LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM070918\
Data File : BM015848.D
Acq On : 09 Jul 2018 18:13
Operator : SJ/JU
Sample : J3888-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : AOC7-BTM-6-6.5

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	5.322	341	346	359	rVB	266894	425647	4.45%	0.889%
2	5.804	421	428	444	rBV	2394138	3715639	38.84%	7.763%
3	7.451	701	708	724	rBV	2521139	4198759	43.89%	8.772%
4	7.828	765	772	787	rBV	2586357	4288428	44.83%	8.959%
5	8.298	845	852	860	rBV	396981	672577	7.03%	1.405%
6	8.622	900	907	921	rBV	1830376	3057523	31.96%	6.388%
7	9.486	1047	1054	1073	rBV	1488024	2512164	26.26%	5.248%
8	11.128	1326	1333	1341	rBV	524133	876885	9.17%	1.832%
9	13.545	1737	1744	1755	rBV	3887541	5506493	57.56%	11.504%
10	14.363	1878	1883	1896	rBV	358944	515763	5.39%	1.078%
11	14.921	1972	1978	1990	rVB2	744959	1141914	11.94%	2.386%
12	16.398	2223	2229	2243	rBV	3529761	4916725	51.40%	10.272%
13	17.645	2435	2441	2453	rBV	978857	1415706	14.80%	2.958%
14	18.486	2576	2584	2595	rBV	495935	691330	7.23%	1.444%
15	19.733	2791	2796	2809	rBV	266639	384109	4.02%	0.802%
16	20.209	2871	2877	2882	rBV	8258320	9565801	100.00%	19.984%
17	21.421	3078	3083	3094	rBV	395971	693749	7.25%	1.449%
18	21.756	3134	3140	3150	rVB	1225852	1696095	17.73%	3.543%
19	24.150	3541	3547	3558	rVB2	780028	1591142	16.63%	3.324%

Sum of corrected areas: 47866449

LSC Report - Integrated Chromatogram

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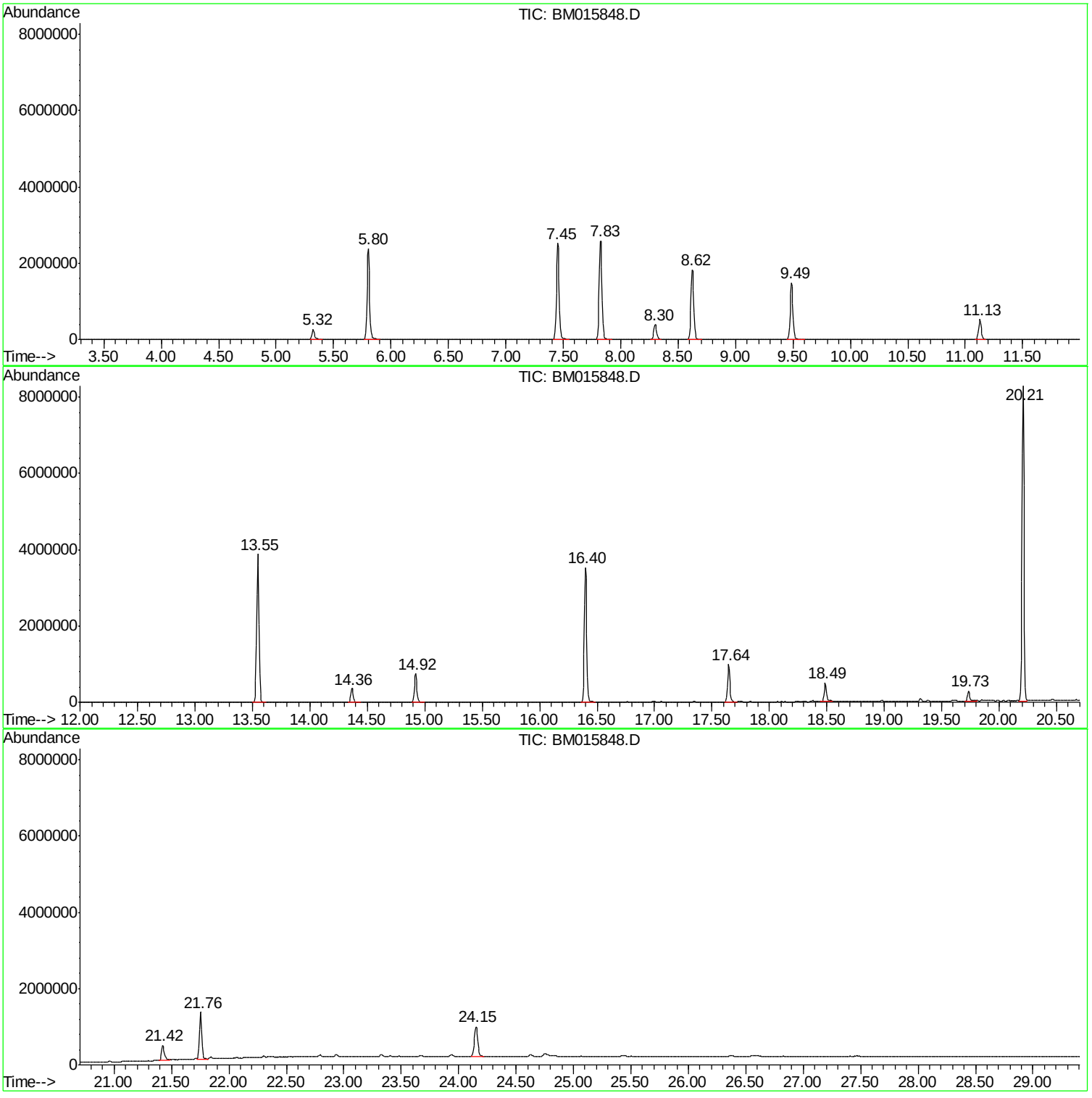
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : AOC7-BTM-6-6.5

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

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



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Instrument : BNA_M
ClientSampleId : AOC7-BTM-6-6.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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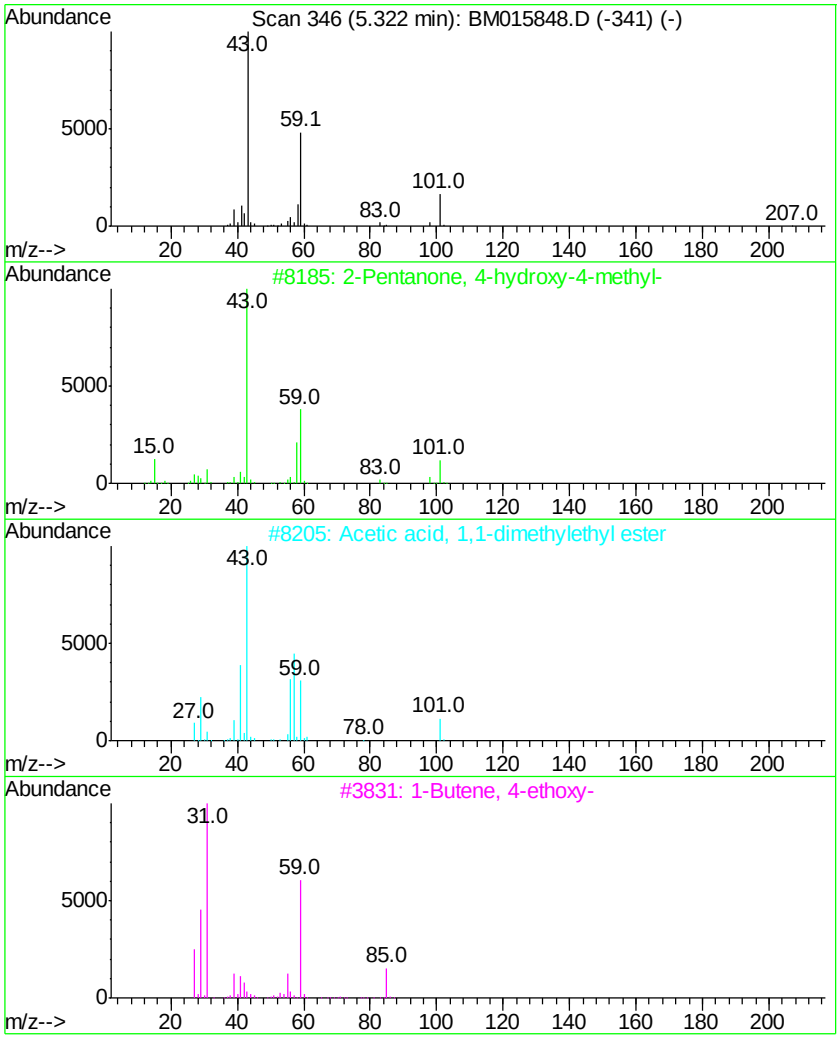
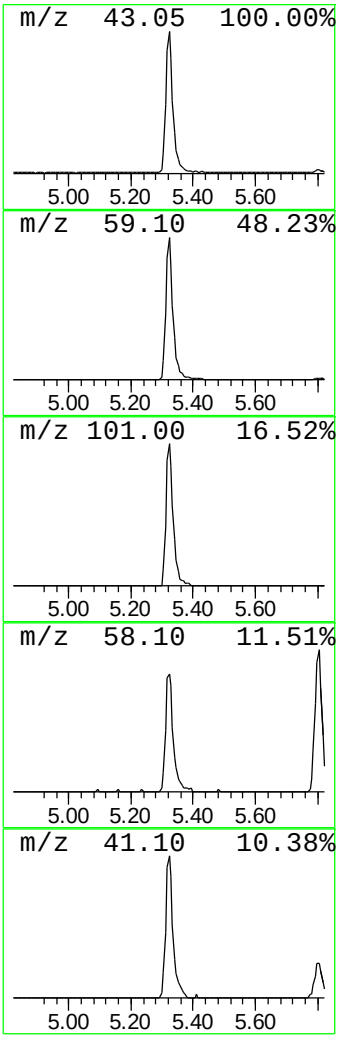
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.32	12.66 ng	425647	1,4-Dichlorobenzene-d4	8.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	Propylamine	59	C3H9N	000107-10-8	9





Library Search Compound Report

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Operator : SJ/JU
Sample : J3888-02
Misc :
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Instrument : BNA_M
ClientSampleId : AOC7-BTM-6-6.5

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

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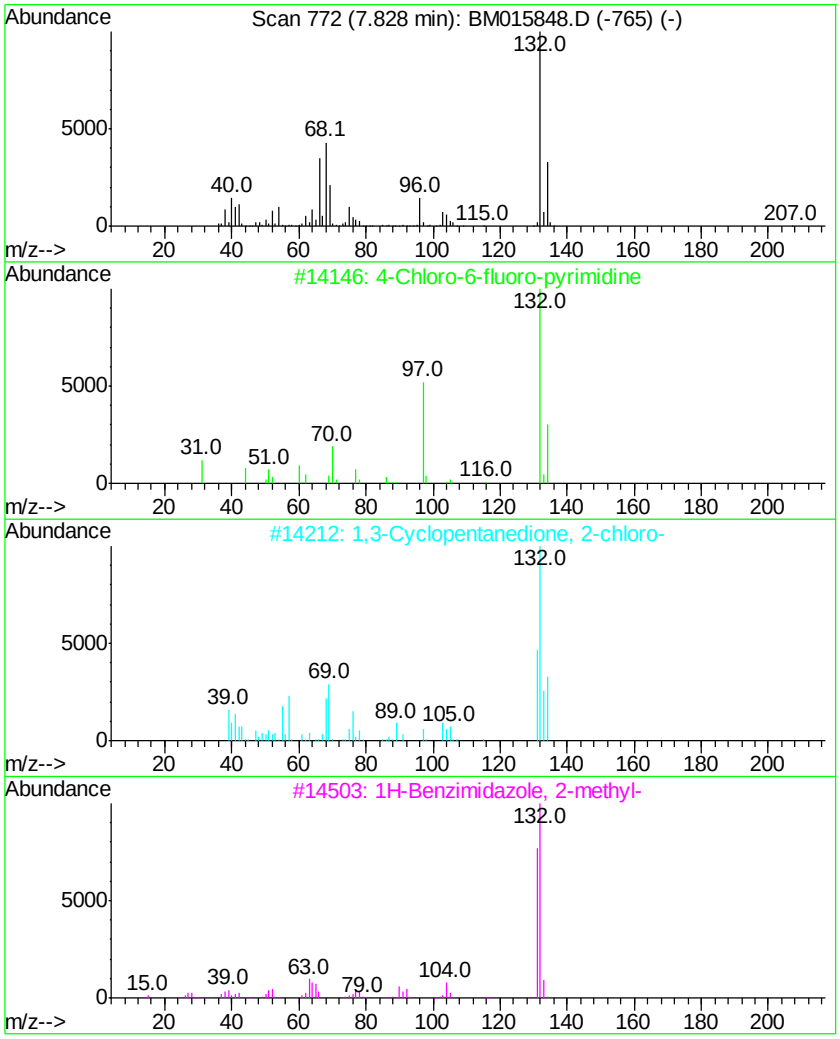
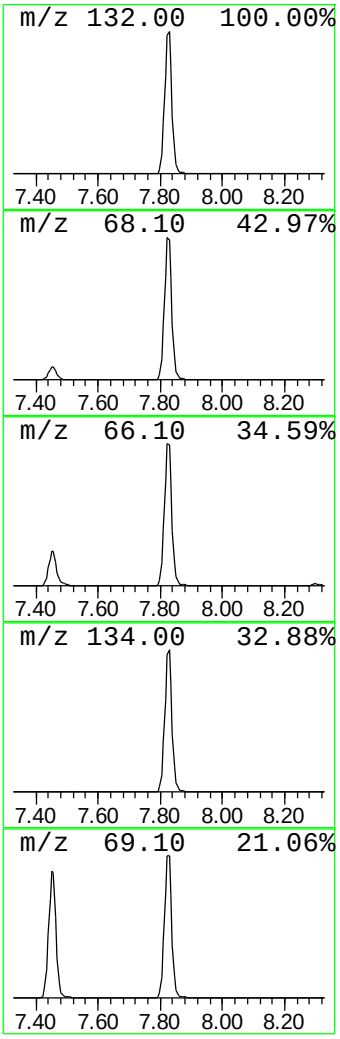
Peak Number 2 unknown7.83 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.83	127.52 ng	4288430	1,4-Dichlorobenzene-d4	8.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	22
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22





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Sample : J3888-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : AOC7-BTM-6-6.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.M
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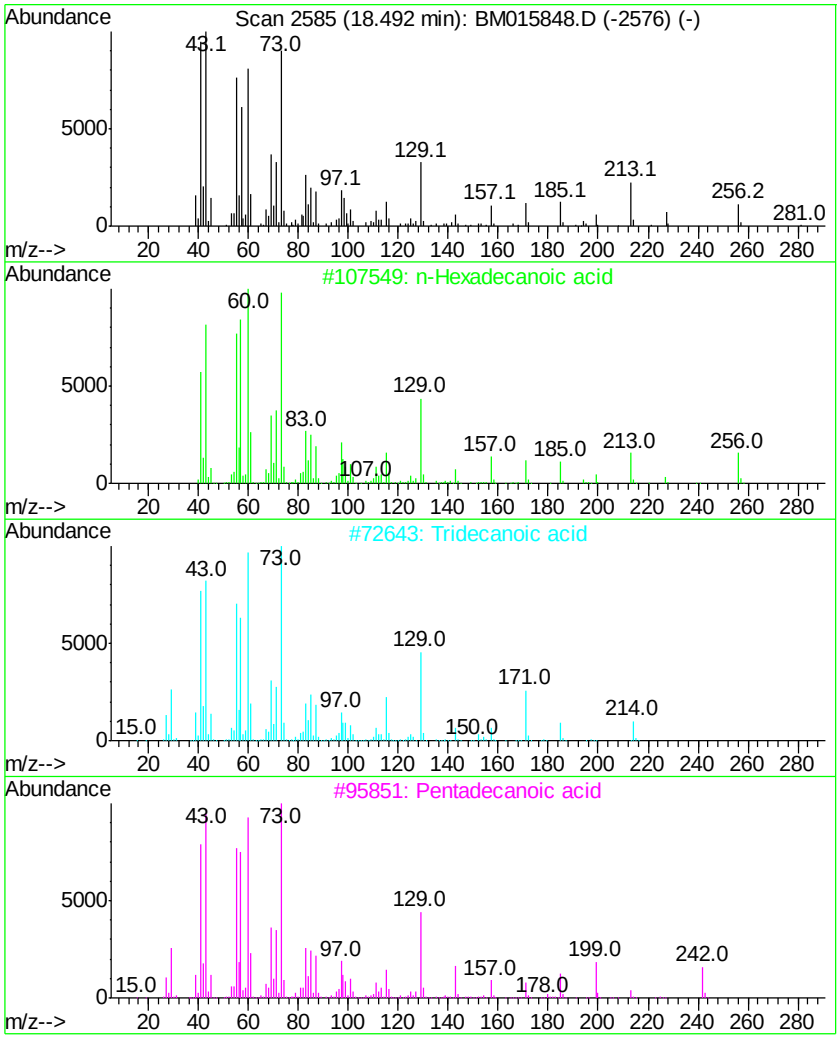
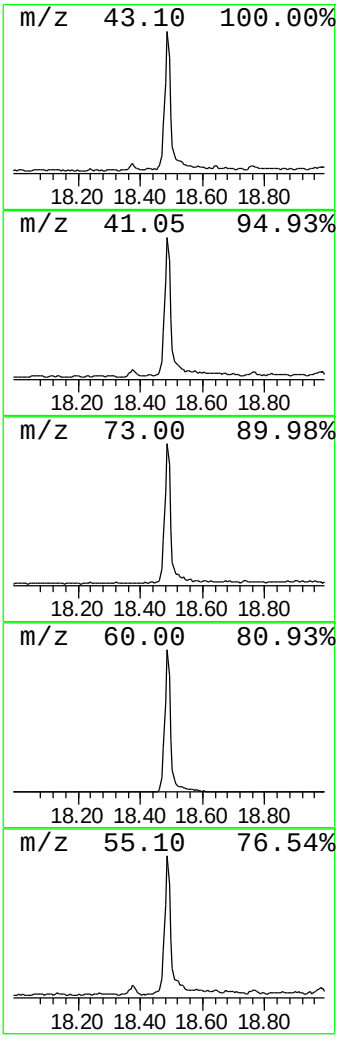
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.49	9.77 ng	691330	Phenanthrene-d10	17.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Undecanoic acid	186	C11H22O2	000112-37-8	58





Library Search Compound Report

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Sample : J3888-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : AOC7-BTM-6-6.5

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

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

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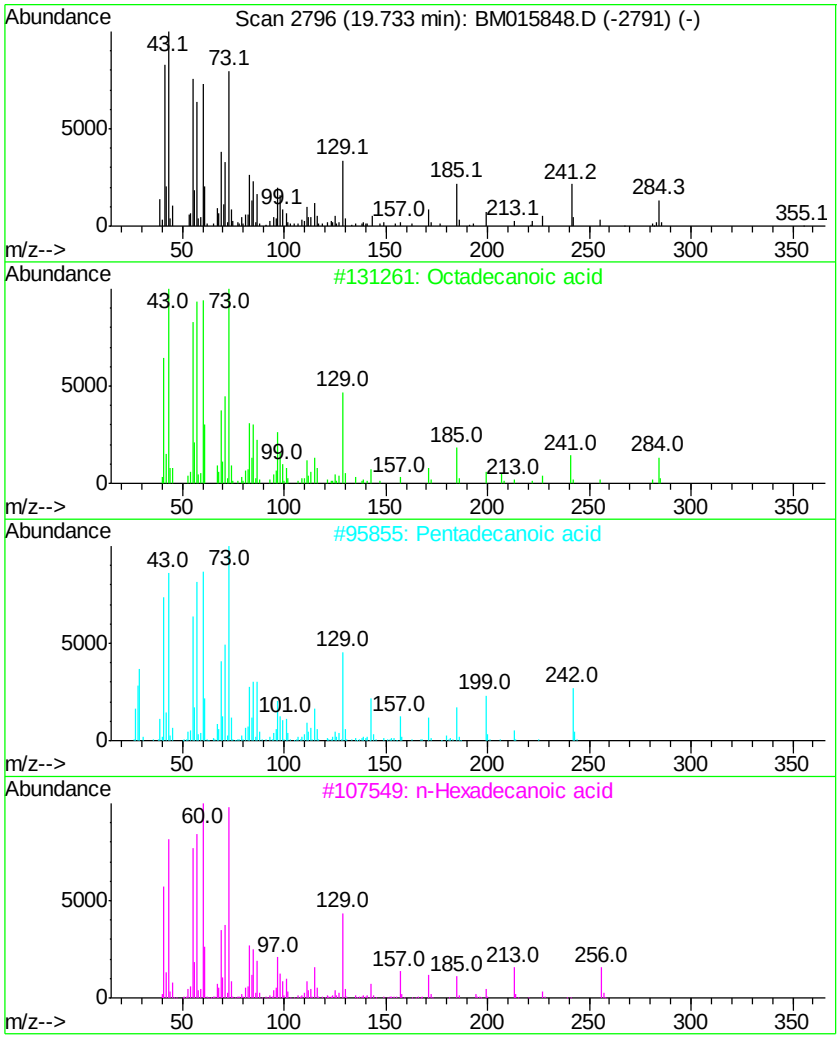
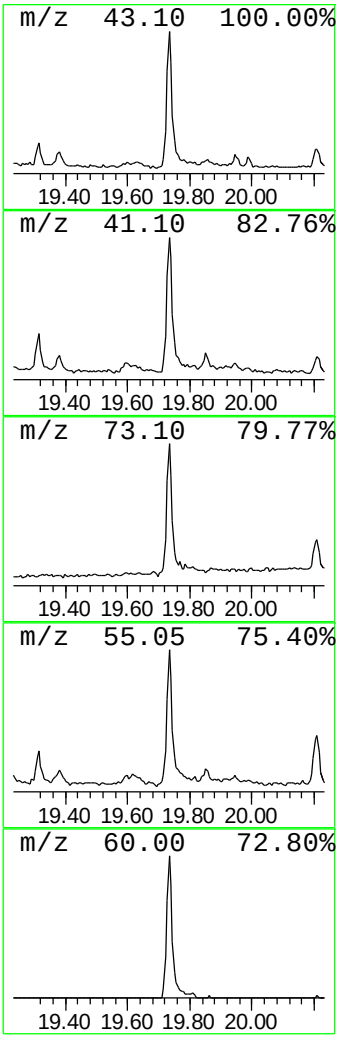
Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.73	4.53 ng	384109	Chrysene-d12	21.76

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	83
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	68
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	62





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Instrument : BNA_M
ClientSampleId : AOC7-BTM-6-6.5

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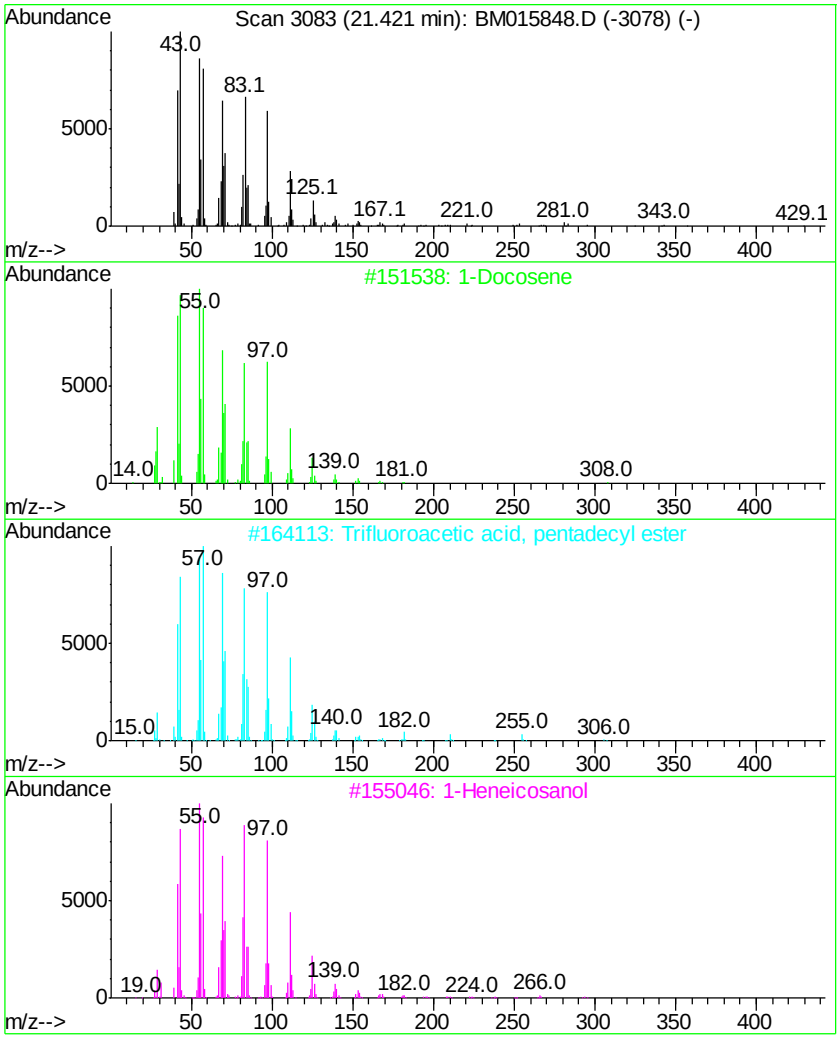
TIC Integration Parameters: LSCINT.P

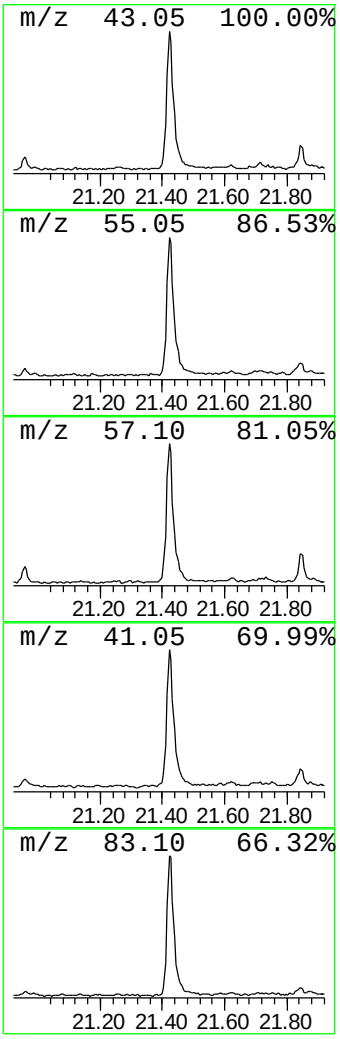
****

Peak Number 5 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.42	8.18 ng	693749	Chrysene-d12	21.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	94
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94





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	12.7	ng	425647	1	8.30	672577	20.0
unknown7.83	7.83	127.5	ng	4288430	1	8.30	672577	20.0
n-Hexadecanoic acid	18.49	9.8	ng	691330	4	17.64	1415710	20.0
Octadecanoic acid	19.73	4.5	ng	384109	5	21.76	1696100	20.0
1-Docosene	21.42	8.2	ng	693749	5	21.76	1696100	20.0