LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
Data File : BF092085.D
Acq On : 4 Jan 2017 23:14
Operator : UM/SJ
Sample : I1004-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-23

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-BF122116.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	2.013	7	11	12	rBV2	26268	61301	1.15%	0.169%
2	4.093	191	193	198	rBV	55380	84682	1.59%	0.234%
3	4.230	203	205	208	rVB	46755	62633	1.18%	0.173%
4	4.801	252	255	265	rBV	766357	955545	17.93%	2.638%
5	5.259	293	295	298	rBV	2197268	2776236	52.10%	7.664%
6	6.322	385	388	395	rBV	2038383	2032468	38.14%	5.610%
7	6.436	395	398	400	rBV	5356350	5328719	100.00%	14.709%
8	6.665	415	418	420	rBV	964882	1298091	24.36%	3.583%
9	6.813	429	431	434	rBV	4148442	4679025	87.81%	12.916%
10	7.236	464	468	470	rBV	3590993	4508425	84.61%	12.445%
11	7.945	527	530	533	rBV	1930521	1719397	32.27%	4.746%
12	9.031	622	625	627	rBV	3429724	3763184	70.62%	10.388%
13	9.693	680	683	685	rBV	958522	815042	15.30%	2.250%
14	10.139	718	722	724	rBV	57642	56315	1.06%	0.155%
15	10.482	749	752	755	rBV2	1900406	2101503	39.44%	5.801%
16	10.608	761	763	768	rVB	65170	77548	1.46%	0.214%
17	11.168	810	812	815	rVB	678231	722278	13.55%	1.994%
18	11.716	858	860	863	rBV	172945	265804	4.99%	0.734%
19	12.505	927	929	931	rBV	365568	331976	6.23%	0.916%
20	12.768	948	952	954	rBV	2435948	3234732	60.70%	8.929%
21	13.660	1028	1030	1034	rBV	63340	72432	1.36%	0.200%
22	13.797	1040	1042	1045	rBV	601899	658077	12.35%	1.817%
23	15.168	1160	1162	1165	rBV	343348	514860	9.66%	1.421%
24	19.409	1530	1533	1535	rBV3	33587	106285	1.99%	0.293%

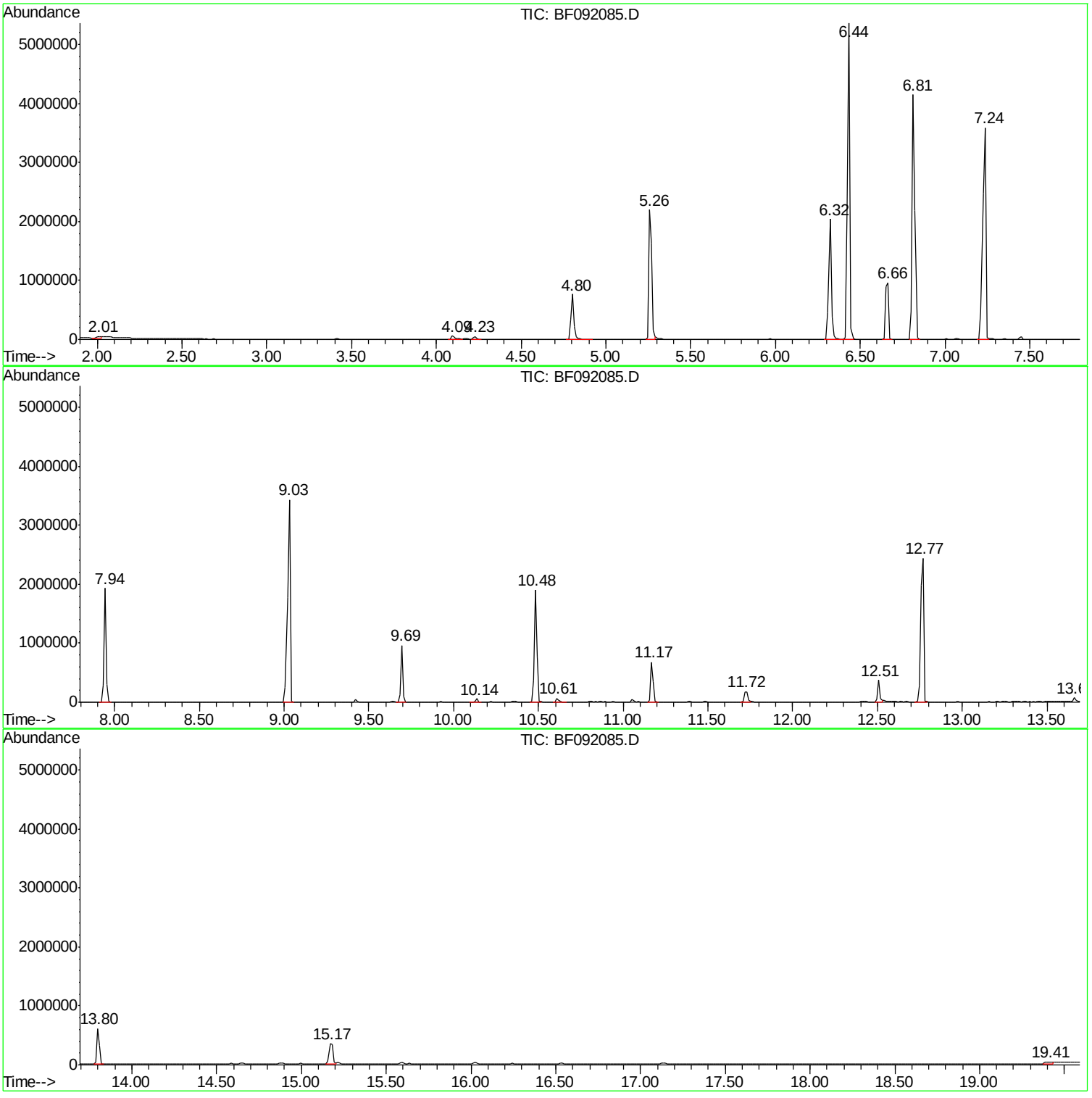
Sum of corrected areas: 36226558

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
Data File : BF092085.D
Acq On : 4 Jan 2017 23:14
Operator : UM/SJ
Sample : I1004-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-23

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
Data File : BF092085.D
Acq On : 4 Jan 2017 23:14
Operator : UM/SJ
Sample : I1004-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-23

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

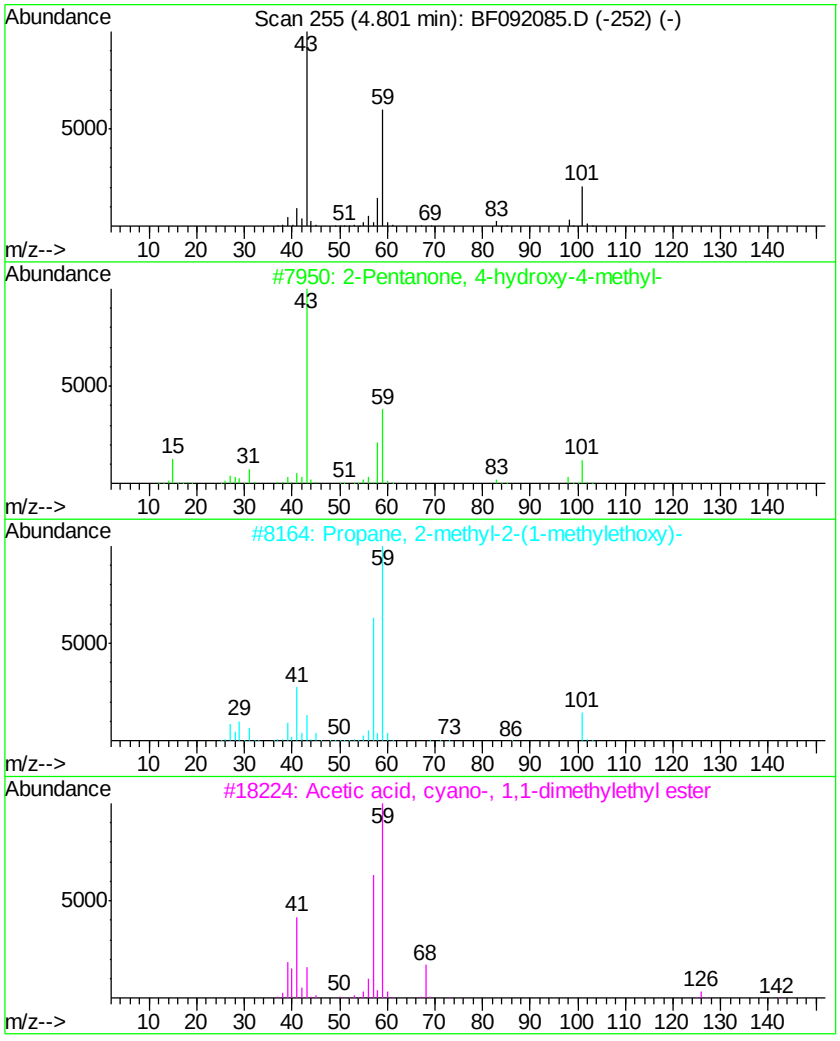
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

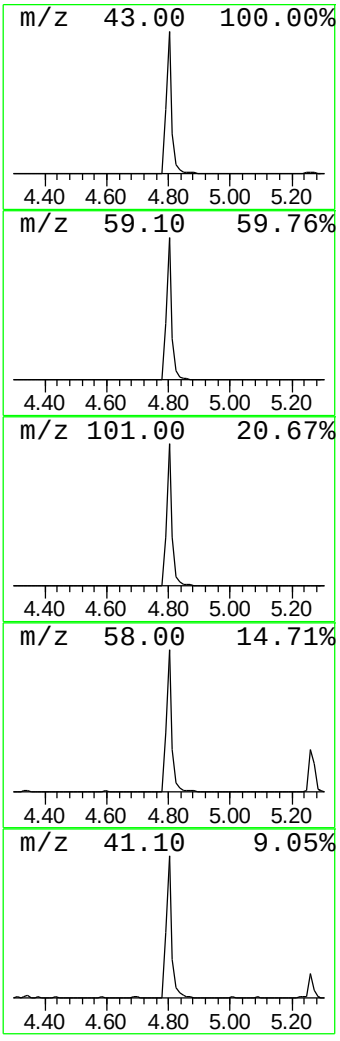
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	14.72 ng	955545	1,4-Dichlorobenzene-d4	6.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
Data File : BF092085.D
Acq On : 4 Jan 2017 23:14
Operator : UM/SJ
Sample : I1004-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-23

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

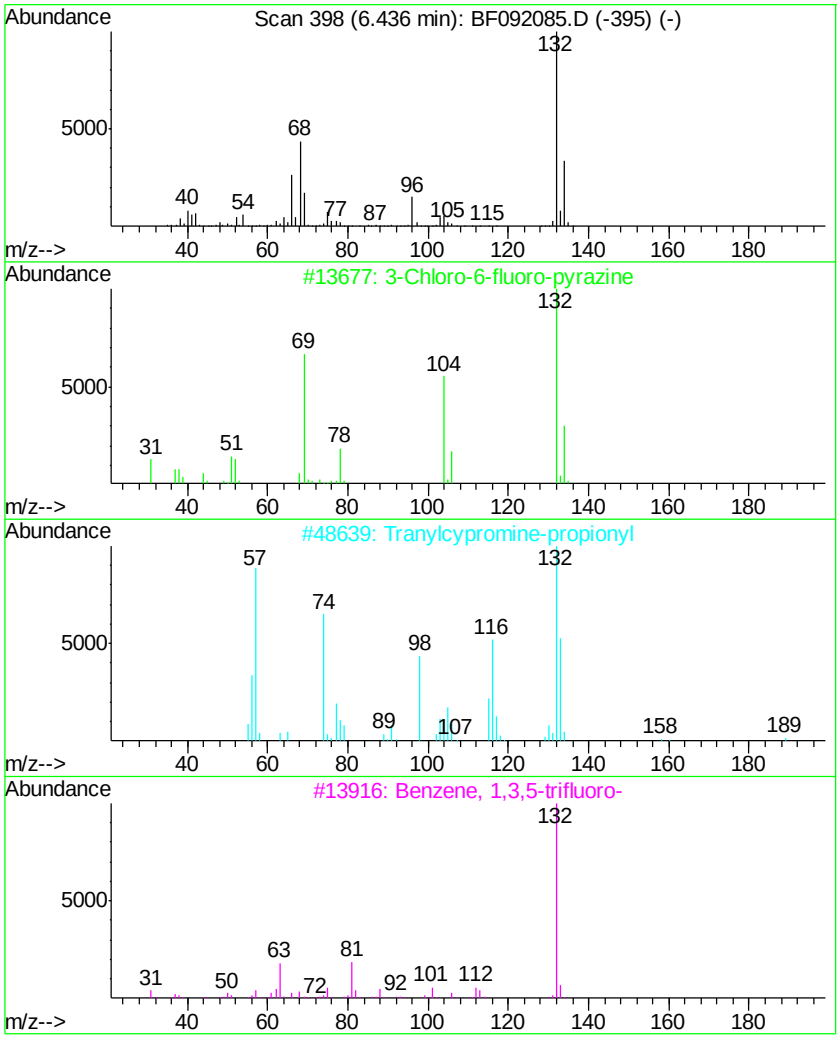
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

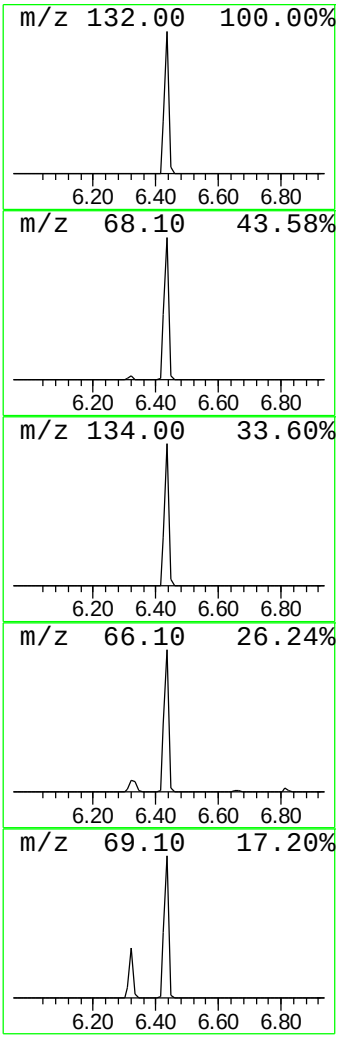
****

Peak Number 2 unknown6.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	82.10 ng	5328720	1,4-Dichlorobenzene-d4	6.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
Data File : BF092085.D
Acq On : 4 Jan 2017 23:14
Operator : UM/SJ
Sample : I1004-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-23

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

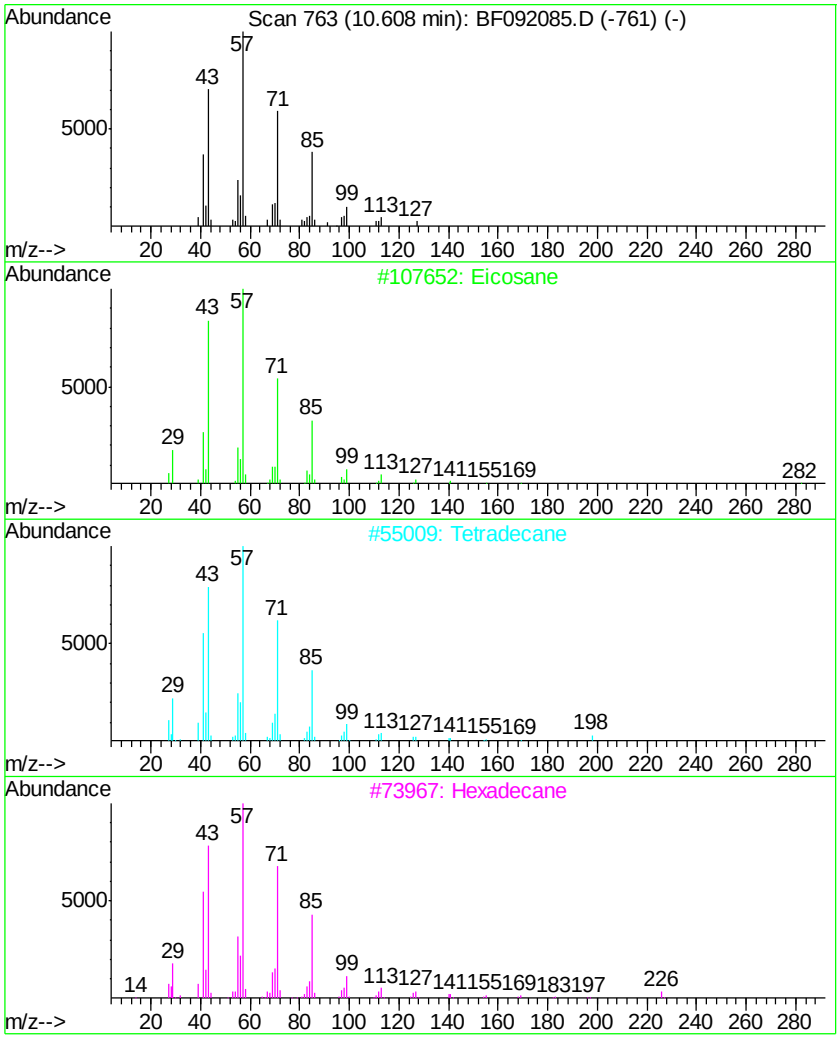
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

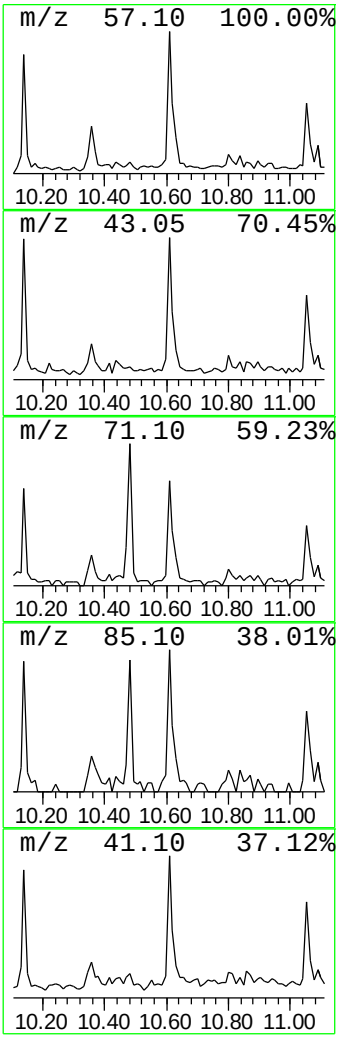
****

Peak Number 4 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.61	2.15 ng	77548	Phenanthrene-d10	11.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Tetradecane	198	C14H30	000629-59-4	90
3	Hexadecane	226	C16H34	000544-76-3	87
4	Tridecane	184	C13H28	000629-50-5	86
5	Heptacosane	380	C27H56	000593-49-7	78





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
Data File : BF092085.D
Acq On : 4 Jan 2017 23:14
Operator : UM/SJ
Sample : I1004-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-23

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

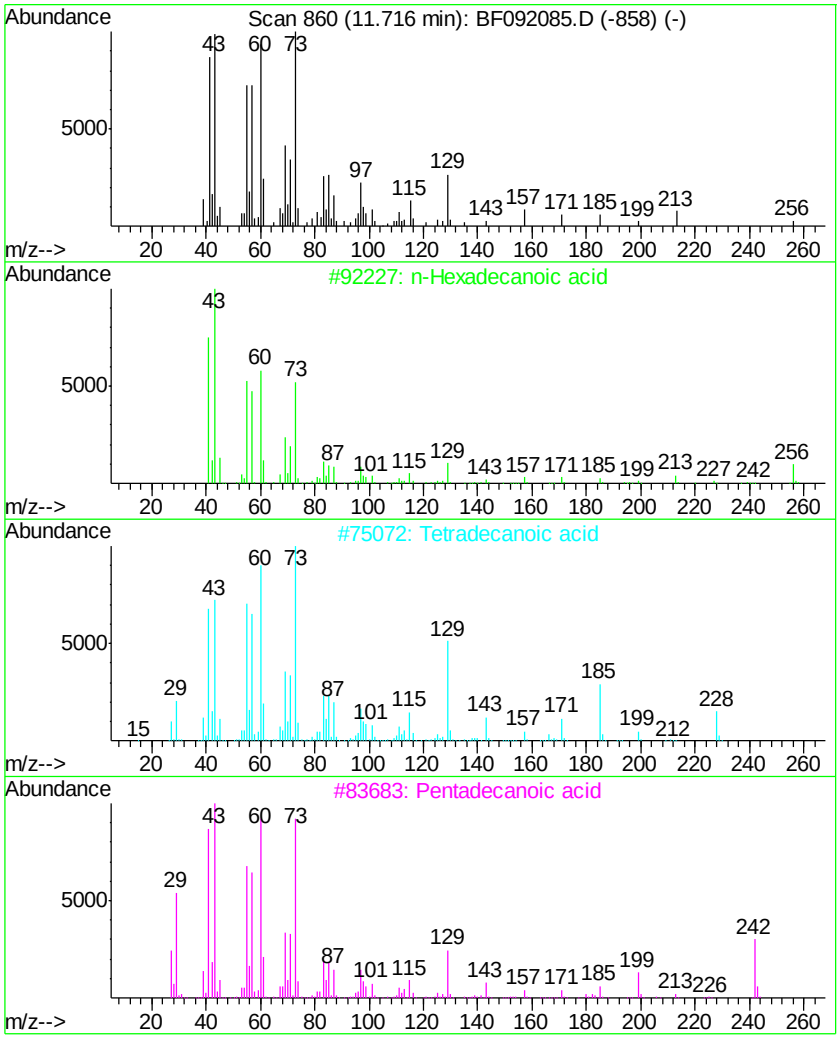
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

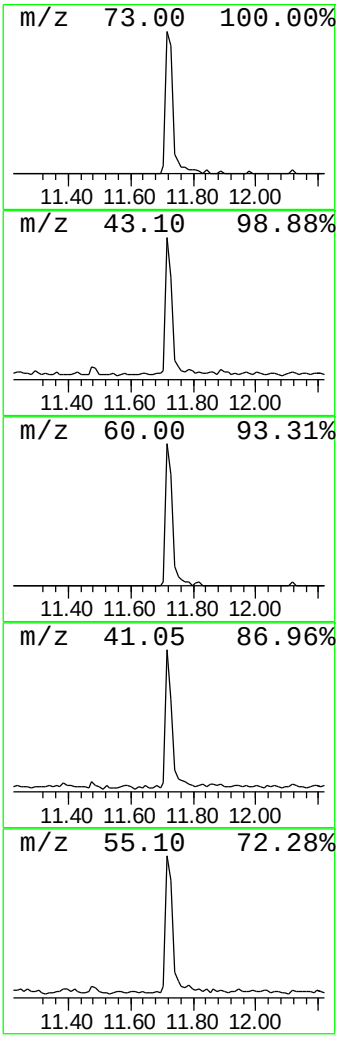
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.72	7.36 ng	265804	Phenanthrene-d10	11.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
Data File : BF092085.D
Acq On : 4 Jan 2017 23:14
Operator : UM/SJ
Sample : I1004-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-23

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

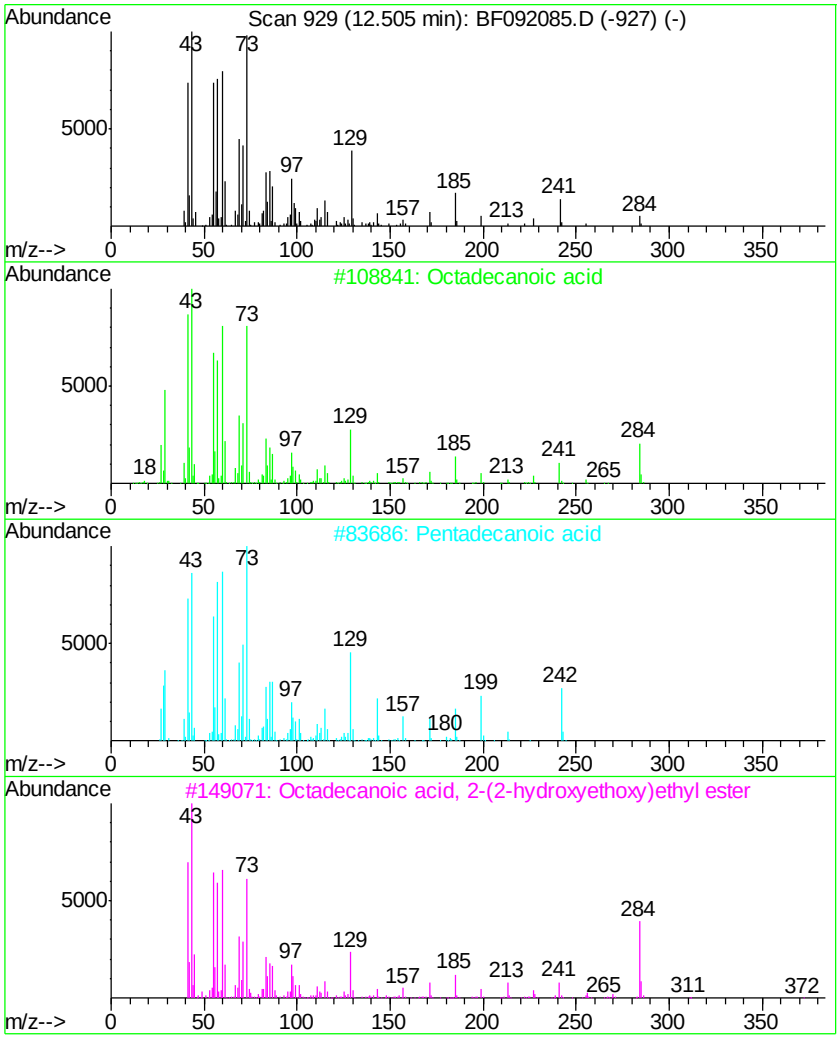
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

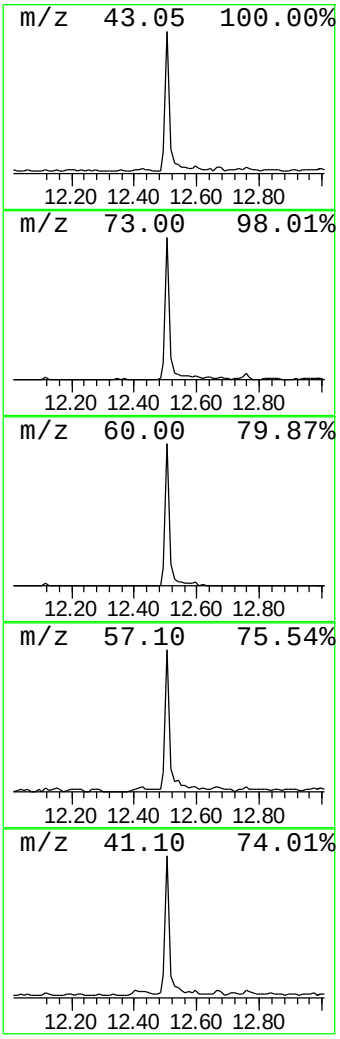
****

Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.51	10.09 ng	331976	Chrysene-d12	13.80

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	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
Data File : BF092085.D
Acq On : 4 Jan 2017 23:14
Operator : UM/SJ
Sample : I1004-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-23

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

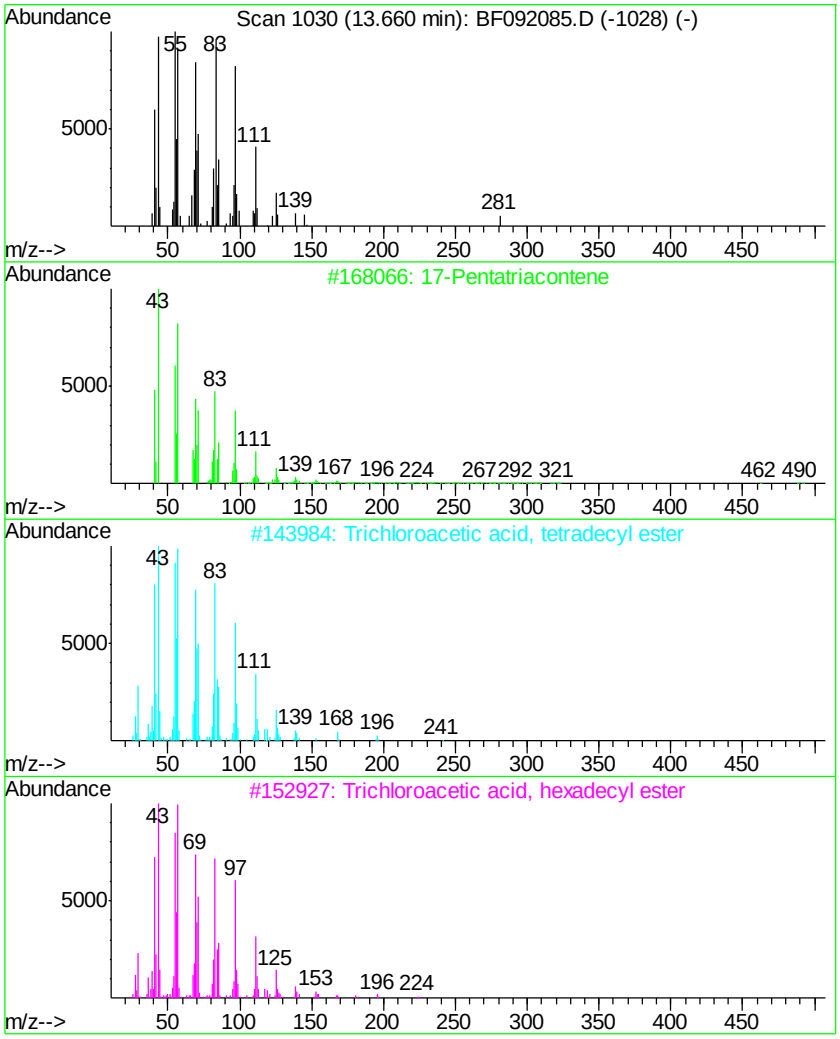
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

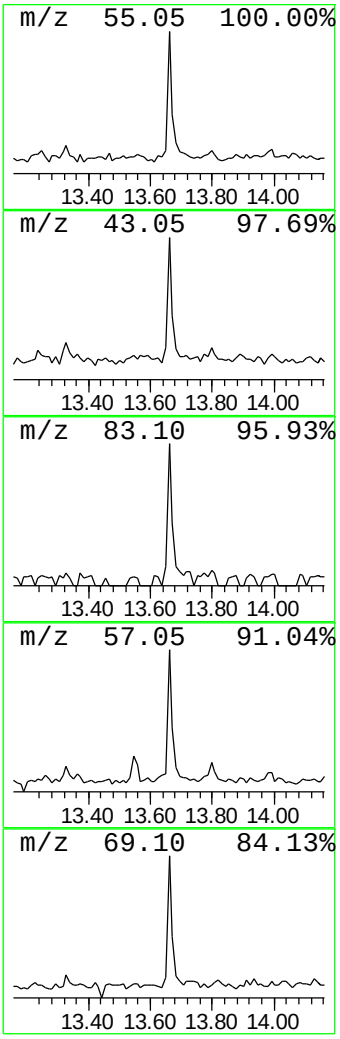
****

Peak Number 7 17-Pentatriacontene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	2.20 ng	72432	Chrysene-d12	13.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	87
2	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	72
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	70
4	1-Docosene	308	C22H44	001599-67-3	64
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	62





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
Data File : BF092085.D
Acq On : 4 Jan 2017 23:14
Operator : UM/SJ
Sample : I1004-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-23

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

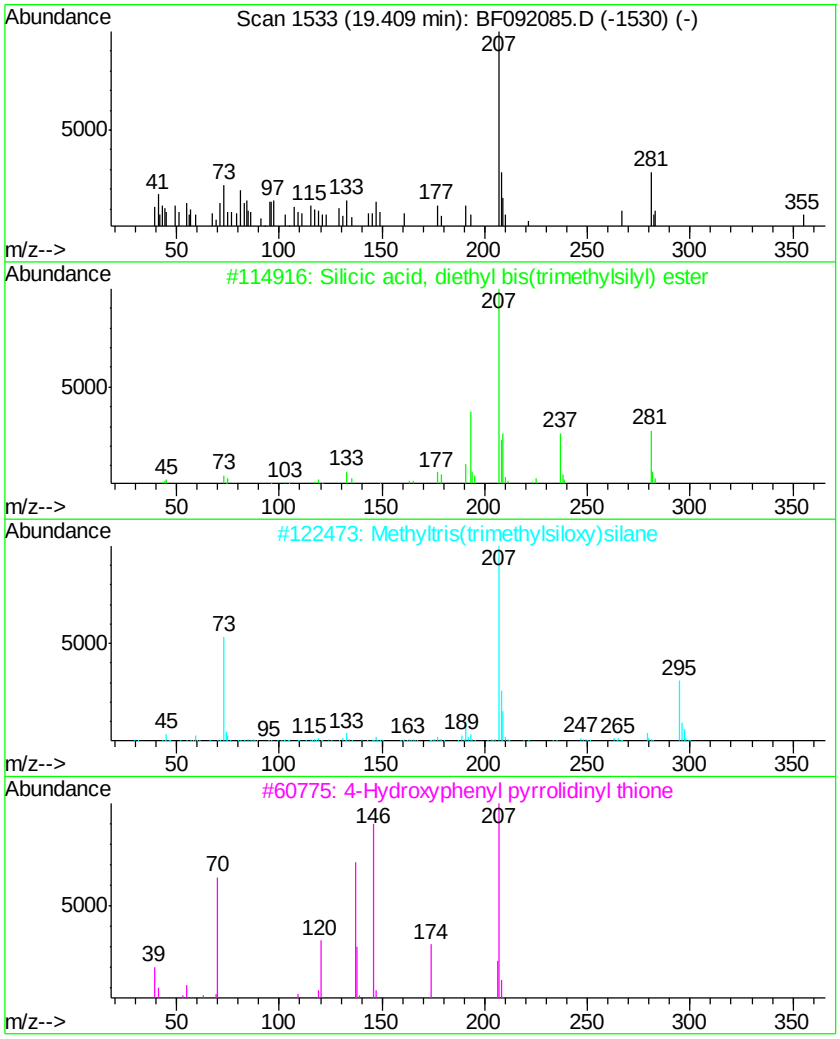
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

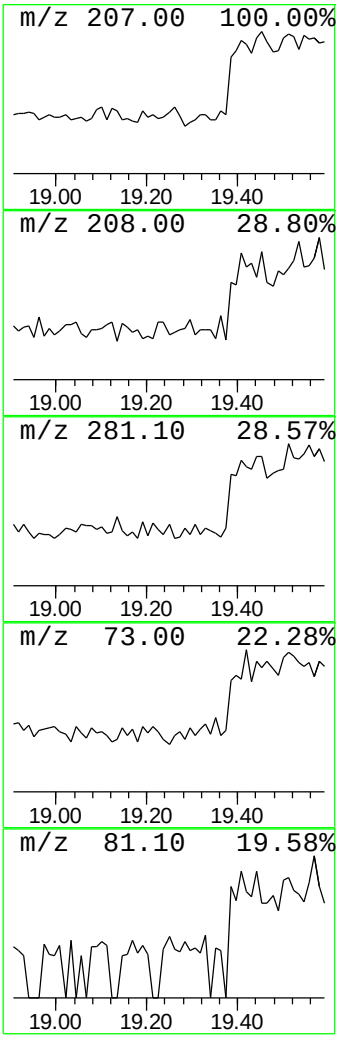
****

Peak Number 8 Silicic acid, diethyl bis(t... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.41	4.13 ng	106285	Perylene-d12	15.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silicic acid, diethyl bis(trimet...	296	C10H28O4Si3	003555-45-1	59
2	Methyltris(trimethylsiloxy)silane	310	C10H30O3Si4	017928-28-8	45
3	4-Hydroxyphenyl pyrrolidinyl thione	207	C11H13NOS	084783-02-8	43
4	1,1,1,3,5,5,5-Heptamethyltrisilo...	222	C7H22O2Si3	001873-88-7	40
5	Cyclotrisiloxane, hexamethyl-	222	C6H18O3Si3	000541-05-9	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010417\
Data File : BF092085.D
Acq On : 4 Jan 2017 23:14
Operator : UM/SJ
Sample : I1004-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-23

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.80	14.7	ng	955545	1	6.66	1298090	20.0
unknown6.44	6.44	82.1	ng	5328720	1	6.66	1298090	20.0
Eicosane	10.61	2.1	ng	77548	4	11.17	722278	20.0
n-Hexadecanoic acid	11.72	7.4	ng	265804	4	11.17	722278	20.0
Octadecanoic acid	12.51	10.1	ng	331976	5	13.80	658077	20.0
17-Pentatriacontene	13.66	2.2	ng	72432	5	13.80	658077	20.0
Silicic acid, die...	19.41	4.1	ng	106285	6	15.18	514860	20.0