LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG011217\
Data File : BG025502.D
Acq On : 13 Jan 2017 4:15
Operator : UM/SJ
Sample : I1135-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : W-41

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-BG122116.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	5.260	406	412	423	rBV	228889	369214	4.38%	1.052%
2	5.741	487	494	505	rBV	712840	1298255	15.39%	3.700%
3	7.363	763	770	780	rBV	460503	907375	10.76%	2.586%
4	7.733	826	833	848	rBV	1286761	2364179	28.02%	6.738%
5	8.203	906	913	922	rBV	246904	444633	5.27%	1.267%
6	8.526	961	968	979	rVB	1183697	2115054	25.07%	6.028%
7	9.384	1106	1114	1124	rBV	1034240	1970360	23.36%	5.616%
8	10.401	1280	1287	1295	rBV6	42899	99167	1.18%	0.283%
9	11.029	1388	1394	1406	rVB	320509	679322	8.05%	1.936%
10	12.886	1706	1710	1717	rVB5	49512	94004	1.11%	0.268%
11	13.444	1798	1805	1813	rBV	2759452	4376892	51.88%	12.475%
12	13.679	1840	1845	1852	rBV2	67895	131021	1.55%	0.373%
13	14.273	1941	1946	1951	rVB	58448	93558	1.11%	0.267%
14	14.825	2034	2040	2050	rVB2	574856	921946	10.93%	2.628%
15	16.317	2286	2294	2307	rBV	2871492	4600968	54.54%	13.114%
16	17.575	2500	2508	2519	rBV	762039	1238385	14.68%	3.530%
17	17.909	2560	2565	2575	rBV5	96806	230386	2.73%	0.657%
18	18.409	2646	2650	2660	rBV7	77743	129071	1.53%	0.368%
19	19.261	2788	2795	2808	rBV2	379003	854861	10.13%	2.437%
20	19.801	2881	2887	2890	rBV5	49094	99045	1.17%	0.282%
21	20.154	2941	2947	2955	rBV	6281805	8436040	100.00%	24.044%
22	20.753	3046	3049	3054	rVB3	60531	91109	1.08%	0.260%
23	21.864	3231	3238	3245	rBV	1022794	1769085	20.97%	5.042%
24	25.260	3807	3816	3834	rVB	568290	1771259	21.00%	5.048%

Sum of corrected areas: 35085189

LSC Report - Integrated Chromatogram

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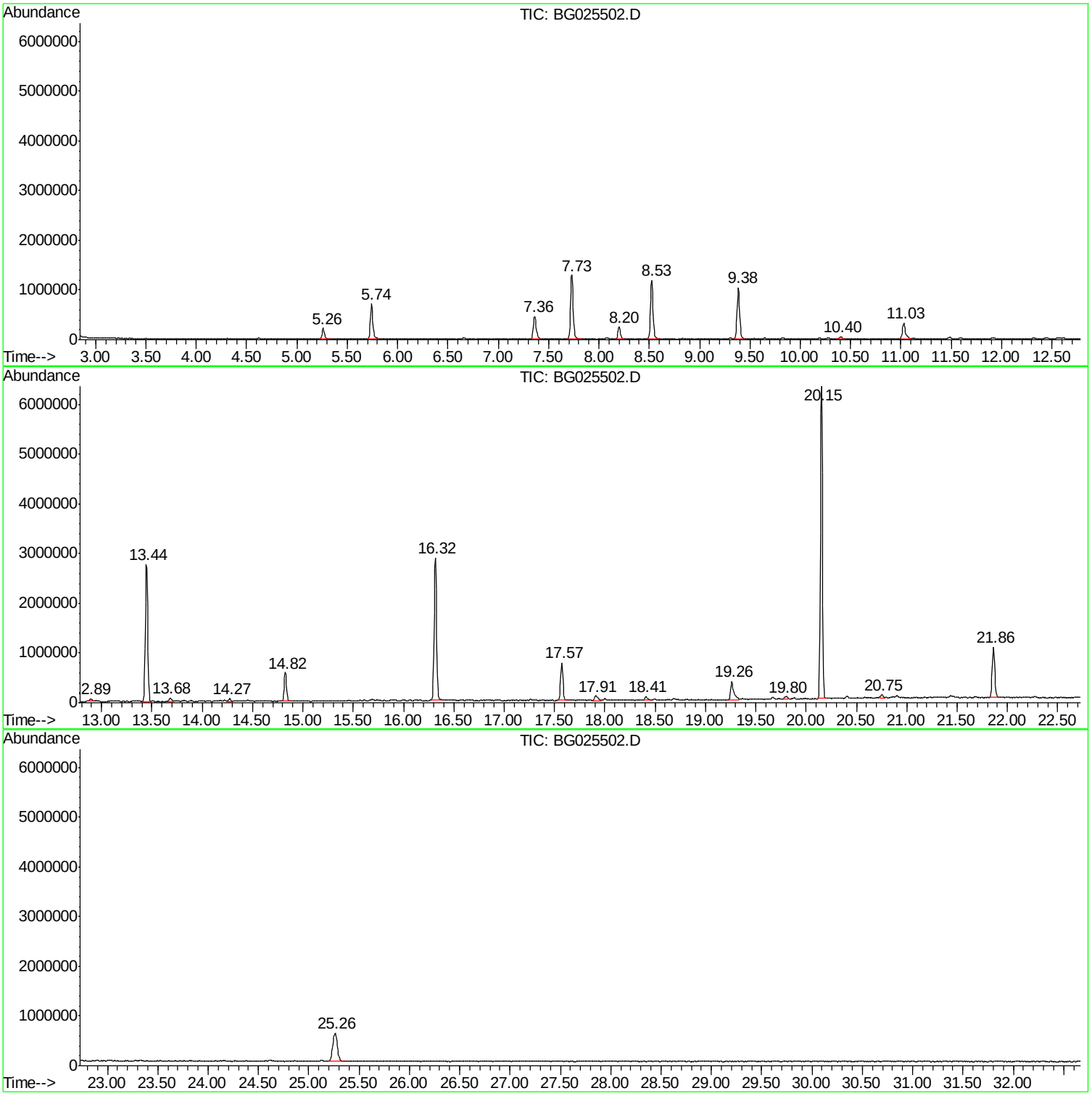
Data File : BG025502.D
Acq On : 13 Jan 2017 4:15
Operator : UM/SJ
Sample : I1135-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : W-41

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.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\BG011217\
Data File : BG025502.D
Acq On : 13 Jan 2017 4:15
Operator : UM/SJ
Sample : I1135-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : W-41

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

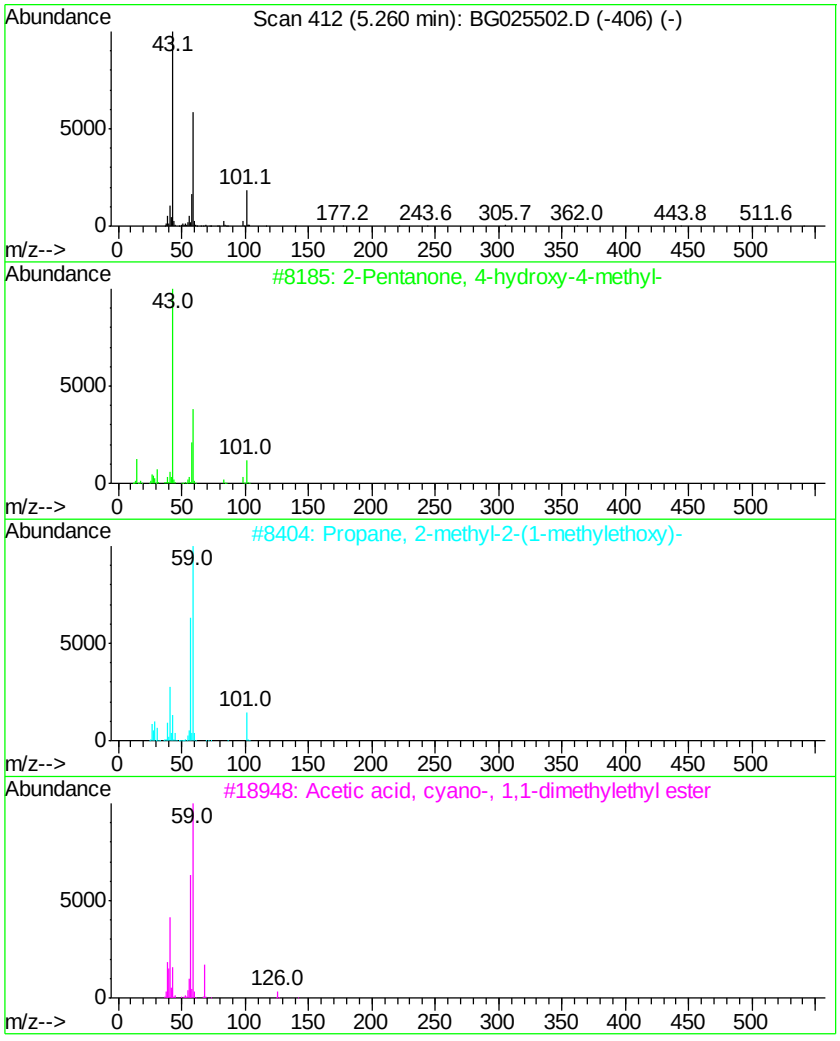
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

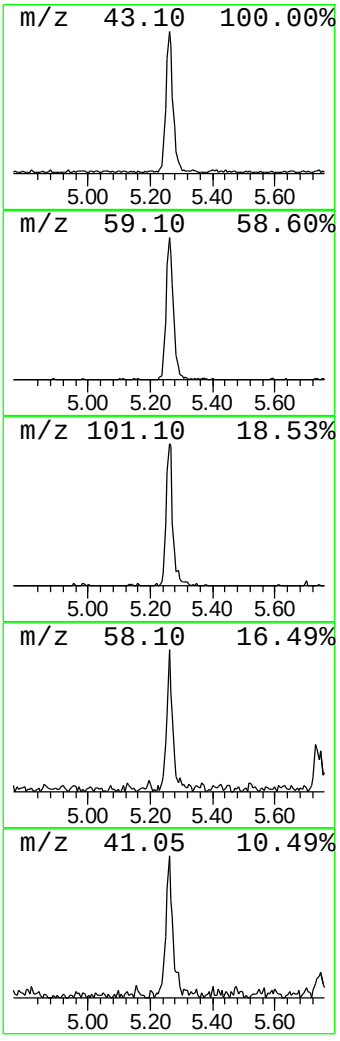
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.26	16.61 ng	369214	1,4-Dichlorobenzene-d4	8.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12





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Data File : BG025502.D
Acq On : 13 Jan 2017 4:15
Operator : UM/SJ
Sample : I1135-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : W-41

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

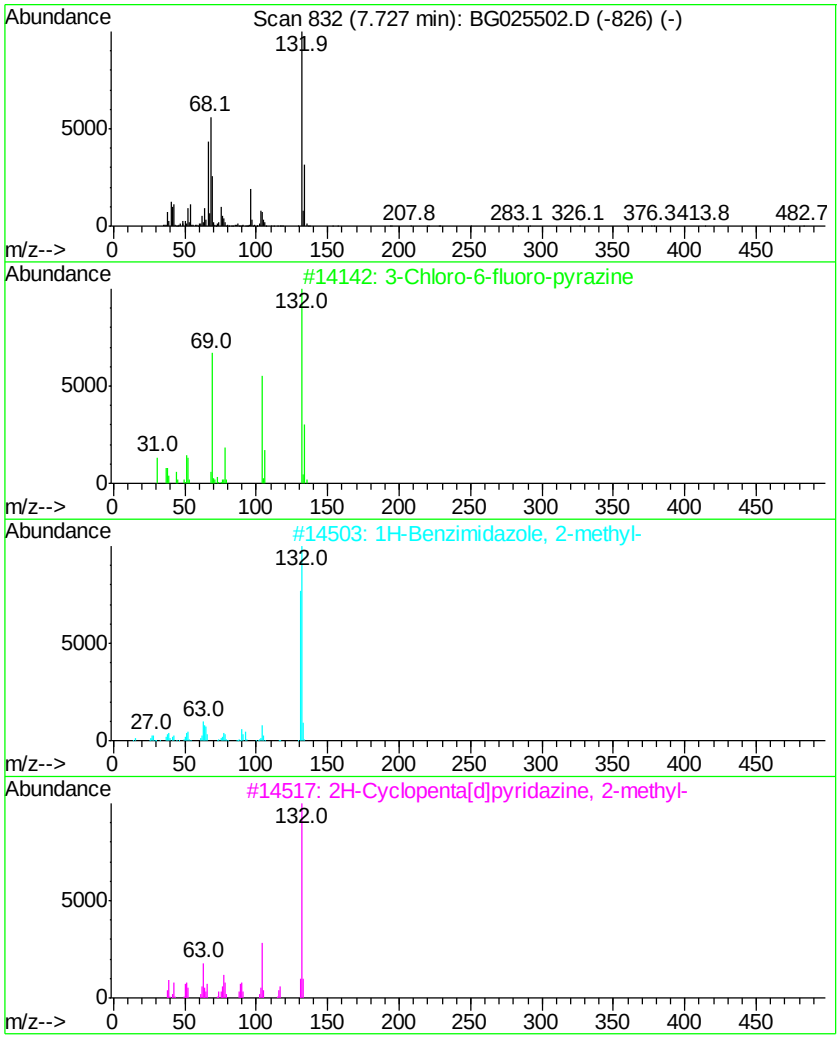
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

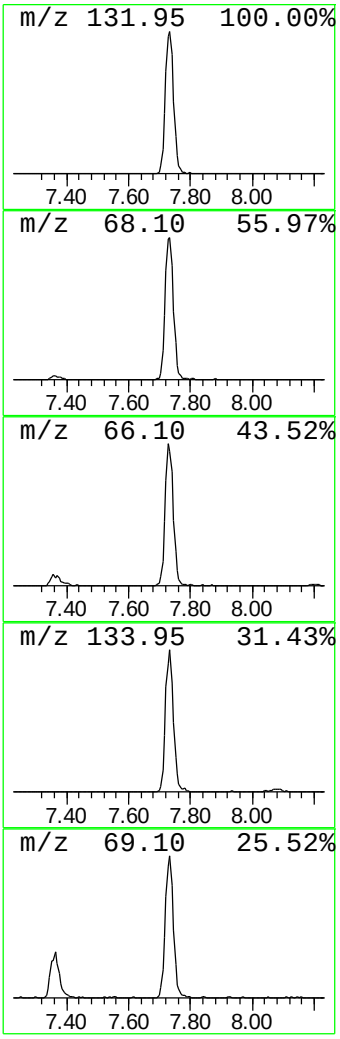
****

Peak Number 2 unknown7.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.73	106.34 ng	2364180	1,4-Dichlorobenzene-d4	8.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	18
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	14
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	10





Data Path : Z:\HPCHEM1\BNA G\DATA\BG011217\
Data File : BG025502.D
Acq On : 13 Jan 2017 4:15
Operator : UM/SJ
Sample : I1135-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : W-41

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

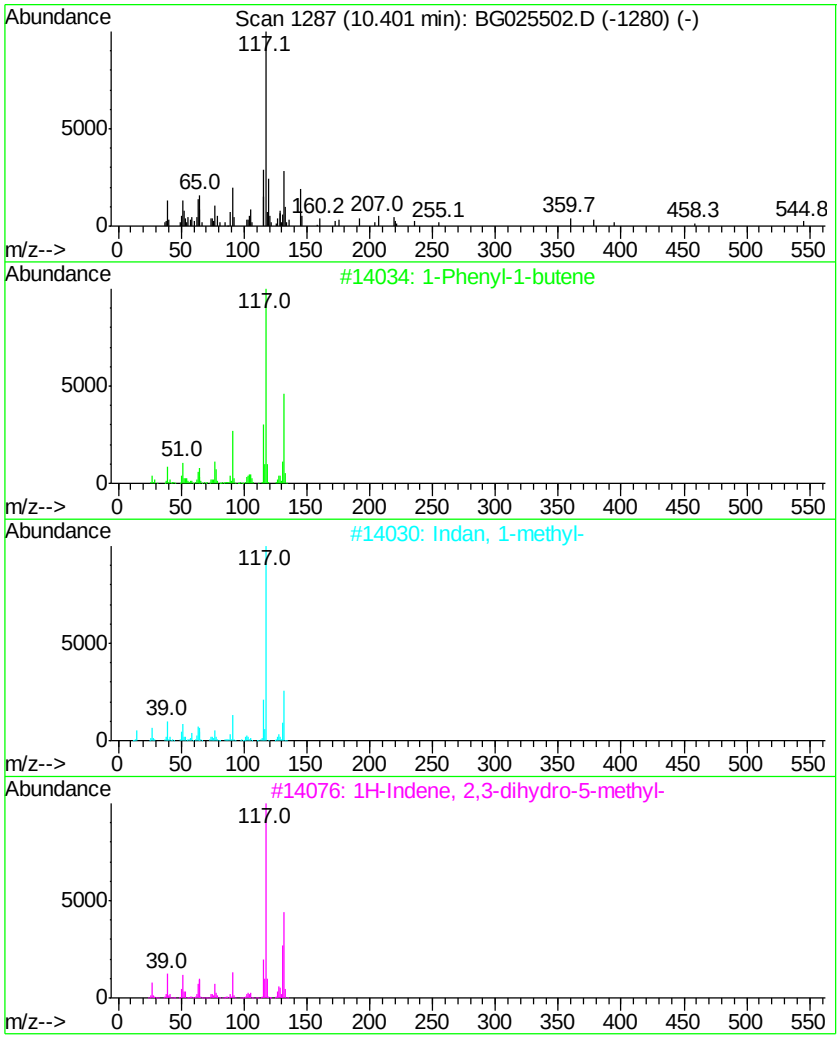
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

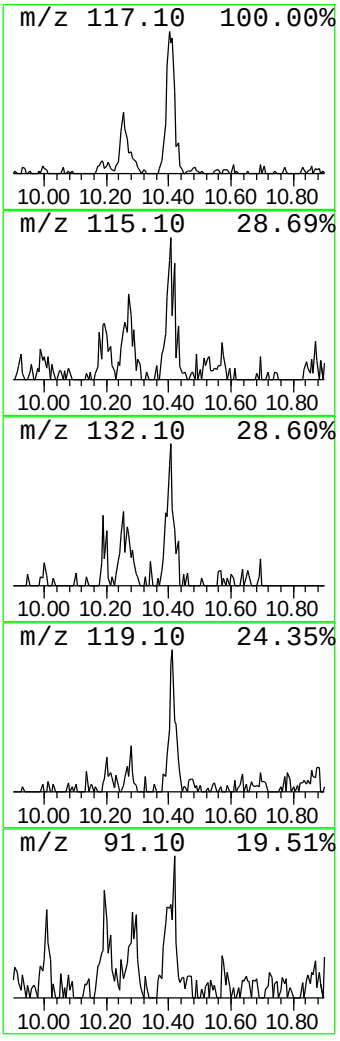
****

Peak Number 4 1-Phenyl-1-butene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.40	2.92 ng	99167	Naphthalene-d8	11.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenyl-1-butene	132	C10H12	000824-90-8	53
2	Indan, 1-methyl-	132	C10H12	000767-58-8	53
3	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	53
4	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	49
5	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	49





Data Path : Z:\HPCHEM1\BNA G\DATA\BG011217\
Data File : BG025502.D
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Operator : UM/SJ
Sample : I1135-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : W-41

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

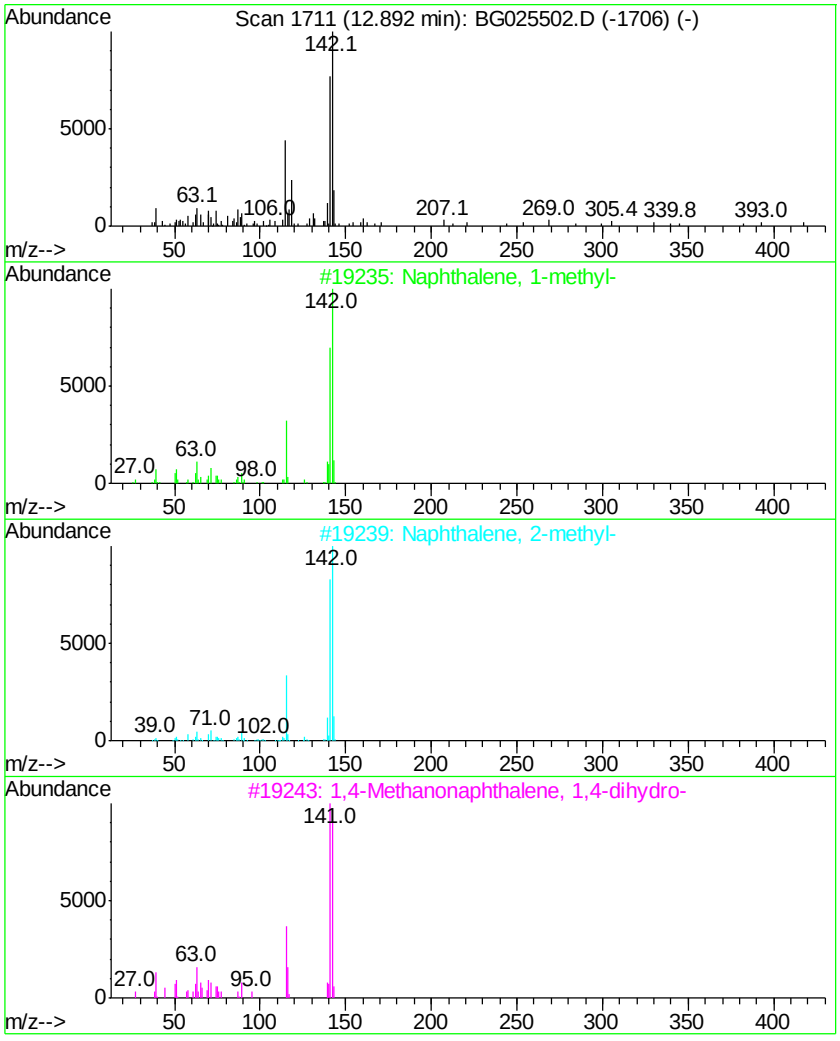
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

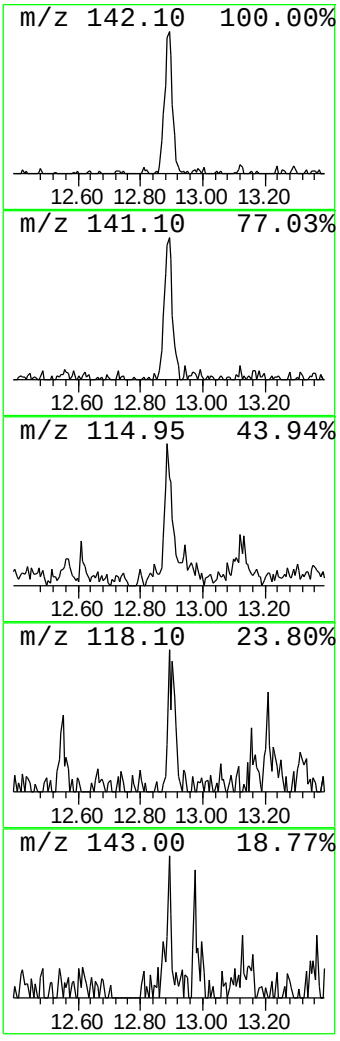
****

Peak Number 5 Naphthalene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.89	2.77 ng	94004	Naphthalene-d8	11.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	86
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	64
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	64
4	Naphthalene, 1-[(2-propenyloxy)m...	198	C14H14O	074685-39-5	64
5	3,4-Difluorobenzaldehyde	142	C7H4F2O	034036-07-2	53





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Data File : BG025502.D
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Operator : UM/SJ
Sample : I1135-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : W-41

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.M
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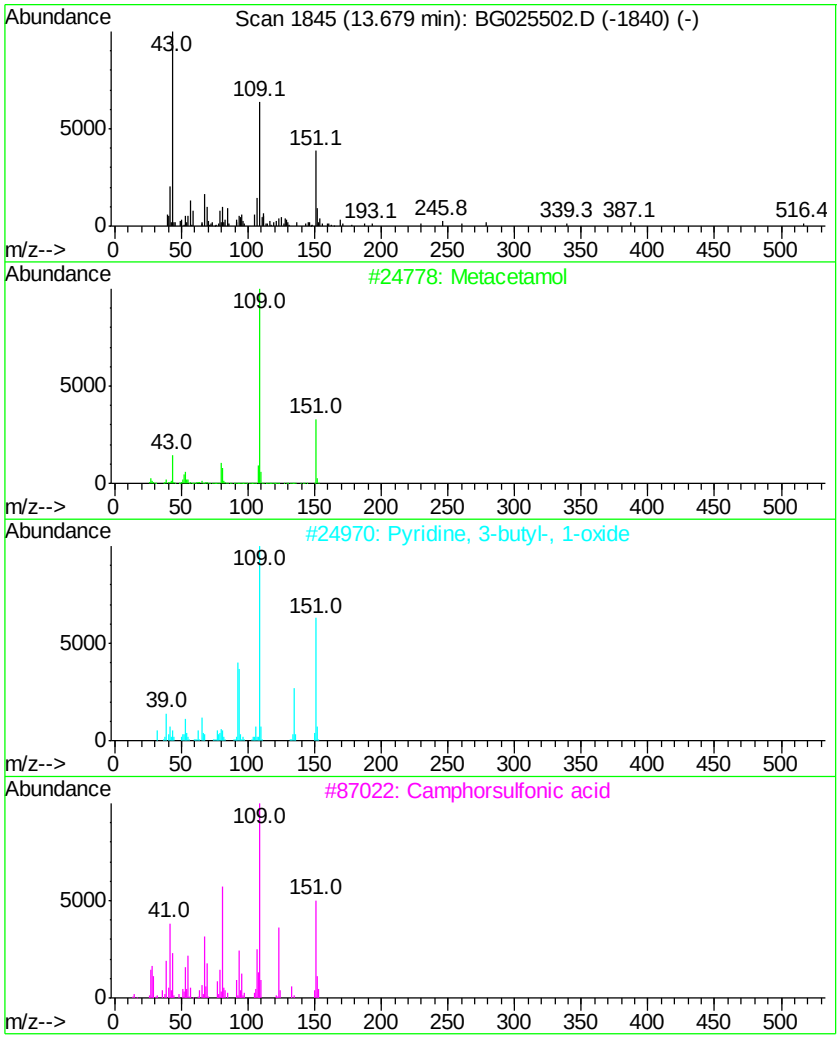
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

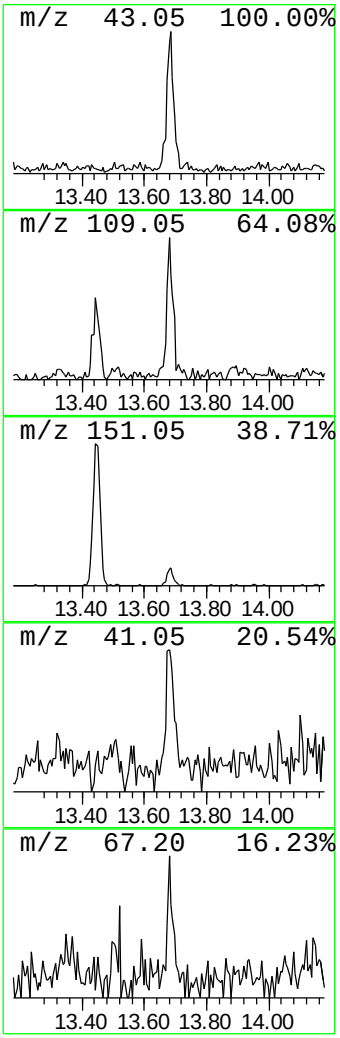
****

Peak Number 6 Metacetamol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	2.84 ng	131021	Acenaphthene-d10	14.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Metacetamol	151	C8H9NO2	000621-42-1	53
2	Pyridine, 3-butyl-, 1-oxide	151	C9H13NO	031396-33-5	53
3	Camphorsulfonic acid	232	C10H16O4S	003144-16-9	45
4	(+)-Camphor-10-sulfonyl chloride	250	C10H15ClO3S	021286-54-4	45
5	Bicyclo[2.2.1]heptane-1-methanes...	232	C10H16O4S	005872-08-2	45





Library Search Compound Report

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Instrument : BNA_G
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

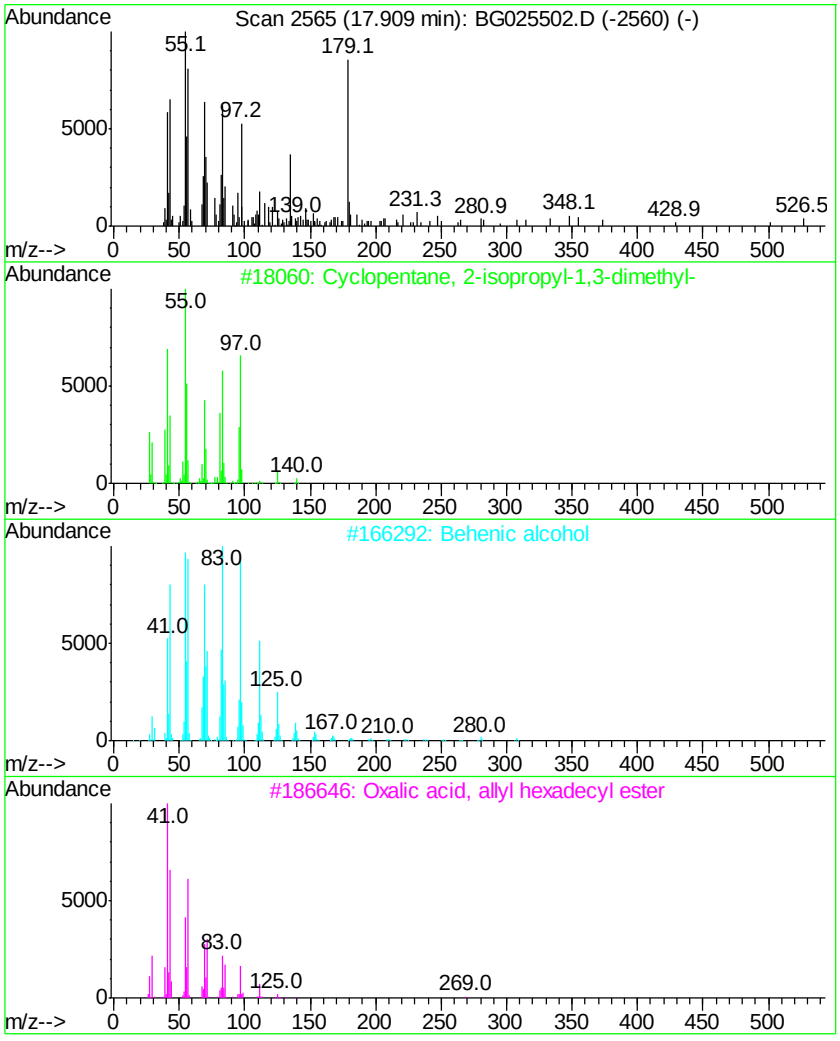
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

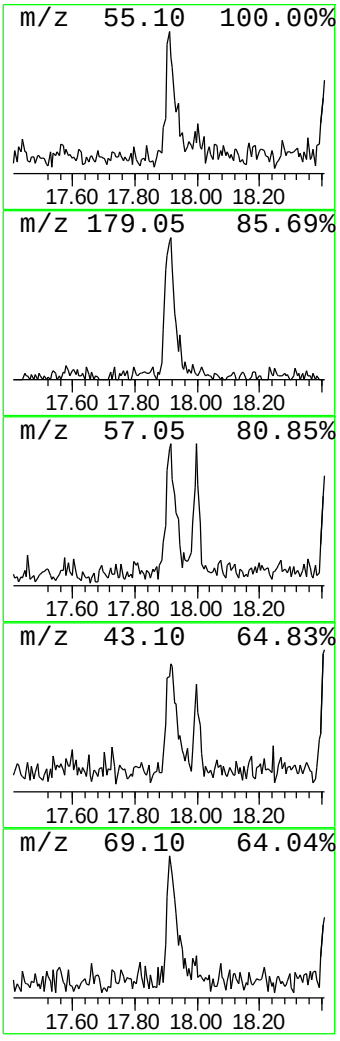
****

Peak Number 7 unknown17.91 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.91	3.72 ng	230386	Phenanthrene-d10	17.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 2-isopropyl-1,3-di...	140	C10H20	032281-85-9	46
2	Behenic alcohol	326	C22H46O	000661-19-8	46
3	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	38
4	Piperazine, 1-(4-ethylbenzenesul...	348	C18H21FN2O2S	1000304-15-2	38
5	1-Hexacosanol	382	C26H54O	000506-52-5	35





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ClientSampleId : W-41

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

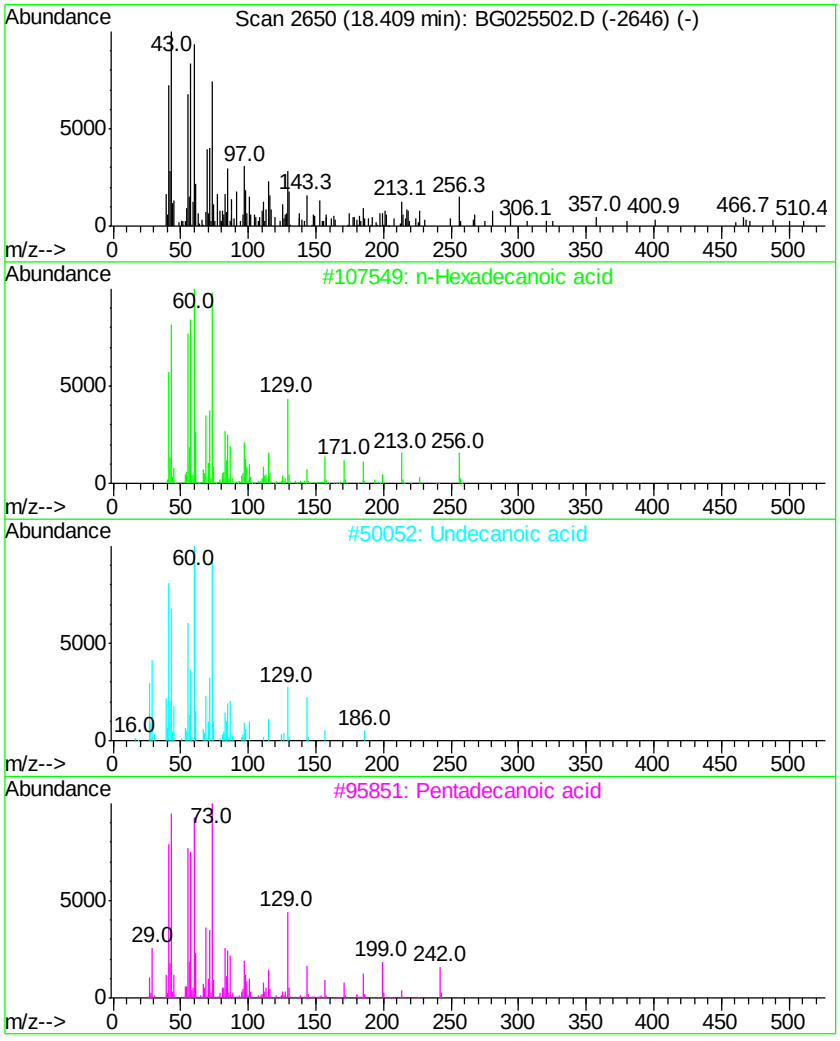
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

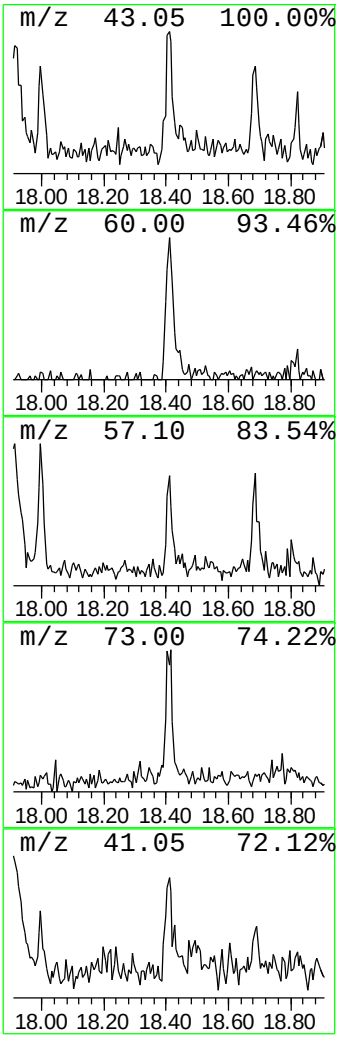
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.41	2.08 ng	129071	Phenanthrene-d10	17.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Undecanoic acid	186	C11H22O2	000112-37-8	70
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59





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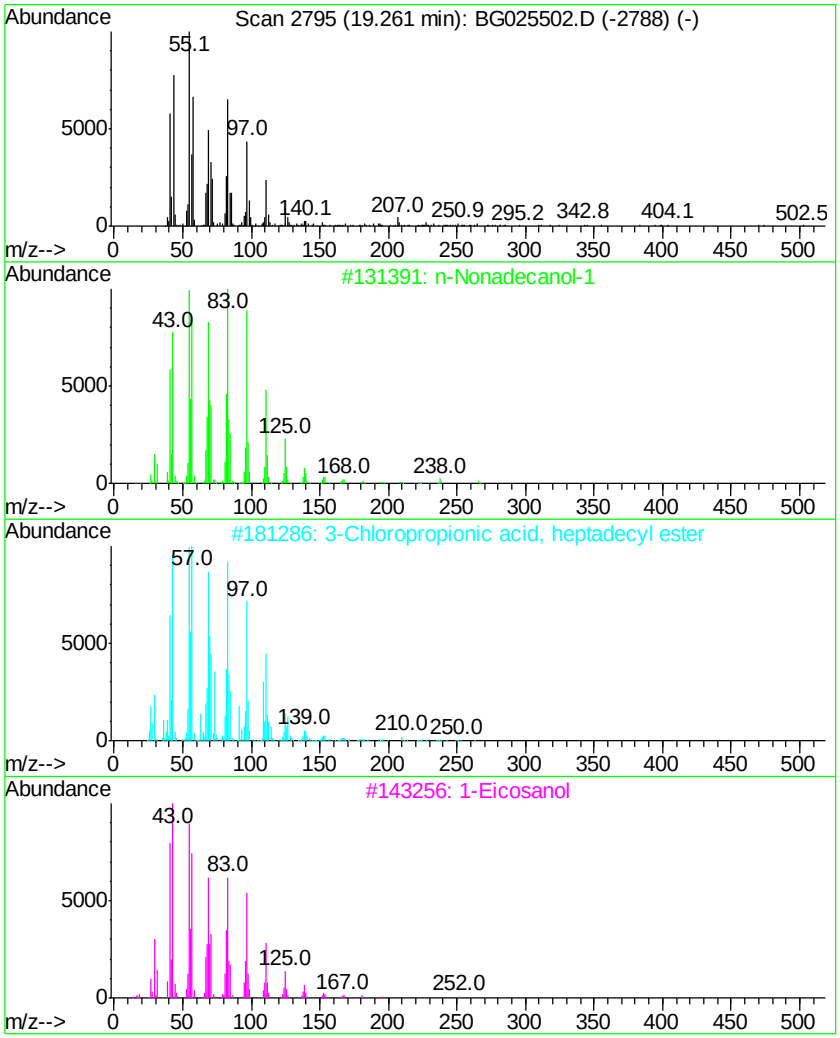
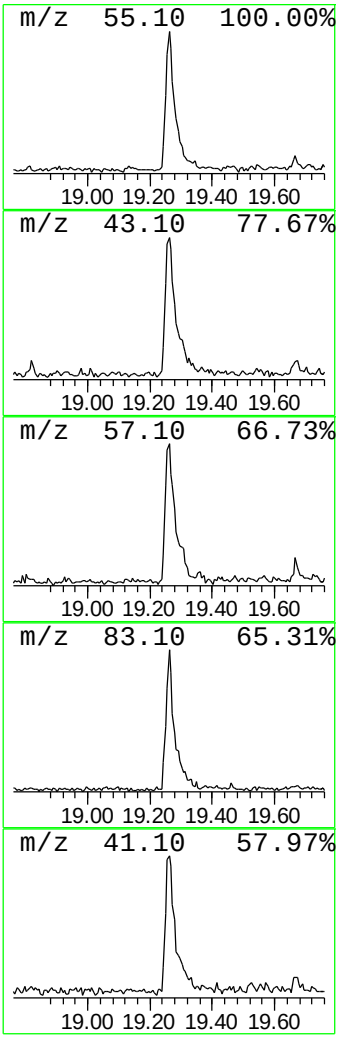
****

Peak Number 9 n-Nonadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.26	13.81 ng	854861	Phenanthrene-d10	17.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
2	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
3	1-Eicosanol	298	C20H42O	000629-96-9	91
4	1-Octadecanol	270	C18H38O	000112-92-5	91
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	91





Tentatively Identified Compound (LSC) summary

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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...	5.26	16.6	ng	369214	1	8.20	444633	20.0
unknown7.73	7.73	106.3	ng	2364180	1	8.20	444633	20.0
1-Phenyl-1-butene	10.40	2.9	ng	99167	2	11.03	679322	20.0
Naphthalene, 1-me...	12.89	2.8	ng	94004	2	11.03	679322	20.0
Metacetamol	13.68	2.8	ng	131021	3	14.82	921946	20.0
unknown17.91	17.91	3.7	ng	230386	4	17.57	1238390	20.0
n-Hexadecanoic acid	18.41	2.1	ng	129071	4	17.57	1238390	20.0
n-Nonadecanol-1	19.26	13.8	ng	854861	4	17.57	1238390	20.0