LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120417\
Data File : BF101095.D
Acq On : 4 Dec 2017 14:02
Operator : SJ/JU
Sample : I6620-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6(5-7)-20171128

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-BF113017.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	5.063	502	506	518	rBV	107450	128388	11.25%	1.138%
2	5.463	570	574	586	rBB	785614	757965	66.42%	6.720%
3	6.481	742	747	759	rBV	968868	925355	81.09%	8.204%
4	6.616	766	770	773	rBV	1047219	892219	78.18%	7.910%
5	6.845	806	809	813	rBV	387204	298448	26.15%	2.646%
6	7.004	832	836	839	rBV	913874	752129	65.91%	6.668%
7	7.410	901	905	908	rBV	624274	574098	50.31%	5.090%
8	8.128	1024	1027	1030	rBV	497209	386544	33.87%	3.427%
9	9.204	1206	1210	1213	rBV	1397732	1141188	100.00%	10.117%
10	9.275	1219	1222	1226	rBV2	18001	16795	1.47%	0.149%
11	9.592	1273	1276	1283	rVB	72948	66235	5.80%	0.587%
12	9.745	1299	1302	1305	rBV	18962	15539	1.36%	0.138%
13	9.804	1307	1312	1316	rVV	39350	32179	2.82%	0.285%
14	9.886	1322	1326	1329	rBV	490405	411019	36.02%	3.644%
15	10.304	1394	1397	1400	rVB	30186	21324	1.87%	0.189%
16	10.528	1429	1435	1437	rBV4	9591	13929	1.22%	0.123%
17	10.675	1456	1460	1463	rBV	410420	344963	30.23%	3.058%
18	10.775	1475	1477	1484	rBV3	21336	28405	2.49%	0.252%
19	11.375	1575	1579	1581	rBV	448922	379518	33.26%	3.365%
20	11.398	1581	1583	1586	rVV	155993	119965	10.51%	1.064%
21	11.445	1586	1591	1596	rVB	31786	26794	2.35%	0.238%
22	11.604	1612	1618	1624	rBV2	19828	20749	1.82%	0.184%
23	11.886	1659	1666	1671	rBV3	41685	77352	6.78%	0.686%
24	11.986	1680	1683	1685	rBV2	25947	27924	2.45%	0.248%
25	12.198	1716	1719	1725	rVB	26141	23369	2.05%	0.207%
26	12.439	1753	1760	1763	rBV2	224003	200647	17.58%	1.779%
27	12.463	1763	1764	1770	rVB2	35878	23425	2.05%	0.208%
28	12.510	1770	1772	1776	rBV	18961	18937	1.66%	0.168%
29	12.586	1782	1785	1789	rBV	287092	238640	20.91%	2.116%
30	12.680	1798	1801	1805	rVB3	19064	21596	1.89%	0.191%
31	12.816	1817	1824	1828	rBV	244158	251775	22.06%	2.232%
32	12.863	1830	1832	1836	rBV2	13399	16584	1.45%	0.147%
33	12.957	1844	1848	1851	rBV	997088	824482	72.25%	7.309%
34	13.033	1856	1861	1865	rBV5	12484	21865	1.92%	0.194%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120417\
Data File : BF101095.D
Acq On : 4 Dec 2017 14:02
Operator : SJ/JU
Sample : I6620-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6(5-7)-20171128

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-BF113017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.122	1873	1876	1877	rBV3	15667	17515	1.53%	0.155%
36	13.145	1878	1880	1883	rVB	21137	19604	1.72%	0.174%
37	13.251	1893	1898	1903	rVB3	19973	35535	3.11%	0.315%
38	13.339	1909	1913	1916	rBV2	14357	20615	1.81%	0.183%
39	13.369	1916	1918	1925	rVV5	26663	29340	2.57%	0.260%
40	13.427	1925	1928	1931	rVV	24135	19160	1.68%	0.170%
41	13.657	1961	1967	1969	rBV	33924	37707	3.30%	0.334%
42	13.763	1981	1985	1988	rBV2	32780	39153	3.43%	0.347%
43	13.816	1991	1994	1996	rBV2	25491	24121	2.11%	0.214%
44	13.839	1996	1998	2001	rVV3	59094	52033	4.56%	0.461%
45	13.980	2017	2022	2024	rBV2	40154	50032	4.38%	0.444%
46	14.016	2024	2028	2031	rVV2	439184	516944	45.30%	4.583%
47	14.039	2031	2032	2039	rVB	121848	109033	9.55%	0.967%
48	14.121	2044	2046	2048	rBV	18526	18197	1.59%	0.161%
49	14.163	2051	2053	2054	rVV2	23333	18892	1.66%	0.167%
50	14.210	2058	2061	2063	rVB	41882	35679	3.13%	0.316%
51	14.363	2085	2087	2089	rBV2	21996	17326	1.52%	0.154%
52	14.598	2125	2127	2130	rBV3	21070	21450	1.88%	0.190%
53	15.063	2202	2206	2209	rBV	152788	222746	19.52%	1.975%
54	15.168	2221	2224	2230	rBV	28900	47722	4.18%	0.423%
55	15.363	2254	2257	2264	rVB	92309	124952	10.95%	1.108%
56	15.427	2264	2268	2273	rBV	115937	154936	13.58%	1.374%
57	15.492	2274	2279	2283	rBV	257135	330419	28.95%	2.929%
58	15.615	2298	2300	2305	rBV5	20023	28048	2.46%	0.249%
59	16.974	2526	2531	2541	rVB3	55518	109785	9.62%	0.973%
60	17.421	2603	2607	2612	rVB2	40704	78470	6.88%	0.696%

Sum of corrected areas: 11279758

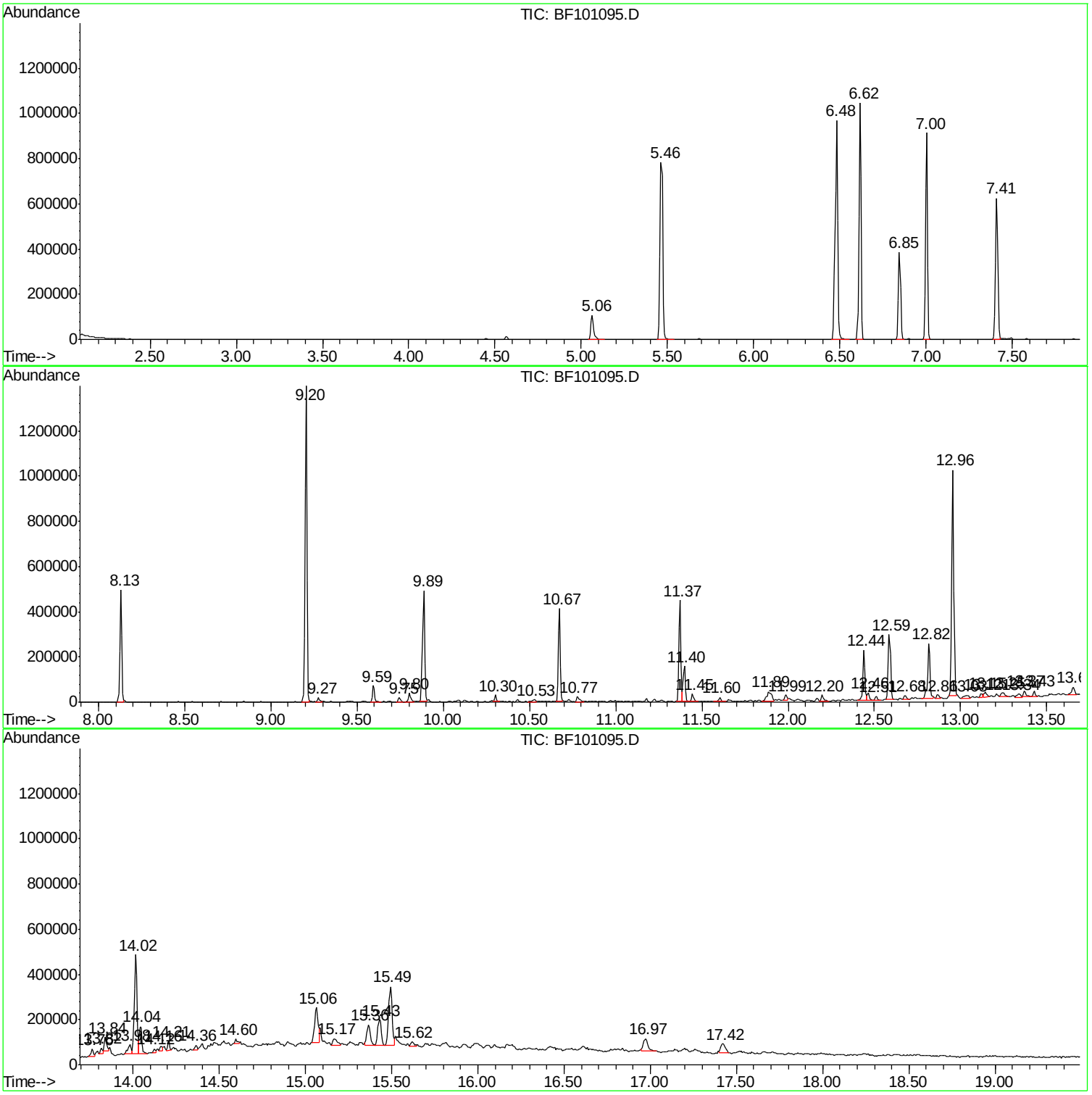
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120417\
Data File : BF101095.D
Acq On : 4 Dec 2017 14:02
Operator : SJ/JU
Sample : I6620-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6(5-7)-20171128

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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\BF120417\
Data File : BF101095.D
Acq On : 4 Dec 2017 14:02
Operator : SJ/JU
Sample : I6620-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6(5-7)-20171128

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

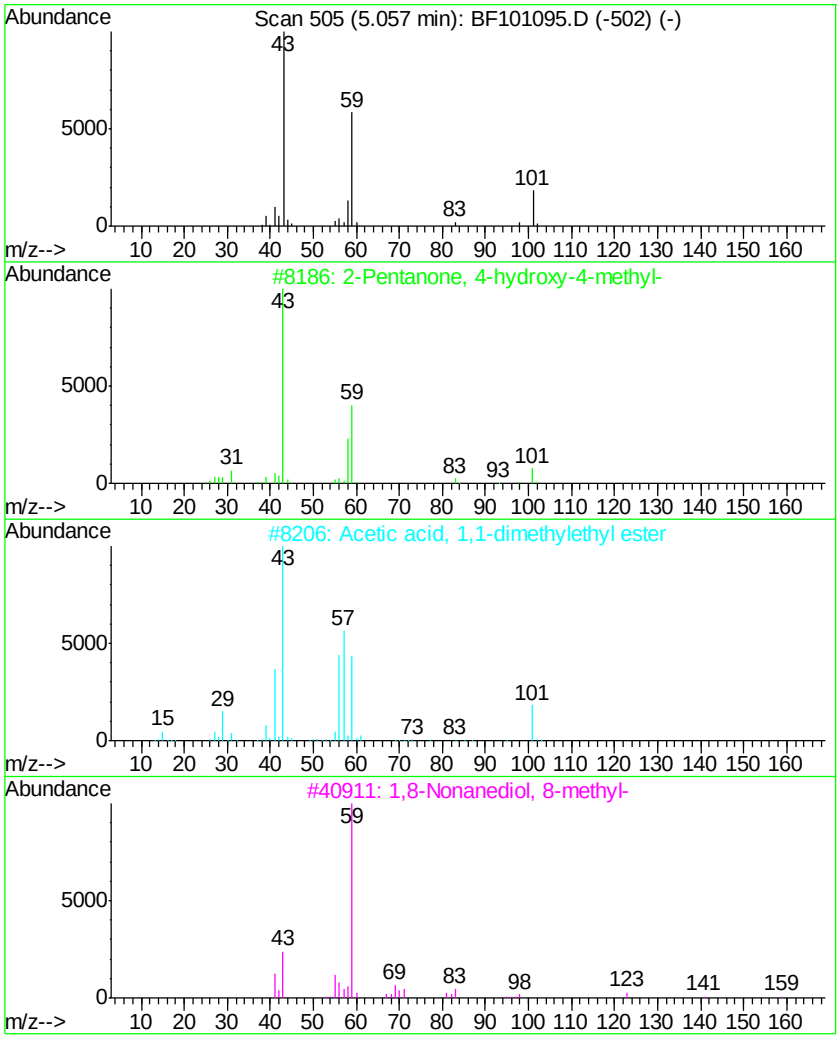
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

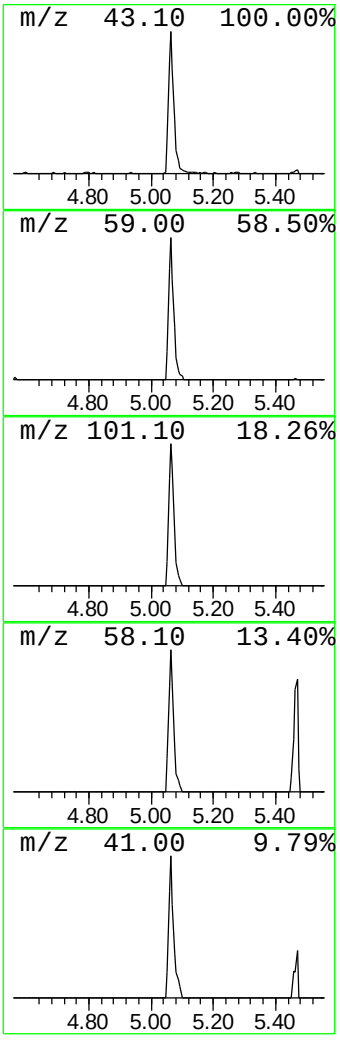
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	8.60 ng	128388	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF120417\
Data File : BF101095.D
Acq On : 4 Dec 2017 14:02
Operator : SJ/JU
Sample : I6620-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6(5-7)-20171128

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

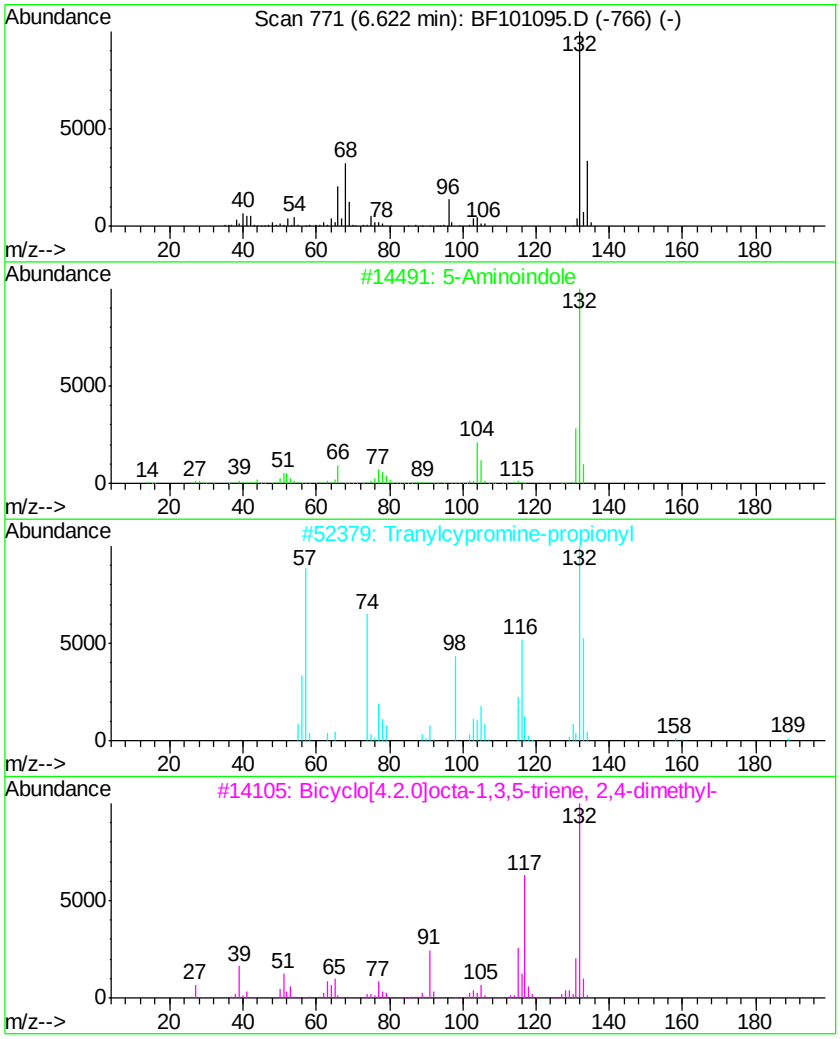
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

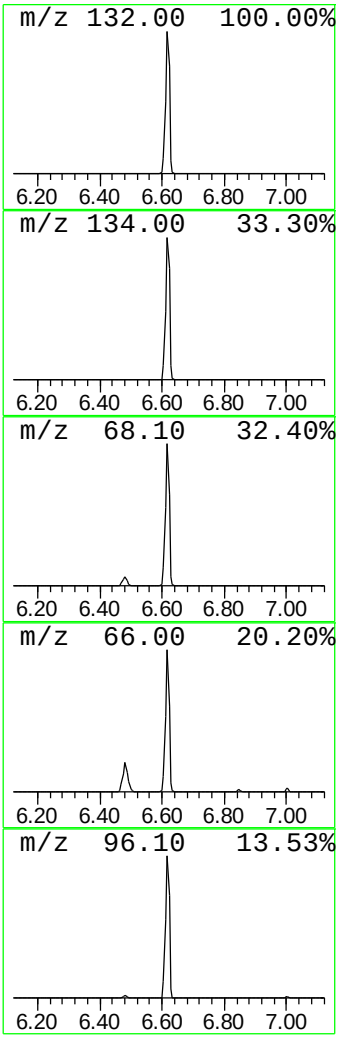
****

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	59.79 ng	892219	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF120417\
Data File : BF101095.D
Acq On : 4 Dec 2017 14:02
Operator : SJ/JU
Sample : I6620-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6(5-7)-20171128

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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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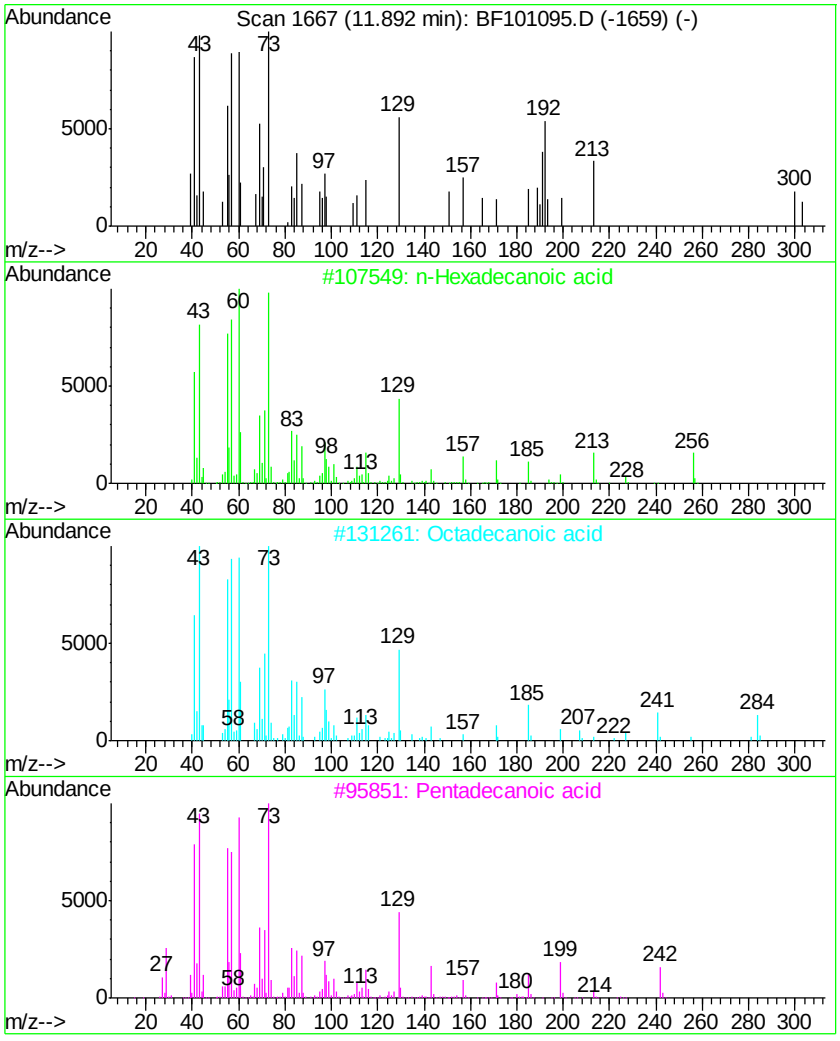
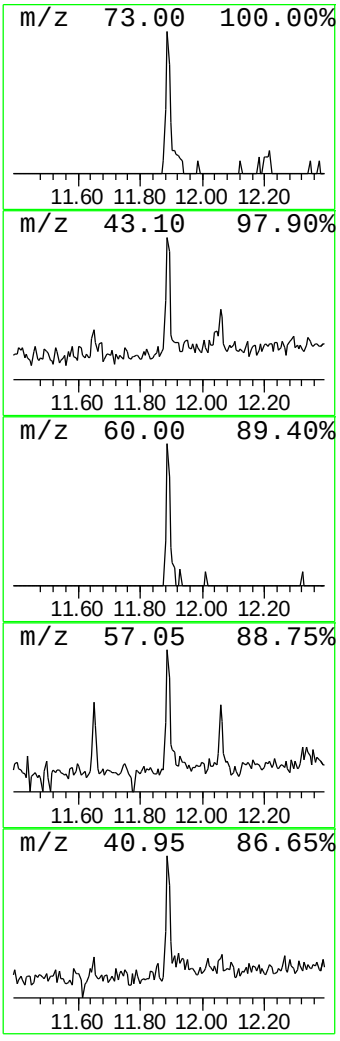
Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	4.08 ng	77352	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
2	Octadecanoic acid	284	C18H36O2	000057-11-4	72
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120417\
Data File : BF101095.D
Acq On : 4 Dec 2017 14:02
Operator : SJ/JU
Sample : I6620-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6(5-7)-20171128

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

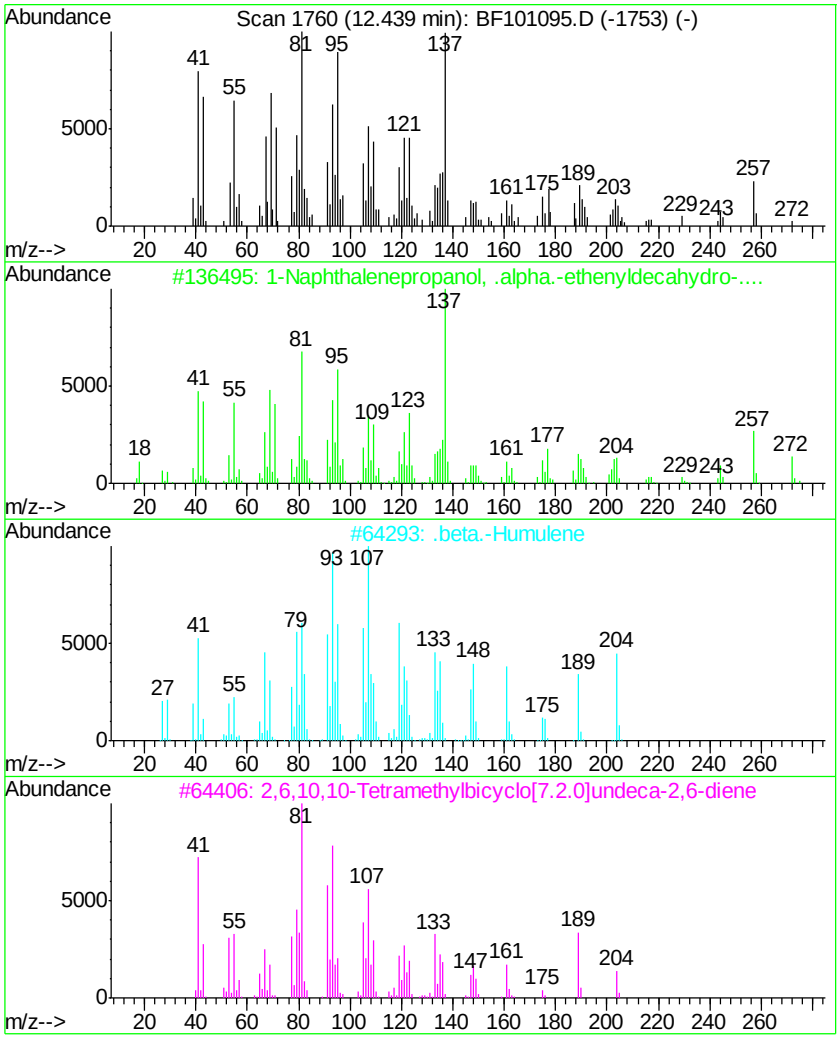
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

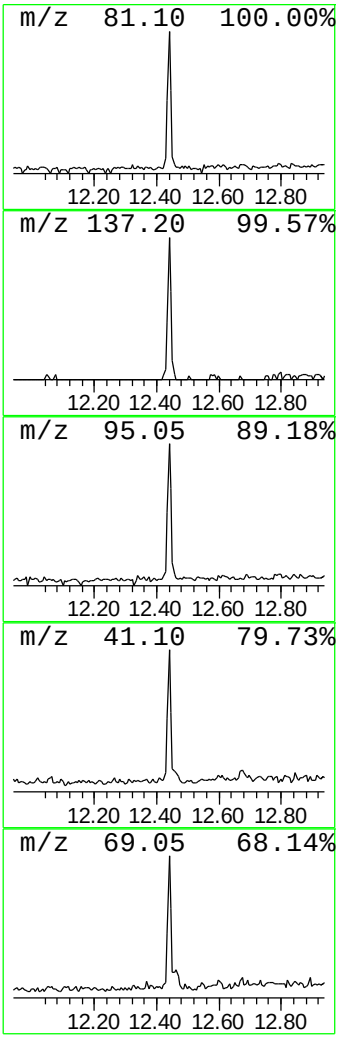
****

Peak Number 5 1-Naphthalenepropanol, .alp... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.44	10.57 ng	200647	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Naphthalenepropanol, .alpha.-e...	290	C20H34O	001438-62-6	76
2	.beta.-Humulene	204	C15H24	000116-04-1	59
3	2,6,10,10-Tetramethylbicyclo[7.2...	204	C15H24	136296-37-2	53
4	cis, cis-3-Ethylbicyclo[4.4.0]de...	166	C12H22	066660-42-2	49
5	Naphthalene, 2-ethyldecahydro-	166	C12H22	001618-23-1	46





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Sample : I6620-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6(5-7)-20171128

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

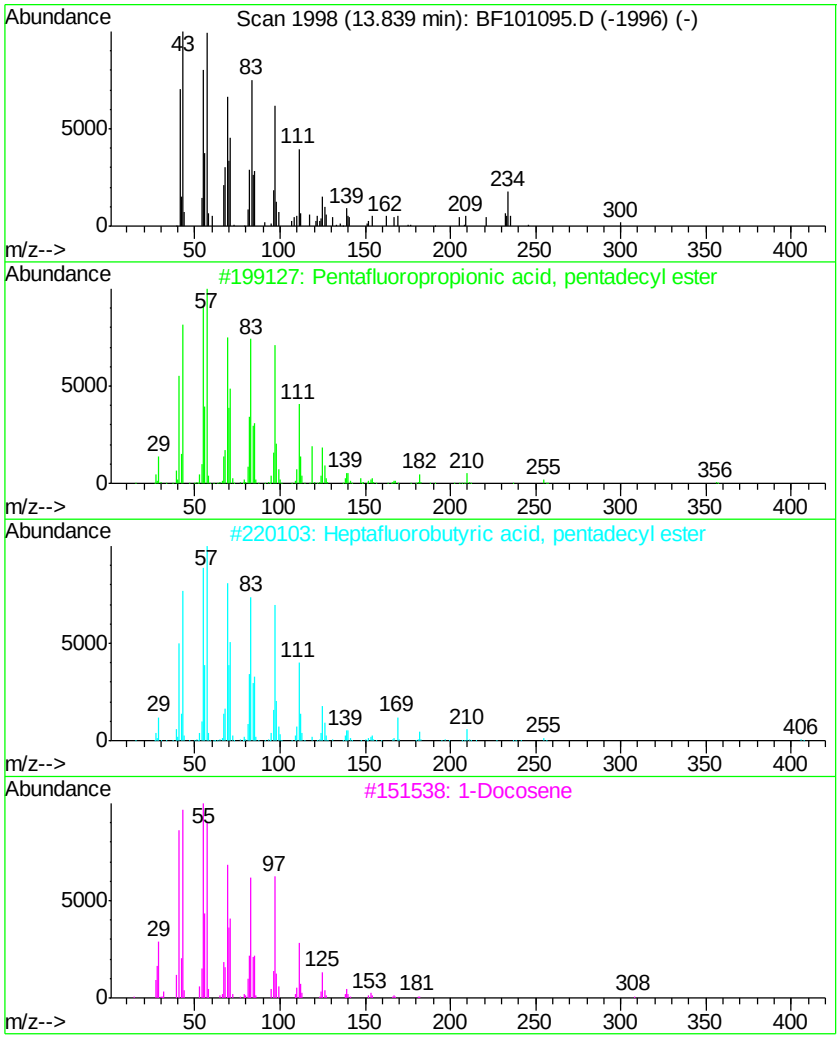
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

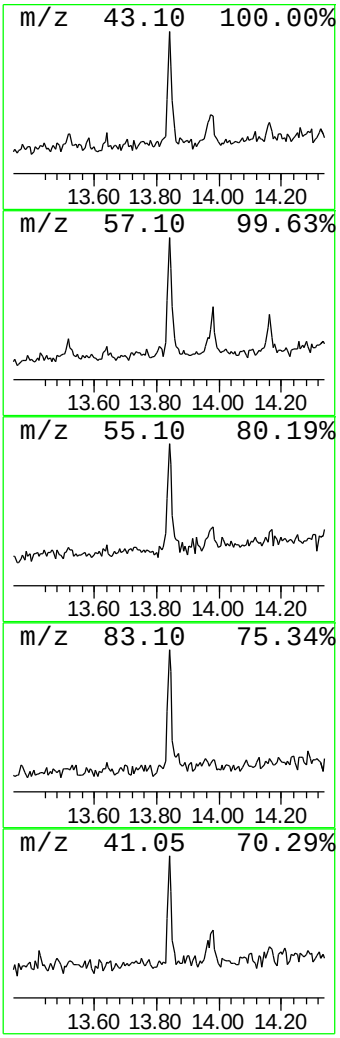
****

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	2.01 ng	52033	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90
3	1-Docosene	308	C22H44	001599-67-3	90
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
5	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	87





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Acq On : 4 Dec 2017 14:02
Operator : SJ/JU
Sample : I6620-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6(5-7)-20171128

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

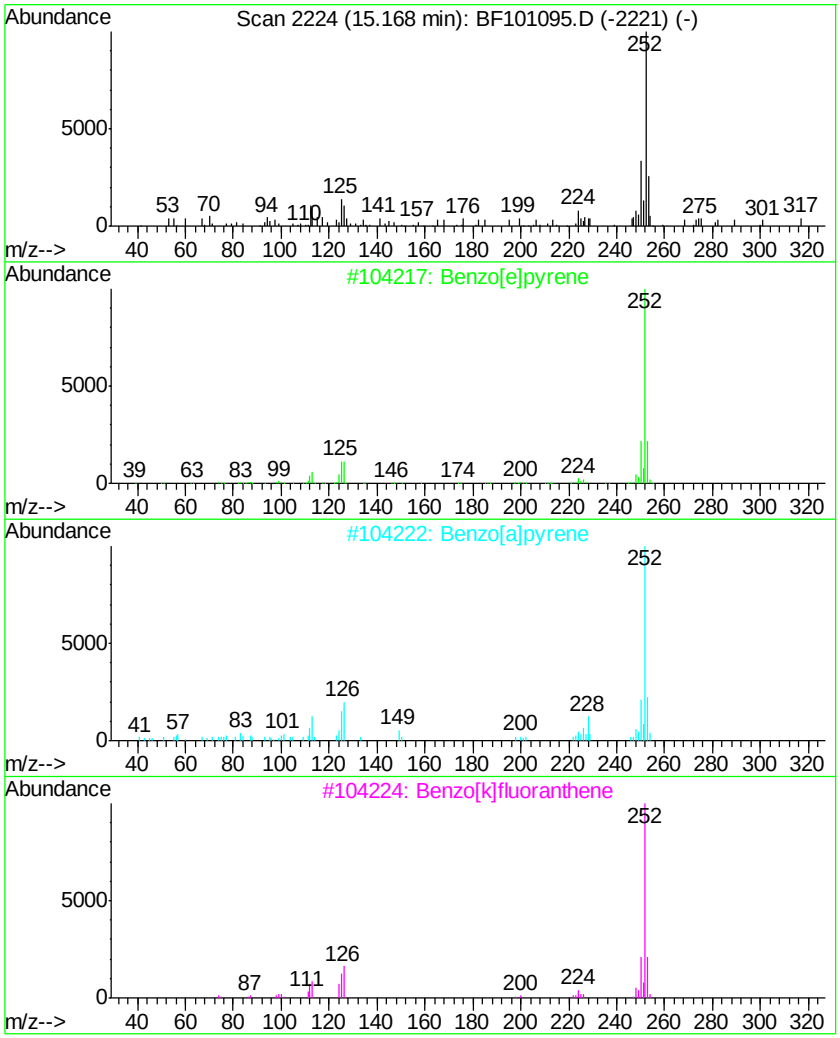
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

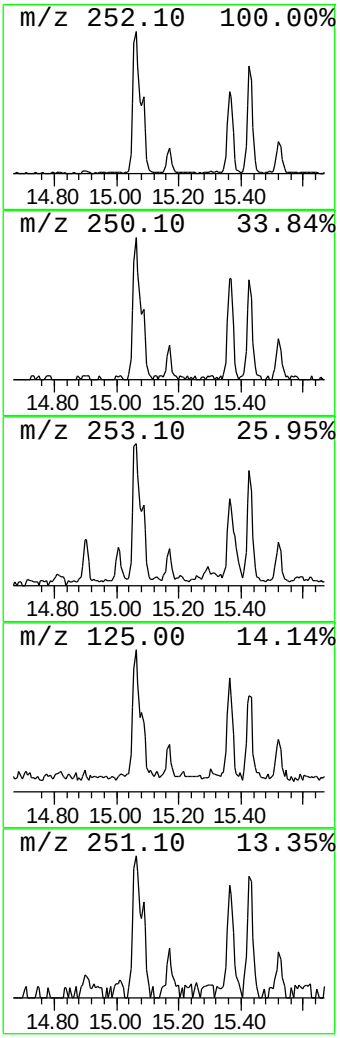
****

Peak Number 7 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	2.89 ng	47722	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	64
2	Benzo[a]pyrene	252	C20H12	000050-32-8	64
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	64
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	64
5	1-Phenyl-3-(4-methoxyphenyl)-2-p...	252	C16H16N2O	003314-43-0	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120417\
Data File : BF101095.D
Acq On : 4 Dec 2017 14:02
Operator : SJ/JU
Sample : I6620-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6(5-7)-20171128

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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...	5.06	8.6	ng	128388	1	6.85	298448	20.0
unknown6.62	6.62	59.8	ng	892219	1	6.85	298448	20.0
n-Hexadecanoic acid	11.89	4.1	ng	77352	4	11.37	379518	20.0
1-Naphthaleneprop...	12.44	10.6	ng	200647	4	11.37	379518	20.0
Pentafluoropropio...	13.84	2.0	ng	52033	5	14.02	516944	20.0
Benzo[e]pyrene	15.17	2.9	ng	47722	6	15.49	330419	20.0