LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051217\
Data File : BM010033.D
Acq On : 12 May 2017 20:53
Operator : SJ/MA
Sample : I3100-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-4-051017

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	316	rBV	101308	154788	2.06%	0.495%
2	5.346	378	384	396	rBV	768426	1208114	16.07%	3.862%
3	6.940	649	655	668	rBV	504578	859270	11.43%	2.747%
4	7.292	708	715	724	rBV	1655189	2601128	34.59%	8.315%
5	7.757	788	794	802	rBV	317511	494690	6.58%	1.581%
6	8.075	840	848	860	rBV	1414441	2239483	29.78%	7.159%
7	8.934	986	994	1004	rBV	1375084	2320589	30.86%	7.418%
8	10.551	1263	1269	1281	rBV	380970	664597	8.84%	2.124%
9	13.021	1682	1689	1702	rBV	3012331	4433063	58.95%	14.171%
10	13.880	1829	1835	1842	rBV2	48308	79565	1.06%	0.254%
11	14.410	1919	1925	1936	rBV2	515624	836787	11.13%	2.675%
12	15.915	2174	2181	2195	rBV	2683994	3879262	51.59%	12.400%
13	17.168	2388	2394	2403	rBV	689375	1028309	13.67%	3.287%
14	17.521	2448	2454	2460	rBV	107412	162803	2.16%	0.520%
15	18.045	2537	2543	2553	rBV2	103163	163975	2.18%	0.524%
16	19.327	2756	2761	2767	rBV2	128781	199485	2.65%	0.638%
17	19.427	2773	2778	2788	rBV2	175133	246074	3.27%	0.787%
18	19.792	2834	2840	2847	rBV	6191700	7519959	100.00%	24.038%
19	20.909	3027	3030	3036	rBV4	100327	150687	2.00%	0.482%
20	21.356	3101	3106	3112	rBV	910908	1169182	15.55%	3.737%
21	23.650	3490	3496	3505	rVB2	443830	871657	11.59%	2.786%

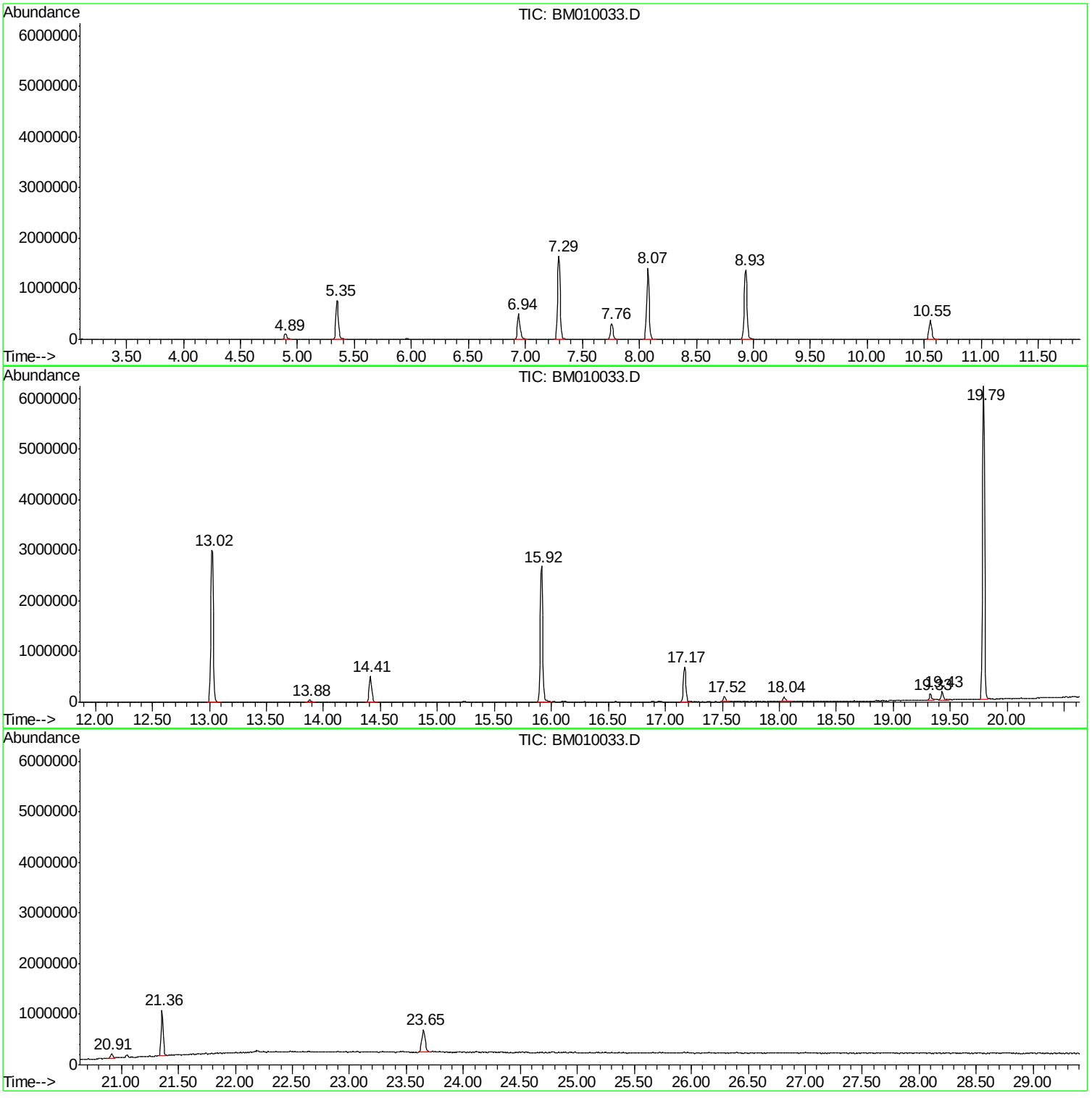
Sum of corrected areas: 31283467

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051217\
Data File : BM010033.D
Acq On : 12 May 2017 20:53
Operator : SJ/MA
Sample : I3100-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-4-051017

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



Data Path : Z:\HPCHEM1\BNA M\DATA\BM051217\
Data File : BM010033.D
Acq On : 12 May 2017 20:53
Operator : SJ/MA
Sample : I3100-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

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ClientSampleId : MW-4-051017

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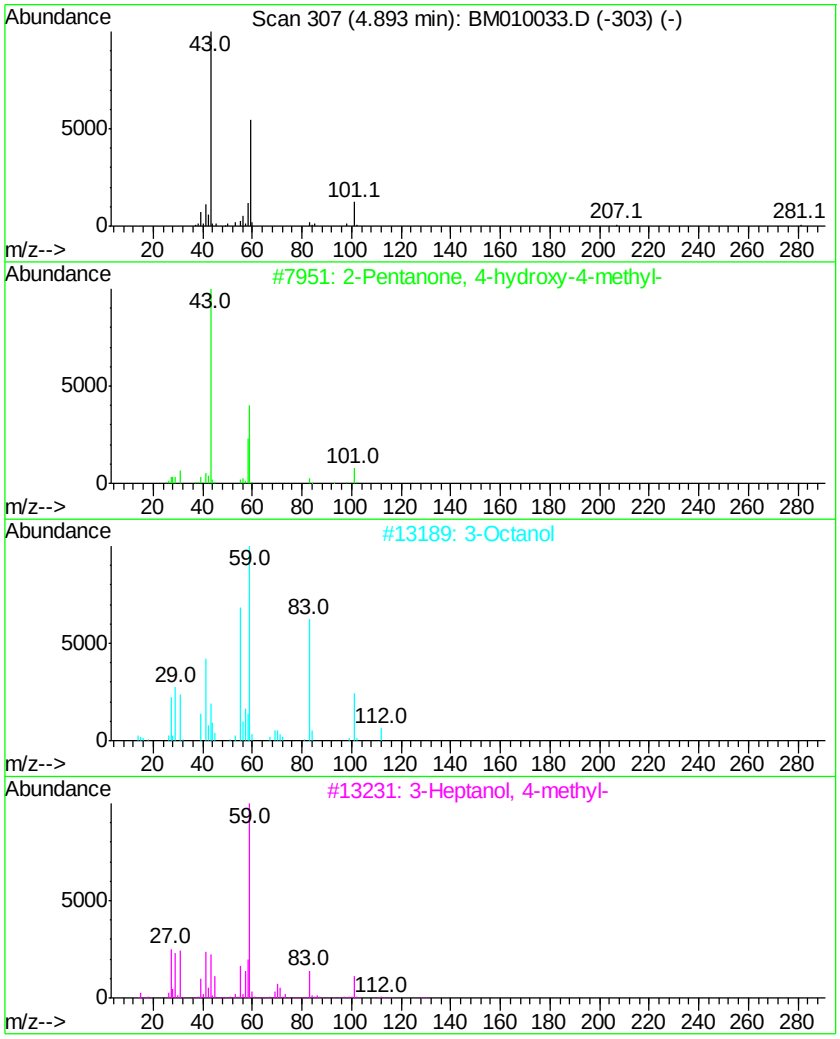
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

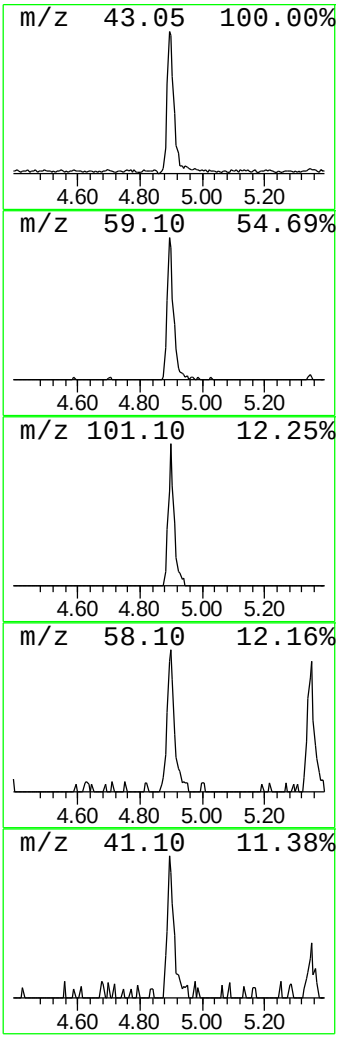
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	6.26 ng	154788	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	3-Octanol	130	C8H18O	000589-98-0	36
3	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25





Library Search Compound Report

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Data File : BM010033.D
Acq On : 12 May 2017 20:53
Operator : SJ/MA
Sample : I3100-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-4-051017

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

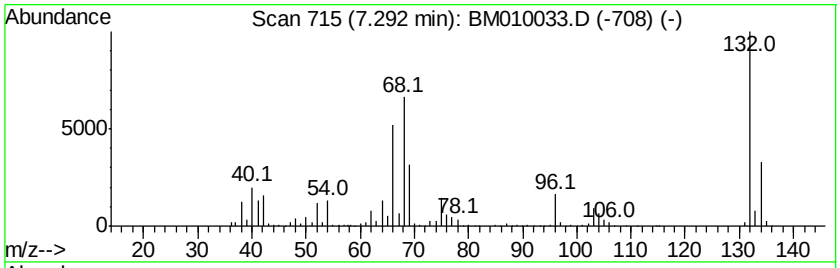
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

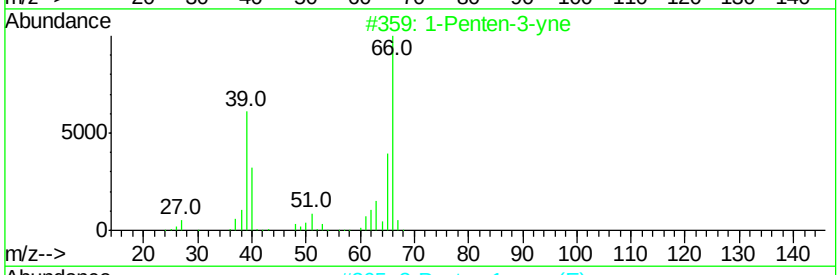
****

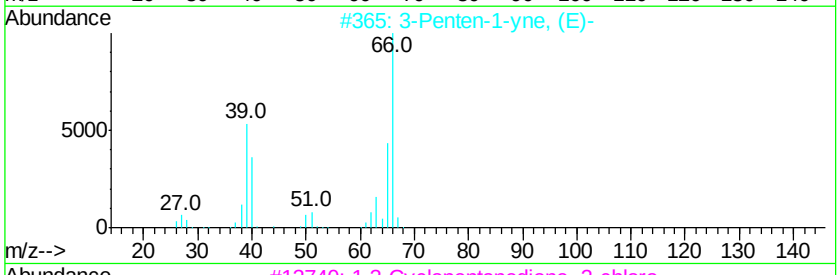
Peak Number 2 unknown7.29 Concentration Rank 1

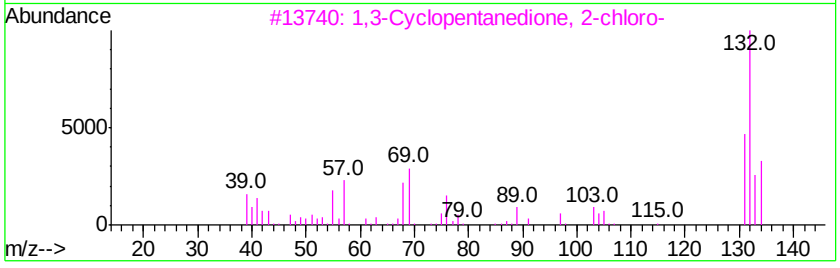
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.29	105.16 ng	2601130	1,4-Dichlorobenzene-d4	7.76

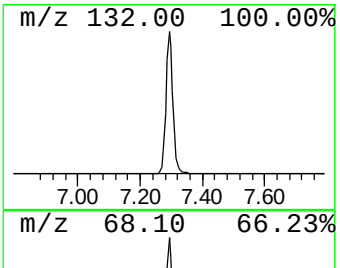
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Penten-3-yne	66	C5H6	000646-05-9	38
2	3-Penten-1-yne, (E)-	66	C5H6	002004-69-5	35
3	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	27
4	3-Penten-1-yne, (Z)-	66	C5H6	001574-40-9	25
5	Propanedinitrile	66	C3H2N2	000109-77-3	25

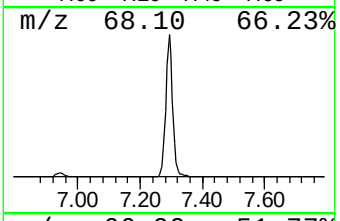


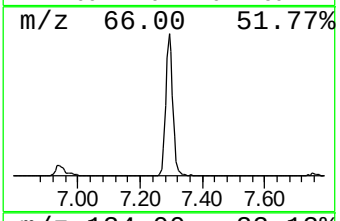


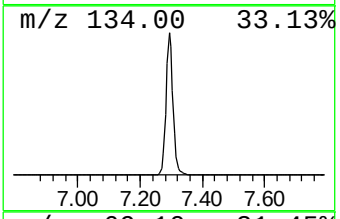


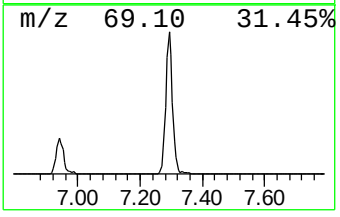












Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051217\
Data File : BM010033.D
Acq On : 12 May 2017 20:53
Operator : SJ/MA
Sample : I3100-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-4-051017

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

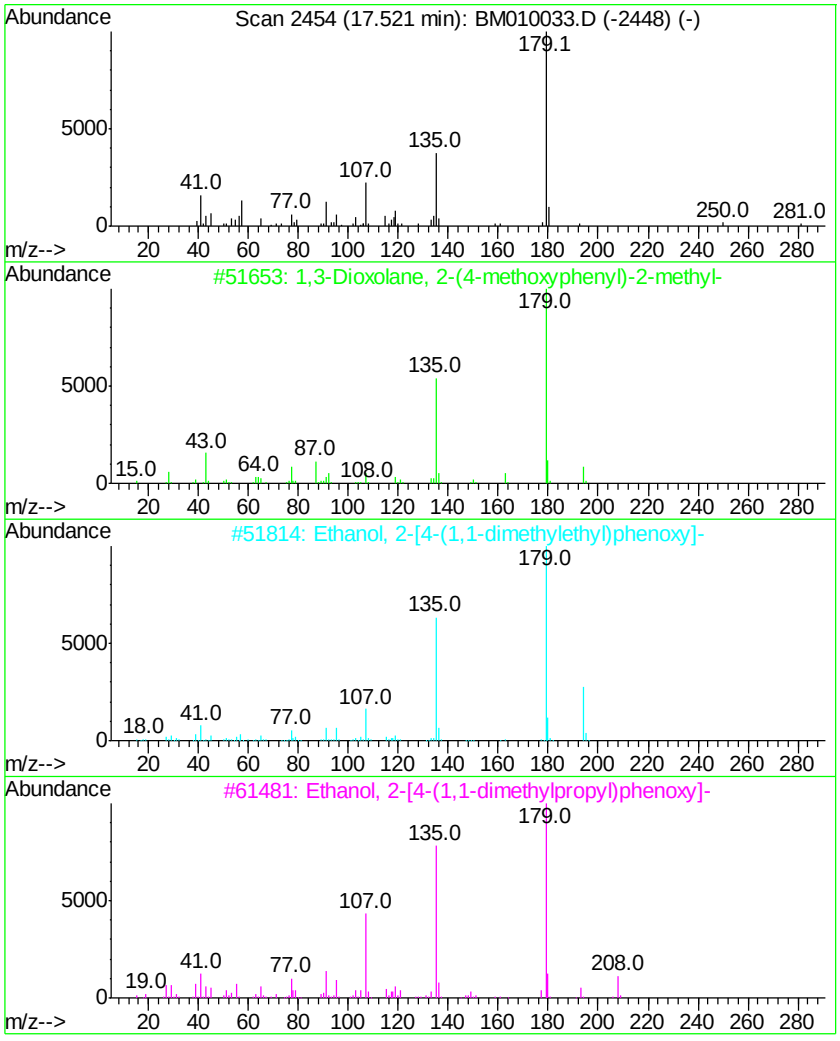
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

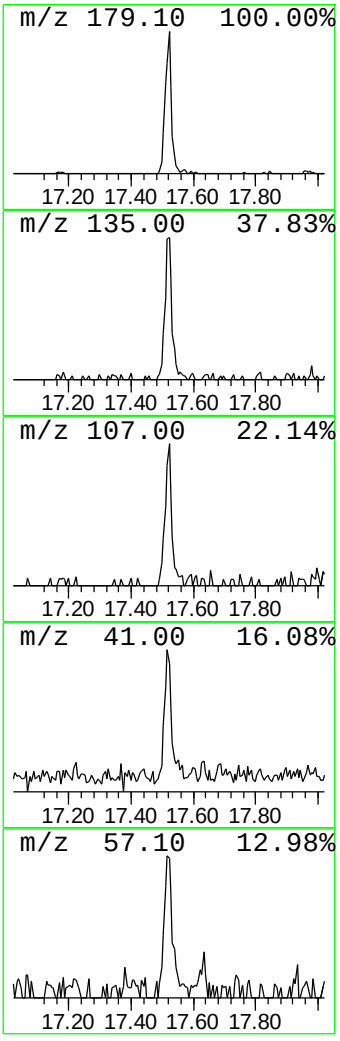
****

Peak Number 4 1,3-Dioxolane, 2-(4-methoxy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.52	3.17 ng	162803	Phenanthrene-d10	17.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-(4-methoxyphenyl...	194	C11H14O3	036881-00-2	64
2	Ethanol, 2-[4-(1,1-dimethylethyl...	194	C12H18O2	000713-46-2	64
3	Ethanol, 2-[4-(1,1-dimethylpropyl...	208	C13H20O2	006382-07-6	56
4	Benzothiazole-6-carboxylic acid	179	C8H5NO2S	003622-35-3	42
5	1-Dimethyl(phenyl)silyloxypropane	194	C11H18OSi	013360-21-9	33





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051217\
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Sample : I3100-03
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ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-4-051017

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

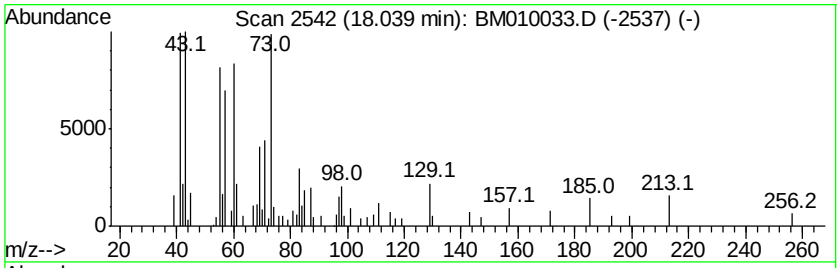
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

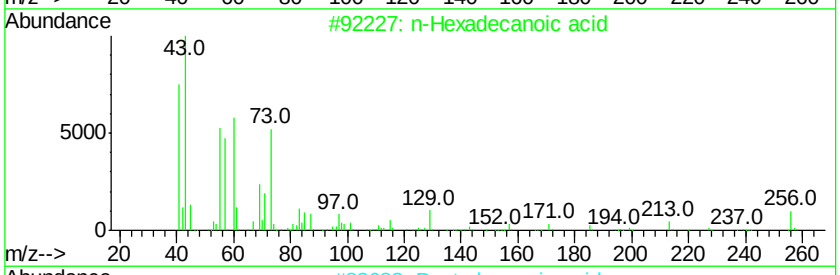
****

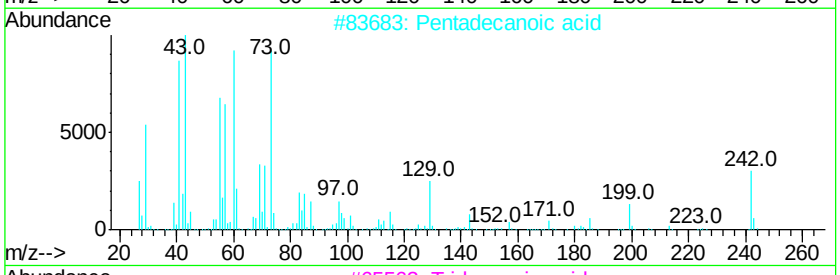
Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

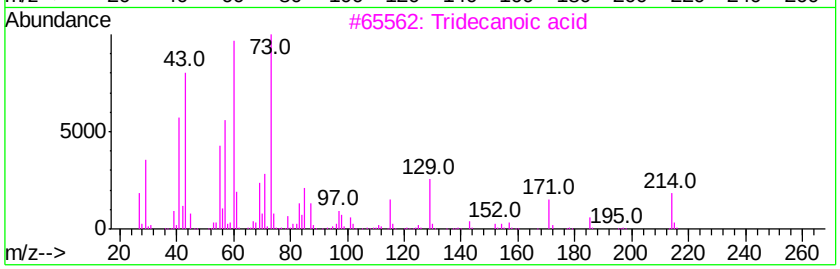
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.04	3.19 ng	163975	Phenanthrene-d10	17.17

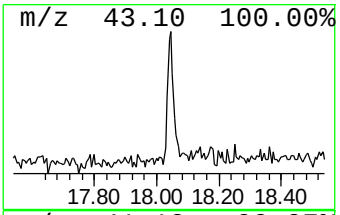
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	Tridecanoic acid	214	C13H26O2	000638-53-9	53
4	Dodecanoic acid	200	C12H24O2	000143-07-7	50
5	n-Decanoic acid	172	C10H20O2	000334-48-5	43

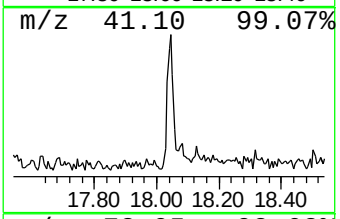


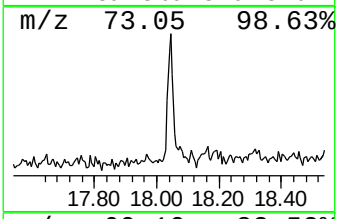


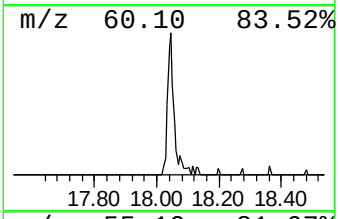


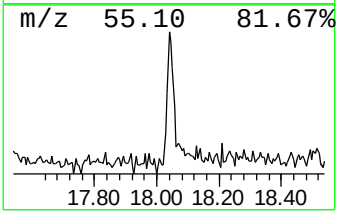












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Instrument : BNA_M
ClientSampleId : MW-4-051017

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

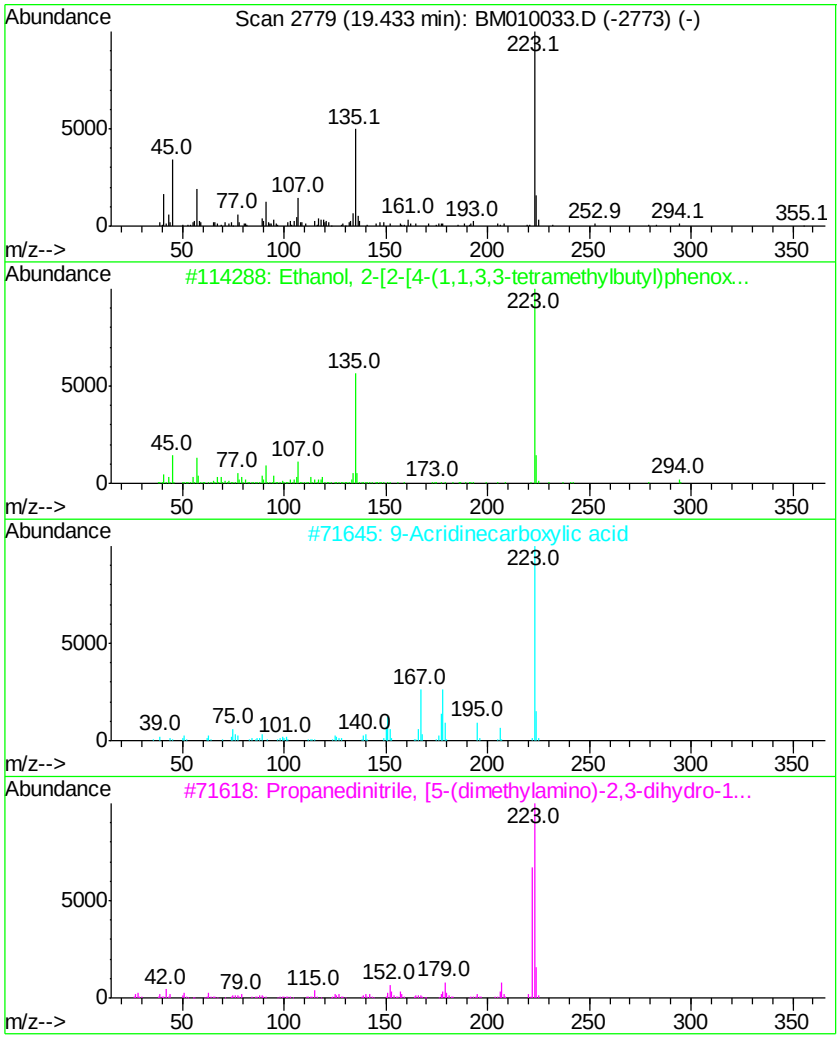
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

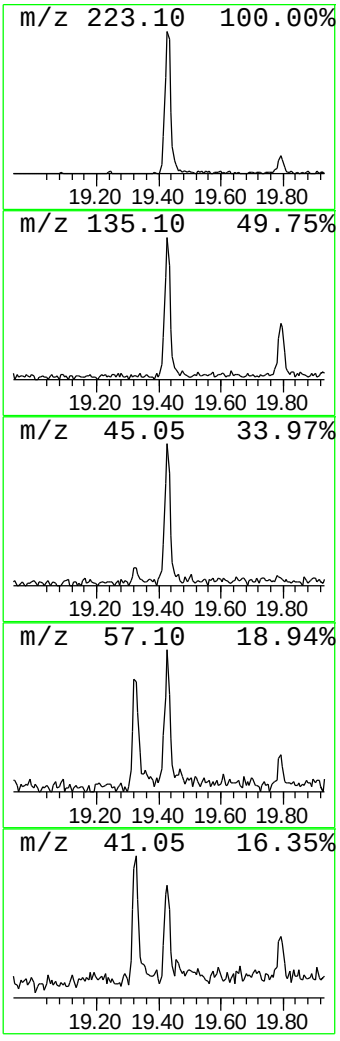
****

Peak Number 7 Ethanol, 2-[2-[4-(1,1,3,3-t... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.43	4.21 ng	246074	Chrysene-d12	21.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	64
2	9-Acridinecarboxylic acid	223	C14H9NO2	005336-90-3	35
3	Propanedinitrile, [5-(dimethylam...	223	C14H13N3	131303-47-4	35
4	2H-1,4-Benzoxazine, 3,4-dihydro-	135	C8H9NO	005735-53-5	11
5	Benzene, 1-(1,3-dimethyl-3-buten...	190	C13H18O	074672-05-2	10





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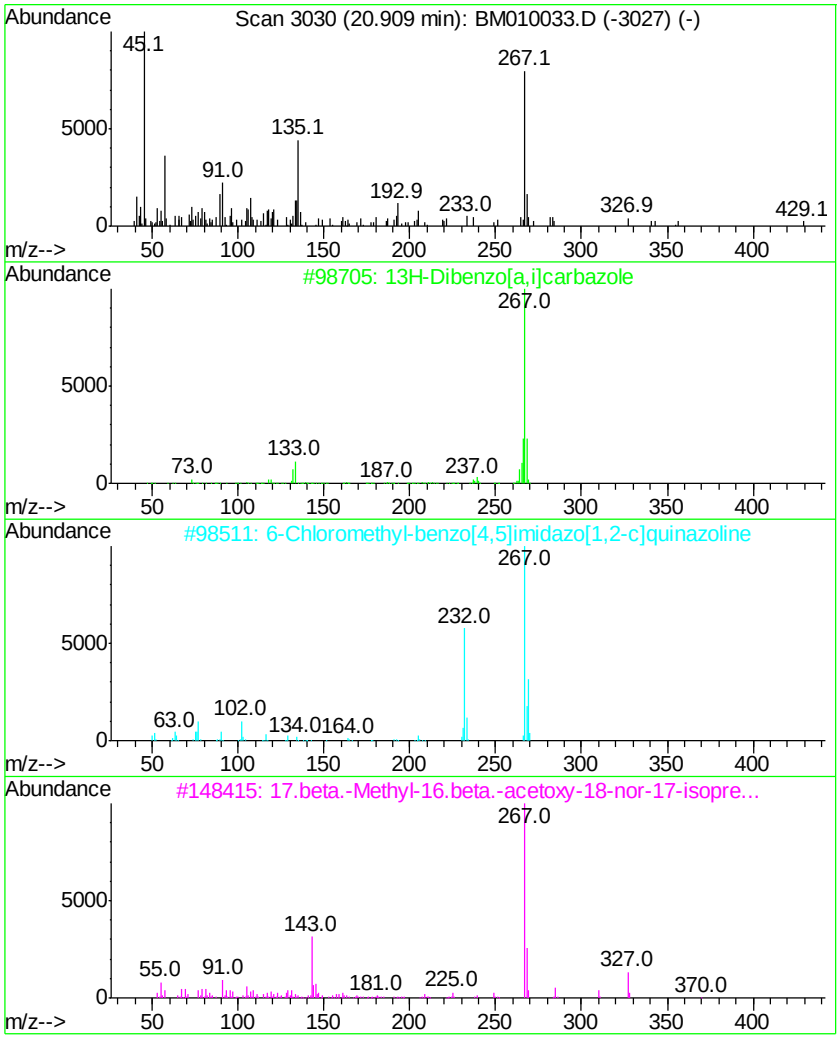
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

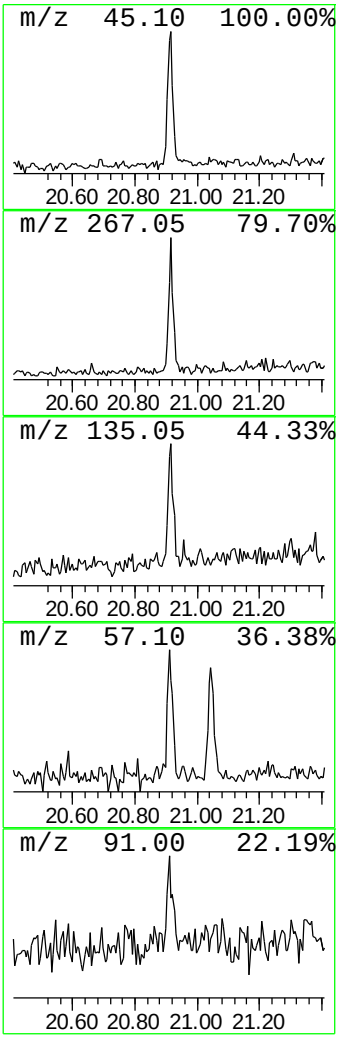
****

Peak Number 8 13H-Dibenzo[a,i]carbazole Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.91	2.58 ng	150687	Chrysene-d12	21.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13H-Dibenzo[a,i]carbazole	267	C20H13N	000239-64-5	43
2	6-Chloromethyl-benzo[4,5]imidazo...	267	C15H10ClN3	070371-92-5	38
3	17.beta.-Methyl-16.beta.-acetoxy...	370	C23H30O4	023925-70-4	37
4	1,3,4-Thiadiazole, 2,2-diethyl-2...	296	C18H20N2S	053067-48-4	37
5	7H-Dibenzo[c,g]carbazole	267	C20H13N	000194-59-2	37





Tentatively Identified Compound (LSC) summary

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Operator : SJ/MA
Sample : I3100-03
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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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.89	6.3	ng	154788	1	7.76	494690	20.0
unknown7.29	7.29	105.2	ng	2601130	1	7.76	494690	20.0
1,3-Dioxolane, 2-...	17.52	3.2	ng	162803	4	17.17	1028310	20.0
n-Hexadecanoic acid	18.04	3.2	ng	163975	4	17.17	1028310	20.0
Ethanol, 2-[2-[4-...	19.43	4.2	ng	246074	5	21.36	1169180	20.0
13H-Dibenzo[a,i]c...	20.91	2.6	ng	150687	5	21.36	1169180	20.0