LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101817\
Data File : BF099636.D
Acq On : 19 Oct 2017 00:01
Operator : SJ/JU
Sample : I5935-13 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-101617-E

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-BF092317.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	5.040	499	502	512	rBV	110174	127766	15.03%	1.354%
2	5.451	569	572	590	rBV	858291	826967	97.29%	8.761%
3	6.469	741	745	759	rBV	833743	809275	95.21%	8.573%
4	6.598	764	767	775	rBV	1041150	849984	100.00%	9.005%
5	6.828	803	806	815	rBV	610256	494855	58.22%	5.242%
6	6.981	829	832	842	rBV	787841	659275	77.56%	6.984%
7	7.392	898	902	914	rBV	513677	452709	53.26%	4.796%
8	8.110	1020	1024	1027	rBV	678924	568252	66.85%	6.020%
9	9.181	1202	1206	1209	rBV	949656	771881	90.81%	8.177%
10	9.251	1215	1218	1221	rBV	12340	10666	1.25%	0.113%
11	9.575	1267	1273	1280	rVB2	22877	28349	3.34%	0.300%
12	9.728	1292	1299	1301	rBV	11474	13012	1.53%	0.138%
13	9.781	1303	1308	1310	rVV3	12242	10958	1.29%	0.116%
14	9.863	1318	1322	1326	rVB	576492	499553	58.77%	5.292%
15	10.651	1453	1456	1466	rVB	435999	369233	43.44%	3.912%
16	10.763	1470	1475	1478	rVV2	11154	15447	1.82%	0.164%
17	11.198	1546	1549	1552	rBV2	9882	9926	1.17%	0.105%
18	11.351	1571	1575	1578	rBV	576400	503831	59.28%	5.337%
19	11.375	1578	1579	1585	rVB3	20744	13651	1.61%	0.145%
20	11.622	1618	1621	1627	rVB	11332	11390	1.34%	0.121%
21	11.863	1657	1662	1663	rBV2	17838	23320	2.74%	0.247%
22	11.880	1663	1665	1668	rVB	18062	14975	1.76%	0.159%
23	11.963	1676	1679	1681	rBV2	14573	15969	1.88%	0.169%
24	11.986	1681	1683	1686	rVB	12143	10058	1.18%	0.107%
25	12.145	1705	1710	1713	rBV6	7613	11181	1.32%	0.118%
26	12.398	1750	1753	1755	rBV	27549	25221	2.97%	0.267%
27	12.492	1765	1769	1772	rBV3	8017	14469	1.70%	0.153%
28	12.563	1778	1781	1784	rBV	32133	30425	3.58%	0.322%
29	12.663	1795	1798	1803	rVB3	13274	16668	1.96%	0.177%
30	12.716	1803	1807	1809	rBV5	13289	19144	2.25%	0.203%
31	12.792	1815	1820	1826	rBV2	58913	73260	8.62%	0.776%
32	12.845	1827	1829	1831	rVV2	14818	10824	1.27%	0.115%
33	12.904	1836	1839	1840	rBV3	12032	11793	1.39%	0.125%
34	12.927	1840	1843	1847	rBV	936149	760564	89.48%	8.057%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101817\
Data File : BF099636.D
Acq On : 19 Oct 2017 00:01
Operator : SJ/JU
Sample : I5935-13 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-101617-E

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-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.010	1853	1857	1858	rBV4	11496	13824	1.63%	0.146%
36	13.110	1870	1874	1875	rBV4	14255	17872	2.10%	0.189%
37	13.145	1878	1880	1882	rVV2	15465	12370	1.46%	0.131%
38	13.227	1892	1894	1897	rVB2	16310	12564	1.48%	0.133%
39	13.321	1907	1910	1911	rBV	13407	9920	1.17%	0.105%
40	13.351	1913	1915	1921	rVB6	16065	25038	2.95%	0.265%
41	13.492	1936	1939	1942	rBV4	15328	14088	1.66%	0.149%
42	13.816	1991	1994	1998	rBV	89453	99795	11.74%	1.057%
43	13.992	2020	2024	2028	rBV	685661	629069	74.01%	6.664%
44	14.433	2097	2099	2103	rBV3	36038	44137	5.19%	0.468%
45	15.463	2269	2274	2278	rVB	362242	475946	55.99%	5.042%

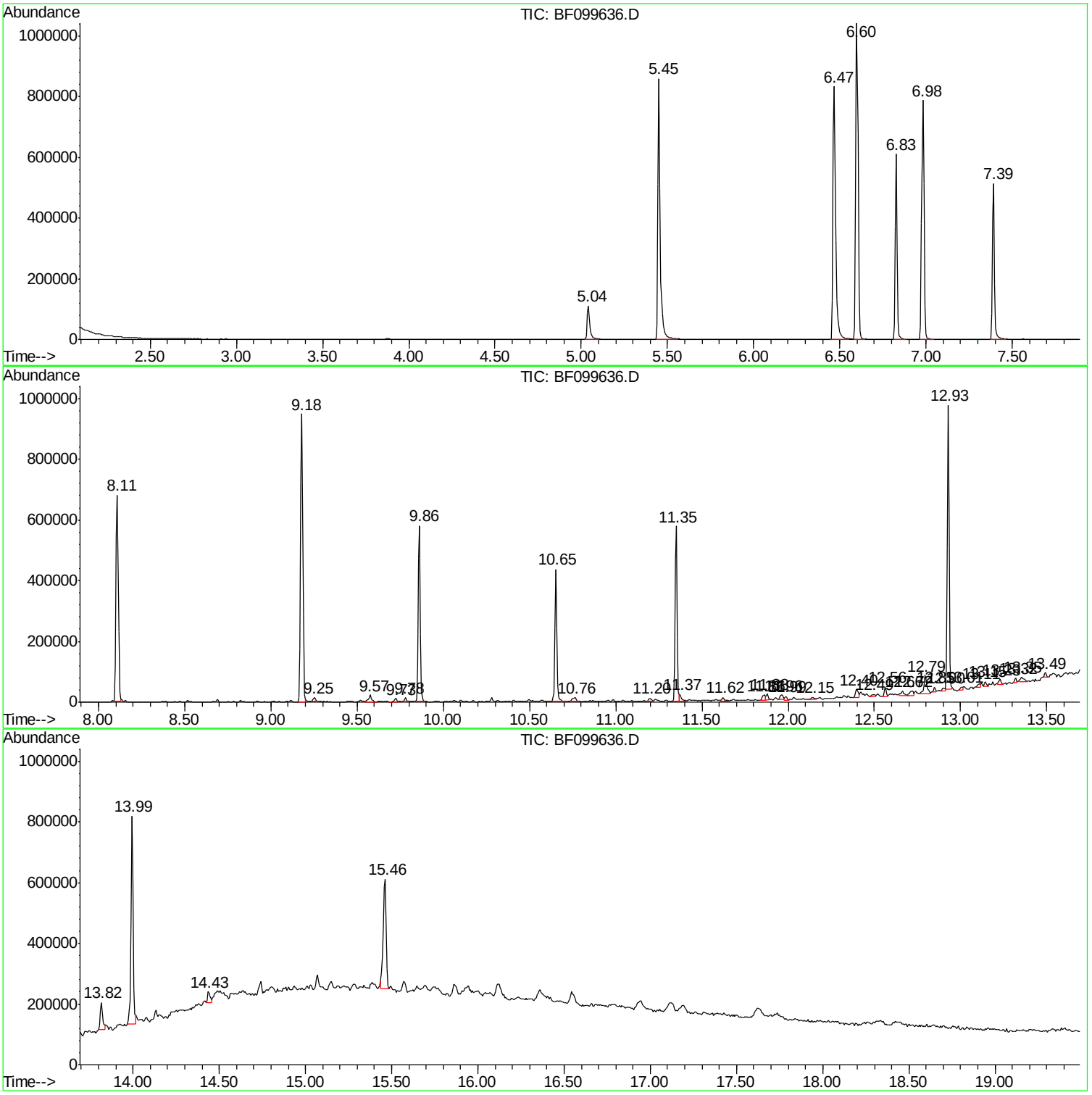
Sum of corrected areas: 9439474

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101817\
Data File : BF099636.D
Acq On : 19 Oct 2017 00:01
Operator : SJ/JU
Sample : I5935-13 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-101617-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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:\HPCHEM1\BNA F\DATA\BF101817\
Data File : BF099636.D
Acq On : 19 Oct 2017 00:01
Operator : SJ/JU
Sample : I5935-13 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-101617-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

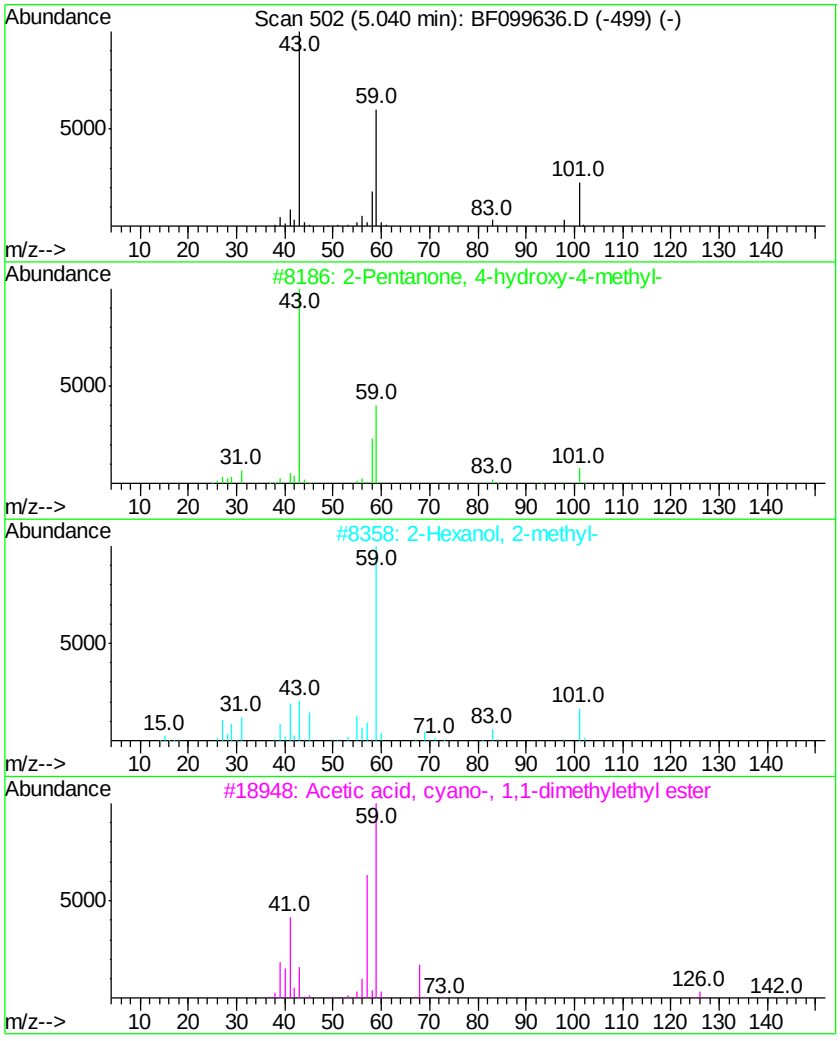
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

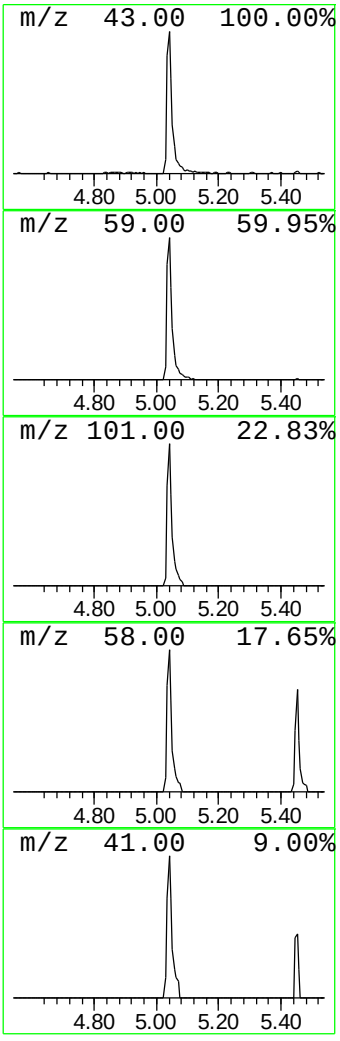
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	5.16 ng	127766	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	10
5	Acetone	58	C3H6O	000067-64-1	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101817\
Data File : BF099636.D
Acq On : 19 Oct 2017 00:01
Operator : SJ/JU
Sample : I5935-13 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-101617-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

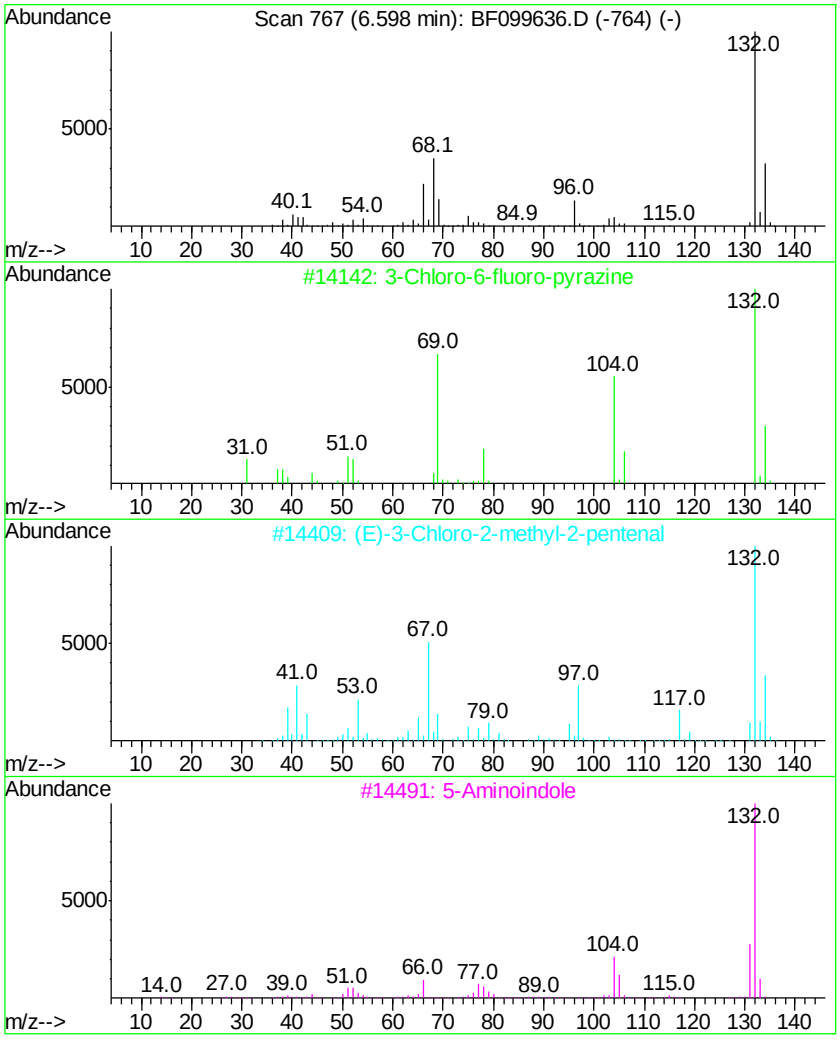
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

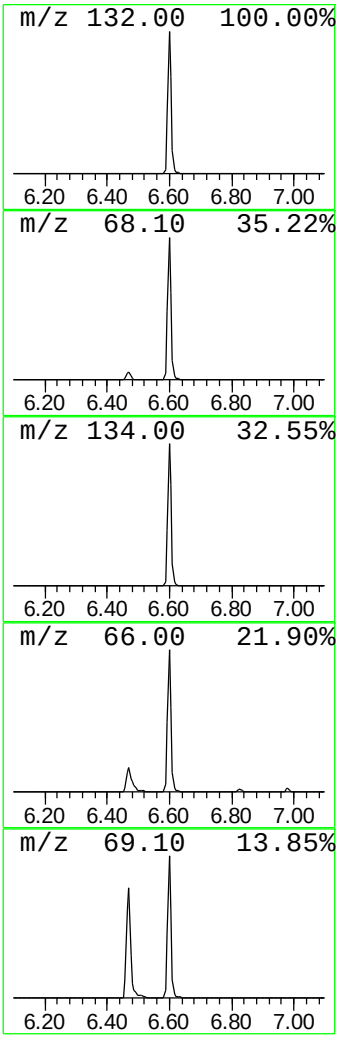
****

Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	34.35 ng	849984	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	1-Aminoindan	133	C9H11N	034698-41-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101817\
Data File : BF099636.D
Acq On : 19 Oct 2017 00:01
Operator : SJ/JU
Sample : I5935-13 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-101617-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

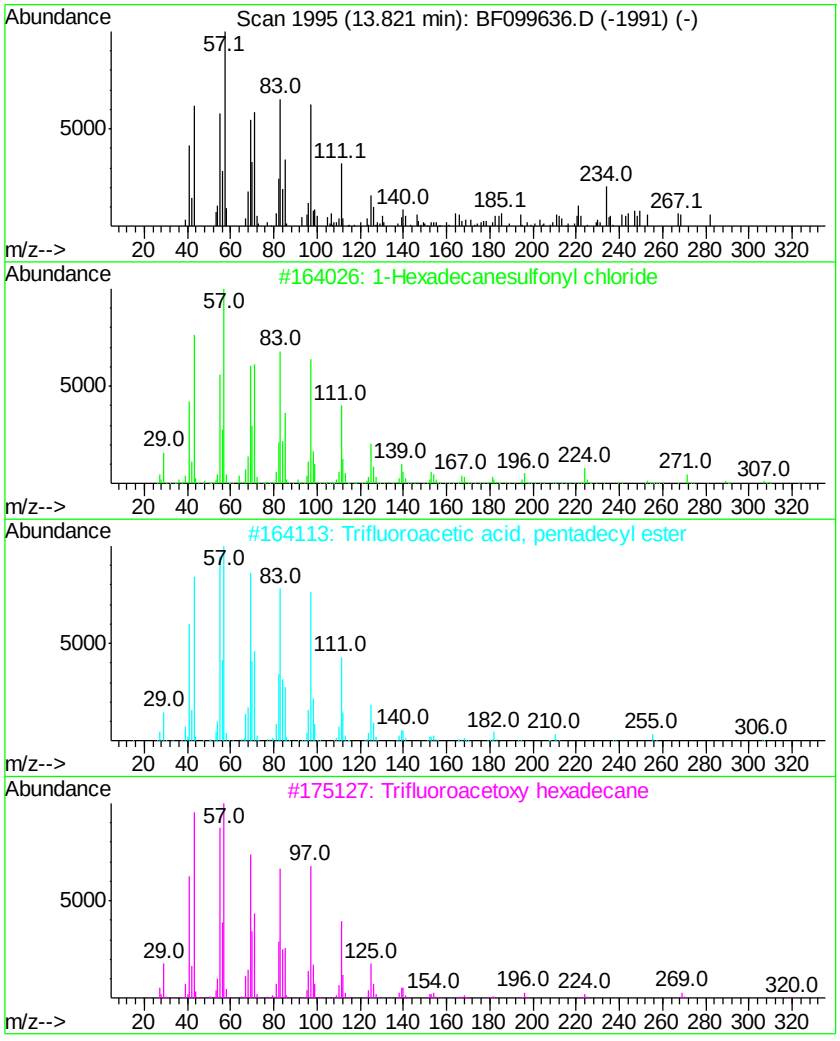
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

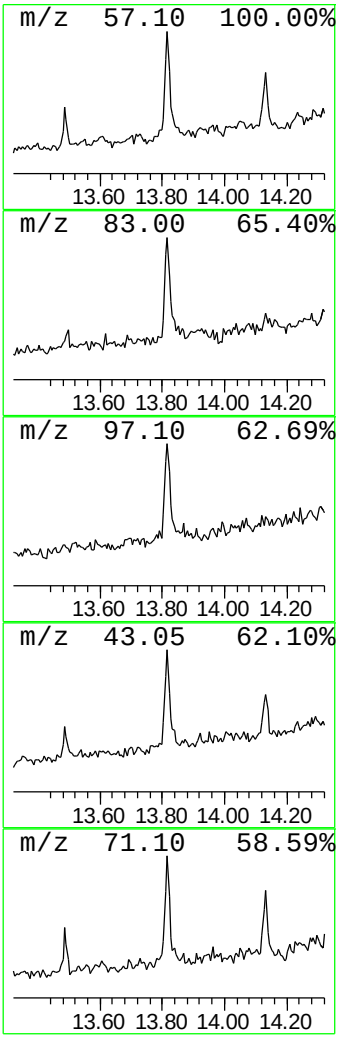
****

Peak Number 5 1-Hexadecanesulfonyl chloride Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	3.17 ng	99795	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	87
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	64
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	64
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	64
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101817\
Data File : BF099636.D
Acq On : 19 Oct 2017 00:01
Operator : SJ/JU
Sample : I5935-13 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-101617-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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...	5.04	5.2	ng	127766	1	6.83	494855	20.0
unknown6.60	6.60	34.4	ng	849984	1	6.83	494855	20.0
1-Hexadecanesulfo...	13.82	3.2	ng	99795	5	13.99	629069	20.0