LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM081617\
Data File : BM011265.D
Acq On : 16 Aug 2017 21:46
Operator : SJ/JU
Sample : I4736-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TWP-37

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	4.469	282	286	291	rBV	107411	144152	1.12%	0.266%
2	4.916	356	362	369	rBV	1163173	1602016	12.49%	2.962%
3	6.340	596	604	611	rBV4	106320	199618	1.56%	0.369%
4	6.475	622	627	640	rVB	800634	1271411	9.91%	2.350%
5	6.816	678	685	692	rBV	1787842	2671058	20.82%	4.938%
6	7.275	757	763	771	rVB	635417	940623	7.33%	1.739%
7	7.587	809	816	824	rBV	2347451	3562400	27.77%	6.586%
8	8.422	951	958	966	rBV	1982167	3166247	24.68%	5.853%
9	9.410	1121	1126	1131	rVB2	94559	135772	1.06%	0.251%
10	10.028	1225	1231	1240	rBV	702327	1142582	8.91%	2.112%
11	10.875	1365	1375	1381	rBV4	129971	241803	1.88%	0.447%
12	12.110	1579	1585	1589	rBV4	192801	302989	2.36%	0.560%
13	12.551	1653	1660	1667	rBV	4206643	6180616	48.18%	11.426%
14	13.422	1803	1808	1812	rBV2	123547	167034	1.30%	0.309%
15	13.945	1890	1897	1905	rBV2	1006268	1594072	12.43%	2.947%
16	14.410	1972	1976	1983	rVB3	122204	173766	1.35%	0.321%
17	14.504	1983	1992	1995	rBV2	190397	515062	4.01%	0.952%
18	14.621	2010	2012	2029	rVB2	297791	813411	6.34%	1.504%
19	15.445	2146	2152	2164	rBV	2922350	4124511	32.15%	7.625%
20	16.704	2360	2366	2372	rBV	1529211	2157446	16.82%	3.988%
21	17.645	2521	2526	2533	rBV	1079728	1442405	11.24%	2.667%
22	17.857	2558	2562	2570	rBV5	173174	351010	2.74%	0.649%
23	18.945	2743	2747	2757	rVB	1284794	1542490	12.02%	2.852%
24	19.374	2814	2820	2825	rBV	10937070	12828851	100.00%	23.716%
25	20.627	3031	3033	3039	rVV5	121414	202294	1.58%	0.374%
26	20.686	3039	3043	3047	rVV3	322845	429691	3.35%	0.794%
27	20.733	3049	3051	3057	rVB	150749	190592	1.49%	0.352%
28	20.927	3079	3084	3088	rBV	2594199	3156194	24.60%	5.835%
29	22.997	3431	3436	3448	rVB	1665931	2843040	22.16%	5.256%

Sum of corrected areas: 54093156

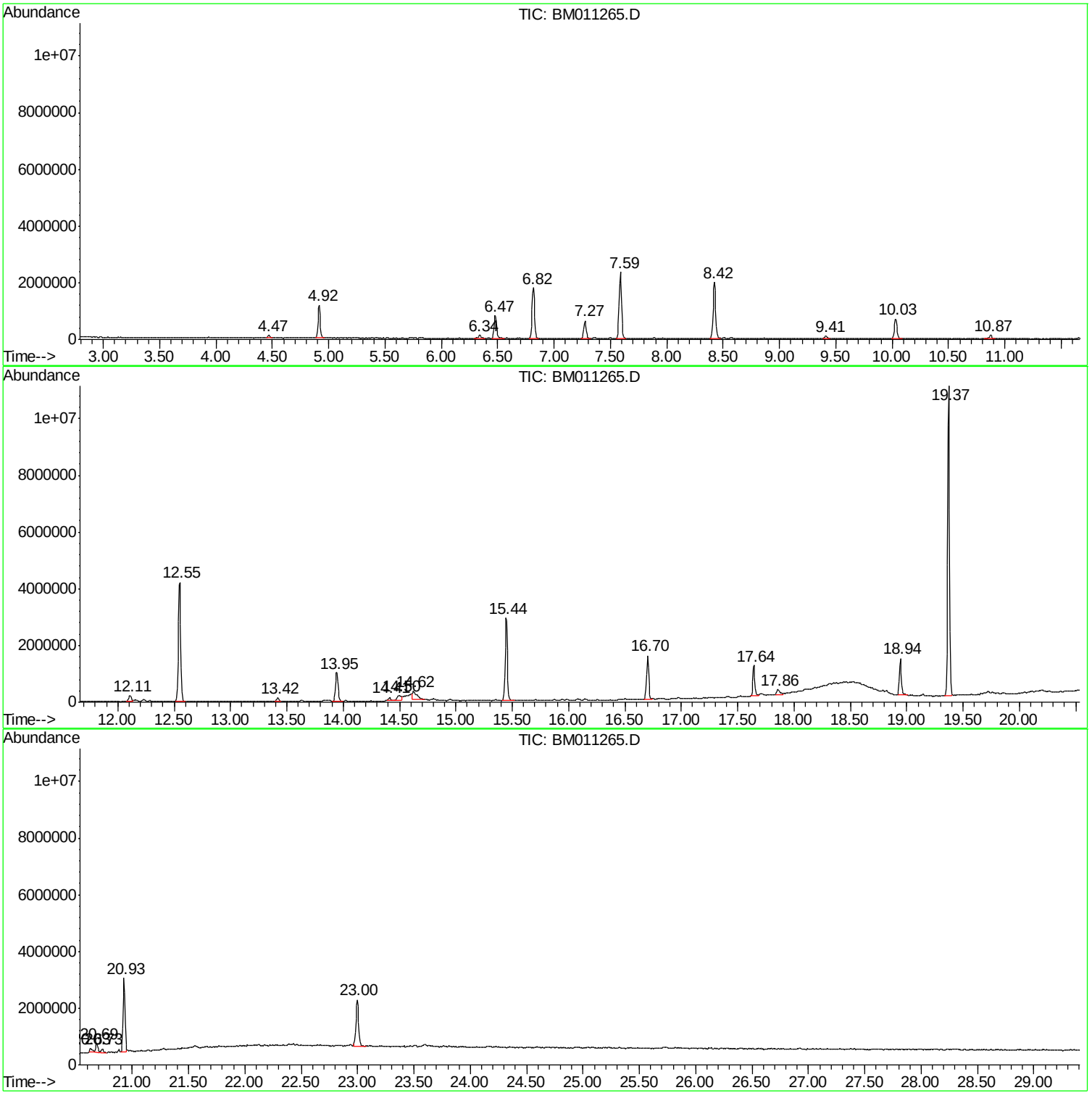
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA M\DATA\BM081617\
Data File : BM011265.D
Acq On : 16 Aug 2017 21:46
Operator : SJ/JU
Sample : I4736-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TWP-37

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 : BM011265.D
Acq On : 16 Aug 2017 21:46
Operator : SJ/JU
Sample : I4736-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TWP-37

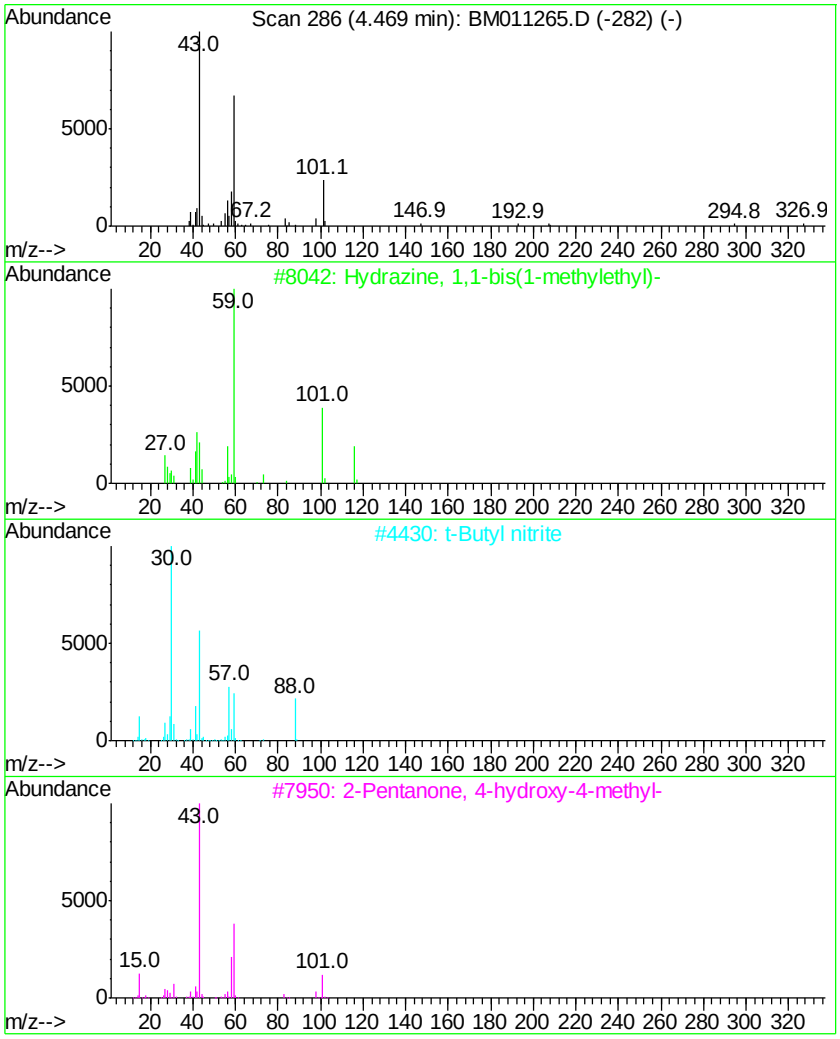
Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM072617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

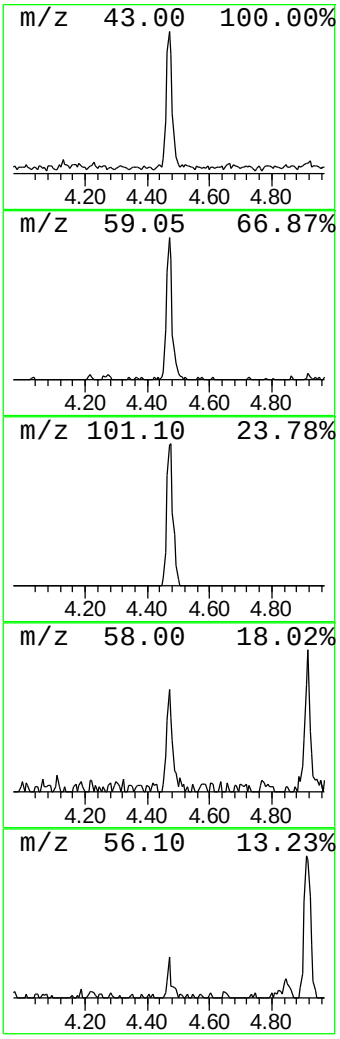
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Hydrazine, 1,1-bis(1-methyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.47	3.07 ng	144152	1,4-Dichlorobenzene-d4	7.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	50
2	t-Butyl nitrite	103	C4H9NO2	000540-80-7	42
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	36
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	30
5	3-Nonanol	144	C9H20O	000624-51-1	28





Data Path : Z:\HPCHEM1\BNA M\DATA\BM081617\
Data File : BM011265.D
Acq On : 16 Aug 2017 21:46
Operator : SJ/JU
Sample : I4736-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TWP-37

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

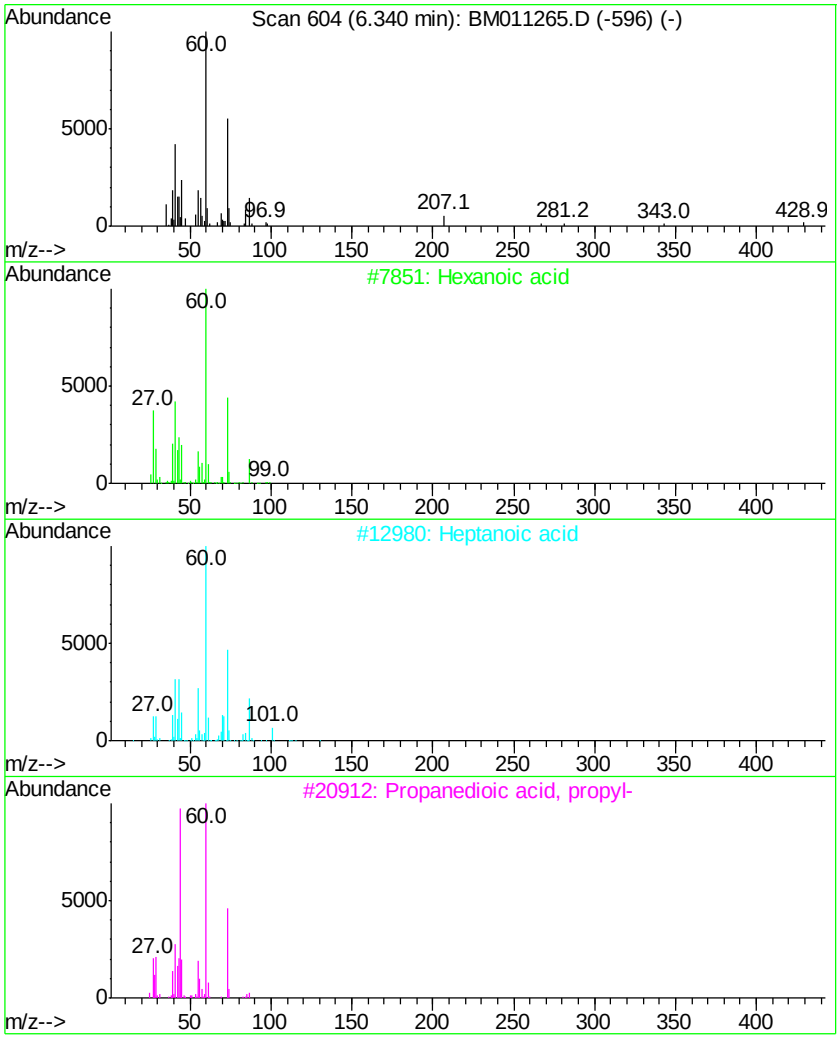
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

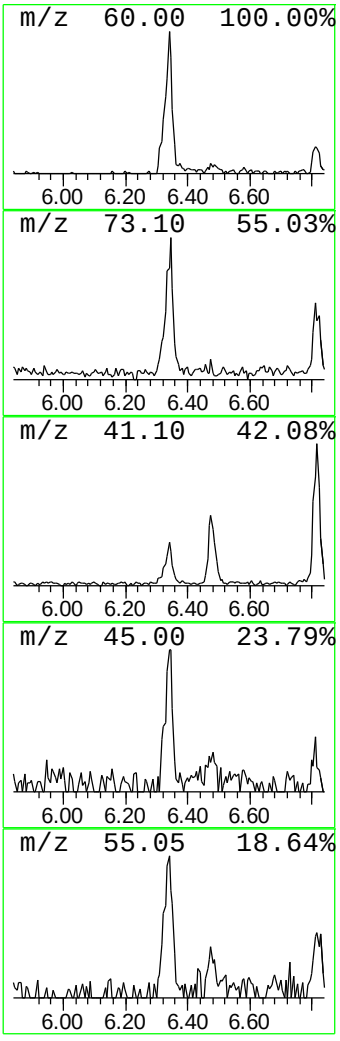
****

Peak Number 2 Hexanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	4.24 ng	199618	1,4-Dichlorobenzene-d4	7.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid	116	C6H12O2	000142-62-1	72
2	Heptanoic acid	130	C7H14O2	000111-14-8	56
3	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	50
4	L-Mannose, 6-deoxy-	164	C6H12O5	003615-41-6	50
5	Pentanoic acid	102	C5H10O2	000109-52-4	45





Data Path : Z:\HPCHEM1\BNA M\DATA\BM081617\
Data File : BM011265.D
Acq On : 16 Aug 2017 21:46
Operator : SJ/JU
Sample : I4736-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TWP-37

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

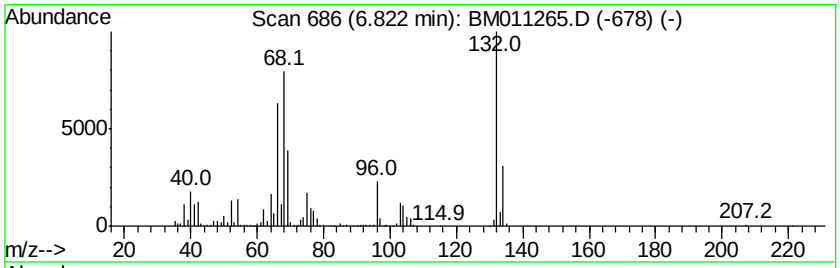
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

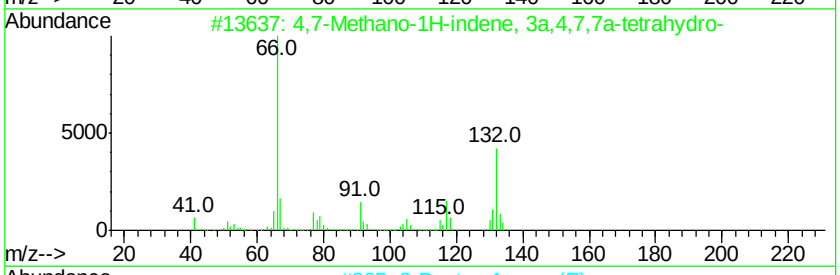
****

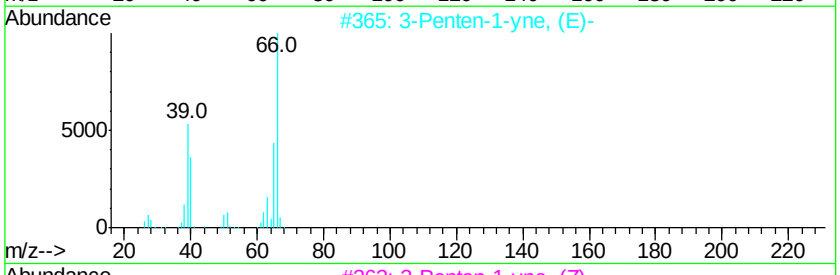
Peak Number 3 unknown6.82 Concentration Rank 2

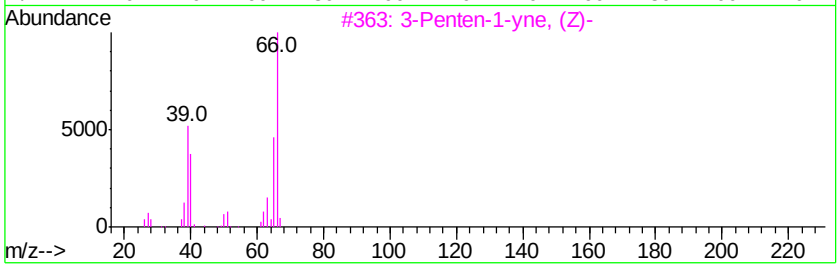
R.T.	EstConc	Area	Relative to ISTD	R.T.
6.82	56.79 ng	2671060	1,4-Dichlorobenzene-d4	7.27

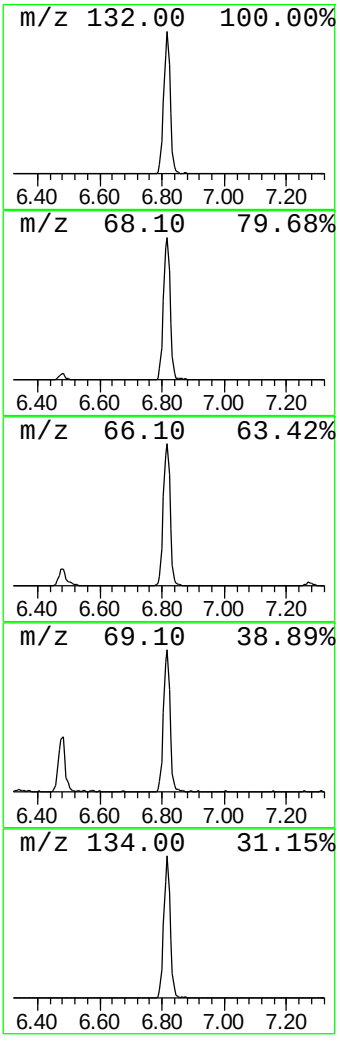
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,7-Methano-1H-indene, 3a,4,7,7a...	132	C10H12	000077-73-6	37
2	3-Penten-1-yne, (E)-	66	C5H6	002004-69-5	25
3	3-Penten-1-yne, (Z)-	66	C5H6	001574-40-9	22
4	1-Penten-3-yne	66	C5H6	000646-05-9	22
5	endo-4-Oxatricyclo[5.2.1.0(2,6)]...	136	C9H12O	001528-23-0	22











Data Path : Z:\HPCHEM1\BNA M\DATA\BM081617\
Data File : BM011265.D
Acq On : 16 Aug 2017 21:46
Operator : SJ/JU
Sample : I4736-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TWP-37

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

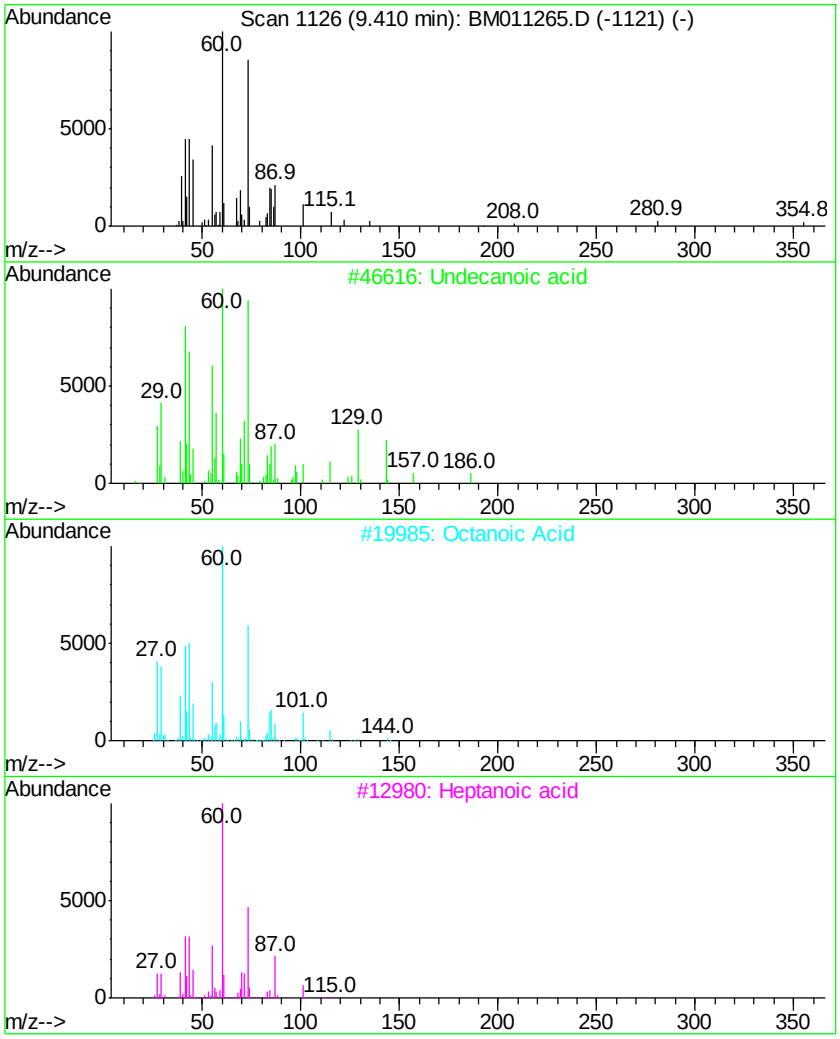
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

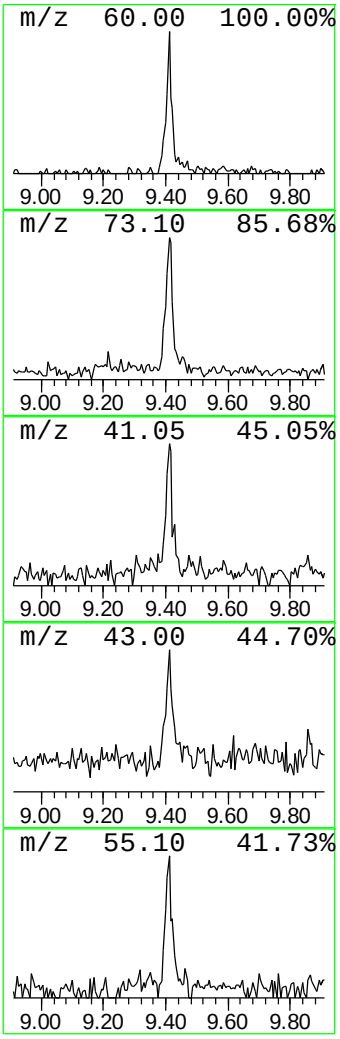
****

Peak Number 5 Undecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.41	2.38 ng	135772	Naphthalene-d8	10.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	59
2	Octanoic Acid	144	C8H16O2	000124-07-2	50
3	Heptanoic acid	130	C7H14O2	000111-14-8	47
4	Nonanoic acid	158	C9H18O2	000112-05-0	38
5	D-Galactose, 6-deoxy-	164	C6H12O5	003615-37-0	38





Data Path : Z:\HPCHEM1\BNA M\DATA\BM081617\
Data File : BM011265.D
Acq On : 16 Aug 2017 21:46
Operator : SJ/JU
Sample : I4736-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TWP-37

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

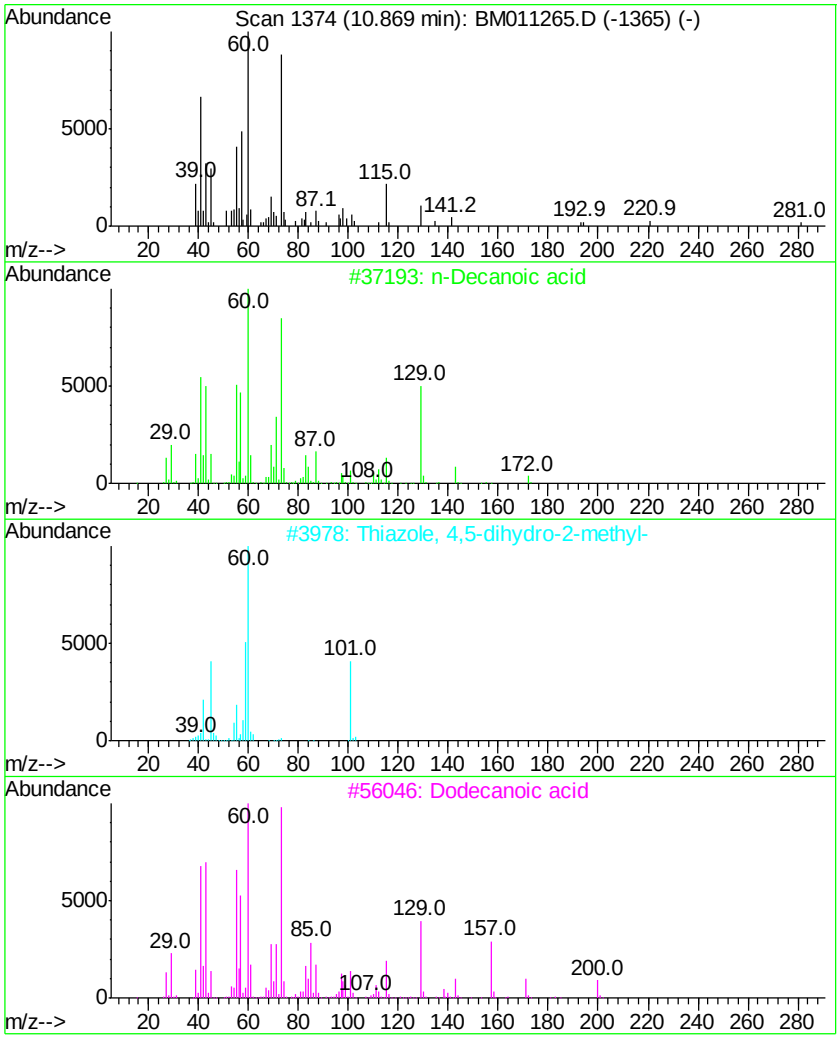
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

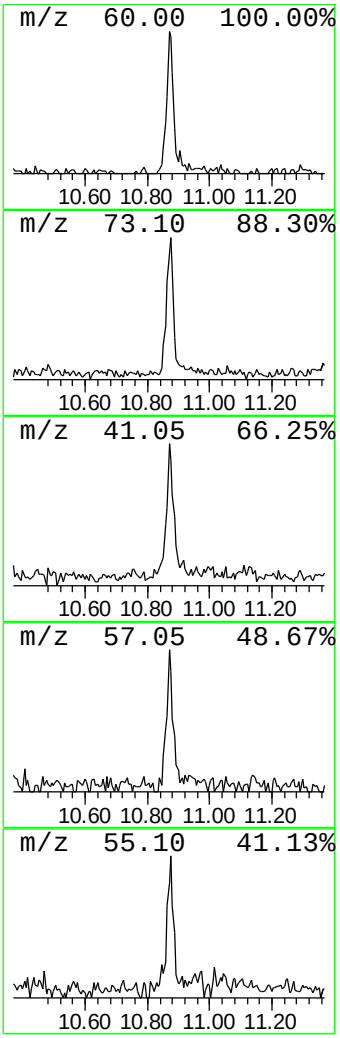
****

Peak Number 6 n-Decanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.87	4.23 ng	241803	Naphthalene-d8	10.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	53
2	Thiazole, 4,5-dihydro-2-methyl-	101	C4H7NS	002346-00-1	47
3	Dodecanoic acid	200	C12H24O2	000143-07-7	45
4	Nonanoic acid	158	C9H18O2	000112-05-0	45
5	Undecanoic acid	186	C11H22O2	000112-37-8	42





Data Path : Z:\HPCHEM1\BNA M\DATA\BM081617\
Data File : BM011265.D
Acq On : 16 Aug 2017 21:46
Operator : SJ/JU
Sample : I4736-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TWP-37

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

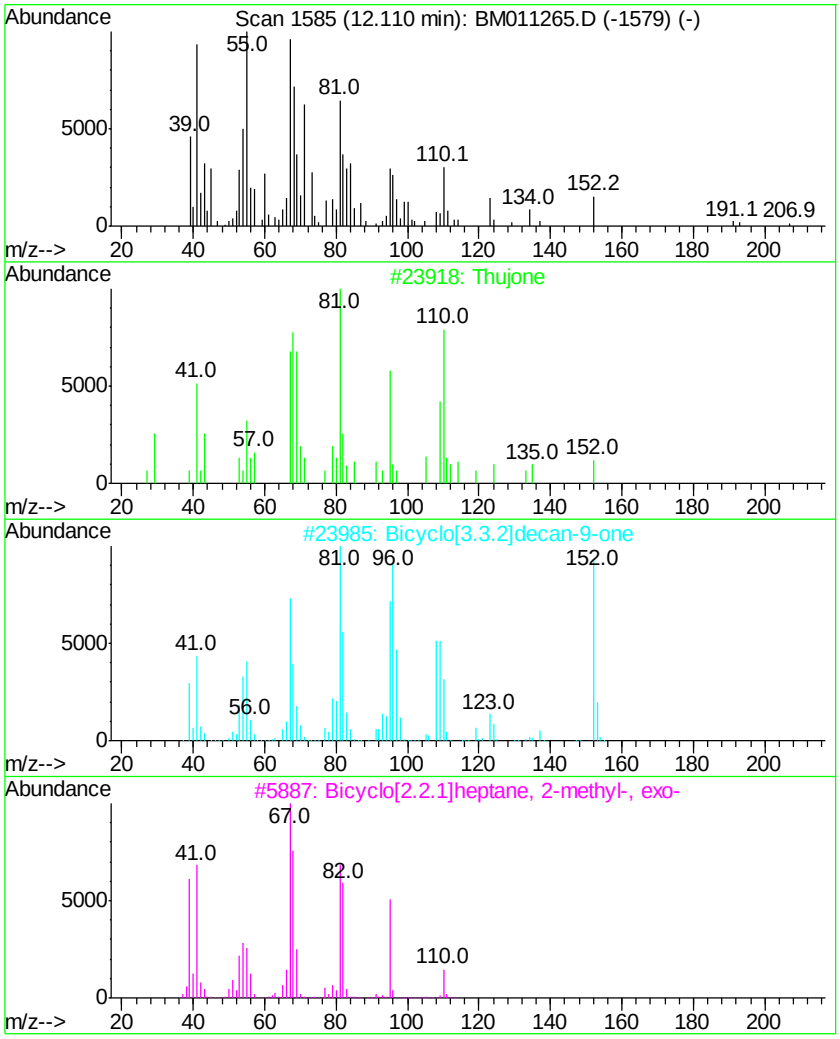
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

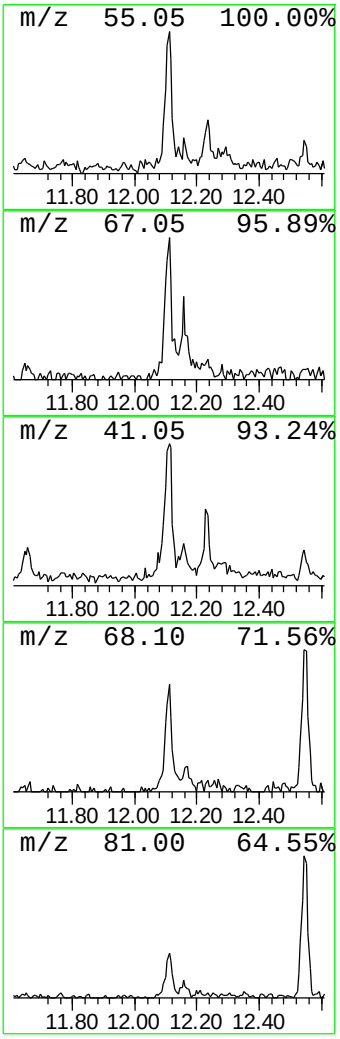
****

Peak Number 7 Thujone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.11	3.80 ng	302989	Acenaphthene-d10	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thujone	152	C10H16O	000546-80-5	50
2	Bicyclo[3.3.2]decan-9-one	152	C10H16O	028054-91-3	50
3	Bicyclo[2.2.1]heptane, 2-methyl-...	110	C8H14	000872-78-6	46
4	Bicyclo[3.1.0]hexan-3-one, 4-met...	152	C10H16O	000471-15-8	45
5	1-Methylcycloheptene	110	C8H14	055308-20-8	43





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM081617\
Data File : BM011265.D
Acq On : 16 Aug 2017 21:46
Operator : SJ/JU
Sample : I4736-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TWP-37

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

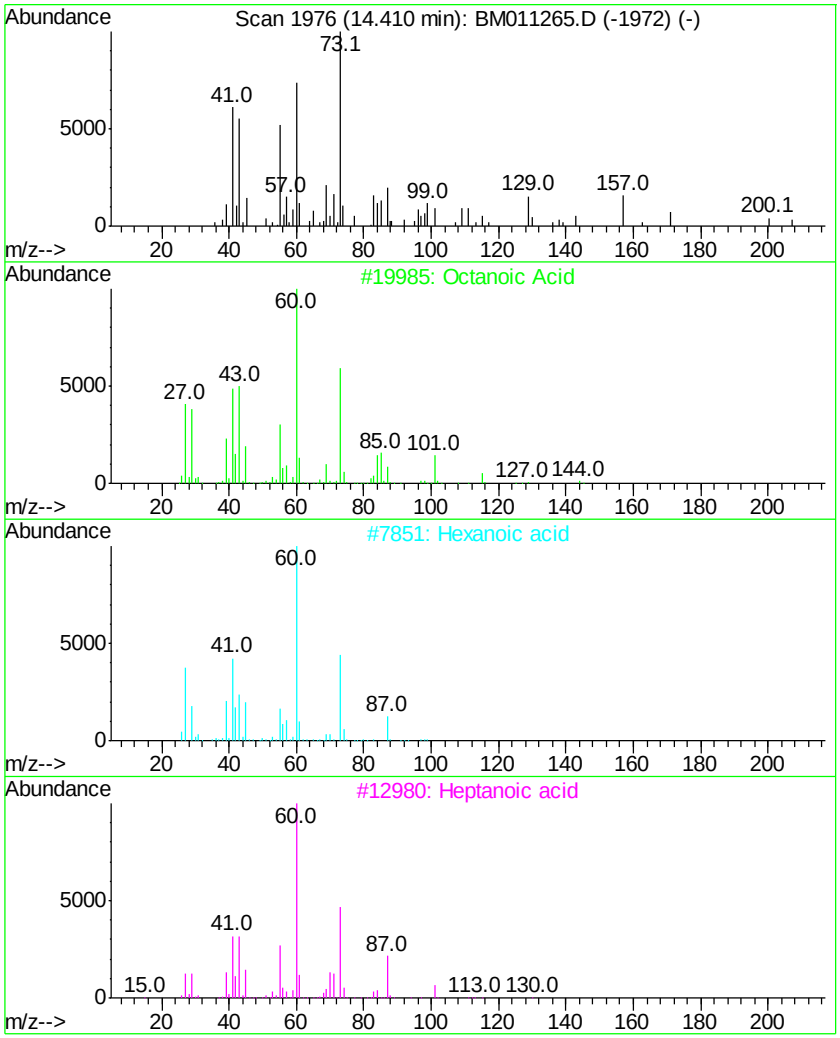
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

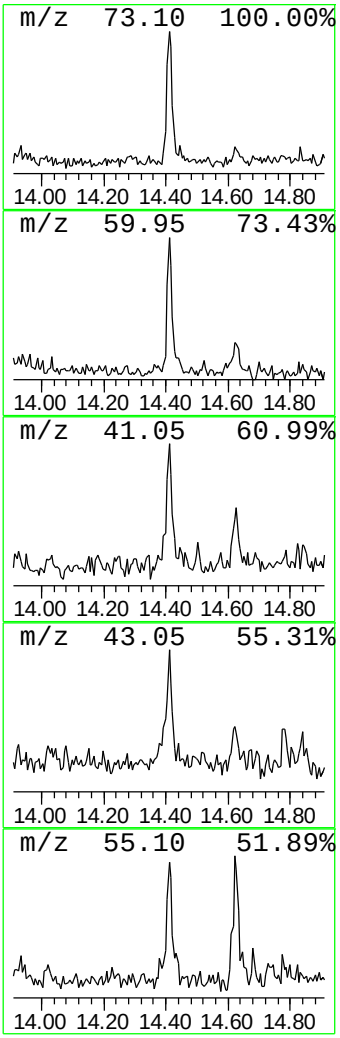
****

Peak Number 8 unknown14.41 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.41	2.18 ng	173766	Acenaphthene-d10	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic Acid	144	C8H16O2	000124-07-2	47
2	Hexanoic acid	116	C6H12O2	000142-62-1	43
3	Heptanoic acid	130	C7H14O2	000111-14-8	40
4	n-Decanoic acid	172	C10H20O2	000334-48-5	40
5	Ethyl .alpha.-d-glucopyranoside	208	C8H16O6	1000127-29-4	38





Data Path : Z:\HPCHEM1\BNA M\DATA\BM081617\
Data File : BM011265.D
Acq On : 16 Aug 2017 21:46
Operator : SJ/JU
Sample : I4736-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TWP-37

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

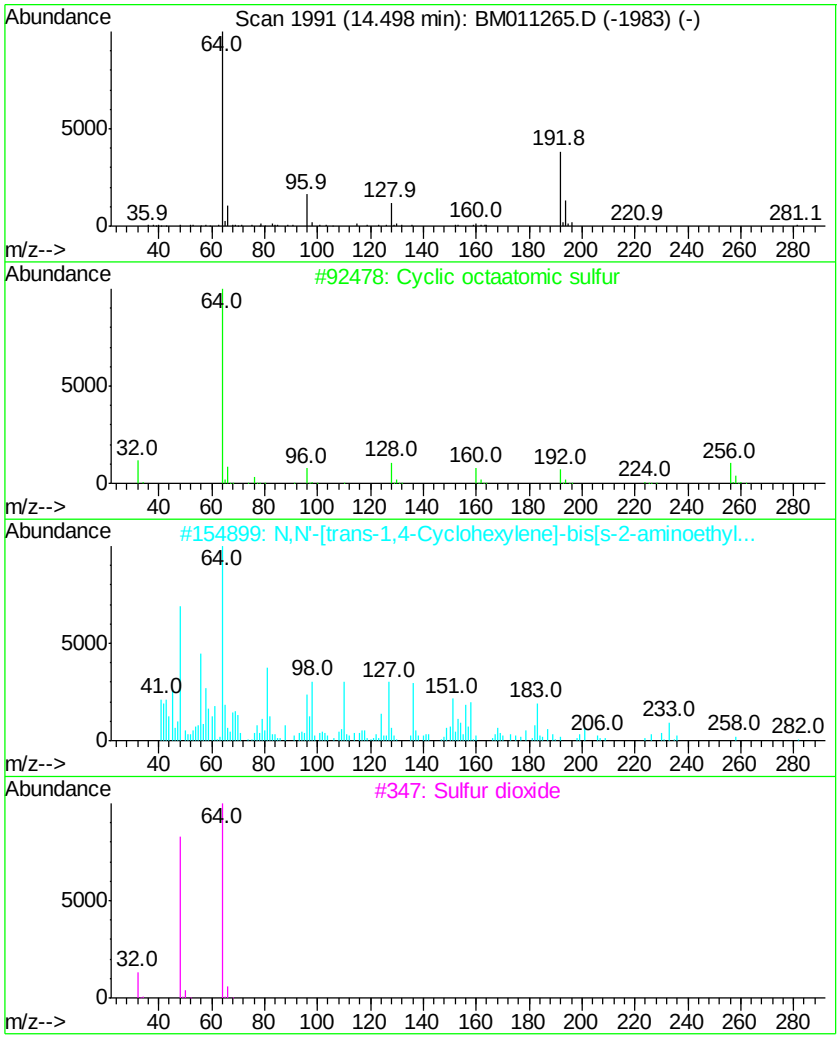
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

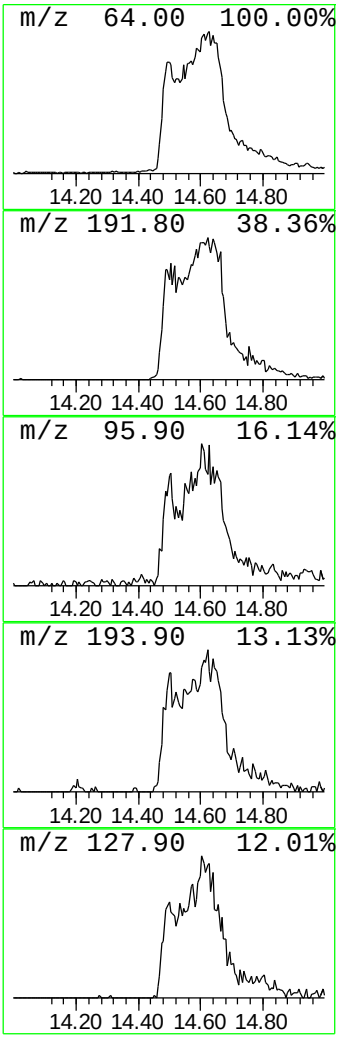
****

Peak Number 9 unknown14.50 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	6.46 ng	515062	Acenaphthene-d10	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclic octaatomic sulfur	256	S8	010544-50-0	40
2	N,N'-[trans-1,4-Cyclohexylene]-b...	394	C10H22N2O6S4	035871-63-7	9
3	Sulfur dioxide	64	O2S	007446-09-5	4
4	Ethyl Chloride	64	C2H5Cl	000075-00-3	4
5	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4





Data Path : Z:\HPCHEM1\BNA M\DATA\BM081617\
Data File : BM011265.D
Acq On : 16 Aug 2017 21:46
Operator : SJ/JU
Sample : I4736-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TWP-37

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

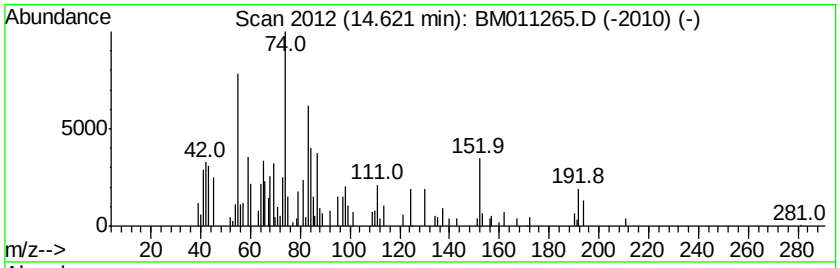
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

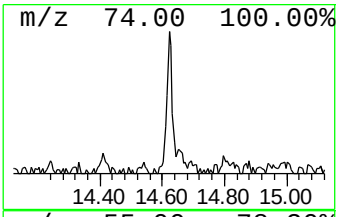
****

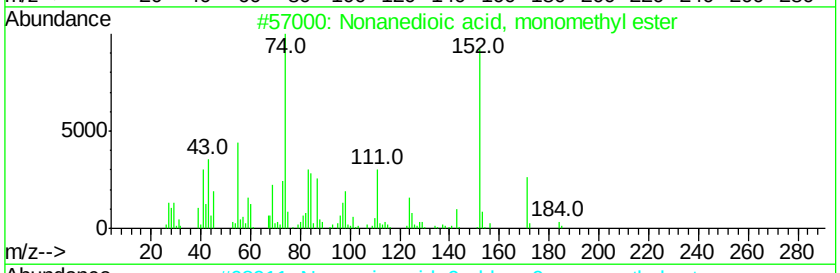
Peak Number 10 unknown14.62 Concentration Rank 4

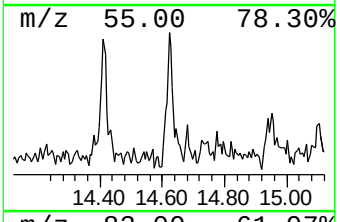
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	10.21 ng	813411	Acenaphthene-d10	13.94

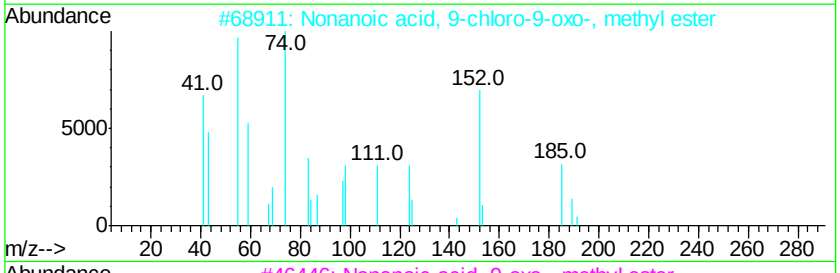
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanedioic acid, monomethyl ester	202	C10H18O4	002104-19-0	43
2	Nonanoic acid, 9-chloro-9-oxo-, ...	220	C10H17ClO3	056555-02-3	27
3	Nonanoic acid, 9-oxo-, methyl ester	186	C10H18O3	001931-63-1	27
4	10-Hydroxydecanoic acid, methyl ...	202	C11H22O3	002640-94-0	27
5	Cyclopentanol, 3-(carbmethoxy)me...	158	C8H14O3	339363-86-9	22

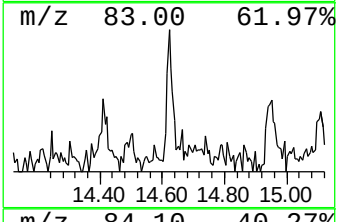


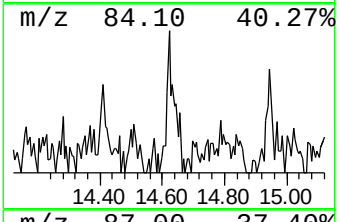


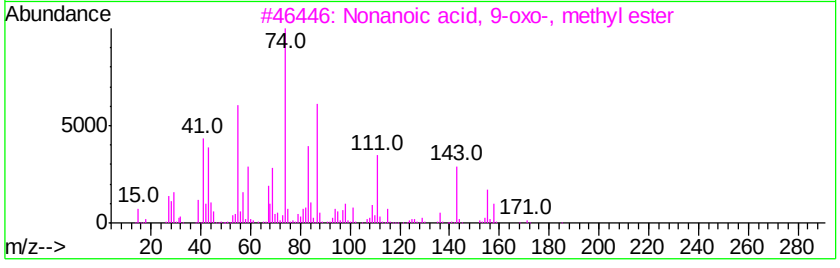


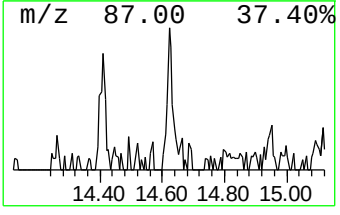












Data Path : Z:\HPCHEM1\BNA M\DATA\BM081617\
Data File : BM011265.D
Acq On : 16 Aug 2017 21:46
Operator : SJ/JU
Sample : I4736-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TWP-37

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

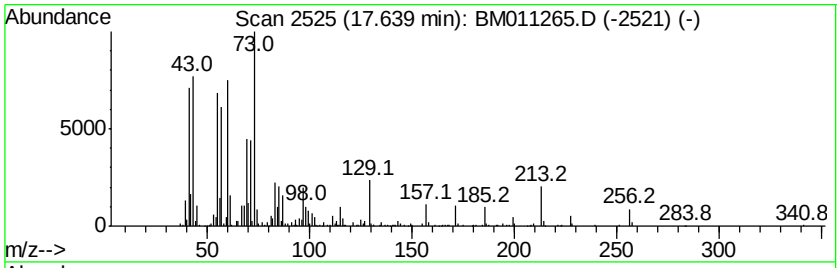
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

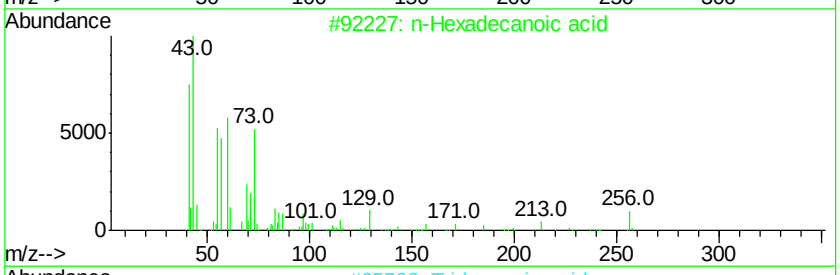
****

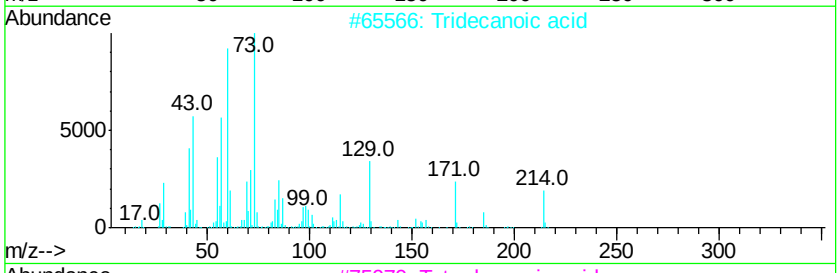
Peak Number 11 n-Hexadecanoic acid Concentration Rank 3

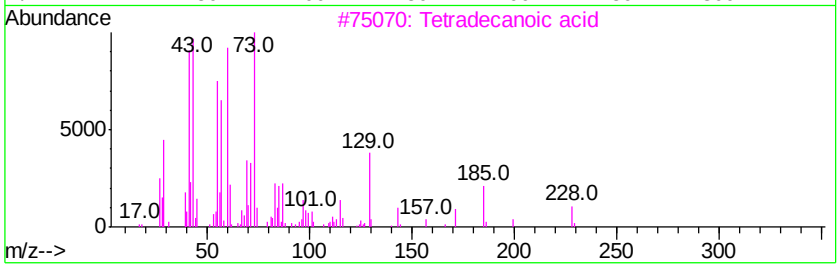
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.64	13.37 ng	1442410	Phenanthrene-d10	16.70

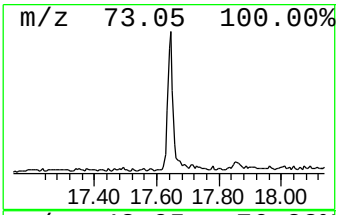
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	64
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
5	Nonanoic acid	158	C9H18O2	000112-05-0	38

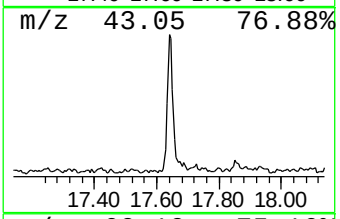


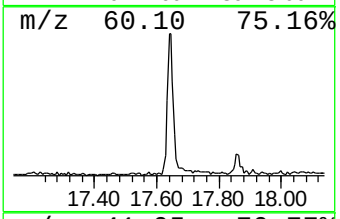


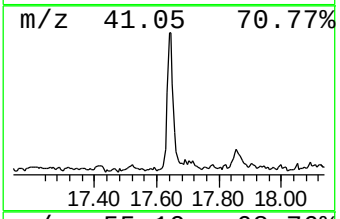


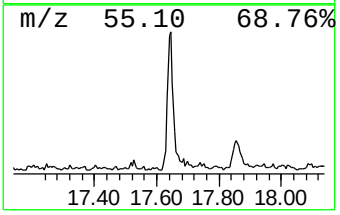












Data Path : Z:\HPCHEM1\BNA M\DATA\BM081617\
Data File : BM011265.D
Acq On : 16 Aug 2017 21:46
Operator : SJ/JU
Sample : I4736-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TWP-37

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

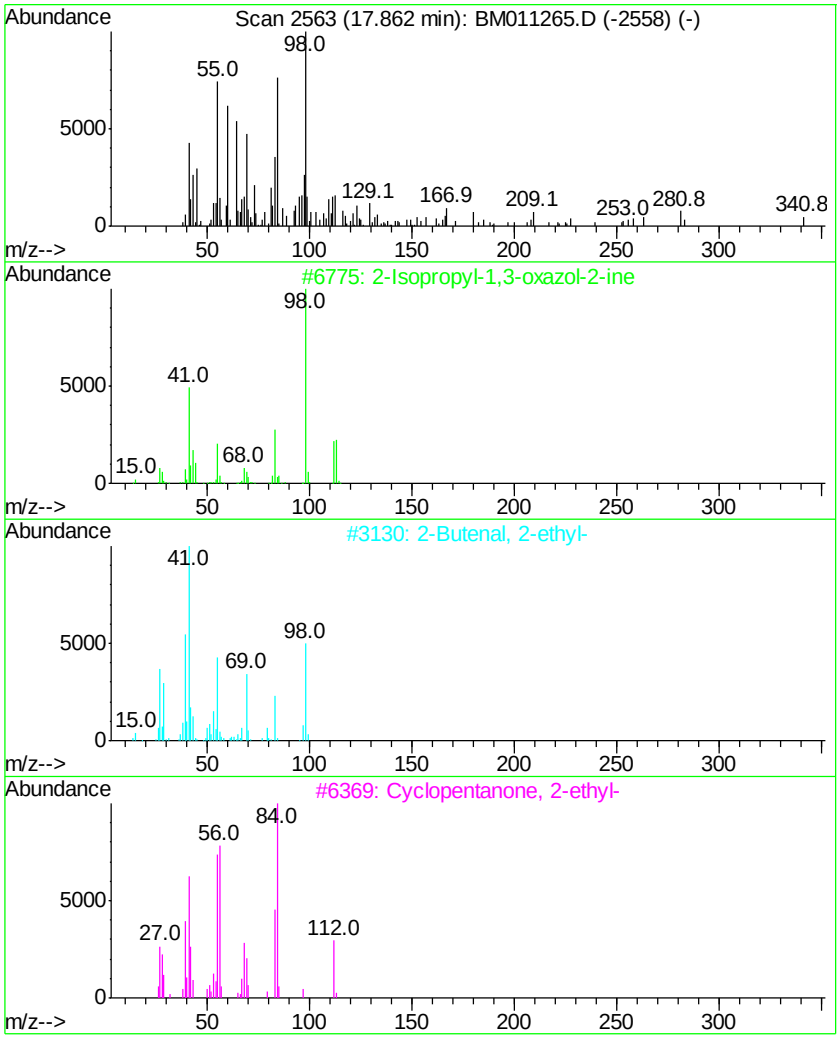
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

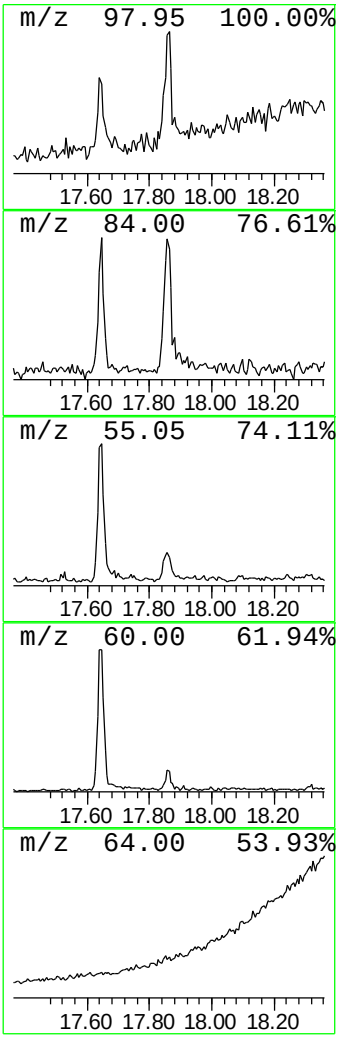
****

Peak Number 12 unknown17.86 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.86	3.25 ng	351010	Phenanthrene-d10	16.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Isopropyl-1,3-oxazol-2-ine	113	C6H11NO	010431-99-9	27
2	2-Butenal, 2-ethyl-	98	C6H10O	019780-25-7	27
3	Cyclopentanone, 2-ethyl-	112	C7H12O	004971-18-0	27
4	2-Ethyl-trans-2-butenal	98	C6H10O	063883-69-2	22
5	3-Furanmethanol	98	C5H6O2	004412-91-3	18





Data Path : Z:\HPCHEM1\BNA M\DATA\BM081617\
Data File : BM011265.D
Acq On : 16 Aug 2017 21:46
Operator : SJ/JU
Sample : I4736-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TWP-37

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

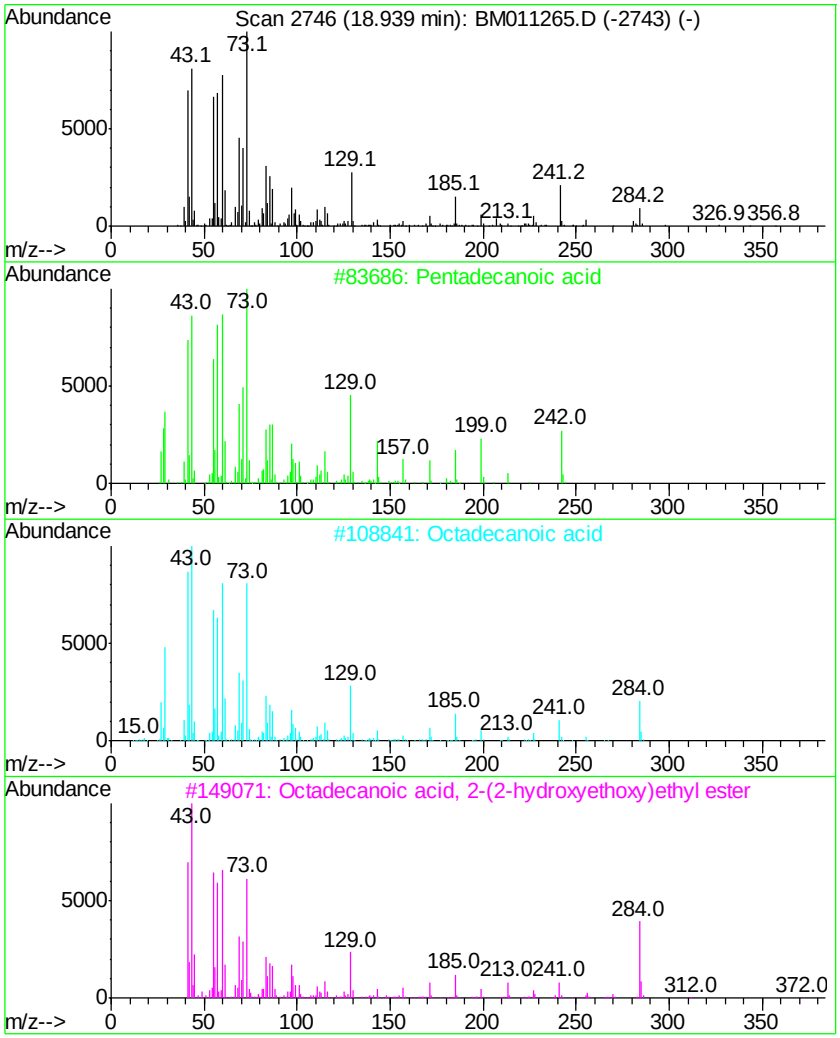
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

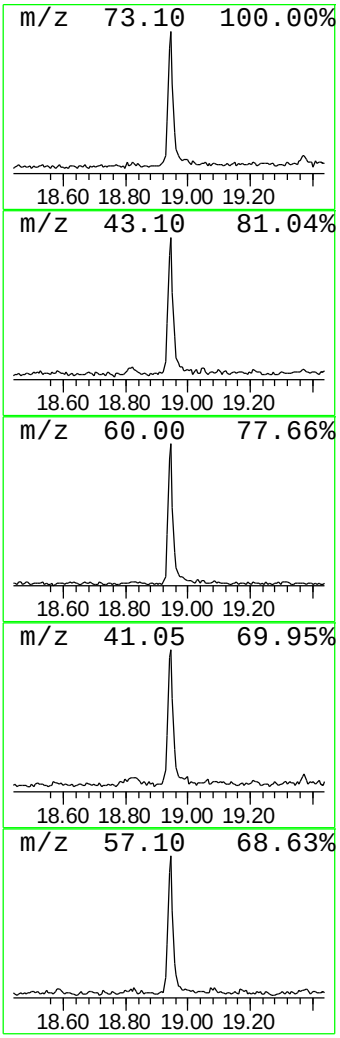
****

Peak Number 13 Pentadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.94	9.77 ng	1542490	Chrysene-d12	20.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
2	Octadecanoic acid	284	C18H36O2	000057-11-4	91
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	78
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	60
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	59





Data Path : Z:\HPCHEM1\BNA M\DATA\BM081617\
Data File : BM011265.D
Acq On : 16 Aug 2017 21:46
Operator : SJ/JU
Sample : I4736-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TWP-37

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

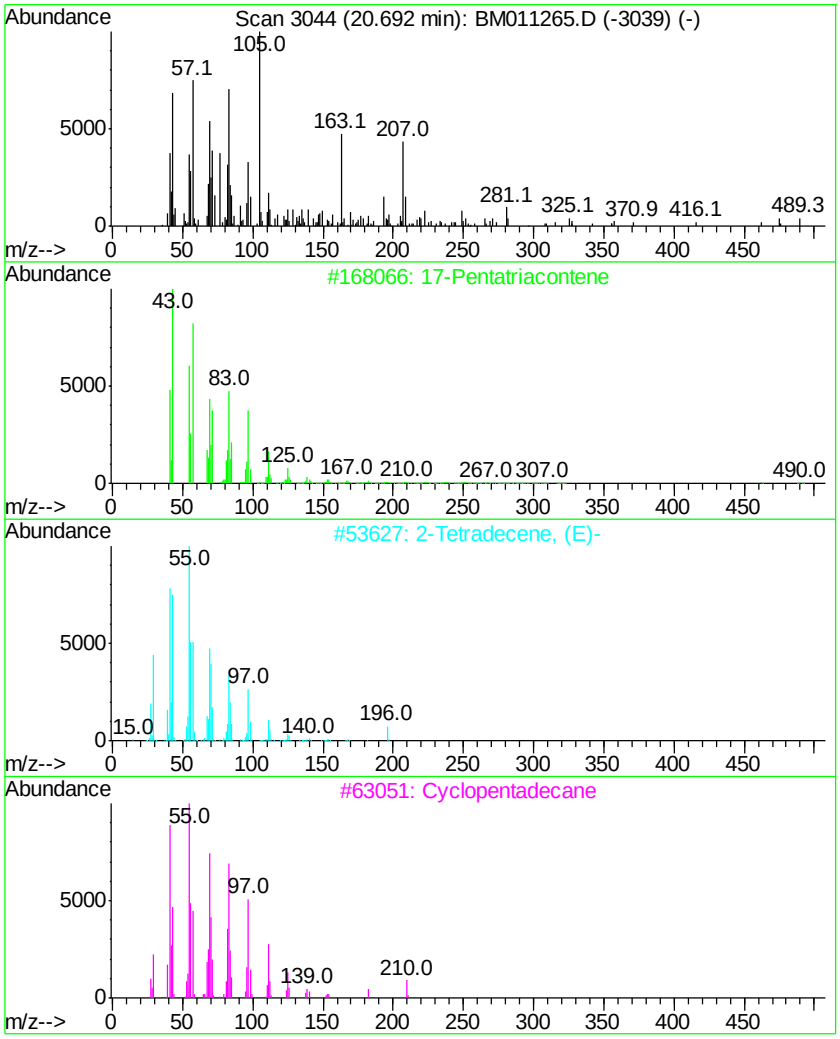
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

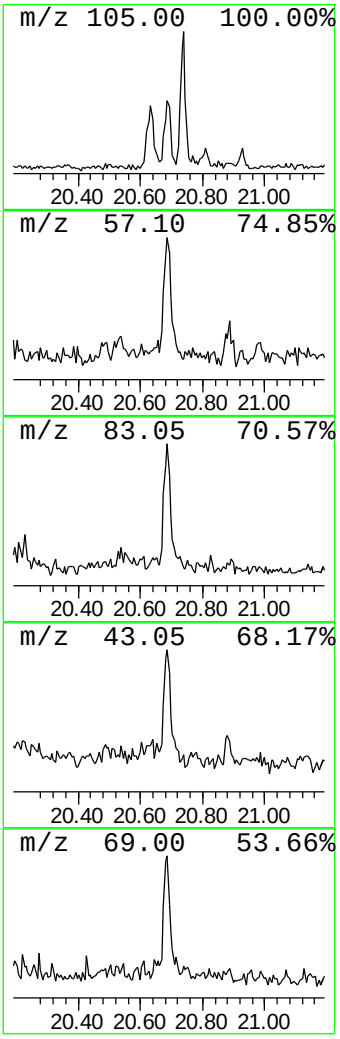
****

Peak Number 14 17-Pentatriacontene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.69	2.72 ng	429691	Chrysene-d12	20.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	62
2	2-Tetradecene, (E)-	196	C14H28	035953-53-8	60
3	Cyclopentadecane	210	C15H30	000295-48-7	47
4	Cyclohexane, 1,1'-(2-propyl-1,3-...	250	C18H34	055030-21-2	41
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	41





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM081617\
Data File : BM011265.D
Acq On : 16 Aug 2017 21:46
Operator : SJ/JU
Sample : I4736-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TWP-37

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
Hydrazine, 1,1-bi...	4.47	3.1	ng	144152	1	7.27	940623	20.0
Hexanoic acid	6.34	4.2	ng	199618	1	7.27	940623	20.0
unknown6.82	6.82	56.8	ng	2671060	1	7.27	940623	20.0
Undecanoic acid	9.41	2.4	ng	135772	2	10.03	1142580	20.0
n-Decanoic acid	10.87	4.2	ng	241803	2	10.03	1142580	20.0
Thujone	12.11	3.8	ng	302989	3	13.94	1594070	20.0
unknown14.41	14.41	2.2	ng	173766	3	13.94	1594070	20.0
unknown14.50	14.50	6.5	ng	515062	3	13.94	1594070	20.0
unknown14.62	14.62	10.2	ng	813411	3	13.94	1594070	20.0
n-Hexadecanoic acid	17.64	13.4	ng	1442410	4	16.70	2157450	20.0
unknown17.86	17.86	3.3	ng	351010	4	16.70	2157450	20.0
Pentadecanoic acid	18.94	9.8	ng	1542490	5	20.93	3156190	20.0
17-Pentatriacontene	20.69	2.7	ng	429691	5	20.93	3156190	20.0