LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026393.D
Acq On : 15 Jun 2020 16:08
Operator : JU/CG
Sample : L3005-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF001MW002-200611

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_M\METHODS\8270-BM060520.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	4.110	202	208	222	rBV	956042	1337241	19.51%	3.944%
2	4.769	315	320	328	rBV	89413	133170	1.94%	0.393%
3	5.040	360	366	381	rBV	594107	859018	12.53%	2.533%
4	6.610	625	633	644	rBV	356138	595652	8.69%	1.757%
5	7.404	758	768	772	rBV	414867	638886	9.32%	1.884%
6	7.434	772	773	779	rVB	66780	76238	1.11%	0.225%
7	7.716	814	821	833	rVB	1353082	2100209	30.64%	6.194%
8	8.551	952	963	973	rBV	1224711	1932582	28.19%	5.700%
9	10.163	1229	1237	1244	rBV	527666	865870	12.63%	2.554%
10	11.469	1452	1459	1465	rBV	61925	109018	1.59%	0.322%
11	12.616	1647	1654	1658	rBV	1145983	1772610	25.86%	5.228%
12	12.669	1658	1663	1675	rVB	3042623	4284023	62.50%	12.635%
13	12.974	1707	1715	1723	rVB	105519	167878	2.45%	0.495%
14	13.527	1803	1809	1816	rBV	448717	620527	9.05%	1.830%
15	14.057	1893	1899	1908	rBV	792695	1150245	16.78%	3.392%
16	15.321	2110	2114	2125	rVB2	39557	70963	1.04%	0.209%
17	15.563	2148	2155	2163	rBV2	2498374	3730420	54.42%	11.002%
18	15.698	2172	2178	2184	rVB4	53324	87705	1.28%	0.259%
19	16.104	2238	2247	2257	rBV	157314	295845	4.32%	0.873%
20	16.810	2362	2367	2380	rVB	1009444	1382918	20.17%	4.079%
21	17.757	2523	2528	2535	rBV5	31287	73336	1.07%	0.216%
22	17.962	2555	2563	2567	rBV3	65875	112316	1.64%	0.331%
23	18.009	2567	2571	2575	rVB2	121939	153886	2.24%	0.454%
24	18.215	2601	2606	2615	rBV2	321112	531413	7.75%	1.567%
25	18.974	2731	2735	2739	rVB	94258	101899	1.49%	0.301%
26	19.233	2774	2779	2783	rBV	149756	195833	2.86%	0.578%
27	19.468	2813	2819	2825	rBV	5757126	6854698	100.00%	20.216%
28	20.768	3036	3040	3052	rBV	390226	512725	7.48%	1.512%
29	21.021	3078	3083	3088	rBV	1231765	1502522	21.92%	4.431%
30	22.174	3276	3279	3284	rVB	115279	136054	1.98%	0.401%
31	23.109	3433	3438	3445	rVB	908975	1521147	22.19%	4.486%

Sum of corrected areas: 33906847

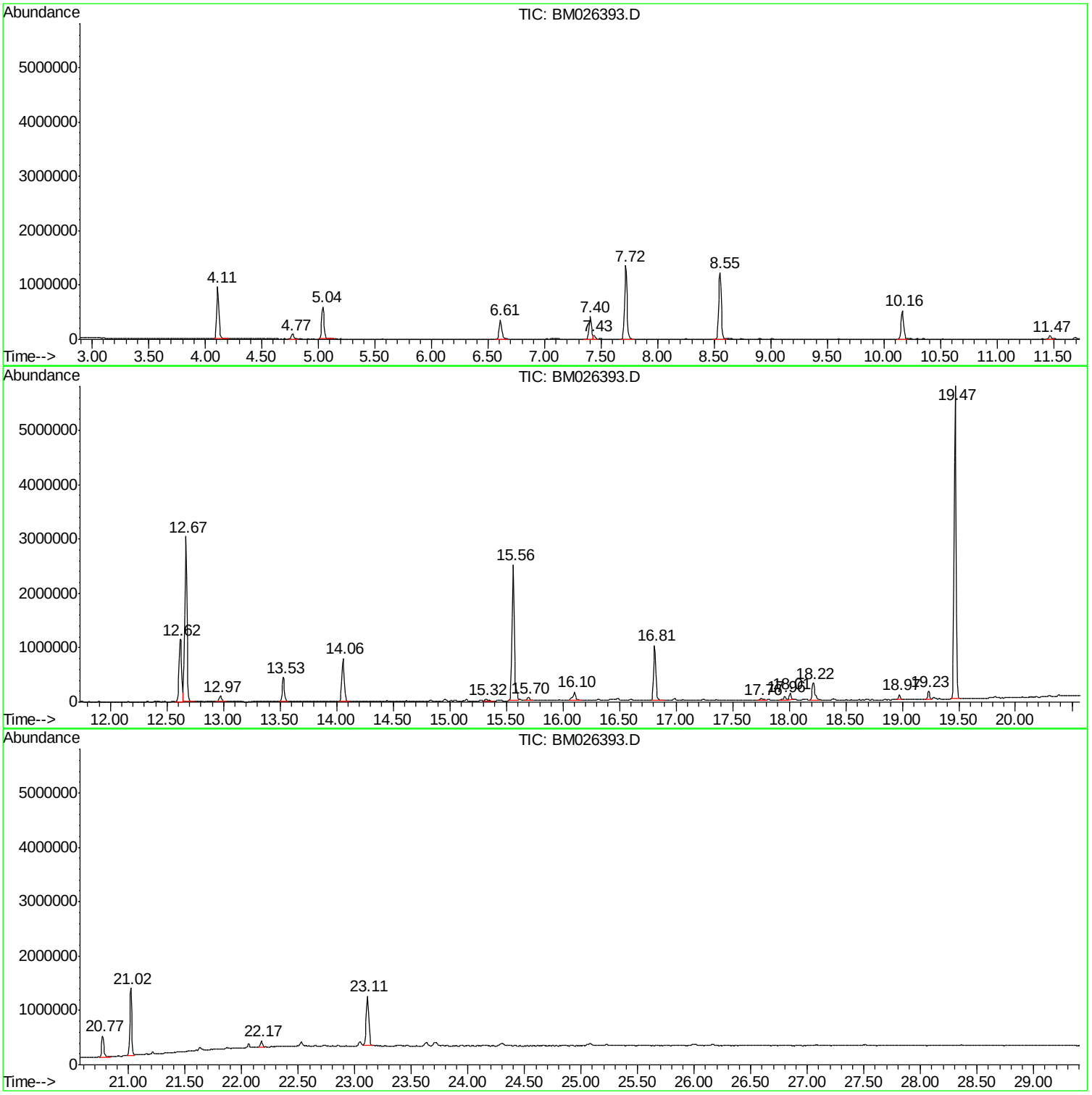
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026393.D
Acq On : 15 Jun 2020 16:08
Operator : JU/CG
Sample : L3005-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LF001MW002-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026393.D
Acq On : 15 Jun 2020 16:08
Operator : JU/CG
Sample : L3005-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF001MW002-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

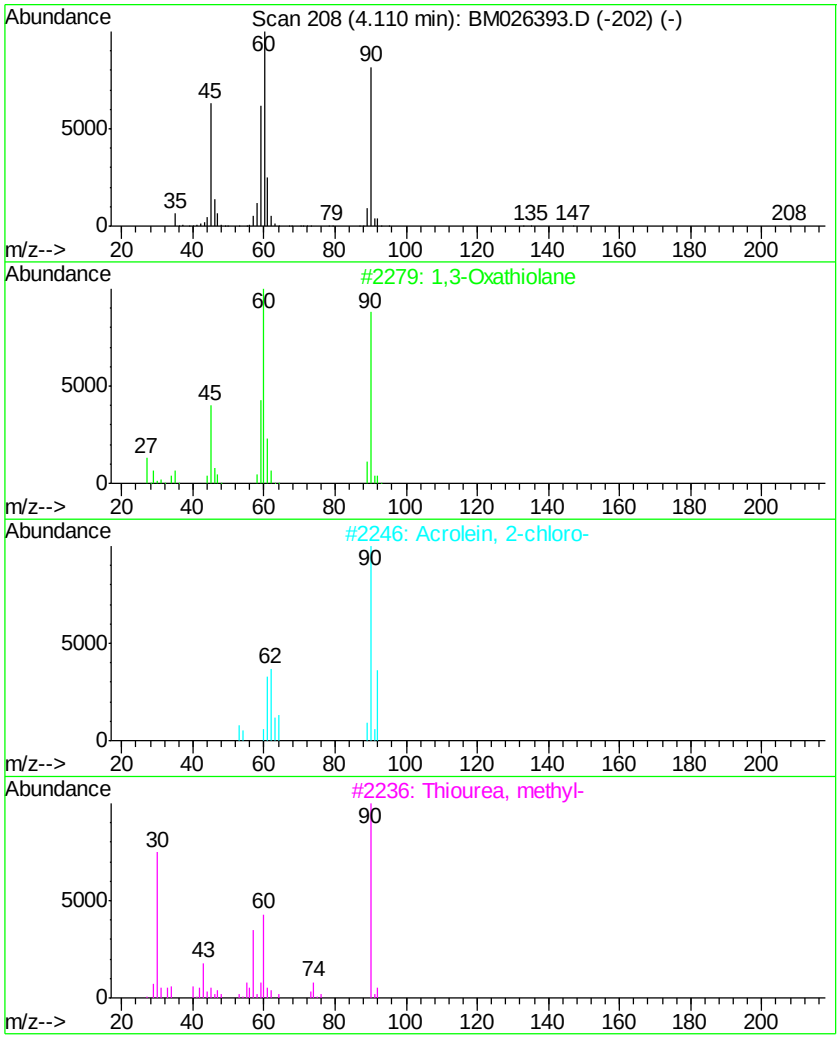
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

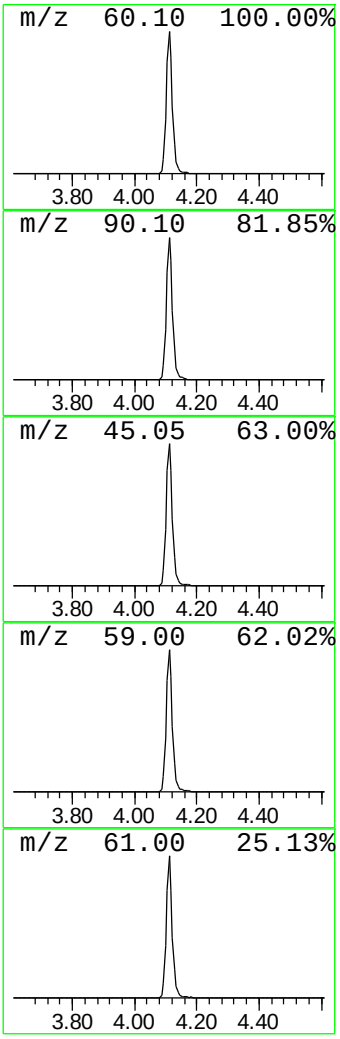
****

Peak Number 1 1,3-Oxathiolane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.11	41.86 ng	1337240	1,4-Dichlorobenzene-d4	7.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Oxathiolane	90	C3H6OS	002094-97-5	90
2	Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	59
3	Thiourea, methyl-	90	C2H6N2S	000598-52-7	50
4	Hydrazinecarboxylic acid, methyl...	90	C2H6N2O2	006294-89-9	38
5	3-Thietanol	90	C3H6OS	010304-16-2	36





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026393.D
Acq On : 15 Jun 2020 16:08
Operator : JU/CG
Sample : L3005-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF001MW002-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

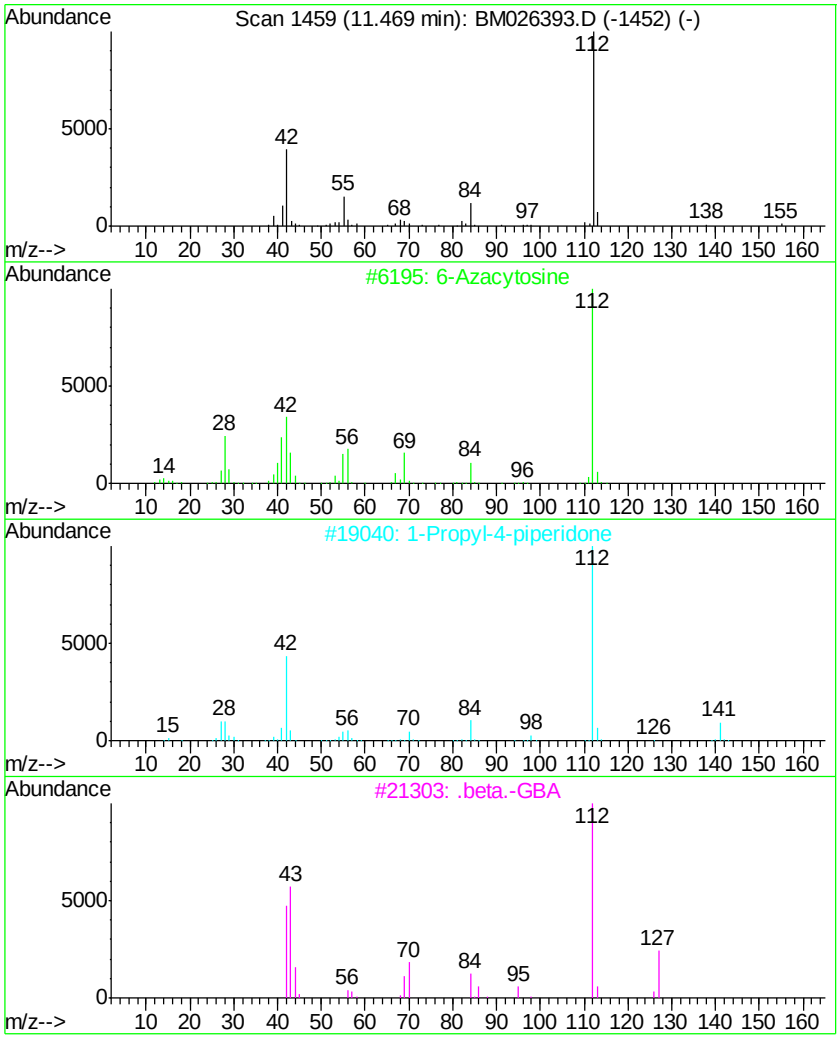
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

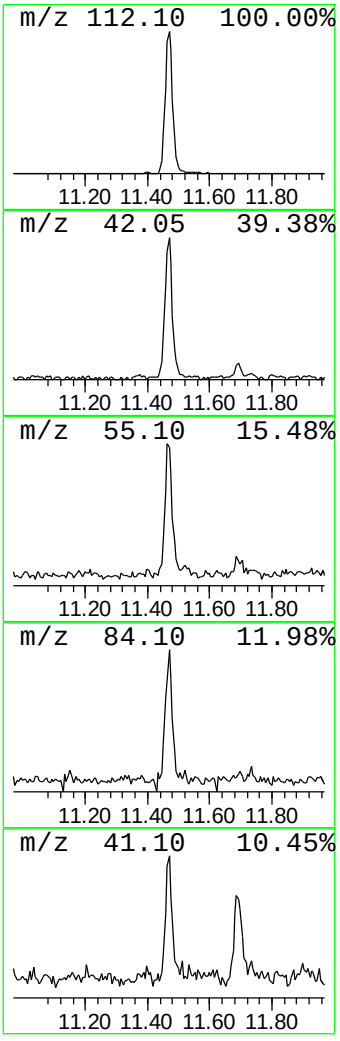
****

Peak Number 4 6-Azacytosine Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.47	2.52 ng	109018	Naphthalene-d8	10.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Azacytosine	112	C3H4N4O	000931-85-1	86
2	1-Propyl-4-piperidone	141	C8H15NO	023133-37-1	43
3	.beta.-GBA	145	C5H11N3O2	000352-83-0	43
4	2-(Hexamethyleneimino)ethanol	143	C8H17NO	020603-00-3	43
5	5-Chloro-3-[.alpha.-hydroxy-.bet...	309	C16H20ClNOS	1000251-01-5	33





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026393.D
Acq On : 15 Jun 2020 16:08
Operator : JU/CG
Sample : L3005-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF001MW002-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

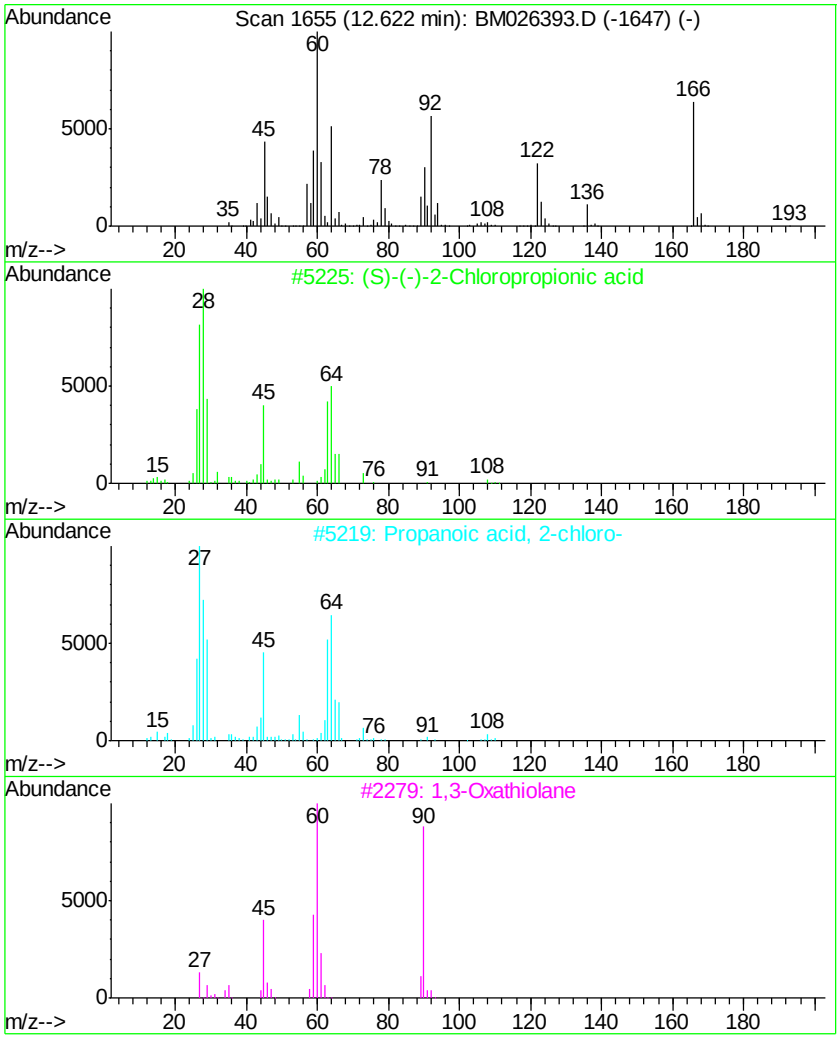
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

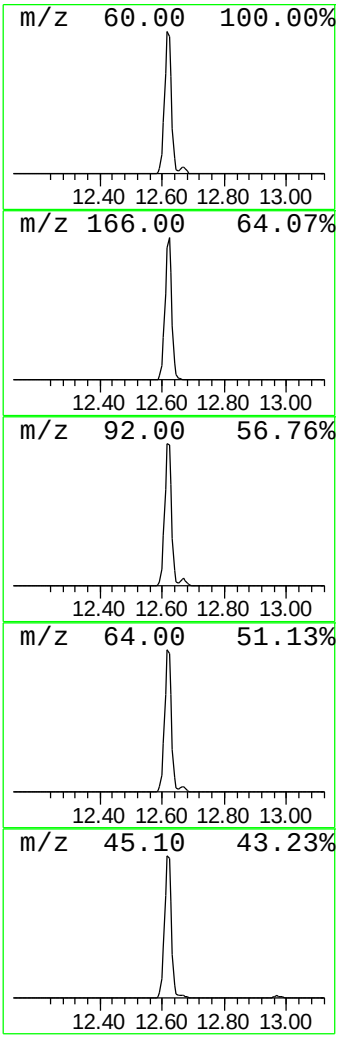
****

Peak Number 5 unknown12.62 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.62	30.82 ng	1772610	Acenaphthene-d10	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(-)-2-Chloropropionic acid	108	C3H5ClO2	029617-66-1	38
2	Propanoic acid, 2-chloro-	108	C3H5ClO2	000598-78-7	27
3	1,3-Oxathiolane	90	C3H6OS	002094-97-5	27
4	3,5-Dimethyl-[1,2]dithiolane 1,1...	166	C5H10O2S2	1000185-07-5	16
5	1,3-Oxathiolane, 2,2-dimethyl-	118	C5H10OS	005684-31-1	14





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026393.D
Acq On : 15 Jun 2020 16:08
Operator : JU/CG
Sample : L3005-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF001MW002-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

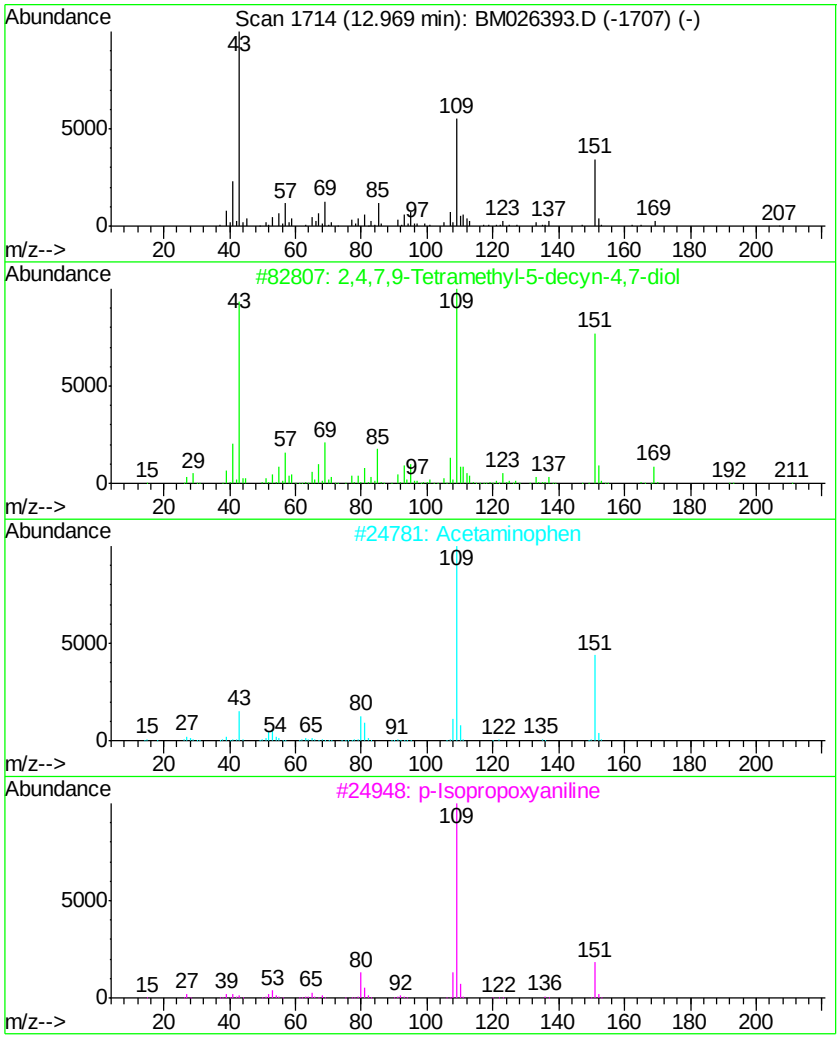
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

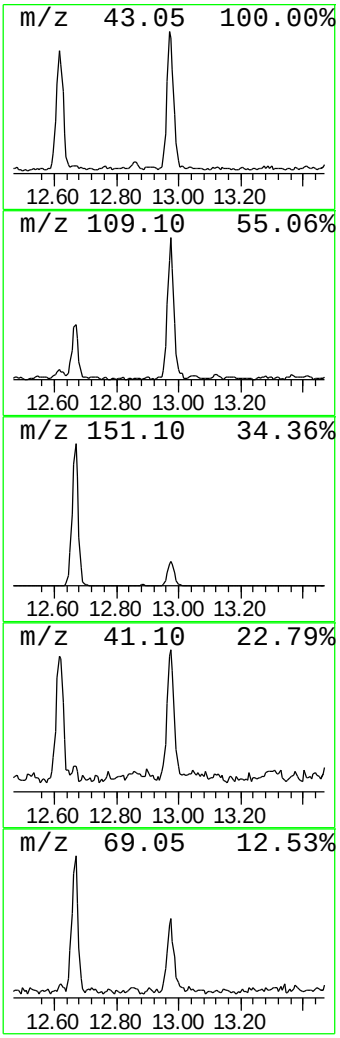
****

Peak Number 6 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.97	2.92 ng	167878	Acenaphthene-d10	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	Acetaminophen	151	C8H9NO2	000103-90-2	53
3	p-Isopropoxyaniline	151	C9H13NO	007664-66-6	53
4	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53
5	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026393.D
Acq On : 15 Jun 2020 16:08
Operator : JU/CG
Sample : L3005-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF001MW002-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

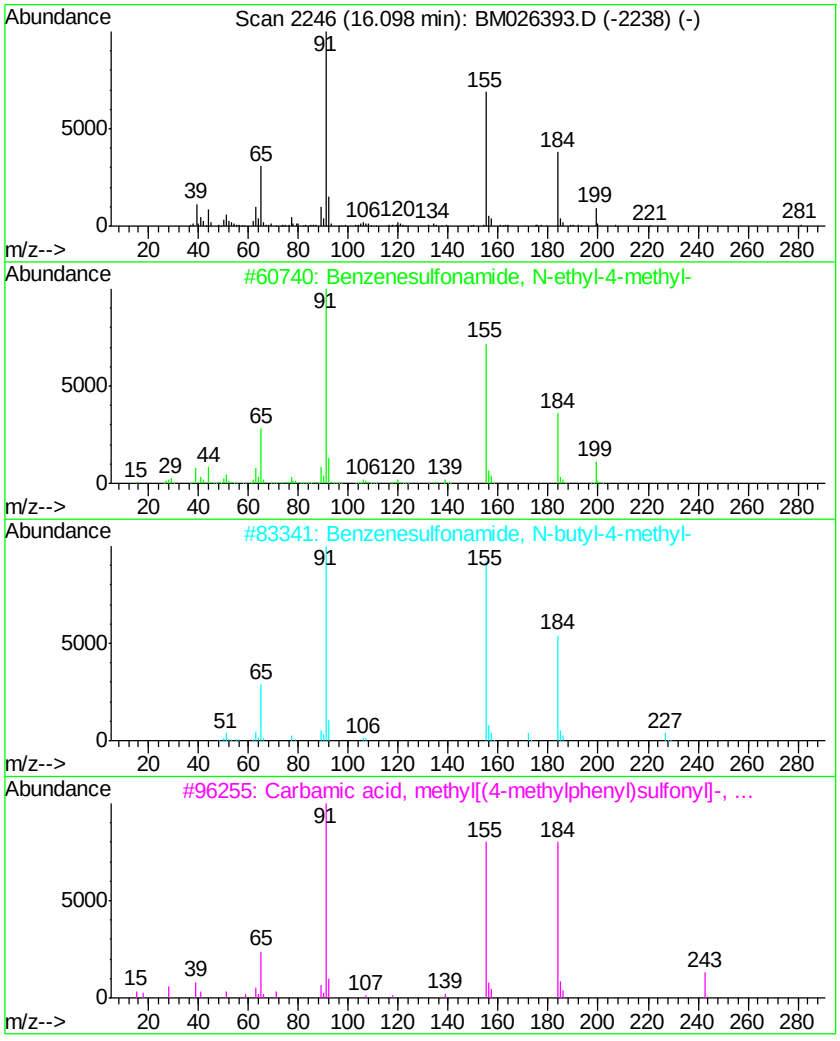
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

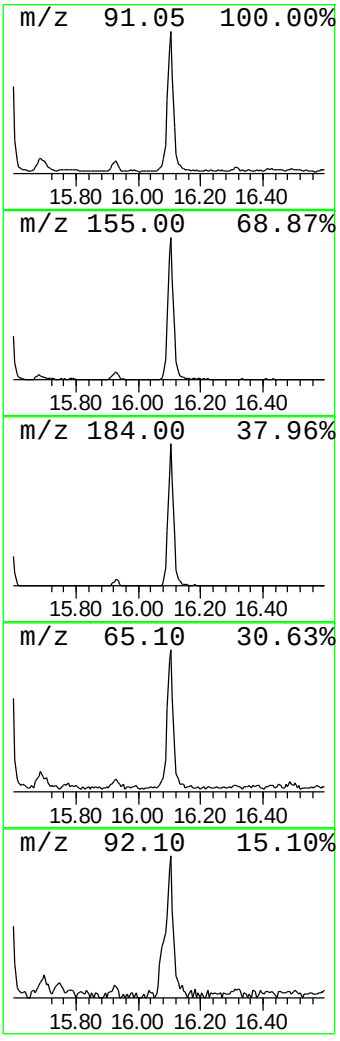
****

Peak Number 7 Benzenesulfonamide, N-ethyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	4.28 ng	295845	Phenanthrene-d10	16.81

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	86
3	Carbamic acid, methyl[(4-methylp...	243	C10H13NO4S	032258-50-7	78
4	4-Methyl-N-[2-(3-nitro-[1,2,4]tr...	311	C11H13N5O4S	1000301-03-5	78
5	Glycine, N-[(4-methylphenyl)sulf...	229	C9H11NO4S	001080-44-0	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026393.D
Acq On : 15 Jun 2020 16:08
Operator : JU/CG
Sample : L3005-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF001MW002-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

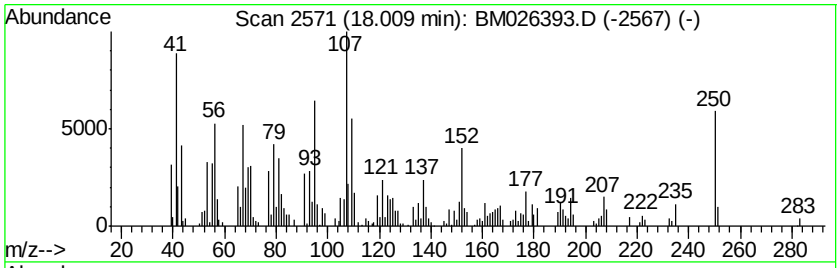
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

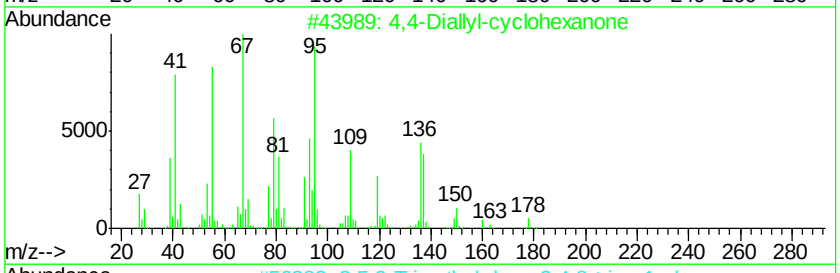
****

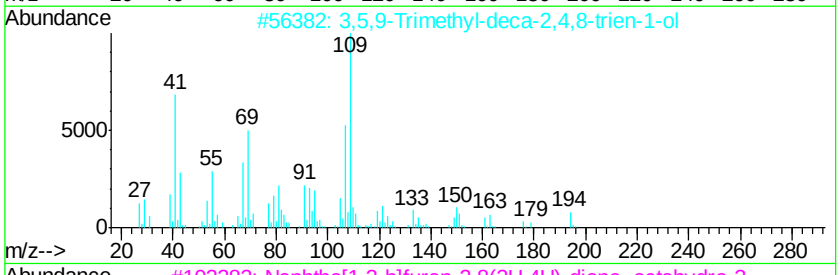
Peak Number 8 unknown18.01 Concentration Rank 11

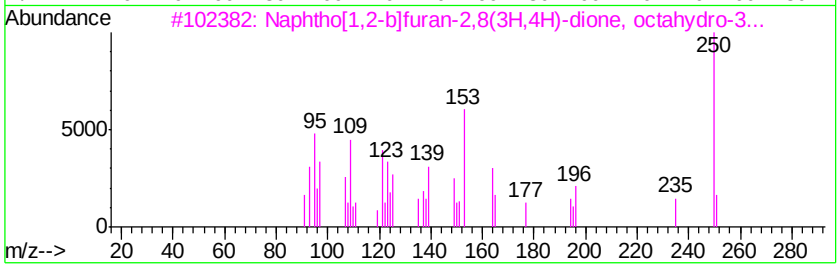
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.01	2.23 ng	153886	Phenanthrene-d10	16.81

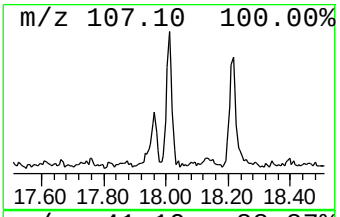
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4-Diallyl-cyclohexanone	178	C12H18O	1000186-50-2	45
2	3,5,9-Trimethyl-deca-2,4,8-trien...	194	C13H22O	1000188-00-3	38
3	Naphtho[1,2-b]furan-2,8(3H,4H)-d...	250	C15H22O3	013902-54-0	30
4	Diisopropylaminoacrylonitryl	152	C9H16N2	038691-28-0	30
5	3-Heptyne, 7-iodo-2,2-dimethyl-	250	C9H15I	055402-07-8	30

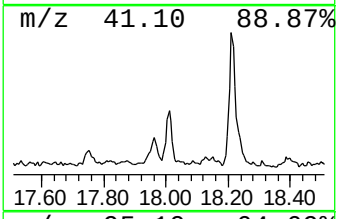


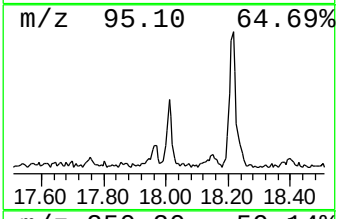


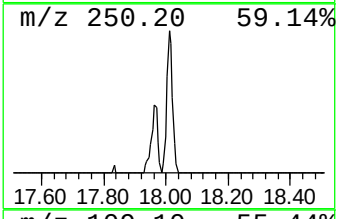


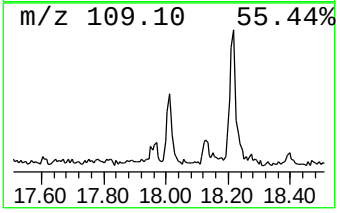












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026393.D
Acq On : 15 Jun 2020 16:08
Operator : JU/CG
Sample : L3005-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF001MW002-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

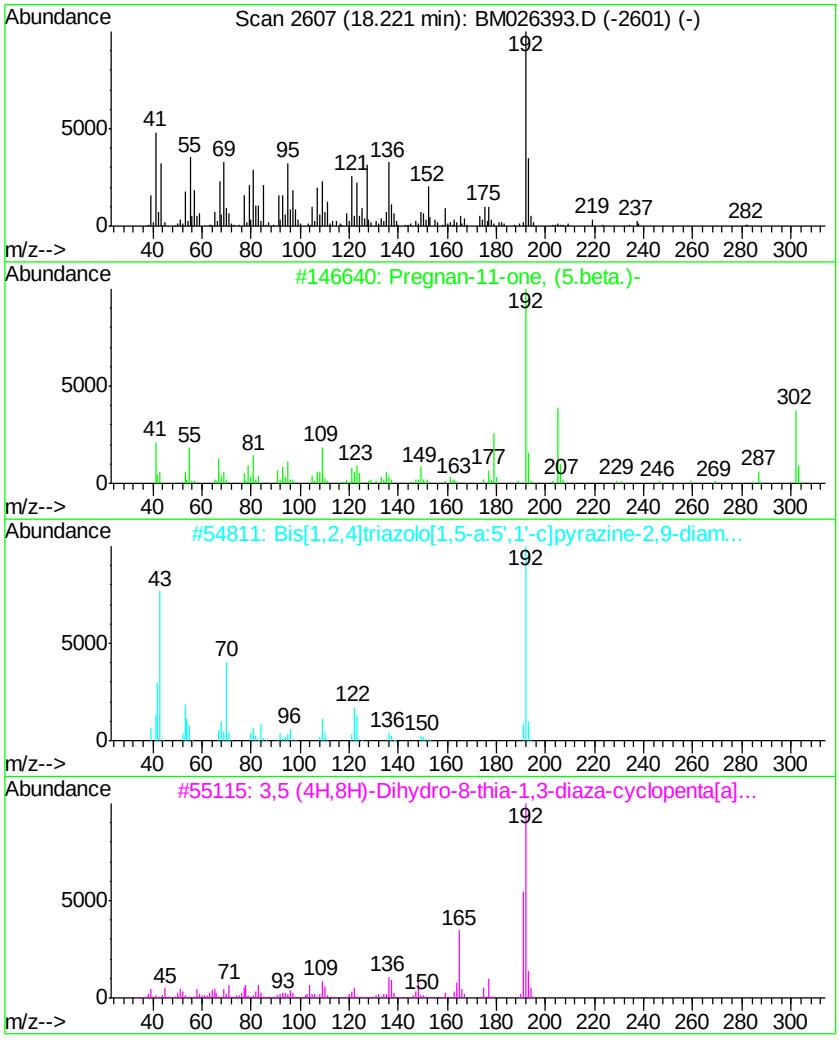
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

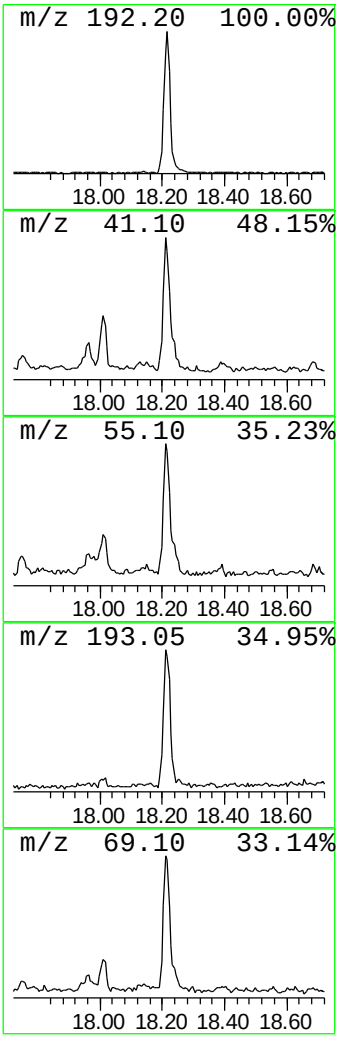
****

Peak Number 9 unknown18.22 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.22	7.69 ng	531413	Phenanthrene-d10	16.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pregnan-11-one, (5.beta.)-	302	C21H34O	026729-46-4	35
2	Bis[1,2,4]triazolo[1,5-a:5',1'-c...	192	C6H8N8	339174-08-2	35
3	3,5 (4H,8H)-Dihydro-8-thia-1,3-d...	192	C9H8N2OS	014346-25-9	30
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	27
5	5,6-Dimethoxy-1-indanone	192	C11H12O3	002107-69-9	27





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026393.D
Acq On : 15 Jun 2020 16:08
Operator : JU/CG
Sample : L3005-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF001MW002-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

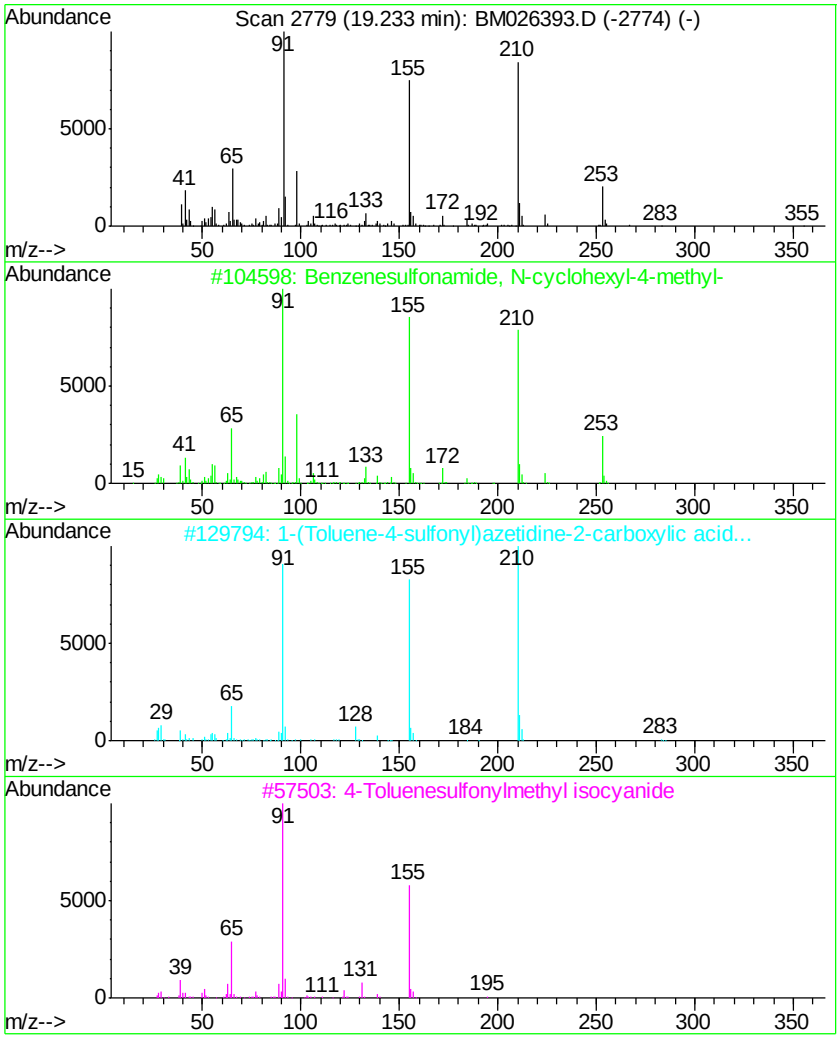
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

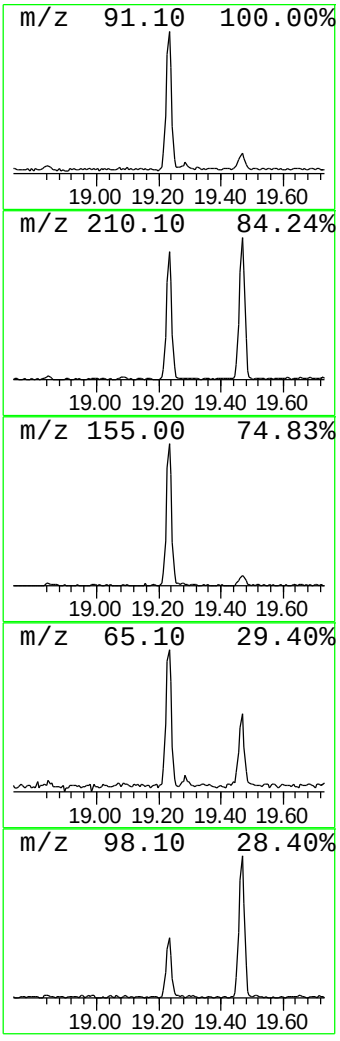
****

Peak Number 10 Benzenesulfonamide, N-cyclo... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.23	2.61 ng	195833	Chrysene-d12	21.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N-cyclohexyl...	253	C13H19NO2S	000080-30-8	98
2	1-(Toluene-4-sulfonyl)azetidine-...	283	C13H17NO4S	1000185-95-4	59
3	4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	38
4	Benzenamine, 4-imidazo[1,2-a]pyr...	210	C12H10N4	1000337-86-0	35
5	4-Amino-5-(3,5-dimethyl-1H-pyraz...	210	C7H10N6S	067130-52-3	30





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026393.D
Acq On : 15 Jun 2020 16:08
Operator : JU/CG
Sample : L3005-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF001MW002-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

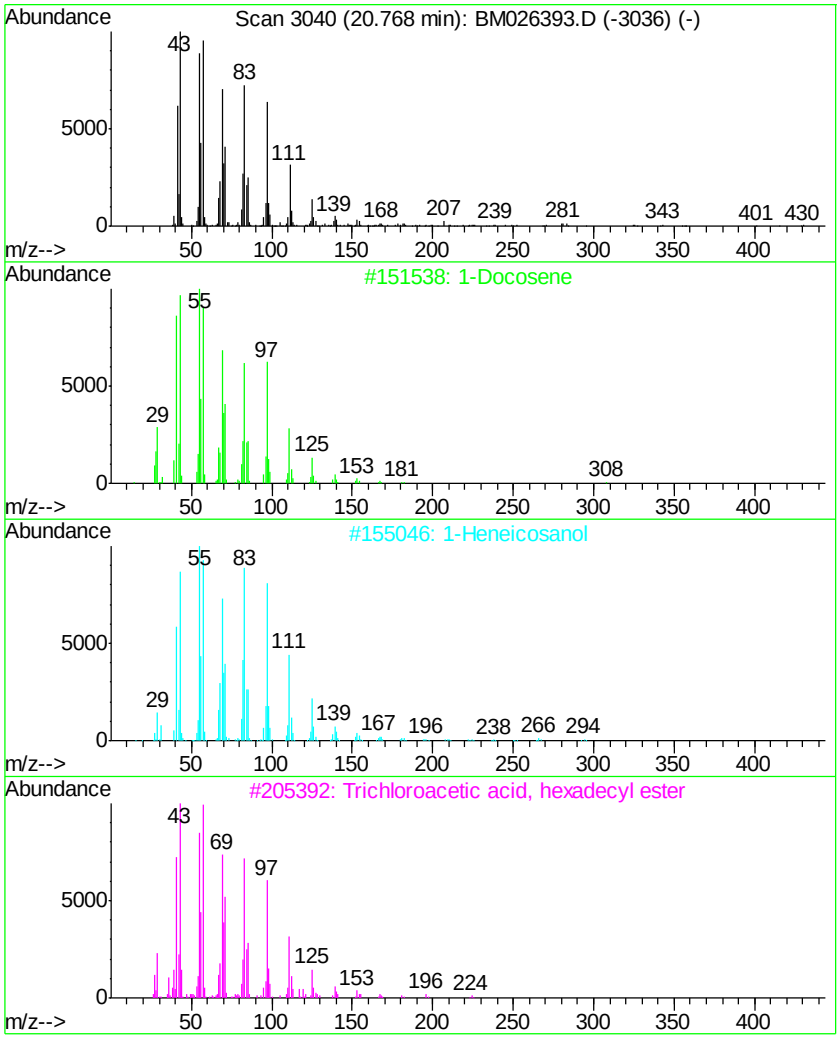
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

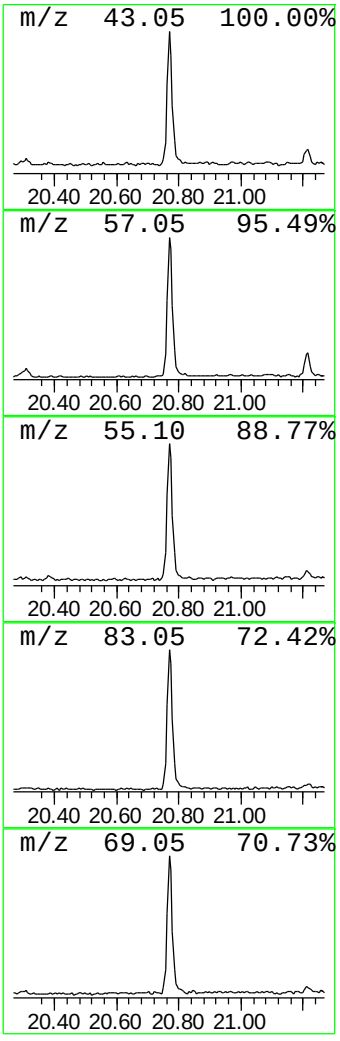
****

Peak Number 11 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.77	6.82 ng	512725	Chrysene-d12	21.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	94
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4	Cyclotetracosane	336	C24H48	000297-03-0	94
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM061520\
Data File : BM026393.D
Acq On : 15 Jun 2020 16:08
Operator : JU/CG
Sample : L3005-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF001MW002-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1,3-Oxathiolane	4.11	41.9	ng	1337240	1	7.40	638886	20.0
6-Azacytosine	11.47	2.5	ng	109018	2	10.16	865870	20.0
unknown12.62	12.62	30.8	ng	1772610	3	14.06	1150250	20.0
2,4,7,9-Tetrameth...	12.97	2.9	ng	167878	3	14.06	1150250	20.0
Benzenesulfonamid...	16.10	4.3	ng	295845	4	16.81	1382920	20.0
unknown18.01	18.01	2.2	ng	153886	4	16.81	1382920	20.0
unknown18.22	18.22	7.7	ng	531413	4	16.81	1382920	20.0
Benzenesulfonamid...	19.23	2.6	ng	195833	5	21.02	1502520	20.0
1-Docosene	20.77	6.8	ng	512725	5	21.02	1502520	20.0