LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011717\
Data File : BF092337.D
Acq On : 18 Jan 2017 1:15
Operator : UM/SJ
Sample : I1162-10
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-48-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-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	4.667	249	252	266	rBV	1331563	2183438	45.16%	5.012%
2	5.147	291	294	313	rBV	3118980	4834895	100.00%	11.097%
3	6.221	385	388	395	rBV	4214576	4733536	97.90%	10.865%
4	6.324	395	397	400	rVV	4548675	4315967	89.27%	9.906%
5	6.553	415	417	420	rBV	1236068	1101500	22.78%	2.528%
6	6.713	428	431	433	rBV	2888274	3492692	72.24%	8.017%
7	7.124	465	467	470	rBV	2543237	2588610	53.54%	5.942%
8	7.844	527	530	532	rBV	1360879	1465730	30.32%	3.364%
9	8.919	621	624	627	rBV	4428207	4288034	88.69%	9.842%
10	9.319	657	659	662	rBV	502061	471003	9.74%	1.081%
11	9.582	680	682	685	rBV	1386341	1541463	31.88%	3.538%
12	10.039	720	722	724	rVB	119235	102004	2.11%	0.234%
13	10.256	738	741	744	rBV	45736	61962	1.28%	0.142%
14	10.370	749	751	754	rBV2	1979496	2721352	56.29%	6.246%
15	10.508	761	763	767	rVB	140617	171968	3.56%	0.395%
16	10.953	800	802	803	rBV	110975	94991	1.96%	0.218%
17	11.068	809	812	814	rBV	1144077	1473546	30.48%	3.382%
18	11.376	837	839	842	rVB	51788	48706	1.01%	0.112%
19	11.616	858	860	864	rBV2	123385	149823	3.10%	0.344%
20	12.485	935	936	939	rVB2	92861	100918	2.09%	0.232%
21	12.645	948	950	953	rBV	2999938	3481248	72.00%	7.990%
22	13.194	995	998	999	rBV	58914	56583	1.17%	0.130%
23	13.571	1028	1031	1039	rBV2	88681	215704	4.46%	0.495%
24	13.685	1039	1041	1044	rBV	855160	1136139	23.50%	2.608%
25	14.211	1082	1087	1091	rBV2	27521	101451	2.10%	0.233%
26	14.336	1096	1098	1101	rVB	1103568	1022646	21.15%	2.347%
27	14.451	1106	1108	1112	rBV2	51701	95771	1.98%	0.220%
28	14.805	1137	1139	1147	rVB2	54495	161553	3.34%	0.371%
29	15.045	1157	1160	1163	rBV	829367	1002483	20.73%	2.301%
30	15.434	1191	1194	1197	rBV	39600	59899	1.24%	0.137%
31	15.514	1197	1201	1207	rVV6	15917	64419	1.33%	0.148%
32	15.845	1227	1230	1238	rVB2	30109	69115	1.43%	0.159%
33	16.325	1269	1272	1277	rVB	26940	54942	1.14%	0.126%
34	16.760	1305	1310	1314	rBV7	13256	51690	1.07%	0.119%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011717\
Data File : BF092337.D
Acq On : 18 Jan 2017 1:15
Operator : UM/SJ
Sample : I1162-10
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-48-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-BF122116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.537	1375	1378	1384	rVB5	17111	52365	1.08%	0.120%

Sum of corrected areas: 43568146

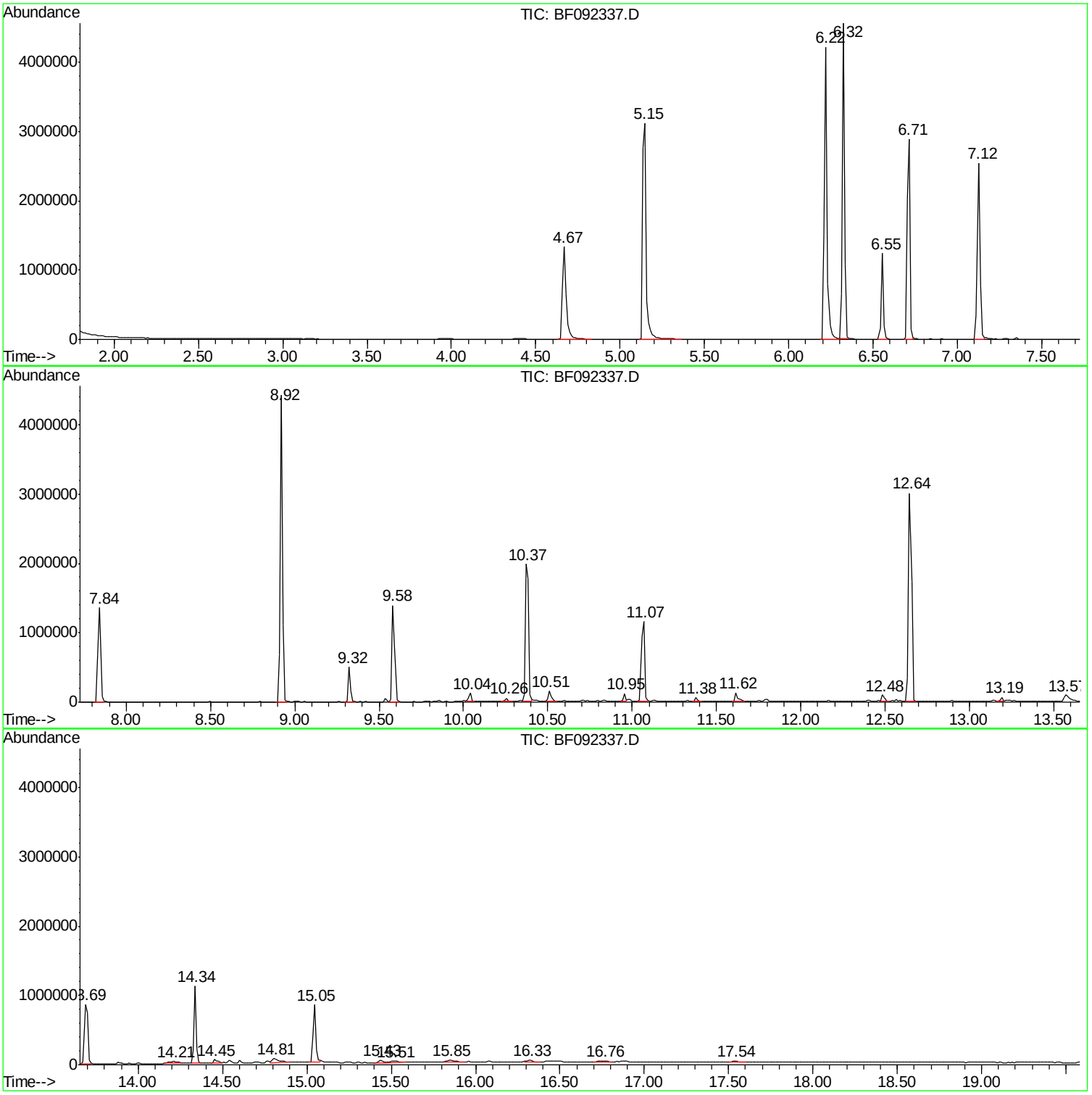
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011717\
Data File : BF092337.D
Acq On : 18 Jan 2017 1:15
Operator : UM/SJ
Sample : I1162-10
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-48-COMP

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011717\
Data File : BF092337.D
Acq On : 18 Jan 2017 1:15
Operator : UM/SJ
Sample : I1162-10
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-48-COMP

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

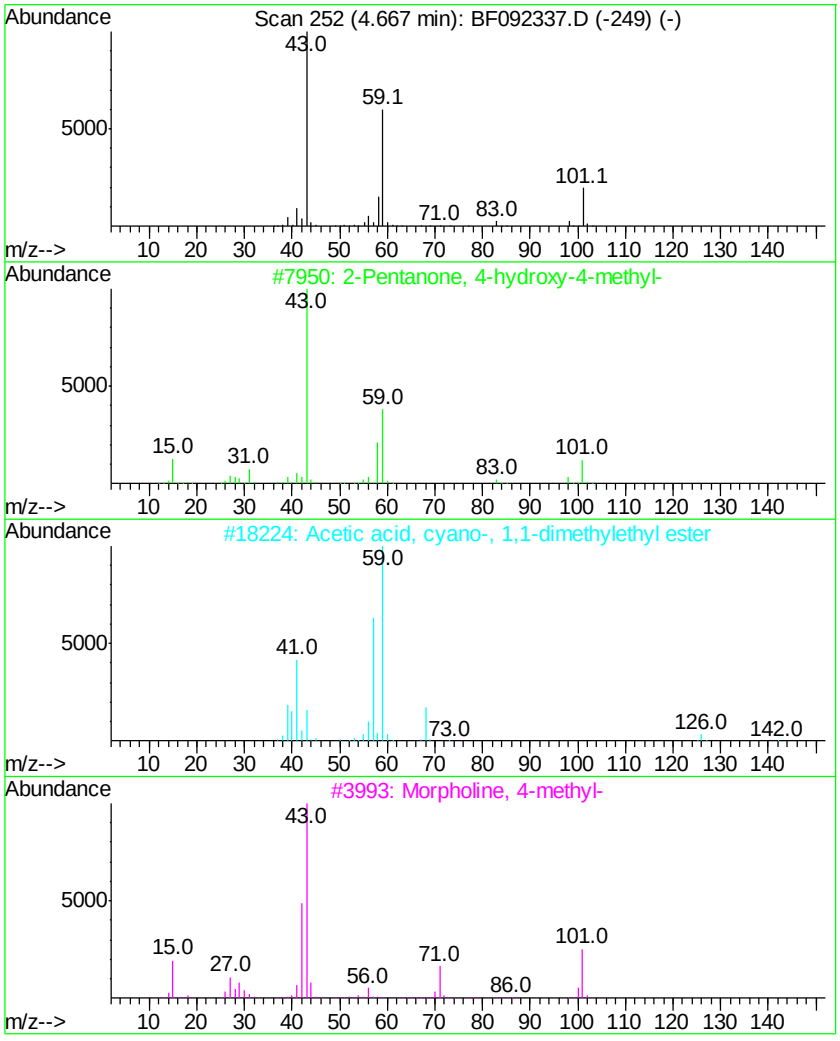
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

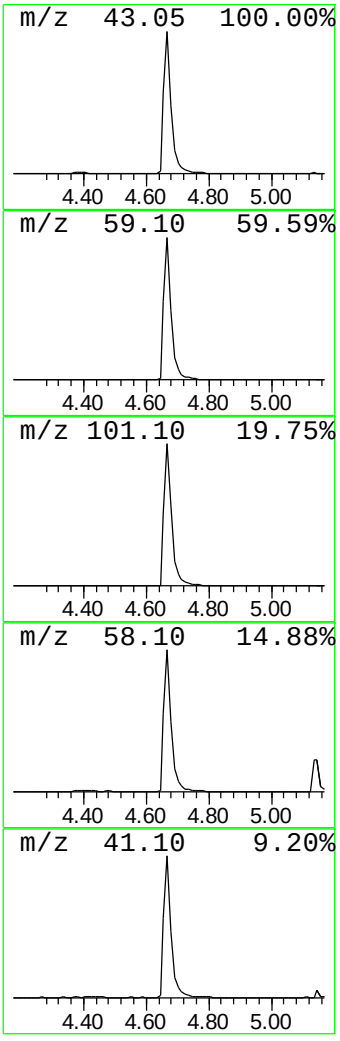
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.67	39.64 ng	2183440	1,4-Dichlorobenzene-d4	6.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	6-Hydroxy-4,4,6-trimethyltetrahy...	191	C7H13NOS2	016504-29-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011717\
Data File : BF092337.D
Acq On : 18 Jan 2017 1:15
Operator : UM/SJ
Sample : I1162-10
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-48-COMP

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

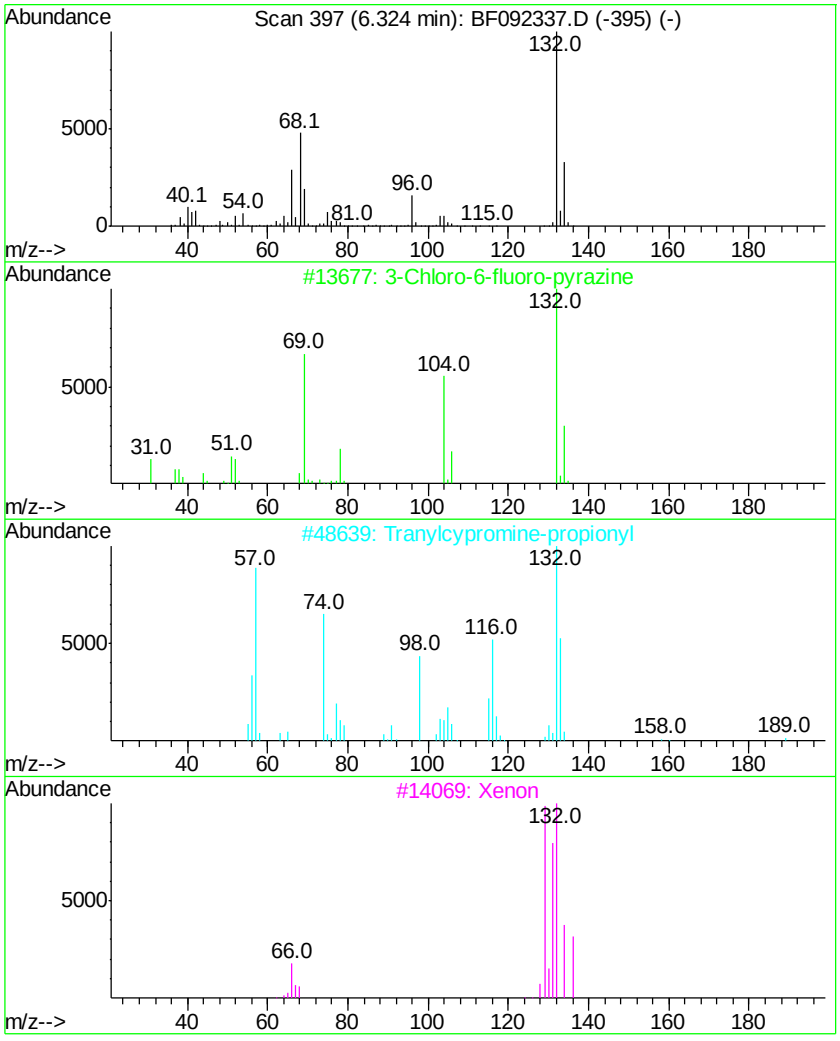
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

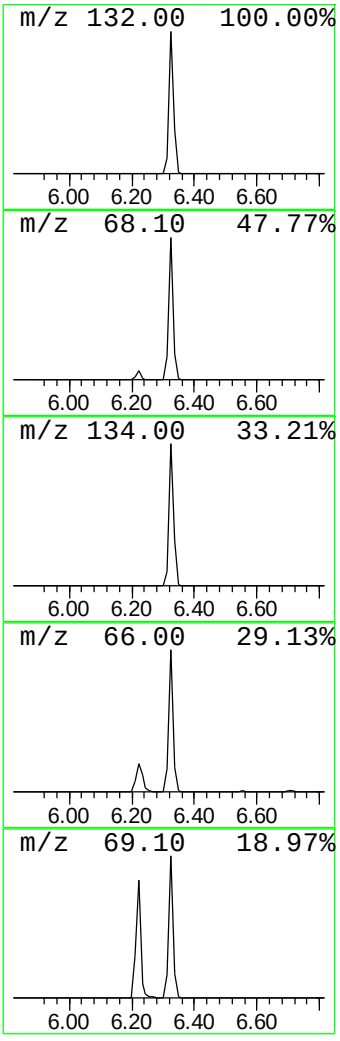
****

Peak Number 2 unknown6.32 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.32	78.37 ng	4315970	1,4-Dichlorobenzene-d4	6.55

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	Xenon	132	Xe	007440-63-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011717\
Data File : BF092337.D
Acq On : 18 Jan 2017 1:15
Operator : UM/SJ
Sample : I1162-10
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-48-COMP

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

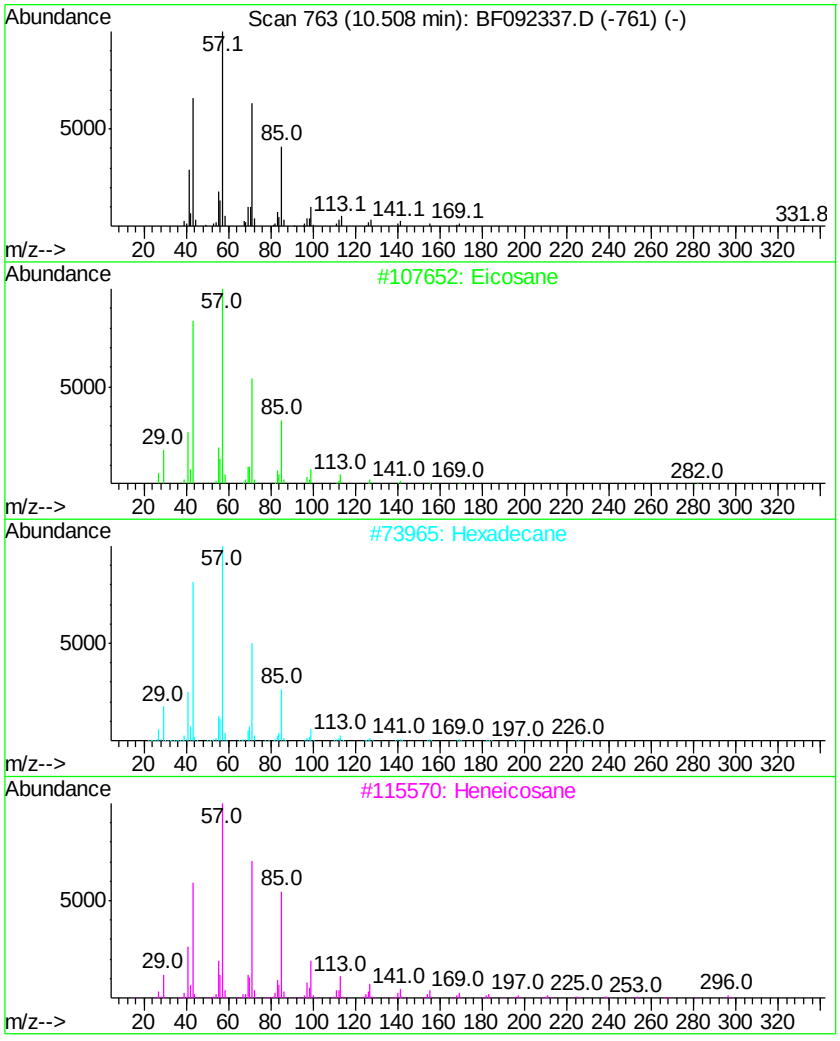
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

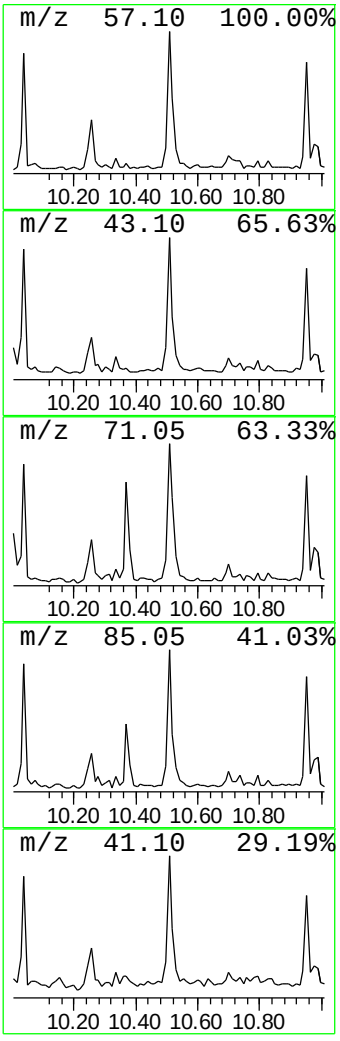
****

Peak Number 4 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.51	2.33 ng	171968	Phenanthrene-d10	11.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Pentadecane	212	C15H32	000629-62-9	86
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011717\
Data File : BF092337.D
Acq On : 18 Jan 2017 1:15
Operator : UM/SJ
Sample : I1162-10
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-48-COMP

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

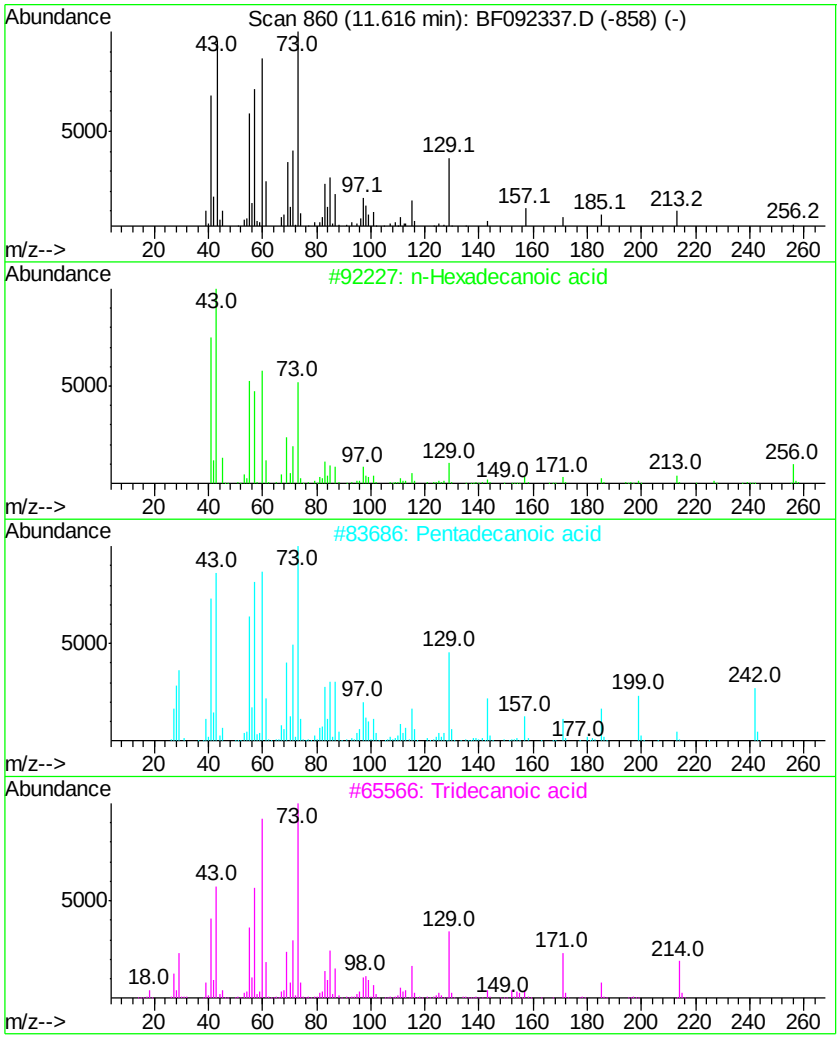
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

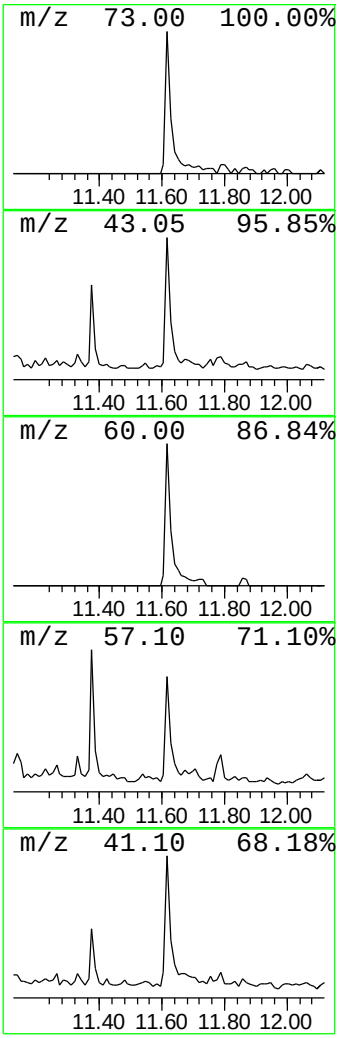
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.62	2.03 ng	149823	Phenanthrene-d10	11.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Amyl Nitrite	117	C5H11NO2	000110-46-3	27





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011717\
Data File : BF092337.D
Acq On : 18 Jan 2017 1:15
Operator : UM/SJ
Sample : I1162-10
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-48-COMP

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

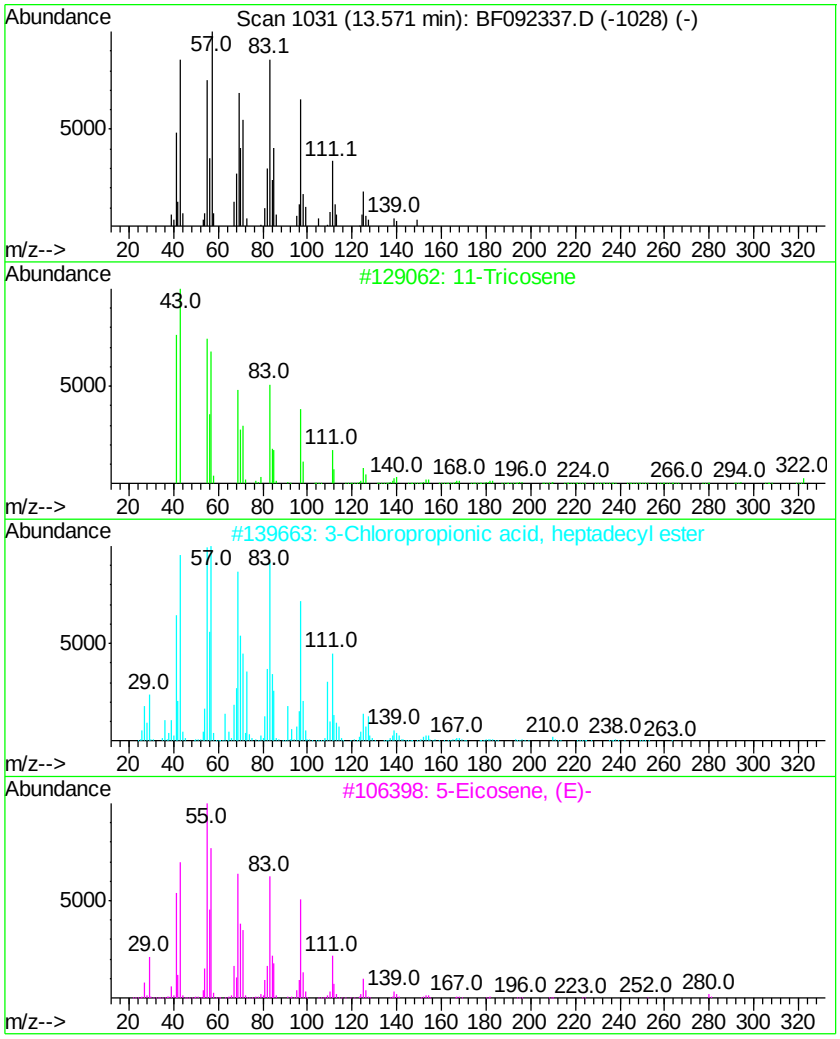
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

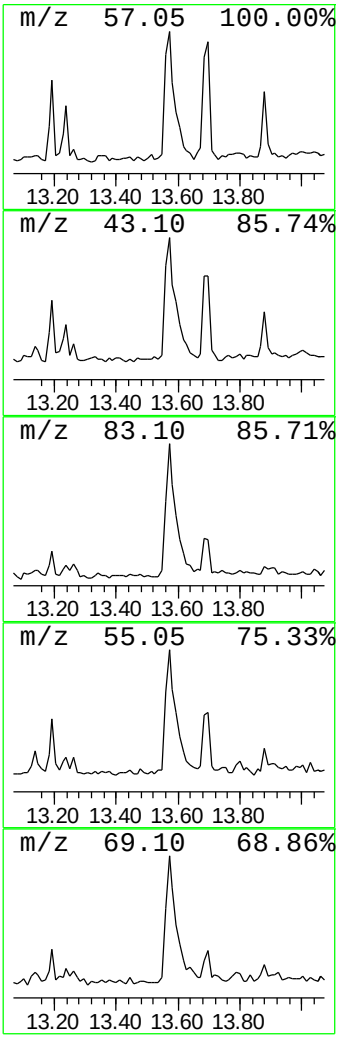
****

Peak Number 6 11-Tricosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.57	3.80 ng	215704	Chrysene-d12	13.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Tricosene	322	C23H46	052078-56-5	86
2	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	81
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	80
4	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	74
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	72





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Acq On : 18 Jan 2017 1:15
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Sample : I1162-10
Misc :
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Instrument : BNA_F
ClientSampleId : SB-48-COMP

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

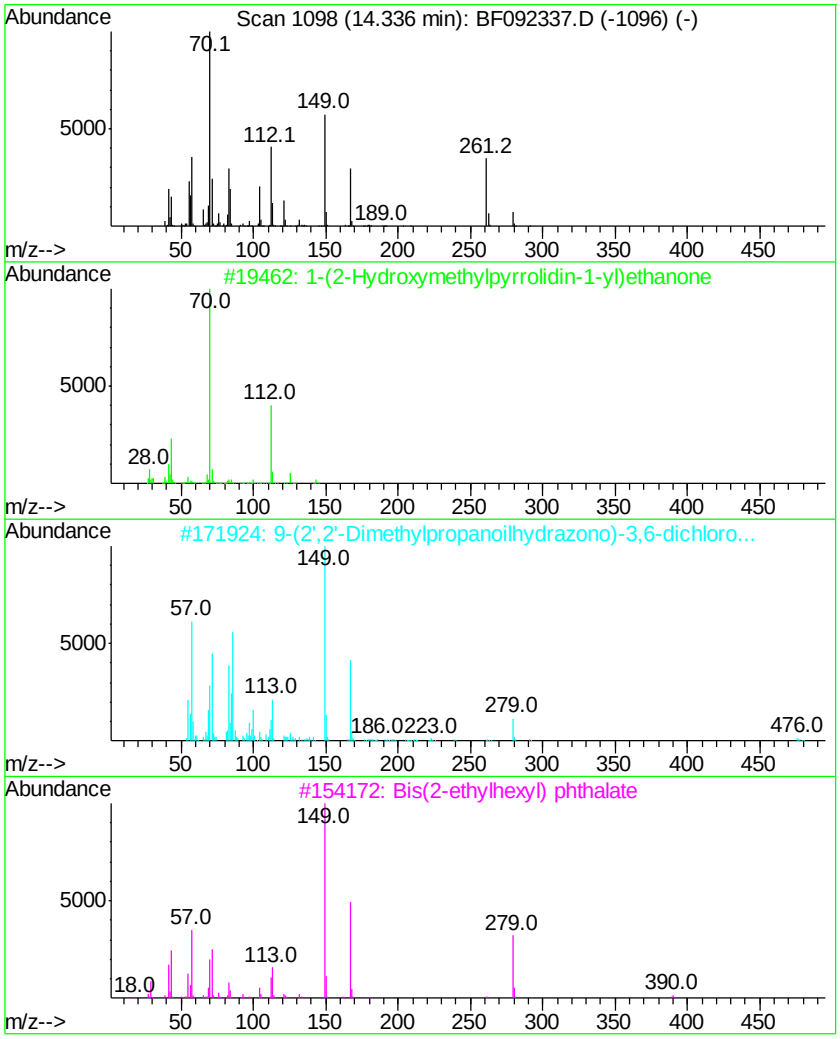
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

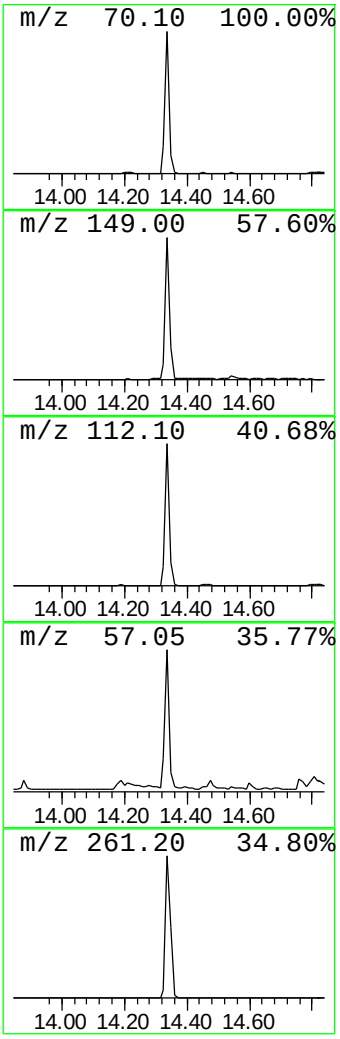
****

Peak Number 7 unknown14.34 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	18.00 ng	1022650	Chrysene-d12	13.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(2-Hydroxymethylpyrrolidin-1-y...	143	C7H13NO2	1000192-83-2	32
2	9-(2',2'-Dimethylpropanoilhydraz...	576	C30H42Cl2N4O3	1000111-04-6	25
3	Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	25
4	4-Nitrobenzoic acid, cyclobutyl ...	221	C11H11NO4	070335-00-1	25
5	1,2-Benzenedicarboxylic acid, di...	390	C24H38O4	027554-26-3	22





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

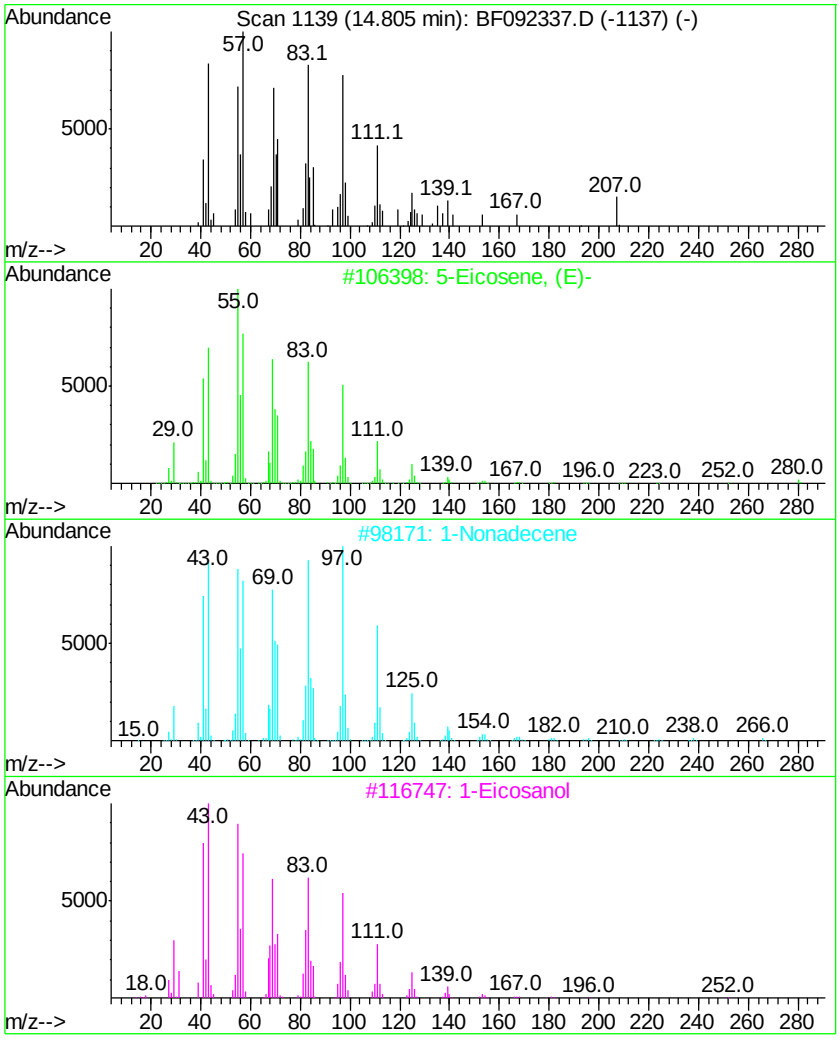
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

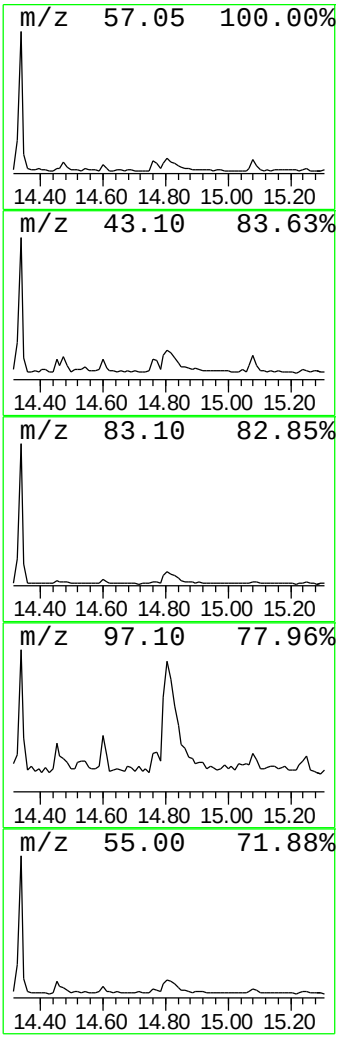
****

Peak Number 8 5-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	3.22 ng	161553	Perylene-d12	15.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	90
2	1-Nonadecene	266	C19H38	018435-45-5	87
3	1-Eicosanol	298	C20H42O	000629-96-9	86
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	86
5	1-Hexadecanol	242	C16H34O	036653-82-4	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011717\
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Acq On : 18 Jan 2017 1:15
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Sample : I1162-10
Misc :
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Instrument : BNA_F
ClientSampleId : SB-48-COMP

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...	4.67	39.6	ng	2183440	1	6.55	1101500	20.0
unknown6.32	6.32	78.4	ng	4315970	1	6.55	1101500	20.0
Eicosane	10.51	2.3	ng	171968	4	11.07	1473550	20.0
n-Hexadecanoic acid	11.62	2.0	ng	149823	4	11.07	1473550	20.0
11-Tricosene	13.57	3.8	ng	215704	5	13.69	1136140	20.0
unknown14.34	14.34	18.0	ng	1022650	5	13.69	1136140	20.0
5-Eicosene, (E)-	14.81	3.2	ng	161553	6	15.05	1002480	20.0