LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100621\
Data File : BG050475.D
Acq On : 6 Oct 2021 19:51
Operator : CG/JU
Sample : M4088-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : WC-20211005-WATER

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-BG100621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG050475.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.790	385	392	401	rBV	346199	564959	18.10%	3.765%
2	7.389	657	664	674	rVB	248100	443553	14.21%	2.956%
3	8.258	802	812	818	rBV	178299	323263	10.36%	2.154%
4	8.487	842	851	857	rBV	67219	122775	3.93%	0.818%
5	9.169	961	967	972	rBV2	20413	38153	1.22%	0.254%
6	9.427	1003	1011	1019	rBV	563180	1029850	32.99%	6.863%
7	10.279	1148	1156	1163	rBV2	34327	72142	2.31%	0.481%
8	10.473	1184	1189	1196	rBV5	15354	34911	1.12%	0.233%
9	10.826	1242	1249	1265	rBV	145609	278414	8.92%	1.855%
10	11.084	1284	1293	1297	rBV	239112	454362	14.56%	3.028%
11	11.131	1297	1301	1308	rVB	143072	259017	8.30%	1.726%
12	12.253	1486	1492	1498	rBV4	23340	40801	1.31%	0.272%
13	12.612	1547	1553	1558	rVB4	19241	33803	1.08%	0.225%
14	12.718	1562	1571	1578	rBV	80174	138856	4.45%	0.925%
15	12.935	1599	1608	1618	rBV	50927	111370	3.57%	0.742%
16	13.499	1697	1704	1712	rBV	1403670	2233919	71.57%	14.886%
17	13.711	1734	1740	1746	rVB2	17082	31283	1.00%	0.208%
18	14.051	1792	1798	1807	rVB6	13009	32827	1.05%	0.219%
19	14.192	1817	1822	1827	rBV2	18578	33012	1.06%	0.220%
20	14.598	1886	1891	1900	rBV2	26882	60046	1.92%	0.400%
21	14.821	1925	1929	1931	rBV	23528	33995	1.09%	0.227%
22	14.874	1932	1938	1945	rVB	383105	629500	20.17%	4.195%
23	15.650	2065	2070	2076	rBV2	32634	61019	1.95%	0.407%
24	16.355	2184	2190	2199	rBV	1007431	1570314	50.31%	10.464%
25	17.371	2360	2363	2371	rVB	89941	131263	4.21%	0.875%
26	17.618	2399	2405	2410	rBV	459706	710010	22.75%	4.731%
27	18.476	2547	2551	2555	rBV2	84444	106359	3.41%	0.709%
28	19.733	2762	2765	2770	rBV4	48985	65450	2.10%	0.436%
29	20.015	2808	2813	2823	rVB	334620	504780	16.17%	3.364%
30	20.209	2840	2846	2852	rVB	2275383	3121363	100.00%	20.800%
31	20.691	2925	2928	2934	rVB3	36975	57821	1.85%	0.385%
32	21.531	3067	3071	3080	rVB4	42598	99039	3.17%	0.660%
33	21.613	3082	3085	3089	rVB	36956	47230	1.51%	0.315%
34	21.913	3130	3136	3143	rVB	425976	729179	23.36%	4.859%
35	25.326	3706	3717	3729	rVB2	261264	802208	25.70%	5.346%

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100621\
Data File : BG050475.D
Acq On : 6 Oct 2021 19:51
Operator : CG/JU
Sample : M4088-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-20211005-WATER

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-BG100621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

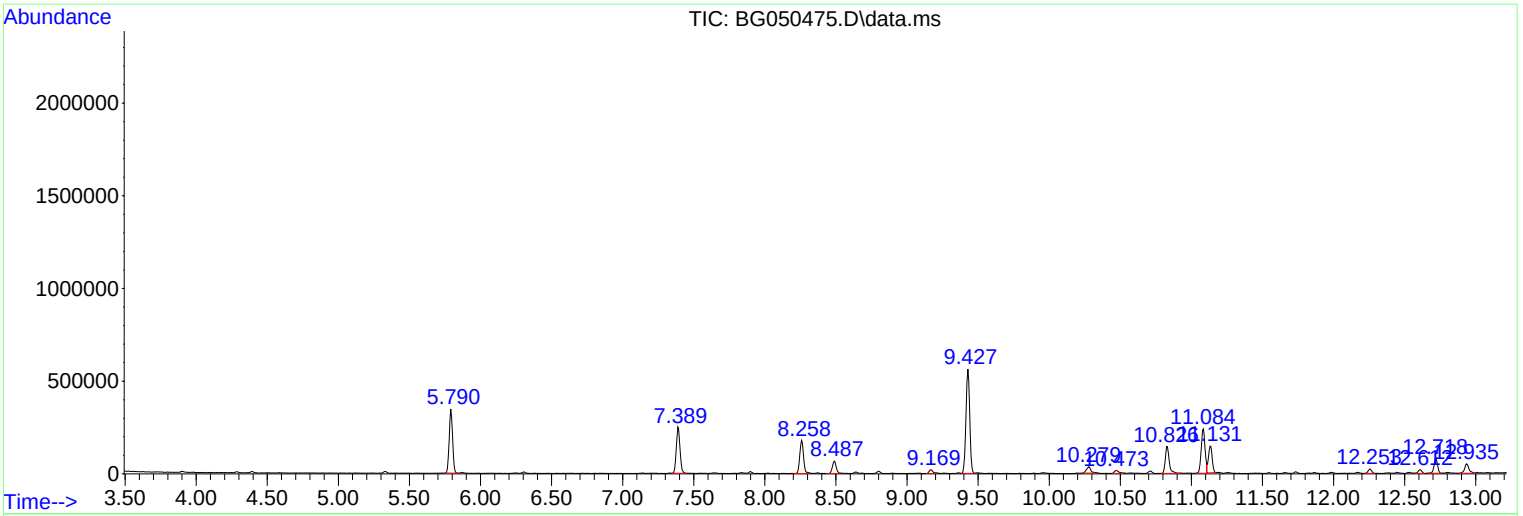
Sum of corrected areas: 15006846

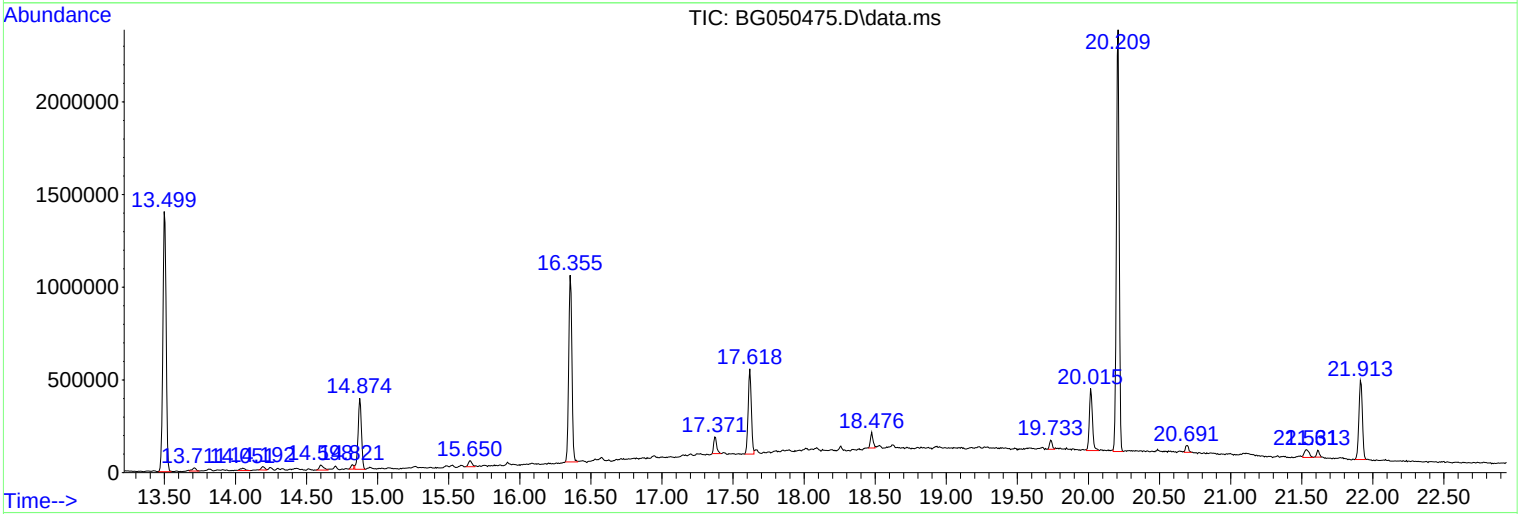
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100621\
Data File : BG050475.D
Acq On : 6 Oct 2021 19:51
Operator : CG/JU
Sample : M4088-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

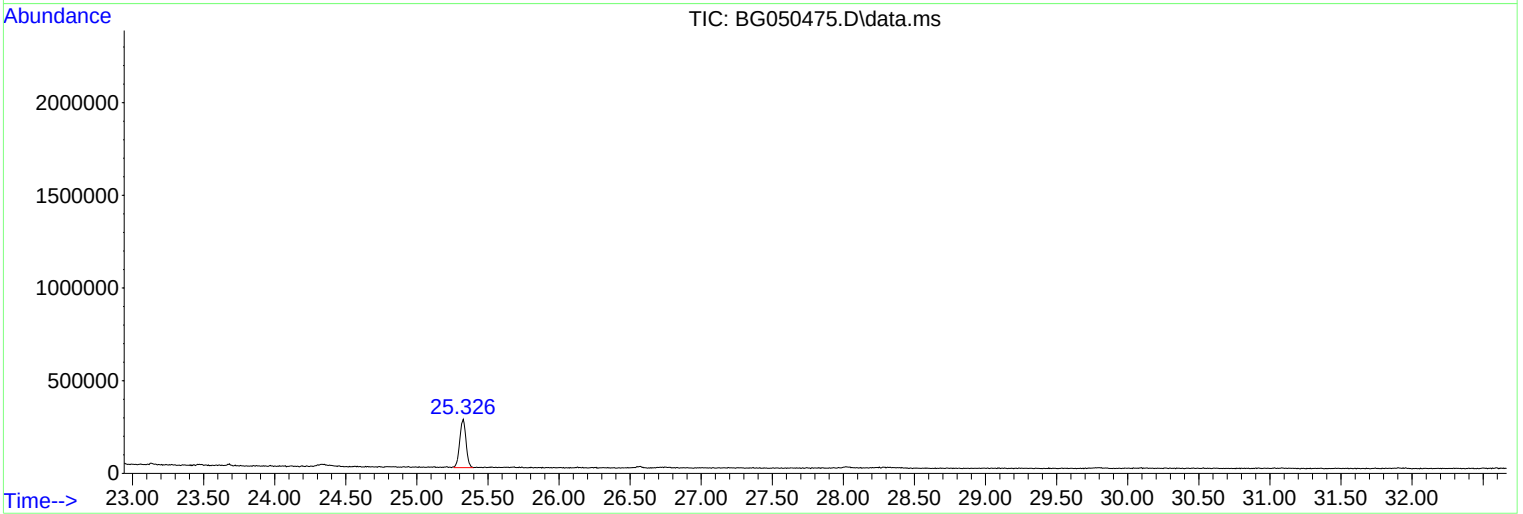
Instrument :
BNA_G
ClientSampleId :
WC-20211005-WATER

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100621\
Data File : BG050475.D
Acq On : 6 Oct 2021 19:51
Operator : CG/JU
Sample : M4088-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : WC-20211005-WATER

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

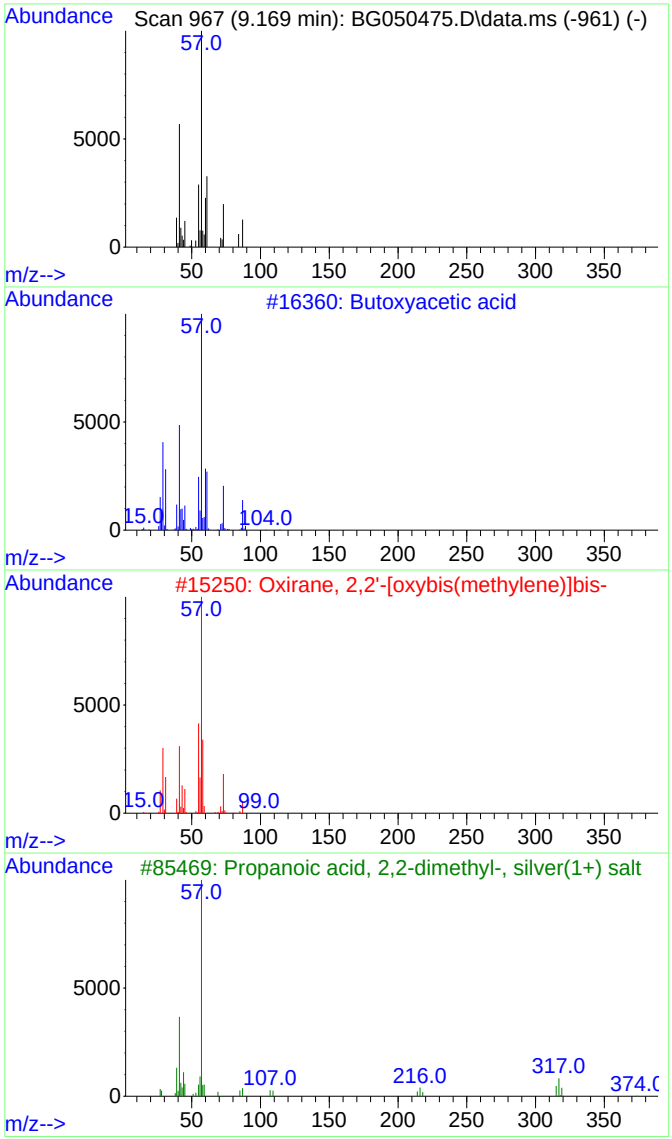
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

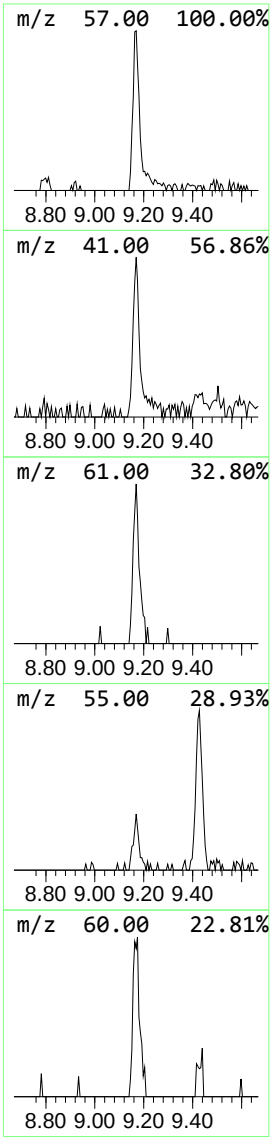
****

Peak Number 1 Butoxyacetic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.169	2.36 ng	38153	1,4-Dichlorobenzene-d4	8.258

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butoxyacetic acid	132	C6H12O3	002516-93-0	78
2	Oxirane, 2,2'-[oxybis(methylene)...	130	C6H10O3	002238-07-5	25
3	Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	14
4	1-Propanol, 2,2-dimethyl-	88	C5H12O	000075-84-3	12
5	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100621\
Data File : BG050475.D
Acq On : 6 Oct 2021 19:51
Operator : CG/JU
Sample : M4088-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : WC-20211005-WATER

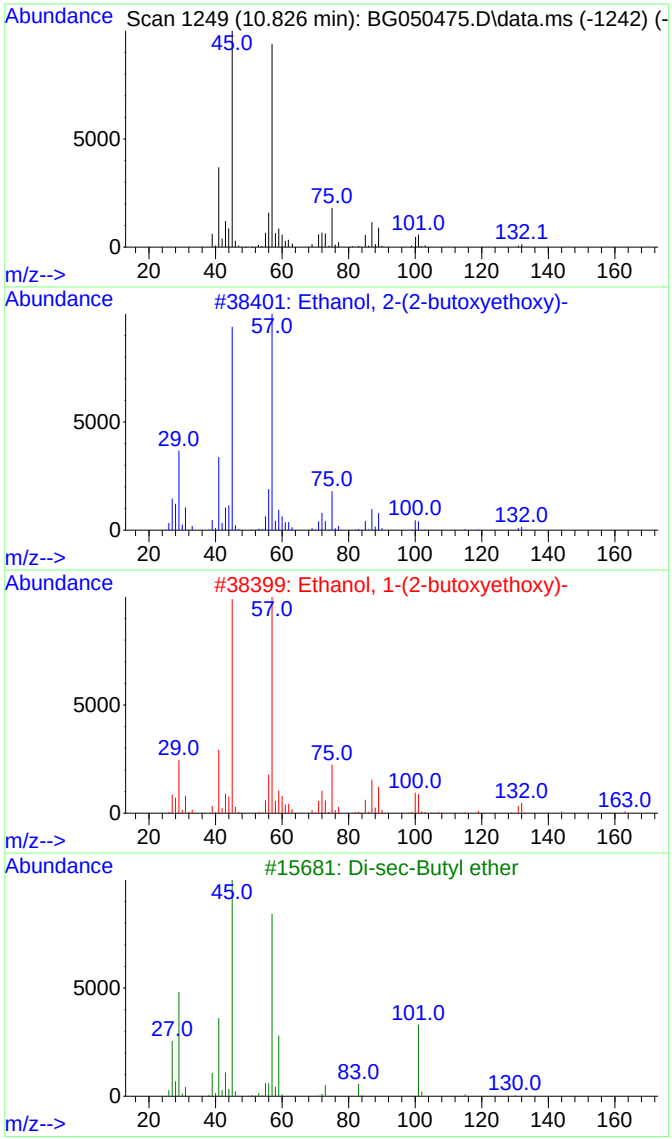
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

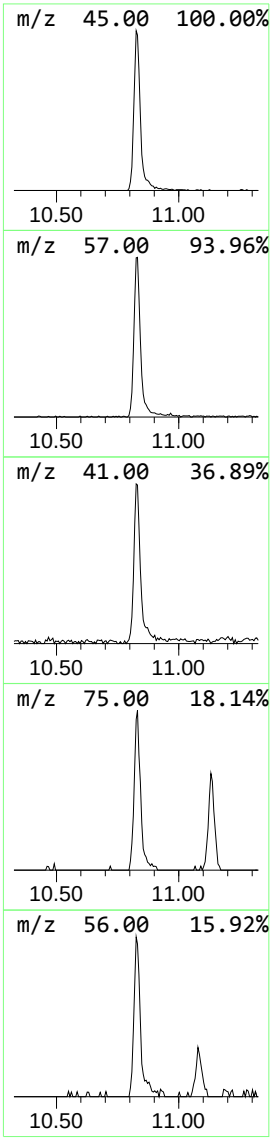
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.826	12.26 ng	278414	Naphthalene-d8	11.084

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Di-sec-Butyl ether	130	C8H18O	006863-58-7	59
4	Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	53
5	Tetraethylene glycol	194	C8H18O5	000112-60-7	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100621\
Data File : BG050475.D
Acq On : 6 Oct 2021 19:51
Operator : CG/JU
Sample : M4088-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : WC-20211005-WATER

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

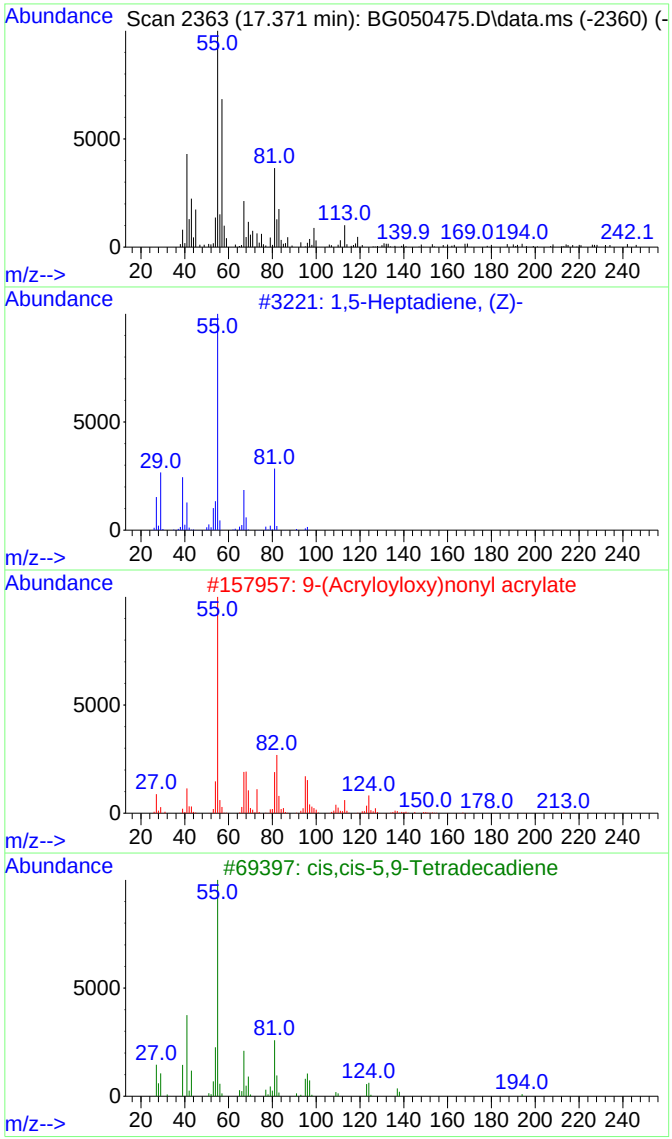
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

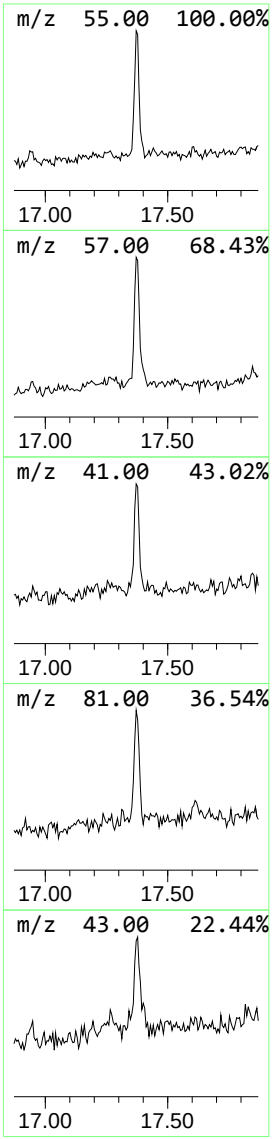
****

Peak Number 3 unknown17.371 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.371	3.70 ng	131263	Phenanthrene-d10	17.618

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5-Heptadiene, (Z)-	96	C7H12	007736-34-7	43
2	9-(Acryloyloxy)nonyl acrylate	268	C15H24O4	107481-28-7	42
3	cis,cis-5,9-Tetradecadiene	194	C14H26	051255-62-0	38
4	6-Nitroundec-5-ene	199	C11H21NO2	1000192-40-3	37
5	Pentanoic acid, 10-undecenyl ester	254	C16H30O2	1000159-93-4	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100621\
Data File : BG050475.D
Acq On : 6 Oct 2021 19:51
Operator : CG/JU
Sample : M4088-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : WC-20211005-WATER

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

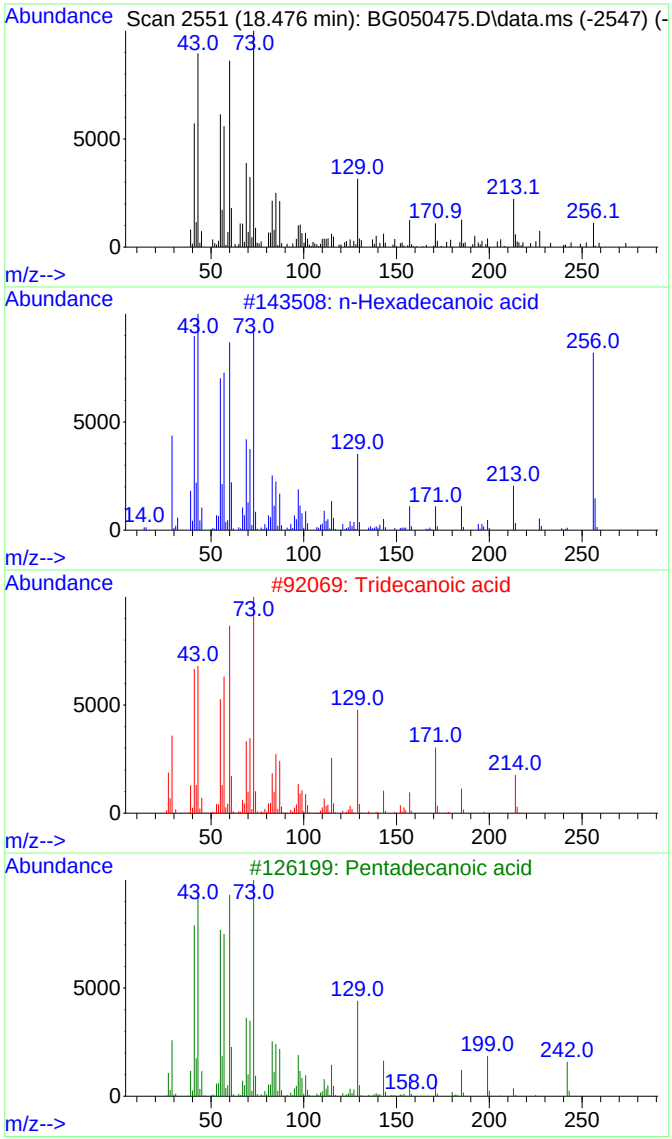
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

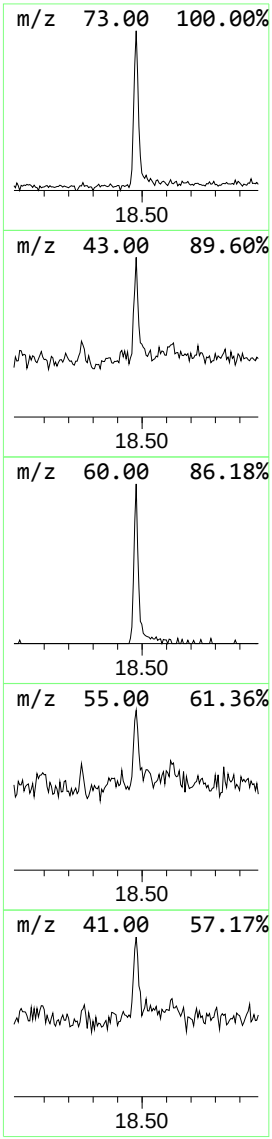
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.476	3.00 ng	106359	Phenanthrene-d10	17.618

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	n-Decanoic acid	172	C10H20O2	000334-48-5	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100621\
Data File : BG050475.D
Acq On : 6 Oct 2021 19:51
Operator : CG/JU
Sample : M4088-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : WC-20211005-WATER

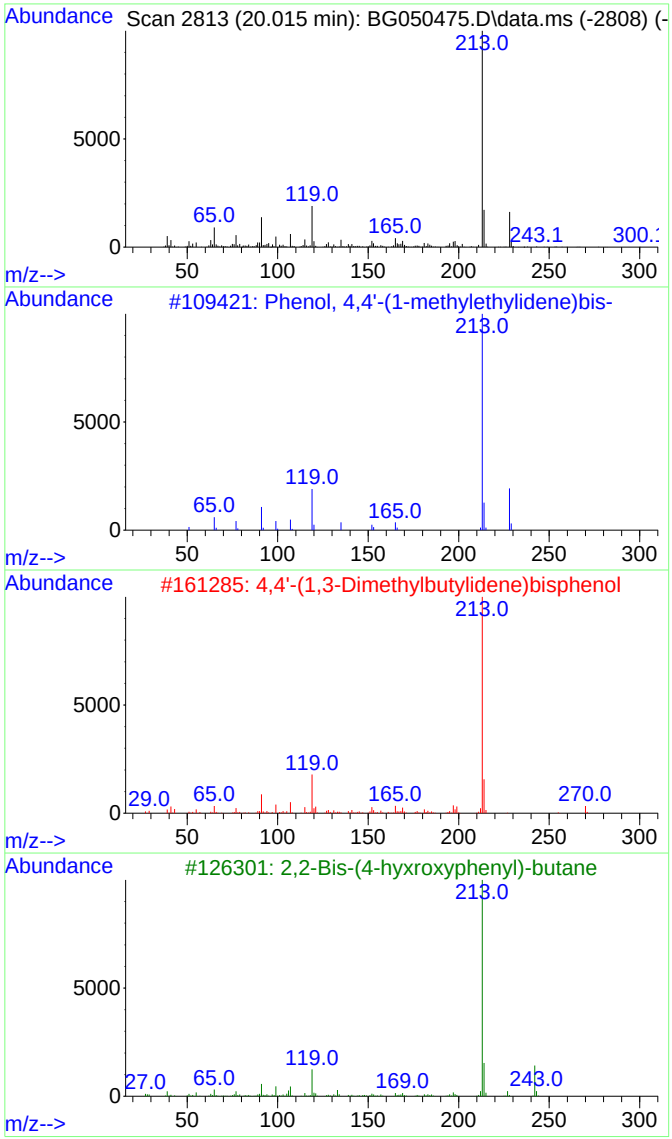
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

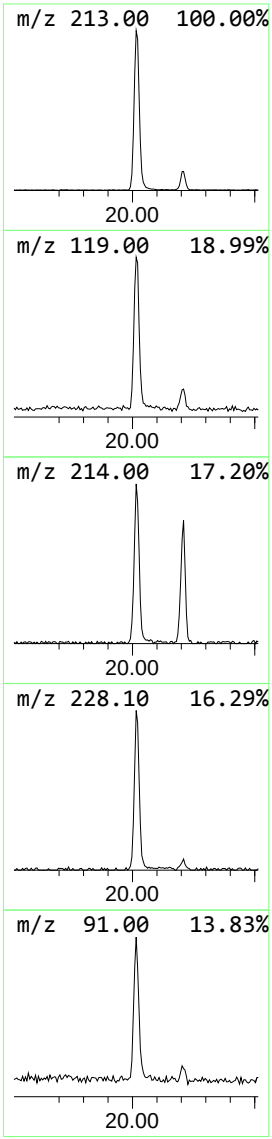
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Phenol, 4,4'-(1-methylethyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.015	13.85 ng	504780	Chrysene-d12	21.913

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	96
2	4,4'-(1,3-Dimethylbutylidene)bis...	270	C18H22O2	006807-17-6	80
3	2,2-Bis-(4-hyxroxyphenyl)-butane	242	C16H18O2	000077-40-7	72
4	3,4'-Isopropylidenediphenol	228	C15H16O2	046765-25-7	60
5	5-Fluoro-2-nitrophenylamine, TMS...	228	C9H13FN2O2Si	1000484-54-5	59





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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : WC-20211005-WATER

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

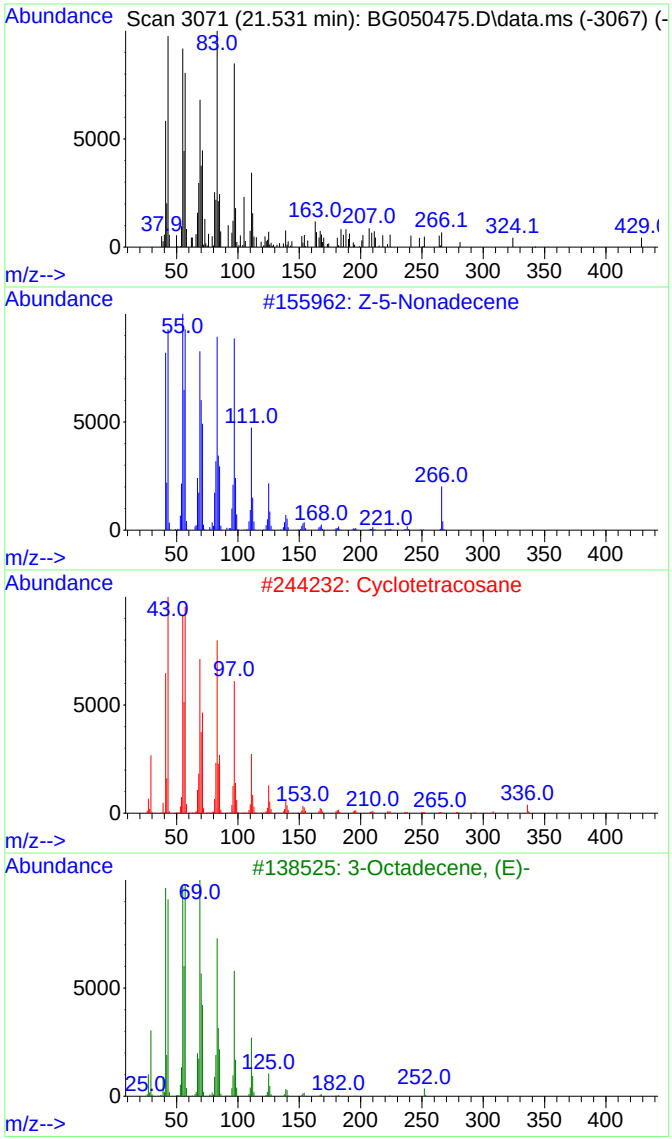
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

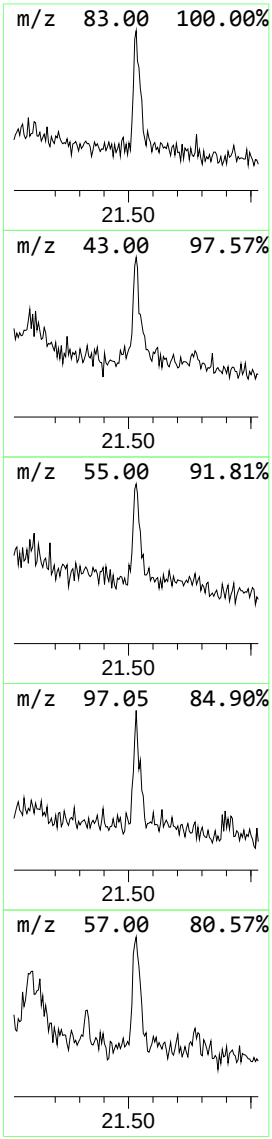
****

Peak Number 6 Z-5-Nonadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.531	2.72 ng	99039	Chrysene-d12	21.913

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Z-5-Nonadecene	266	C19H38	1000131-11-8	91
2	Cyclotetracosane	336	C24H48	000297-03-0	91
3	3-Octadecene, (E)-	252	C18H36	007206-19-1	87
4	Cetene	224	C16H32	000629-73-2	83
5	1-Tricosanol	340	C23H48O	003133-01-5	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100621\
Data File : BG050475.D
Acq On : 6 Oct 2021 19:51
Operator : CG/JU
Sample : M4088-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-20211005-WATER

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.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
Butoxyacetic acid	9.169	2.4	ng	38153	1	8.258	323263	20.0
Ethanol, 2-(2-b...	10.826	12.3	ng	278414	2	11.084	454362	20.0
unknown17.371	17.371	3.7	ng	131263	4	17.618	710010	20.0
n-Hexadecanoic ...	18.476	3.0	ng	106359	4	17.618	710010	20.0
Phenol, 4,4'-(1...	20.015	13.9	ng	504780	5	21.913	729179	20.0
Z-5-Nonadecene	21.531	2.7	ng	99039	5	21.913	729179	20.0