LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
Data File : BM016353.D
Acq On : 14 Aug 2018 14:12
Operator : SJ/JU
Sample : J4442-51
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SP-1-6

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:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.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	5.169	314	320	332	rBV	111779	174348	9.50%	1.283%
2	5.645	396	401	415	rBV	777804	1190147	64.83%	8.755%
3	7.287	674	680	694	rBV	783032	1268826	69.11%	9.334%
4	7.645	735	741	758	rBB	883264	1388832	75.65%	10.217%
5	8.116	815	821	830	rBB	176618	283029	15.42%	2.082%
6	8.433	869	875	885	rBB	612111	993896	54.14%	7.311%
7	9.304	1016	1023	1035	rBV	457977	763303	41.58%	5.615%
8	10.927	1293	1299	1307	rBV	199186	341467	18.60%	2.512%
9	13.368	1708	1714	1722	rBV	1004049	1453279	79.16%	10.691%
10	13.498	1731	1736	1742	rBV4	9371	19423	1.06%	0.143%
11	14.145	1841	1846	1849	rBV2	14146	21759	1.19%	0.160%
12	14.210	1849	1857	1861	rVB2	60630	101669	5.54%	0.748%
13	14.551	1910	1915	1920	rBV2	16848	26176	1.43%	0.193%
14	14.751	1943	1949	1958	rVB2	261097	410559	22.36%	3.020%
15	15.504	2072	2077	2081	rBV5	13966	23358	1.27%	0.172%
16	15.951	2146	2153	2158	rBV2	19417	35556	1.94%	0.262%
17	16.239	2196	2202	2216	rBV	992328	1424493	77.59%	10.479%
18	16.427	2227	2234	2239	rBV	45373	81669	4.45%	0.601%
19	17.245	2368	2373	2378	rVB	19688	30023	1.64%	0.221%
20	17.492	2409	2415	2425	rVB	310751	466258	25.40%	3.430%
21	18.339	2554	2559	2567	rBV	109185	161418	8.79%	1.187%
22	19.597	2769	2773	2778	rBV2	49263	67544	3.68%	0.497%
23	20.068	2848	2853	2858	rBV	1612708	1835850	100.00%	13.505%
24	20.339	2897	2899	2903	rVB5	19730	20137	1.10%	0.148%
25	21.291	3058	3061	3068	rVB5	58327	99043	5.39%	0.729%
26	21.621	3112	3117	3123	rBV	340140	460818	25.10%	3.390%
27	23.950	3508	3513	3519	rVB	242649	450797	24.56%	3.316%

Sum of corrected areas: 13593677

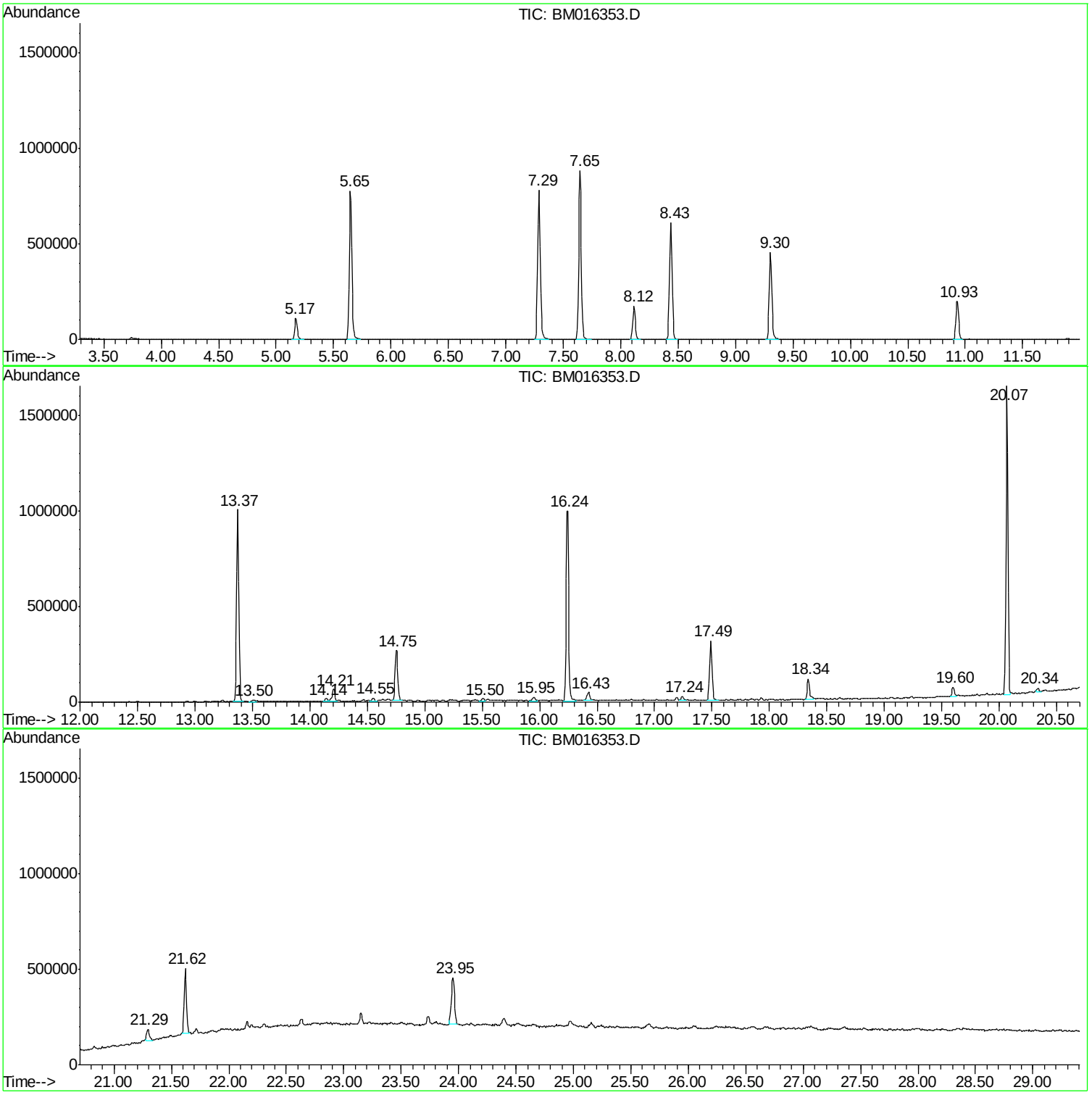
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
Data File : BM016353.D
Acq On : 14 Aug 2018 14:12
Operator : SJ/JU
Sample : J4442-51
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SP-1-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
Data File : BM016353.D
Acq On : 14 Aug 2018 14:12
Operator : SJ/JU
Sample : J4442-51
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SP-1-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

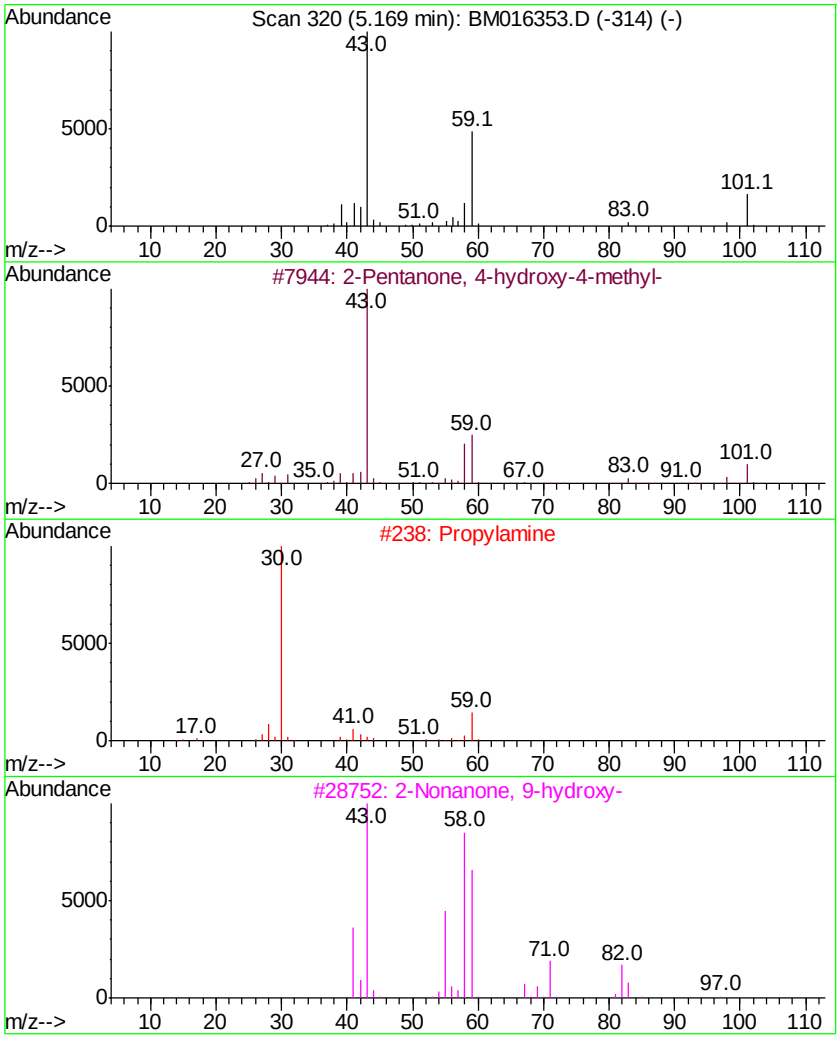
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

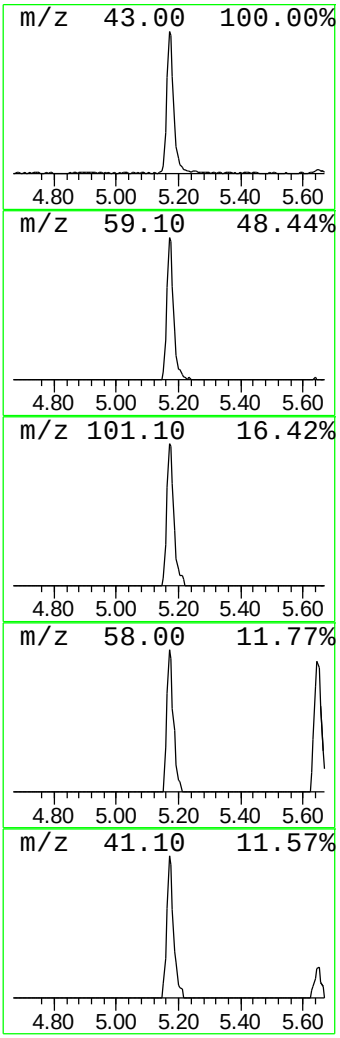
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	12.32 ng	174348	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propylamine	59	C3H9N	000107-10-8	42
3	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	36
4	Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	25
5	Butane	58	C4H10	000106-97-8	22





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
Data File : BM016353.D
Acq On : 14 Aug 2018 14:12
Operator : SJ/JU
Sample : J4442-51
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SP-1-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

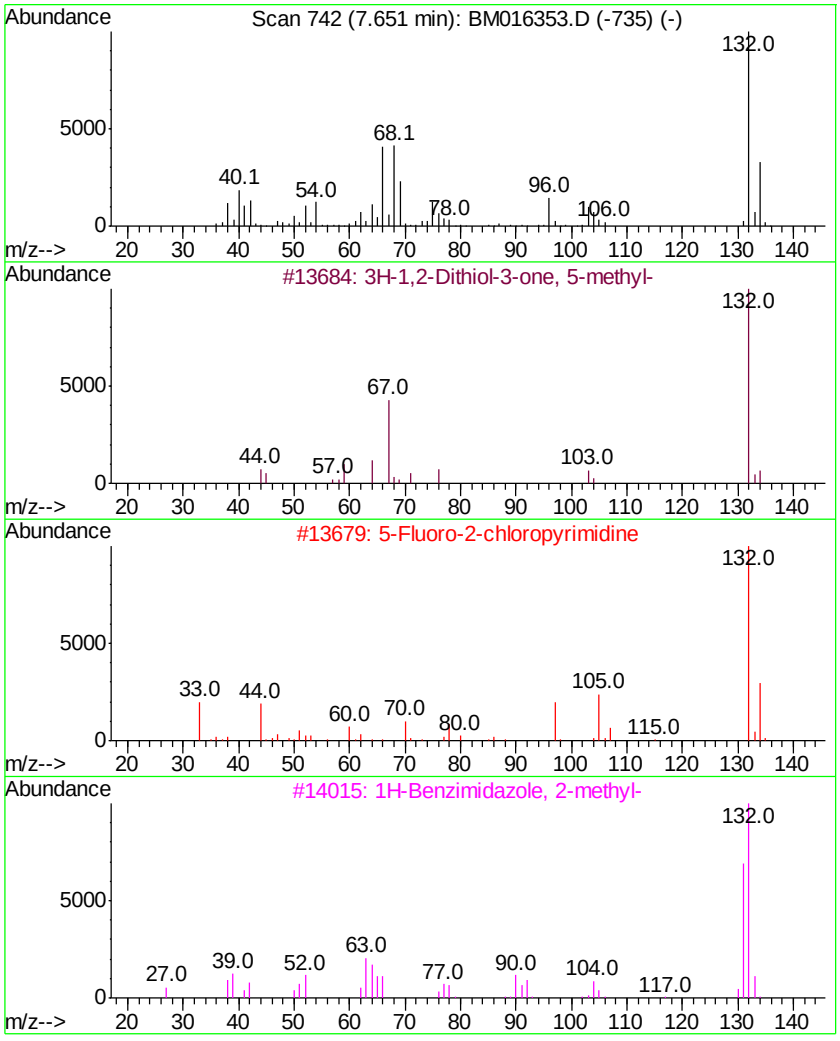
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

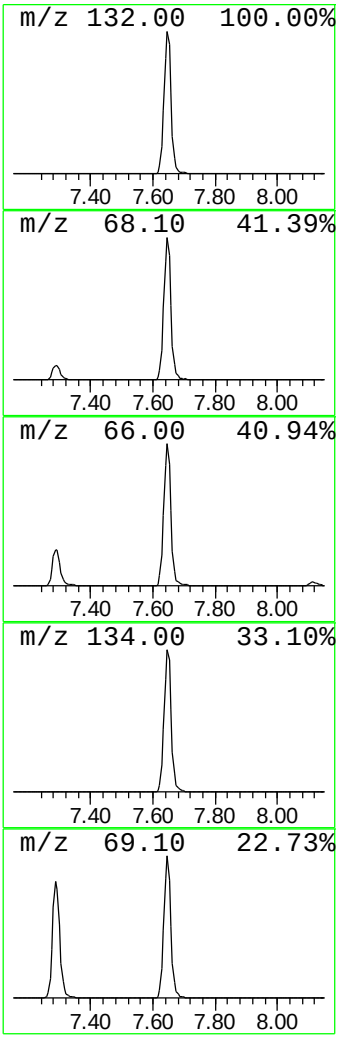
****

Peak Number 2 unknown7.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	98.14 ng	1388830	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
4	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
Data File : BM016353.D
Acq On : 14 Aug 2018 14:12
Operator : SJ/JU
Sample : J4442-51
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SP-1-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

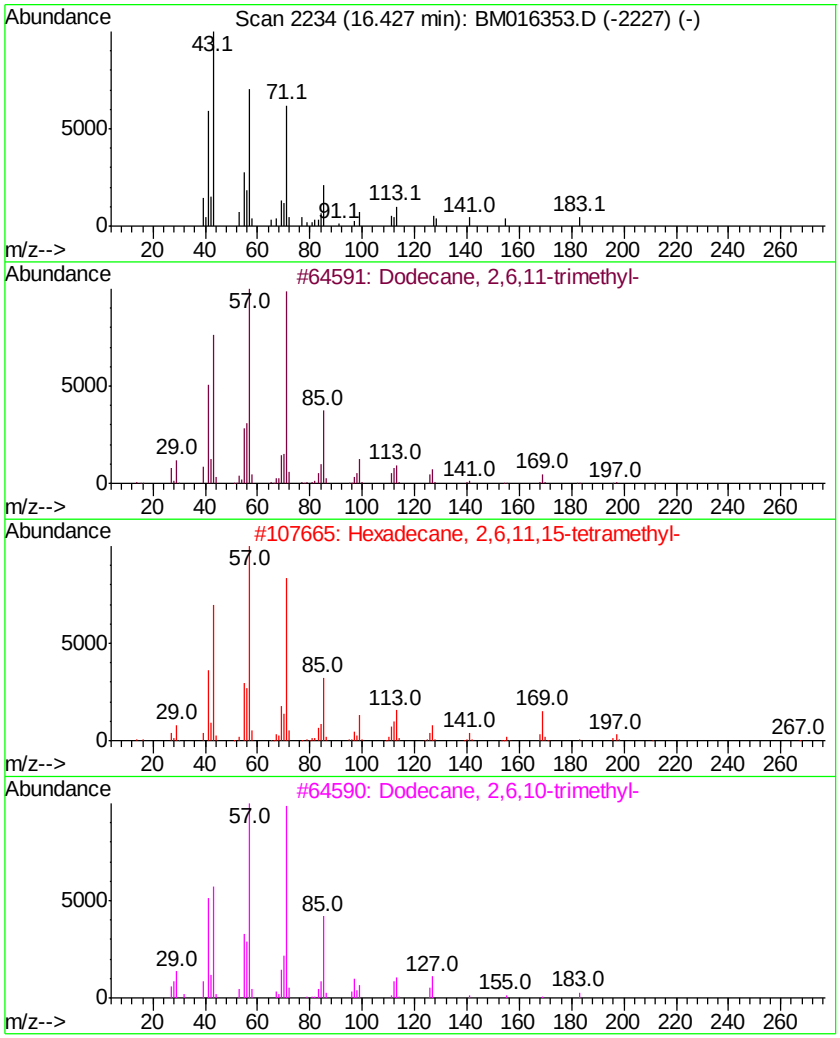
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

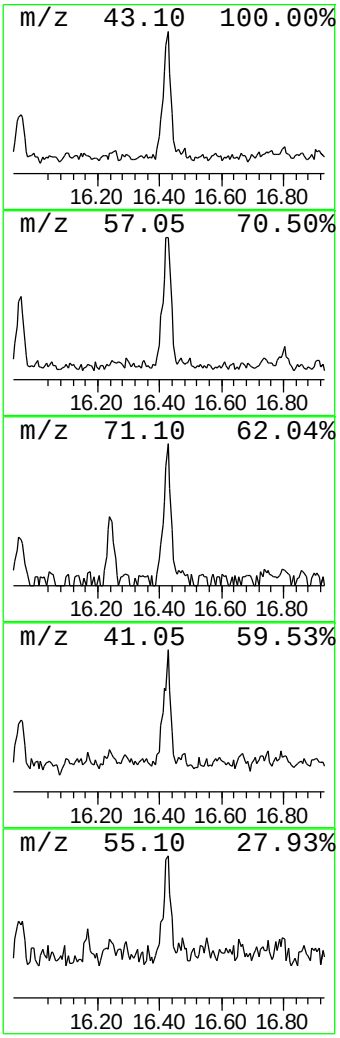
****

Peak Number 4 Dodecane, 2,6,11-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.43	3.50 ng	81669	Phenanthrene-d10	17.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	72
2	Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	64
3	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	64
4	Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	59
5	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	59





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
Data File : BM016353.D
Acq On : 14 Aug 2018 14:12
Operator : SJ/JU
Sample : J4442-51
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SP-1-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

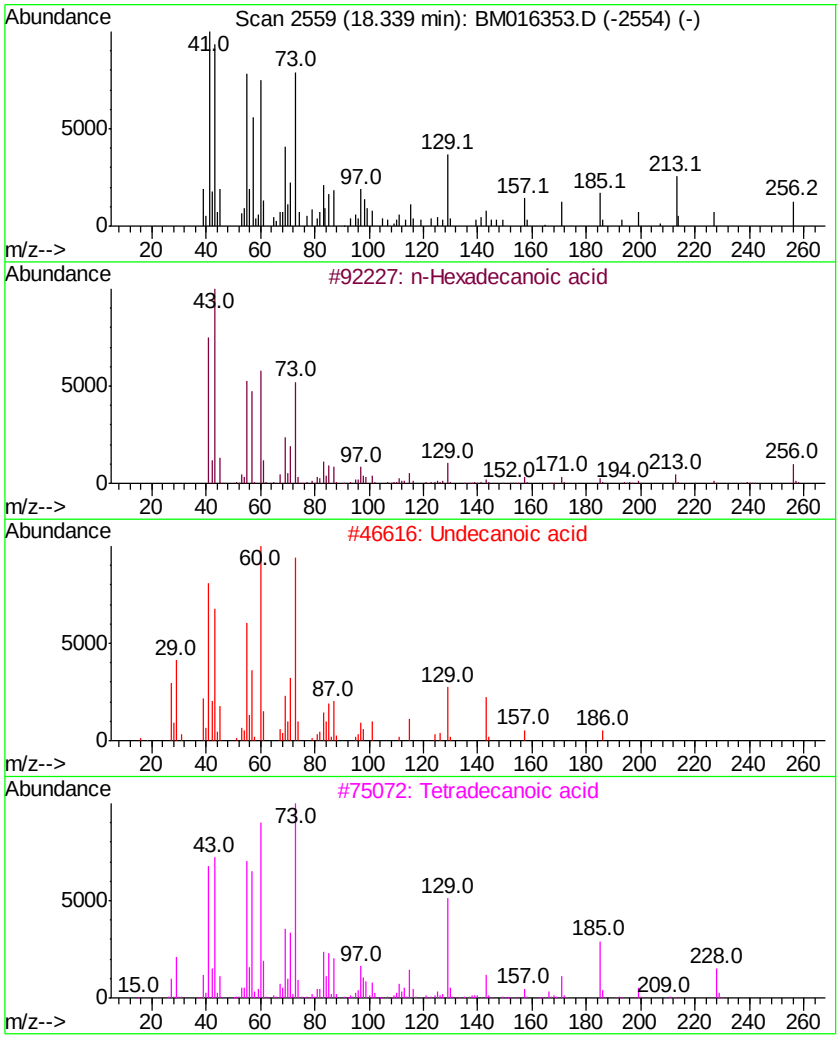
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

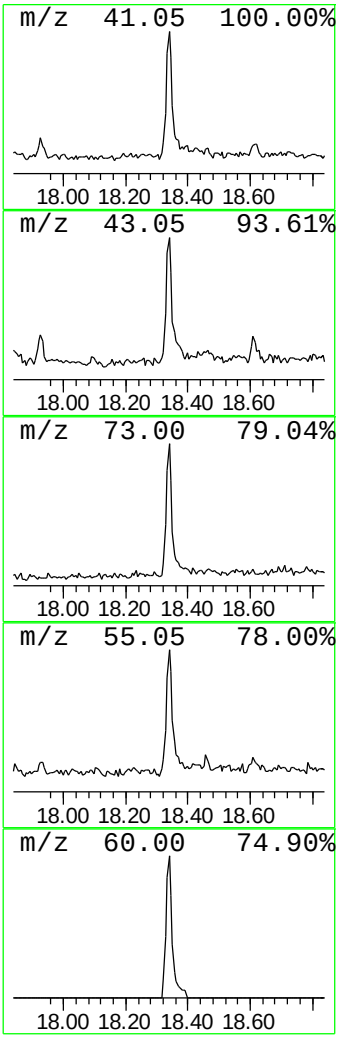
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.34	6.92 ng	161418	Phenanthrene-d10	17.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
2	Undecanoic acid	186	C11H22O2	000112-37-8	78
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Dodecanoic acid	200	C12H24O2	000143-07-7	52
5	n-Decanoic acid	172	C10H20O2	000334-48-5	49





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
Data File : BM016353.D
Acq On : 14 Aug 2018 14:12
Operator : SJ/JU
Sample : J4442-51
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SP-1-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

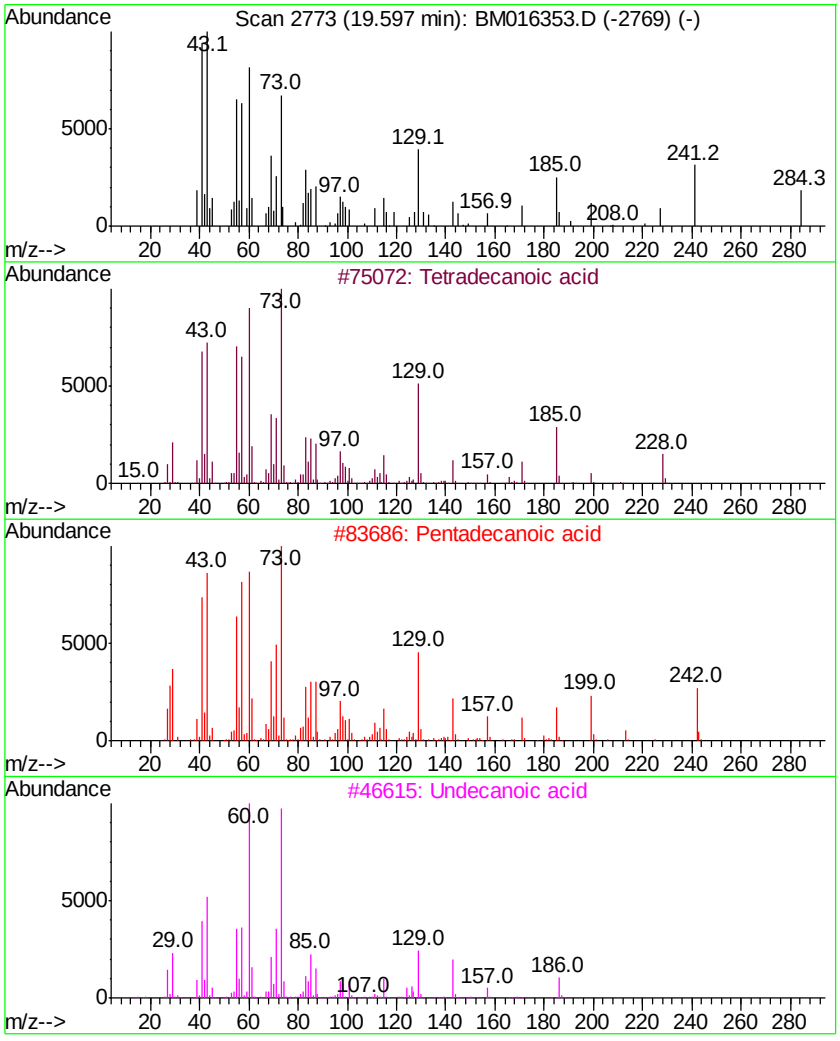
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

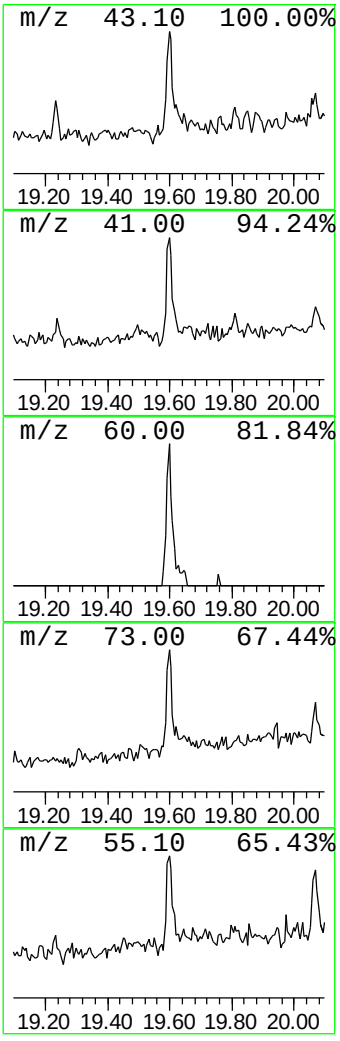
****

Peak Number 6 Tetradecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.60	2.93 ng	67544	Chrysene-d12	21.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	46
3	Undecanoic acid	186	C11H22O2	000112-37-8	46
4	n-Decanoic acid	172	C10H20O2	000334-48-5	43
5	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
Data File : BM016353.D
Acq On : 14 Aug 2018 14:12
Operator : SJ/JU
Sample : J4442-51
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SP-1-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

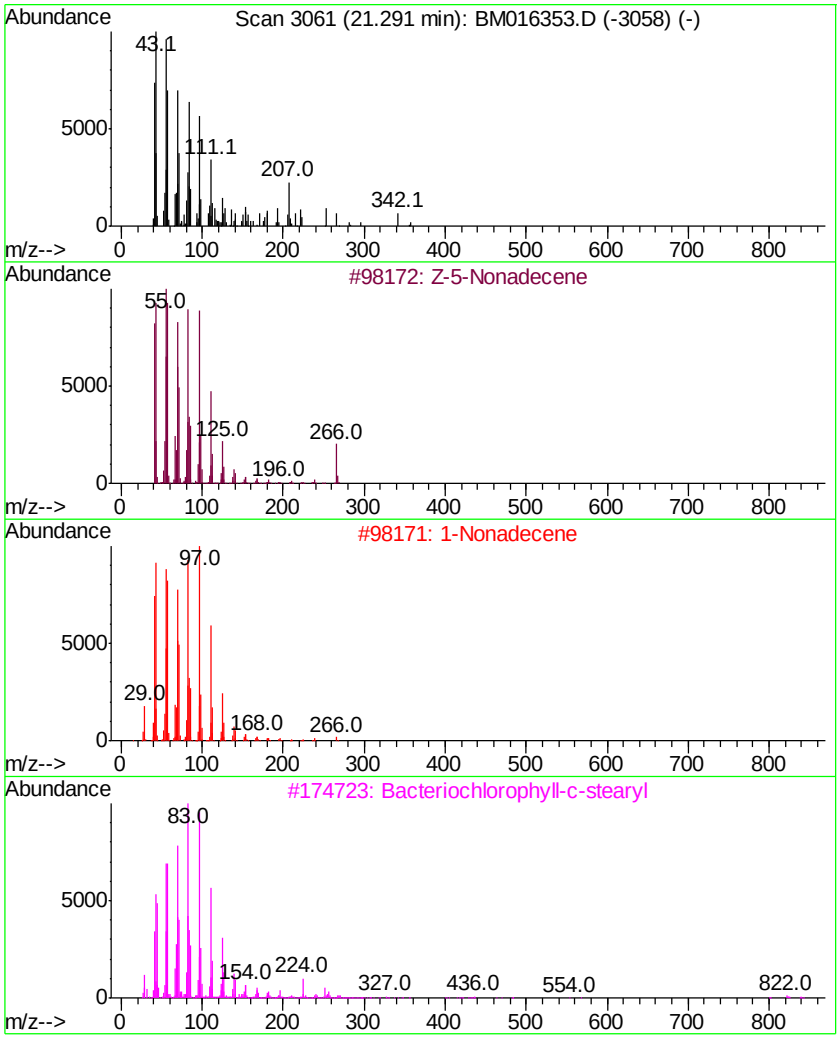
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

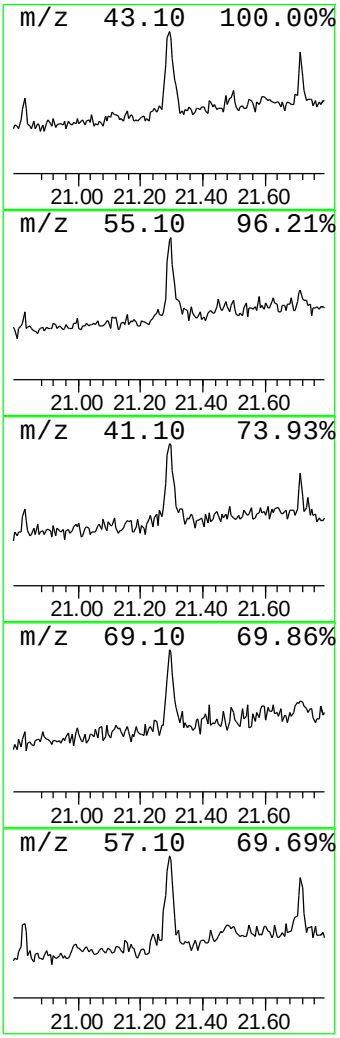
****

Peak Number 7 Z-5-Nonadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.29	4.30 ng	99043	Chrysene-d12	21.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Z-5-Nonadecene	266	C19H38	1000131-11-8	86
2	1-Nonadecene	266	C19H38	018435-45-5	86
3	Bacteriochlorophyll-c-stearyl	841	C52H72MgN4O4	1000164-49-7	62
4	9-Nonadecene	266	C19H38	031035-07-1	62
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	62





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM081418\
Data File : BM016353.D
Acq On : 14 Aug 2018 14:12
Operator : SJ/JU
Sample : J4442-51
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SP-1-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.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...	5.17	12.3	ng	174348	1	8.12	283029	20.0
unknown7.65	7.65	98.1	ng	1388830	1	8.12	283029	20.0
Dodecane, 2,6,11-...	16.43	3.5	ng	81669	4	17.49	466258	20.0
n-Hexadecanoic acid	18.34	6.9	ng	161418	4	17.49	466258	20.0
Tetradecanoic acid	19.60	2.9	ng	67544	5	21.62	460818	20.0
Z-5-Nonadecene	21.29	4.3	ng	99043	5	21.62	460818	20.0