LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
Data File : BF096509.D
Acq On : 6 Jul 2017 3:47
Operator : SJ/MA
Sample : I3975-01
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B7-0-2

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-BF070117.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	3.045	156	163	168	rBV2	14089	25098	1.05%	0.111%
2	4.904	474	479	488	rBV	263844	348822	14.63%	1.539%
3	5.328	546	551	554	rBV	2485640	2334127	97.90%	10.300%
4	6.351	720	725	736	rVB	2249792	2384224	100.00%	10.521%
5	6.481	743	747	751	rBV	2234939	2281134	95.68%	10.066%
6	6.716	783	787	790	rBV	737642	673895	28.26%	2.974%
7	6.869	809	813	817	rBV	1957048	1763190	73.95%	7.781%
8	7.275	876	882	885	rBV	1531039	1367590	57.36%	6.035%
9	7.992	1000	1004	1007	rBV	1035522	931577	39.07%	4.111%
10	9.074	1183	1188	1191	rBV	2604897	2205756	92.51%	9.734%
11	9.169	1200	1204	1207	rVB2	48218	42233	1.77%	0.186%
12	9.469	1251	1255	1258	rBV	505972	453656	19.03%	2.002%
13	9.698	1290	1294	1298	rBV	53118	45674	1.92%	0.202%
14	9.751	1298	1303	1306	rBV	710783	682131	28.61%	3.010%
15	10.192	1375	1378	1381	rVB	65943	55205	2.32%	0.244%
16	10.533	1432	1436	1441	rBV	1128346	1024652	42.98%	4.522%
17	10.669	1456	1459	1466	rVB	74156	91928	3.86%	0.406%
18	11.116	1532	1535	1538	rBV3	43524	45964	1.93%	0.203%
19	11.227	1551	1554	1556	rBV	763159	625185	26.22%	2.759%
20	11.251	1556	1558	1561	rVV	192749	144007	6.04%	0.635%
21	11.304	1561	1567	1570	rVB	60486	60385	2.53%	0.266%
22	11.539	1604	1607	1609	rBV2	29241	26477	1.11%	0.117%
23	11.757	1642	1644	1648	rVB	40320	38945	1.63%	0.172%
24	11.804	1648	1652	1654	rBV3	27183	28627	1.20%	0.126%
25	11.839	1654	1658	1660	rBV2	54444	58628	2.46%	0.259%
26	12.280	1729	1733	1736	rBV3	28232	37106	1.56%	0.164%
27	12.439	1756	1760	1763	rBV	259626	242381	10.17%	1.070%
28	12.574	1779	1783	1784	rBV4	20323	27219	1.14%	0.120%
29	12.662	1792	1798	1802	rBV	222792	282493	11.85%	1.247%
30	12.704	1804	1805	1808	rVB2	34598	25092	1.05%	0.111%
31	12.786	1816	1819	1820	rBV2	29475	25381	1.06%	0.112%
32	12.815	1820	1824	1827	rVV	1806310	1633276	68.50%	7.207%
33	12.886	1831	1836	1839	rBV6	31100	46463	1.95%	0.205%
34	12.998	1852	1855	1858	rVB2	55973	61202	2.57%	0.270%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
Data File : BF096509.D
Acq On : 6 Jul 2017 3:47
Operator : SJ/MA
Sample : I3975-01
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B7-0-2

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-BF070117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.033	1858	1861	1863	rBV3	28006	36919	1.55%	0.163%
36	13.062	1863	1866	1869	rVV	67918	69713	2.92%	0.308%
37	13.098	1869	1872	1876	rVB3	28784	45605	1.91%	0.201%
38	13.298	1901	1906	1913	rVB	356139	367682	15.42%	1.623%
39	13.351	1913	1915	1918	rBV3	20606	28420	1.19%	0.125%
40	13.404	1921	1924	1927	rVV3	42171	43148	1.81%	0.190%
41	13.639	1962	1964	1967	rBV4	26817	32967	1.38%	0.145%
42	13.721	1974	1978	1986	rVB2	233367	286247	12.01%	1.263%
43	13.862	1997	2002	2005	rBV	738263	829754	34.80%	3.662%
44	13.886	2005	2006	2008	rVB	111618	60078	2.52%	0.265%
45	14.045	2031	2033	2035	rVB	45542	36519	1.53%	0.161%
46	14.351	2083	2085	2090	rBV	42991	48127	2.02%	0.212%
47	14.645	2133	2135	2139	rBV3	39527	40348	1.69%	0.178%
48	14.868	2171	2173	2184	rVB	78570	163427	6.85%	0.721%
49	15.209	2229	2231	2236	rVB	55784	62633	2.63%	0.276%
50	15.274	2237	2242	2245	rBV	329816	389570	16.34%	1.719%

Sum of corrected areas: 22660880

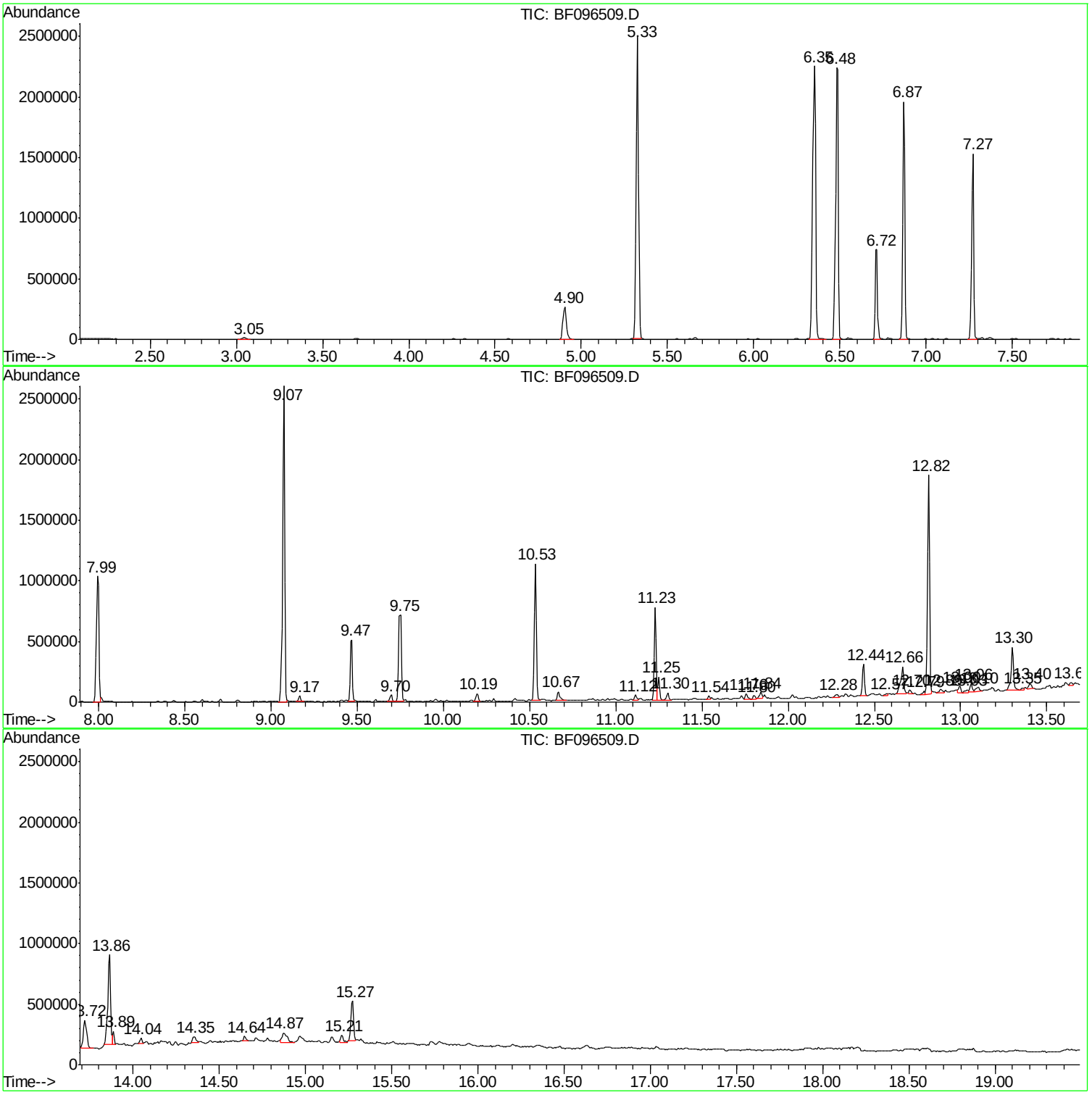
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
Data File : BF096509.D
Acq On : 6 Jul 2017 3:47
Operator : SJ/MA
Sample : I3975-01
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B7-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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\BF070517\
Data File : BF096509.D
Acq On : 6 Jul 2017 3:47
Operator : SJ/MA
Sample : I3975-01
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B7-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

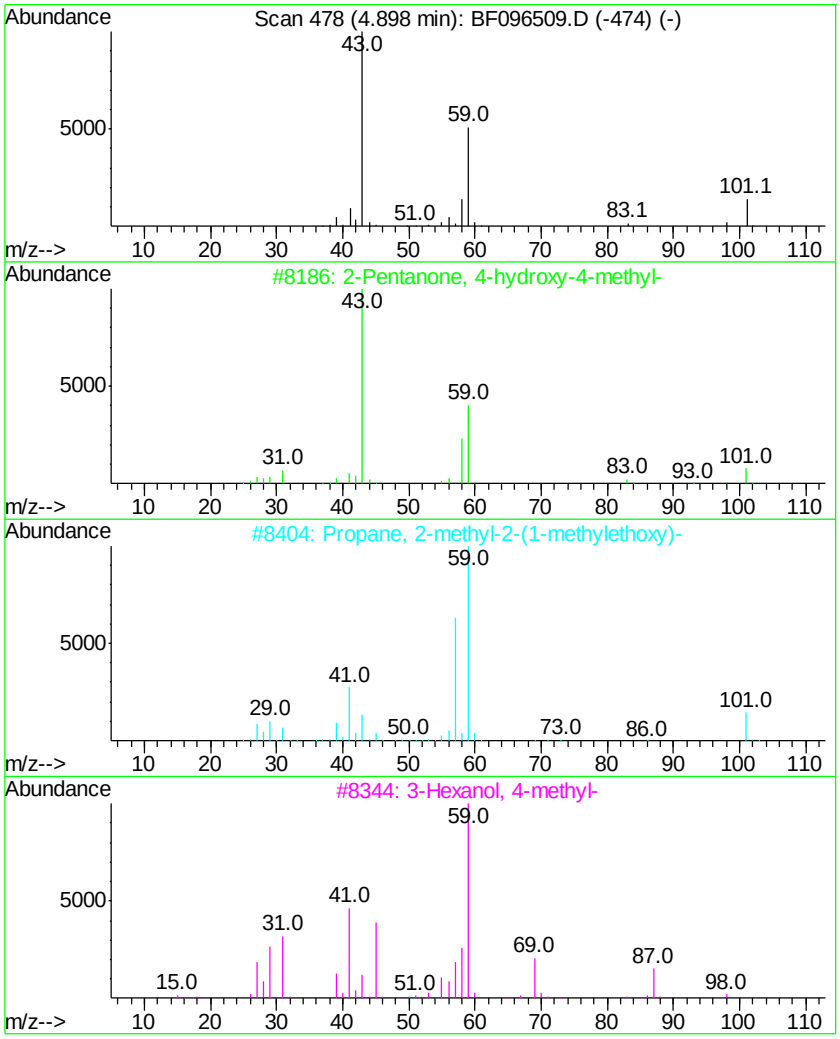
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

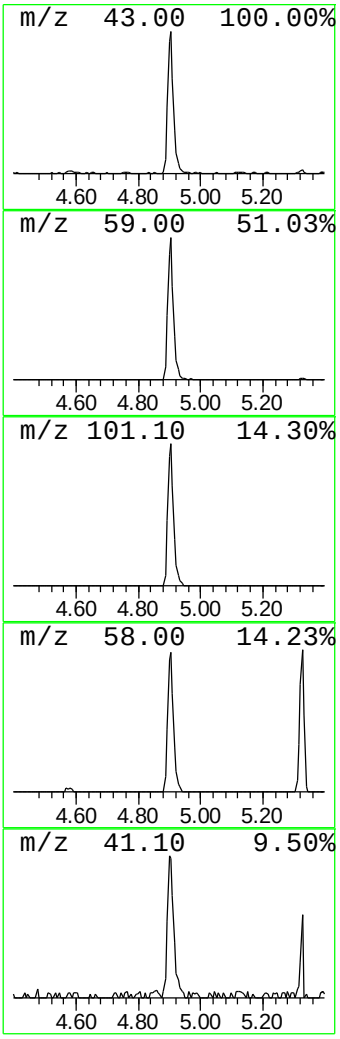
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	10.35 ng	348822	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	3-Hexanol	102	C6H14O	000623-37-0	33
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
Data File : BF096509.D
Acq On : 6 Jul 2017 3:47
Operator : SJ/MA
Sample : I3975-01
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B7-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

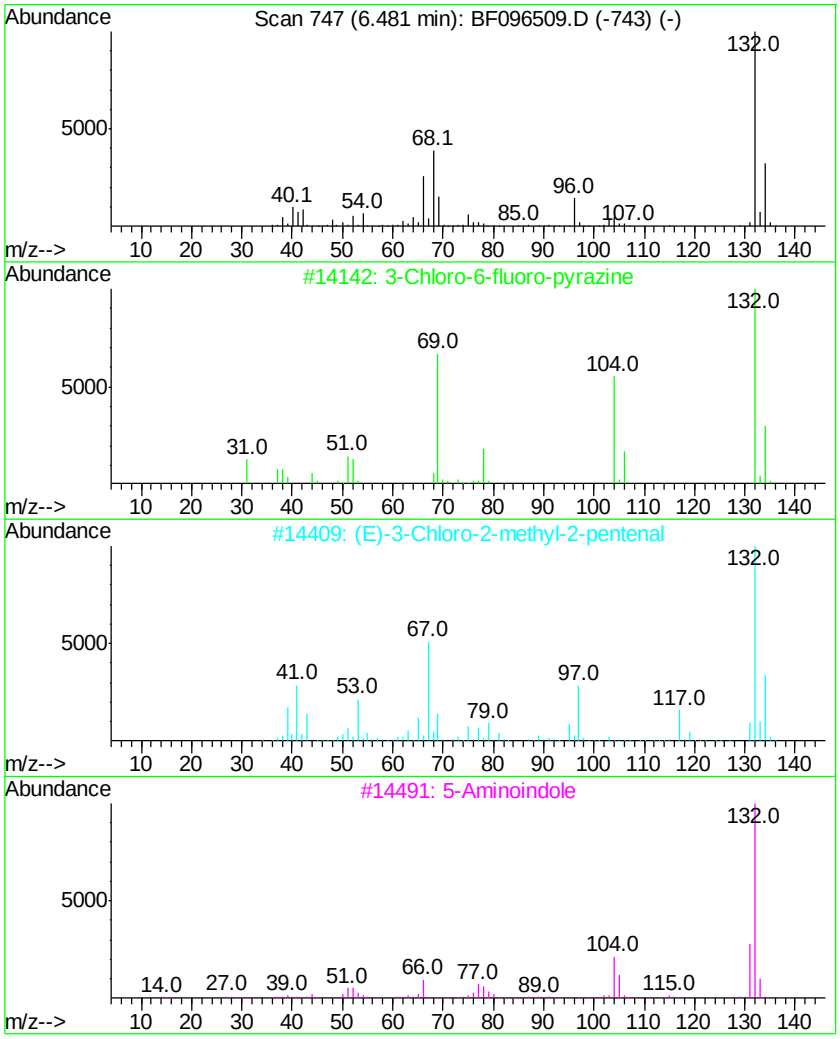
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

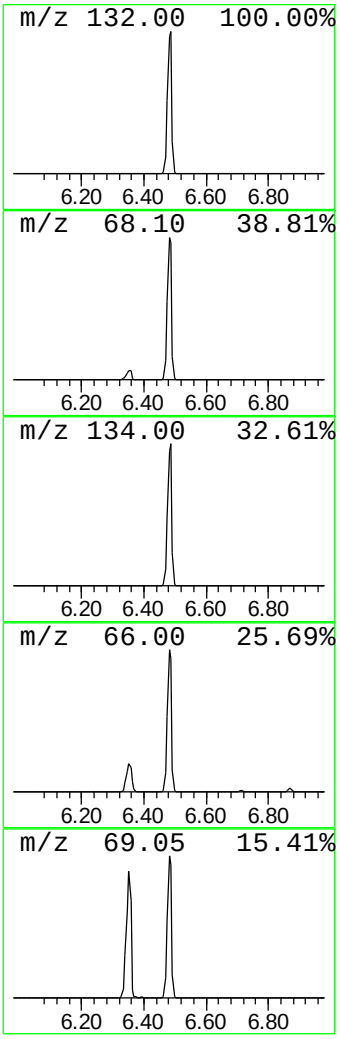
****

Peak Number 2 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	67.70 ng	2281130	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
Data File : BF096509.D
Acq On : 6 Jul 2017 3:47
Operator : SJ/MA
Sample : I3975-01
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B7-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

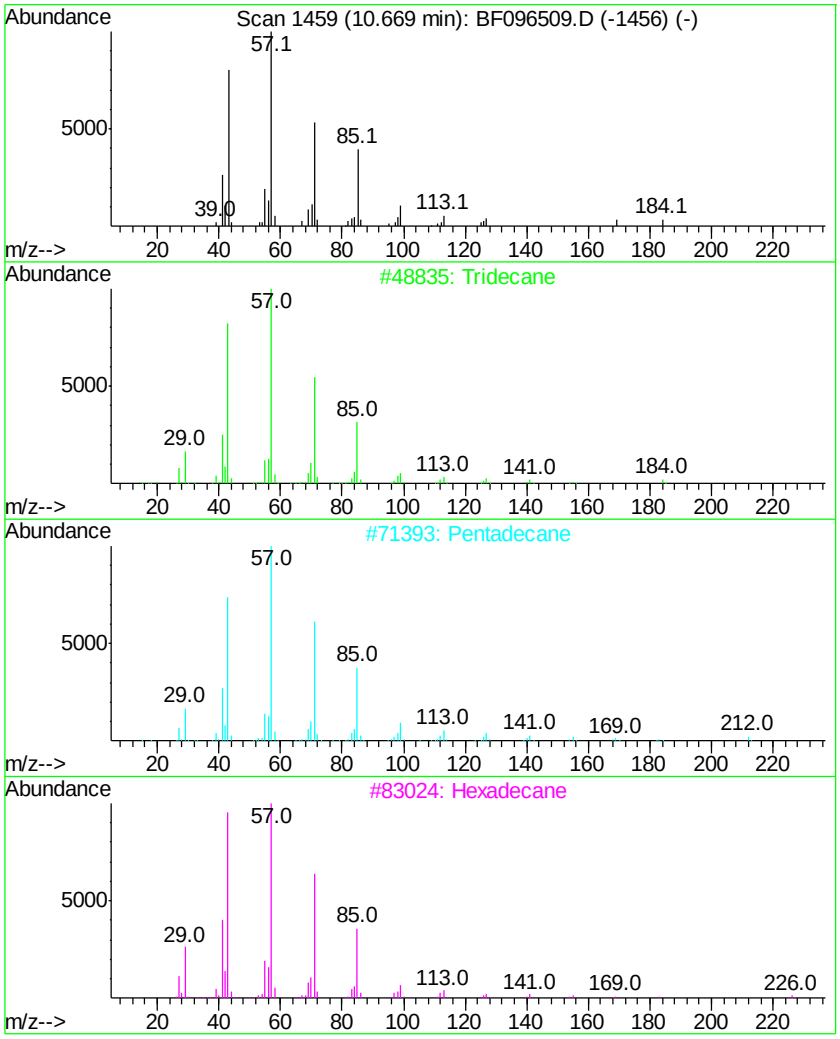
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

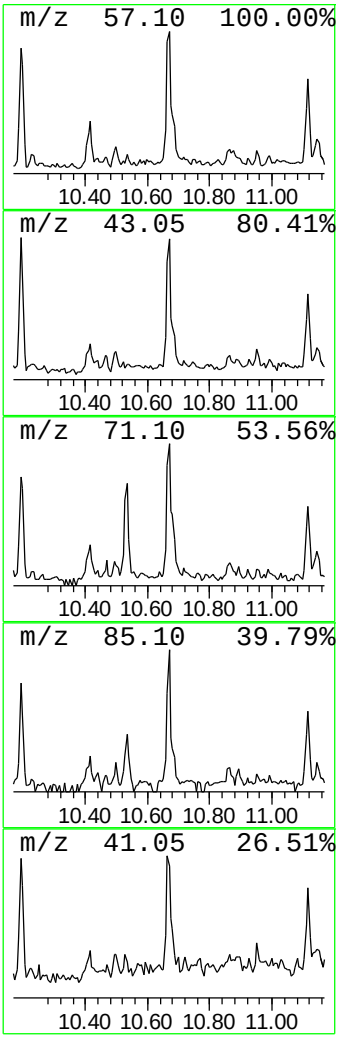
****

Peak Number 4 Tridecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	2.94 ng	91928	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	90
2	Pentadecane	212	C15H32	000629-62-9	86
3	Hexadecane	226	C16H34	000544-76-3	86
4	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
Data File : BF096509.D
Acq On : 6 Jul 2017 3:47
Operator : SJ/MA
Sample : I3975-01
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B7-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

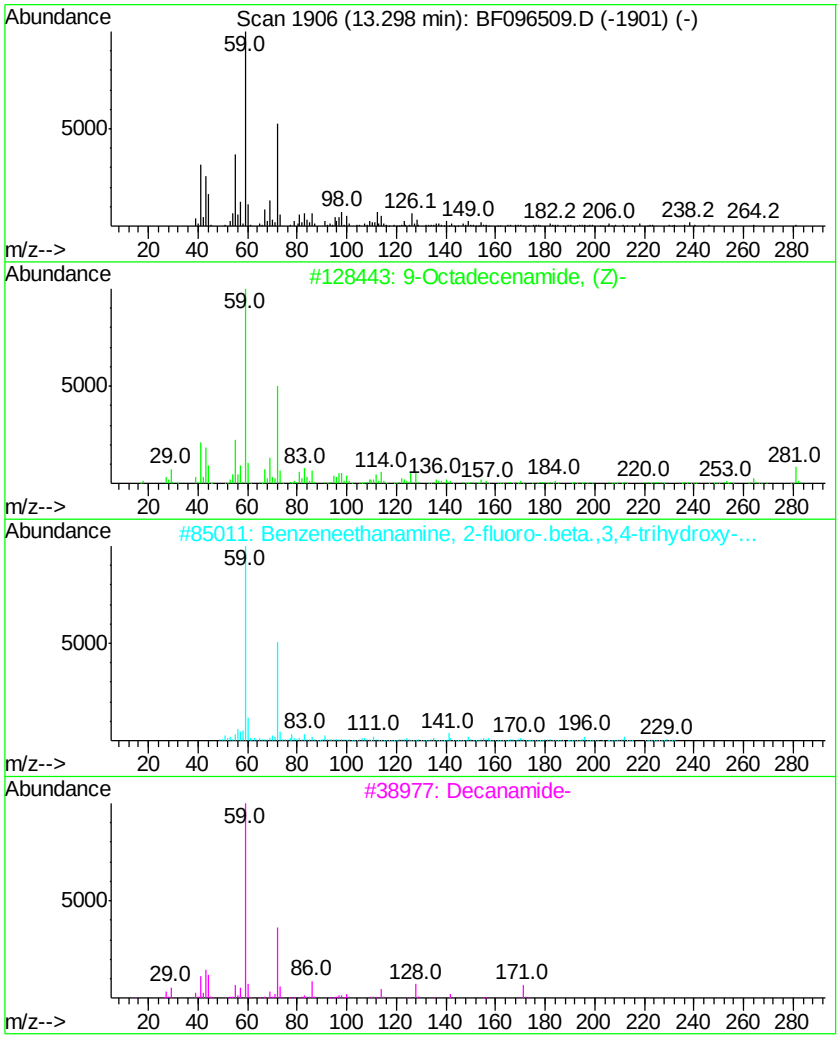
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

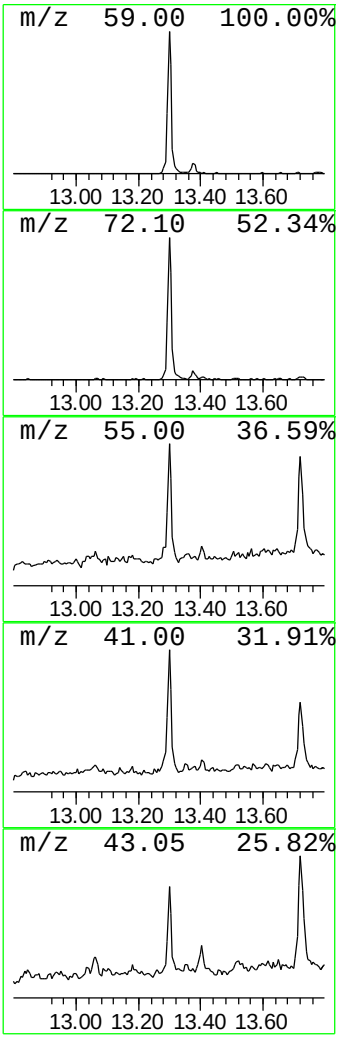
****

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.30	8.86 ng	367682	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	64
3	Decanamide-	171	C10H21NO	002319-29-1	56
4	Nonanamide	157	C9H19NO	001120-07-6	50
5	Silane, hexyl-	116	C6H16Si	001072-14-6	47





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
Data File : BF096509.D
Acq On : 6 Jul 2017 3:47
Operator : SJ/MA
Sample : I3975-01
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B7-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

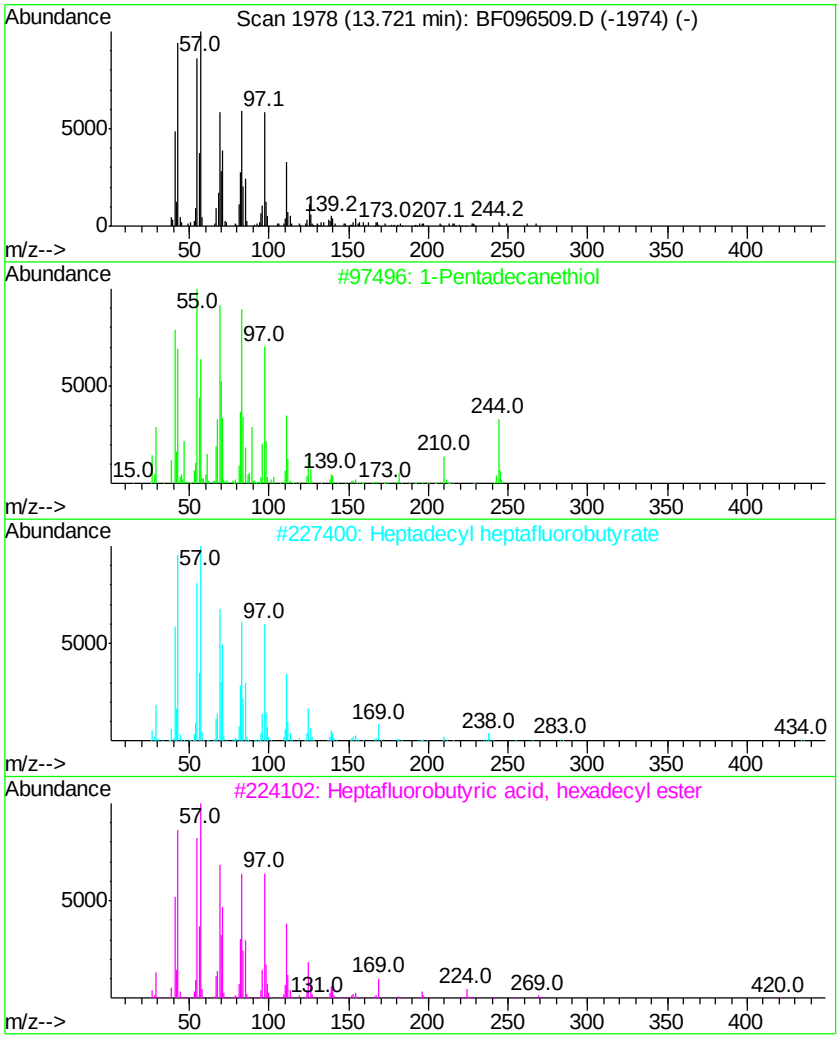
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

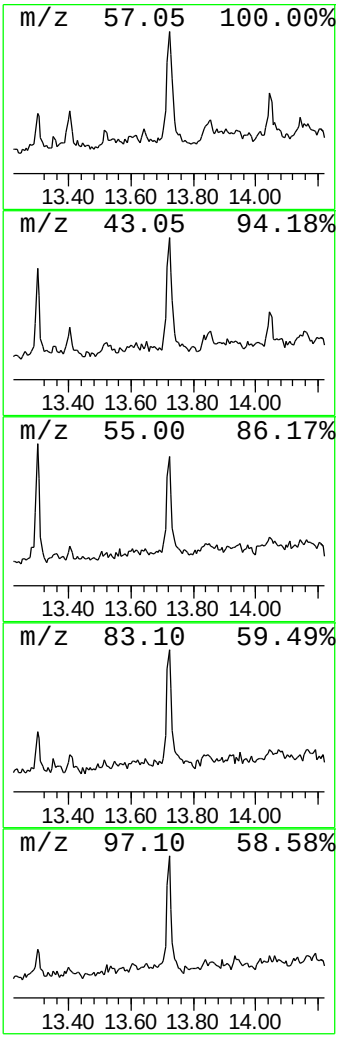
****

Peak Number 6 1-Pentadecanethiol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	6.90 ng	286247	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentadecanethiol	244	C15H32S	025276-70-4	94
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
Data File : BF096509.D
Acq On : 6 Jul 2017 3:47
Operator : SJ/MA
Sample : I3975-01
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B7-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

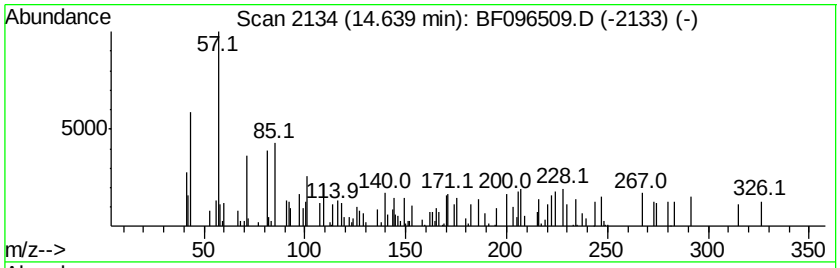
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

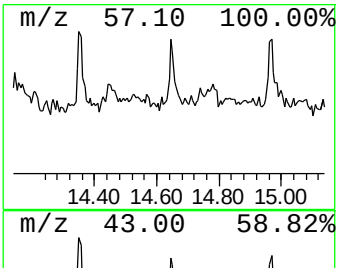
****

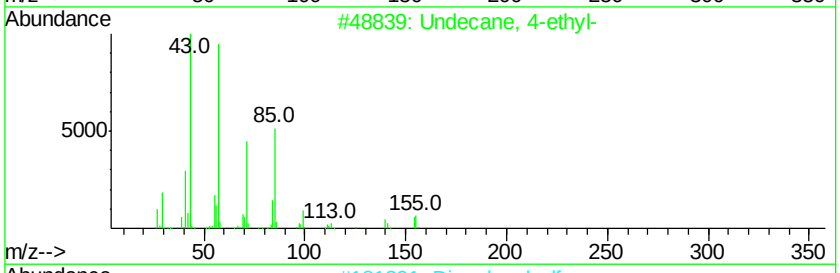
Peak Number 7 unknown14.64 Concentration Rank 7

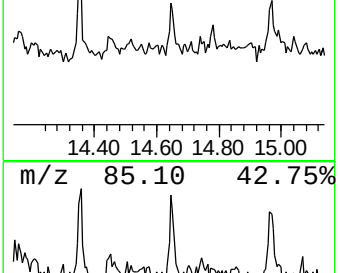
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.07 ng	40348	Perylene-d12	15.27

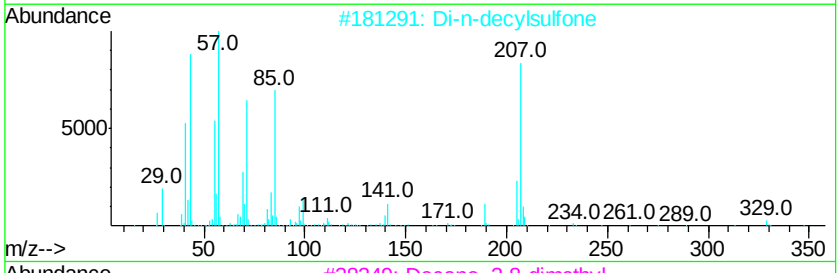
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 4-ethyl-	184	C13H28	017312-59-3	47
2	Di-n-decylsulfone	346	C20H42O2S	111530-37-1	47
3	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	47
4	Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	47
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	47

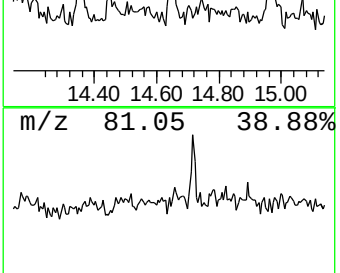


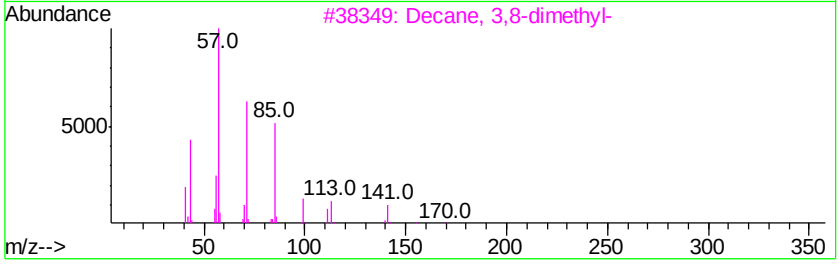


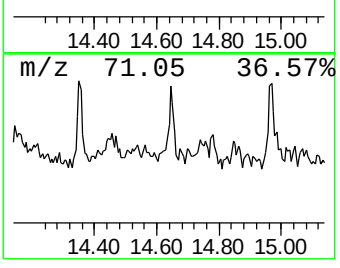












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070517\
Data File : BF096509.D
Acq On : 6 Jul 2017 3:47
Operator : SJ/MA
Sample : I3975-01
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B7-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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...	4.90	10.4	ng	348822	1	6.72	673895	20.0
unknown6.48	6.48	67.7	ng	2281130	1	6.72	673895	20.0
Tridecane	10.67	2.9	ng	91928	4	11.23	625185	20.0
9-Octadecenamide,...	13.30	8.9	ng	367682	5	13.86	829754	20.0
1-Pentadecanethiol	13.72	6.9	ng	286247	5	13.86	829754	20.0
unknown14.64	14.64	2.1	ng	40348	6	15.27	389570	20.0