LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096532.D
Acq On : 6 Jul 2017 14:47
Operator : SJ/MA
Sample : I4053-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-070317-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-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	3.069	165	167	182	rBV	31730	76260	2.91%	0.329%
2	4.904	474	479	489	rBV	284631	385204	14.70%	1.660%
3	5.328	546	551	554	rBV	2414310	2498139	95.34%	10.766%
4	6.357	715	726	735	rBV	2286601	2620112	100.00%	11.291%
5	6.487	743	748	751	rBV	2577812	2463326	94.02%	10.616%
6	6.716	783	787	790	rBV	794550	726653	27.73%	3.131%
7	6.869	809	813	817	rBV	1986727	1878557	71.70%	8.096%
8	7.275	877	882	885	rBV	1664338	1531663	58.46%	6.601%
9	7.381	893	900	906	rVB	52169	62235	2.38%	0.268%
10	7.998	1000	1005	1008	rBV	1034231	954036	36.41%	4.111%
11	9.075	1183	1188	1191	rBV	2920104	2583936	98.62%	11.135%
12	9.469	1251	1255	1258	rBV	691959	571742	21.82%	2.464%
13	9.751	1298	1303	1306	rBV	1029152	902727	34.45%	3.890%
14	10.192	1375	1378	1381	rVB	47191	40524	1.55%	0.175%
15	10.416	1409	1416	1418	rBV	21003	28529	1.09%	0.123%
16	10.533	1432	1436	1445	rVB	1161192	1048382	40.01%	4.518%
17	10.669	1456	1459	1467	rVB	71170	90483	3.45%	0.390%
18	11.116	1531	1535	1538	rBV2	65089	58605	2.24%	0.253%
19	11.227	1551	1554	1557	rBV	823980	761603	29.07%	3.282%
20	11.251	1557	1558	1561	rVV	116666	70900	2.71%	0.306%
21	11.298	1561	1566	1570	rVB2	39916	45983	1.76%	0.198%
22	11.539	1604	1607	1611	rBV2	26524	29539	1.13%	0.127%
23	11.839	1655	1658	1661	rBV	25927	29454	1.12%	0.127%
24	12.439	1756	1760	1764	rVB	252537	208092	7.94%	0.897%
25	12.557	1778	1780	1785	rBV5	31782	44363	1.69%	0.191%
26	12.663	1793	1798	1803	rBV	191464	231035	8.82%	0.996%
27	12.816	1820	1824	1828	rBV	1648893	1552737	59.26%	6.691%
28	13.063	1864	1866	1868	rVB2	42311	34416	1.31%	0.148%
29	13.721	1975	1978	1987	rVB3	141818	157316	6.00%	0.678%
30	13.863	1998	2002	2005	rBV	726302	740494	28.26%	3.191%
31	14.357	2083	2086	2090	rBV	148471	164781	6.29%	0.710%
32	14.986	2191	2193	2198	rVB	180487	198173	7.56%	0.854%
33	15.280	2239	2243	2246	rBV	366417	414693	15.83%	1.787%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096532.D
Acq On : 6 Jul 2017 14:47
Operator : SJ/MA
Sample : I4053-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-070317-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-BF070117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 23204692

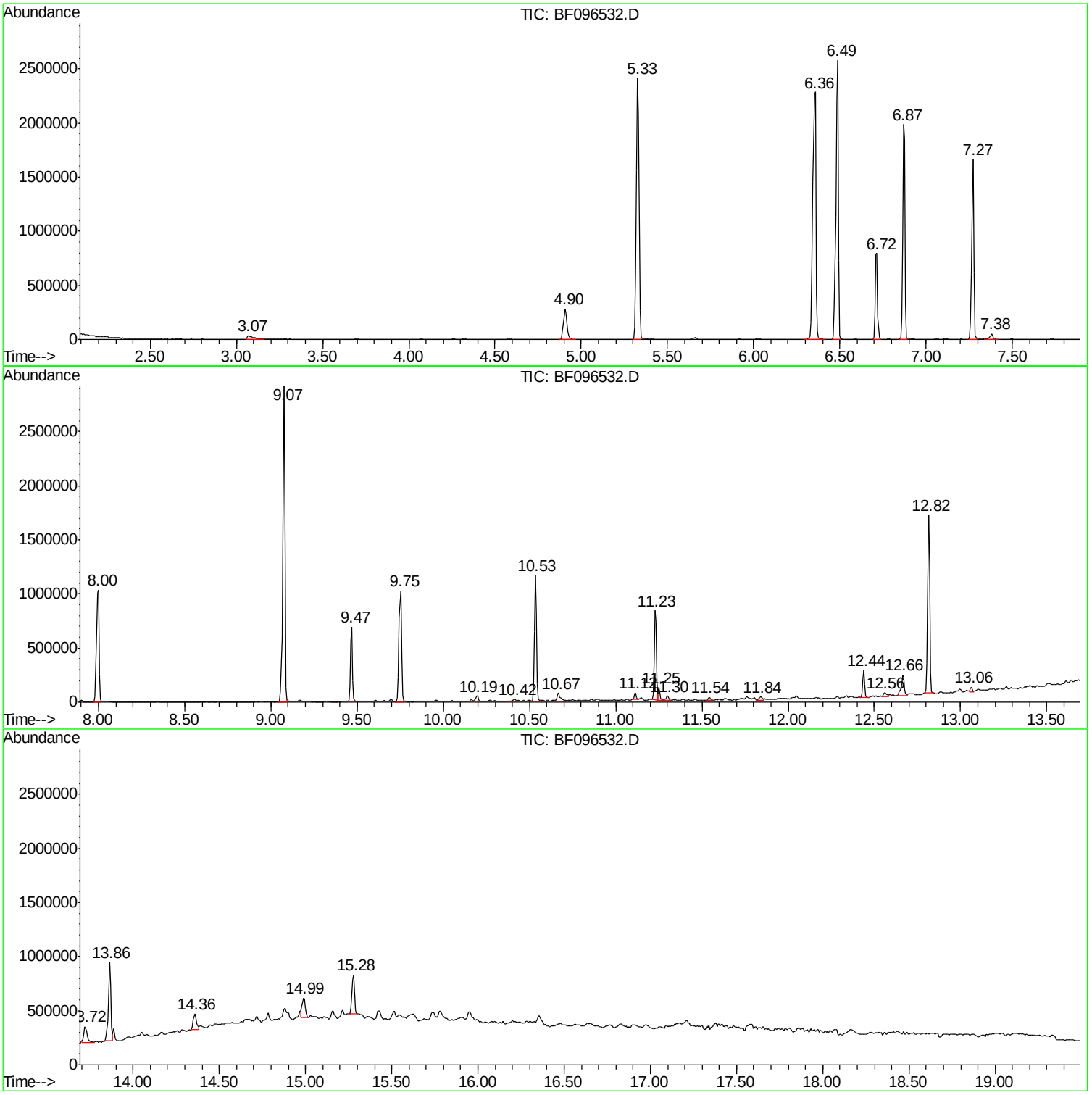
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096532.D
Acq On : 6 Jul 2017 14:47
Operator : SJ/MA
Sample : I4053-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-070317-E

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\BF070617\
Data File : BF096532.D
Acq On : 6 Jul 2017 14:47
Operator : SJ/MA
Sample : I4053-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-070317-E

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

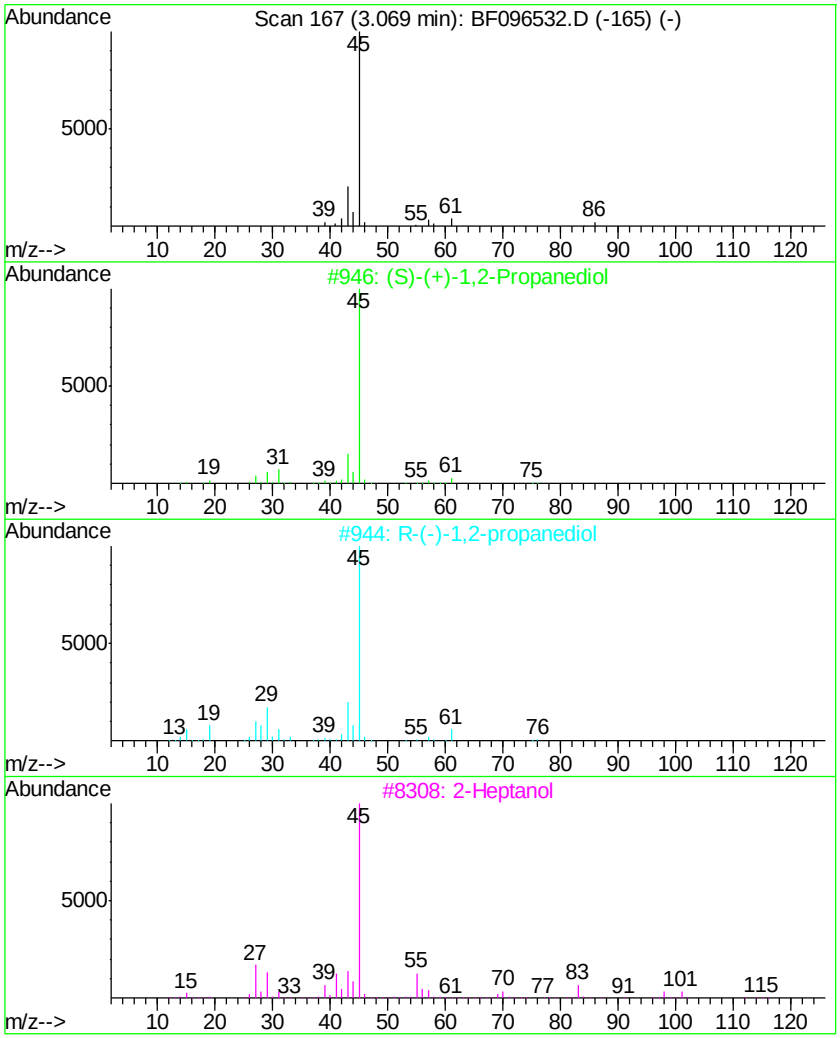
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

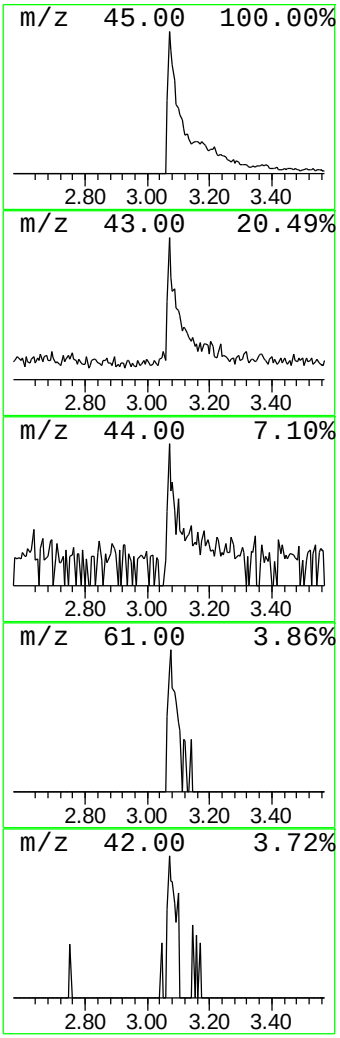
****

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.07	2.10 ng	76260	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
3	2-Heptanol	116	C7H16O	000543-49-7	9
4	3-Ethyl-2-pentanol	116	C7H16O	000609-27-8	9
5	Butanenitrile, 2-(methoxymethoxy)	129	C6H11NO2	1000196-86-5	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096532.D
Acq On : 6 Jul 2017 14:47
Operator : SJ/MA
Sample : I4053-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-070317-E

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

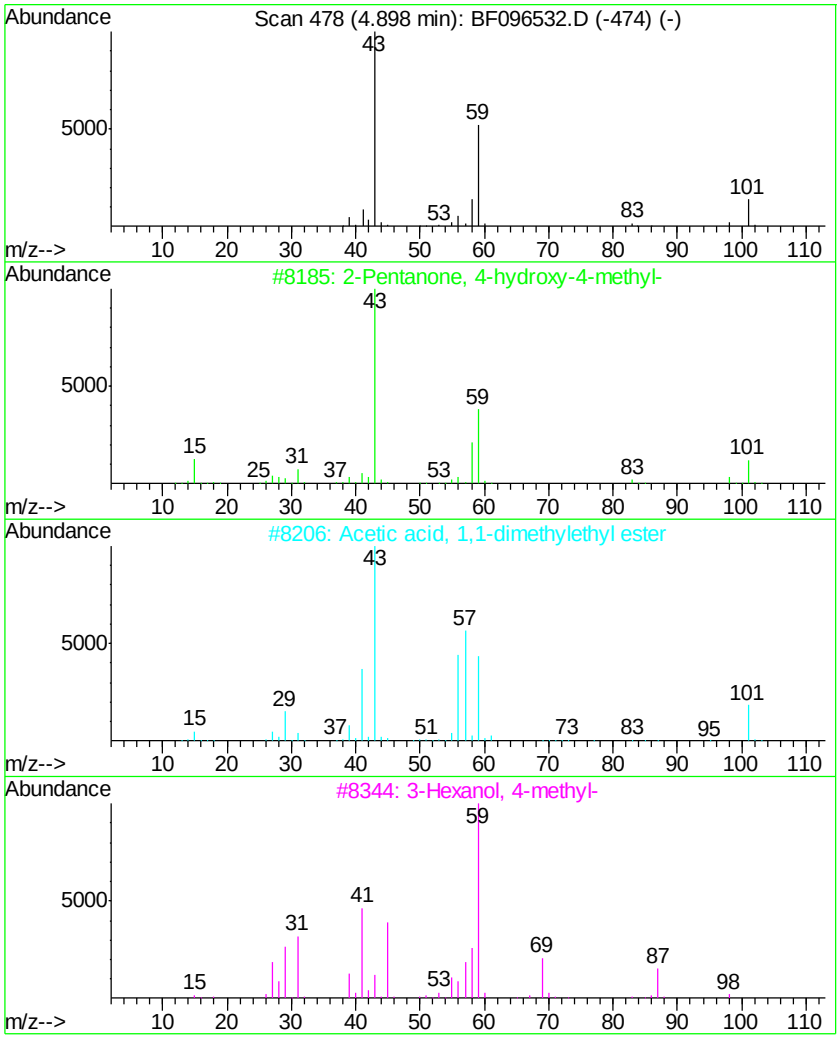
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

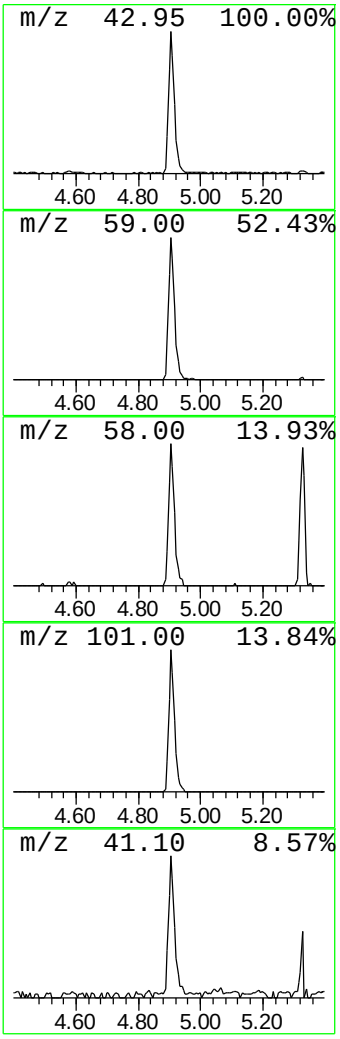
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	10.60 ng	385204	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	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096532.D
Acq On : 6 Jul 2017 14:47
Operator : SJ/MA
Sample : I4053-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-070317-E

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

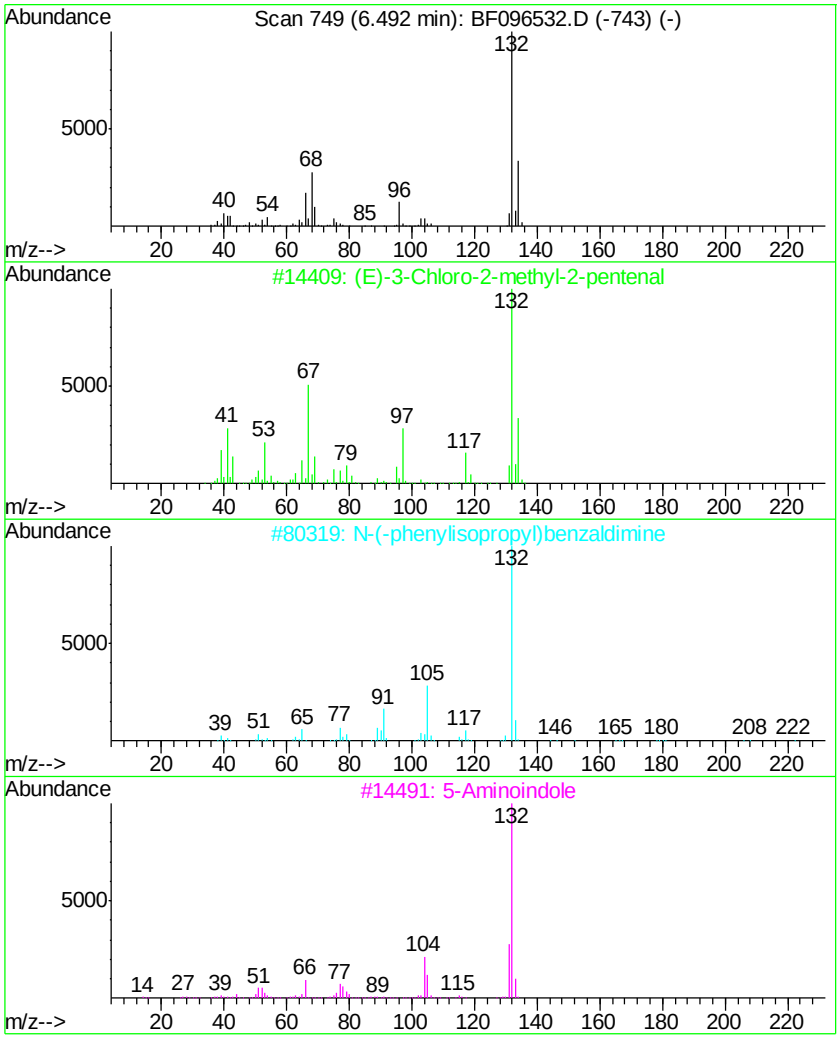
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

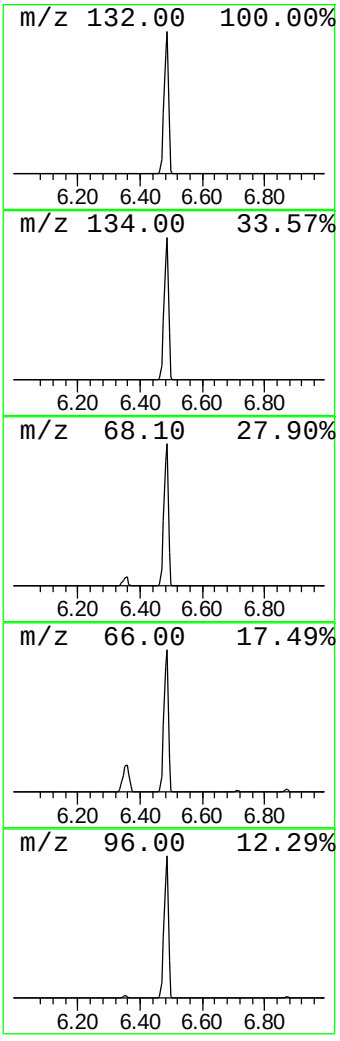
****

Peak Number 3 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	67.80 ng	2463330	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	N-(-phenylisopropyl)benzaldimine	223	C16H17N	1000379-01-3	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096532.D
Acq On : 6 Jul 2017 14:47
Operator : SJ/MA
Sample : I4053-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-070317-E

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

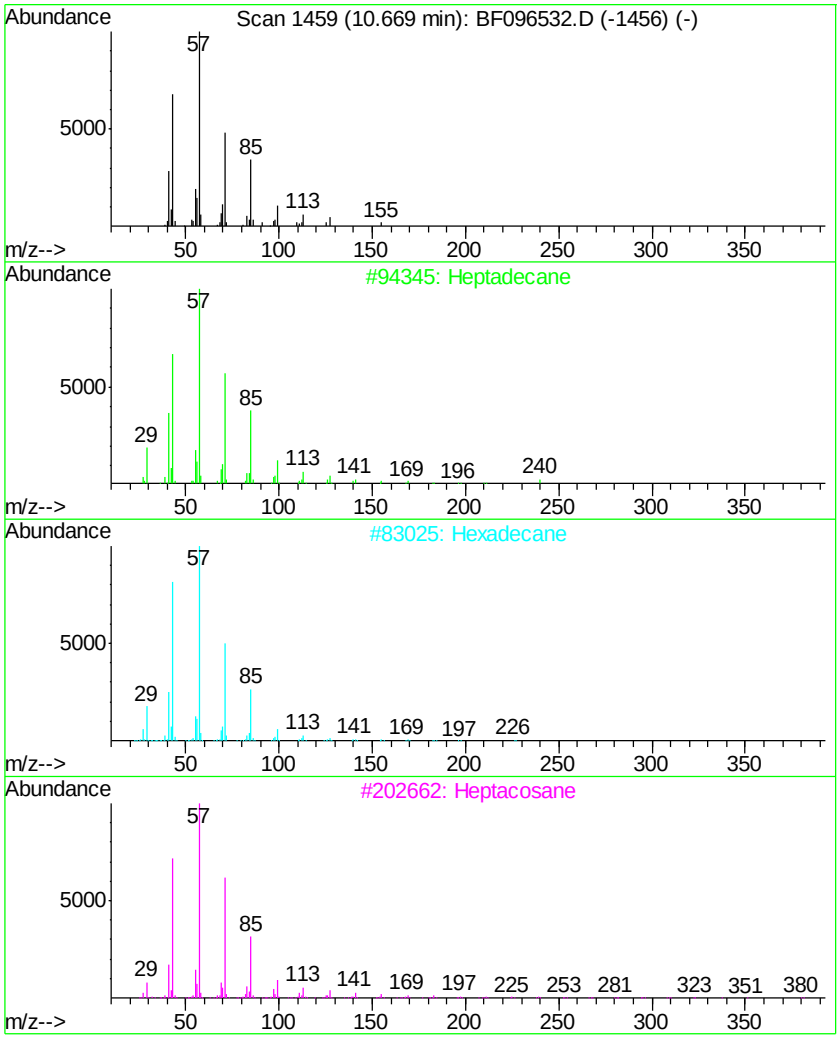
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

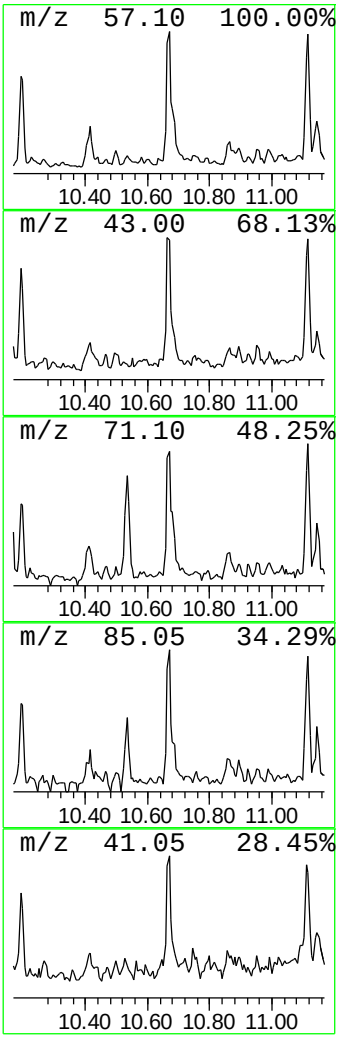
****

Peak Number 5 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	2.38 ng	90483	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	80
2	Hexadecane	226	C16H34	000544-76-3	78
3	Heptacosane	380	C27H56	000593-49-7	78
4	Pentadecane	212	C15H32	000629-62-9	72
5	Tetracosane	338	C24H50	000646-31-1	72





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096532.D
Acq On : 6 Jul 2017 14:47
Operator : SJ/MA
Sample : I4053-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-070317-E

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

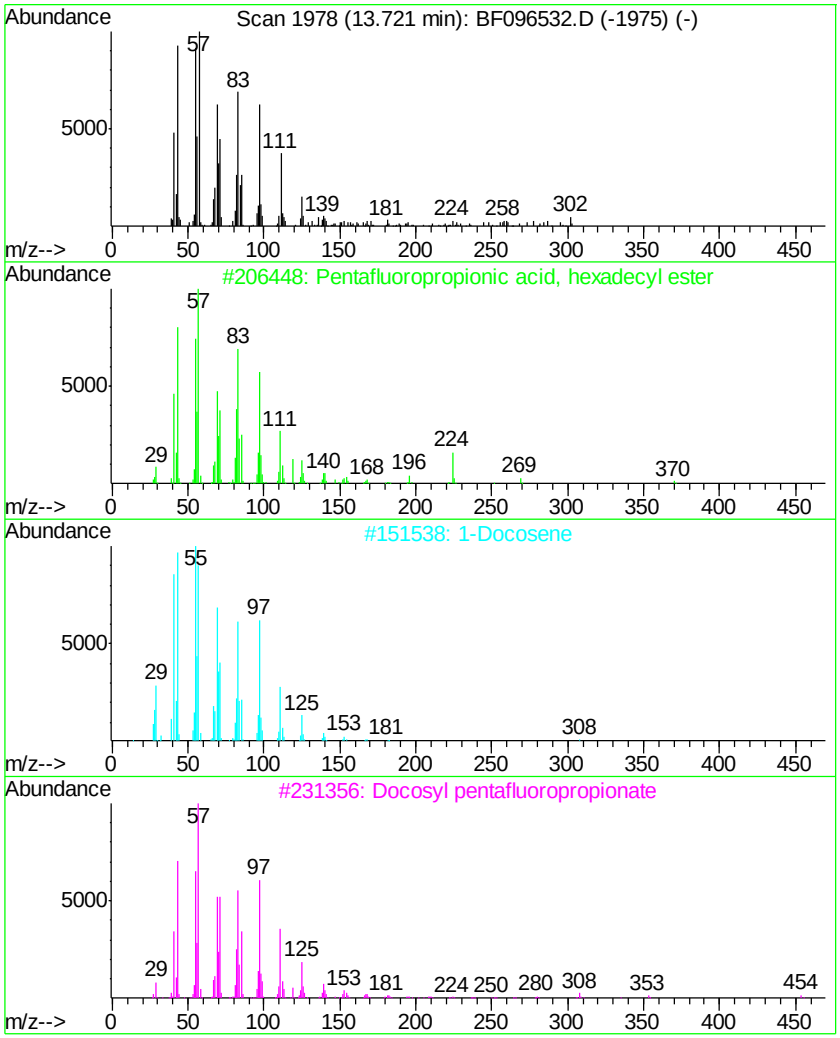
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

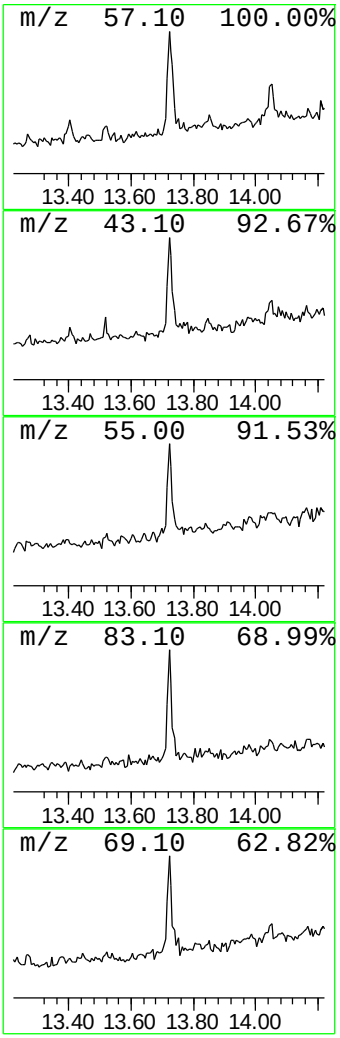
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	4.25 ng	157316	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
2	1-Docosene	308	C22H44	001599-67-3	90
3	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	87
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	87
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	87





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096532.D
Acq On : 6 Jul 2017 14:47
Operator : SJ/MA
Sample : I4053-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-070317-E

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

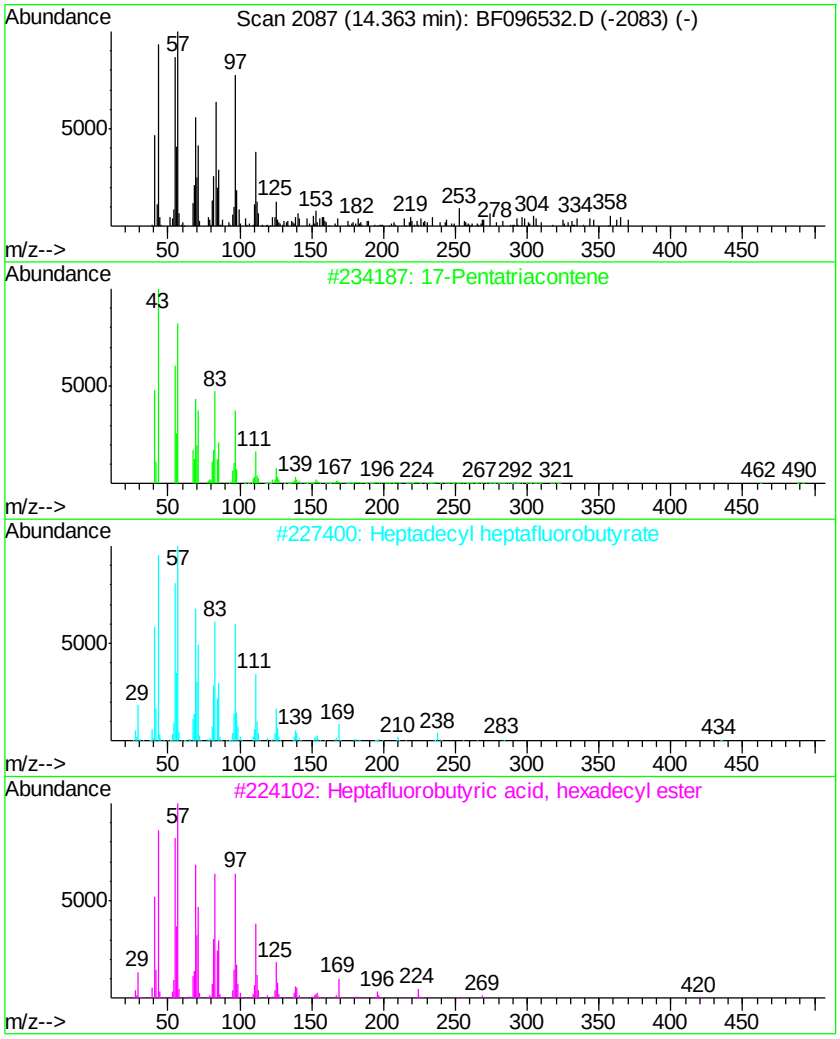
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

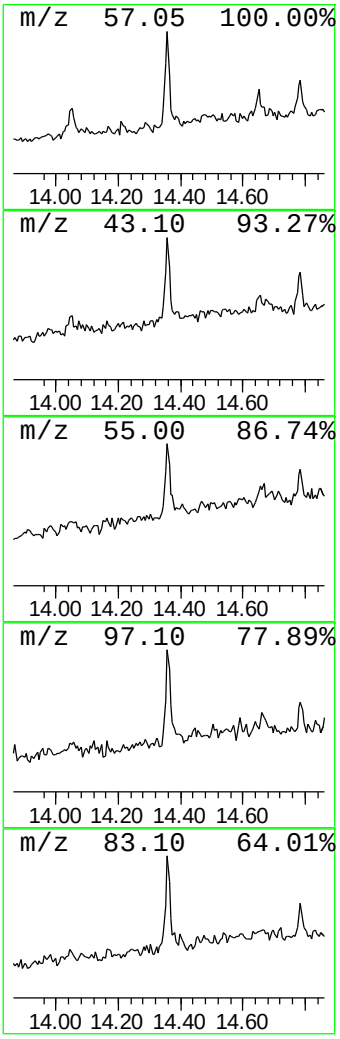
****

Peak Number 7 17-Pentatriacontene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	4.45 ng	164781	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	87
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	83
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	74
4	Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	68
5	1-Hexacosanol	382	C26H54O	000506-52-5	68





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Acq On : 6 Jul 2017 14:47
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Sample : I4053-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-070317-E

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

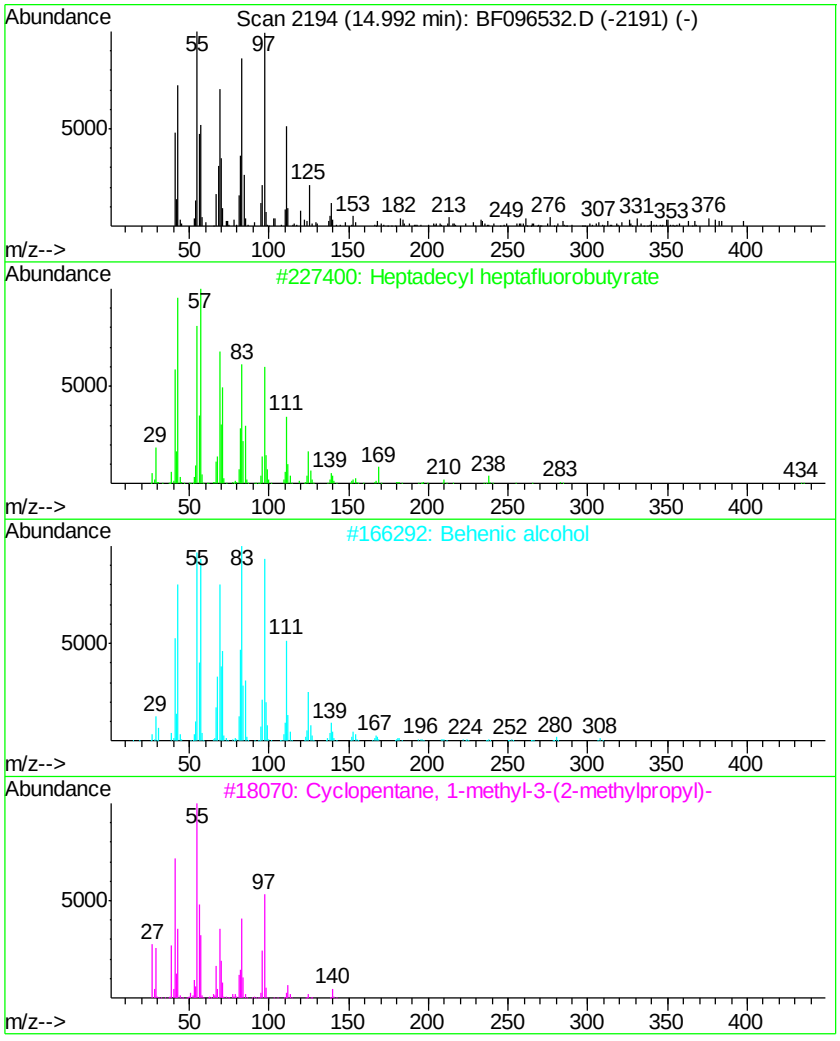
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

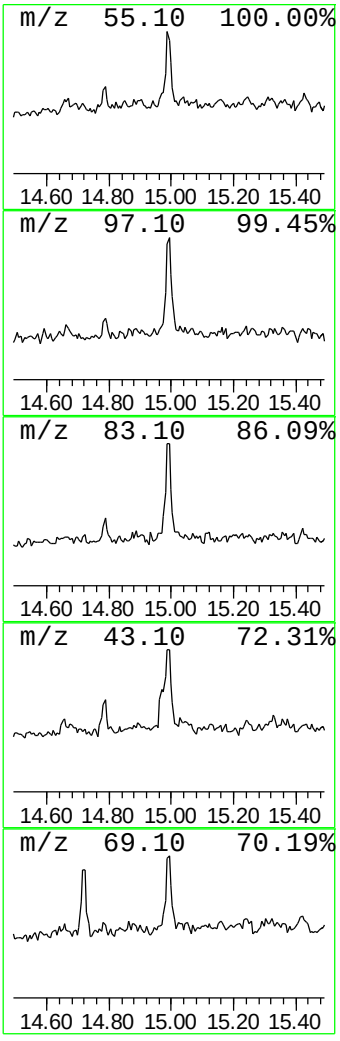
****

Peak Number 8 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	9.56 ng	198173	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
2	Behenic alcohol	326	C22H46O	000661-19-8	78
3	Cyclopentane, 1-methyl-3-(2-meth...	140	C10H20	029053-04-1	68
4	4-Methyl-E-9-octadecene	266	C19H38	1000130-87-1	64
5	1-Heptacosanol	396	C27H56O	002004-39-9	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096532.D
Acq On : 6 Jul 2017 14:47
Operator : SJ/MA
Sample : I4053-13
Misc :
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Instrument : BNA_F
ClientSampleId : CL-02-070317-E

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
(S)-(+)-1,2-Propa...	3.07	2.1	ng	76260	1	6.72	726653	20.0
2-Pentanone, 4-hy...	4.90	10.6	ng	385204	1	6.72	726653	20.0
unknown6.49	6.49	67.8	ng	2463330	1	6.72	726653	20.0
Heptadecane	10.67	2.4	ng	90483	4	11.23	761603	20.0
Pentafluoropropio...	13.72	4.3	ng	157316	5	13.86	740494	20.0
17-Pentatriacontene	14.36	4.5	ng	164781	5	13.86	740494	20.0
Heptadecyl heptaf...	14.99	9.6	ng	198173	6	15.28	414693	20.0