LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA G\DATA\BG122617\
Data File : BG031766.D
Acq On : 26 Dec 2017 17:53
Operator : SJ/JU
Sample : I7040-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-6

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-BG122117.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	3.434	19	25	35	rBV	87072	180574	4.47%	1.034%
2	3.528	35	41	49	rVB	30931	51254	1.27%	0.294%
3	5.726	406	415	422	rBV2	27866	49403	1.22%	0.283%
4	6.225	493	500	511	rBV	300055	523418	12.95%	2.997%
5	7.900	778	785	793	rBV	196657	360796	8.93%	2.066%
6	8.317	848	856	866	rBV	604733	1072934	26.55%	6.144%
7	8.805	931	939	949	rVB	127991	236550	5.85%	1.355%
8	9.145	989	997	1010	rVB	550899	1018856	25.21%	5.835%
9	10.003	1135	1143	1153	rBV	388389	721845	17.86%	4.134%
10	11.689	1420	1430	1438	rBV	188929	366183	9.06%	2.097%
11	13.505	1736	1739	1750	rVB7	15362	41885	1.04%	0.240%
12	14.063	1826	1834	1844	rBV	1516745	2499927	61.87%	14.316%
13	14.639	1921	1932	1937	rBV	18911	58594	1.45%	0.336%
14	15.203	2020	2028	2038	rBV	18071	61096	1.51%	0.350%
15	15.438	2056	2068	2078	rBV2	337463	652883	16.16%	3.739%
16	15.861	2136	2140	2146	rBV7	24954	49613	1.23%	0.284%
17	15.955	2152	2156	2161	rVB7	26173	46434	1.15%	0.266%
18	16.020	2161	2167	2174	rBV9	43432	106573	2.64%	0.610%
19	16.642	2268	2273	2278	rBV9	19127	40916	1.01%	0.234%
20	16.907	2311	2318	2329	rVB	1299607	2145429	53.10%	12.286%
21	18.170	2526	2533	2539	rVB2	478610	776902	19.23%	4.449%
22	18.987	2668	2672	2679	rBV2	57591	86315	2.14%	0.494%
23	20.226	2878	2883	2888	rBV	101640	148865	3.68%	0.853%
24	20.702	2957	2964	2972	rBV	2979570	4040728	100.00%	23.140%
25	21.607	3114	3118	3124	rVB	61517	94482	2.34%	0.541%
26	22.512	3265	3272	3283	rVB2	513806	982143	24.31%	5.624%
27	26.266	3898	3911	3926	rBV	320369	1047408	25.92%	5.998%

Sum of corrected areas: 17462006

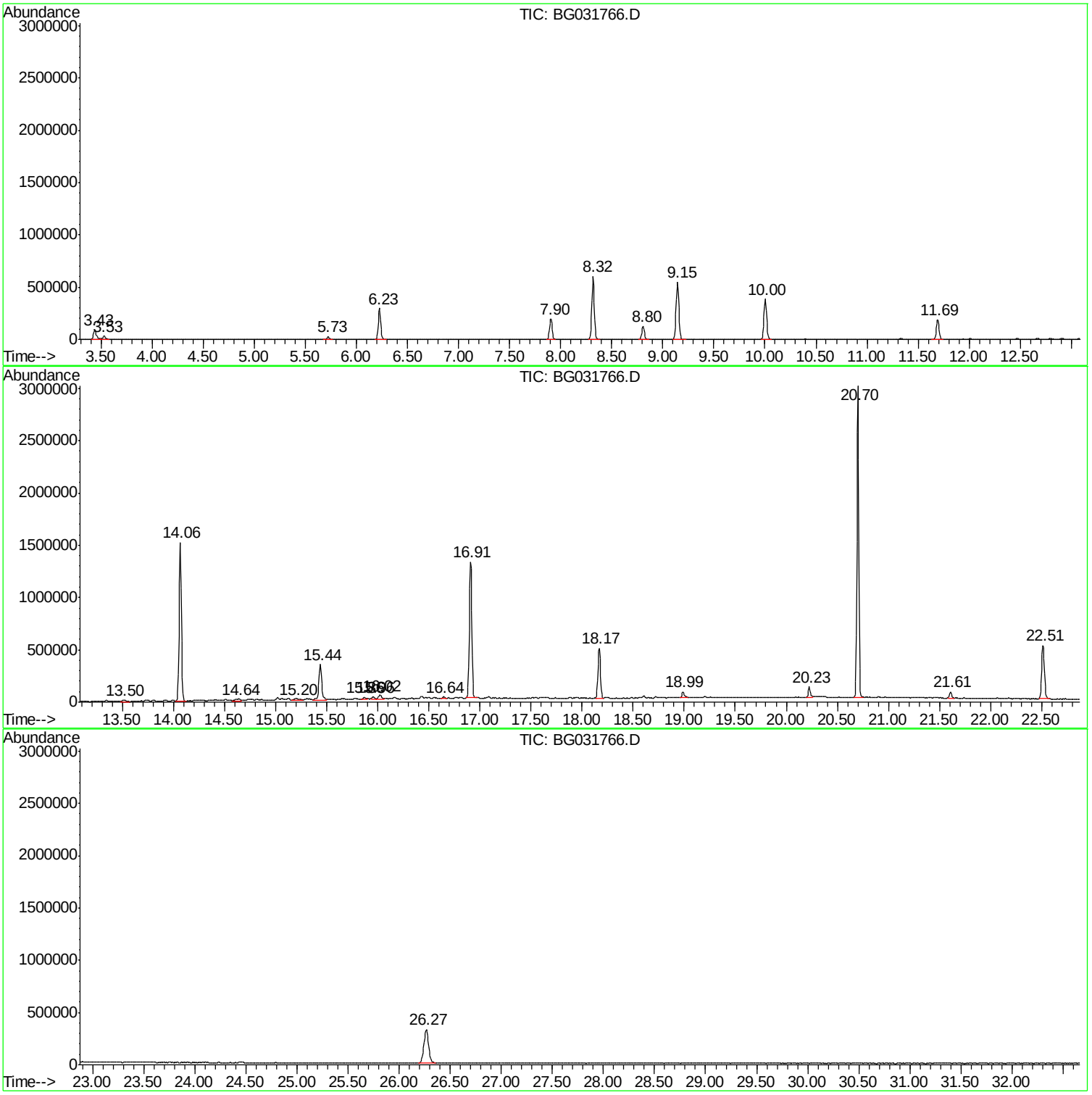
LSC Report - Integrated Chromatogram

Data Path : U:\HPCHEM1\BNA G\DATA\BG122617\
Data File : BG031766.D
Acq On : 26 Dec 2017 17:53
Operator : SJ/JU
Sample : I7040-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-6

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : U:\HPCHEM1\BNA G\DATA\BG122617\
Data File : BG031766.D
Acq On : 26 Dec 2017 17:53
Operator : SJ/JU
Sample : I7040-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-6

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

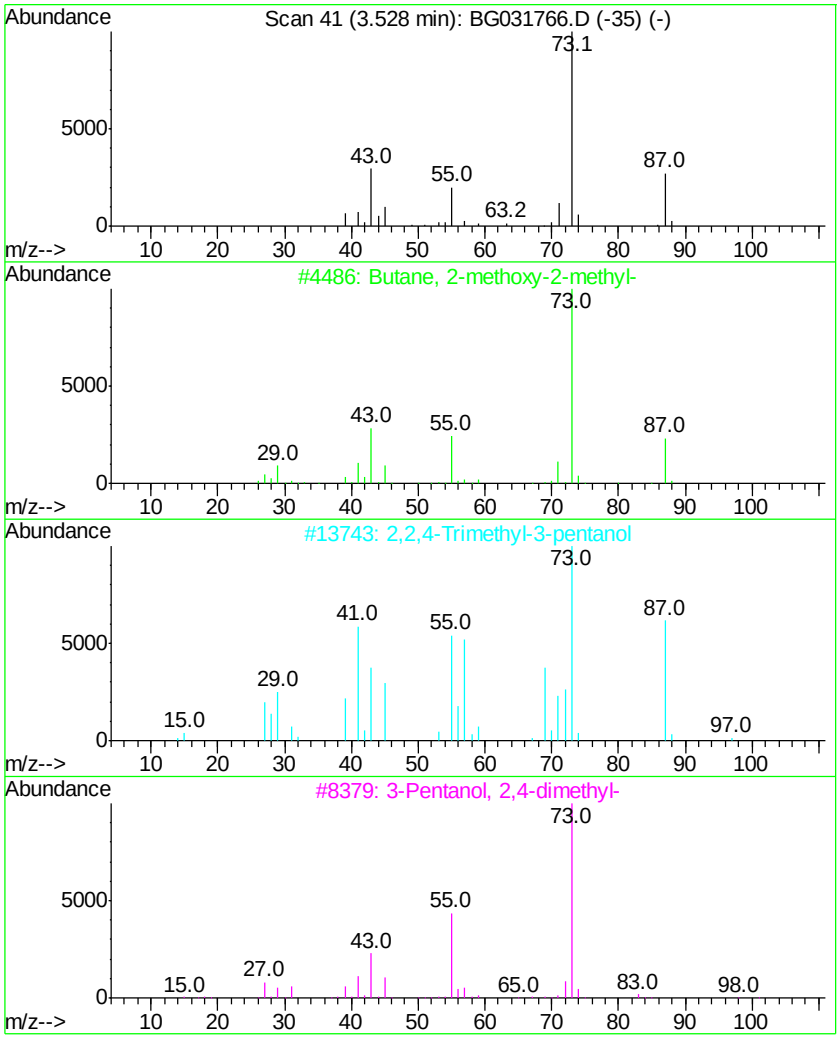
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

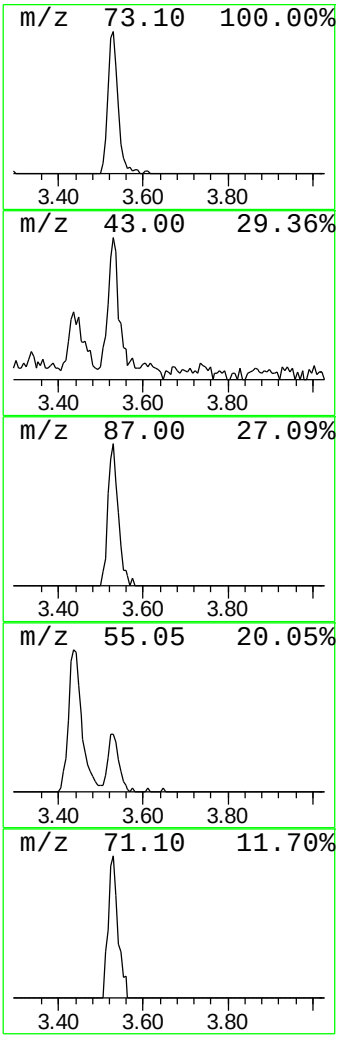
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.53	4.33 ng	51254	1,4-Dichlorobenzene-d4	8.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	56
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	9





Data Path : U:\HPCHEM1\BNA G\DATA\BG122617\
Data File : BG031766.D
Acq On : 26 Dec 2017 17:53
Operator : SJ/JU
Sample : I7040-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-6

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.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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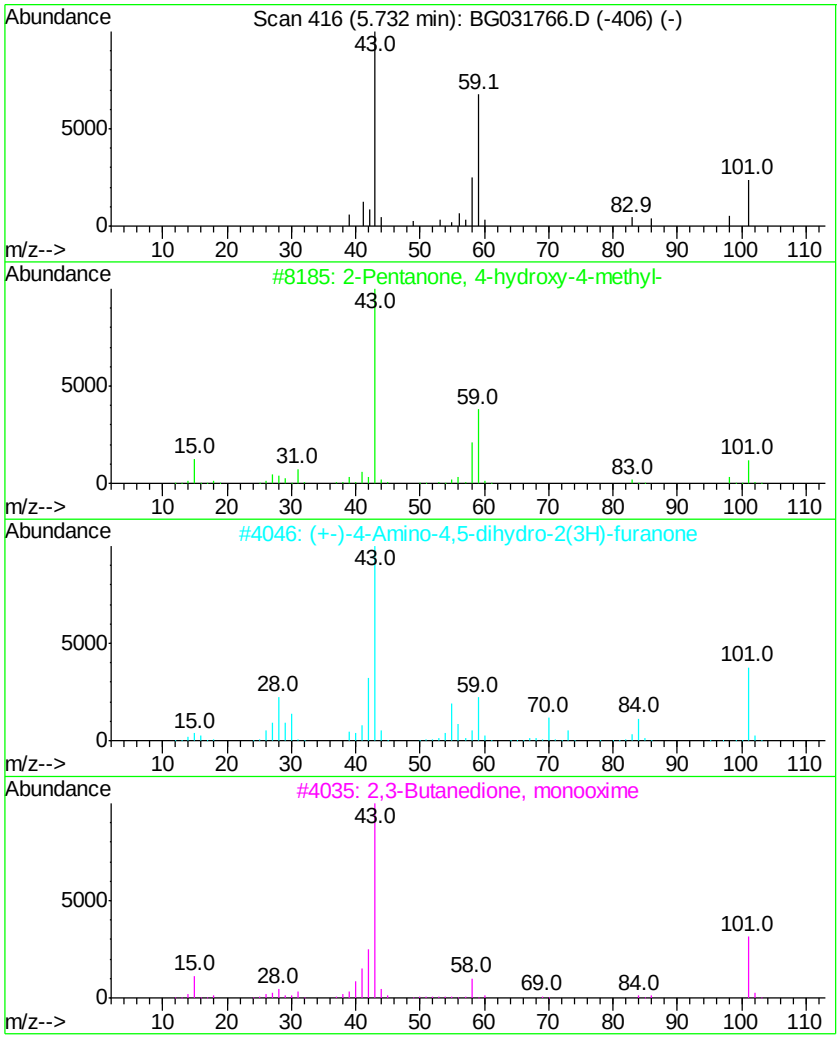
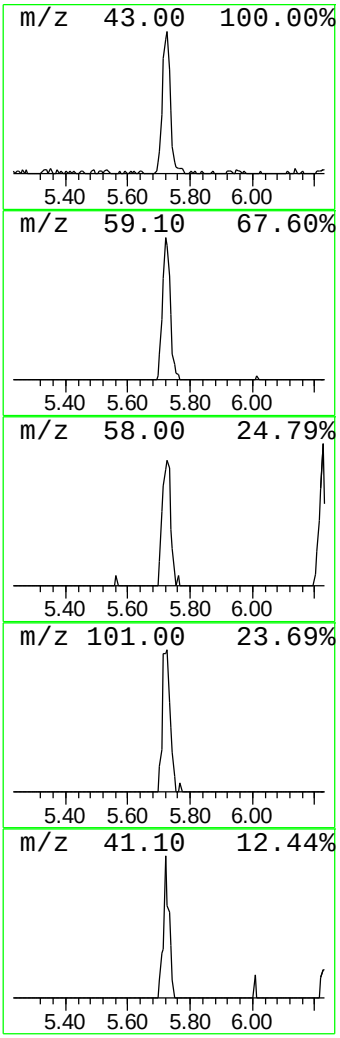
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.73	4.18 ng	49403	1,4-Dichlorobenzene-d4	8.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	43
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	37
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	23
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	22





Data Path : U:\HPCHEM1\BNA G\DATA\BG122617\
Data File : BG031766.D
Acq On : 26 Dec 2017 17:53
Operator : SJ/JU
Sample : I7040-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-6

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.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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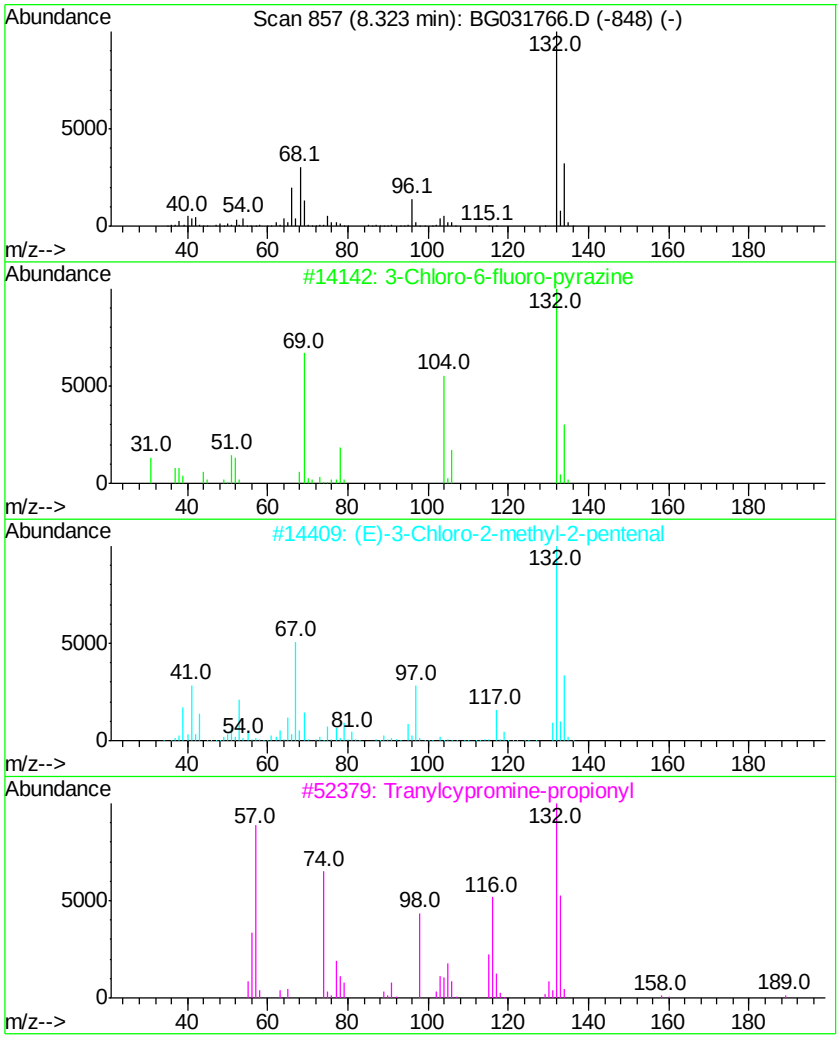
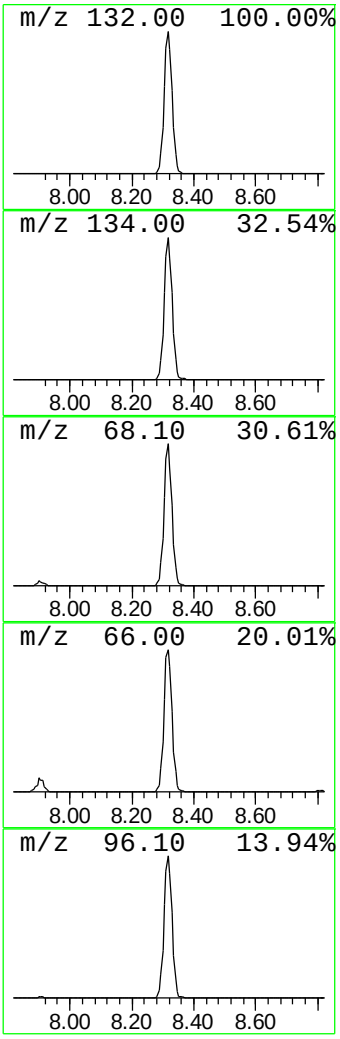
Peak Number 4 unknown8.32 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.32	90.72 ng	1072930	1,4-Dichlorobenzene-d4	8.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	N-(-phenylisopropyl)benzaldimine	223	C16H17N	1000379-01-3	12
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : U:\HPCHEM1\BNA G\DATA\BG122617\
Data File : BG031766.D
Acq On : 26 Dec 2017 17:53
Operator : SJ/JU
Sample : I7040-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-6

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.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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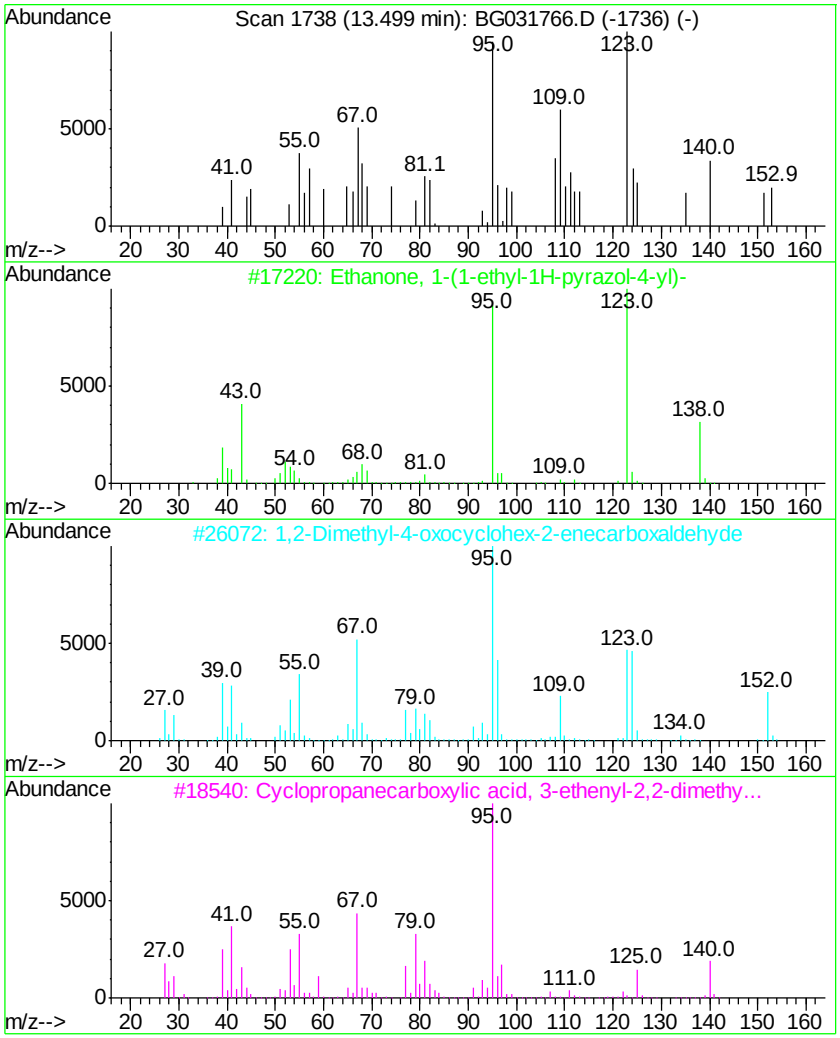
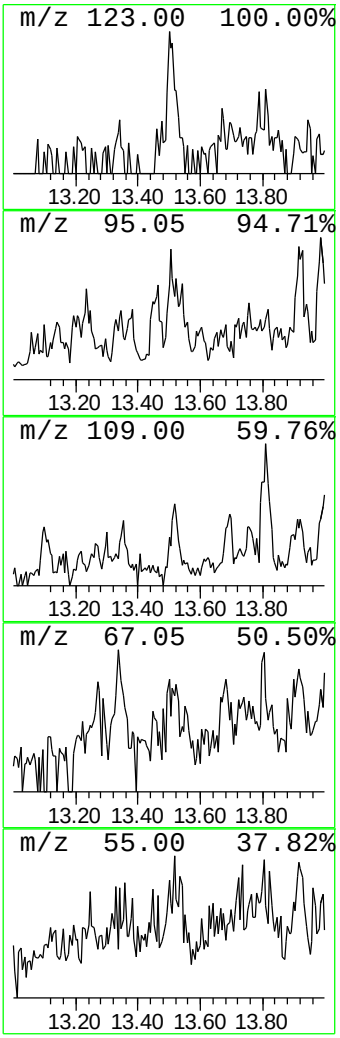
Peak Number 6 unknown13.50 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	2.29 ng	41885	Naphthalene-d8	11.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-(1-ethyl-1H-pyrazol-...	138	C7H10N2O	1000316-95-0	43
2	1,2-Dimethyl-4-oxocyclohex-2-ene...	152	C9H12O2	1000187-01-2	38
3	Cyclopropanecarboxylic acid, 3-e...	140	C8H12O2	067528-58-9	38
4	5-Methyl-5-hexen-3-yn-2-ol	110	C7H10O	068017-33-4	30
5	trans,trans-1,7-Dimethylspiro[4....	166	C12H22	1000111-72-6	27





Data Path : U:\HPCHEM1\BNA G\DATA\BG122617\
Data File : BG031766.D
Acq On : 26 Dec 2017 17:53
Operator : SJ/JU
Sample : I7040-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-6

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

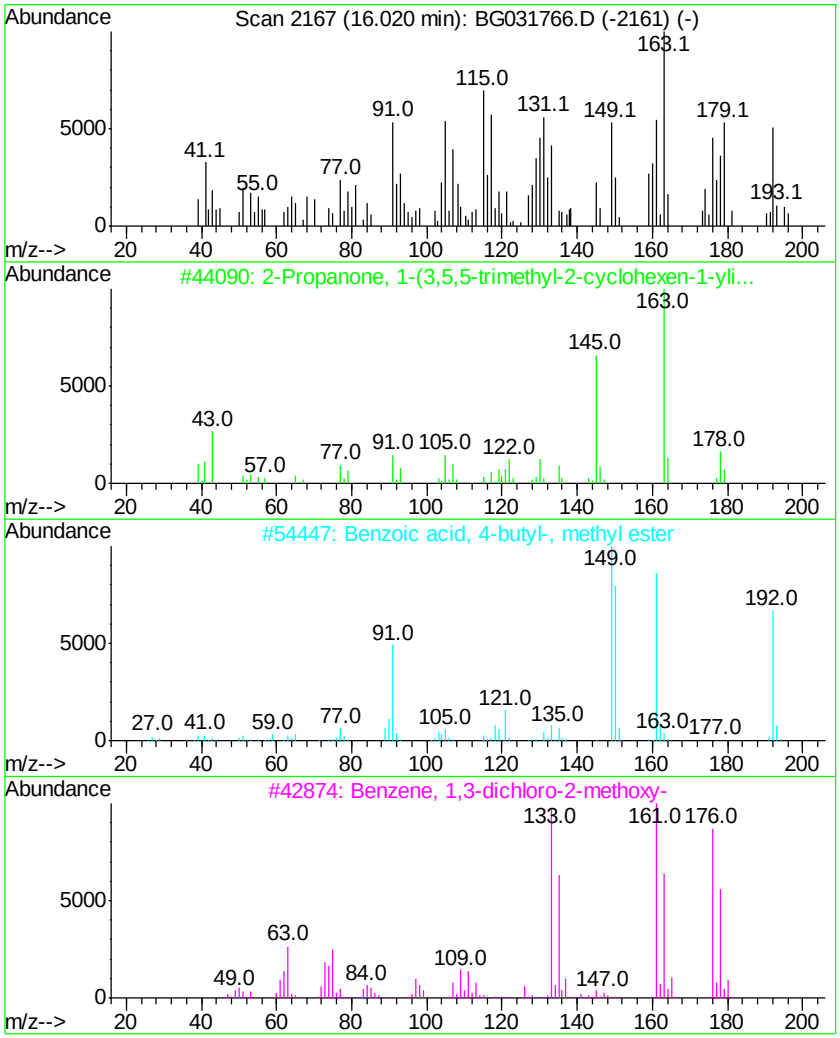
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

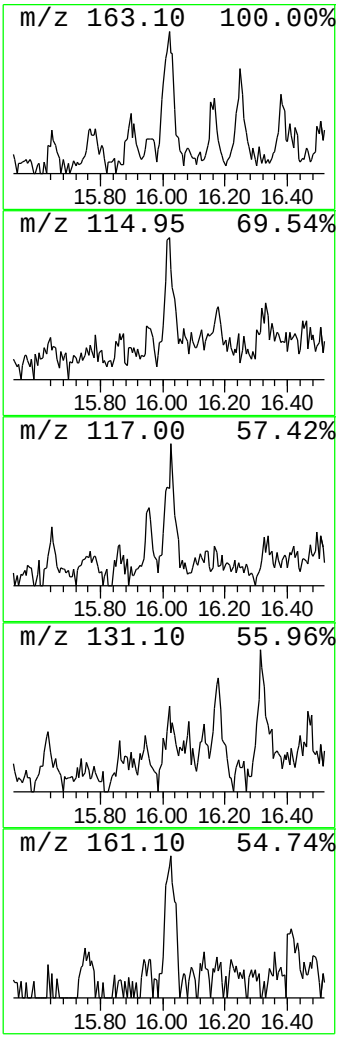
****

Peak Number 7 unknown16.02 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	3.26 ng	106573	Acenaphthene-d10	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanone, 1-(3,5,5-trimethyl-...	178	C12H18O	016695-72-0	25
2	Benzoic acid, 4-butyl-, methyl e...	192	C12H16O2	020651-69-8	18
3	Benzene, 1,3-dichloro-2-methoxy-	176	C7H6Cl2O	001984-65-2	18
4	2-Propenal, 3-(3,4-dimethoxyphen...	192	C11H12O3	004497-40-9	15
5	1H-Indene, 2,3-dihydro-5-nitro-	163	C9H9NO2	007436-07-9	14





Data Path : U:\HPCHEM1\BNA G\DATA\BG122617\
Data File : BG031766.D
Acq On : 26 Dec 2017 17:53
Operator : SJ/JU
Sample : I7040-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-6

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

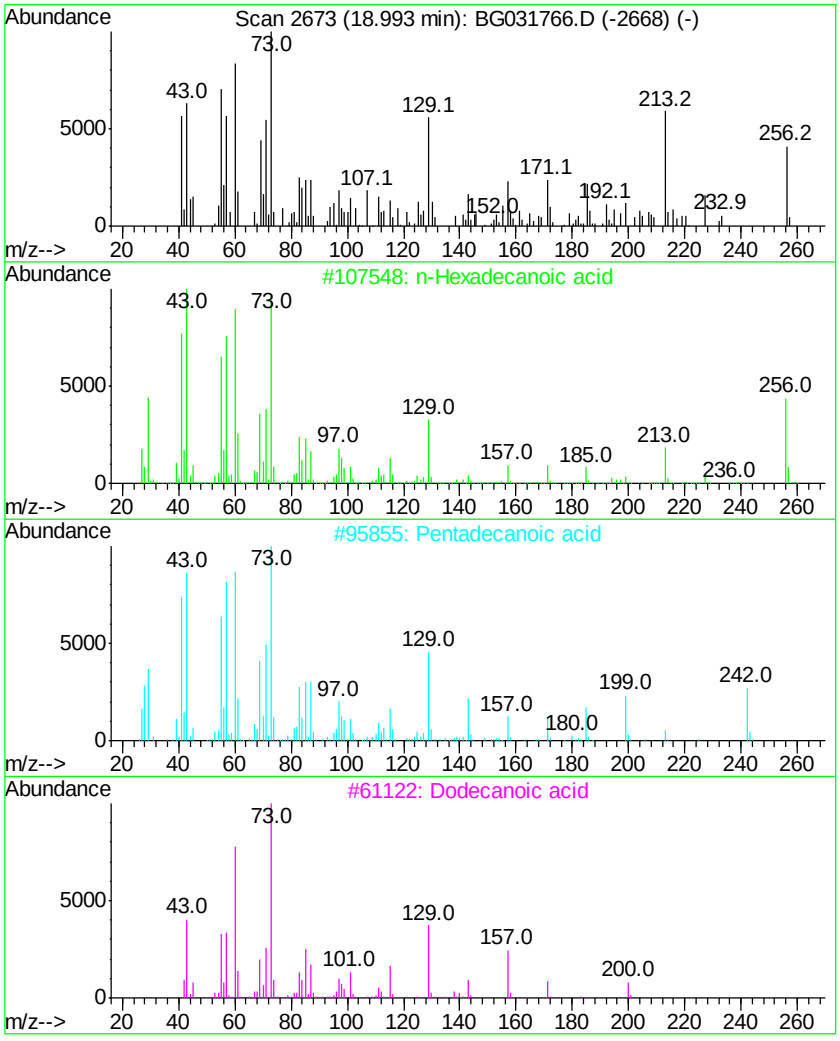
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

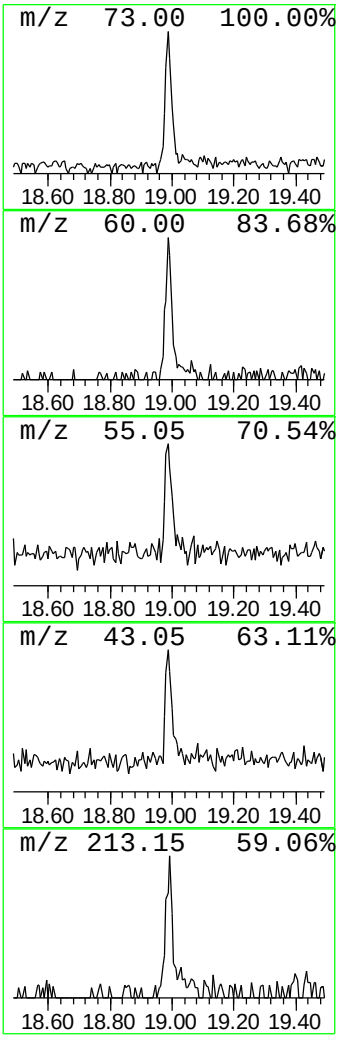
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.99	2.22 ng	86315	Phenanthrene-d10	18.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	Dodecanoic acid	200	C12H24O2	000143-07-7	60
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Tridecanoic acid	214	C13H26O2	000638-53-9	53





Data Path : U:\HPCHEM1\BNA G\DATA\BG122617\
Data File : BG031766.D
Acq On : 26 Dec 2017 17:53
Operator : SJ/JU
Sample : I7040-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-6

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

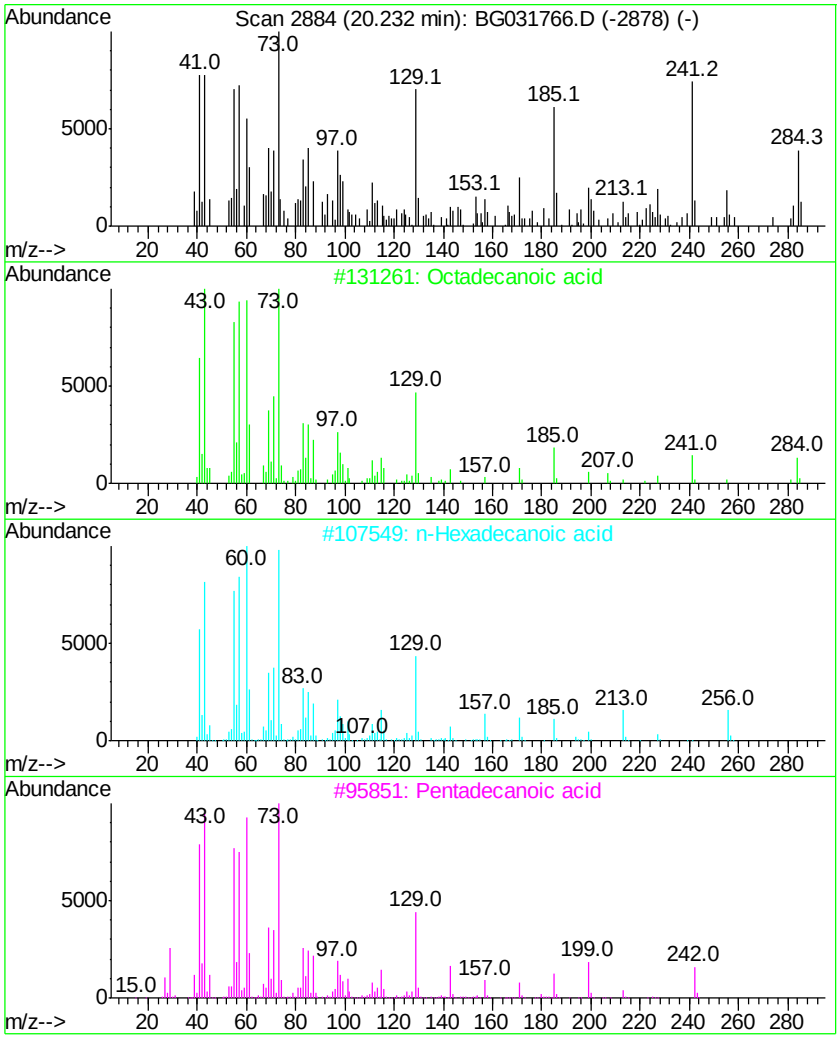
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

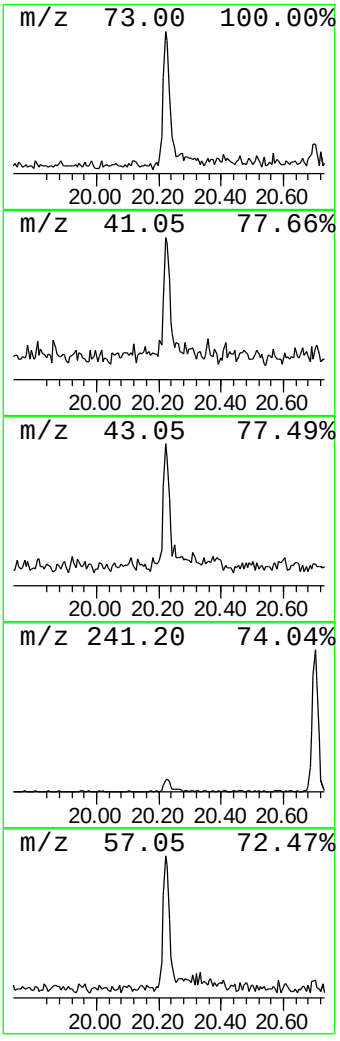
****

Peak Number 9 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.23	3.83 ng	148865	Phenanthrene-d10	18.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	78
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4	n-Decanoic acid	172	C10H20O2	000334-48-5	46
5	Dodecanoic acid	200	C12H24O2	000143-07-7	46





Tentatively Identified Compound (LSC) summary

Data Path : U:\HPCHEM1\BNA_G\DATA\BG122617\
Data File : BG031766.D
Acq On : 26 Dec 2017 17:53
Operator : SJ/JU
Sample : I7040-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-6

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.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
Butane, 2-methoxy...	3.53	4.3	ng	51254	1	8.80	236550	20.0
2-Pentanone, 4-hy...	5.73	4.2	ng	49403	1	8.80	236550	20.0
unknown8.32	8.32	90.7	ng	1072930	1	8.80	236550	20.0
unknown13.50	13.50	2.3	ng	41885	2	11.69	366183	20.0
unknown16.02	16.02	3.3	ng	106573	3	15.43	652883	20.0
n-Hexadecanoic acid	18.99	2.2	ng	86315	4	18.17	776902	20.0
Octadecanoic acid	20.23	3.8	ng	148865	4	18.17	776902	20.0