LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM122018\
Data File : BM018335.D
Acq On : 20 Dec 2018 18:08
Operator : JU/SJ
Sample : J6353-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS007-0002-01

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-BM121518.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	4.675	299	304	311	rBV	79950	112005	2.69%	0.295%
2	5.122	373	380	394	rBV	1966268	2859691	68.78%	7.532%
3	5.504	439	445	453	rBV2	27440	44811	1.08%	0.118%
4	6.687	639	646	660	rBV	1936244	3309678	79.61%	8.717%
5	7.022	696	703	718	rBV	2086764	3529316	84.89%	9.295%
6	7.287	743	748	760	rVB2	24866	48670	1.17%	0.128%
7	7.481	774	781	788	rBV	532022	830473	19.97%	2.187%
8	7.792	828	834	844	rBV	1204719	1896740	45.62%	4.995%
9	8.639	971	978	991	rBV	1100714	1831490	44.05%	4.824%
10	10.245	1244	1251	1257	rBV	675530	1134784	27.29%	2.989%
11	10.298	1257	1260	1268	rVB3	27884	58703	1.41%	0.155%
12	10.627	1310	1316	1324	rBV	101192	185806	4.47%	0.489%
13	11.286	1426	1428	1438	rVB6	25109	47174	1.13%	0.124%
14	12.339	1603	1607	1615	rVB4	30918	52284	1.26%	0.138%
15	12.745	1669	1676	1683	rBV	1880739	2736214	65.81%	7.206%
16	13.616	1818	1824	1830	rBV	186126	284847	6.85%	0.750%
17	14.039	1887	1896	1907	rBV2	96424	294319	7.08%	0.775%
18	14.139	1907	1913	1923	rVB2	995610	1532678	36.86%	4.037%
19	15.651	2164	2170	2179	rBV	2344670	3383587	81.38%	8.911%
20	16.686	2342	2346	2350	rBV2	129633	195260	4.70%	0.514%
21	16.904	2378	2383	2389	rBV	1286146	1818523	43.74%	4.789%
22	17.821	2535	2539	2547	rVB	974951	1337215	32.16%	3.522%
23	19.115	2756	2759	2769	rBV	616402	877050	21.10%	2.310%
24	19.386	2800	2805	2812	rBV	1024143	1413712	34.00%	3.723%
25	19.562	2830	2835	2844	rVB	3461803	4157564	100.00%	10.950%
26	20.850	3051	3054	3059	rVB	605669	695896	16.74%	1.833%
27	21.133	3098	3102	3109	rVB	1361199	1770187	42.58%	4.662%
28	23.291	3465	3469	3477	rVB2	836478	1530758	36.82%	4.032%

Sum of corrected areas: 37969435

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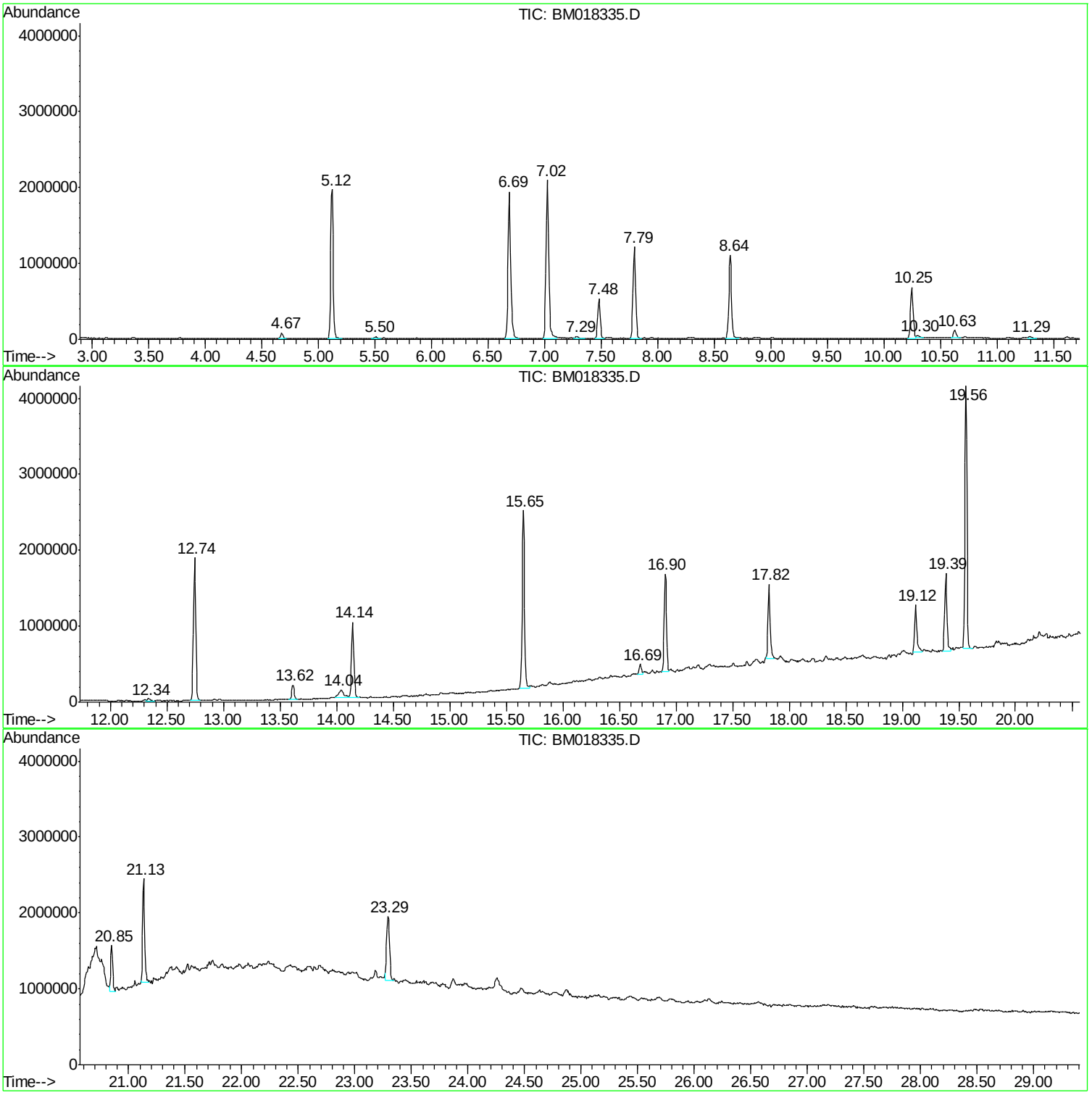
Instrument :
BNA_M
ClientSampleId :
P001-SS007-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.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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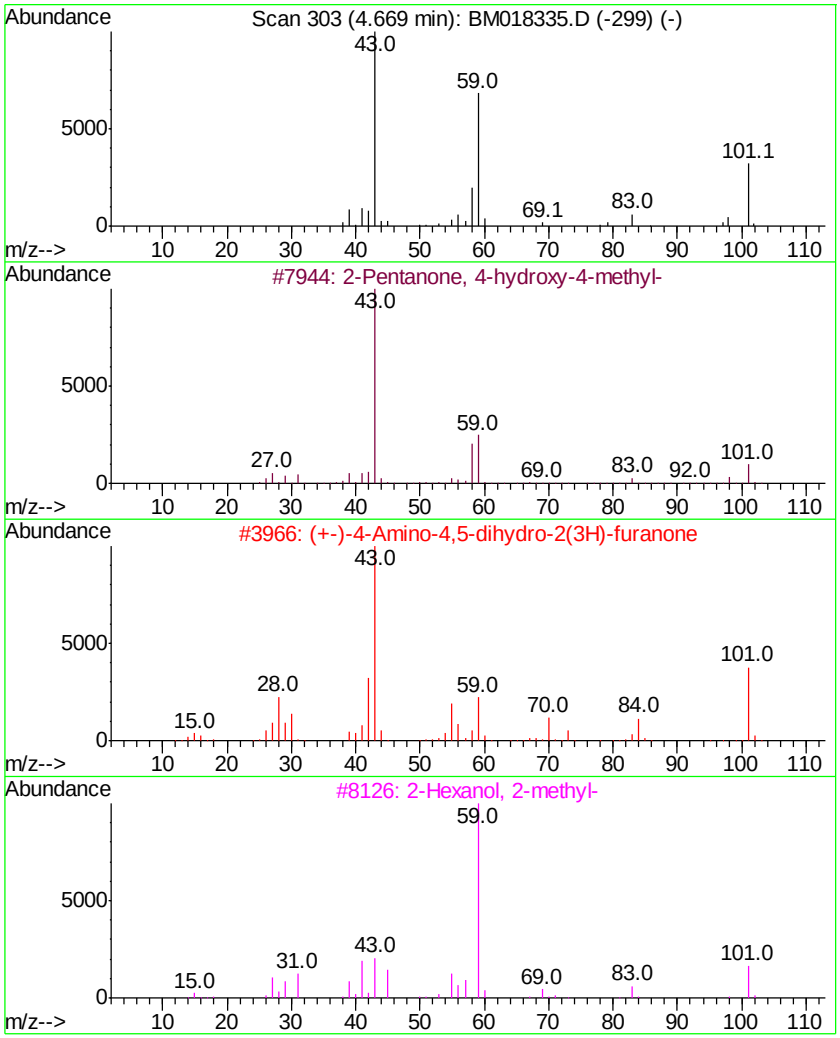
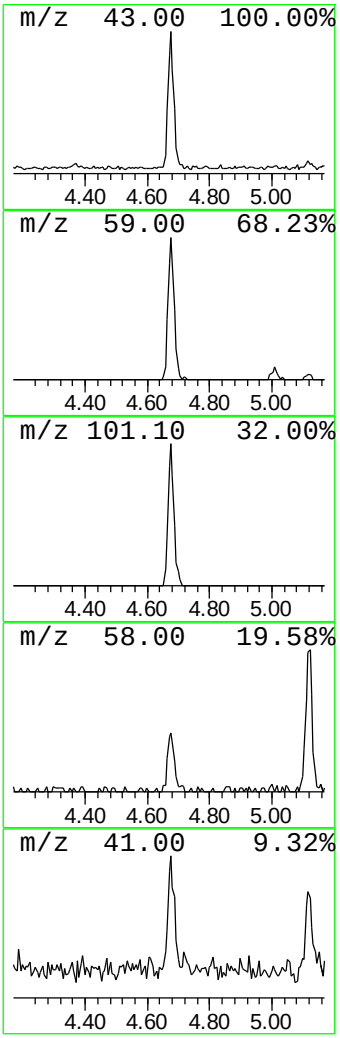
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.67	2.70 ng	112005	1,4-Dichlorobenzene-d4	7.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	53
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	47
4	Guanidine	59	CH5N3	000113-00-8	47
5	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	38





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ClientSampleId : P001-SS007-0002-01

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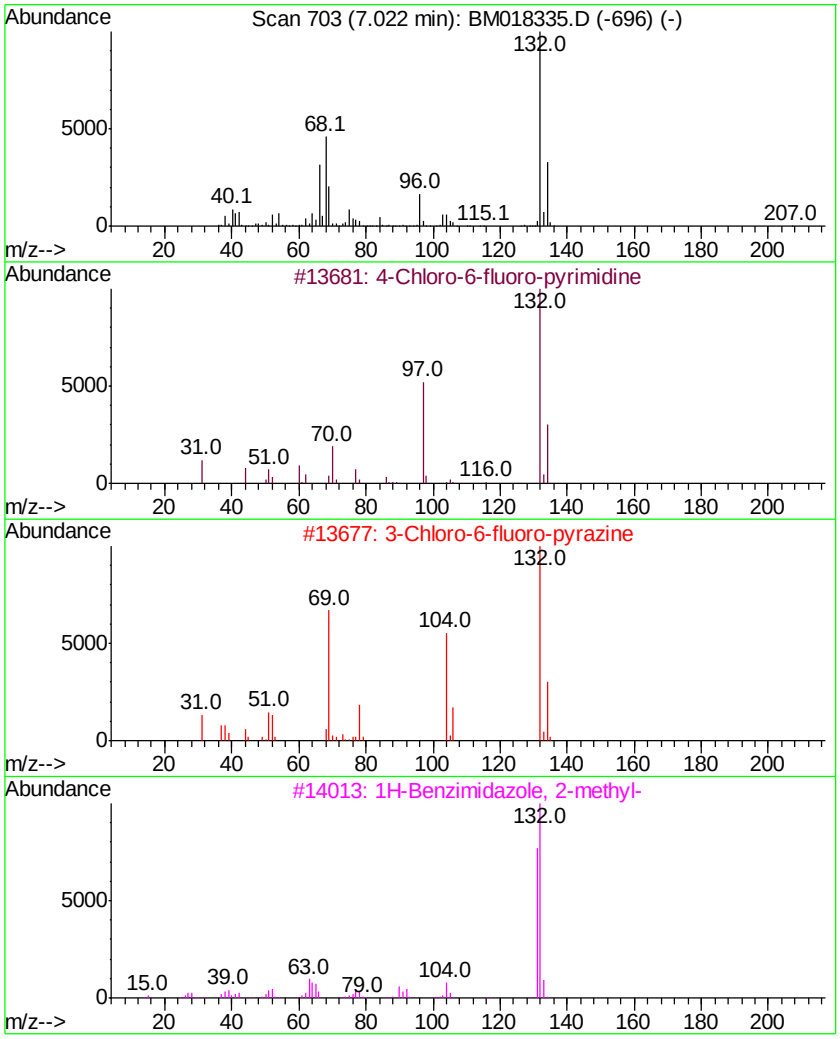
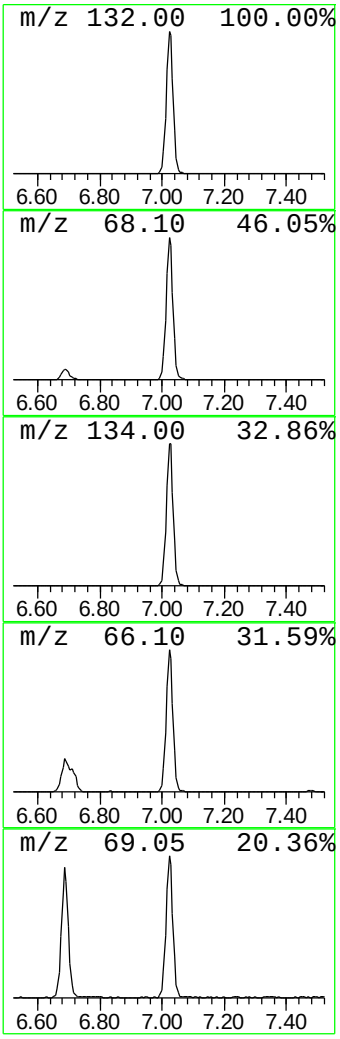
Peak Number 2 unknown7.02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.02	85.00 ng	3529320	1,4-Dichlorobenzene-d4	7.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





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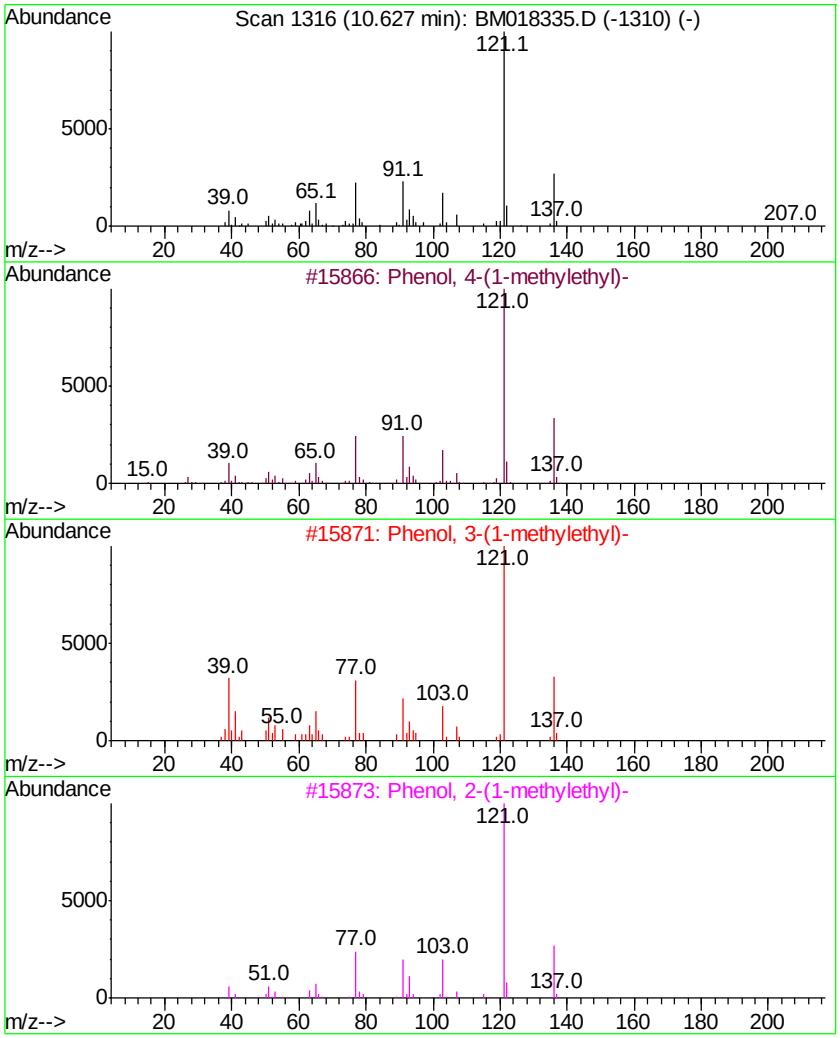
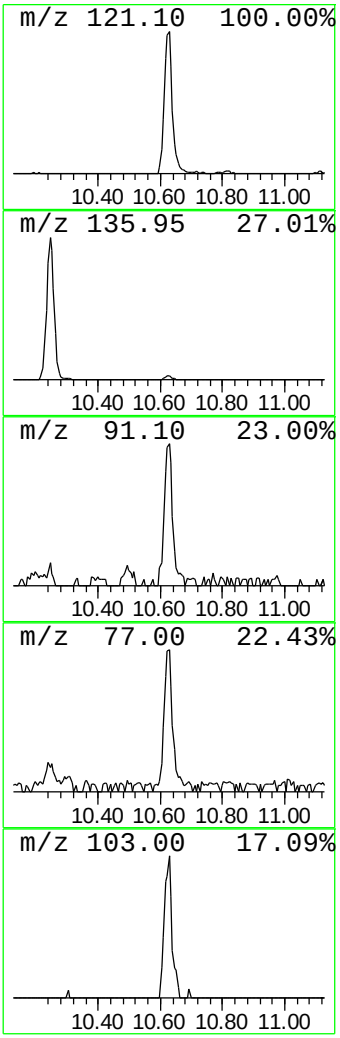
Peak Number 4 Phenol, 4-(1-methylethyl)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	3.27 ng	185806	Naphthalene-d8	10.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1-methylethyl)-	136	C9H12O	000099-89-8	96
2	Phenol, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	93
3	Phenol, 2-(1-methylethyl)-	136	C9H12O	000088-69-7	91
4	Phenol, 4-ethyl-3-methyl-	136	C9H12O	001123-94-0	87
5	Phenol, 2-(1-methylethyl)-, meth...	193	C11H15NO2	002631-40-5	86





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Instrument : BNA_M
ClientSampleId : P001-SS007-0002-01

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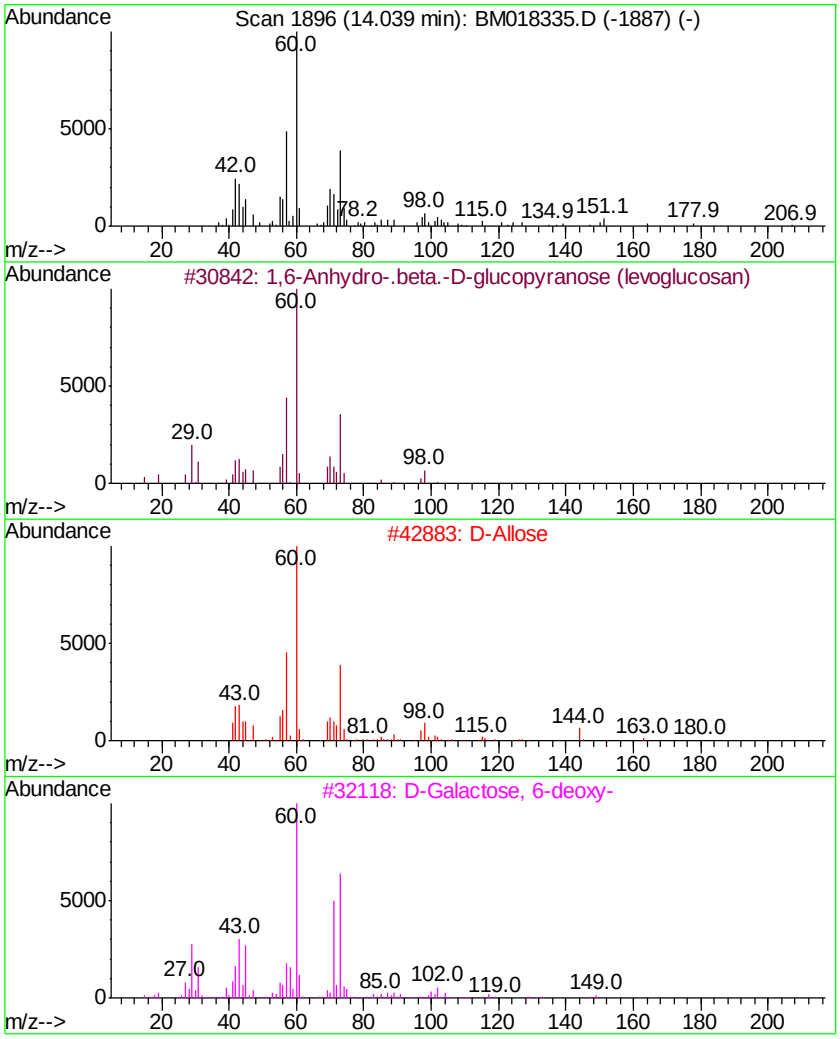
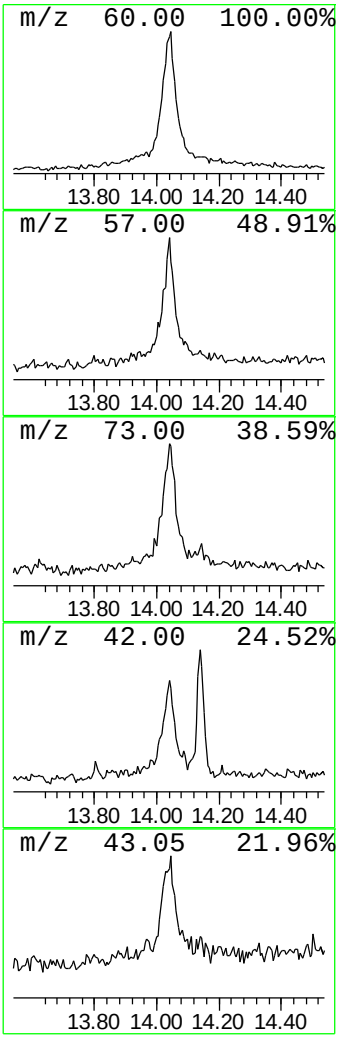
****

Peak Number 5 1,6-Anhydro-.beta.-D-glucop... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	3.84 ng	294319	Acenaphthene-d10	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	80
2	D-Allose	180	C6H12O6	002595-97-3	64
3	D-Galactose, 6-deoxy-	164	C6H12O5	003615-37-0	59
4	Hexanoic acid	116	C6H12O2	000142-62-1	53
5	Heptanoic acid	130	C7H14O2	000111-14-8	53





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Instrument : BNA_M
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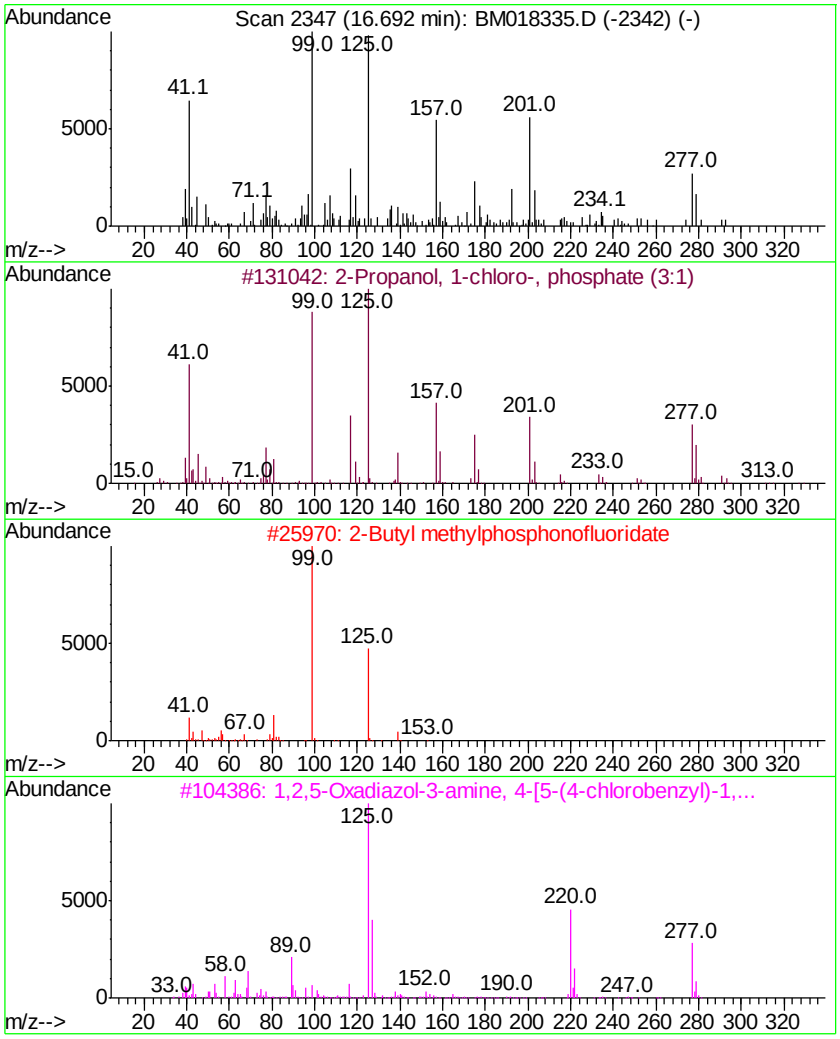
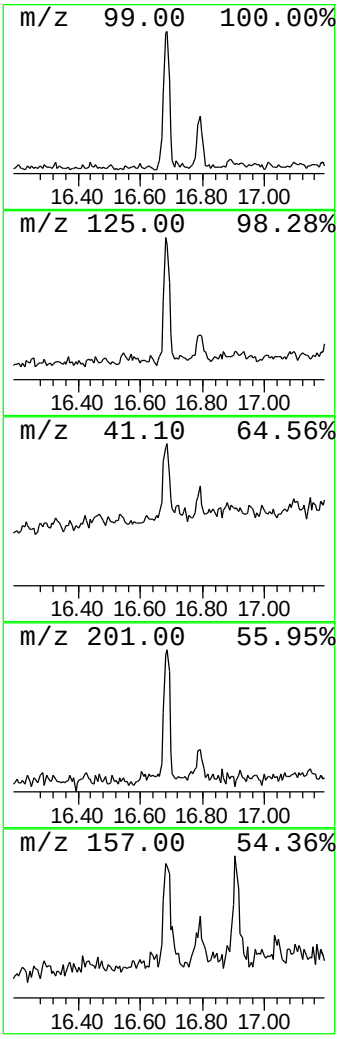
****

Peak Number 6 2-Propanol, 1-chloro-, phos... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.69	2.15 ng	195260	Phenanthrene-d10	16.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-chloro-, phosphate...	326	C9H18Cl3O4P	013674-84-5	76
2	2-Butyl methylphosphonofluoridate	154	C5H12FO2P	000352-52-3	43
3	1,2,5-Oxadiazol-3-amine, 4-[5-(4...	277	C11H8ClN5O2	1000276-59-0	12
4	4-Methyl-2-pentyl methylphosphon...	182	C7H16FO2P	000352-53-4	10
5	n-Hexyl methylphosphonofluoridate	182	C7H16FO2P	113548-89-3	10





Library Search Compound Report

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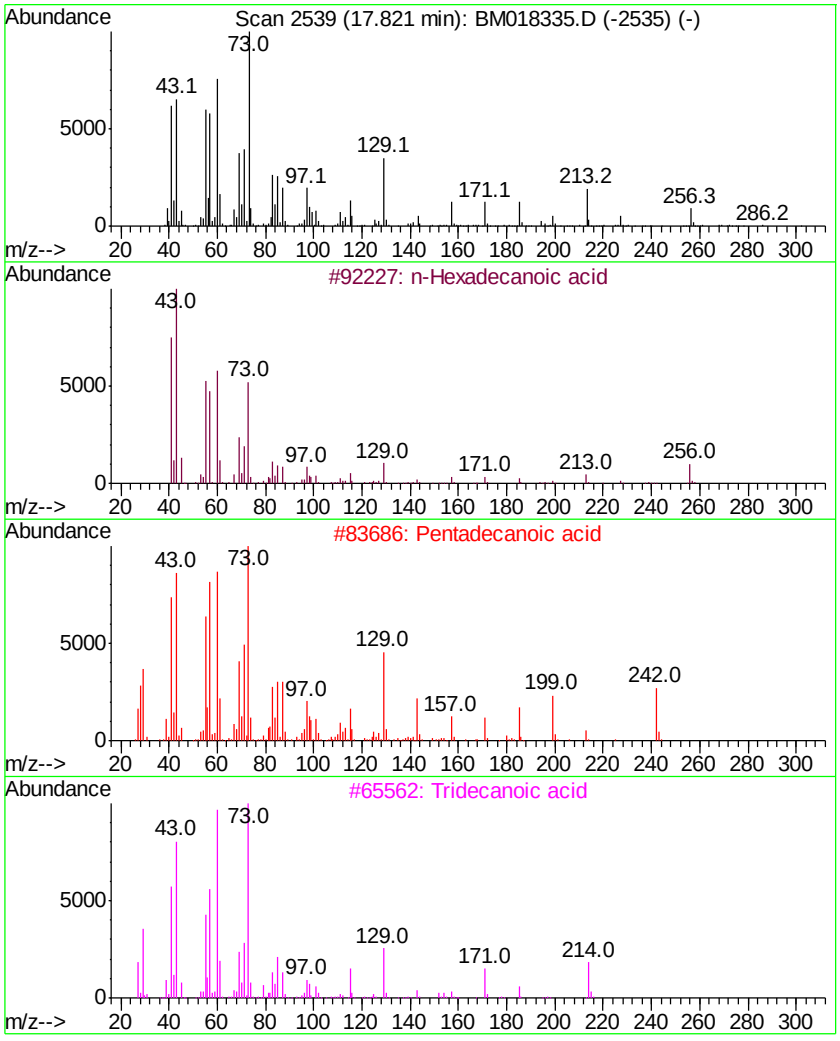
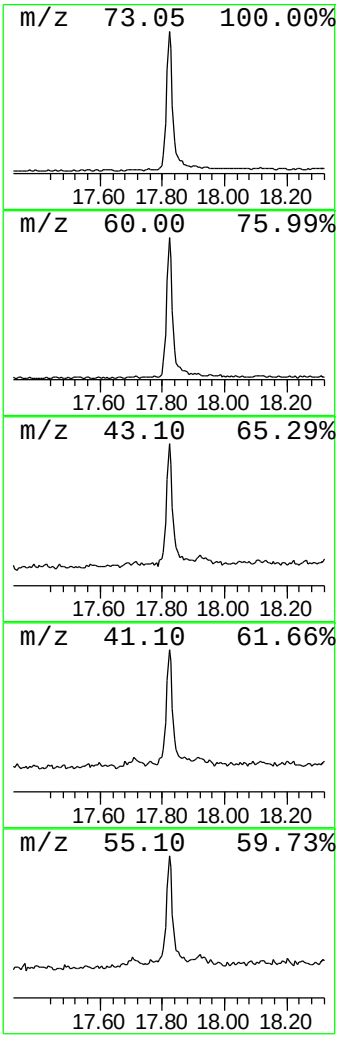
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.82	14.71 ng	1337220	Phenanthrene-d10	16.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	Hexadecane	226	C16H34	000544-76-3	11





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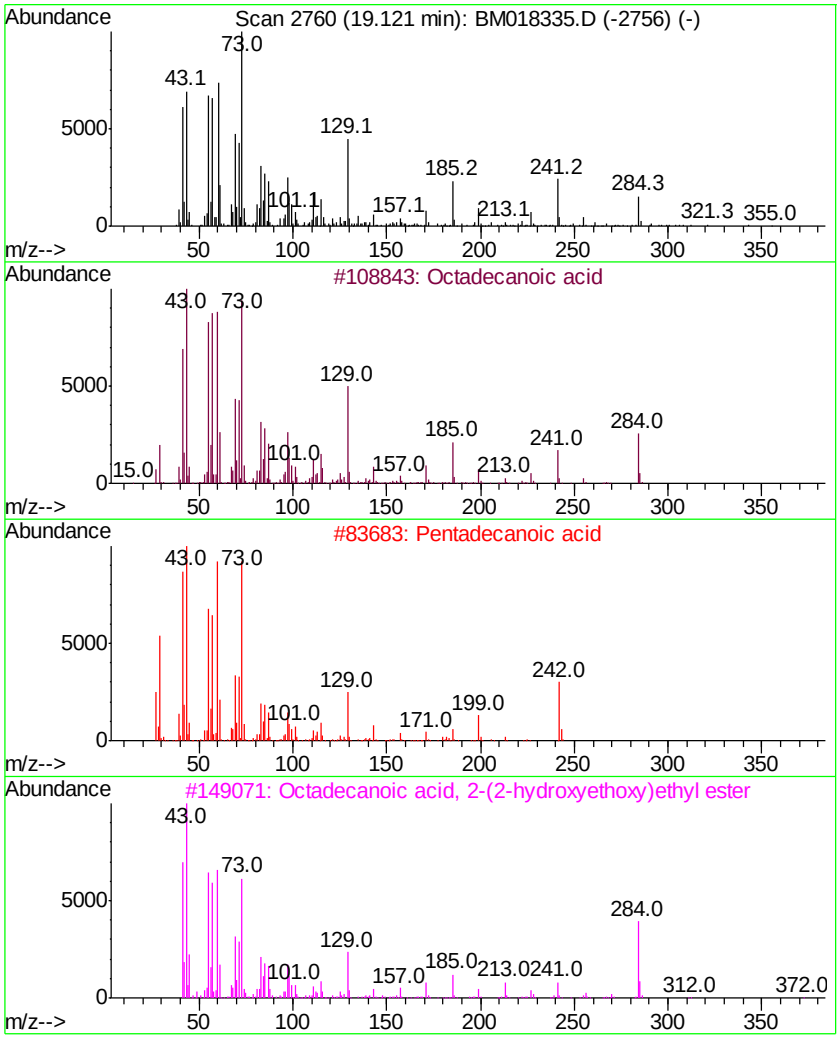
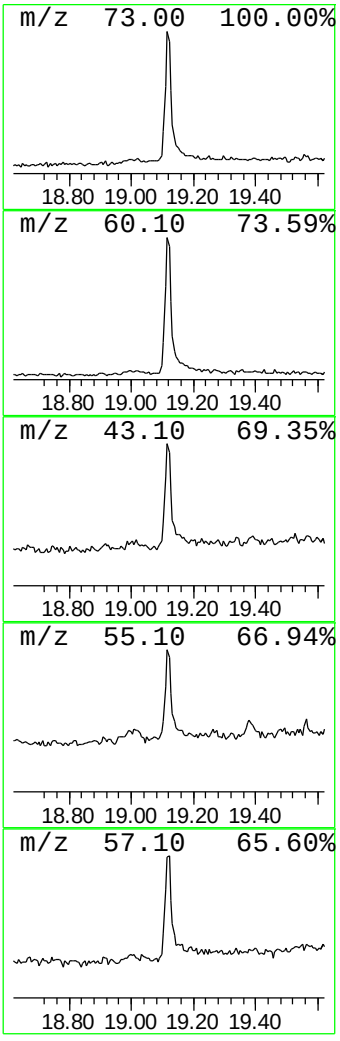
Peak Number 8 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.12	9.91 ng	877050	Chrysene-d12	21.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





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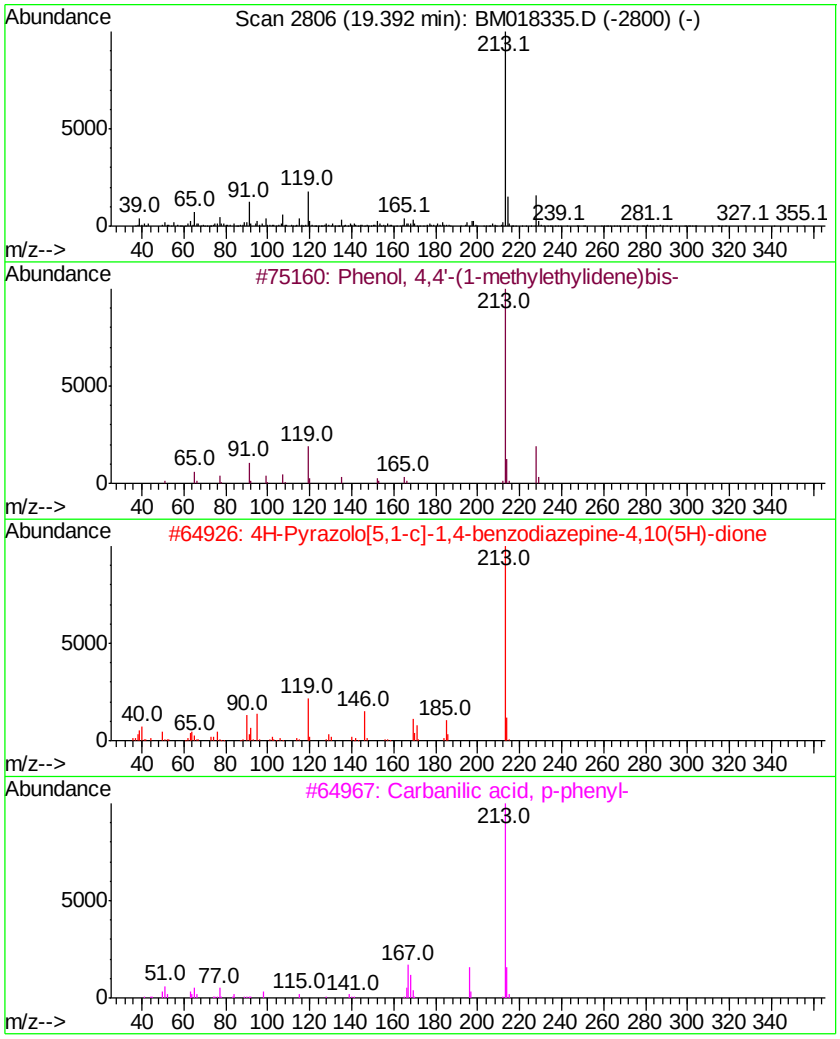
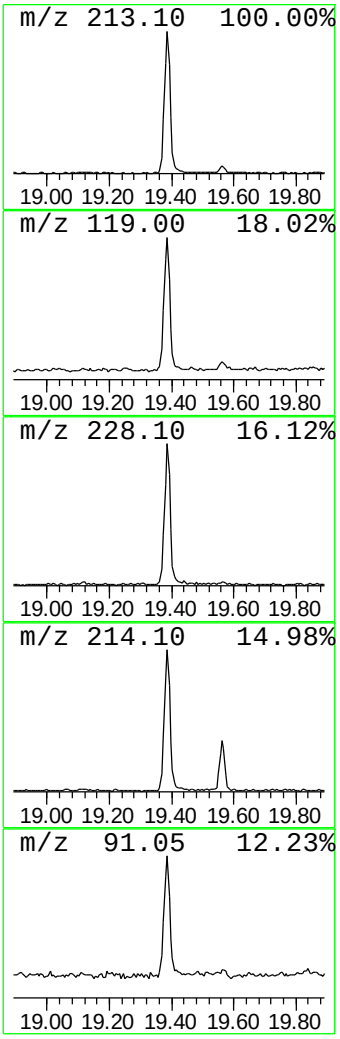
****

Peak Number 9 Phenol, 4,4'-(1-methylethyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.39	15.97 ng	1413710	Chrysene-d12	21.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	97
2	4H-Pyrazolo[5,1-c]-1,4-benzodiaz...	213	C11H7N3O2	1000277-20-1	59
3	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	49
4	Carbamic acid, [1,1'-biphenyl]-3...	213	C13H11NO2	055030-29-0	47
5	1,4-Puran, 5,6-dihydro-3-[3-indo...	213	C14H15NO	1000128-72-9	40





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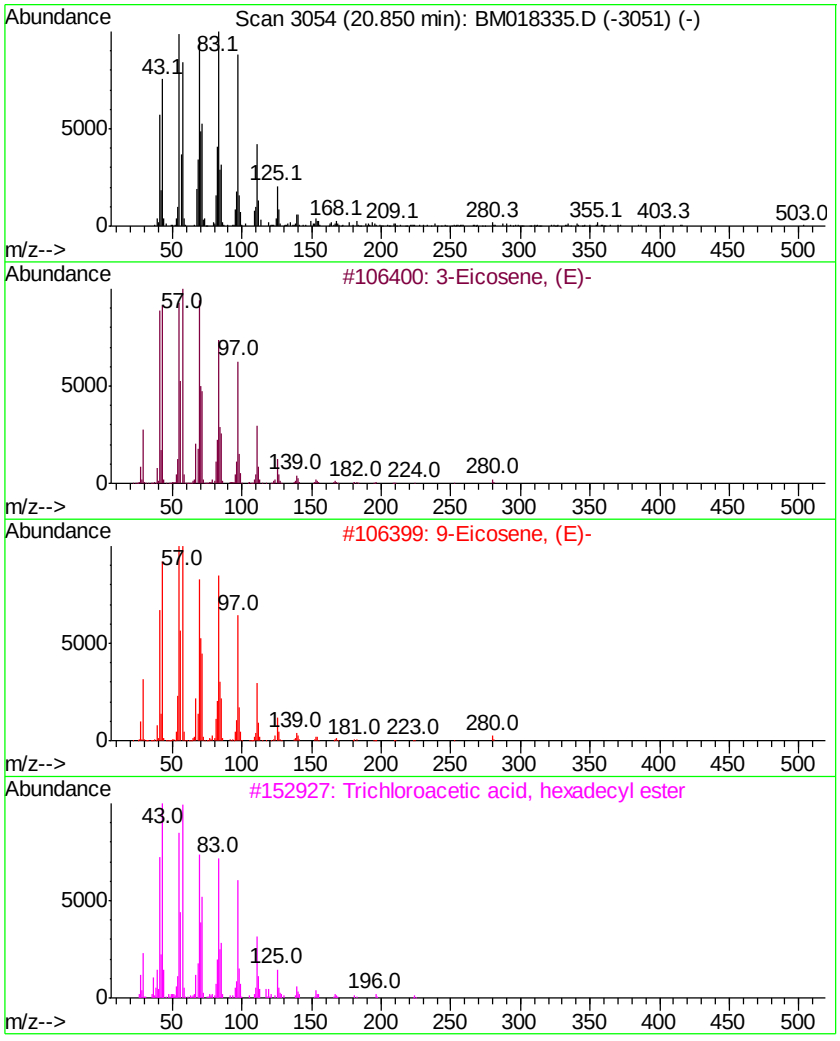
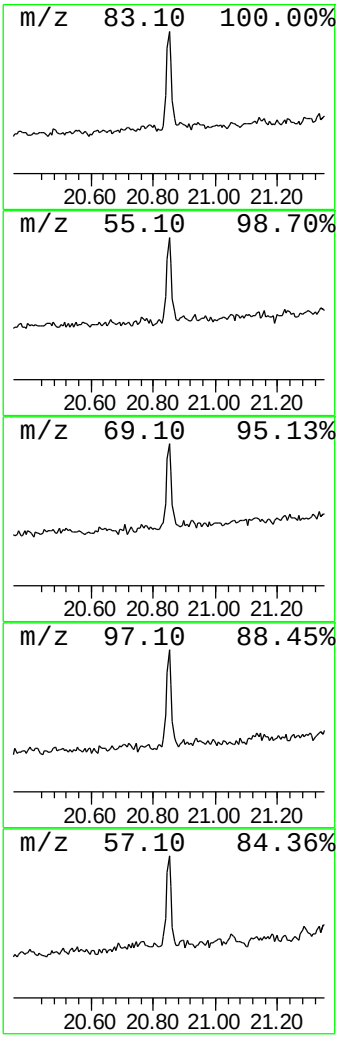
****

Peak Number 10 3-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.85	7.86 ng	695896	Chrysene-d12	21.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	94
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	93
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	90
5	1-Docosene	308	C22H44	001599-67-3	76





Tentatively Identified Compound (LSC) summary

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Acq On : 20 Dec 2018 18:08
Operator : JU/SJ
Sample : J6353-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS007-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.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
2-Pentanone, 4-hy...	4.67	2.7	ng	112005	1	7.48	830473	20.0
unknown7.02	7.02	85.0	ng	3529320	1	7.48	830473	20.0
Phenol, 4-(1-meth...	10.63	3.3	ng	185806	2	10.25	1134780	20.0
1,6-Anhydro-.beta...	14.04	3.8	ng	294319	3	14.14	1532680	20.0
2-Propanol, 1-chl...	16.69	2.1	ng	195260	4	16.90	1818520	20.0
n-Hexadecanoic acid	17.82	14.7	ng	1337220	4	16.90	1818520	20.0
Octadecanoic acid	19.12	9.9	ng	877050	5	21.13	1770190	20.0
Phenol, 4,4'-(1-m...	19.39	16.0	ng	1413710	5	21.13	1770190	20.0
3-Eicosene, (E)-	20.85	7.9	ng	695896	5	21.13	1770190	20.0