LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG011718\
Data File : BG032114.D
Acq On : 17 Jan 2018 23:36
Operator : SJ/JU
Sample : J1163-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-2-(0-4)

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_G\METHODS\8270-BG011218.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	3.391	12	17	27	rBV	35227	67439	1.62%	0.347%
2	3.479	27	32	39	rVB	27745	42640	1.02%	0.219%
3	5.665	396	404	412	rBV	34911	58669	1.41%	0.302%
4	6.170	483	490	499	rBV	610241	1050715	25.25%	5.404%
5	7.850	766	776	787	rBV	621573	1184842	28.47%	6.094%
6	8.256	837	845	854	rBV	664272	1204250	28.94%	6.194%
7	8.743	920	928	936	rBV	151531	270717	6.51%	1.392%
8	9.078	977	985	997	rBV	546164	998225	23.99%	5.134%
9	9.942	1123	1132	1141	rBV	366566	695335	16.71%	3.576%
10	11.628	1411	1419	1432	rVB	199597	389306	9.36%	2.002%
11	12.886	1627	1633	1642	rVB2	34745	56755	1.36%	0.292%
12	14.008	1813	1824	1835	rBV	1381449	2247569	54.01%	11.561%
13	14.801	1953	1959	1966	rBV	152913	220298	5.29%	1.133%
14	15.377	2051	2057	2069	rVB3	360524	613876	14.75%	3.158%
15	16.710	2278	2284	2291	rBV	208597	307505	7.39%	1.582%
16	16.857	2301	2309	2319	rBV	1324096	2100191	50.47%	10.802%
17	18.115	2515	2523	2532	rBV2	536975	885739	21.29%	4.556%
18	18.931	2657	2662	2668	rBV2	87188	135519	3.26%	0.697%
19	20.165	2869	2872	2881	rBV4	32328	53250	1.28%	0.274%
20	20.647	2948	2954	2964	rBV	2958937	4161310	100.00%	21.404%
21	21.987	3177	3182	3195	rBV	173681	279980	6.73%	1.440%
22	22.445	3252	3260	3269	rBV2	622480	1165947	28.02%	5.997%
23	26.152	3877	3891	3906	rBV2	367764	1196766	28.76%	6.156%
24	27.627	4134	4142	4151	rBV2	14582	54930	1.32%	0.283%

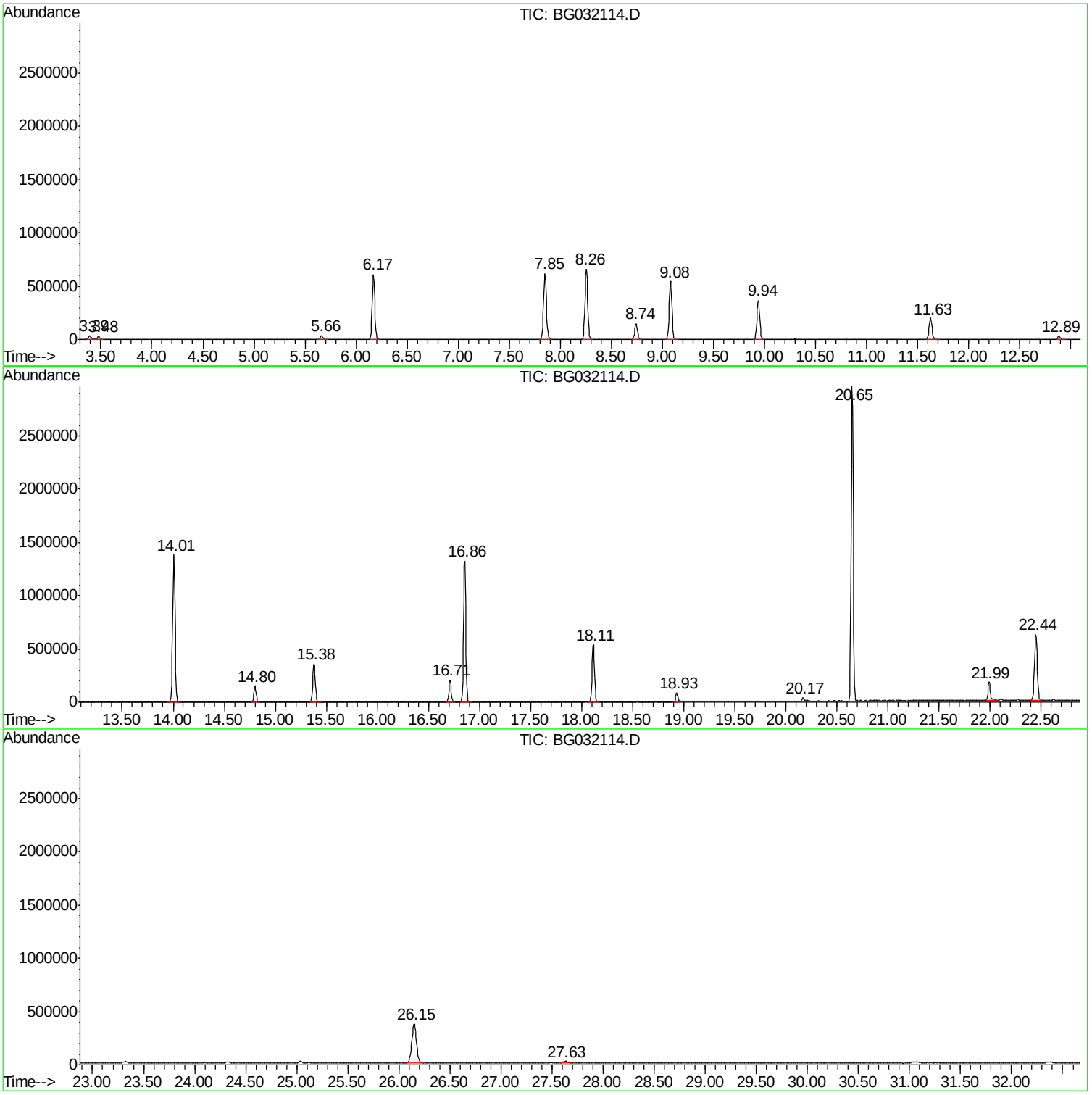
Sum of corrected areas: 19441773

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG011718\
Data File : BG032114.D
Acq On : 17 Jan 2018 23:36
Operator : SJ/JU
Sample : J1163-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-2-(0-4)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BG032114.D
Acq On : 17 Jan 2018 23:36
Operator : SJ/JU
Sample : J1163-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-2-(0-4)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

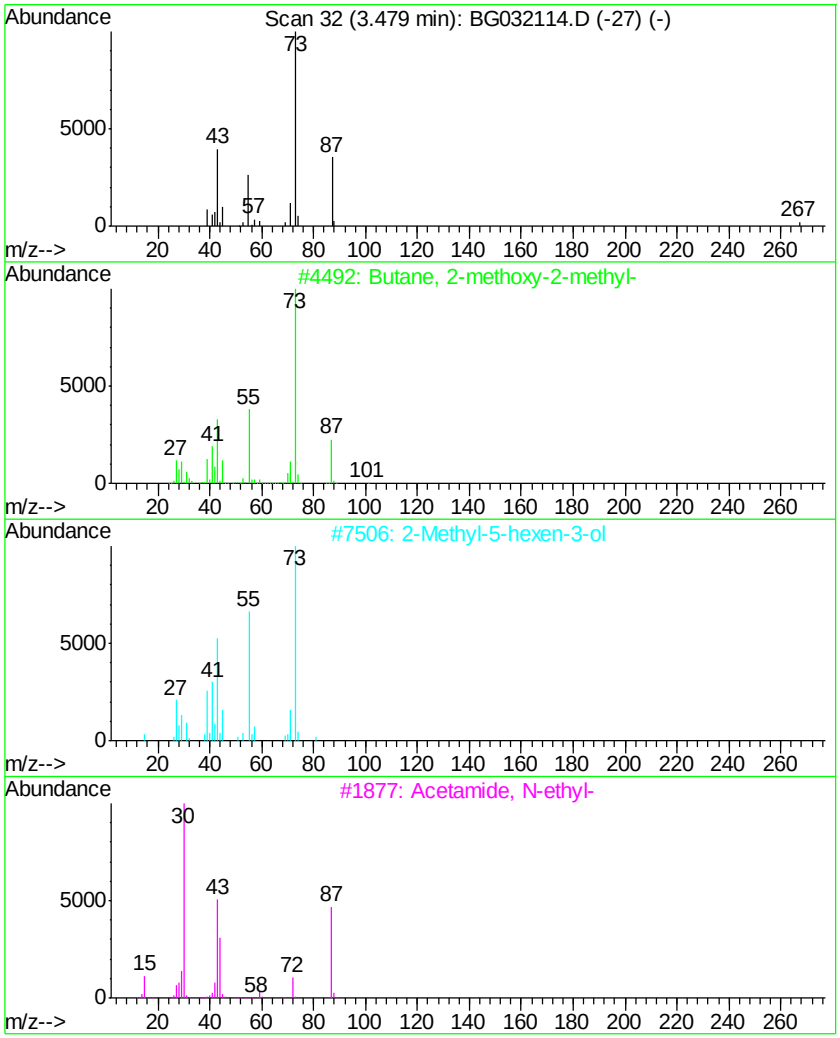
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

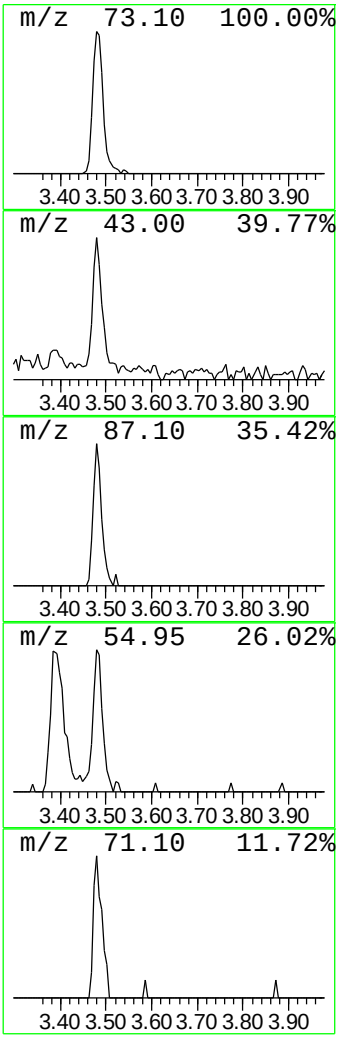
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.48	3.15 ng	42640	1,4-Dichlorobenzene-d4	8.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	16
4	3-Hexanol, 3-methyl-	116	C7H16O	000597-96-6	9
5	3-Pentanol, 2,3-dimethyl-	116	C7H16O	000595-41-5	9





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG011718\
Data File : BG032114.D
Acq On : 17 Jan 2018 23:36
Operator : SJ/JU
Sample : J1163-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-2-(0-4)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

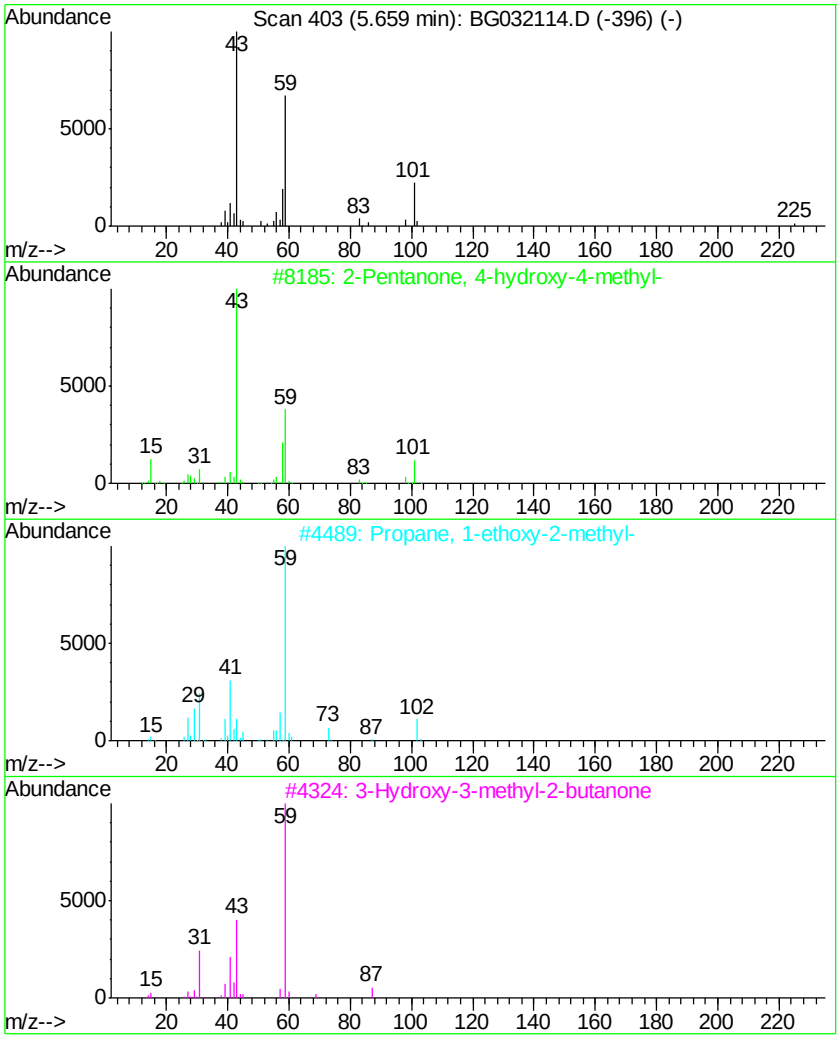
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

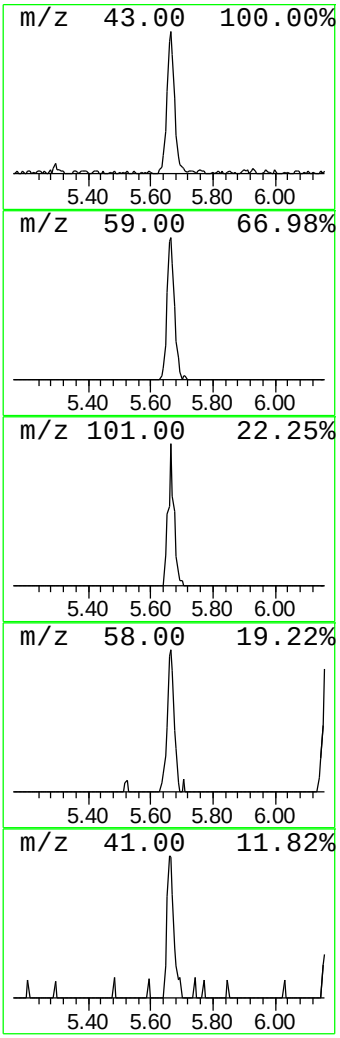
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.66	4.33 ng	58669	1,4-Dichlorobenzene-d4	8.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	38
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
4	2,4-Pentanedione, 3-(1-methyleth...	142	C8H14O2	001540-38-1	12
5	Acetone	58	C3H6O	000067-64-1	10





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG011718\
Data File : BG032114.D
Acq On : 17 Jan 2018 23:36
Operator : SJ/JU
Sample : J1163-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-2-(0-4)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

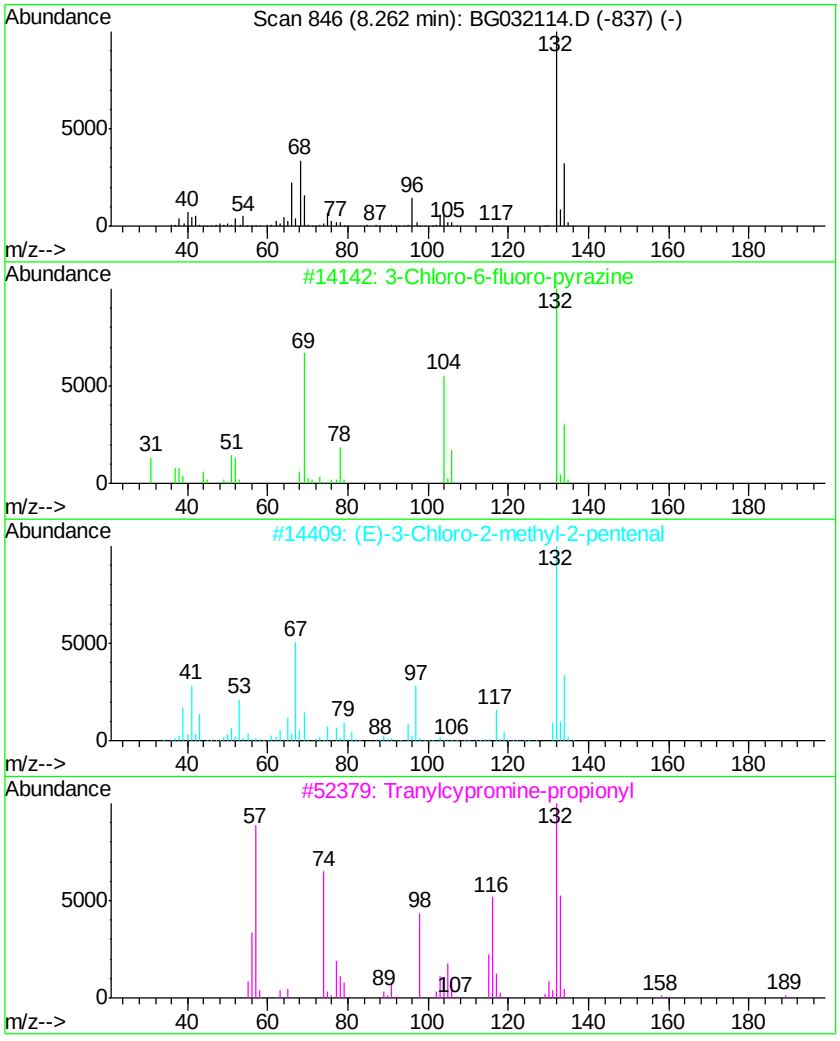
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

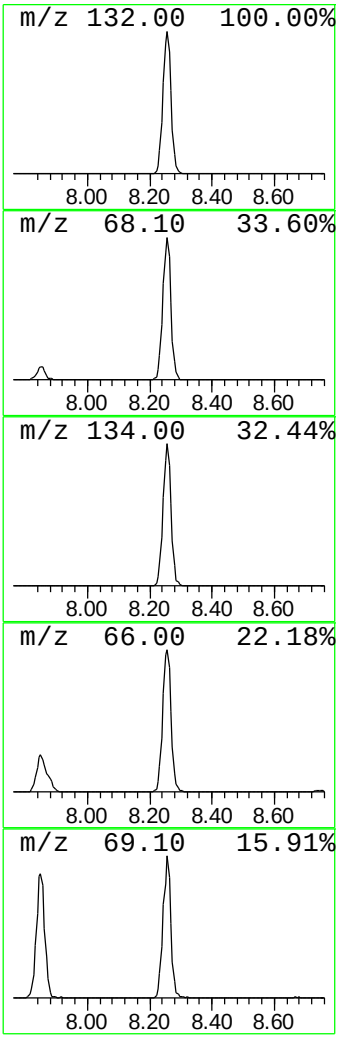
****

Peak Number 4 unknown8.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.26	88.97 ng	1204250	1,4-Dichlorobenzene-d4	8.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG011718\
Data File : BG032114.D
Acq On : 17 Jan 2018 23:36
Operator : SJ/JU
Sample : J1163-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-2-(0-4)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

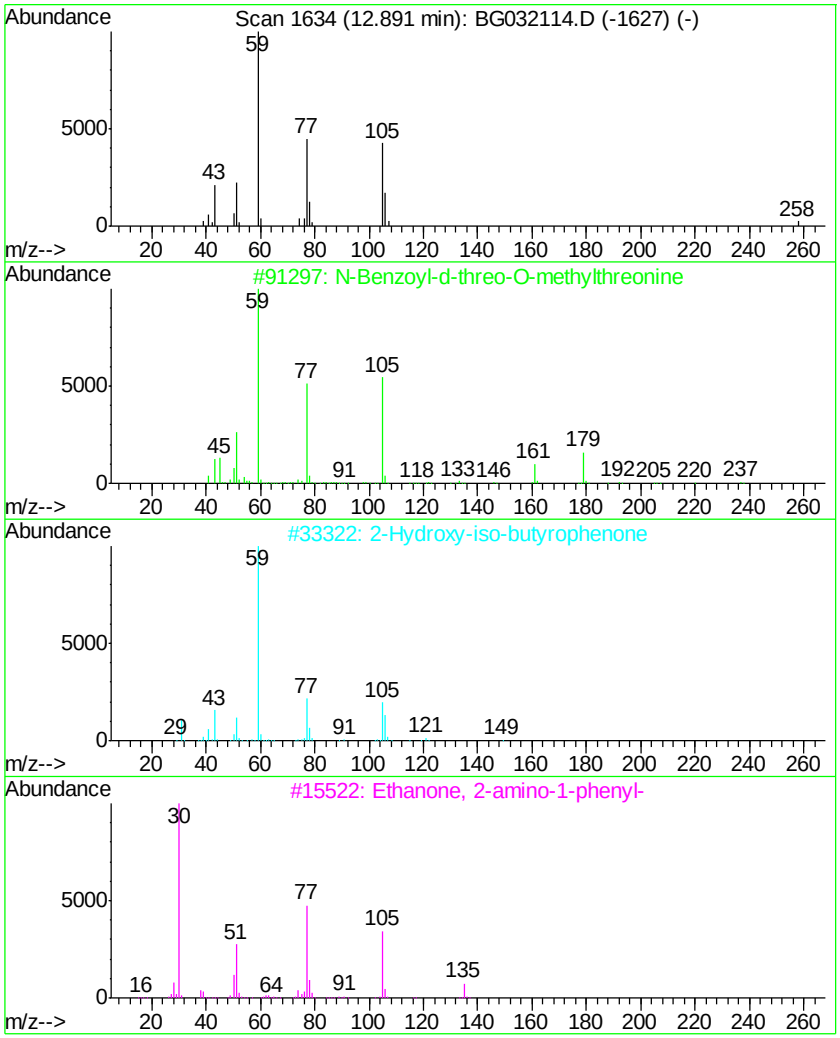
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

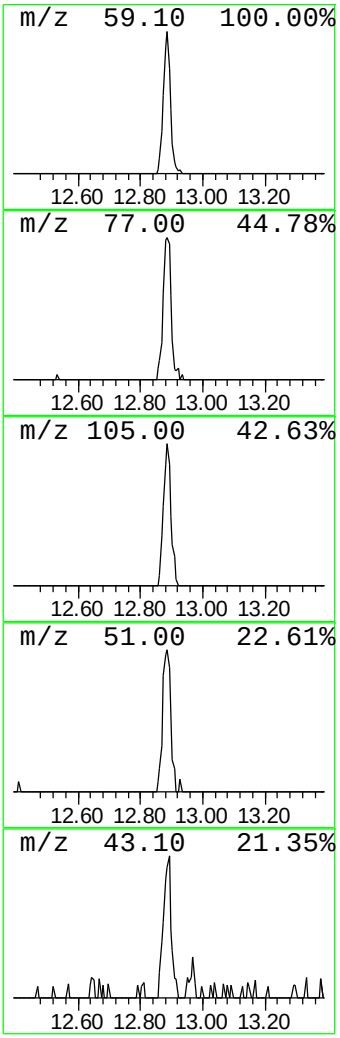
****

Peak Number 6 N-Benzoyl-d-threo-O-methylt... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.89	2.92 ng	56755	Naphthalene-d8	11.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-Benzoyl-d-threo-O-methylthreonine	237	C12H15NO4	131644-54-7	50
2	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	25
3	Ethanone, 2-amino-1-phenyl-	135	C8H9NO	000613-89-8	16
4	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	9
5	Propanedioic acid, (benzoylhydra...	282	C12H14N2O6	1000142-99-9	9





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG011718\
Data File : BG032114.D
Acq On : 17 Jan 2018 23:36
Operator : SJ/JU
Sample : J1163-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-2-(0-4)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

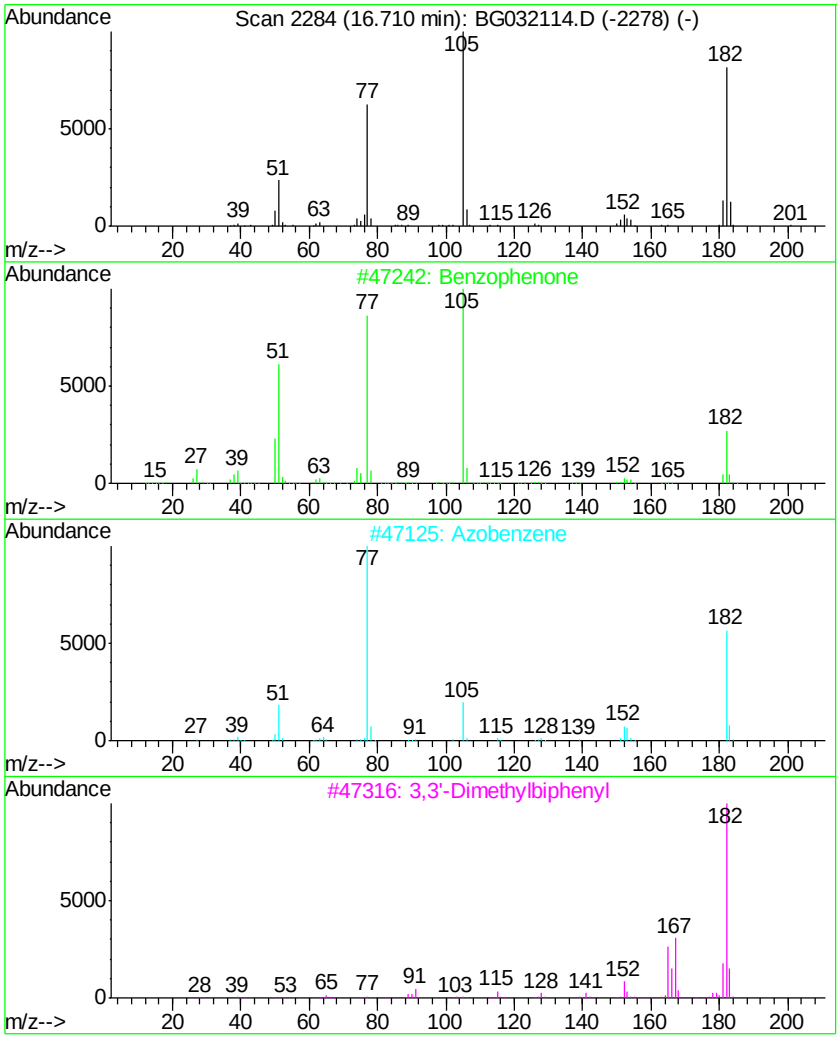
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

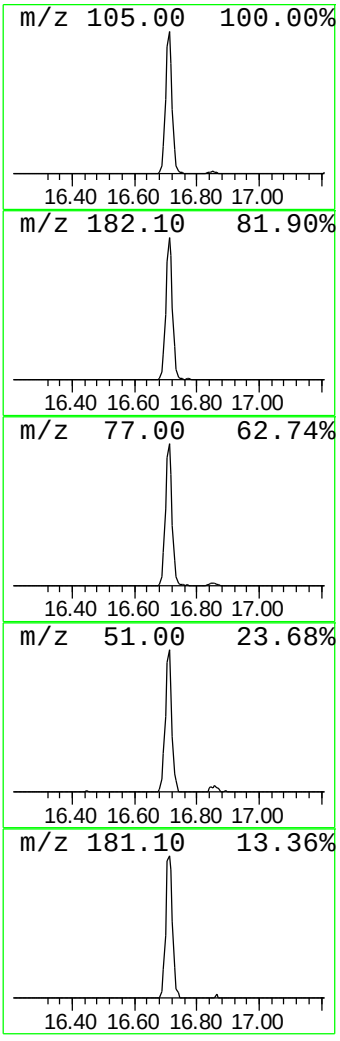
****

Peak Number 7 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.71	10.02 ng	307505	Acenaphthene-d10	15.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Azobenzene	182	C12H10N2	000103-33-3	72
3	3,3'-Dimethylbiphenyl	182	C14H14	000612-75-9	43
4	2,4,6-Trimethoxytoluene	182	C10H14O3	014107-97-2	43
5	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	35





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG011718\
Data File : BG032114.D
Acq On : 17 Jan 2018 23:36
Operator : SJ/JU
Sample : J1163-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-2-(0-4)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

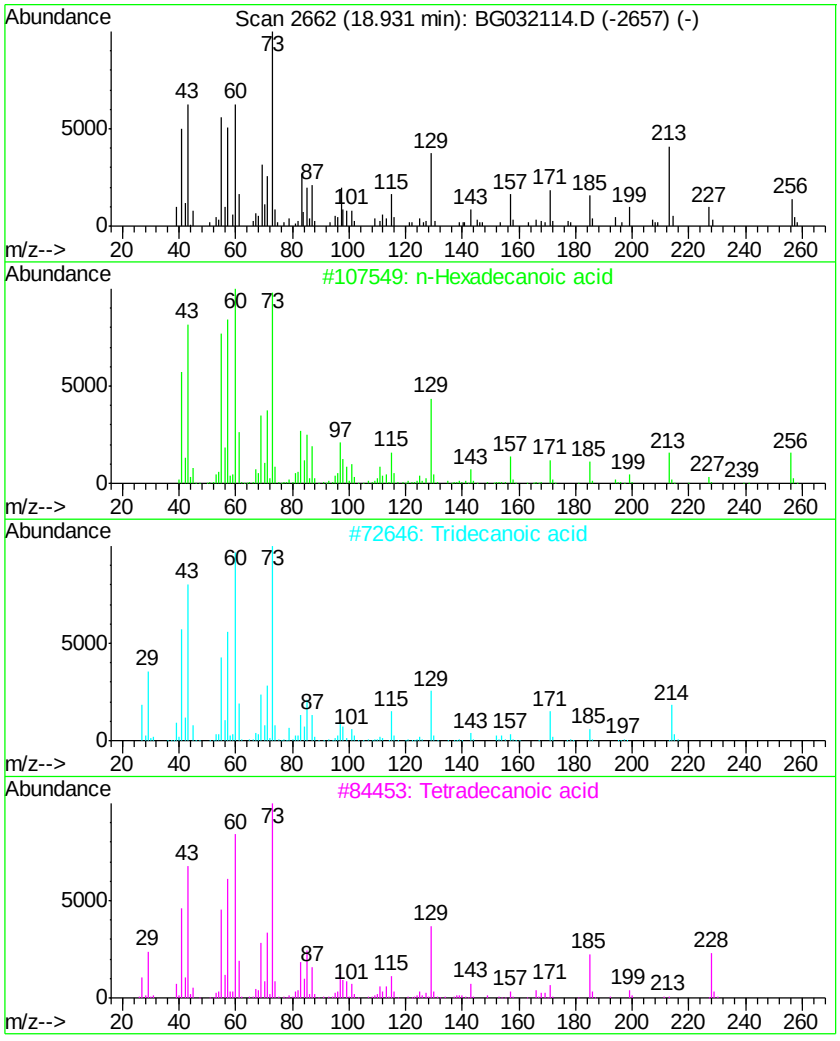
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

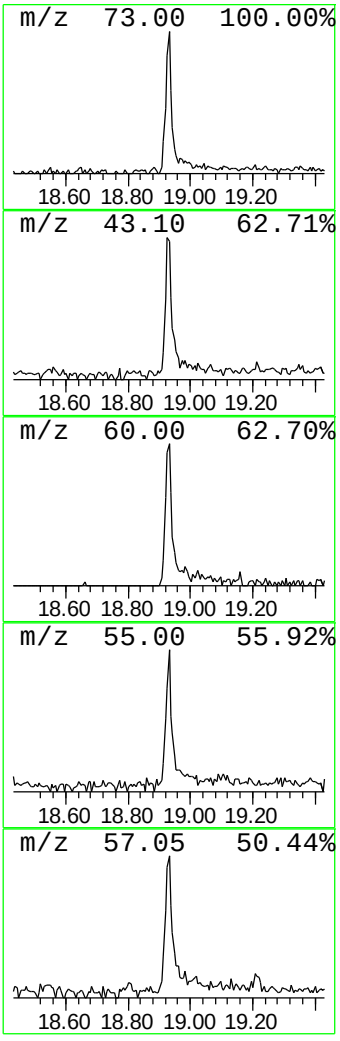
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.93	3.06 ng	135519	Phenanthrene-d10	18.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
4	n-Decanoic acid	172	C10H20O2	000334-48-5	42
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	38





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Data File : BG032114.D
Acq On : 17 Jan 2018 23:36
Operator : SJ/JU
Sample : J1163-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-2-(0-4)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

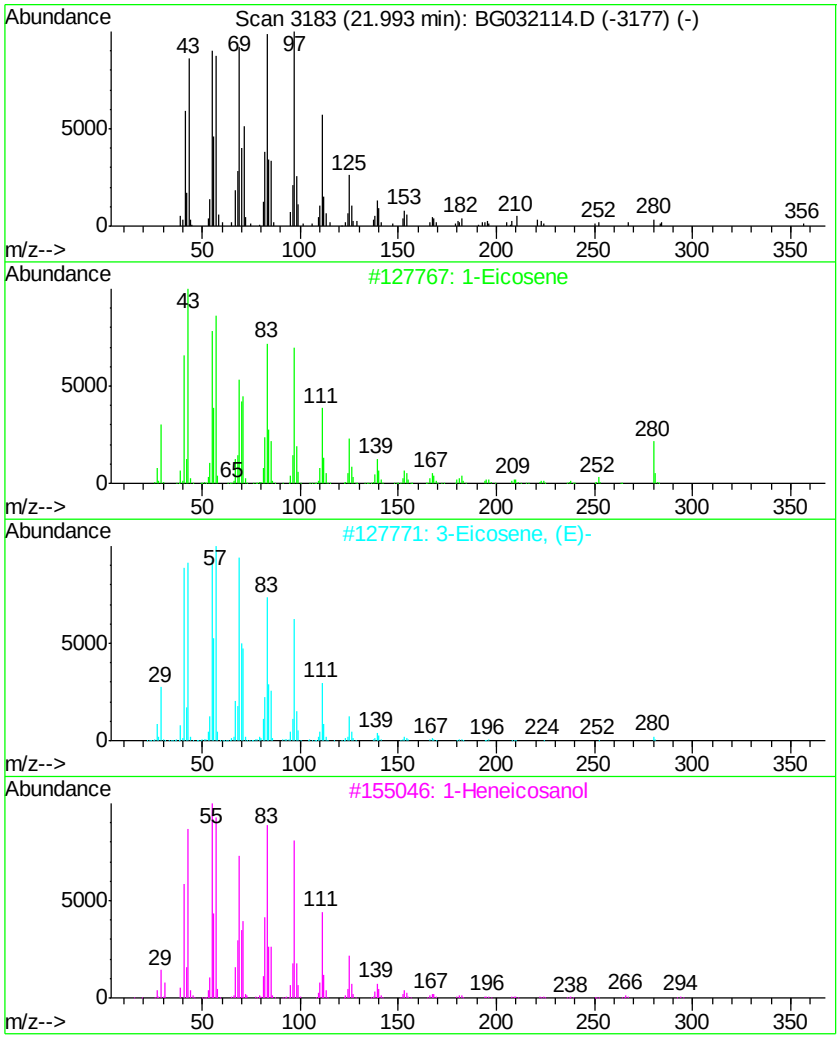
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

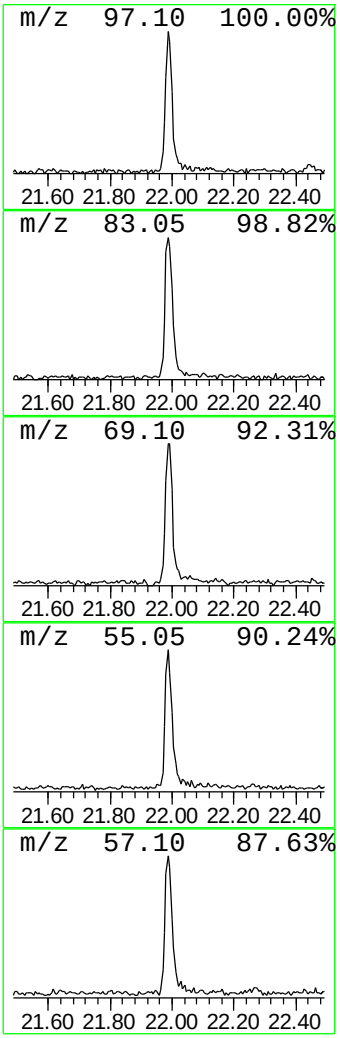
****

Peak Number 9 1-Eicosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.99	4.80 ng	279980	Chrysene-d12	22.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosene	280	C20H40	003452-07-1	98
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	96
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
5	Behenic alcohol	326	C22H46O	000661-19-8	95





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG011718\
Data File : BG032114.D
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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
Butane, 2-methoxy...	3.48	3.1	ng	42640	1	8.74	270717	20.0
2-Pentanone, 4-hy...	5.66	4.3	ng	58669	1	8.74	270717	20.0
unknown8.26	8.26	89.0	ng	1204250	1	8.74	270717	20.0
N-Benzoyl-d-threo...	12.89	2.9	ng	56755	2	11.63	389306	20.0
Benzophenone	16.71	10.0	ng	307505	3	15.38	613876	20.0
n-Hexadecanoic acid	18.93	3.1	ng	135519	4	18.11	885739	20.0
1-Eicosene	21.99	4.8	ng	279980	5	22.44	1165950	20.0