LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122618\
Data File : BF111714.D
Acq On : 26 Dec 2018 14:23
Operator : JU/SJ
Sample : J6498-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1218-S-AB-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_F\METHODS\8270-BF121918.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	2.199	15	19	25	rVB2	70279	106550	2.95%	0.289%
2	3.428	226	228	242	rBV	27408	63037	1.75%	0.171%
3	5.116	508	515	522	rBV	157647	196014	5.43%	0.532%
4	5.534	581	586	589	rBV	3353828	2952646	81.85%	8.011%
5	6.539	751	757	761	rBV	3115592	3340350	92.60%	9.063%
6	6.675	775	780	783	rBV	3768339	3178083	88.10%	8.623%
7	6.898	815	818	822	rVB	1120501	1001339	27.76%	2.717%
8	7.057	841	845	849	rBV	2936299	2457715	68.13%	6.668%
9	7.457	908	913	916	rBV	2344016	1979942	54.89%	5.372%
10	8.180	1032	1036	1039	rBV	1465698	1266216	35.10%	3.435%
11	8.892	1154	1157	1161	rVB	108227	84135	2.33%	0.228%
12	8.992	1171	1174	1177	rBV	64910	48314	1.34%	0.131%
13	9.257	1214	1219	1222	rBV	4164420	3607326	100.00%	9.787%
14	9.645	1282	1285	1288	rVB	455187	375708	10.42%	1.019%
15	9.933	1331	1334	1338	rBV	1478937	1387962	38.48%	3.766%
16	9.969	1338	1340	1343	rVB	224819	164352	4.56%	0.446%
17	10.139	1365	1369	1372	rBV	129686	104554	2.90%	0.284%
18	10.480	1424	1427	1433	rVB	133990	109535	3.04%	0.297%
19	10.721	1464	1468	1472	rBV	2690369	2334592	64.72%	6.334%
20	11.421	1583	1587	1589	rBV	1678880	1399445	38.79%	3.797%
21	11.445	1589	1591	1594	rVV	637611	477487	13.24%	1.295%
22	11.492	1594	1599	1603	rVV	155200	141787	3.93%	0.385%
23	11.645	1620	1625	1628	rBV2	79293	78300	2.17%	0.212%
24	11.945	1673	1676	1680	rVB2	127641	133539	3.70%	0.362%
25	12.033	1688	1691	1694	rBV	78087	82040	2.27%	0.223%
26	12.633	1789	1793	1796	rBV	565167	448567	12.43%	1.217%
27	12.863	1826	1832	1834	rBV2	388120	424569	11.77%	1.152%
28	13.004	1852	1856	1859	rVB	4077525	3493477	96.84%	9.478%
29	13.074	1864	1868	1872	rBV3	22027	40035	1.11%	0.109%
30	13.192	1885	1888	1890	rBV	52422	46252	1.28%	0.125%
31	13.480	1935	1937	1941	rBV3	45044	46080	1.28%	0.125%
32	13.692	1971	1973	1978	rVB2	40301	42650	1.18%	0.116%
33	13.898	2005	2008	2014	rVB	325102	367711	10.19%	0.998%
34	14.057	2029	2035	2038	rBV2	1509669	1648527	45.70%	4.473%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122618\
Data File : BF111714.D
Acq On : 26 Dec 2018 14:23
Operator : JU/SJ
Sample : J6498-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1218-S-AB-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_F\METHODS\8270-BF121918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.080	2038	2039	2043	rVB	160491	126960	3.52%	0.344%
36	14.162	2051	2053	2056	rBV	54936	55051	1.53%	0.149%
37	14.221	2060	2063	2066	rBV	85321	80239	2.22%	0.218%
38	14.533	2112	2116	2120	rBV3	183151	192977	5.35%	0.524%
39	14.704	2142	2145	2150	rBV2	100584	108150	3.00%	0.293%
40	14.839	2166	2168	2172	rVB	100393	97490	2.70%	0.265%
41	14.921	2179	2182	2185	rBV	94786	94425	2.62%	0.256%
42	15.104	2210	2213	2216	rBV	111355	156293	4.33%	0.424%
43	15.186	2224	2227	2230	rBV	147972	155924	4.32%	0.423%
44	15.415	2263	2266	2271	rVB	70246	97425	2.70%	0.264%
45	15.474	2273	2276	2281	rVV	112147	139775	3.87%	0.379%
46	15.545	2283	2288	2291	rVV	950863	1206531	33.45%	3.274%
47	15.574	2291	2293	2301	rVB	134941	178016	4.93%	0.483%
48	15.780	2325	2328	2333	rVB2	87672	112946	3.13%	0.306%
49	16.021	2366	2369	2374	rVB	84205	110282	3.06%	0.299%
50	16.839	2503	2508	2516	rVB2	168838	316198	8.77%	0.858%

Sum of corrected areas: 36857518

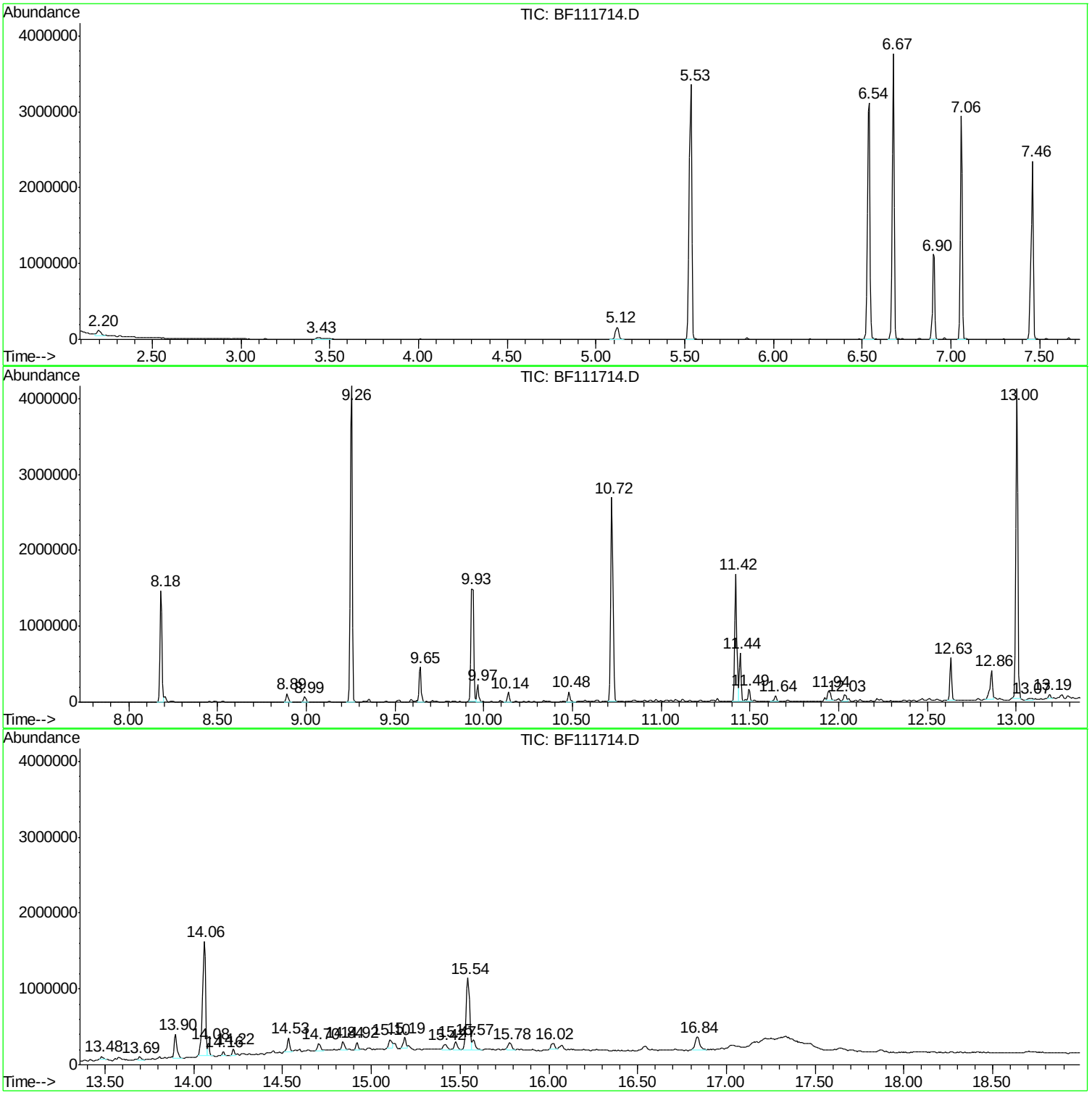
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122618\
Data File : BF111714.D
Acq On : 26 Dec 2018 14:23
Operator : JU/SJ
Sample : J6498-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1218-S-AB-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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\BF122618\
Data File : BF111714.D
Acq On : 26 Dec 2018 14:23
Operator : JU/SJ
Sample : J6498-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1218-S-AB-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

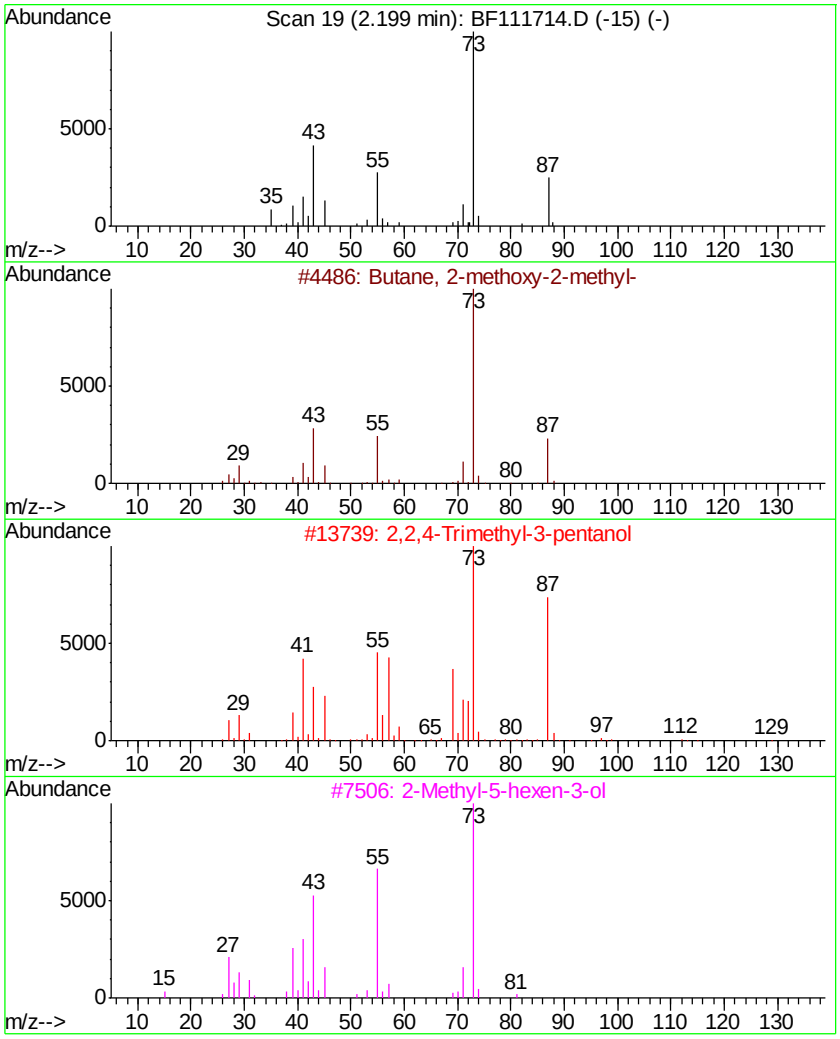
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

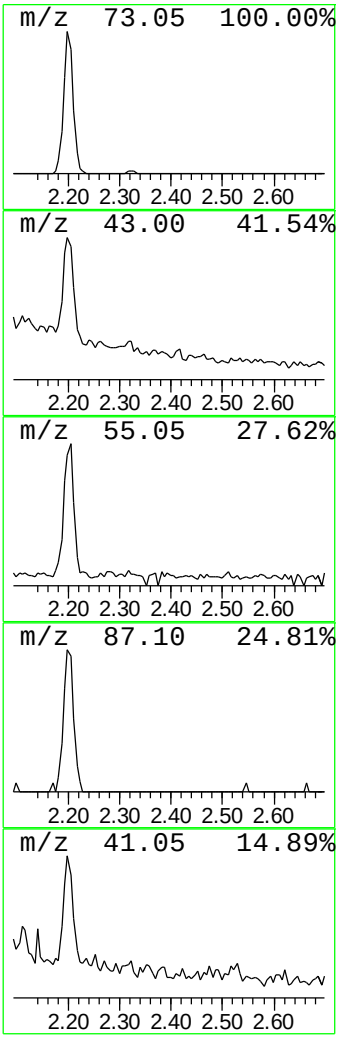
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	2.13 ng	106550	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
5	1-Propene-1-thiol	74	C3H6S	000925-89-3	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122618\
Data File : BF111714.D
Acq On : 26 Dec 2018 14:23
Operator : JU/SJ
Sample : J6498-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1218-S-AB-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

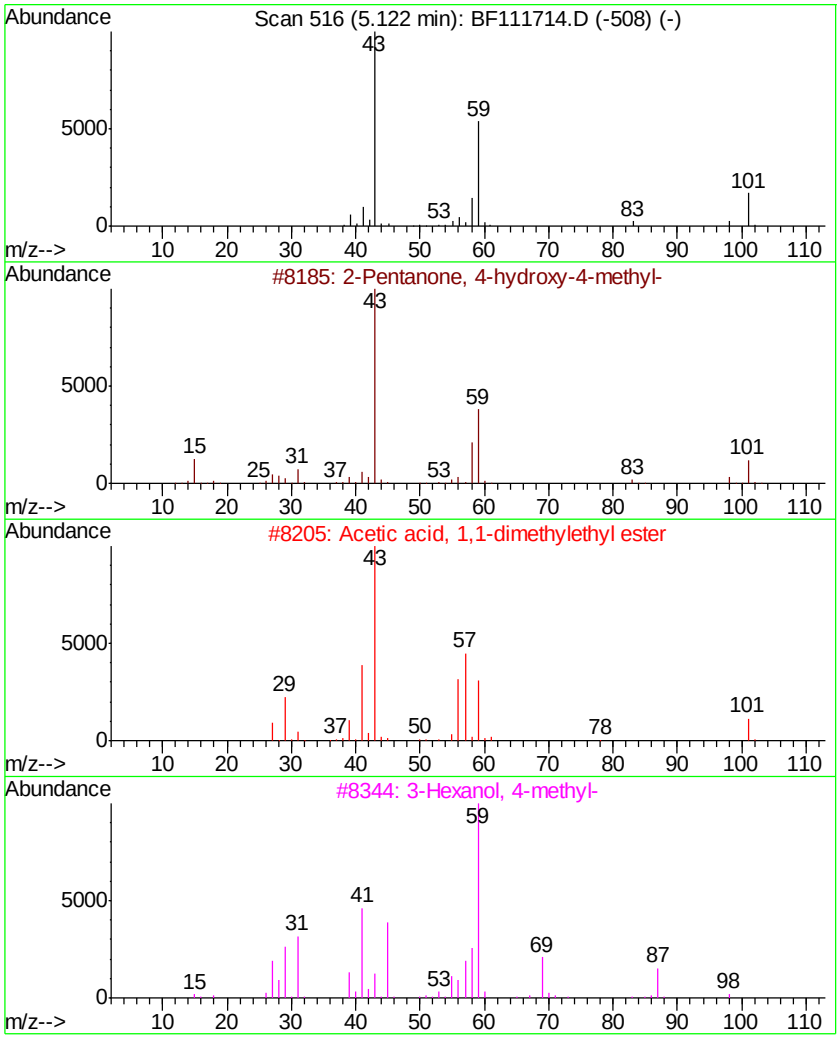
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

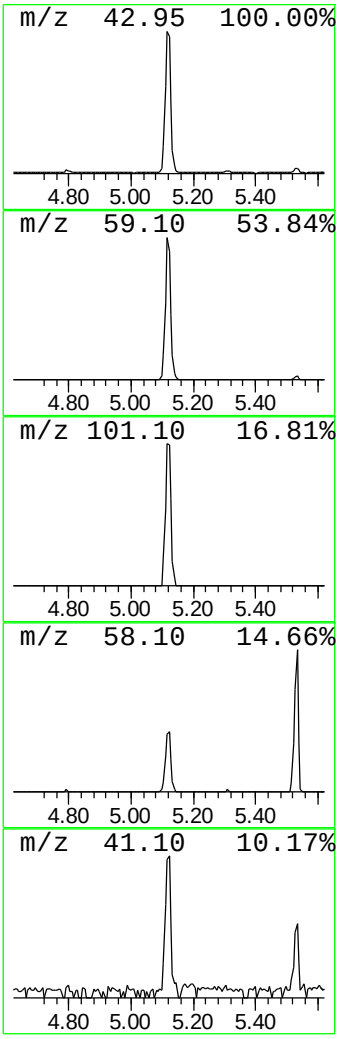
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	3.92 ng	196014	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122618\
Data File : BF111714.D
Acq On : 26 Dec 2018 14:23
Operator : JU/SJ
Sample : J6498-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1218-S-AB-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

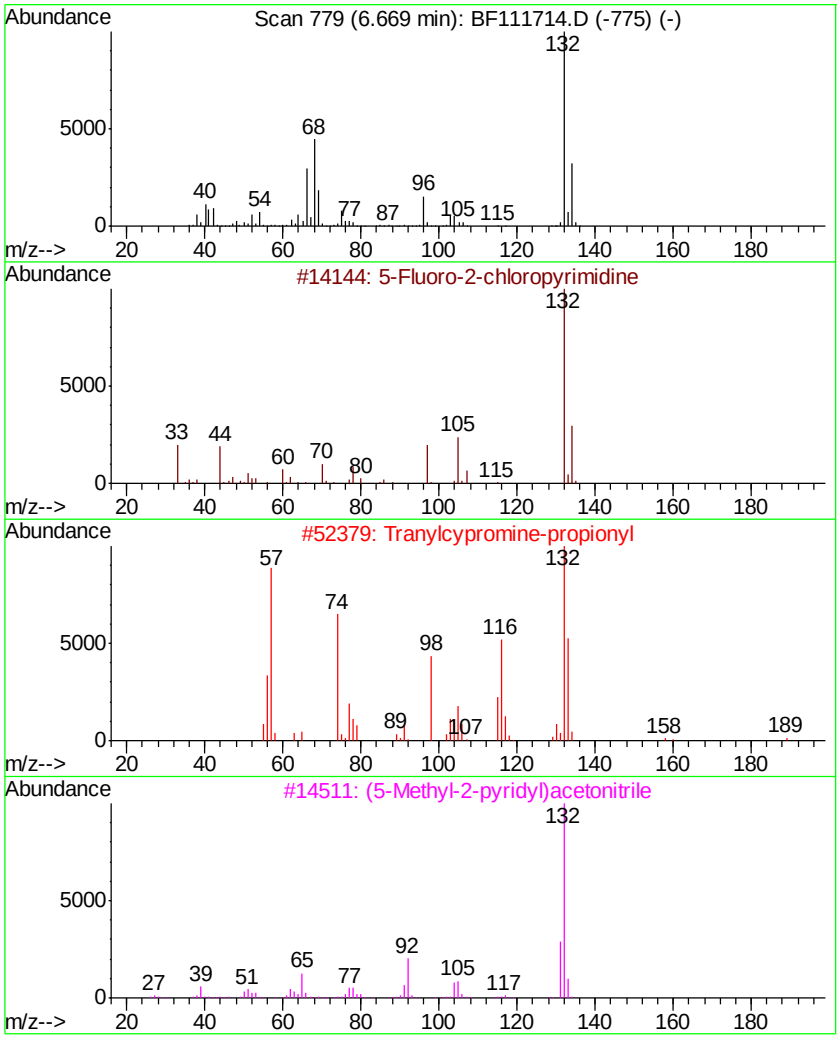
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

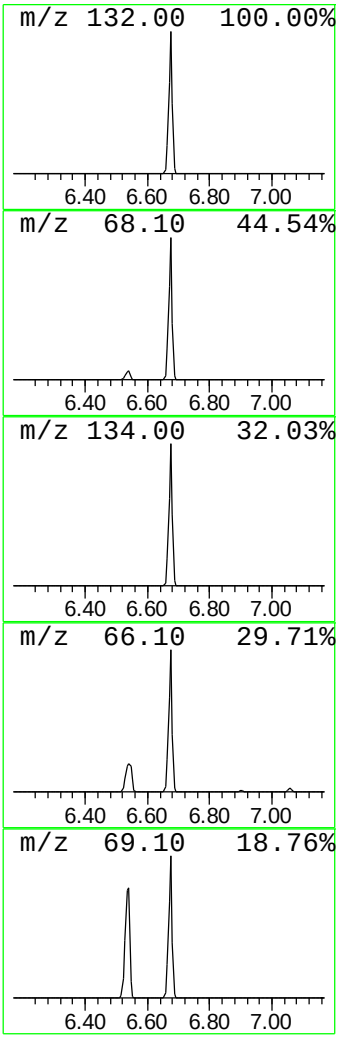
****

Peak Number 3 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	63.48 ng	3178080	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122618\
Data File : BF111714.D
Acq On : 26 Dec 2018 14:23
Operator : JU/SJ
Sample : J6498-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1218-S-AB-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

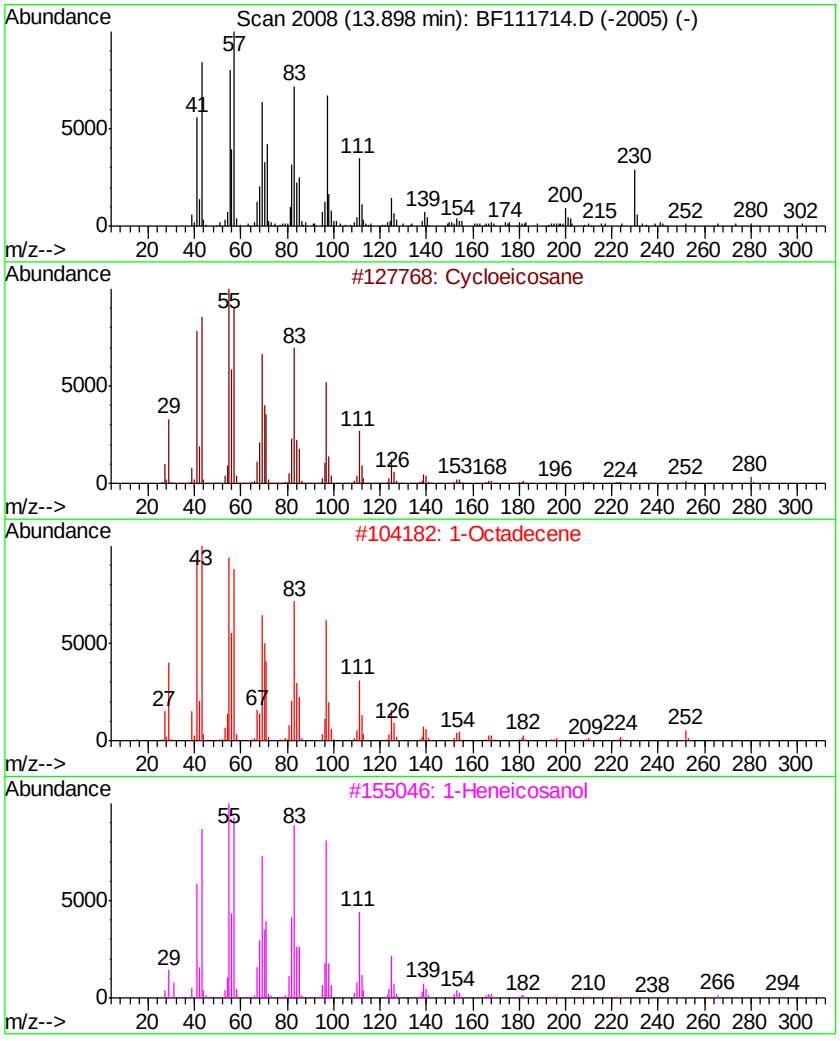
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

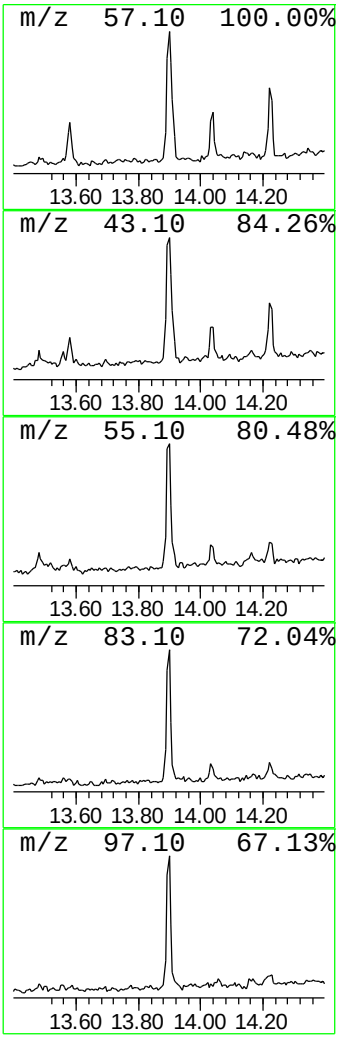
****

Peak Number 5 Cycloeicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	4.46 ng	367711	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloeicosane	280	C20H40	000296-56-0	98
2	1-Octadecene	252	C18H36	000112-88-9	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	93
5	Behenic alcohol	326	C22H46O	000661-19-8	93





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122618\
Data File : BF111714.D
Acq On : 26 Dec 2018 14:23
Operator : JU/SJ
Sample : J6498-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1218-S-AB-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

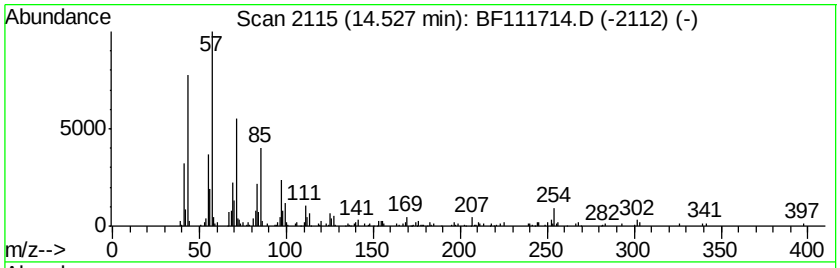
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

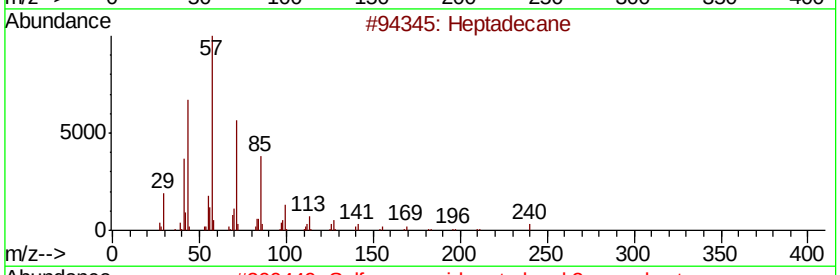
****

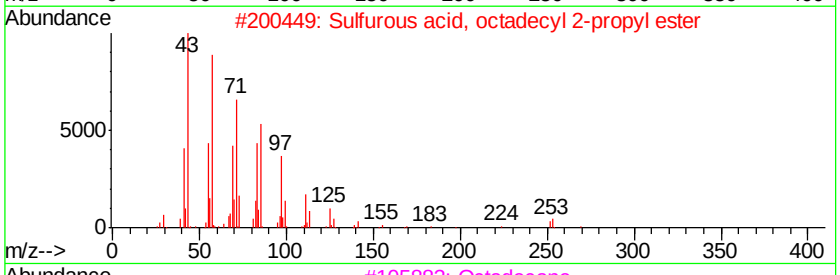
Peak Number 6 Sulfurous acid, octadecyl 2... Concentration Rank 7

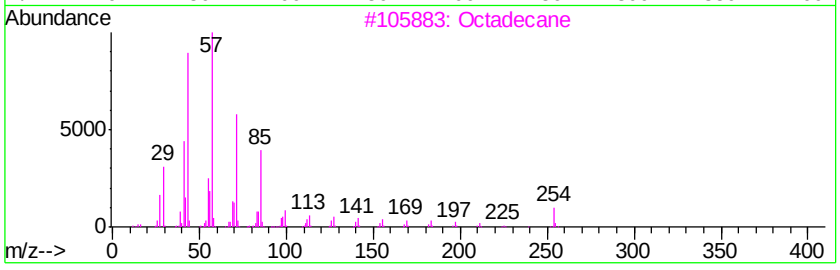
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	2.34 ng	192977	Chrysene-d12	14.06

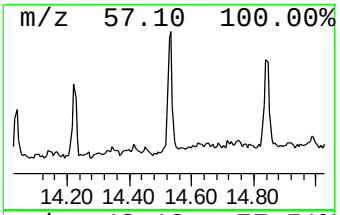
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	92
2	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	87
3	Octadecane	254	C18H38	000593-45-3	86
4	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	81
5	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	74

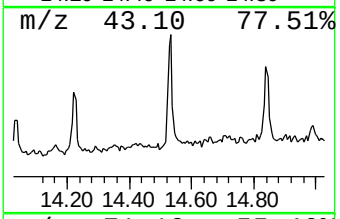


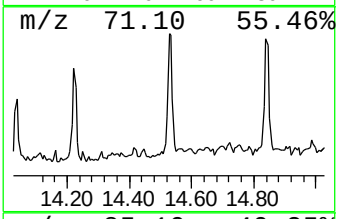


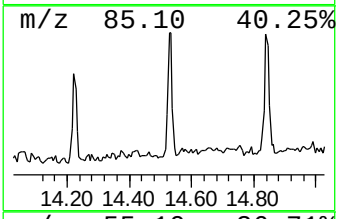


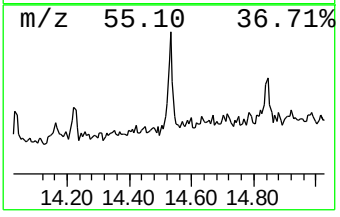












Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122618\
Data File : BF111714.D
Acq On : 26 Dec 2018 14:23
Operator : JU/SJ
Sample : J6498-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1218-S-AB-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

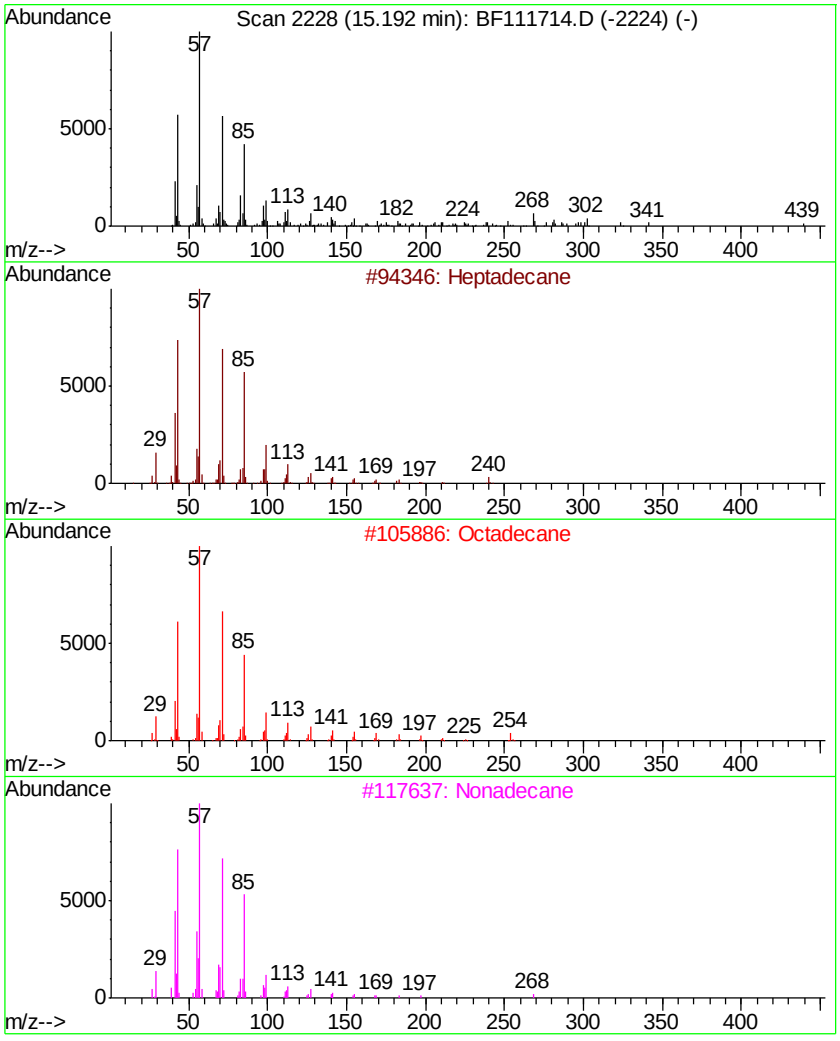
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

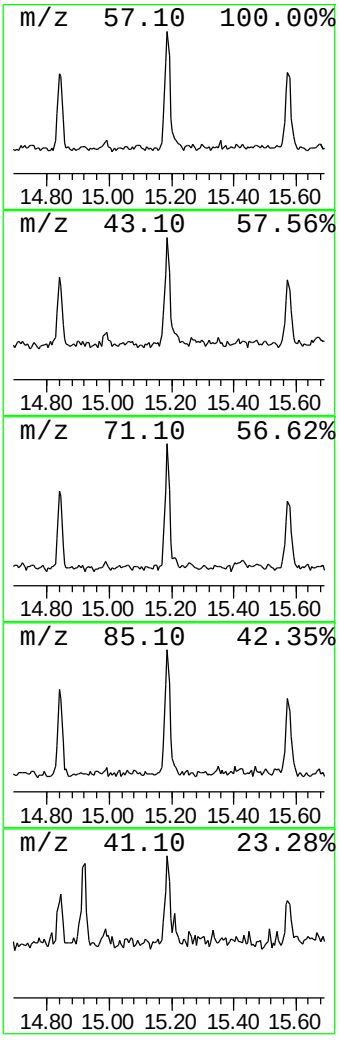
****

Peak Number 7 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.19	2.58 ng	155924	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	94
2	Octadecane	254	C18H38	000593-45-3	94
3	Nonadecane	268	C19H40	000629-92-5	94
4	Hexacosane	366	C26H54	000630-01-3	90
5	Octacosane	394	C28H58	000630-02-4	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122618\
Data File : BF111714.D
Acq On : 26 Dec 2018 14:23
Operator : JU/SJ
Sample : J6498-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1218-S-AB-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

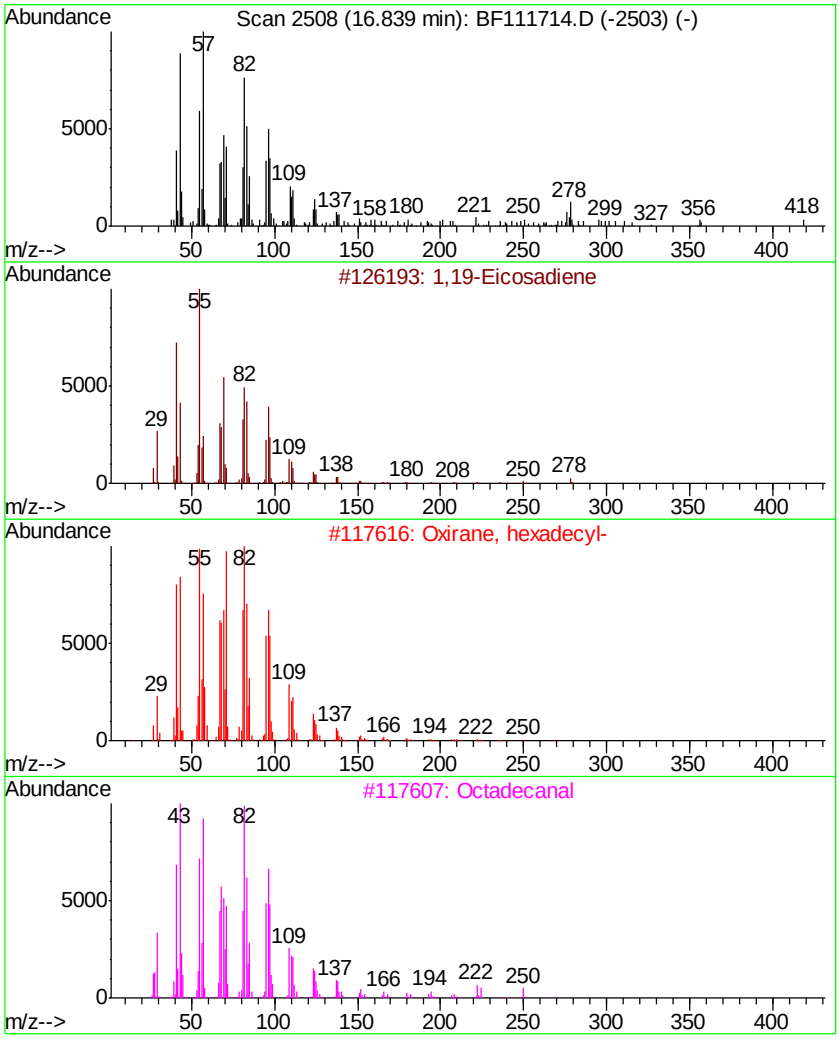
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

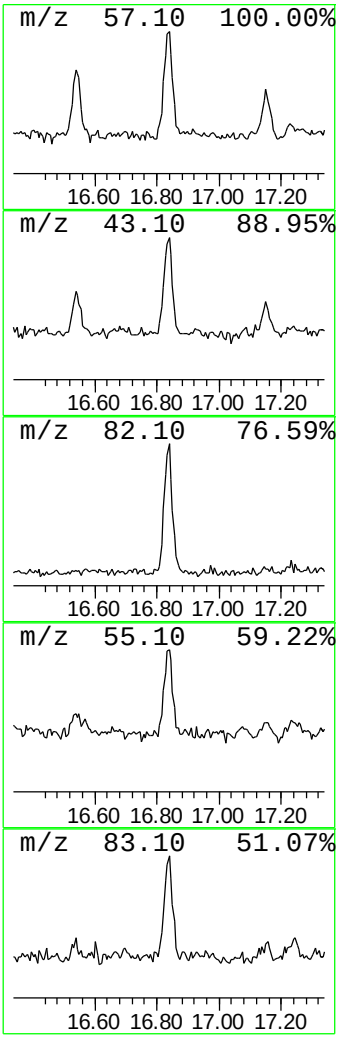
****

Peak Number 8 1,19-Eicosadiene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.84	5.24 ng	316198	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	93
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3	Octadecanal	268	C18H36O	000638-66-4	90
4	Tetradecanal	212	C14H28O	000124-25-4	90
5	(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	89





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF122618\
Data File : BF111714.D
Acq On : 26 Dec 2018 14:23
Operator : JU/SJ
Sample : J6498-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1218-S-AB-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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...	2.20	2.1	ng	106550	1	6.90	1001340	20.0
2-Pentanone, 4-hy...	5.12	3.9	ng	196014	1	6.90	1001340	20.0
unknown6.67	6.67	63.5	ng	3178080	1	6.90	1001340	20.0
Cycloeicosane	13.90	4.5	ng	367711	5	14.06	1648530	20.0
Sulfurous acid, o...	14.53	2.3	ng	192977	5	14.06	1648530	20.0
Heptadecane	15.19	2.6	ng	155924	6	15.54	1206530	20.0
1,19-Eicosadiene	16.84	5.2	ng	316198	6	15.54	1206530	20.0