LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051217\
Data File : BM010032.D
Acq On : 12 May 2017 20:17
Operator : SJ/MA
Sample : I3100-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PMW-1A-051017

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	303	307	315	rBV	129157	187635	2.26%	0.592%
2	5.351	379	385	395	rBV	752933	1208482	14.56%	3.813%
3	6.939	650	655	668	rVB	501709	843124	10.16%	2.660%
4	7.292	709	715	726	rBV	1614994	2533068	30.53%	7.992%
5	7.757	788	794	803	rBV	296035	483298	5.82%	1.525%
6	8.075	838	848	857	rBV	1389409	2198648	26.50%	6.937%
7	8.933	987	994	1006	rBV	1319817	2215412	26.70%	6.990%
8	10.551	1257	1269	1276	rBV	390696	687015	8.28%	2.168%
9	13.021	1683	1689	1698	rBV	2887112	4353057	52.46%	13.735%
10	13.874	1828	1834	1839	rBV	69716	107058	1.29%	0.338%
11	14.415	1920	1926	1933	rBV3	518290	836227	10.08%	2.639%
12	15.915	2174	2181	2197	rBV	2782406	4027022	48.53%	12.706%
13	17.168	2388	2394	2405	rVB	750344	1069655	12.89%	3.375%
14	18.045	2538	2543	2552	rBV	102610	159563	1.92%	0.503%
15	19.321	2757	2760	2768	rBV3	101371	150687	1.82%	0.475%
16	19.792	2834	2840	2846	rBV	6818049	8297529	100.00%	26.181%
17	21.044	3049	3053	3059	rBV7	66202	99918	1.20%	0.315%
18	21.356	3101	3106	3112	rBV	996334	1277278	15.39%	4.030%
19	23.650	3490	3496	3506	rVB	484924	958467	11.55%	3.024%

Sum of corrected areas: 31693143

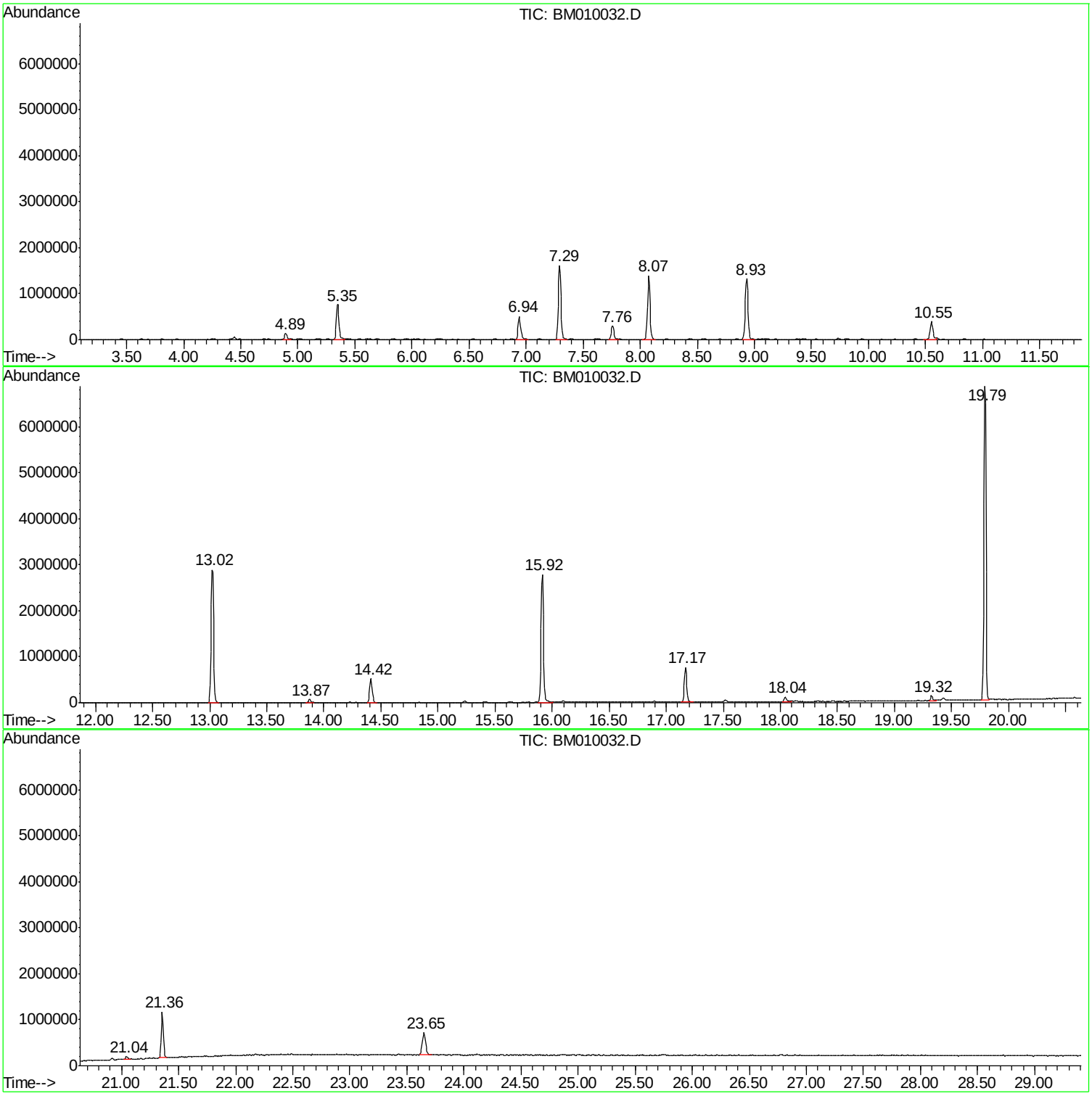
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051217\
Data File : BM010032.D
Acq On : 12 May 2017 20:17
Operator : SJ/MA
Sample : I3100-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PMW-1A-051017

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\BM051217\
Data File : BM010032.D
Acq On : 12 May 2017 20:17
Operator : SJ/MA
Sample : I3100-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PMW-1A-051017

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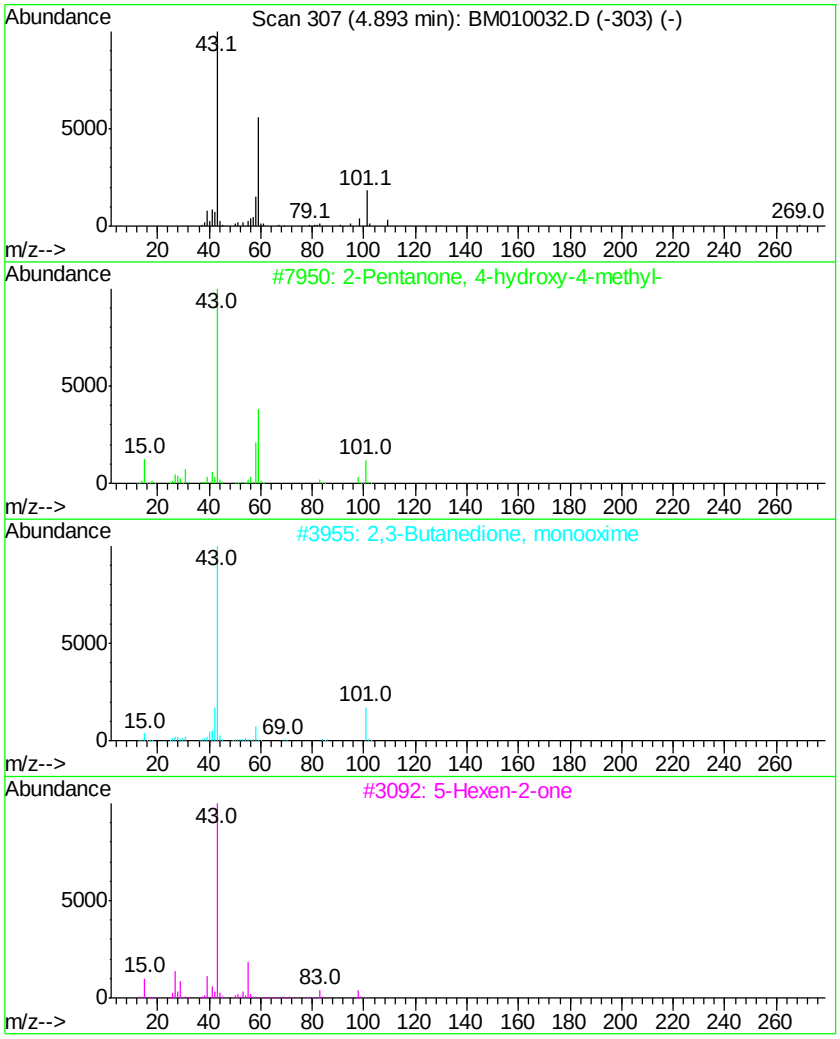
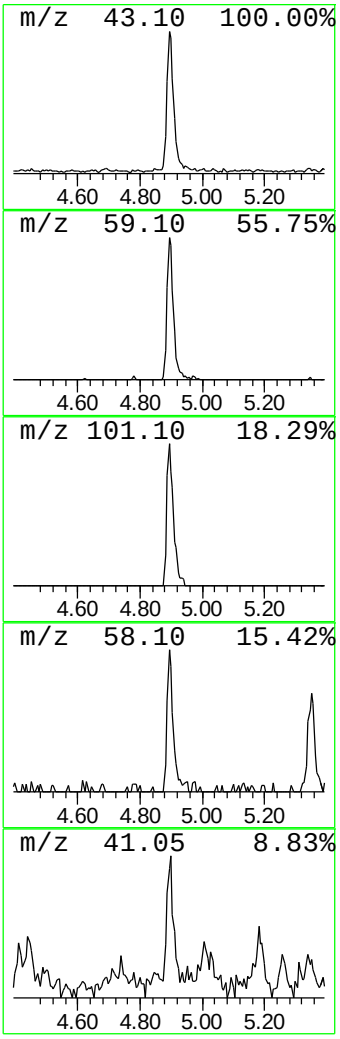
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	7.76 ng	187635	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	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3	5-Hexen-2-one	98	C6H10O	000109-49-9	10
4	Acetamide	59	C2H5NO	000060-35-5	9
5	2-Propanone, 1-cyclopropyl-	98	C6H10O	004160-75-2	9





Library Search Compound Report

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Data File : BM010032.D
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Sample : I3100-02
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PMW-1A-051017

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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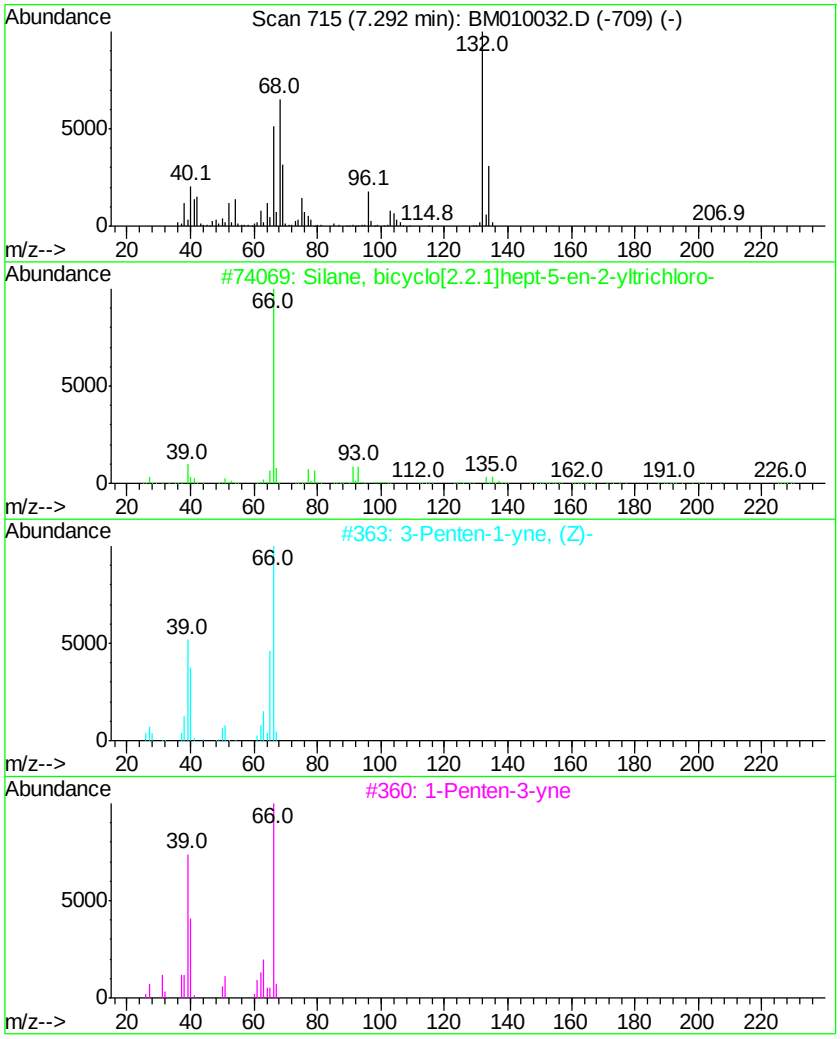
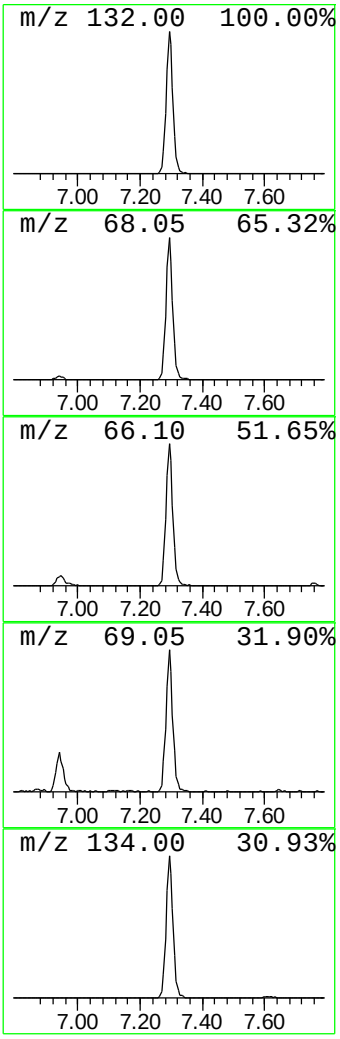
Peak Number 2 unknown7.29 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.29	104.82 ng	2533070	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, bicyclo[2.2.1]hept-5-en-...	226	C7H9Cl3Si	014319-64-3	35
2	3-Penten-1-yne, (Z)-	66	C5H6	001574-40-9	35
3	1-Penten-3-yne	66	C5H6	000646-05-9	35
4	5-Norbornene-2-methanol	124	C8H12O	000095-12-5	25
5	1,4,4a,8a-Tetrahydro-1,4-methano...	174	C11H10O2	001200-89-1	25





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051217\
Data File : BM010032.D
Acq On : 12 May 2017 20:17
Operator : SJ/MA
Sample : I3100-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PMW-1A-051017

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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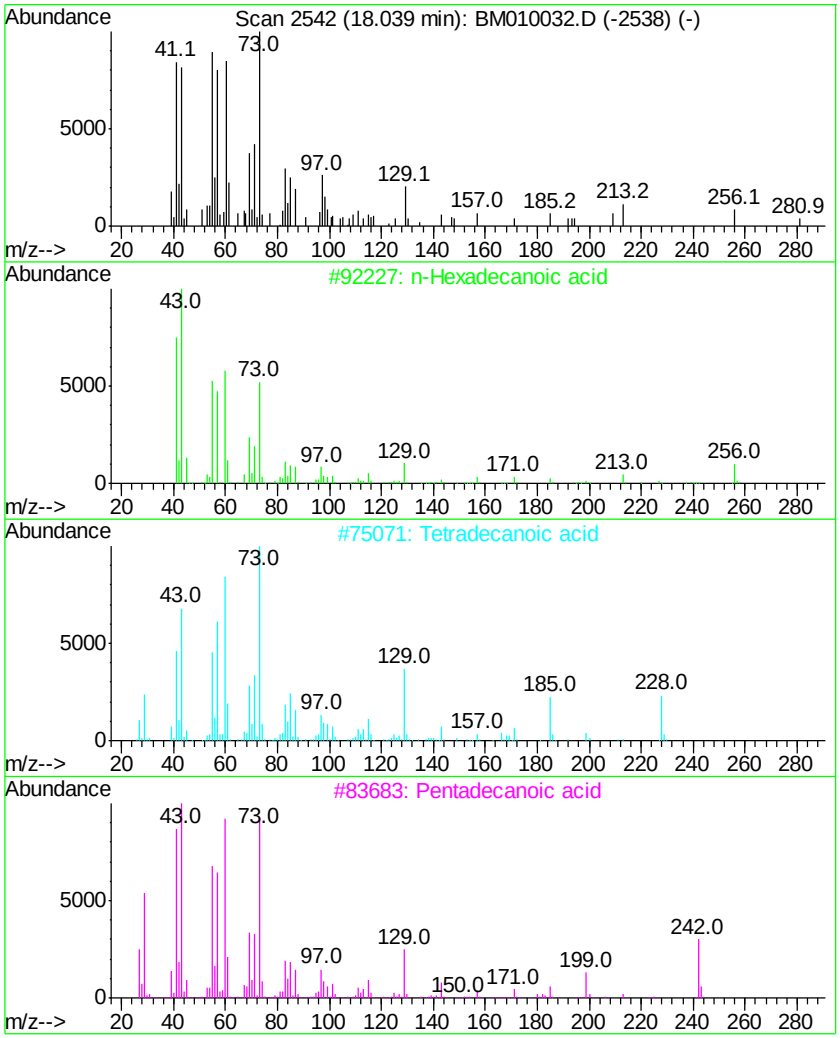
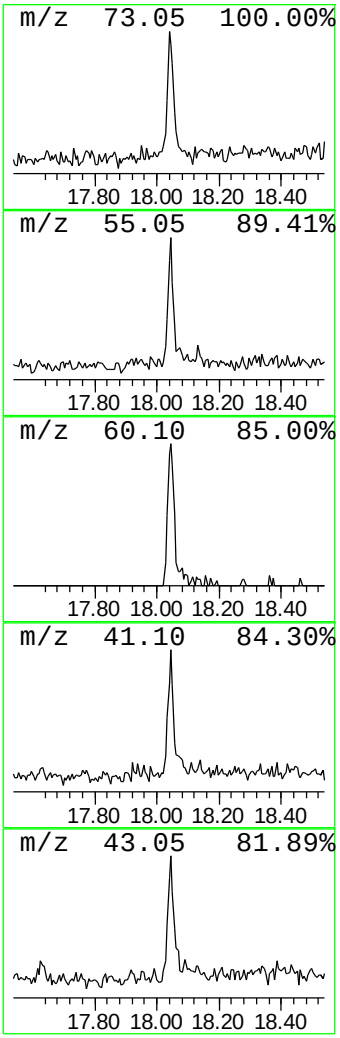
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.04	2.98 ng	159563	Phenanthrene-d10	17.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Undecanoic acid	186	C11H22O2	000112-37-8	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





Library Search Compound Report

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Data File : BM010032.D
Acq On : 12 May 2017 20:17
Operator : SJ/MA
Sample : I3100-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PMW-1A-051017

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

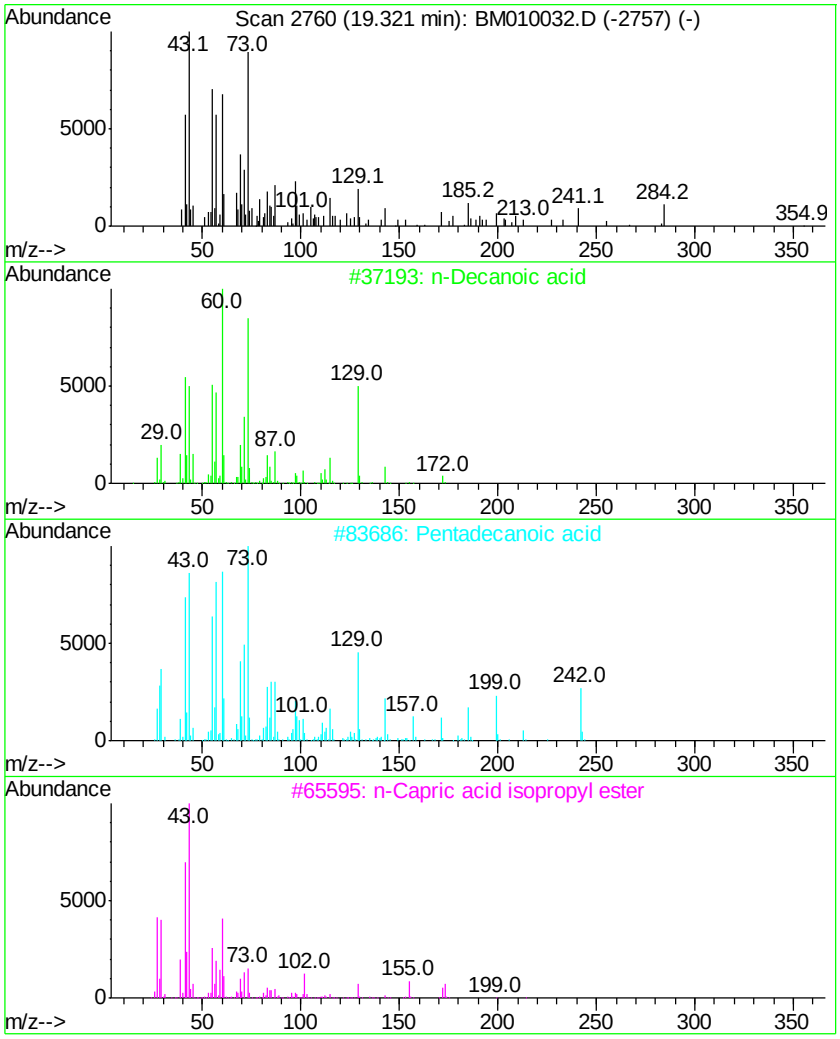
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

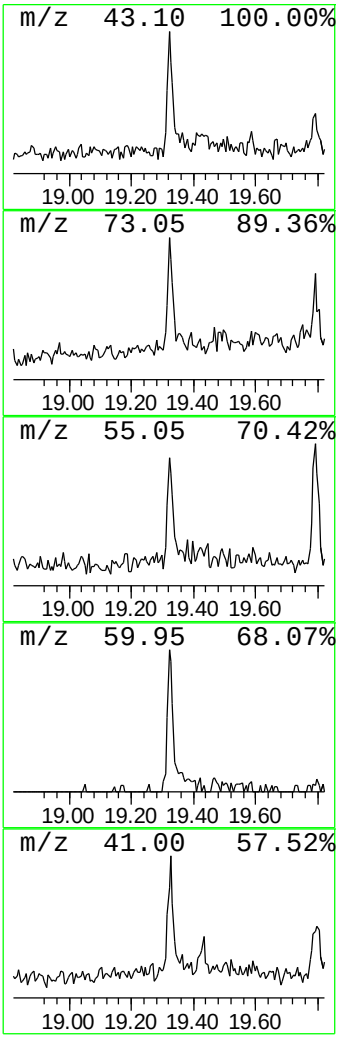
****

Peak Number 5 n-Decanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.32	2.36 ng	150687	Chrysene-d12	21.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	50
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	50
3	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	38
4	Tridecanoic acid	214	C13H26O2	000638-53-9	38
5	Heptanoic acid	130	C7H14O2	000111-14-8	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM051217\
Data File : BM010032.D
Acq On : 12 May 2017 20:17
Operator : SJ/MA
Sample : I3100-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PMW-1A-051017

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	4.89	7.8	ng	187635	1	7.76	483298	20.0
unknown7.29	7.29	104.8	ng	2533070	1	7.76	483298	20.0
n-Hexadecanoic acid	18.04	3.0	ng	159563	4	17.17	1069660	20.0
n-Decanoic acid	19.32	2.4	ng	150687	5	21.36	1277280	20.0