LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
Data File : BF084639.D
Acq On : 29 Jan 2016 16:41
Operator : SJ/IZ
Sample : H1257-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B016(12-12.5)

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-BF012916.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	4.190	181	184	190	rBV	352831	428452	8.38%	0.964%
2	4.899	241	246	248	rBV	3120852	5110571	100.00%	11.503%
3	5.321	280	283	286	rBV	3974383	3798099	74.32%	8.549%
4	5.721	316	318	321	rBV	352685	338876	6.63%	0.763%
5	6.373	372	375	377	rBV	3940331	4407296	86.24%	9.920%
6	6.487	383	385	388	rBV	3412082	3864929	75.63%	8.699%
7	6.727	403	406	408	rBV	746022	1026041	20.08%	2.309%
8	6.876	417	419	422	rBV	3177654	2860392	55.97%	6.438%
9	7.287	452	455	458	rBV	2499784	2367816	46.33%	5.330%
10	8.007	516	518	520	rBV	1633550	1413556	27.66%	3.182%
11	9.093	610	613	615	rBV	3183143	4247030	83.10%	9.559%
12	9.482	645	647	650	rBV	440360	423231	8.28%	0.953%
13	9.756	669	671	674	rVB	1490654	1525531	29.85%	3.434%
14	10.202	708	710	712	rVB	95287	77514	1.52%	0.174%
15	10.545	737	740	743	rVV	2492532	2459807	48.13%	5.537%
16	10.671	749	751	756	rVB	73922	105739	2.07%	0.238%
17	11.242	798	801	803	rBV	1253355	1262411	24.70%	2.842%
18	12.831	937	940	942	rBV	3791020	4221499	82.60%	9.502%
19	13.745	1017	1020	1029	rBV	293113	866165	16.95%	1.950%
20	13.871	1029	1031	1033	rBV	1831307	1669573	32.67%	3.758%
21	14.408	1075	1078	1086	rVB5	16234	57451	1.12%	0.129%
22	14.717	1103	1105	1108	rBV	189626	188912	3.70%	0.425%
23	15.254	1149	1152	1155	rBV	1268592	1461101	28.59%	3.289%
24	15.688	1187	1190	1194	rBV	62431	89354	1.75%	0.201%
25	15.791	1194	1199	1206	rBV7	33164	156004	3.05%	0.351%

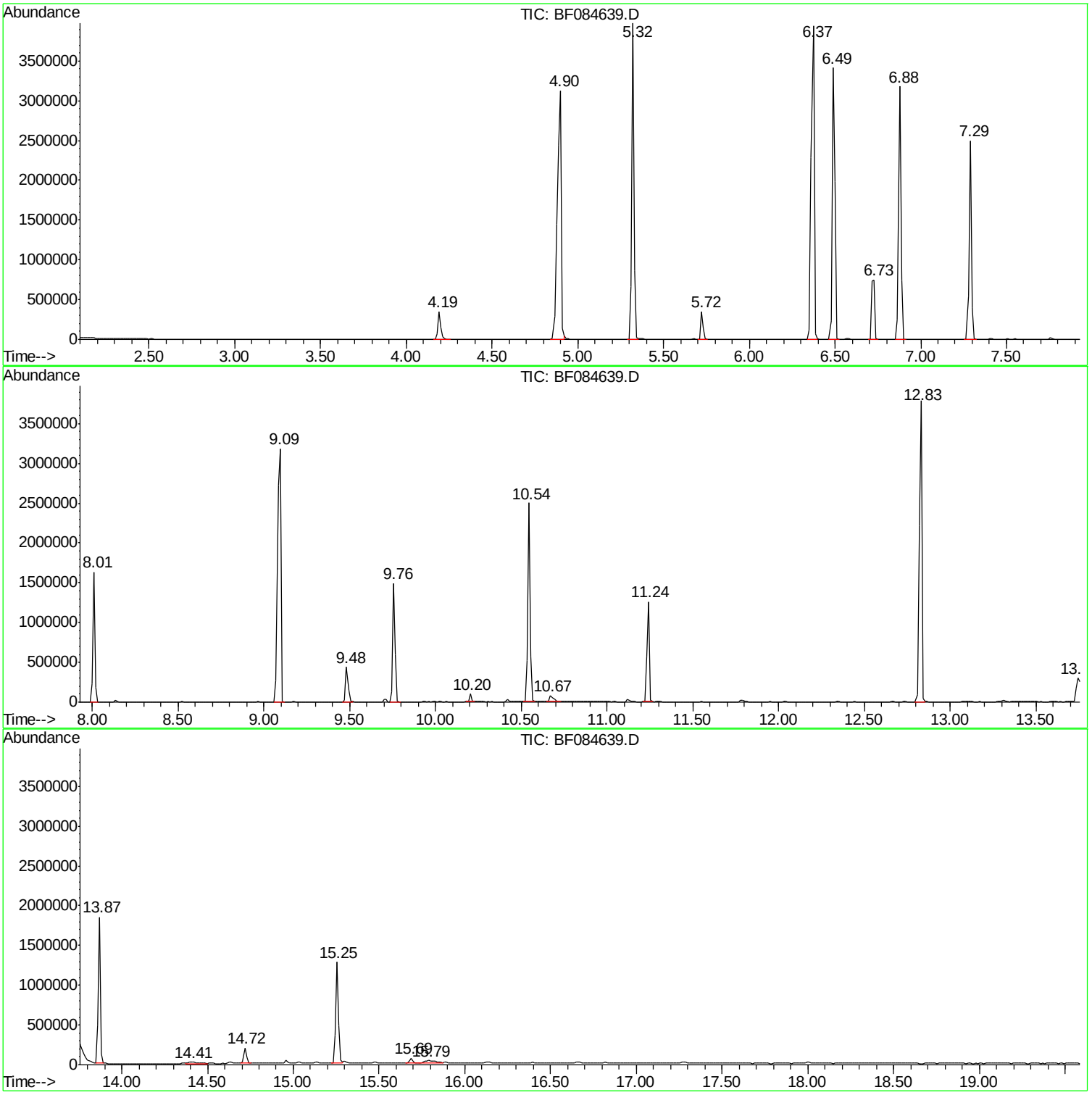
Sum of corrected areas: 44427350

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
Data File : BF084639.D
Acq On : 29 Jan 2016 16:41
Operator : SJ/IZ
Sample : H1257-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B016(12-12.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
Data File : BF084639.D
Acq On : 29 Jan 2016 16:41
Operator : SJ/IZ
Sample : H1257-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B016(12-12.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

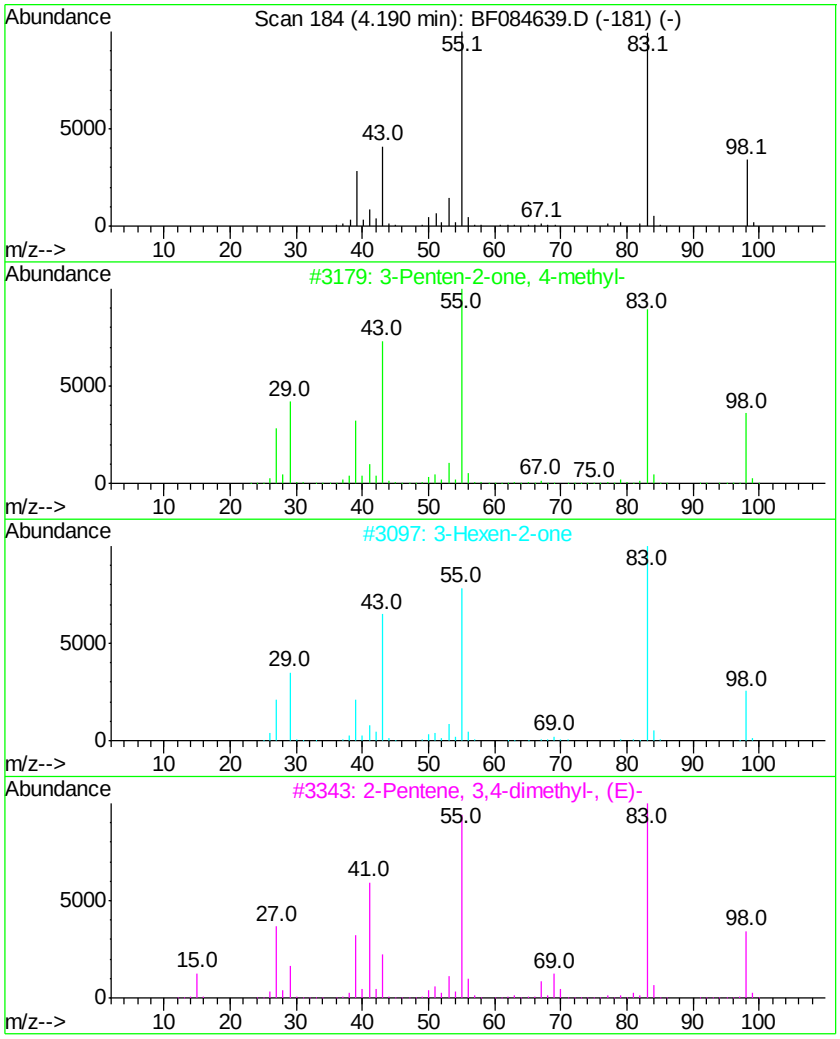
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

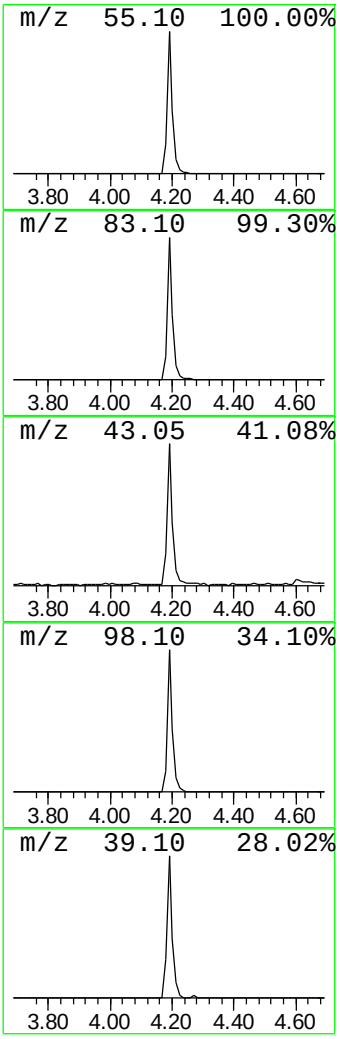
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.19	8.35 ng	428452	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
Data File : BF084639.D
Acq On : 29 Jan 2016 16:41
Operator : SJ/IZ
Sample : H1257-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B016(12-12.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

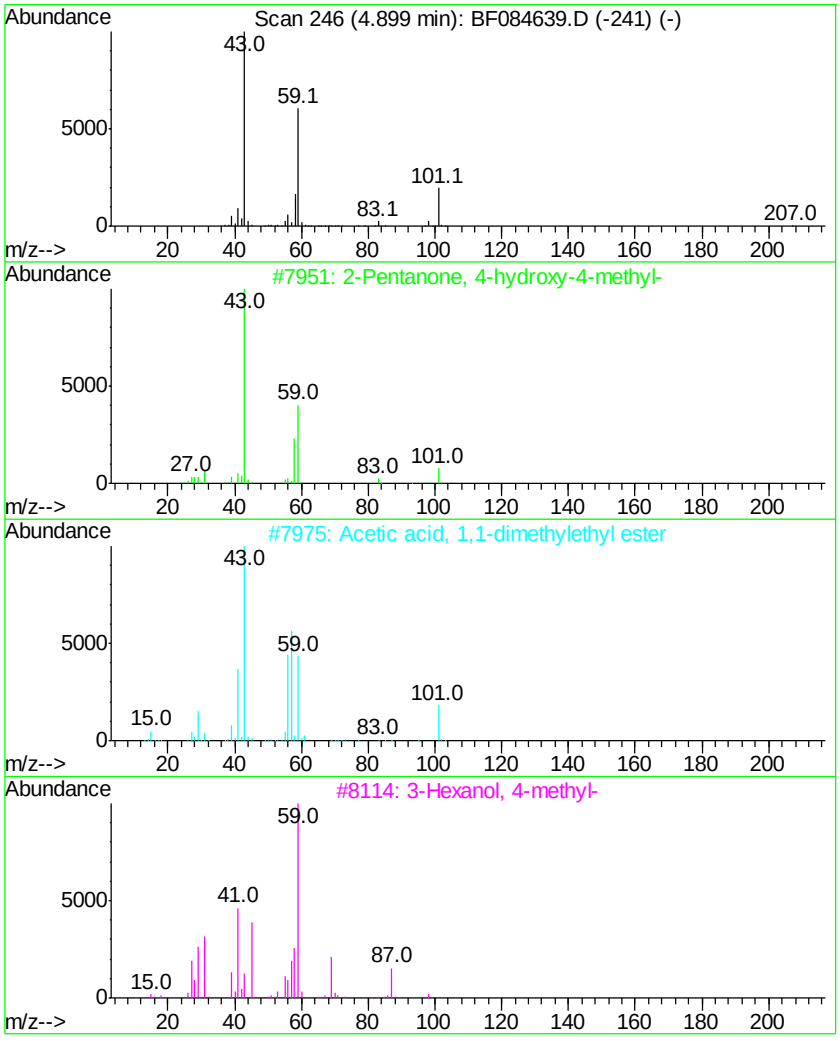
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

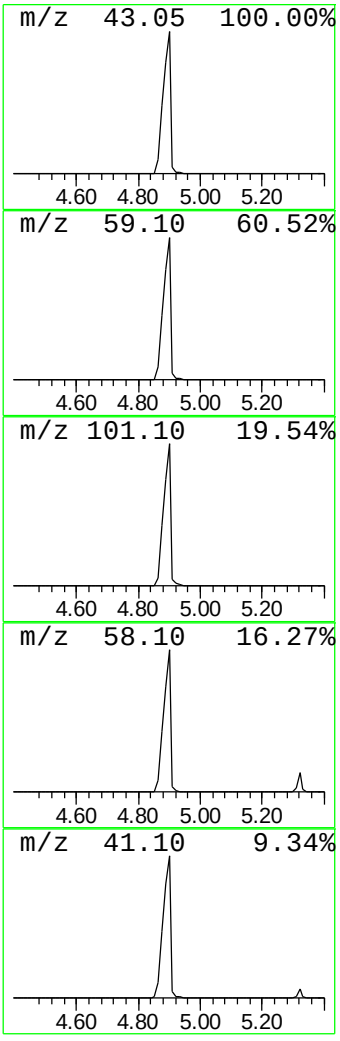
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	99.62 ng	5110570	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
Data File : BF084639.D
Acq On : 29 Jan 2016 16:41
Operator : SJ/IZ
Sample : H1257-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B016(12-12.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

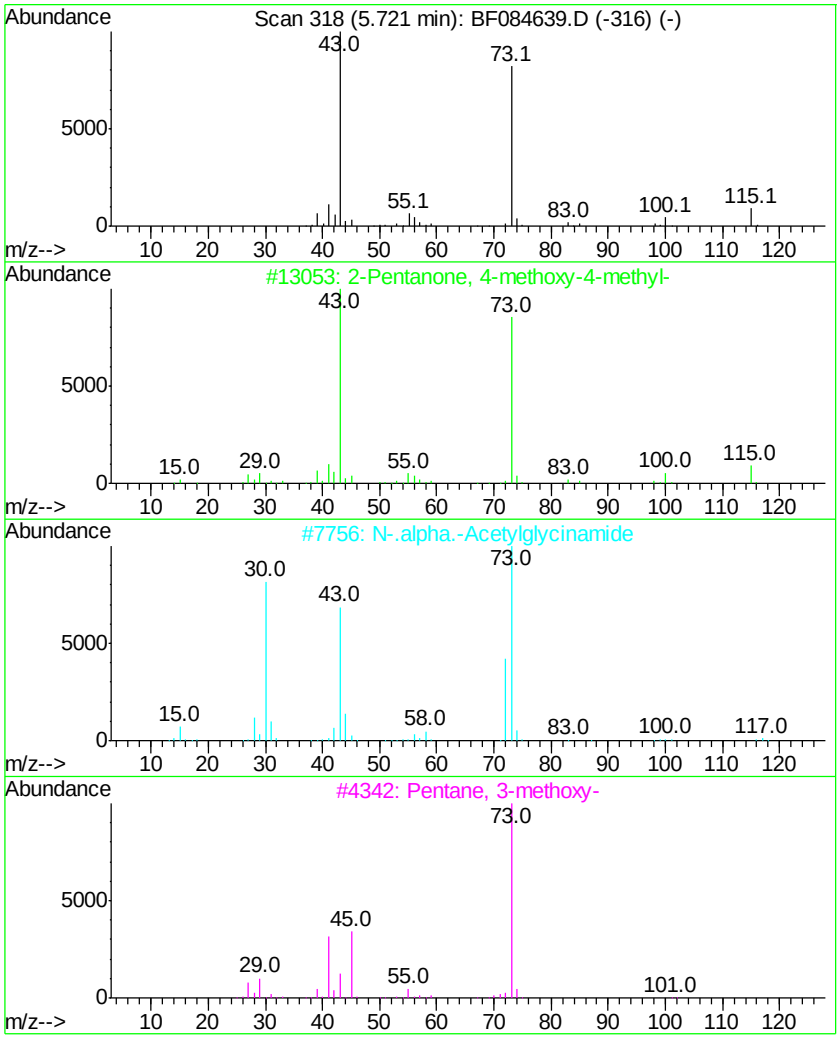
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

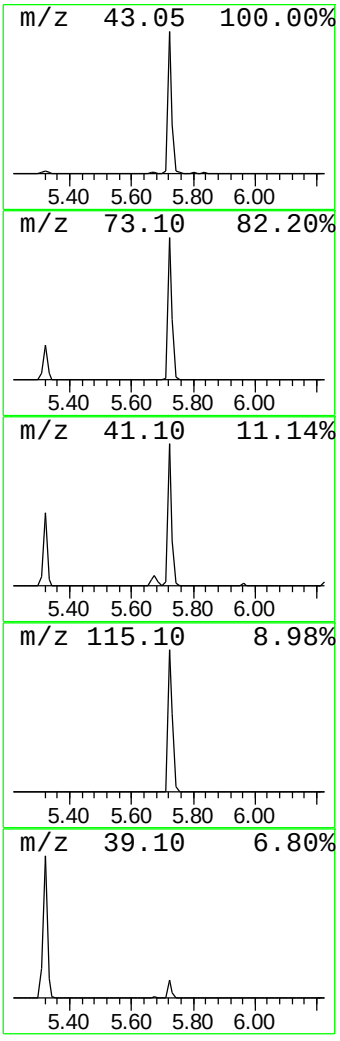
****

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	6.61 ng	338876	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	43
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4	N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	10
5	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
Data File : BF084639.D
Acq On : 29 Jan 2016 16:41
Operator : SJ/IZ
Sample : H1257-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B016(12-12.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

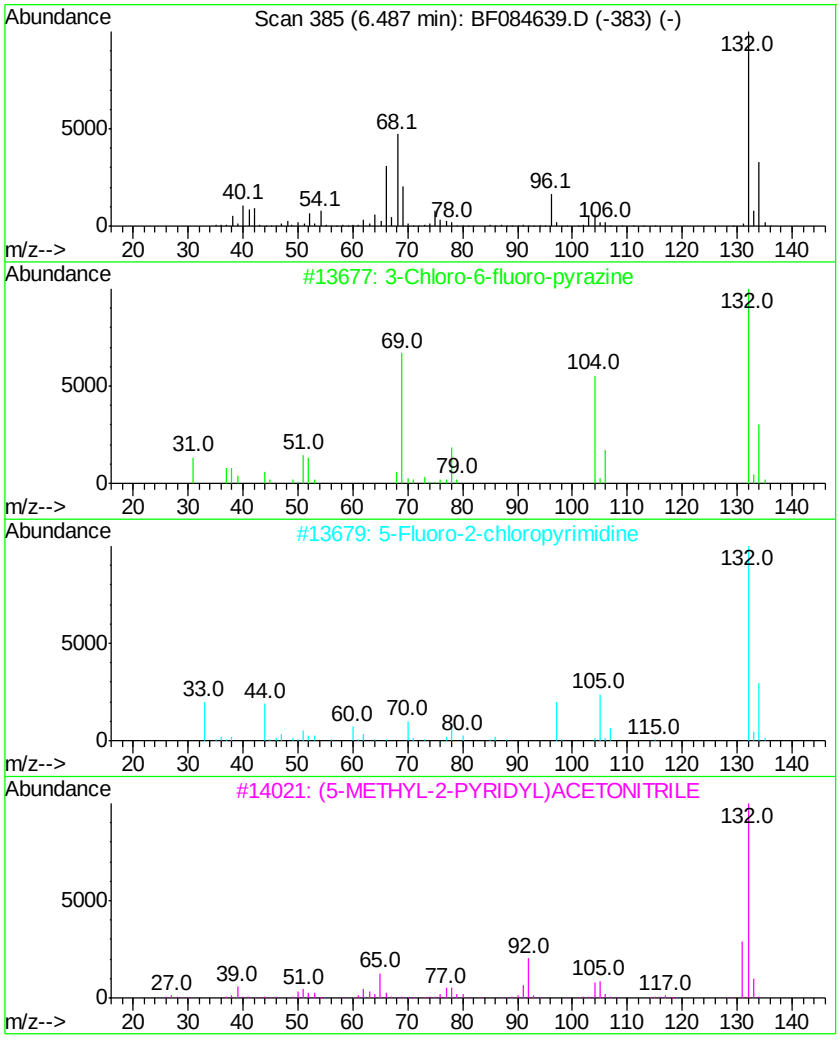
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

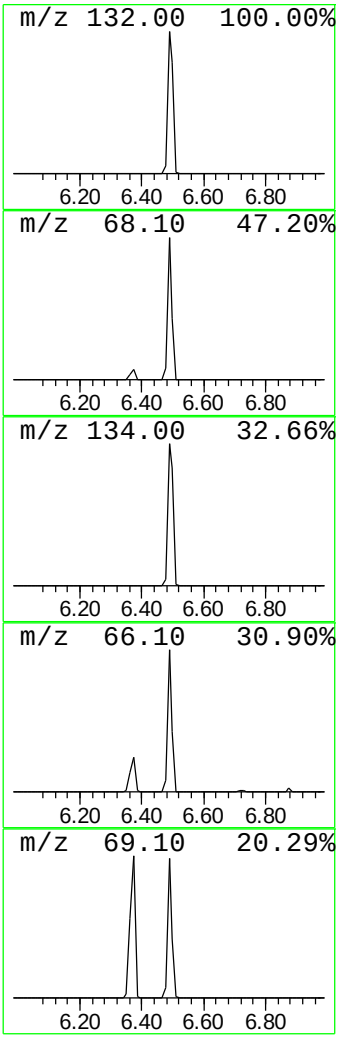
****

Peak Number 4 unknown6.49 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	75.34 ng	3864930	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Xenon	132	Xe	007440-63-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
Data File : BF084639.D
Acq On : 29 Jan 2016 16:41
Operator : SJ/IZ
Sample : H1257-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B016(12-12.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

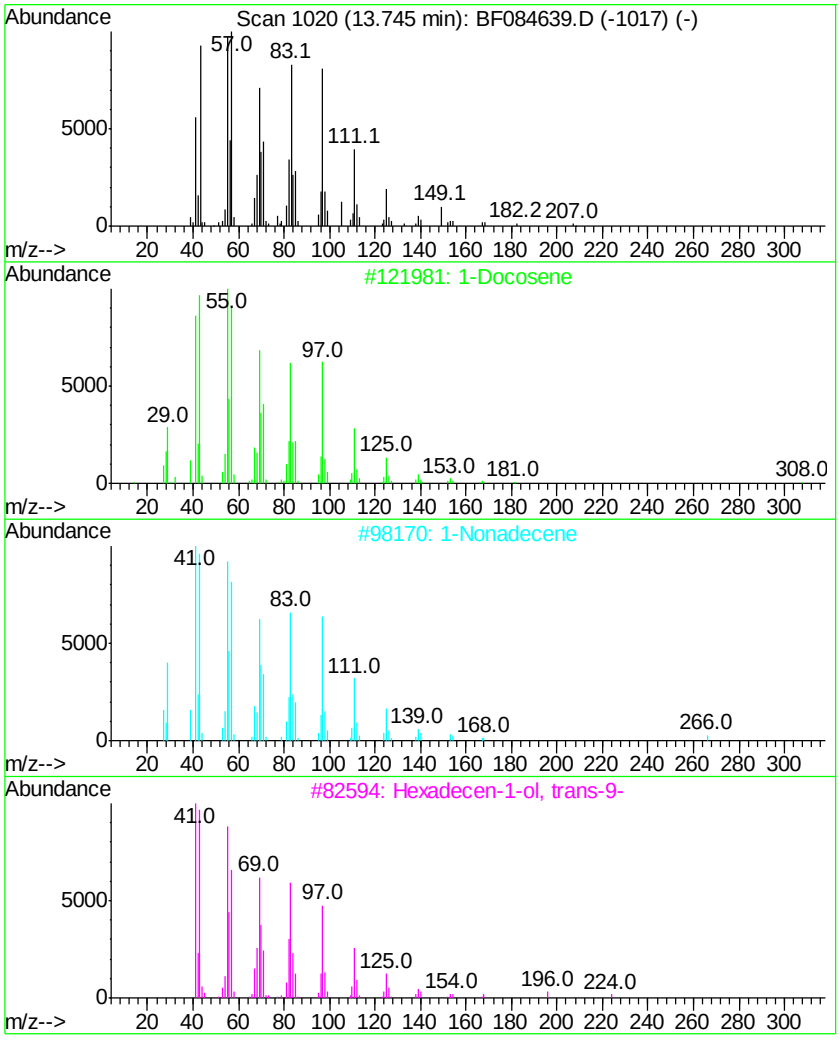
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

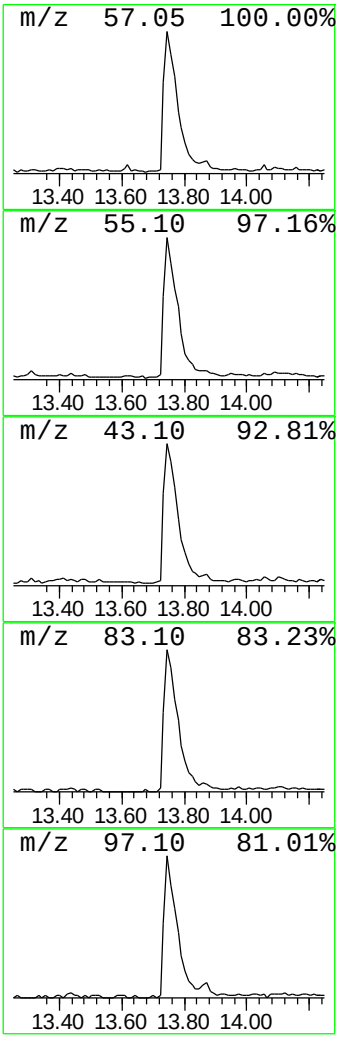
****

Peak Number 6 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	10.38 ng	866165	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	94
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	Hexadecen-1-ol, trans-9-	240	C16H32O	064437-47-4	87
4	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	80
5	2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	74





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
Data File : BF084639.D
Acq On : 29 Jan 2016 16:41
Operator : SJ/IZ
Sample : H1257-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B016(12-12.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

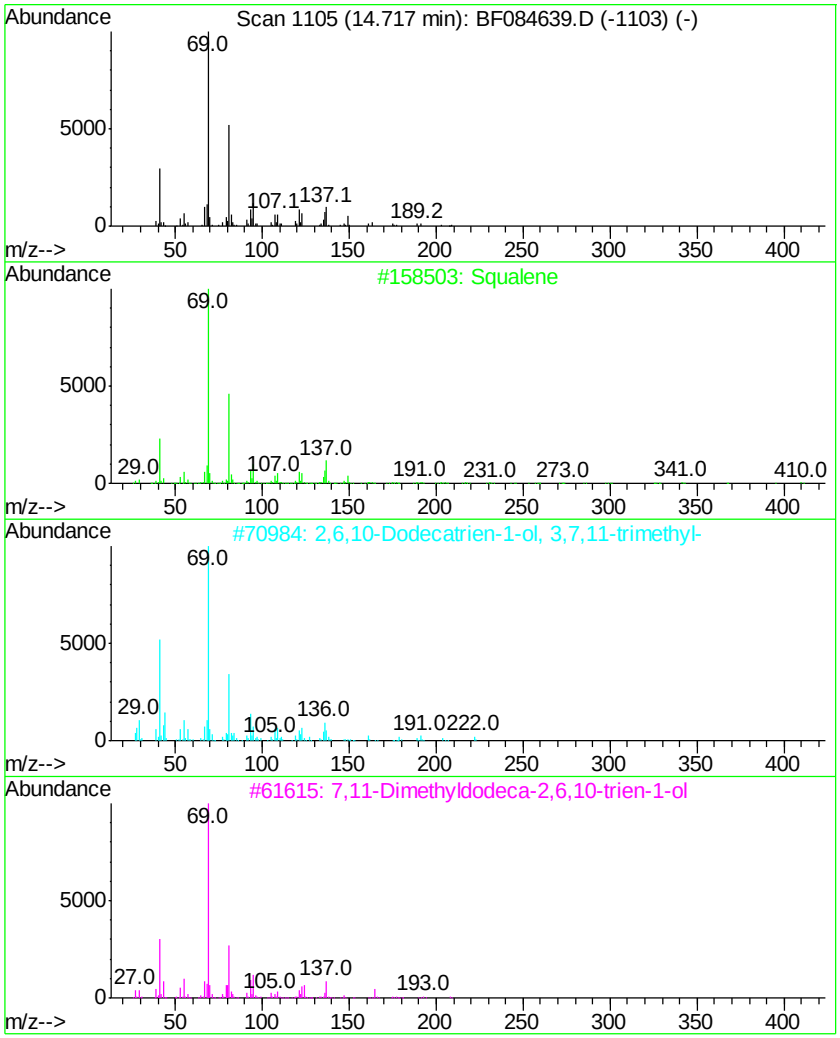
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

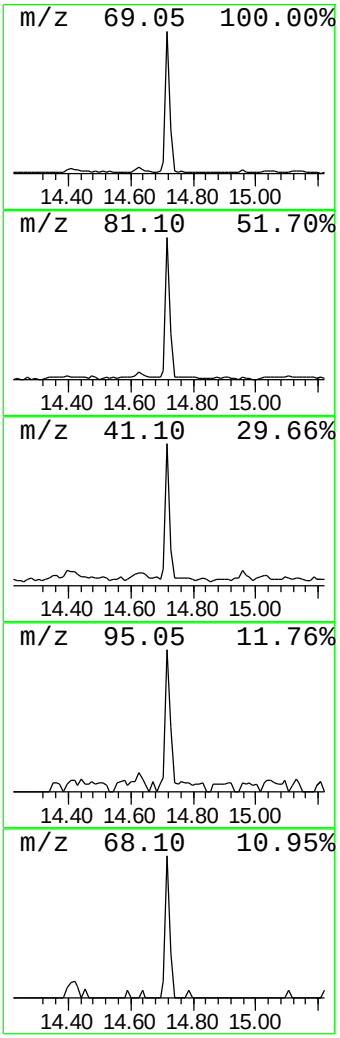
****

Peak Number 7 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	2.59 ng	188912	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	87
2	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
Data File : BF084639.D
Acq On : 29 Jan 2016 16:41
Operator : SJ/IZ
Sample : H1257-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B016(12-12.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

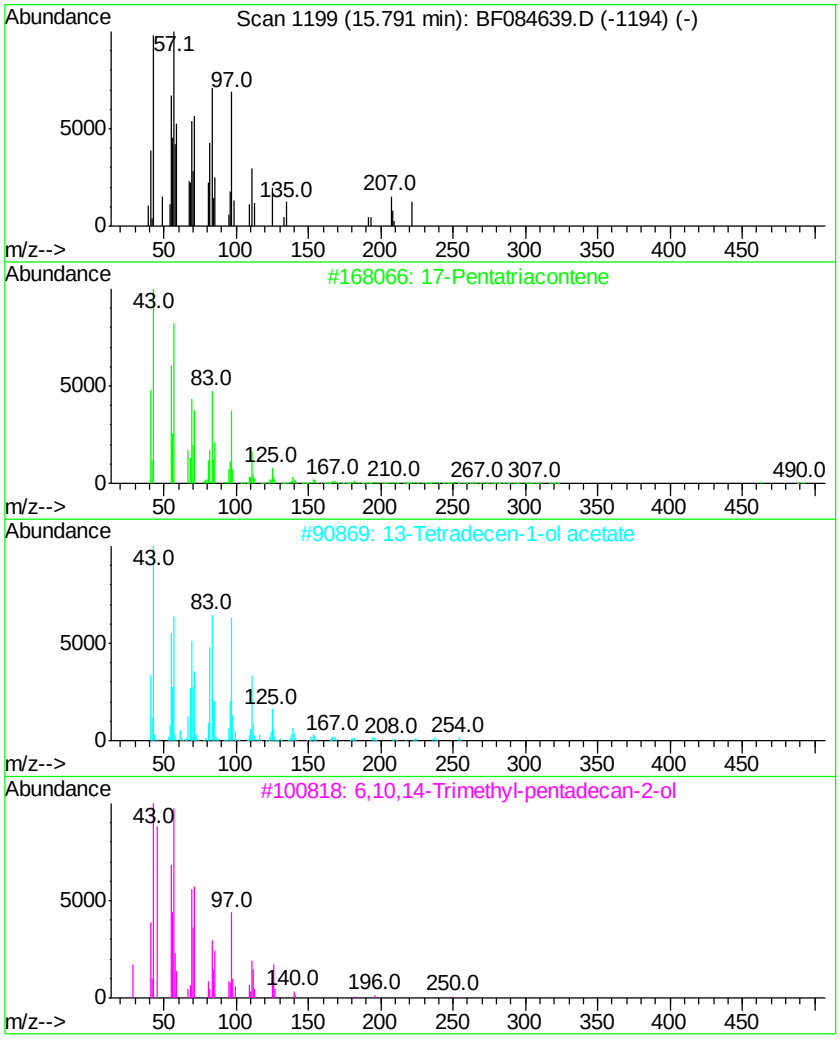
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

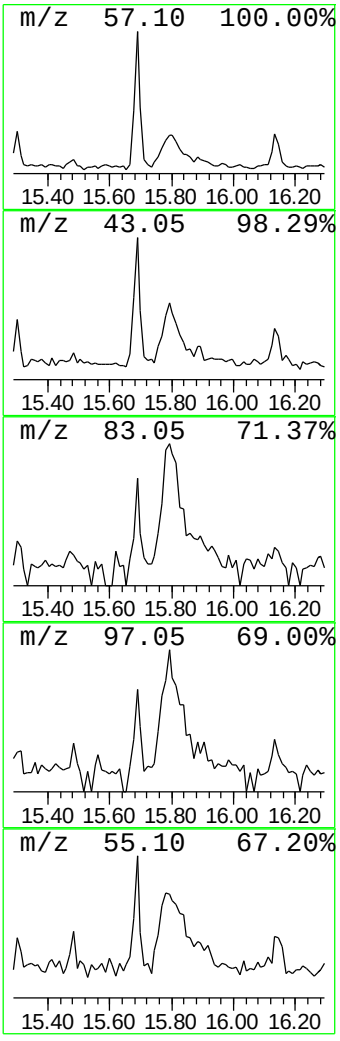
****

Peak Number 8 unknown15.79 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	2.14 ng	156004	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	49
2	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	43
3	6,10,14-Trimethyl-pentadecan-2-ol	270	C18H38O	1000143-49-8	38
4	Dodecane, 5-cyclohexyl-	252	C18H36	013151-85-4	38
5	Dodecane, 6-cyclohexyl-	252	C18H36	013151-86-5	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012916\
Data File : BF084639.D
Acq On : 29 Jan 2016 16:41
Operator : SJ/IZ
Sample : H1257-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B016(12-12.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.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
3-Penten-2-one, 4...	4.19	8.3	ng	428452	1	6.73	1026040	20.0
2-Pentanone, 4-hy...	4.90	99.6	ng	5110570	1	6.73	1026040	20.0
2-Pentanone, 4-me...	5.72	6.6	ng	338876	1	6.73	1026040	20.0
unknown6.49	6.49	75.3	ng	3864930	1	6.73	1026040	20.0
1-Docosene	13.75	10.4	ng	866165	5	13.87	1669570	20.0
Squalene	14.72	2.6	ng	188912	6	15.25	1461100	20.0
unknown15.79	15.79	2.1	ng	156004	6	15.25	1461100	20.0