LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101015\
Data File : BG019145.D
Acq On : 11 Oct 2015 8:34
Operator : UM/NP
Sample : G3971-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CS-7

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-BG101015.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	2.996	22	27	47	rVB	1072854	1397156	95.71%	16.087%
2	3.143	47	52	60	rBV	21323	32862	2.25%	0.378%
3	3.214	60	64	70	rBV	48938	60642	4.15%	0.698%
4	4.536	283	289	300	rBV	161210	231604	15.87%	2.667%
5	5.147	385	393	402	rBV	948499	1459835	100.00%	16.809%
6	7.191	733	741	750	rBV	59014	103227	7.07%	1.189%
7	8.032	877	884	890	rBV	69988	113349	7.76%	1.305%
8	8.355	932	939	947	rVB	174415	294891	20.20%	3.395%
9	9.189	1074	1081	1089	rBV	159558	276510	18.94%	3.184%
10	10.834	1354	1361	1369	rVB	101699	179007	12.26%	2.061%
11	13.284	1770	1778	1785	rBV	475804	731104	50.08%	8.418%
12	13.555	1816	1824	1831	rBV2	9752	15589	1.07%	0.179%
13	14.107	1910	1918	1926	rBV	58422	82248	5.63%	0.947%
14	14.659	2005	2012	2024	rVB2	182143	289171	19.81%	3.330%
15	16.363	2298	2302	2310	rVB	25323	38319	2.62%	0.441%
16	17.162	2433	2438	2442	rBV	12343	15861	1.09%	0.183%
17	17.403	2473	2479	2486	rBV	250214	371413	25.44%	4.277%
18	17.573	2499	2508	2516	rBV5	11197	23441	1.61%	0.270%
19	17.685	2521	2527	2536	rVB	355421	481212	32.96%	5.541%
20	17.779	2536	2543	2547	rBV2	23425	32015	2.19%	0.369%
21	18.496	2658	2665	2671	rVB3	91455	192820	13.21%	2.220%
22	18.590	2676	2681	2690	rBV7	8742	19269	1.32%	0.222%
23	19.148	2772	2776	2781	rBV5	16890	27319	1.87%	0.315%
24	19.965	2913	2915	2918	rBV3	15851	21439	1.47%	0.247%
25	20.018	2919	2924	2930	rVB	911445	1177594	80.67%	13.559%
26	21.674	3201	3206	3212	rBV	270284	458964	31.44%	5.285%
27	23.167	3456	3460	3470	rVB	93115	170794	11.70%	1.967%
28	24.912	3751	3757	3767	rVB	148426	387132	26.52%	4.458%

Sum of corrected areas: 8684787

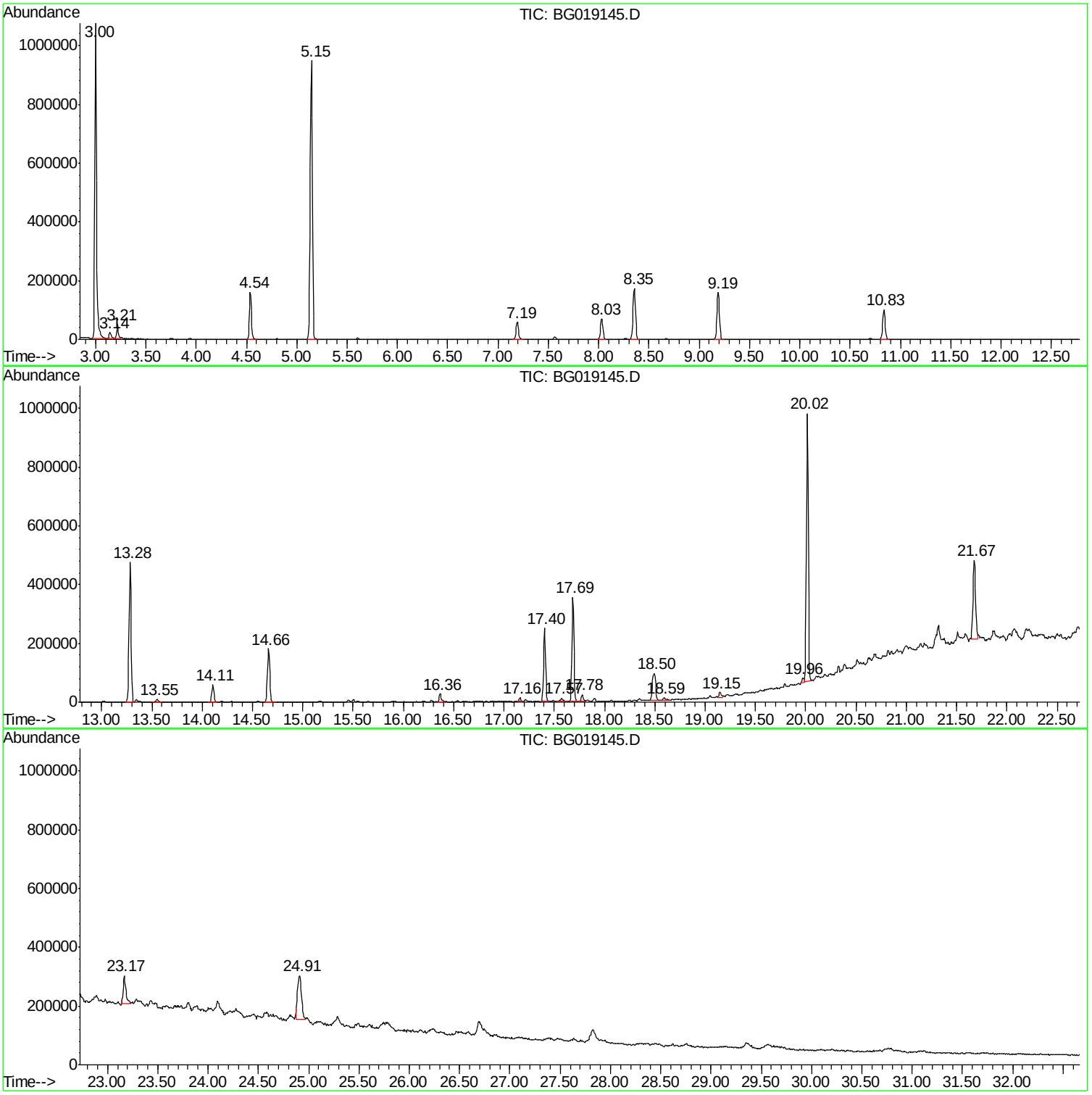
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101015\
Data File : BG019145.D
Acq On : 11 Oct 2015 8:34
Operator : UM/NP
Sample : G3971-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CS-7

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101015\
Data File : BG019145.D
Acq On : 11 Oct 2015 8:34
Operator : UM/NP
Sample : G3971-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CS-7

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

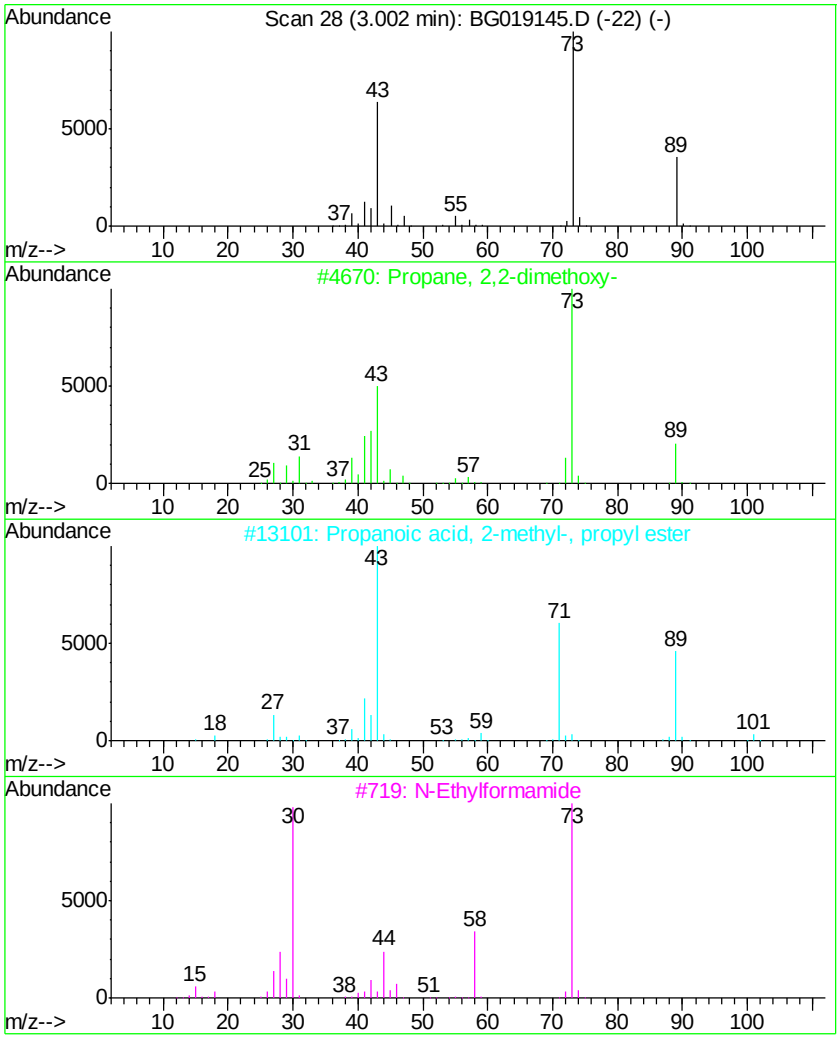
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

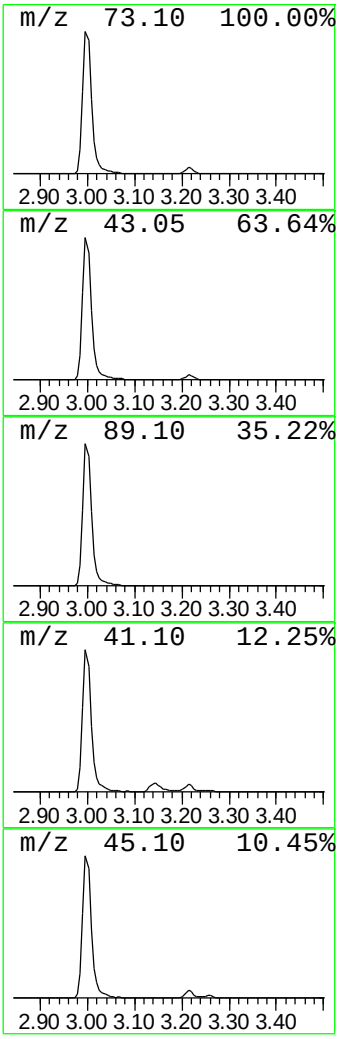
****

Peak Number 1 unknown3.00 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.00	246.52 ng	1397160	1,4-Dichlorobenzene-d4	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	39
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	12
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101015\
Data File : BG019145.D
Acq On : 11 Oct 2015 8:34
Operator : UM/NP
Sample : G3971-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CS-7

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101015.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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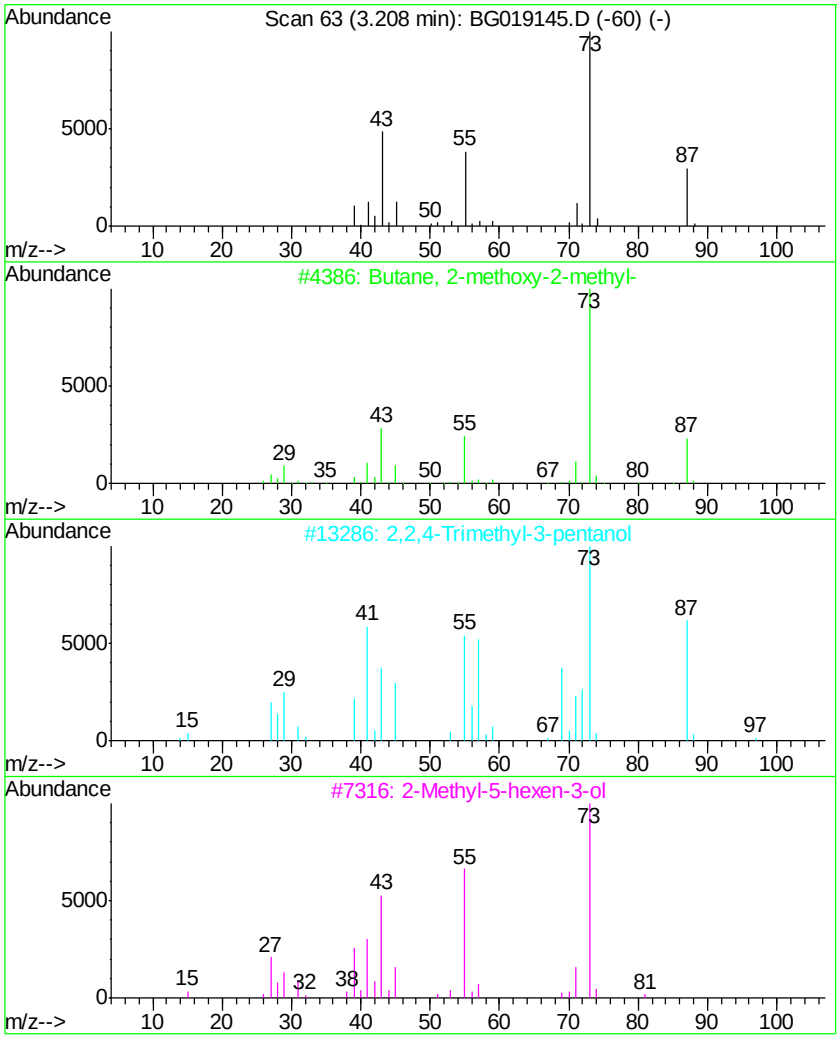
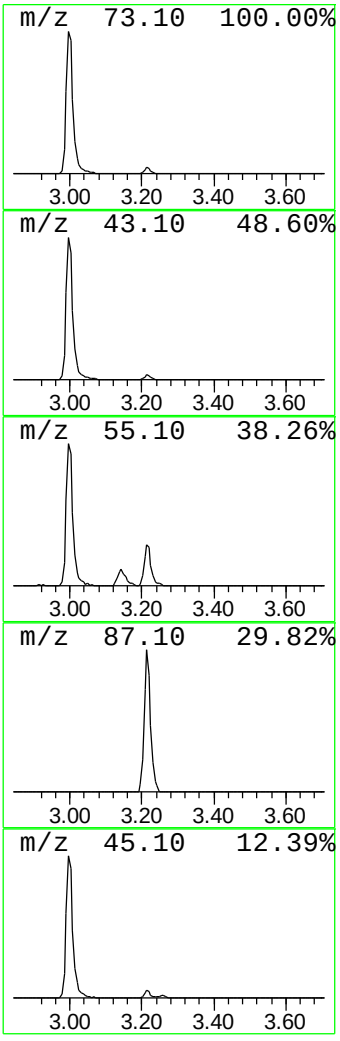
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.21	10.70 ng	60642	1,4-Dichlorobenzene-d4	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	28
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101015\
Data File : BG019145.D
Acq On : 11 Oct 2015 8:34
Operator : UM/NP
Sample : G3971-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CS-7

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

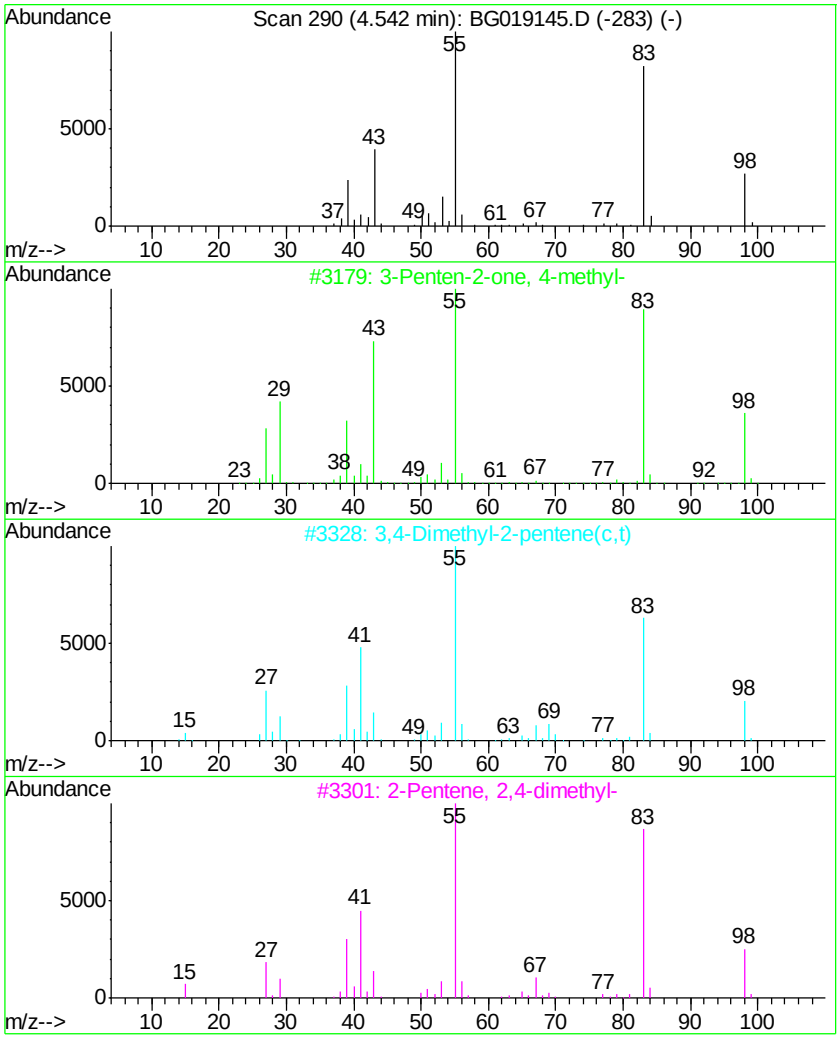
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

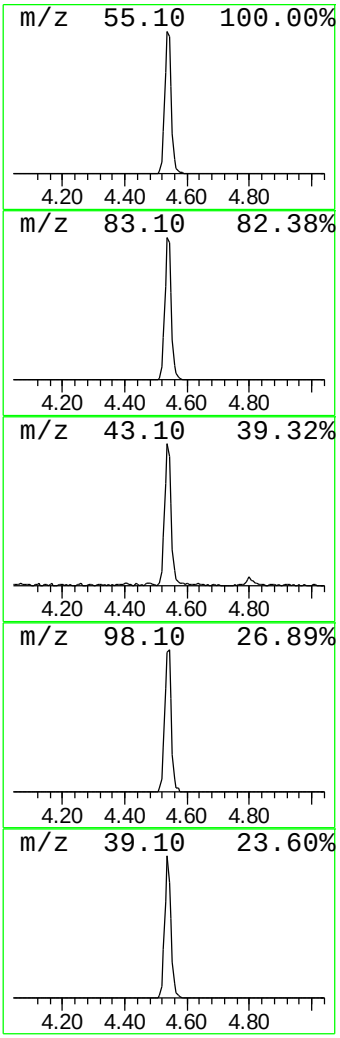
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.54	40.87 ng	231604	1,4-Dichlorobenzene-d4	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	3-Hexen-2-one	98	C6H10O	000763-93-9	80





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101015\
Data File : BG019145.D
Acq On : 11 Oct 2015 8:34
Operator : UM/NP
Sample : G3971-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CS-7

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

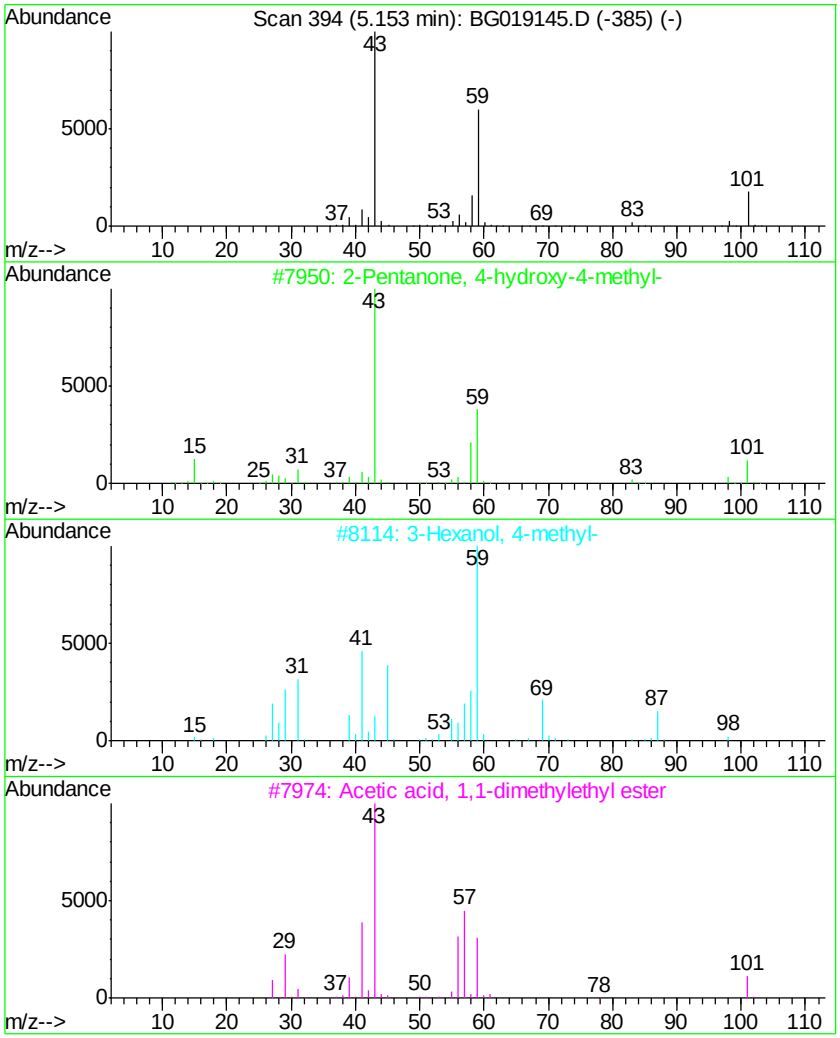
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

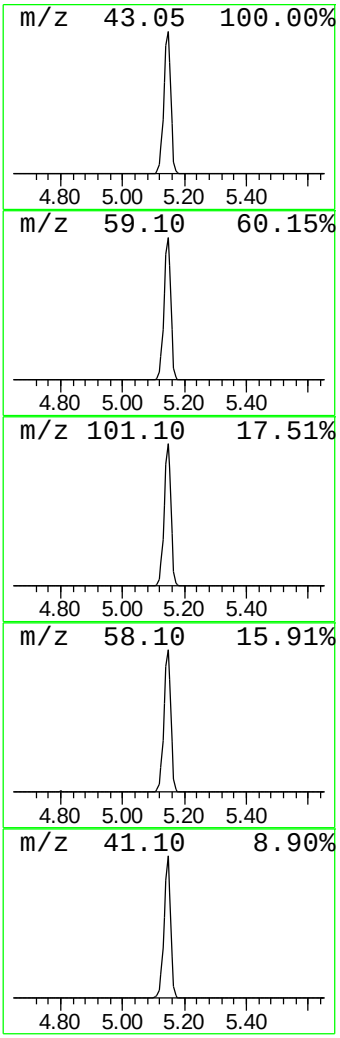
****

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	257.58 ng	1459840	1,4-Dichlorobenzene-d4	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101015\
Data File : BG019145.D
Acq On : 11 Oct 2015 8:34
Operator : UM/NP
Sample : G3971-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CS-7

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

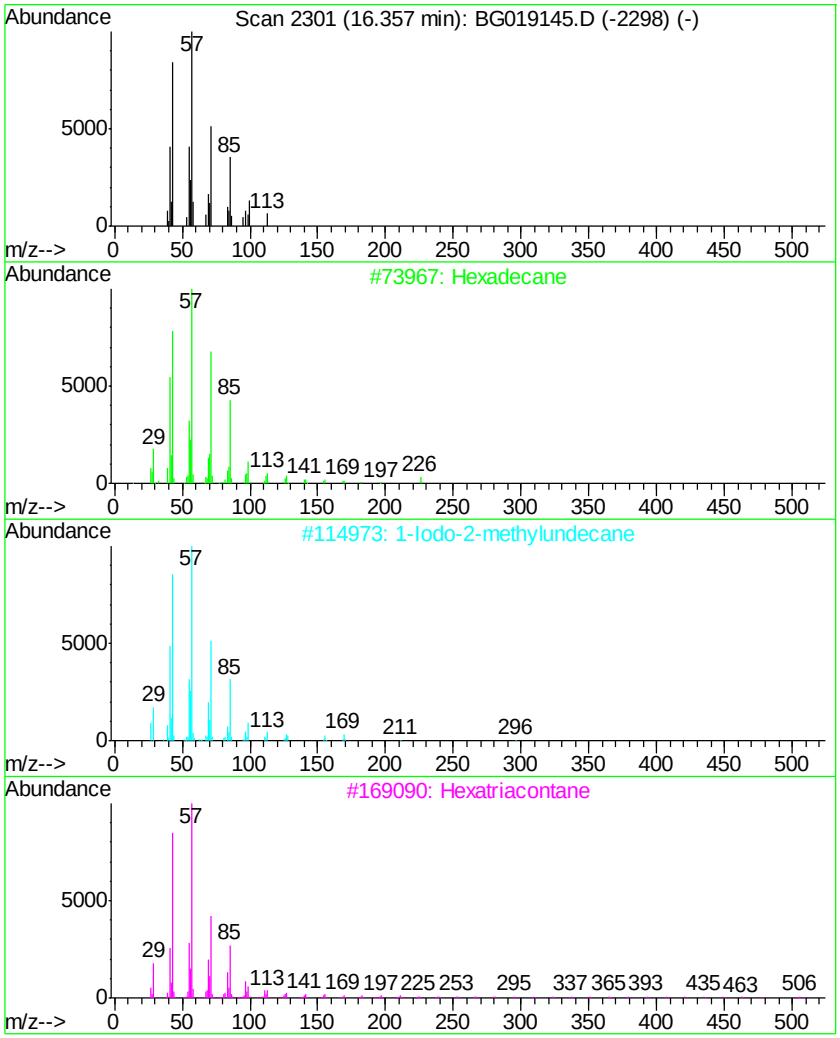
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

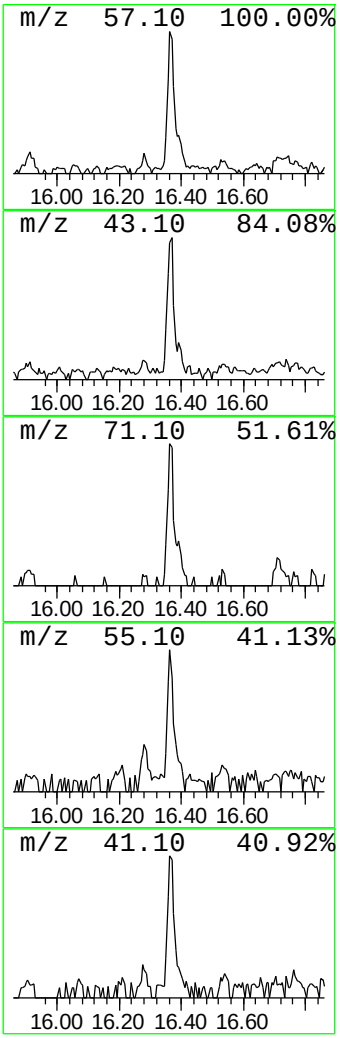
****

Peak Number 7 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.36	2.06 ng	38319	Phenanthrene-d10	17.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	86
3	Hexatriacontane	507	C36H74	000630-06-8	72
4	Dotriacontane	451	C32H66	000544-85-4	72
5	Eicosane	282	C20H42	000112-95-8	72





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101015\
Data File : BG019145.D
Acq On : 11 Oct 2015 8:34
Operator : UM/NP
Sample : G3971-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CS-7

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

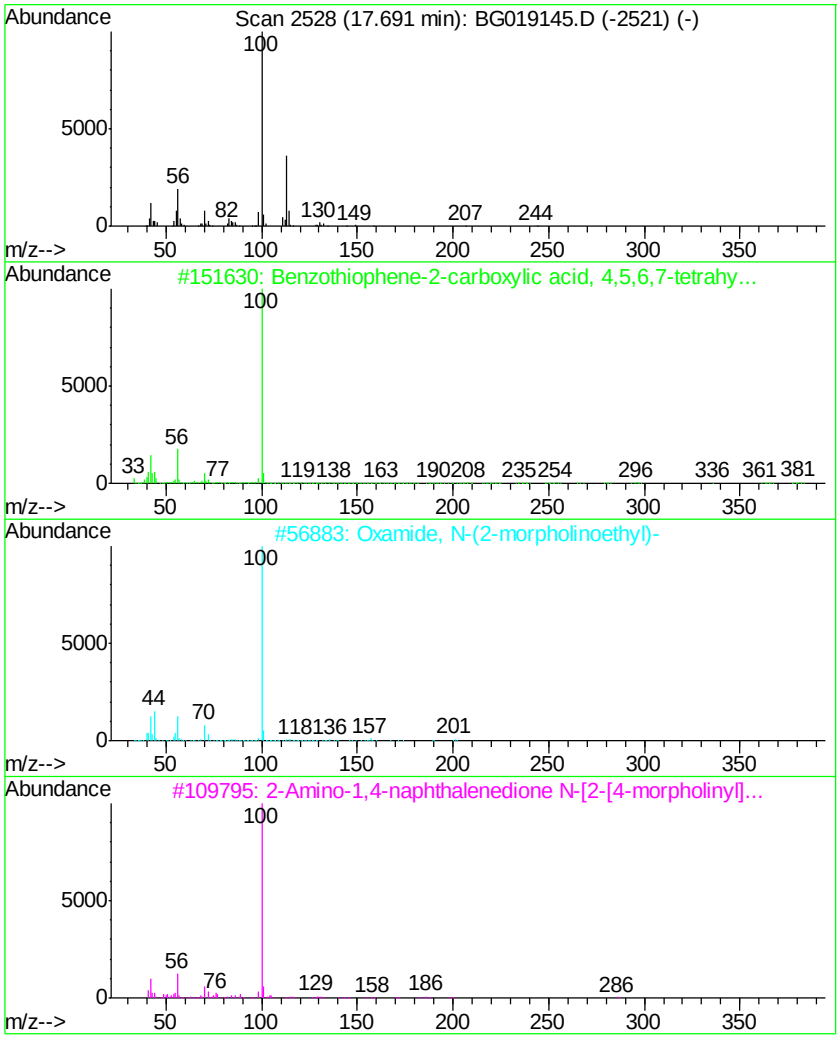
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

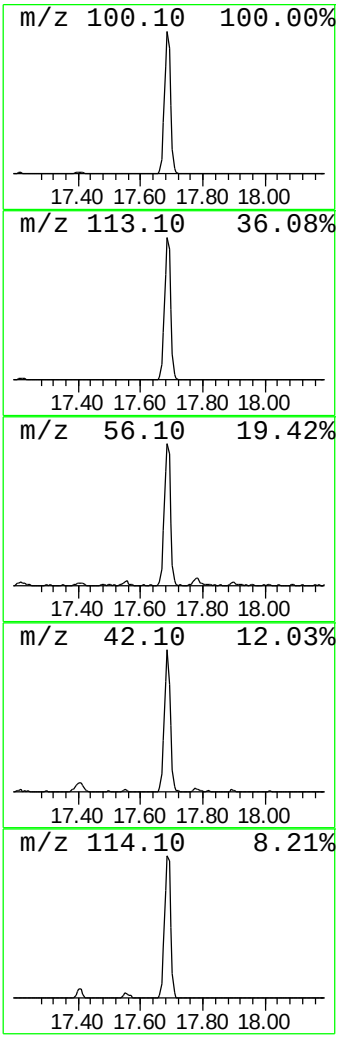
****

Peak Number 8 Benzothiophene-2-carboxylic... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.69	25.91 ng	481212	Phenanthrene-d10	17.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiophene-2-carboxylic acid...	381	C17H23N3O5S	1000260-55-7	59
2	Oxamide, N-(2-morpholinoethyl)-	201	C8H15N3O3	1000277-15-3	59
3	2-Amino-1,4-naphthalenedione N-[...	286	C16H18N2O3	038528-37-9	59
4	Benzothiazol-2(3H)-one, 3-(4-mor...	250	C12H14N2O2S	077708-55-5	59
5	1,4-Bis(morpholinoacetyl)piperazine	340	C16H28N4O4	022764-36-9	59





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Sample : G3971-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CS-7

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

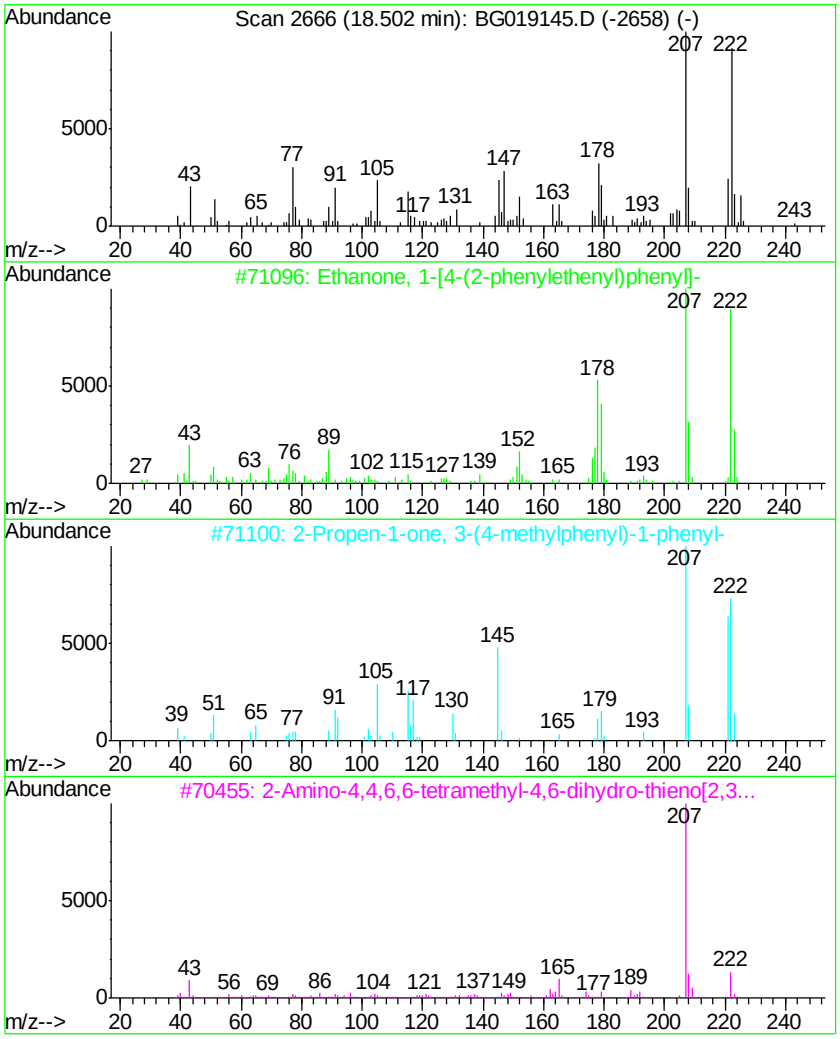
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

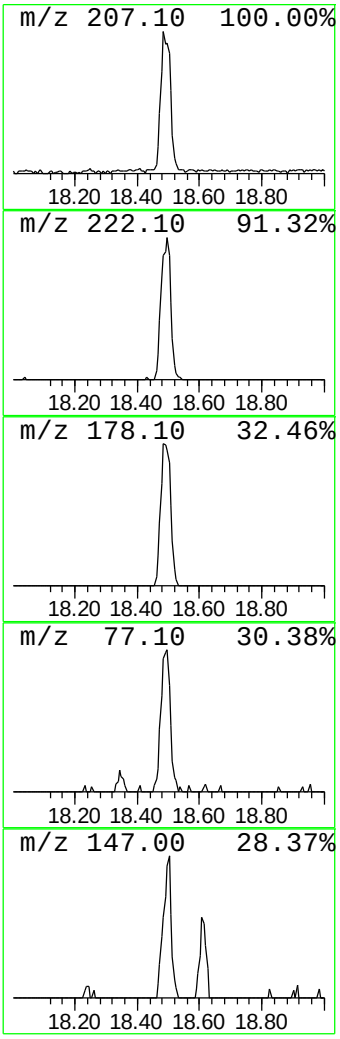
****

Peak Number 9 Ethanone, 1-[4-(2-phenyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.50	10.38 ng	192820	Phenanthrene-d10	17.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-[4-(2-phenylethenyl)...	222	C16H14O	003112-03-6	58
2	2-Propen-1-one, 3-(4-methylpheny...	222	C16H14O	004224-87-7	58
3	2-Amino-4,4,6,6-tetramethyl-4,6-...	222	C11H14N2OS	1000275-36-2	49
4	1,4-Benzenediol, 2,5-bis(1,1-dim...	222	C14H22O2	000088-58-4	47
5	4-Phenyl-3,4-dihydroisoquinoline	207	C15H13N	006187-58-2	27





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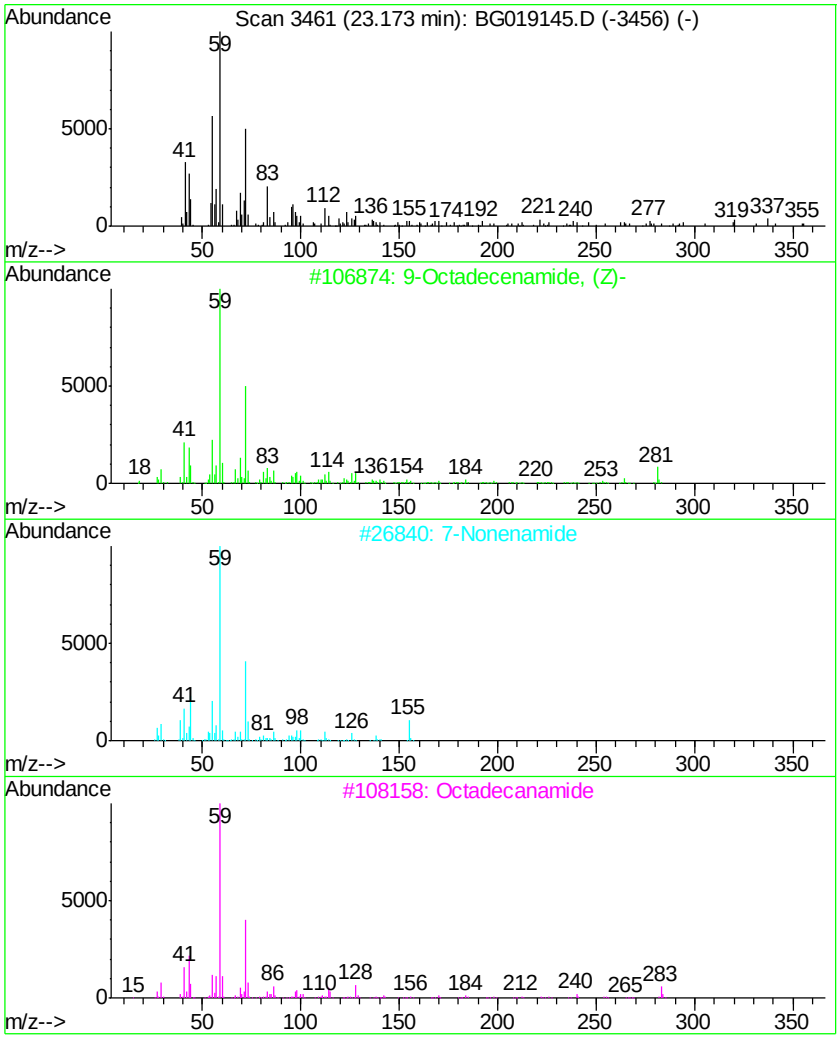
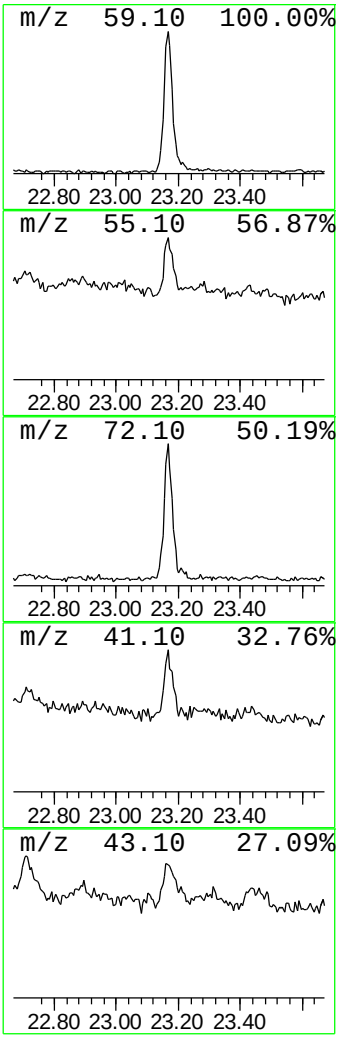
****

Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.17	7.44 ng	170794	Chrysene-d12	21.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	74
2	7-Nonenamide	155	C9H17NO	090949-53-4	70
3	Octadecanamide	283	C18H37NO	000124-26-5	64
4	Tetradecanamide	227	C14H29NO	000638-58-4	64
5	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101015\
Data File : BG019145.D
Acq On : 11 Oct 2015 8:34
Operator : UM/NP
Sample : G3971-01
Misc :
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Instrument : BNA_G
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101015.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
unknown3.00	3.00	246.5	ng	1397160	1	8.03	113349	20.0
Butane, 2-methoxy...	3.21	10.7	ng	60642	1	8.03	113349	20.0
3-Penten-2-one, 4...	4.54	40.9	ng	231604	1	8.03	113349	20.0
2-Pentanone, 4-hy...	5.15	257.6	ng	1459840	1	8.03	113349	20.0
Hexadecane	16.36	2.1	ng	38319	4	17.40	371413	20.0
Benzothiophene-2-...	17.69	25.9	ng	481212	4	17.40	371413	20.0
Ethanone, 1-[4-(2...	18.50	10.4	ng	192820	4	17.40	371413	20.0
9-Octadecenamide,...	23.17	7.4	ng	170794	5	21.67	458964	20.0