LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051017\
Data File : BM009975.D
Acq On : 10 May 2017 17:46
Operator : SJ/MA
Sample : I3058-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF017MW001-170508

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:\HPCHEM1\BNA_M\METHODS\8270-BM050517.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	4.422	220	227	242	rBV	4477290	6388616	100.00%	16.693%
2	4.898	303	308	318	rVB	118420	172935	2.71%	0.452%
3	5.357	380	386	397	rBV	681219	1060473	16.60%	2.771%
4	6.951	651	657	668	rBV	430283	737715	11.55%	1.928%
5	7.304	709	717	727	rBV	1405839	2264366	35.44%	5.917%
6	7.769	790	796	808	rVB	305251	493891	7.73%	1.291%
7	8.086	842	850	862	rBV	1164259	1894614	29.66%	4.951%
8	8.939	988	995	1004	rBV	1201884	1960925	30.69%	5.124%
9	9.022	1004	1009	1013	rVB3	42286	73804	1.16%	0.193%
10	10.563	1260	1271	1281	rBV	408248	703707	11.02%	1.839%
11	11.857	1487	1491	1498	rBV	49320	89082	1.39%	0.233%
12	13.033	1680	1691	1697	rBV	2757110	4500488	70.45%	11.760%
13	13.733	1803	1810	1817	rBV6	24359	67039	1.05%	0.175%
14	13.880	1830	1835	1841	rBV2	89477	133926	2.10%	0.350%
15	14.421	1920	1927	1936	rVB2	591014	923410	14.45%	2.413%
16	15.168	2048	2054	2062	rBV	54369	94585	1.48%	0.247%
17	15.921	2176	2182	2192	rBV	2693774	3934490	61.59%	10.281%
18	16.462	2269	2274	2280	rBV	125311	198898	3.11%	0.520%
19	17.174	2389	2395	2405	rBV2	832066	1212484	18.98%	3.168%
20	17.345	2420	2424	2428	rBV3	57144	85002	1.33%	0.222%
21	18.056	2540	2545	2549	rBV5	79728	120497	1.89%	0.315%
22	18.151	2558	2561	2567	rVB3	49550	67693	1.06%	0.177%
23	19.268	2747	2751	2759	rBV	513942	666559	10.43%	1.742%
24	19.333	2759	2762	2767	rVV6	56050	71975	1.13%	0.188%
25	19.574	2799	2803	2808	rBV2	95383	116690	1.83%	0.305%
26	19.627	2808	2812	2818	rBV2	90803	126408	1.98%	0.330%
27	19.803	2836	2842	2852	rBV	5082615	6302939	98.66%	16.469%
28	20.580	2971	2974	2979	rVB7	47172	72987	1.14%	0.191%
29	21.050	3050	3054	3058	rBV4	167876	205715	3.22%	0.538%
30	21.250	3086	3088	3093	rVB2	110129	108788	1.70%	0.284%
31	21.368	3103	3108	3114	rVB	1288961	1602627	25.09%	4.188%
32	22.191	3244	3248	3252	rVB2	300303	388860	6.09%	1.016%
33	23.662	3492	3498	3506	rVB2	733873	1428569	22.36%	3.733%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051017\
Data File : BM009975.D
Acq On : 10 May 2017 17:46
Operator : SJ/MA
Sample : I3058-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF017MW001-170508

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:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

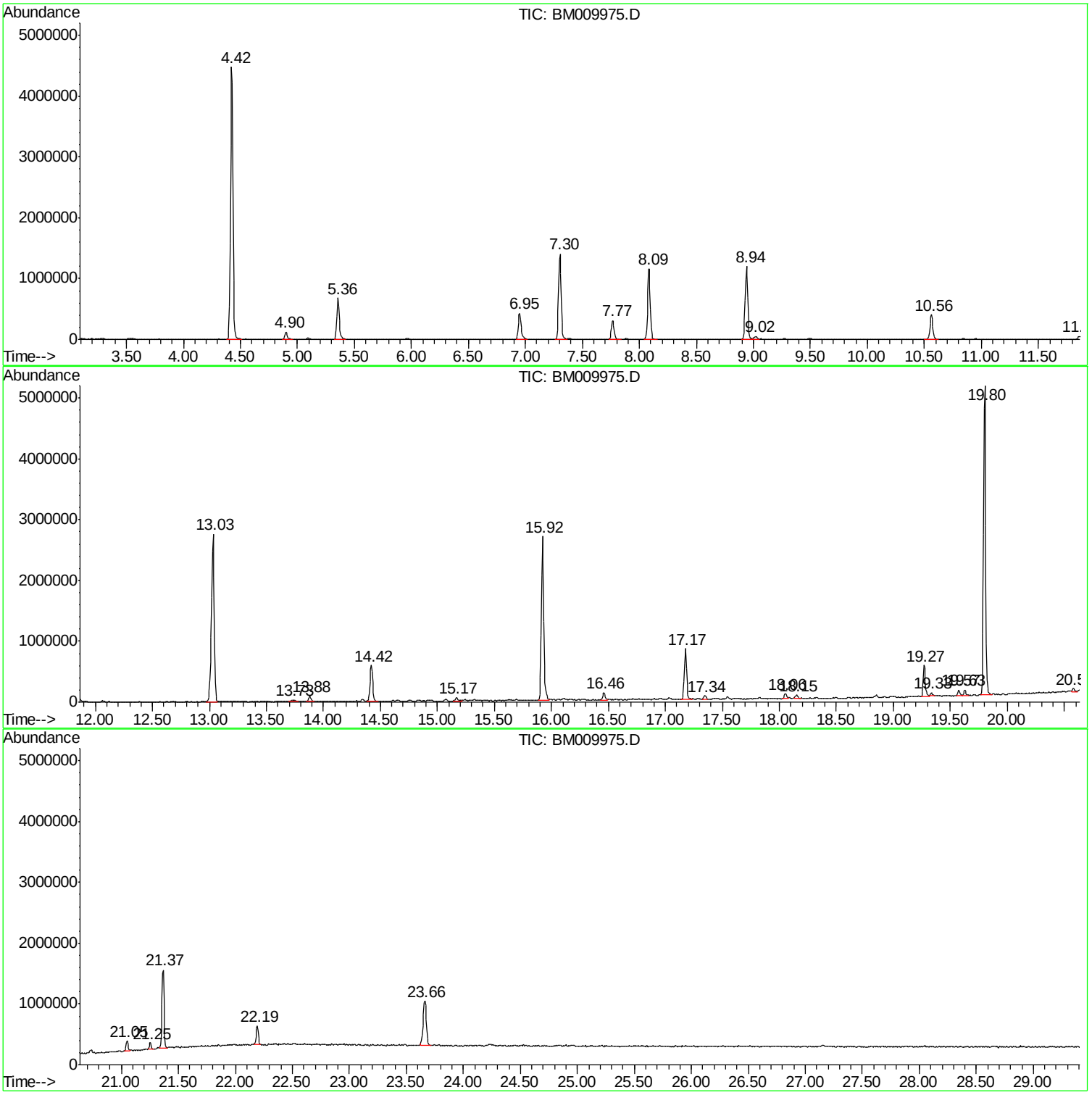
Sum of corrected areas: 38270757

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051017\
Data File : BM009975.D
Acq On : 10 May 2017 17:46
Operator : SJ/MA
Sample : I3058-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF017MW001-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051017\
Data File : BM009975.D
Acq On : 10 May 2017 17:46
Operator : SJ/MA
Sample : I3058-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LF017MW001-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

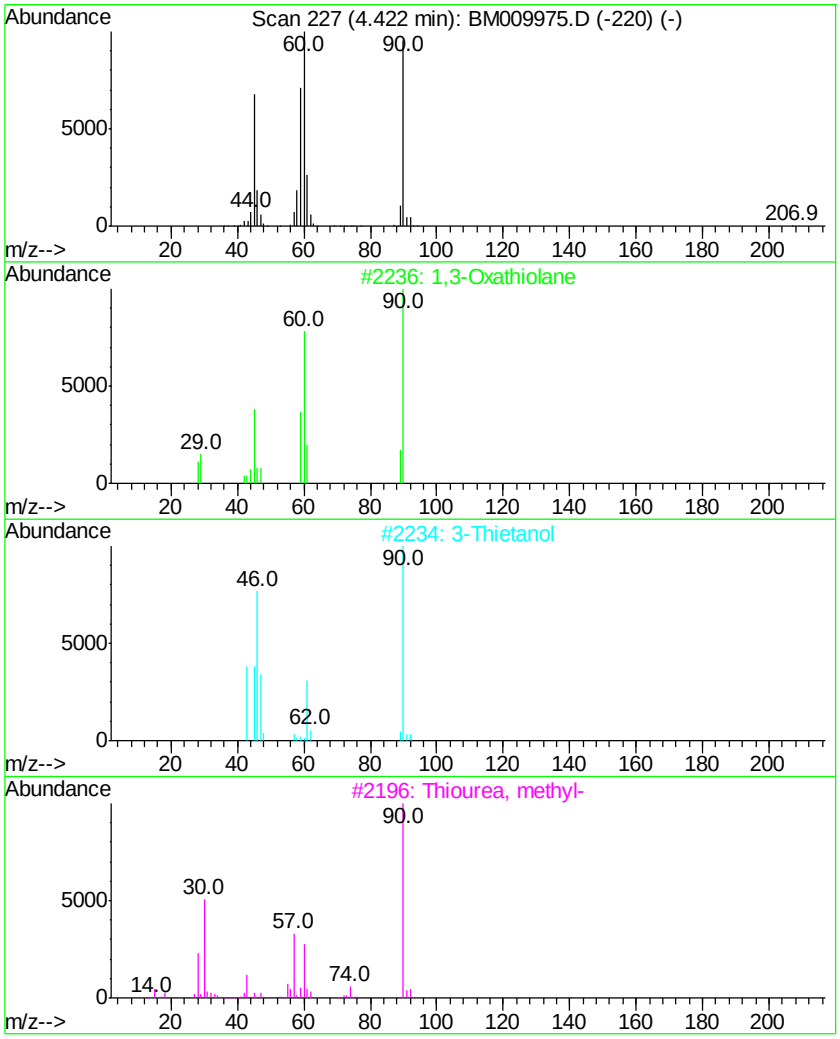
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

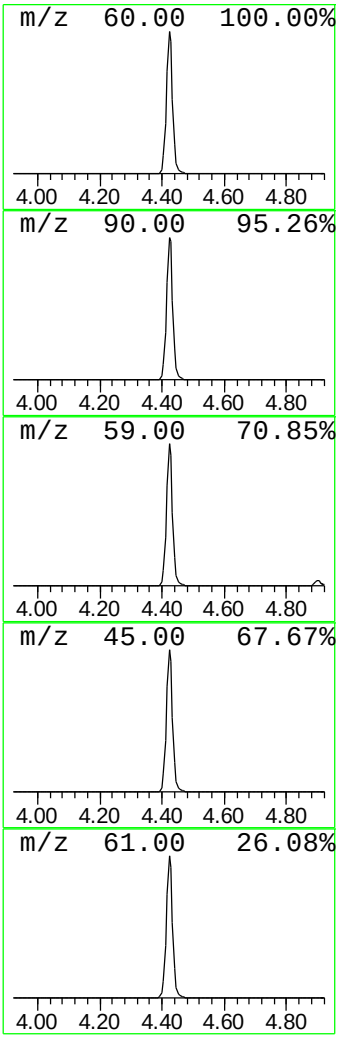
****

Peak Number 1 1,3-Oxathiolane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.42	258.71 ng	6388620	1,4-Dichlorobenzene-d4	7.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Oxathiolane	90	C3H6OS	002094-97-5	56
2	3-Thietanol	90	C3H6OS	010304-16-2	53
3	Thiourea, methyl-	90	C2H6N2S	000598-52-7	50
4	Hydrazinecarboxylic acid, methyl...	90	C2H6N2O2	006294-89-9	38
5	Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	38





Data Path : Z:\HPCHEM1\BNA M\DATA\BM051017\
Data File : BM009975.D
Acq On : 10 May 2017 17:46
Operator : SJ/MA
Sample : I3058-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF017MW001-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

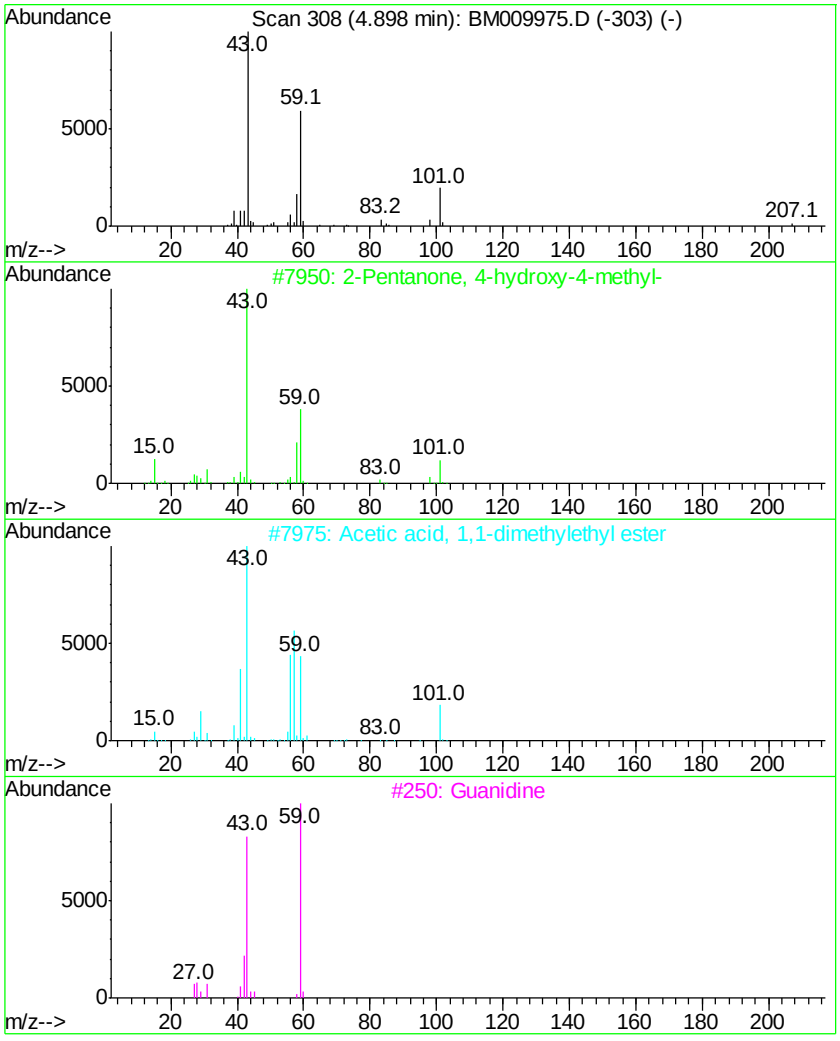
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

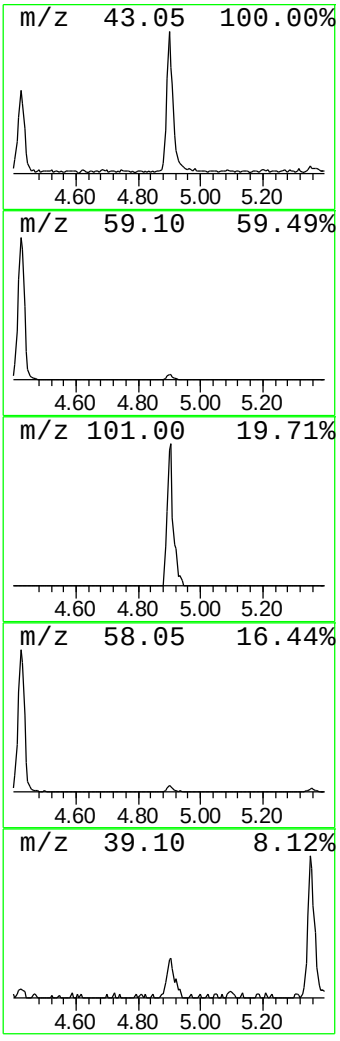
****

Peak Number 2 unknown4.90 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	7.00 ng	172935	1,4-Dichlorobenzene-d4	7.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Guanidine	59	CH5N3	000113-00-8	38
4	Dimethadione	129	C5H7NO3	000695-53-4	36
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32





Data Path : Z:\HPCHEM1\BNA M\DATA\BM051017\
Data File : BM009975.D
Acq On : 10 May 2017 17:46
Operator : SJ/MA
Sample : I3058-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF017MW001-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

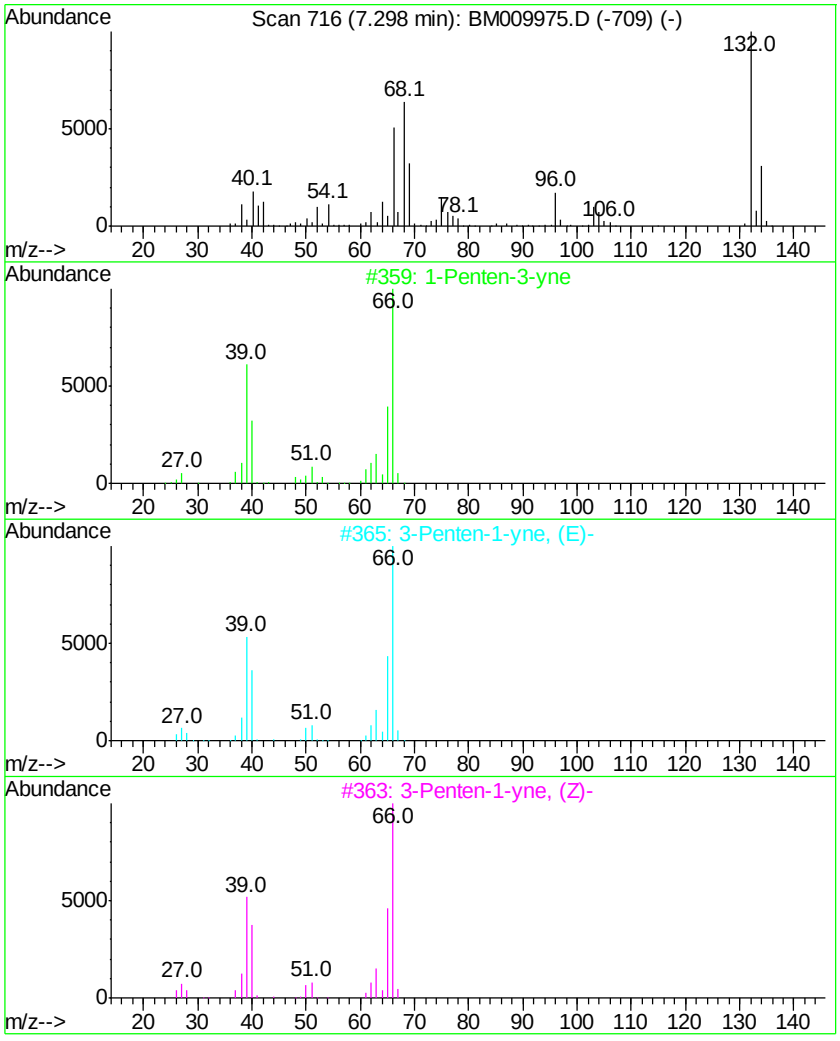
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

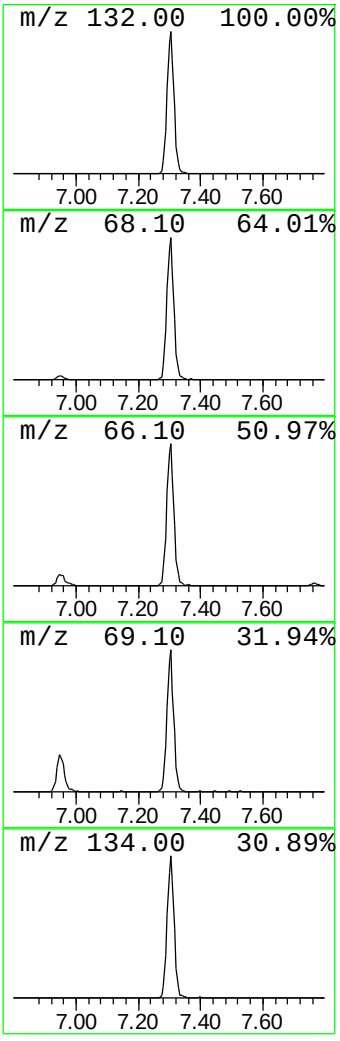
****

Peak Number 3 unknown7.30 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.30	91.70 ng	2264370	1,4-Dichlorobenzene-d4	7.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Penten-3-yne	66	C5H6	000646-05-9	38
2	3-Penten-1-yne, (E)-	66	C5H6	002004-69-5	35
3	3-Penten-1-yne, (Z)-	66	C5H6	001574-40-9	35
4	1,3-Cyclopentadiene	66	C5H6	000542-92-7	25
5	Silane, bicyclo[2.2.1]hept-5-en-...	226	C7H9Cl3Si	014319-64-3	17





Data Path : Z:\HPCHEM1\BNA M\DATA\BM051017\
Data File : BM009975.D
Acq On : 10 May 2017 17:46
Operator : SJ/MA
Sample : I3058-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF017MW001-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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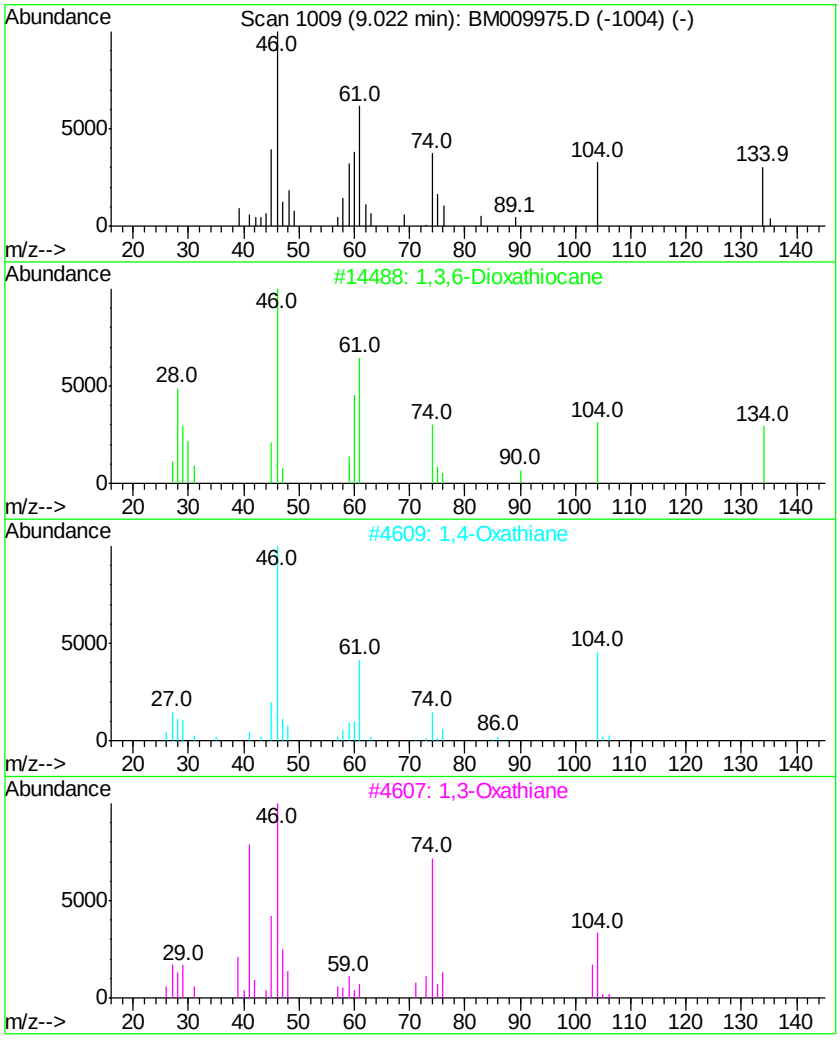
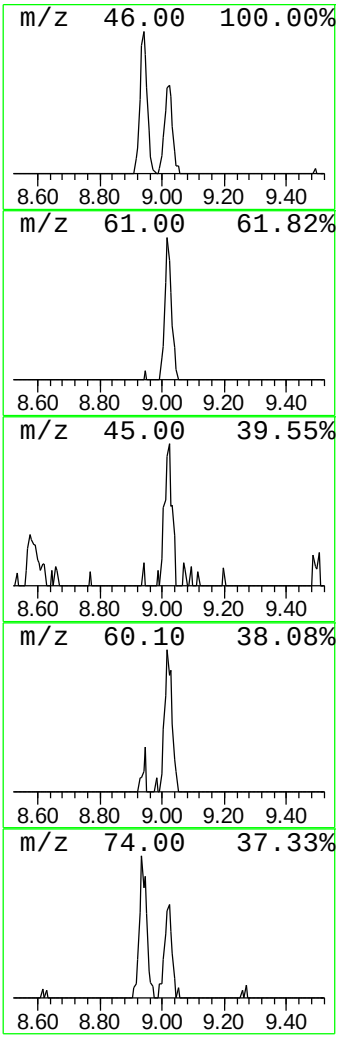
Peak Number 5 1,3,6-Dioxathiocane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.02	2.99 ng	73804	1,4-Dichlorobenzene-d4	7.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,6-Dioxathiocane	134	C5H10O2S	002094-92-0	70
2	1,4-Oxathiane	104	C4H8OS	015980-15-1	43
3	1,3-Oxathiane	104	C4H8OS	000646-12-8	38
4	Butane, 1-(methylthio)-	104	C5H12S	000628-29-5	30
5	Trimethylphosphine	76	C3H9P	000594-09-2	18





Data Path : Z:\HPCHEM1\BNA M\DATA\BM051017\
Data File : BM009975.D
Acq On : 10 May 2017 17:46
Operator : SJ/MA
Sample : I3058-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF017MW001-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

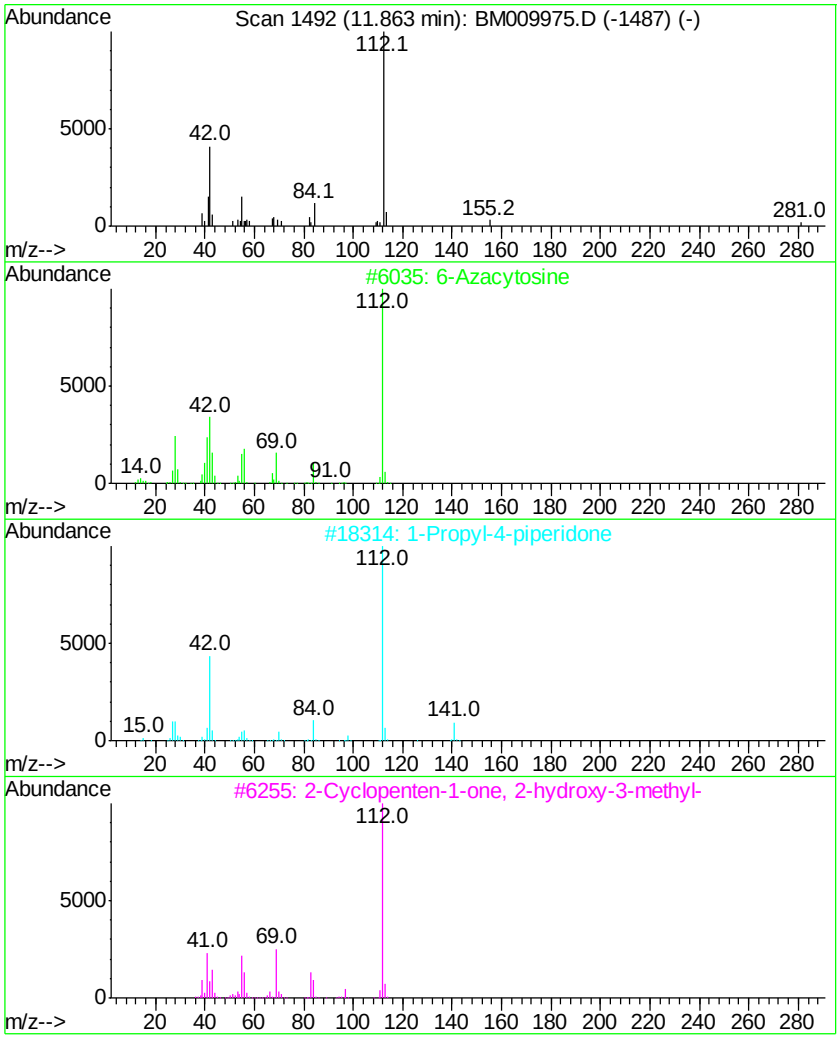
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

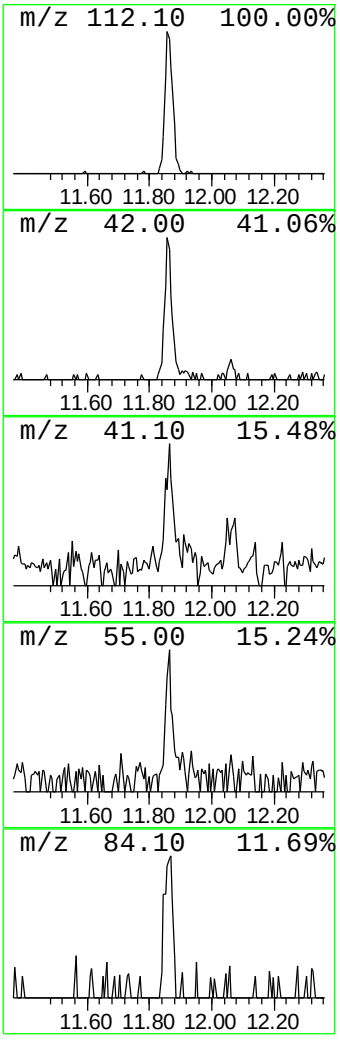
****

Peak Number 6 6-Azacytosine Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	2.53 ng	89082	Naphthalene-d8	10.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Azacytosine	112	C3H4N4O	000931-85-1	78
2	1-Propyl-4-piperidone	141	C8H15NO	023133-37-1	56
3	2-Cyclopenten-1-one, 2-hydroxy-3...	112	C6H8O2	000080-71-7	50
4	Uracil	112	C4H4N2O2	000066-22-8	50
5	2-Hydroxymethyl-2-methyl-pyrroli...	143	C7H13NO2	1000189-82-1	43





Data Path : Z:\HPCHEM1\BNA M\DATA\BM051017\
Data File : BM009975.D
Acq On : 10 May 2017 17:46
Operator : SJ/MA
Sample : I3058-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF017MW001-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

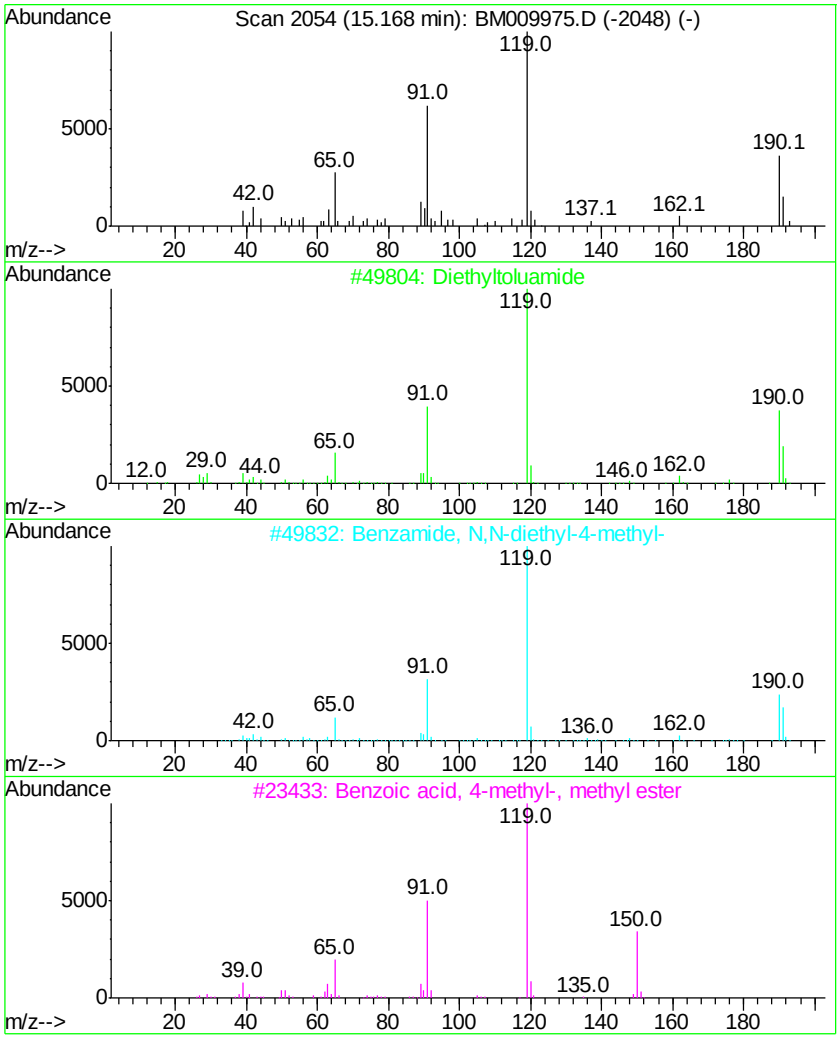
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

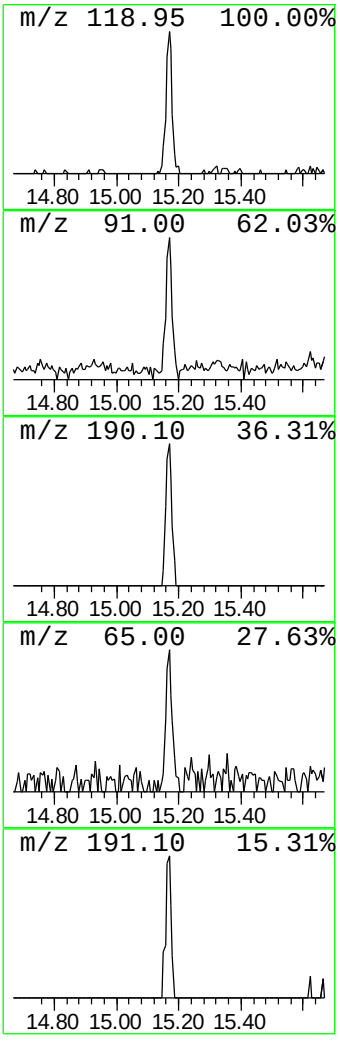
****

Peak Number 7 Diethyltoluamide Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	2.05 ng	94585	Acenaphthene-d10	14.42

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	78
3	Benzoic acid, 4-methyl-, methyl ...	150	C9H10O2	000099-75-2	53
4	Benzhydrazide, 4-methyl-N2-[1-me...	303	C12H13N7O3	324021-25-2	50
5	1-Propanone, 2-methyl-1-(2-methy...	162	C11H14O	002040-21-3	50





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051017\
Data File : BM009975.D
Acq On : 10 May 2017 17:46
Operator : SJ/MA
Sample : I3058-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF017MW001-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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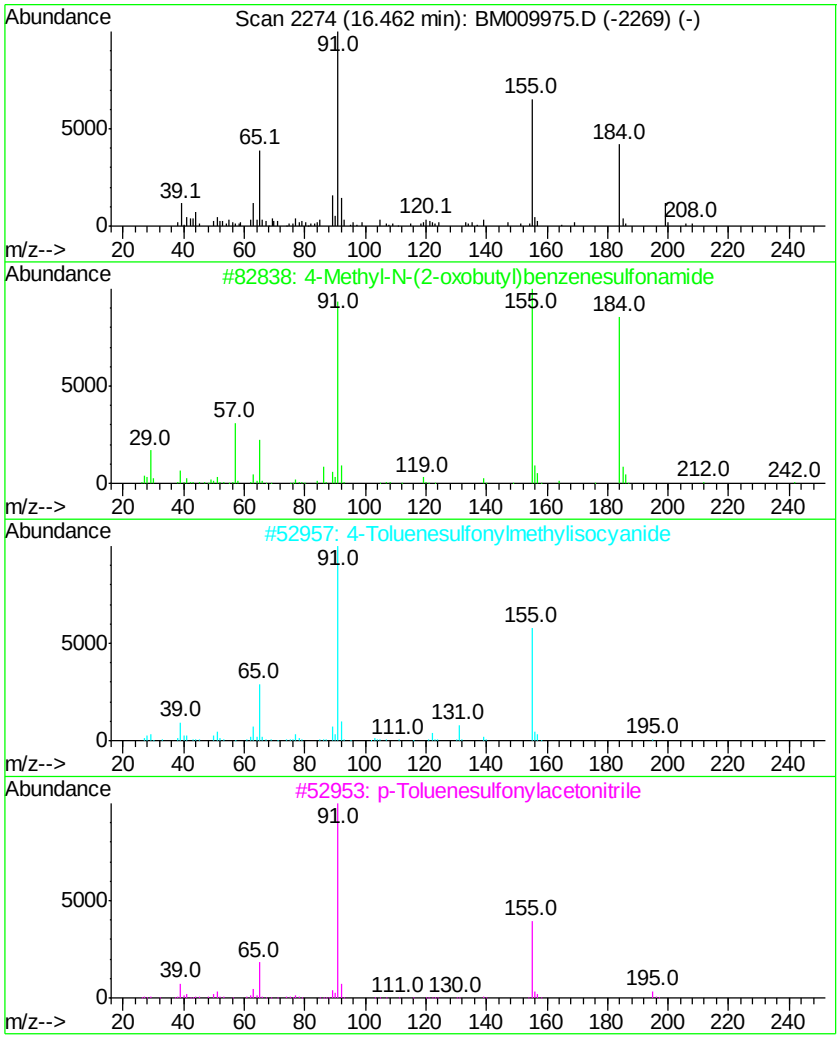
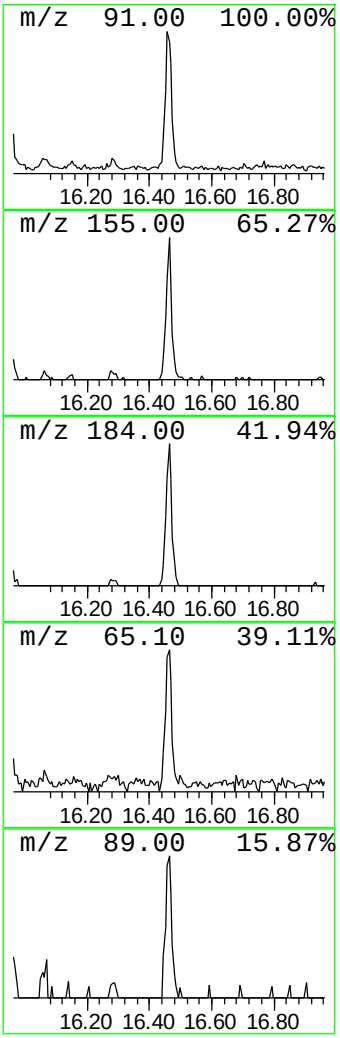
Peak Number 8 4-Methyl-N-(2-oxobutyl)benz... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.46	3.28 ng	198898	Phenanthrene-d10	17.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methyl-N-(2-oxobutyl)benzenesu...	241	C11H15NO3S	1000192-14-5	78
2	4-Toluenesulfonylmethylisocyanide	195	C9H9NO2S	036635-61-7	64
3	p-Toluenesulfonylacetonitrile	195	C9H9NO2S	005697-44-9	59
4	Pyridine-2-carbonitrile, 3,5,6-t...	375	C13H8Cl3N3O2S	255713-77-0	59
5	Benzene, (phenoxymethyl)-	184	C13H12O	000946-80-5	58





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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF017MW001-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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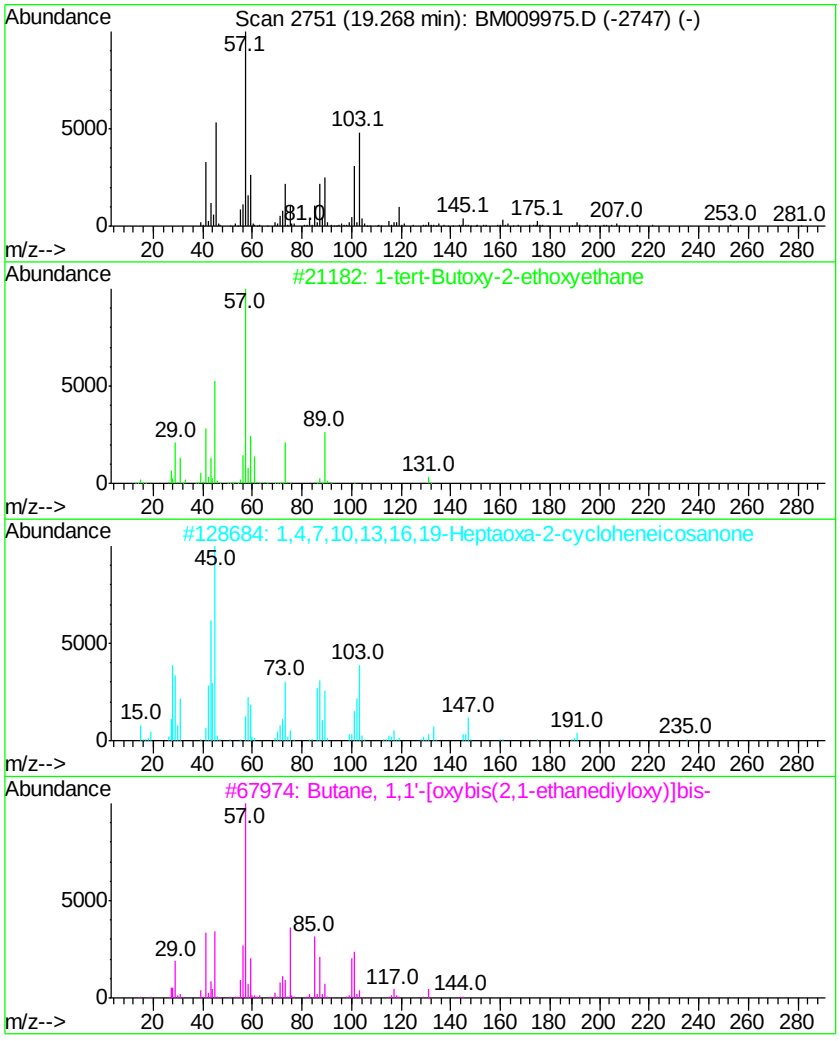
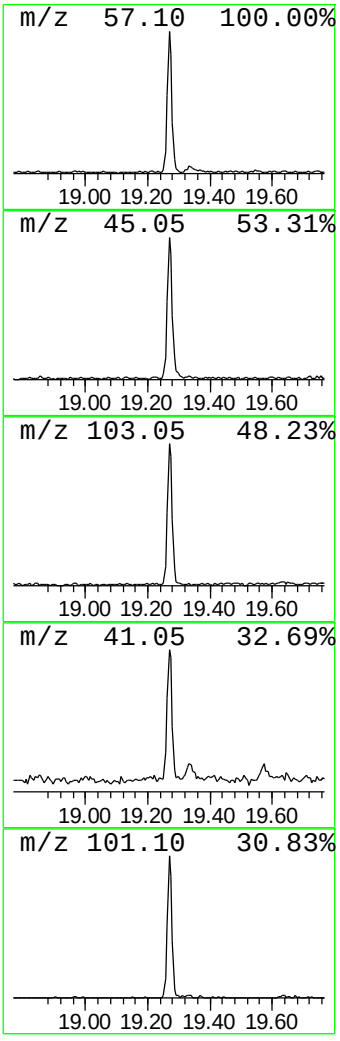
Peak Number 9 unknown19.27 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.27	10.99 ng	666559	Phenanthrene-d10	17.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-tert-Butoxy-2-ethoxyethane	146	C8H18O2	051422-54-9	43
2	1,4,7,10,13,16,19-Heptaoxa-2-cyc...	322	C14H26O8	083410-52-0	38
3	Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	37
4	Di-sec-butyl ether	130	C8H18O	006863-58-7	35
5	Carbonic acid, bis(1-methylpropy...	174	C9H18O3	000623-63-2	35





Data Path : Z:\HPCHEM1\BNA M\DATA\BM051017\
Data File : BM009975.D
Acq On : 10 May 2017 17:46
Operator : SJ/MA
Sample : I3058-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF017MW001-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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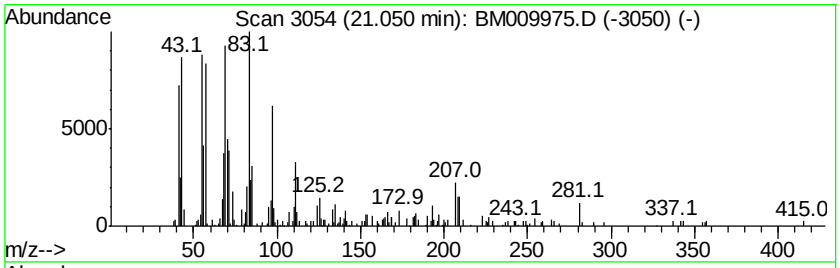
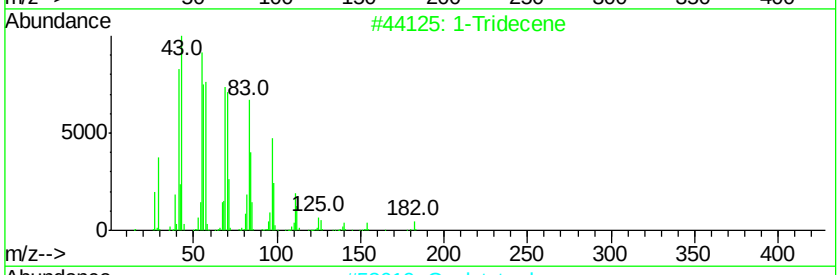
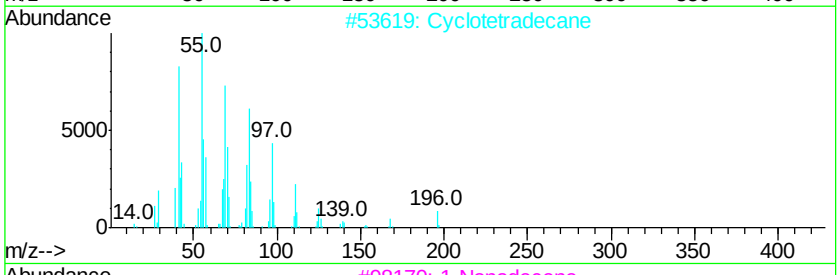
Peak Number 10 1-Tridecene Concentration Rank 9

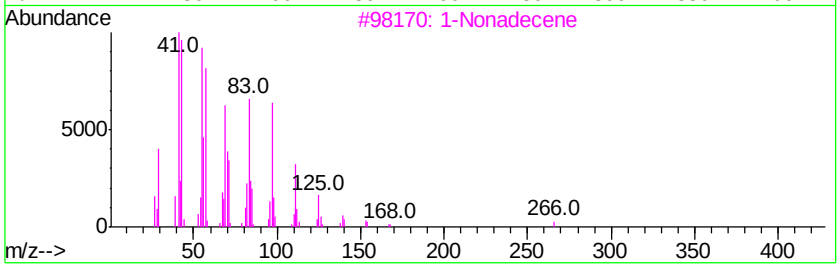
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.05	2.57 ng	205715	Chrysene-d12	21.37

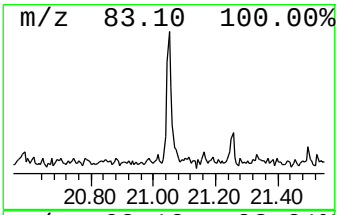
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tridecene	182	C13H26	002437-56-1	74
2	Cyclotetradecane	196	C14H28	000295-17-0	64
3	1-Nonadecene	266	C19H38	018435-45-5	64
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	58
5	Cyclopentane, 1-pentyl-2-propyl-	182	C13H26	062199-51-3	55

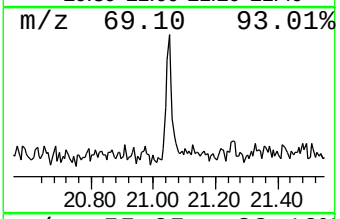


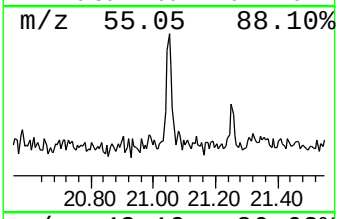


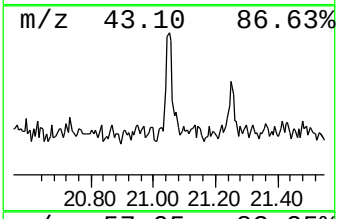


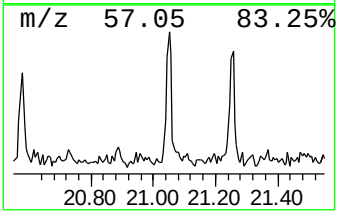












Data Path : Z:\HPCHEM1\BNA M\DATA\BM051017\
Data File : BM009975.D
Acq On : 10 May 2017 17:46
Operator : SJ/MA
Sample : I3058-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF017MW001-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

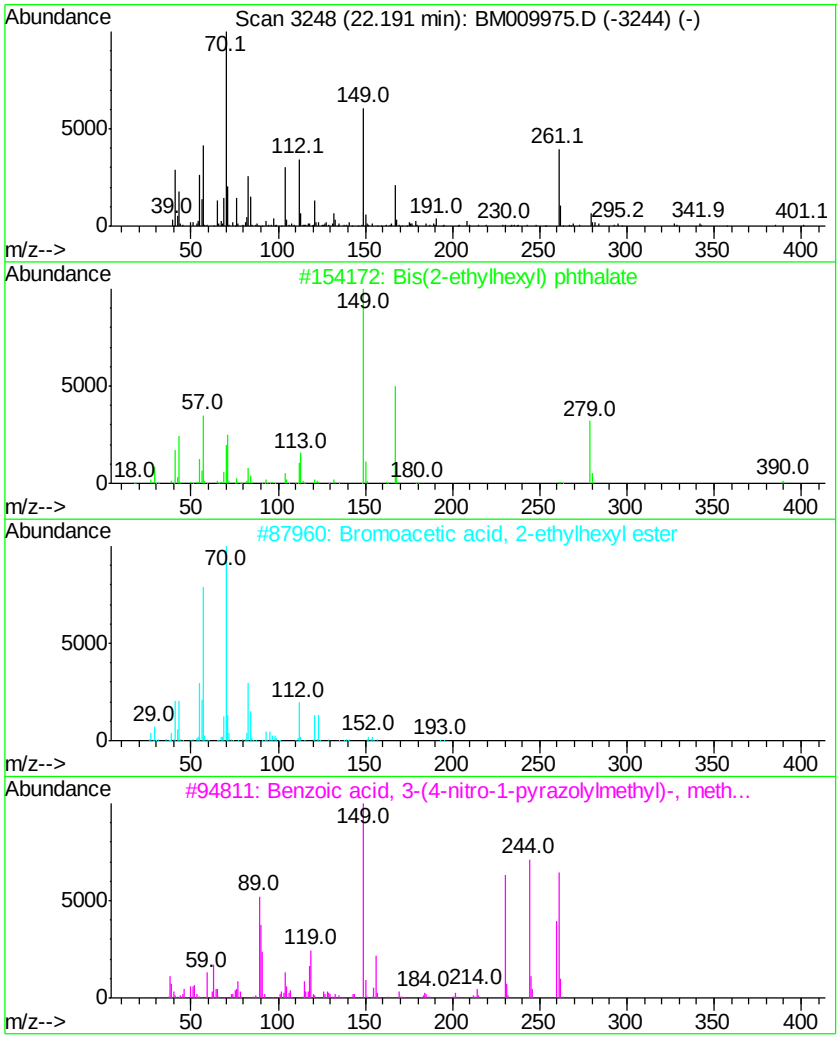
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

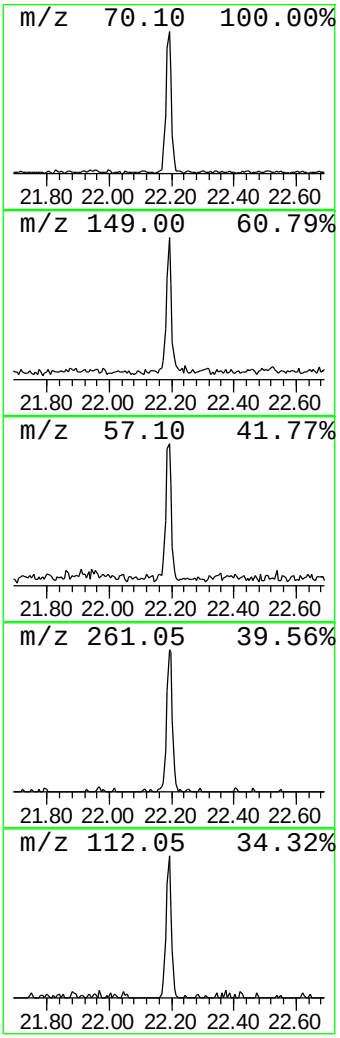
****

Peak Number 11 unknown22.19 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.19	4.85 ng	388860	Chrysene-d12	21.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	32
2	Bromoacetic acid, 2-ethylhexyl e...	250	C10H19BrO2	068144-73-0	27
3	Benzoic acid, 3-(4-nitro-1-pyraz...	261	C12H11N3O4	1000273-84-4	22
4	1,2-Benzenedicarboxylic acid, di...	390	C24H38O4	027554-26-3	22
5	Di-n-octyl phthalate	390	C24H38O4	000117-84-0	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM051017\
Data File : BM009975.D
Acq On : 10 May 2017 17:46
Operator : SJ/MA
Sample : I3058-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF017MW001-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1,3-Oxathiolane	4.42	258.7	ng	6388620	1	7.77	493891	20.0
unknown4.90	4.90	7.0	ng	172935	1	7.77	493891	20.0
unknown7.30	7.30	91.7	ng	2264370	1	7.77	493891	20.0
1,3,6-Dioxathiocane	9.02	3.0	ng	73804	1	7.77	493891	20.0
6-Azacytosine	11.86	2.5	ng	89082	2	10.56	703707	20.0
Diethyltoluamide	15.17	2.0	ng	94585	3	14.42	923410	20.0
4-Methyl-N-(2-oxo...	16.46	3.3	ng	198898	4	17.17	1212480	20.0
unknown19.27	19.27	11.0	ng	666559	4	17.17	1212480	20.0
1-Tridecene	21.05	2.6	ng	205715	5	21.37	1602630	20.0
unknown22.19	22.19	4.8	ng	388860	5	21.37	1602630	20.0