LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050917\
Data File : BF095040.D
Acq On : 10 May 2017 00:56
Operator : SJ/MA
Sample : I3027-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-2-3-COMP

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-BF050217.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	4.119	367	371	386	rBV	101594	222438	7.62%	0.868%
2	5.054	525	530	553	rBV	362805	751681	25.75%	2.934%
3	5.689	633	638	670	rBV	1214478	2540968	87.04%	9.918%
4	7.278	903	908	922	rBV	1391998	2390874	81.90%	9.332%
5	7.389	922	927	946	rVB	1751657	2919211	100.00%	11.394%
6	7.713	978	982	992	rVB	514384	573164	19.63%	2.237%
7	7.954	1018	1023	1034	rBV	1692980	1975202	67.66%	7.709%
8	8.613	1130	1135	1154	rBV	1086700	1549477	53.08%	6.048%
9	9.730	1321	1325	1343	rBV	563567	750756	25.72%	2.930%
10	11.507	1621	1627	1641	rBV	2222159	2828335	96.89%	11.039%
11	12.024	1711	1715	1722	rBV	62167	69109	2.37%	0.270%
12	12.201	1741	1745	1755	rBV	138300	188730	6.47%	0.737%
13	12.560	1801	1806	1818	rBV2	604957	862505	29.55%	3.366%
14	12.824	1843	1851	1855	rBV	28963	32612	1.12%	0.127%
15	12.871	1855	1859	1863	rBV2	29875	37185	1.27%	0.145%
16	13.401	1946	1949	1956	rBV3	32584	61186	2.10%	0.239%
17	13.859	2021	2027	2040	rBV	1156265	1694026	58.03%	6.612%
18	14.171	2076	2080	2083	rBV	40990	48572	1.66%	0.190%
19	14.906	2200	2205	2210	rBV2	24624	31131	1.07%	0.122%
20	14.965	2210	2215	2231	rVB	519426	798905	27.37%	3.118%
21	15.936	2373	2380	2394	rBV	232093	321013	11.00%	1.253%
22	17.018	2559	2564	2577	rBV2	136089	201215	6.89%	0.785%
23	17.130	2580	2583	2588	rVB	38412	42360	1.45%	0.165%
24	17.289	2605	2610	2614	rBV	1921966	2308710	79.09%	9.011%
25	17.983	2721	2728	2737	rBV	807425	956187	32.75%	3.732%
26	18.089	2743	2746	2754	rVB	41139	55977	1.92%	0.218%
27	18.530	2817	2821	2833	rBV2	70292	145825	5.00%	0.569%
28	18.630	2834	2838	2846	rVV	533448	612594	20.98%	2.391%
29	19.653	3008	3012	3017	rBV3	39695	60608	2.08%	0.237%
30	20.041	3075	3078	3081	rBV4	26551	32321	1.11%	0.126%
31	20.300	3117	3122	3129	rBV	381537	520267	17.82%	2.031%
32	20.759	3198	3200	3205	rBV3	34242	37343	1.28%	0.146%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050917\
Data File : BF095040.D
Acq On : 10 May 2017 00:56
Operator : SJ/MA
Sample : I3027-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-2-3-COMP

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-BF050217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 25620487

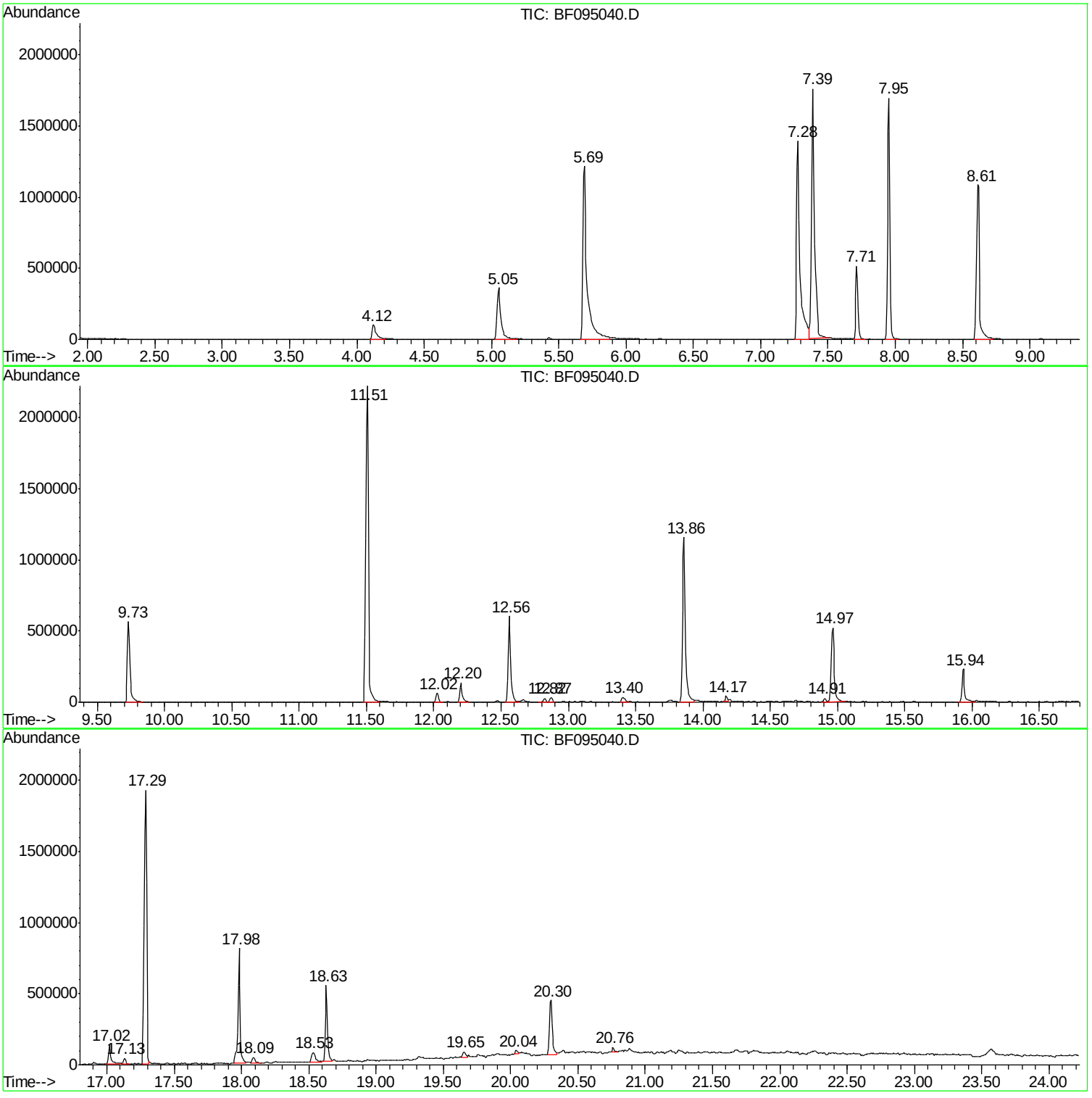
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050917\
Data File : BF095040.D
Acq On : 10 May 2017 00:56
Operator : SJ/MA
Sample : I3027-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-2-3-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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\BF050917\
Data File : BF095040.D
Acq On : 10 May 2017 00:56
Operator : SJ/MA
Sample : I3027-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-2-3-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

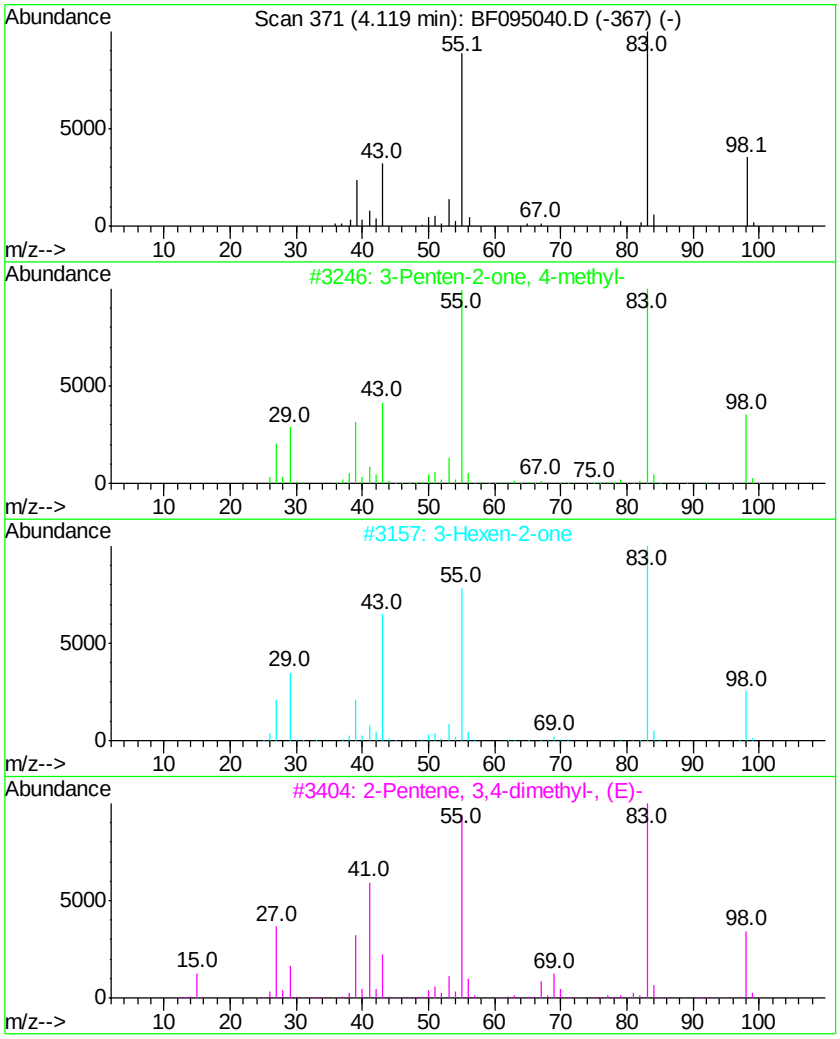
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

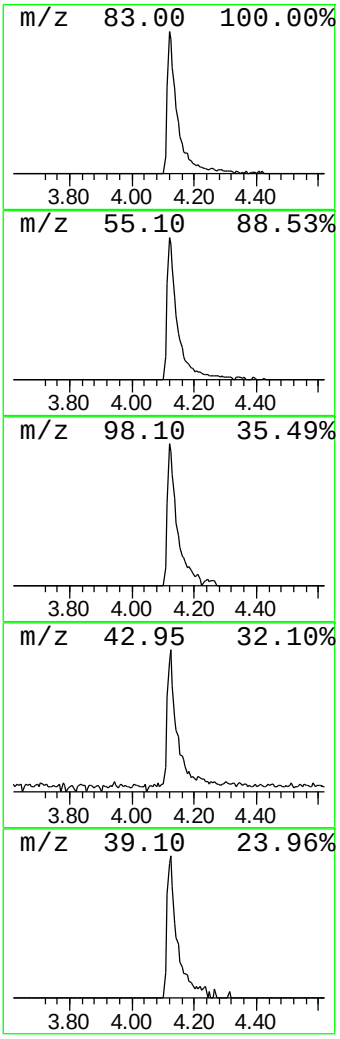
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.12	7.76 ng	222438	1,4-Dichlorobenzene-d4	7.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	78





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050917\
Data File : BF095040.D
Acq On : 10 May 2017 00:56
Operator : SJ/MA
Sample : I3027-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-2-3-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

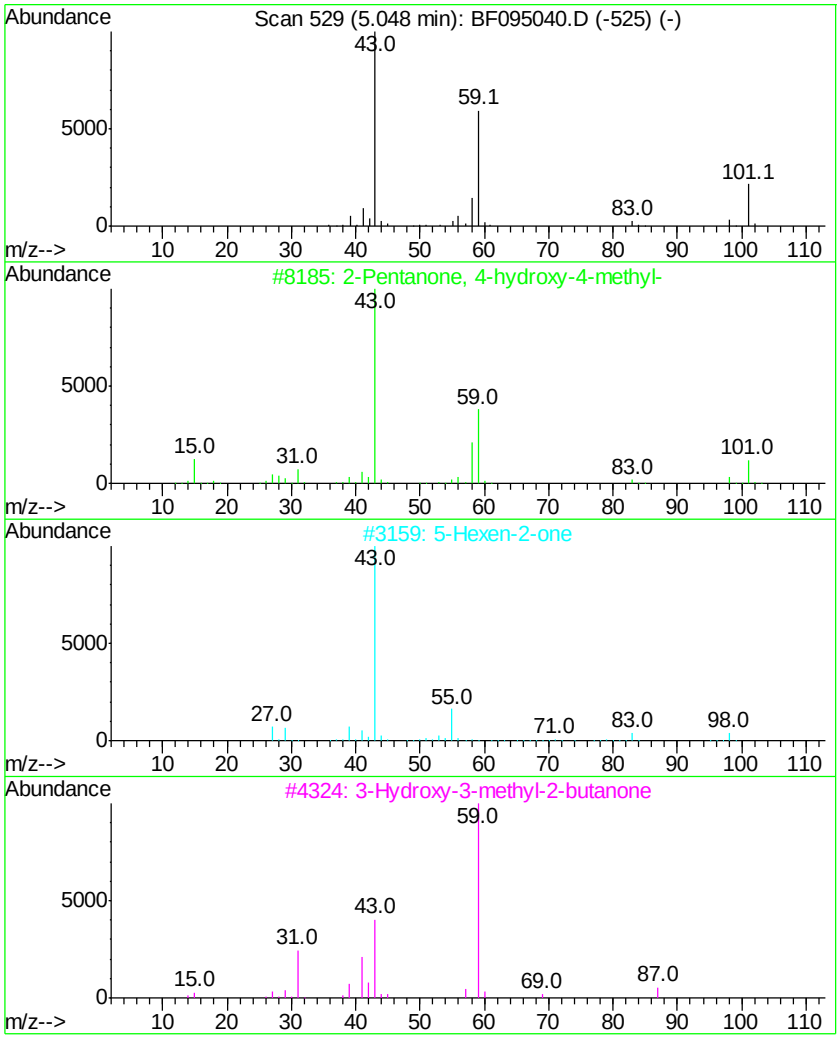
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

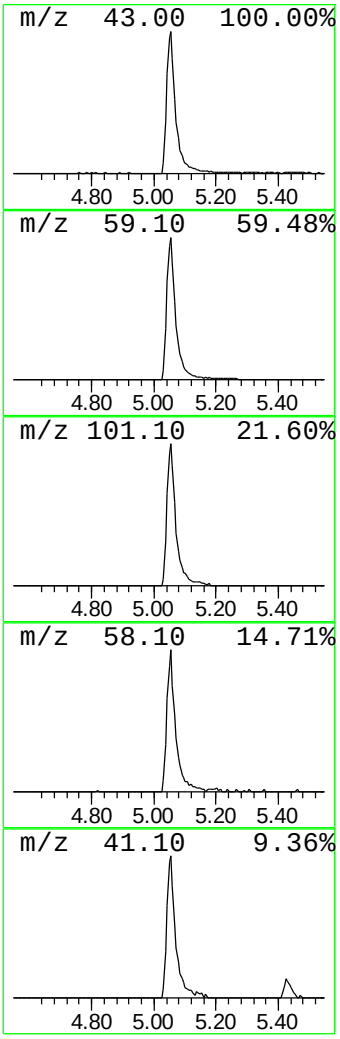
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	26.23 ng	751681	1,4-Dichlorobenzene-d4	7.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9
5	3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050917\
Data File : BF095040.D
Acq On : 10 May 2017 00:56
Operator : SJ/MA
Sample : I3027-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-2-3-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

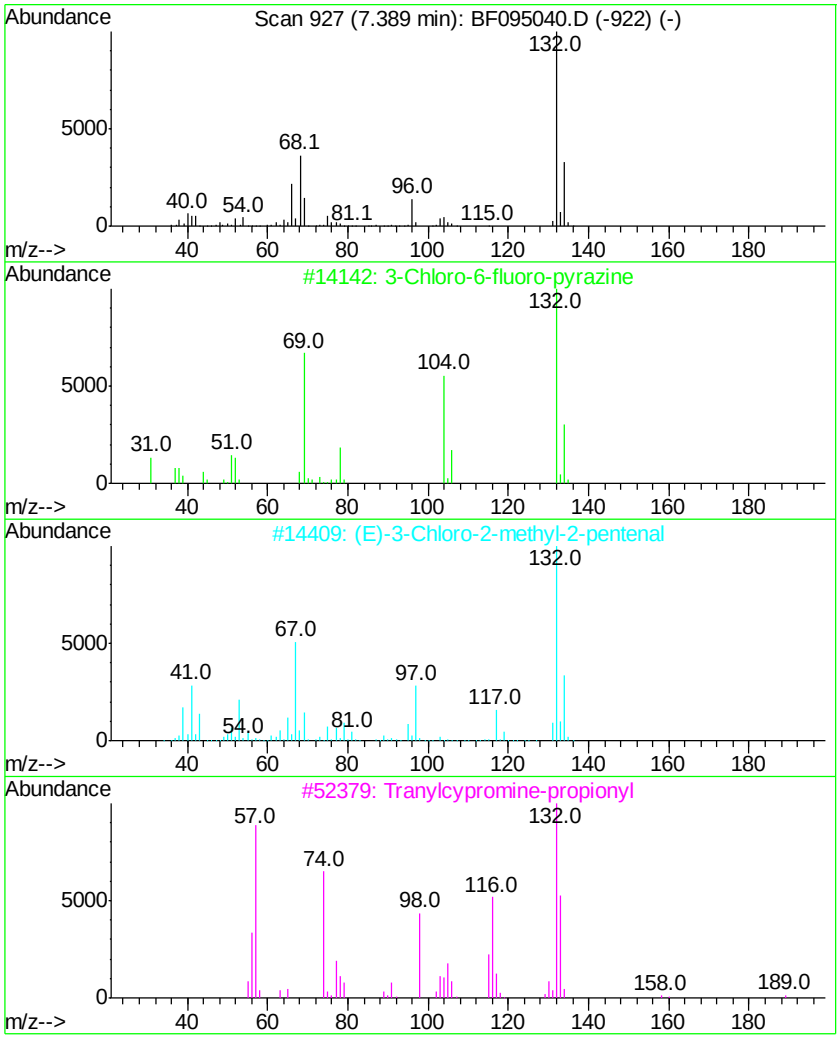
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

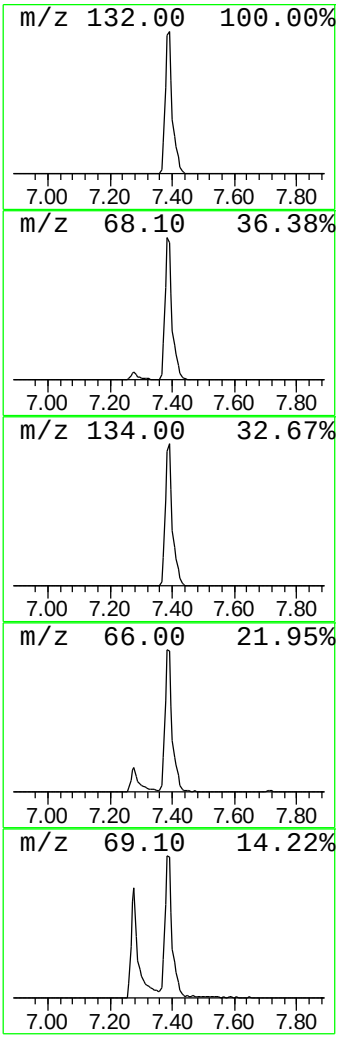
****

Peak Number 3 unknown7.39 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.39	101.86 ng	2919210	1,4-Dichlorobenzene-d4	7.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050917\
Data File : BF095040.D
Acq On : 10 May 2017 00:56
Operator : SJ/MA
Sample : I3027-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-2-3-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

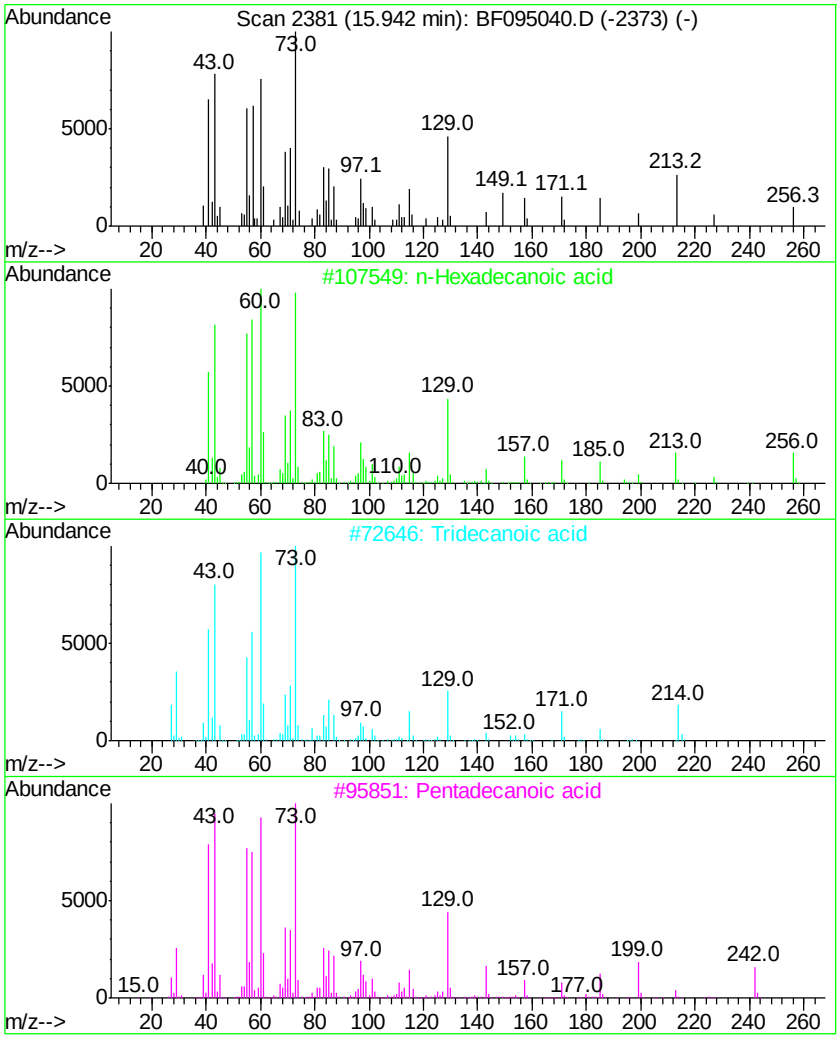
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

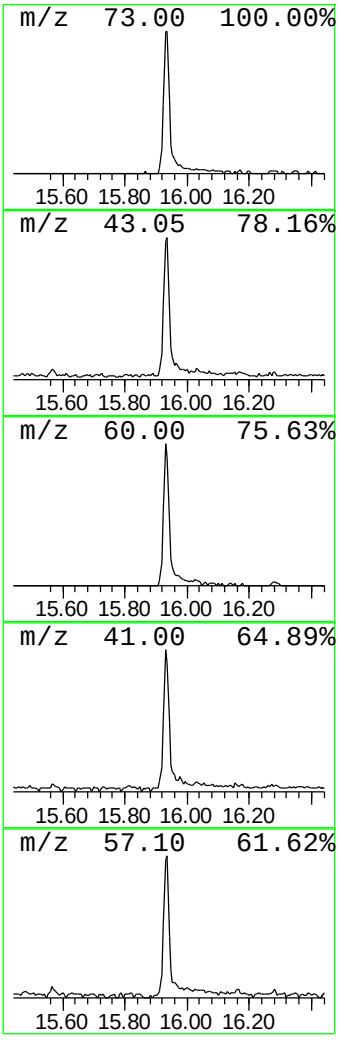
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	8.04 ng	321013	Phenanthrene-d10	14.97

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	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050917\
Data File : BF095040.D
Acq On : 10 May 2017 00:56
Operator : SJ/MA
Sample : I3027-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-2-3-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

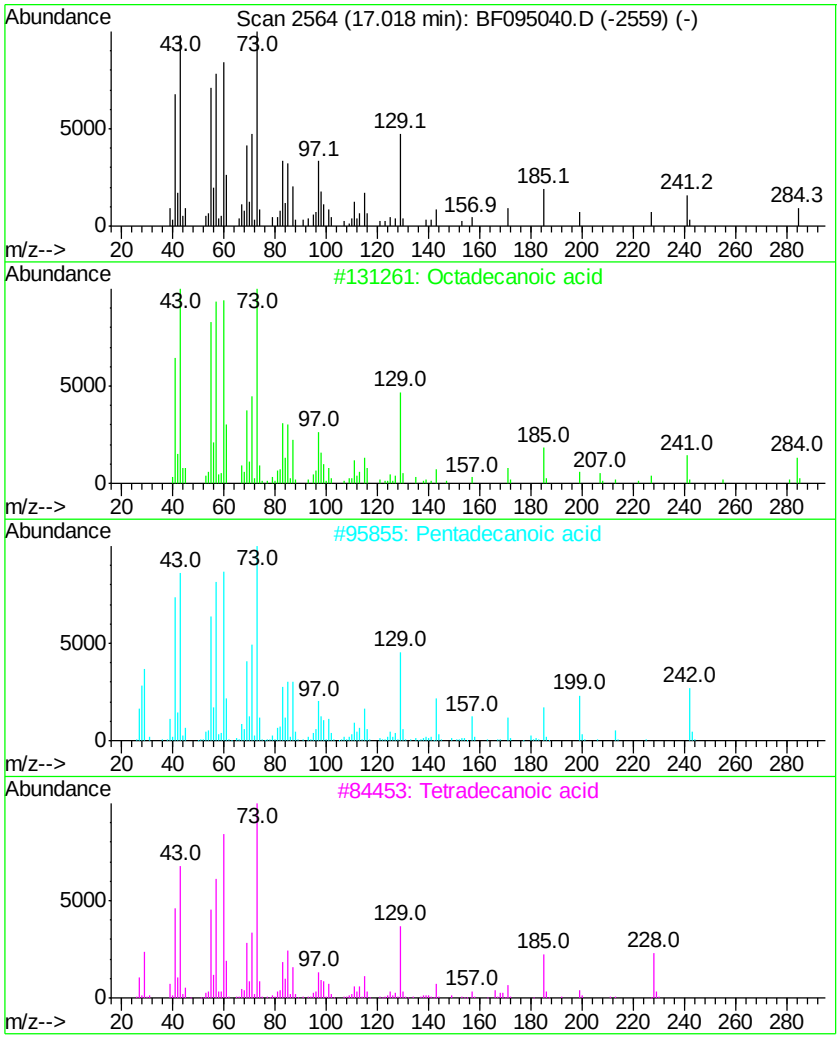
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

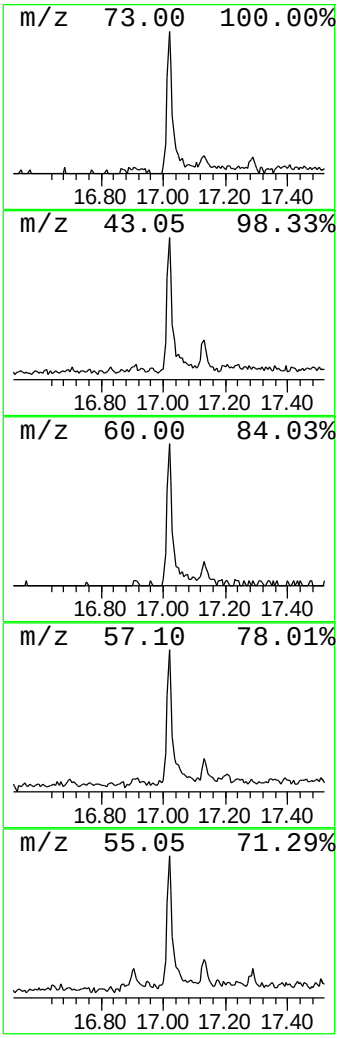
****

Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.02	6.57 ng	201215	Chrysene-d12	18.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050917\
Data File : BF095040.D
Acq On : 10 May 2017 00:56
Operator : SJ/MA
Sample : I3027-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-2-3-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

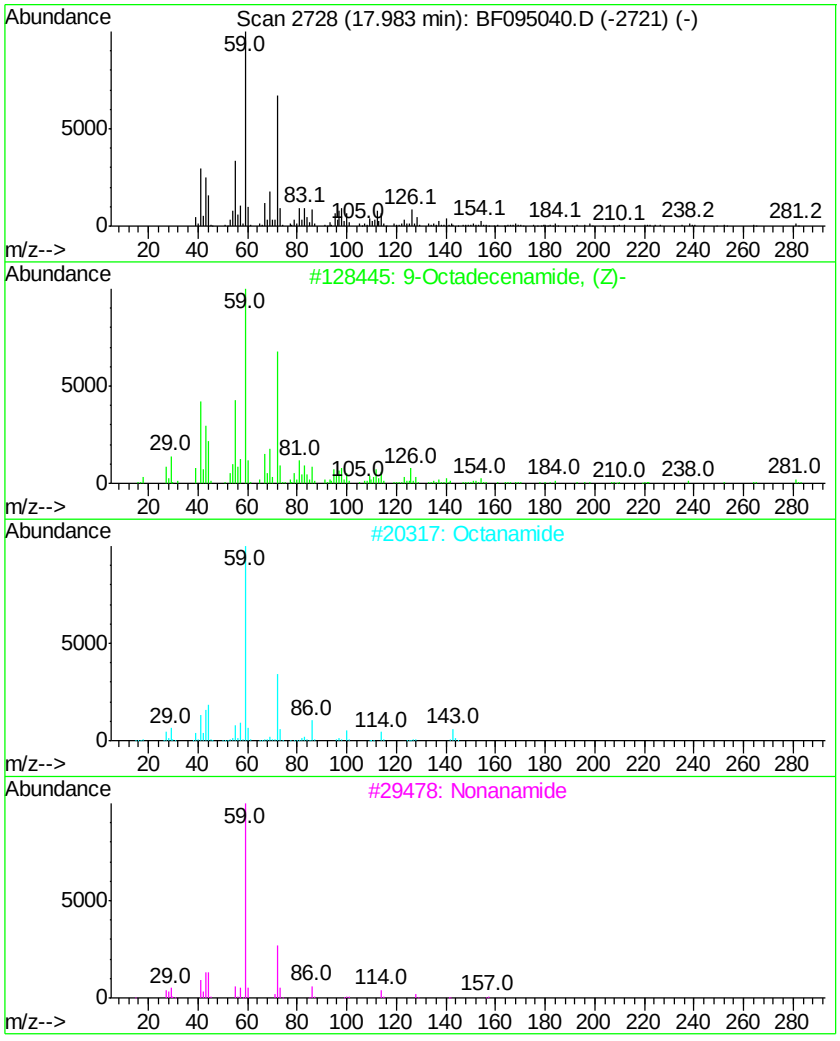
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

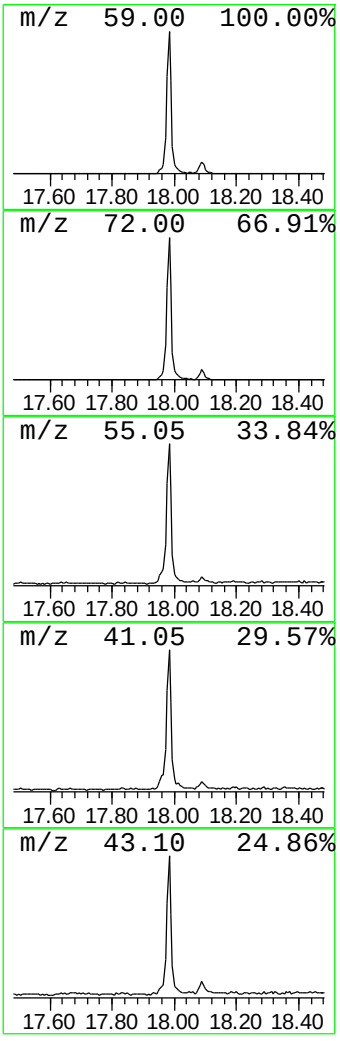
****

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.98	31.22 ng	956187	Chrysene-d12	18.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2	Octanamide	143	C8H17NO	000629-01-6	53
3	Nonanamide	157	C9H19NO	001120-07-6	53
4	Dodecanamide	199	C12H25NO	001120-16-7	53
5	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	50





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050917\
Data File : BF095040.D
Acq On : 10 May 2017 00:56
Operator : SJ/MA
Sample : I3027-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-2-3-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

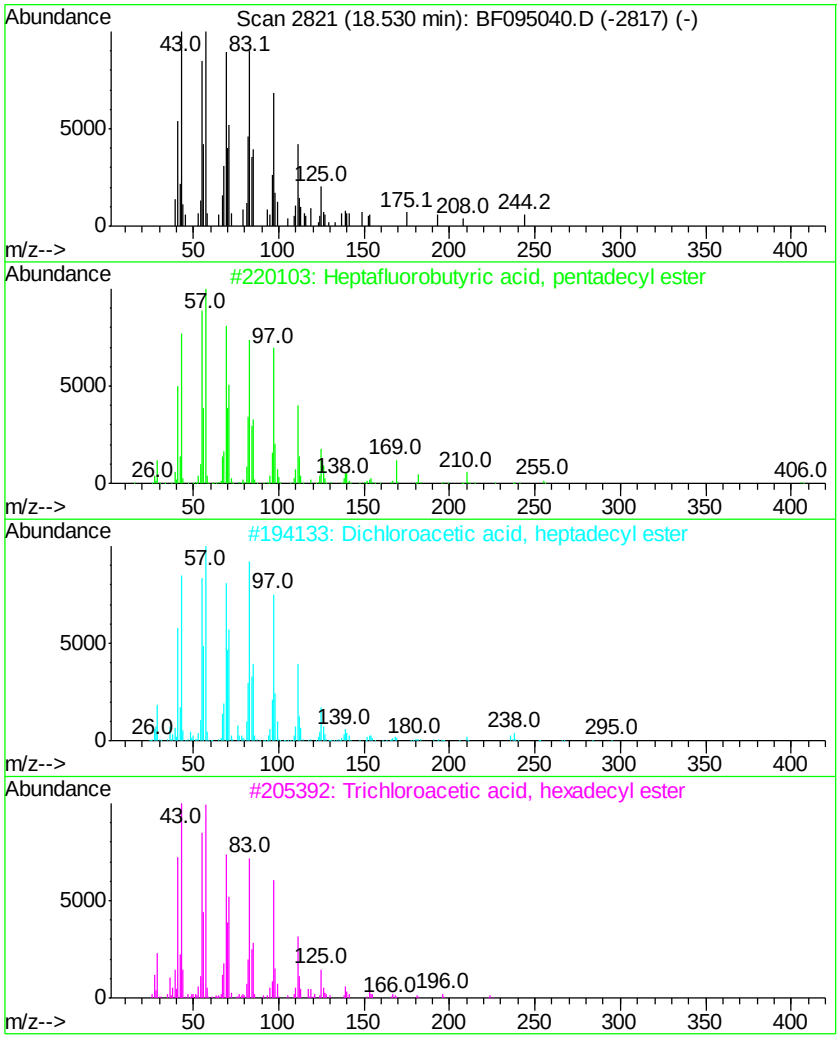
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

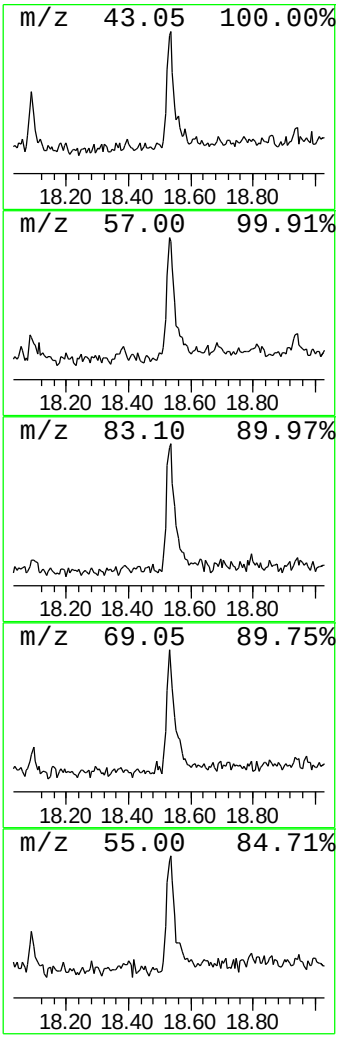
****

Peak Number 8 Heptafluorobutyric acid, pe... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.53	4.76 ng	145825	Chrysene-d12	18.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
4	Behenic alcohol	326	C22H46O	000661-19-8	90
5	1-Heneicosanol	312	C21H44O	015594-90-8	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050917\
Data File : BF095040.D
Acq On : 10 May 2017 00:56
Operator : SJ/MA
Sample : I3027-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-2-3-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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
3-Penten-2-one, 4...	4.12	7.8	ng	222438	1	7.71	573164	20.0
2-Pentanone, 4-hy...	5.05	26.2	ng	751681	1	7.71	573164	20.0
unknown7.39	7.39	101.9	ng	2919210	1	7.71	573164	20.0
n-Hexadecanoic acid	15.94	8.0	ng	321013	4	14.97	798905	20.0
Octadecanoic acid	17.02	6.6	ng	201215	5	18.63	612594	20.0
9-Octadecenamide,...	17.98	31.2	ng	956187	5	18.63	612594	20.0
Heptafluorobutyri...	18.53	4.8	ng	145825	5	18.63	612594	20.0