LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042522\
Data File : BG053310.D
Acq On : 25 Apr 2022 15:50
Operator : CG/JU
Sample : N2481-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-12

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: BG053310.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.192	302	307	313	rBV2	23565	37926	1.16%	0.327%
2	5.674	382	389	401	rVB	338191	549724	16.79%	4.744%
3	7.266	652	660	671	rBV	228081	410177	12.53%	3.540%
4	7.630	717	722	727	rBV	23666	36886	1.13%	0.318%
5	7.683	727	731	738	rVB	23702	37759	1.15%	0.326%
6	7.871	757	763	773	rBV	38287	65663	2.01%	0.567%
7	8.106	795	803	809	rBV	101291	177801	5.43%	1.534%
8	8.159	809	812	824	rVB2	23378	36644	1.12%	0.316%
9	9.269	993	1001	1011	rVB	428302	764688	23.36%	6.599%
10	10.920	1274	1282	1288	rBV	135349	247044	7.55%	2.132%
11	13.094	1645	1652	1660	rBV	47991	82998	2.54%	0.716%
12	13.352	1686	1696	1704	rBV	1128925	1859167	56.80%	16.044%
13	13.569	1727	1733	1745	rVB	229596	349995	10.69%	3.020%
14	14.727	1924	1930	1939	rBV	220919	365518	11.17%	3.154%
15	15.531	2061	2067	2073	rVB	32051	46724	1.43%	0.403%
16	16.066	2153	2158	2162	rBV3	32113	44735	1.37%	0.386%
17	16.219	2177	2184	2194	rBV	1023709	1530239	46.75%	13.205%
18	17.476	2391	2398	2406	rVB	325760	497381	15.19%	4.292%
19	18.134	2505	2510	2514	rVB2	53120	67544	2.06%	0.583%
20	20.078	2835	2841	2848	rBV	2503927	3273332	100.00%	28.248%
21	21.758	3120	3127	3138	rBV	317424	554645	16.94%	4.786%
22	25.054	3679	3688	3699	rVB2	187251	551329	16.84%	4.758%

Sum of corrected areas: 11587919

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042522\
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Acq On : 25 Apr 2022 15:50
Operator : CG/JU
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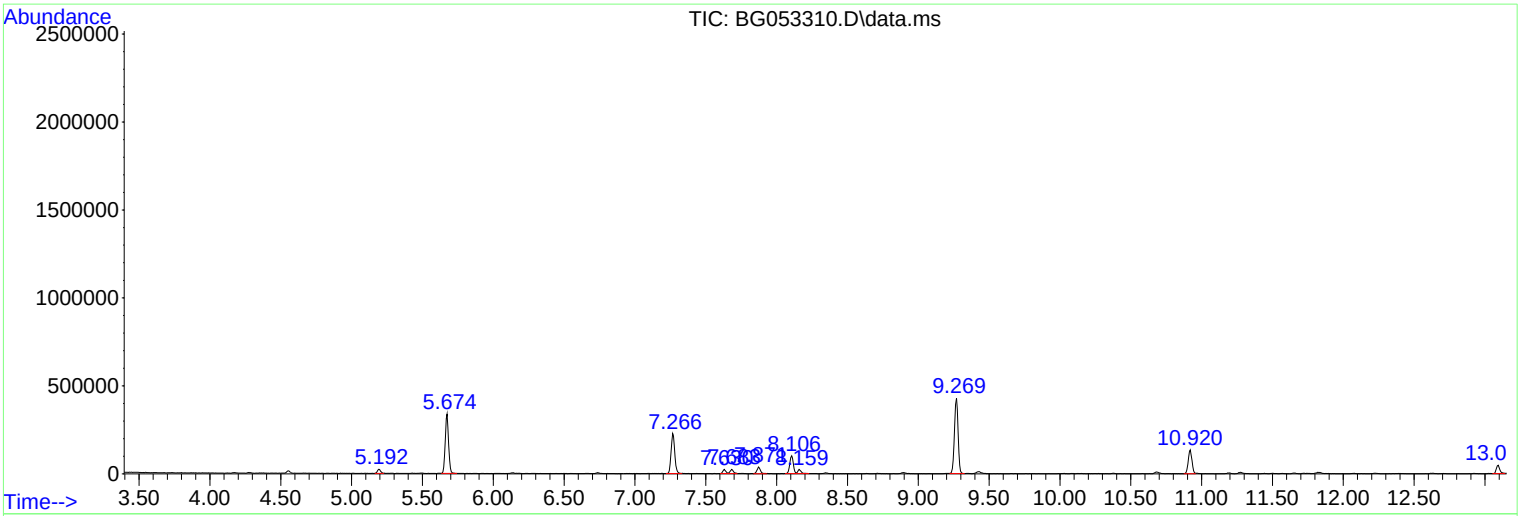
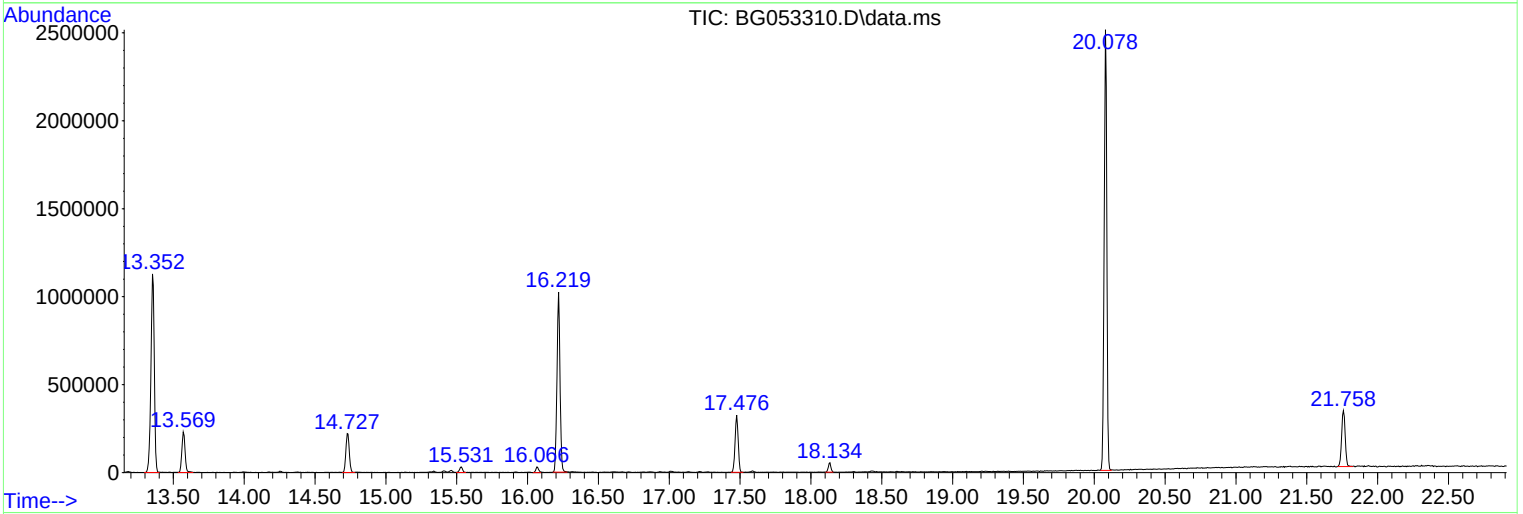
Misc :
ALS Vial : 7 Sample Multiplier: 1

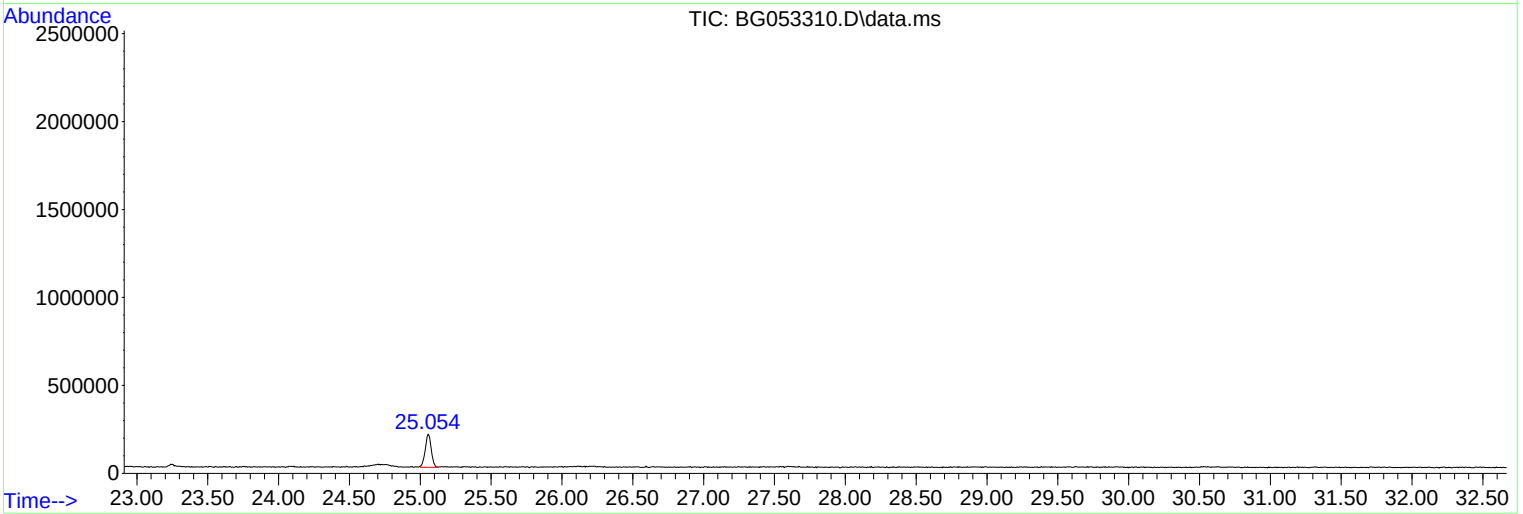
Instrument :
BNA_G
ClientSampleId :
MW-12

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 : BG053310.D
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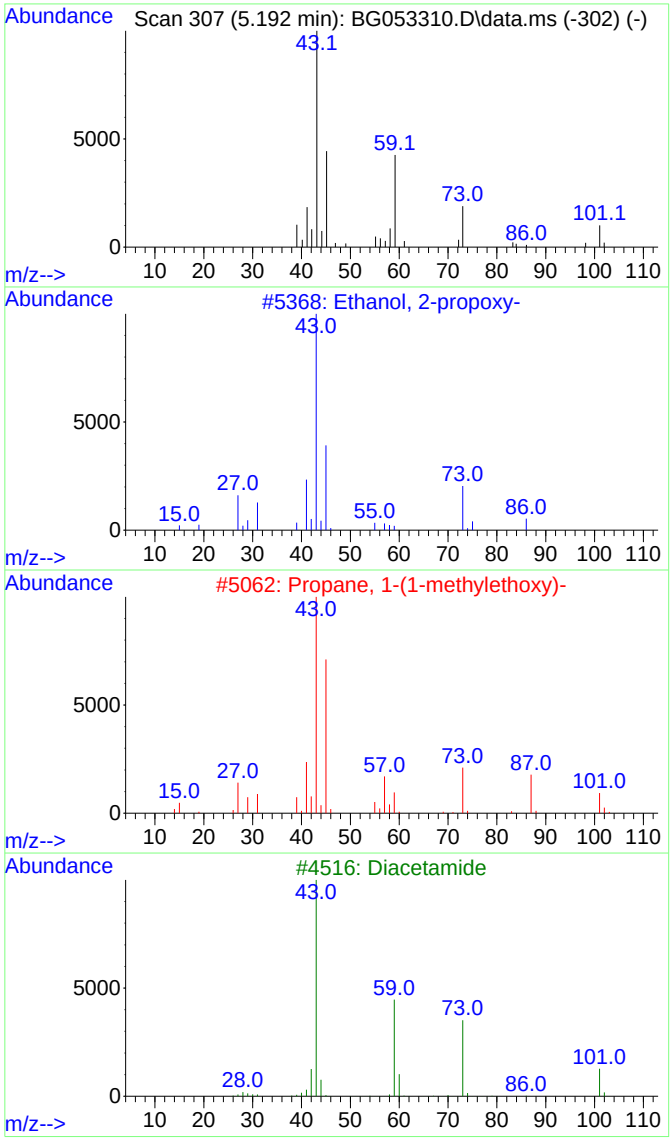
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

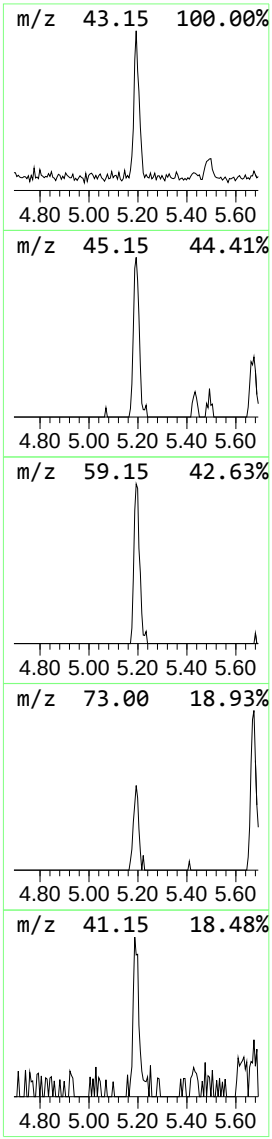
****

Peak Number 1 unknown5.192 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.192	4.27 ng	37926	1,4-Dichlorobenzene-d4	8.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-propoxy-	104	C5H12O2	002807-30-9	43
2	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	43
3	Diacetamide	101	C4H7NO2	000625-77-4	16
4	Formamide, N-butyl-	101	C5H11NO	000871-71-6	9
5	Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9





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Data File : BG053310.D
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Operator : CG/JU
Sample : N2481-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-12

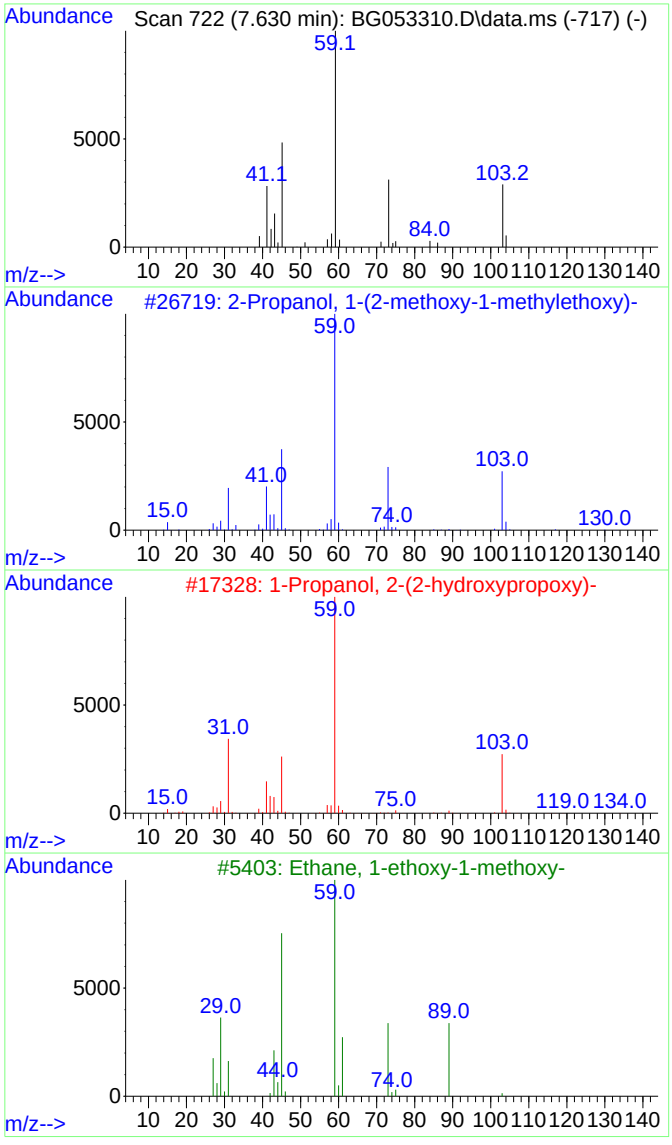
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

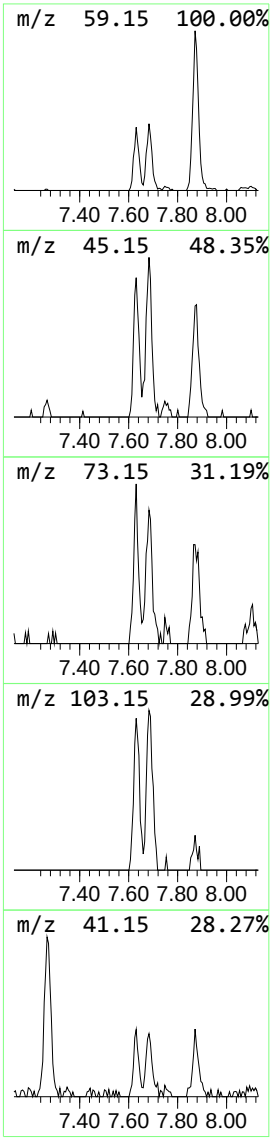
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.630	4.15 ng	36886	1,4-Dichlorobenzene-d4	8.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	59
3	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	45
4	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	42
5	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042522\
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Acq On : 25 Apr 2022 15:50
Operator : CG/JU
Sample : N2481-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-12

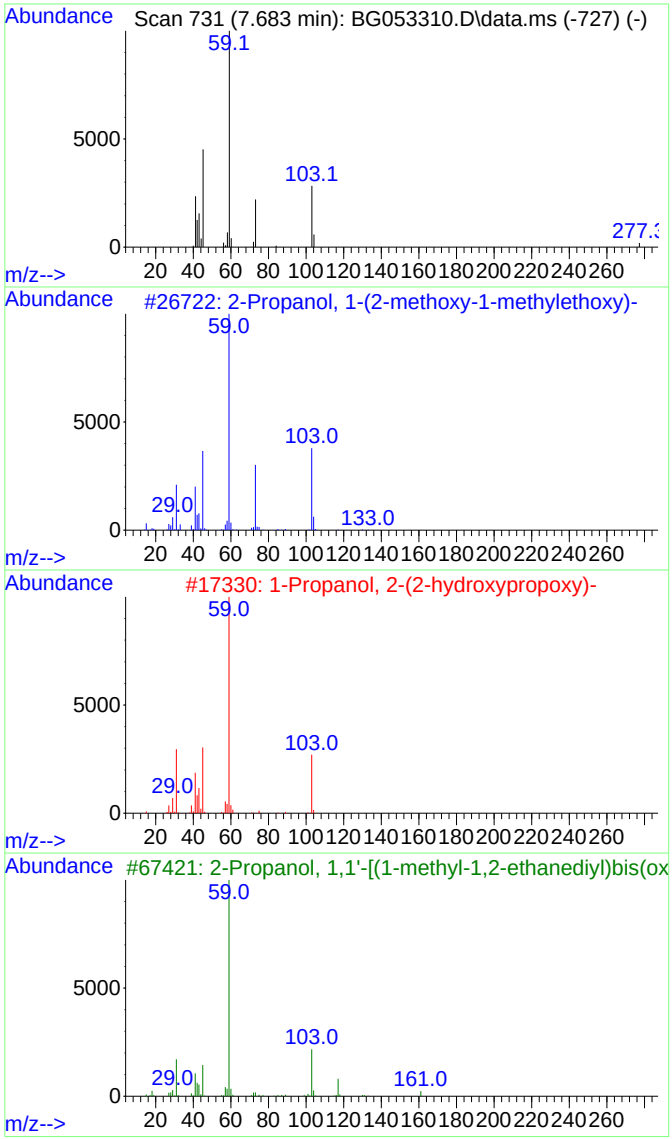
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

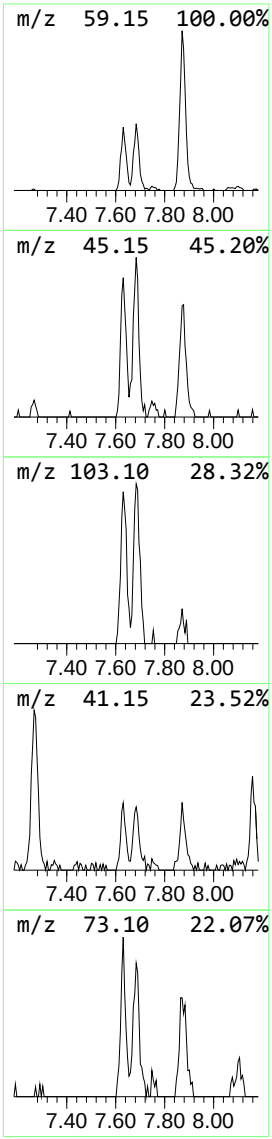
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.683	4.25 ng	37759	1,4-Dichlorobenzene-d4	8.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	72
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
3	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	42
4	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	38
5	Ethyl 2,5,8,11,14,17,20-heptaoxa...	382	C17H34O9	1000366-80-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042522\
Data File : BG053310.D
Acq On : 25 Apr 2022 15:50
Operator : CG/JU
Sample : N2481-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-12

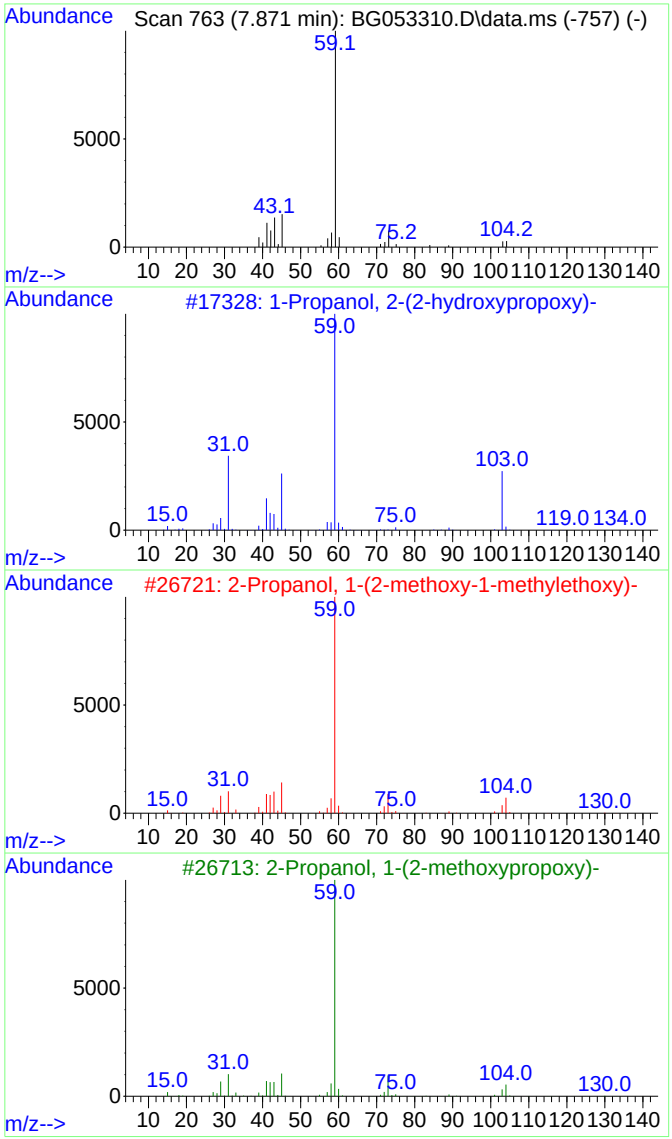
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

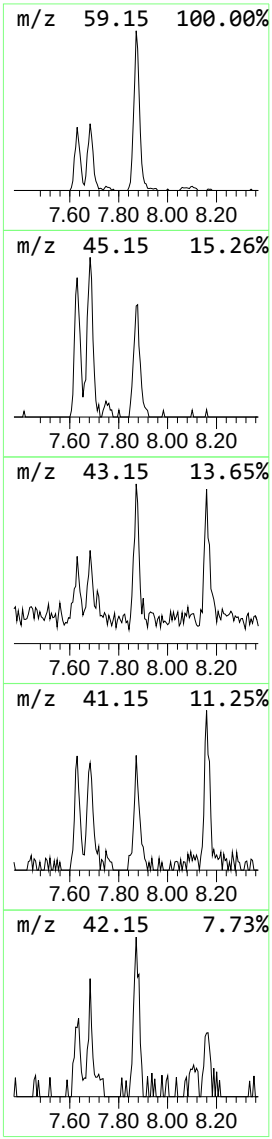
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Dipropylene glycol (isomer 2) Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.871	7.39 ng	65663	1,4-Dichlorobenzene-d4	8.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78
2	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	74
3	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	74
4	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	64
5	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042522\
Data File : BG053310.D
Acq On : 25 Apr 2022 15:50
Operator : CG/JU
Sample : N2481-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-12

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

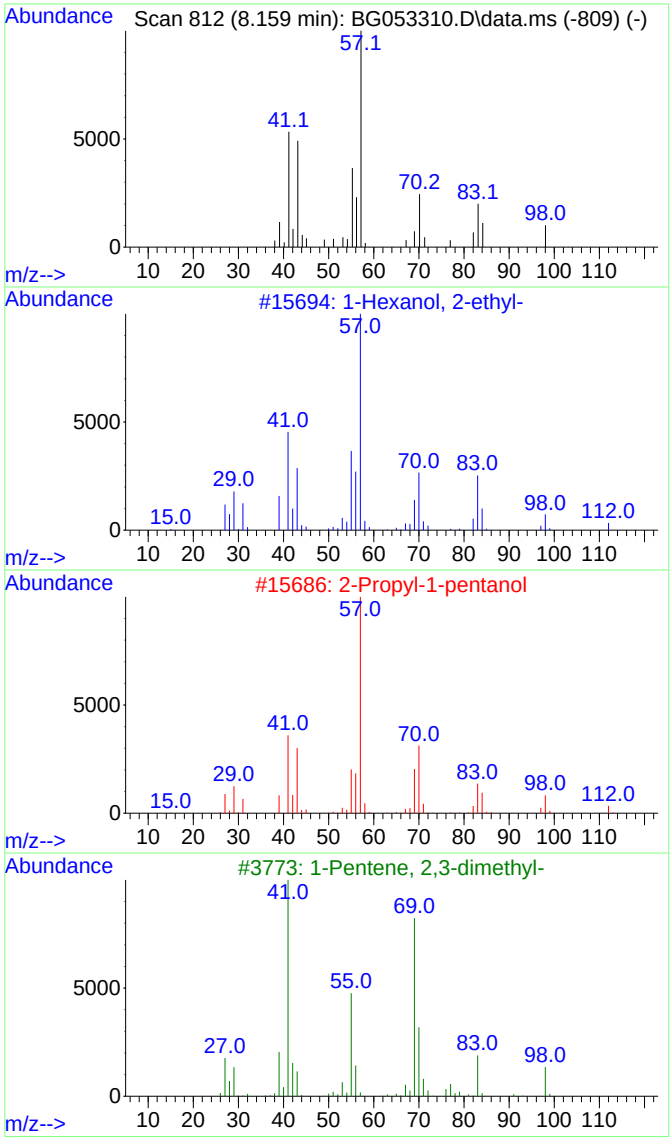
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

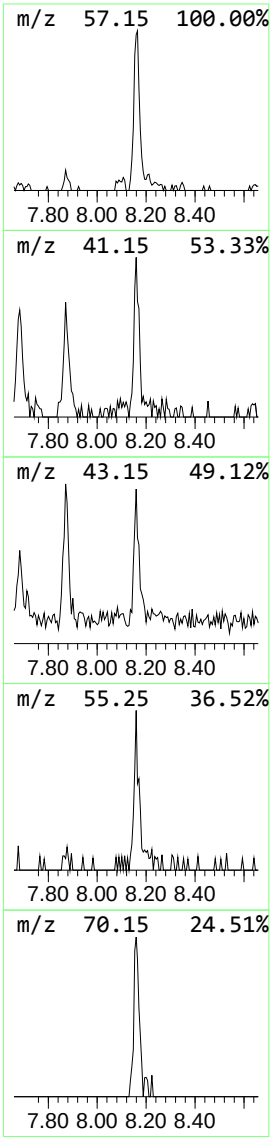
****

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.159	4.12 ng	36644	1,4-Dichlorobenzene-d4	8.106

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	42
3	1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	30
4	Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	25
5	Bicyclo[3.1.0]hexan-2-ol	98	C6H10O	1000194-18-6	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042522\
Data File : BG053310.D
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Sample : N2481-01
Misc :
ALS Vial : 7 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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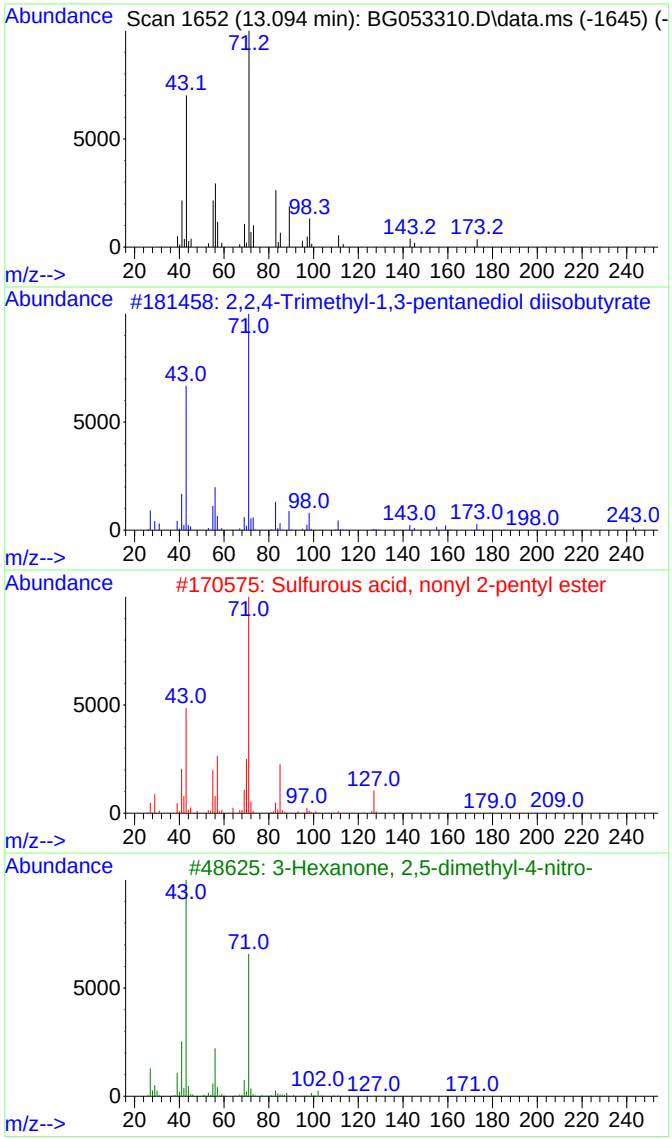
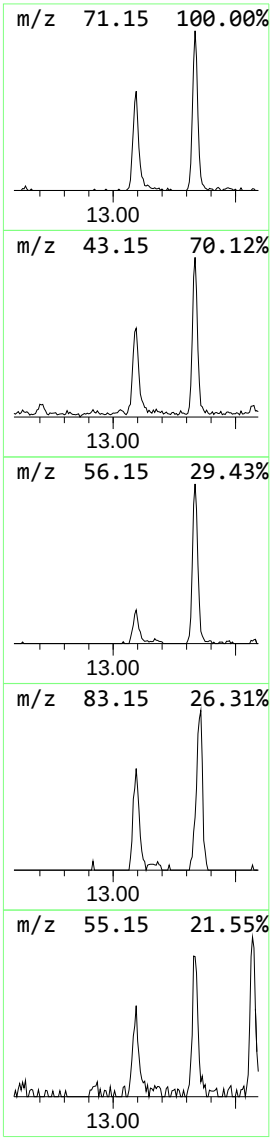
****

Peak Number 6 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.094	4.54 ng	82998	Acenaphthene-d10	14.727

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	90
2	Sulfurous acid, nonyl 2-pentyl e...	278	C14H30O3S	1010309-15-8	43
3	3-Hexanone, 2,5-dimethyl-4-nitro-	173	C8H15NO3	059906-54-6	43
4	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	42
5	Propanoic acid, 2-methyl-, 2-eth...	286	C16H30O4	074367-30-9	42





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Operator : CG/JU
Sample : N2481-01
Misc :
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Instrument :
BNA_G
ClientSampleId :
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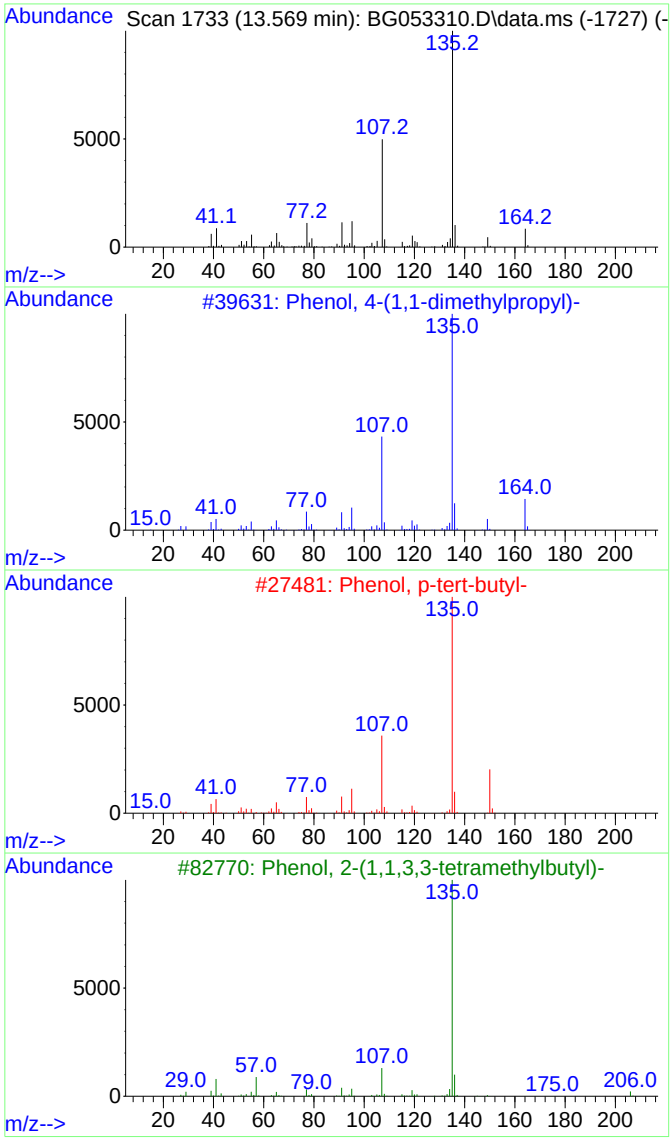
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

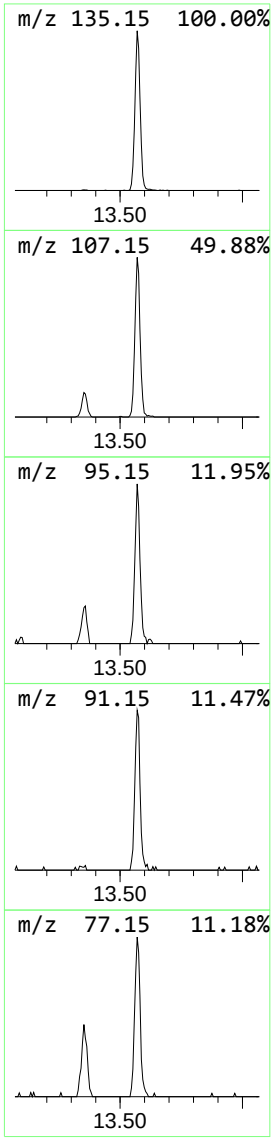
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.569	19.15 ng	349995	Acenaphthene-d10	14.727

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	94
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	86
3	Phenol, 2-(1,1,3,3-tetramethylbu...	206	C14H22O	003884-95-5	64
4	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	64
5	Imidazo[1,2-c]pyrimidin-5-ol	135	C6H5N3O	055662-66-3	64





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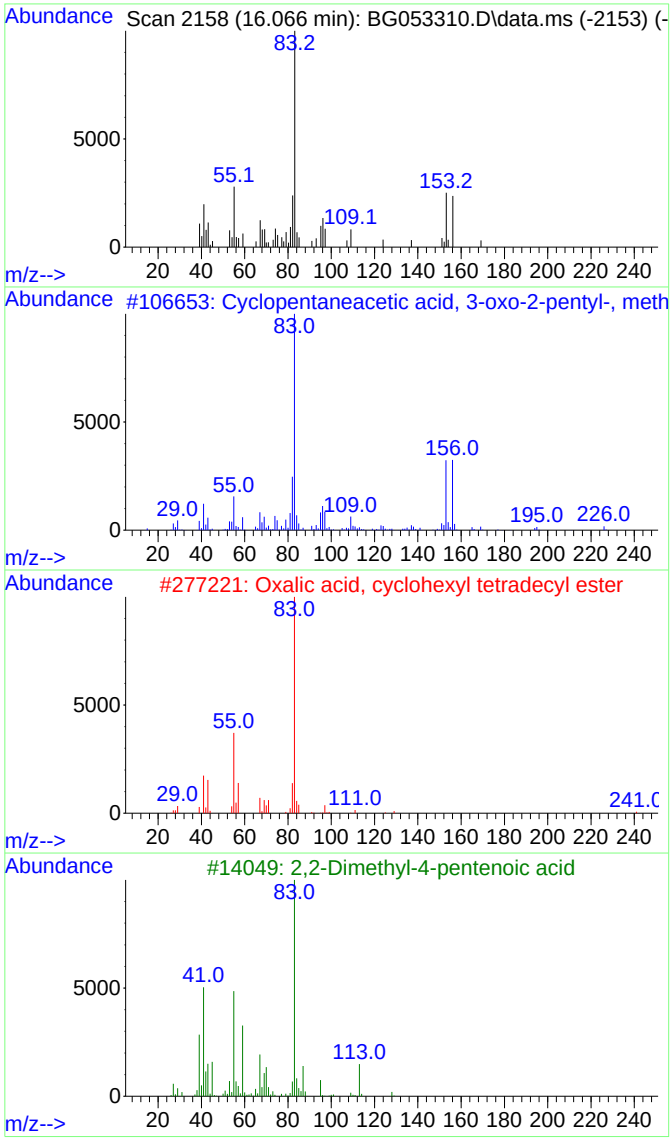
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

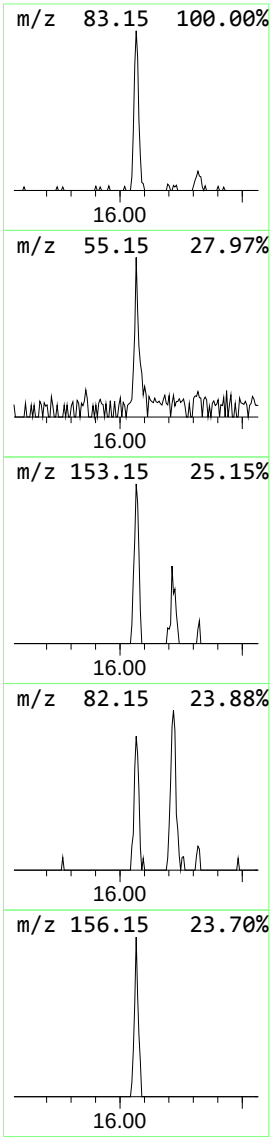
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Cyclopentaneacetic acid, 3-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.066	2.45 ng	44735	Acenaphthene-d10	14.727

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	90
2	Oxalic acid, cyclohexyl tetradec...	368	C22H40O4	1000309-31-5	38
3	2,2-Dimethyl-4-pentenoic acid	128	C7H12O2	016386-93-9	38
4	2,6-Dimethyl-6-nitro-2-hepten-4-one	185	C9H15NO3	073583-56-9	37
5	Cyclohexane, 1,1'-(1,4-butanediy...	222	C16H30	006165-44-2	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042522\
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Acq On : 25 Apr 2022 15:50
Operator : CG/JU
Sample : N2481-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-12

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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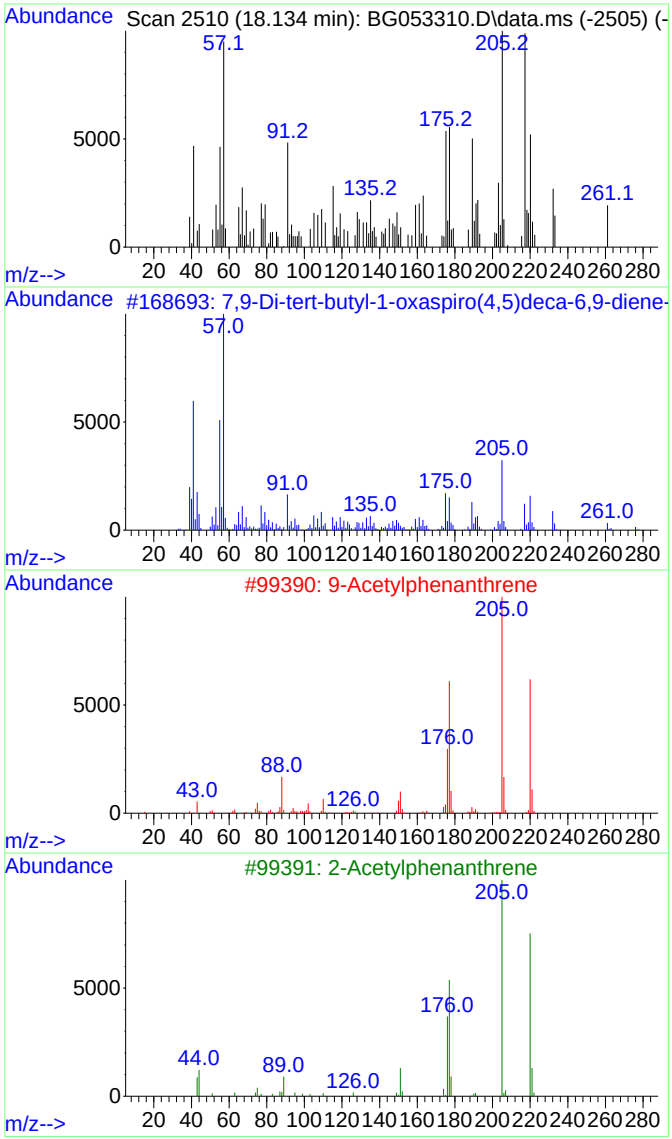
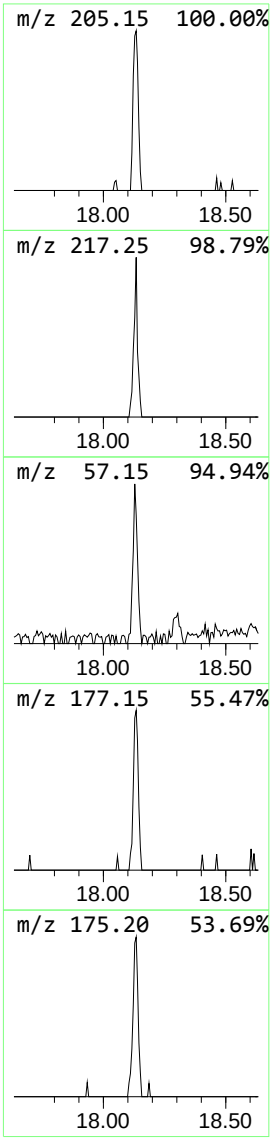
****
Peak Number 9 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.134	2.72 ng	67544	Phenanthrene-d10	17.476

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	9-Acetylphenanthrene	220	C16H12O	002039-77-2	42
3	2-Acetylphenanthrene	220	C16H12O	005960-69-0	42
4	3-Acetylphenanthrene	220	C16H12O	002039-76-1	38
5	Ethanone, 1-(9-anthracenyl)-	220	C16H12O	000784-04-3	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042522\
Data File : BG053310.D
Acq On : 25 Apr 2022 15:50
Operator : CG/JU
Sample : N2481-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-12

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
unknown5.192	5.192	4.3	ng	37926	1	8.106	177801	20.0
1-Propanol, 2-(...	7.630	4.2	ng	36886	1	8.106	177801	20.0
2-Propanol, 1-(...	7.683	4.3	ng	37759	1	8.106	177801	20.0
Dipropylene gly...	7.871	7.4	ng	65663	1	8.106	177801	20.0
1-Hexanol, 2-et...	8.159	4.1	ng	36644	1	8.106	177801	20.0
2,2,4-Trimethyl...	13.094	4.5	ng	82998	3	14.727	365518	20.0
Phenol, 4-(1,1-...	13.569	19.1	ng	349995	3	14.727	365518	20.0
Cyclopentaneace...	16.066	2.5	ng	44735	3	14.727	365518	20.0
7,9-Di-tert-but...	18.134	2.7	ng	67544	4	17.476	497381	20.0