LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG121115\
Data File : BG020081.D
Acq On : 10 Dec 2015 18:35
Operator : UM/SJ
Sample : G4683-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S30-15

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-BG120215.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	2.987	21	25	40	rBV	318078	465944	26.74%	4.619%
2	5.185	393	399	407	rBV	87851	130130	7.47%	1.290%
3	5.661	470	480	488	rBV	396303	643834	36.95%	6.382%
4	7.265	744	753	762	rBV	441888	763511	43.81%	7.568%
5	7.641	809	817	828	rBV	431906	727546	41.75%	7.212%
6	8.111	890	897	903	rBV	69391	113290	6.50%	1.123%
7	8.434	945	952	960	rBV	292428	499561	28.67%	4.952%
8	9.280	1087	1096	1105	rVB	265406	475596	27.29%	4.714%
9	10.925	1369	1376	1384	rBV	98430	175359	10.06%	1.738%
10	13.363	1782	1791	1798	rBV	709195	1067119	61.23%	10.578%
11	14.180	1925	1930	1936	rBV	188119	276165	15.85%	2.737%
12	14.738	2019	2025	2032	rVB2	166230	263293	15.11%	2.610%
13	15.567	2162	2166	2172	rVB	20159	24721	1.42%	0.245%
14	15.954	2226	2232	2239	rBV5	11697	23523	1.35%	0.233%
15	16.225	2269	2278	2285	rBV	677023	1012573	58.10%	10.037%
16	16.307	2287	2292	2299	rVB	35813	56911	3.27%	0.564%
17	16.424	2308	2312	2324	rBV2	20837	36596	2.10%	0.363%
18	17.218	2442	2447	2452	rBV	13814	18647	1.07%	0.185%
19	17.482	2485	2492	2497	rBV2	223173	341652	19.60%	3.387%
20	18.352	2635	2640	2645	rBV	65705	90400	5.19%	0.896%
21	19.204	2782	2785	2788	rBV3	21263	24459	1.40%	0.242%
22	19.521	2836	2839	2845	rVB	17372	26089	1.50%	0.259%
23	19.615	2851	2855	2860	rBV4	29015	41877	2.40%	0.415%
24	19.756	2875	2879	2885	rVB4	16746	35215	2.02%	0.349%
25	19.885	2897	2901	2908	rVB	41895	71054	4.08%	0.704%
26	20.085	2928	2935	2940	rBV	1281319	1742682	100.00%	17.274%
27	20.761	3046	3050	3053	rBV6	14743	26282	1.51%	0.261%
28	21.377	3152	3155	3165	rVB2	35476	56179	3.22%	0.557%
29	21.754	3213	3219	3224	rBV	271057	448586	25.74%	4.447%
30	25.032	3769	3777	3787	rVB	143616	409440	23.49%	4.059%

Sum of corrected areas: 10088234

Data Path : Z:\HPCHEM1\BNA G\DATA\BG121115\
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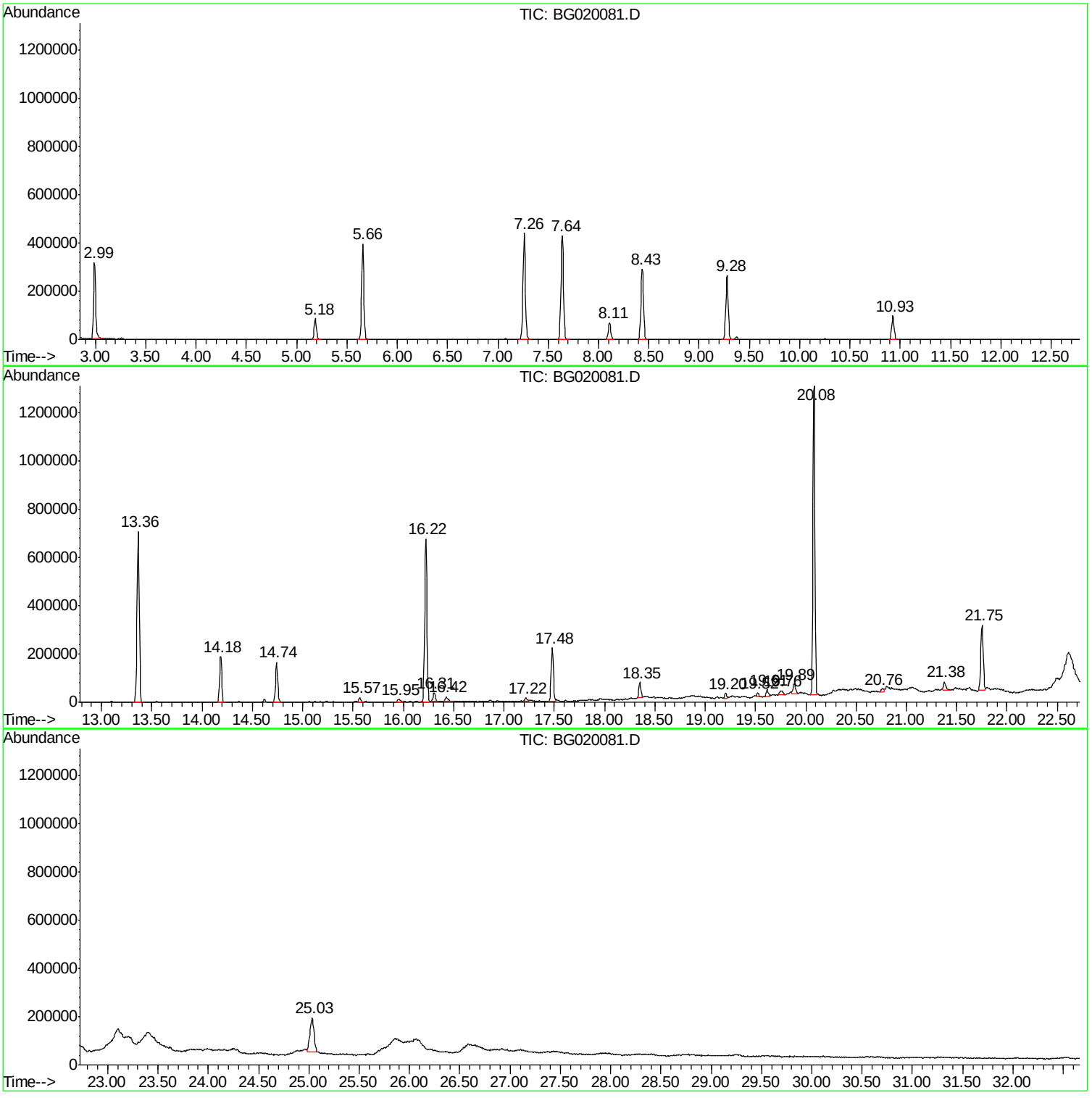
Operator : UM/SJ
Sample : G4683-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S30-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

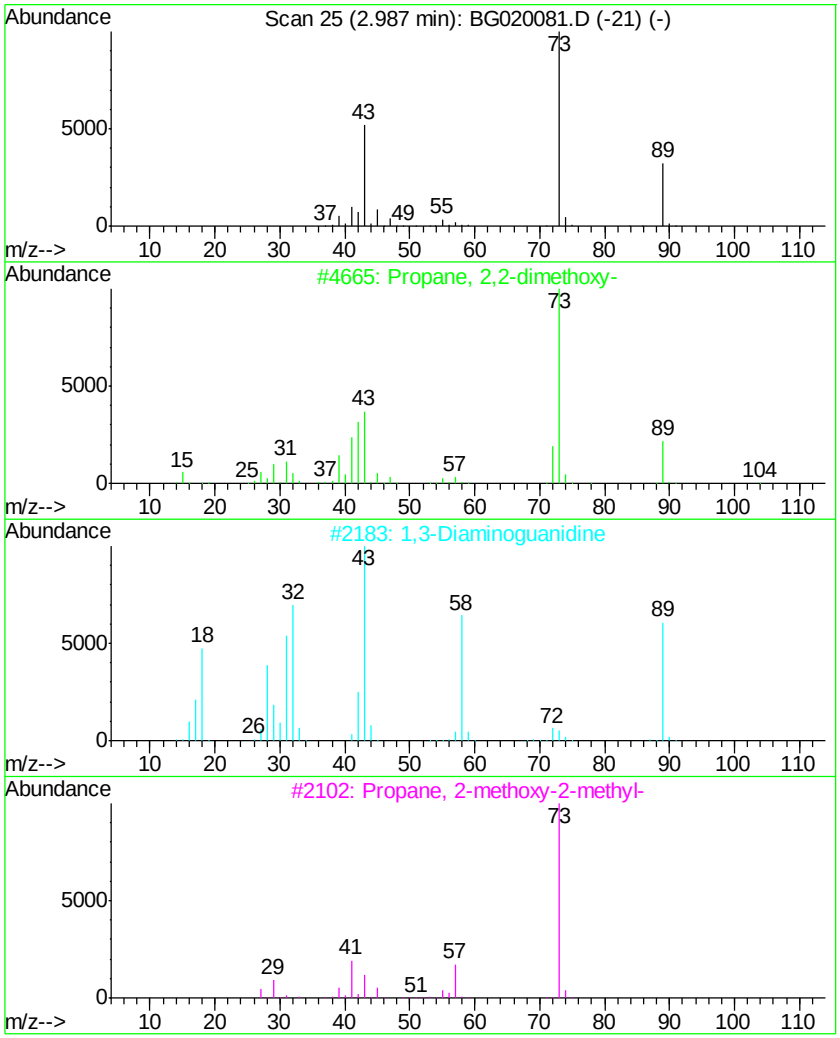
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

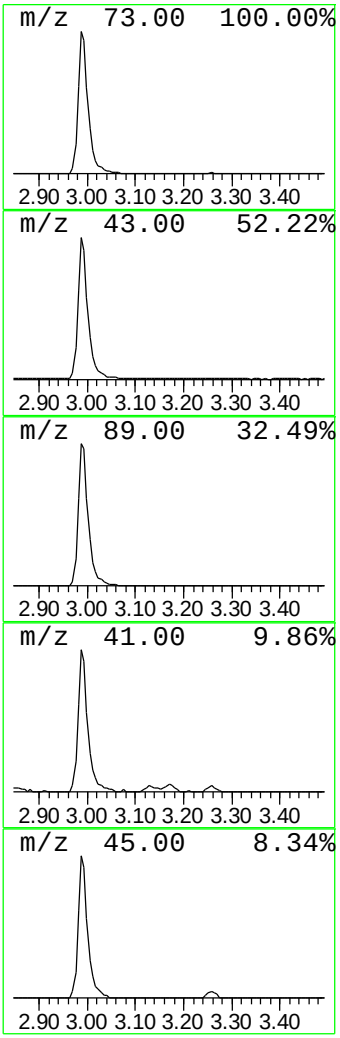
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	82.26 ng	465944	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
3	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	5
5	Guanidine, methyl-	73	C2H7N3	000471-29-4	5





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Data File : BG020081.D
Acq On : 10 Dec 2015 18:35
Operator : UM/SJ
Sample : G4683-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S30-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

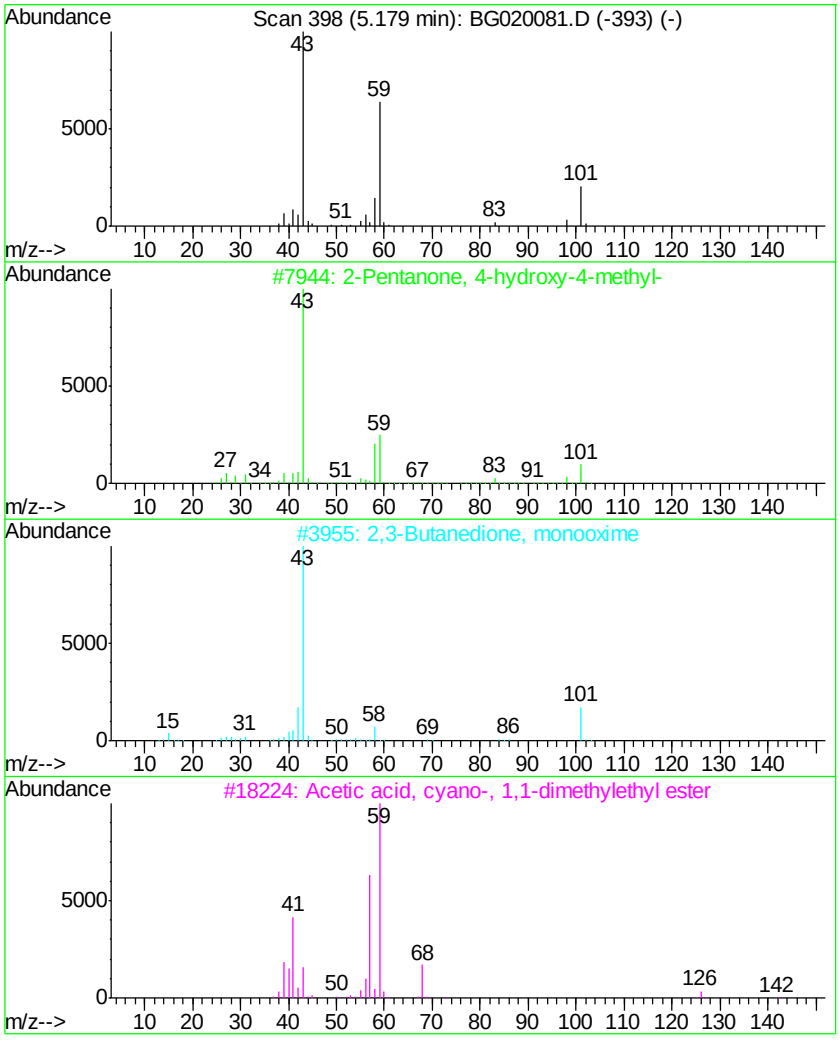
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

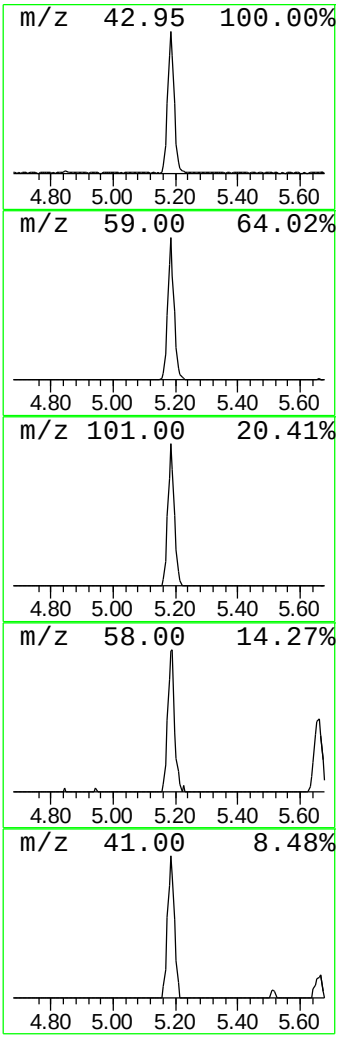
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	22.97 ng	130130	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	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4	3-Hexanol	102	C6H14O	000623-37-0	28
5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG121115\
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Sample : G4683-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S30-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

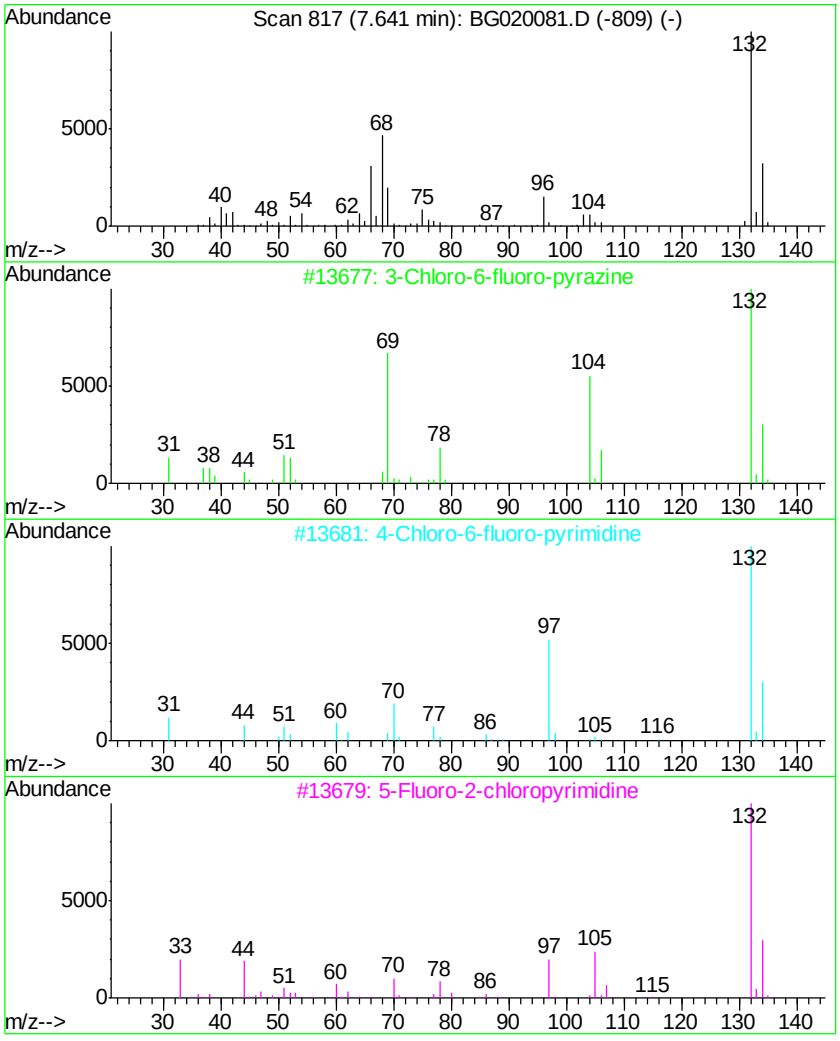
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

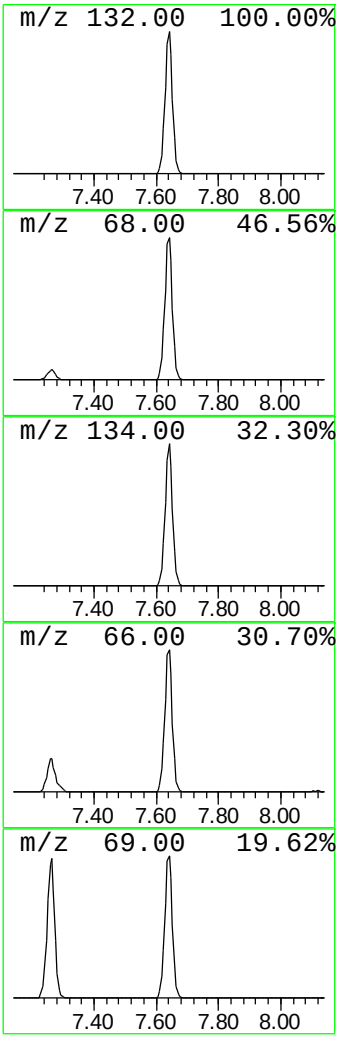
****

Peak Number 3 unknown7.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	128.44 ng	727546	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	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Data Path : Z:\HPCHEM1\BNA G\DATA\BG121115\
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Operator : UM/SJ
Sample : G4683-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S30-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

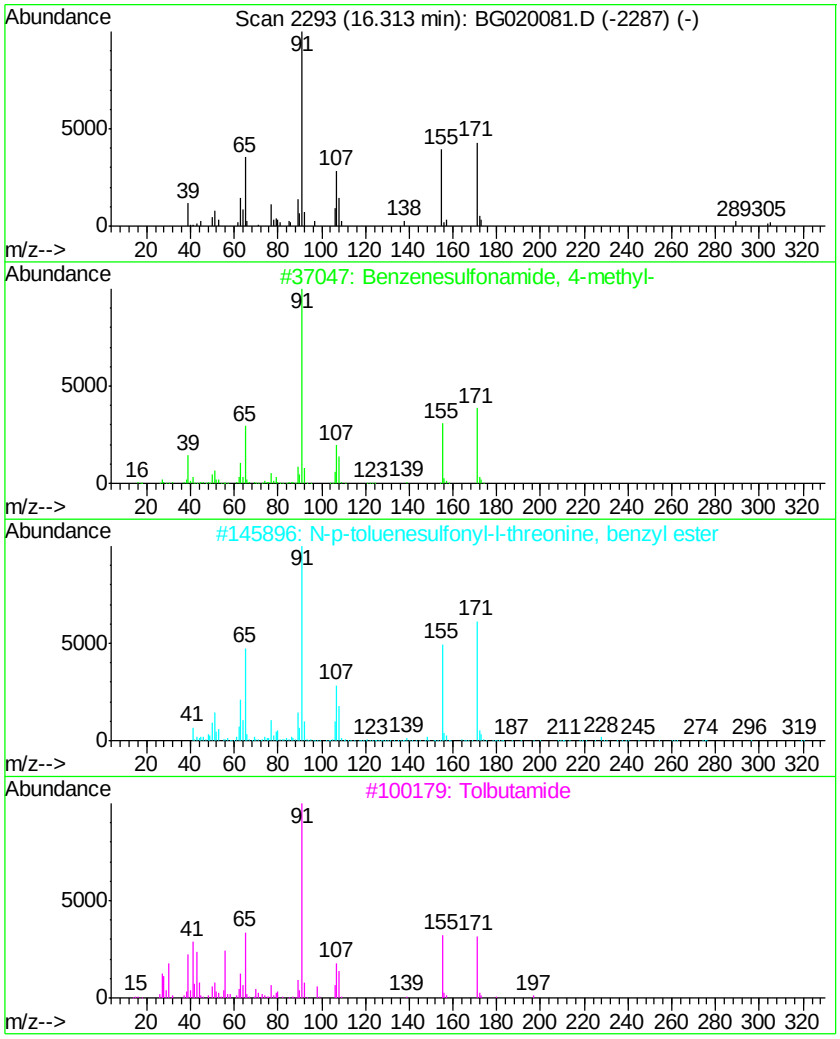
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

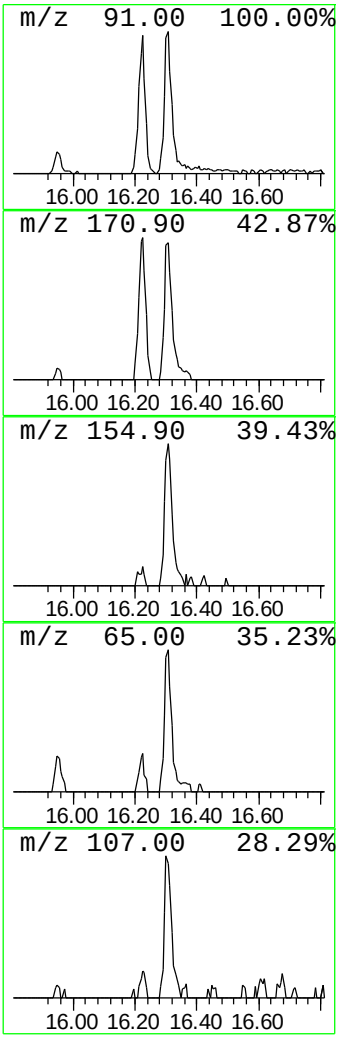
****

Peak Number 5 Benzenesulfonamide, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.31	3.33 ng	56911	Phenanthrene-d10	17.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	97
2	N-p-toluenesulfonyl-l-threonine,...	363	C18H21NO5S	1000130-34-4	91
3	Tolbutamide	270	C12H18N2O3S	000064-77-7	91
4	Thiosulfuric acid, S-[2-[3-(4-me...	381	C12H19N3O5S3	1000255-60-3	83
5	O-p-toluenesulfonyll-N-acetylser...	315	C13H17NO6S	1000126-44-8	72





Data Path : Z:\HPCHEM1\BNA G\DATA\BG121115\
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Sample : G4683-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S30-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

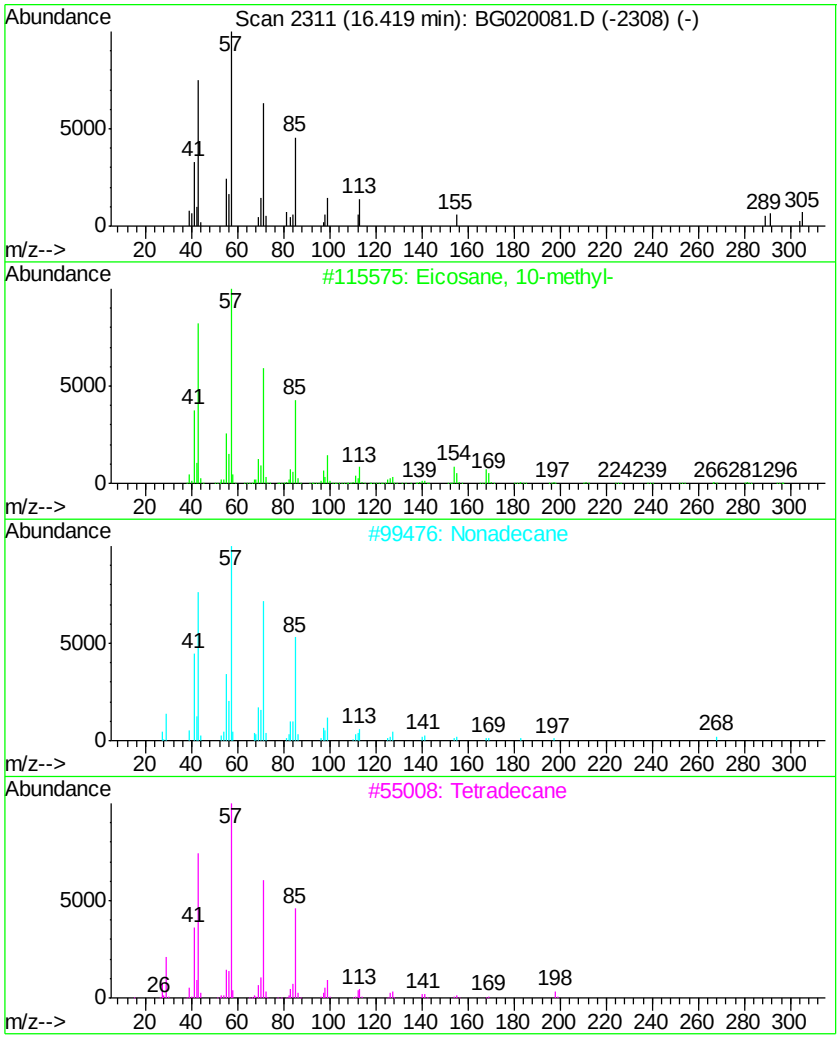
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

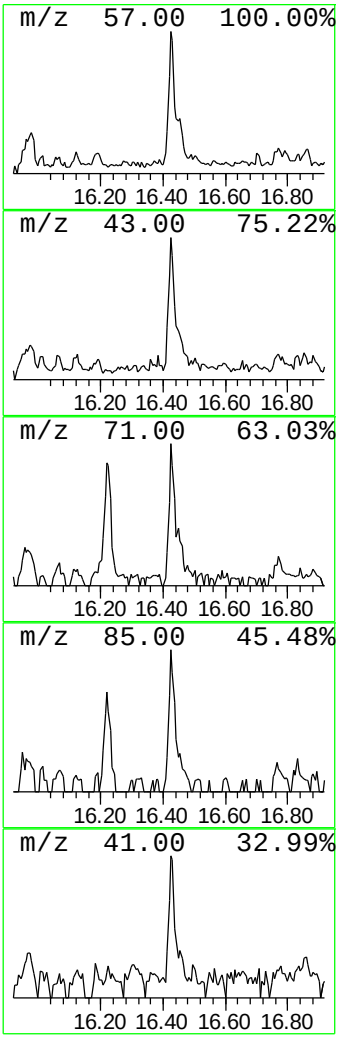
****

Peak Number 6 Eicosane, 10-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.42	2.14 ng	36596	Phenanthrene-d10	17.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 10-methyl-	296	C21H44	054833-23-7	80
2	Nonadecane	268	C19H40	000629-92-5	80
3	Tetradecane	198	C14H30	000629-59-4	80
4	Heptadecane	240	C17H36	000629-78-7	80
5	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	80





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Operator : UM/SJ
Sample : G4683-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S30-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

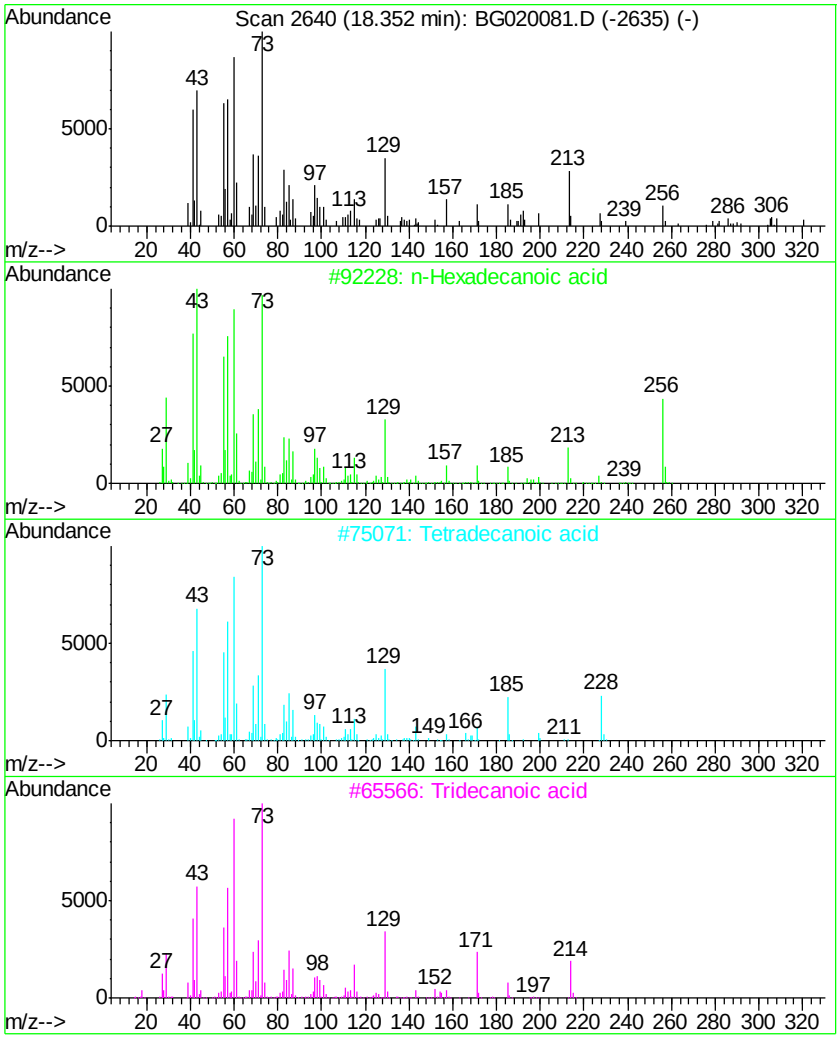
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

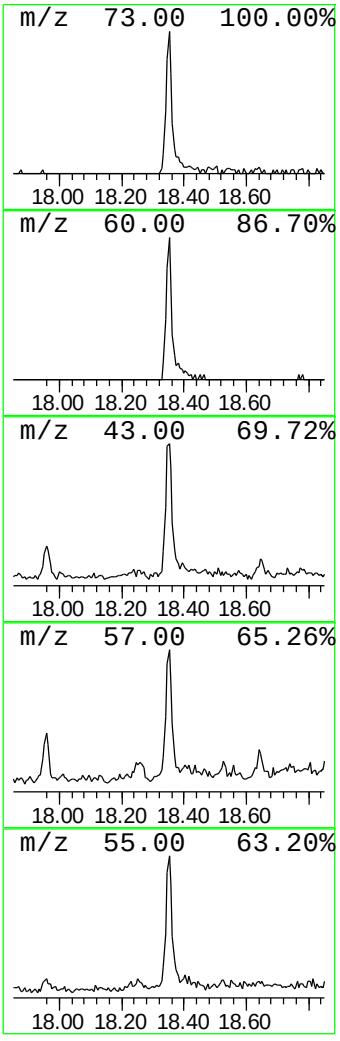
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.35	5.29 ng	90400	Phenanthrene-d10	17.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	59
5	Undecanoic acid	186	C11H22O2	000112-37-8	53





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Operator : UM/SJ
Sample : G4683-08
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Instrument : BNA_G
ClientSampleId : S30-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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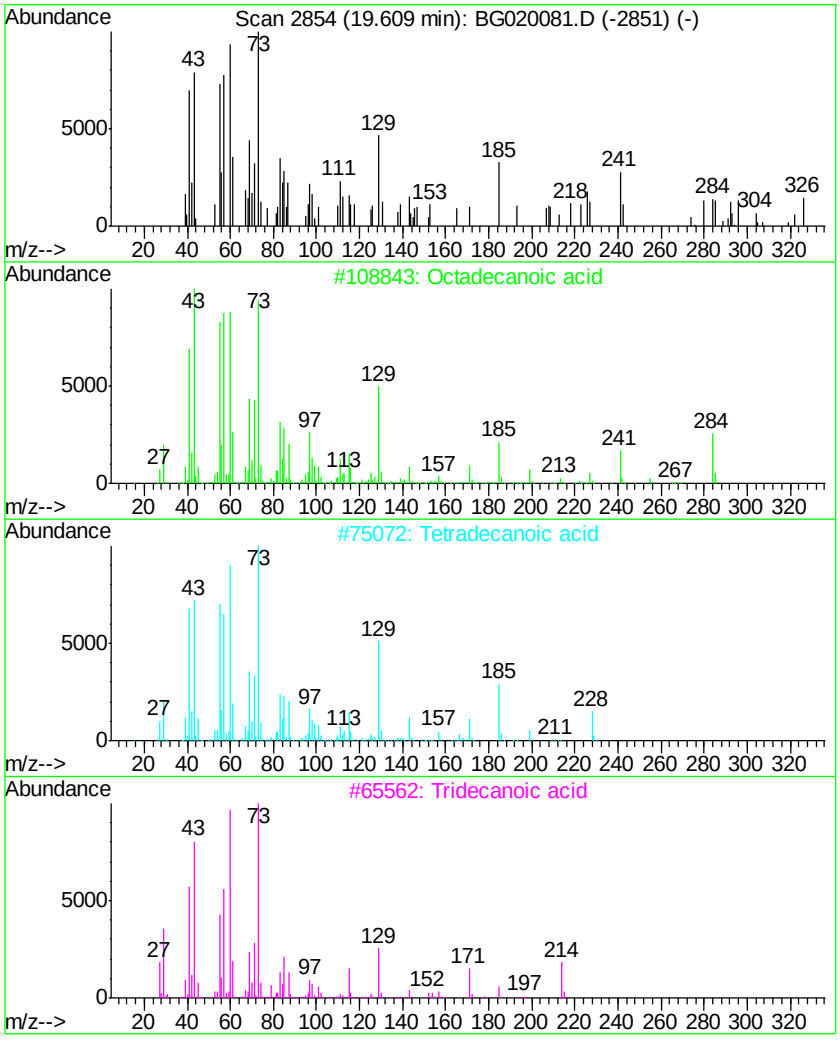
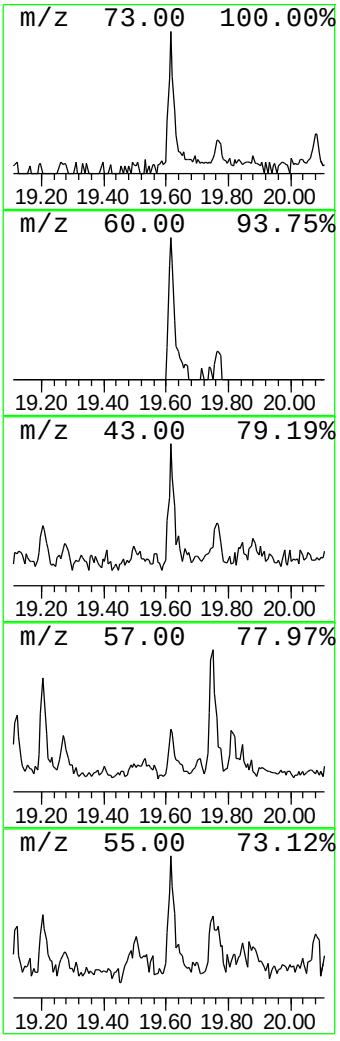
****

Peak Number 8 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.61	2.45 ng	41877	Phenanthrene-d10	17.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	53
5	Dodecanoic acid	200	C12H24O2	000143-07-7	52





Library Search Compound Report

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

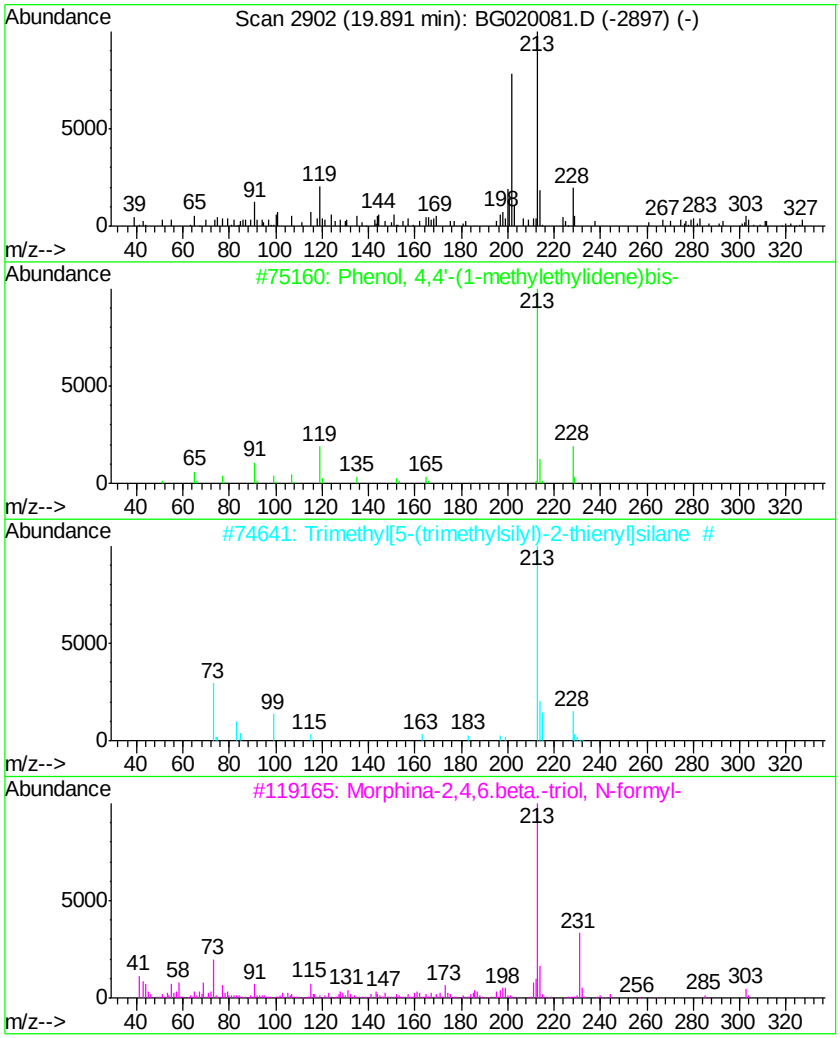
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

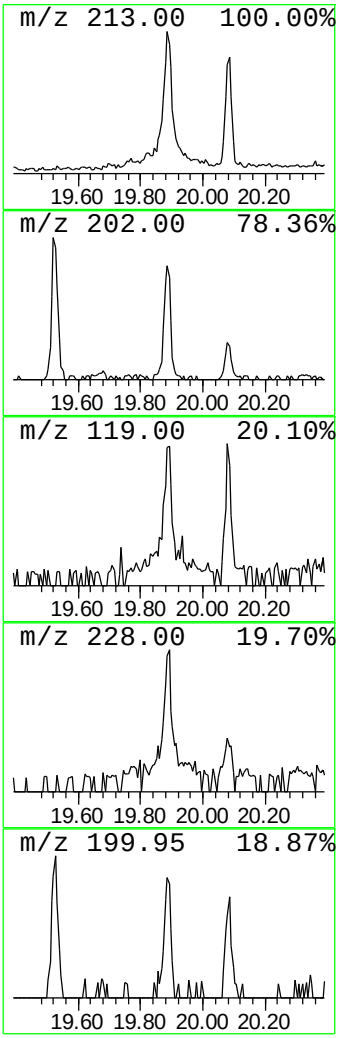
****

Peak Number 9 unknown19.89 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.89	3.17 ng	71054	Chrysene-d12	21.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	41
2	Trimethyl[5-(trimethylsilyl)-2-t...	228	C10H20SSi2	017906-71-7	38
3	Morphina-2,4,6.beta.-triol, N-fo...	303	C17H21NO4	1000129-09-2	38
4	Morphina-2,4,6.alpha.-triol, N-f...	303	C17H21NO4	1000129-09-3	35
5	2,2-Bis-(4-hyxroxyphenyl)-butane	242	C16H18O2	000077-40-7	35





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Operator : UM/SJ
Sample : G4683-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S30-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

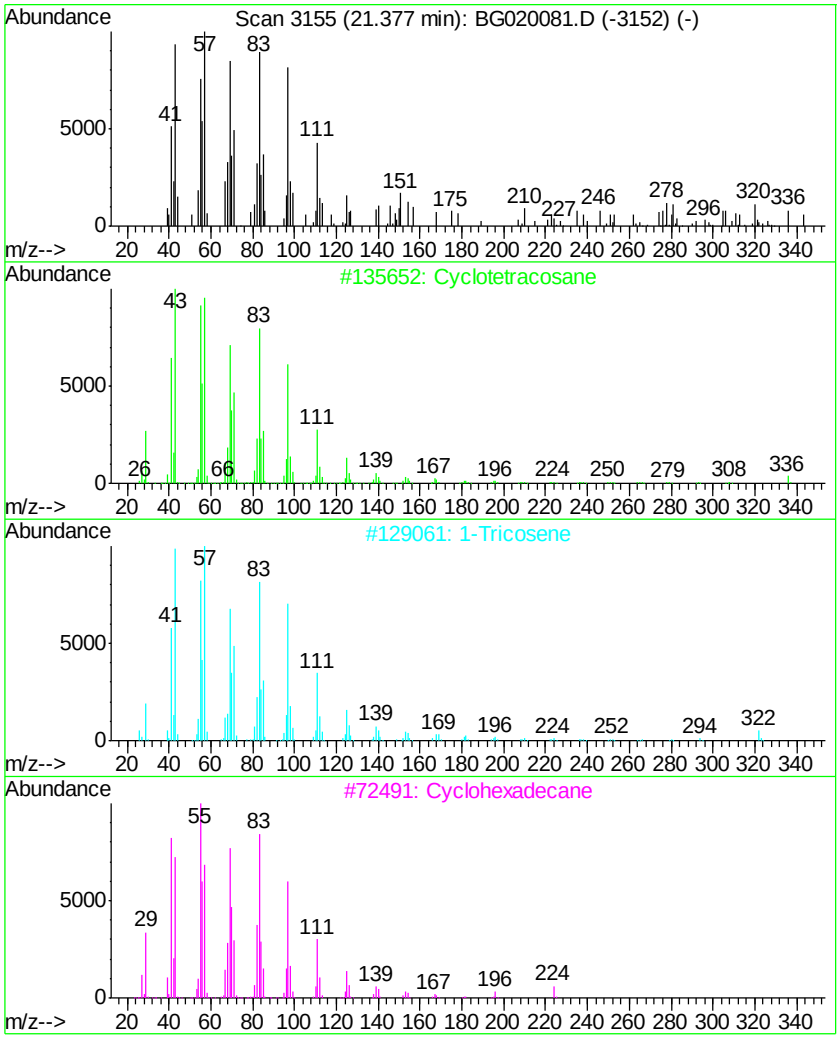
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

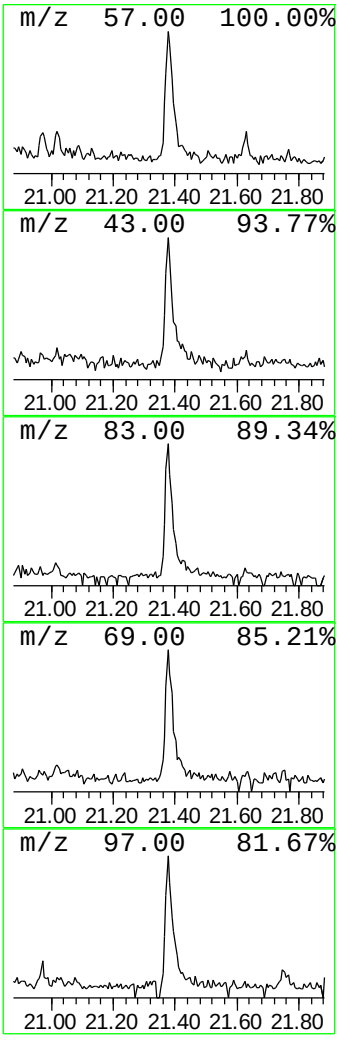
****

Peak Number 10 Cyclotetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.38	2.50 ng	56179	Chrysene-d12	21.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	98
2	1-Tricosene	322	C23H46	018835-32-0	97
3	Cyclohexadecane	224	C16H32	000295-65-8	96
4	9-Tricosene, (Z)-	322	C23H46	027519-02-4	95
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG121115\
Data File : BG020081.D
Acq On : 10 Dec 2015 18:35
Operator : UM/SJ
Sample : G4683-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S30-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 2,2-dime...	2.99	82.3	ng	465944	1	8.11	113290	20.0
2-Pentanone, 4-hy...	5.18	23.0	ng	130130	1	8.11	113290	20.0
unknown7.64	7.64	128.4	ng	727546	1	8.11	113290	20.0
Benzenesulfonamid...	16.31	3.3	ng	56911	4	17.48	341652	20.0
Eicosane, 10-methyl-	16.42	2.1	ng	36596	4	17.48	341652	20.0
n-Hexadecanoic acid	18.35	5.3	ng	90400	4	17.48	341652	20.0
Octadecanoic acid	19.61	2.5	ng	41877	4	17.48	341652	20.0
unknown19.89	19.89	3.2	ng	71054	5	21.75	448586	20.0
Cyclotetracosane	21.38	2.5	ng	56179	5	21.75	448586	20.0