LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM072617\
Data File : BM010992.D
Acq On : 27 Jul 2017 04:00
Operator : SJ/JU
Sample : I4391-03
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BU-02-072117-A

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-BM072617.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	3.440	108	111	121	rVB	340663	402251	2.56%	0.439%
2	4.016	204	209	215	rBV	776285	951311	6.05%	1.038%
3	4.128	223	228	234	rBV	559300	757547	4.82%	0.827%
4	4.593	301	307	315	rBV	251132	377749	2.40%	0.412%
5	5.034	376	382	389	rBV	5614924	7652781	48.69%	8.354%
6	6.593	635	647	660	rBV2	4777085	8503185	54.11%	9.282%
7	6.934	697	705	713	rBV	5732157	8683048	55.25%	9.479%
8	7.393	775	783	790	rBV	1006960	1534102	9.76%	1.675%
9	7.704	829	836	846	rBV	4389675	6759043	43.01%	7.378%
10	7.963	875	880	888	rVB3	160178	266187	1.69%	0.291%
11	8.540	970	978	987	rVB	3751196	5878388	37.40%	6.417%
12	8.981	1048	1053	1069	rBV2	183950	333354	2.12%	0.364%
13	10.151	1243	1252	1257	rBV	1180907	1936876	12.32%	2.114%
14	10.198	1257	1260	1268	rVB2	118481	183708	1.17%	0.201%
15	11.469	1470	1476	1482	rBV	98445	170035	1.08%	0.186%
16	12.657	1671	1678	1685	rBV	8629684	12663507	80.58%	13.824%
17	14.045	1908	1914	1922	rBV2	1364095	2152712	13.70%	2.350%
18	15.551	2163	2170	2180	rBV	8013708	10633251	67.66%	11.608%
19	16.804	2377	2383	2389	rBV2	2092497	2830038	18.01%	3.089%
20	19.027	2757	2761	2768	rBV	163823	246891	1.57%	0.270%
21	19.468	2827	2836	2842	rBV	13347157	15716056	100.00%	17.156%
22	21.021	3095	3100	3107	rBV	1744245	2230407	14.19%	2.435%
23	23.139	3456	3460	3468	rVB5	334129	742922	4.73%	0.811%

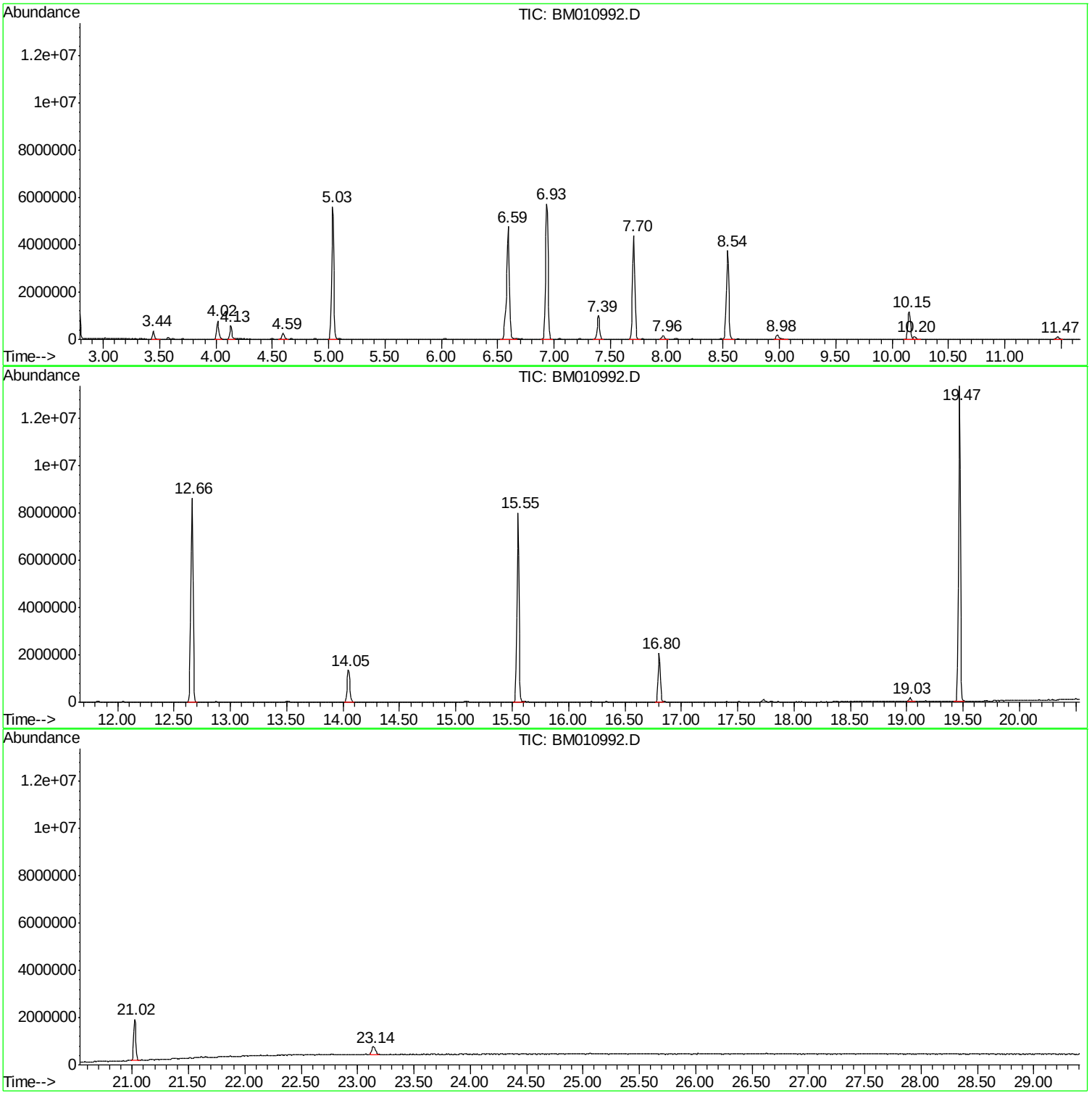
Sum of corrected areas: 91605349

Data Path : Z:\HPCHEM1\BNA M\DATA\BM072617\
Data File : BM010992.D
Acq On : 27 Jul 2017 04:00
Operator : SJ/JU
Sample : I4391-03
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BU-02-072117-A

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM072617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA M\DATA\BM072617\
Data File : BM010992.D
Acq On : 27 Jul 2017 04:00
Operator : SJ/JU
Sample : I4391-03
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BU-02-072117-A

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM072617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

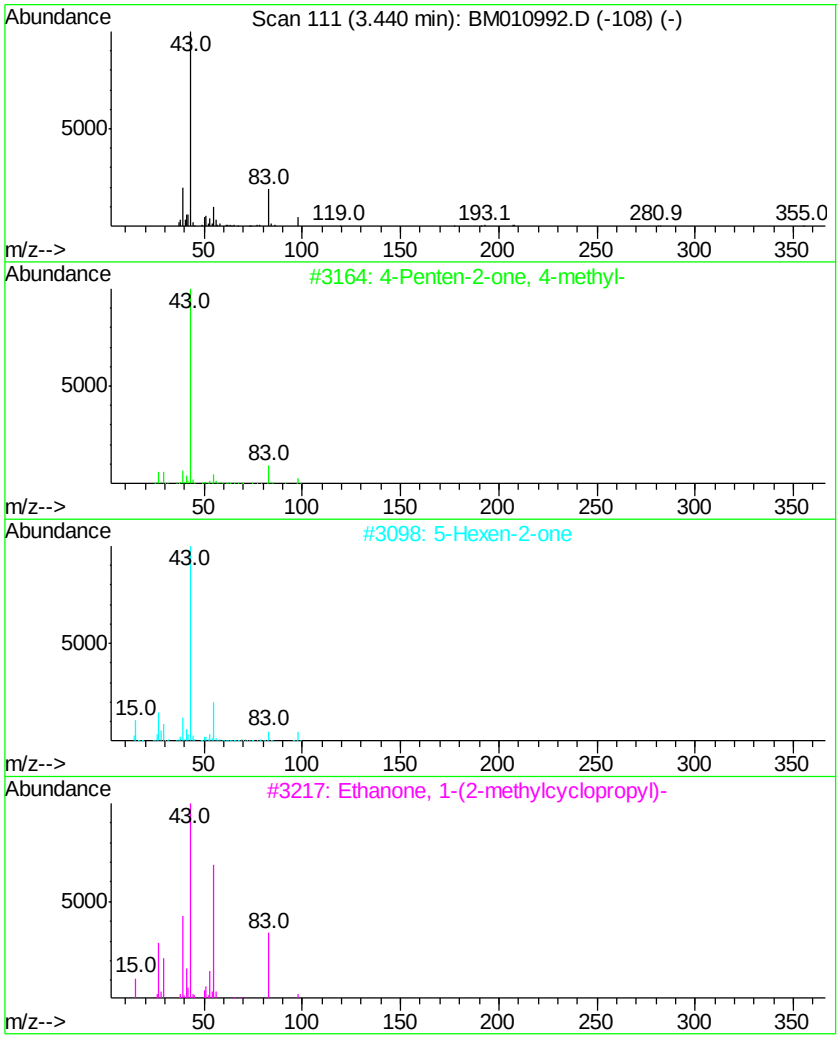
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

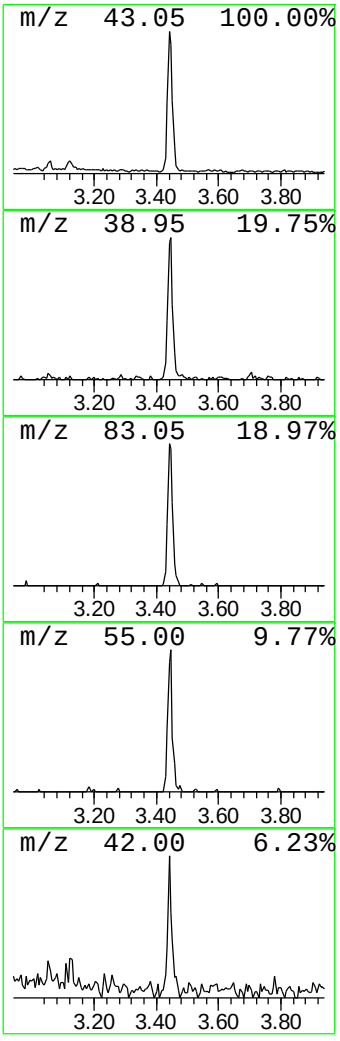
****

Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.44	5.24 ng	402251	1,4-Dichlorobenzene-d4	7.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	50
2	5-Hexen-2-one	98	C6H10O	000109-49-9	42
3	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	25
4	2-Propanone, 1-cyclopropyl-	98	C6H10O	004160-75-2	9
5	3,5-Hexadien-2-ol	98	C6H10O	003280-51-1	9





Data Path : Z:\HPCHEM1\BNA M\DATA\BM072617\
Data File : BM010992.D
Acq On : 27 Jul 2017 04:00
Operator : SJ/JU
Sample : I4391-03
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BU-02-072117-A

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM072617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

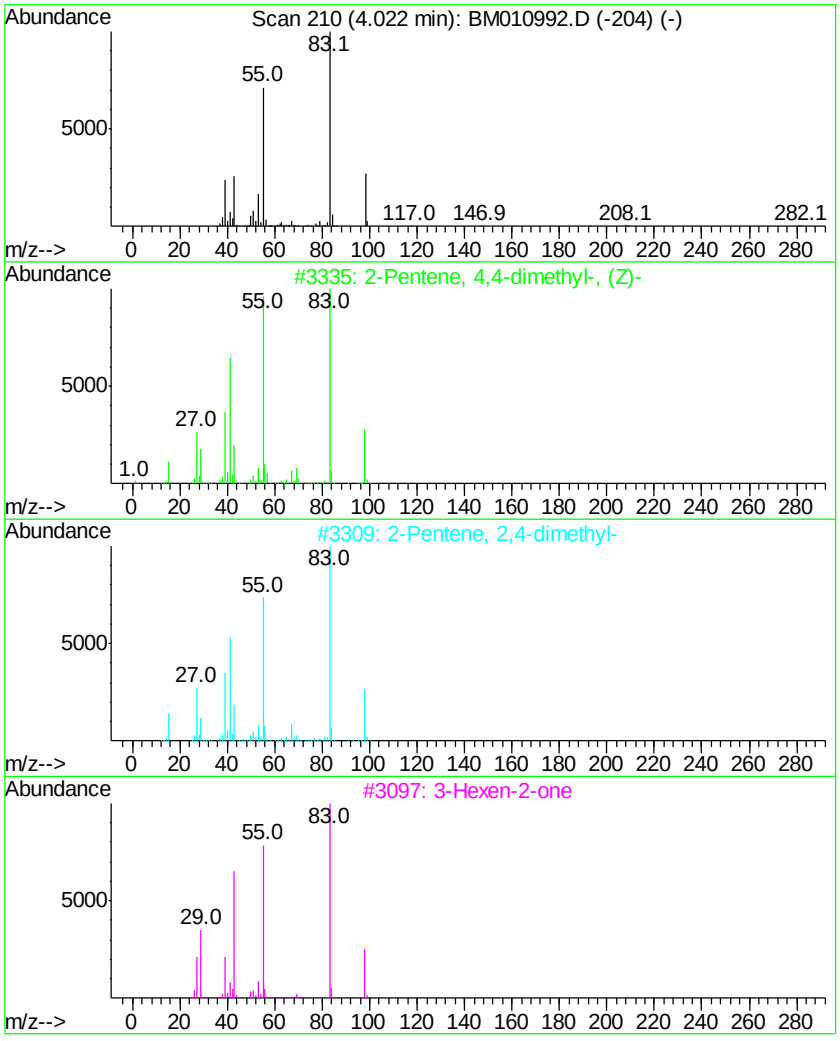
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

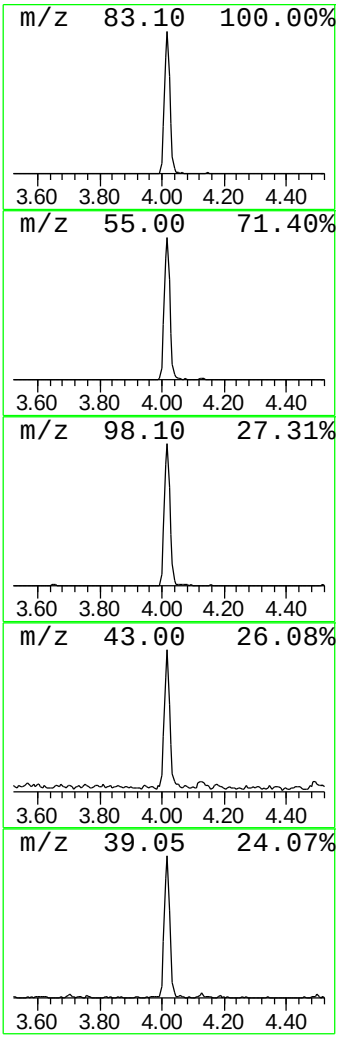
****

Peak Number 2 2-Pentene, 4,4-dimethyl-, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.02	12.40 ng	951311	1,4-Dichlorobenzene-d4	7.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	90
2	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	90
3	3-Hexen-2-one	98	C6H10O	000763-93-9	86
4	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	86
5	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78





Data Path : Z:\HPCHEM1\BNA M\DATA\BM072617\
Data File : BM010992.D
Acq On : 27 Jul 2017 04:00
Operator : SJ/JU
Sample : I4391-03
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BU-02-072117-A

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM072617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

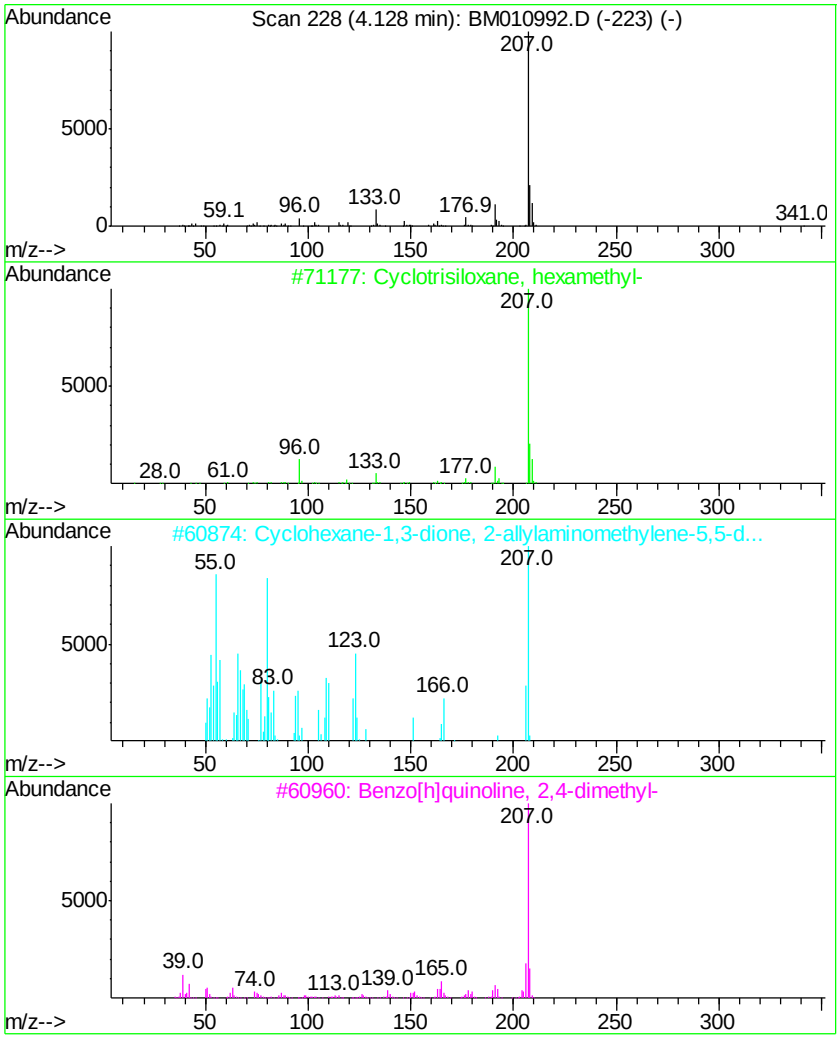
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

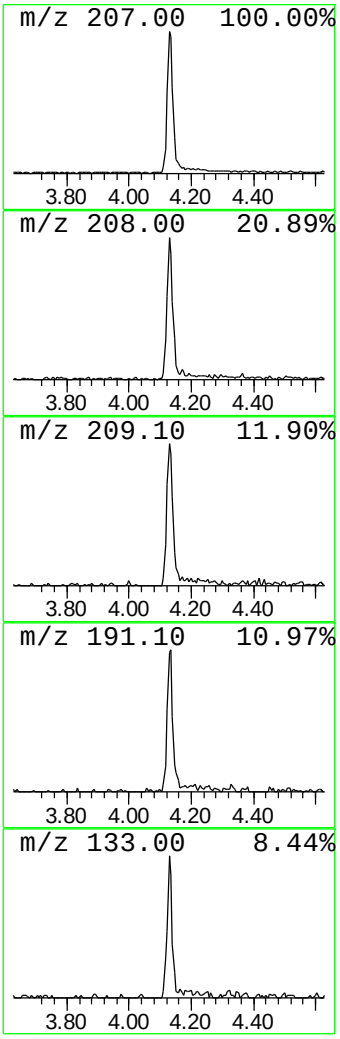
****

Peak Number 3 Cyclotrisiloxane, hexamethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.13	9.88 ng	757547	1,4-Dichlorobenzene-d4	7.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotrisiloxane, hexamethyl-	222	C6H18O3Si3	000541-05-9	87
2	Cyclohexane-1,3-dione, 2-allylam...	207	C12H17NO2	104926-37-6	43
3	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	39
4	Benz[b]-1,4-oxazepine-4(5H)-thio...	207	C11H13NOS	1000258-63-4	38
5	2-Methyl-7-phenylindole	207	C15H13N	001140-08-5	38





Data Path : Z:\HPCHEM1\BNA M\DATA\BM072617\
Data File : BM010992.D
Acq On : 27 Jul 2017 04:00
Operator : SJ/JU
Sample : I4391-03
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BU-02-072117-A

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM072617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

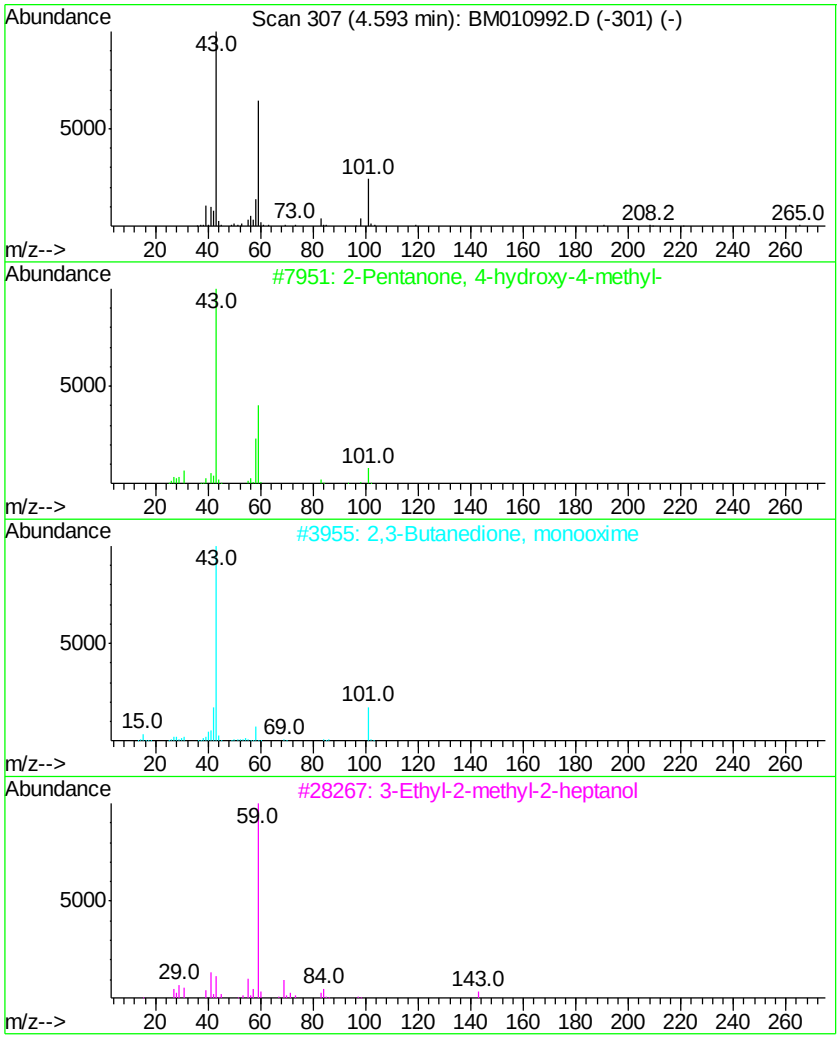
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

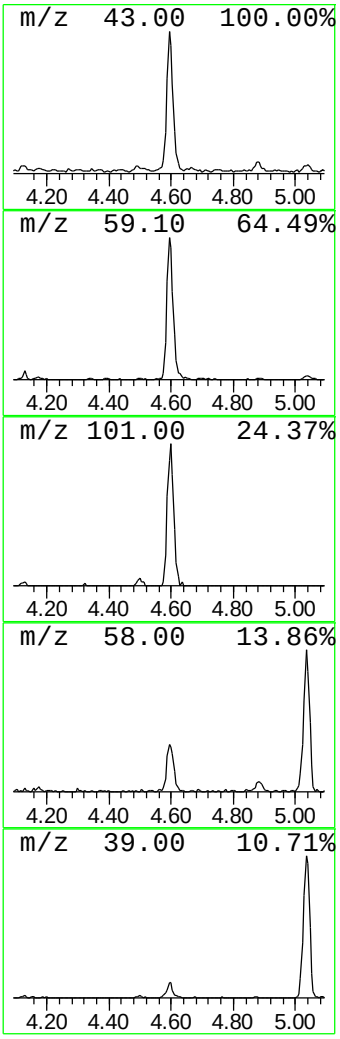
****

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.59	4.92 ng	377749	1,4-Dichlorobenzene-d4	7.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	3-Ethyl-2-methyl-2-heptanol	158	C10H22O	019780-59-7	12
4	5-Hydroxypentanehydroxylamine, N...	245	C11H19NO5	104556-13-0	12
5	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	12





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM072617\
Data File : BM010992.D
Acq On : 27 Jul 2017 04:00
Operator : SJ/JU
Sample : I4391-03
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BU-02-072117-A

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM072617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

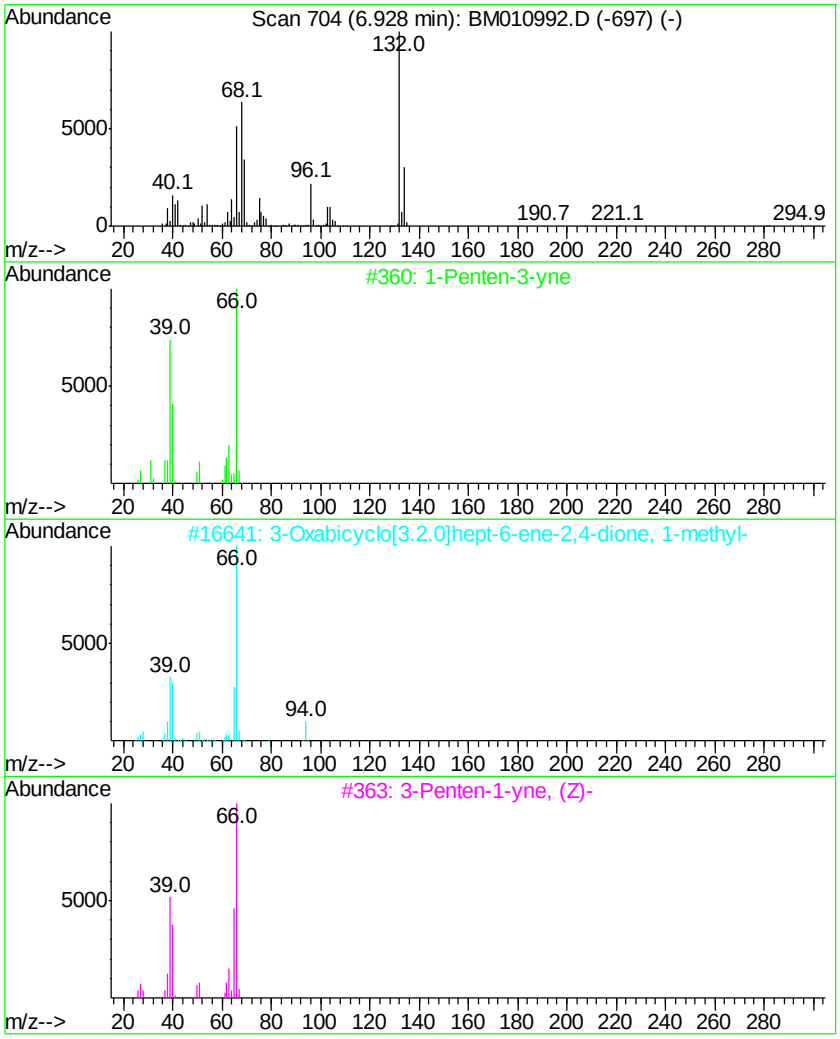
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

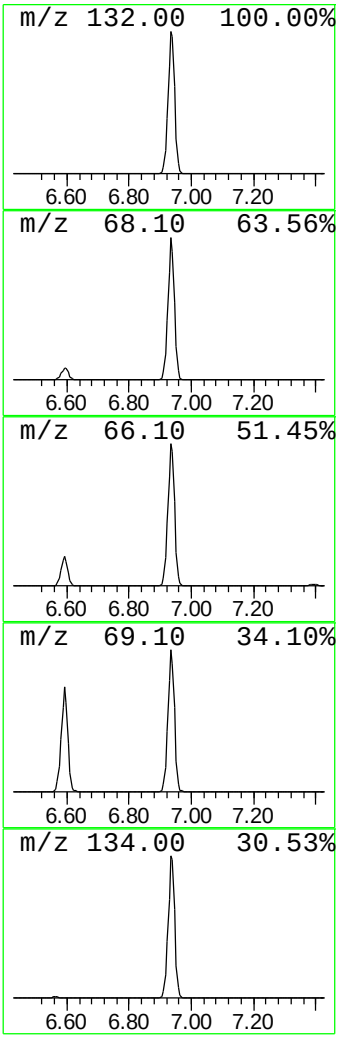
****

Peak Number 5 unknown6.93 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.93	113.20 ng	8683050	1,4-Dichlorobenzene-d4	7.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Penten-3-yne	66	C5H6	000646-05-9	38
2	3-Oxabicyclo[3.2.0]hept-6-ene-2,...	138	C7H6O3	064197-88-2	35
3	3-Penten-1-yne, (Z)-	66	C5H6	001574-40-9	25
4	Silane, bicyclo[2.2.1]hept-5-en-...	226	C7H9Cl3Si	014319-64-3	25
5	Bicyclo[3.2.0]hept-2-en-6-one	108	C7H8O	013173-09-6	25





Data Path : Z:\HPCHEM1\BNA M\DATA\BM072617\
Data File : BM010992.D
Acq On : 27 Jul 2017 04:00
Operator : SJ/JU
Sample : I4391-03
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BU-02-072117-A

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM072617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

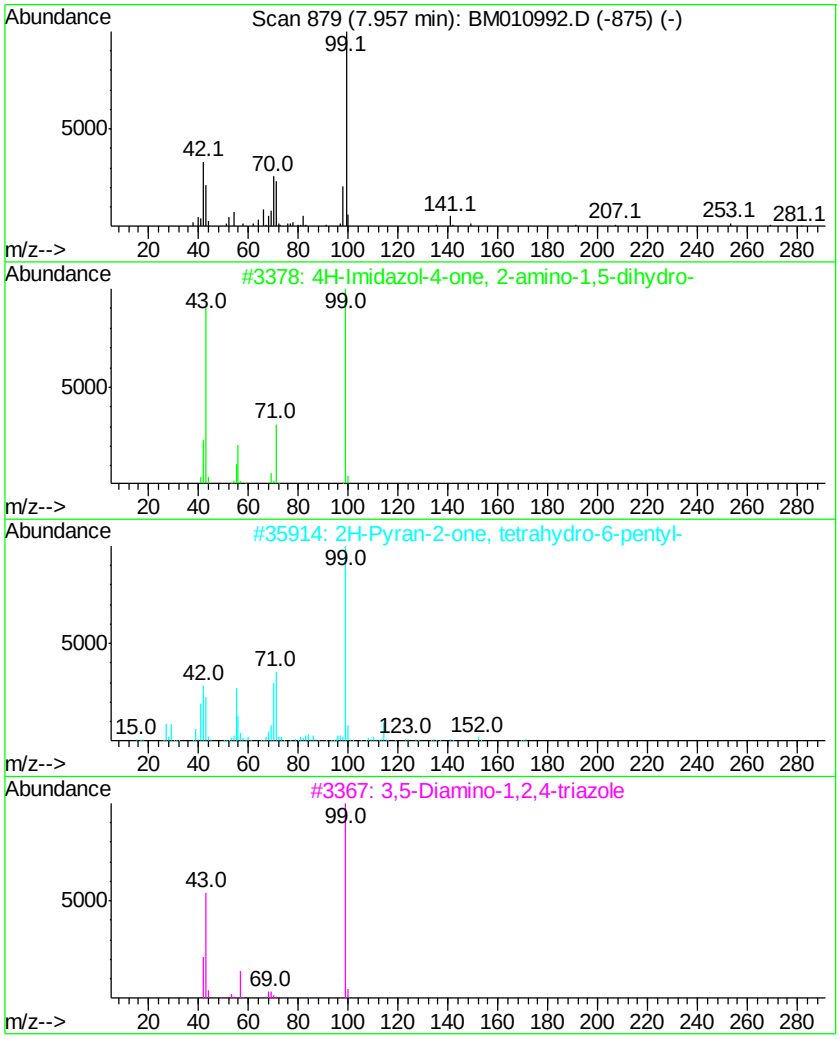
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

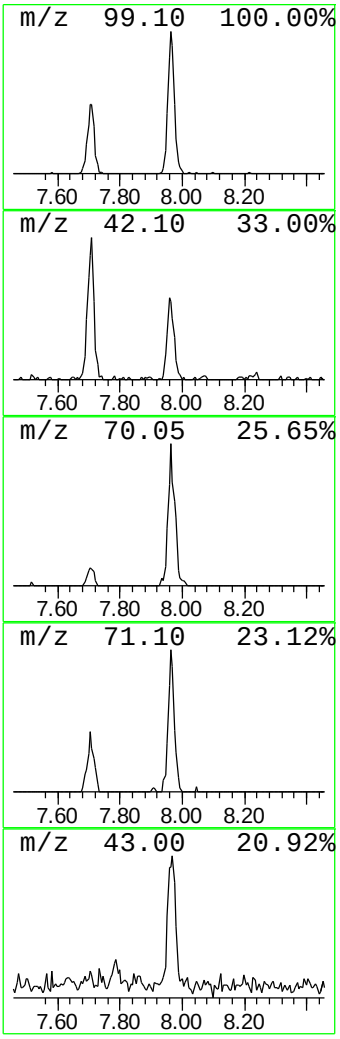
****

Peak Number 7 4H-Imidazol-4-one, 2-amino-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.96	3.47 ng	266187	1,4-Dichlorobenzene-d4	7.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Imidazol-4-one, 2-amino-1,5-d...	99	C3H5N3O	000503-86-6	53
2	2H-Pyran-2-one, tetrahydro-6-pen...	170	C10H18O2	000705-86-2	50
3	3,5-Diamino-1,2,4-triazole	99	C2H5N5	001455-77-2	43
4	2-Piperidinone	99	C5H9NO	000675-20-7	42
5	2H-Pyran-2-one, 6-hexyltetrahydro-	184	C11H20O2	000710-04-3	36





Data Path : Z:\HPCHEM1\BNA M\DATA\BM072617\
Data File : BM010992.D
Acq On : 27 Jul 2017 04:00
Operator : SJ/JU
Sample : I4391-03
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BU-02-072117-A

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM072617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

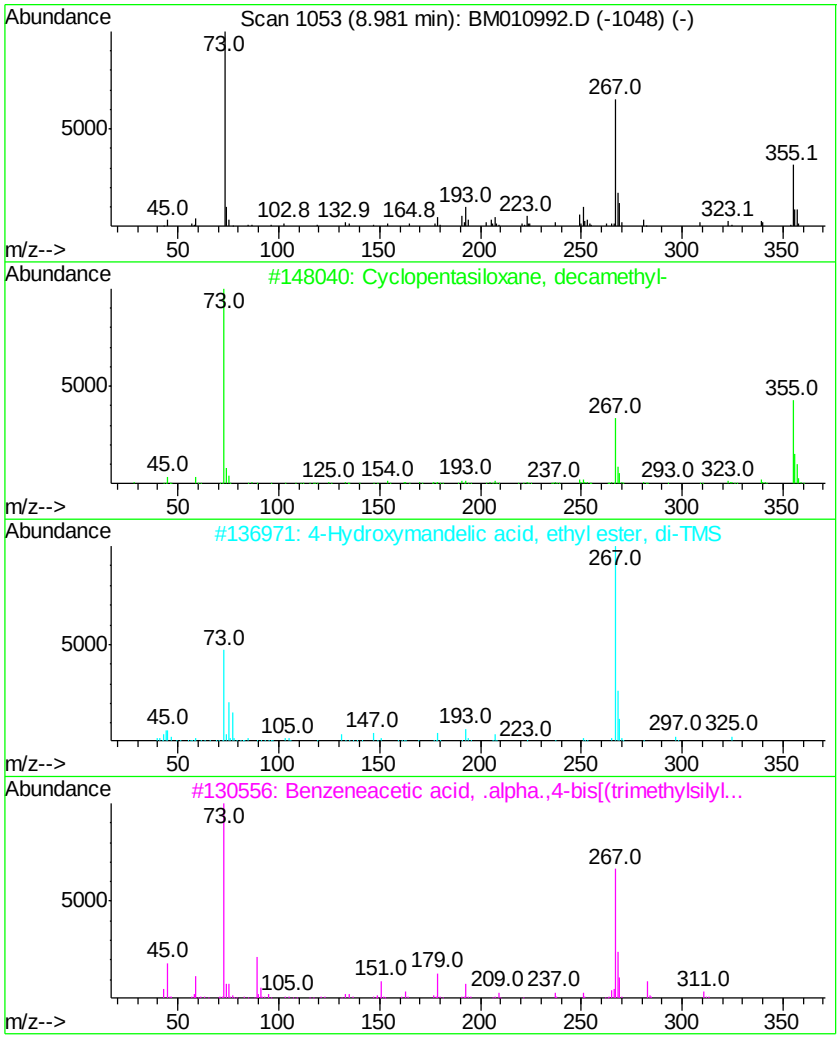
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

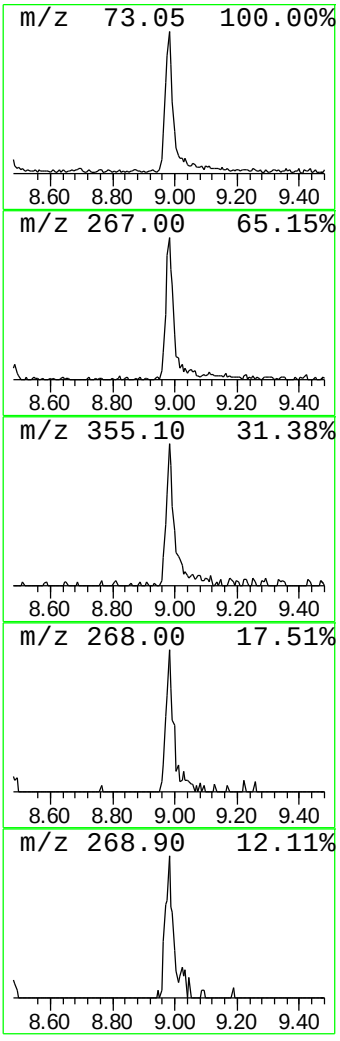
****

Peak Number 8 Cyclopentasiloxane, decamet... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.98	3.44 ng	333354	Naphthalene-d8	10.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	72
2	4-Hydroxymandelic acid, ethyl es...	340	C16H28O4Si2	1000071-53-3	50
3	Benzeneacetic acid, .alpha.,4-bi...	326	C15H26O4Si2	055334-40-2	47
4	Silanamine, 1,1,1-trimethyl-N-[2...	369	C17H35NO2Si3	068595-60-8	42
5	Benzenemethanol, .alpha.-(aminom...	369	C17H35NO2Si3	056145-08-5	42





Data Path : Z:\HPCHEM1\BNA M\DATA\BM072617\
Data File : BM010992.D
Acq On : 27 Jul 2017 04:00
Operator : SJ/JU
Sample : I4391-03
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BU-02-072117-A

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM072617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

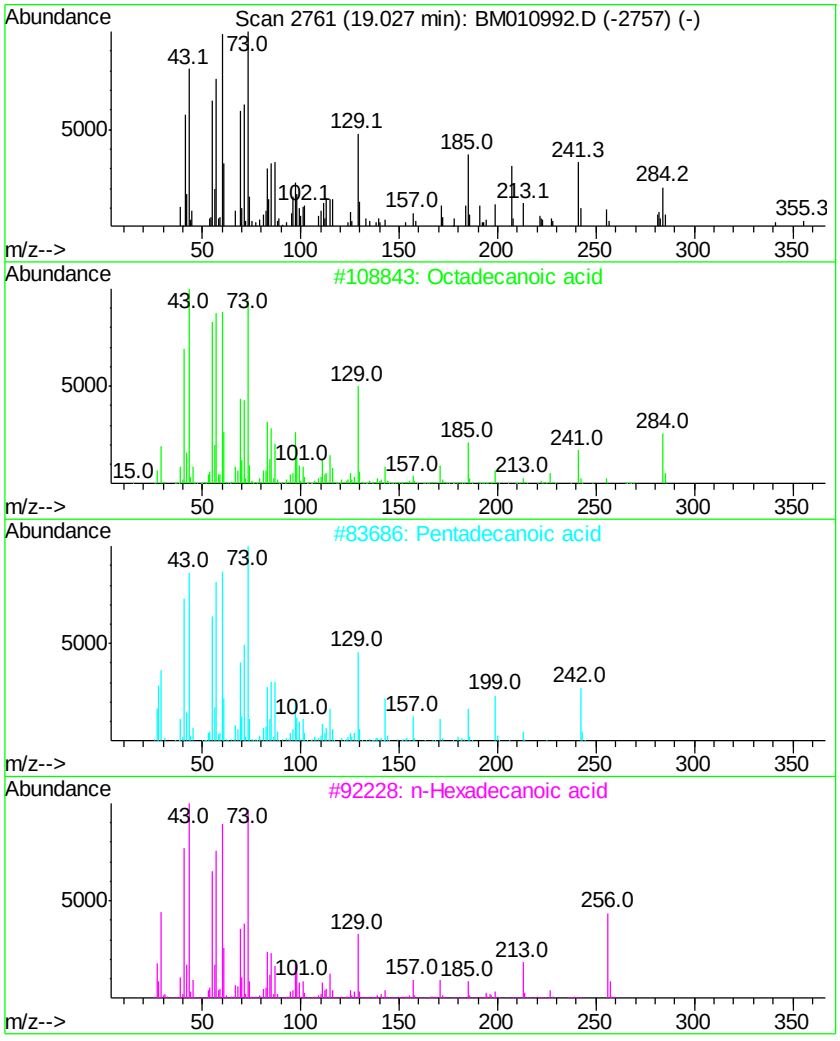
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

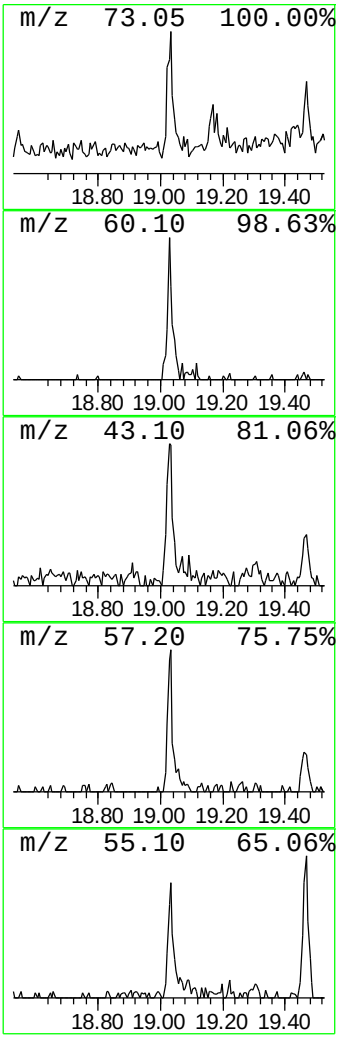
****

Peak Number 9 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.03	2.21 ng	246891	Chrysene-d12	21.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM072617\
Data File : BM010992.D
Acq On : 27 Jul 2017 04:00
Operator : SJ/JU
Sample : I4391-03
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BU-02-072117-A

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM072617.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
4-Penten-2-one, 4...	3.44	5.2	ng	402251	1	7.39	1534100	20.0
2-Pentene, 4,4-di...	4.02	12.4	ng	951311	1	7.39	1534100	20.0
Cyclotrisiloxane,...	4.13	9.9	ng	757547	1	7.39	1534100	20.0
2-Pentanone, 4-hy...	4.59	4.9	ng	377749	1	7.39	1534100	20.0
unknown6.93	6.93	113.2	ng	8683050	1	7.39	1534100	20.0
4H-Imidazol-4-one...	7.96	3.5	ng	266187	1	7.39	1534100	20.0
Cyclopentasiloxan...	8.98	3.4	ng	333354	2	10.15	1936880	20.0
Octadecanoic acid	19.03	2.2	ng	246891	5	21.02	2230410	20.0