LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM050719\
Data File : BM020173.D
Acq On : 07 May 2019 20:04
Operator : JU/SJ
Sample : K2697-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-1-20190502

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-BM043019.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	5.369	396	405	414	rBV	1444106	2051004	21.15%	4.533%
2	6.951	665	674	687	rBV	854913	1388094	14.31%	3.068%
3	7.322	730	737	750	rBV	2345050	3742212	38.59%	8.271%
4	7.787	809	816	822	rBV	464128	722075	7.45%	1.596%
5	8.104	862	870	877	rBV	1988190	3208705	33.09%	7.092%
6	8.957	1007	1015	1022	rBV	1693484	2832886	29.21%	6.261%
7	10.580	1283	1291	1298	rBV	550488	910216	9.39%	2.012%
8	13.051	1703	1711	1719	rBV	4049364	5858793	60.42%	12.949%
9	14.292	1916	1922	1935	rVB3	50886	140993	1.45%	0.312%
10	14.433	1939	1946	1952	rVV2	786353	1205932	12.44%	2.665%
11	14.498	1952	1957	1964	rVB	176412	278162	2.87%	0.615%
12	15.921	2193	2199	2212	rBV	3444973	5147761	53.09%	11.377%
13	16.157	2233	2239	2244	rBV6	115180	280653	2.89%	0.620%
14	16.310	2261	2265	2269	rVB2	101433	134881	1.39%	0.298%
15	16.533	2299	2303	2308	rBV	219683	296857	3.06%	0.656%
16	16.621	2313	2318	2324	rBV8	65111	144088	1.49%	0.318%
17	16.704	2329	2332	2337	rVB4	106392	146514	1.51%	0.324%
18	16.809	2346	2350	2357	rVB	191120	258453	2.67%	0.571%
19	17.015	2380	2385	2393	rVB	308101	436303	4.50%	0.964%
20	17.180	2408	2413	2418	rBV2	1016325	1411713	14.56%	3.120%
21	17.309	2432	2435	2444	rVB	142775	222952	2.30%	0.493%
22	17.704	2500	2502	2511	rVB6	55557	137757	1.42%	0.304%
23	17.804	2516	2519	2527	rVB5	66621	112495	1.16%	0.249%
24	17.945	2537	2543	2547	rBV7	90647	184786	1.91%	0.408%
25	18.062	2559	2563	2572	rVB	266649	391213	4.03%	0.865%
26	19.339	2777	2780	2787	rVB3	177034	236580	2.44%	0.523%
27	19.803	2853	2859	2865	rBV	7979189	9697133	100.00%	21.432%
28	21.362	3119	3124	3130	rBV	1369230	1775234	18.31%	3.924%
29	23.650	3507	3513	3520	rVB	965784	1890782	19.50%	4.179%

Sum of corrected areas: 45245227

LSC Report - Integrated Chromatogram

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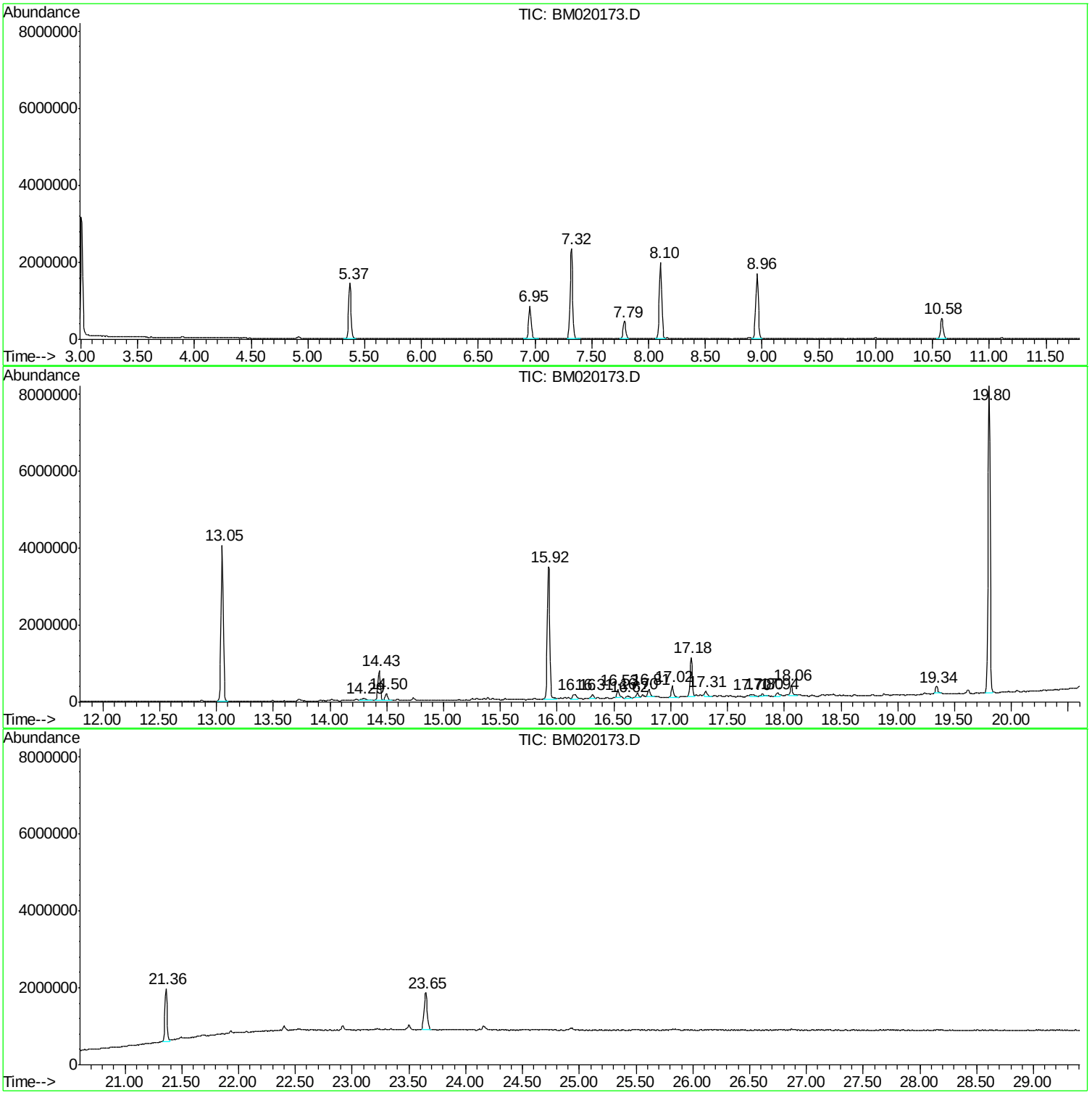
Operator : JU/SJ
Sample : K2697-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-1-20190502

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.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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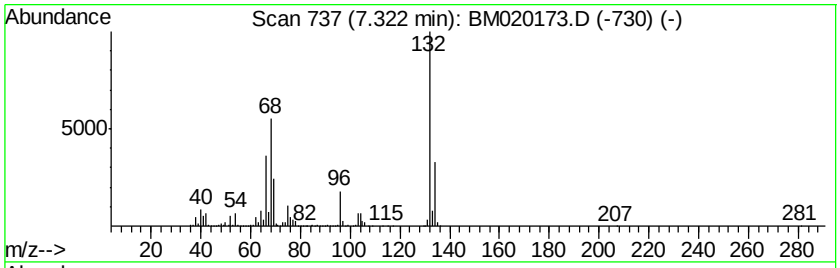
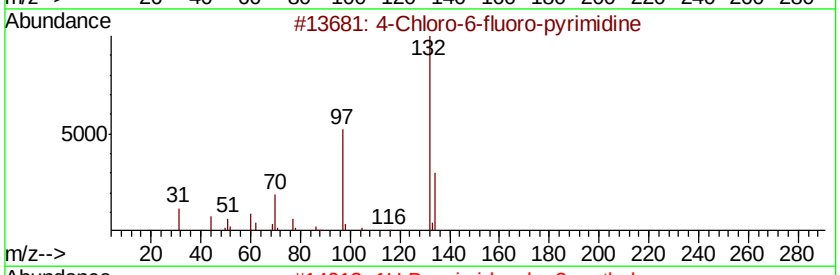
****

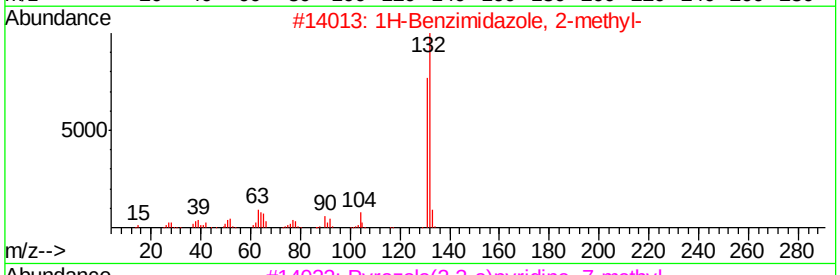
Peak Number 1 unknown7.32 Concentration Rank 1

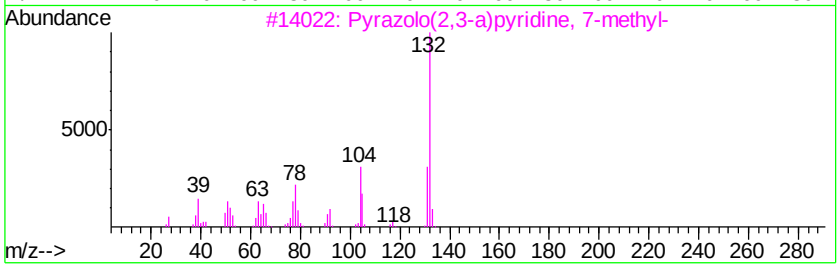
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.32	103.65 ng	3742210	1,4-Dichlorobenzene-d4	7.79

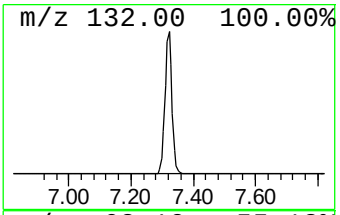
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22
4	5-Aminoindole	132	C8H8N2	005192-03-0	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12

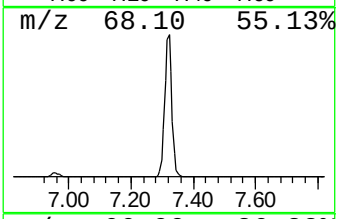


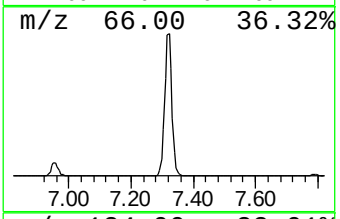


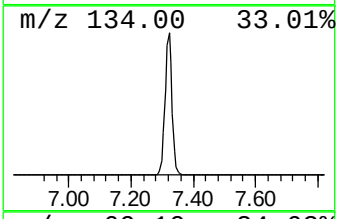


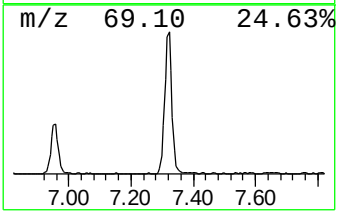












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Instrument : BNA_M
ClientSampleId : MW-1-20190502

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.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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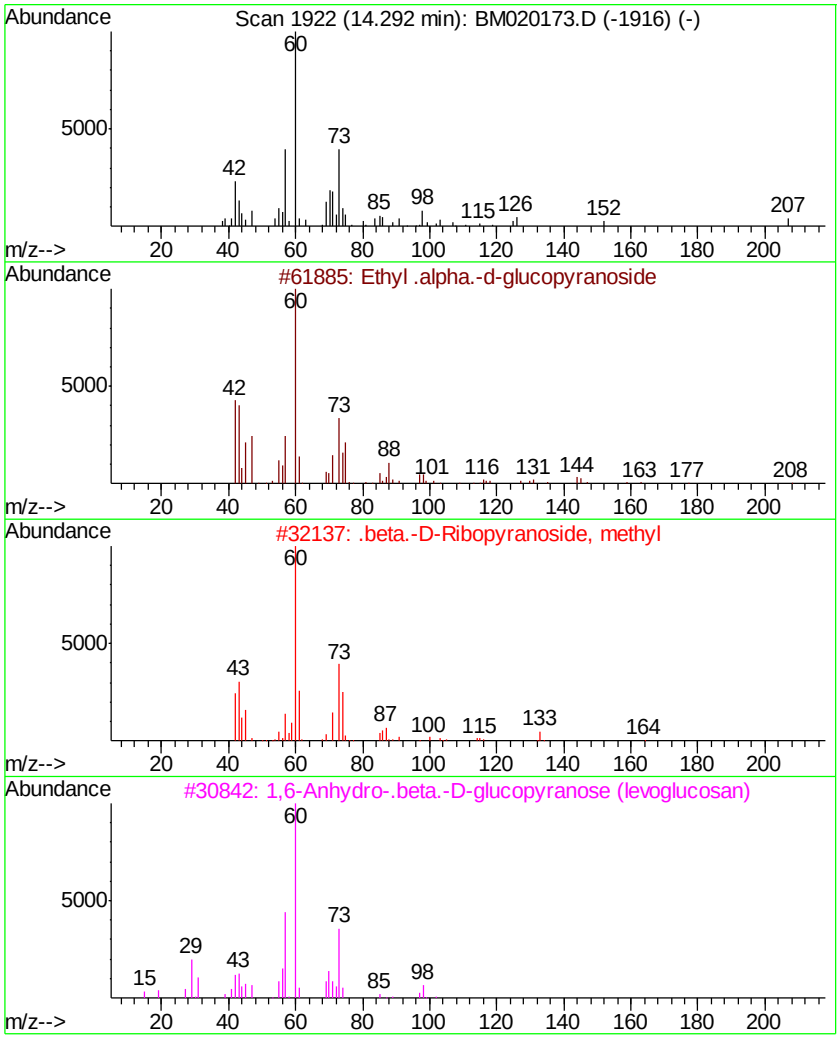
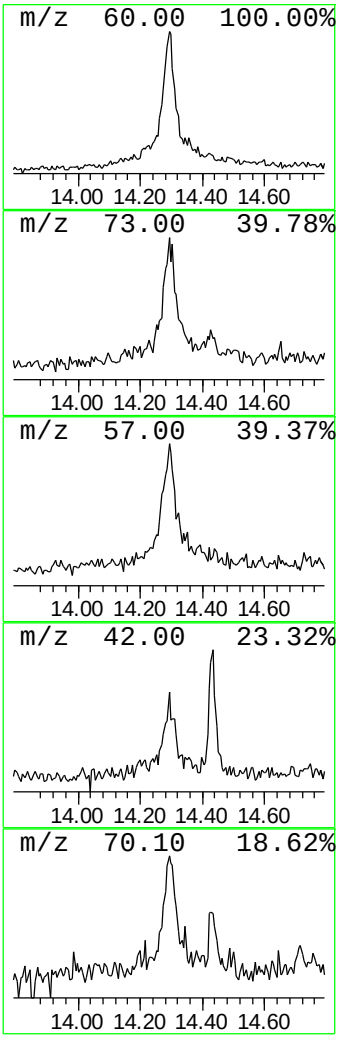
Peak Number 3 Ethyl .alpha.-d-glucopyrano... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.29	2.34 ng	140993	Acenaphthene-d10	14.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl .alpha.-d-glucopyranoside	208	C8H16O6	1000127-29-4	64
2	.beta.-D-Ribopyranoside, methyl	164	C6H12O5	017289-61-1	50
3	1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	45
4	Methyl .beta.-d-galactopyranoside	194	C7H14O6	1000126-04-6	42
5	D-Allose	180	C6H12O6	002595-97-3	38





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Instrument : BNA_M
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
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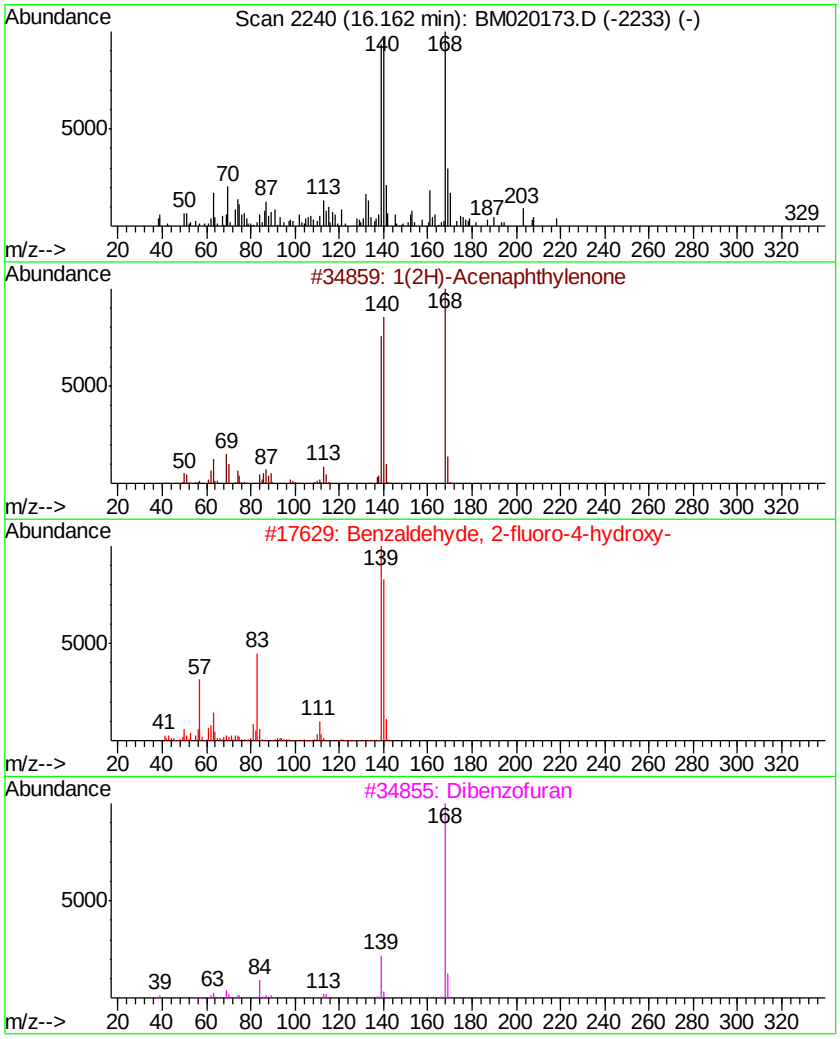
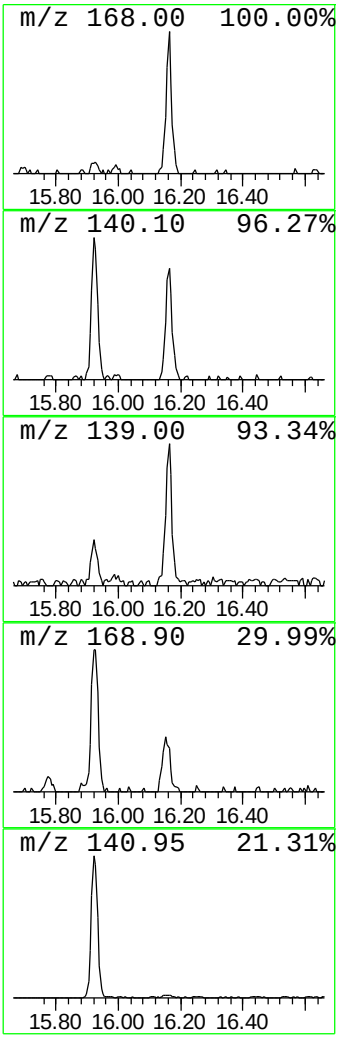
****

Peak Number 4 1(2H)-Acenaphthylenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.16	3.98 ng	280653	Phenanthrene-d10	17.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1(2H)-Acenaphthylenone	168	C12H8O	002235-15-6	76
2	Benzaldehyde, 2-fluoro-4-hydroxy-	140	C7H5FO2	000348-27-6	41
3	Dibenzofuran	168	C12H8O	000132-64-9	38
4	2,5-Thiophenedicarboxaldehyde	140	C6H4O2S	000932-95-6	35
5	Cyclobuta[de]naphthalene	140	C11H8	024973-91-9	35





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Sample : K2697-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-1-20190502

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
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TIC Library : C:\DATABASE\NIST02.L
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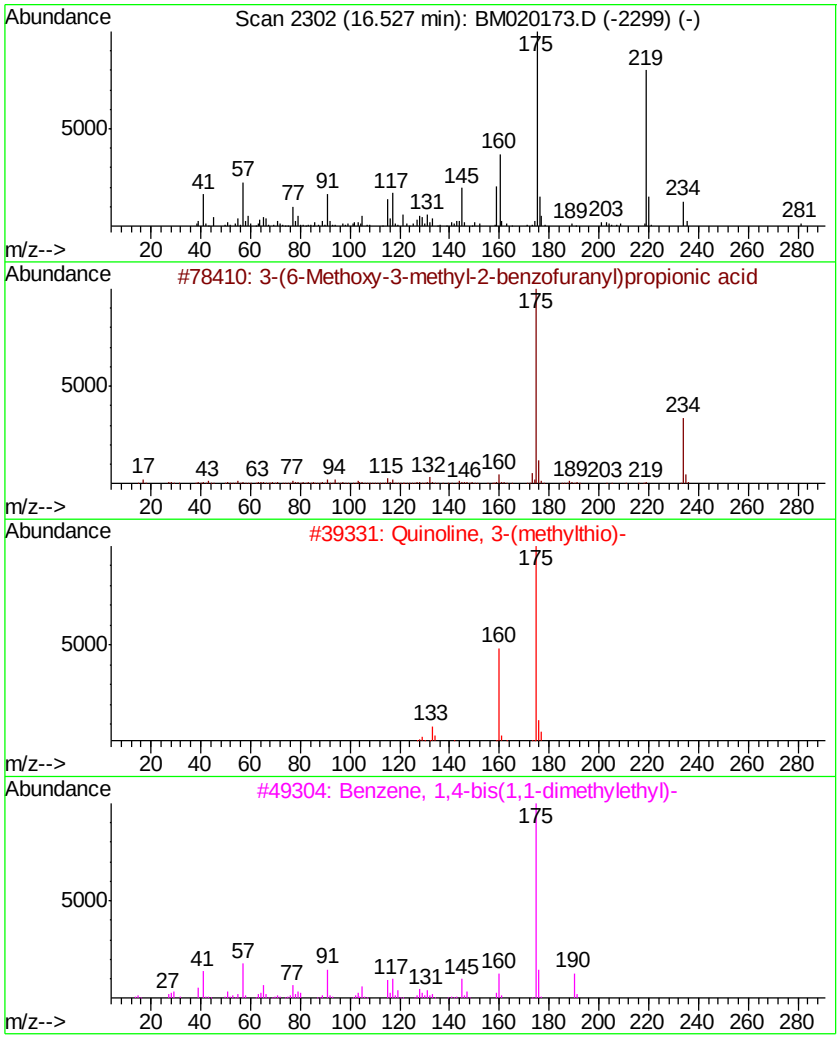
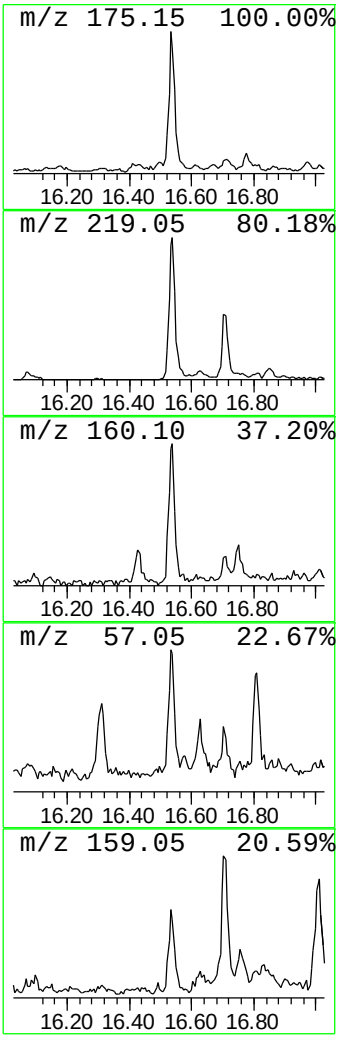
****

Peak Number 5 unknown16.53 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	4.21 ng	296857	Phenanthrene-d10	17.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(6-Methoxy-3-methyl-2-benzofur...	234	C13H14O4	010410-30-7	47
2	Quinoline, 3-(methylthio)-	175	C10H9NS	051934-46-4	46
3	Benzene, 1,4-bis(1,1-dimethyleth...	190	C14H22	001012-72-2	43
4	7-Amino-4-methyl-1,8-naphthyridi...	175	C9H9N3O	001569-15-9	38
5	1H-Indole-2,3-dione, 1-methyl-, ...	175	C9H9N3O	003265-23-4	38





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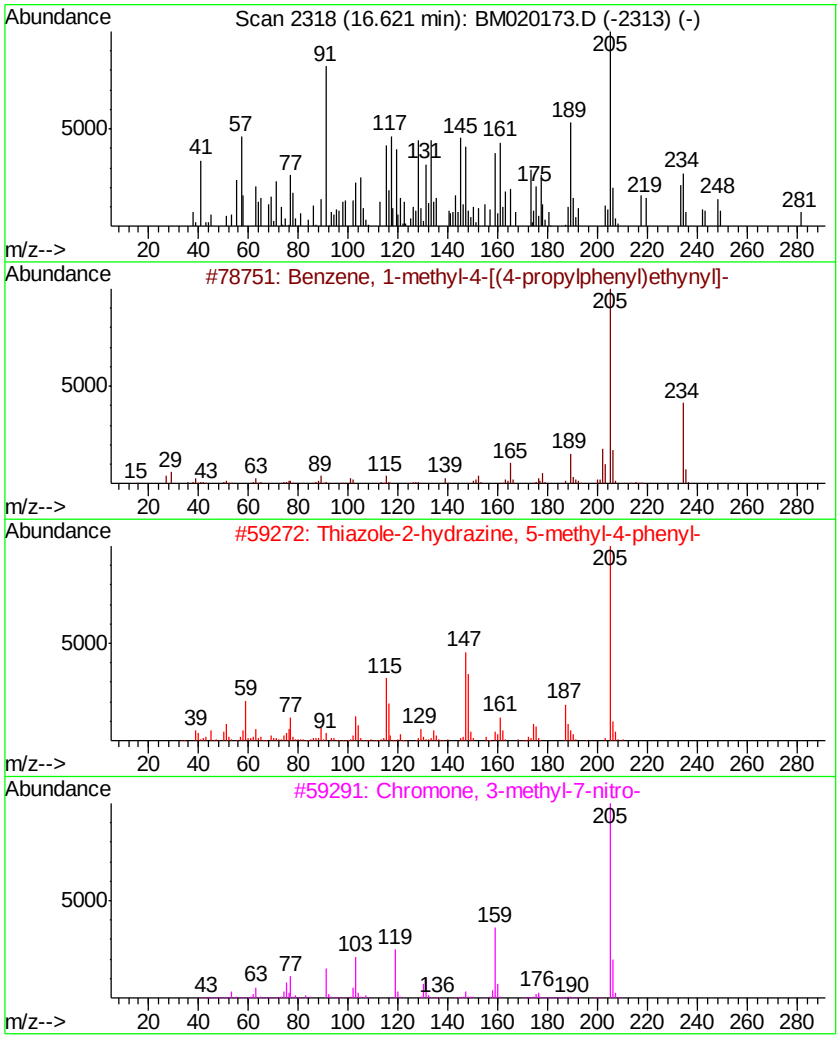
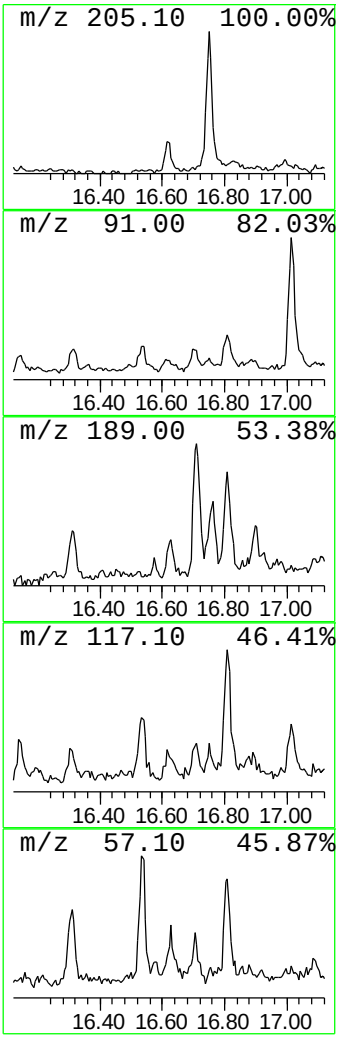
****

Peak Number 6 unknown16.62 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.62	2.04 ng	144088	Phenanthrene-d10	17.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-4-[(4-propylph...	234	C18H18	184161-94-2	38
2	Thiazole-2-hydrazine, 5-methyl-4...	205	C10H11N3S	137506-14-0	25
3	Chromone, 3-methyl-7-nitro-	205	C10H7NO4	253668-57-4	15
4	Tricyclo[5.1.0.0(2,4)]oct-5-ene-...	234	C15H22O2	074793-63-8	12
5	Pyrimidin-4(3H)-one, 2-amino-6-(...	205	C10H8FN3O	098305-63-6	11





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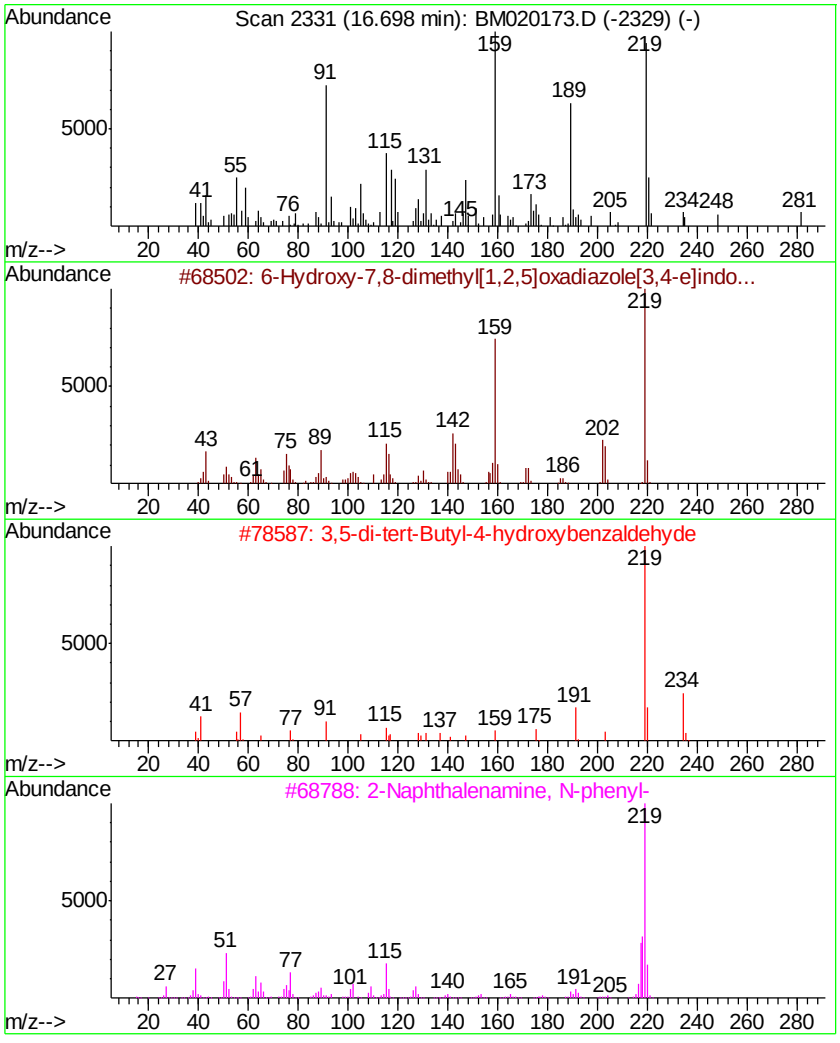
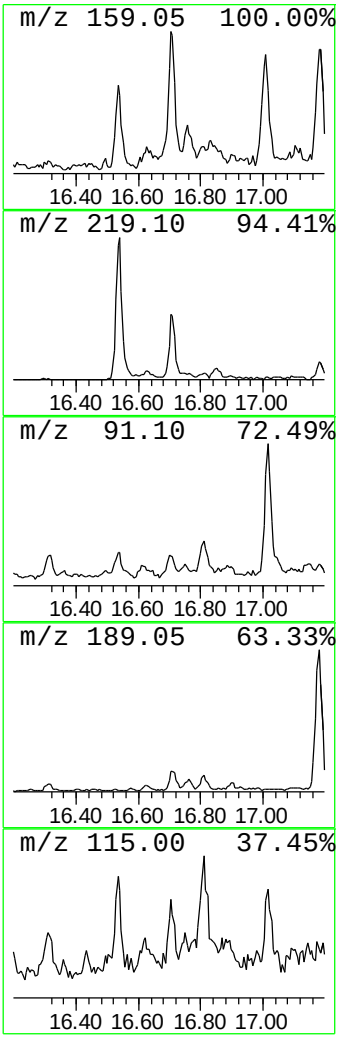
Peak Number 7 unknown16.70 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.70	2.08 ng	146514	Phenanthrene-d10	17.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Hydroxy-7,8-dimethyl[1,2,5]oxa...	219	C10H9N3O3	164356-01-8	47
2	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	41
3	2-Naphthalenamine, N-phenyl-	219	C16H13N	000135-88-6	35
4	2(1H)-Quinolinone, 4-methyl-	159	C10H9NO	000607-66-9	25
5	Pyrido[3,4-d]pyrimidine-2,4(1H,3...	219	C11H13N3O2	022389-81-7	25





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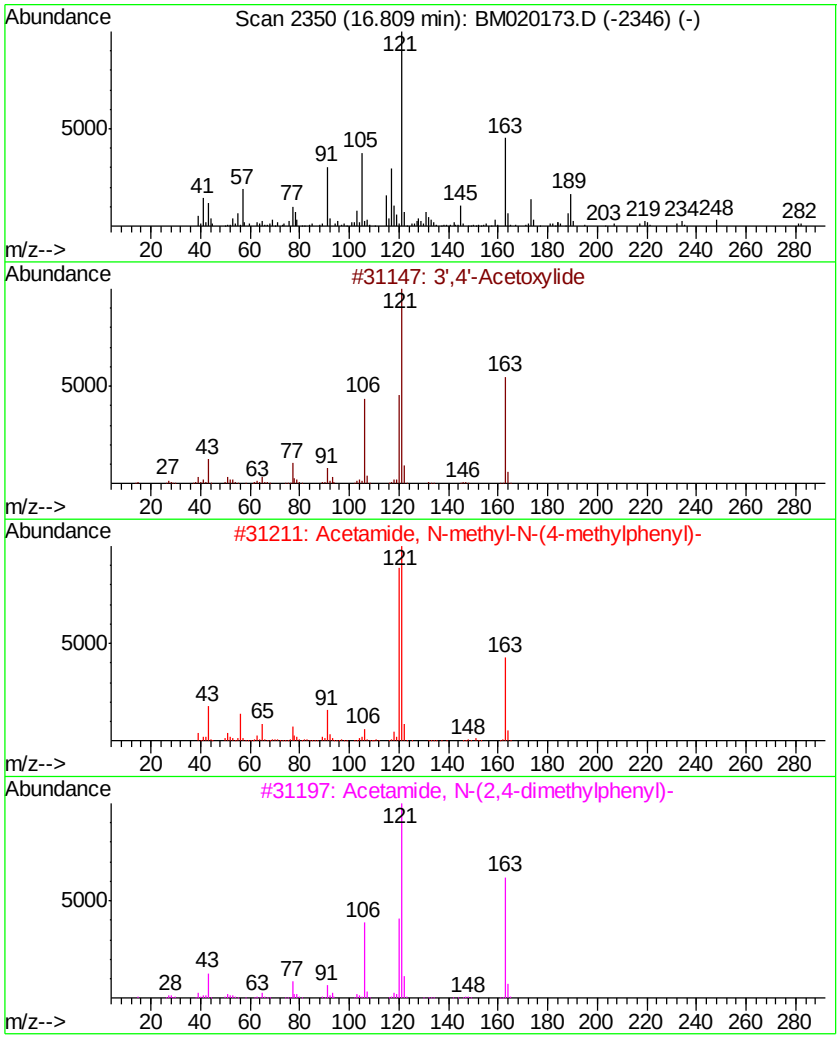
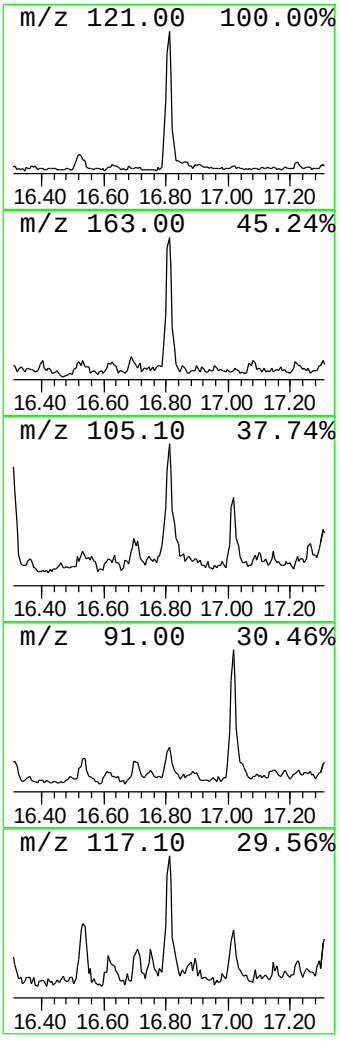
Peak Number 8 unknown16.81 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.81	3.66 ng	258453	Phenanthrene-d10	17.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3',4'-Acetoxylide	163	C10H13NO	002198-54-1	49
2	Acetamide, N-methyl-N-(4-methylp...	163	C10H13NO	000612-03-3	47
3	Acetamide, N-(2,4-dimethylphenyl)-	163	C10H13NO	002050-43-3	46
4	1,2-Bis(p-acetoxyphenyl)ethanedione	326	C18H14O6	093655-79-9	43
5	N'-(4,.gamma.-Dihydroxycinnamyli...	282	C16H14N2O3	1000225-23-0	38





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Misc :
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Instrument : BNA_M
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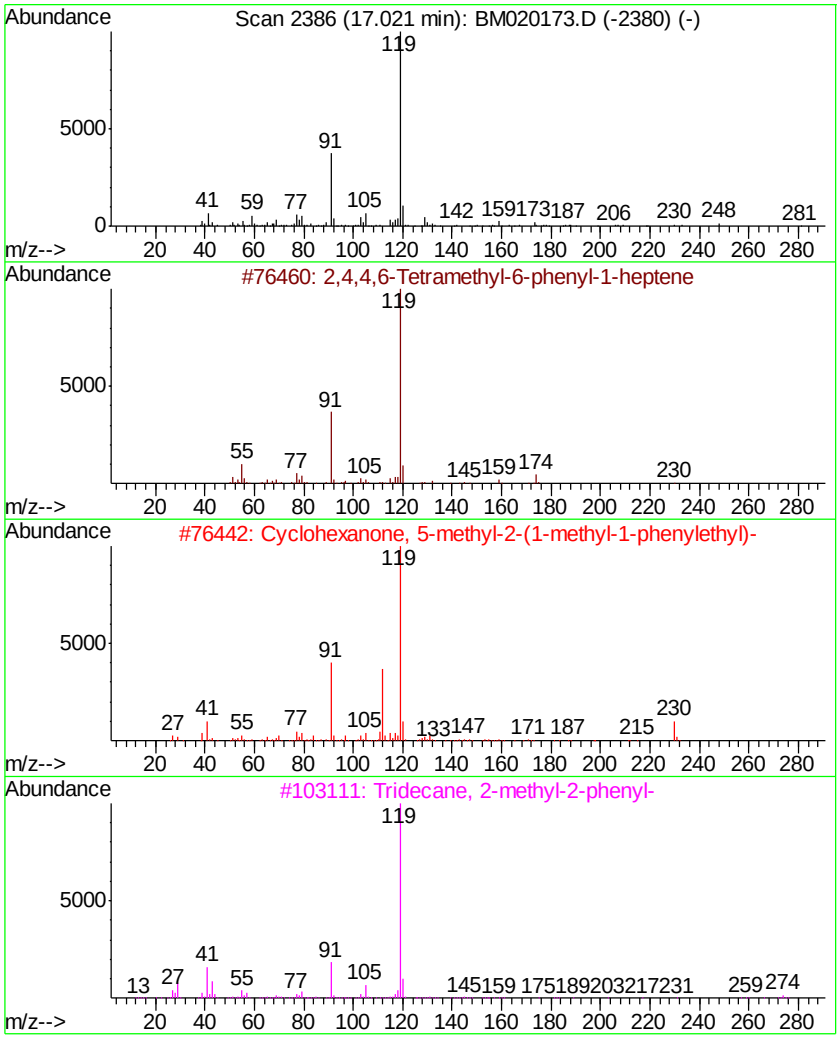
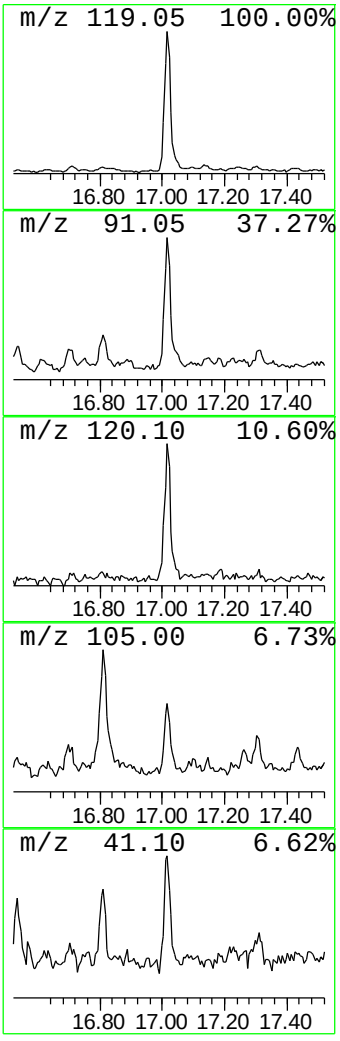
Peak Number 9 2,4,4,6-Tetramethyl-6-pheny... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.02	6.18 ng	436303	Phenanthrene-d10	17.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6-Tetramethyl-6-phenyl-1-h...	230	C17H26	1000293-27-9	72
2	Cyclohexanone, 5-methyl-2-(1-met...	230	C16H22O	097275-48-4	72
3	Tridecane, 2-methyl-2-phenyl-	274	C20H34	027854-41-7	72
4	Benzene, (1,1-dimethylbutyl)-	162	C12H18	001985-57-5	72
5	Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	72





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM050719\
Data File : BM020173.D
Acq On : 07 May 2019 20:04
Operator : JU/SJ
Sample : K2697-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-1-20190502

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

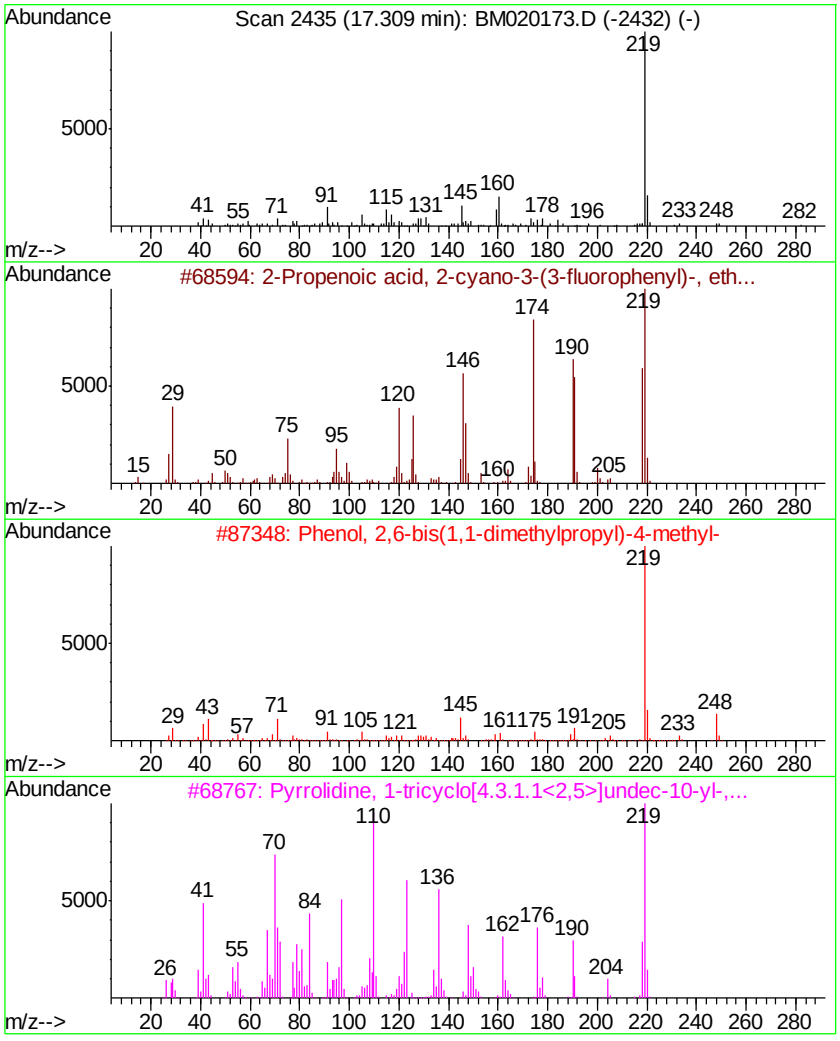
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

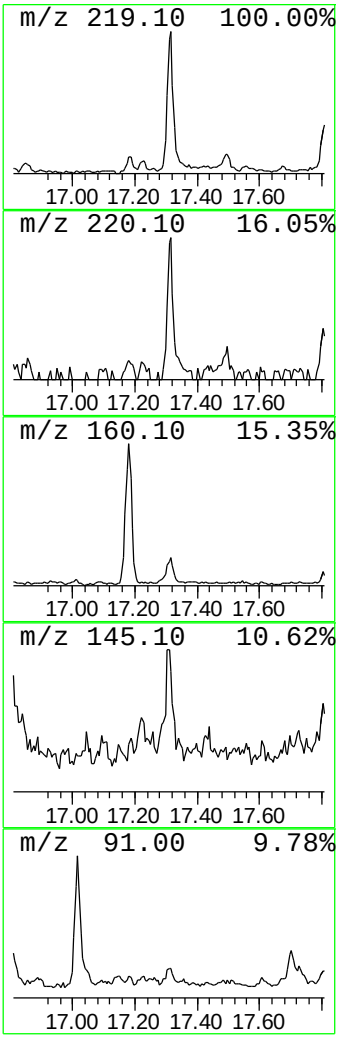
****

Peak Number 10 2-Propenoic acid, 2-cyano-3... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.31	3.16 ng	222952	Phenanthrene-d10	17.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenoic acid, 2-cyano-3-(3-f...	219	C12H10FNO2	019310-52-2	72
2	Phenol, 2,6-bis(1,1-dimethylprop...	248	C17H28O	056103-67-4	64
3	Pyrrolidine, 1-tricyclo[4.3.1.1<...	219	C15H25N	085538-51-8	53
4	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	42
5	5-(4-Ethoxy-phenyl)-5-methyl-imi...	234	C12H14N2O3	1000297-64-8	42





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Data File : BM020173.D
Acq On : 07 May 2019 20:04
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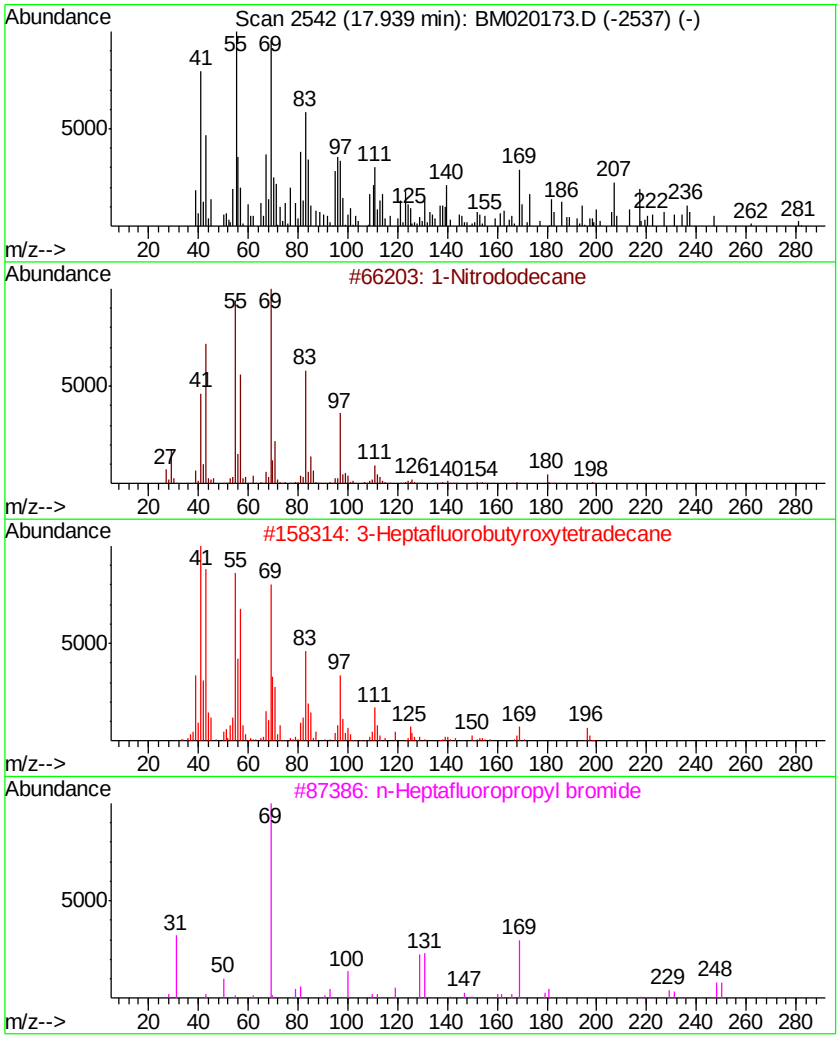
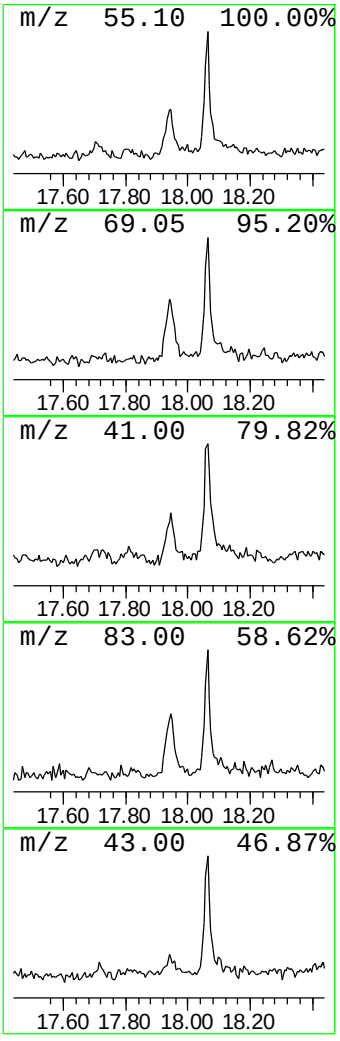
Peak Number 11 unknown17.94 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.94	2.62 ng	184786	Phenanthrene-d10	17.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nitrododecane	215	C12H25NO2	016891-99-9	46
2	3-Heptafluorobutyroxytetradecane	410	C18H29F7O2	1000245-49-8	46
3	n-Heptafluoropropyl bromide	248	C3BrF7	000422-85-5	38
4	2,6-Octadienal, 3,7-dimethyl-	152	C10H16O	005392-40-5	38
5	2H-Quinolizine-1-methanol, octah...	169	C10H19NO	000486-70-4	35





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Data File : BM020173.D
Acq On : 07 May 2019 20:04
Operator : JU/SJ
Sample : K2697-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-1-20190502

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
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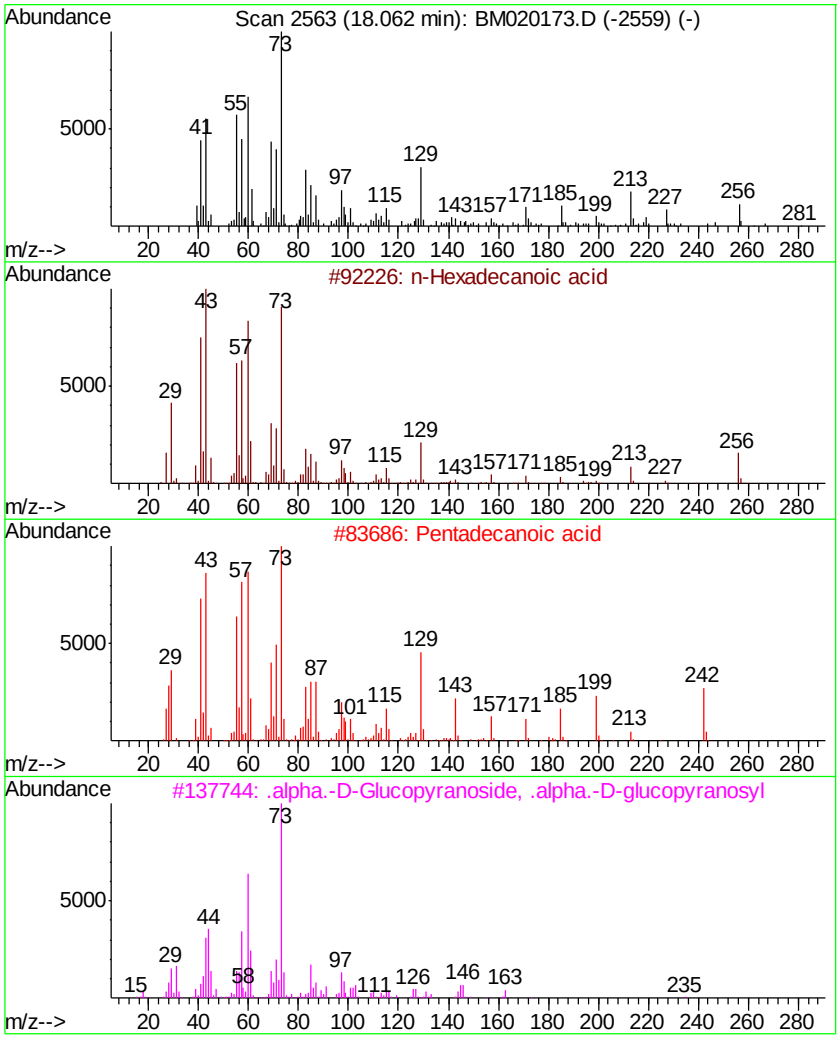
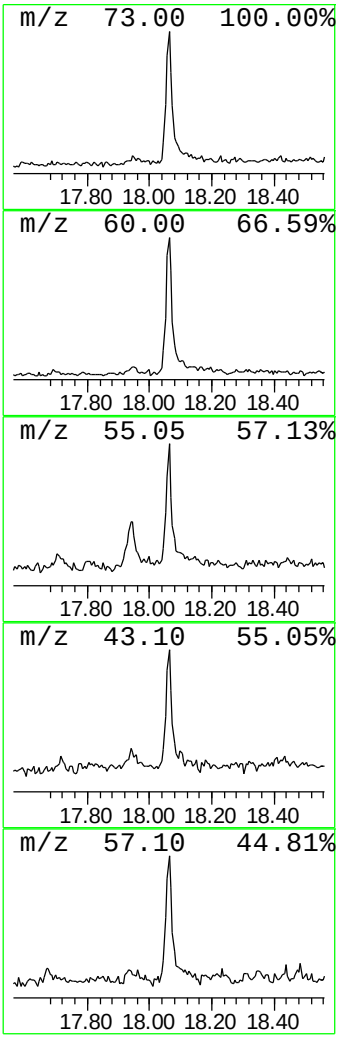
Peak Number 12 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.06	5.54 ng	391213	Phenanthrene-d10	17.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	52
3	.alpha.-D-Glucopyranoside, .alph...	342	C12H22O11	000099-20-7	43
4	Nonanoic acid	158	C9H18O2	000112-05-0	30
5	Decane, 2,3,6-trimethyl-	184	C13H28	062238-12-4	18





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Data File : BM020173.D
Acq On : 07 May 2019 20:04
Operator : JU/SJ
Sample : K2697-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-1-20190502

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.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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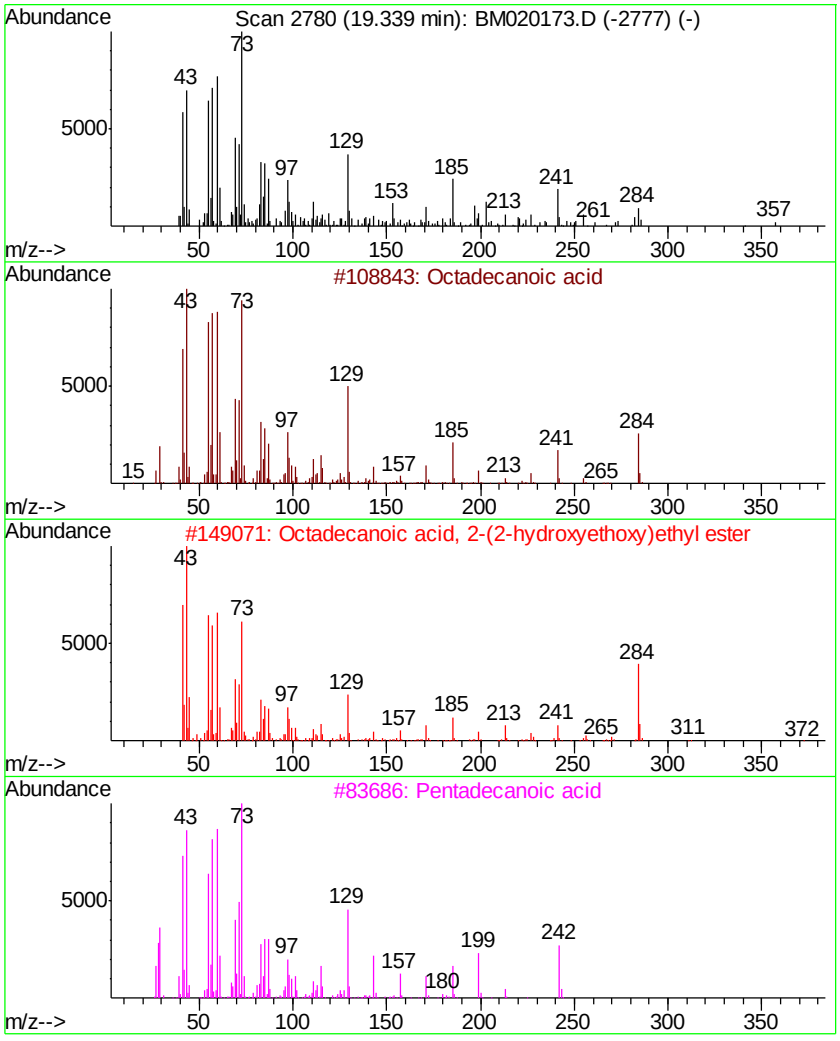
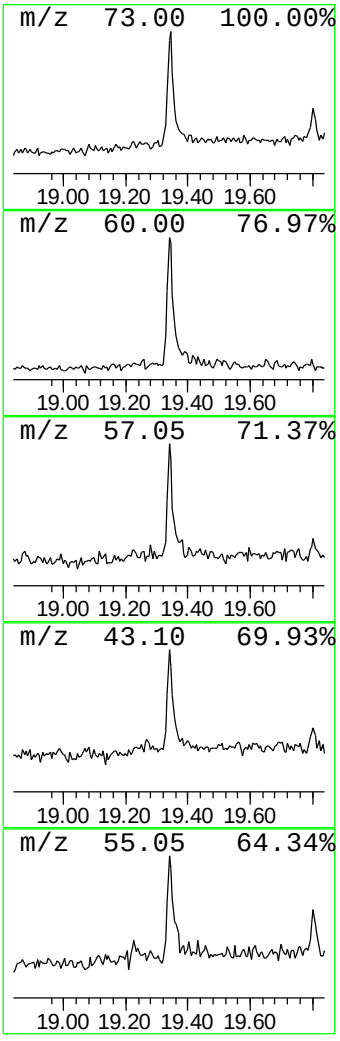
Peak Number 13 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.34	2.67 ng	236580	Chrysene-d12	21.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM050719\
Data File : BM020173.D
Acq On : 07 May 2019 20:04
Operator : JU/SJ
Sample : K2697-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-1-20190502

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.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
unknown7.32	7.32	103.7	ng	3742210	1	7.79	722075	20.0
Ethyl .alpha.-d-g...	14.29	2.3	ng	140993	3	14.43	1205930	20.0
1(2H)-Acenaphthyl...	16.16	4.0	ng	280653	4	17.18	1411710	20.0
unknown16.53	16.53	4.2	ng	296857	4	17.18	1411710	20.0
unknown16.62	16.62	2.0	ng	144088	4	17.18	1411710	20.0
unknown16.70	16.70	2.1	ng	146514	4	17.18	1411710	20.0
unknown16.81	16.81	3.7	ng	258453	4	17.18	1411710	20.0
2,4,4,6-Tetrameth...	17.02	6.2	ng	436303	4	17.18	1411710	20.0
2-Propenoic acid,...	17.31	3.2	ng	222952	4	17.18	1411710	20.0
unknown17.94	17.94	2.6	ng	184786	4	17.18	1411710	20.0
n-Hexadecanoic acid	18.06	5.5	ng	391213	4	17.18	1411710	20.0
Octadecanoic acid	19.34	2.7	ng	236580	5	21.36	1775230	20.0