LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG011218\
Data File : BG032022.D
Acq On : 13 Jan 2018 3:33
Operator : SJ/JU
Sample : J1096-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-02-BOTTOM

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	3.417	16	22	31	rVV2	36565	71662	1.81%	0.364%
2	3.505	31	37	44	rVB	25147	40568	1.02%	0.206%
3	5.032	288	297	306	rBV	21576	40045	1.01%	0.203%
4	5.691	402	409	418	rBV	50154	86435	2.18%	0.439%
5	6.196	486	495	506	rBV	624223	1076044	27.11%	5.461%
6	7.876	769	781	793	rBV	634967	1189201	29.96%	6.036%
7	8.288	841	851	859	rBV	665608	1236972	31.17%	6.278%
8	8.775	927	934	944	rVB	167207	312581	7.88%	1.586%
9	9.110	983	991	1000	rBV	541789	997139	25.12%	5.061%
10	9.968	1127	1137	1145	rBV	371342	701756	17.68%	3.562%
11	11.654	1416	1424	1441	rBV	241538	462957	11.67%	2.350%
12	14.034	1821	1829	1843	rVB	1423952	2294161	57.81%	11.644%
13	14.827	1958	1964	1970	rBV	169212	257750	6.49%	1.308%
14	15.244	2030	2035	2044	rVB3	33410	44562	1.12%	0.226%
15	15.403	2055	2062	2071	rVB2	434706	727159	18.32%	3.691%
16	16.184	2191	2195	2201	rVB	37224	50476	1.27%	0.256%
17	16.877	2306	2313	2326	rBV	1227497	1939985	48.88%	9.846%
18	17.042	2336	2341	2352	rVB2	32105	58139	1.46%	0.295%
19	18.135	2520	2527	2540	rBV2	631822	1015311	25.58%	5.153%
20	18.951	2661	2666	2675	rBV2	74019	111813	2.82%	0.567%
21	20.673	2952	2959	2969	rBV	2795682	3968713	100.00%	20.142%
22	22.018	3181	3188	3198	rBV	175493	298682	7.53%	1.516%
23	22.477	3258	3266	3278	rBV	633582	1221673	30.78%	6.200%
24	24.128	3539	3547	3559	rBV4	99179	251635	6.34%	1.277%
25	26.202	3887	3900	3914	rBV2	381453	1247886	31.44%	6.333%

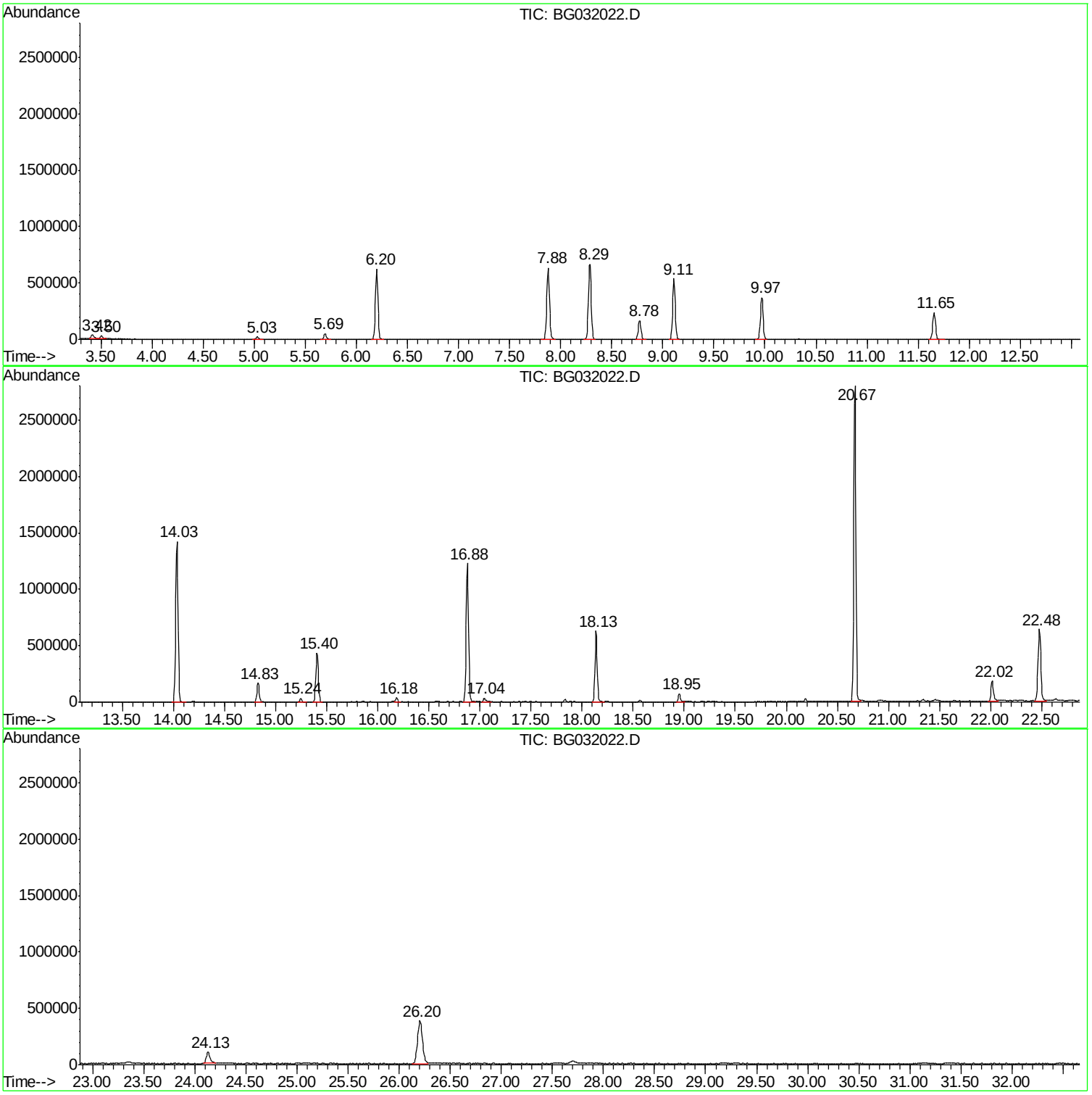
Sum of corrected areas: 19703305

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG011218\
Data File : BG032022.D
Acq On : 13 Jan 2018 3:33
Operator : SJ/JU
Sample : J1096-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-02-BOTTOM

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



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG011218\
Data File : BG032022.D
Acq On : 13 Jan 2018 3:33
Operator : SJ/JU
Sample : J1096-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-02-BOTTOM

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

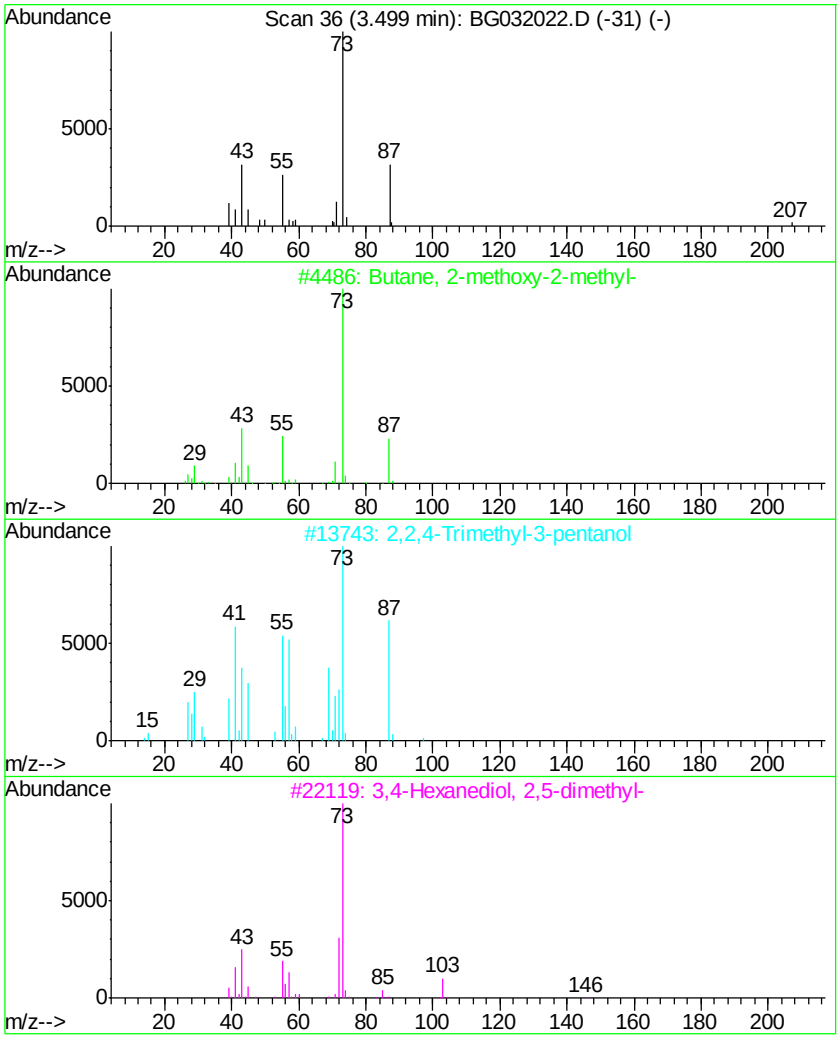
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

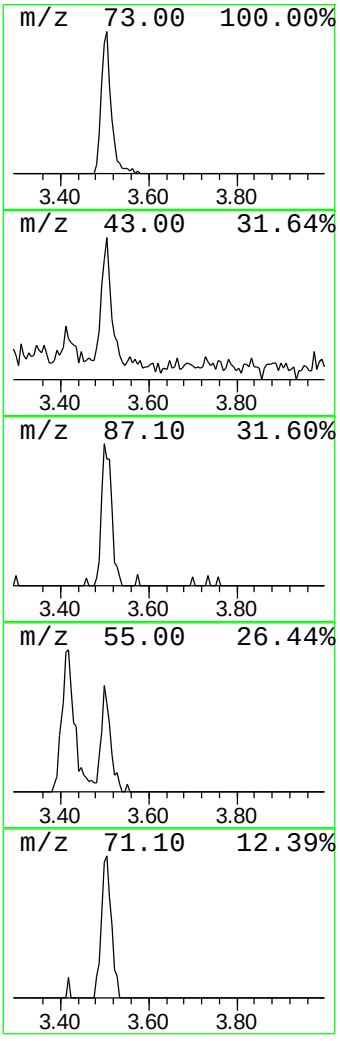
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.50	2.60 ng	40568	1,4-Dichlorobenzene-d4	8.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	59
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9
3	3,4-Hexanediol, 2,5-dimethyl-	146	C8H18O2	022607-11-0	9
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	7
5	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG011218\
Data File : BG032022.D
Acq On : 13 Jan 2018 3:33
Operator : SJ/JU
Sample : J1096-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-02-BOTTOM

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

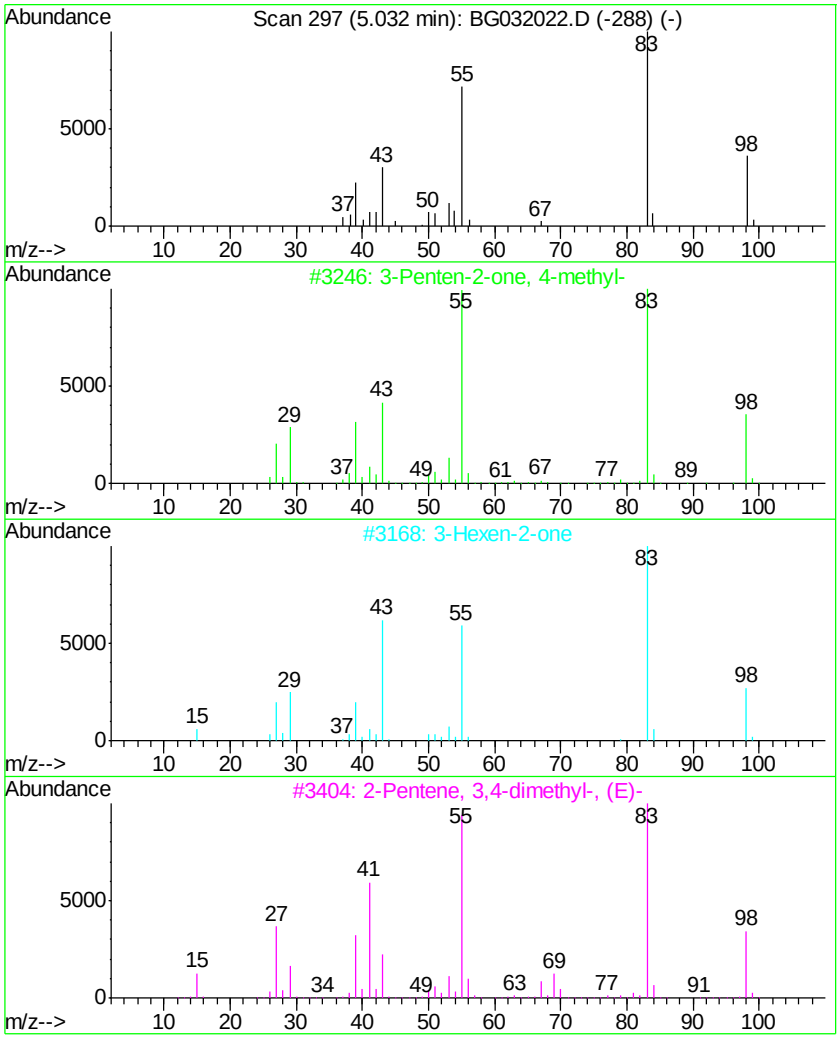
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

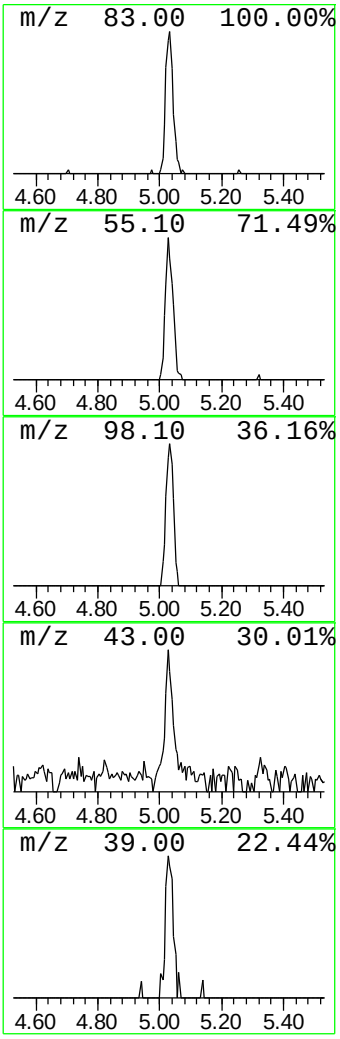
****

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	2.56 ng	40045	1,4-Dichlorobenzene-d4	8.78

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	86
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





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Data File : BG032022.D
Acq On : 13 Jan 2018 3:33
Operator : SJ/JU
Sample : J1096-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-02-BOTTOM

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

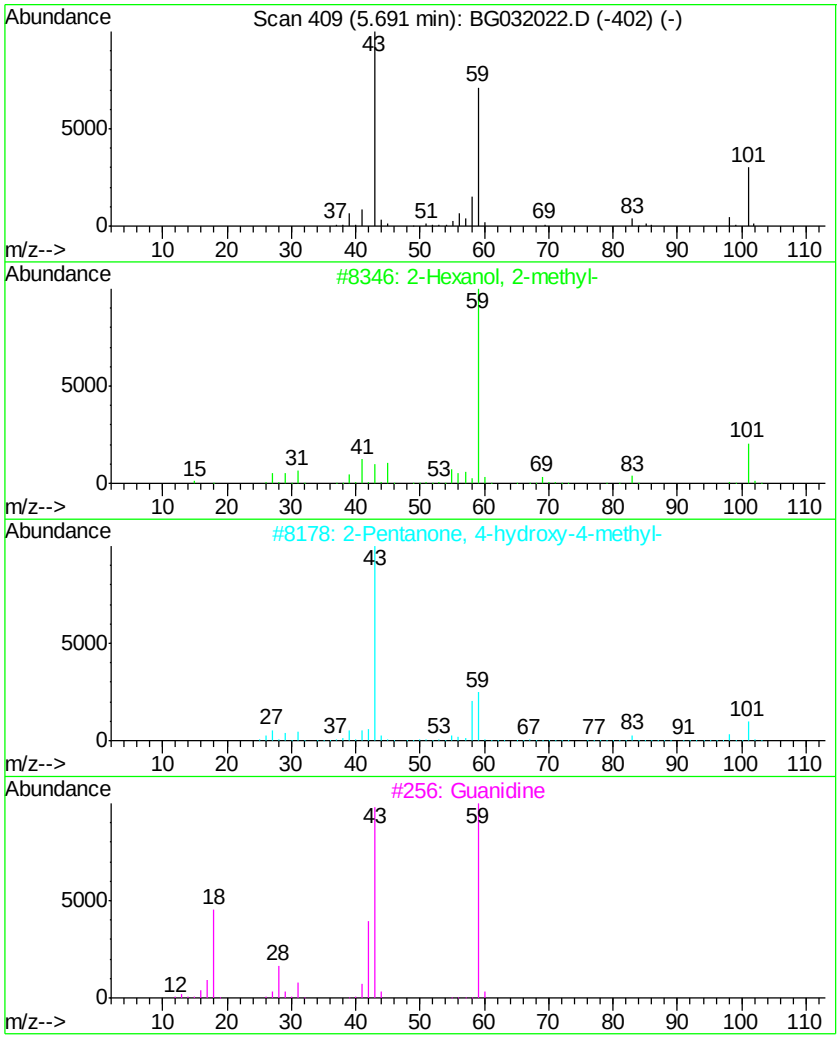
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

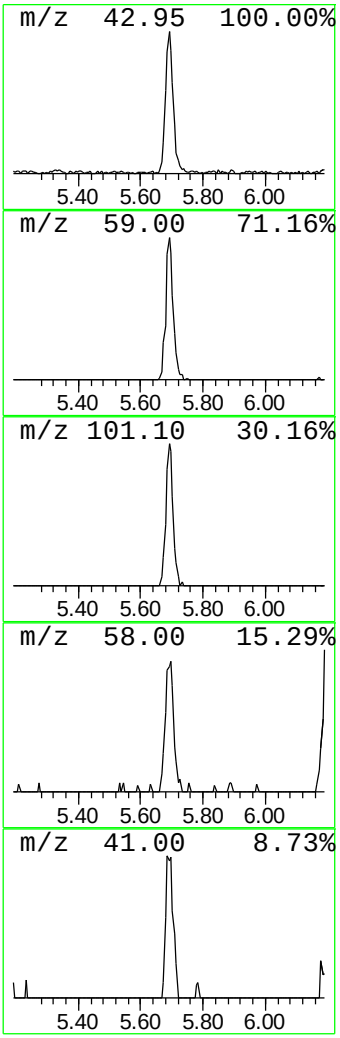
****

Peak Number 4 2-Hexanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.69	5.53 ng	86435	1,4-Dichlorobenzene-d4	8.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	50
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
3	Guanidine	59	CH5N3	000113-00-8	43
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	25
5	3-Hexanol	102	C6H14O	000623-37-0	17





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG011218\
Data File : BG032022.D
Acq On : 13 Jan 2018 3:33
Operator : SJ/JU
Sample : J1096-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-02-BOTTOM

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

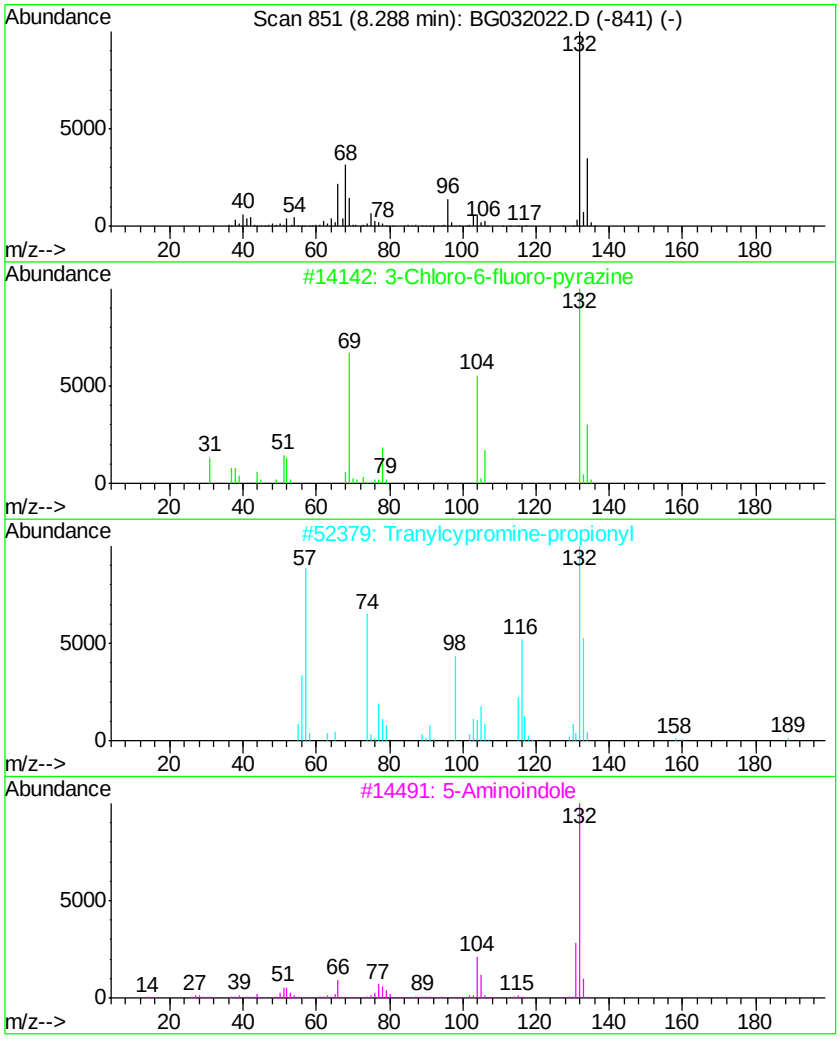
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

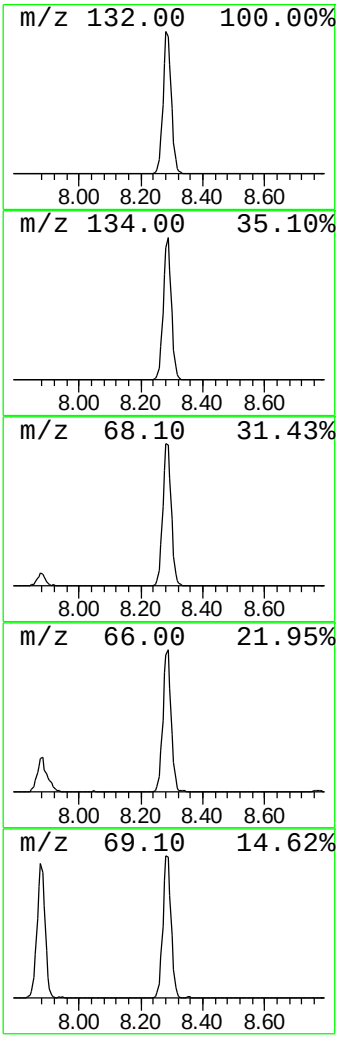
****

Peak Number 5 unknown8.29 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.29	79.15 ng	1236970	1,4-Dichlorobenzene-d4	8.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	16
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG011218\
Data File : BG032022.D
Acq On : 13 Jan 2018 3:33
Operator : SJ/JU
Sample : J1096-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-02-BOTTOM

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

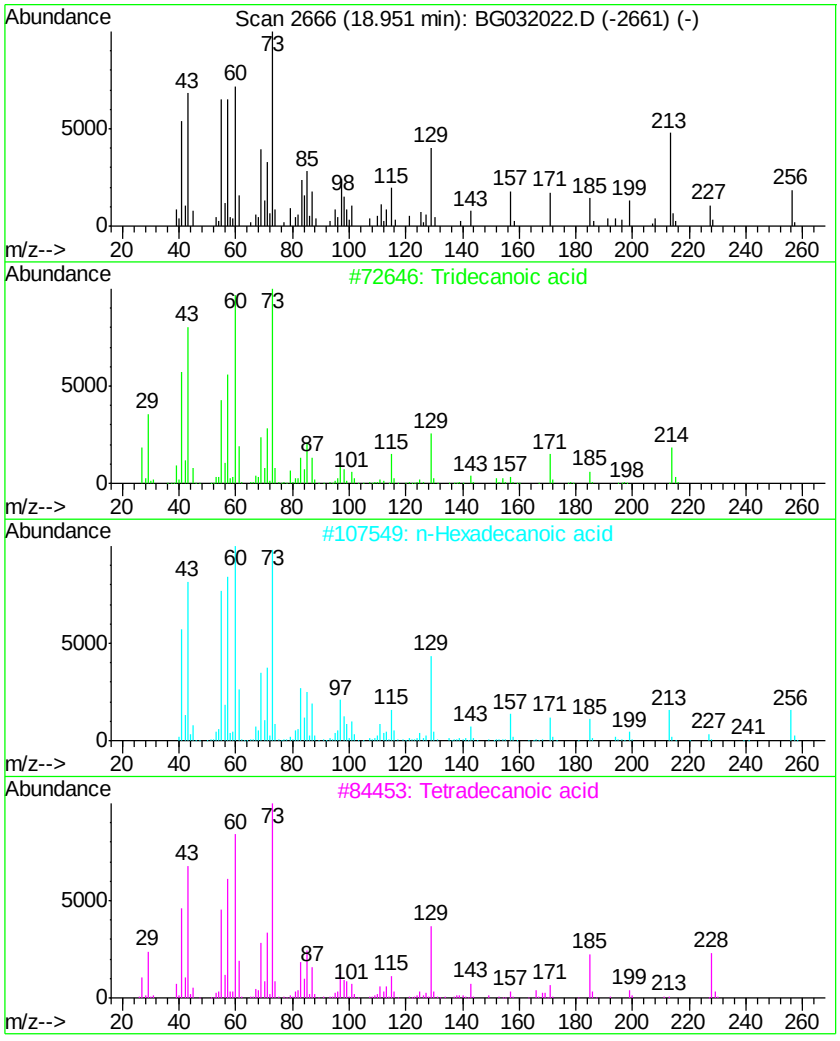
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

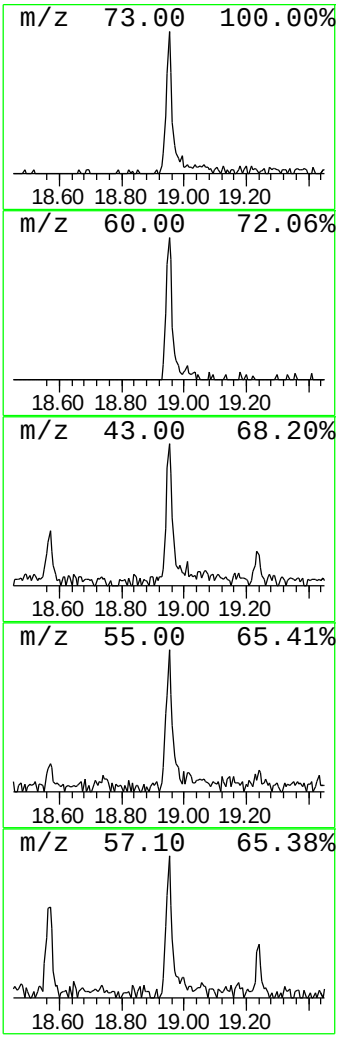
****

Peak Number 7 Tridecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.95	2.20 ng	111813	Phenanthrene-d10	18.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	93
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	49
5	Dodecanoic acid	200	C12H24O2	000143-07-7	43





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG011218\
Data File : BG032022.D
Acq On : 13 Jan 2018 3:33
Operator : SJ/JU
Sample : J1096-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-02-BOTTOM

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

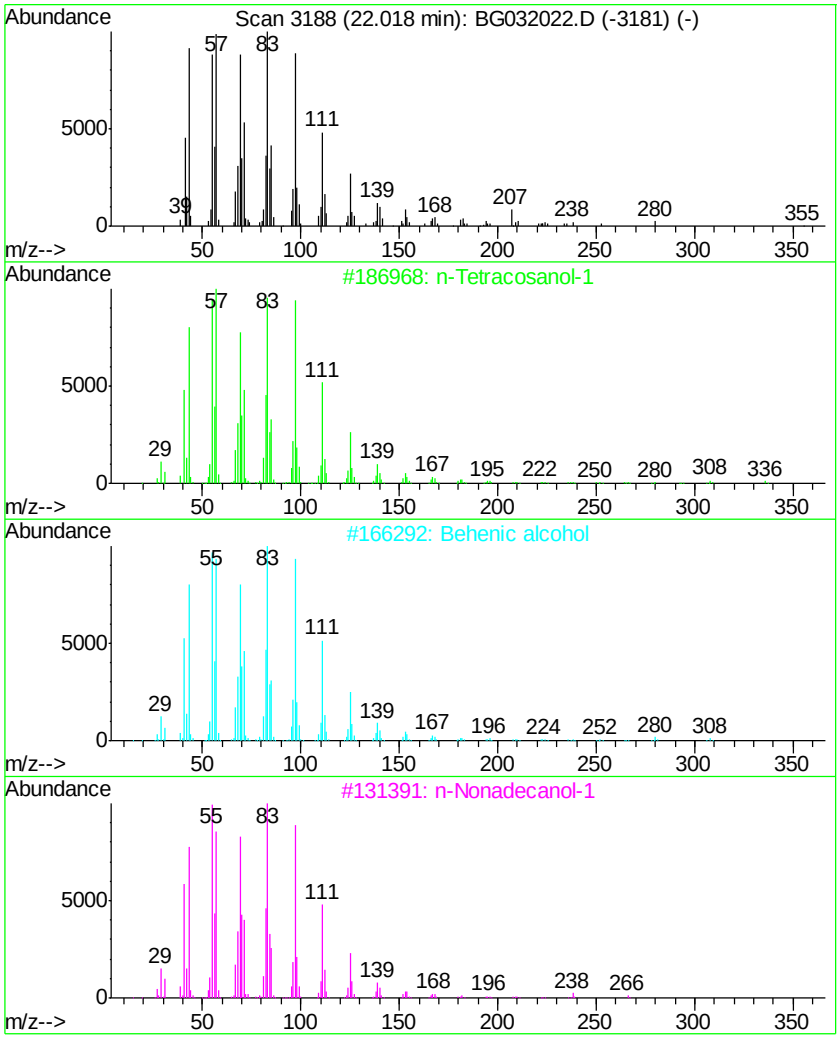
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

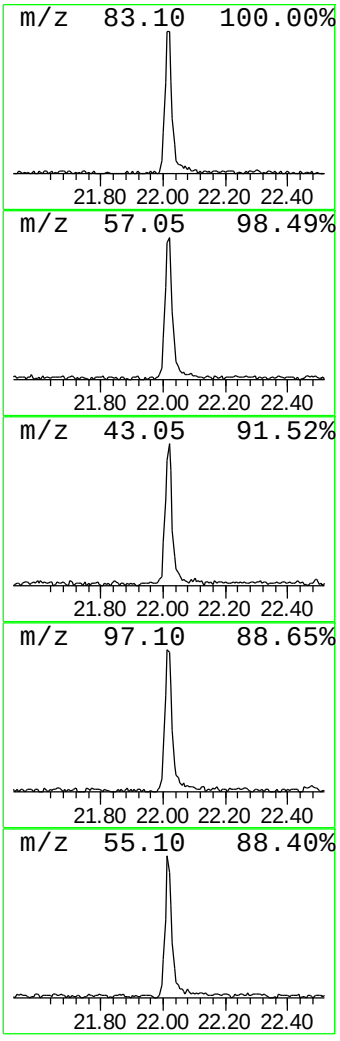
****

Peak Number 8 n-Tetracosanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.02	4.89 ng	298682	Chrysene-d12	22.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
4	1-Heptacosanol	396	C27H56O	002004-39-9	93
5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	90





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG011218\
Data File : BG032022.D
Acq On : 13 Jan 2018 3:33
Operator : SJ/JU
Sample : J1096-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-02-BOTTOM

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

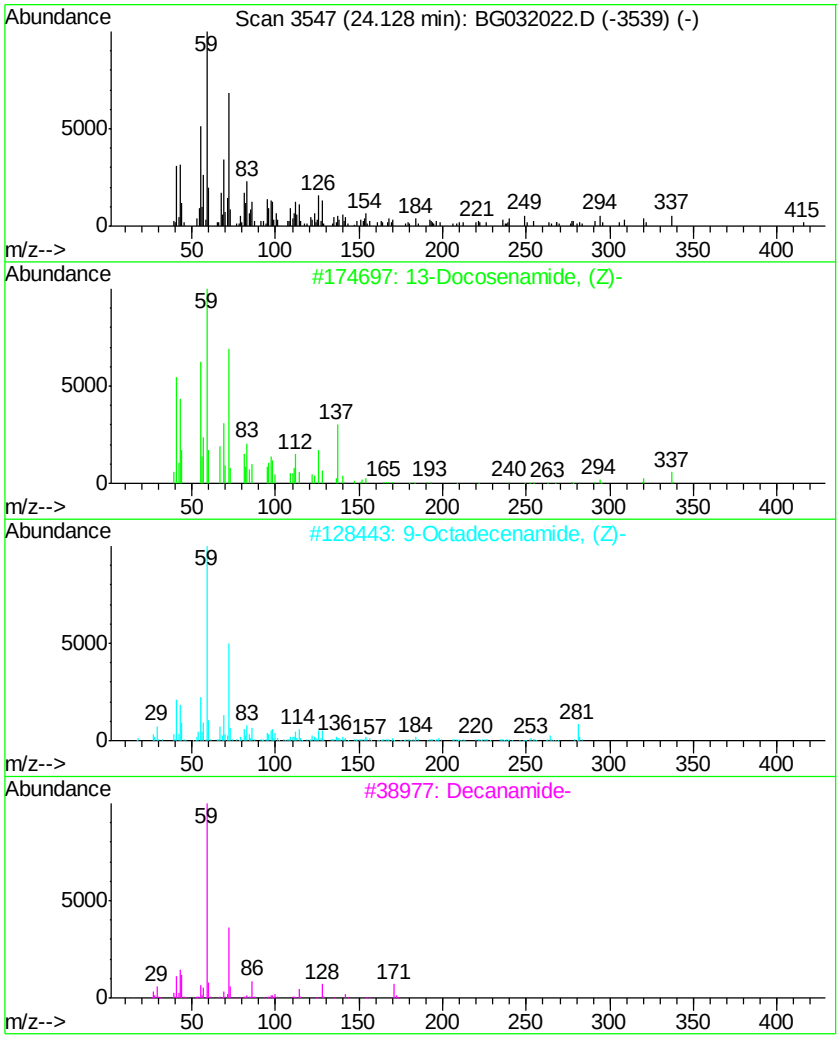
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

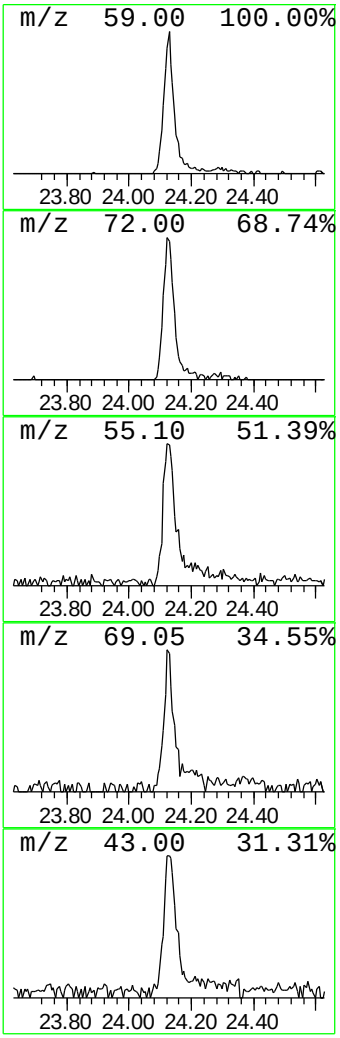
****

Peak Number 9 13-Docosenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.13	4.12 ng	251635	Chrysene-d12	22.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	94
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	68
3	Decanamide-	171	C10H21NO	002319-29-1	59
4	Dodecanamide	199	C12H25NO	001120-16-7	47
5	trans-13-Docosenamide	337	C22H43NO	010436-09-6	45





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG011218\
Data File : BG032022.D
Acq On : 13 Jan 2018 3:33
Operator : SJ/JU
Sample : J1096-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-02-BOTTOM

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	3.50	2.6	ng	40568	1	8.78	312581	20.0
3-Penten-2-one, 4...	5.03	2.6	ng	40045	1	8.78	312581	20.0
2-Hexanol, 2-methyl-	5.69	5.5	ng	86435	1	8.78	312581	20.0
unknown8.29	8.29	79.2	ng	1236970	1	8.78	312581	20.0
Tridecanoic acid	18.95	2.2	ng	111813	4	18.13	1015310	20.0
n-Tetracosanol-1	22.02	4.9	ng	298682	5	22.48	1221670	20.0
13-Docosenamide, ...	24.13	4.1	ng	251635	5	22.48	1221670	20.0