LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060817\
Data File : BG027326.D
Acq On : 8 Jun 2017 20:57
Operator : SJ/MA
Sample : I3460-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-113

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-BG060517.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	5.703	338	343	352	rVB	47698	81433	1.86%	0.386%
2	6.144	409	418	431	rVB	490459	863934	19.71%	4.091%
3	7.689	673	681	693	rBV	345161	647190	14.77%	3.065%
4	8.089	741	749	760	rBV	871435	1599572	36.50%	7.575%
5	8.559	818	829	838	rBV	162383	297680	6.79%	1.410%
6	8.882	875	884	899	rVB	621877	1183348	27.00%	5.604%
7	9.722	1017	1027	1040	rBV	601698	1173142	26.77%	5.555%
8	11.373	1300	1308	1313	rBV	259748	510373	11.65%	2.417%
9	11.426	1313	1317	1324	rVB	146446	272161	6.21%	1.289%
10	12.989	1572	1583	1591	rBV	37865	76844	1.75%	0.364%
11	13.206	1613	1620	1628	rVB2	44869	80347	1.83%	0.380%
12	13.764	1706	1715	1723	rBV	1855636	2992476	68.28%	14.170%
13	15.133	1942	1948	1955	rBV2	405541	708886	16.18%	3.357%
14	15.198	1955	1959	1966	rVB	67723	106314	2.43%	0.503%
15	15.527	2009	2015	2020	rBV	28018	51101	1.17%	0.242%
16	16.179	2121	2126	2131	rVB	49364	80396	1.83%	0.381%
17	16.620	2194	2201	2209	rBV	1584350	2530728	57.75%	11.984%
18	17.889	2410	2417	2422	rBV2	527128	889048	20.29%	4.210%
19	18.283	2480	2484	2491	rVB	52133	84487	1.93%	0.400%
20	18.729	2556	2560	2568	rBV	122582	194188	4.43%	0.920%
21	19.986	2771	2774	2782	rVB	99214	136093	3.11%	0.644%
22	20.468	2849	2856	2864	rVB	3110981	4382437	100.00%	20.752%
23	21.831	3084	3088	3102	rVB2	64307	133137	3.04%	0.630%
24	22.272	3156	3163	3174	rVB	546365	1061619	24.22%	5.027%
25	25.962	3779	3791	3802	rVB2	298517	980828	22.38%	4.645%

Sum of corrected areas: 21117762

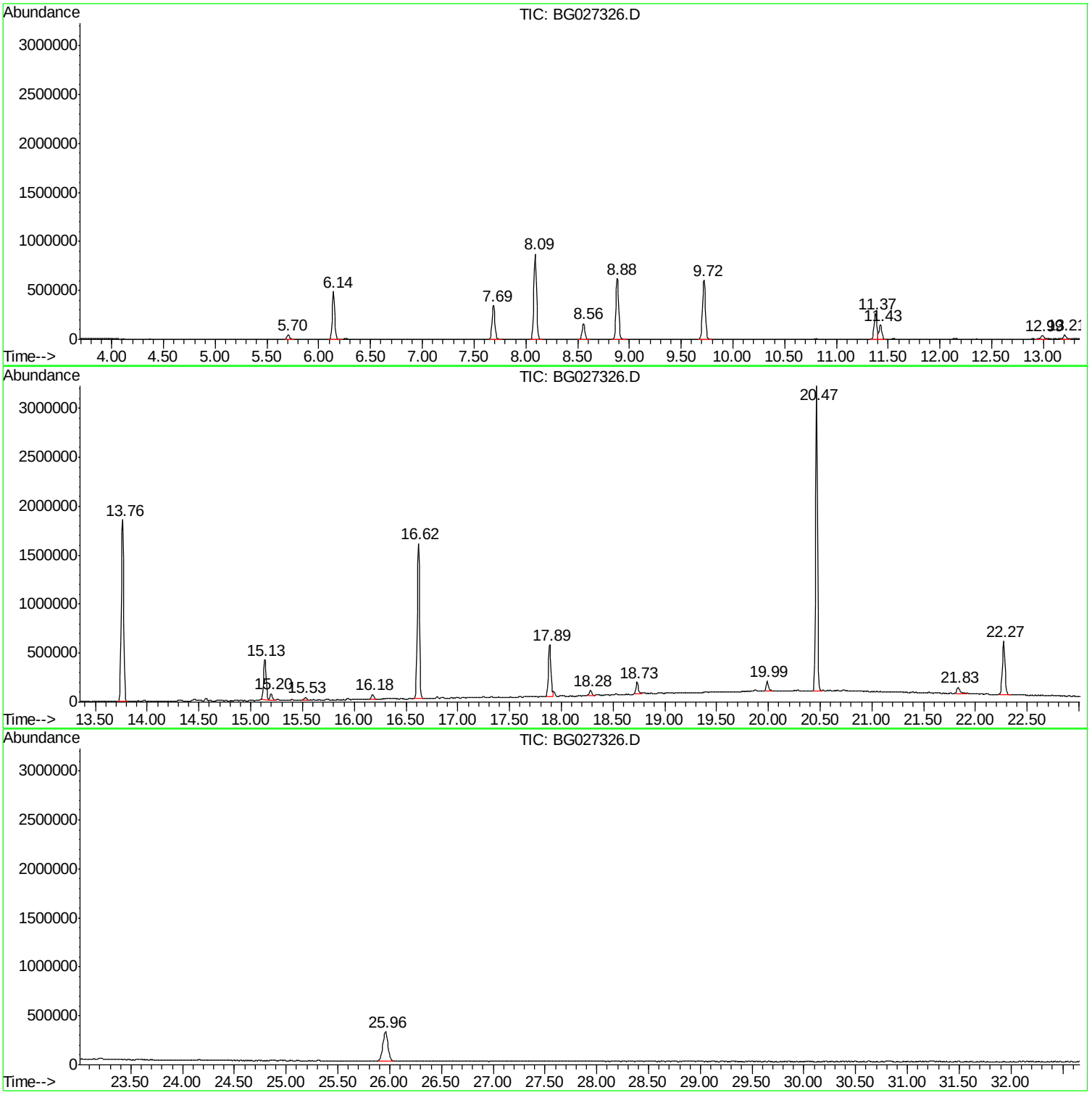
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060817\
Data File : BG027326.D
Acq On : 8 Jun 2017 20:57
Operator : SJ/MA
Sample : I3460-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-113

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.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:\HPCHEM1\BNA_G\DATA\BG060817\
Data File : BG027326.D
Acq On : 8 Jun 2017 20:57
Operator : SJ/MA
Sample : I3460-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-113

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

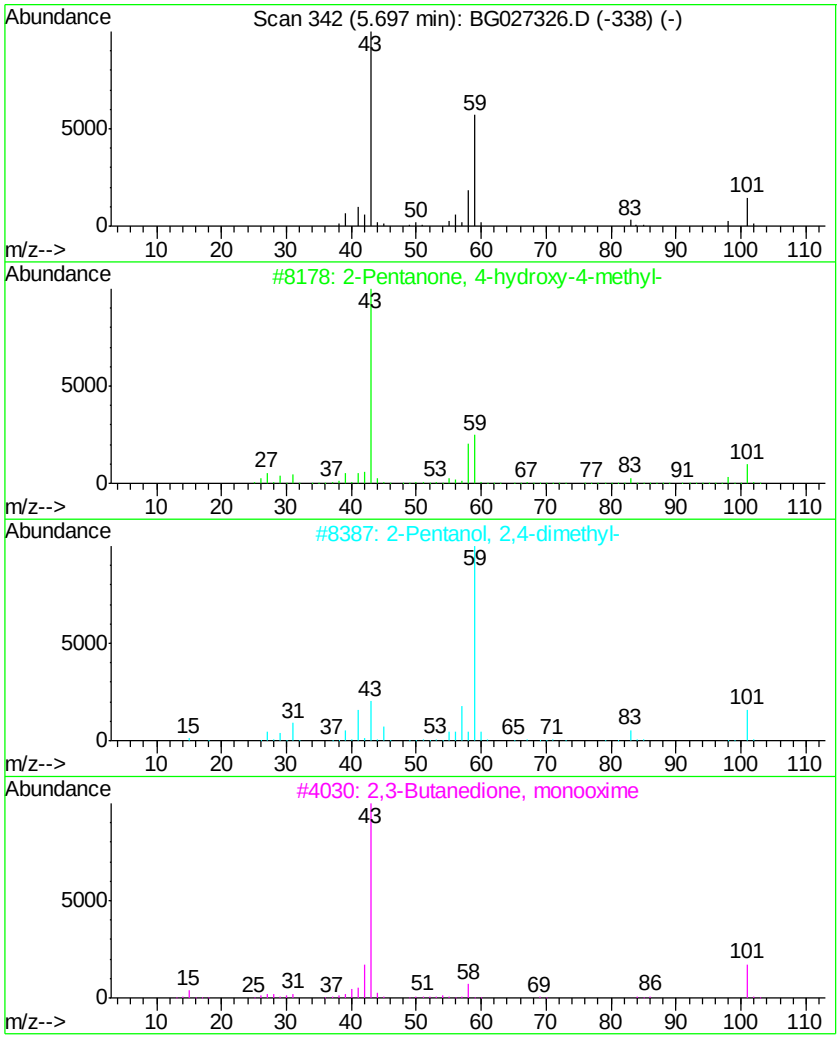
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

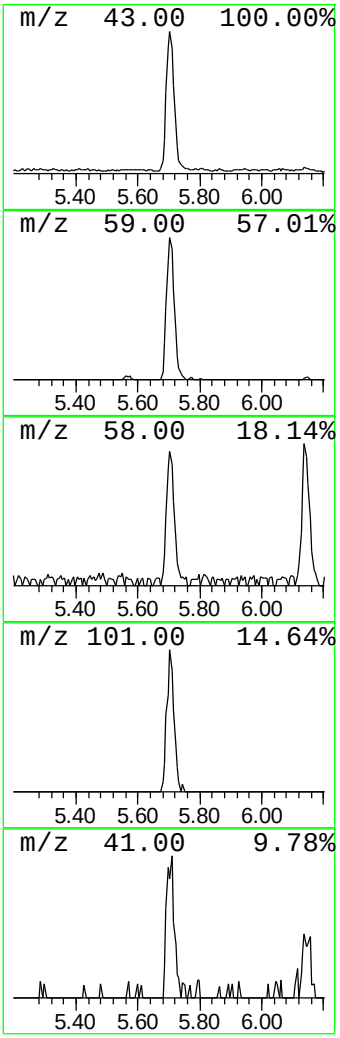
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.70	5.47 ng	81433	1,4-Dichlorobenzene-d4	8.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	50
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060817\
Data File : BG027326.D
Acq On : 8 Jun 2017 20:57
Operator : SJ/MA
Sample : I3460-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-113

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

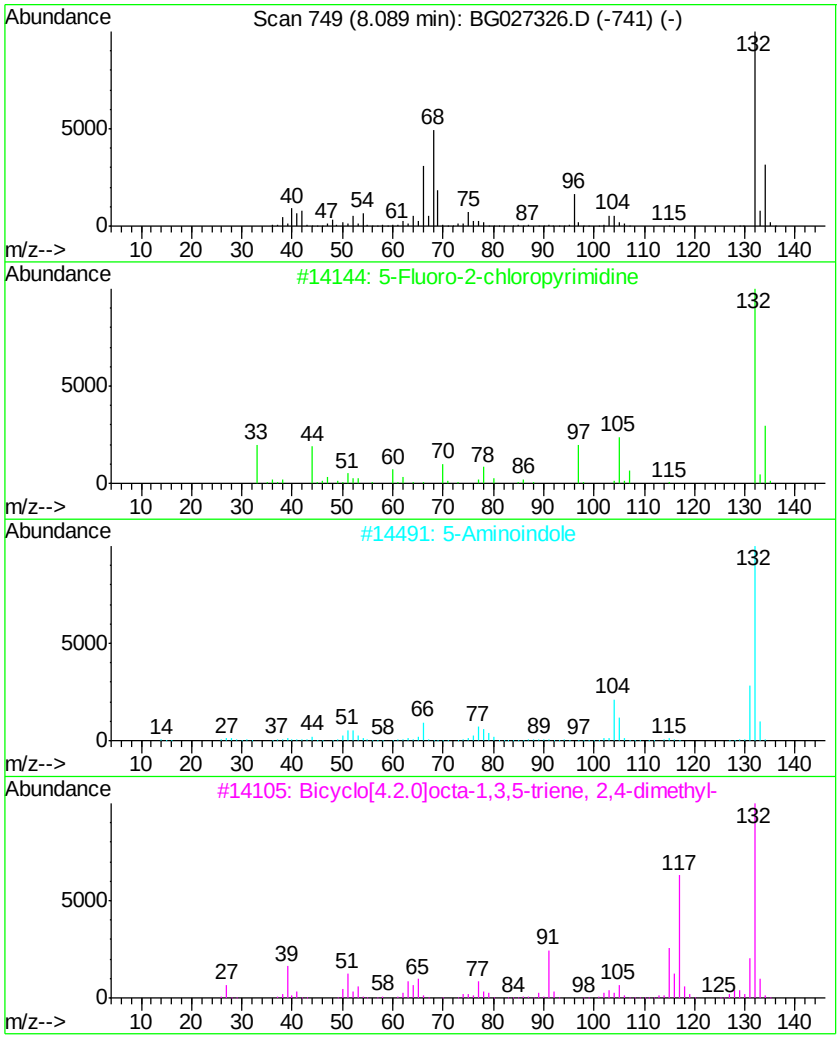
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

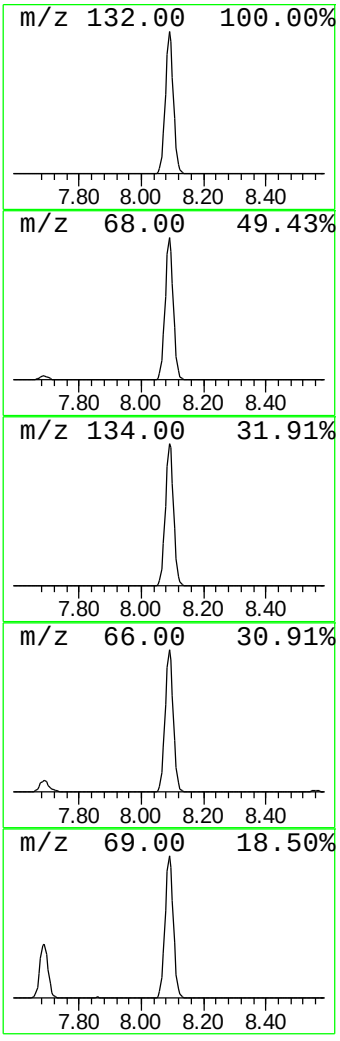
****

Peak Number 2 unknown8.09 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.09	107.47 ng	1599570	1,4-Dichlorobenzene-d4	8.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	Xenon	132	Xe	007440-63-3	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060817\
Data File : BG027326.D
Acq On : 8 Jun 2017 20:57
Operator : SJ/MA
Sample : I3460-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-113

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

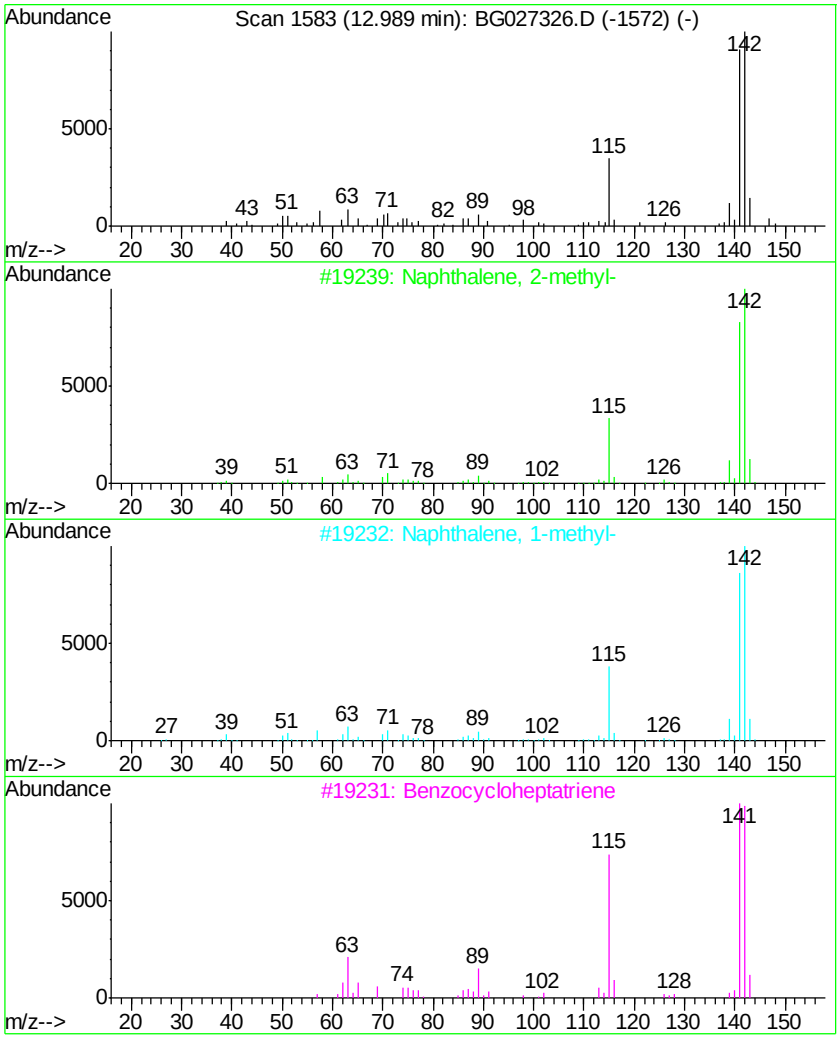
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

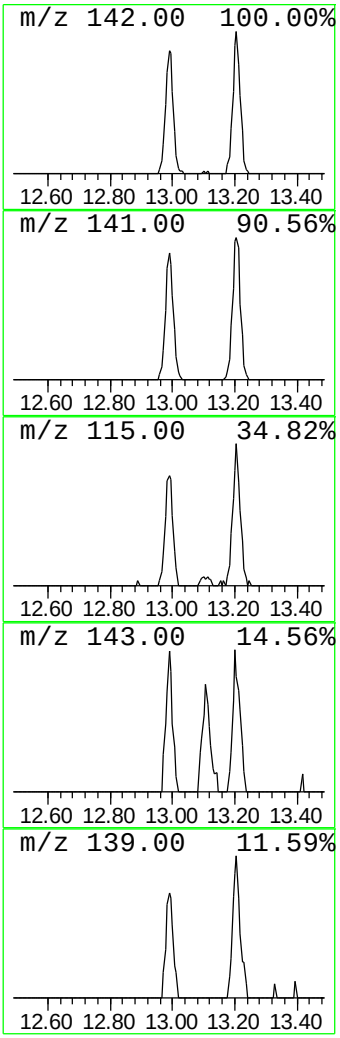
****

Peak Number 4 Naphthalene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.99	3.01 ng	76844	Naphthalene-d8	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
3	Benzocycloheptatriene	142	C11H10	000264-09-5	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	59





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060817\
Data File : BG027326.D
Acq On : 8 Jun 2017 20:57
Operator : SJ/MA
Sample : I3460-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-113

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

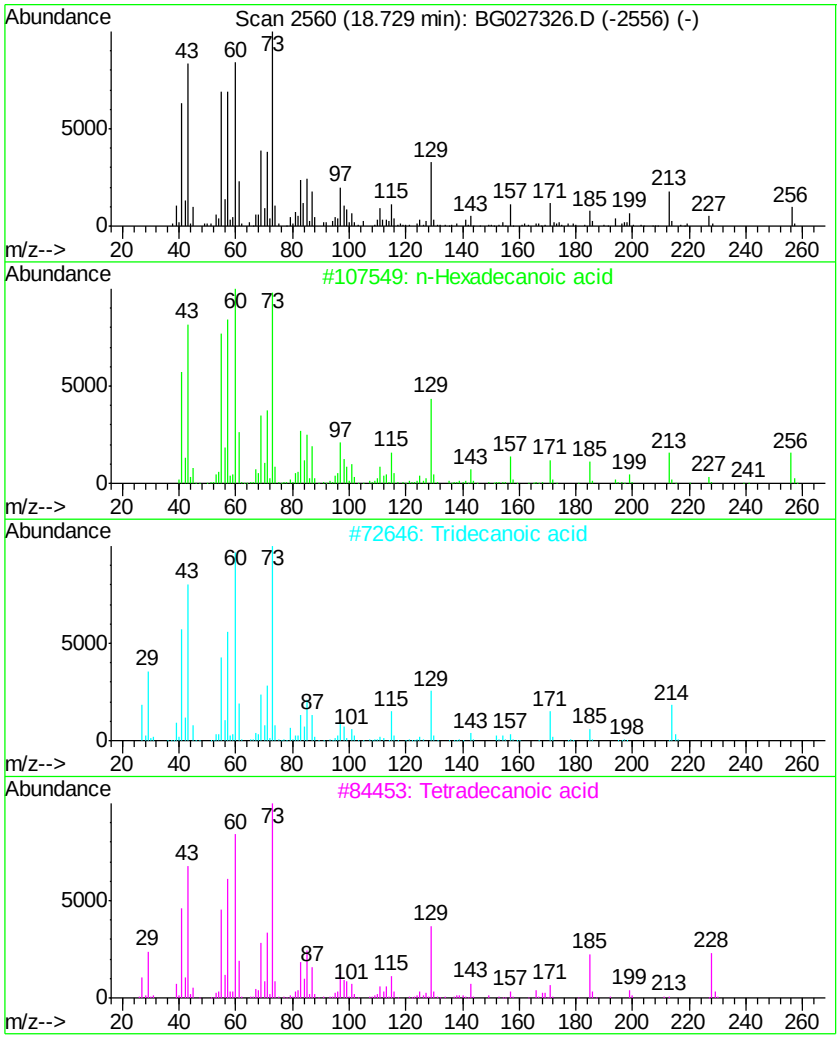
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

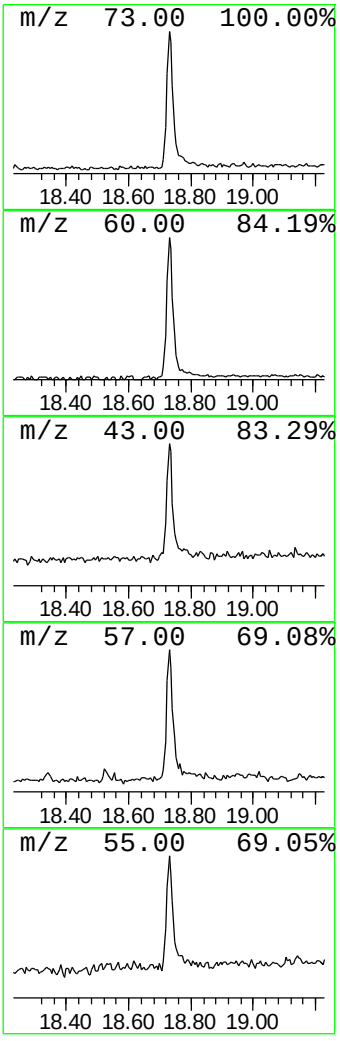
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.73	4.37 ng	194188	Phenanthrene-d10	17.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060817\
Data File : BG027326.D
Acq On : 8 Jun 2017 20:57
Operator : SJ/MA
Sample : I3460-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-113

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

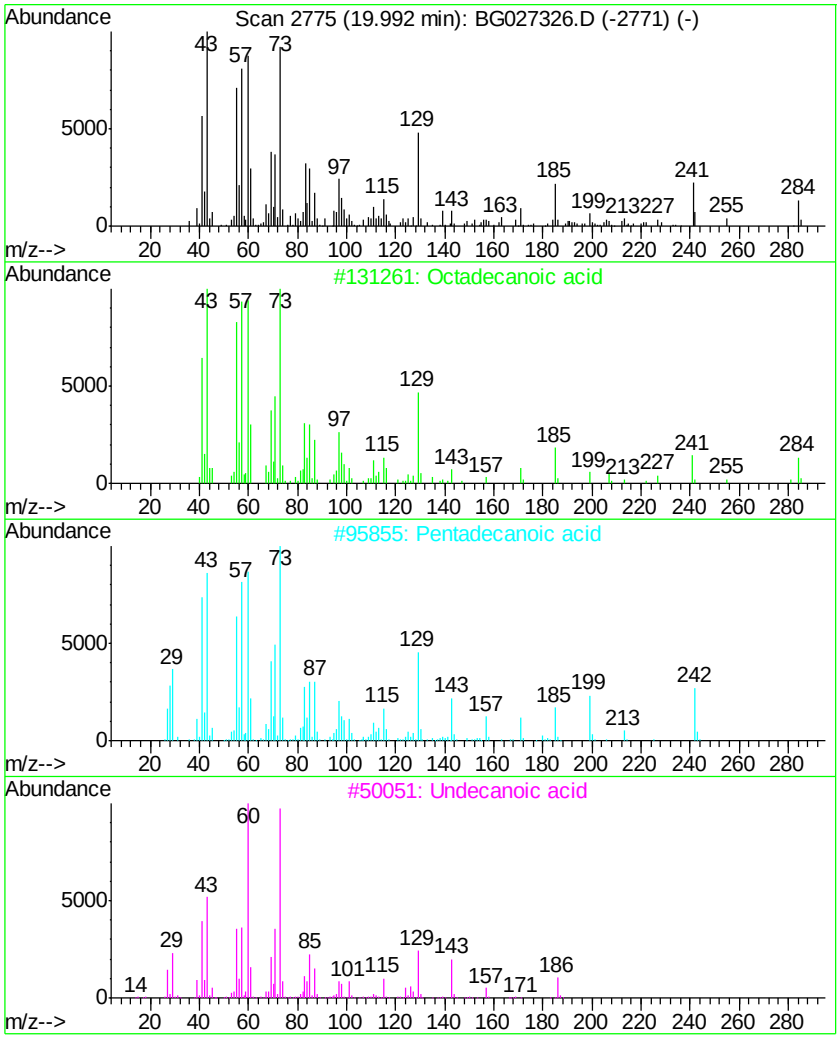
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

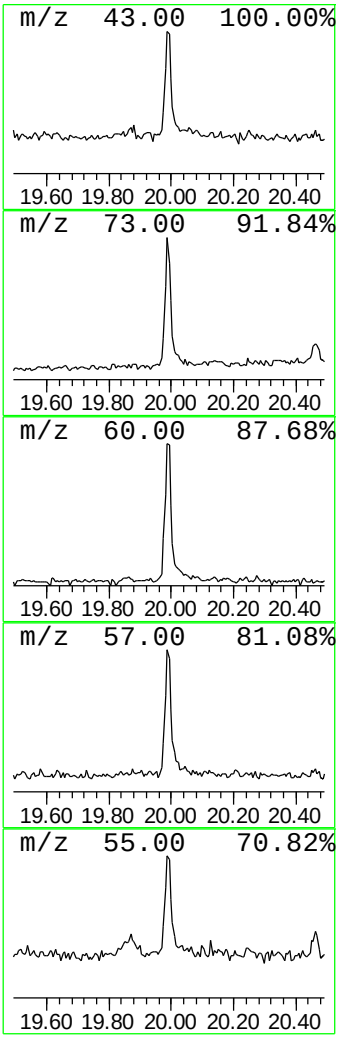
****

Peak Number 8 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.99	3.06 ng	136093	Phenanthrene-d10	17.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Undecanoic acid	186	C11H22O2	000112-37-8	76
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060817\
Data File : BG027326.D
Acq On : 8 Jun 2017 20:57
Operator : SJ/MA
Sample : I3460-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-113

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

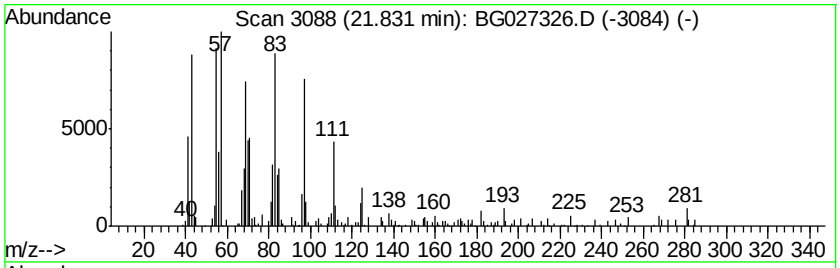
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

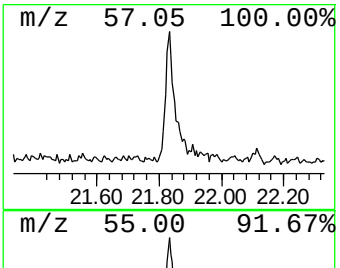
****

Peak Number 9 n-Tetracosanol-1 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.83	2.51 ng	133137	Chrysene-d12	22.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4	1-Heptacosanol	396	C27H56O	002004-39-9	90
5	1-Heneicosanol	312	C21H44O	015594-90-8	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060817\
Data File : BG027326.D
Acq On : 8 Jun 2017 20:57
Operator : SJ/MA
Sample : I3460-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-113

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.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...	5.70	5.5	ng	81433	1	8.56	297680	20.0
unknown8.09	8.09	107.5	ng	1599570	1	8.56	297680	20.0
Naphthalene, 1-me...	12.99	3.0	ng	76844	2	11.37	510373	20.0
n-Hexadecanoic acid	18.73	4.4	ng	194188	4	17.89	889048	20.0
Octadecanoic acid	19.99	3.1	ng	136093	4	17.89	889048	20.0
n-Tetracosanol-1	21.83	2.5	ng	133137	5	22.27	1061620	20.0