LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041218\
Data File : BF104449.D
Acq On : 12 Apr 2018 14:28
Operator : JU/SJ
Sample : J2163-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-01-041118-D

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-BF040618.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	5.028	491	500	510	rBV	113232	155021	4.78%	0.450%
2	5.422	562	567	570	rBV	2676488	2989261	92.20%	8.671%
3	5.745	619	622	629	rVB	37452	36504	1.13%	0.106%
4	6.075	674	678	689	rVB	38089	61578	1.90%	0.179%
5	6.440	735	740	743	rBV	2543363	3018547	93.10%	8.756%
6	6.581	758	764	767	rBV	3048672	3081442	95.04%	8.939%
7	6.810	799	803	806	rBV	964014	851317	26.26%	2.469%
8	6.963	825	829	832	rBV	2610589	2388148	73.66%	6.927%
9	7.375	893	899	902	rBV	2013512	1946679	60.04%	5.647%
10	8.092	1015	1021	1024	rBV	1412316	1189567	36.69%	3.451%
11	9.169	1198	1204	1207	rBV	3573233	3242150	100.00%	9.405%
12	9.557	1267	1270	1274	rBV	270791	246413	7.60%	0.715%
13	9.704	1292	1295	1300	rBV	69819	68590	2.12%	0.199%
14	9.775	1304	1307	1310	rVB	99688	74759	2.31%	0.217%
15	9.845	1315	1319	1323	rVV	1317030	1258776	38.83%	3.651%
16	10.045	1349	1353	1358	rVB4	19571	37076	1.14%	0.108%
17	10.092	1358	1361	1365	rBV4	27682	34370	1.06%	0.100%
18	10.275	1389	1392	1395	rVB	152336	114607	3.53%	0.332%
19	10.498	1425	1430	1436	rBV2	45333	66186	2.04%	0.192%
20	10.639	1447	1454	1457	rBV	2112216	2001818	61.74%	5.807%
21	10.751	1470	1473	1482	rVB	139689	172553	5.32%	0.501%
22	11.198	1544	1549	1552	rBV	86389	79744	2.46%	0.231%
23	11.227	1552	1554	1560	rVB	42800	42963	1.33%	0.125%
24	11.339	1568	1573	1575	rBV	1197360	1166016	35.96%	3.382%
25	11.357	1575	1576	1579	rVV	177737	118942	3.67%	0.345%
26	11.410	1583	1585	1588	rVB	69126	51124	1.58%	0.148%
27	11.557	1605	1610	1617	rBV5	37927	87330	2.69%	0.253%
28	11.863	1659	1662	1667	rBV	296253	238412	7.35%	0.692%
29	11.951	1673	1677	1679	rBV	69489	71523	2.21%	0.207%
30	12.033	1685	1691	1694	rBV4	42117	62633	1.93%	0.182%
31	12.386	1747	1751	1753	rBV3	53631	69658	2.15%	0.202%
32	12.416	1753	1756	1758	rBV2	86218	93536	2.88%	0.271%
33	12.474	1763	1766	1771	rVB2	36079	37688	1.16%	0.109%
34	12.551	1775	1779	1782	rVV	608591	493910	15.23%	1.433%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041218\
Data File : BF104449.D
Acq On : 12 Apr 2018 14:28
Operator : JU/SJ
Sample : J2163-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-01-041118-D

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-BF040618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.645	1792	1795	1798	rBV2	77153	71693	2.21%	0.208%
36	12.780	1812	1818	1823	rBV	586137	613597	18.93%	1.780%
37	12.927	1838	1843	1846	rVB	2597060	2389313	73.70%	6.931%
38	12.998	1852	1855	1858	rVB2	36873	47629	1.47%	0.138%
39	13.086	1867	1870	1871	rBV2	38590	42464	1.31%	0.123%
40	13.110	1871	1874	1876	rVB	78301	71940	2.22%	0.209%
41	13.174	1883	1885	1887	rVB	62509	43268	1.33%	0.126%
42	13.210	1888	1891	1894	rBV2	69705	69262	2.14%	0.201%
43	13.333	1909	1912	1915	rBV	44381	45990	1.42%	0.133%
44	13.616	1957	1960	1964	rVB	47462	52483	1.62%	0.152%
45	13.727	1976	1979	1982	rBV2	48202	50430	1.56%	0.146%
46	13.757	1982	1984	1986	rBV	49257	35144	1.08%	0.102%
47	13.780	1986	1988	1991	rBV2	50973	54678	1.69%	0.159%
48	13.816	1991	1994	1998	rVV2	471662	461487	14.23%	1.339%
49	13.980	2016	2022	2025	rBV2	983593	1278137	39.42%	3.708%
50	14.010	2025	2027	2032	rVB	332297	297549	9.18%	0.863%
51	14.086	2038	2040	2043	rVB	78724	60501	1.87%	0.175%
52	14.374	2087	2089	2091	rVB	68201	52006	1.60%	0.151%
53	14.463	2102	2104	2108	rVB2	90419	93534	2.88%	0.271%
54	14.504	2108	2111	2112	rBV2	55993	52259	1.61%	0.152%
55	15.027	2196	2200	2203	rBV	431134	627471	19.35%	1.820%
56	15.133	2215	2218	2223	rVB	108471	105462	3.25%	0.306%
57	15.327	2248	2251	2257	rVB	247378	319469	9.85%	0.927%
58	15.392	2258	2262	2268	rVB	348144	434837	13.41%	1.261%
59	15.457	2268	2273	2276	rBV	593377	785336	24.22%	2.278%
60	15.962	2356	2359	2365	rVB4	81825	119812	3.70%	0.348%
61	16.904	2514	2519	2525	rVB2	160914	307208	9.48%	0.891%
62	17.351	2589	2595	2601	rBV	128828	241885	7.46%	0.702%

Sum of corrected areas: 34473685

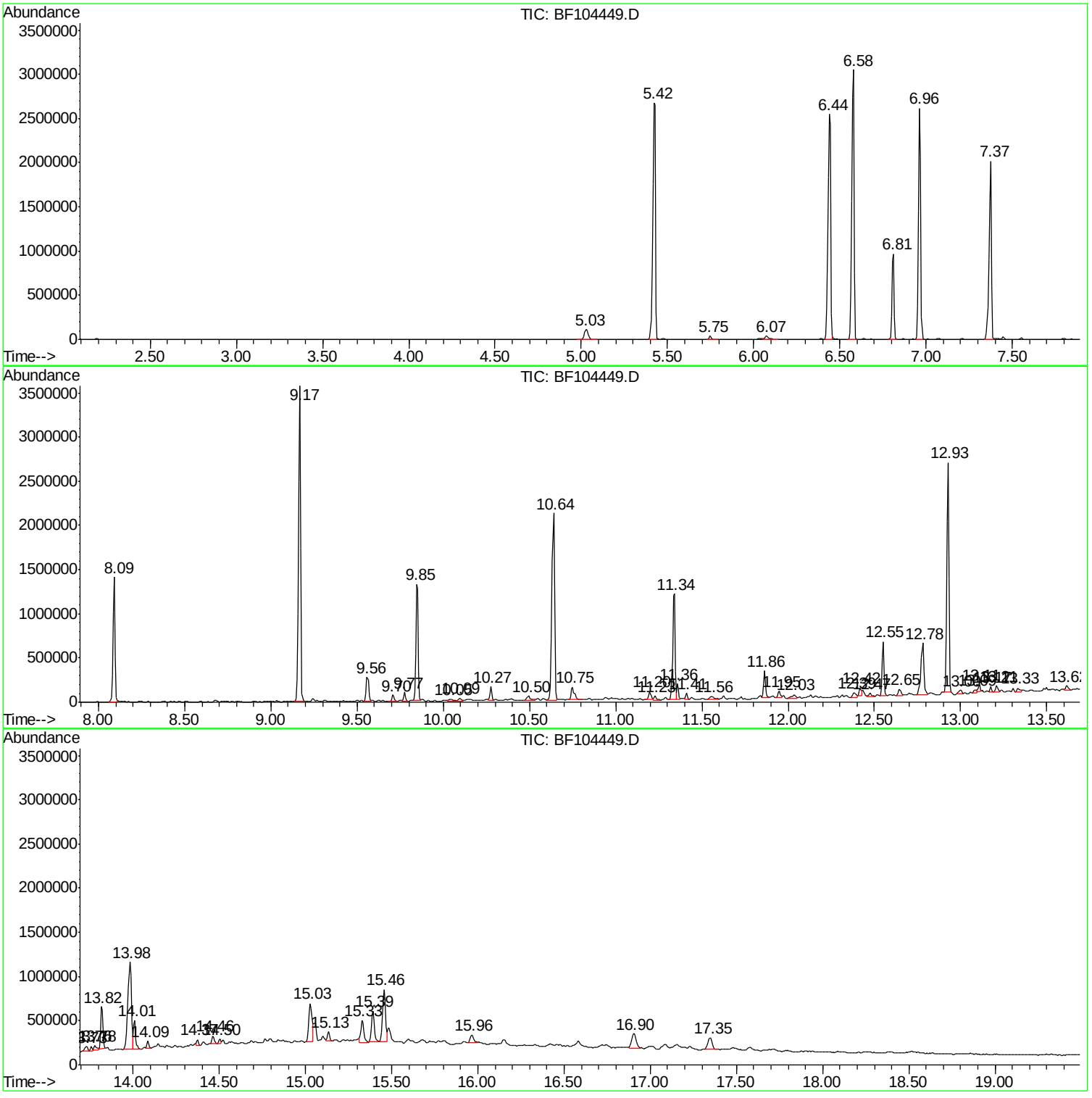
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041218\
Data File : BF104449.D
Acq On : 12 Apr 2018 14:28
Operator : JU/SJ
Sample : J2163-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-01-041118-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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\BF041218\
Data File : BF104449.D
Acq On : 12 Apr 2018 14:28
Operator : JU/SJ
Sample : J2163-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-01-041118-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

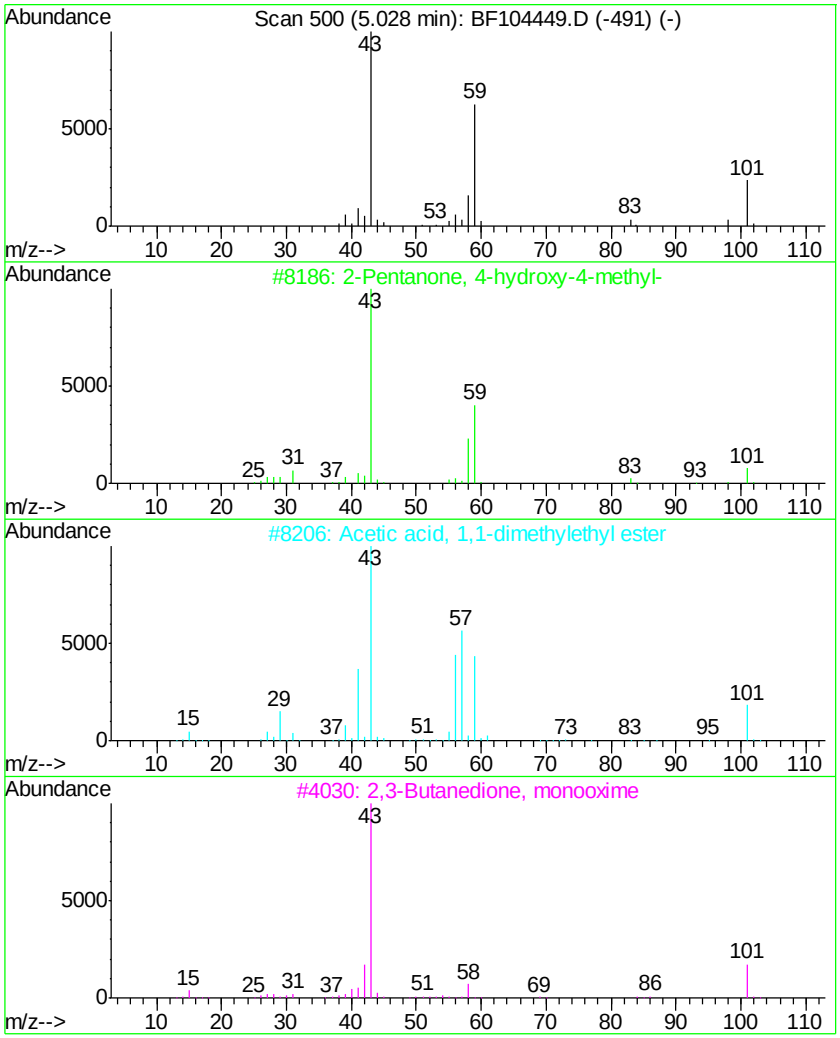
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

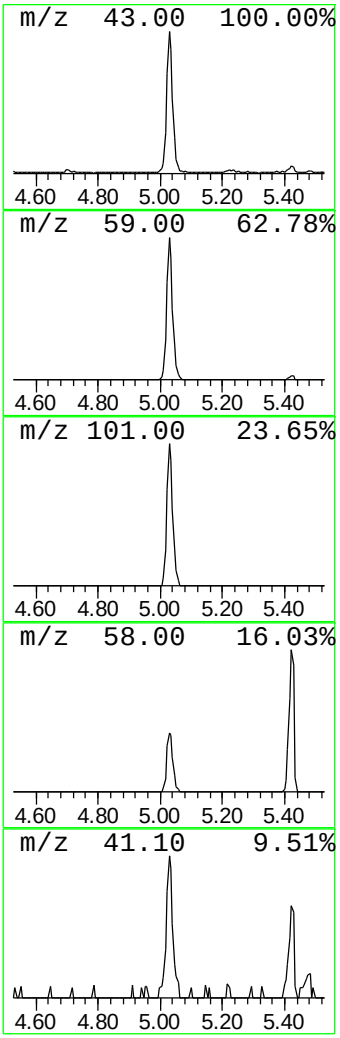
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	3.64 ng	155021	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041218\
Data File : BF104449.D
Acq On : 12 Apr 2018 14:28
Operator : JU/SJ
Sample : J2163-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-01-041118-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

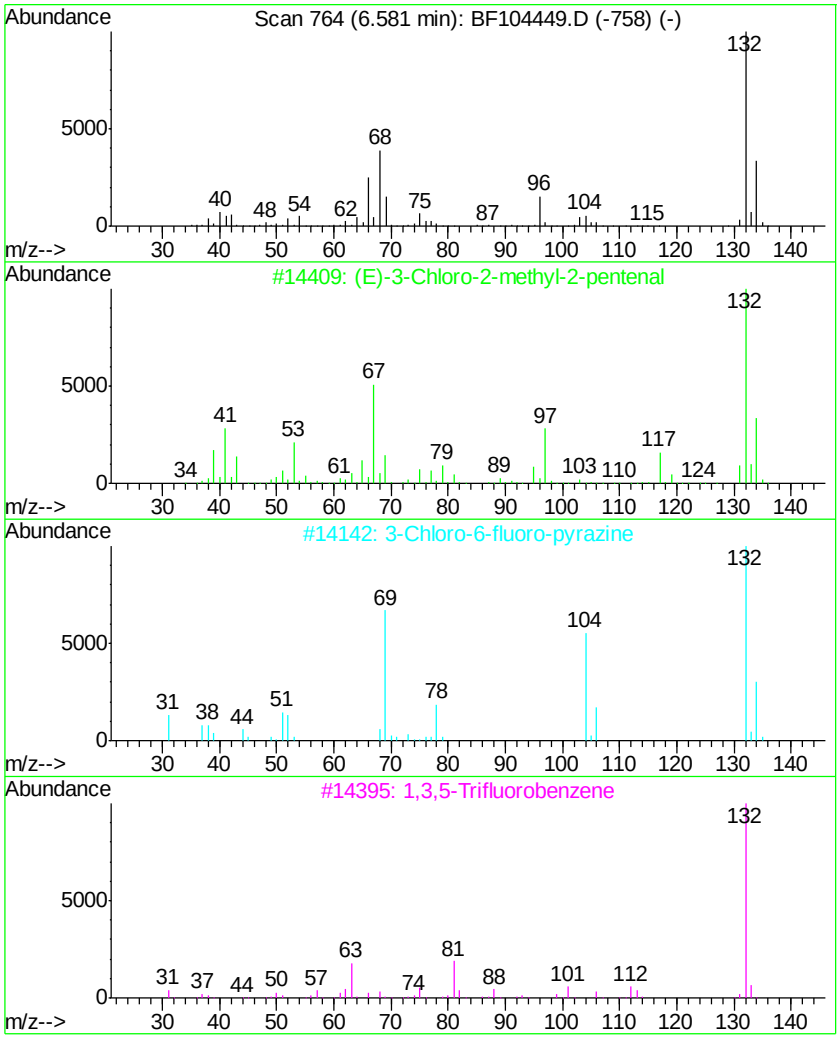
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

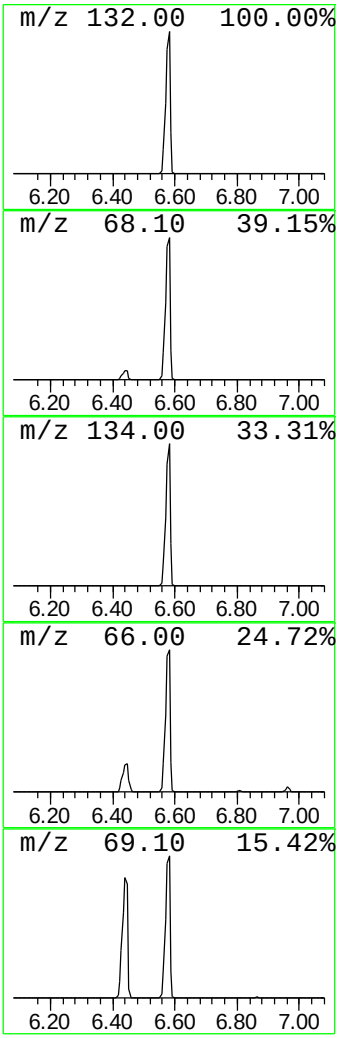
****

Peak Number 2 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	72.39 ng	3081440	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041218\
Data File : BF104449.D
Acq On : 12 Apr 2018 14:28
Operator : JU/SJ
Sample : J2163-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-01-041118-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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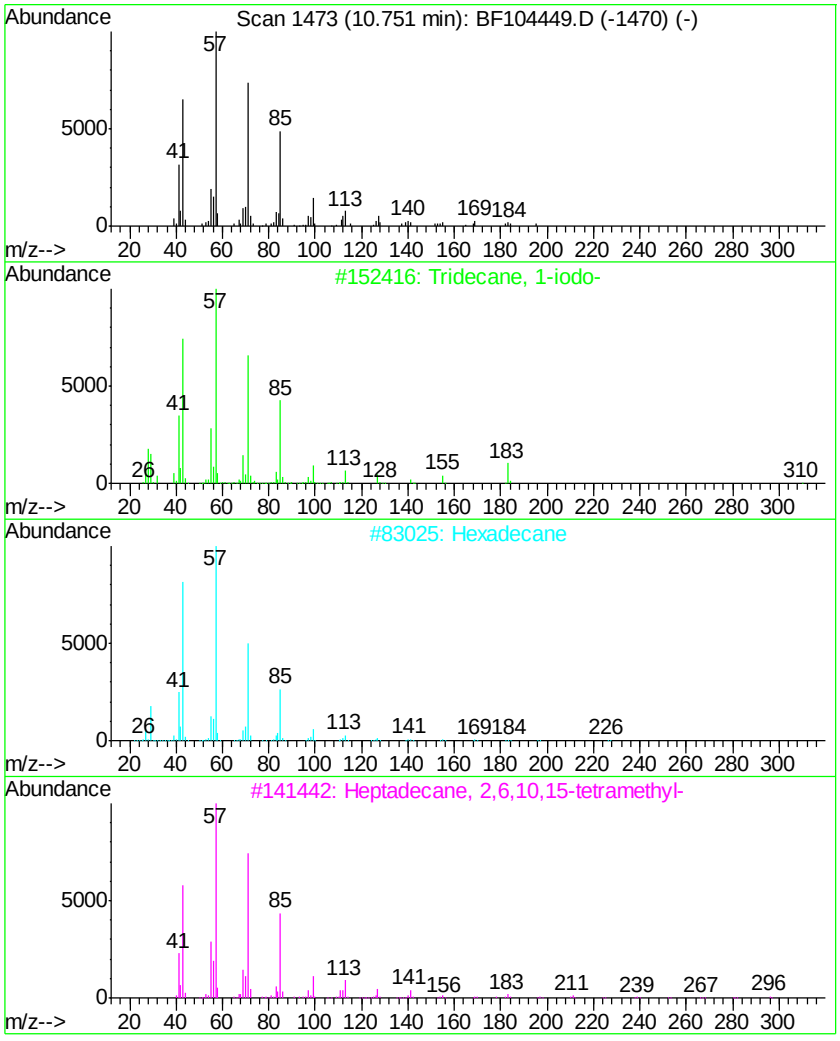
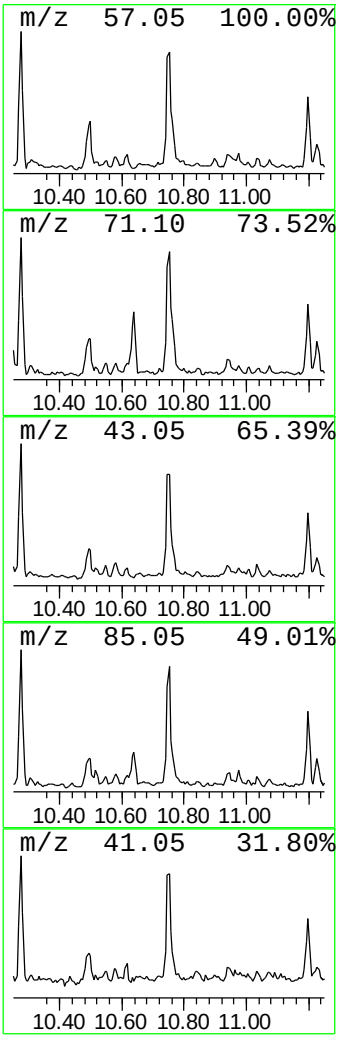
Peak Number 4 Tridecane, 1-iodo- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	2.96 ng	172553	Phenanthrene-d10	11.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	87
5	Octadecane	254	C18H38	000593-45-3	86





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041218\
Data File : BF104449.D
Acq On : 12 Apr 2018 14:28
Operator : JU/SJ
Sample : J2163-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-01-041118-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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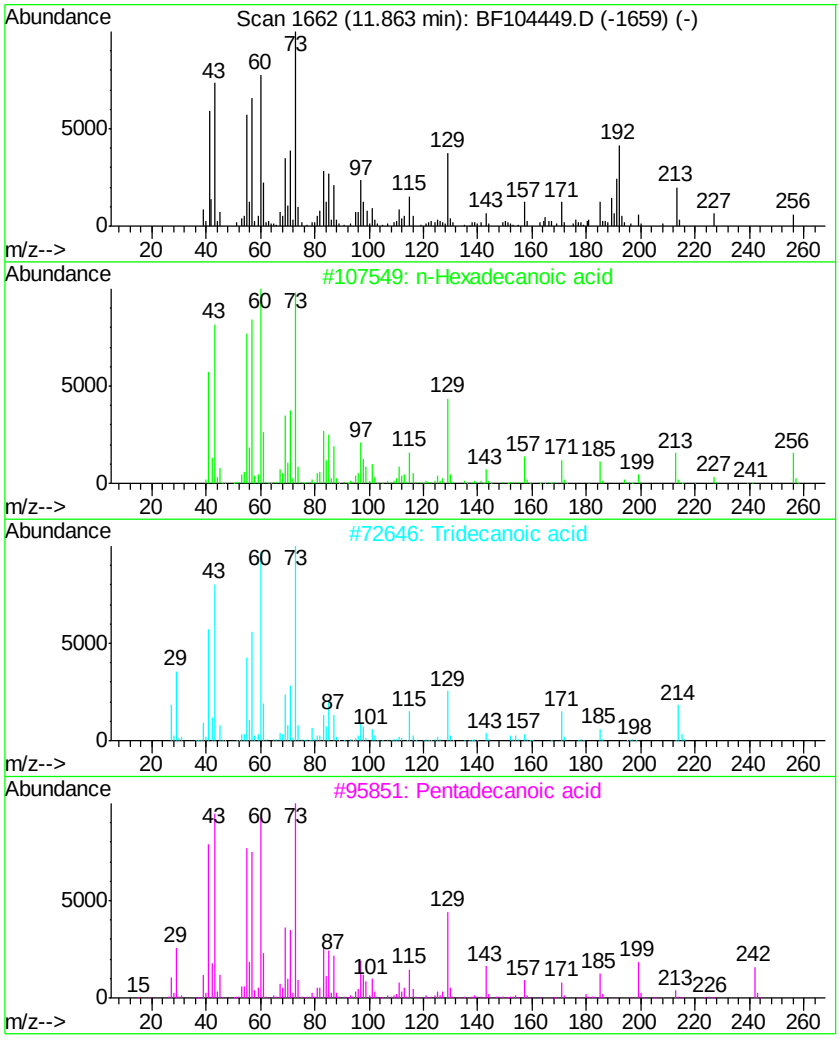
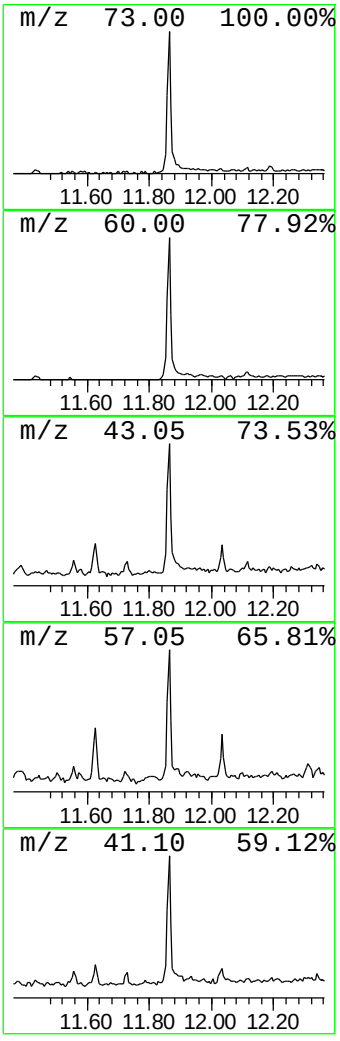
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	4.09 ng	238412	Phenanthrene-d10	11.34

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	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





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Data File : BF104449.D
Acq On : 12 Apr 2018 14:28
Operator : JU/SJ
Sample : J2163-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-01-041118-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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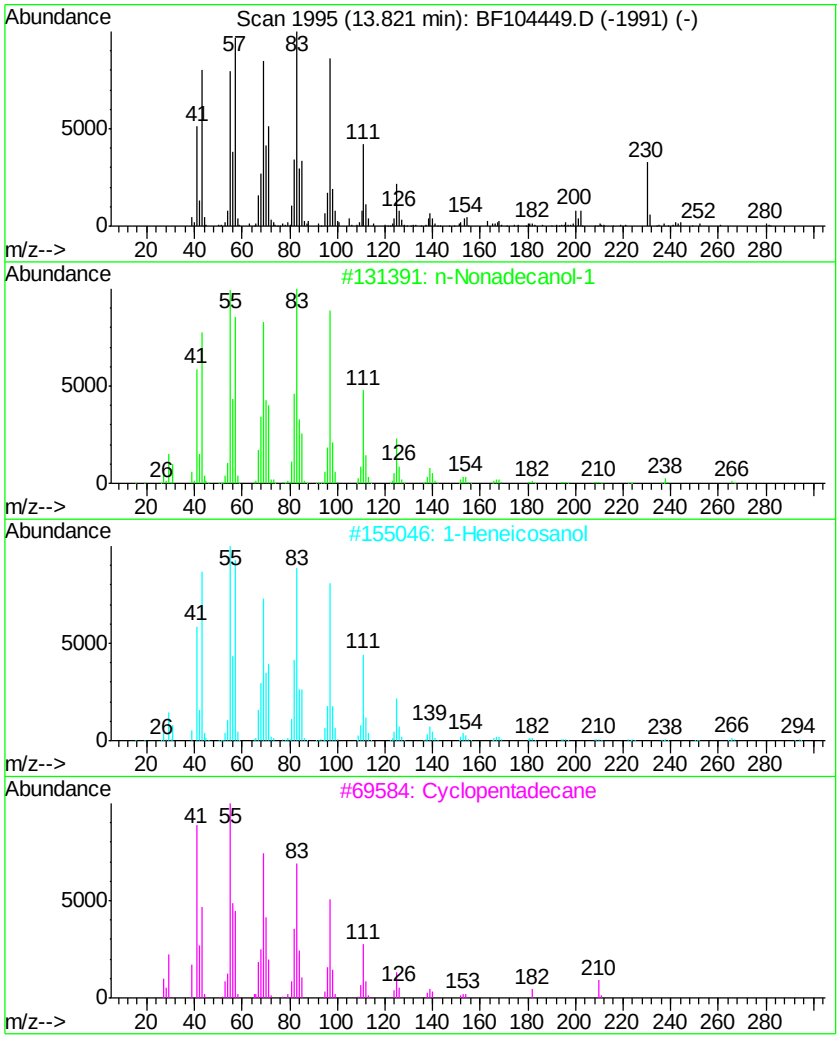
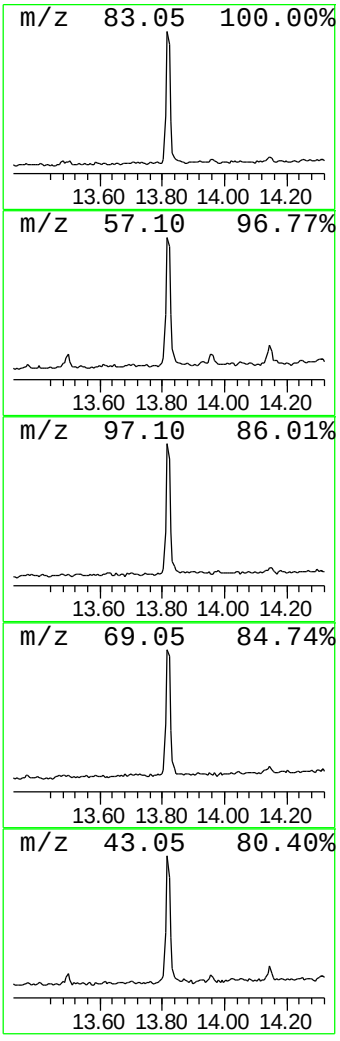
Peak Number 6 n-Nonadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	7.22 ng	461487	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Cyclopentadecane	210	C15H30	000295-48-7	93
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
5	Behenic alcohol	326	C22H46O	000661-19-8	91





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Data File : BF104449.D
Acq On : 12 Apr 2018 14:28
Operator : JU/SJ
Sample : J2163-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-01-041118-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

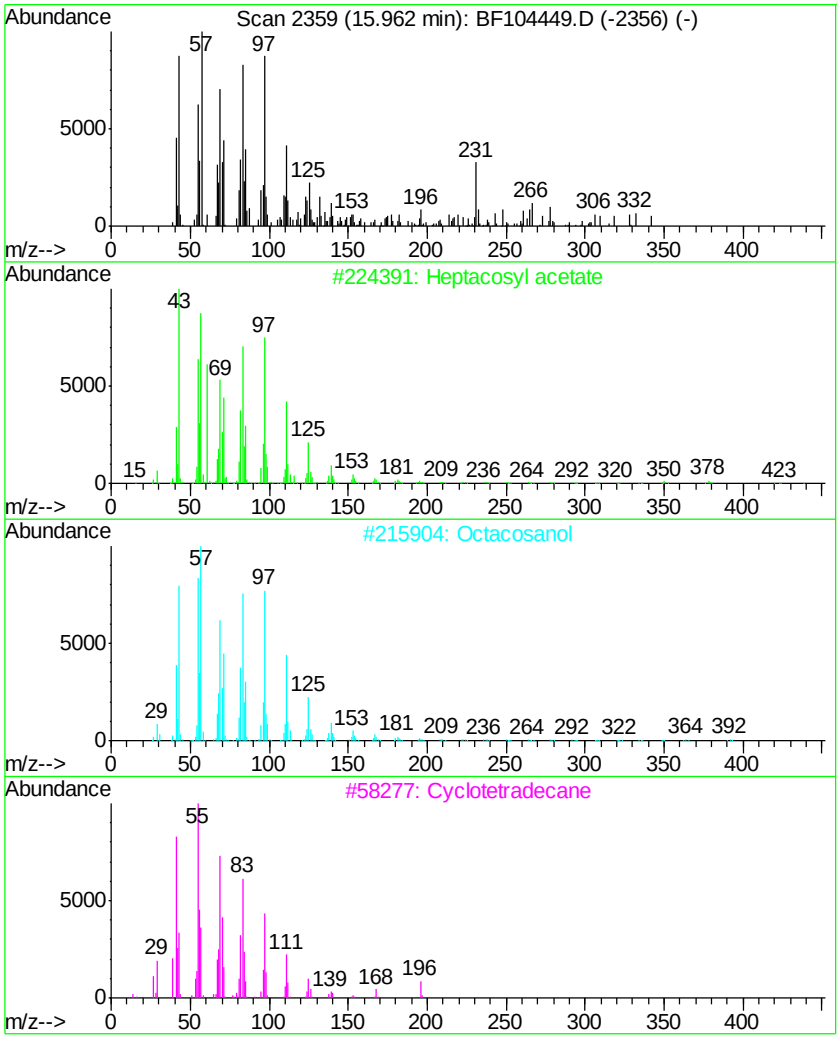
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

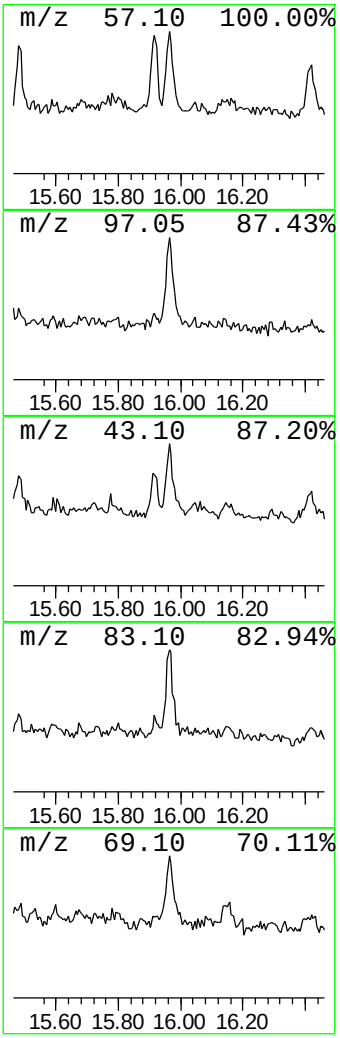
****

Peak Number 9 Heptacosyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	3.05 ng	119812	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosyl acetate	438	C29H58O2	1000351-78-2	93
2	Octacosanol	410	C28H58O	000557-61-9	91
3	Cyclotetradecane	196	C14H28	000295-17-0	90
4	9-Nonadecene	266	C19H38	031035-07-1	90
5	1-Nonadecene	266	C19H38	018435-45-5	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041218\
Data File : BF104449.D
Acq On : 12 Apr 2018 14:28
Operator : JU/SJ
Sample : J2163-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-01-041118-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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...	5.03	3.6	ng	155021	1	6.81	851317	20.0
unknown6.58	6.58	72.4	ng	3081440	1	6.81	851317	20.0
Tridecane, 1-iodo-	10.75	3.0	ng	172553	4	11.34	1166020	20.0
n-Hexadecanoic acid	11.86	4.1	ng	238412	4	11.34	1166020	20.0
n-Nonadecanol-1	13.82	7.2	ng	461487	5	13.98	1278140	20.0
Heptacosyl acetate	15.96	3.0	ng	119812	6	15.46	785336	20.0