LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011320\
Data File : BF118541.D
Acq On : 13 Jan 2020 20:09
Operator : JU
Sample : L1106-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CIY1-SB-02-03-0-32

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-BF010820.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	5.010	493	497	507	rBV	148782	172098	13.35%	1.180%
2	5.434	565	569	592	rBV	1076678	1148420	89.06%	7.877%
3	6.457	739	743	761	rBV	1115560	1063898	82.51%	7.297%
4	6.587	761	765	774	rVB	1496608	1223762	94.91%	8.393%
5	6.816	800	804	813	rBV	467286	399189	30.96%	2.738%
6	6.969	827	830	840	rBV	1342433	1075632	83.42%	7.377%
7	7.381	896	900	915	rBV	944080	812507	63.01%	5.573%
8	8.098	1019	1022	1036	rBV	554824	479640	37.20%	3.290%
9	9.175	1202	1205	1209	rBV	1733925	1289438	100.00%	8.844%
10	9.575	1270	1273	1277	rBV	147526	110139	8.54%	0.755%
11	9.857	1318	1321	1325	rBV	615072	547133	42.43%	3.753%
12	10.657	1453	1457	1469	rBV	1124388	1060089	82.21%	7.271%
13	10.769	1472	1476	1485	rVB	44545	48967	3.80%	0.336%
14	10.945	1504	1506	1510	rBV2	20105	20199	1.57%	0.139%
15	11.080	1525	1529	1533	rBV2	18774	18914	1.47%	0.130%
16	11.351	1572	1575	1578	rBV	687378	584692	45.34%	4.010%
17	11.374	1578	1579	1584	rVB	103113	87578	6.79%	0.601%
18	11.433	1584	1589	1591	rBV	23570	27585	2.14%	0.189%
19	11.874	1662	1664	1671	rVB3	67242	74017	5.74%	0.508%
20	11.933	1671	1674	1677	rVB2	21297	19922	1.55%	0.137%
21	11.969	1677	1680	1682	rBV	26944	25254	1.96%	0.173%
22	12.122	1704	1706	1709	rVB	23619	17297	1.34%	0.119%
23	12.404	1749	1754	1757	rBV4	20945	27630	2.14%	0.190%
24	12.569	1779	1782	1785	rBV	167404	160492	12.45%	1.101%
25	12.804	1815	1822	1825	rBV	168262	190298	14.76%	1.305%
26	12.939	1841	1845	1848	rBV	1135246	1047478	81.24%	7.184%
27	13.021	1855	1859	1863	rBV4	16690	30339	2.35%	0.208%
28	13.410	1922	1925	1931	rVB	84004	80249	6.22%	0.550%
29	13.651	1962	1966	1970	rVB5	12029	16932	1.31%	0.116%
30	13.757	1978	1984	1986	rBV6	13537	20414	1.58%	0.140%
31	13.833	1993	1997	2000	rBV3	82825	99460	7.71%	0.682%
32	14.004	2022	2026	2029	rBV2	450725	419318	32.52%	2.876%
33	14.027	2029	2030	2033	rVB	52969	41835	3.24%	0.287%
34	14.151	2048	2051	2055	rBV2	22401	28760	2.23%	0.197%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011320\
Data File : BF118541.D
Acq On : 13 Jan 2020 20:09
Operator : JU
Sample : L1106-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CIY1-SB-02-03-0-32

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-BF010820.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.192	2055	2058	2061	rVV	41331	34771	2.70%	0.238%
36	14.351	2082	2085	2088	rBV2	24060	28552	2.21%	0.196%
37	14.457	2100	2103	2106	rBV	34581	39935	3.10%	0.274%
38	14.757	2151	2154	2157	rBV	38603	41229	3.20%	0.283%
39	14.833	2164	2167	2175	rVB	320258	333173	25.84%	2.285%
40	14.904	2175	2179	2181	rBV5	11919	18304	1.42%	0.126%
41	15.051	2200	2204	2208	rBV	70570	106325	8.25%	0.729%
42	15.262	2235	2240	2243	rBV6	24150	48911	3.79%	0.335%
43	15.351	2251	2255	2261	rBV2	67166	94165	7.30%	0.646%
44	15.421	2264	2267	2272	rVB	71734	83053	6.44%	0.570%
45	15.480	2272	2277	2285	rBV	492440	666250	51.67%	4.570%
46	15.904	2346	2349	2354	rVB	70073	92480	7.17%	0.634%
47	16.404	2430	2434	2438	rBV2	50919	89138	6.91%	0.611%
48	16.986	2528	2533	2545	rVB5	51322	172289	13.36%	1.182%
49	17.862	2679	2682	2683	rBV3	35522	34008	2.64%	0.233%
50	18.927	2854	2863	2870	rBV7	64340	227978	17.68%	1.564%

Sum of corrected areas: 14580136

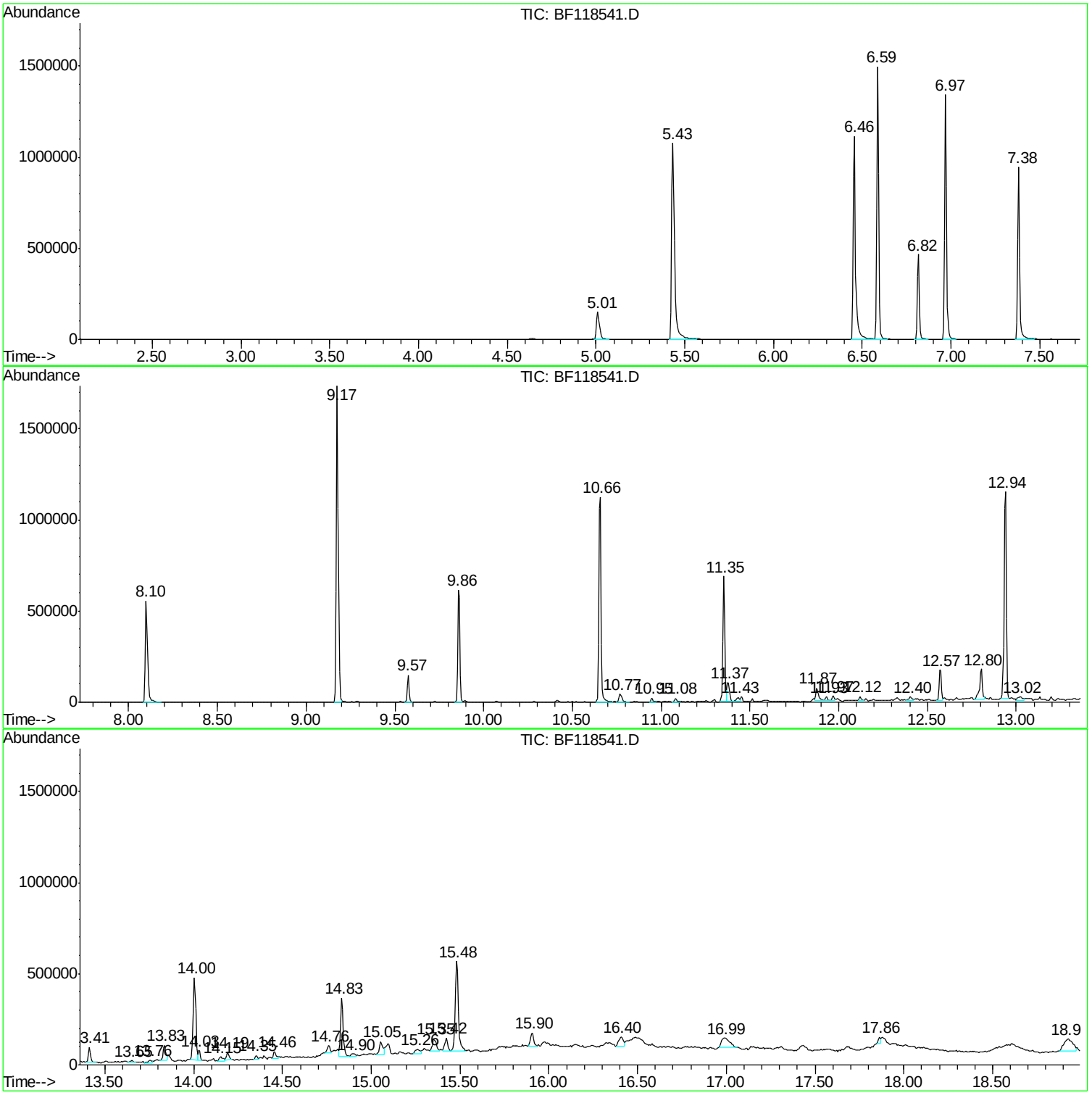
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011320\
Data File : BF118541.D
Acq On : 13 Jan 2020 20:09
Operator : JU
Sample : L1106-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CIY1-SB-02-03-0-32

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011320\
Data File : BF118541.D
Acq On : 13 Jan 2020 20:09
Operator : JU
Sample : L1106-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CIY1-SB-02-03-0-32

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

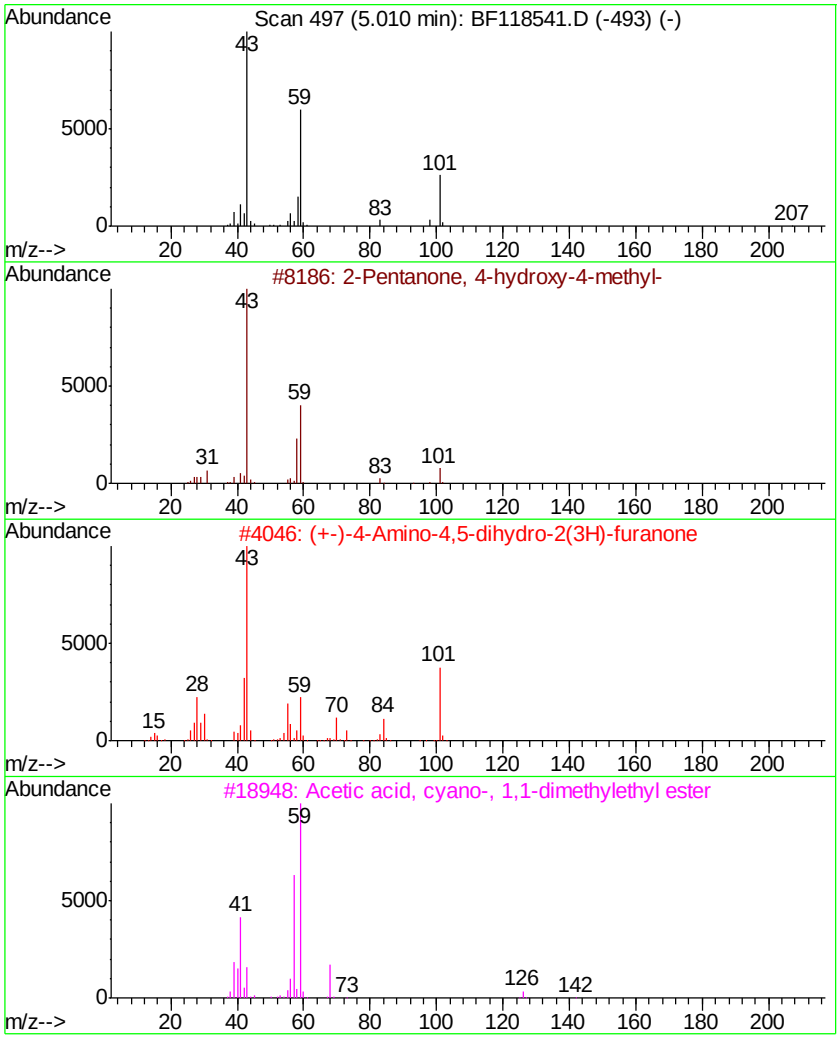
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

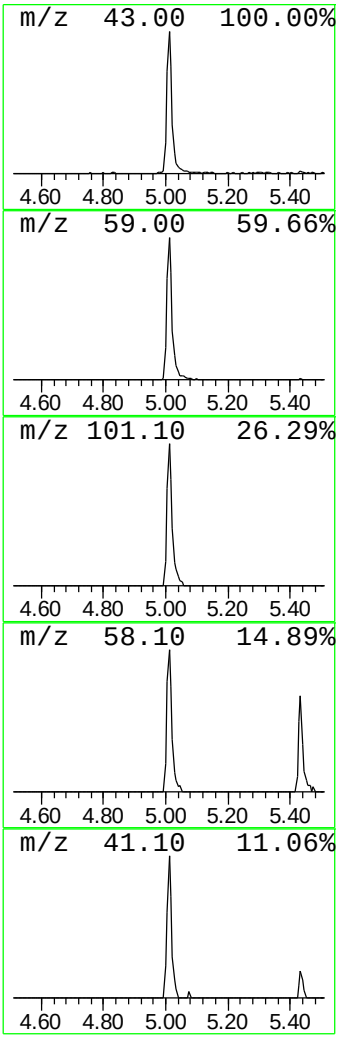
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	8.62 ng	172098	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011320\
Data File : BF118541.D
Acq On : 13 Jan 2020 20:09
Operator : JU
Sample : L1106-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CIY1-SB-02-03-0-32

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

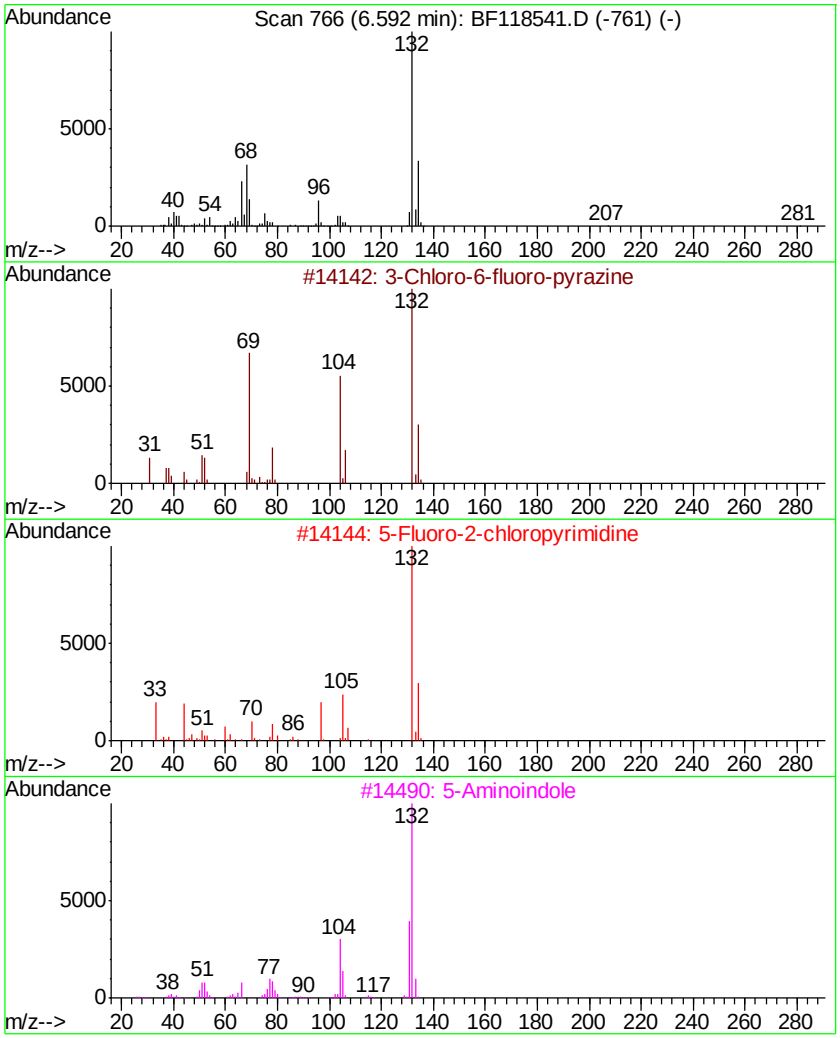
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

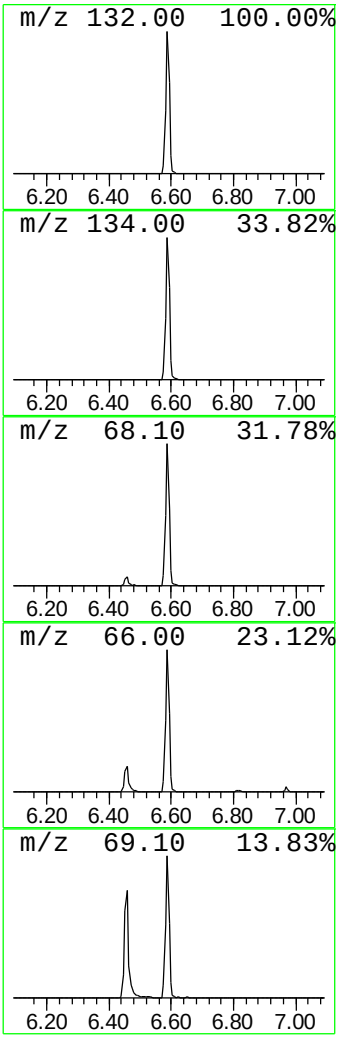
****

Peak Number 2 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	61.31 ng	1223760	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	25
3	5-Aminoindole	132	C8H8N2	005192-03-0	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011320\
Data File : BF118541.D
Acq On : 13 Jan 2020 20:09
Operator : JU
Sample : L1106-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CIY1-SB-02-03-0-32

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010820.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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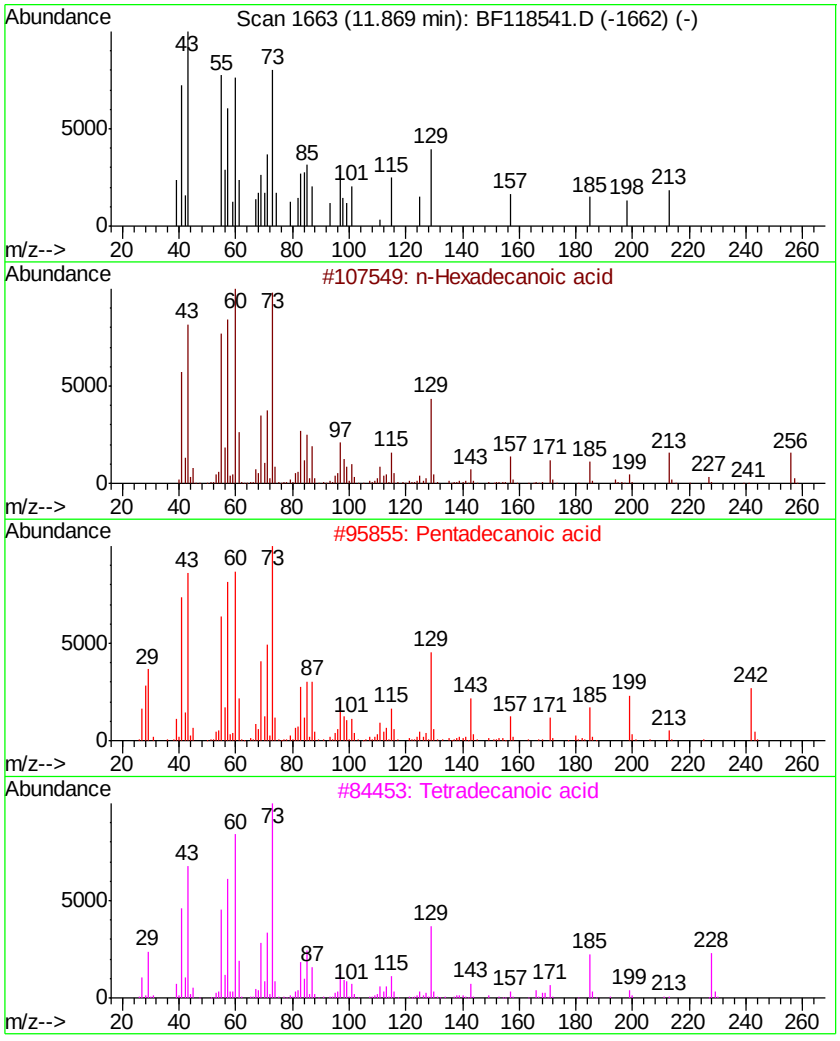
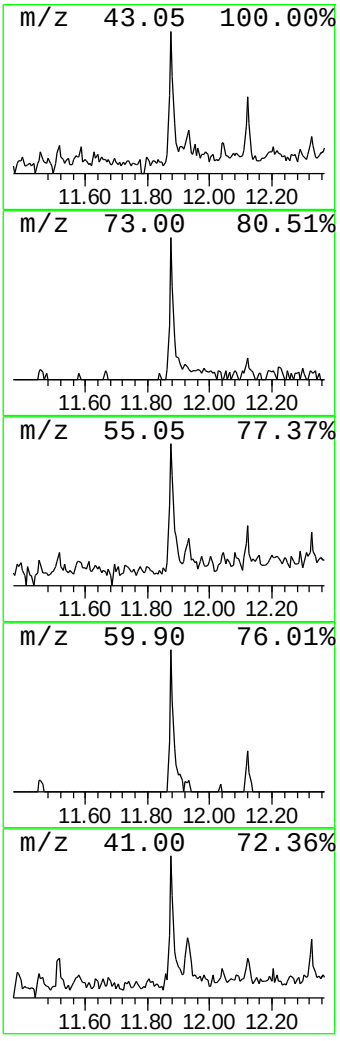
Peak Number 4 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	2.53 ng	74017	Phenanthrene-d10	11.35

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	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	59
5	n-Decanoic acid	172	C10H20O2	000334-48-5	59





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011320\
Data File : BF118541.D
Acq On : 13 Jan 2020 20:09
Operator : JU
Sample : L1106-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CIY1-SB-02-03-0-32

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

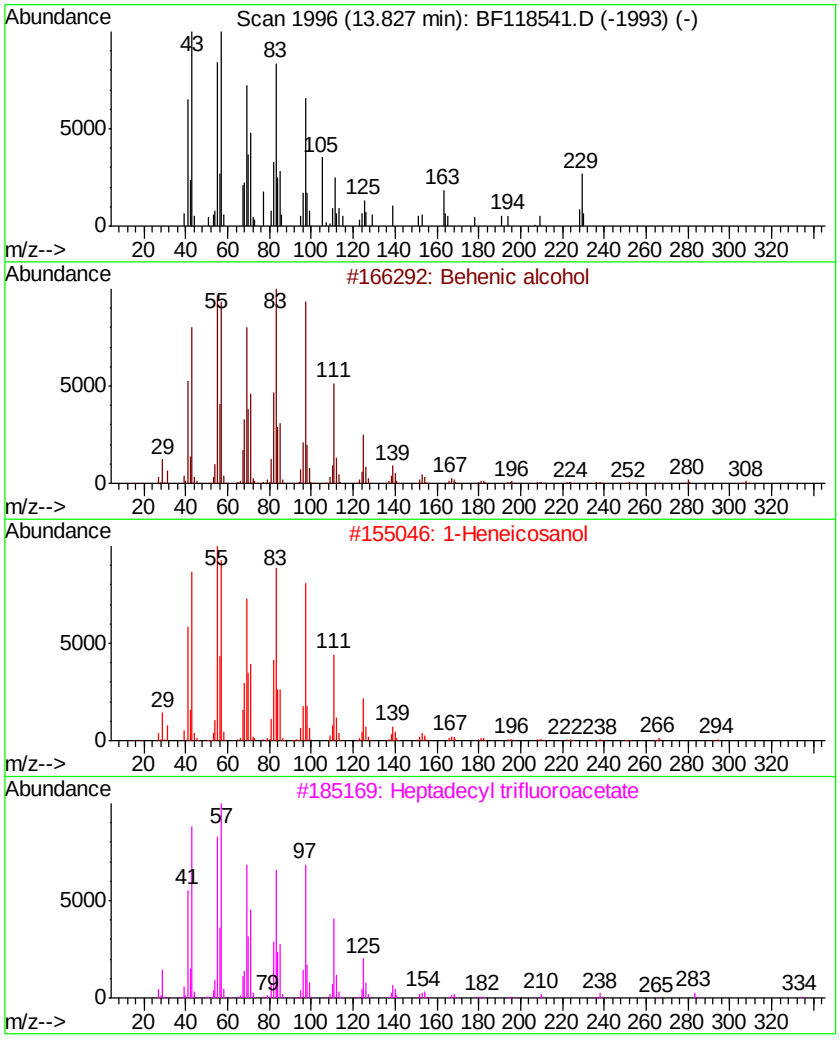
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

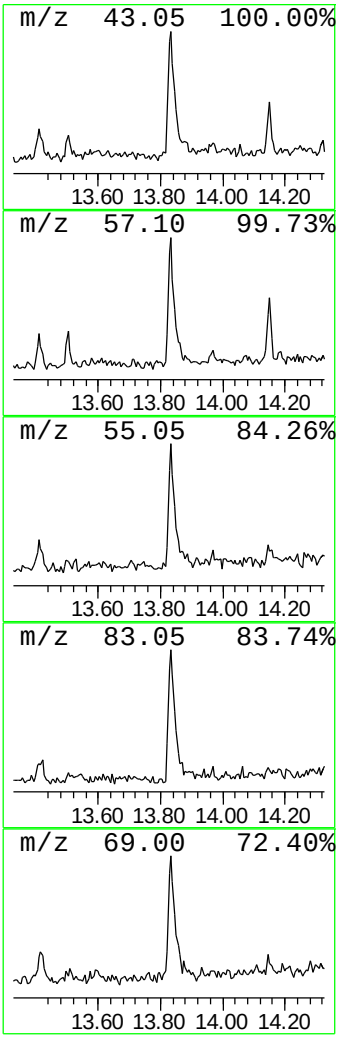
****

Peak Number 5 Behenic alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	4.74 ng	99460	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	93
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	92
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011320\
Data File : BF118541.D
Acq On : 13 Jan 2020 20:09
Operator : JU
Sample : L1106-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CIY1-SB-02-03-0-32

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

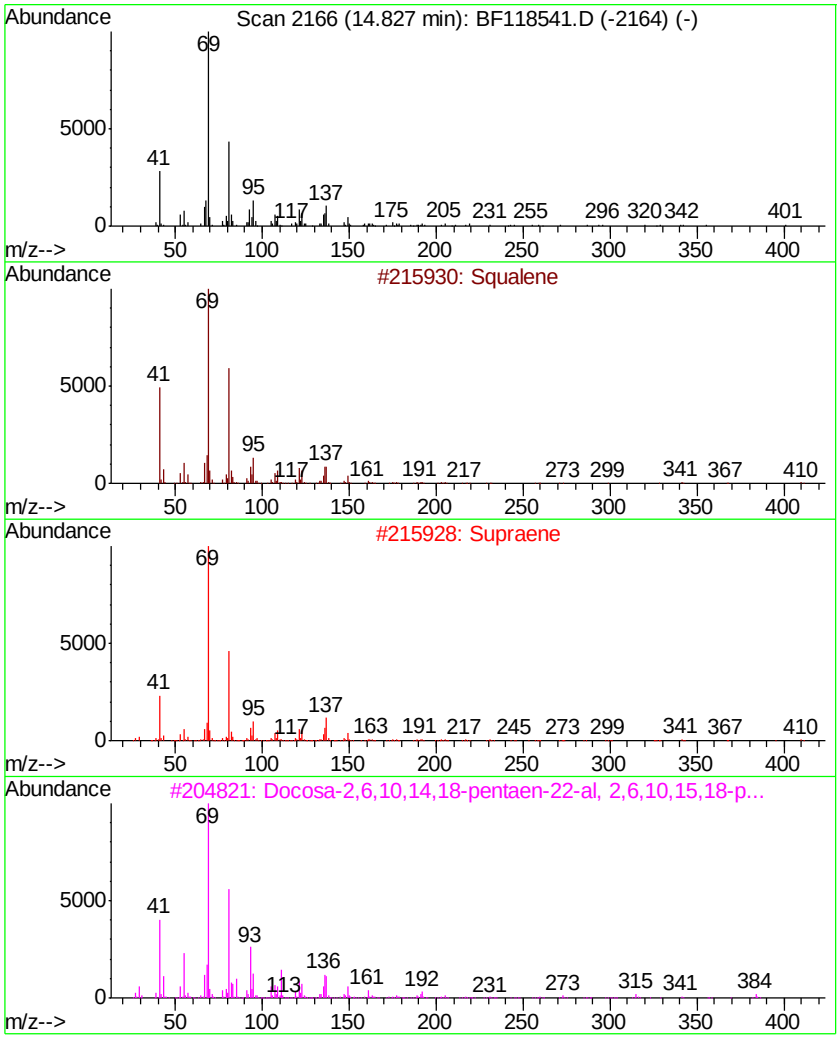
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

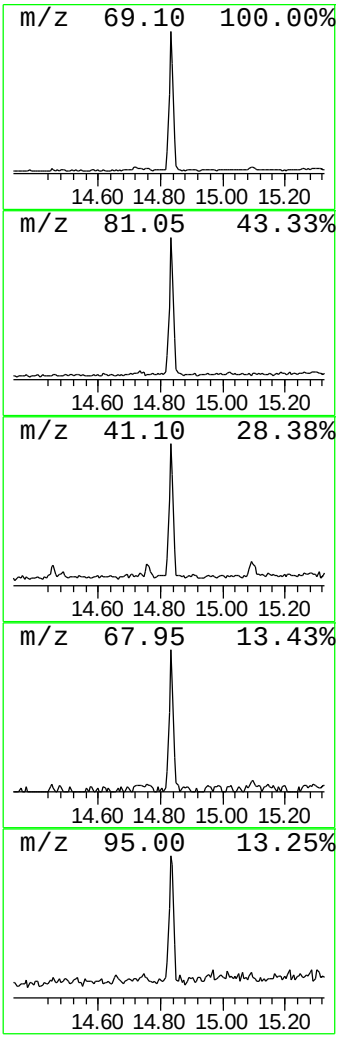
****

Peak Number 6 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	10.00 ng	333173	Perylene-d12	15.48

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	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	72
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011320\
Data File : BF118541.D
Acq On : 13 Jan 2020 20:09
Operator : JU
Sample : L1106-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CIY1-SB-02-03-0-32

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010820.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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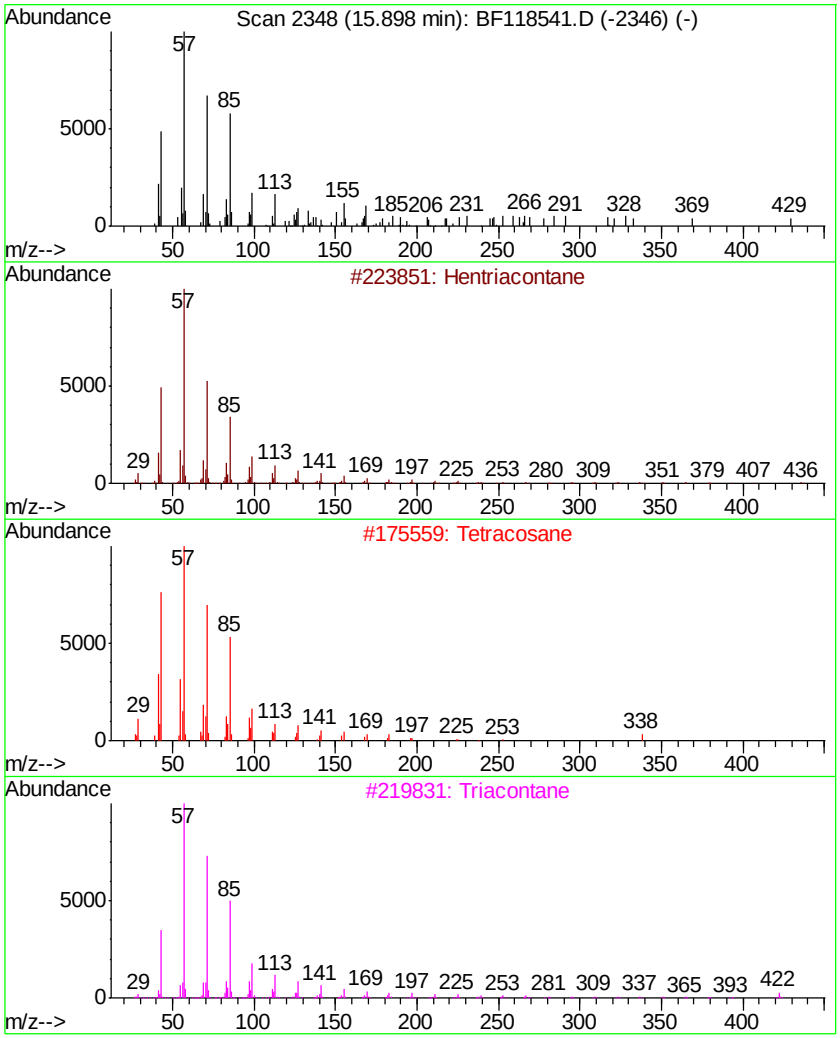
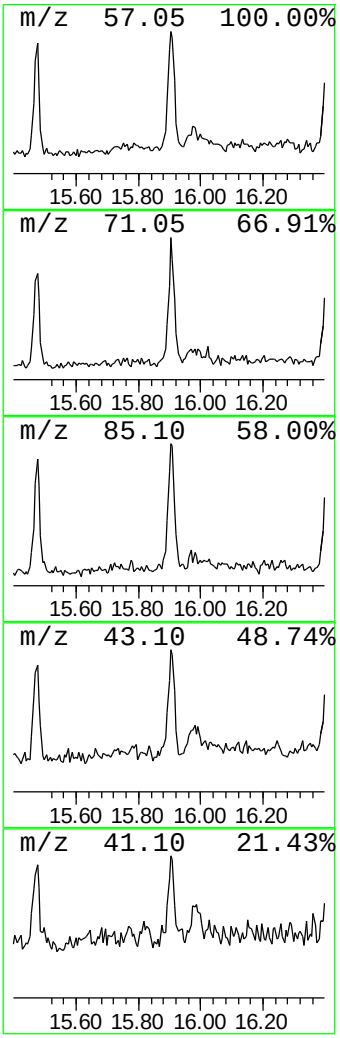
Peak Number 8 Hentriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.90	2.78 ng	92480	Perylene-d12	15.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	74
2	Tetracosane	338	C24H50	000646-31-1	74
3	Triacontane	422	C30H62	000638-68-6	74
4	6,6-Diethylhexadecane	282	C20H42	1000360-41-4	72
5	Eicosane, 2-methyl-	296	C21H44	001560-84-5	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011320\
Data File : BF118541.D
Acq On : 13 Jan 2020 20:09
Operator : JU
Sample : L1106-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CIY1-SB-02-03-0-32

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010820.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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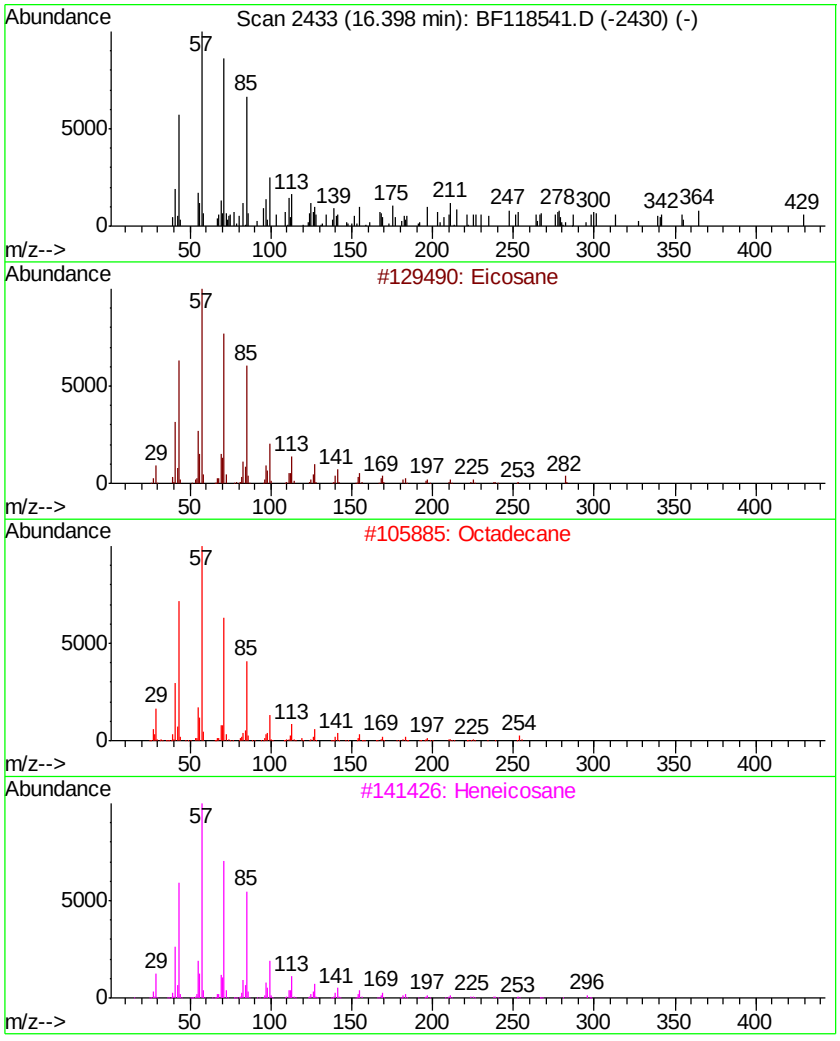
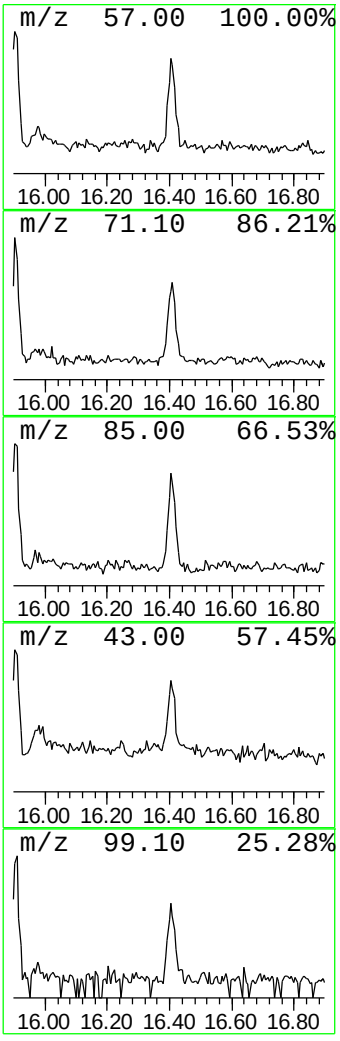
Peak Number 9 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.40	2.68 ng	89138	Perylene-d12	15.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Octadecane	254	C18H38	000593-45-3	83
3	Heneicosane	296	C21H44	000629-94-7	58
4	Octacosane	394	C28H58	000630-02-4	58
5	Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	58





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011320\
Data File : BF118541.D
Acq On : 13 Jan 2020 20:09
Operator : JU
Sample : L1106-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CIY1-SB-02-03-0-32

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010820.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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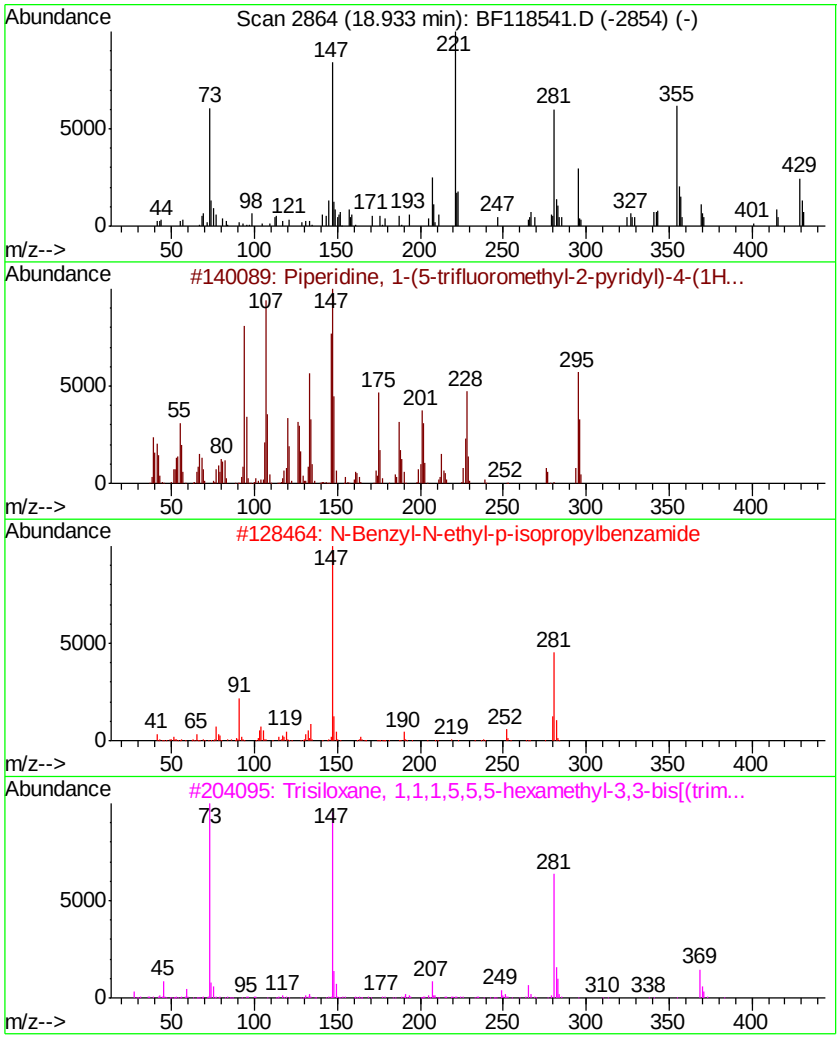
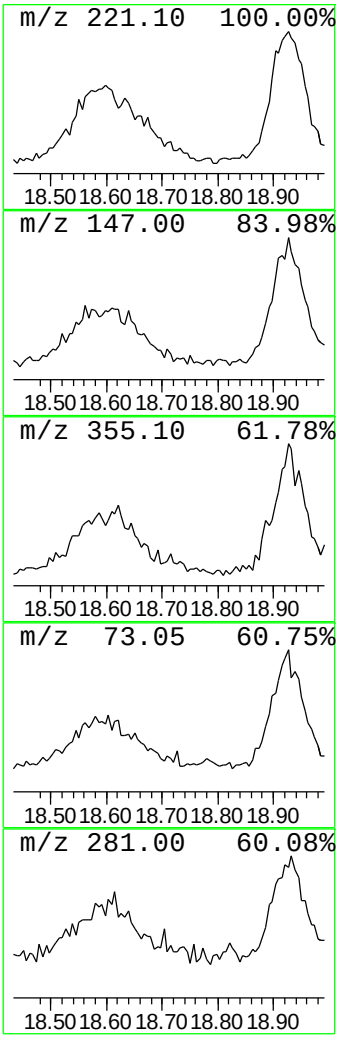
Peak Number 10 Piperidine, 1-(5-trifluorom... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.93	6.84 ng	227978	Perylene-d12	15.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Piperidine, 1-(5-trifluoromethyl...	295	C15H16F3N3	1000268-74-7	91
2	N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	25
3	Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	25
4	Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	22
5	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	14





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF011320\
Data File : BF118541.D
Acq On : 13 Jan 2020 20:09
Operator : JU
Sample : L1106-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CIY1-SB-02-03-0-32

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010820.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...	5.01	8.6	ng	172098	1	6.82	399189	20.0
unknown6.59	6.59	61.3	ng	1223760	1	6.82	399189	20.0
n-Hexadecanoic acid	11.87	2.5	ng	74017	4	11.35	584692	20.0
Behenic alcohol	13.83	4.7	ng	99460	5	14.00	419318	20.0
Squalene	14.83	10.0	ng	333173	6	15.48	666250	20.0
Hentriacontane	15.90	2.8	ng	92480	6	15.48	666250	20.0
Eicosane	16.40	2.7	ng	89138	6	15.48	666250	20.0
Piperidine, 1-(5-...	18.93	6.8	ng	227978	6	15.48	666250	20.0