LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051617\
Data File : BM010063.D
Acq On : 16 May 2017 21:03
Operator : SJ/MA
Sample : I3171-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : WS-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:\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	4.287	199	204	223	rBV	1283279	1748387	29.09%	6.370%
2	4.892	301	307	319	rBV	2077223	2812679	46.80%	10.248%
3	5.345	379	384	397	rBV	522745	806447	13.42%	2.938%
4	5.945	480	486	499	rBV	320746	486407	8.09%	1.772%
5	6.934	646	654	672	rBV	331197	597803	9.95%	2.178%
6	7.286	707	714	728	rBV	873986	1436821	23.91%	5.235%
7	7.757	787	794	801	rBV	223084	366006	6.09%	1.334%
8	8.069	841	847	857	rBV	1114086	1797540	29.91%	6.549%
9	8.928	986	993	1009	rBV	1073153	1791292	29.81%	6.527%
10	10.545	1262	1268	1284	rBV	269530	482726	8.03%	1.759%
11	13.021	1682	1689	1702	rBV	2296009	3359238	55.89%	12.239%
12	13.874	1829	1834	1841	rBV2	56644	92367	1.54%	0.337%
13	14.410	1919	1925	1935	rBV3	375566	602101	10.02%	2.194%
14	15.909	2173	2180	2195	rBV	1322411	1993669	33.17%	7.264%
15	16.092	2207	2211	2220	rVB2	46300	69324	1.15%	0.253%
16	17.162	2387	2393	2402	rBV2	533514	793315	13.20%	2.890%
17	18.039	2537	2542	2549	rBV2	102857	150392	2.50%	0.548%
18	19.321	2754	2760	2765	rBV	91864	139560	2.32%	0.508%
19	19.786	2833	2839	2845	rBV	4911423	6009944	100.00%	21.897%
20	21.044	3049	3053	3060	rBV3	115945	181464	3.02%	0.661%
21	21.350	3100	3105	3112	rBV	731717	983842	16.37%	3.585%
22	23.644	3489	3495	3504	rVB2	358961	744984	12.40%	2.714%

Sum of corrected areas: 27446308

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051617\
Data File : BM010063.D
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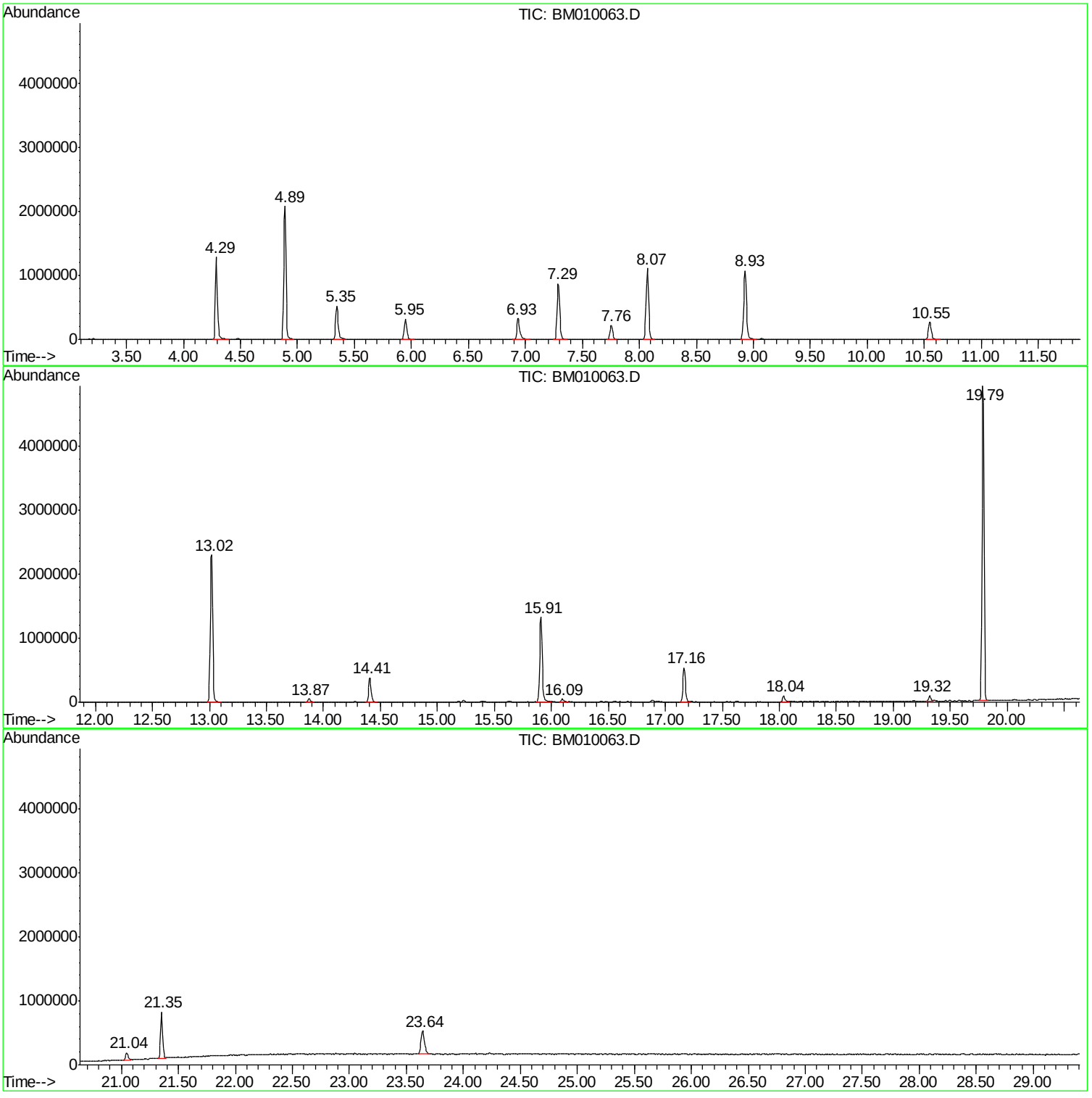
Operator : SJ/MA
Sample : I3171-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : WS-5

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\BM051617\
Data File : BM010063.D
Acq On : 16 May 2017 21:03
Operator : SJ/MA
Sample : I3171-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : WS-5

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

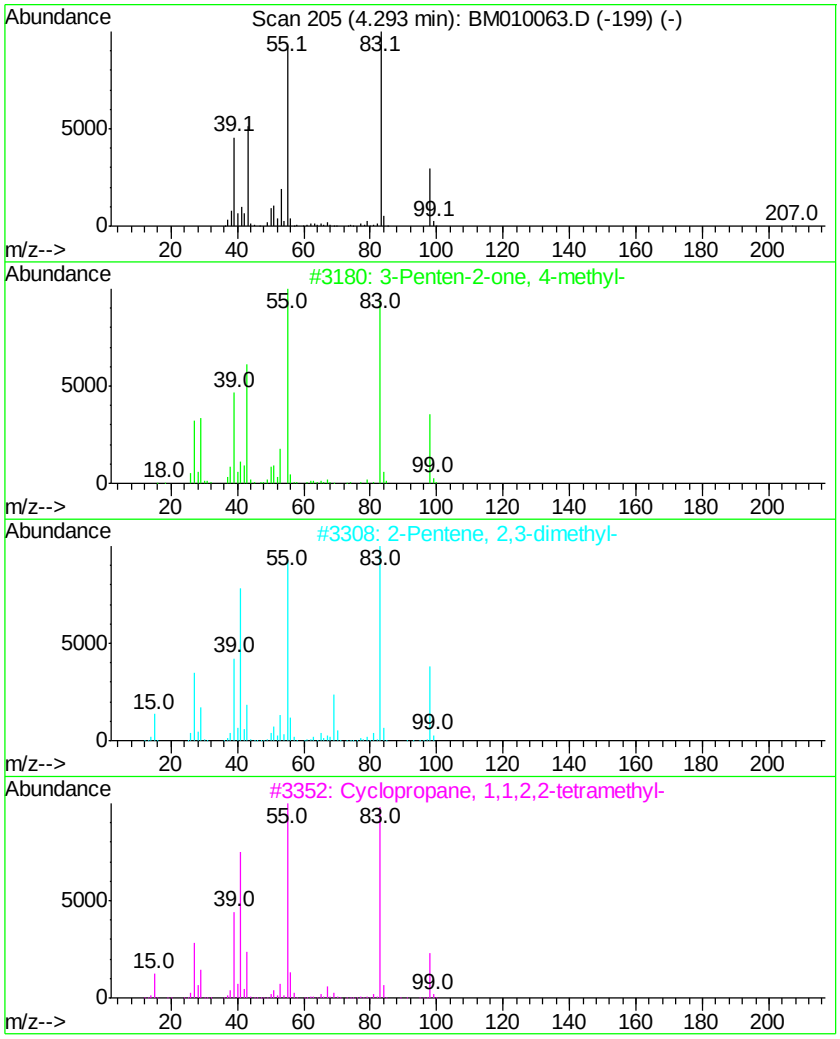
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

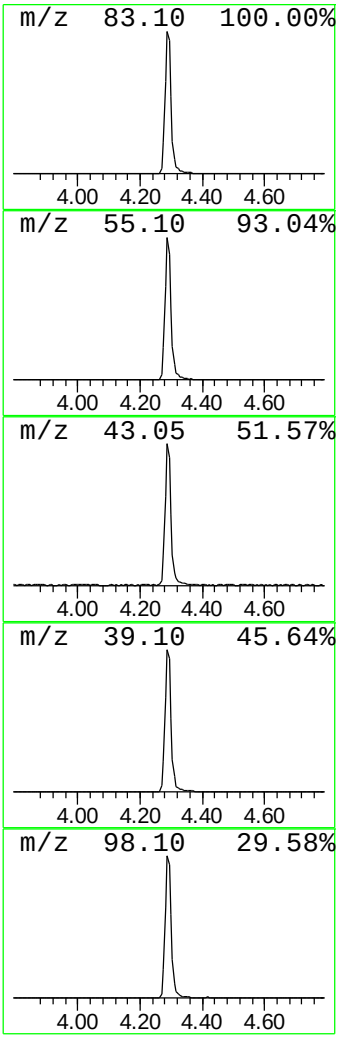
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.29	95.54 ng	1748390	1,4-Dichlorobenzene-d4	7.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	81
2	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	72
3	Cyclopropane, 1,1,2,2-tetramethyl-	98	C7H14	004127-47-3	72
4	1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	59
5	3-Hexen-2-one	98	C6H10O	000763-93-9	53





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051617\
Data File : BM010063.D
Acq On : 16 May 2017 21:03
Operator : SJ/MA
Sample : I3171-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : WS-5

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

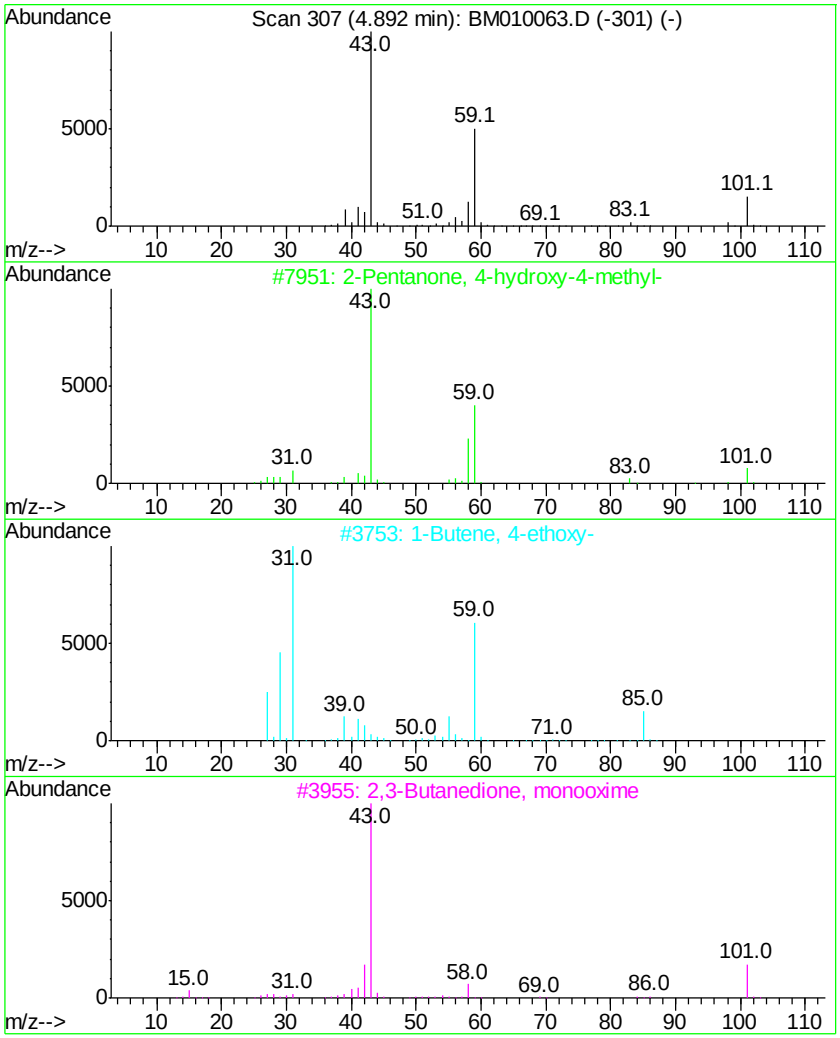
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

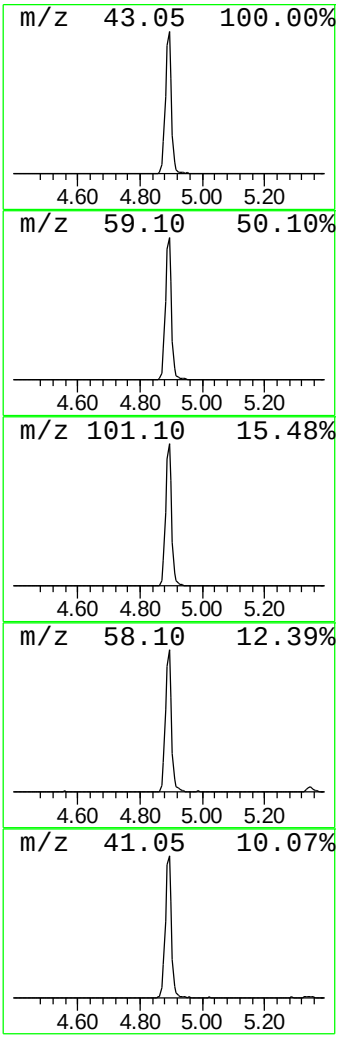
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	153.70 ng	2812680	1,4-Dichlorobenzene-d4	7.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Butane	58	C4H10	000106-97-8	9
5	Propylamine	59	C3H9N	000107-10-8	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051617\
Data File : BM010063.D
Acq On : 16 May 2017 21:03
Operator : SJ/MA
Sample : I3171-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : WS-5

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

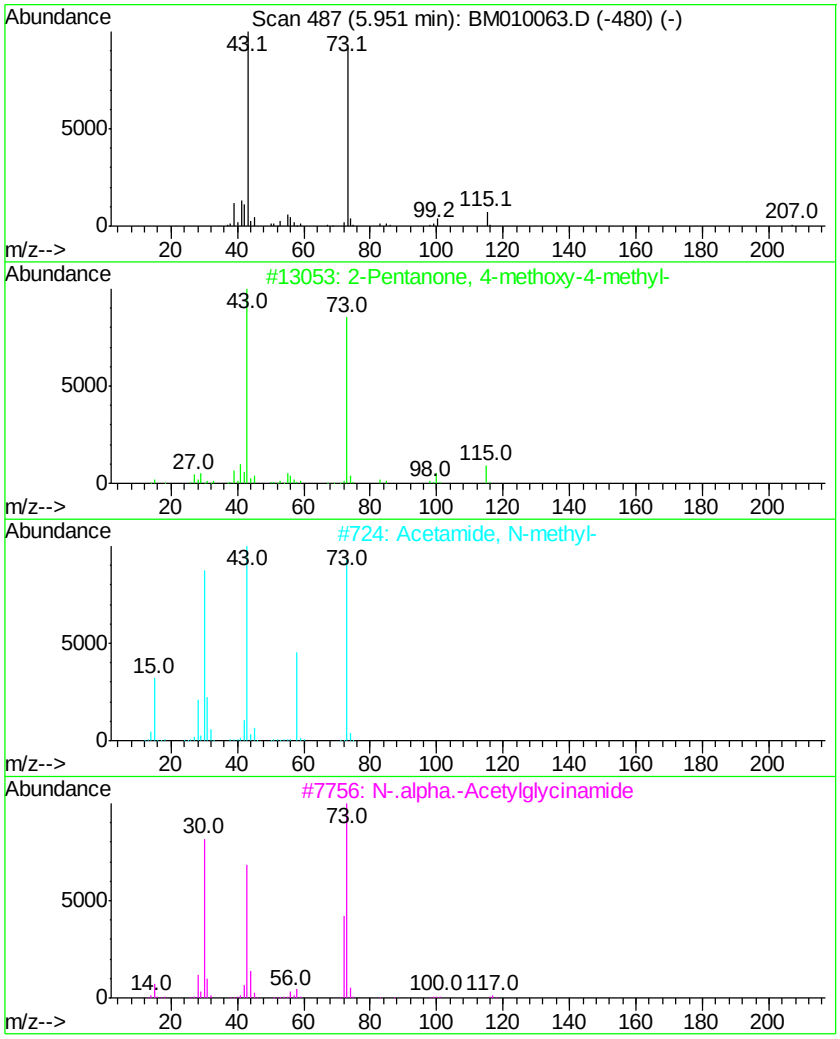
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

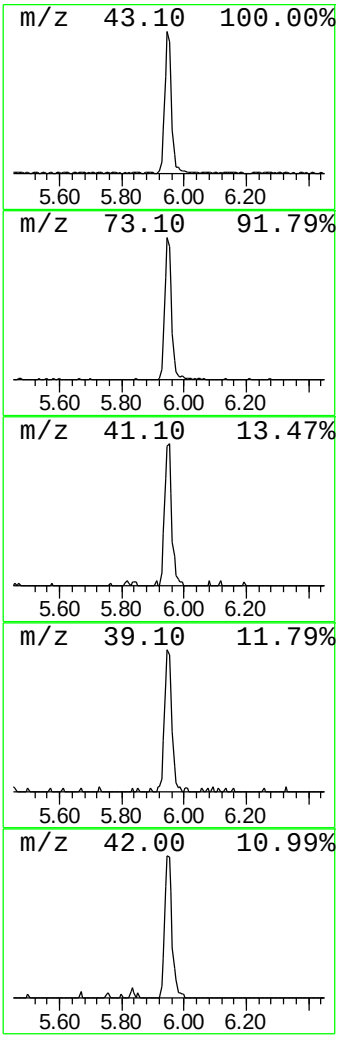
****

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.95	26.58 ng	486407	1,4-Dichlorobenzene-d4	7.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	64
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	53
3	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	50
4	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	35
5	N-Ethylformamide	73	C3H7NO	000627-45-2	32





Data Path : Z:\HPCHEM1\BNA M\DATA\BM051617\
Data File : BM010063.D
Acq On : 16 May 2017 21:03
Operator : SJ/MA
Sample : I3171-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : WS-5

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

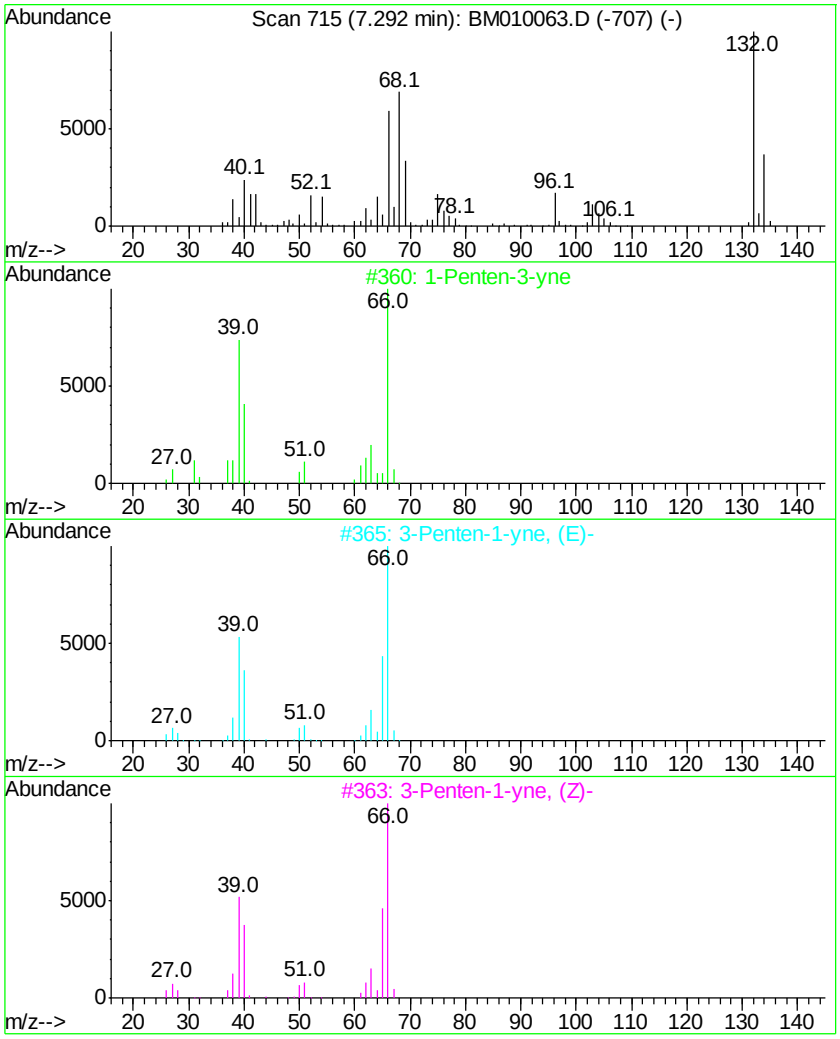
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

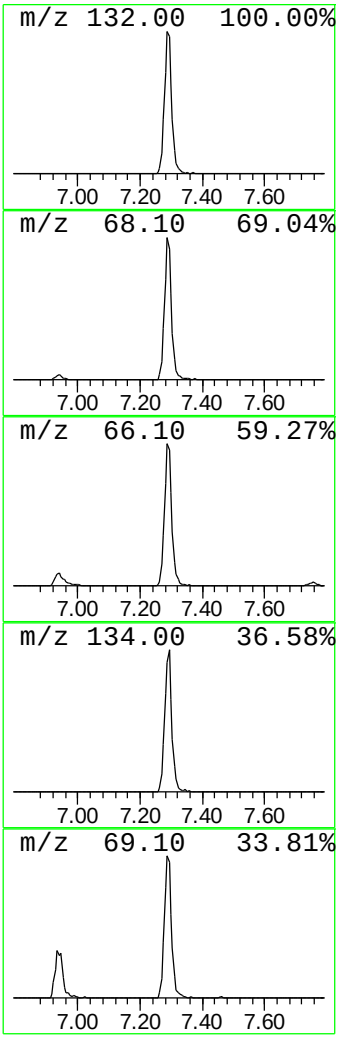
****

Peak Number 4 unknown7.29 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.29	78.51 ng	1436820	1,4-Dichlorobenzene-d4	7.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Penten-3-yne	66	C5H6	000646-05-9	30
2	3-Penten-1-yne, (E)-	66	C5H6	002004-69-5	27
3	3-Penten-1-yne, (Z)-	66	C5H6	001574-40-9	27
4	Bicyclo[2.2.1]hept-2-ene, 5-ethe...	120	C9H12	003048-64-4	16
5	3-Oxabicyclo[3.2.0]hept-6-ene-2,...	138	C7H6O3	064197-88-2	16





Data Path : Z:\HPCHEM1\BNA M\DATA\BM051617\
Data File : BM010063.D
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Operator : SJ/MA
Sample : I3171-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : WS-5

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

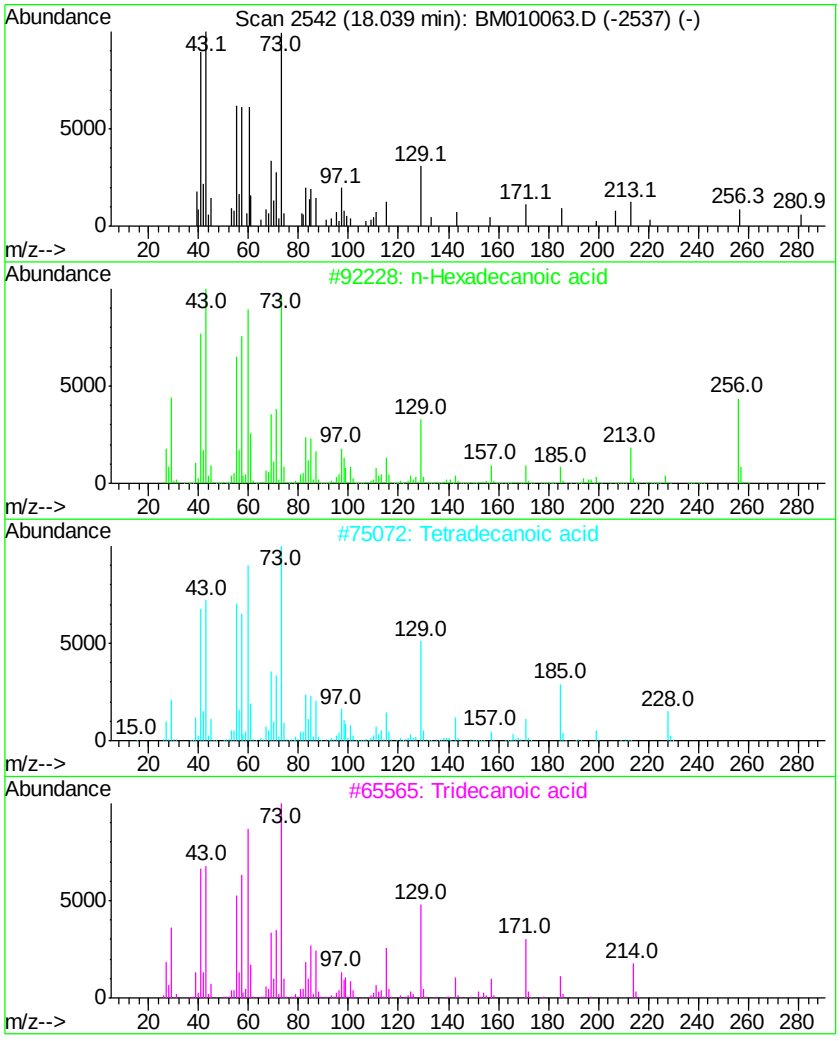
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

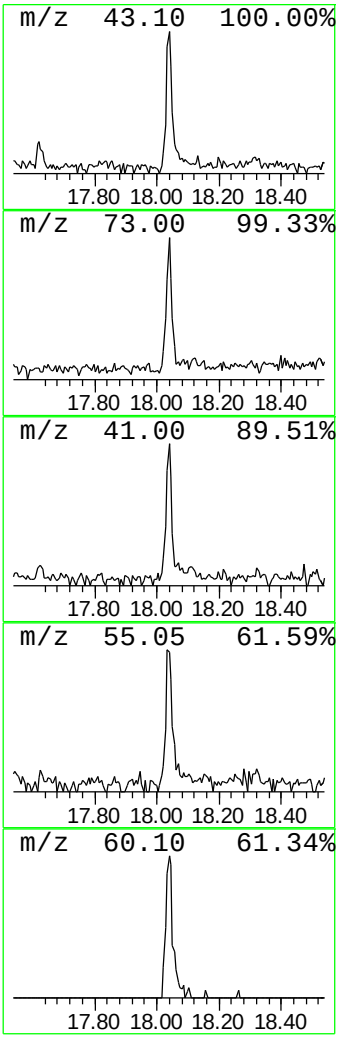
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.04	3.79 ng	150392	Phenanthrene-d10	17.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
3	Tridecanoic acid	214	C13H26O2	000638-53-9	53
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	47
5	n-Decanoic acid	172	C10H20O2	000334-48-5	38





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Sample : I3171-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : WS-5

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

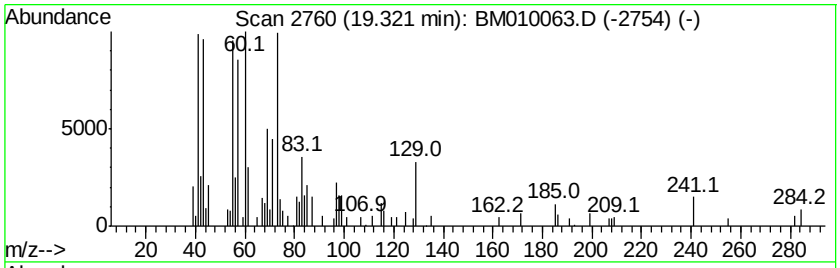
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

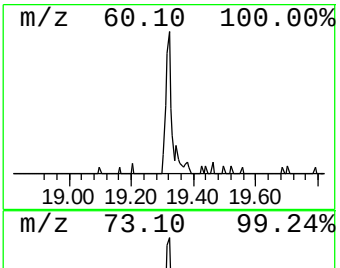
****

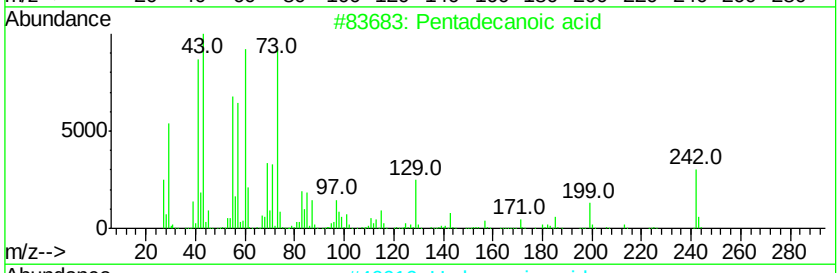
Peak Number 7 Pentadecanoic acid Concentration Rank 8

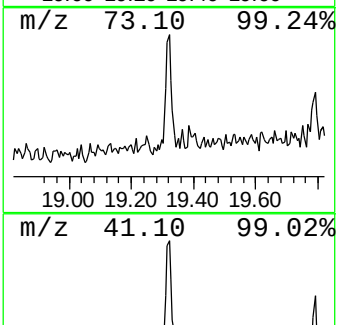
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.32	2.84 ng	139560	Chrysene-d12	21.35

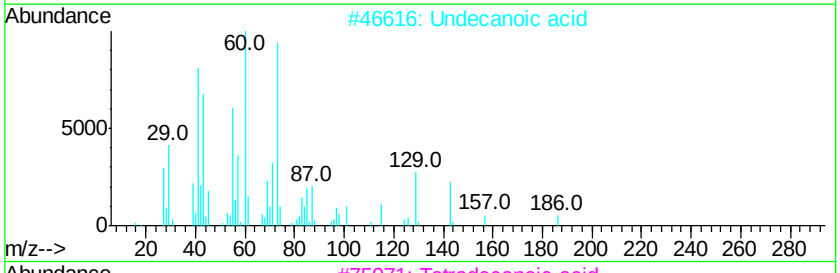
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
2	Undecanoic acid	186	C11H22O2	000112-37-8	72
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	53
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53

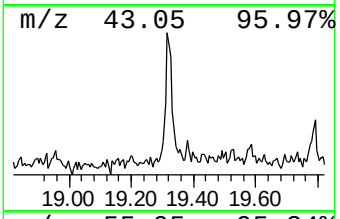


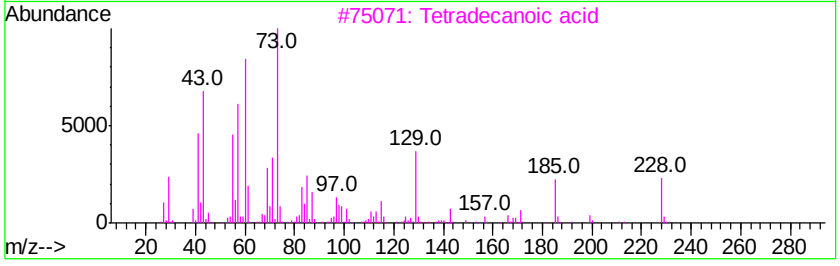


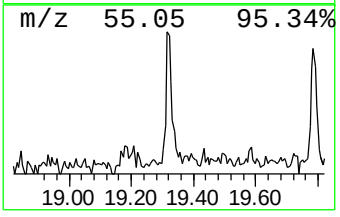












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Instrument : BNA_M
ClientSampleId : WS-5

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

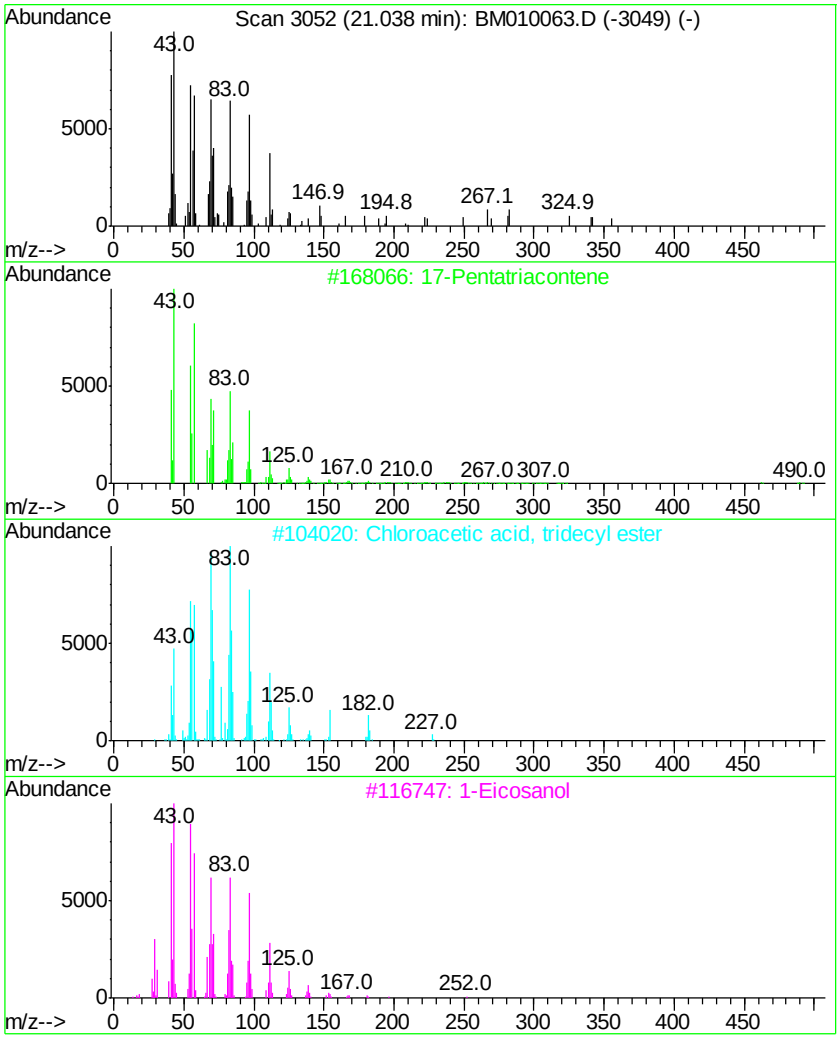
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

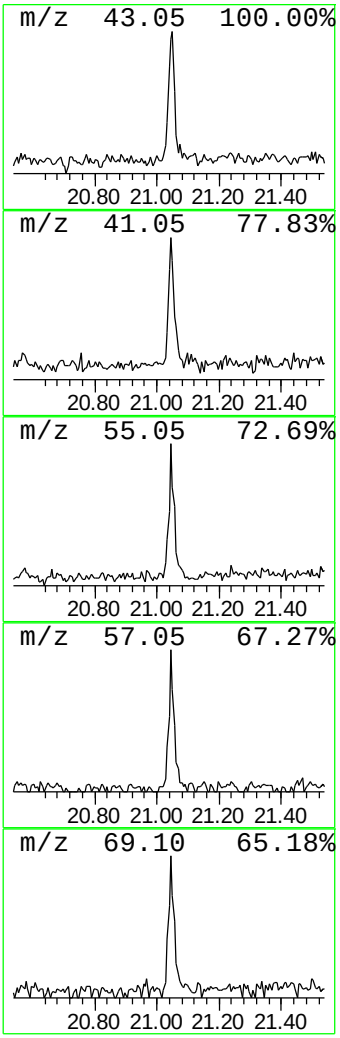
****

Peak Number 8 17-Pentatriacontene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.04	3.69 ng	181464	Chrysene-d12	21.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	80
2	Chloroacetic acid, tridecyl ester	276	C15H29ClO2	018277-85-5	74
3	1-Eicosanol	298	C20H42O	000629-96-9	64
4	Cyclotetracosane	336	C24H48	000297-03-0	52
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	1000280-07-5	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM051617\
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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.29	95.5	ng	1748390	1	7.75	366006	20.0
2-Pentanone, 4-hy...	4.89	153.7	ng	2812680	1	7.75	366006	20.0
2-Pentanone, 4-me...	5.95	26.6	ng	486407	1	7.75	366006	20.0
unknown7.29	7.29	78.5	ng	1436820	1	7.75	366006	20.0
n-Hexadecanoic acid	18.04	3.8	ng	150392	4	17.16	793315	20.0
Pentadecanoic acid	19.32	2.8	ng	139560	5	21.35	983842	20.0
17-Pentatriacontene	21.04	3.7	ng	181464	5	21.35	983842	20.0