LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051117\
Data File : BM010004.D
Acq On : 12 May 2017 02:54
Operator : SJ/MA
Sample : I3079-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : AOC50MW002-170509

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:\HPCHEM1\BNA_M\METHODS\8270-BM051117.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	4.893	302	307	318	rBV	197188	292568	4.12%	0.903%
2	5.351	380	385	394	rBV	432119	659866	9.29%	2.037%
3	5.463	397	404	418	rVV	1777726	2615960	36.84%	8.074%
4	6.939	648	655	670	rBV	388989	704215	9.92%	2.173%
5	7.298	708	716	728	rBV	1152944	1888030	26.59%	5.827%
6	7.763	789	795	803	rBV	247598	407247	5.73%	1.257%
7	8.081	842	849	859	rBV	979659	1594292	22.45%	4.921%
8	8.933	986	994	1008	rBV	1062160	1785449	25.14%	5.510%
9	10.563	1262	1271	1272	rBV	400795	675432	9.51%	2.085%
10	11.439	1408	1420	1434	rBV	980740	1838431	25.89%	5.674%
11	13.027	1682	1690	1697	rBV	2608840	3618814	50.96%	11.169%
12	13.539	1771	1777	1788	rBV	290669	468758	6.60%	1.447%
13	14.415	1919	1926	1937	rBV2	524696	803927	11.32%	2.481%
14	15.815	2157	2164	2169	rBV2	79274	118257	1.67%	0.365%
15	15.874	2169	2174	2176	rVV	143727	210589	2.97%	0.650%
16	15.915	2176	2181	2195	rVB	2440483	3433629	48.35%	10.597%
17	17.168	2388	2394	2406	rBV	698115	1053460	14.84%	3.251%
18	18.045	2538	2543	2550	rBV	217486	304965	4.29%	0.941%
19	19.250	2744	2748	2756	rVB3	104114	166135	2.34%	0.513%
20	19.327	2757	2761	2771	rVB2	154271	208056	2.93%	0.642%
21	19.797	2835	2841	2847	rBV	5889648	7101165	100.00%	21.917%
22	21.050	3050	3054	3059	rBV5	80110	97491	1.37%	0.301%
23	21.356	3101	3106	3115	rBV	989477	1368138	19.27%	4.223%
24	23.650	3490	3496	3505	rBV	498396	985989	13.88%	3.043%

Sum of corrected areas: 32400863

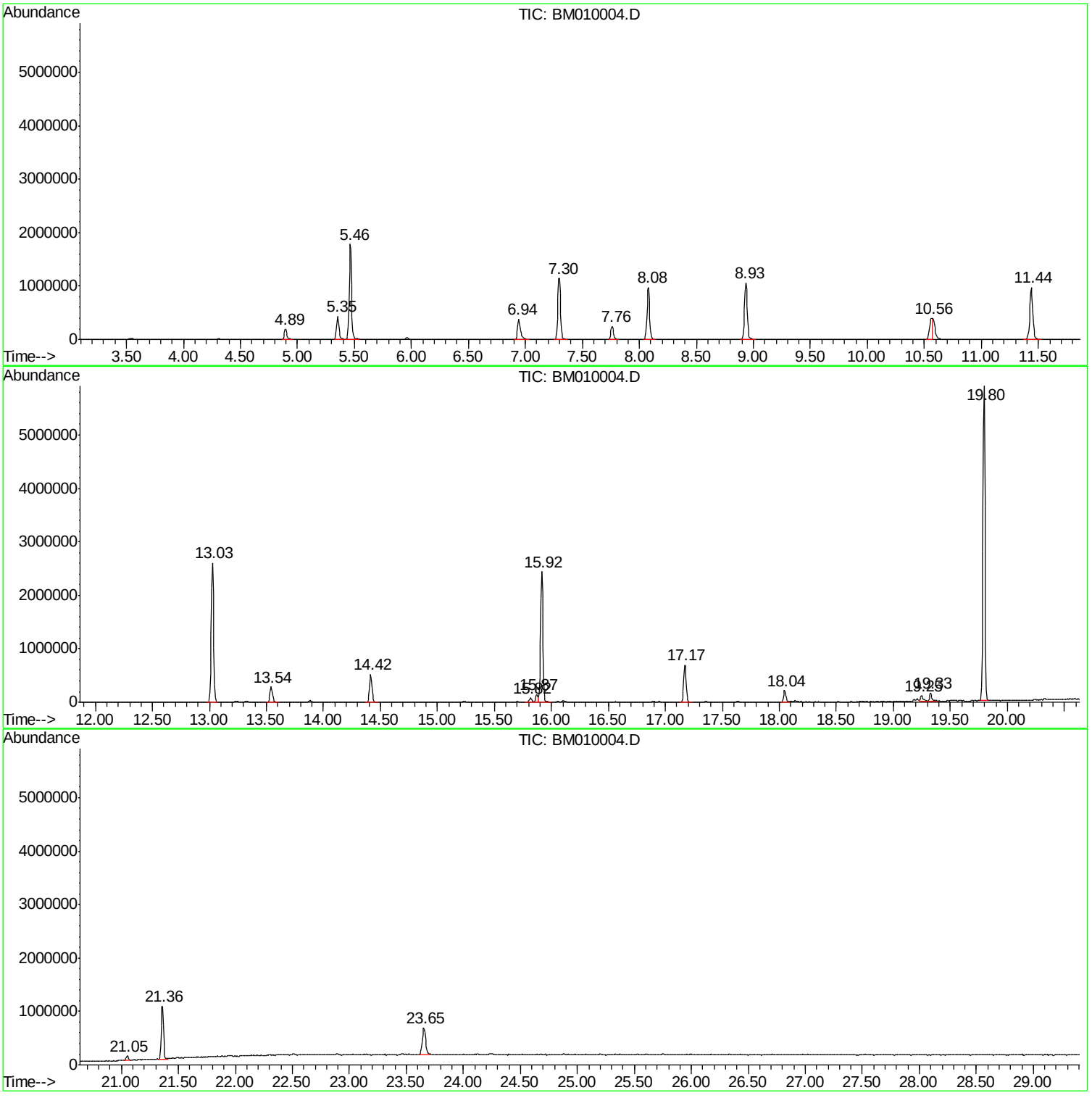
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051117\
Data File : BM010004.D
Acq On : 12 May 2017 02:54
Operator : SJ/MA
Sample : I3079-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AOC50MW002-170509

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.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

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051117\
Data File : BM010004.D
Acq On : 12 May 2017 02:54
Operator : SJ/MA
Sample : I3079-01
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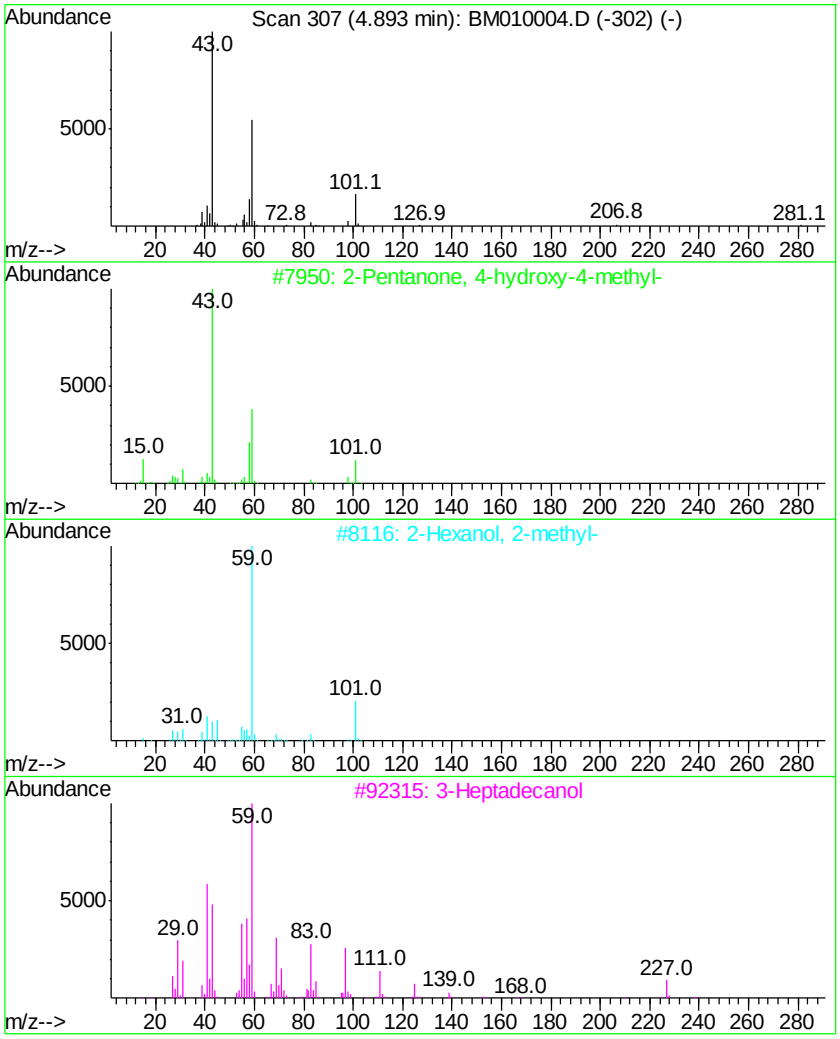
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

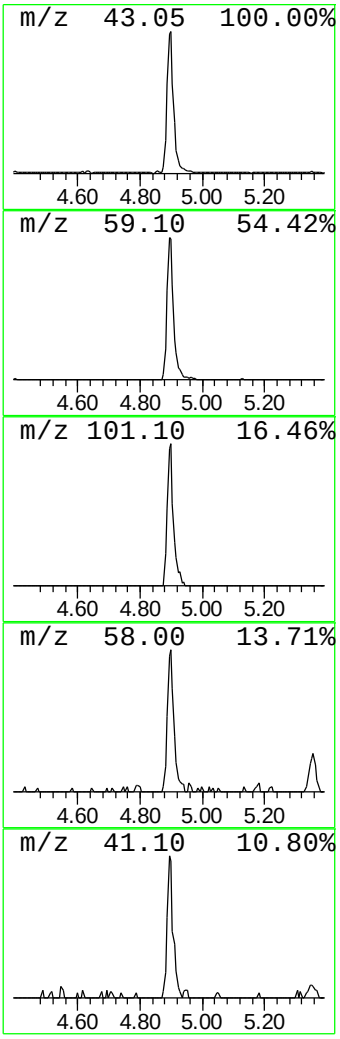
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	14.37 ng	292568	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3	3-Heptadecanol	256	C17H36O	084534-30-5	28
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051117\
Data File : BM010004.D
Acq On : 12 May 2017 02:54
Operator : SJ/MA
Sample : I3079-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : AOC50MW002-170509

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

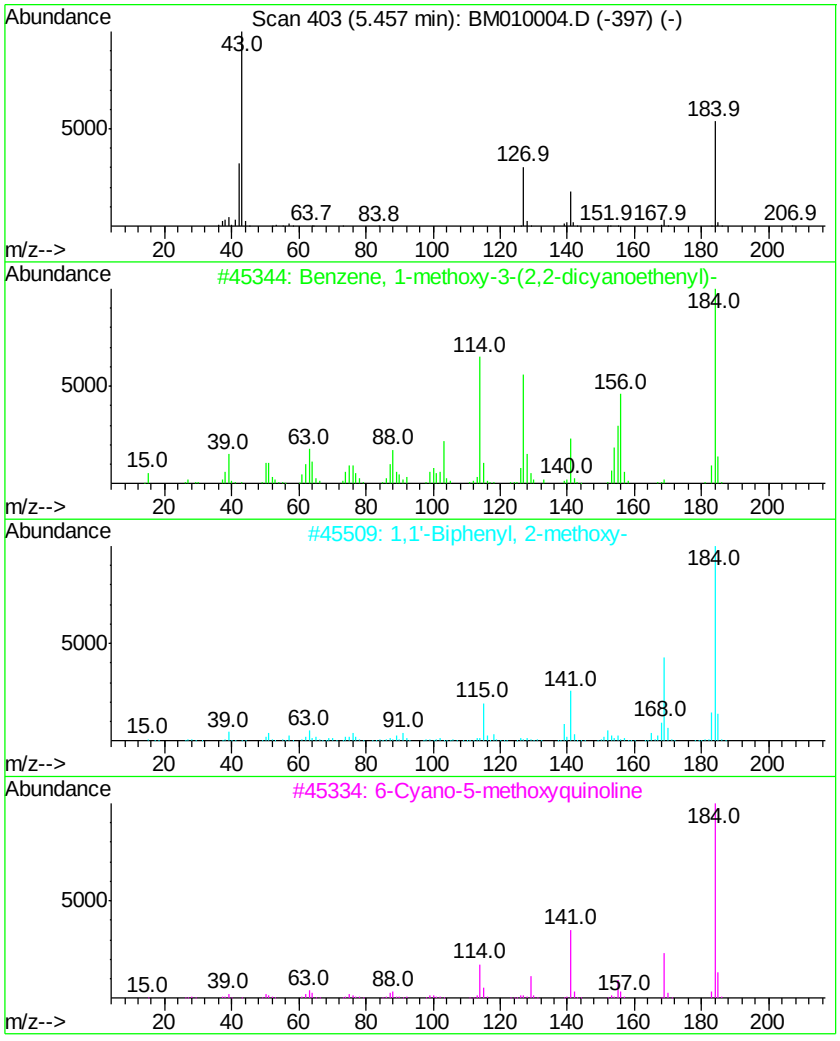
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

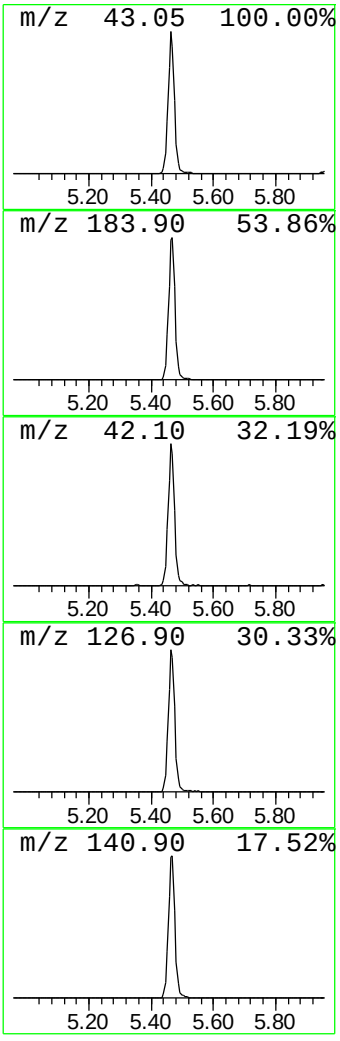
****

Peak Number 2 unknown5.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.46	128.47 ng	2615960	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methoxy-3-(2,2-dicyan...	184	C11H8N2O	002972-72-7	25
2	1,1'-Biphenyl, 2-methoxy-	184	C13H12O	000086-26-0	9
3	6-Cyano-5-methoxyquinoline	184	C11H8N2O	1000241-27-7	9
4	4H-1,3-Oxazine, 5,6-dihydro-2,4,...	141	C8H15NO	026939-18-4	9
5	2-Amino-5-nitropyrimidine	140	C4H4N4O2	003073-77-6	9





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Acq On : 12 May 2017 02:54
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Sample : I3079-01
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ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : AOC50MW002-170509

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.M
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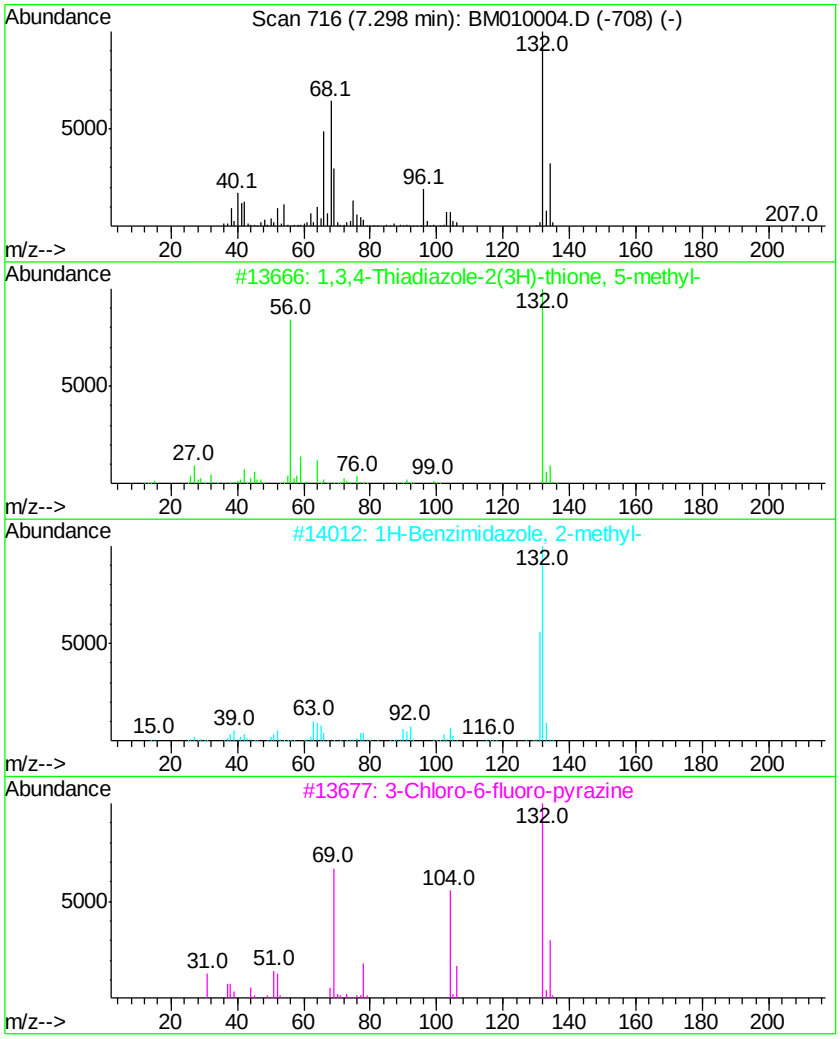
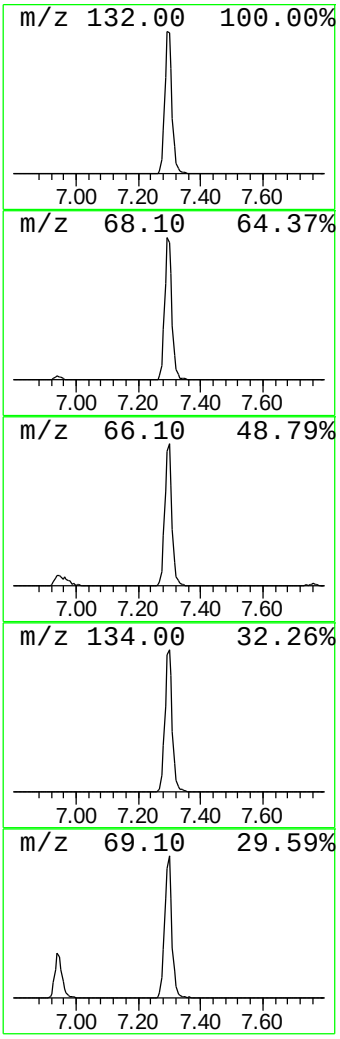
****

Peak Number 3 unknown7.30 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.30	92.72 ng	1888030	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	14
5	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14





Data Path : Z:\HPCHEM1\BNA M\DATA\BM051117\
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Operator : SJ/MA
Sample : I3079-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : AOC50MW002-170509

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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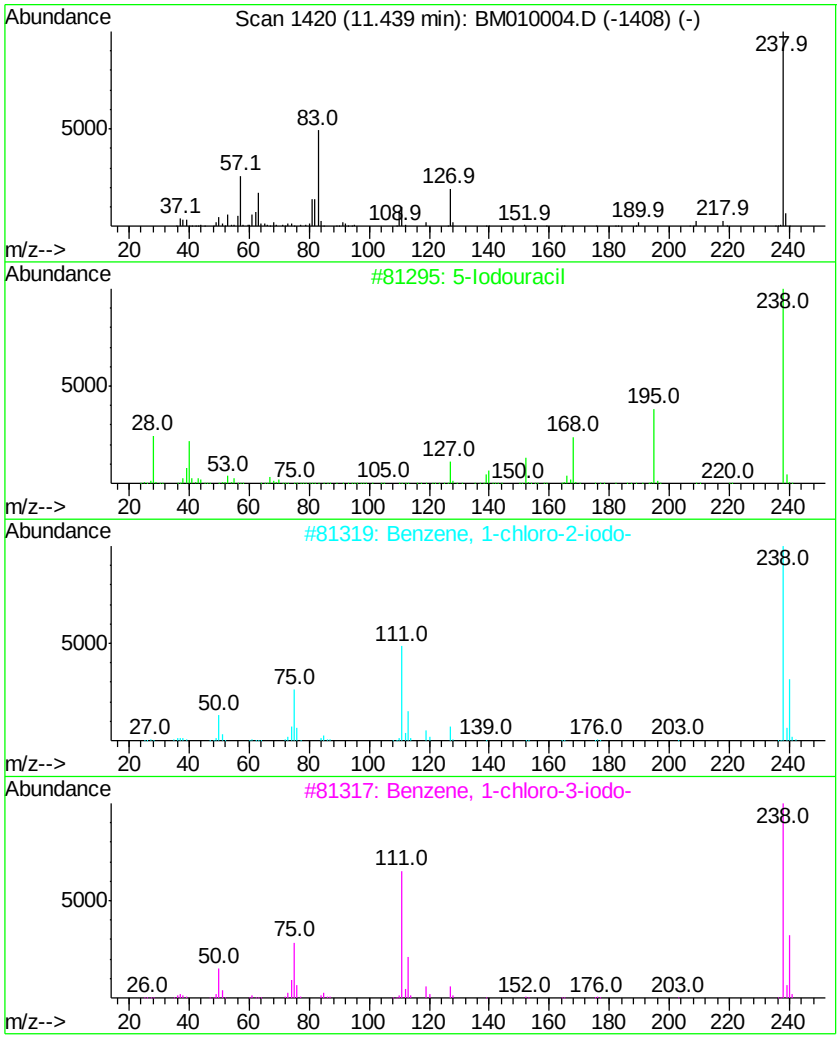
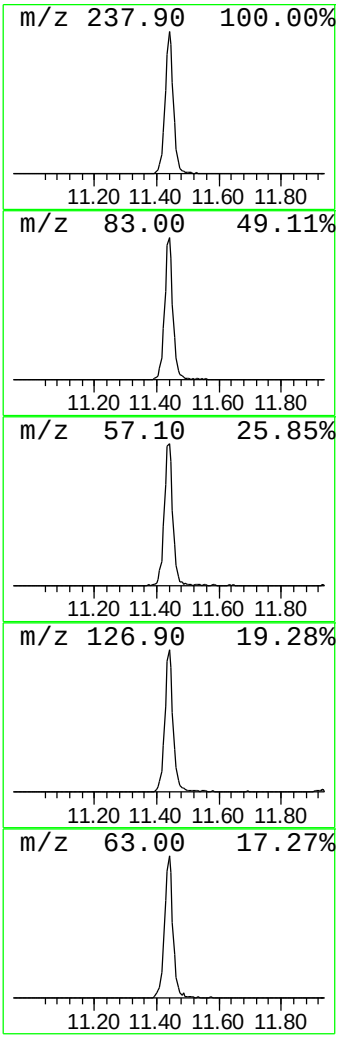
****

Peak Number 5 unknown11.44 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.44	54.44 ng	1838430	Naphthalene-d8	10.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Iodouracil	238	C4H3IN2O2	000696-07-1	38
2	Benzene, 1-chloro-2-iodo-	238	C6H4ClI	000615-41-8	9
3	Benzene, 1-chloro-3-iodo-	238	C6H4ClI	000625-99-0	9
4	9,10-Anthracenedione, 1,4-diamino-	238	C14H10N2O2	000128-95-0	9
5	Benzene, 1-chloro-4-iodo-	238	C6H4ClI	000637-87-6	9





Data Path : Z:\HPCHEM1\BNA M\DATA\BM051117\
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Sample : I3079-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : AOC50MW002-170509

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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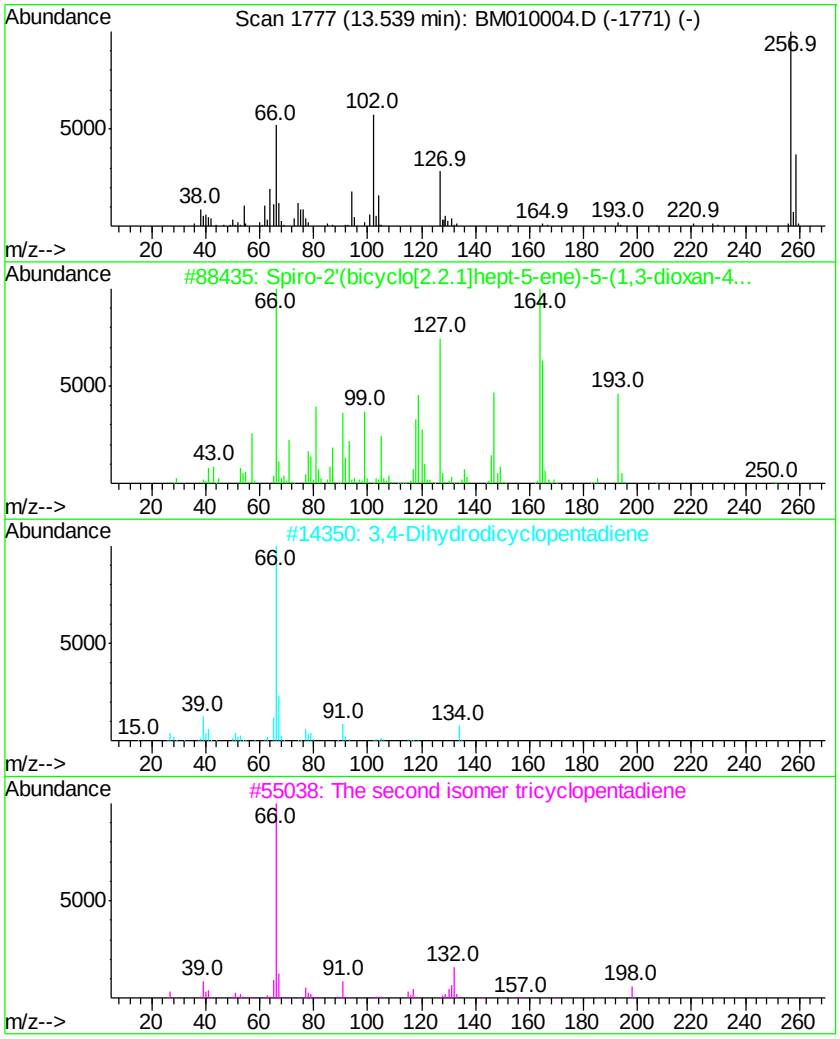
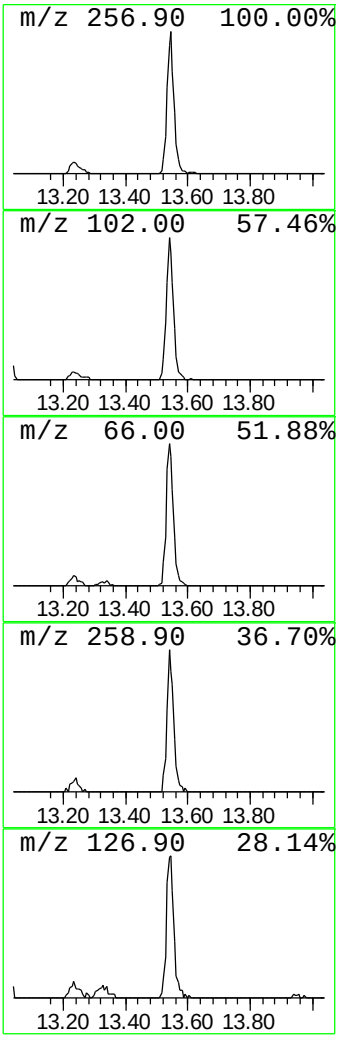
****

Peak Number 6 unknown13.54 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.54	11.66 ng	468758	Acenaphthene-d10	14.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Spiro-2'(bicyclo[2.2.1]hept-5-en...	250	C15H22O3	1000188-54-9	25
2	3,4-Dihydrodicyclopentadiene	134	C10H14	1000113-53-5	16
3	The second isomer tricyclopentad...	198	C15H18	1000222-21-1	16
4	4,7-Methano-1H-indene, 3a,4,7,7a...	132	C10H12	000077-73-6	16
5	Bicyclo[2.2.2]oct-7-ene-2,5-dione	136	C8H8O2	017660-74-1	12





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051117\
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Sample : I3079-01
Misc :
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Instrument : BNA_M
ClientSampleId : AOC50MW002-170509

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.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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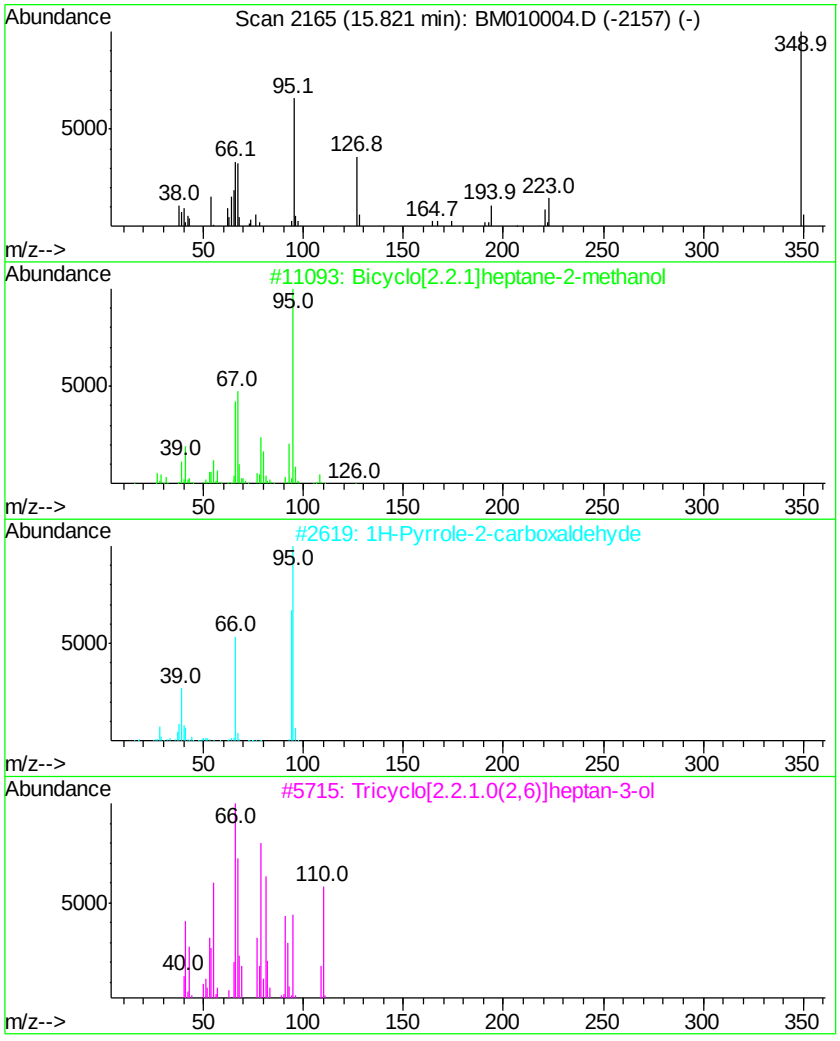
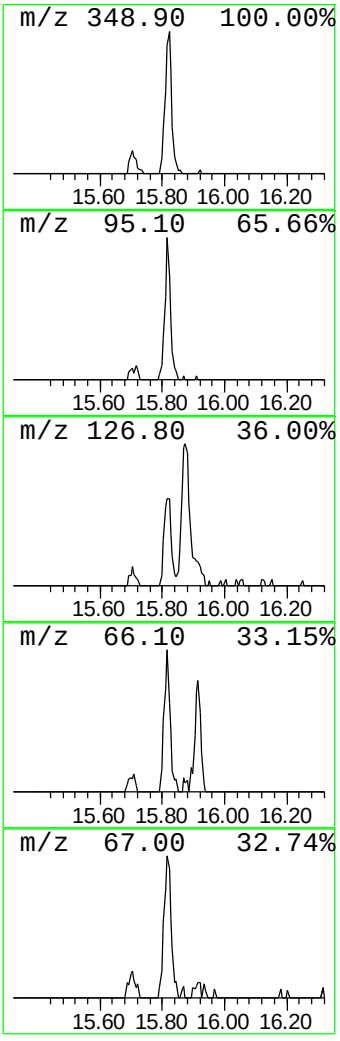
Peak Number 7 unknown15.82 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.82	2.25 ng	118257	Phenanthrene-d10	17.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptane-2-methanol	126	C8H14O	005240-72-2	43
2	1H-Pyrrole-2-carboxaldehyde	95	C5H5NO	001003-29-8	32
3	Tricyclo[2.2.1.0(2,6)]heptan-3-ol	110	C7H10O	000695-04-5	12
4	Bicyclo[2.2.1]hept-5-ene-2-carbo...	131	C9H9N	112893-81-9	12
5	2-Cyclohexen-1-one, oxime	111	C6H9NO	003349-62-0	12





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TIC Library : C:\DATABASE\NIST02.L
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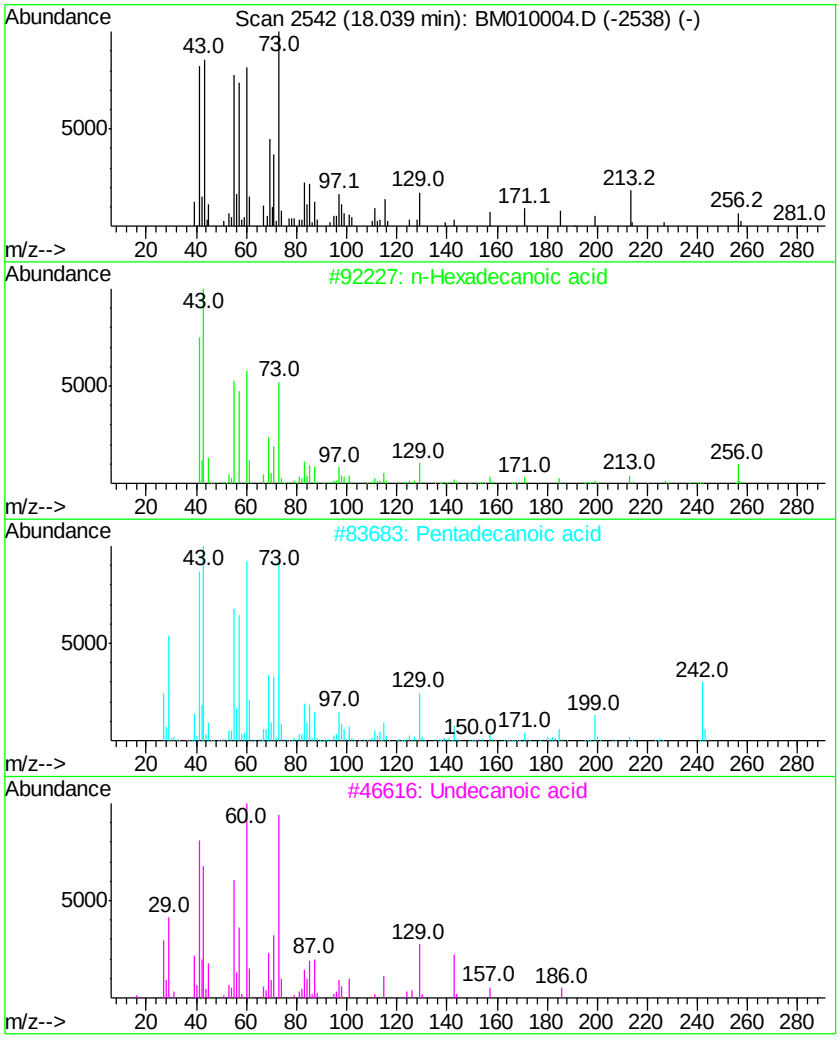
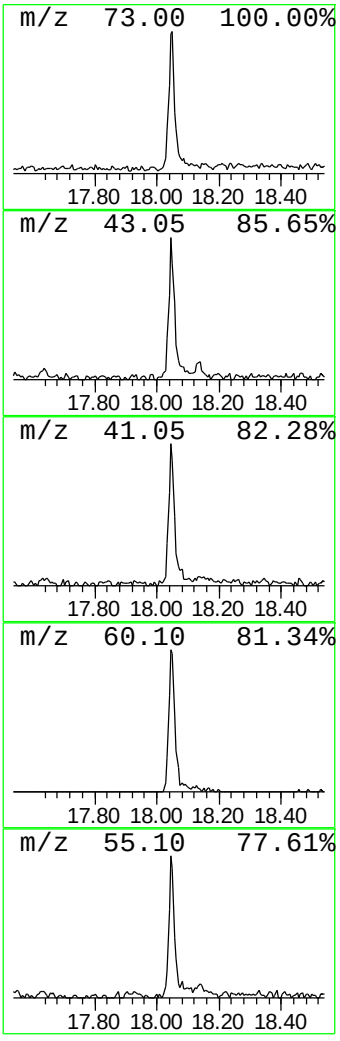
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.04	5.79 ng	304965	Phenanthrene-d10	17.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Undecanoic acid	186	C11H22O2	000112-37-8	72
4	12-Bromododecanoic acid	278	C12H23BrO2	073367-80-3	72
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





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TIC Library : C:\DATABASE\NIST02.L
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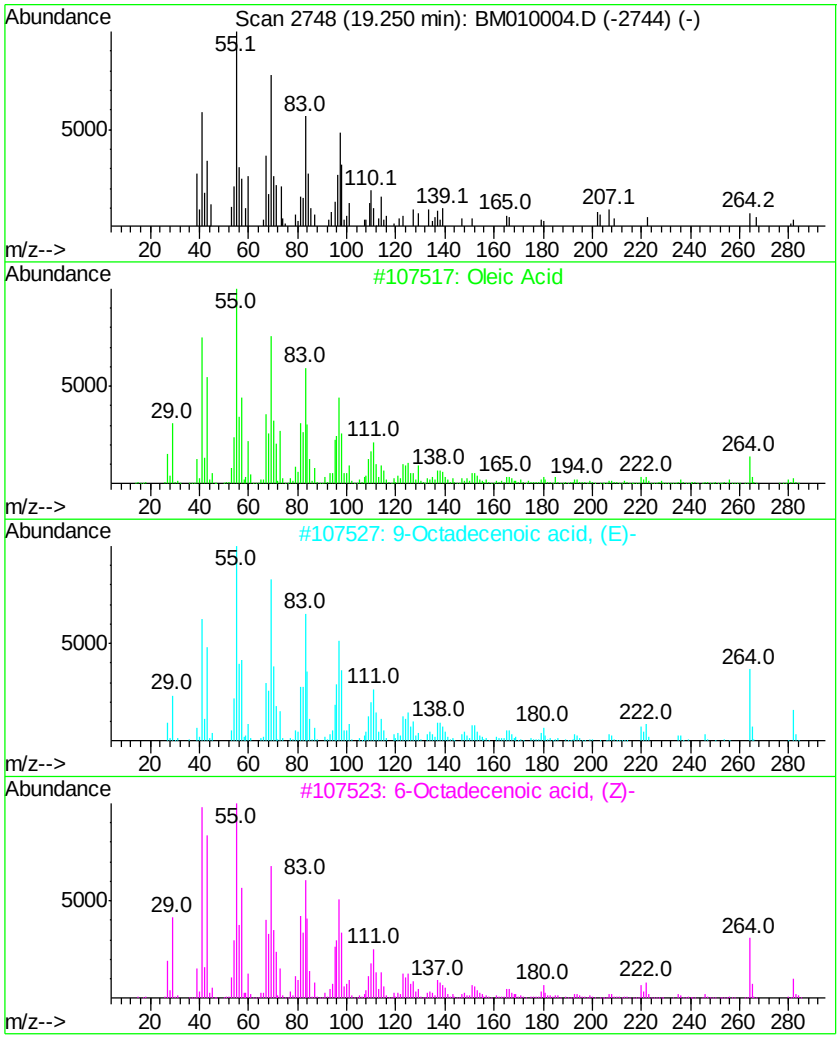
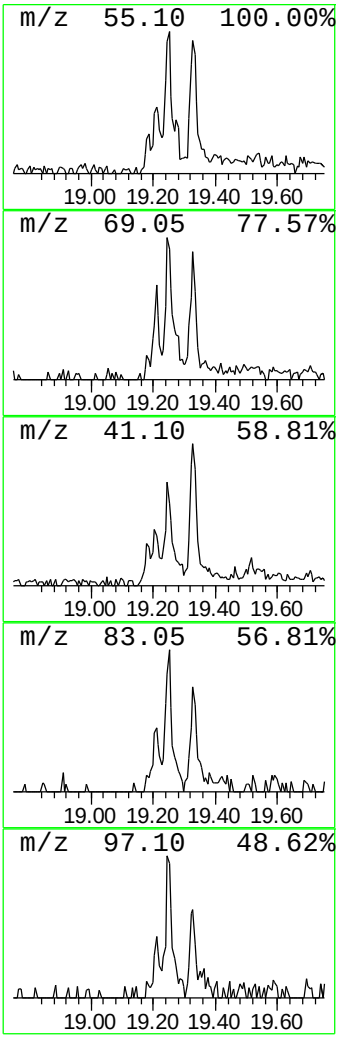
Peak Number 9 Oleic Acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.25	3.15 ng	166135	Phenanthrene-d10	17.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oleic Acid	282	C18H34O2	000112-80-1	93
2	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	89
3	6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	43
4	3-Undecanol, 2,3-dimethyl-	200	C13H28O	1000149-68-6	43
5	3,7-Nonadien-2-one, 4,8-dimethyl-	166	C11H18O	000817-88-9	38





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Instrument : BNA_M
ClientSampleId : AOC50MW002-170509

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

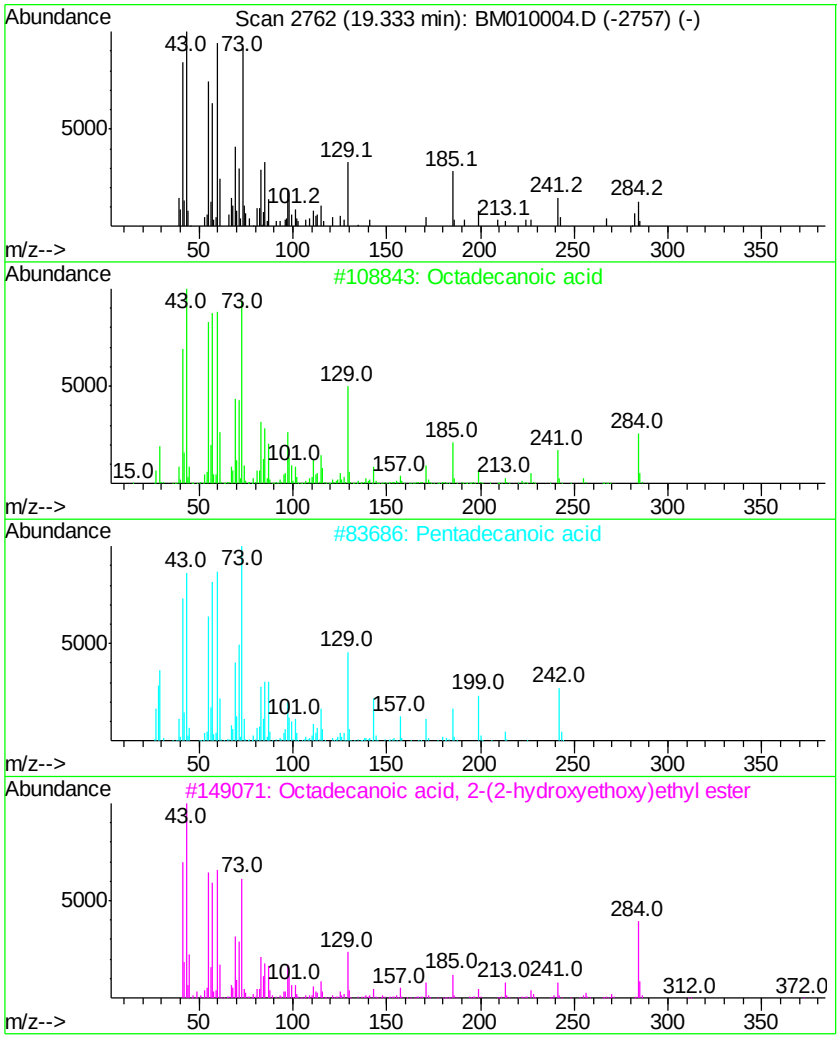
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

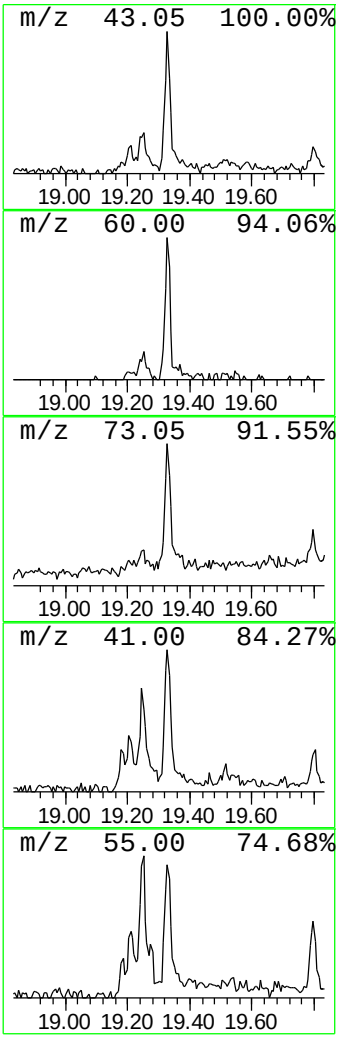
****

Peak Number 10 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.33	3.04 ng	208056	Chrysene-d12	21.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM051117\
Data File : BM010004.D
Acq On : 12 May 2017 02:54
Operator : SJ/MA
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Misc :
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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.89	14.4	ng	292568	1	7.76	407247	20.0
unknown5.46	5.46	128.5	ng	2615960	1	7.76	407247	20.0
unknown7.30	7.30	92.7	ng	1888030	1	7.76	407247	20.0
unknown11.44	11.44	54.4	ng	1838430	2	10.56	675432	20.0
unknown13.54	13.54	11.7	ng	468758	3	14.42	803927	20.0
unknown15.82	15.82	2.3	ng	118257	4	17.17	1053460	20.0
n-Hexadecanoic acid	18.04	5.8	ng	304965	4	17.17	1053460	20.0
Oleic Acid	19.25	3.1	ng	166135	4	17.17	1053460	20.0
Octadecanoic acid	19.33	3.0	ng	208056	5	21.36	1368140	20.0