LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM081617\
Data File : BM011257.D
Acq On : 16 Aug 2017 16:25
Operator : SJ/JU
Sample : I4798-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DRUM-1-6-COMP

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	4.475	281	287	294	rVB	238043	344343	2.24%	0.502%
2	4.916	356	362	370	rBV	3070759	4166119	27.09%	6.070%
3	6.481	620	628	642	rVB	2751930	4177385	27.17%	6.086%
4	6.816	679	685	694	rVB	3259230	4791871	31.16%	6.981%
5	7.275	755	763	769	rBV	599713	893638	5.81%	1.302%
6	7.357	769	777	783	rBV	306873	465479	3.03%	0.678%
7	7.586	809	816	825	rBV	2310321	3514803	22.86%	5.121%
8	8.422	951	958	966	rBV	2052433	3185906	20.72%	4.642%
9	8.616	979	991	996	rBV2	307390	690234	4.49%	1.006%
10	10.027	1224	1231	1238	rBV	649791	1105241	7.19%	1.610%
11	12.551	1653	1660	1667	rBV	4570161	6548223	42.58%	9.540%
12	13.945	1891	1897	1904	rVB2	976437	1458916	9.49%	2.126%
13	14.804	2034	2043	2049	rBV2	128686	241518	1.57%	0.352%
14	15.451	2146	2153	2162	rBV	5131897	7038558	45.77%	10.255%
15	16.703	2360	2366	2372	rBV	1531042	2108195	13.71%	3.071%
16	17.639	2519	2525	2533	rBV	811214	1299832	8.45%	1.894%
17	17.703	2533	2536	2542	rVB	177107	273906	1.78%	0.399%
18	18.780	2710	2719	2723	rBV4	245363	477356	3.10%	0.695%
19	18.821	2723	2726	2731	rVB6	106603	176261	1.15%	0.257%
20	18.945	2742	2747	2757	rBV	1091103	1712292	11.13%	2.495%
21	19.374	2814	2820	2832	rBV	12581740	15377594	100.00%	22.404%
22	20.633	3029	3034	3039	rBV	214066	335909	2.18%	0.489%
23	20.686	3039	3043	3047	rBV	293180	422655	2.75%	0.616%
24	20.739	3048	3052	3061	rVB	748470	956080	6.22%	1.393%
25	20.886	3073	3077	3079	rBV3	190535	217981	1.42%	0.318%
26	20.927	3079	3084	3089	rVV	2781782	3618815	23.53%	5.272%
27	22.997	3430	3436	3443	rBV2	1781954	3039200	19.76%	4.428%

Sum of corrected areas: 68638310

LSC Report - Integrated Chromatogram

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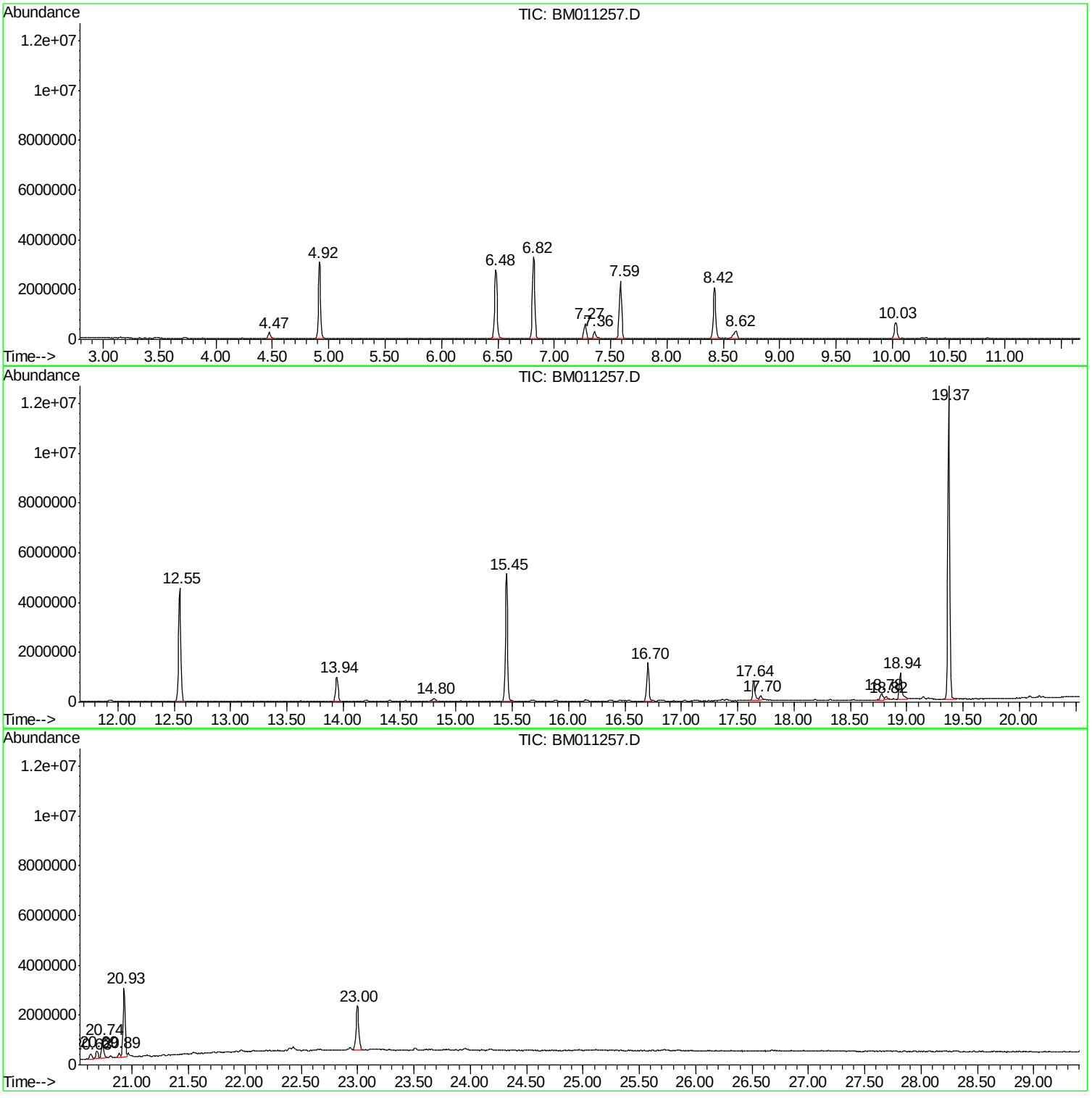
Data File : BM011257.D
Acq On : 16 Aug 2017 16:25
Operator : SJ/JU
Sample : I4798-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DRUM-1-6-COMP

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\BM081617\
Data File : BM011257.D
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Instrument : BNA_M
ClientSampleId : DRUM-1-6-COMP

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

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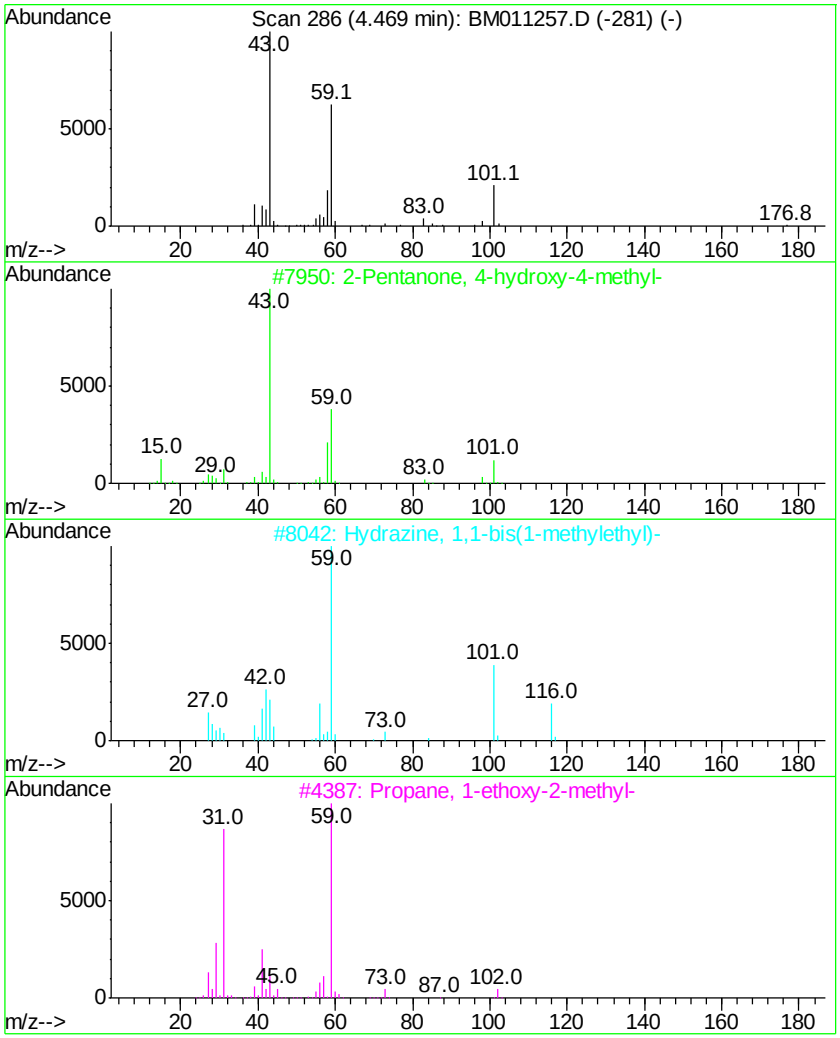
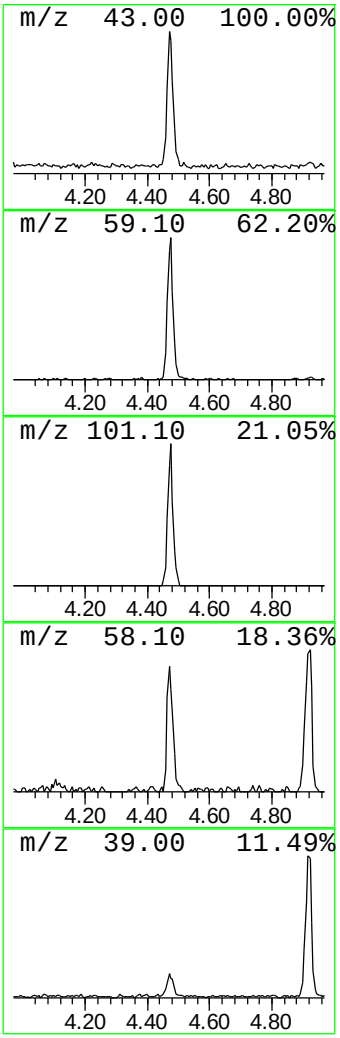
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.47	7.71 ng	344343	1,4-Dichlorobenzene-d4	7.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	40
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	27
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	17





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Operator : SJ/JU
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Instrument : BNA_M
ClientSampleId : DRUM-1-6-COMP

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

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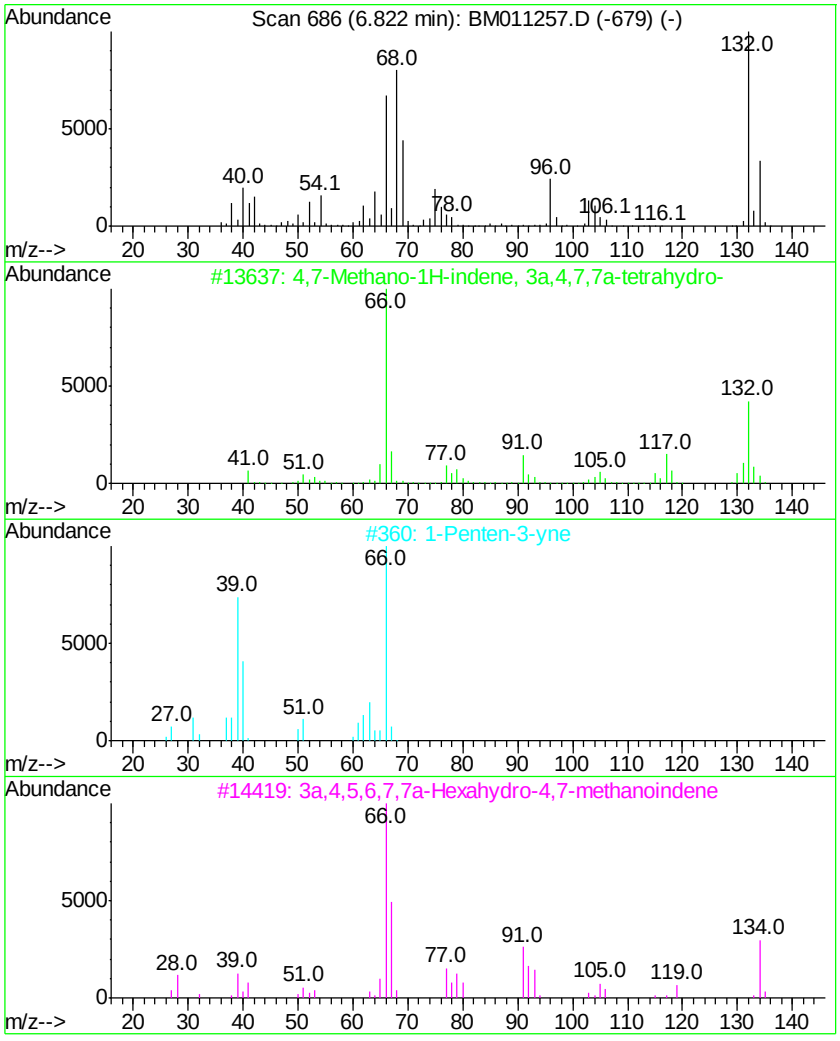
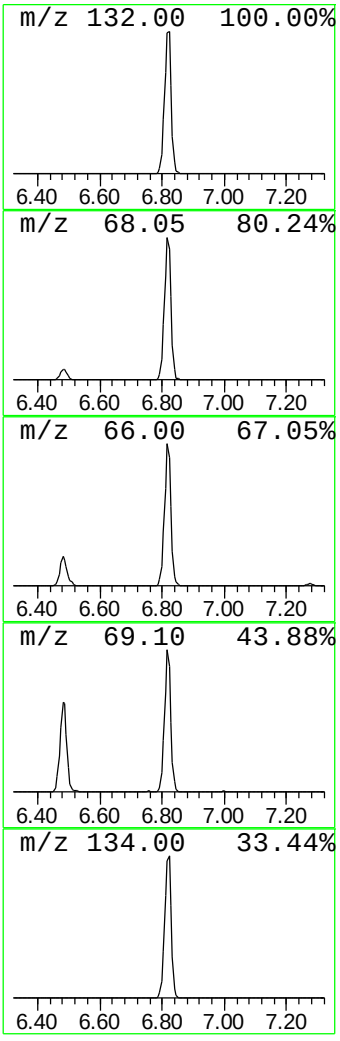
Peak Number 2 4,7-Methano-1H-indene, 3a,4... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.82	107.24 ng	4791870	1,4-Dichlorobenzene-d4	7.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,7-Methano-1H-indene, 3a,4,7,7a...	132	C10H12	000077-73-6	50
2	1-Penten-3-yne	66	C5H6	000646-05-9	43
3	3a,4,5,6,7,7a-Hexahydro-4,7-meth...	134	C10H14	004488-57-7	43
4	3-Hexenedinitrile	106	C6H6N2	001119-85-3	38
5	3-Penten-1-yne, (Z)-	66	C5H6	001574-40-9	38





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM081617\
Data File : BM011257.D
Acq On : 16 Aug 2017 16:25
Operator : SJ/JU
Sample : I4798-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DRUM-1-6-COMP

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

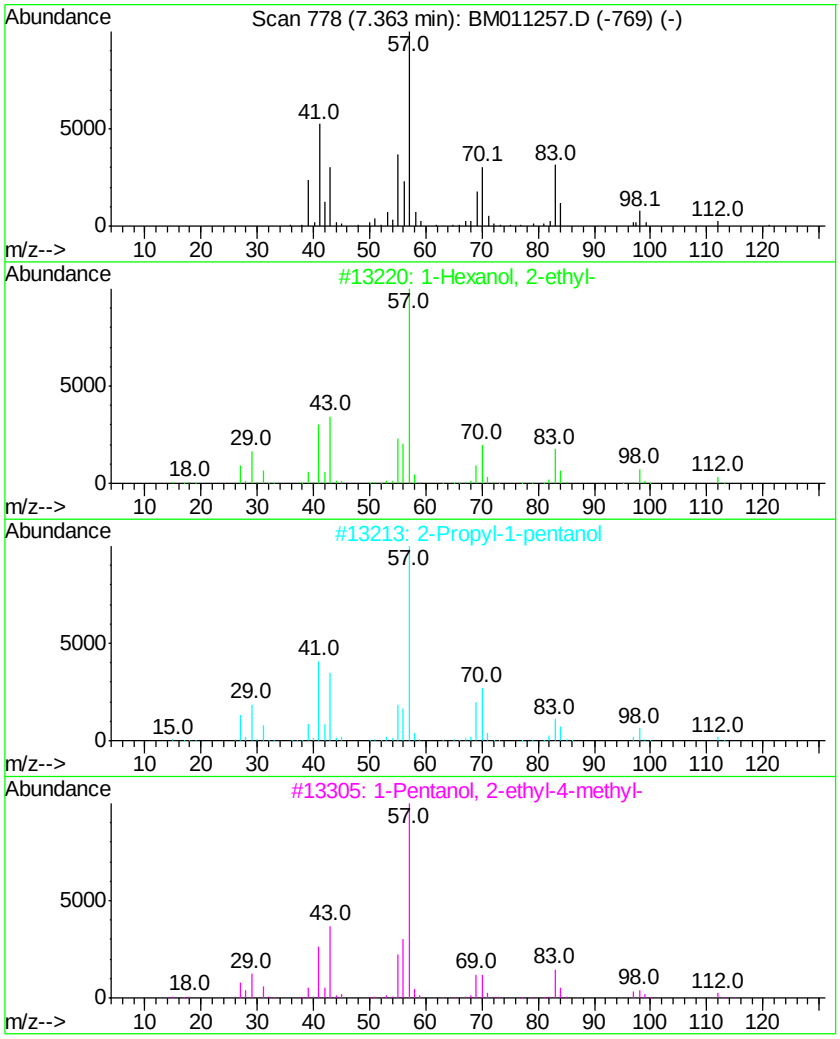
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

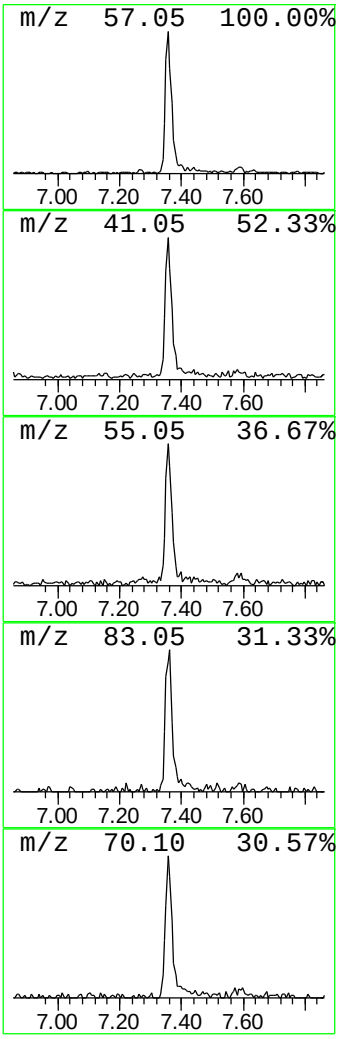
****

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.36	10.42 ng	465479	1,4-Dichlorobenzene-d4	7.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	64
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50
4	Bicyclo[3.1.0]hexan-2-ol	98	C6H10O	1000194-18-6	43
5	Pentafluoropropionic acid, 2-eth...	276	C11H17F5O2	1000280-14-6	42





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM081617\
Data File : BM011257.D
Acq On : 16 Aug 2017 16:25
Operator : SJ/JU
Sample : I4798-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DRUM-1-6-COMP

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

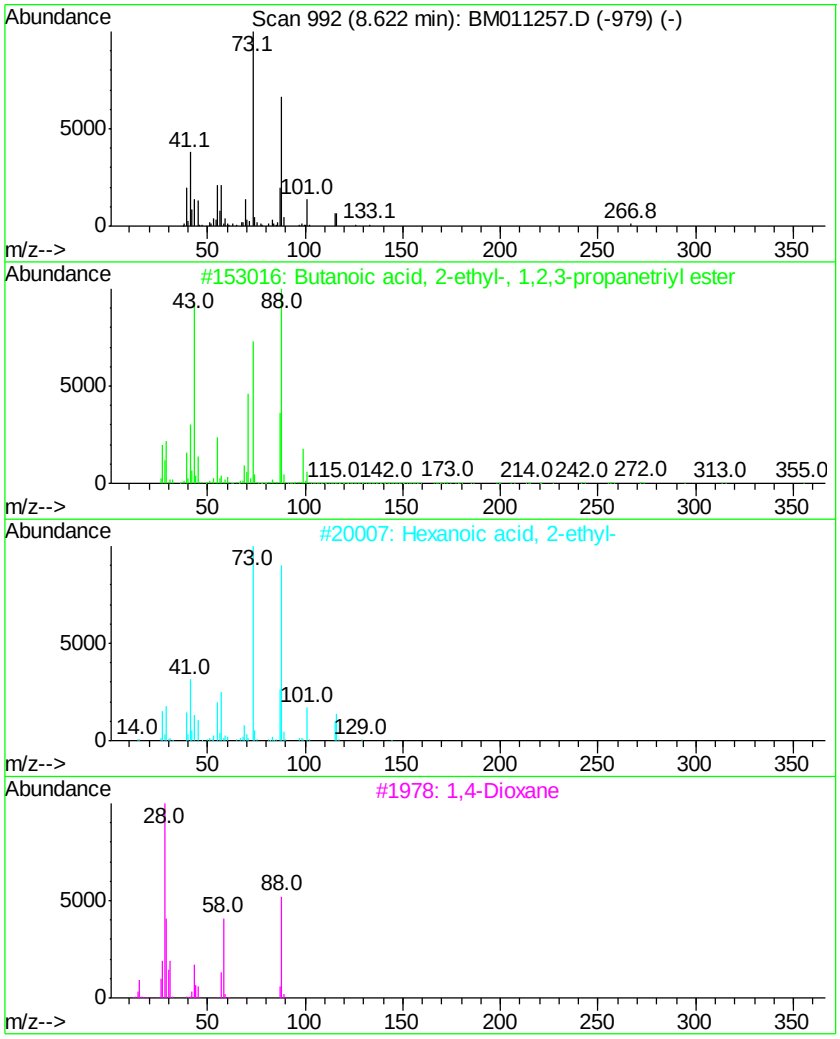
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

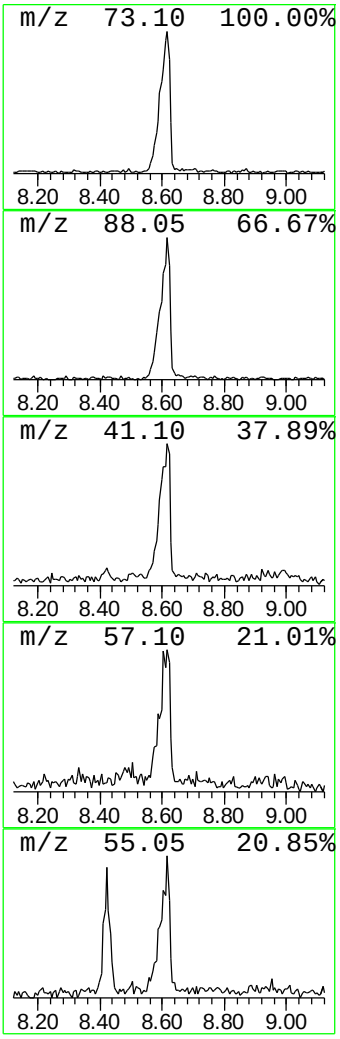
****

Peak Number 5 unknown8.62 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.62	15.45 ng	690234	1,4-Dichlorobenzene-d4	7.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	45
2	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	45
3	1,4-Dioxane	88	C4H8O2	000123-91-1	38
4	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	37
5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	27





Data Path : Z:\HPCHEM1\BNA M\DATA\BM081617\
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Acq On : 16 Aug 2017 16:25
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Sample : I4798-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DRUM-1-6-COMP

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM072617.M
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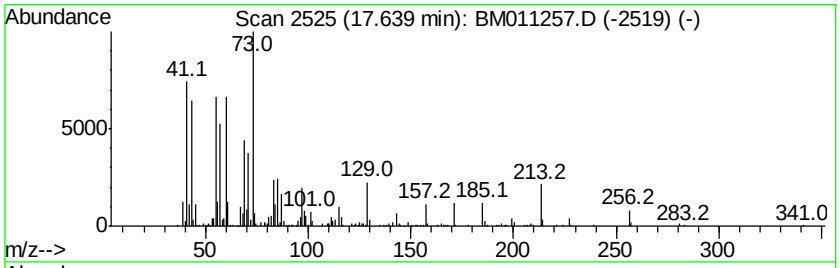
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

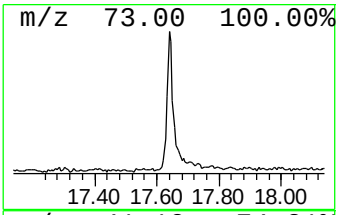
****

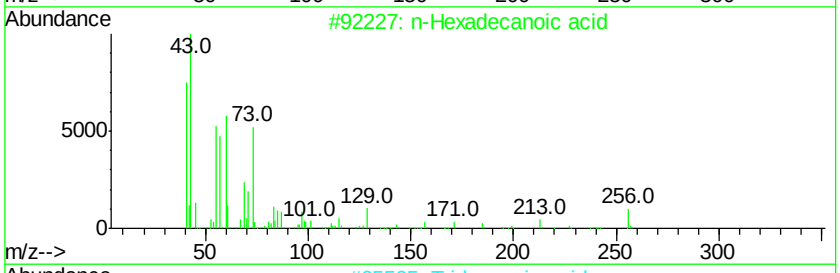
Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

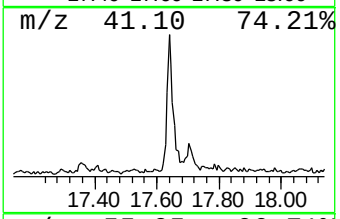
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.64	12.33 ng	1299830	Phenanthrene-d10	16.70

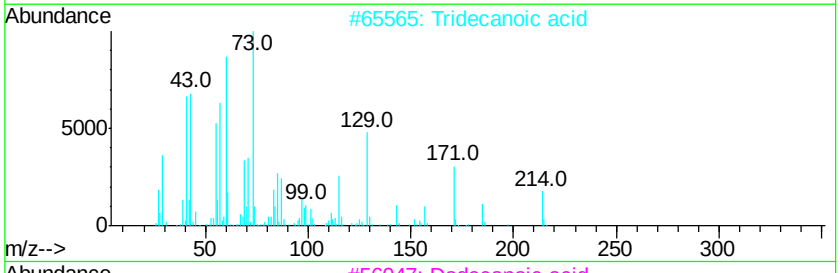
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	58
3	Dodecanoic acid	200	C12H24O2	000143-07-7	50
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	43

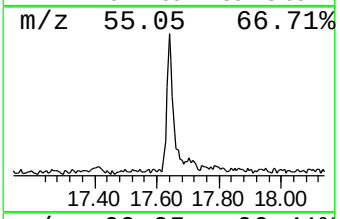


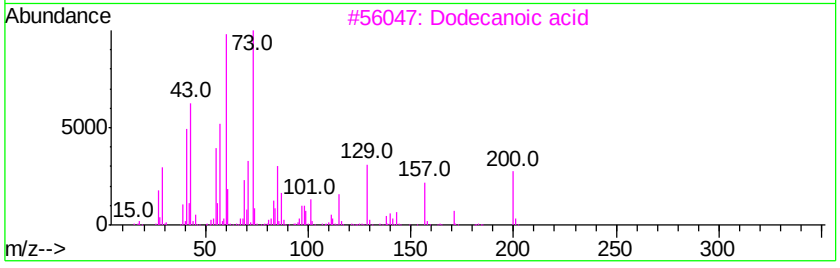


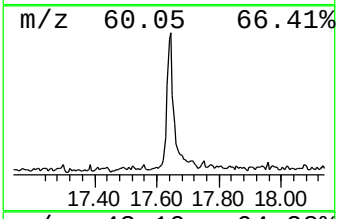


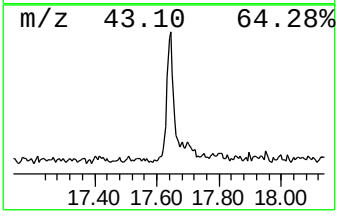












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Instrument : BNA_M
ClientSampleId : DRUM-1-6-COMP

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

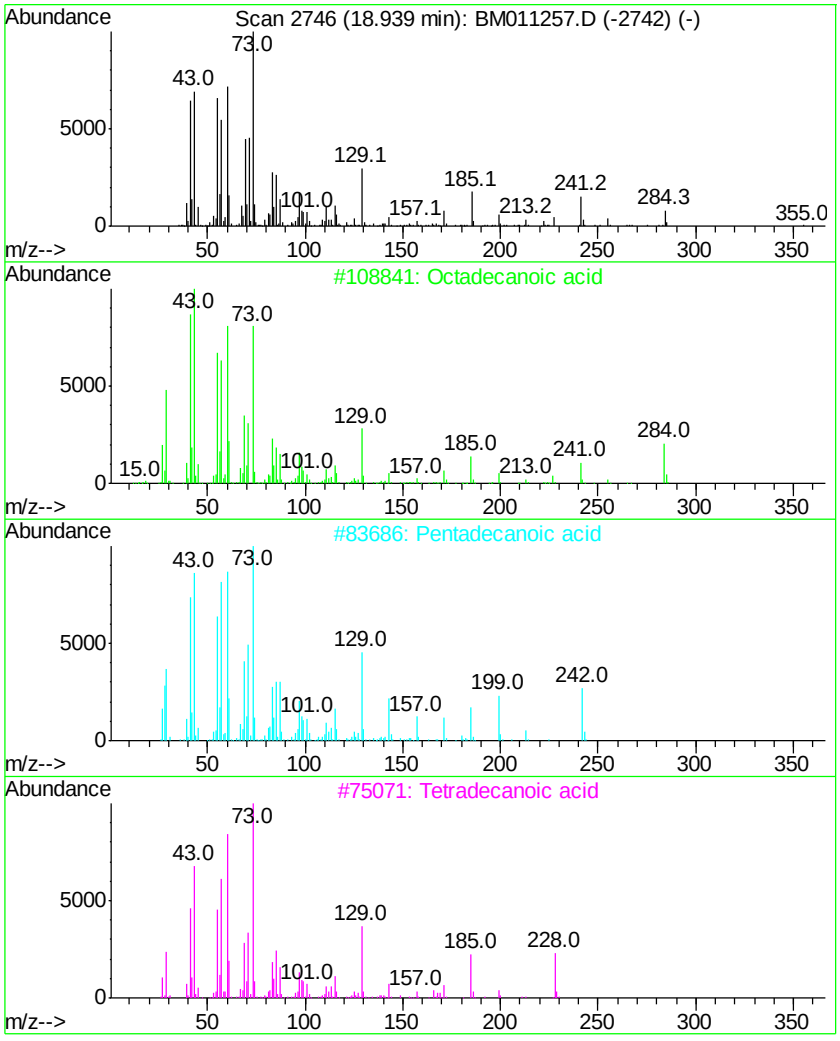
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

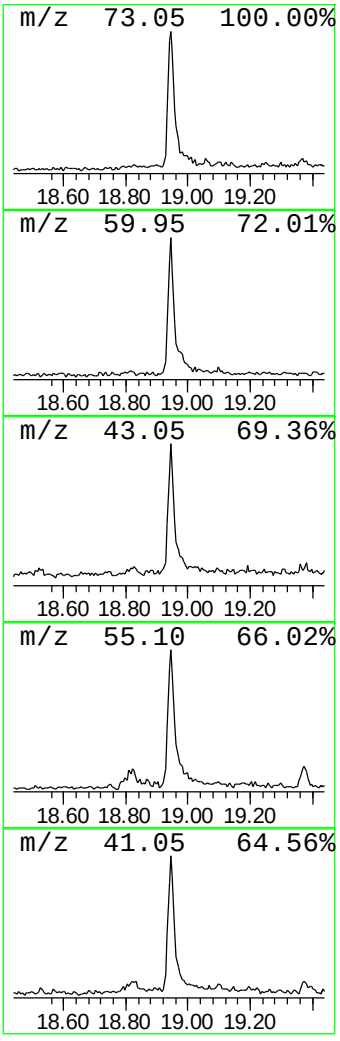
****

Peak Number 8 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.94	9.46 ng	1712290	Chrysene-d12	20.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	90
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	52
5	n-Decanoic acid	172	C10H20O2	000334-48-5	46





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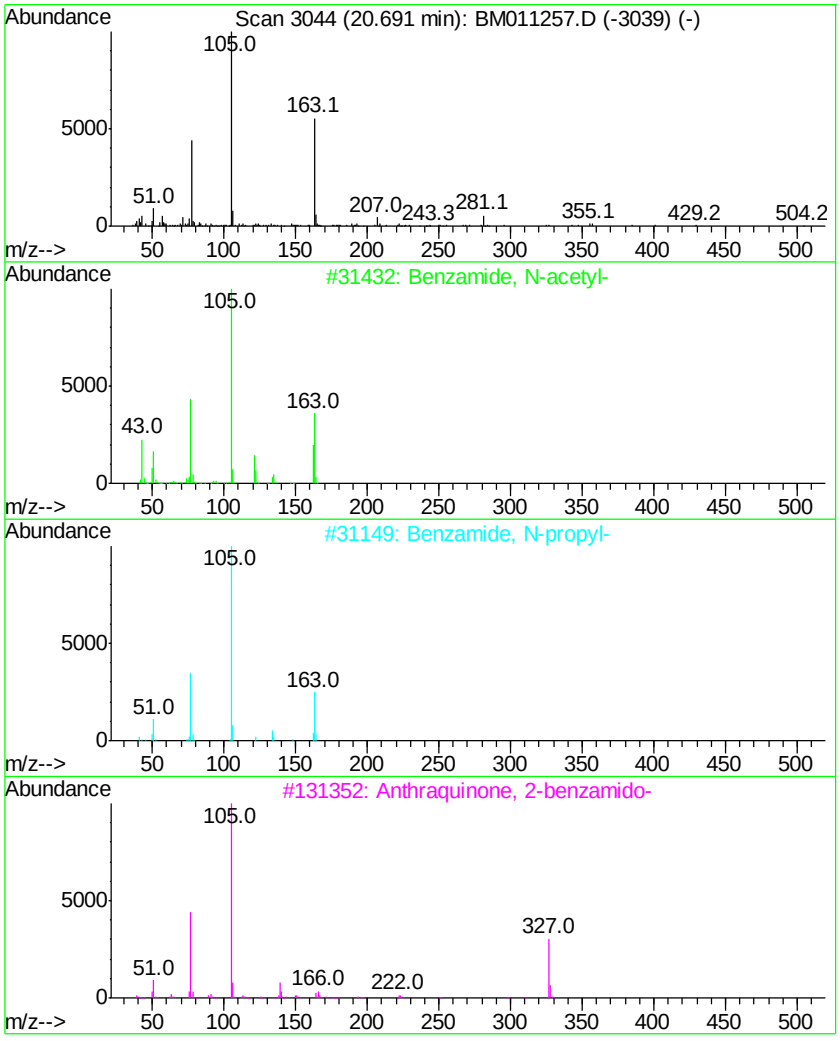
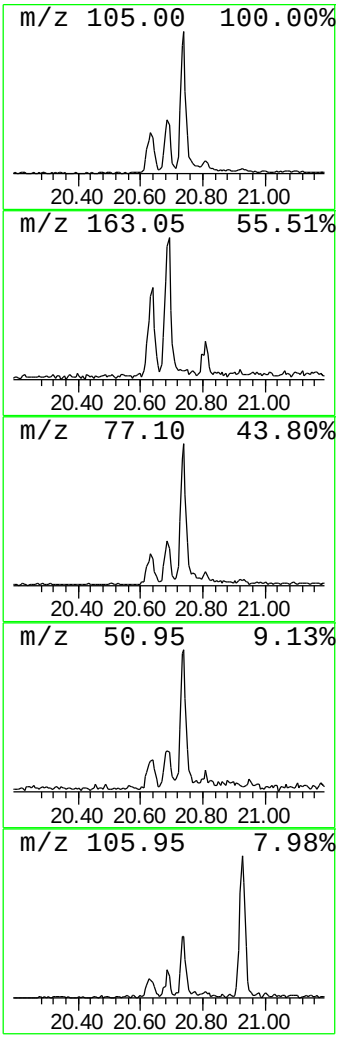
****

Peak Number 9 Benzamide, N-acetyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.69	2.34 ng	422655	Chrysene-d12	20.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	72
2	Benzamide, N-propyl-	163	C10H13NO	010546-70-0	56
3	Anthraquinone, 2-benzamido-	327	C21H13NO3	052869-18-8	46
4	1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	45
5	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	43





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Data File : BM011257.D
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Sample : I4798-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DRUM-1-6-COMP

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
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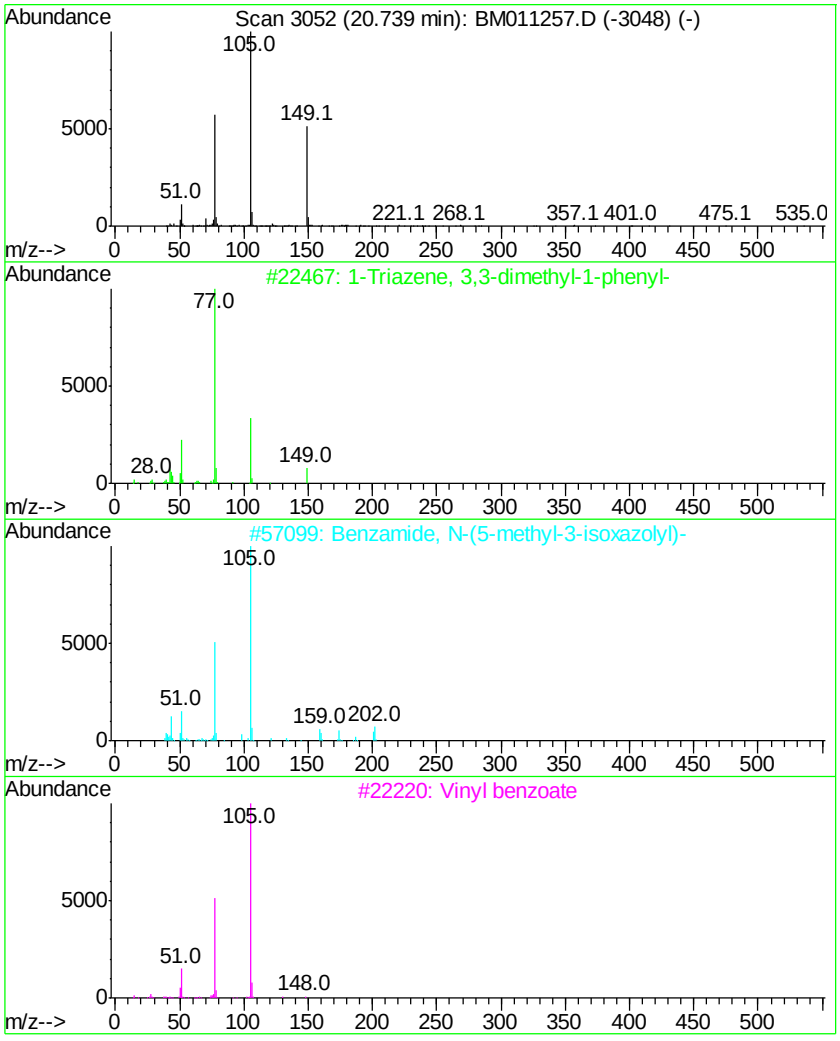
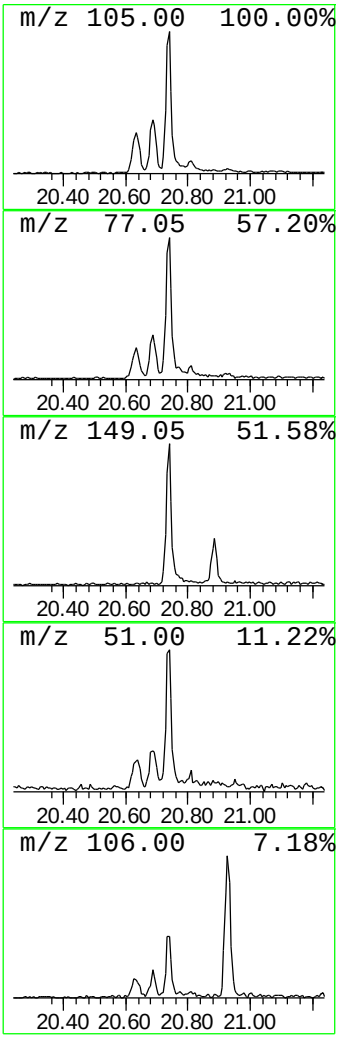
****

Peak Number 10 1-Triazene, 3,3-dimethyl-1-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.74	5.28 ng	956080	Chrysene-d12	20.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Triazene, 3,3-dimethyl-1-phenyl-	149	C8H11N3	007227-91-0	53
2	Benzamide, N-(5-methyl-3-isoxazo...	202	C11H10N2O2	013053-85-5	47
3	Vinyl benzoate	148	C9H8O2	000769-78-8	47
4	1,3,4-Oxadiazin-6-one, 5-isoprop...	216	C12H12N2O2	173973-78-9	47
5	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM081617\
Data File : BM011257.D
Acq On : 16 Aug 2017 16:25
Operator : SJ/JU
Sample : I4798-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DRUM-1-6-COMP

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
2-Pentanone, 4-hy...	4.47	7.7	ng	344343	1	7.27	893638	20.0
4,7-Methano-1H-in...	6.82	107.2	ng	4791870	1	7.27	893638	20.0
1-Hexanol, 2-ethyl-	7.36	10.4	ng	465479	1	7.27	893638	20.0
unknown8.62	8.62	15.4	ng	690234	1	7.27	893638	20.0
n-Hexadecanoic acid	17.64	12.3	ng	1299830	4	16.70	2108200	20.0
Octadecanoic acid	18.94	9.5	ng	1712290	5	20.93	3618820	20.0
Benzamide, N-acetyl-	20.69	2.3	ng	422655	5	20.93	3618820	20.0
1-Triazene, 3,3-d...	20.74	5.3	ng	956080	5	20.93	3618820	20.0