LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071118\
Data File : BM015893.D
Acq On : 11 Jul 2018 17:45
Operator : SJ/JU
Sample : J3906-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CB-7-8-6-ST-WW-3@2.5

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-BM070518.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	5.316	339	345	358	rBV	290699	442738	8.22%	1.173%
2	5.798	420	427	443	rBV	2374896	3569190	66.28%	9.456%
3	7.445	700	707	728	rBV	2360280	4044169	75.10%	10.714%
4	7.816	763	770	786	rBV	2551453	4054144	75.28%	10.740%
5	8.292	845	851	858	rBV	394824	657893	12.22%	1.743%
6	8.616	899	906	920	rBV	1715777	2804758	52.08%	7.431%
7	9.480	1046	1053	1066	rBV	1354192	2281550	42.37%	6.044%
8	11.116	1325	1331	1343	rBV	466108	814969	15.13%	2.159%
9	13.539	1736	1743	1755	rBV	3130450	4399838	81.70%	11.656%
10	14.357	1877	1882	1896	rBV	473934	678804	12.60%	1.798%
11	14.915	1970	1977	1984	rBV2	609163	964605	17.91%	2.555%
12	16.392	2222	2228	2242	rBV	2668447	3658347	67.93%	9.692%
13	17.639	2434	2440	2452	rVB	728116	1032733	19.18%	2.736%
14	18.480	2577	2583	2593	rBV	212147	318553	5.92%	0.844%
15	19.727	2790	2795	2804	rBV	100885	146922	2.73%	0.389%
16	20.203	2870	2876	2885	rVB	4506007	5385281	100.00%	14.267%
17	21.415	3078	3082	3085	rBV2	61152	97760	1.82%	0.259%
18	21.503	3093	3097	3104	rBV	157952	211371	3.92%	0.560%
19	21.750	3134	3139	3144	rBV	774994	1043466	19.38%	2.764%
20	22.927	3335	3339	3345	rVB	119027	171740	3.19%	0.455%
21	24.144	3540	3546	3557	rVB2	496610	967507	17.97%	2.563%

Sum of corrected areas: 37746338

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Misc :
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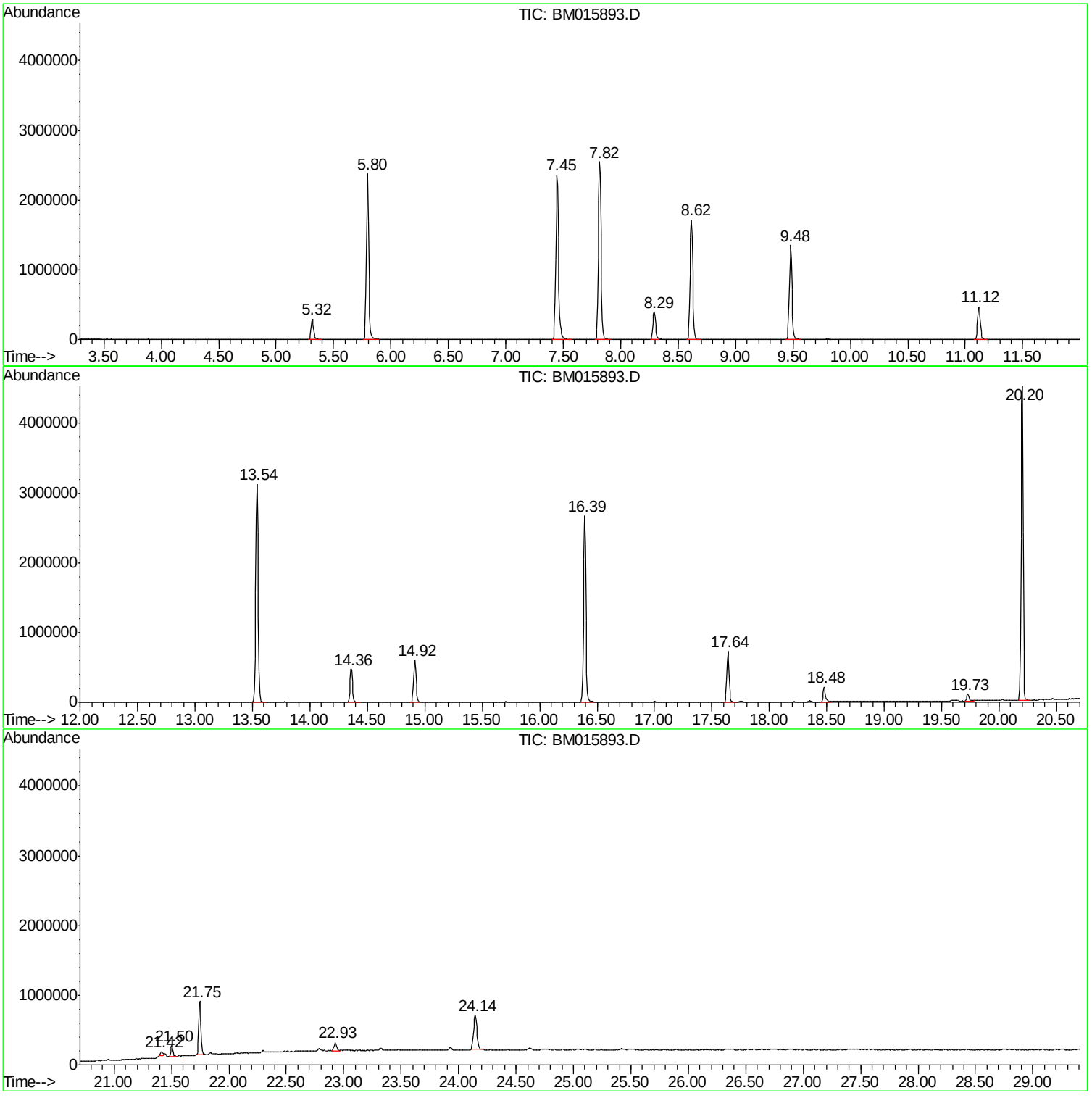
Instrument :
BNA_M
ClientSampleId :
CB-7-8-6-ST-WW-3@2.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.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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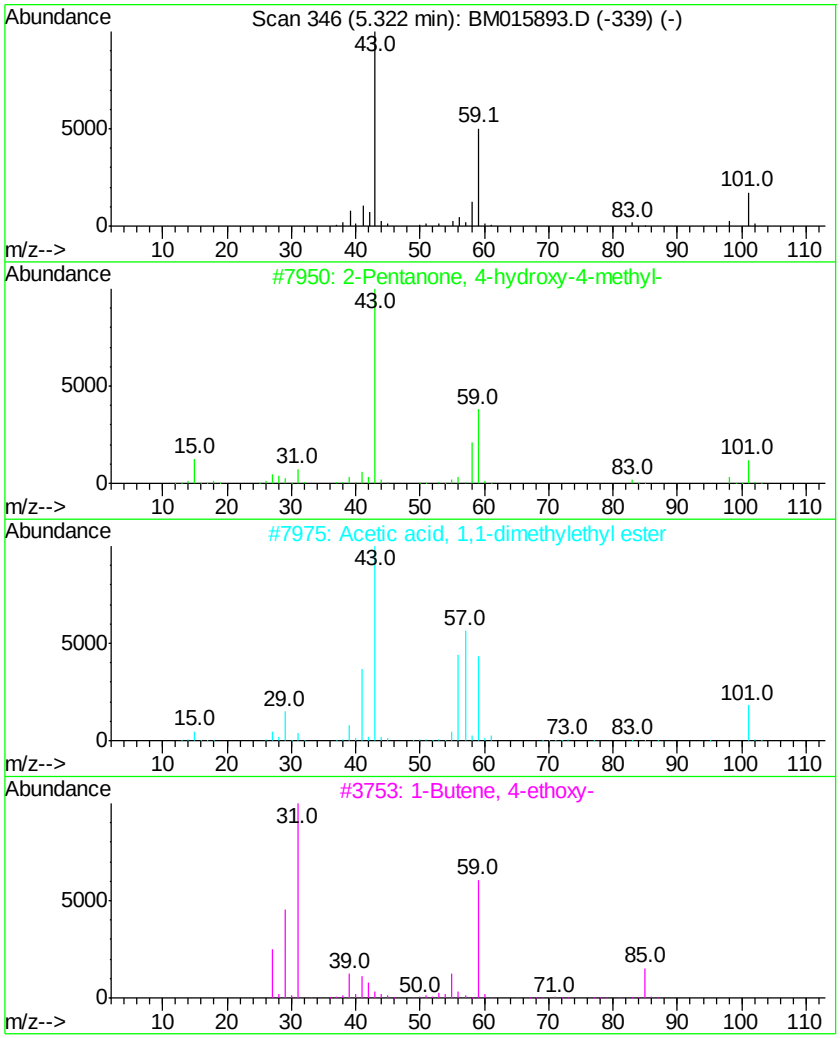
TIC Integration Parameters: LSCINT.P

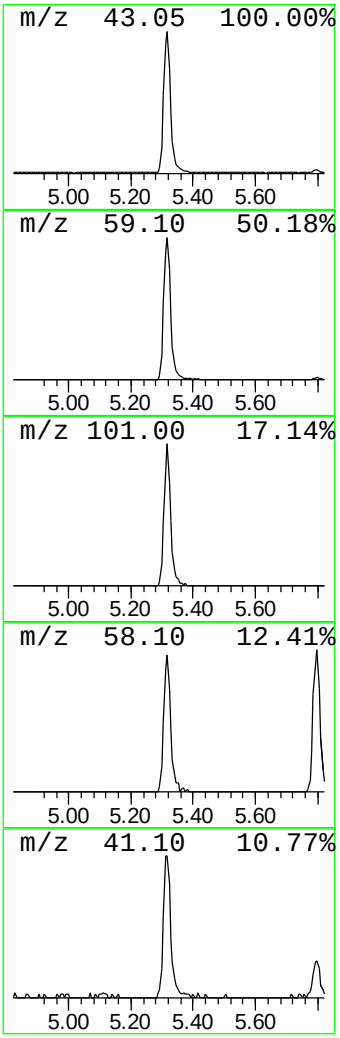
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.32	13.46 ng	442738	1,4-Dichlorobenzene-d4	8.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CB-7-8-6-ST-WW-3@2.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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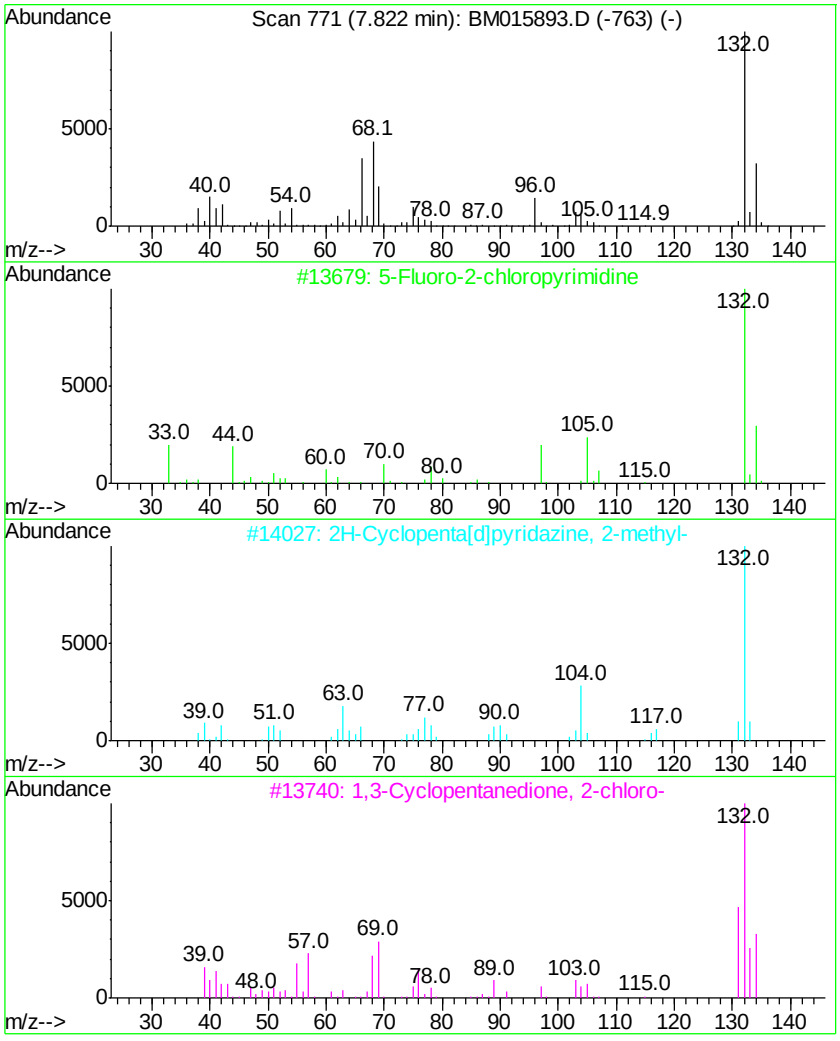
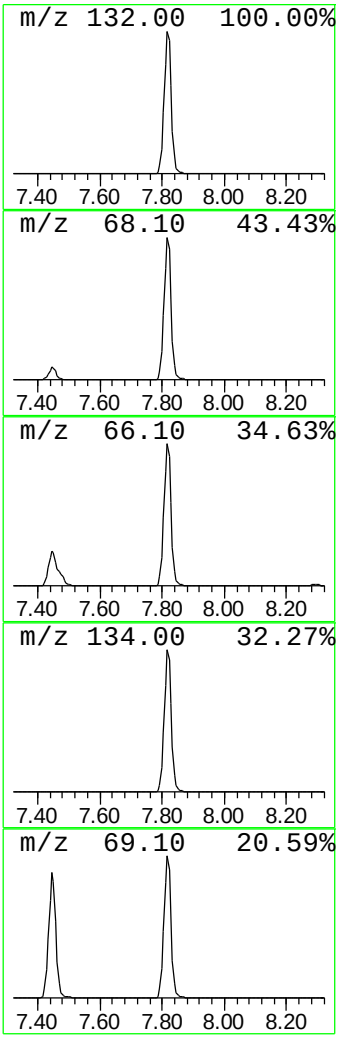
Peak Number 2 unknown7.82 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.82	123.25 ng	4054140	1,4-Dichlorobenzene-d4	8.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	27
3	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	23
4	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	22
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22





Library Search Compound Report

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Data File : BM015893.D
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Operator : SJ/JU
Sample : J3906-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CB-7-8-6-ST-WW-3@2.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.M
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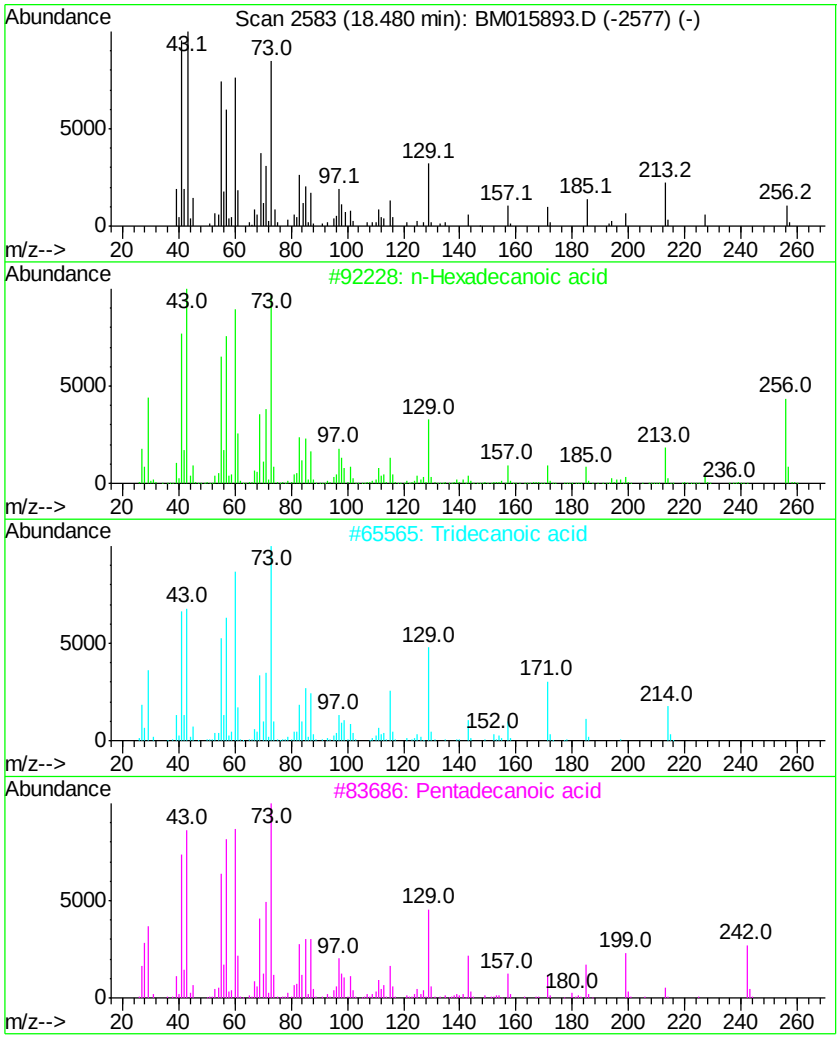
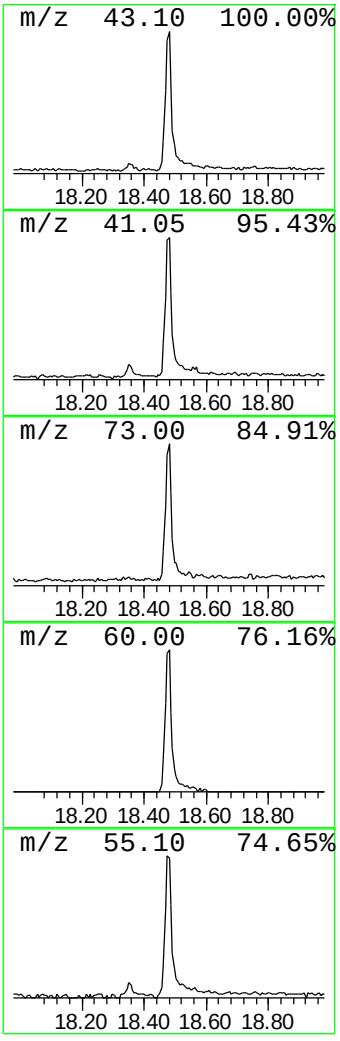
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.48	6.17 ng	318553	Phenanthrene-d10	17.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Dodecanoic acid	200	C12H24O2	000143-07-7	50





Library Search Compound Report

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Data File : BM015893.D
Acq On : 11 Jul 2018 17:45
Operator : SJ/JU
Sample : J3906-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CB-7-8-6-ST-WW-3@2.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.M
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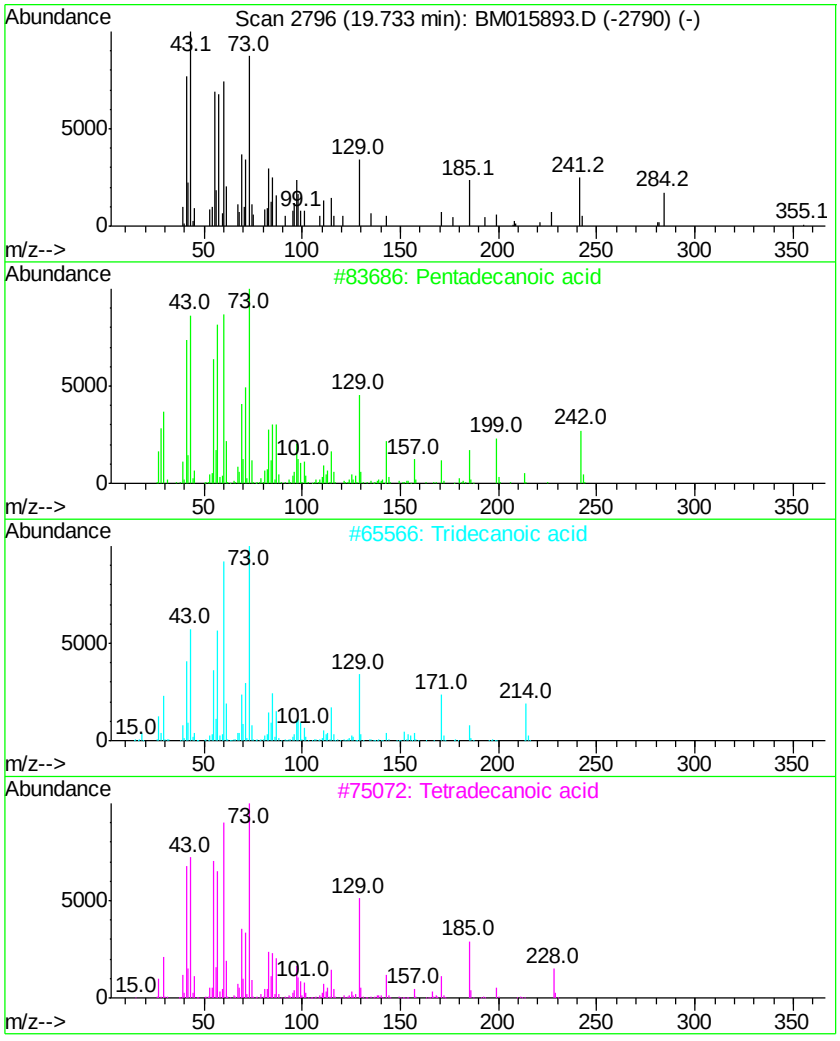
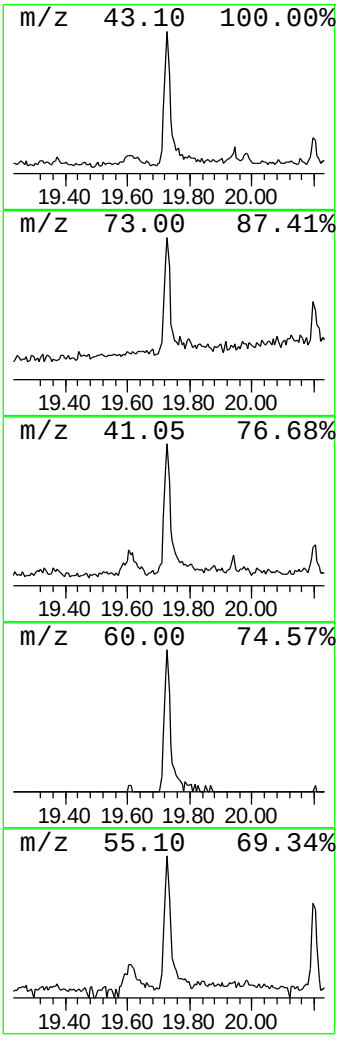
Peak Number 5 Pentadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.73	2.82 ng	146922	Chrysene-d12	21.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	62
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50
5	Undecanoic acid	186	C11H22O2	000112-37-8	38





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Operator : SJ/JU
Sample : J3906-06
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Instrument : BNA_M
ClientSampleId : CB-7-8-6-ST-WW-3@2.5

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

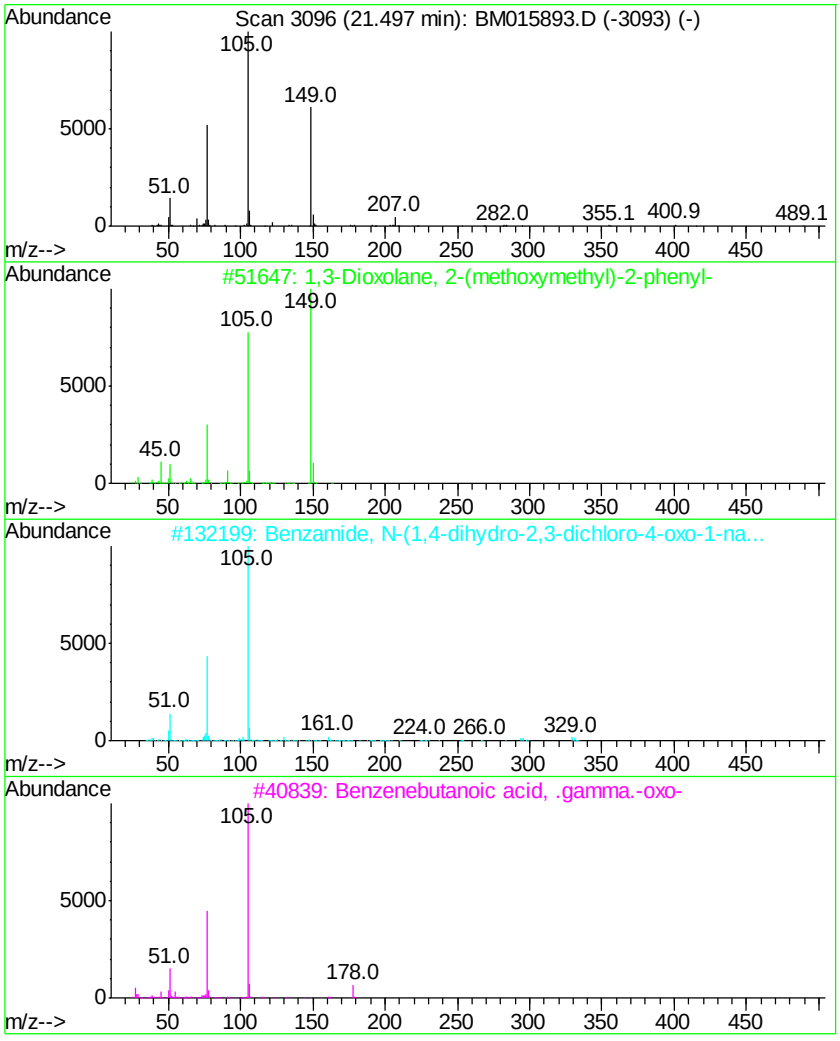
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

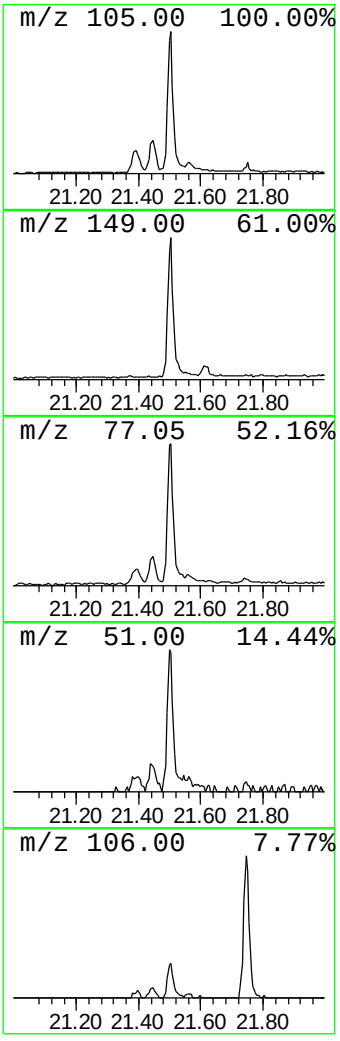
****

Peak Number 6 1,3-Dioxolane, 2-(methoxyme... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.50	4.05 ng	211371	Chrysene-d12	21.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	78
2	Benzamide, N-(1,4-dihydro-2,3-di...	329	C17H9Cl2NO2	307553-57-7	47
3	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	43
4	1,3,4-Oxadiazin-6-one, 5-isoprop...	216	C12H12N2O2	173973-78-9	43
5	Vinyl benzoate	148	C9H8O2	000769-78-8	43





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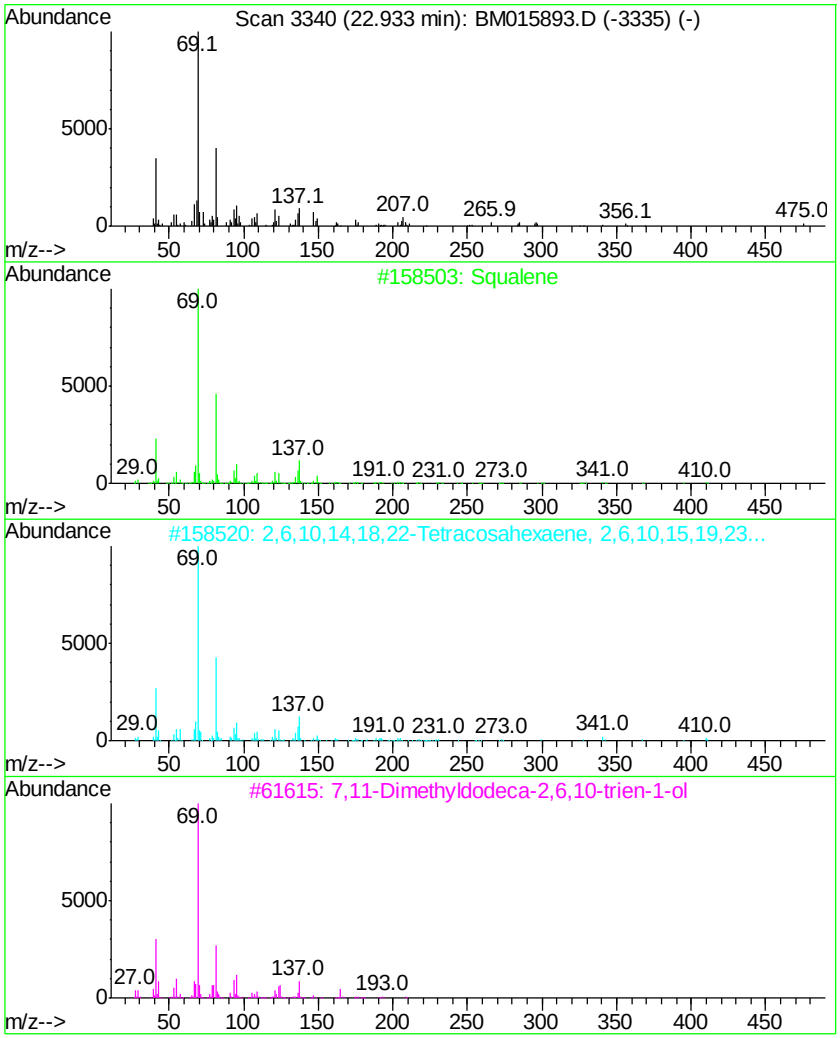
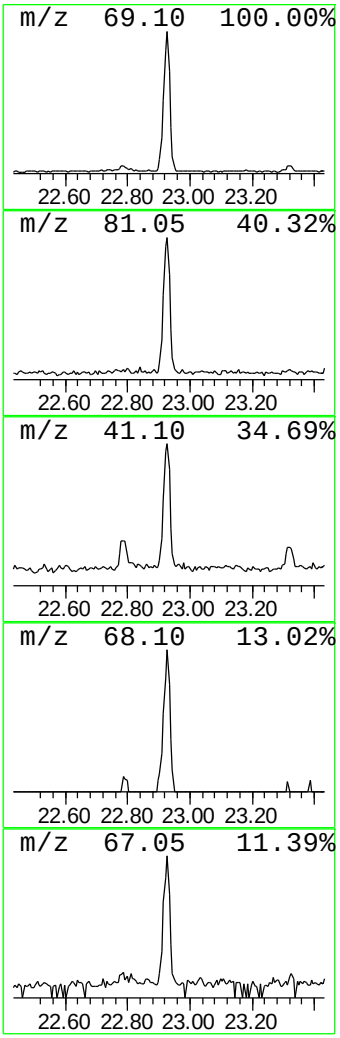
Peak Number 7 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.93	3.29 ng	171740	Chrysene-d12	21.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	83
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	72
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	59
5	Farnesol isomer a	222	C15H26O	1000108-92-4	58





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.32	13.5	ng	442738	1	8.29	657893	20.0
unknown7.82	7.82	123.3	ng	4054140	1	8.29	657893	20.0
n-Hexadecanoic acid	18.48	6.2	ng	318553	4	17.64	1032730	20.0
Pentadecanoic acid	19.73	2.8	ng	146922	5	21.75	1043470	20.0
1,3-Dioxolane, 2-...	21.50	4.0	ng	211371	5	21.75	1043470	20.0
Squalene	22.93	3.3	ng	171740	5	21.75	1043470	20.0