LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032818\
Data File : BF104009.D
Acq On : 28 Mar 2018 14:59
Operator : JU/SJ
Sample : J2075-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-107(12-13)

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_F\METHODS\8270-BF032818.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	2.310	34	38	45	rVB	110631	157074	4.01%	0.445%
2	5.222	529	533	545	rBV	65439	127085	3.24%	0.360%
3	5.604	594	598	632	rBV	1928588	3409811	86.96%	9.656%
4	6.604	763	768	787	rBV	2122481	3373182	86.02%	9.553%
5	6.739	787	791	819	rVB	2755633	3597436	91.74%	10.188%
6	6.963	826	829	851	rVB	579476	764660	19.50%	2.165%
7	7.116	851	855	879	rBV	2223020	2730230	69.63%	7.732%
8	7.527	920	925	935	rBV	1657008	2091526	53.34%	5.923%
9	8.245	1043	1047	1069	rBV	910955	1074856	27.41%	3.044%
10	8.727	1125	1129	1133	rBV	119949	98324	2.51%	0.278%
11	9.316	1224	1229	1239	rBV	3545600	3921170	100.00%	11.104%
12	9.651	1282	1286	1289	rVB	429184	378970	9.66%	1.073%
13	9.710	1289	1296	1306	rBV	357869	393205	10.03%	1.114%
14	9.910	1326	1330	1334	rBV	52487	47493	1.21%	0.134%
15	9.998	1341	1345	1357	rBV	1077758	1193868	30.45%	3.381%
16	10.410	1413	1415	1418	rVB2	82913	66164	1.69%	0.187%
17	10.798	1476	1481	1493	rBV	2235558	2576360	65.70%	7.296%
18	10.886	1493	1496	1505	rVB	72634	102861	2.62%	0.291%
19	11.333	1568	1572	1574	rBV	50852	40609	1.04%	0.115%
20	11.498	1596	1600	1612	rBV	1088518	1232571	31.43%	3.491%
21	11.698	1629	1634	1640	rBV2	58380	72738	1.86%	0.206%
22	12.004	1680	1686	1694	rBV	494422	617555	15.75%	1.749%
23	12.515	1770	1773	1777	rBV	58922	56150	1.43%	0.159%
24	12.574	1777	1783	1791	rVB3	82946	111813	2.85%	0.317%
25	12.709	1800	1806	1811	rBV7	21649	47897	1.22%	0.136%
26	12.786	1815	1819	1823	rBV	130108	153776	3.92%	0.435%
27	13.086	1864	1870	1873	rBV	3418237	3810127	97.17%	10.790%
28	13.951	2014	2017	2023	rBV	506609	515994	13.16%	1.461%
29	14.145	2046	2050	2060	rBV	1189884	1188734	30.32%	3.366%
30	14.598	2123	2127	2130	rBV	45747	67324	1.72%	0.191%
31	14.756	2150	2154	2160	rVB9	36141	56419	1.44%	0.160%
32	14.986	2190	2193	2197	rVB	188279	181330	4.62%	0.514%
33	15.686	2305	2312	2324	rVB	606518	944504	24.09%	2.675%
34	16.180	2391	2396	2402	rBV2	58067	109930	2.80%	0.311%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032818\
Data File : BF104009.D
Acq On : 28 Mar 2018 14:59
Operator : JU/SJ
Sample : J2075-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-107(12-13)

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_F\METHODS\8270-BF032818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 35311746

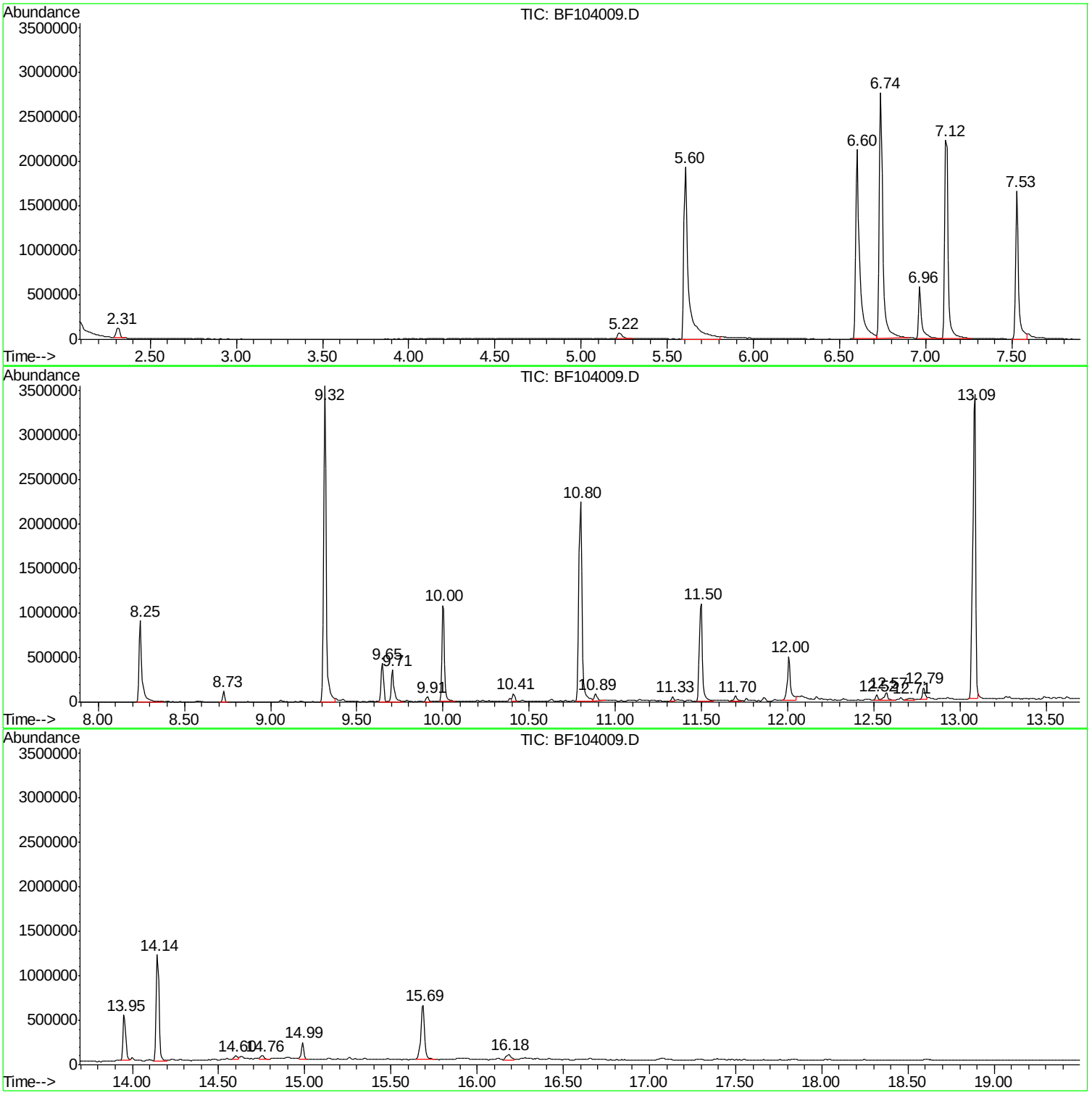
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032818\
Data File : BF104009.D
Acq On : 28 Mar 2018 14:59
Operator : JU/SJ
Sample : J2075-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-107(12-13)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032818\
Data File : BF104009.D
Acq On : 28 Mar 2018 14:59
Operator : JU/SJ
Sample : J2075-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-107(12-13)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

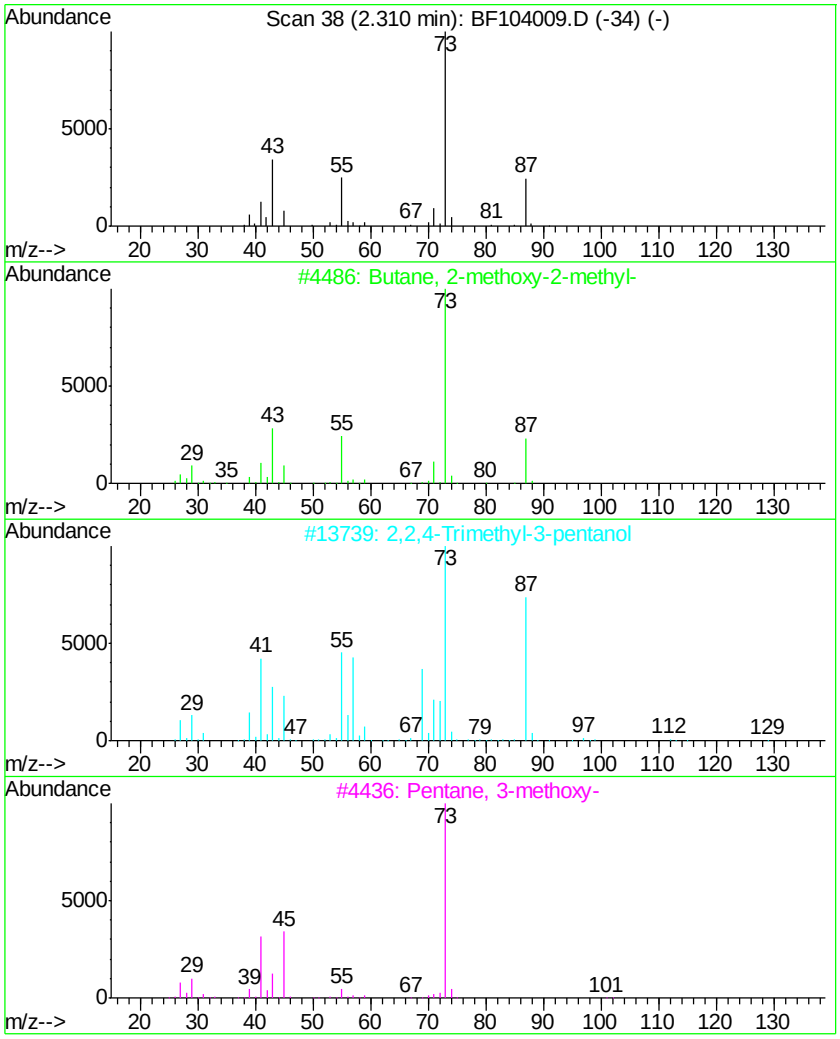
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

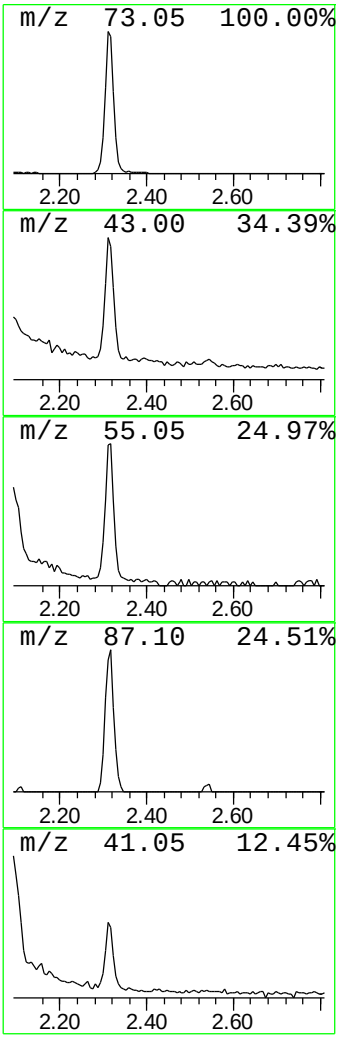
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.31	4.11 ng	157074	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	86
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





Data Path : Z:\HPCHEM1\BNA F\DATA\BF032818\
Data File : BF104009.D
Acq On : 28 Mar 2018 14:59
Operator : JU/SJ
Sample : J2075-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-107(12-13)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

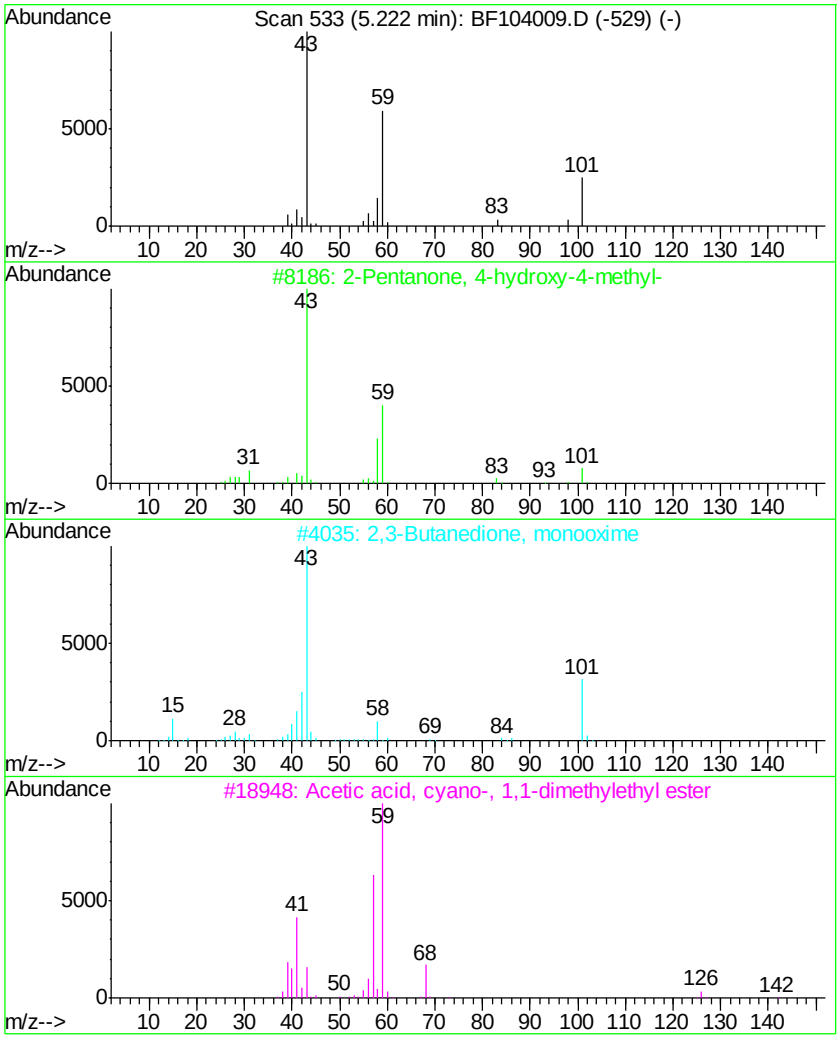
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

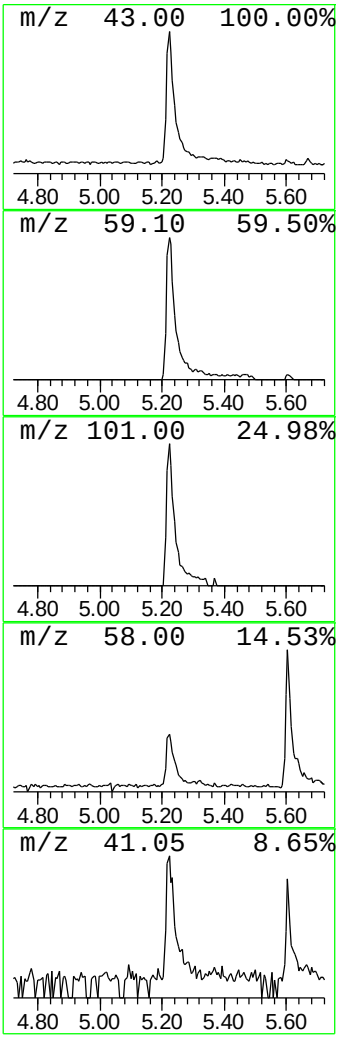
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	3.32 ng	127085	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF032818\
Data File : BF104009.D
Acq On : 28 Mar 2018 14:59
Operator : JU/SJ
Sample : J2075-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-107(12-13)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.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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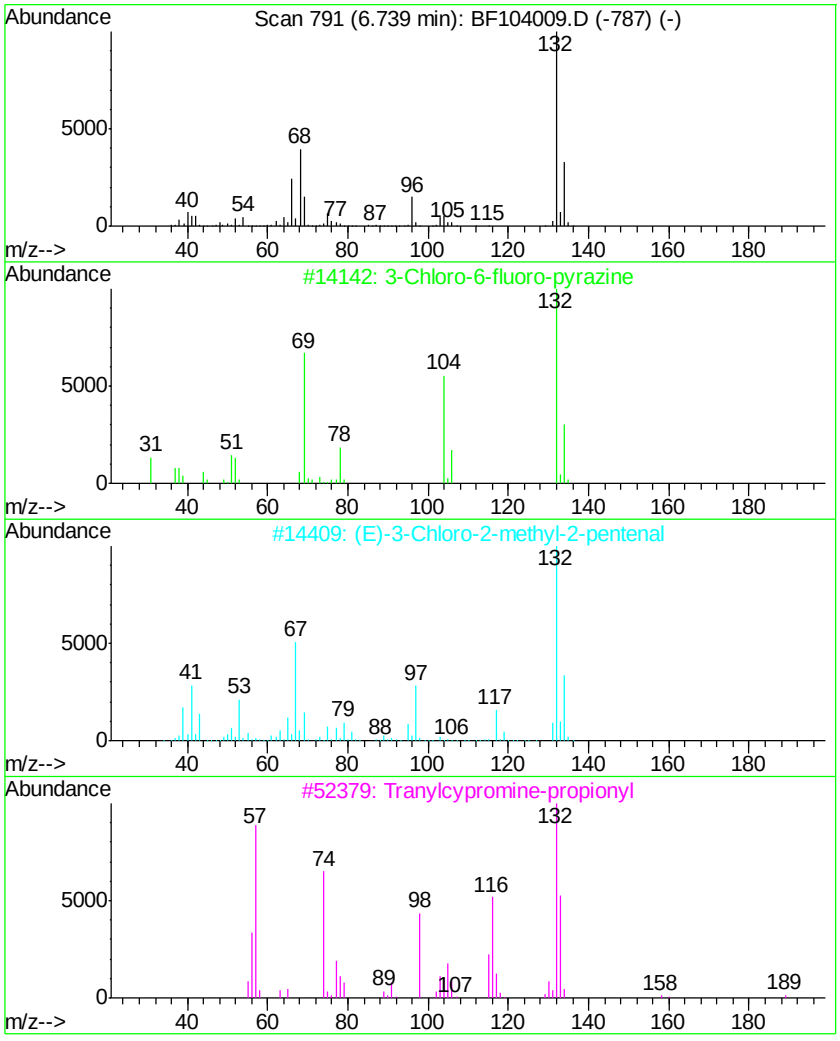
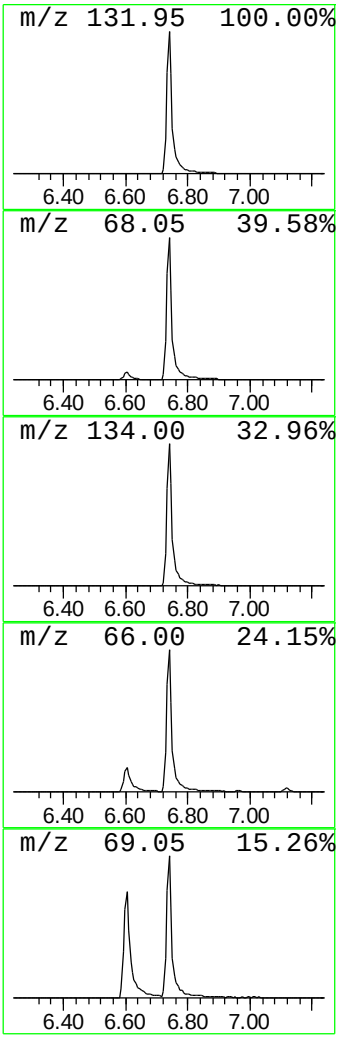
Peak Number 3 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	94.09 ng	3597440	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF032818\
Data File : BF104009.D
Acq On : 28 Mar 2018 14:59
Operator : JU/SJ
Sample : J2075-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-107(12-13)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.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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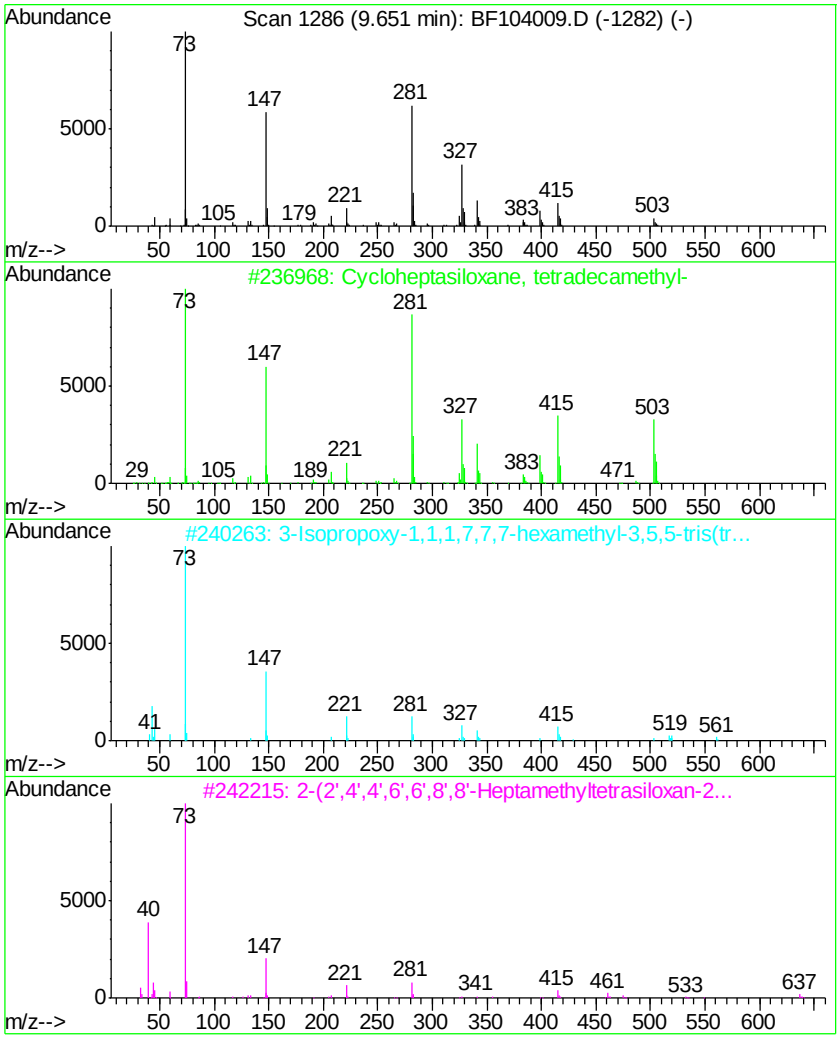
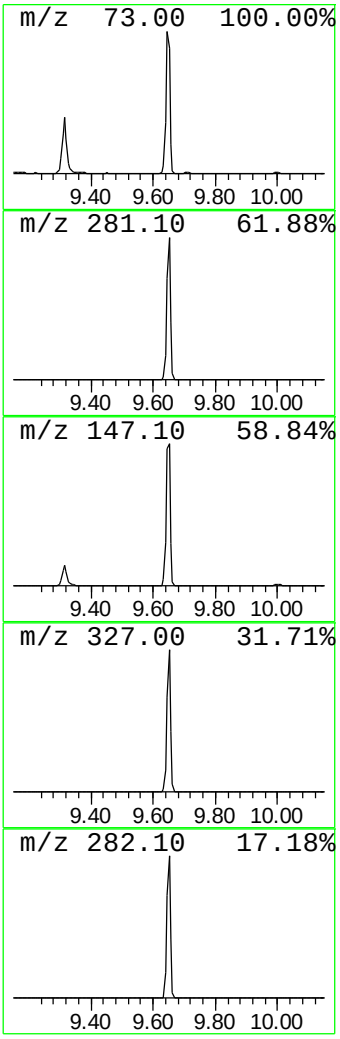
Peak Number 5 Cycloheptasiloxane, tetrade... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.65	6.35 ng	378970	Acenaphthene-d10	10.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloheptasiloxane, tetradecamet...	518	C14H42O7Si7	000107-50-6	93
2	3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	59
3	2-(2',4',4',6',6',8',8'-Heptamet...	652	C16H48O10Si9	145344-72-5	37
4	Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	37
5	Hexasiloxane, 1,1,3,3,5,5,7,7,9,...	430	C12H38O5Si6	000995-82-4	27





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032818\
Data File : BF104009.D
Acq On : 28 Mar 2018 14:59
Operator : JU/SJ
Sample : J2075-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-107(12-13)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

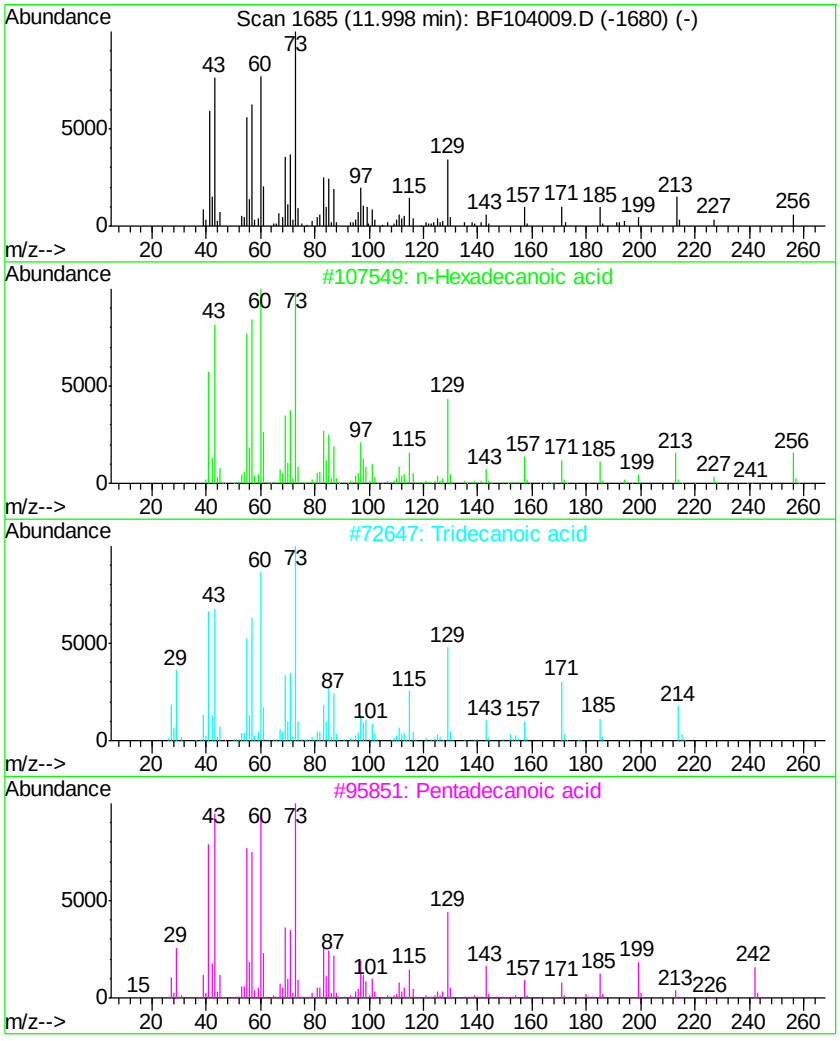
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

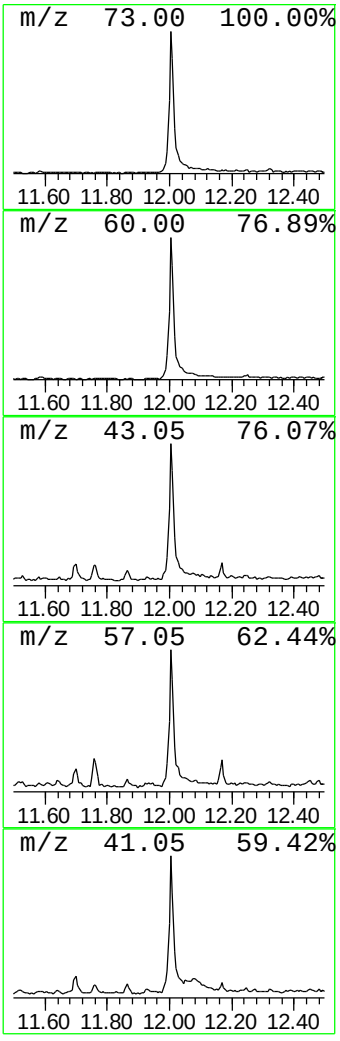
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	10.02 ng	617555	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





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Data File : BF104009.D
Acq On : 28 Mar 2018 14:59
Operator : JU/SJ
Sample : J2075-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-107(12-13)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.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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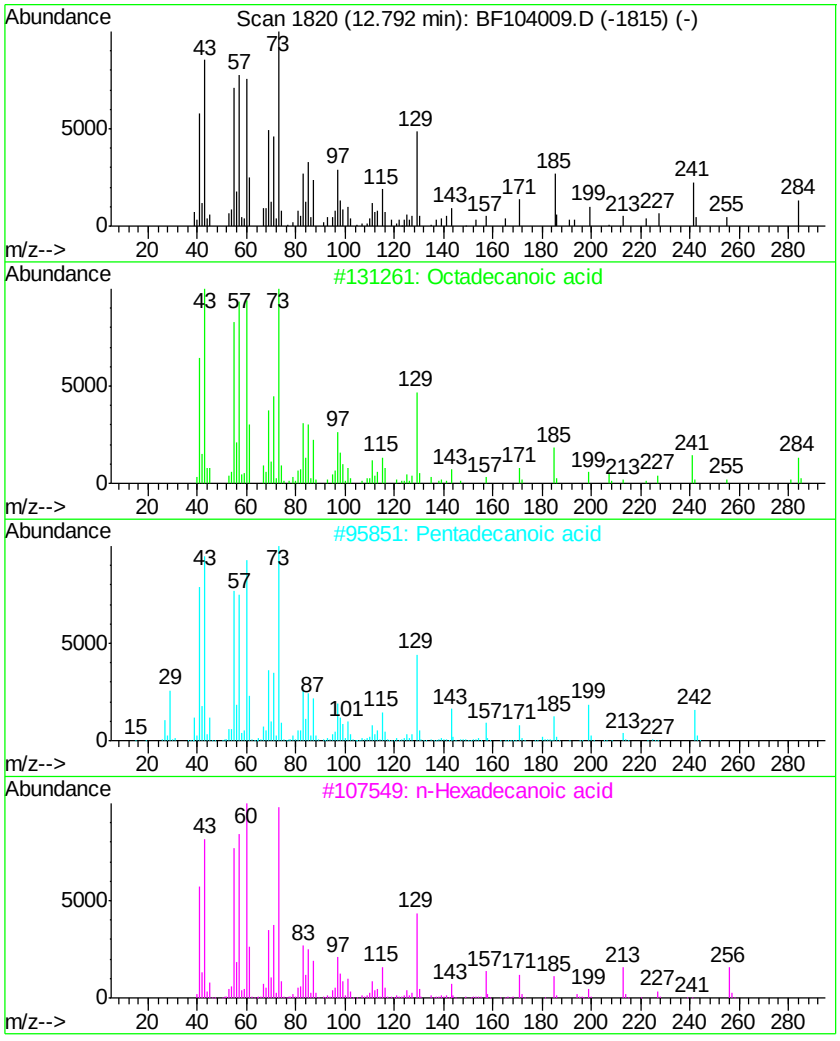
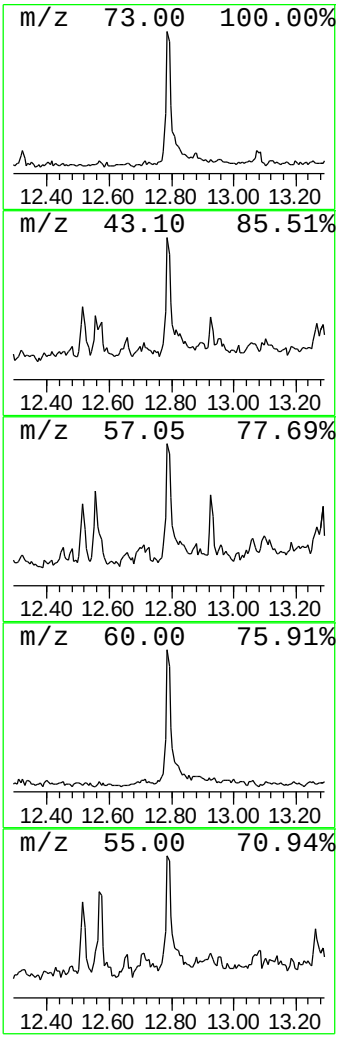
Peak Number 7 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	2.50 ng	153776	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	92
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	52





Data Path : Z:\HPCHEM1\BNA F\DATA\BF032818\
Data File : BF104009.D
Acq On : 28 Mar 2018 14:59
Operator : JU/SJ
Sample : J2075-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-107(12-13)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.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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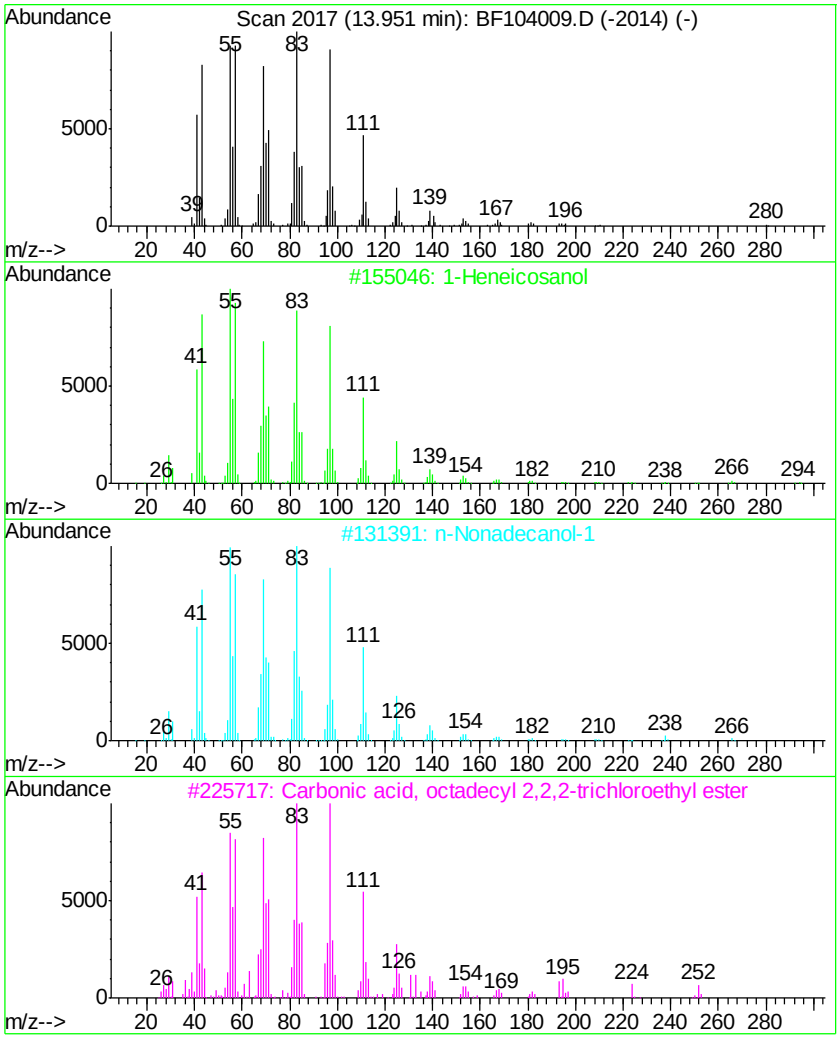
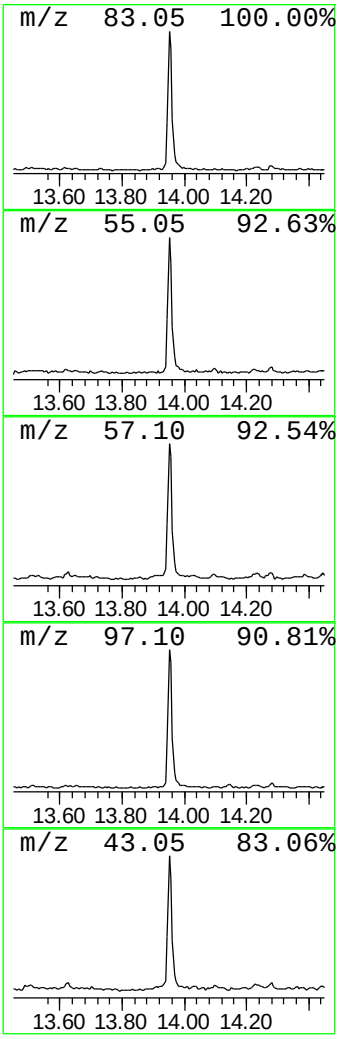
Peak Number 8 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	8.68 ng	515994	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	94
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93





Data Path : Z:\HPCHEM1\BNA F\DATA\BF032818\
Data File : BF104009.D
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Sample : J2075-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-107(12-13)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.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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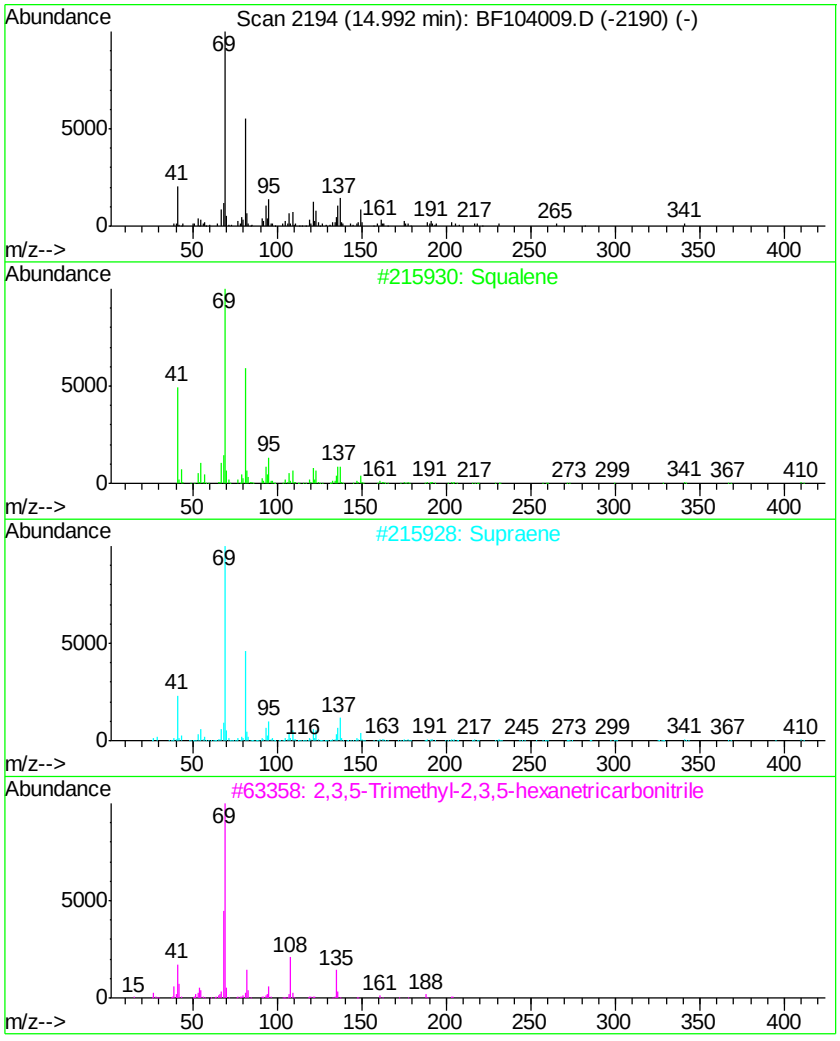
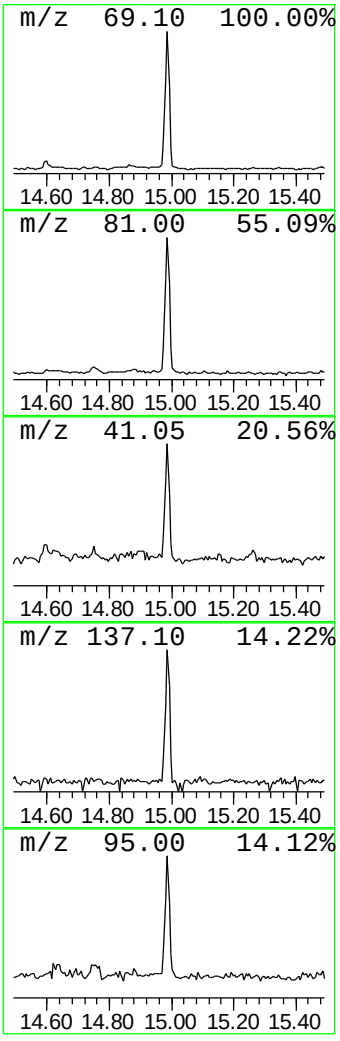
Peak Number 9 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	3.84 ng	181330	Perylene-d12	15.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50
4	Cyclopropanecarboxylic acid, 3-m...	176	C11H12O2	1000307-52-1	49
5	3,6-Dimethyl-1-heptyn-3-ol	140	C9H16O	019549-98-5	47





Data Path : Z:\HPCHEM1\BNA F\DATA\BF032818\
Data File : BF104009.D
Acq On : 28 Mar 2018 14:59
Operator : JU/SJ
Sample : J2075-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-107(12-13)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.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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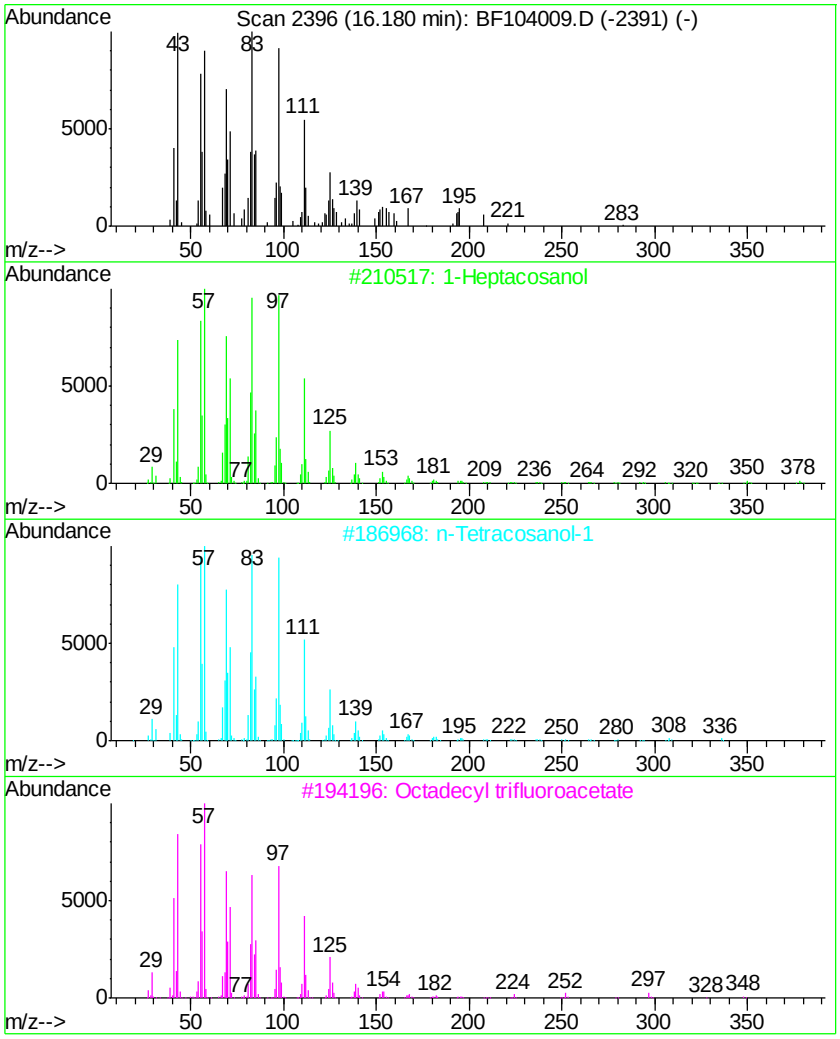
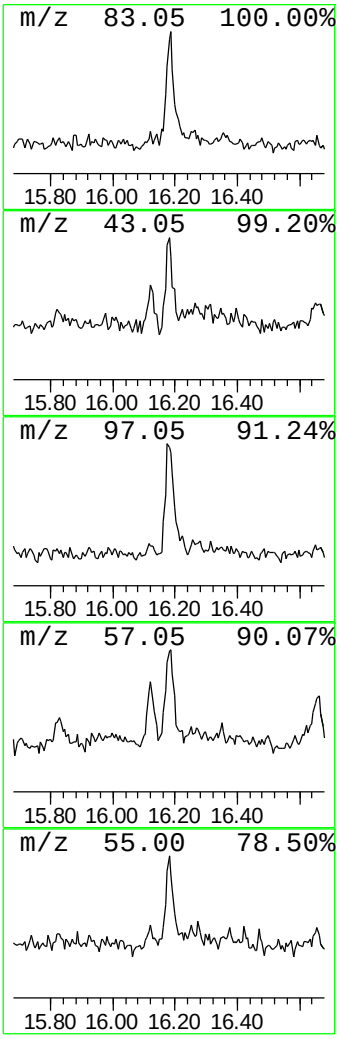
Peak Number 10 1-Heptacosanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	2.33 ng	109930	Perylene-d12	15.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4	Heptacosyl acetate	438	C29H58O2	1000351-78-2	91
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032818\
Data File : BF104009.D
Acq On : 28 Mar 2018 14:59
Operator : JU/SJ
Sample : J2075-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-107(12-13)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.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
Butane, 2-methoxy...	2.31	4.1	ng	157074	1	6.96	764660	20.0
2-Pentanone, 4-hy...	5.22	3.3	ng	127085	1	6.96	764660	20.0
unknown6.74	6.74	94.1	ng	3597440	1	6.96	764660	20.0
Cycloheptasiloxan...	9.65	6.3	ng	378970	3	10.00	1193870	20.0
n-Hexadecanoic acid	12.00	10.0	ng	617555	4	11.50	1232570	20.0
Octadecanoic acid	12.79	2.5	ng	153776	4	11.50	1232570	20.0
1-Heneicosanol	13.95	8.7	ng	515994	5	14.14	1188730	20.0
Squalene	14.99	3.8	ng	181330	6	15.69	944504	20.0
1-Heptacosanol	16.18	2.3	ng	109930	6	15.69	944504	20.0