LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101218\
Data File : BF109833.D
Acq On : 12 Oct 2018 15:04
Operator : JU/SJ
Sample : J5371-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100818-TIPC-F-U-B

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_F\METHODS\8270-BF100818.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	4.887	473	476	485	rBV	66670	85583	2.05%	0.363%
2	5.310	545	548	575	rBV	448708	731752	17.50%	3.101%
3	6.340	720	723	740	rBV	289157	564989	13.51%	2.394%
4	6.463	740	744	766	rVV	1512023	1725445	41.26%	7.311%
5	6.692	780	783	805	rBV	416941	601075	14.37%	2.547%
6	6.851	805	810	832	rBV	2283073	2502349	59.84%	10.603%
7	7.263	875	880	904	rBV	1471342	2180830	52.15%	9.241%
8	7.975	997	1001	1021	rBV	560055	769838	18.41%	3.262%
9	9.051	1178	1184	1221	rBV	3539995	4181543	100.00%	17.719%
10	9.445	1247	1251	1259	rBV	69379	75361	1.80%	0.319%
11	9.722	1293	1298	1325	rBV	919063	990509	23.69%	4.197%
12	10.510	1428	1432	1452	rBV	1440687	1758667	42.06%	7.452%
13	11.198	1546	1549	1560	rBV	804931	993568	23.76%	4.210%
14	11.739	1637	1641	1653	rBV2	71055	119296	2.85%	0.506%
15	12.786	1814	1819	1845	rBV	3563979	4014911	96.02%	17.013%
16	13.704	1967	1975	1986	rBV5	31391	108350	2.59%	0.459%
17	13.827	1992	1996	2015	rVB	663879	844161	20.19%	3.577%
18	14.298	2070	2076	2081	rBV	79828	81920	1.96%	0.347%
19	14.592	2120	2126	2131	rBV	129573	128833	3.08%	0.546%
20	14.663	2134	2138	2145	rVB	40751	46648	1.12%	0.198%
21	14.904	2174	2179	2189	rBV	131551	147655	3.53%	0.626%
22	15.227	2229	2234	2250	rBV2	362902	744685	17.81%	3.156%
23	15.645	2299	2305	2314	rBV	83337	124687	2.98%	0.528%
24	16.098	2377	2382	2390	rVB2	44629	76807	1.84%	0.325%

Sum of corrected areas: 23599462

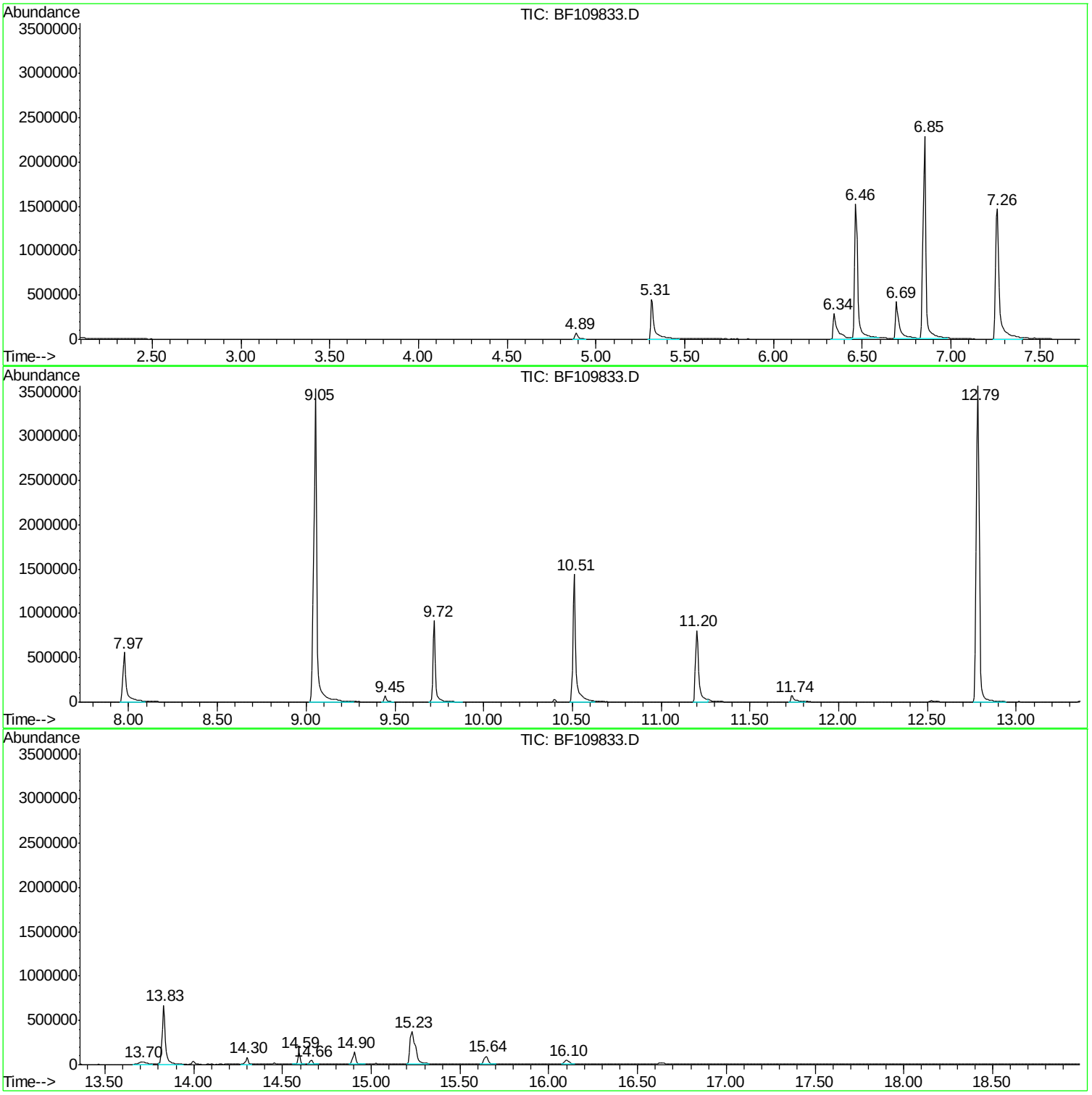
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101218\
Data File : BF109833.D
Acq On : 12 Oct 2018 15:04
Operator : JU/SJ
Sample : J5371-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100818-TIPC-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Data File : BF109833.D
Acq On : 12 Oct 2018 15:04
Operator : JU/SJ
Sample : J5371-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100818-TIPC-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

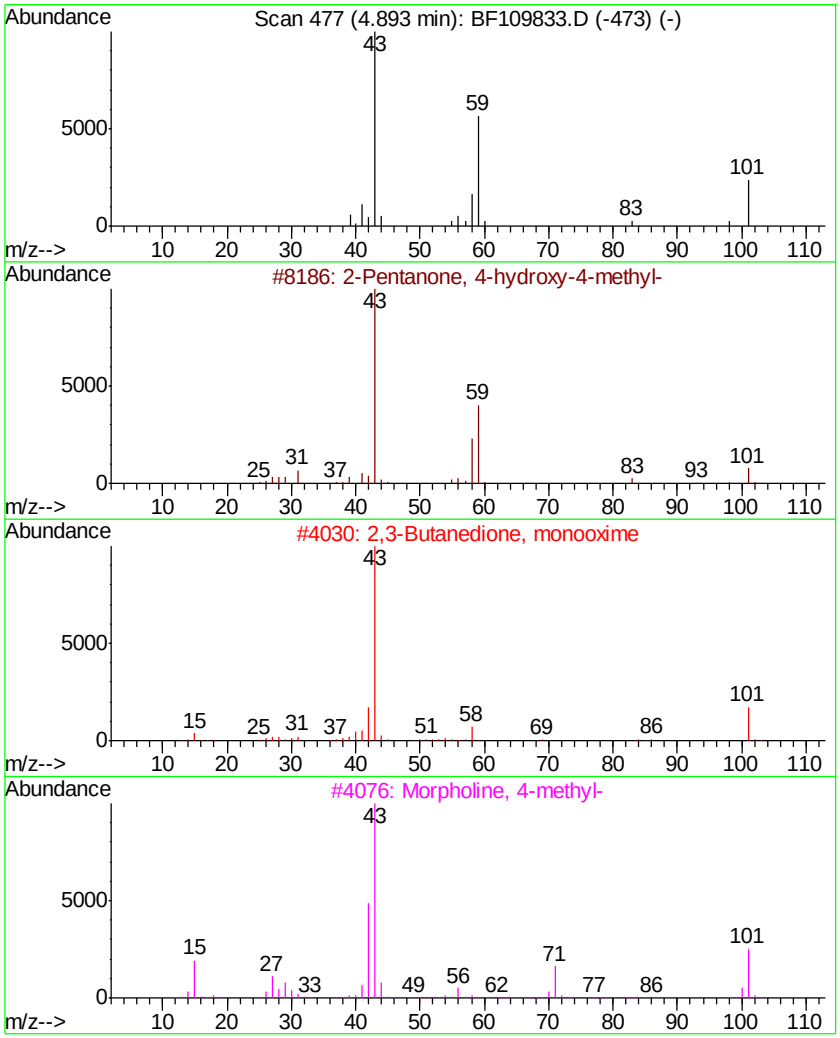
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

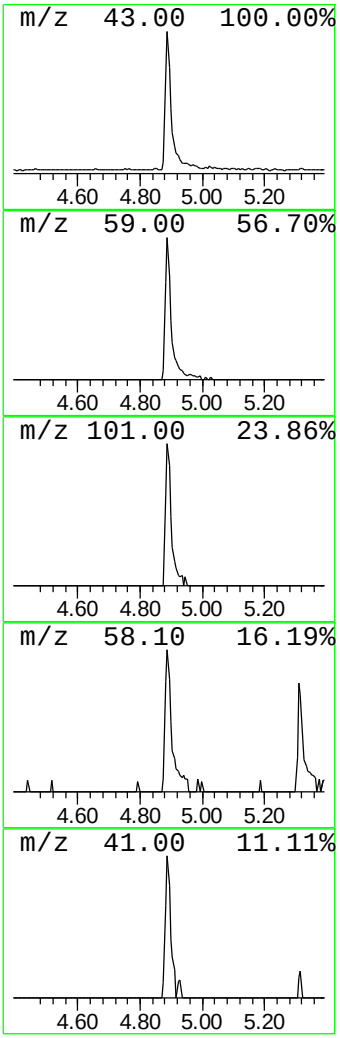
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	2.85 ng	85583	1,4-Dichlorobenzene-d4	6.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101218\
Data File : BF109833.D
Acq On : 12 Oct 2018 15:04
Operator : JU/SJ
Sample : J5371-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100818-TIPC-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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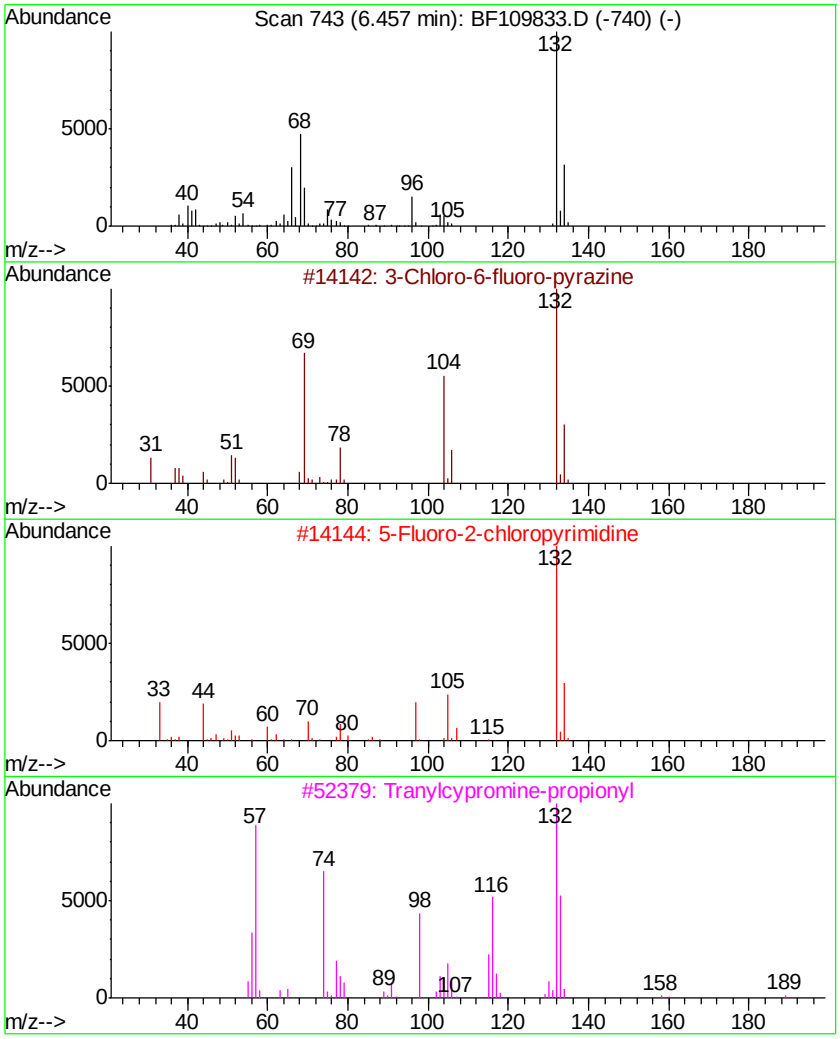
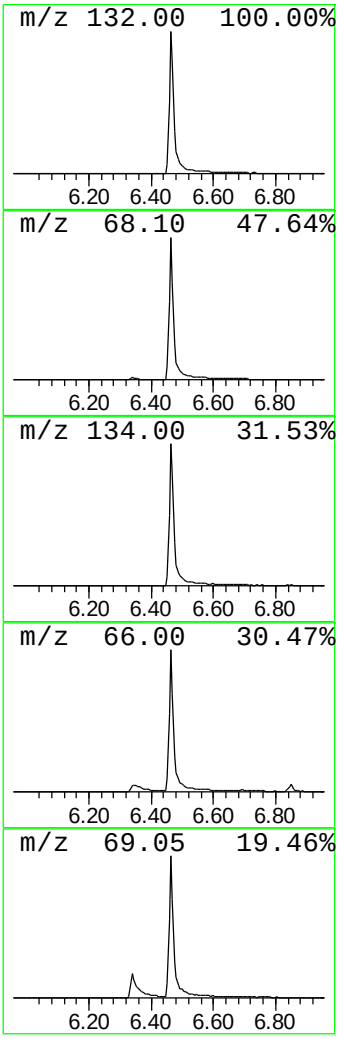
Peak Number 2 unknown6.46 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	57.41 ng	1725450	1,4-Dichlorobenzene-d4	6.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101218\
Data File : BF109833.D
Acq On : 12 Oct 2018 15:04
Operator : JU/SJ
Sample : J5371-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100818-TIPC-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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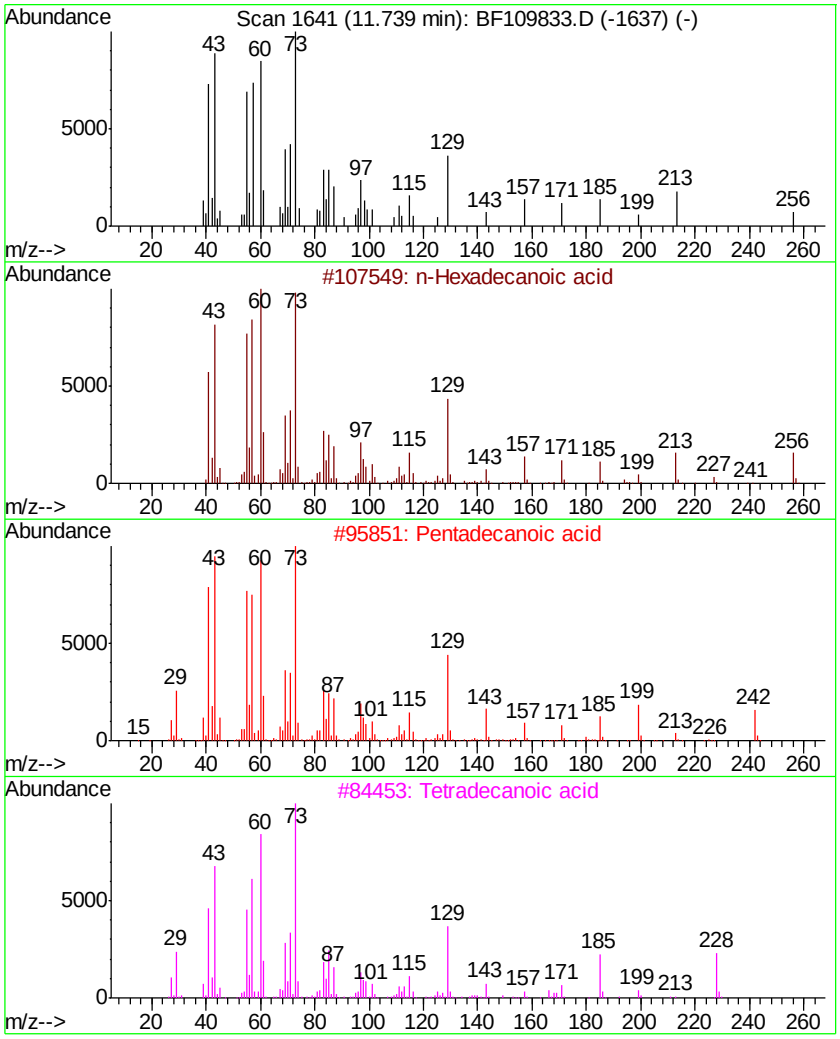
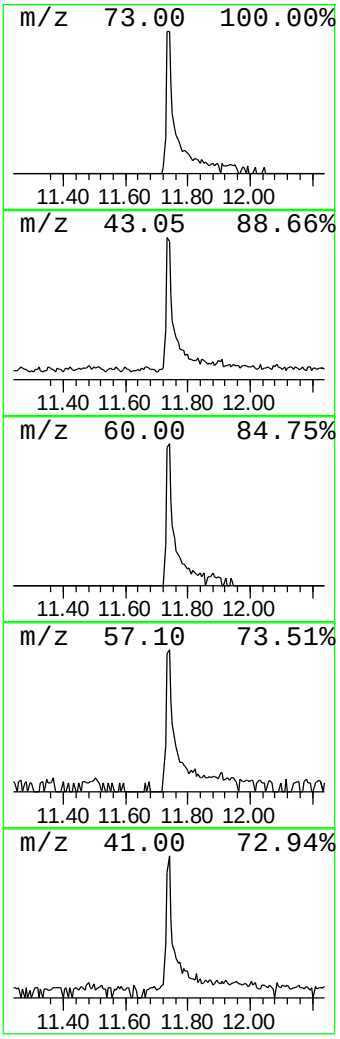
Peak Number 4 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.74	2.40 ng	119296	Phenanthrene-d10	11.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64





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Operator : JU/SJ
Sample : J5371-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100818-TIPC-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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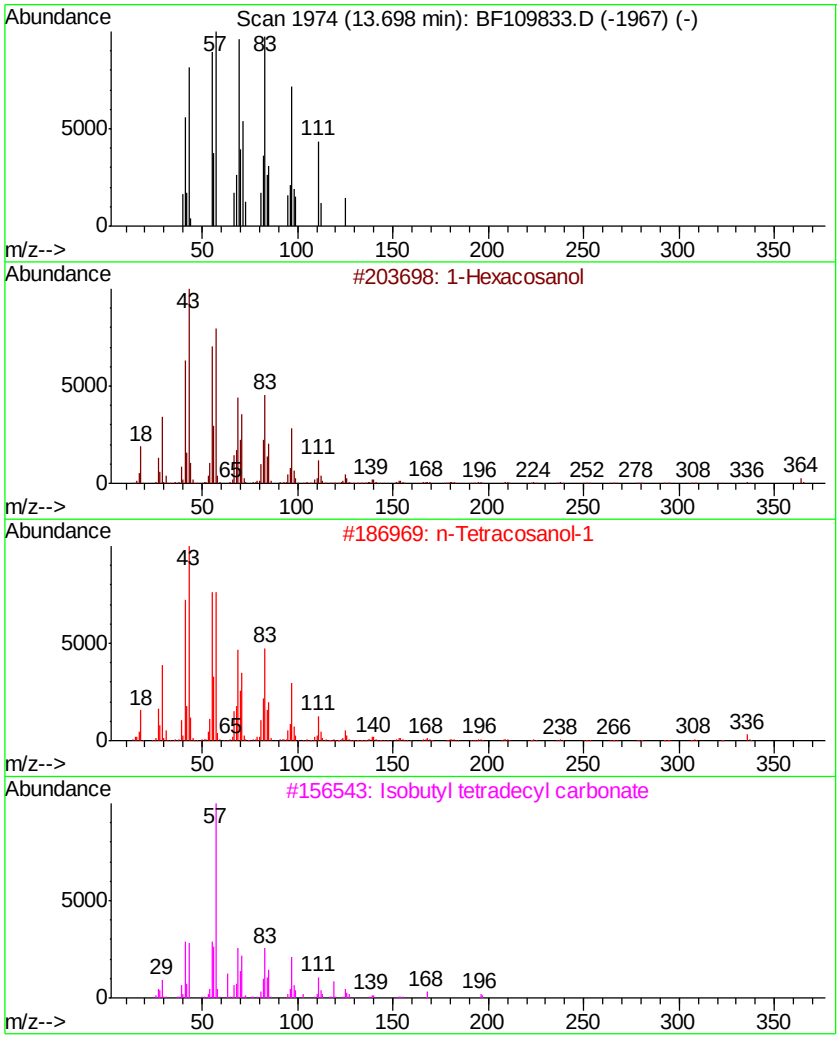
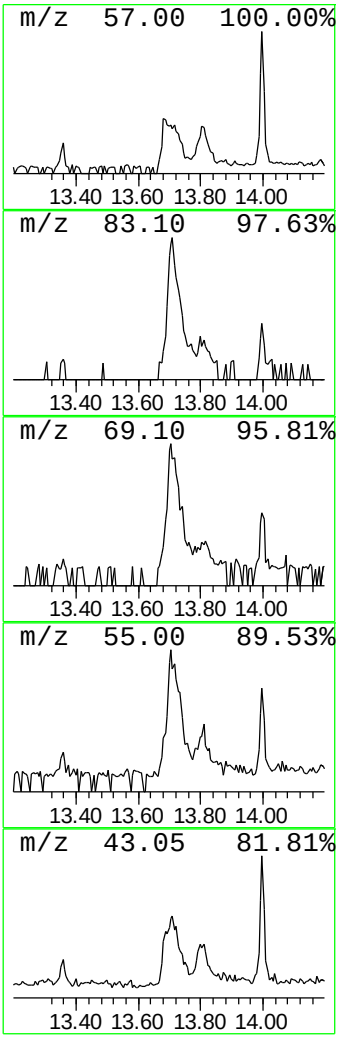
Peak Number 5 1-Hexacosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	2.57 ng	108350	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosanol	382	C26H54O	000506-52-5	90
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
3	Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	64
4	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	46
5	Sulfurous acid, cyclohexylmethyl...	416	C24H48O3S	1000309-22-5	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101218\
Data File : BF109833.D
Acq On : 12 Oct 2018 15:04
Operator : JU/SJ
Sample : J5371-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100818-TIPC-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

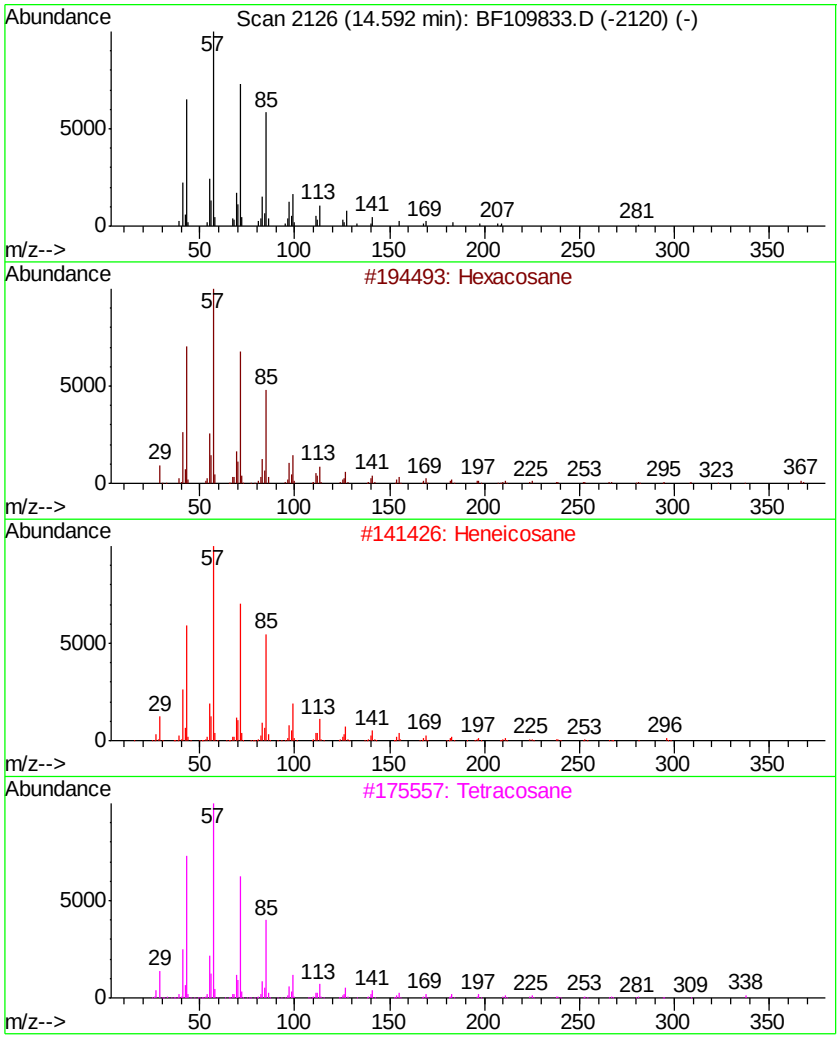
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

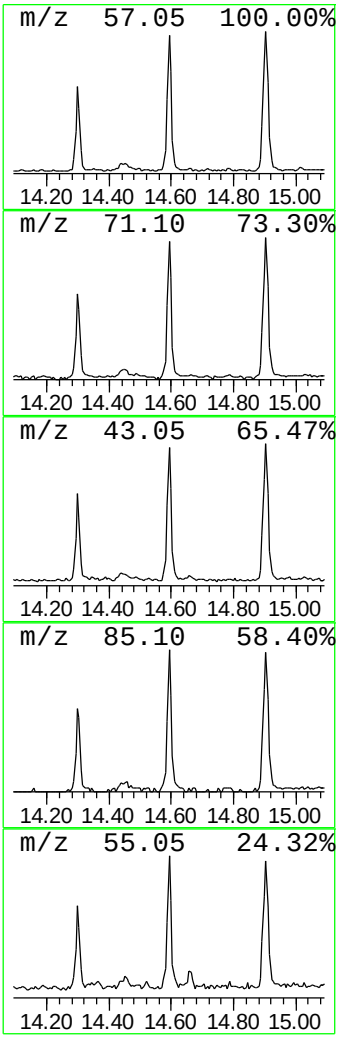
****

Peak Number 6 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	3.46 ng	128833	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Nonadecane	268	C19H40	000629-92-5	90
5	Octadecane	254	C18H38	000593-45-3	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101218\
Data File : BF109833.D
Acq On : 12 Oct 2018 15:04
Operator : JU/SJ
Sample : J5371-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100818-TIPC-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

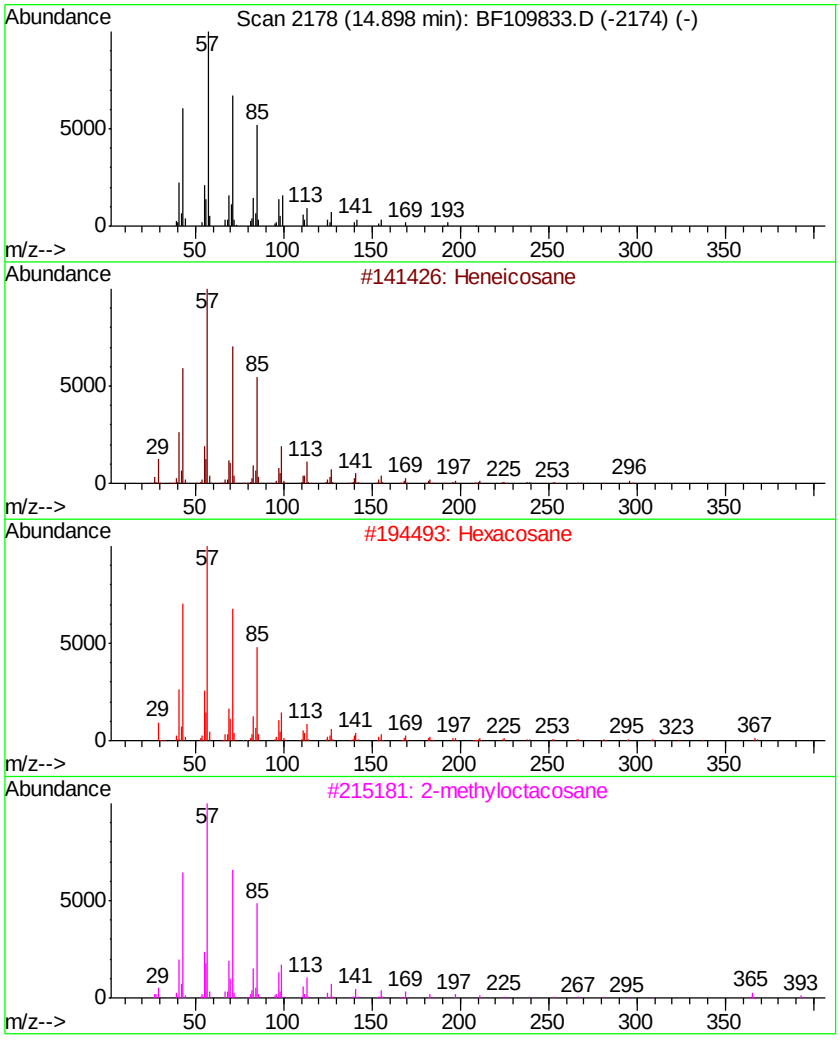
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

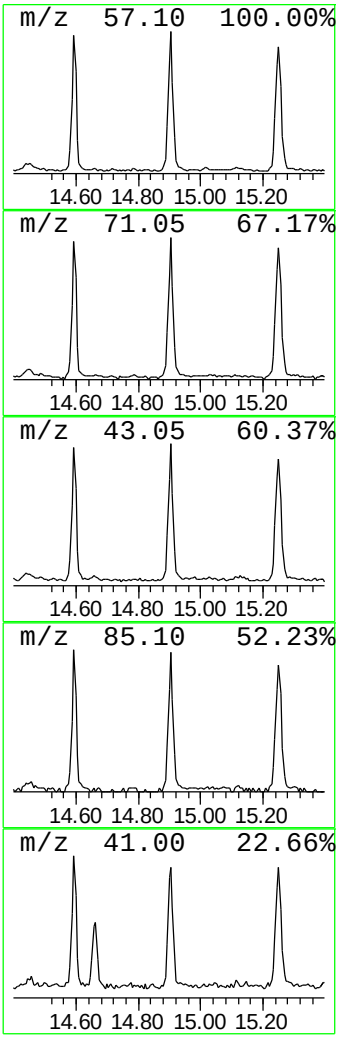
****

Peak Number 7 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.90	3.97 ng	147655	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5	Heptadecane	240	C17H36	000629-78-7	91





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Sample : J5371-09
Misc :
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Instrument : BNA_F
ClientSampleId : 100818-TIPC-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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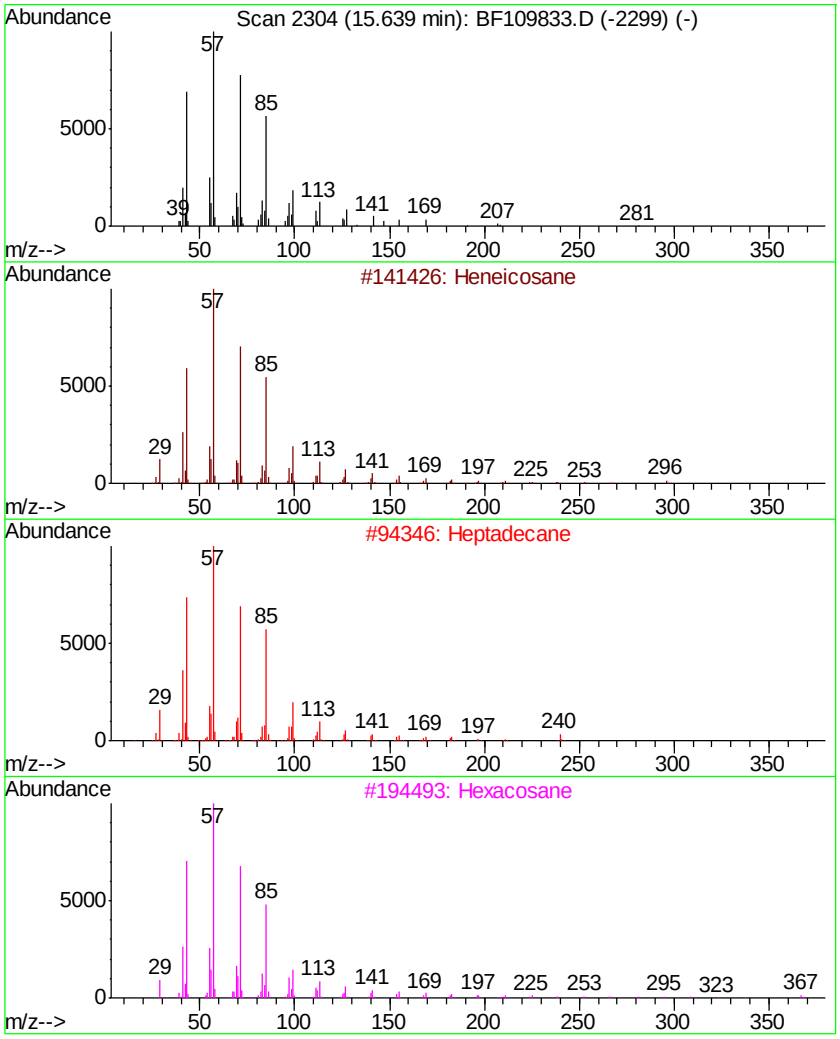
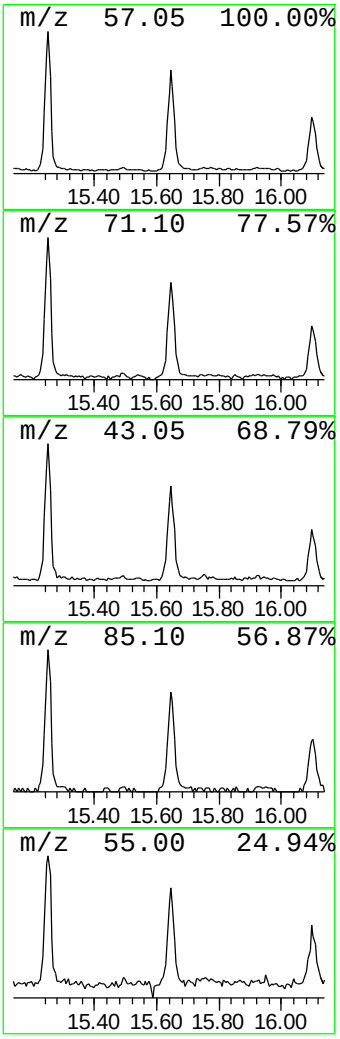
Peak Number 8 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.64	3.35 ng	124687	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Octadecane	254	C18H38	000593-45-3	90
5	2-methyloctacosane	408	C29H60	1000376-72-8	90





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Sample : J5371-09
Misc :
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Instrument : BNA_F
ClientSampleId : 100818-TIPC-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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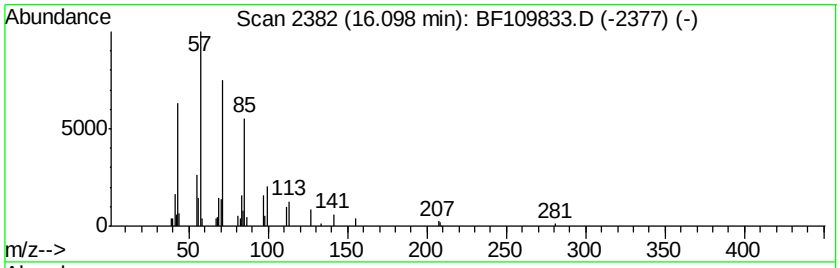
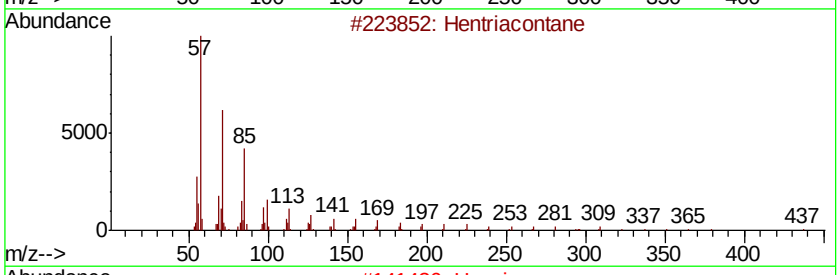
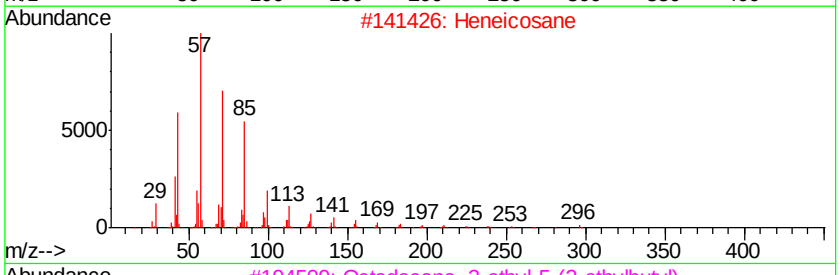
Peak Number 9 Hentriacontane Concentration Rank 9

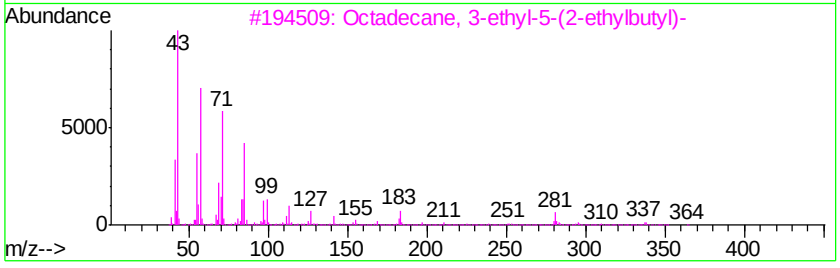
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	2.06 ng	76807	Perylene-d12	15.23

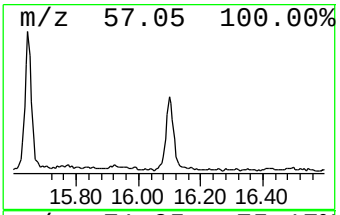
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	90
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90

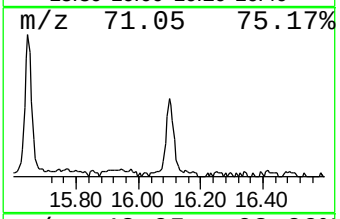


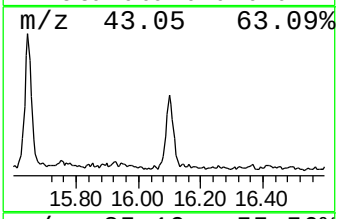


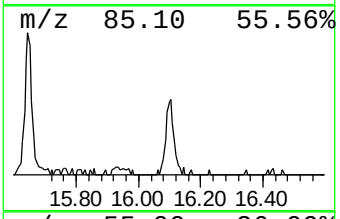


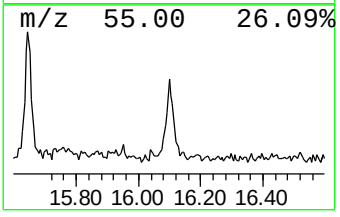












Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101218\
Data File : BF109833.D
Acq On : 12 Oct 2018 15:04
Operator : JU/SJ
Sample : J5371-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100818-TIPC-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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	2.9	ng	85583	1	6.69	601075	20.0
unknown6.46	6.46	57.4	ng	1725450	1	6.69	601075	20.0
n-Hexadecanoic acid	11.74	2.4	ng	119296	4	11.20	993568	20.0
1-Hexacosanol	13.70	2.6	ng	108350	5	13.83	844161	20.0
Hexacosane	14.59	3.5	ng	128833	6	15.23	744685	20.0
Heneicosane	14.90	4.0	ng	147655	6	15.23	744685	20.0
Heptadecane	15.64	3.4	ng	124687	6	15.23	744685	20.0
Hentriacontane	16.10	2.1	ng	76807	6	15.23	744685	20.0