LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062320\
Data File : BG045838.D
Acq On : 23 Jun 2020 13:35
Operator : CG/JU
Sample : L3033-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SS043MW011-200615

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-BG061520.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.372	41	48	63	rVB	312654	605570	3.02%	1.159%
2	4.541	237	247	266	rBV	4190342	8492824	42.40%	16.256%
3	5.223	355	363	378	rBV	748777	1372445	6.85%	2.627%
4	5.528	407	415	429	rVB	218046	412940	2.06%	0.790%
5	7.144	684	690	704	rBV	145772	312760	1.56%	0.599%
6	7.337	712	723	733	rBV	135669	238652	1.19%	0.457%
7	7.913	814	821	826	rBV2	186345	361795	1.81%	0.692%
8	8.242	869	877	893	rVB	594074	1098255	5.48%	2.102%
9	9.082	1013	1020	1028	rVV	460320	845562	4.22%	1.618%
10	10.721	1292	1299	1305	rBV	237928	445259	2.22%	0.852%
11	13.188	1703	1719	1726	rBV	9142078	20029694	100.00%	38.338%
12	14.017	1855	1860	1871	rVB	173019	274267	1.37%	0.525%
13	14.563	1947	1953	1960	rBV	386789	622370	3.11%	1.191%
14	15.309	2073	2080	2085	rBV	548595	791838	3.95%	1.516%
15	15.456	2099	2105	2116	rBV2	209623	463597	2.31%	0.887%
16	16.067	2202	2209	2223	rBV2	1023684	1897353	9.47%	3.632%
17	16.202	2225	2232	2237	rBV	1421354	2249558	11.23%	4.306%
18	16.590	2293	2298	2306	rBV	207619	309888	1.55%	0.593%
19	17.318	2415	2422	2429	rBV	465643	754785	3.77%	1.445%
20	18.152	2558	2564	2572	rBV	464568	832696	4.16%	1.594%
21	19.274	2749	2755	2762	rBV	415854	578512	2.89%	1.107%
22	19.415	2775	2779	2785	rVB2	298135	397068	1.98%	0.760%
23	19.762	2833	2838	2842	rBV	441662	651380	3.25%	1.247%
24	19.932	2861	2867	2873	rBV	2328619	3181069	15.88%	6.089%
25	20.866	3021	3026	3035	rVB	552176	800515	4.00%	1.532%
26	21.230	3083	3088	3096	rBV	208235	313547	1.57%	0.600%
27	21.571	3140	3146	3157	rBV2	522576	853719	4.26%	1.634%
28	22.458	3289	3297	3304	rBV	909427	1656136	8.27%	3.170%
29	24.702	3666	3679	3695	rBV3	370701	1401195	7.00%	2.682%

Sum of corrected areas: 52245249

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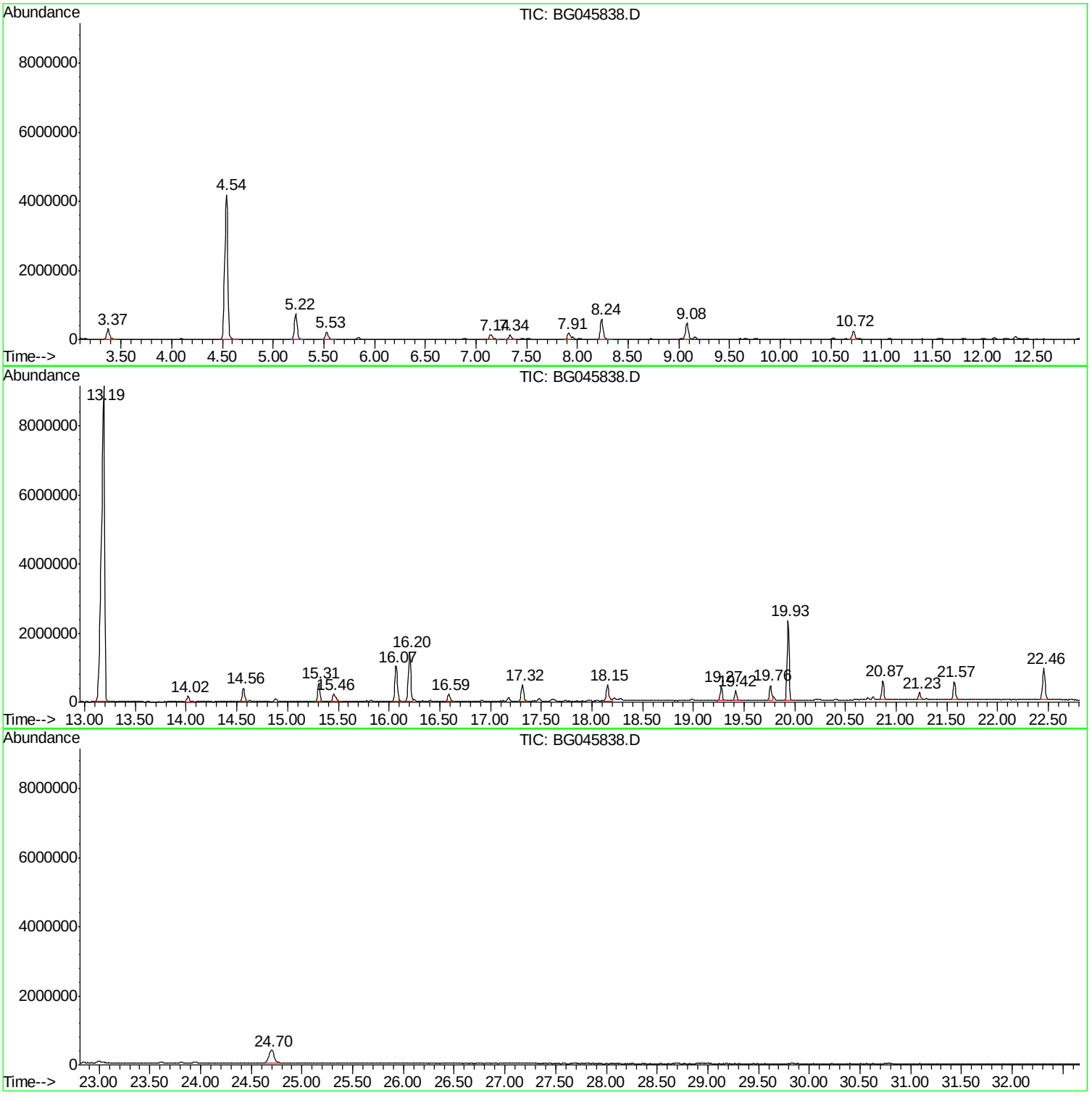
Sample : L3033-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SS043MW011-200615

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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TIC Library : C:\Database\NIST11.L
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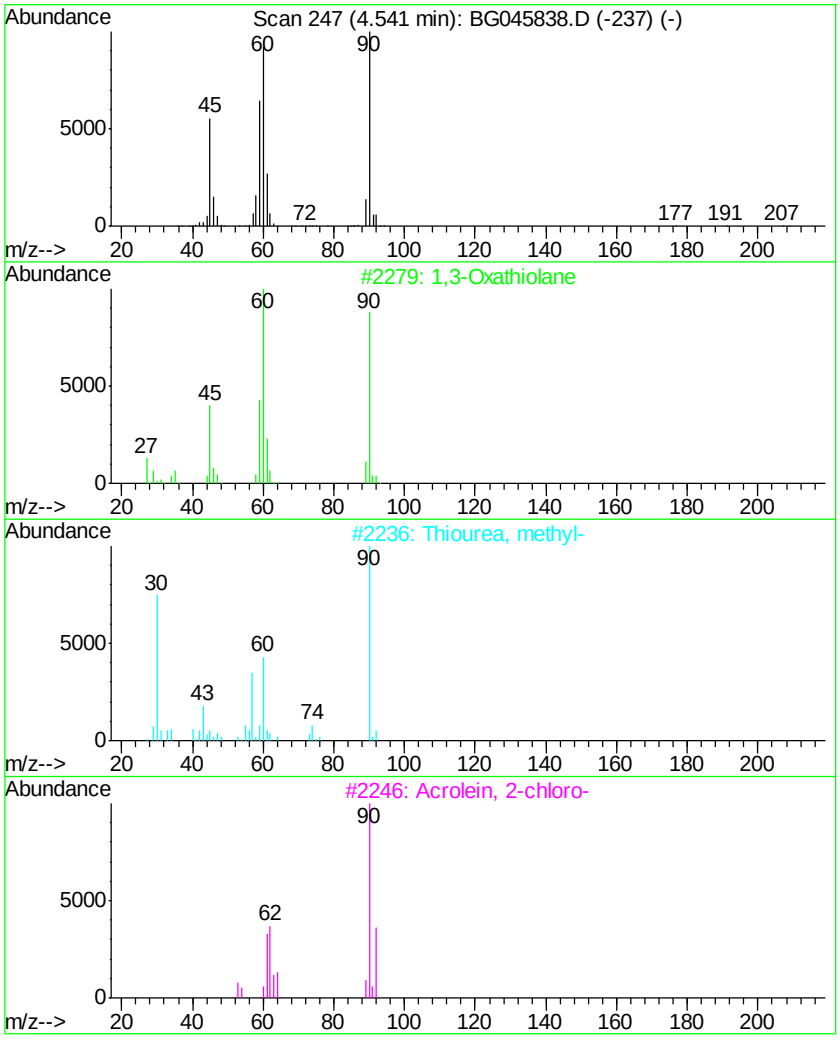
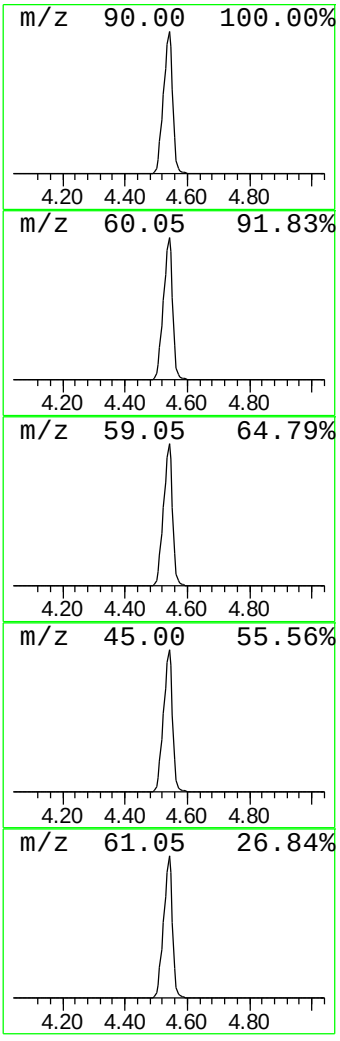
****

Peak Number 1 1,3-Oxathiolane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.54	469.48 ng	8492820	1,4-Dichlorobenzene-d4	7.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Oxathiolane	90	C3H6OS	002094-97-5	91
2	Thiourea, methyl-	90	C2H6N2S	000598-52-7	50
3	Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	36
4	Thiirane	60	C2H4S	000420-12-2	18
5	3-Thietanol	90	C3H6OS	010304-16-2	9





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Operator : CG/JU
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Misc :
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Instrument : BNA_G
ClientSampleId : SS043MW011-200615

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

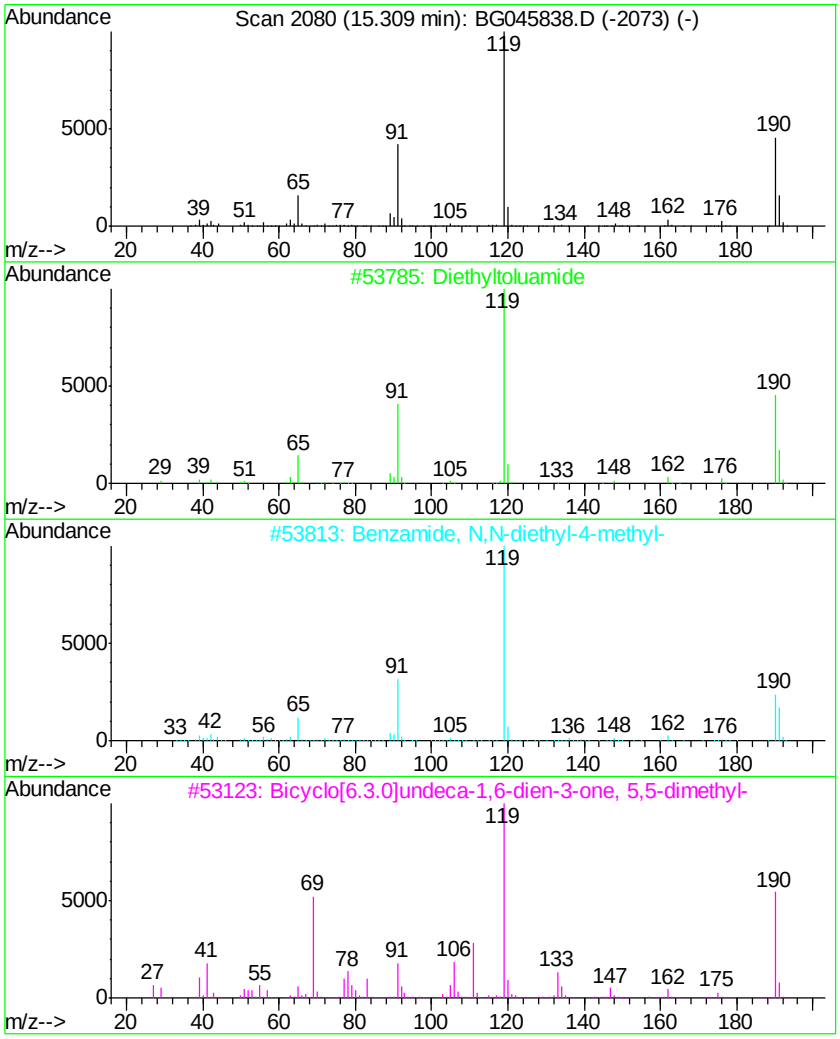
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

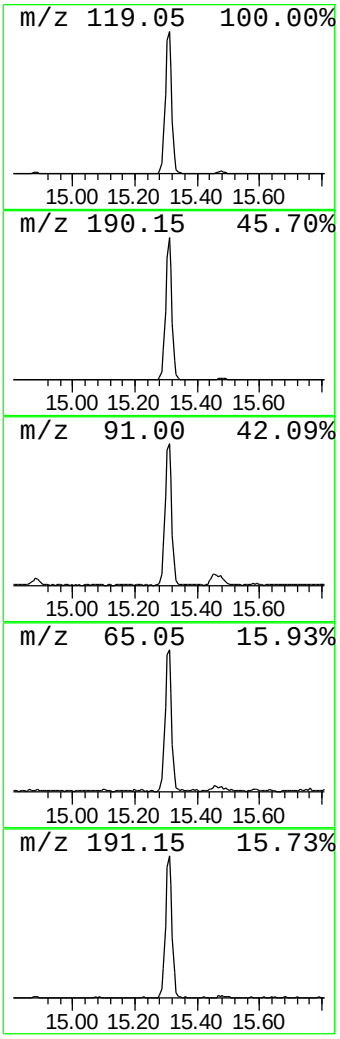
****

Peak Number 3 Diethyltoluamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	25.45 ng	791838	Acenaphthene-d10	14.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyltoluamide	191	C12H17NO	000134-62-3	96
2	Benzamide, N,N-diethyl-4-methyl-	191	C12H17NO	002728-05-4	93
3	Bicyclo[6.3.0]undeca-1,6-dien-3-...	190	C13H18O	1000164-02-3	78
4	N-[1-(Dimethylamino)-2,2,2-trich...	308	C12H15Cl3N2O	300814-41-9	53
5	Benzamide, N-(1,1-dimethylethyl)...	191	C12H17NO	042498-32-8	53





Library Search Compound Report

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Misc :
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Instrument : BNA_G
ClientSampleId : SS043MW011-200615

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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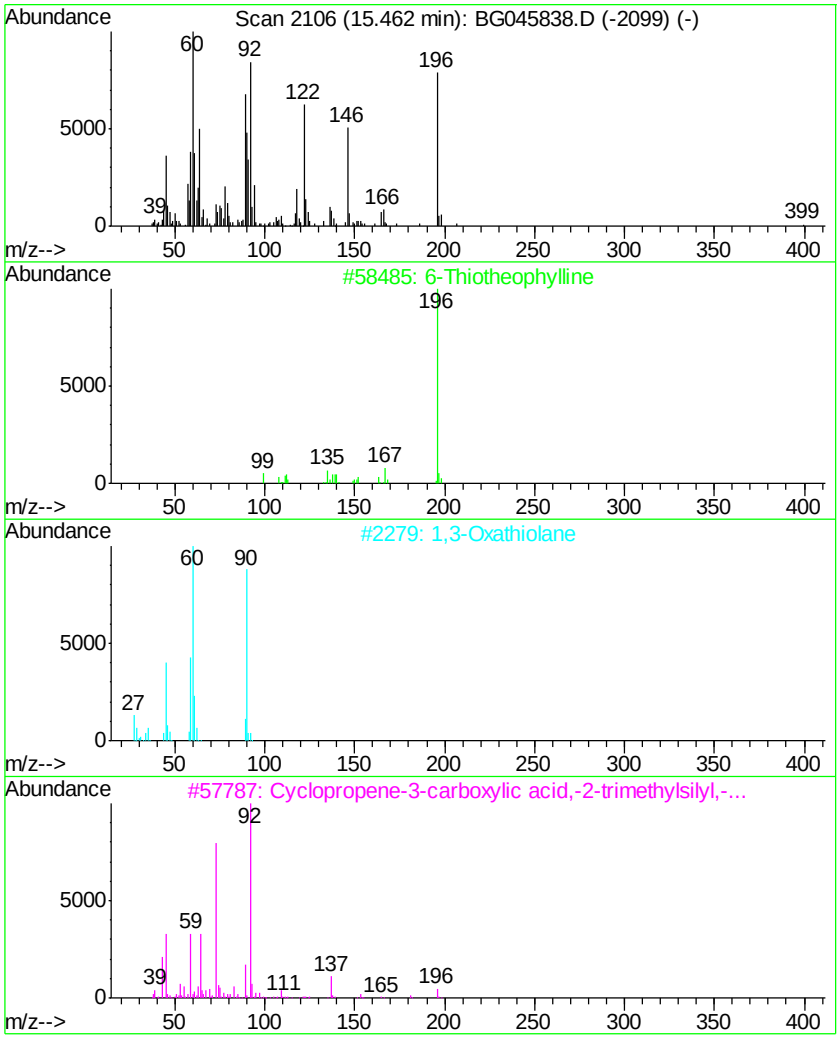
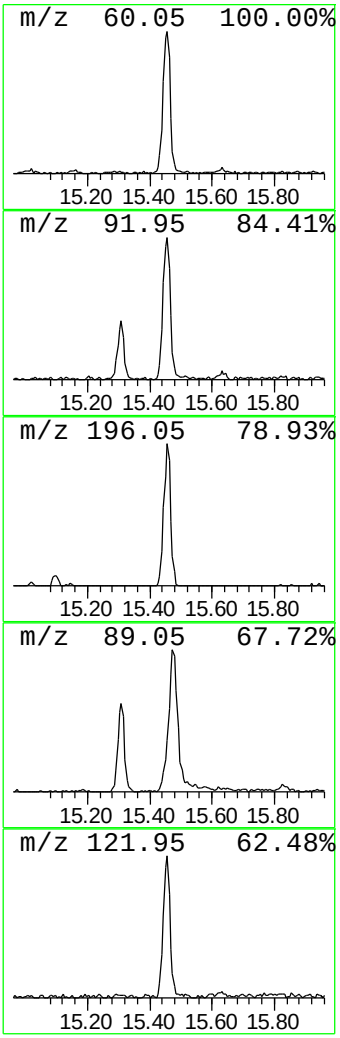
****

Peak Number 4 unknown15.46 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.46	14.90 ng	463597	Acenaphthene-d10	14.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Thiotheophylline	196	C7H8N4OS	002398-70-1	38
2	1,3-Oxathiolane	90	C3H6OS	002094-97-5	22
3	Cyclopropene-3-carboxylic acid,-...	196	C10H16O2Si	180261-20-5	22
4	Thiazole, 4,5-dihydro-2-methyl-	101	C4H7NS	002346-00-1	11
5	Propanoic acid, 2-chloro-	108	C3H5ClO2	000598-78-7	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062320\
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Sample : L3033-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SS043MW011-200615

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

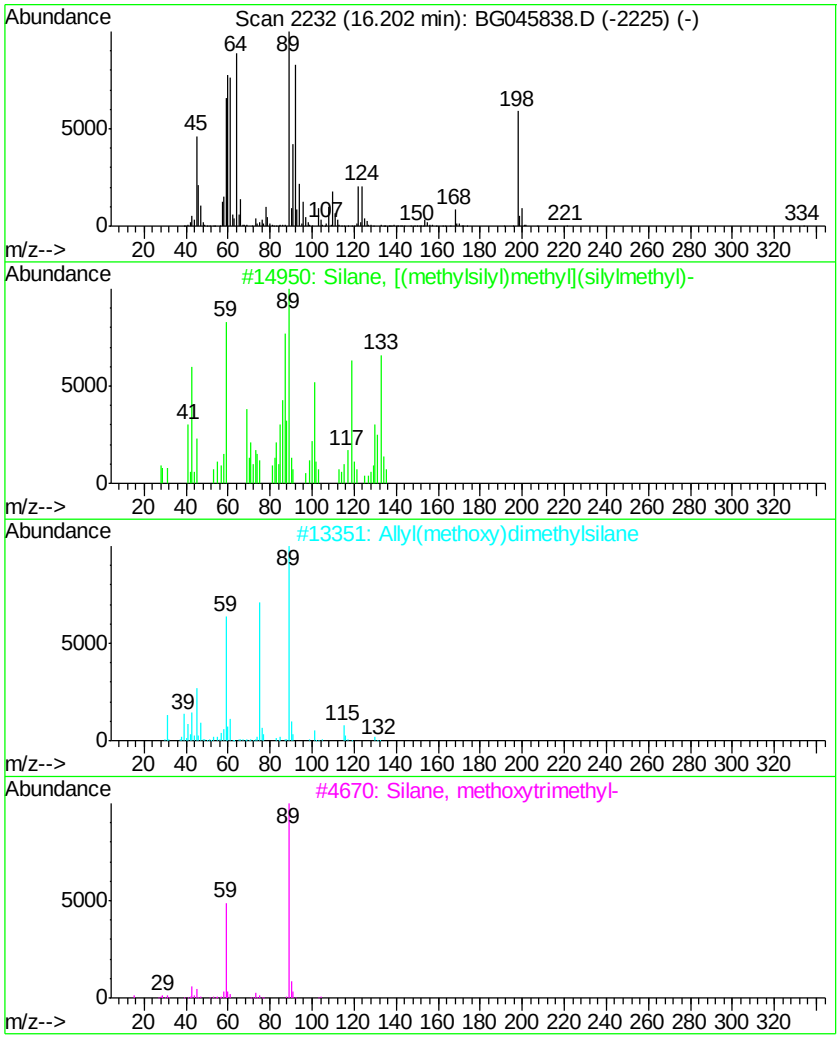
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

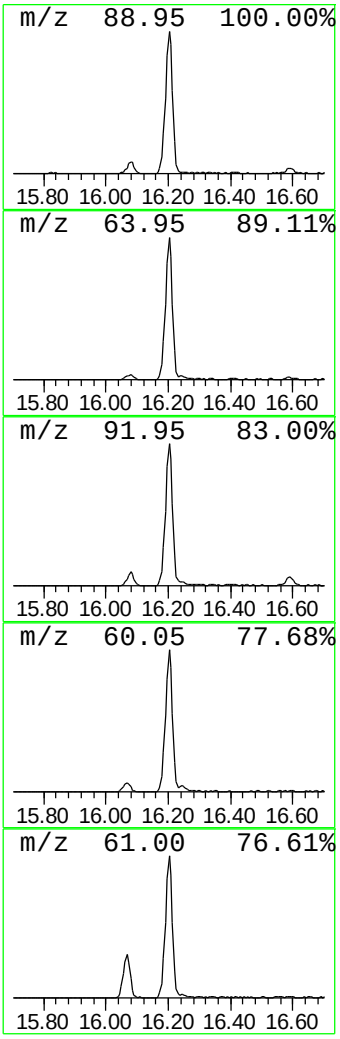
****

Peak Number 5 unknown16.20 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.20	59.61 ng	2249560	Phenanthrene-d10	17.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, [(methylsilyl)methyl(si...	134	C3H14Si3	005695-49-8	22
2	Allyl(methoxy)dimethylsilane	130	C6H14OSi	030535-30-9	22
3	Silane, methoxytrimethyl-	104	C4H12OSi	001825-61-2	22
4	Tetrazolo[1,5-b]pyridazine, 6-ch...	155	C4H2ClN5	021413-15-0	14
5	Ether, bis[2-(ethylthio)ethyl]	194	C8H18OS2	005648-30-6	12





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062320\
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Misc :
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Instrument : BNA_G
ClientSampleId : SS043MW011-200615

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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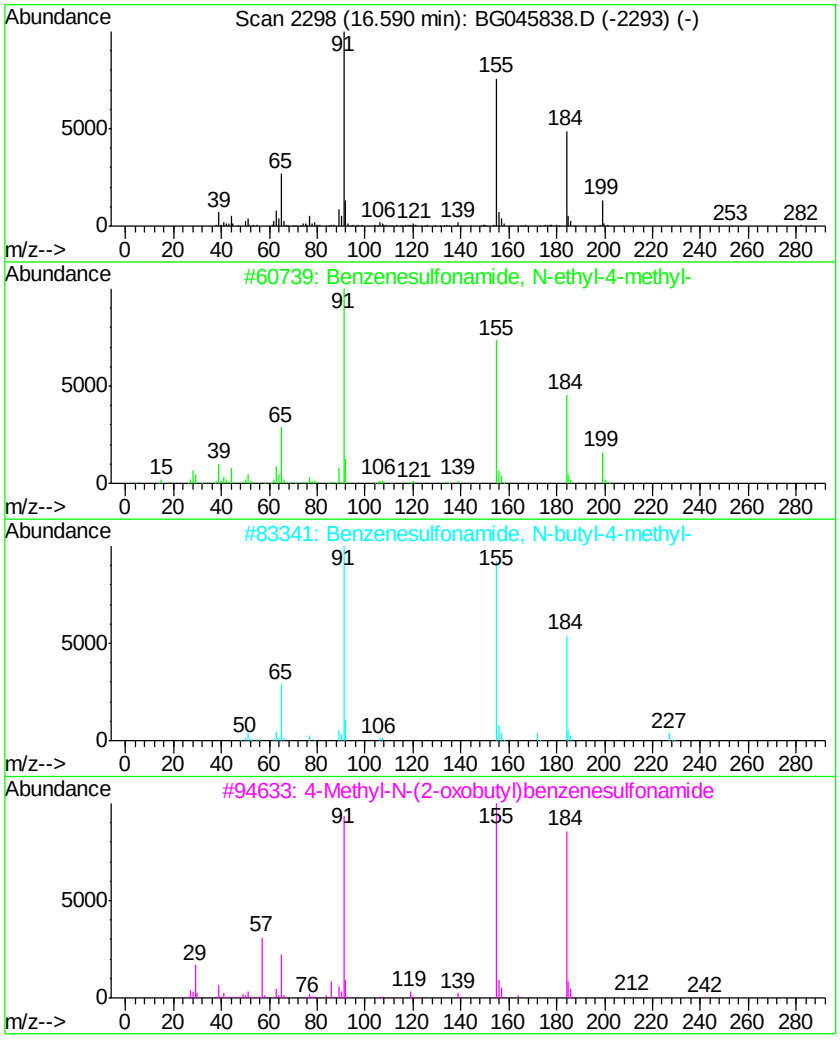
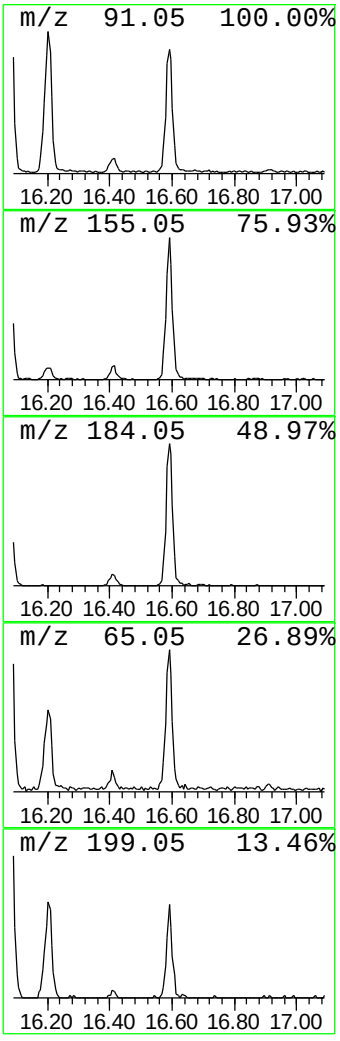
****

Peak Number 6 Benzenesulfonamide, N-ethyl... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.59	8.21 ng	309888	Phenanthrene-d10	17.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N-ethyl-4-me...	199	C9H13NO2S	000080-39-7	98
2	Benzenesulfonamide, N-butyl-4-me...	227	C11H17NO2S	001907-65-9	91
3	4-Methyl-N-(2-oxobutyl)benzenesu...	241	C11H15NO3S	1000192-14-5	90
4	Carbamic acid, methyl[(4-methylp...	243	C10H13NO4S	032258-50-7	83
5	(Toluene-4-sulfonylamino)acetic ...	299	C13H17NO5S	1000191-28-9	72





Library Search Compound Report

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Instrument : BNA_G
ClientSampleId : SS043MW011-200615

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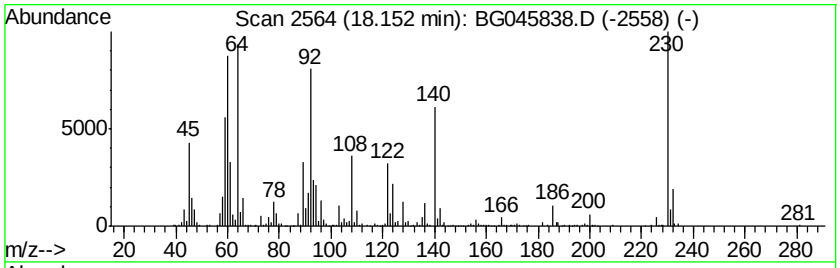
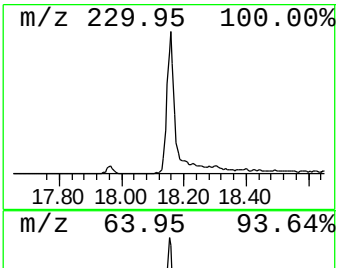
****

Peak Number 7 unknown18.15 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.15	22.06 ng	832696	Phenanthrene-d10	17.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclic octaatomic sulfur	256	S8	010544-50-0	35
2	1,2,5,6-Tetrathiocane	184	C4H8S4	001940-01-8	28
3	Benzenediazonium, 2-hydroxy-, hy...	120	C6H4N2O	029906-36-3	25
4	Ethyl trifluoromethyl trisulfide	194	C3H5F3S3	055882-01-4	25
5	2-Sulfamyl-4,4'-diformamidodiphe...	383	C14H13N3O6S2	1000256-33-9	17





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Instrument : BNA_G
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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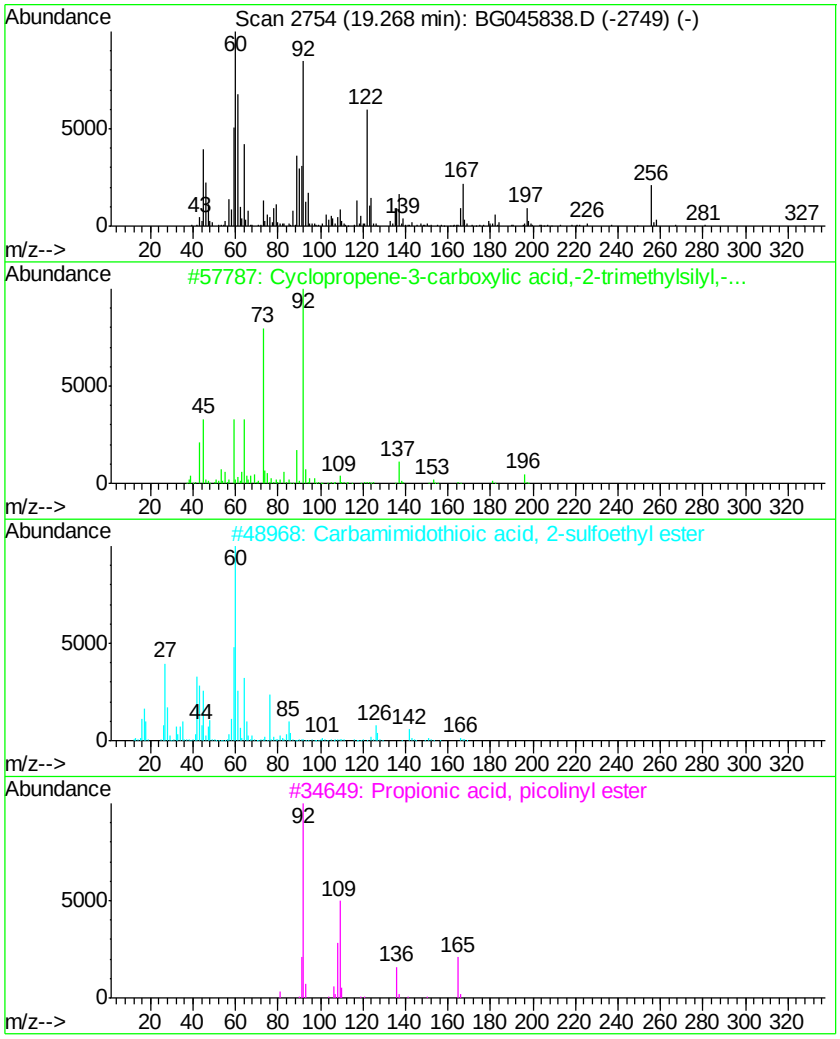
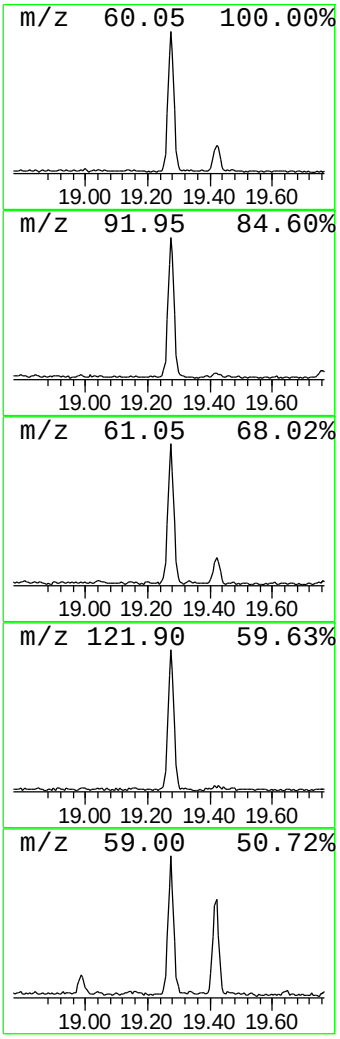
****

Peak Number 8 unknown19.27 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.27	15.33 ng	578512	Phenanthrene-d10	17.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropene-3-carboxylic acid,-...	196	C10H16O2Si	180261-20-5	32
2	Carbamimidothioic acid, 2-sulfoe...	184	C3H8N2O3S2	025985-57-3	25
3	Propionic acid, picolinyl ester	165	C9H11NO2	1000334-80-0	12
4	1,3-Oxathiolane	90	C3H6OS	002094-97-5	10
5	Benzeneethanol, .alpha.,.alpha.-...	150	C10H14O	000100-86-7	10





Library Search Compound Report

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TIC Library : C:\Database\NIST11.L
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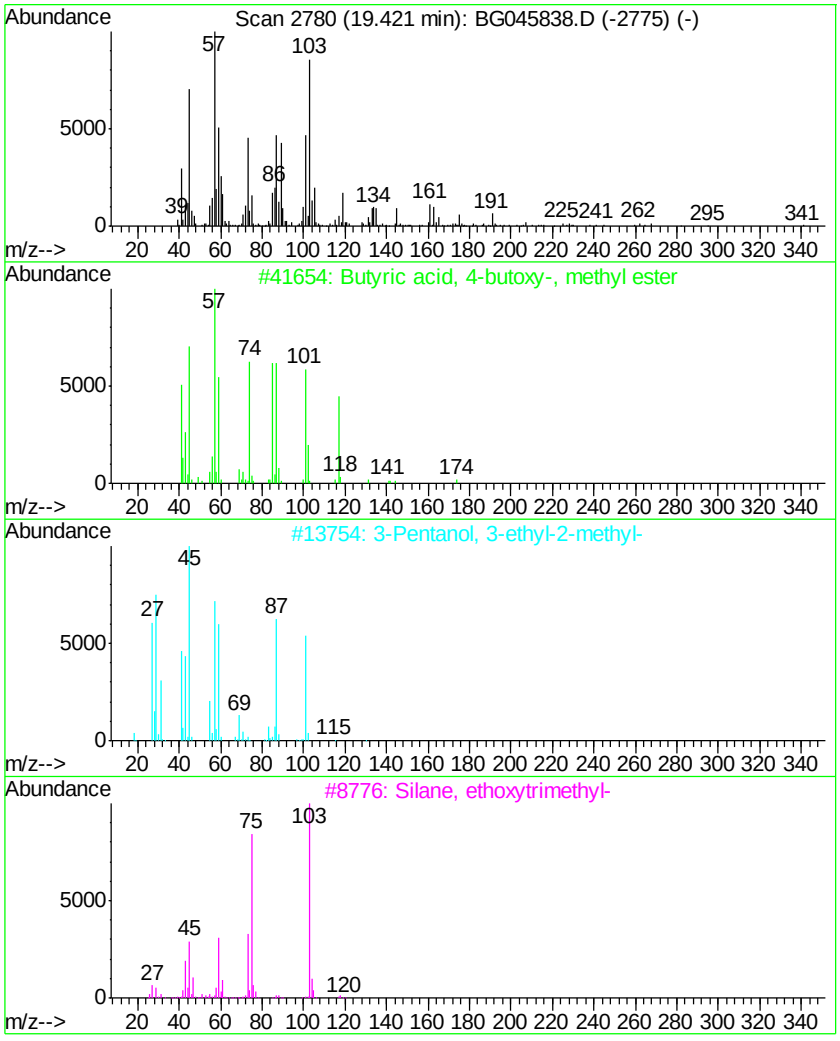
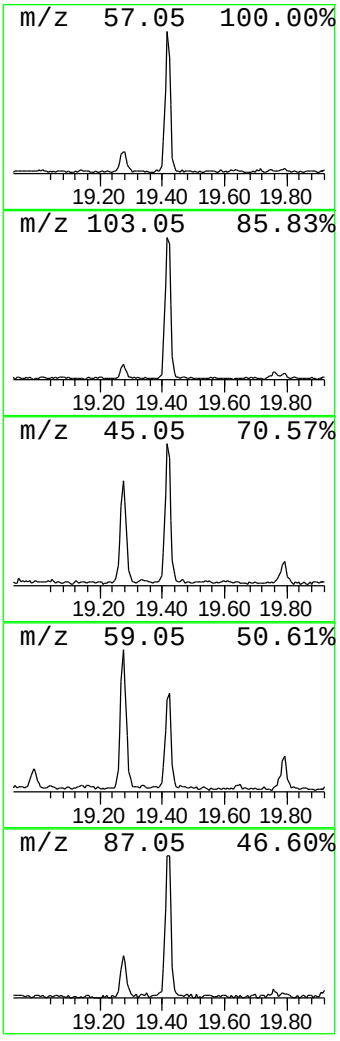
****

Peak Number 9 unknown19.42 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.42	10.52 ng	397068	Phenanthrene-d10	17.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyric acid, 4-butoxy-, methyl ...	174	C9H18O3	029006-06-2	49
2	3-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	000597-05-7	47
3	Silane, ethoxytrimethyl-	118	C5H14OSi	001825-62-3	43
4	Butanedioic acid, 2,3-dimethoxy-...	206	C8H14O6	056145-21-2	43
5	Allyl(ethoxy)dimethylsilane	144	C7H16OSi	018269-47-1	43





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Sample : L3033-03
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Instrument : BNA_G
ClientSampleId : SS043MW011-200615

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

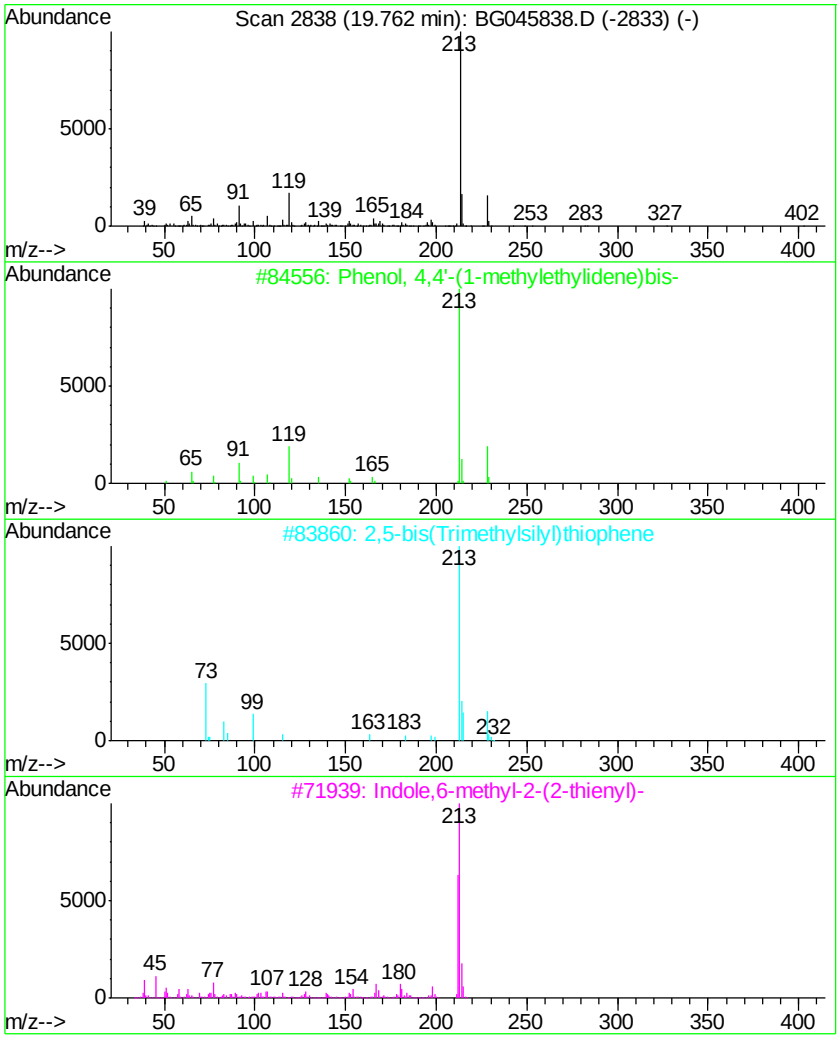
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

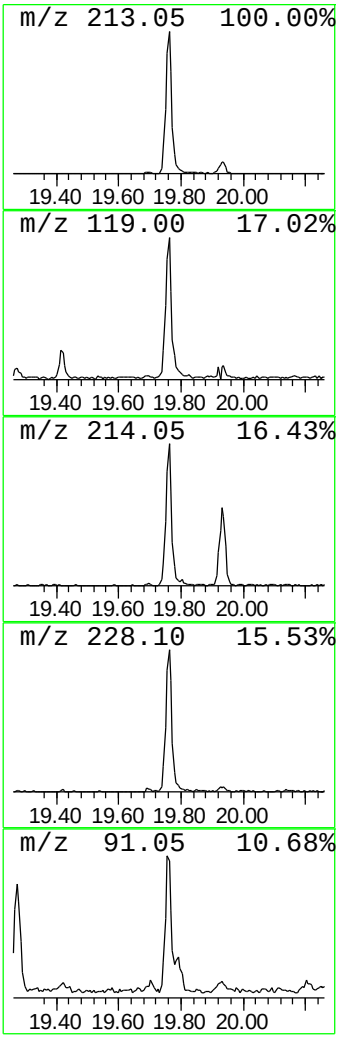
****

Peak Number 10 Phenol, 4,4'-(1-methylethyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.76	15.26 ng	651380	Chrysene-d12	21.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	98
2	2,5-bis(Trimethylsilyl)thiophene	228	C10H20SSi2	017906-71-7	45
3	Indole,6-methyl-2-(2-thienyl)-	213	C13H11NS	296245-70-0	40
4	Phenol, 2,4'-isopropylidenedi-	228	C15H16O2	000837-08-1	38
5	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	38





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062320\
Data File : BG045838.D
Acq On : 23 Jun 2020 13:35
Operator : CG/JU
Sample : L3033-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SS043MW011-200615

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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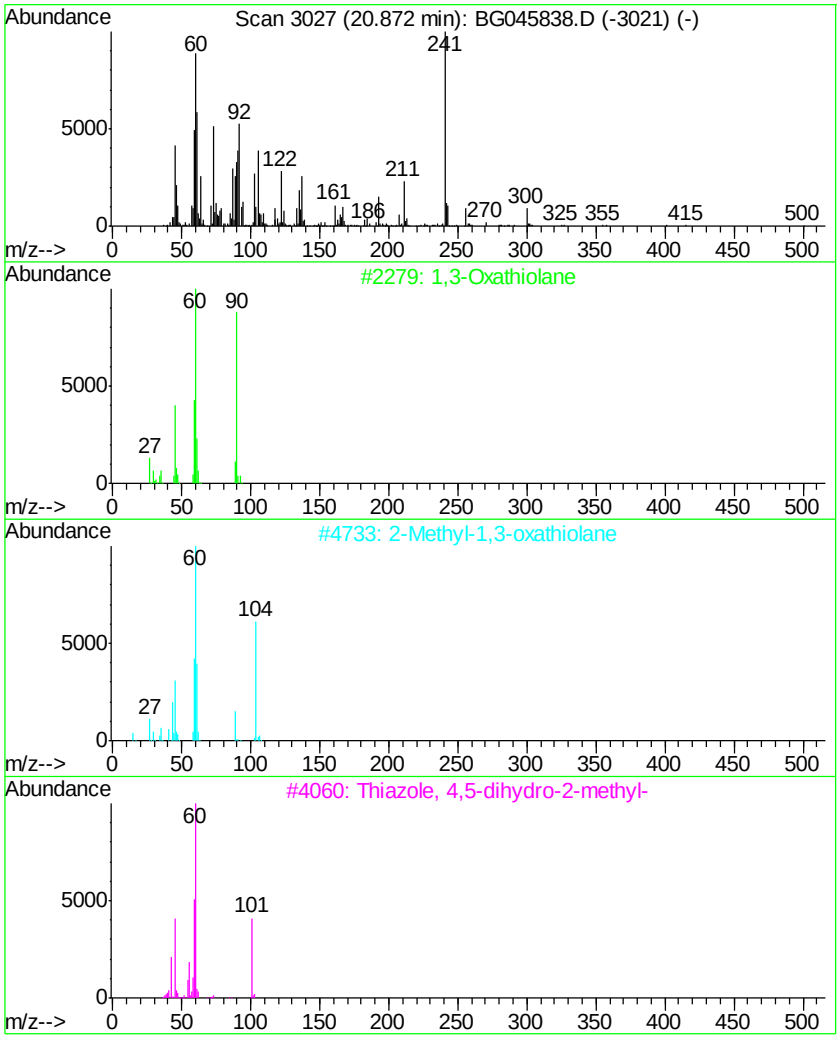
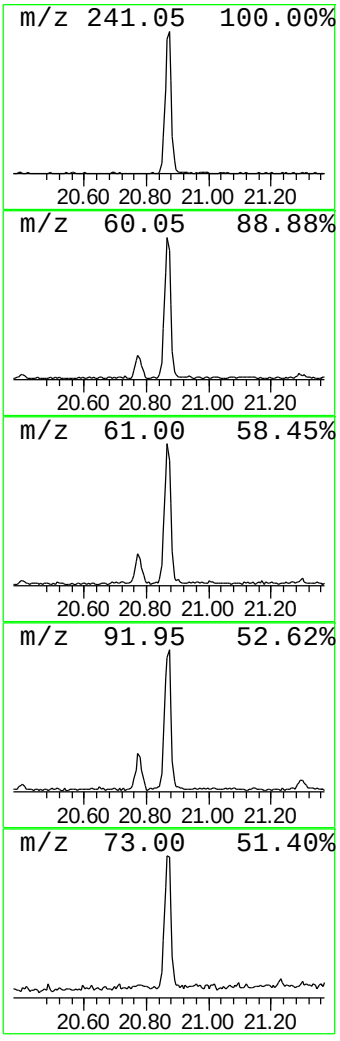
Peak Number 11 unknown20.87 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.87	18.75 ng	800515	Chrysene-d12	21.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Oxathiolane	90	C3H6OS	002094-97-5	22
2	2-Methyl-1,3-oxathiolane	104	C4H8OS	017642-74-9	22
3	Thiazole, 4,5-dihydro-2-methyl-	101	C4H7NS	002346-00-1	22
4	1-Methyl-1-n-decyloxy-1-silacyclo...	256	C15H32OSi	1000216-91-2	18
5	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	18





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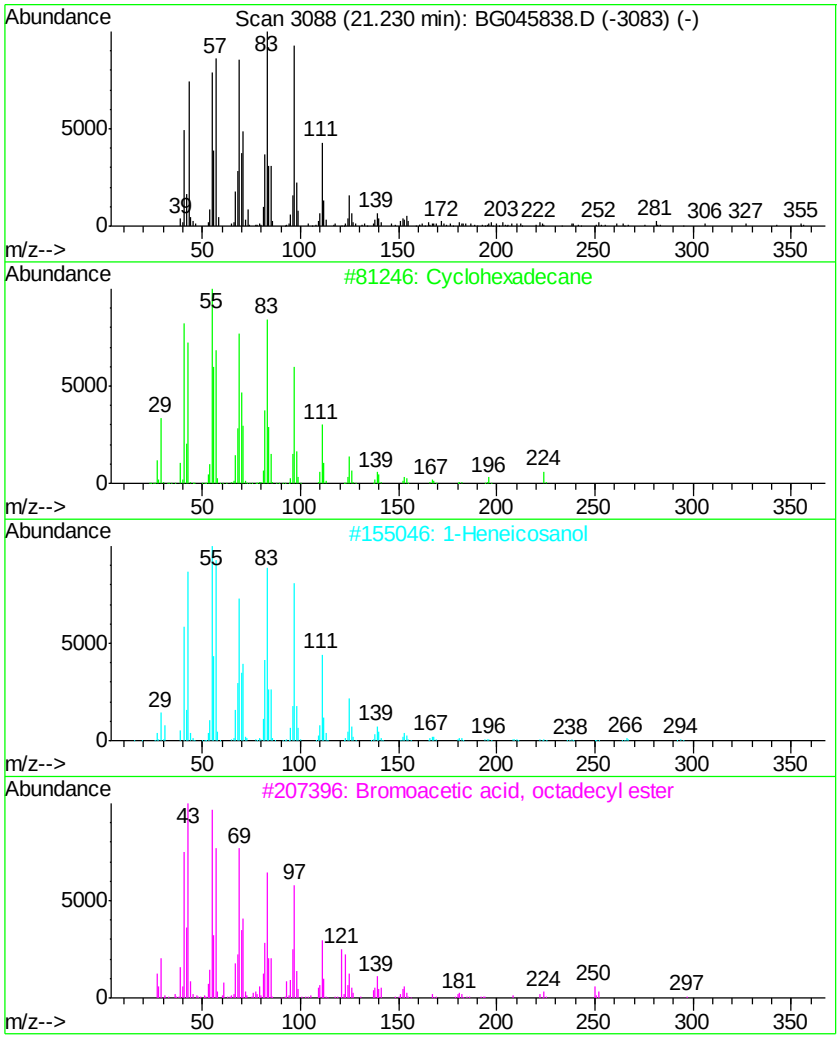
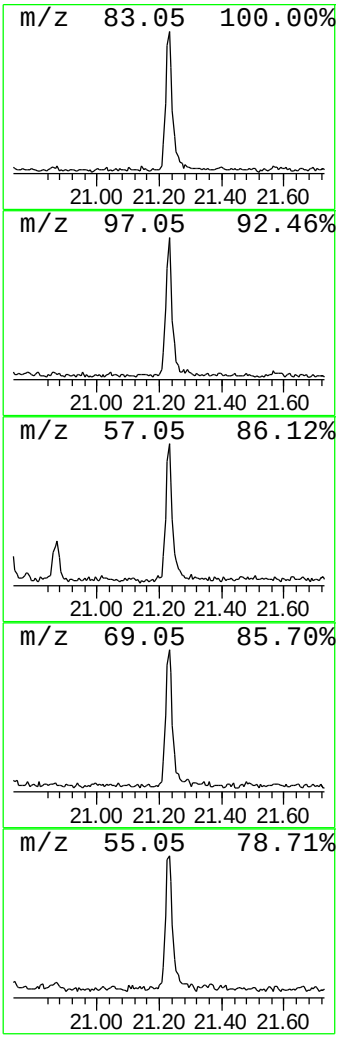
Peak Number 12 Cyclohexadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.23	7.35 ng	313547	Chrysene-d12	21.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	94
3	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
4	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	91





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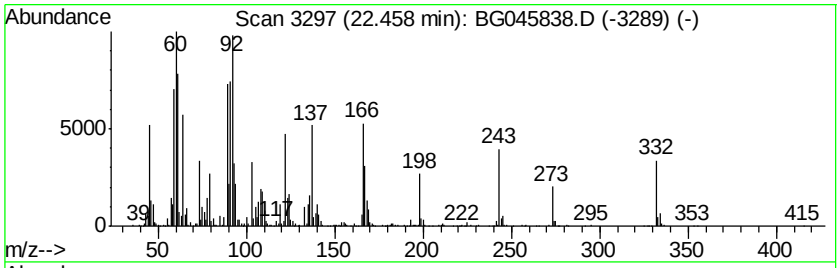
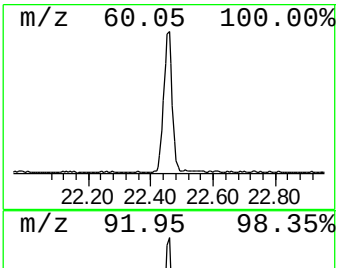
Peak Number 13 unknown22.46 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.46	38.80 ng	1656140	Chrysene-d12	21.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	S-2-[2-[6-Methoxy-4-quinolyloxyl...	358	C14H18N2O5S2	1000254-97-4	14
2	Thiosulfuric acid (H2S2o3), S-[2...	321	C8H20NO6PS2	062209-41-0	10
3	S-2-[3-Succinimidopropylaminolet...	296	C9H16N2O5S2	031701-75-4	9
4	Fluoroacetic acid, ethoxycarbony...	164	C6H9FO4	1000305-93-6	9
5	1,2,5,6-Tetrathiocane	184	C4H8S4	001940-01-8	9





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1,3-Oxathiolane	4.54	469.5	ng	8492820	1	7.92	361795	20.0
Diethyltoluamide	15.31	25.4	ng	791838	3	14.56	622370	20.0
unknown15.46	15.46	14.9	ng	463597	3	14.56	622370	20.0
unknown16.20	16.20	59.6	ng	2249560	4	17.32	754785	20.0
Benzenesulfonamid...	16.59	8.2	ng	309888	4	17.32	754785	20.0
unknown18.15	18.15	22.1	ng	832696	4	17.32	754785	20.0
unknown19.27	19.27	15.3	ng	578512	4	17.32	754785	20.0
unknown19.42	19.42	10.5	ng	397068	4	17.32	754785	20.0
Phenol, 4,4'-(1-m...	19.76	15.3	ng	651380	5	21.57	853719	20.0
unknown20.87	20.87	18.8	ng	800515	5	21.57	853719	20.0
Cyclohexadecane	21.23	7.3	ng	313547	5	21.57	853719	20.0
unknown22.46	22.46	38.8	ng	1656140	5	21.57	853719	20.0