LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087685.D
Acq On : 5 Jun 2016 3:09
Operator : UM/SJ
Sample : H3383-03
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTH-WALL-5BGL

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-BF060416.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	1.770	11	16	18	rBV	4242900	8183032	100.00%	18.800%
2	1.907	26	28	48	rVB	1514459	3243617	39.64%	7.452%
3	2.158	48	50	84	rVB	104975	351881	4.30%	0.808%
4	5.050	301	303	311	rBV	207199	347142	4.24%	0.798%
5	5.462	335	339	341	rBV	2878619	3461243	42.30%	7.952%
6	6.490	425	429	431	rBV	2893897	3616861	44.20%	8.310%
7	6.627	438	441	443	rBV	3101935	3387485	41.40%	7.783%
8	6.856	459	461	464	rBV	860824	727971	8.90%	1.673%
9	7.016	472	475	477	rBV	2854311	2608793	31.88%	5.994%
10	7.428	507	511	513	rBV	1740733	2413593	29.50%	5.545%
11	8.148	571	574	576	rBV	787570	975537	11.92%	2.241%
12	9.222	665	668	671	rBV	3196012	3484889	42.59%	8.006%
13	9.611	700	702	705	rVB	222315	229094	2.80%	0.526%
14	9.896	725	727	730	rVB	1224671	1093639	13.36%	2.513%
15	10.685	793	796	799	rBV	2239600	2407557	29.42%	5.531%
16	11.382	854	857	859	rVB	1107827	1131796	13.83%	2.600%
17	11.919	901	904	906	rBV	277765	334820	4.09%	0.769%
18	12.697	970	972	979	rBV	117157	141095	1.72%	0.324%
19	12.971	993	996	998	rBV	3225080	3473211	42.44%	7.980%
20	14.011	1084	1087	1089	rVB	1090186	1008601	12.33%	2.317%
21	14.868	1160	1162	1165	rBV	150955	149189	1.82%	0.343%
22	15.440	1209	1212	1215	rBV	603609	754825	9.22%	1.734%

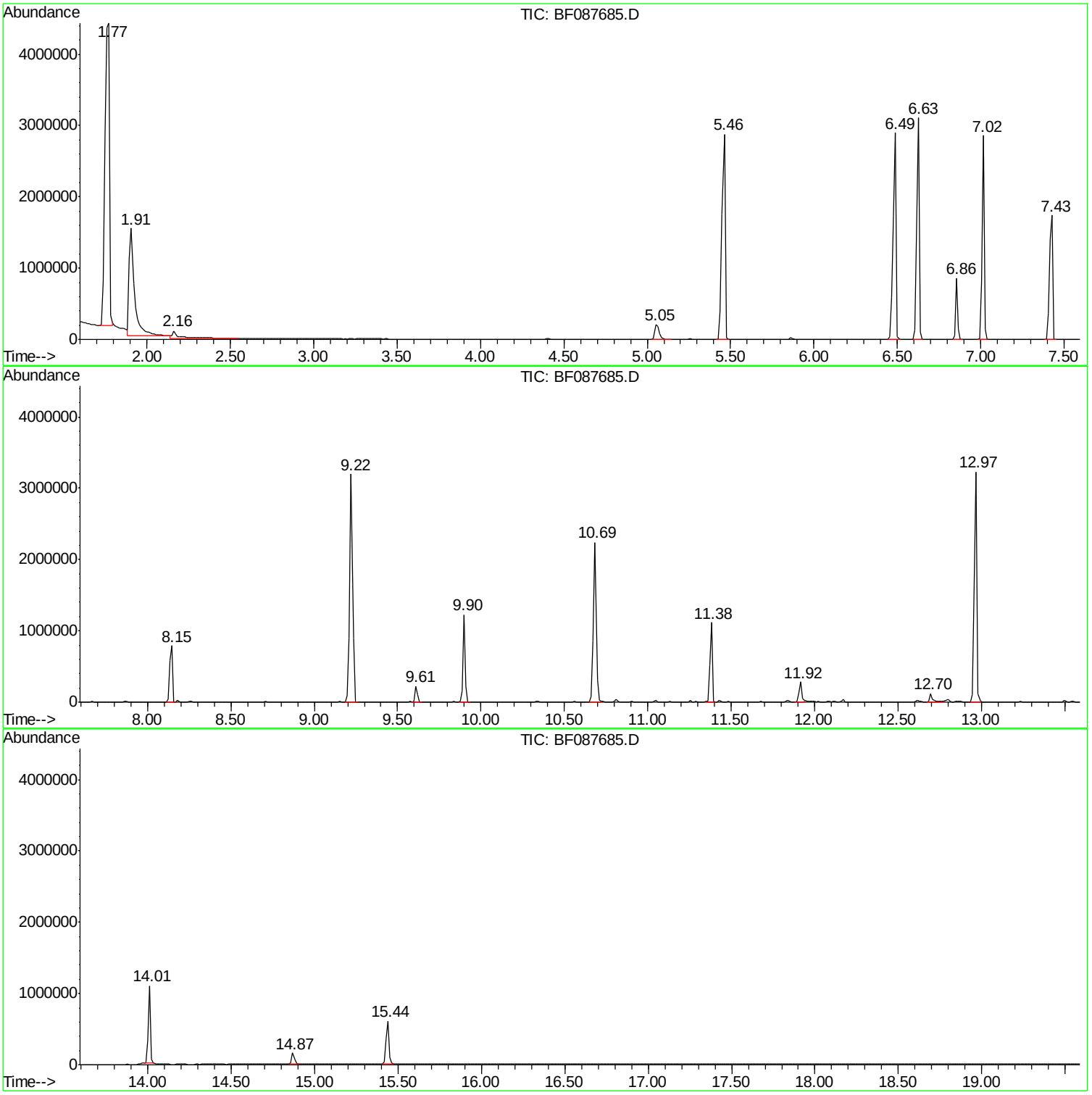
Sum of corrected areas: 43525871

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087685.D
Acq On : 5 Jun 2016 3:09
Operator : UM/SJ
Sample : H3383-03
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SOUTH-WALL-5BGL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.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\BF060416\
Data File : BF087685.D
Acq On : 5 Jun 2016 3:09
Operator : UM/SJ
Sample : H3383-03
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTH-WALL-5BGL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

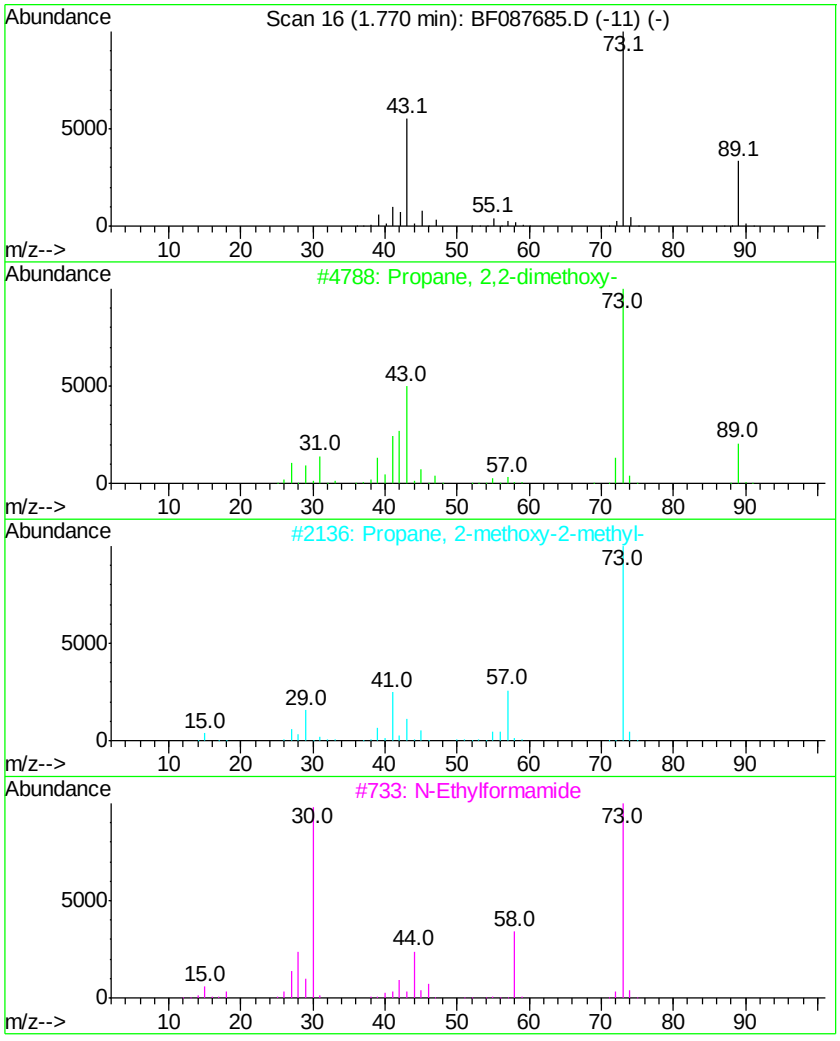
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

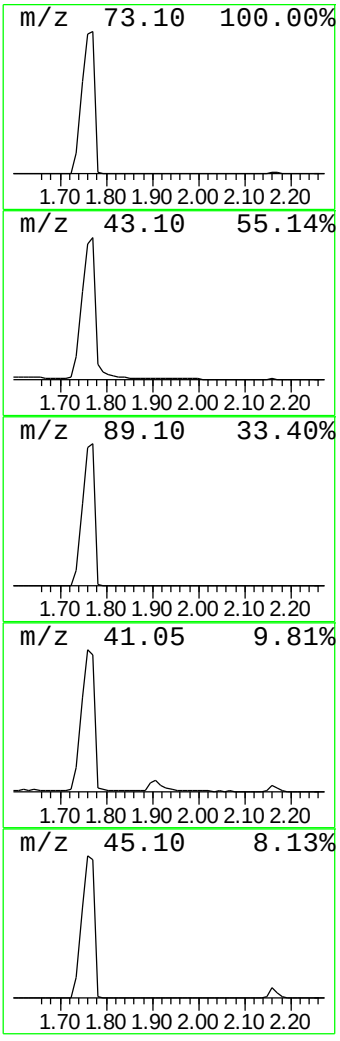
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.77	224.82 ng	8183030	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	50
2	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	17
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087685.D
Acq On : 5 Jun 2016 3:09
Operator : UM/SJ
Sample : H3383-03
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTH-WALL-5BGL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

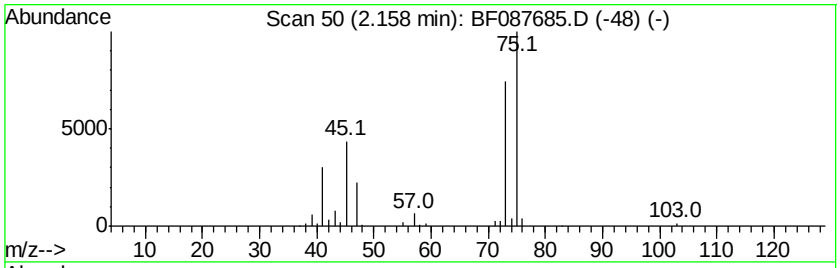
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

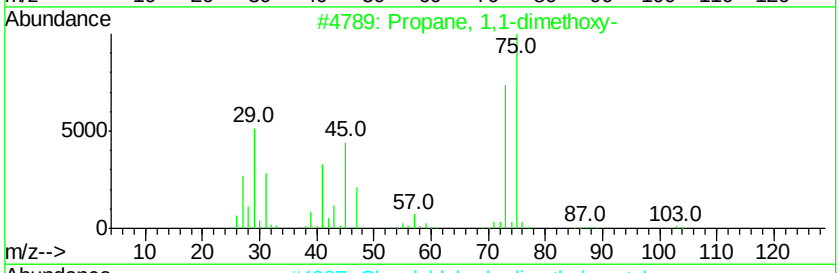
****

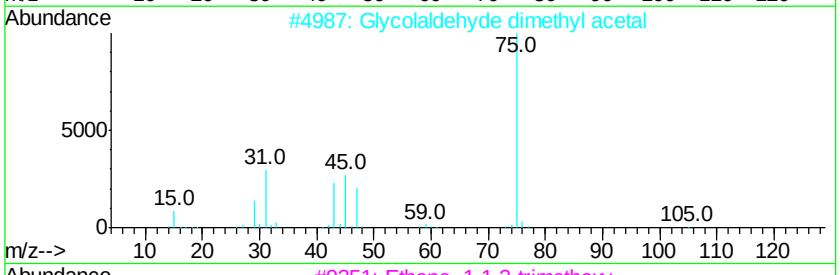
Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 5

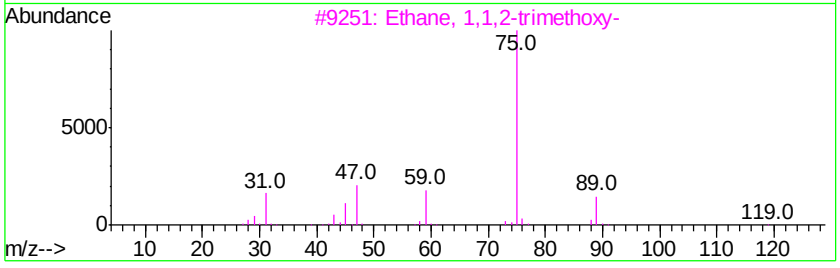
R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	9.67 ng	351881	1,4-Dichlorobenzene-d4	6.86

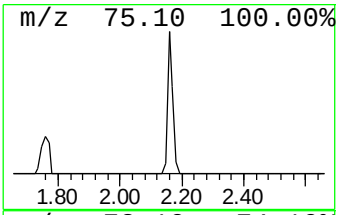
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	36
3	Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	33
4	Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	28
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12

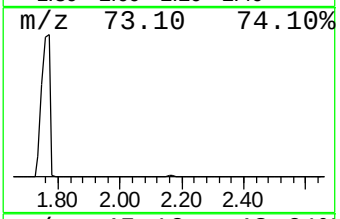


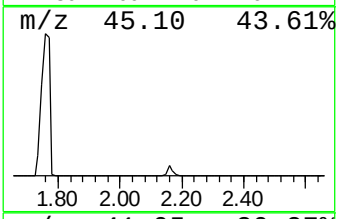


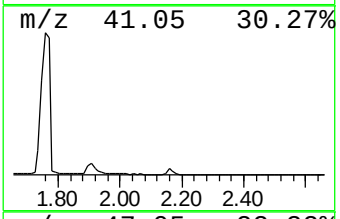


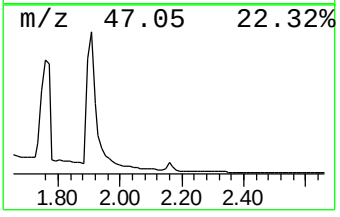












Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087685.D
Acq On : 5 Jun 2016 3:09
Operator : UM/SJ
Sample : H3383-03
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SOUTH-WALL-5BGL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

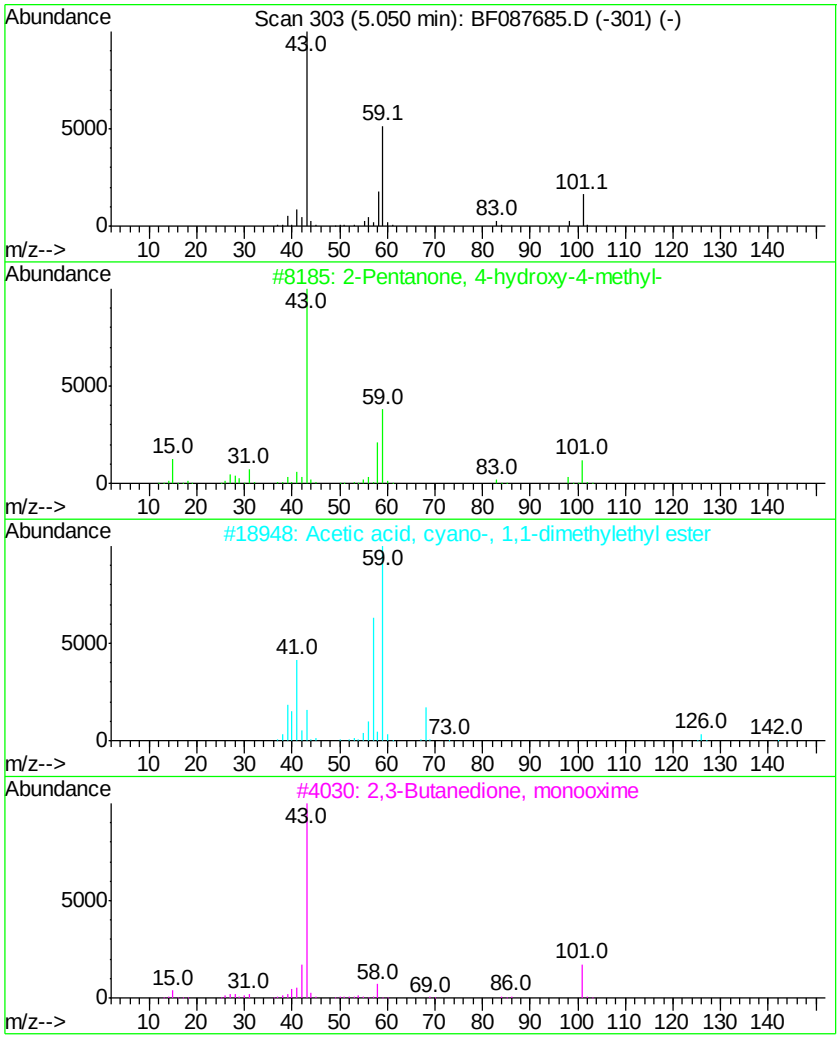
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

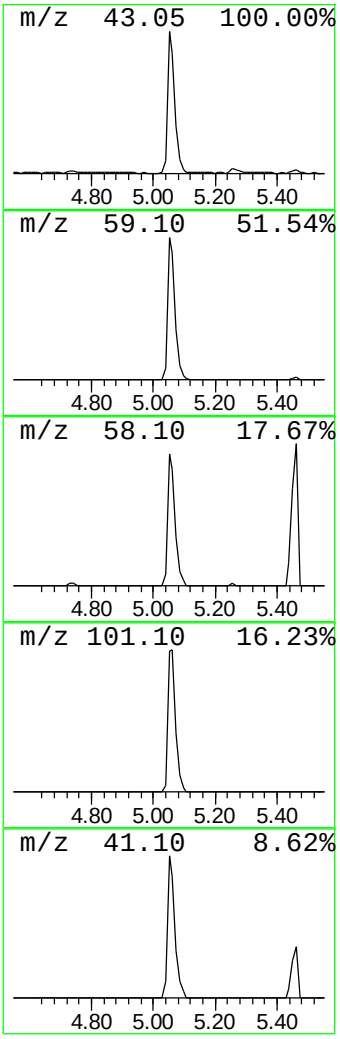
****

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	9.54 ng	347142	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087685.D
Acq On : 5 Jun 2016 3:09
Operator : UM/SJ
Sample : H3383-03
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTH-WALL-5BGL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

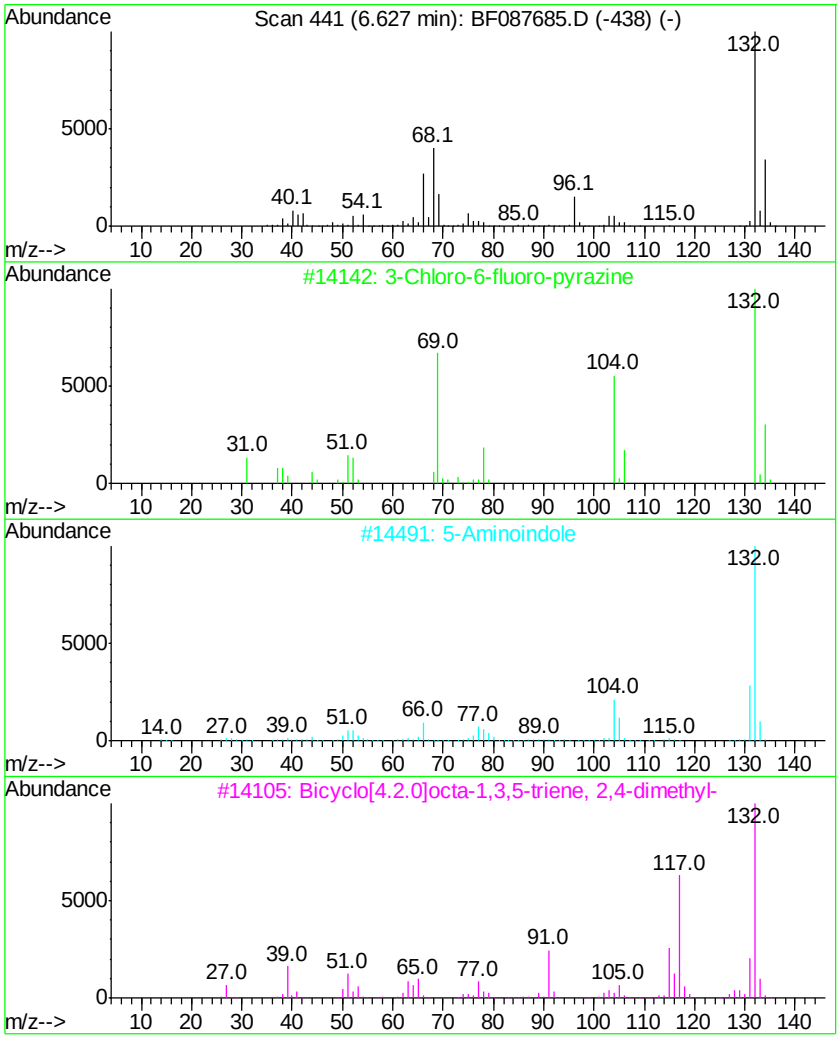
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

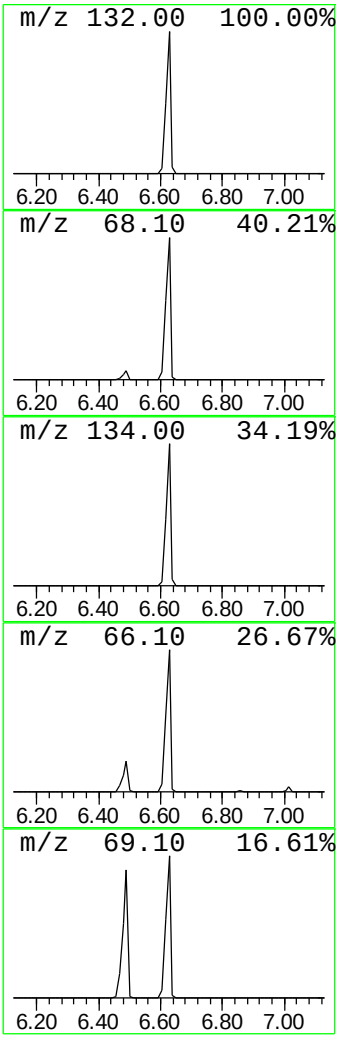
****

Peak Number 5 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	93.07 ng	3387490	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087685.D
Acq On : 5 Jun 2016 3:09
Operator : UM/SJ
Sample : H3383-03
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTH-WALL-5BGL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

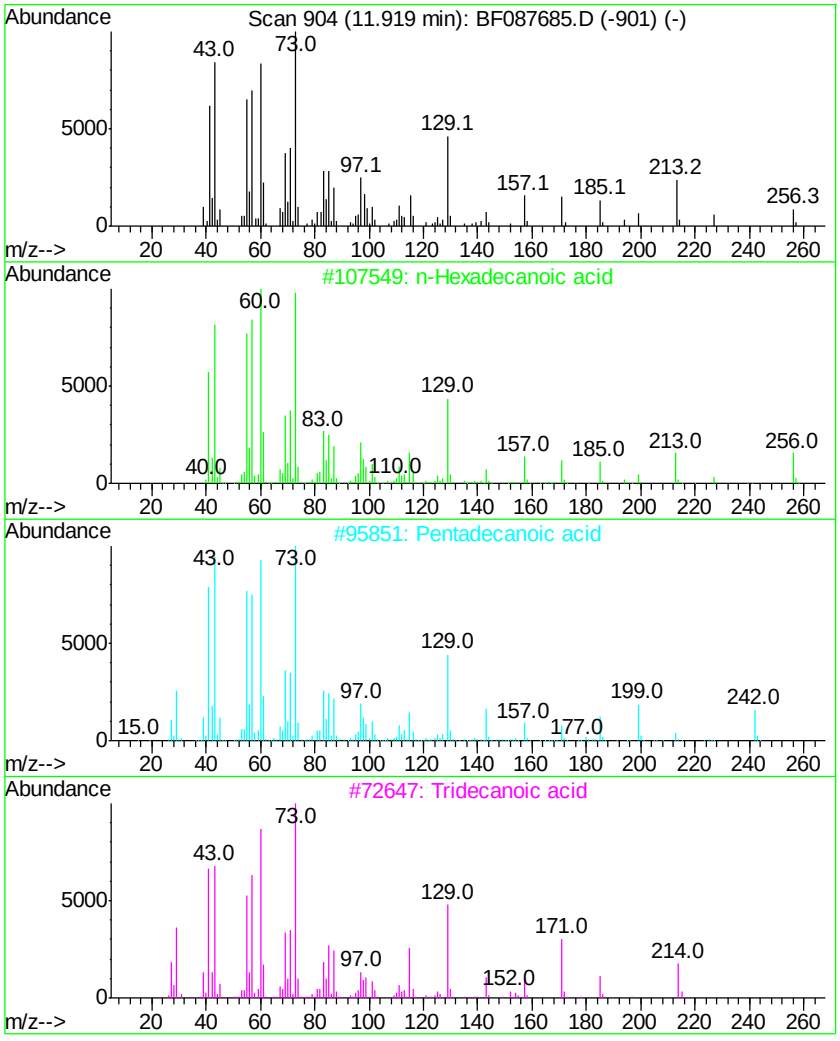
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

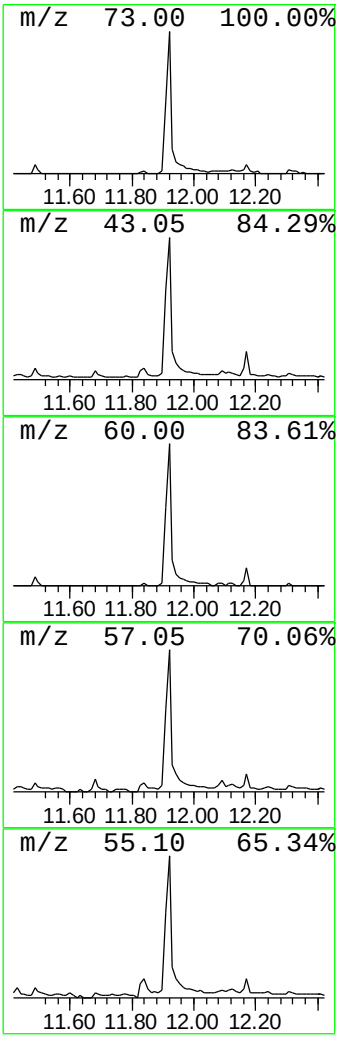
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	5.92 ng	334820	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	83
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Undecanoic acid	186	C11H22O2	000112-37-8	68





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087685.D
Acq On : 5 Jun 2016 3:09
Operator : UM/SJ
Sample : H3383-03
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTH-WALL-5BGL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

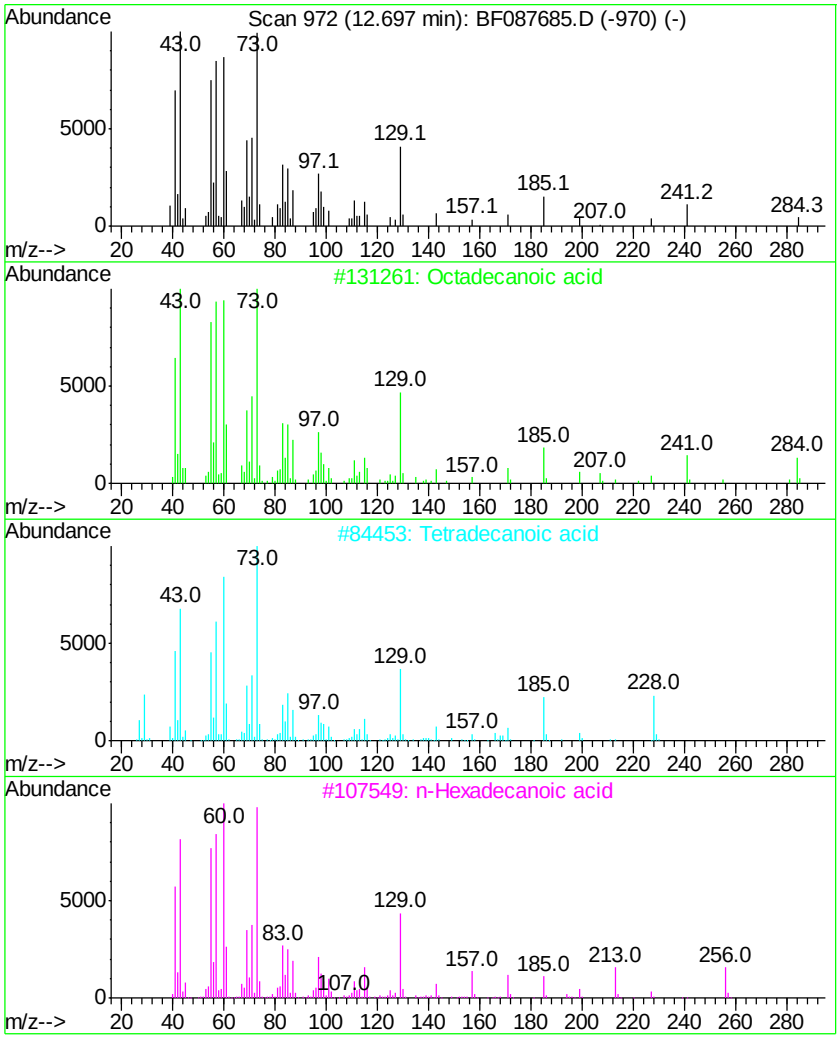
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

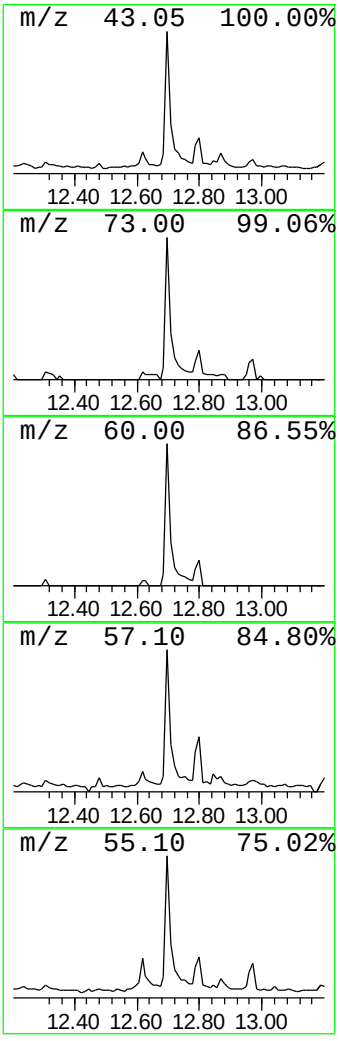
****

Peak Number 8 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	2.80 ng	141095	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	52
4	n-Decanoic acid	172	C10H20O2	000334-48-5	52
5	Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	20





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087685.D
Acq On : 5 Jun 2016 3:09
Operator : UM/SJ
Sample : H3383-03
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTH-WALL-5BGL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

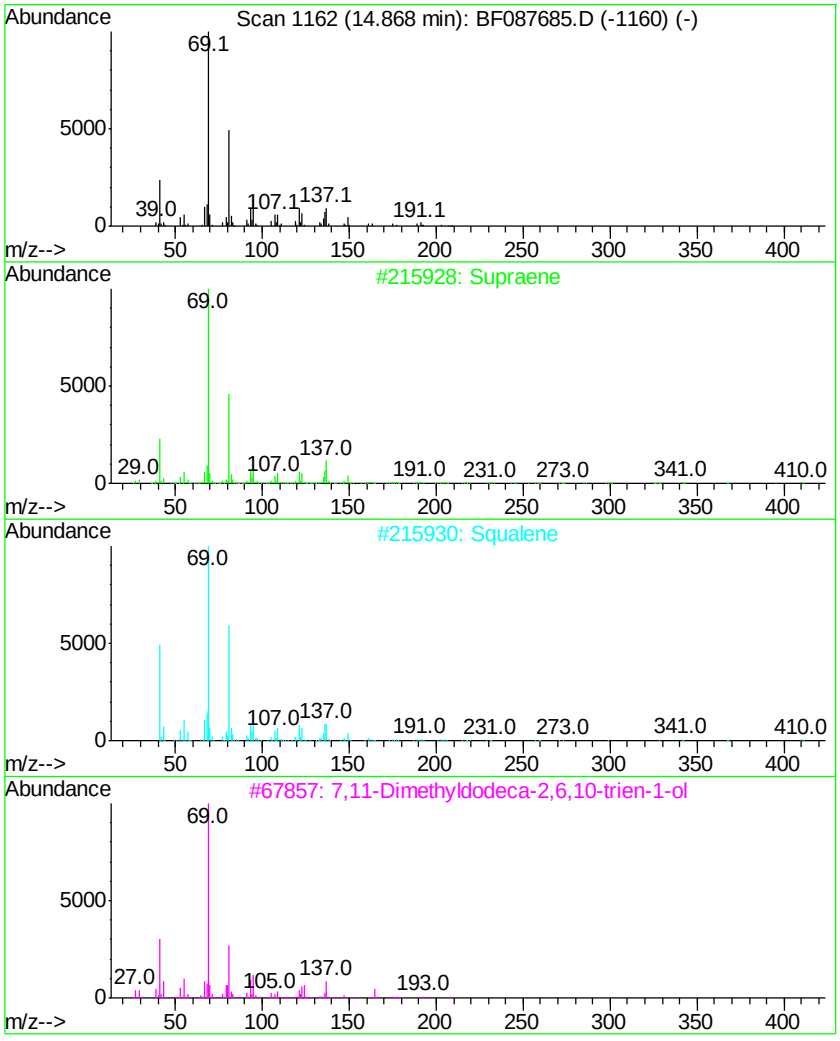
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

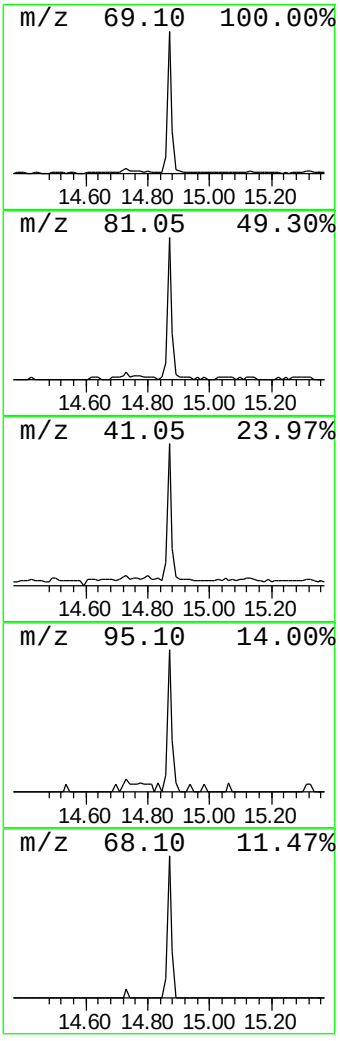
****

Peak Number 9 Supraene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	3.95 ng	149189	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	91
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4	Methanone, dicyclopropyl-	110	C7H10O	001121-37-5	50
5	2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060416\
Data File : BF087685.D
Acq On : 5 Jun 2016 3:09
Operator : UM/SJ
Sample : H3383-03
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTH-WALL-5BGL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.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
Propane, 2,2-dime...	1.77	224.8	ng	8183030	1	6.86	727971	20.0
Propane, 1,1-dime...	2.16	9.7	ng	351881	1	6.86	727971	20.0
2-Pentanone, 4-hy...	5.05	9.5	ng	347142	1	6.86	727971	20.0
unknown6.63	6.63	93.1	ng	3387490	1	6.86	727971	20.0
n-Hexadecanoic acid	11.92	5.9	ng	334820	4	11.38	1131800	20.0
Octadecanoic acid	12.70	2.8	ng	141095	5	14.01	1008600	20.0
Supraene	14.87	4.0	ng	149189	6	15.44	754825	20.0