LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010318\
Data File : BF101859.D
Acq On : 3 Jan 2018 14:56
Operator : SJ/JU
Sample : I6680-23 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-122917-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:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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	4.998	492	495	509	rBV	33920	81102	6.50%	0.527%
2	5.398	560	563	592	rBV	529813	1247775	100.00%	8.105%
3	6.422	734	737	755	rBV	594275	1216933	97.53%	7.905%
4	6.545	755	758	764	rVV	992200	1184521	94.93%	7.694%
5	6.769	793	796	809	rBV	671535	745867	59.78%	4.845%
6	6.922	819	822	837	rBV	840297	1001439	80.26%	6.505%
7	7.345	891	894	918	rBV	388482	787139	63.08%	5.113%
8	8.051	1011	1014	1030	rBV	718104	880616	70.57%	5.720%
9	8.628	1108	1112	1121	rBV	38479	48661	3.90%	0.316%
10	9.122	1193	1196	1204	rBV	1368082	1225121	98.18%	7.958%
11	9.186	1204	1207	1211	rVB	24249	24605	1.97%	0.160%
12	9.504	1257	1261	1263	rBV3	14308	16249	1.30%	0.106%
13	9.528	1263	1265	1269	rVB	83159	71797	5.75%	0.466%
14	9.610	1274	1279	1283	rBV5	9519	15213	1.22%	0.099%
15	9.681	1288	1291	1295	rBV	26871	30033	2.41%	0.195%
16	9.716	1295	1297	1301	rVB	29960	24216	1.94%	0.157%
17	9.804	1308	1312	1326	rVB	823452	768604	61.60%	4.992%
18	10.128	1361	1367	1371	rBV8	6996	16622	1.33%	0.108%
19	10.216	1379	1382	1385	rBV2	34325	27265	2.19%	0.177%
20	10.339	1400	1403	1406	rBV4	12607	14795	1.19%	0.096%
21	10.375	1406	1409	1413	rVB3	11892	15846	1.27%	0.103%
22	10.433	1414	1419	1422	rBV2	17232	22588	1.81%	0.147%
23	10.522	1431	1434	1438	rBV	89694	82157	6.58%	0.534%
24	10.604	1445	1448	1459	rBV	425481	532493	42.68%	3.459%
25	10.686	1459	1462	1467	rVB2	33459	40981	3.28%	0.266%
26	10.910	1493	1500	1503	rBV8	6951	13443	1.08%	0.087%
27	11.133	1535	1538	1540	rBV	26381	23283	1.87%	0.151%
28	11.163	1540	1543	1545	rVB	18261	17273	1.38%	0.112%
29	11.298	1562	1566	1570	rBV	712803	708173	56.75%	4.600%
30	11.392	1579	1582	1589	rVB	19993	28146	2.26%	0.183%
31	11.563	1607	1611	1613	rBV2	23046	22734	1.82%	0.148%
32	11.663	1626	1628	1633	rVB	22762	21042	1.69%	0.137%
33	11.739	1638	1641	1644	rVB5	13565	16337	1.31%	0.106%
34	11.810	1649	1653	1656	rBV2	139751	159255	12.76%	1.034%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010318\
Data File : BF101859.D
Acq On : 3 Jan 2018 14:56
Operator : SJ/JU
Sample : I6680-23 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-122917-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:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.839	1656	1658	1664	rVB	35576	44946	3.60%	0.292%
36	11.922	1669	1672	1674	rVV2	35427	41258	3.31%	0.268%
37	11.963	1678	1679	1682	rVB	21715	18229	1.46%	0.118%
38	12.145	1707	1710	1713	rVB5	14469	15573	1.25%	0.101%
39	12.280	1730	1733	1736	rBV2	17151	17774	1.42%	0.115%
40	12.351	1742	1745	1750	rBV3	101451	136752	10.96%	0.888%
41	12.522	1770	1774	1780	rBV	153382	171011	13.71%	1.111%
42	12.592	1782	1786	1791	rBV2	101594	137352	11.01%	0.892%
43	12.669	1797	1799	1801	rBV2	20318	20970	1.68%	0.136%
44	12.733	1806	1810	1811	rBV3	46485	53633	4.30%	0.348%
45	12.751	1811	1813	1817	rVB	165103	158743	12.72%	1.031%
46	12.874	1830	1834	1838	rBV	1083140	972832	77.97%	6.319%
47	13.080	1867	1869	1873	rVB2	48714	48513	3.89%	0.315%
48	13.286	1901	1904	1907	rBV4	36293	60436	4.84%	0.393%
49	13.421	1925	1927	1931	rBV	42799	35422	2.84%	0.230%
50	13.751	1980	1983	1987	rBV2	164955	169205	13.56%	1.099%
51	13.951	2012	2017	2020	rBV2	742370	927940	74.37%	6.027%
52	14.992	2191	2194	2198	rBV2	191751	250814	20.10%	1.629%
53	15.357	2254	2256	2261	rVB2	175392	212528	17.03%	1.380%
54	15.415	2262	2266	2273	rBV	574401	769157	61.64%	4.996%

Sum of corrected areas: 15395412

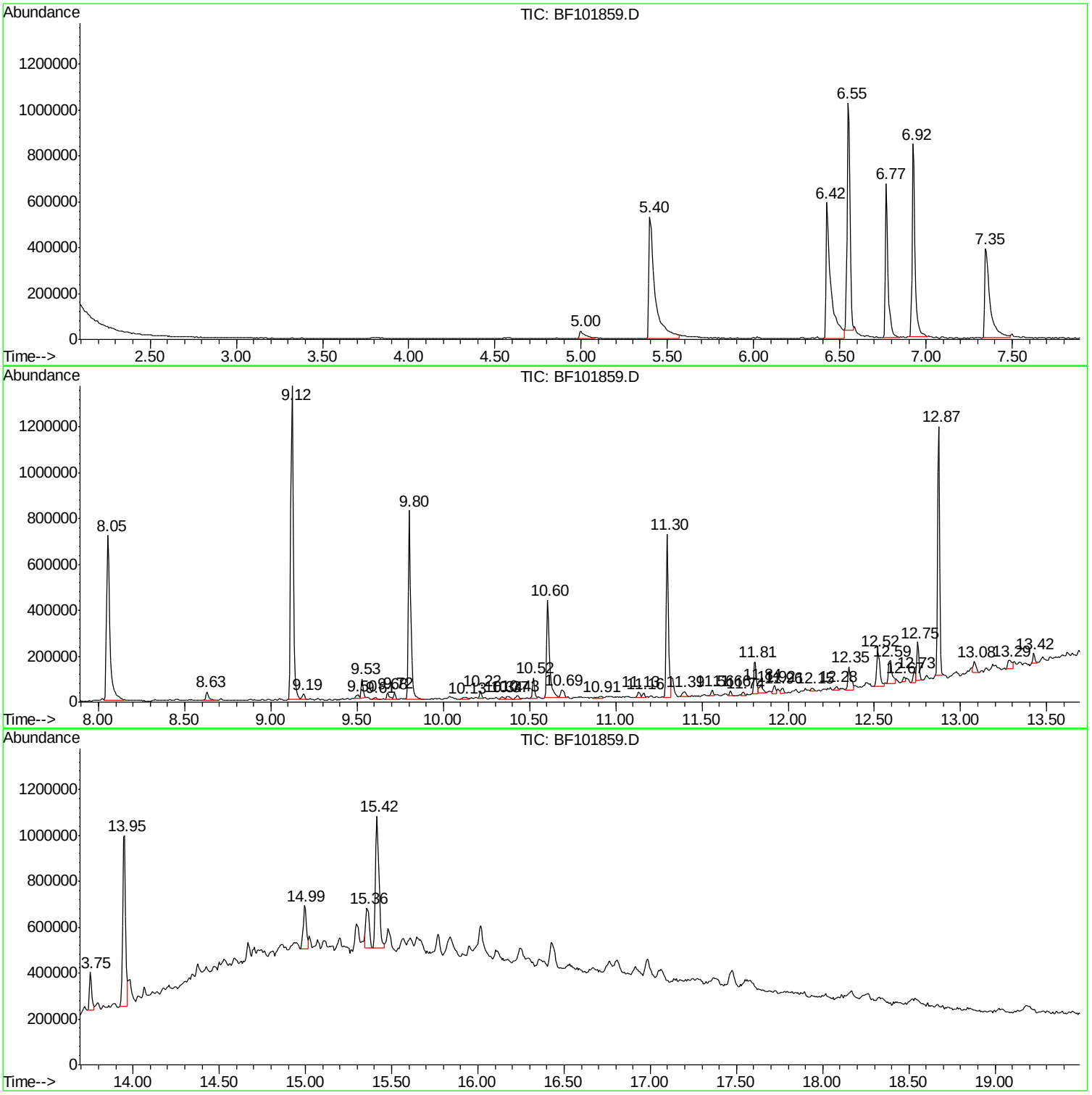
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010318\
Data File : BF101859.D
Acq On : 3 Jan 2018 14:56
Operator : SJ/JU
Sample : I6680-23 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-122917-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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\BF010318\
Data File : BF101859.D
Acq On : 3 Jan 2018 14:56
Operator : SJ/JU
Sample : I6680-23 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-122917-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

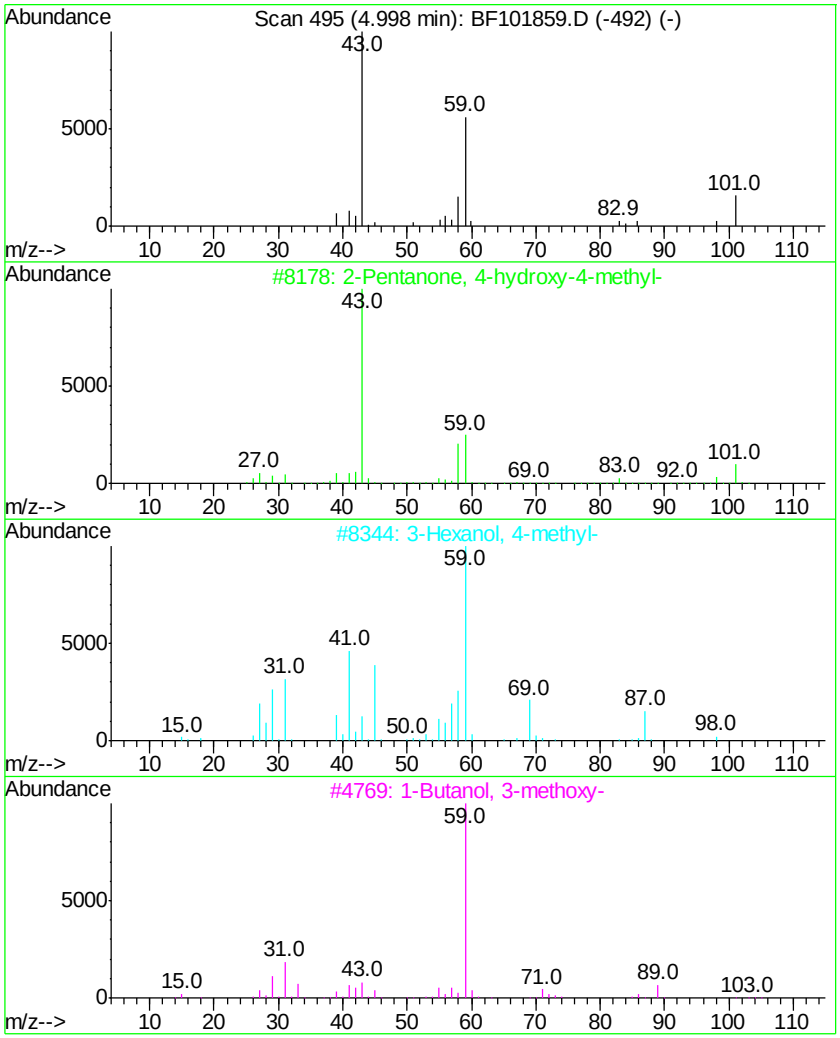
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

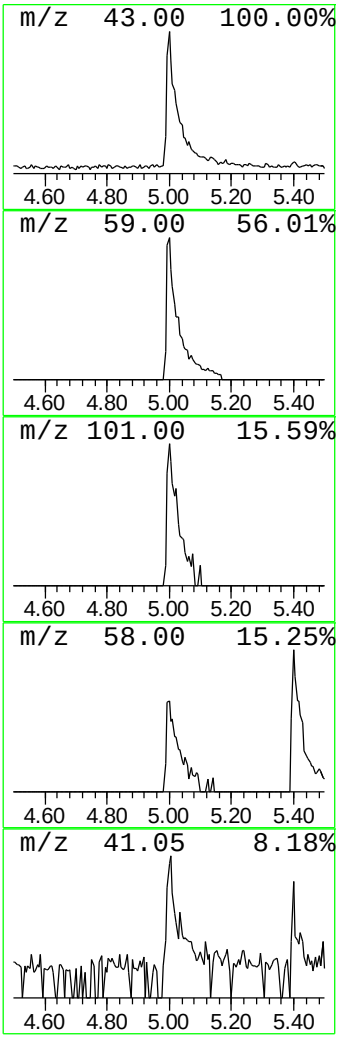
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	2.17 ng	81102	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	17
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	9
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010318\
Data File : BF101859.D
Acq On : 3 Jan 2018 14:56
Operator : SJ/JU
Sample : I6680-23 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-122917-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

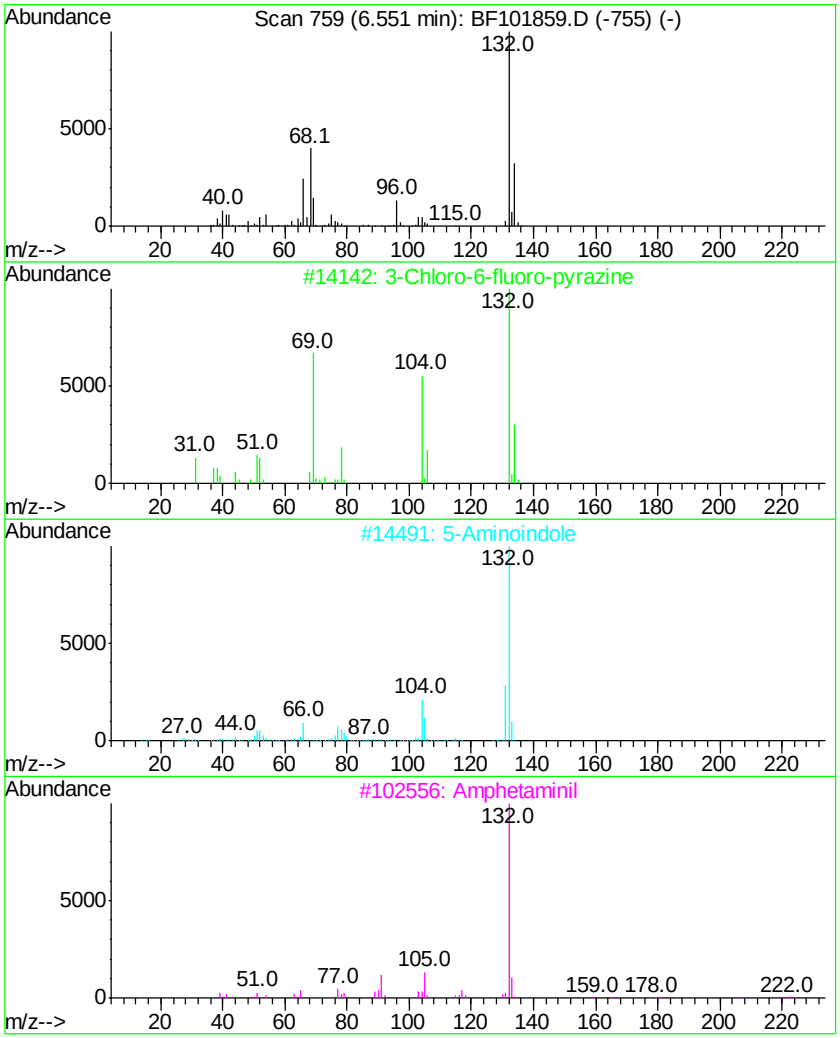
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

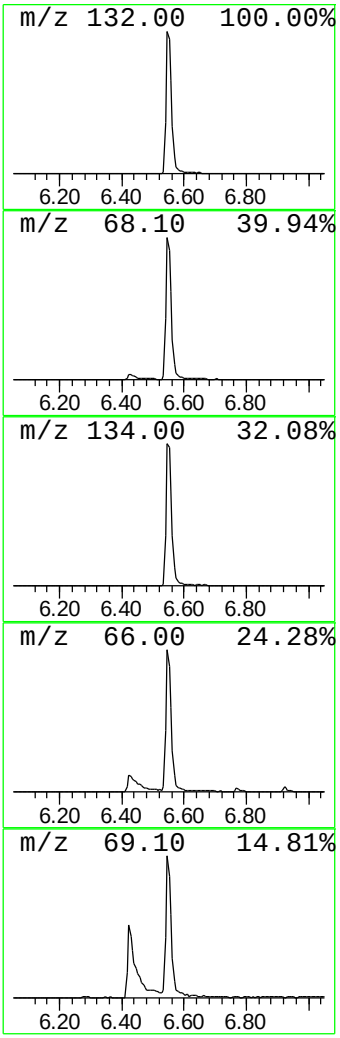
****

Peak Number 2 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	31.76 ng	1184520	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Amphetaminil	250	C17H18N2	017590-01-1	10
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010318\
Data File : BF101859.D
Acq On : 3 Jan 2018 14:56
Operator : SJ/JU
Sample : I6680-23 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-122917-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

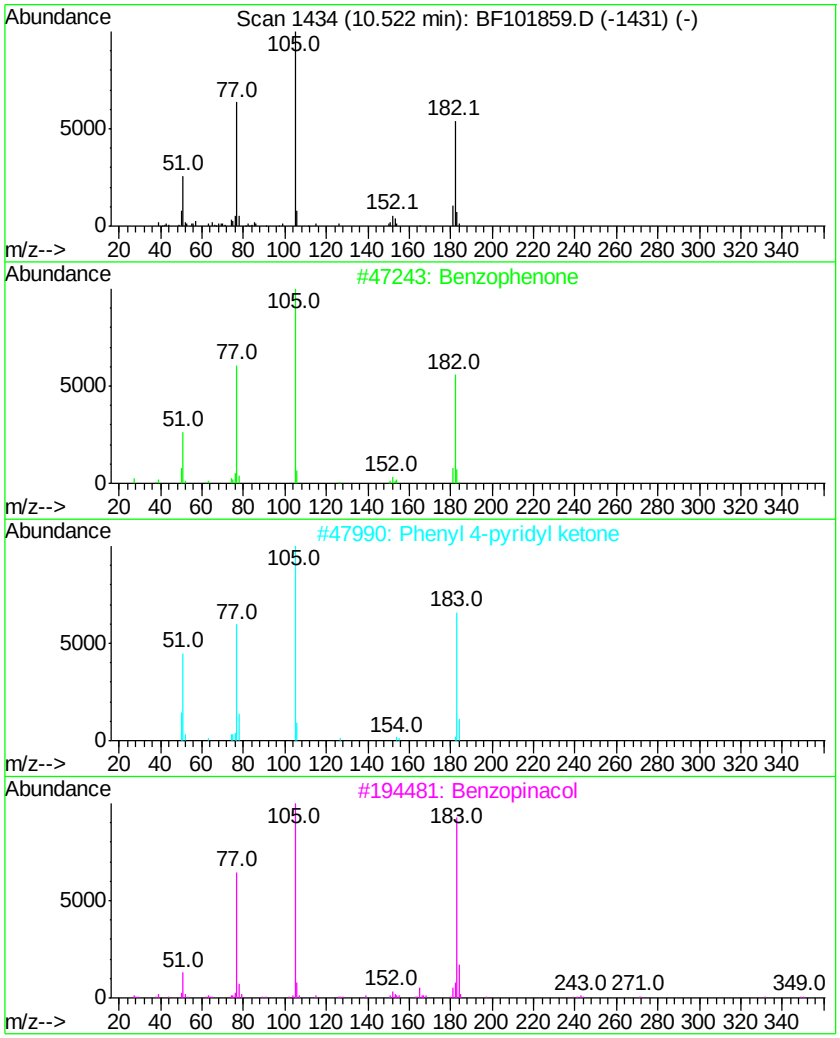
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

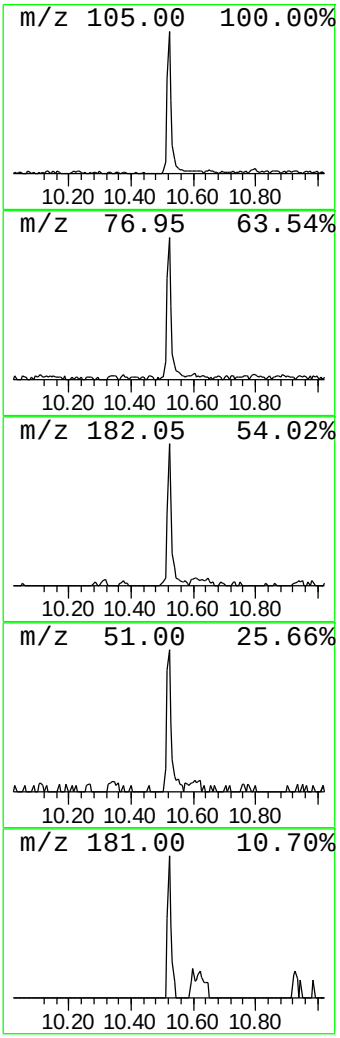
****

Peak Number 4 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.52	2.14 ng	82157	Acenaphthene-d10	9.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	53
3	Benzopinacol	366	C26H22O2	000464-72-2	50
4	Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	47
5	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	43





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010318\
Data File : BF101859.D
Acq On : 3 Jan 2018 14:56
Operator : SJ/JU
Sample : I6680-23 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-122917-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

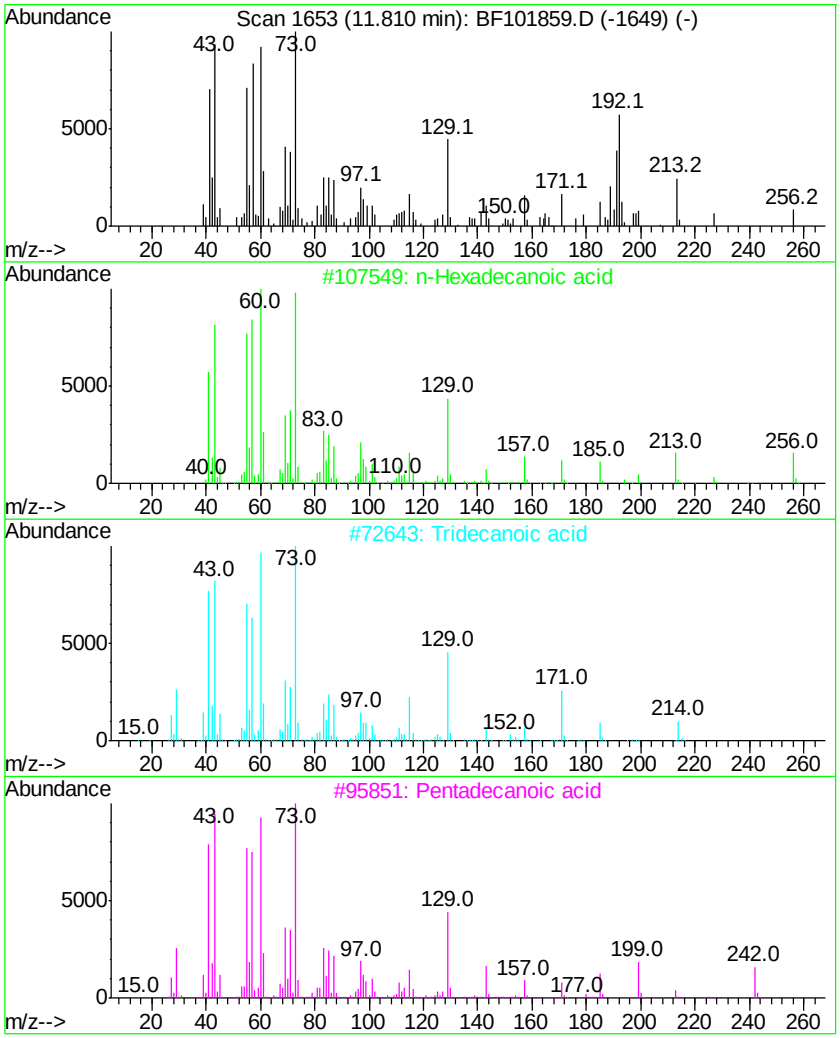
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

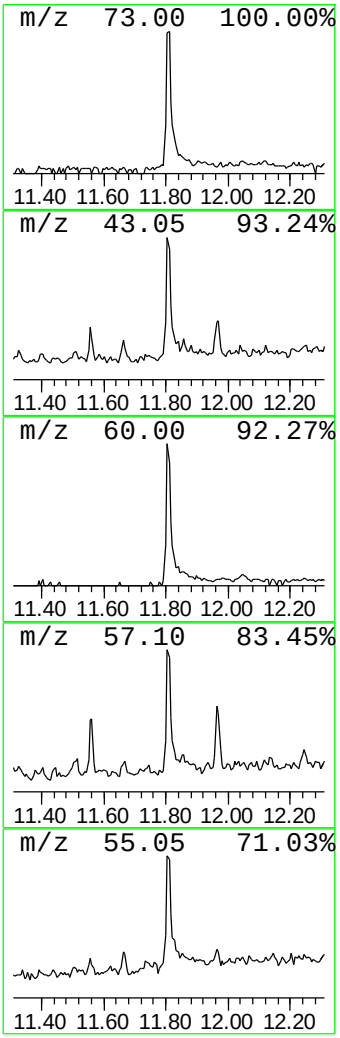
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.81	4.50 ng	159255	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
2	Tridecanoic acid	214	C13H26O2	000638-53-9	78
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	60
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	53
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	53





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010318\
Data File : BF101859.D
Acq On : 3 Jan 2018 14:56
Operator : SJ/JU
Sample : I6680-23 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-122917-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

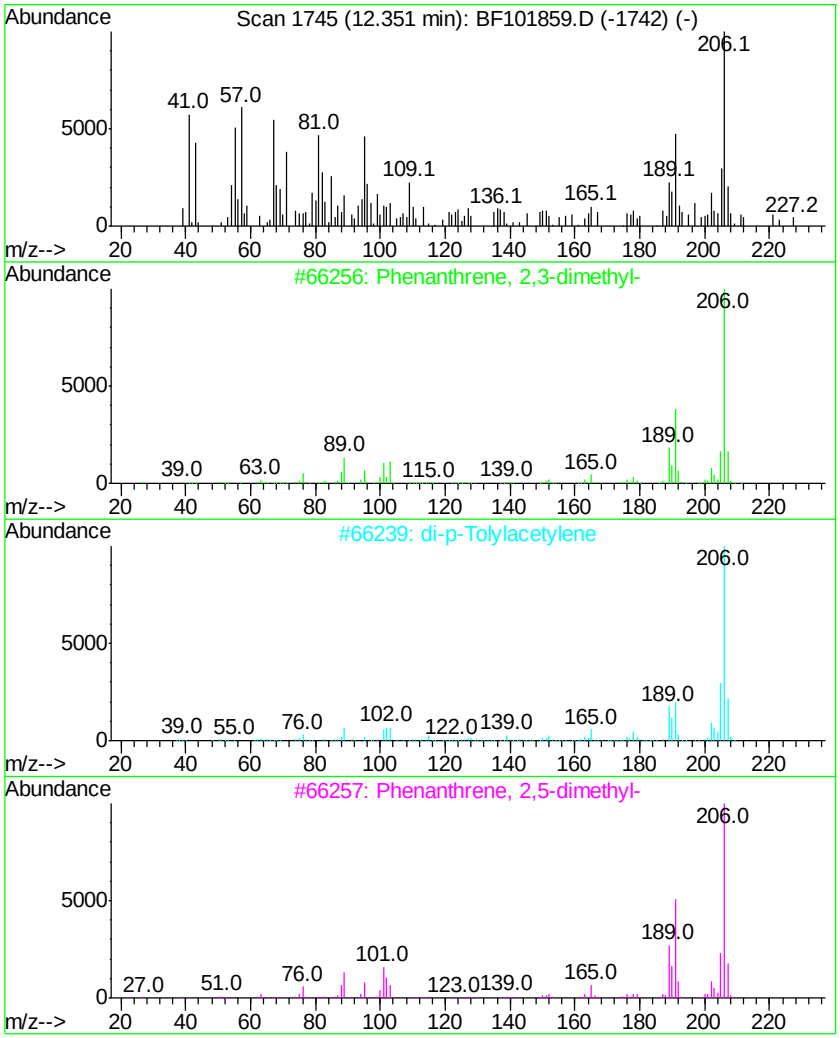
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

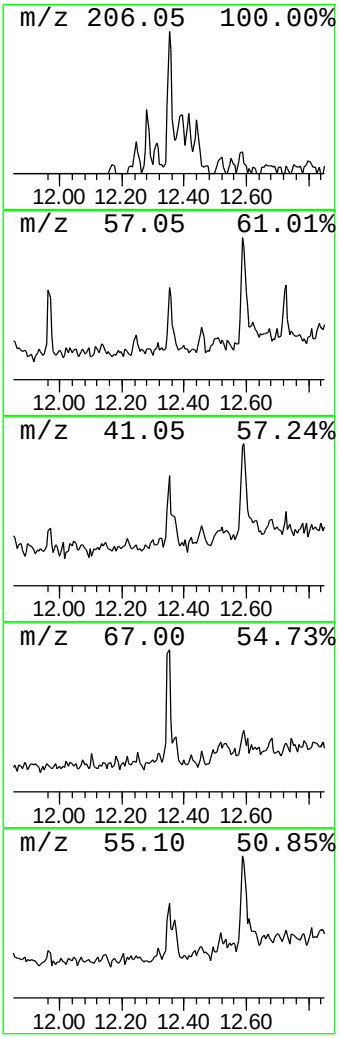
****

Peak Number 6 Phenanthrene, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.35	3.86 ng	136752	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	91
2	di-p-Tolylacetylene	206	C16H14	002789-88-0	90
3	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	90
4	Phenanthrene, 2,7-dimethyl-	206	C16H14	001576-69-8	89
5	Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010318\
Data File : BF101859.D
Acq On : 3 Jan 2018 14:56
Operator : SJ/JU
Sample : I6680-23 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-122917-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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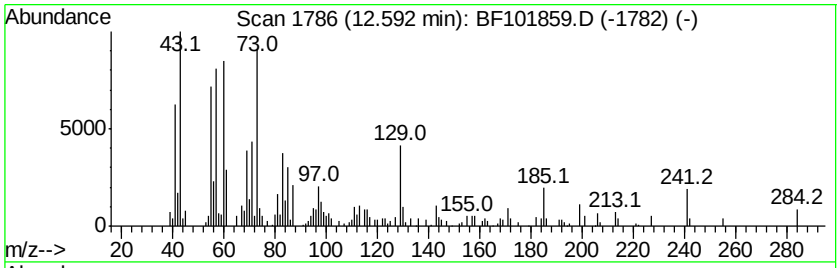
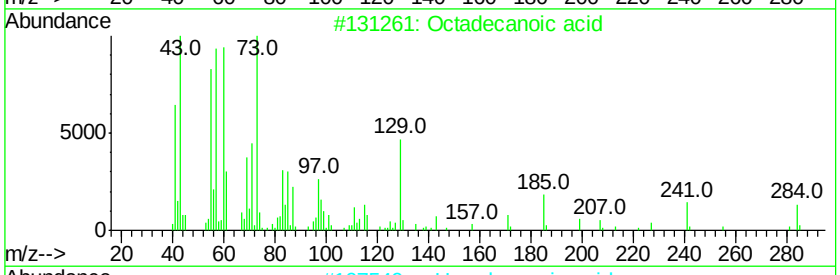
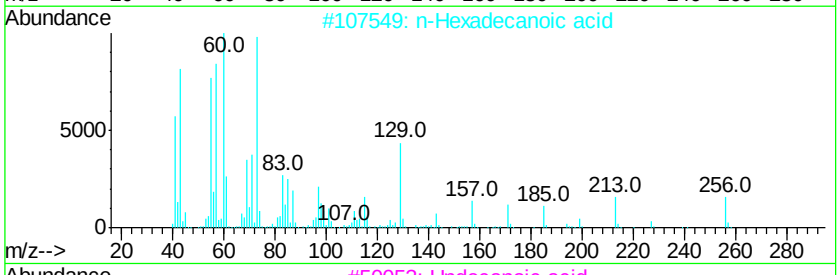
Peak Number 7 Octadecanoic acid Concentration Rank 4

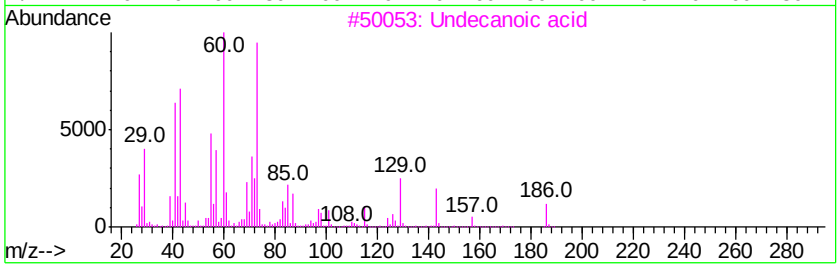
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.59	3.88 ng	137352	Phenanthrene-d10	11.30

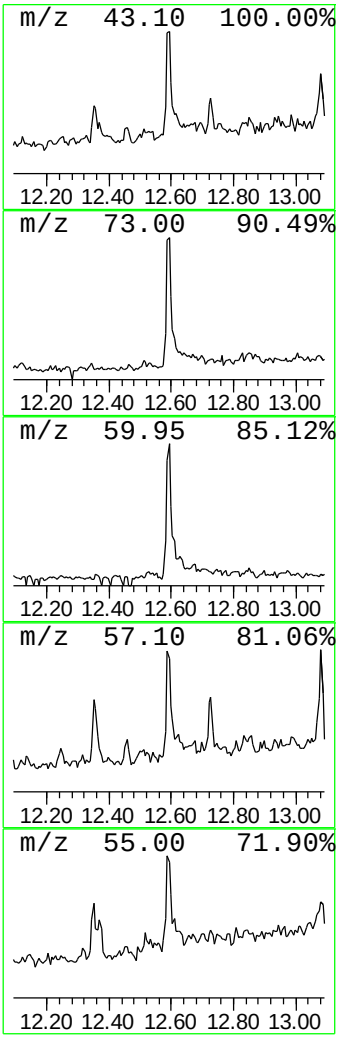
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3	Undecanoic acid	186	C11H22O2	000112-37-8	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64











Data Path : Z:\HPCHEM1\BNA F\DATA\BF010318\
Data File : BF101859.D
Acq On : 3 Jan 2018 14:56
Operator : SJ/JU
Sample : I6680-23 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-122917-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

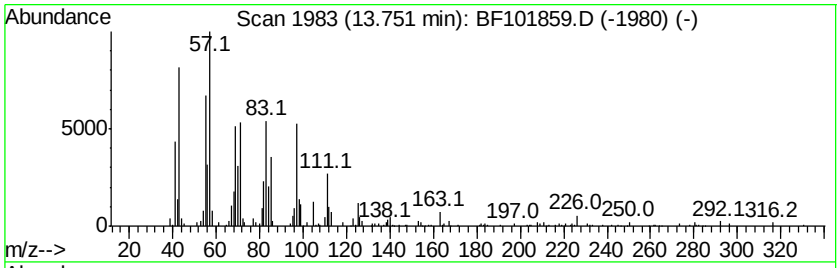
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

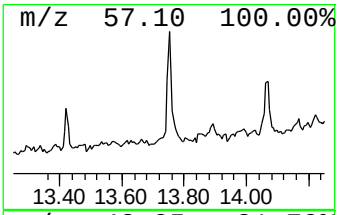
****

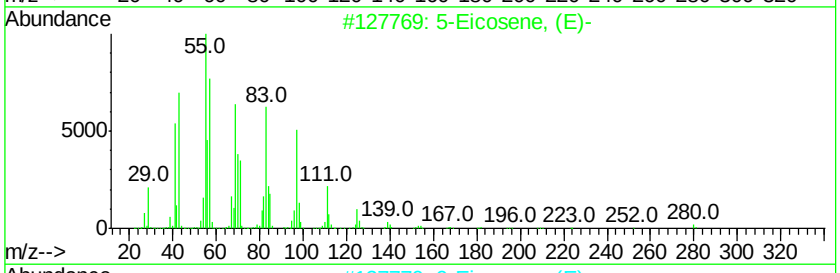
Peak Number 8 5-Eicosene, (E)- Concentration Rank 6

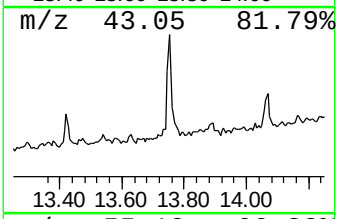
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	3.65 ng	169205	Chrysene-d12	13.95

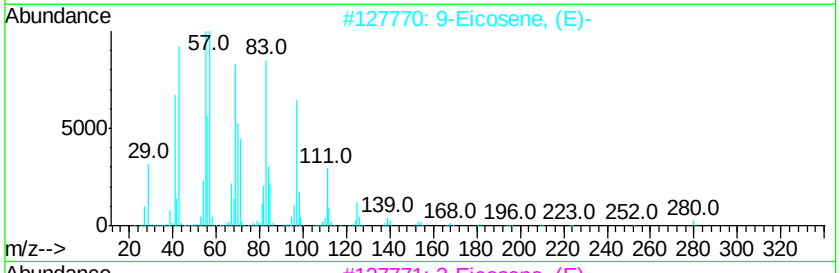
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	96
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	93
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	93
4	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	93
5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91

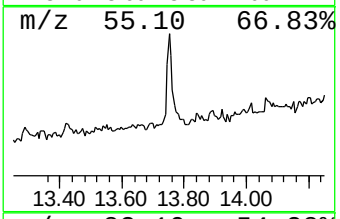


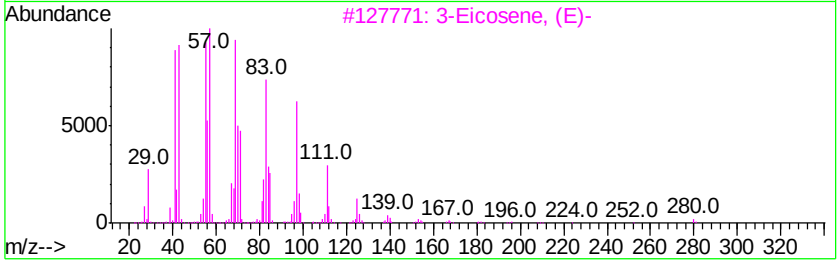


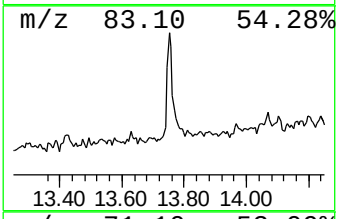


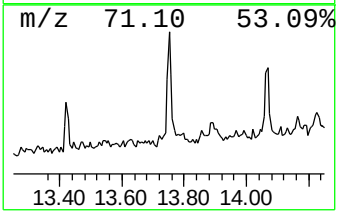












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010318\
Data File : BF101859.D
Acq On : 3 Jan 2018 14:56
Operator : SJ/JU
Sample : I6680-23 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-122917-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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...	5.00	2.2	ng	81102	1	6.77	745867	20.0
unknown6.55	6.55	31.8	ng	1184520	1	6.77	745867	20.0
Benzophenone	10.52	2.1	ng	82157	3	9.80	768604	20.0
n-Hexadecanoic acid	11.81	4.5	ng	159255	4	11.30	708173	20.0
Phenanthrene, 2,3...	12.35	3.9	ng	136752	4	11.30	708173	20.0
Octadecanoic acid	12.59	3.9	ng	137352	4	11.30	708173	20.0
5-Eicosene, (E)-	13.75	3.6	ng	169205	5	13.95	927940	20.0