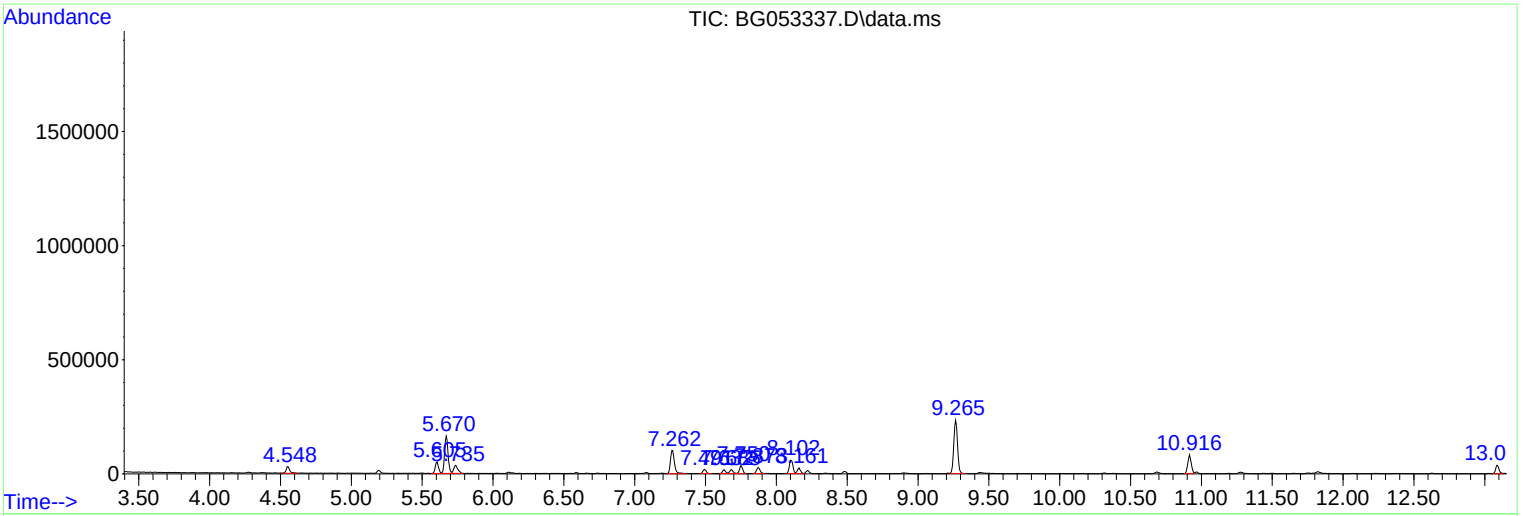
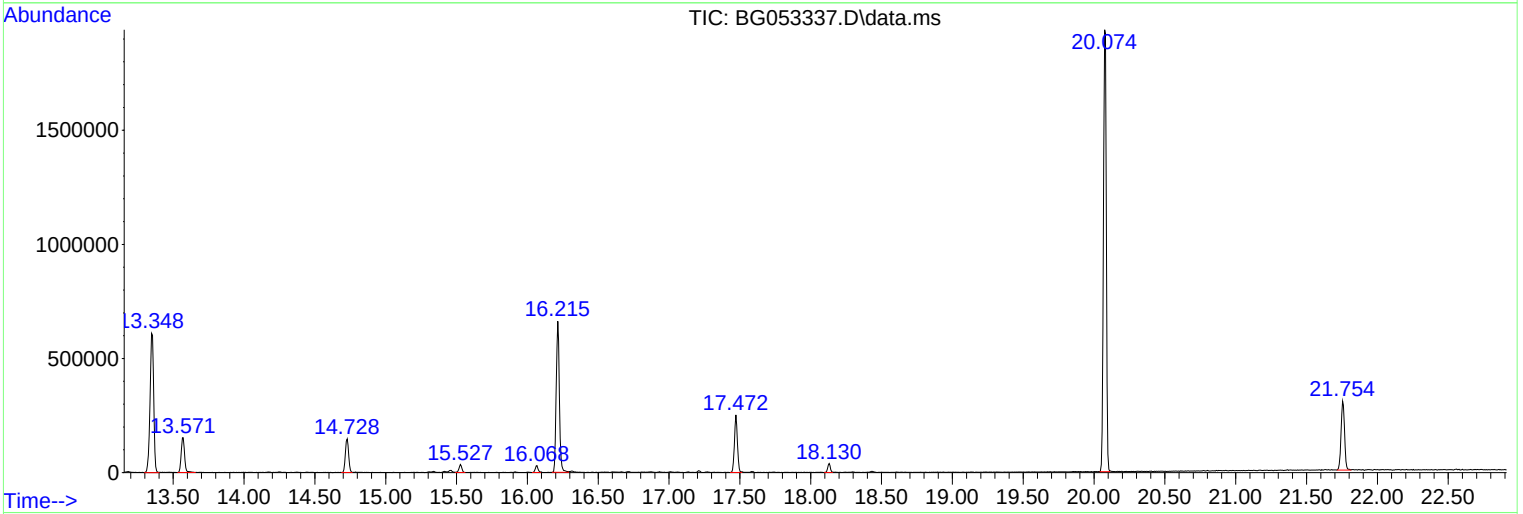
Misc :
ALS Vial : 18 Sample Multiplier: 1

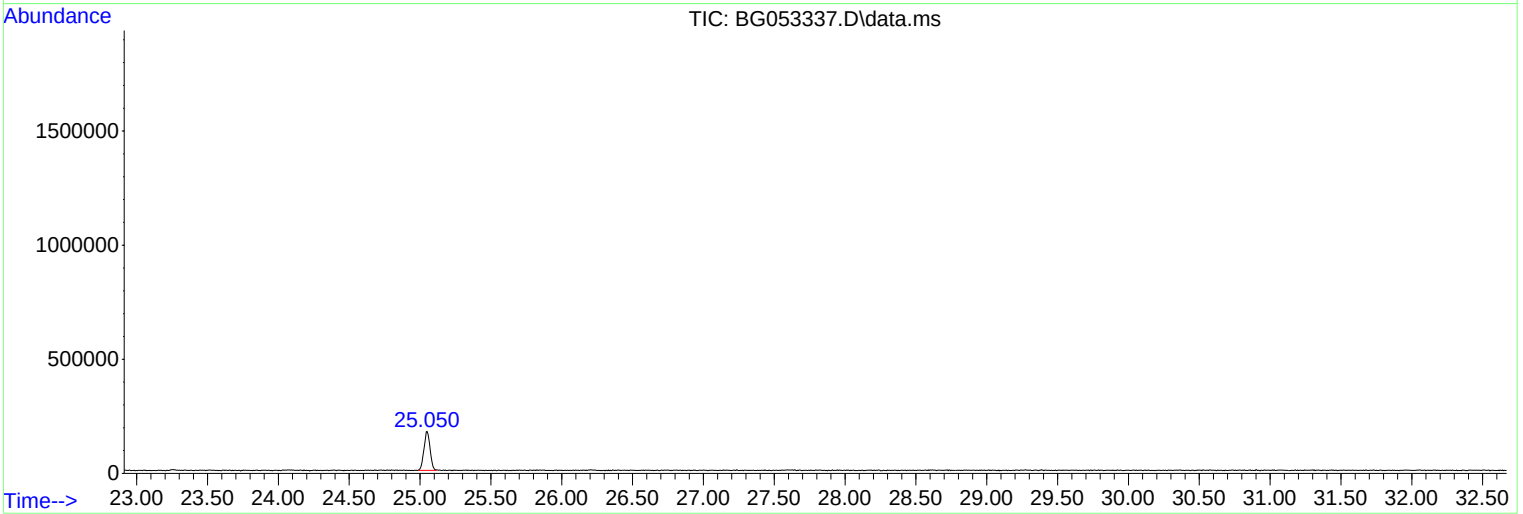
Instrument :
BNA_G
ClientSampleId :
SPN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.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 : BG053337.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

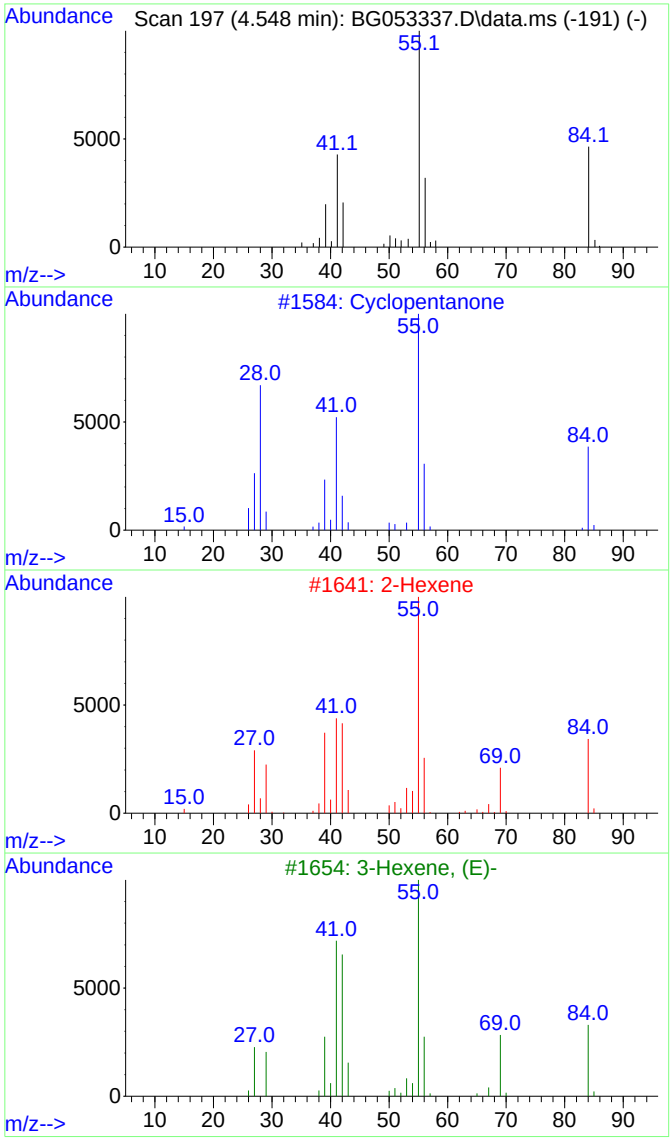
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

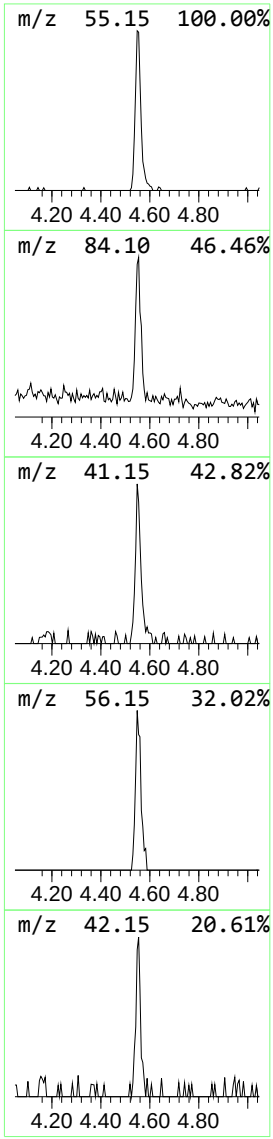
****

Peak Number 1 Cyclopentanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.548	9.81 ng	50837	1,4-Dichlorobenzene-d4	8.102

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	58
3	3-Hexene, (E)-	84	C6H12	013269-52-8	53
4	2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	53
5	3-Hexene	84	C6H12	000592-47-2	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
Data File : BG053337.D
Acq On : 27 Apr 2022 2:00
Operator : CG/JU
Sample : N2482-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

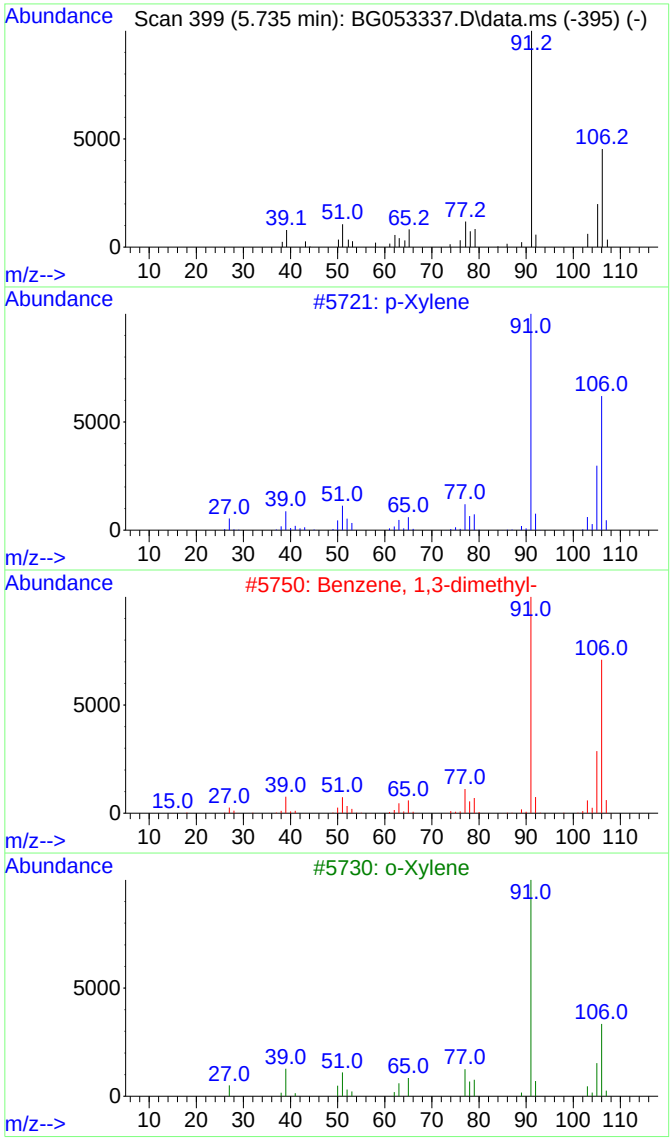
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

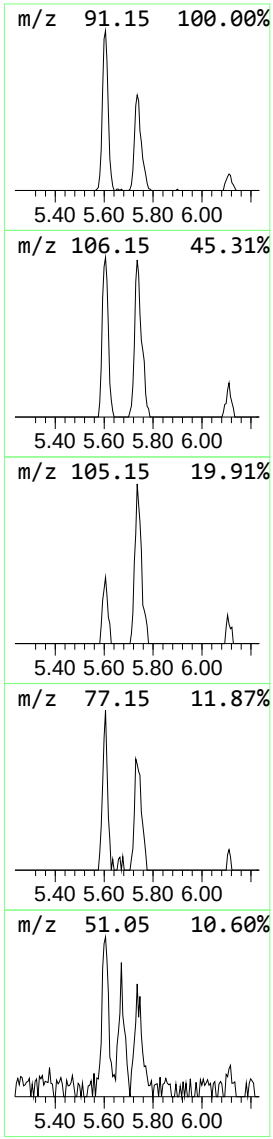
****

Peak Number 3 p-Xylene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.735	13.61 ng	70527	1,4-Dichlorobenzene-d4	8.102

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Xylene	106	C8H10	000106-42-3	94
2	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	91
3	o-Xylene	106	C8H10	000095-47-6	91
4	1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	91
5	Ethylbenzene	106	C8H10	000100-41-4	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
Data File : BG053337.D
Acq On : 27 Apr 2022 2:00
Operator : CG/JU
Sample : N2482-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-1

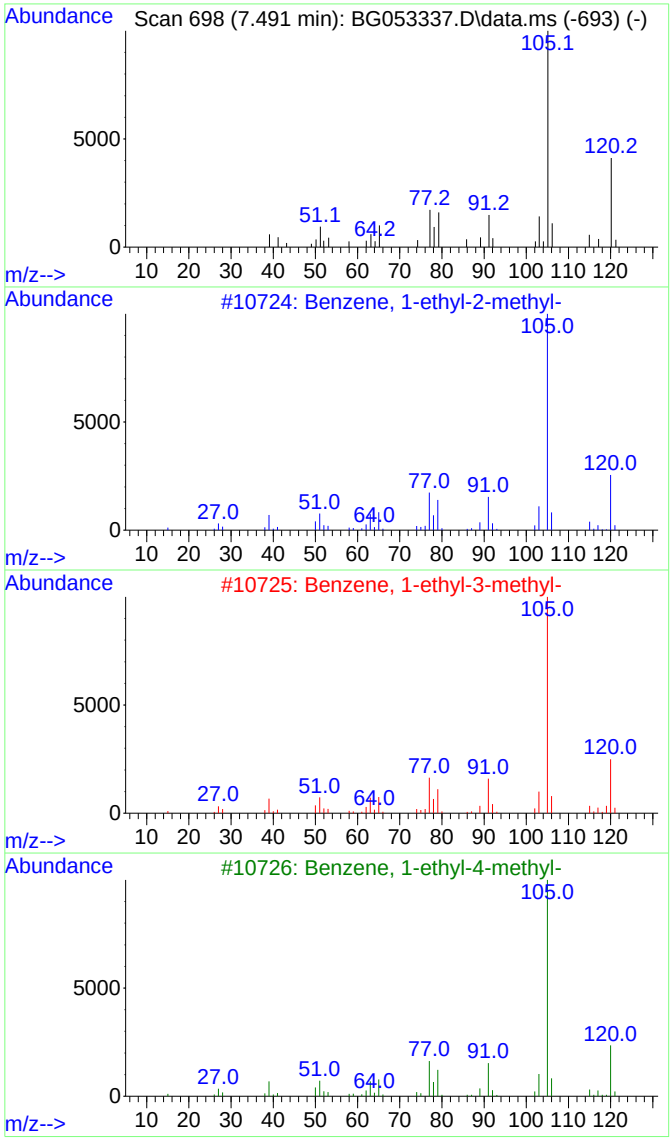
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

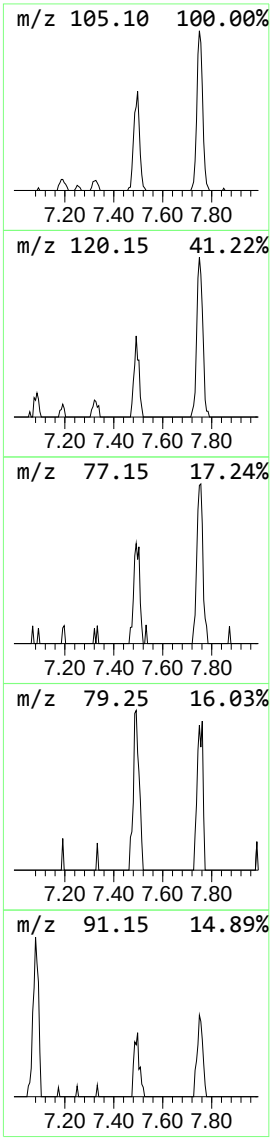
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.491	5.81 ng	30106	1,4-Dichlorobenzene-d4	8.102

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	87
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
Data File : BG053337.D
Acq On : 27 Apr 2022 2:00
Operator : CG/JU
Sample : N2482-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-1

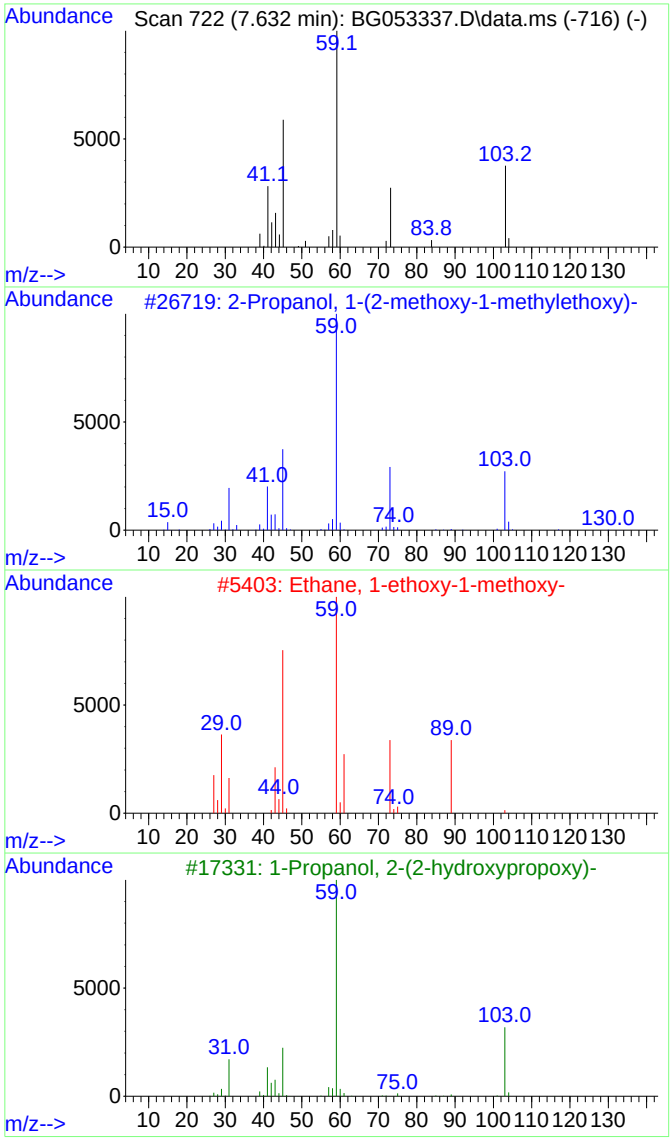
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

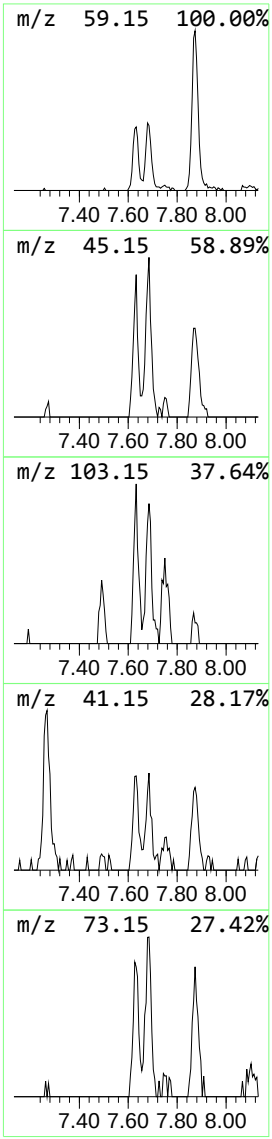
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.632	5.45 ng	28214	1,4-Dichlorobenzene-d4	8.102

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	72
2	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	59
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	59
4	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	59
5	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
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Operator : CG/JU
Sample : N2482-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

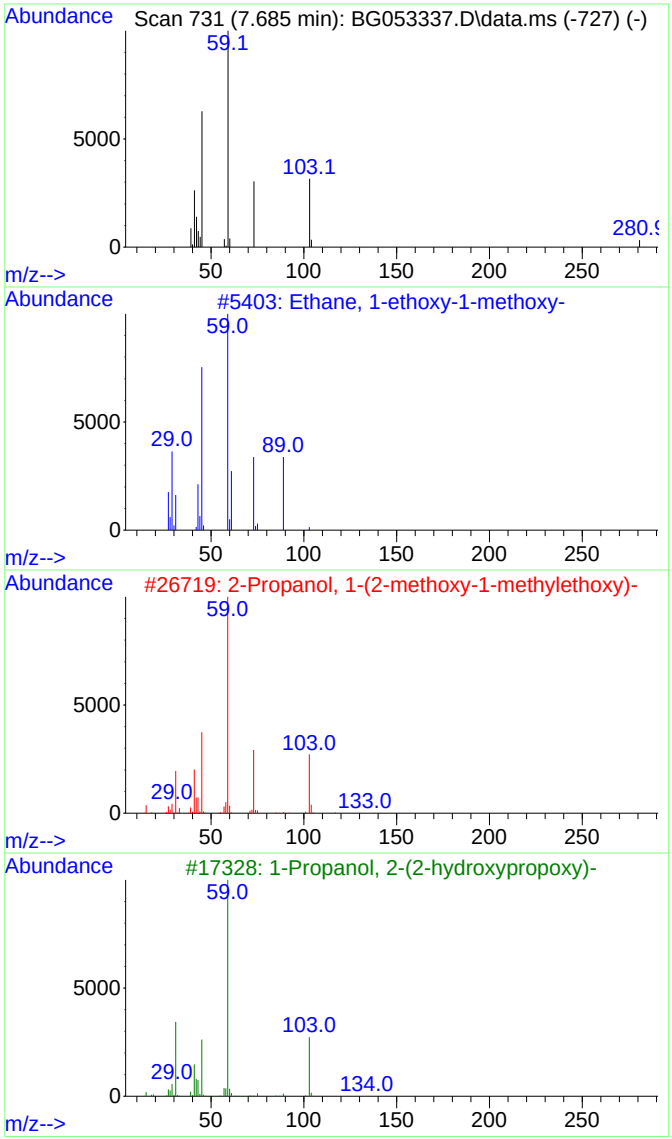
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

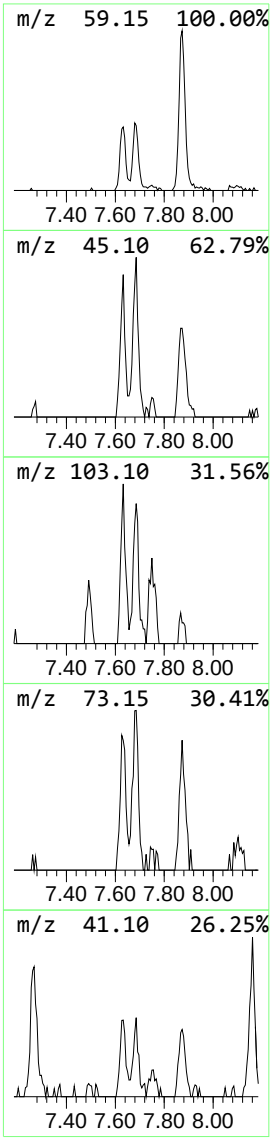
****

Peak Number 6 Ethane, 1-ethoxy-1-methoxy- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.685	5.59 ng	28953	1,4-Dichlorobenzene-d4	8.102

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	50
2	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	50
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	42
4	Acetaldoxime	59	C2H5NO	000107-29-9	38
5	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	36





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Operator : CG/JU
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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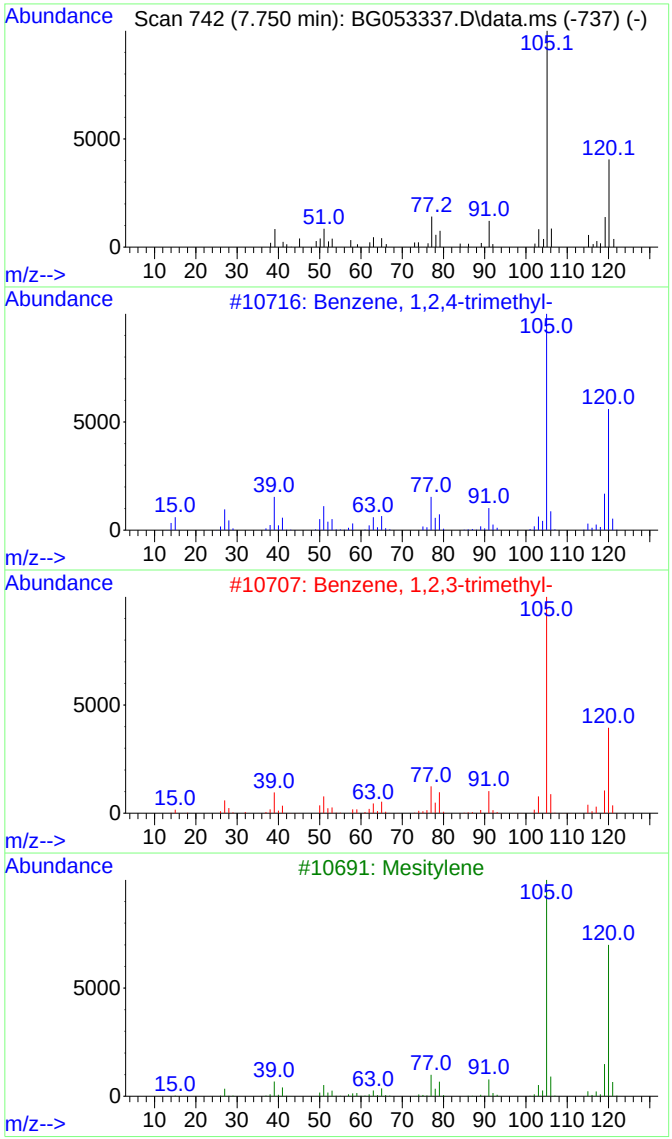
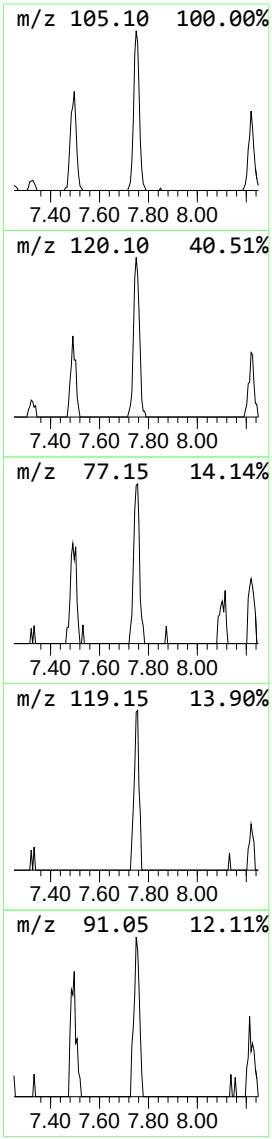
****

Peak Number 7 Benzene, 1,2,4-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.750	10.70 ng	55420	1,4-Dichlorobenzene-d4	8.102

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	95
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90





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Data File : BG053337.D
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Operator : CG/JU
Sample : N2482-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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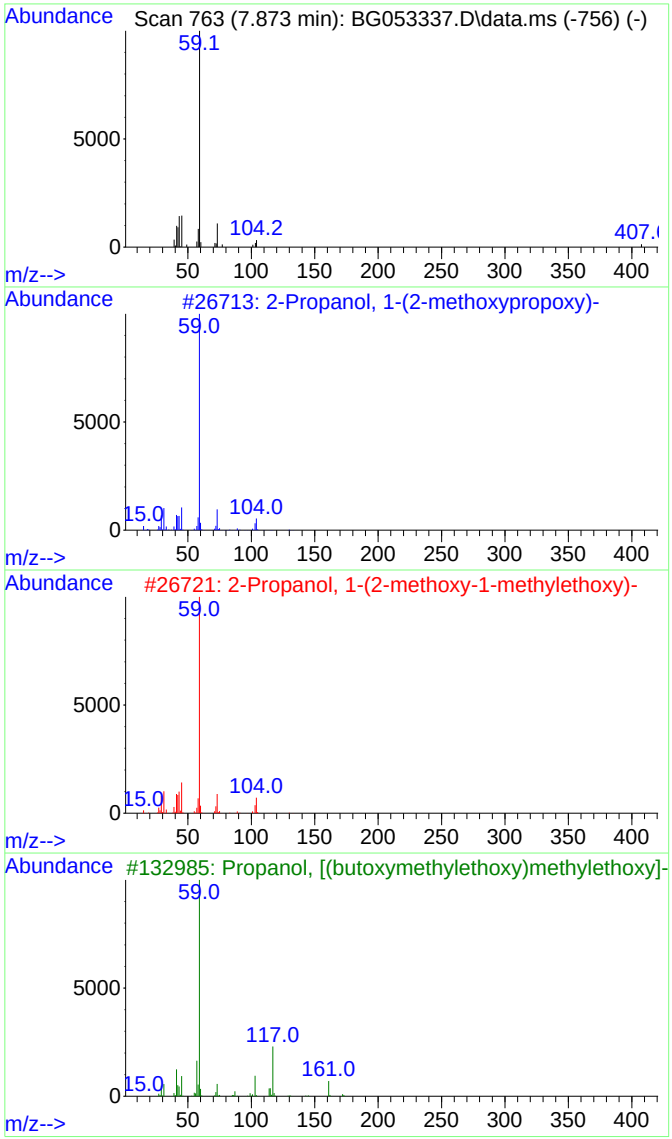
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

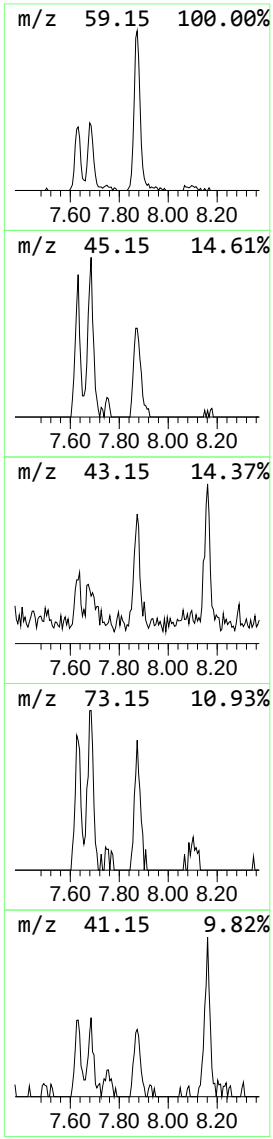
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2-Propanol, 1-(2-methoxypro... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.873	9.17 ng	47529	1,4-Dichlorobenzene-d4	8.102

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	78
2	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	64
3	Propanol, [(butoxymethylethoxy)m...	248	C13H28O4	055934-93-5	43
4	Butanoic acid, 3-methoxy-	118	C5H10O3	010024-70-1	43
5	4,8,12,16-tetraoxaeicosan-1-ol	306	C16H34O5	1010397-63-6	43





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TIC Library : C:\Database\NIST20.L
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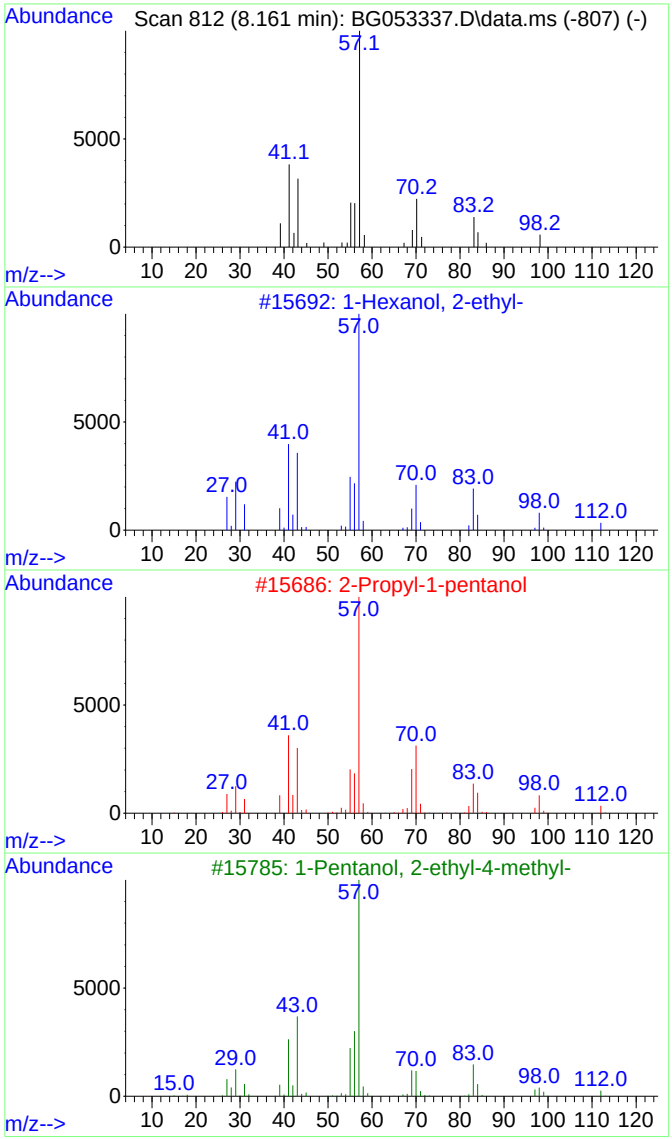
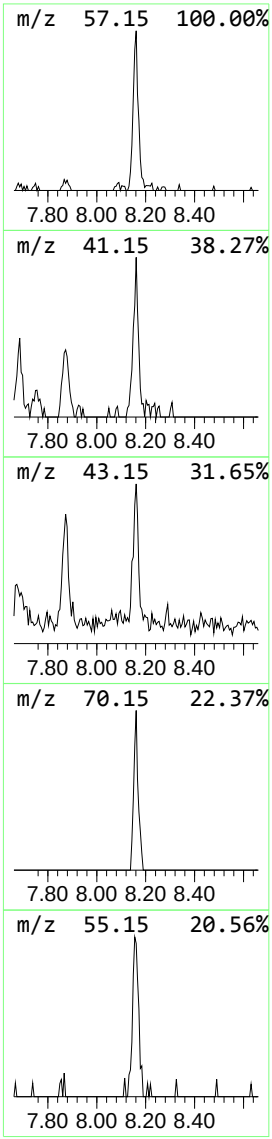
****
Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.161	7.76 ng	40215	1,4-Dichlorobenzene-d4	8.102

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	38
4	Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	38
5	Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	38





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Operator : CG/JU
Sample : N2482-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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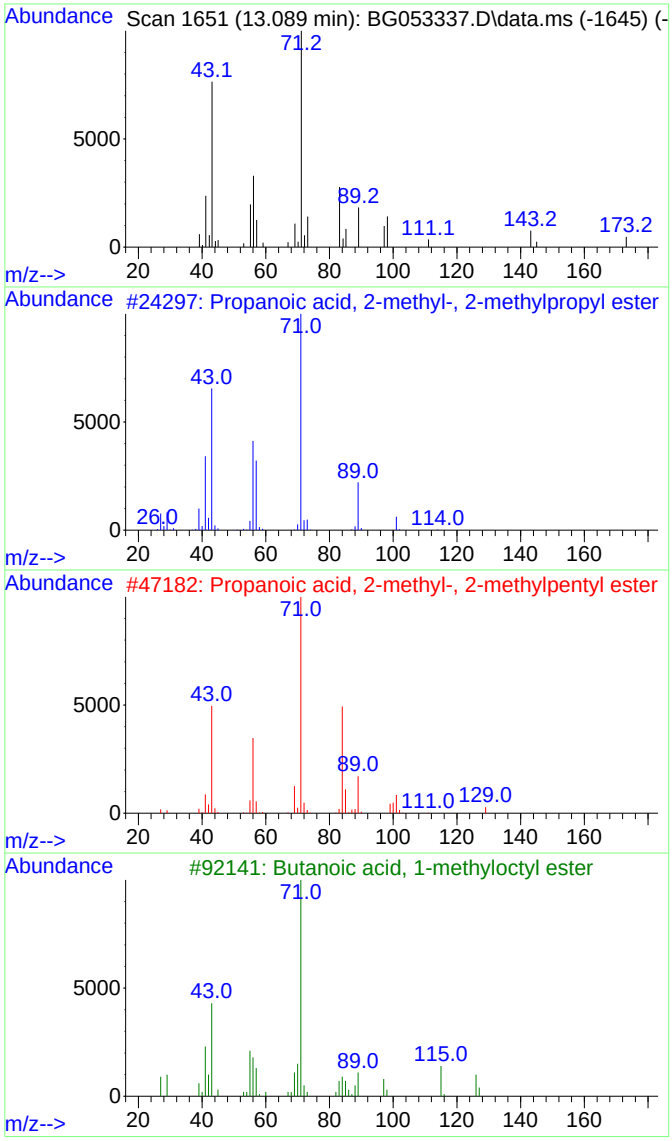
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

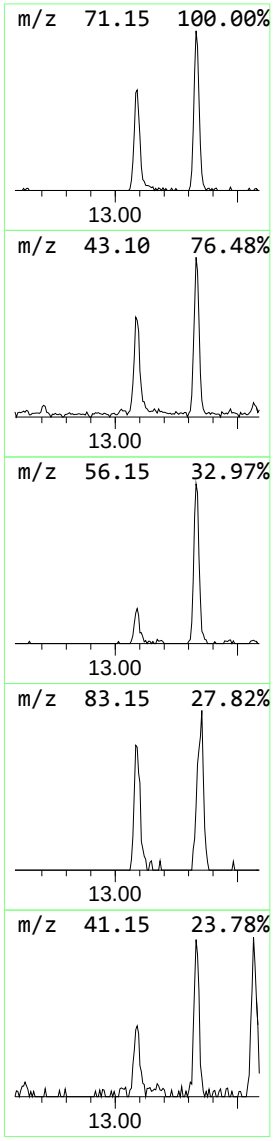
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Propanoic acid, 2-methyl-, ... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.089	5.39 ng	62682	Acenaphthene-d10	14.728

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	50
2	Propanoic acid, 2-methyl-, 2-met...	172	C10H20O2	084254-82-0	50
3	Butanoic acid, 1-methyloctyl ester	214	C13H26O2	069727-42-0	50
4	5-Nonanol, 2-methylpropionate	214	C13H26O2	1000463-47-6	43
5	Pentane, 2,2'-oxybis-	158	C10H22O	056762-00-6	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
Data File : BG053337.D
Acq On : 27 Apr 2022 2:00
Operator : CG/JU
Sample : N2482-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-1

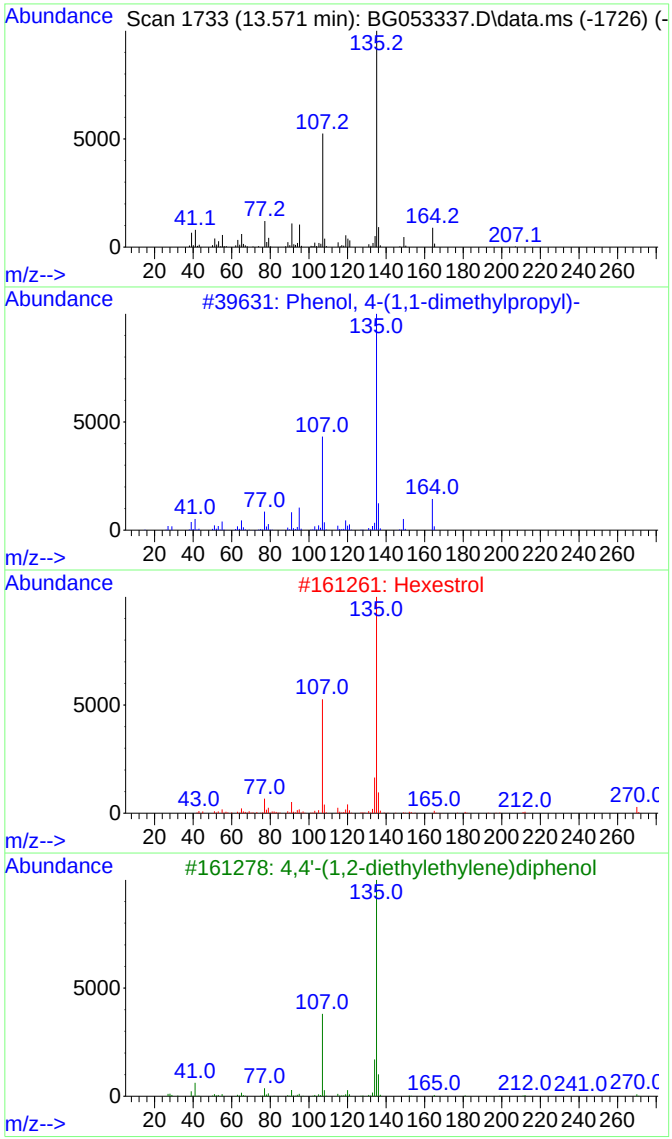
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

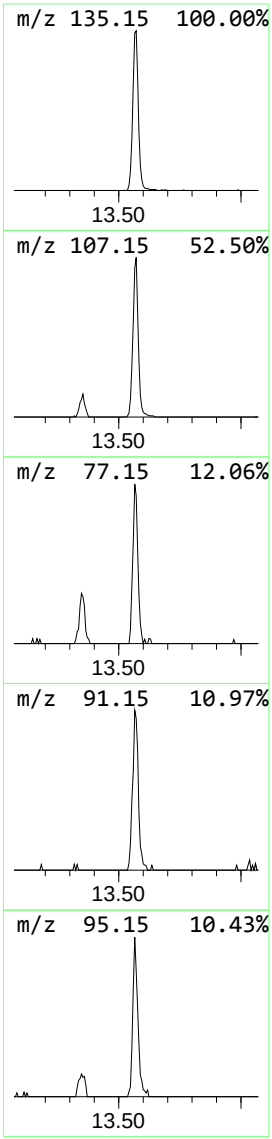
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.571	21.14 ng	245786	Acenaphthene-d10	14.728

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	94
2	Hexestrol	270	C18H22O2	000084-16-2	72
3	4,4'-(1,2-diethylethylene)diphenol	270	C18H22O2	005635-50-7	64
4	Phenol, 2-(1,1,3,3-tetramethylbu...	206	C14H22O	003884-95-5	64
5	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
Data File : BG053337.D
Acq On : 27 Apr 2022 2:00
Operator : CG/JU
Sample : N2482-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-1

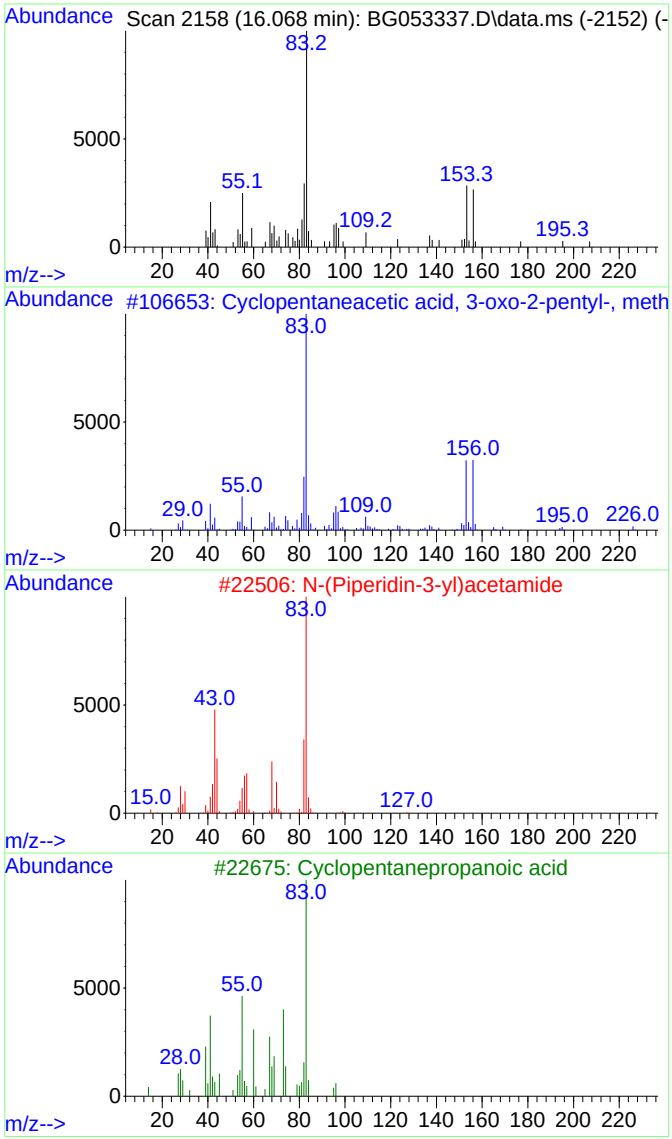
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

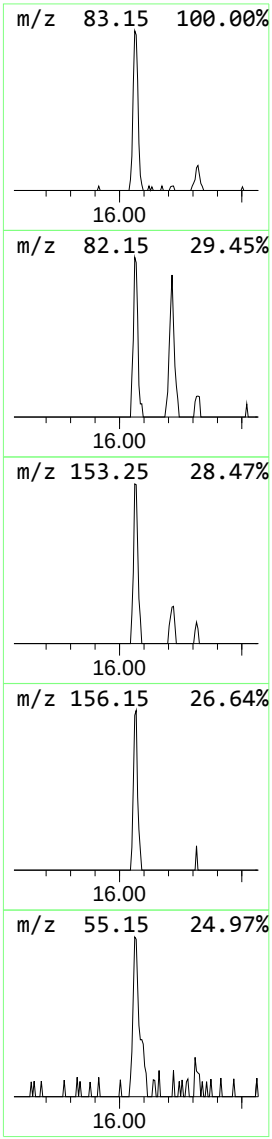
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Cyclopentaneacetic acid, 3-... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.068	3.61 ng	41940	Acenaphthene-d10	14.728

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	86
2	N-(Piperidin-3-yl)acetamide	142	C7H14N2O	005810-55-9	43
3	Cyclopentanepropanoic acid	142	C8H14O2	000140-77-2	43
4	Isocitronellol	156	C10H20O	018479-52-2	38
5	Prop-2-ynyl (E)-2-methylbut-2-en...	138	C8H10O2	1000373-72-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
Data File : BG053337.D
Acq On : 27 Apr 2022 2:00
Operator : CG/JU
Sample : N2482-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPN-1

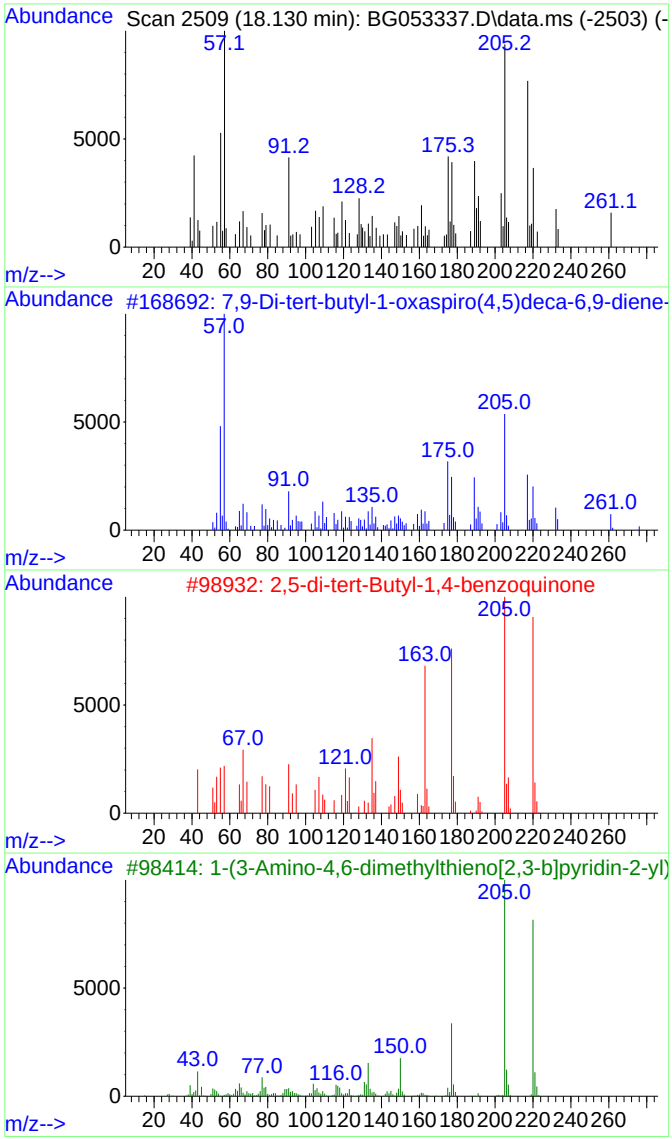
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

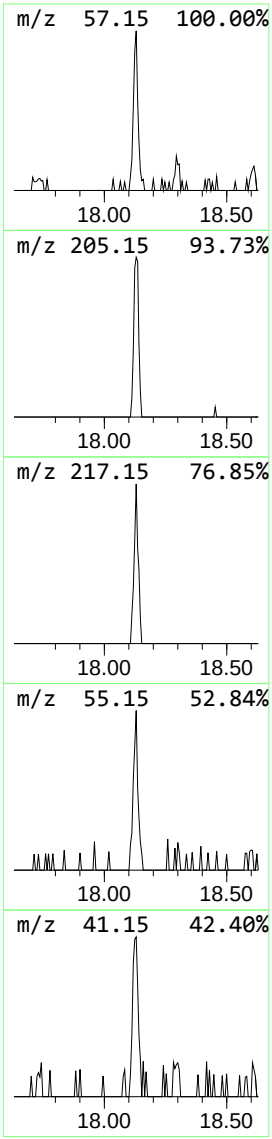
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.130	2.73 ng	49952	Phenanthrene-d10	17.472

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	74
2	2,5-di-tert-Butyl-1,4-benzoquinone	220	C14H20O2	002460-77-7	48
3	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	41
4	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	38
5	(1R,3aR,5aR,9aS)-1,4,4,7-Tetrame...	220	C15H24O	104188-25-2	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
Data File : BG053337.D
Acq On : 27 Apr 2022 2:00
Operator : CG/JU
Sample : N2482-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.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
Cyclopentanone	4.548	9.8	ng	50837	1	8.102	103613	20.0
p-Xylene	5.735	13.6	ng	70527	1	8.102	103613	20.0
Benzene, 1-ethy...	7.491	5.8	ng	30106	1	8.102	103613	20.0
2-Propanol, 1-(...	7.632	5.5	ng	28214	1	8.102	103613	20.0
Ethane, 1-ethox...	7.685	5.6	ng	28953	1	8.102	103613	20.0
Benzene, 1,2,4-...	7.750	10.7	ng	55420	1	8.102	103613	20.0
2-Propanol, 1-(...	7.873	9.2	ng	47529	1	8.102	103613	20.0
1-Hexanol, 2-et...	8.161	7.8	ng	40215	1	8.102	103613	20.0
Propanoic acid,...	13.089	5.4	ng	62682	3	14.728	232562	20.0
Phenol, 4-(1,1-...	13.571	21.1	ng	245786	3	14.728	232562	20.0
Cyclopentaneace...	16.068	3.6	ng	41940	3	14.728	232562	20.0
7,9-Di-tert-but...	18.130	2.7	ng	49952	4	17.472	365716	20.0