LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051054.D
Acq On : 15 Nov 2021 23:30
Operator : CG/JU
Sample : M4573-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MBR2

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-BG111321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG051054.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.761	380	387	396	rBV	421304	702889	23.30%	4.273%
2	7.371	653	661	672	rBV	278791	494494	16.39%	3.006%
3	8.223	798	806	812	rBV	138650	250378	8.30%	1.522%
4	9.398	998	1006	1014	rBV	521030	945970	31.36%	5.750%
5	10.797	1238	1244	1254	rBV	91690	176606	5.85%	1.074%
6	11.049	1278	1287	1296	rBV	202759	370259	12.27%	2.251%
7	13.470	1689	1699	1707	rBV	1307271	2089582	69.27%	12.702%
8	13.717	1735	1741	1746	rVB	25494	37798	1.25%	0.230%
9	14.851	1924	1934	1942	rVB	340692	553356	18.34%	3.364%
10	15.585	2054	2059	2064	rBV2	34914	54316	1.80%	0.330%
11	16.337	2180	2187	2196	rBV	1068058	1607585	53.29%	9.772%
12	16.654	2234	2241	2246	rBV2	21693	36641	1.21%	0.223%
13	17.001	2288	2300	2308	rVV	655724	1032295	34.22%	6.275%
14	17.101	2311	2317	2324	rVV	69374	106307	3.52%	0.646%
15	17.201	2328	2334	2342	rBV	50122	76871	2.55%	0.467%
16	17.595	2391	2401	2409	rBV	431816	707122	23.44%	4.298%
17	18.223	2503	2508	2512	rBV	21790	31398	1.04%	0.191%
18	18.323	2517	2525	2531	rVB	1104128	1787959	59.27%	10.869%
19	18.446	2540	2546	2549	rBV	48940	68389	2.27%	0.416%
20	18.476	2549	2551	2556	rVB3	40325	52666	1.75%	0.320%
21	18.593	2566	2571	2576	rBV3	26352	40738	1.35%	0.248%
22	18.958	2628	2633	2639	rVV	254385	377005	12.50%	2.292%
23	19.046	2643	2648	2653	rVV3	48027	68378	2.27%	0.416%
24	19.105	2653	2658	2664	rVB	178513	246524	8.17%	1.499%
25	19.510	2722	2727	2732	rVB4	19251	30957	1.03%	0.188%
26	20.186	2836	2842	2848	rBV	2279503	3016481	100.00%	18.336%
27	20.462	2884	2889	2894	rVB	71836	98181	3.25%	0.597%
28	20.532	2897	2901	2906	rBV3	26140	37222	1.23%	0.226%
29	21.496	3059	3065	3074	rBV6	32436	74625	2.47%	0.454%
30	21.895	3127	3133	3139	rVB	369535	632064	20.95%	3.842%
31	25.303	3703	3713	3725	rVB2	208799	645648	21.40%	3.925%

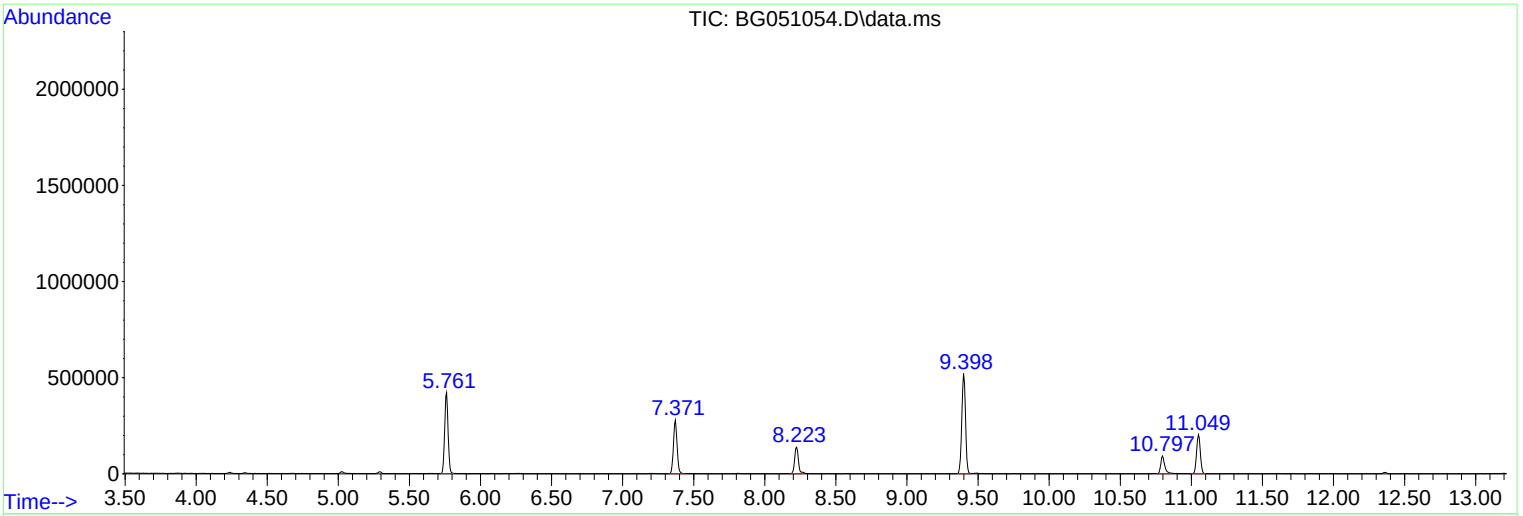
Sum of corrected areas: 16450704

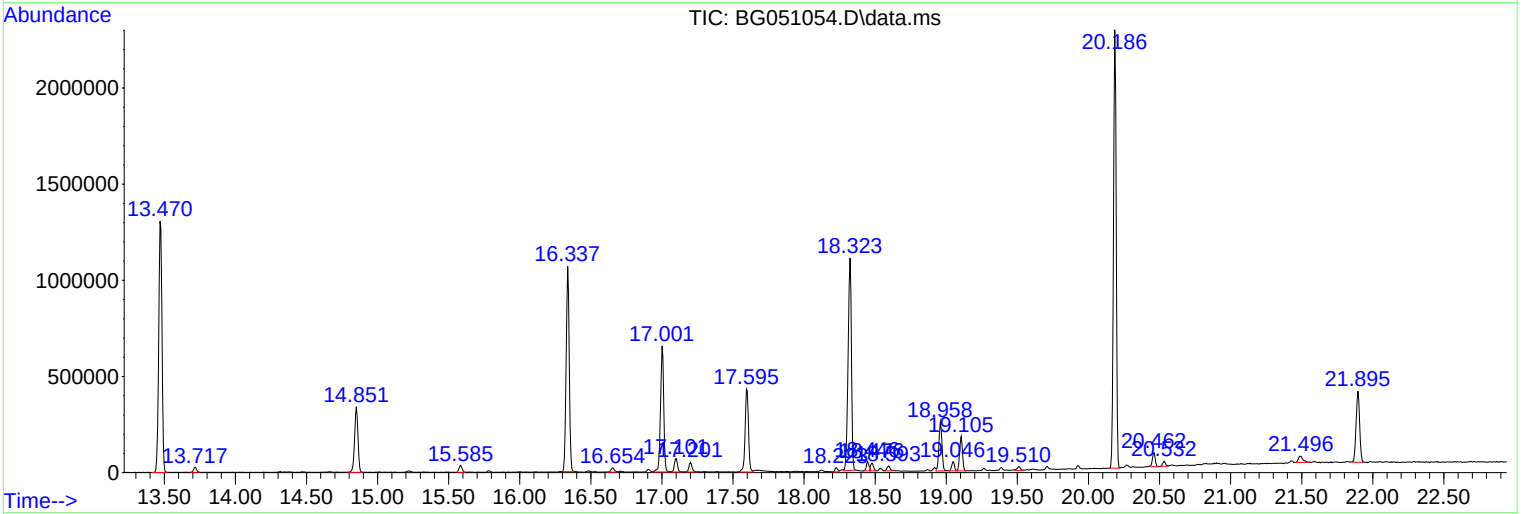
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051054.D
Acq On : 15 Nov 2021 23:30
Operator : CG/JU
Sample : M4573-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

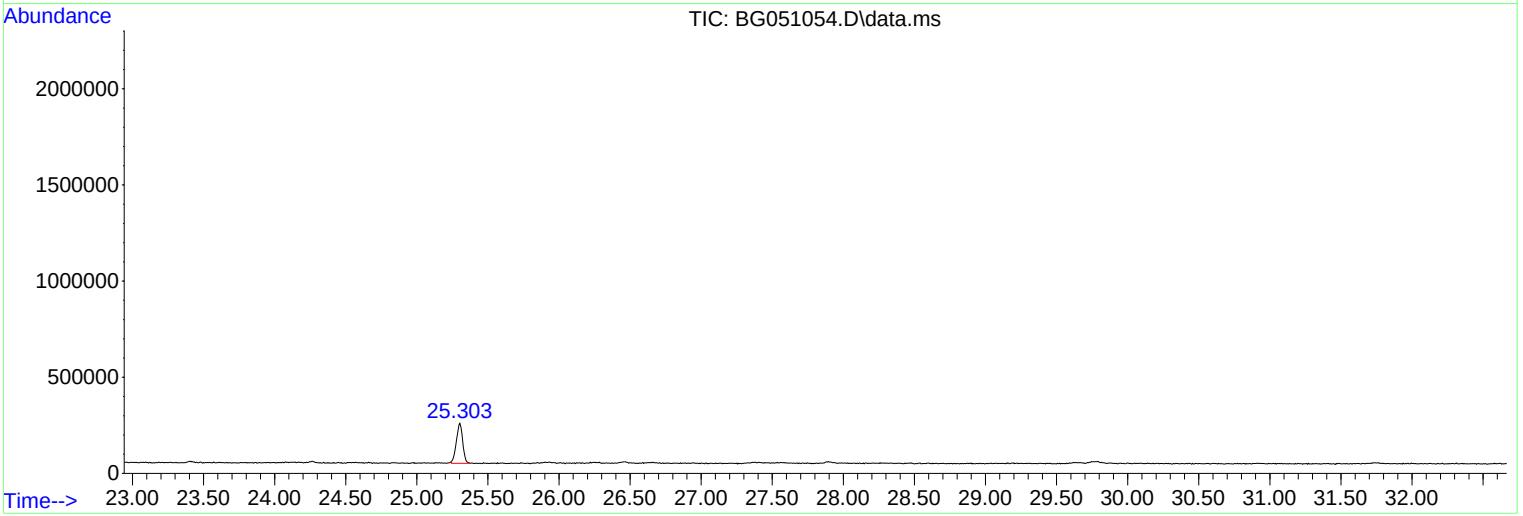
Instrument :
BNA_G
ClientSampleId :
MBR2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.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 : BG051054.D
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Operator : CG/JU
Sample : M4573-02
Misc :
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Instrument :
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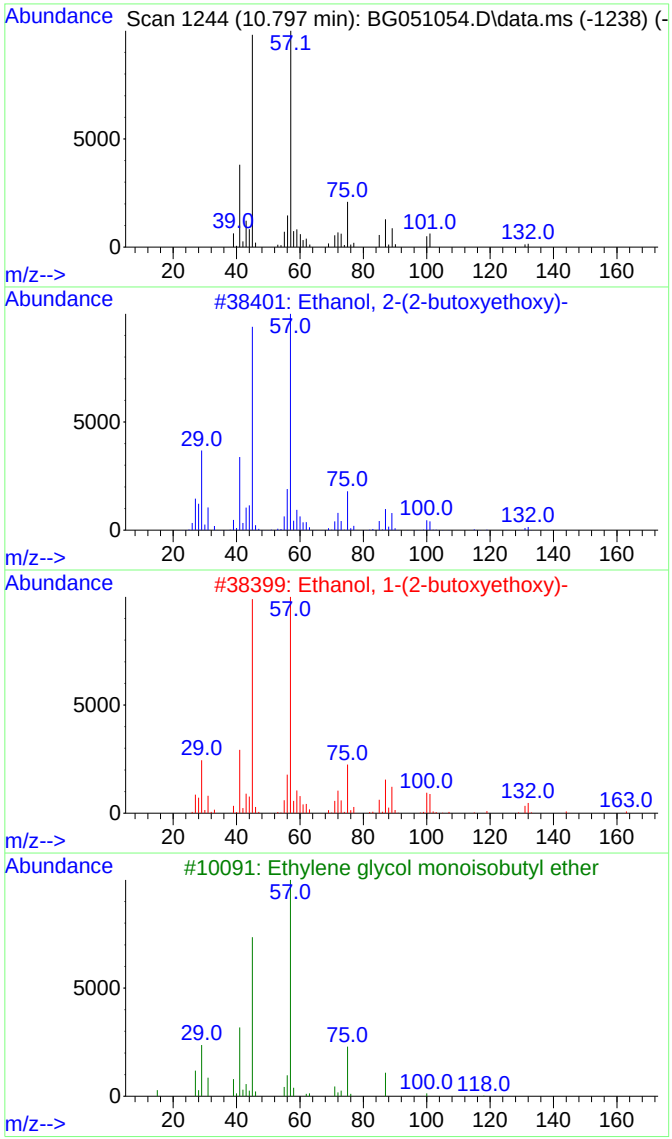
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

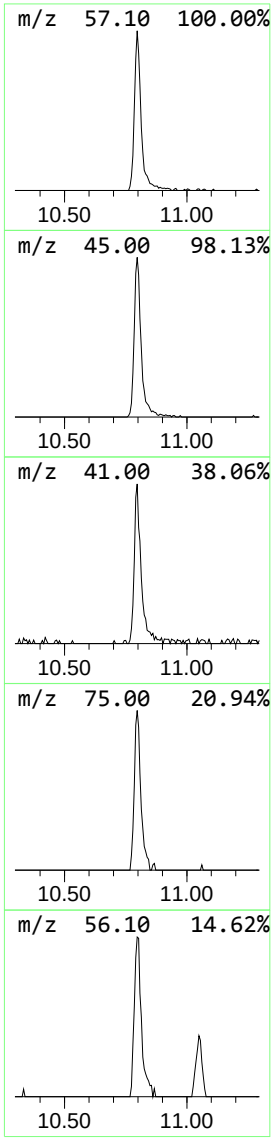
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.797	9.54 ng	176606	Naphthalene-d8	11.049

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	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	72
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53





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Data File : BG051054.D
Acq On : 15 Nov 2021 23:30
Operator : CG/JU
Sample : M4573-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MBR2

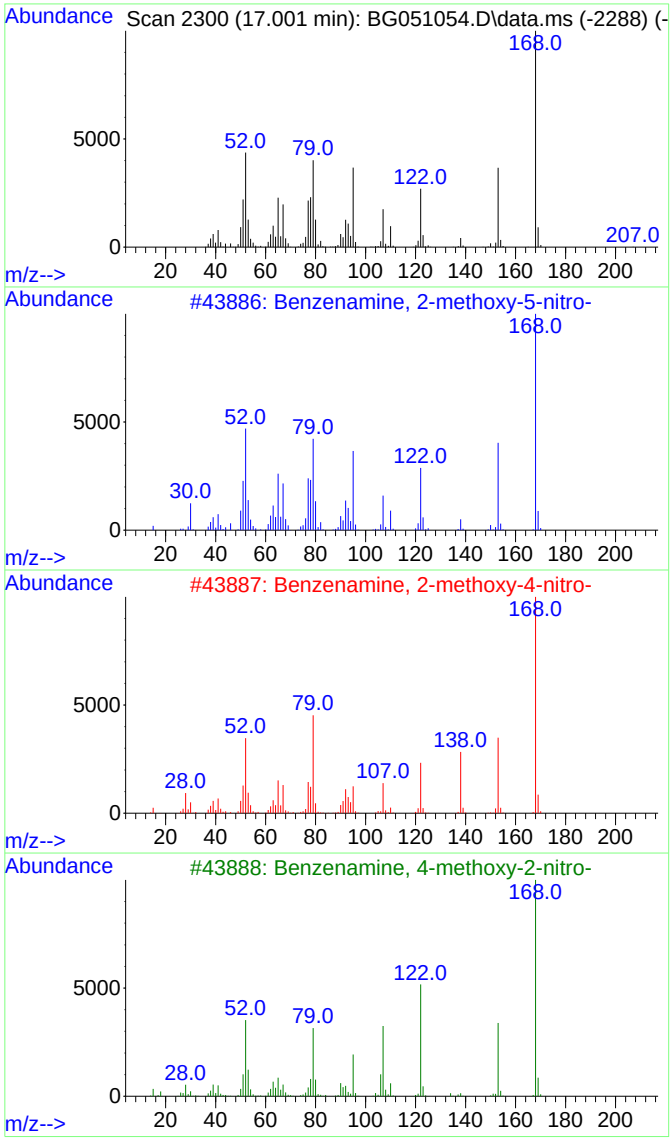
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

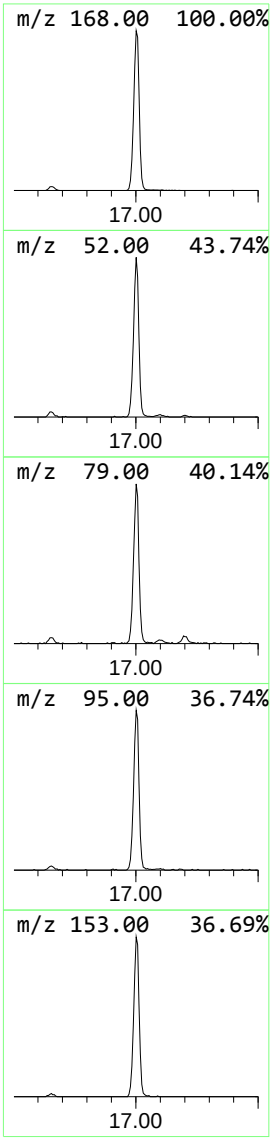
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzenamine, 2-methoxy-5-ni... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.001	29.20 ng	1032300	Phenanthrene-d10	17.595

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 2-methoxy-5-nitro-	168	C7H8N2O3	000099-59-2	98
2	Benzenamine, 2-methoxy-4-nitro-	168	C7H8N2O3	000097-52-9	94
3	Benzenamine, 4-methoxy-2-nitro-	168	C7H8N2O3	000096-96-8	87
4	p-Anisidine, 3-nitro-,	168	C7H8N2O3	000577-72-0	83
5	Benzenamine, 3-methoxy-5-nitro-	168	C7H8N2O3	000586-10-7	74





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Data File : BG051054.D
Acq On : 15 Nov 2021 23:30
Operator : CG/JU
Sample : M4573-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MBR2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

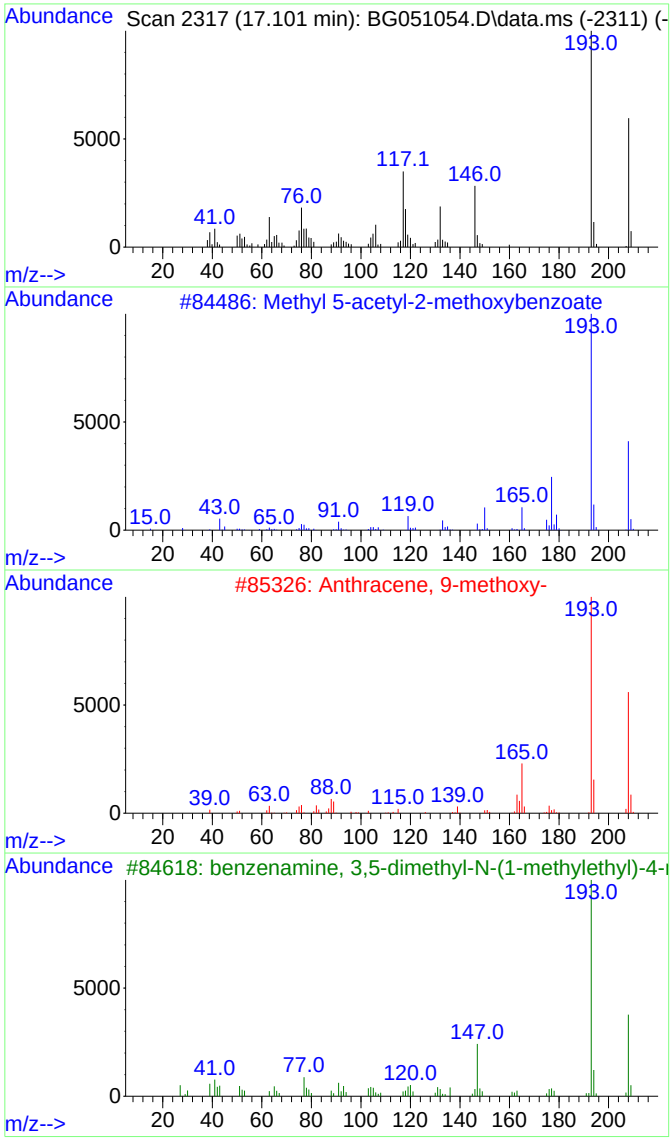
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

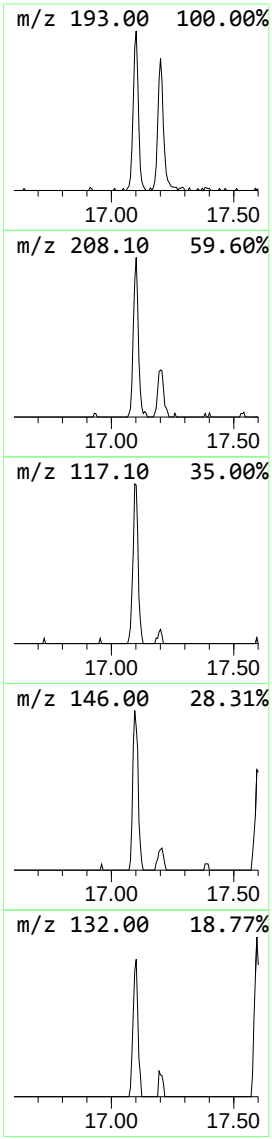
****

Peak Number 3 unknown17.101 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.101	3.01 ng	106307	Phenanthrene-d10	17.595

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 5-acetyl-2-methoxybenzoate	208	C11H12O4	039971-36-3	49
2	Anthracene, 9-methoxy-	208	C15H12O	002395-96-2	47
3	benzenamine, 3,5-dimethyl-N-(1-m...	208	C11H16N2O2	1000400-57-7	47
4	Ethanol, 2-[4-(1,1-dimethylethyl...	208	C13H20O2	054934-87-1	47
5	4-Nitrocinnamic acid	193	C9H7NO4	000619-89-6	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051054.D
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Operator : CG/JU
Sample : M4573-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MBR2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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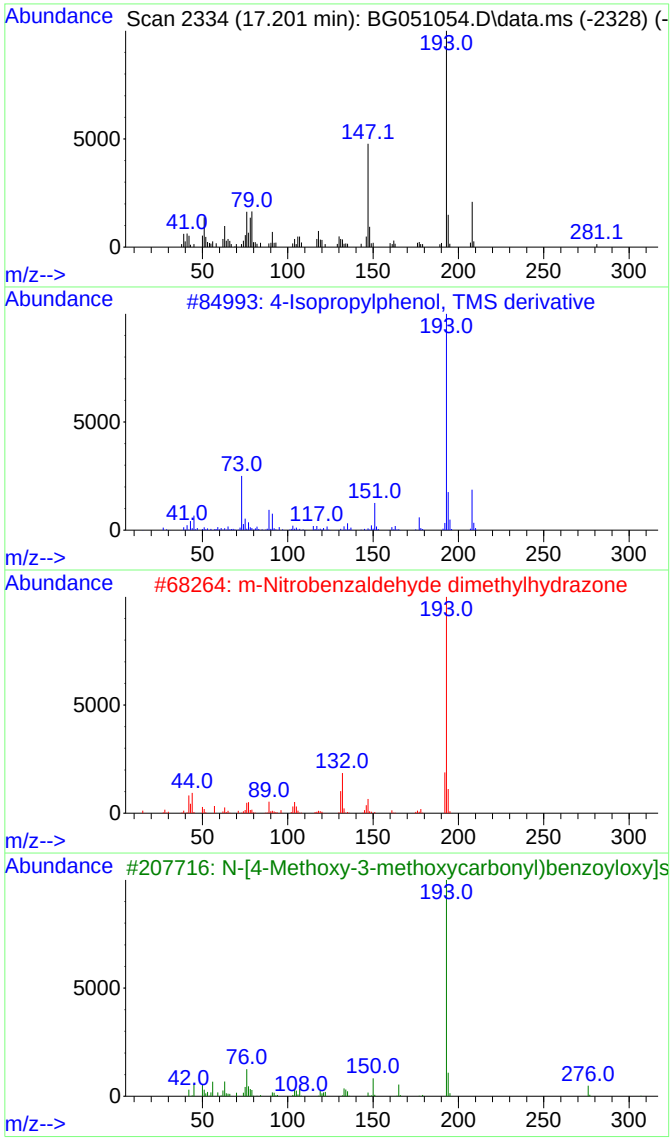
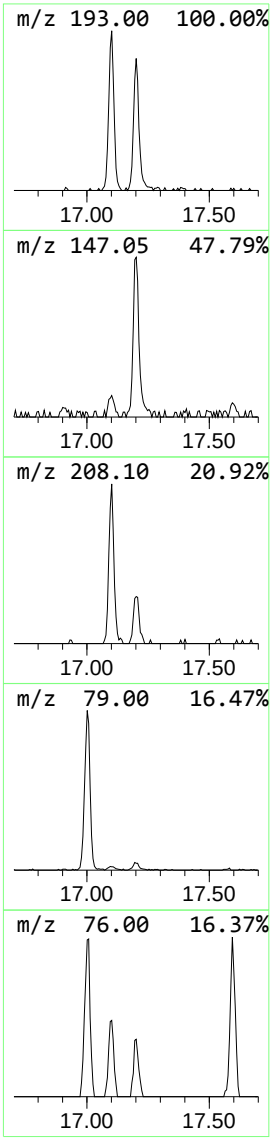
****

Peak Number 4 unknown17.201 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.201	2.17 ng	76871	Phenanthrene-d10	17.595

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Isopropylphenol, TMS derivative	208	C12H20OSi	1000373-17-4	46
2	m-Nitrobenzaldehyde dimethylhydr...	193	C9H11N3O2	032787-76-1	43
3	N-[4-Methoxy-3-methoxycarbonyl)b...	307	C14H13NO7	541528-00-1	43
4	Benzaldehyde, p-nitro-, dimethyl...	193	C9H11N3O2	010424-92-7	43
5	3-Methyl-2-oxo-2,3-dihydro-1,3-b...	193	C9H7NO4	154780-52-6	43





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Sample : M4573-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MBR2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
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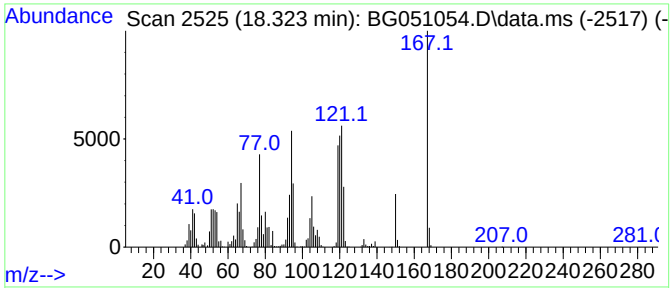
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

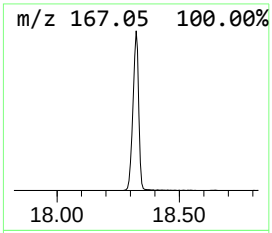
****

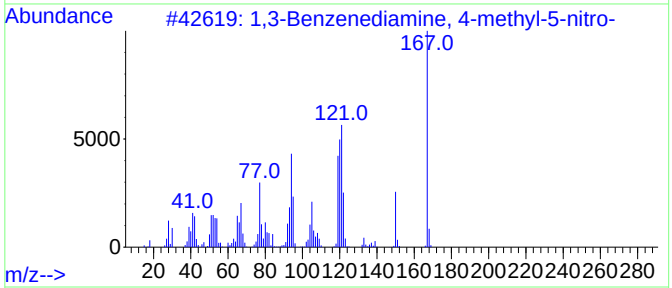
Peak Number 5 1,3-Benzenediamine, 4-methy... Concentration Rank 1

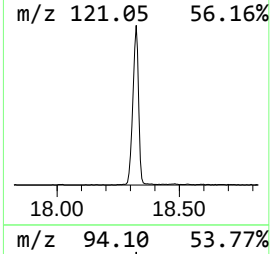
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.323	50.57 ng	1787960	Phenanthrene-d10	17.595

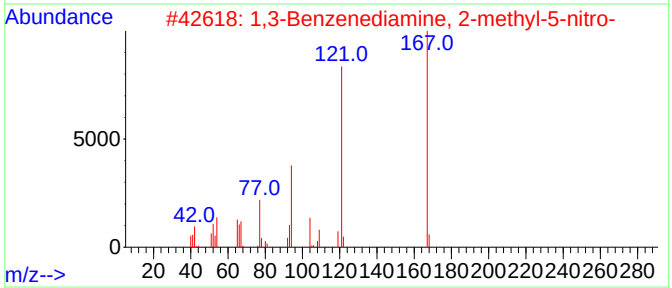
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenediamine, 4-methyl-5-n...	167	C7H9N3O2	006629-29-4	98
2	1,3-Benzenediamine, 2-methyl-5-n...	167	C7H9N3O2	059229-75-3	43
3	4-Pyridinecarboxaldehyde, 3-hydr...	167	C8H9NO3	000066-72-8	41
4	3,5-Pyridinedicarboxylic acid	167	C7H5NO4	000499-81-0	38
5	5-Methyl-2-nitroanisole	167	C8H9NO3	038512-82-2	35

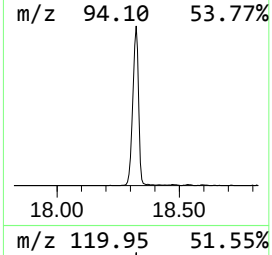


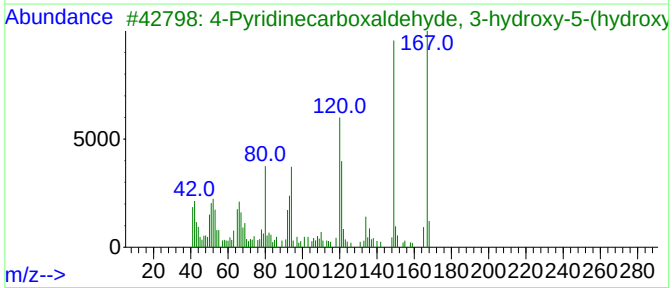


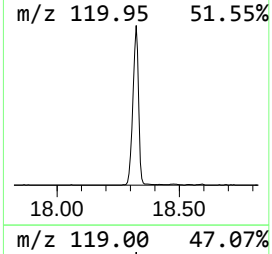


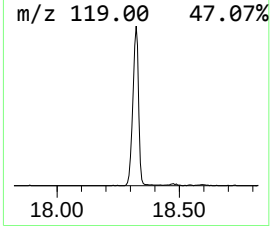












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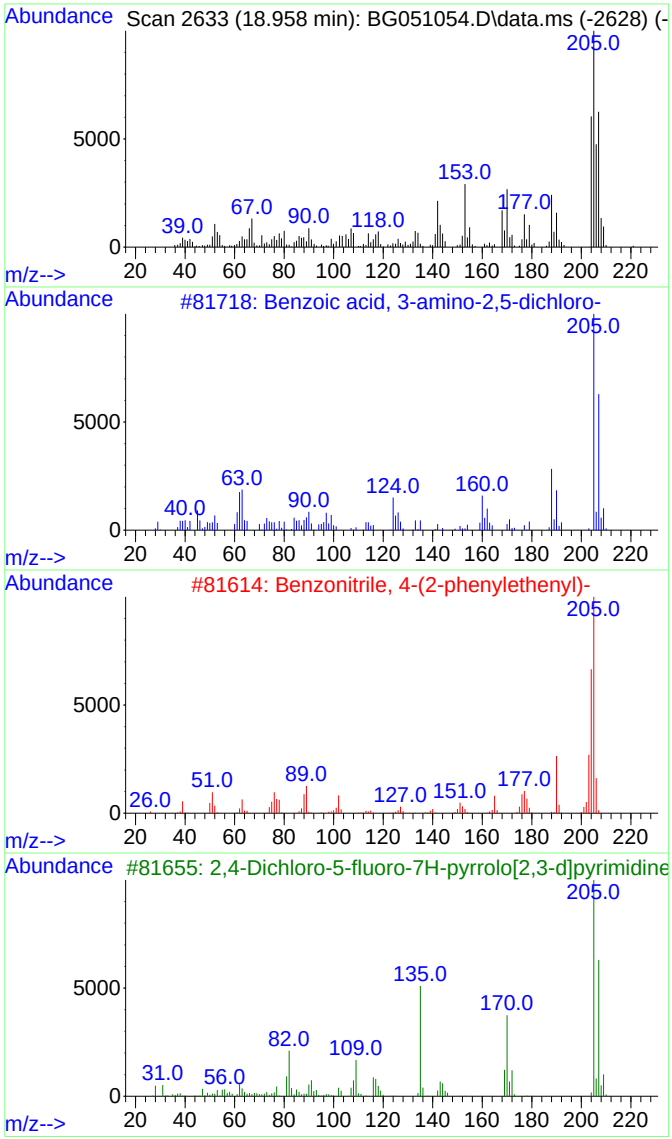
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

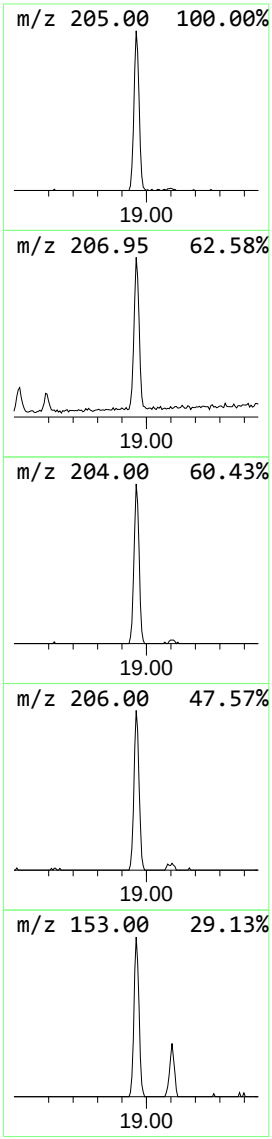
****

Peak Number 6 unknown18.958 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.958	10.66 ng	377005	Phenanthrene-d10	17.595

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 3-amino-2,5-dichloro-	205	C7H5Cl2NO2	000133-90-4	45
2	Benzonitrile, 4-(2-phenylethenyl)-	205	C15H11N	001552-58-5	38
3	2,4-Dichloro-5-fluoro-7H-pyrrolo...	205	C6H2Cl2FN3	1053228-29-7	38
4	Benzenamine, 4-(1-methyl-2-imida...	205	C10H11N3S	133303-54-5	35
5	Pyridine, 3,5-dichloro-4-methoxy...	205	C8H9Cl2NO	051050-42-1	35





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Sample : M4573-02
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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

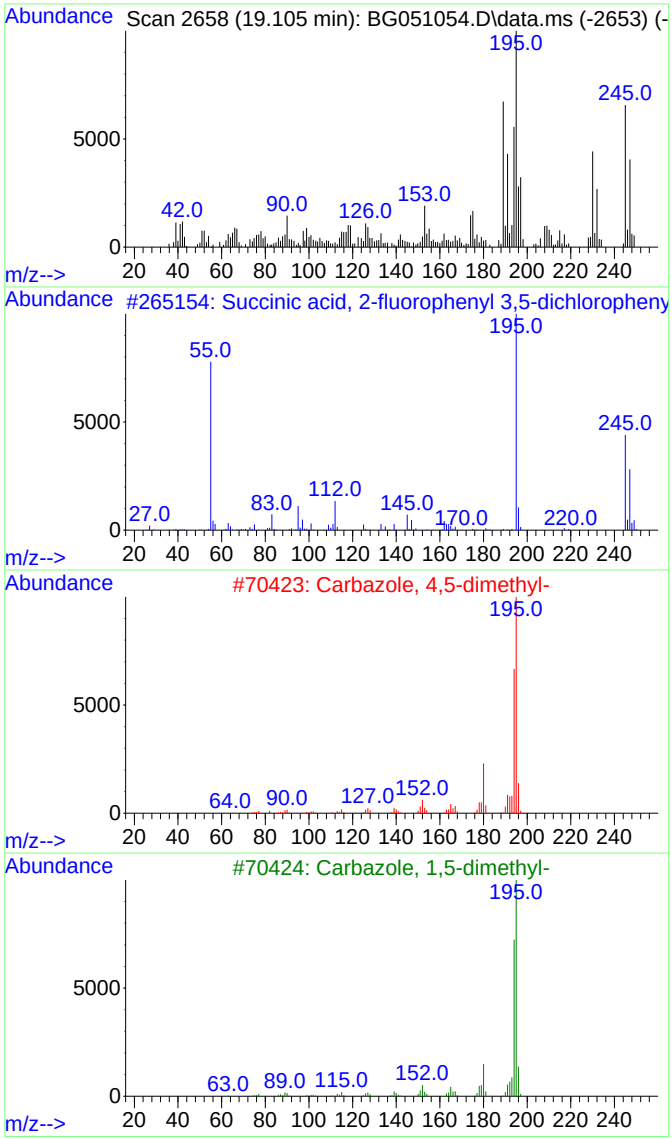
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

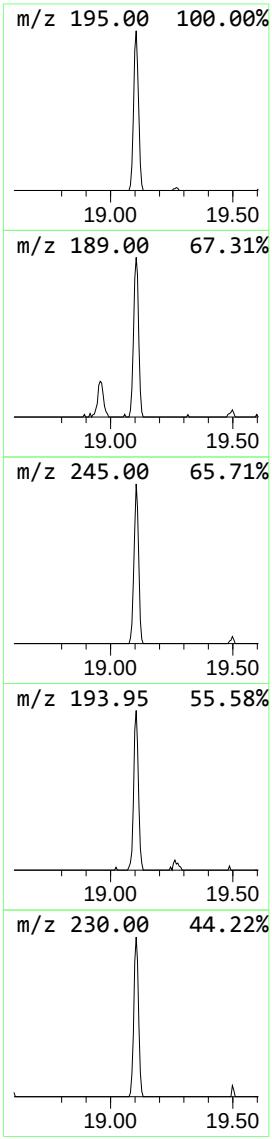
****

Peak Number 7 unknown19.105 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.105	6.97 ng	246524	Phenanthrene-d10	17.595

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Succinic acid, 2-fluorophenyl 3,...	356	C16H11Cl2FO4	1000390-15-1	38
2	Carbazole, 4,5-dimethyl-	195	C14H13N	018992-66-0	30
3	Carbazole, 1,5-dimethyl-	195	C14H13N	051640-60-9	25
4	2-Methyldipyrrolo[1,2-a:2',1'-c]...	195	C12H9N3	1010305-64-5	25
5	Carbazole, 2,5-dimethyl-	195	C14H13N	078787-79-8	25





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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MBR2

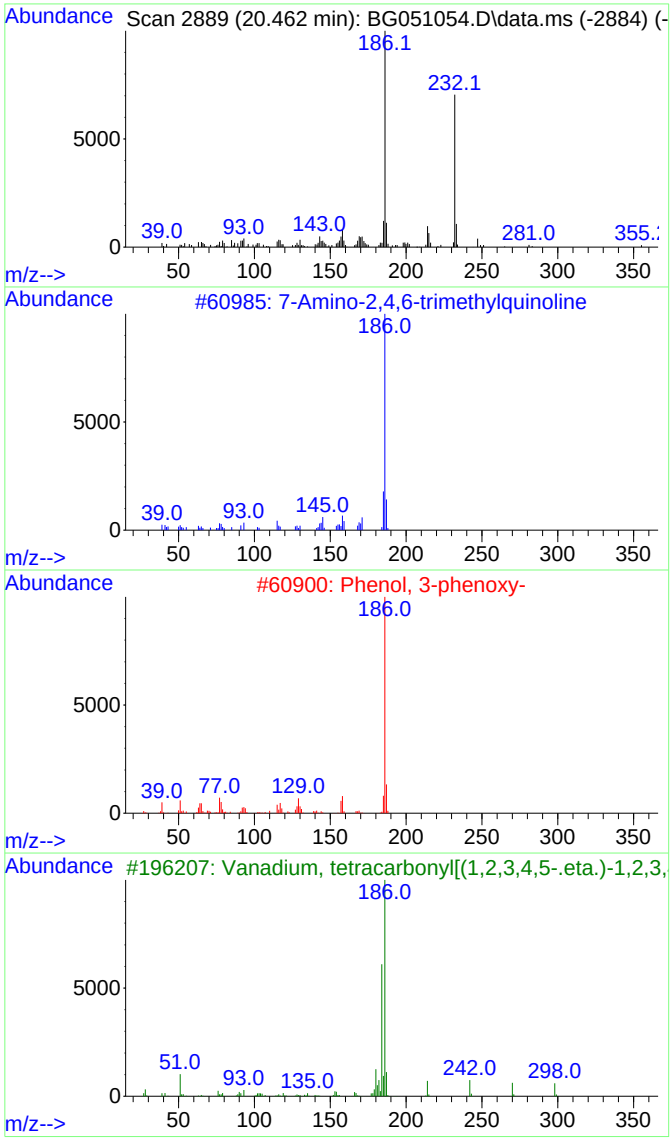
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

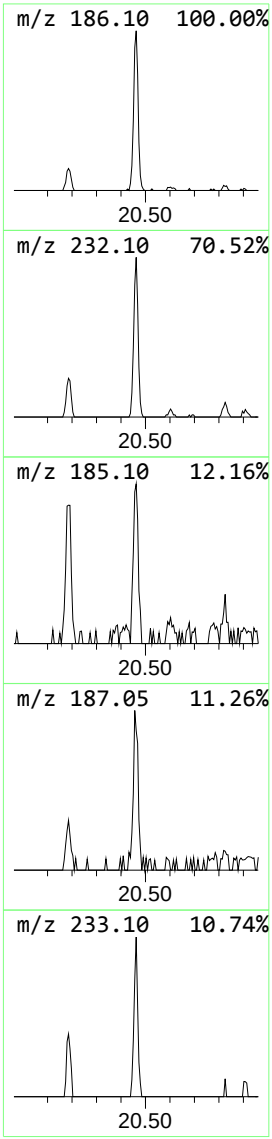
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 7-Amino-2,4,6-trimethylquin... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.462	3.11 ng	98181	Chrysene-d12	21.895

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Amino-2,4,6-trimethylquinoline	186	C12H14N2	1000427-99-9	91
2	Phenol, 3-phenoxy-	186	C12H10O2	000713-68-8	49
3	Vanadium, tetracarbonyl[(1,2,3,4...	298	C14H15O4V	084270-55-3	47
4	[1,1'-Biphenyl]-2,3-diol	186	C12H10O2	001133-63-7	46
5	2,3(2H)-Imidazole-2-one[b]quinox...	186	C9H6N4O	054108-04-2	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051054.D
Acq On : 15 Nov 2021 23:30
Operator : CG/JU
Sample : M4573-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MBR2

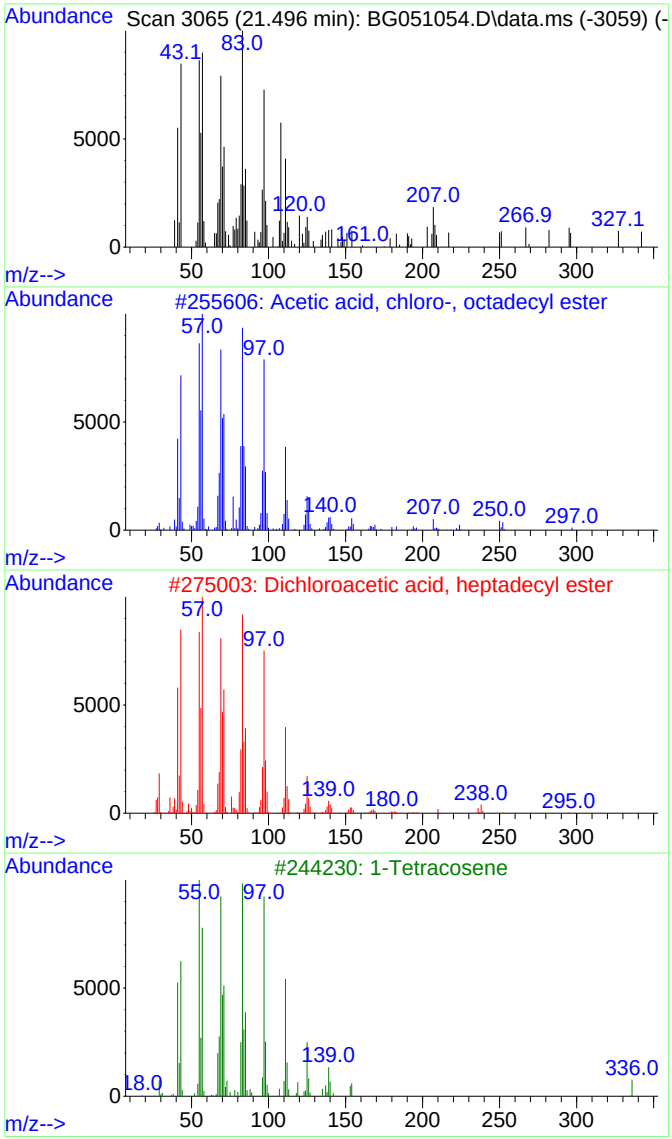
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

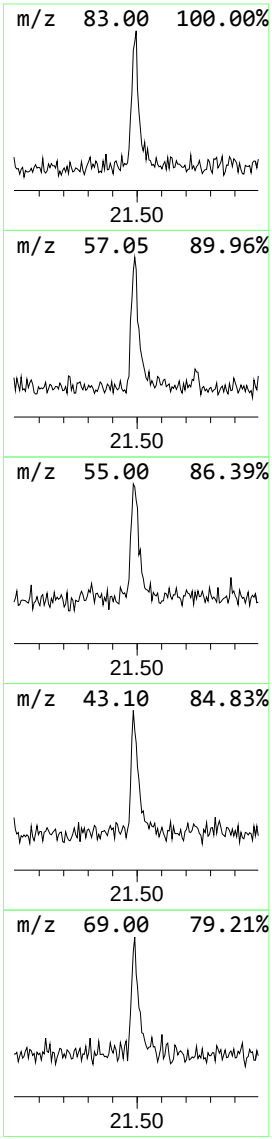
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Acetic acid, chloro-, octad... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.496	2.36 ng	74625	Chrysene-d12	21.895

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	93
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
3	1-Tetracosene	336	C24H48	010192-32-2	81
4	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	81
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051054.D
Acq On : 15 Nov 2021 23:30
Operator : CG/JU
Sample : M4573-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MBR2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.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
Ethanol, 2-(2-b...	10.797	9.5	ng	176606	2	11.049	370259	20.0
Benzenamine, 2-...	17.001	29.2	ng	1032300	4	17.595	707122	20.0
unknown17.101	17.101	3.0	ng	106307	4	17.595	707122	20.0
unknown17.201	17.201	2.2	ng	76871	4	17.595	707122	20.0
1,3-Benzenediam...	18.323	50.6	ng	1787960	4	17.595	707122	20.0
unknown18.958	18.958	10.7	ng	377005	4	17.595	707122	20.0
unknown19.105	19.105	7.0	ng	246524	4	17.595	707122	20.0
7-Amino-2,4,6-t...	20.462	3.1	ng	98181	5	21.895	632064	20.0
Acetic acid, ch...	21.496	2.4	ng	74625	5	21.895	632064	20.0