LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102318\
Data File : BG037504.D
Acq On : 24 Oct 2018 10:16
Operator : JU/SJ
Sample : J5621-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SA-SB-01B

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.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	5.189	317	323	331	rBV	47144	79771	3.40%	0.436%
2	5.647	394	401	411	rBV	760612	1251934	53.39%	6.845%
3	7.251	665	674	687	rBV2	838186	1660817	70.82%	9.081%
4	7.633	730	739	749	rBV	759191	1368484	58.36%	7.483%
5	8.103	812	819	831	rBV	211524	377963	16.12%	2.067%
6	8.426	865	874	885	rBV	487189	876093	37.36%	4.790%
7	9.284	1010	1020	1030	rBV	481301	911633	38.88%	4.985%
8	10.929	1291	1300	1311	rBV	315207	587922	25.07%	3.215%
9	13.361	1705	1714	1724	rBV	946122	1471641	62.76%	8.047%
10	14.184	1846	1854	1860	rBV	167845	249304	10.63%	1.363%
11	14.736	1941	1948	1958	rBV2	542405	917611	39.13%	5.017%
12	16.223	2194	2201	2209	rBV	931657	1440091	61.41%	7.874%
13	17.486	2407	2416	2422	rBV2	712724	1170681	49.92%	6.401%
14	17.592	2428	2434	2446	rVB7	14132	32288	1.38%	0.177%
15	18.338	2556	2561	2569	rBV	103694	167542	7.14%	0.916%
16	19.531	2759	2764	2771	rVB	42060	58939	2.51%	0.322%
17	19.607	2773	2777	2784	rBV4	42193	64551	2.75%	0.353%
18	19.889	2821	2825	2832	rVB	44082	70387	3.00%	0.385%
19	20.083	2851	2858	2865	rBV	1738072	2345033	100.00%	12.822%
20	21.370	3072	3077	3086	rBV	135214	212370	9.06%	1.161%
21	21.769	3137	3145	3152	rBV	682577	1226922	52.32%	6.709%
22	21.928	3169	3172	3177	rVB2	26550	39679	1.69%	0.217%
23	22.551	3274	3278	3287	rBV3	35438	65584	2.80%	0.359%
24	23.261	3393	3399	3407	rVB3	55659	108851	4.64%	0.595%
25	24.090	3536	3540	3548	rVB2	63432	139339	5.94%	0.762%
26	25.101	3701	3712	3732	rVB2	377214	1271880	54.24%	6.954%
27	26.246	3901	3907	3916	rVB3	42995	121725	5.19%	0.666%

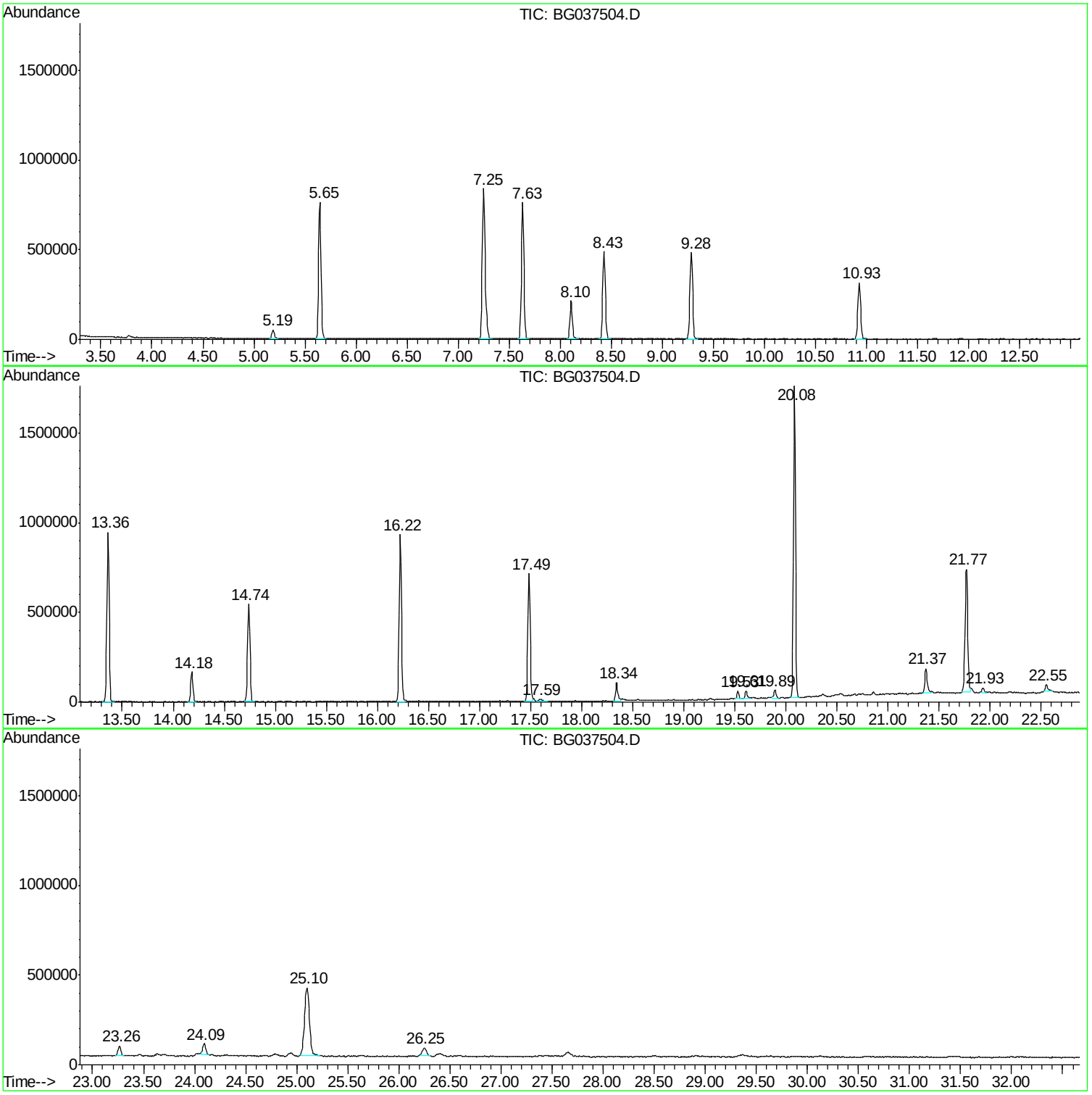
Sum of corrected areas: 18289035

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102318\
Data File : BG037504.D
Acq On : 24 Oct 2018 10:16
Operator : JU/SJ
Sample : J5621-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SA-SB-01B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102318\
Data File : BG037504.D
Acq On : 24 Oct 2018 10:16
Operator : JU/SJ
Sample : J5621-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SA-SB-01B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

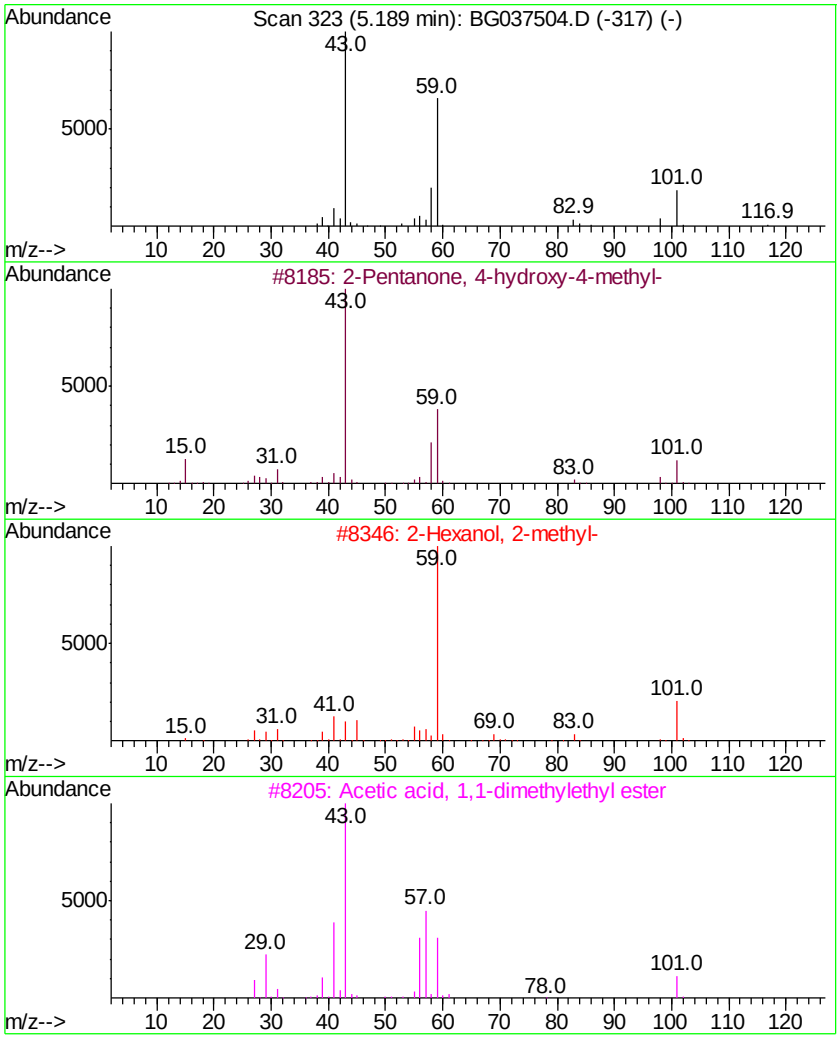
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

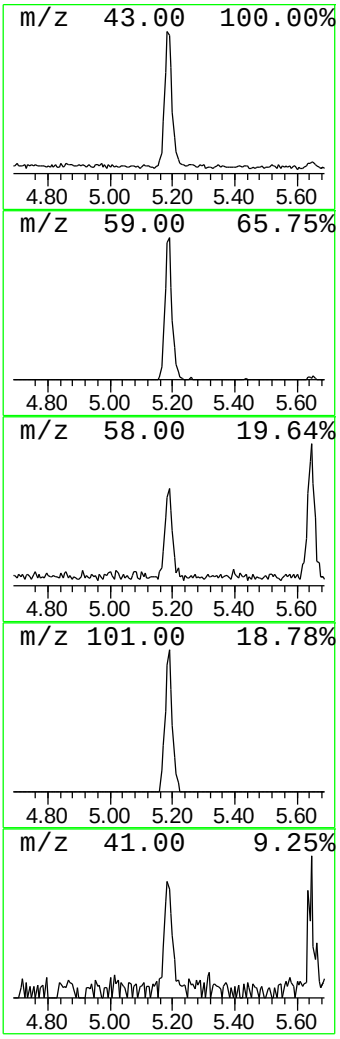
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	4.22 ng	79771	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	37
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102318\
Data File : BG037504.D
Acq On : 24 Oct 2018 10:16
Operator : JU/SJ
Sample : J5621-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SA-SB-01B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

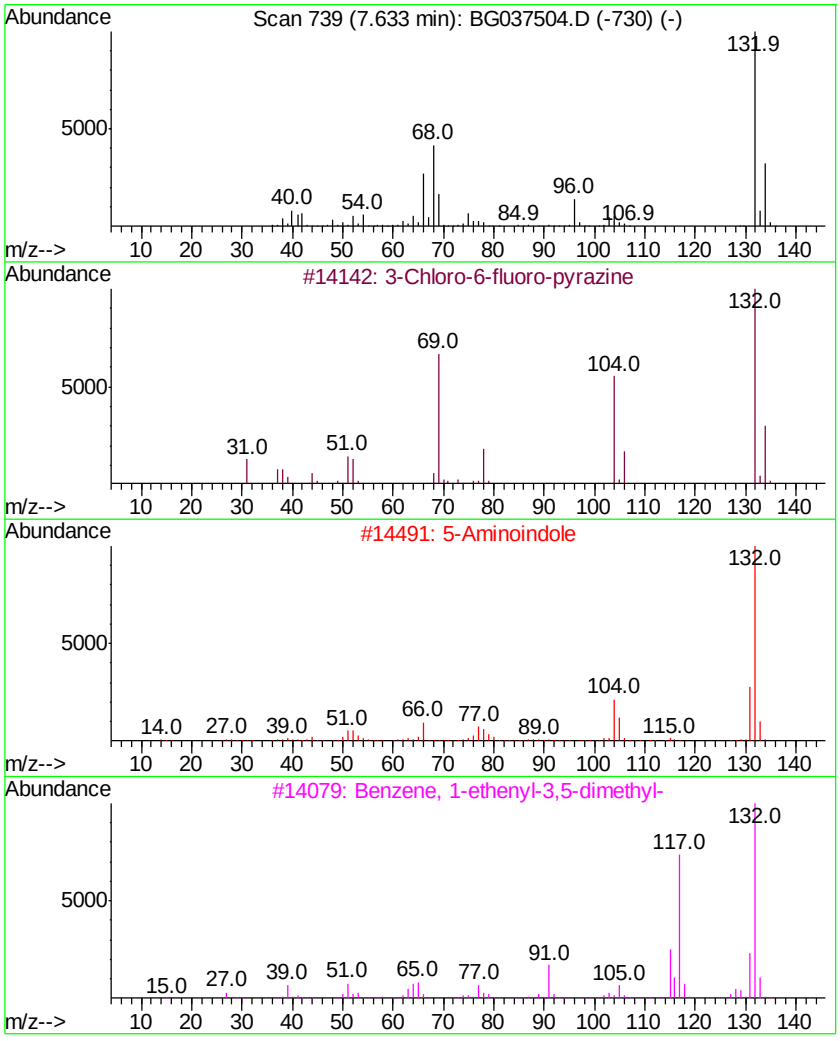
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

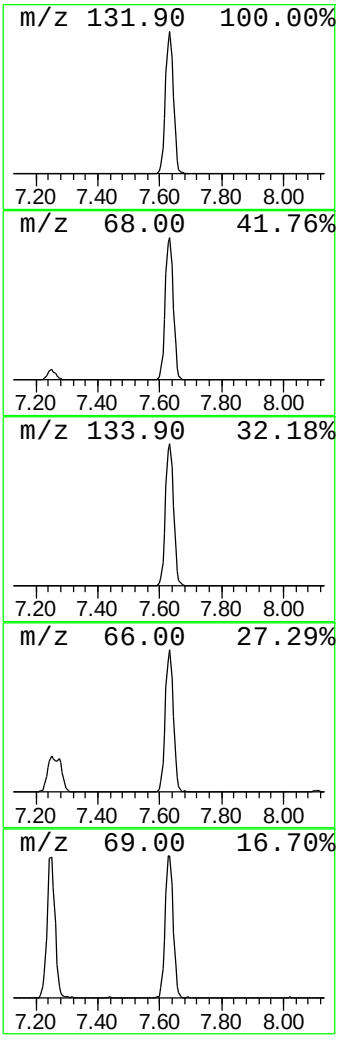
****

Peak Number 2 unknown7.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.63	72.41 ng	1368480	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102318\
Data File : BG037504.D
Acq On : 24 Oct 2018 10:16
Operator : JU/SJ
Sample : J5621-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SA-SB-01B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

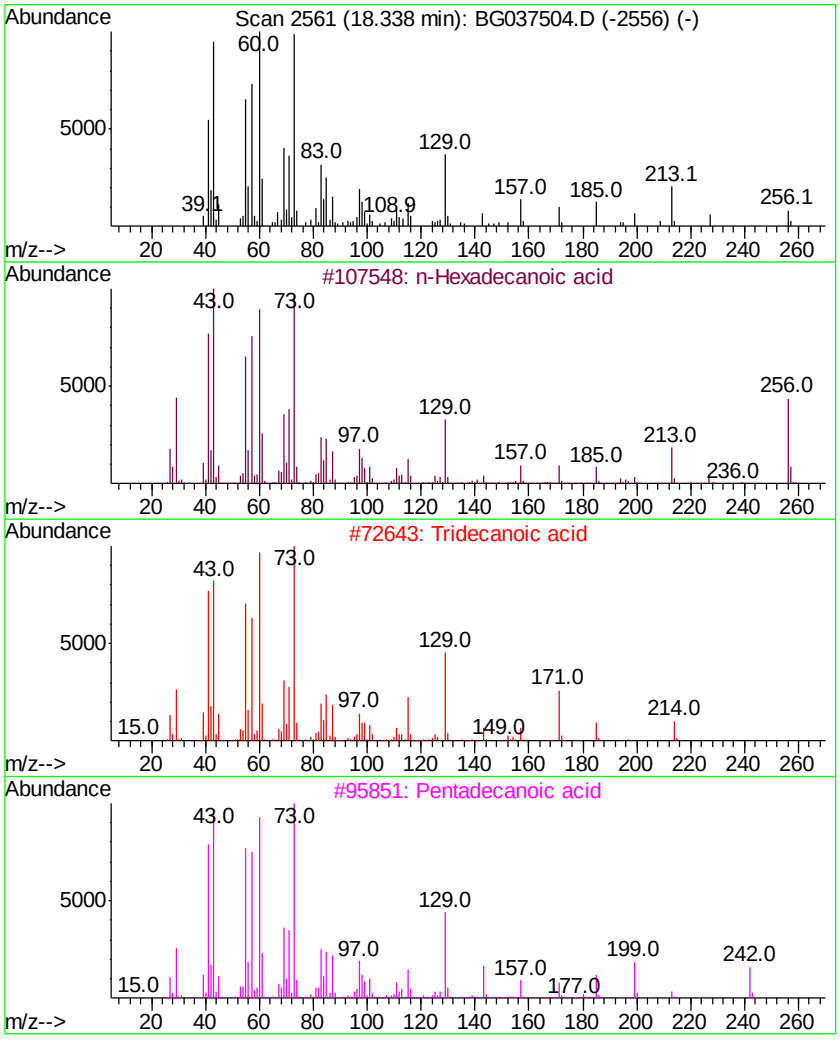
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

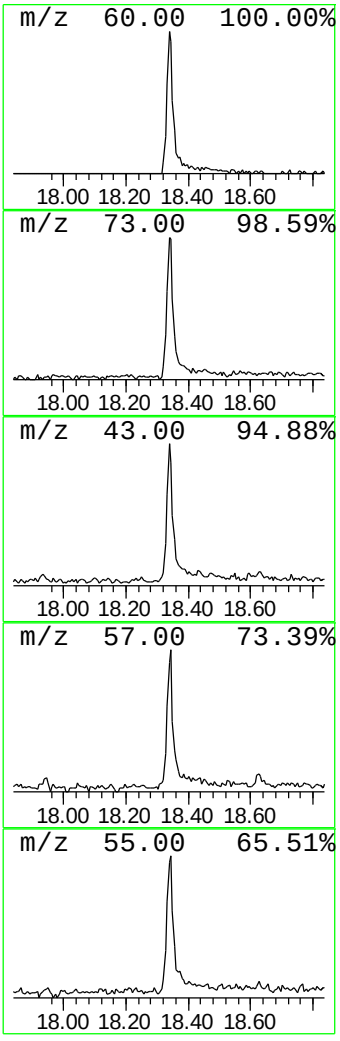
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.34	2.86 ng	167542	Phenanthrene-d10	17.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	55





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102318\
Data File : BG037504.D
Acq On : 24 Oct 2018 10:16
Operator : JU/SJ
Sample : J5621-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SA-SB-01B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

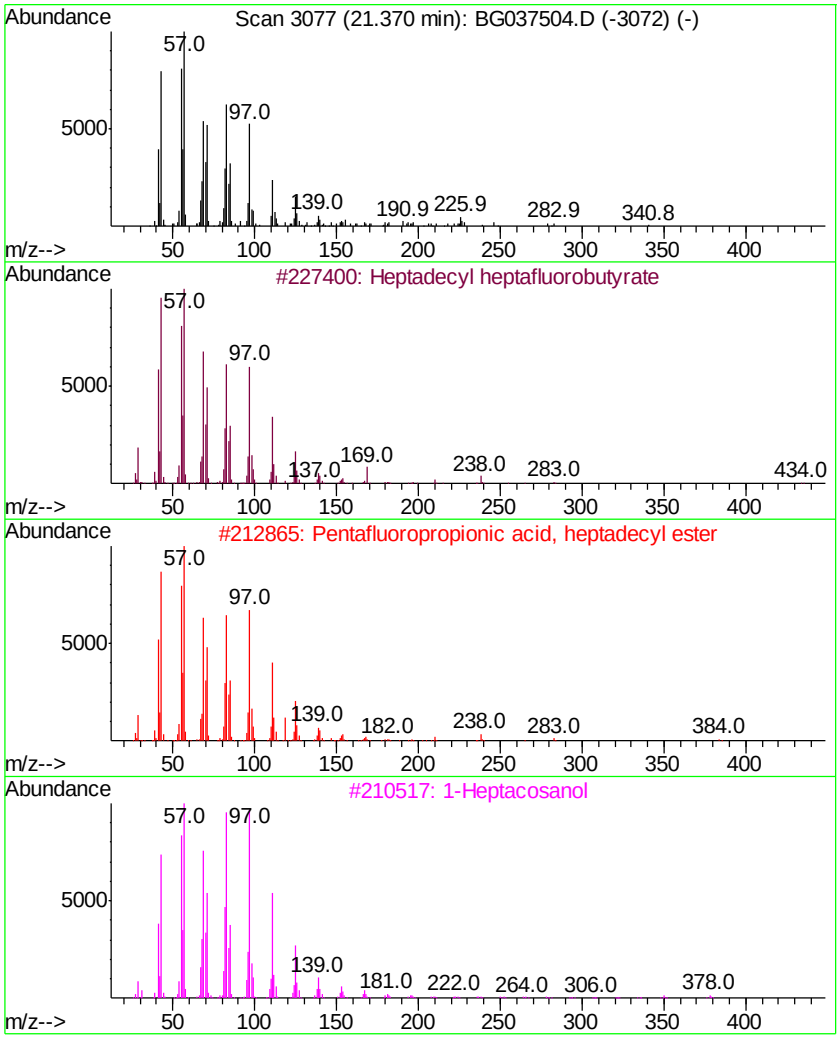
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

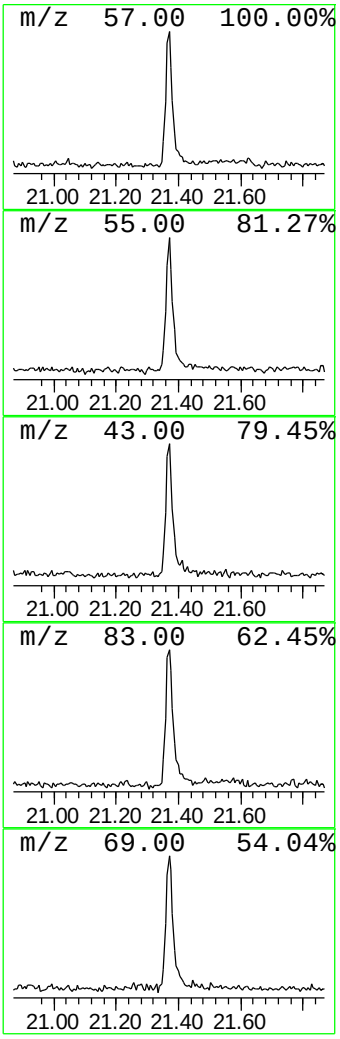
****

Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.37	3.46 ng	212370	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
3	1-Heptacosanol	396	C27H56O	002004-39-9	91
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
5	Cyclotetradecane	196	C14H28	000295-17-0	89





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102318\
Data File : BG037504.D
Acq On : 24 Oct 2018 10:16
Operator : JU/SJ
Sample : J5621-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SA-SB-01B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

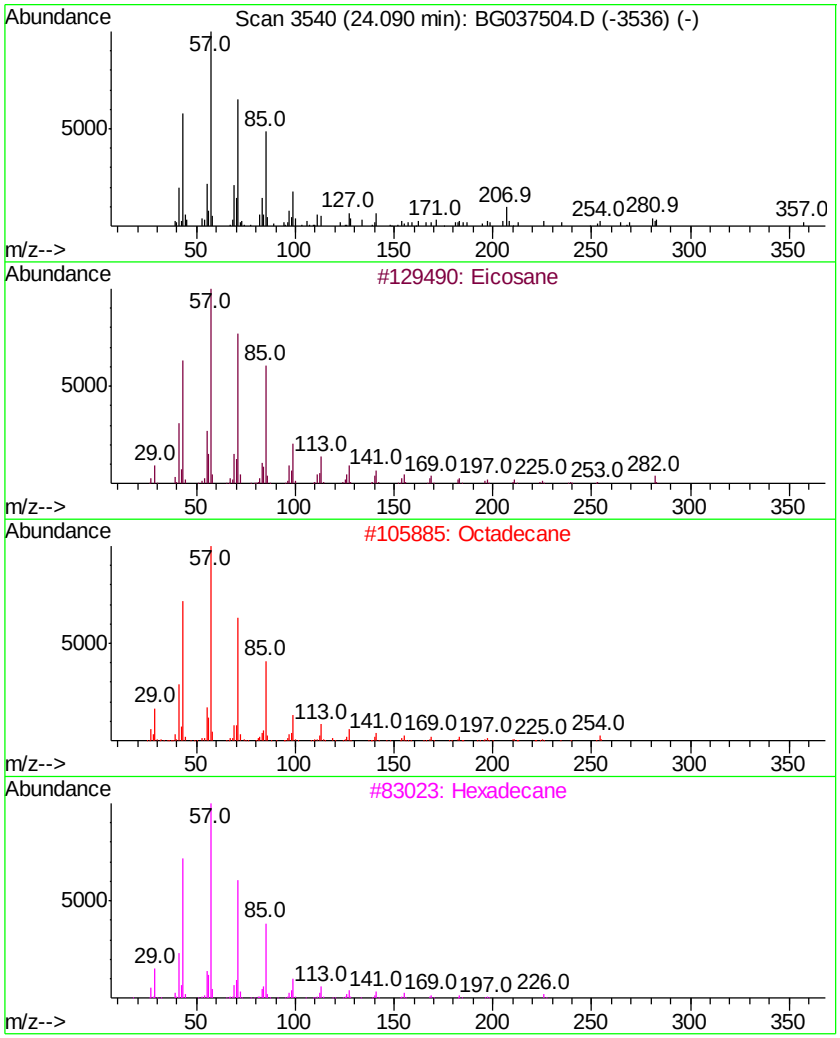
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

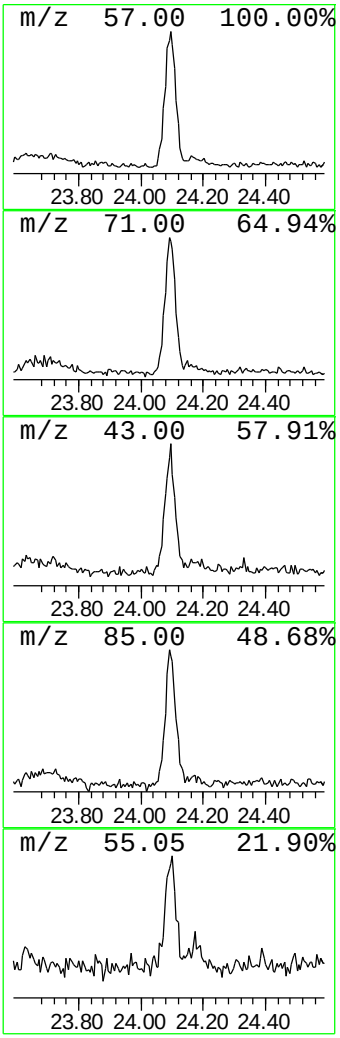
****

Peak Number 6 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.09	2.19 ng	139339	Perylene-d12	25.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Octadecane	254	C18H38	000593-45-3	81
3	Hexadecane	226	C16H34	000544-76-3	81
4	Eicosane, 2-methyl-	296	C21H44	001560-84-5	80
5	Nonadecane	268	C19H40	000629-92-5	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG102318\
Data File : BG037504.D
Acq On : 24 Oct 2018 10:16
Operator : JU/SJ
Sample : J5621-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SA-SB-01B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.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
2-Pentanone, 4-hy...	5.19	4.2	ng	79771	1	8.11	377963	20.0
unknown7.63	7.63	72.4	ng	1368480	1	8.11	377963	20.0
n-Hexadecanoic acid	18.34	2.9	ng	167542	4	17.49	1170680	20.0
Heptadecyl heptaf...	21.37	3.5	ng	212370	5	21.77	1226920	20.0
Eicosane	24.09	2.2	ng	139339	6	25.11	1271880	20.0