LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082418\
Data File : BM016596.D
Acq On : 24 Aug 2018 19:51
Operator : SJ/JU
Sample : J4617-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
N48969

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-BM082118.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	5.551	379	385	404	rBV	601143	1150656	5.41%	1.537%
2	7.187	657	663	680	rBV	347417	729981	3.43%	0.975%
3	7.534	716	722	740	rBV	1701330	2908566	13.68%	3.885%
4	8.004	795	802	813	rBV	509627	904809	4.26%	1.208%
5	8.322	849	856	871	rBV	2128552	3462736	16.29%	4.625%
6	9.192	997	1004	1021	rBV	1158541	2107464	9.91%	2.815%
7	10.810	1273	1279	1294	rBV	591593	1123292	5.28%	1.500%
8	13.263	1690	1696	1703	rBV	5778984	8126569	38.23%	10.854%
9	13.969	1811	1816	1820	rBV	464058	682220	3.21%	0.911%
10	14.027	1824	1826	1832	rVB2	245107	327051	1.54%	0.437%
11	14.110	1835	1840	1843	rBV	608245	869607	4.09%	1.161%
12	14.145	1843	1846	1851	rVB5	177926	278246	1.31%	0.372%
13	14.439	1892	1896	1901	rVB	334298	449057	2.11%	0.600%
14	14.580	1915	1920	1922	rBV4	179047	298370	1.40%	0.399%
15	14.645	1926	1931	1937	rVB2	2458812	3437758	16.17%	4.591%
16	15.398	2055	2059	2064	rBV3	641725	1010104	4.75%	1.349%
17	16.145	2180	2186	2200	rBV	7685586	11191753	52.64%	14.948%
18	17.392	2394	2398	2403	rVB	2367490	3256950	15.32%	4.350%
19	18.256	2543	2545	2554	rVB5	1172545	1729101	8.13%	2.309%
20	19.980	2833	2838	2847	rVB	18124442	21259610	100.00%	28.394%
21	21.215	3045	3048	3054	rVB2	502000	644654	3.03%	0.861%
22	21.533	3098	3102	3111	rVB	3590449	4612410	21.70%	6.160%
23	23.815	3484	3490	3500	rVB	2233348	4311597	20.28%	5.759%

Sum of corrected areas: 74872561

LSC Report - Integrated Chromatogram

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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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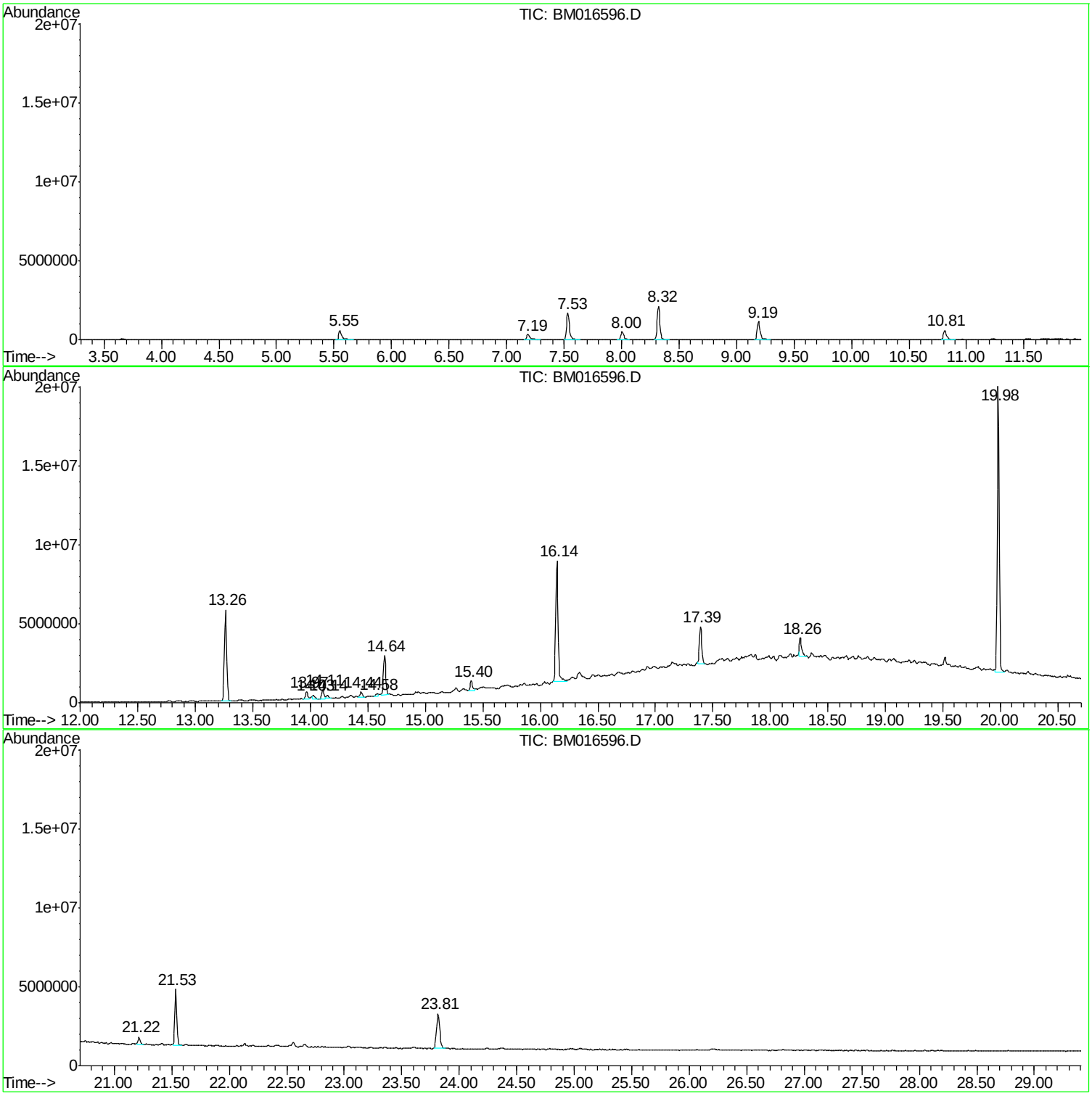
ClientSampleId :
N48969

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082118.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

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Operator : SJ/JU
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Misc :
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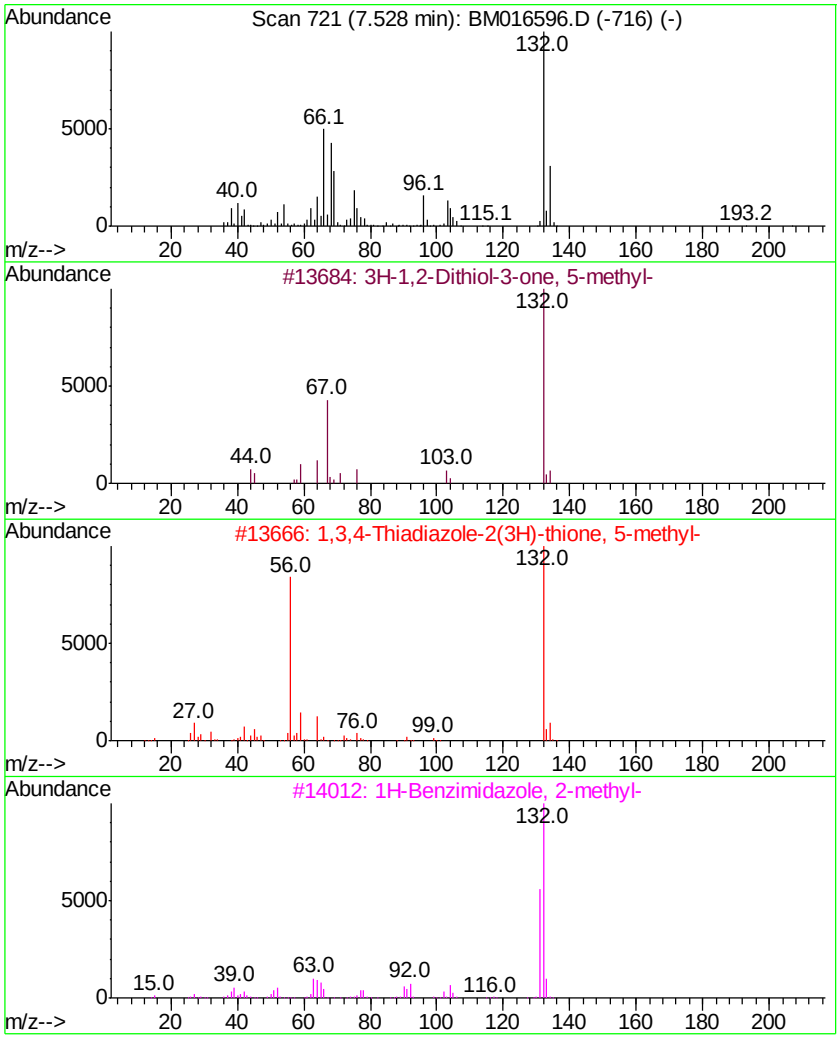
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

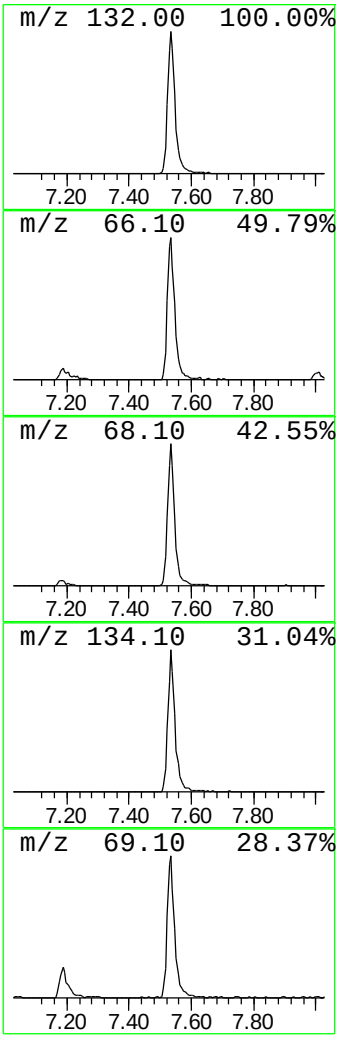
****

Peak Number 1 unknown7.53 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.53	64.29 ng	2908570	1,4-Dichlorobenzene-d4	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	22
2	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1H-Tetrazaborole, 5-chloro-4,5-d...	132	C2H6BClN4	021960-49-6	10





Library Search Compound Report

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BNA_M
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082118.M
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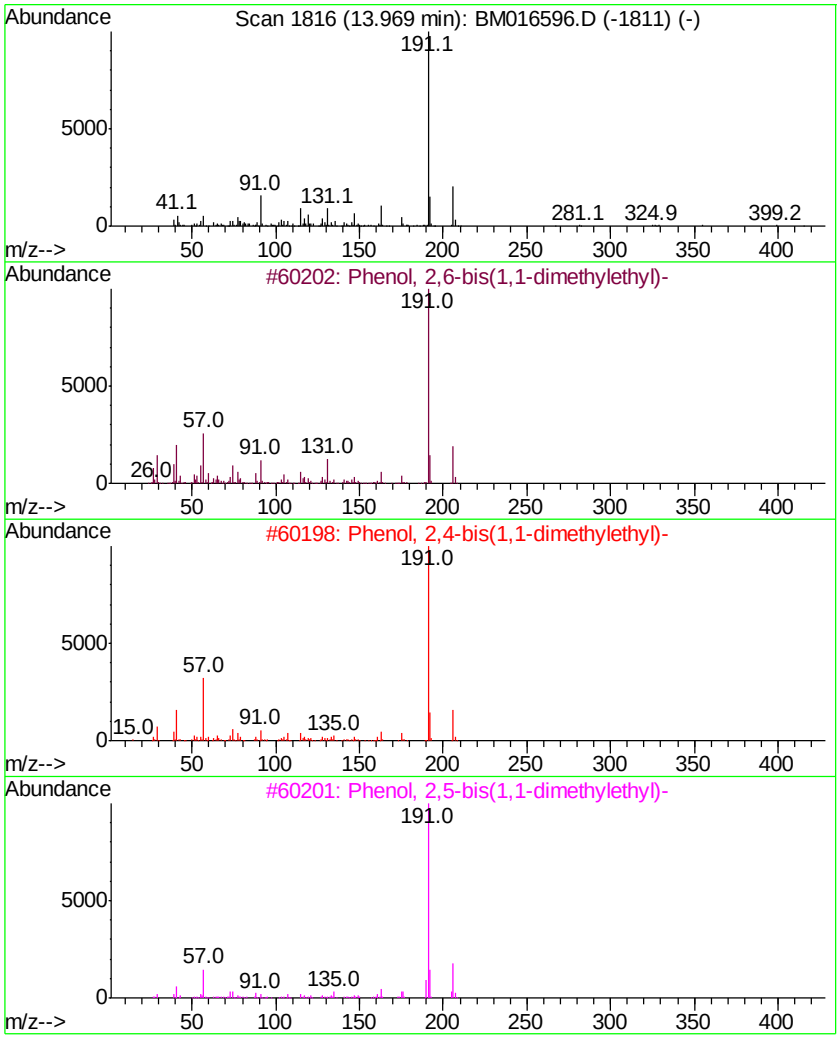
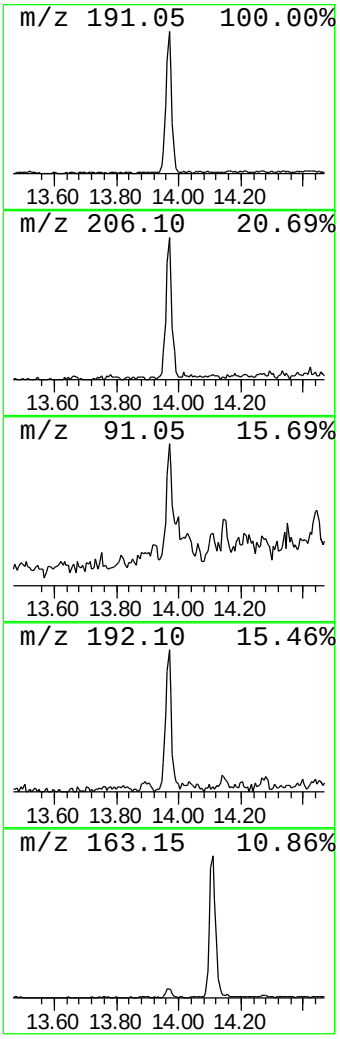
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	3.97 ng	682220	Acenaphthene-d10	14.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	91
2	Phenol, 2,4-bis(1,1-dimethylethyl)-	206	C14H22O	000096-76-4	87
3	Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	72
4	Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	72
5	Phenanthrene, 9-ethyl-	206	C16H14	003674-75-7	53





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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
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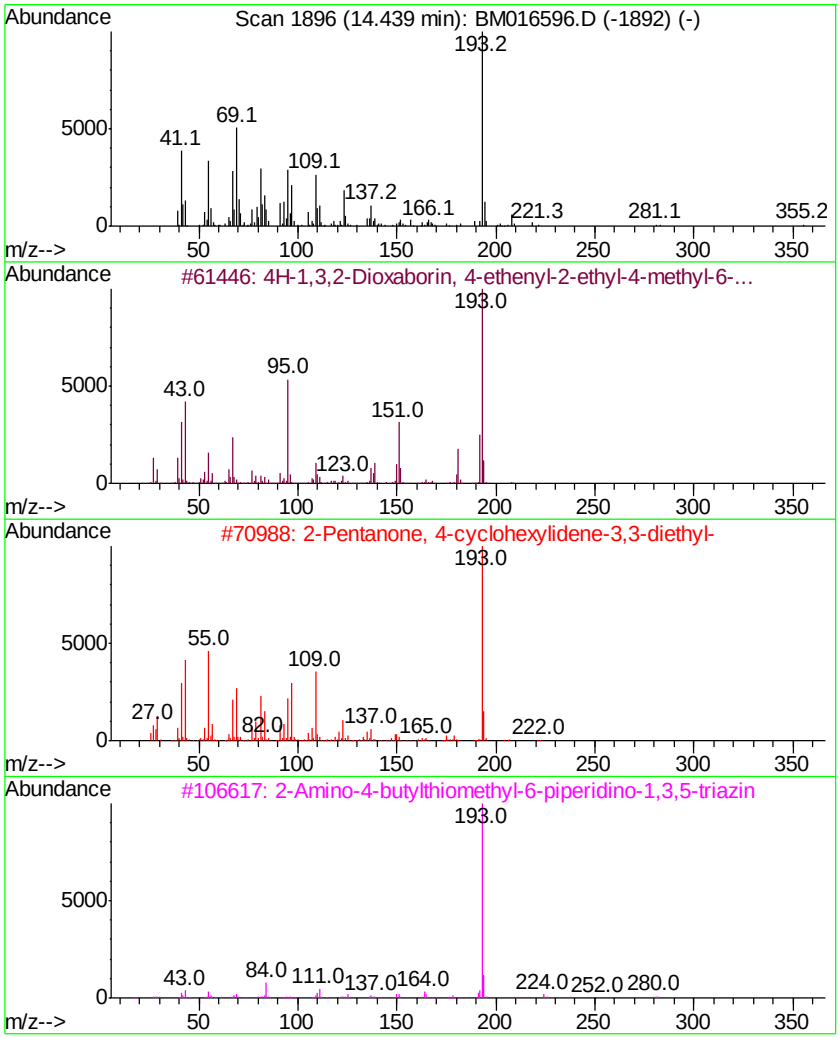
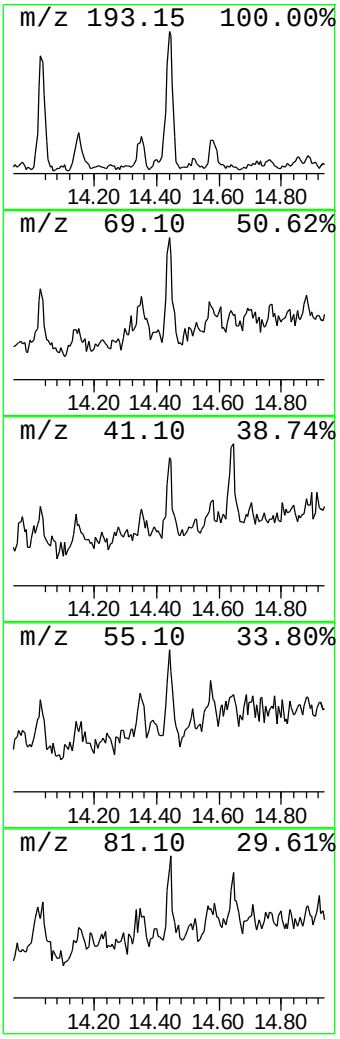
****

Peak Number 4 4H-1,3,2-Dioxaborin, 4-ethe... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.44	2.61 ng	449057	Acenaphthene-d10	14.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-1,3,2-Dioxaborin, 4-ethenyl-2...	208	C12H21BO2	074630-04-9	50
2	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	45
3	2-Amino-4-butylthiomethyl-6-pipe...	281	C13H23N5S	022362-21-6	38
4	6-Methylphenanthridine	193	C14H11N	003955-65-5	35
5	2-Amino-4-benzylthiomethyl-6-pip...	315	C16H21N5S	022362-19-2	35





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TIC Library : C:\DATABASE\NIST02.L
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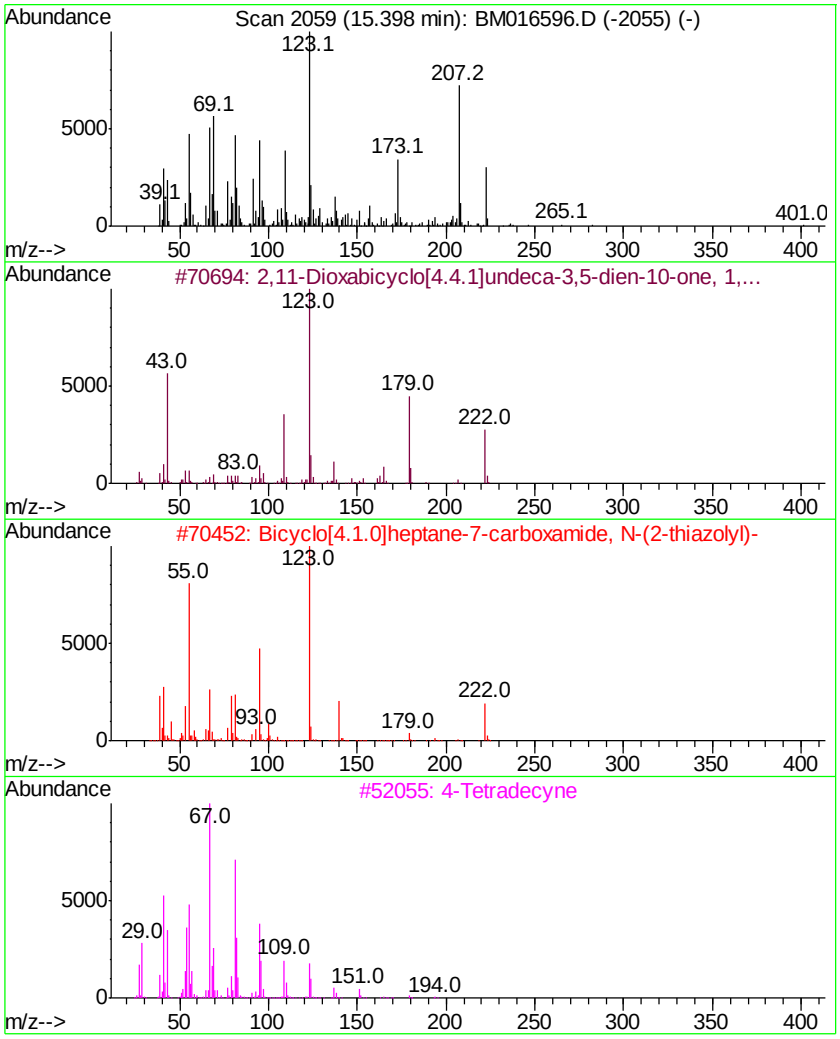
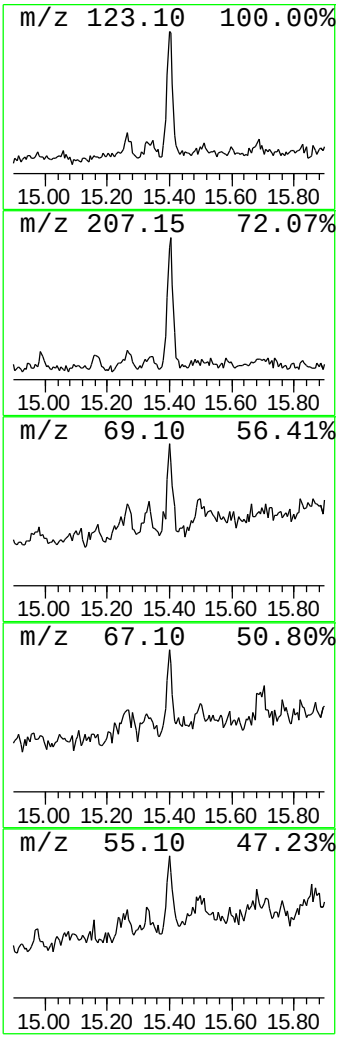
Peak Number 5 unknown15.40 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.40	5.88 ng	1010100	Acenaphthene-d10	14.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,11-Dioxabicyclo[4.4.1]undeca-3...	222	C13H18O3	070412-52-1	45
2	Bicyclo[4.1.0]heptane-7-carboxam...	222	C11H14N2OS	329912-72-3	38
3	4-Tetradecyne	194	C14H26	060212-33-1	35
4	2-Cyclopenten-1-one, 3,4,5,5-tet...	138	C9H14O	090611-02-2	35
5	Benzoyl chloride, 3-fluoro-	158	C7H4ClFO	001711-07-5	30





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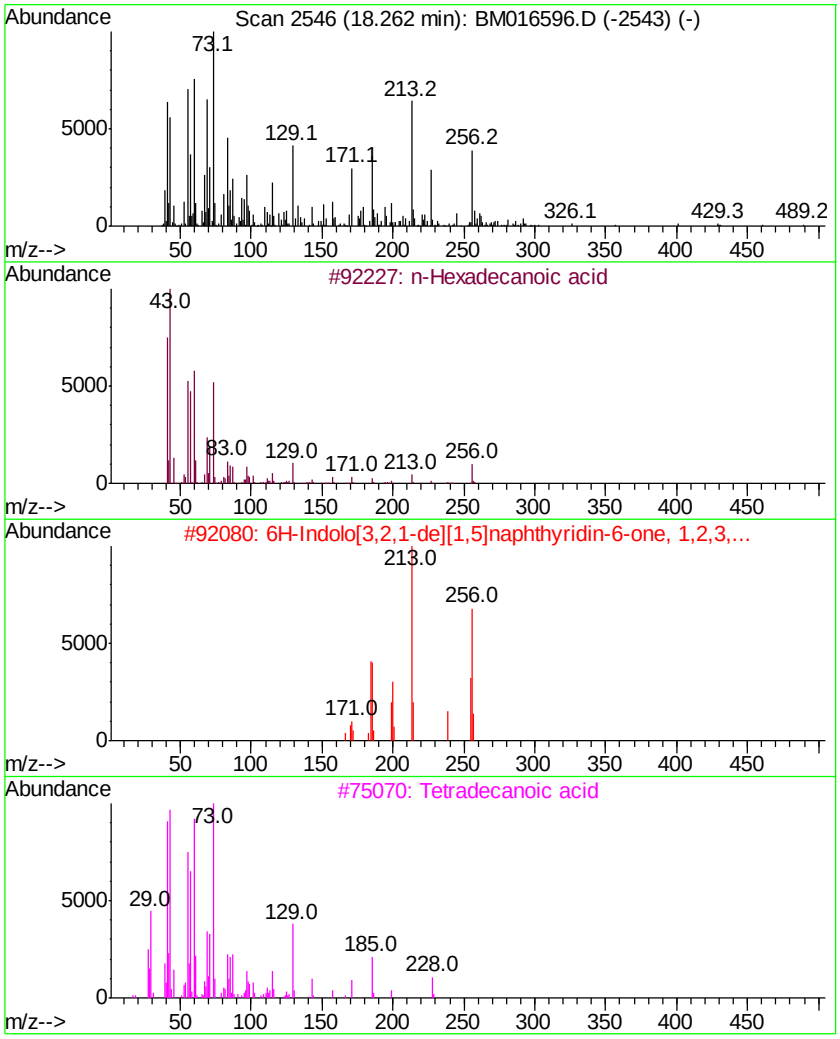
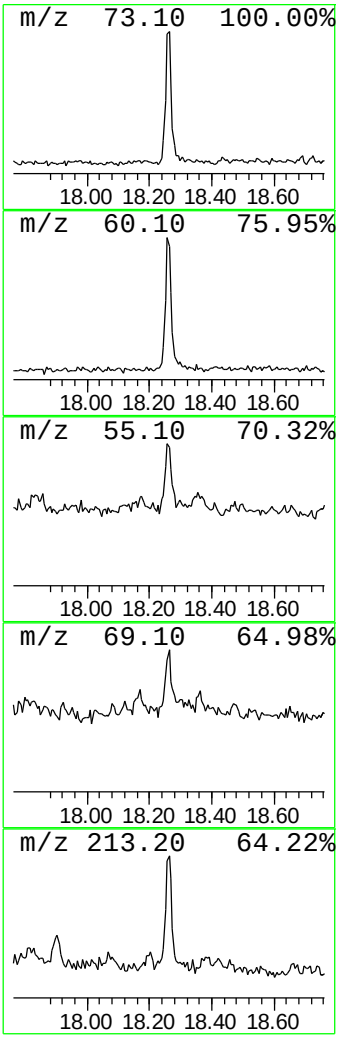
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.26	10.62 ng	1729100	Phenanthrene-d10	17.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	6H-Indolo[3,2,1-de][1,5]naphthyr...	256	C15H16N2O2	050630-67-6	52
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
4	9-Bromononanoic acid	236	C9H17BrO2	041059-02-3	47
5	Tridecanoic acid	214	C13H26O2	000638-53-9	43





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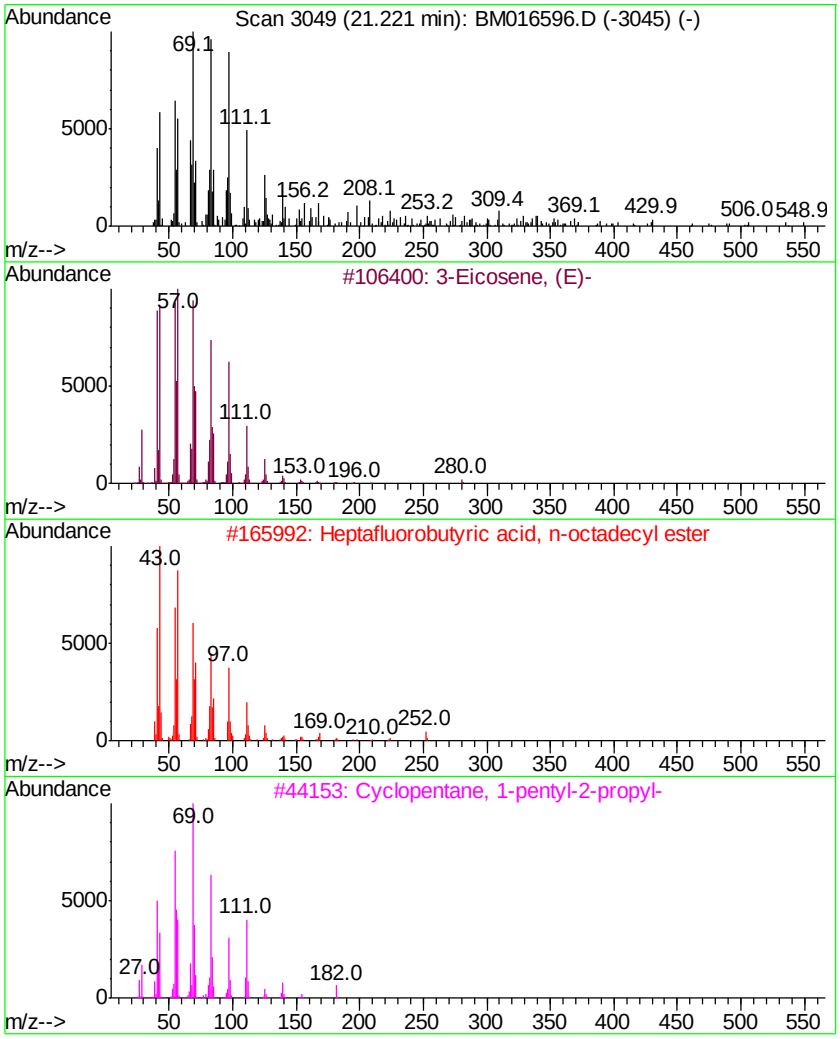
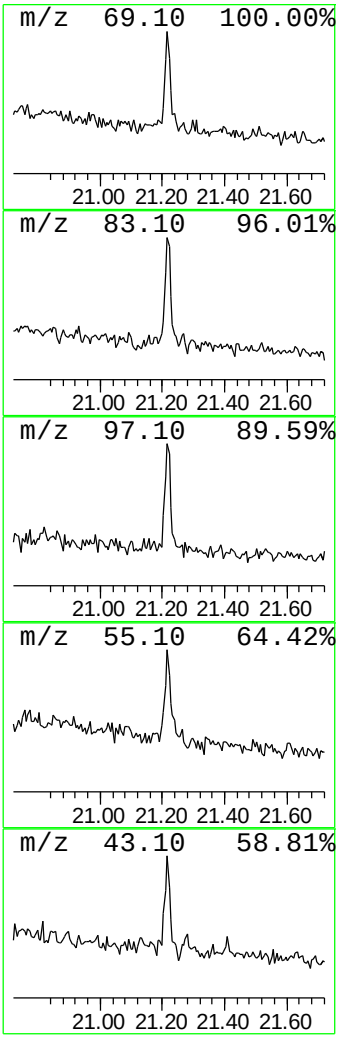
****

Peak Number 7 3-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.22	2.80 ng	644654	Chrysene-d12	21.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	89
2	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	72
3	Cyclopentane, 1-pentyl-2-propyl-	182	C13H26	062199-51-3	58
4	Cyclohexane, (1-butylhexadecyl)-	364	C26H52	004443-59-8	56
5	9-Tricosene, (Z)-	322	C23H46	027519-02-4	55





Tentatively Identified Compound (LSC) summary

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
unknown7.53	7.53	64.3	ng	2908570	1	8.00	904809	20.0
Phenol, 2,6-bis(1...	13.97	4.0	ng	682220	3	14.65	3437760	20.0
4H-1,3,2-Dioxabor...	14.44	2.6	ng	449057	3	14.65	3437760	20.0
unknown15.40	15.40	5.9	ng	1010100	3	14.65	3437760	20.0
n-Hexadecanoic acid	18.26	10.6	ng	1729100	4	17.39	3256950	20.0
3-Eicosene, (E)-	21.22	2.8	ng	644654	5	21.53	4612410	20.0