LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081122\
Data File : BG054603.D
Acq On : 11 Aug 2022 13:45
Operator : CG/JU
Sample : N3971-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-24

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: BG054603.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.089	11	17	34	rVB	263490	449499	25.00%	7.186%
2	4.405	235	241	251	rBV	48632	82167	4.57%	1.314%
3	5.051	345	351	359	rBV2	16111	27557	1.53%	0.441%
4	5.556	431	437	451	rVB	110091	195347	10.86%	3.123%
5	6.602	610	615	620	rBV2	18007	29651	1.65%	0.474%
6	7.172	706	712	724	rVB	70174	135199	7.52%	2.161%
7	7.971	842	848	854	rBV	48038	81336	4.52%	1.300%
8	9.134	1040	1046	1057	rVB	146108	273730	15.22%	4.376%
9	10.780	1319	1326	1334	rBV	60659	108300	6.02%	1.731%
10	11.708	1477	1484	1496	rVB2	30855	67135	3.73%	1.073%
11	12.965	1691	1698	1707	rBV	15038	26828	1.49%	0.429%
12	13.230	1734	1743	1751	rBV	483750	786709	43.75%	12.576%
13	13.465	1776	1783	1796	rBV	118017	190775	10.61%	3.050%
14	14.610	1972	1978	1985	rBV	116687	181546	10.10%	2.902%
15	15.351	2099	2104	2108	rVB	12862	19071	1.06%	0.305%
16	16.109	2227	2233	2246	rBV	465529	737582	41.02%	11.791%
17	16.690	2325	2332	2340	rBV2	21088	33061	1.84%	0.529%
18	17.360	2440	2446	2453	rBV	171008	266782	14.84%	4.265%
19	18.012	2553	2557	2562	rBV2	21651	27216	1.51%	0.435%
20	19.969	2884	2890	2896	rBV	1347761	1798253	100.00%	28.746%
21	21.626	3166	3172	3182	rVB	212800	367780	20.45%	5.879%
22	24.834	3709	3718	3730	rVB2	128494	370037	20.58%	5.915%

Sum of corrected areas: 6255561

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Misc :
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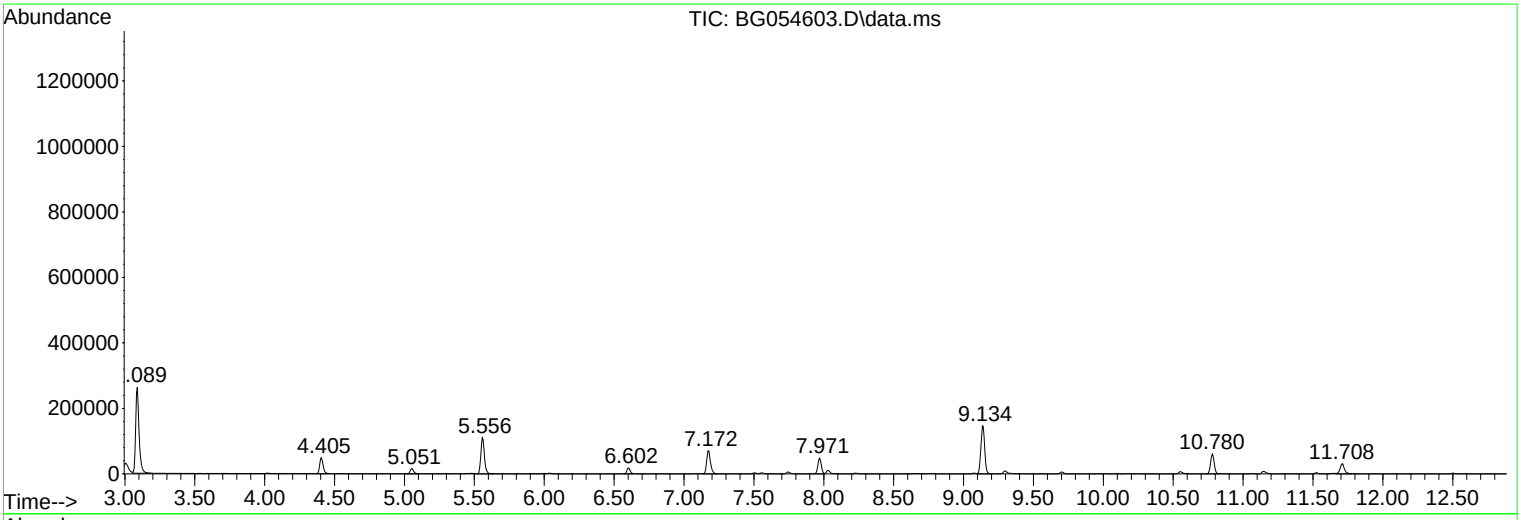
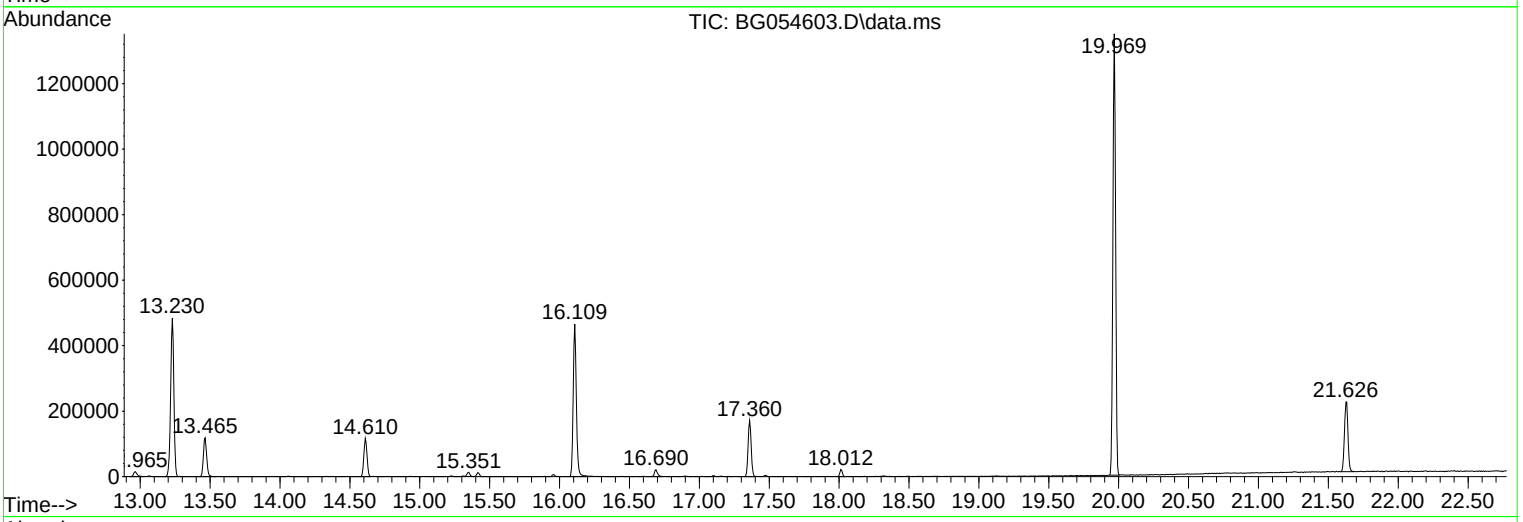
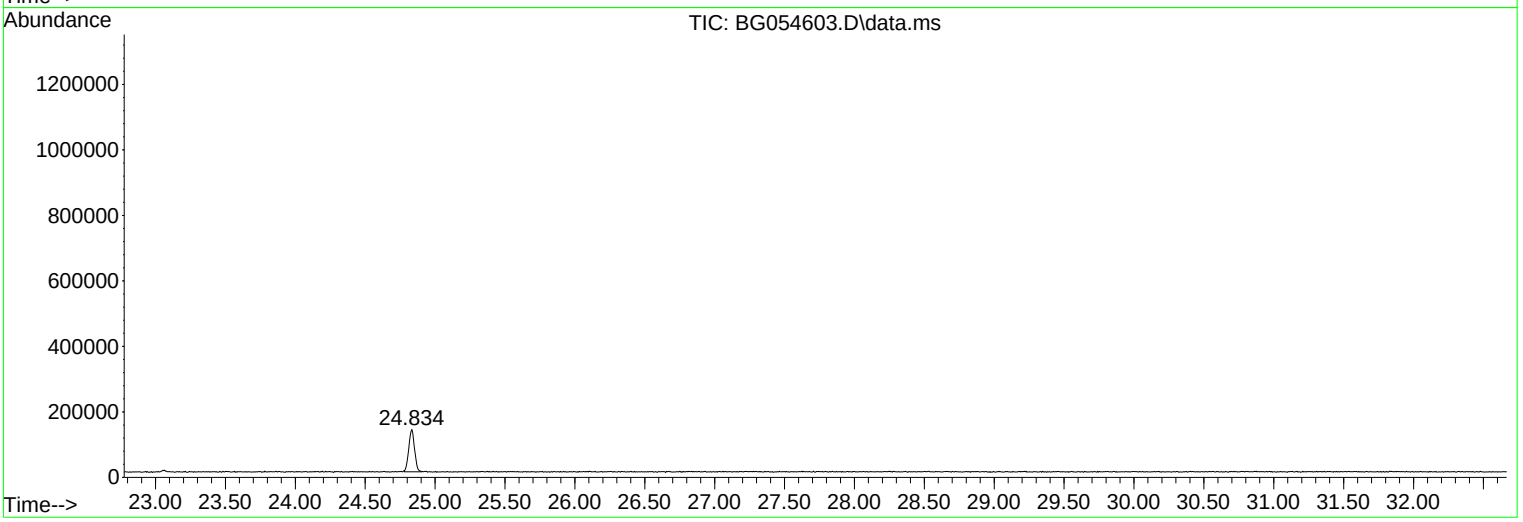
Instrument :
BNA_G
ClientSampleId :
MW-24

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

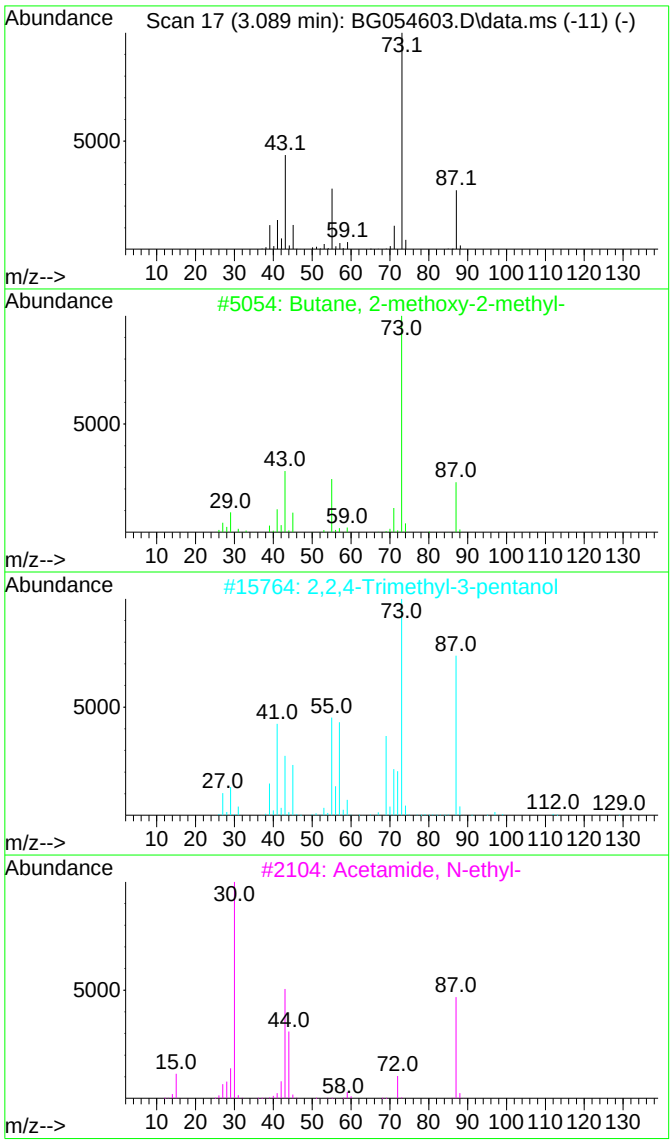
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

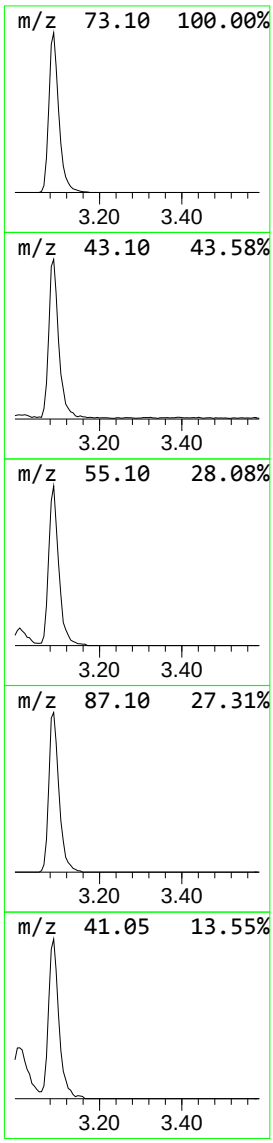
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.089	110.53 ng	449499	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	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Acq On : 11 Aug 2022 13:45
Operator : CG/JU
Sample : N3971-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

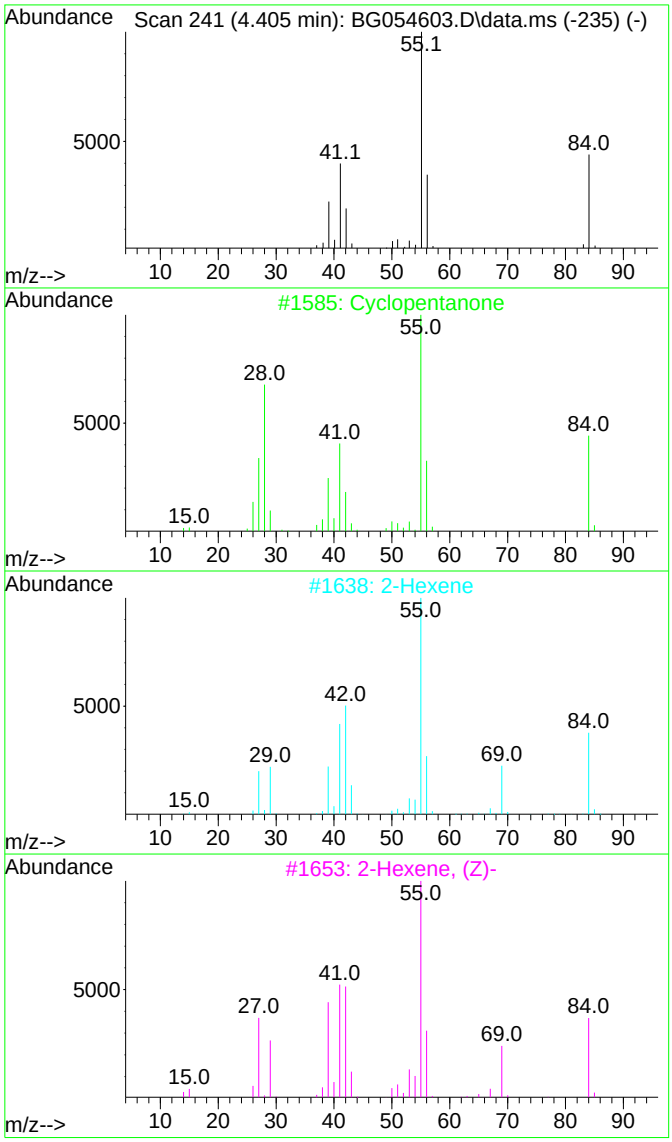
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

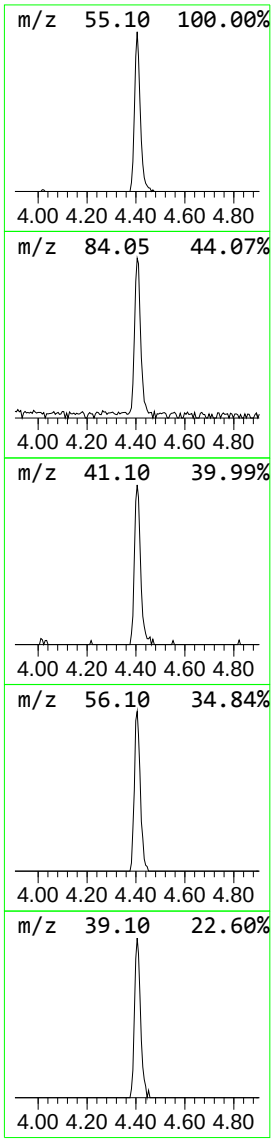
****

Peak Number 2 Cyclopentanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.405	20.20 ng	82167	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	64
3	2-Hexene, (Z)-	84	C6H12	007688-21-3	59
4	2-Ethylacrolein	84	C5H8O	000922-63-4	58
5	3-Hexene, (Z)-	84	C6H12	007642-09-3	50





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Misc :
ALS Vial : 7 Sample Multiplier: 1

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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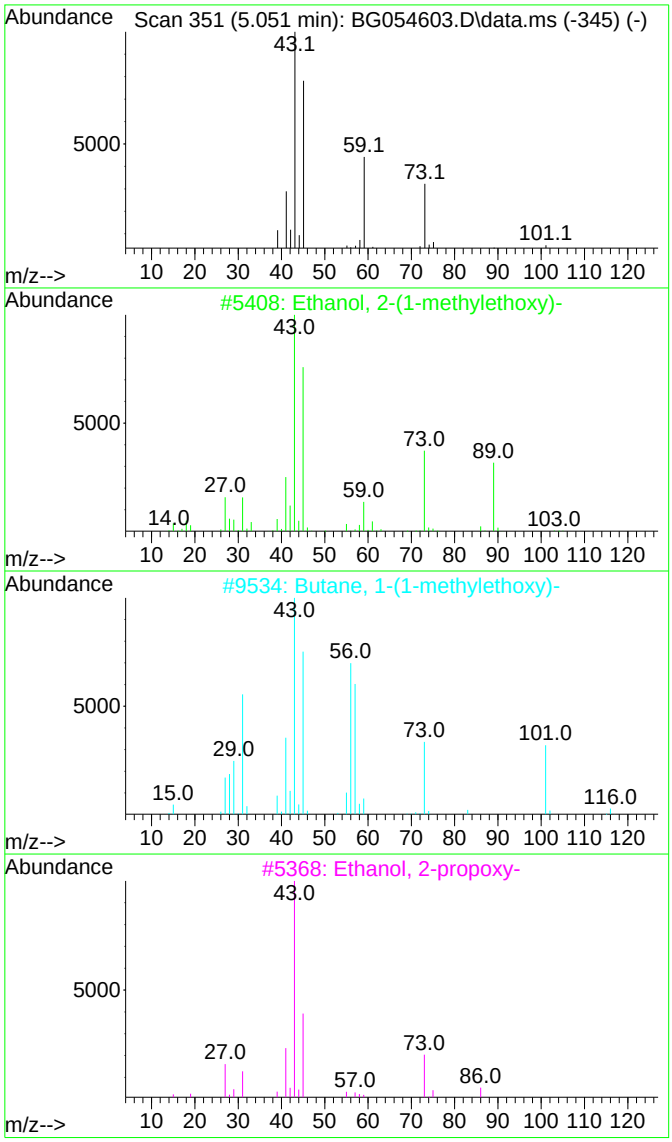
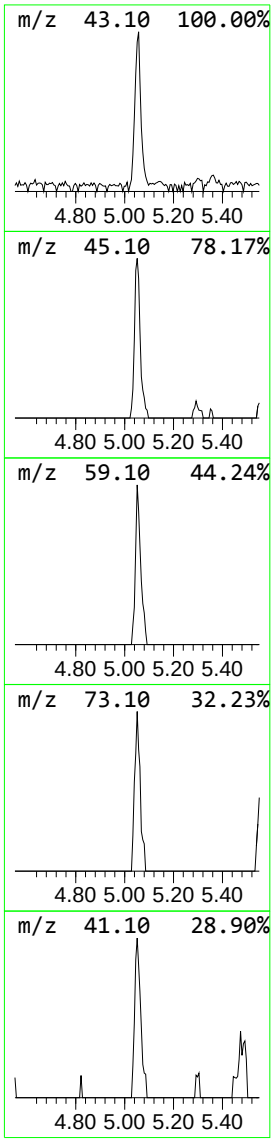
****

Peak Number 3 unknown5.051 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.051	6.78 ng	27557	1,4-Dichlorobenzene-d4	7.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	45
2	Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	42
3	Ethanol, 2-propoxy-	104	C5H12O2	002807-30-9	38
4	Diacetamide	101	C4H7NO2	000625-77-4	38
5	2-O-Mesyl arabinose	228	C6H12O7S	1000130-06-0	36





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Instrument :
BNA_G
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

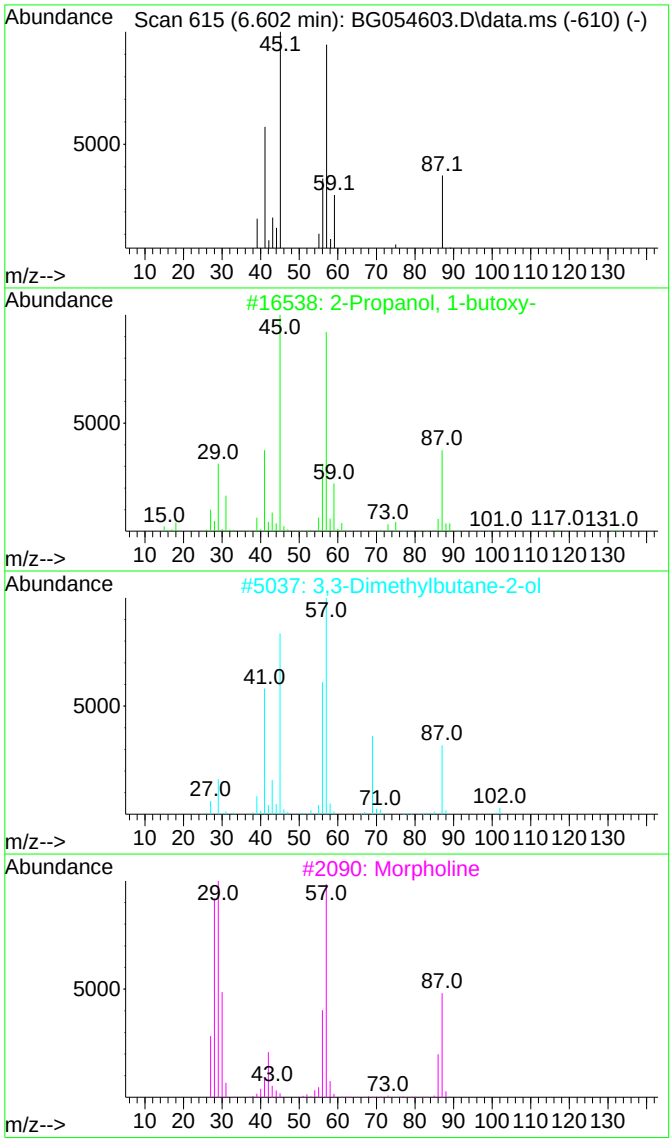
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

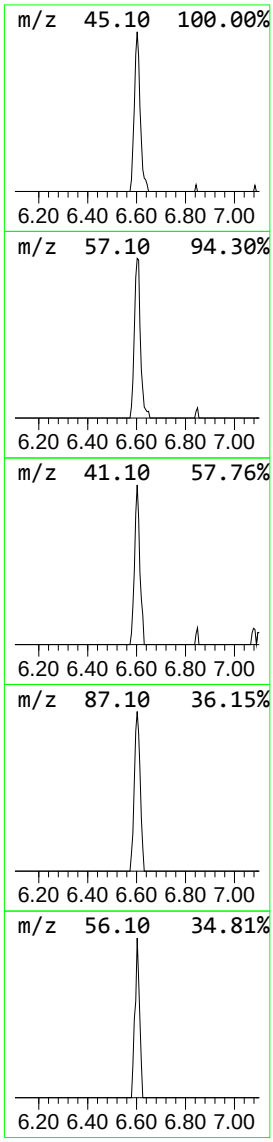
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.602	7.29 ng	29651	1,4-Dichlorobenzene-d4	7.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	78
2	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	36
3	Morpholine	87	C4H9NO	000110-91-8	12
4	1-Butanol, 3,3-dimethyl-	102	C6H14O	000624-95-3	10
5	Acetaldehyde, O-ethyloxime-	87	C4H9NO	1000288-34-6	10





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ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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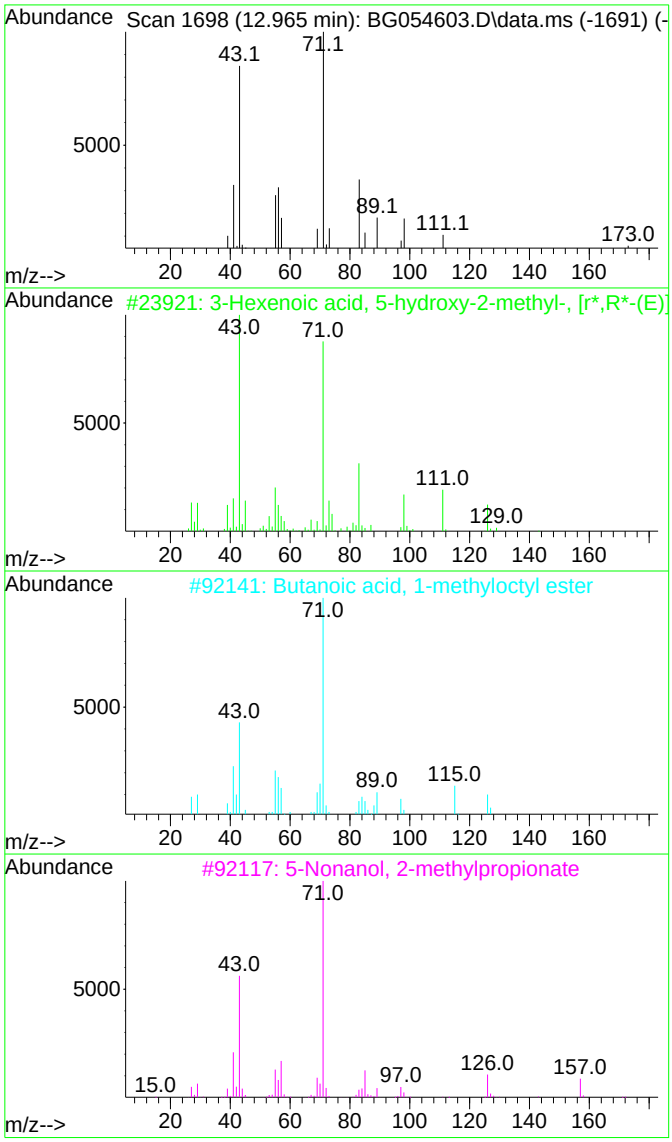
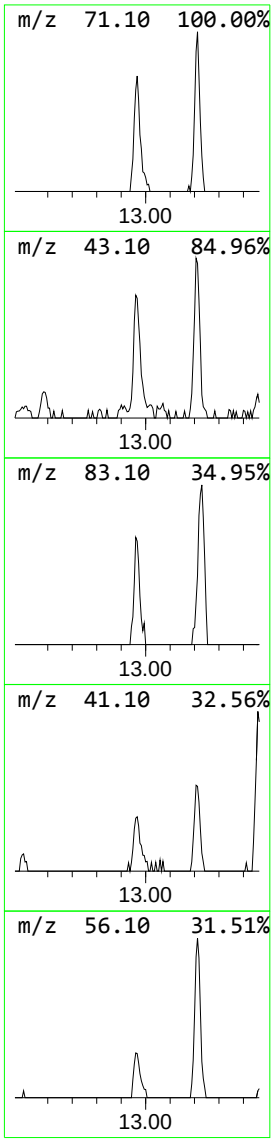
****
Peak Number 5 3-Hexenoic acid, 5-hydroxy-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.965	2.96 ng	26828	Acenaphthene-d10	14.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexenoic acid, 5-hydroxy-2-met...	144	C7H12O3	110678-36-9	64
2	Butanoic acid, 1-methyloctyl ester	214	C13H26O2	069727-42-0	50
3	5-Nonanol, 2-methylpropionate	214	C13H26O2	1000463-47-6	47
4	Carbonic acid, decyl nonyl ester	328	C20H40O3	1000383-15-8	45
5	Butyric acid, dodecyl ester	256	C16H32O2	003724-61-6	45





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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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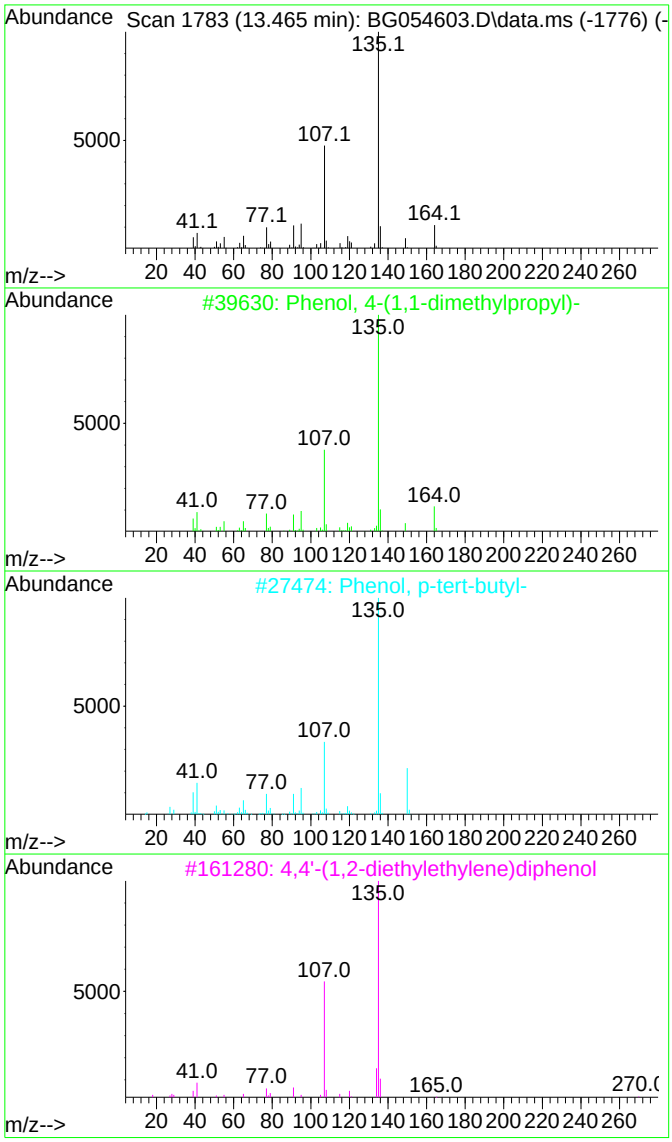
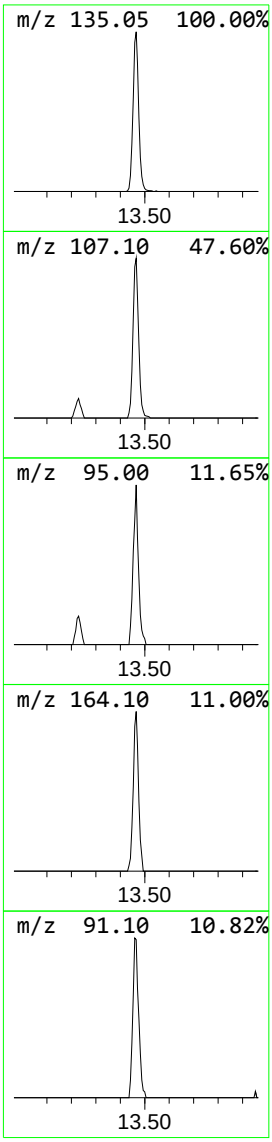
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.465	21.02 ng	190775	Acenaphthene-d10	14.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	93
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	86
3	4,4'-(1,2-diethylethylene)diphenol	270	C18H22O2	005635-50-7	72
4	Hexestrol, O-trifluoroacetyl-	366	C20H21F3O3	1000365-31-7	72
5	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	72





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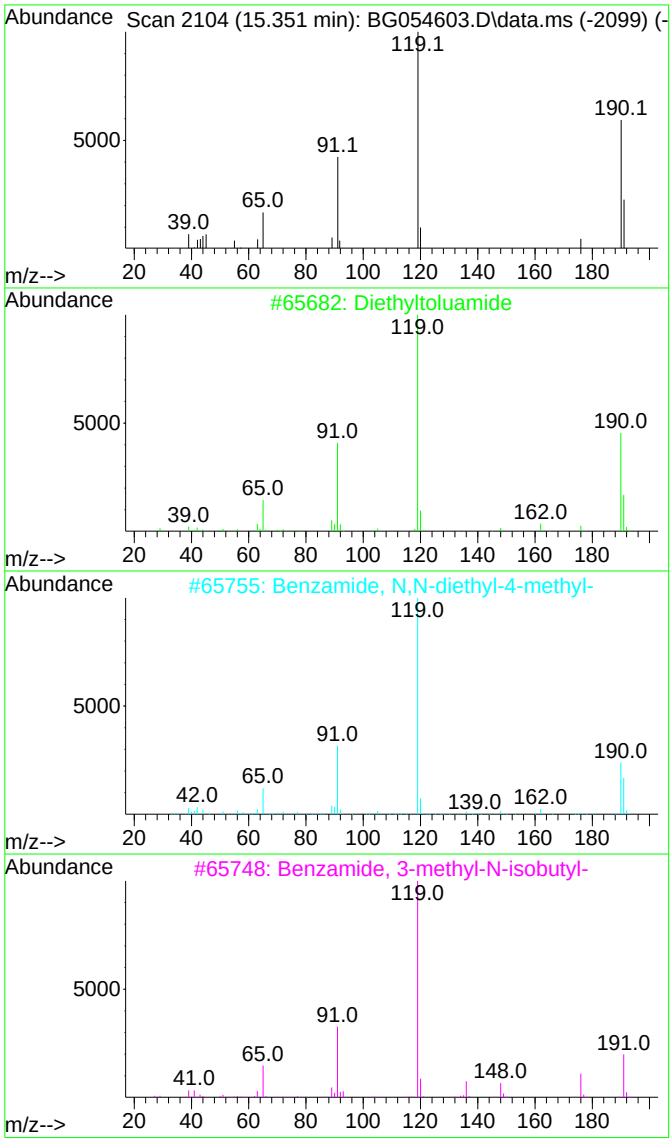
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

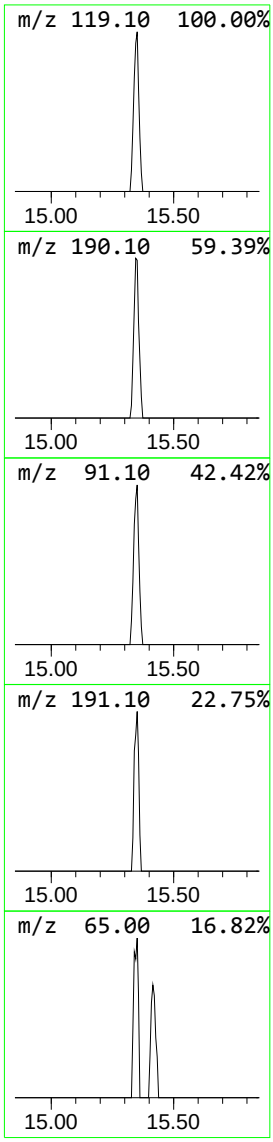
****

Peak Number 7 Diethyltoluamide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.351	2.10 ng	19071	Acenaphthene-d10	14.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyltoluamide	191	C12H17NO	000134-62-3	91
2	Benzamide, N,N-diethyl-4-methyl-	191	C12H17NO	002728-05-4	80
3	Benzamide, 3-methyl-N-isobutyl-	191	C12H17NO	1000407-41-0	64
4	Benzoic acid, 3-methyl-, pentafl...	302	C14H7F5O2	1000355-70-7	50
5	1-Propanone, 2-methyl-1-(2-methy...	162	C11H14O	002040-21-3	50





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TIC Library : C:\Database\NIST20.L
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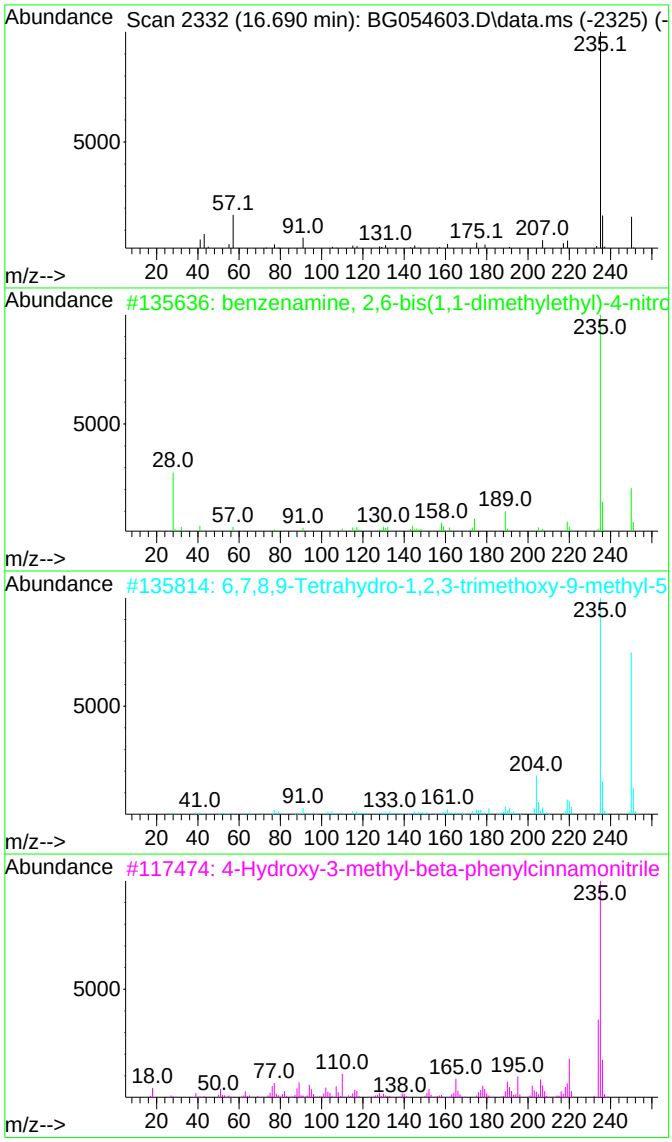
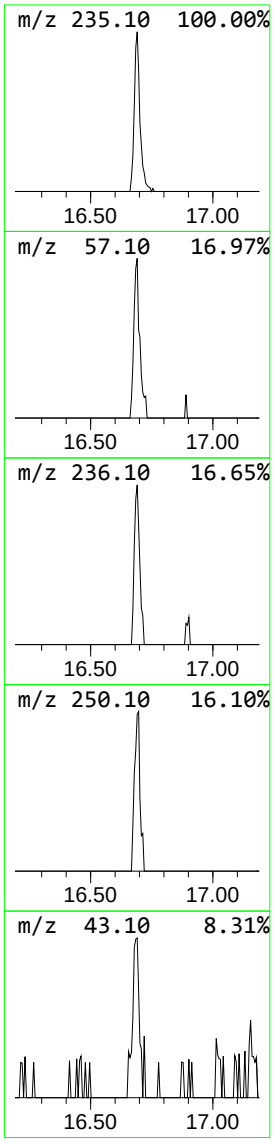
****
Peak Number 8 benzenamine, 2,6-bis(1,1-di... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.690	2.48 ng	33061	Phenanthrene-d10	17.360

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	benzenamine, 2,6-bis(1,1-dimethy...	250	C14H22N2O2	1000401-37-0	72
2	6,7,8,9-Tetrahydro-1,2,3-trimeth...	250	C15H22O3	1000242-60-6	72
3	4-Hydroxy-3-methyl-beta-phenylci...	235	C16H13NO	016299-28-8	64
4	Imidazo[1',2'-a]pyrido[3,2-c]qui...	235	C14H9N3O	129011-77-4	64
5	Indole, 2-(2-toluoyl)-	235	C16H13NO	001026-19-3	59





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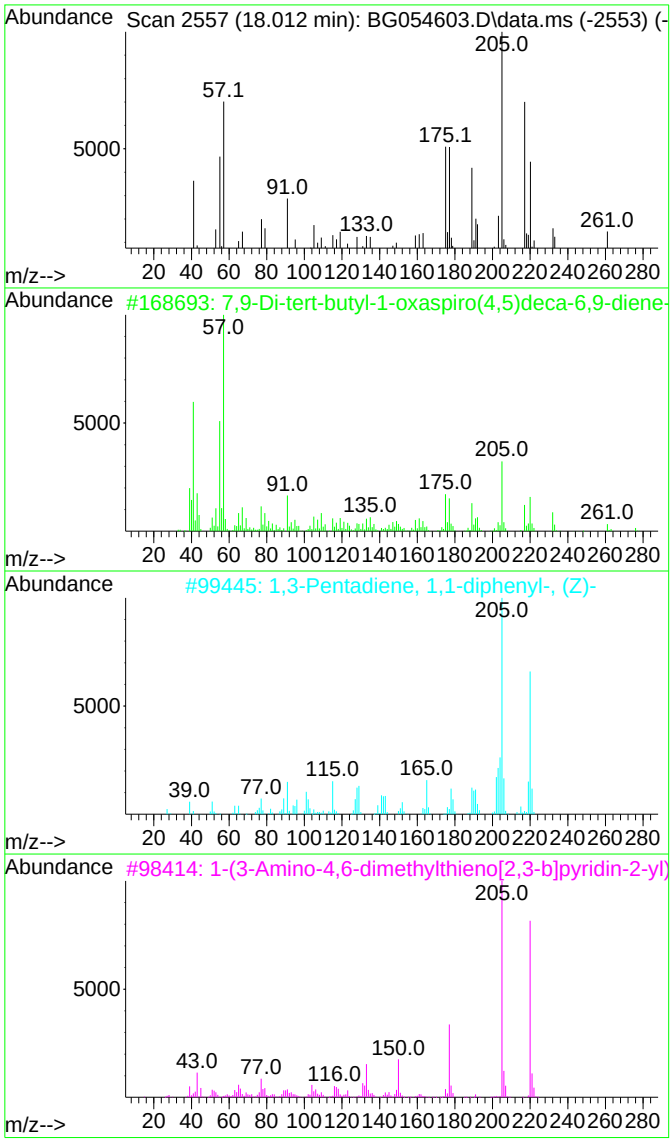
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

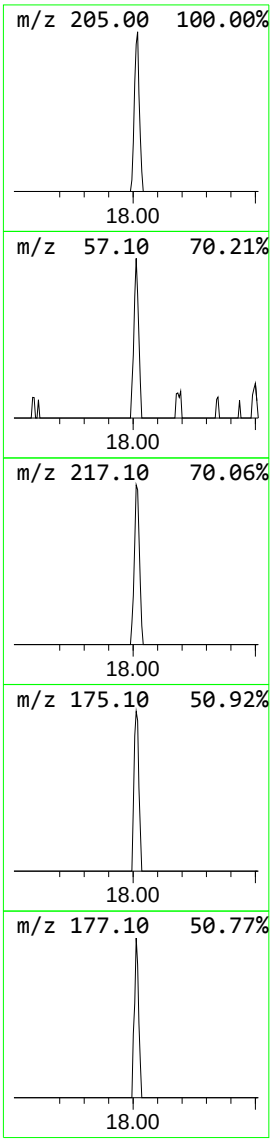
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.012	2.04 ng	27216	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	80
3	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	45
4	9-Acetylphenanthrene	220	C16H12O	002039-77-2	43
5	3,5-Cyclohexadiene-1,2-dione, 3,...	220	C14H20O2	003383-21-9	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081122\
Data File : BG054603.D
Acq On : 11 Aug 2022 13:45
Operator : CG/JU
Sample : N3971-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-24

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...	3.089	110.5	ng	449499	1	7.971	81336	20.0
Cyclopentanone	4.405	20.2	ng	82167	1	7.971	81336	20.0
unknown5.051	5.051	6.8	ng	27557	1	7.971	81336	20.0
2-Propanol, 1-b...	6.602	7.3	ng	29651	1	7.971	81336	20.0
3-Hexenoic acid...	12.965	3.0	ng	26828	3	14.610	181546	20.0
Phenol, 4-(1,1-...	13.465	21.0	ng	190775	3	14.610	181546	20.0
Diethyltoluamide	15.351	2.1	ng	19071	3	14.610	181546	20.0
benzenamine, 2,...	16.690	2.5	ng	33061	4	17.360	266782	20.0
7,9-Di-tert-but...	18.012	2.0	ng	27216	4	17.360	266782	20.0