LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG050515\
Data File : BG016886.D
Acq On : 6 May 2015 4:57
Operator : TP/IZ
Sample : G2114-09
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GRID-3(12-23)

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-BG050515.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	2.788	13	17	36	rBV	5958686	8141998	100.00%	24.502%
2	2.923	36	40	49	rVB	161503	304650	3.74%	0.917%
3	3.005	50	54	59	rVB	170926	209523	2.57%	0.631%
4	4.921	375	380	387	rBV	137332	199227	2.45%	0.600%
5	5.385	453	459	470	rVB	1241862	1802293	22.14%	5.424%
6	6.966	720	728	738	rVB	1349806	2085281	25.61%	6.275%
7	7.336	783	791	799	rBV	1231262	1939721	23.82%	5.837%
8	7.806	863	871	877	rBV	312471	502290	6.17%	1.512%
9	8.123	918	925	934	rVB	814791	1299977	15.97%	3.912%
10	8.957	1059	1067	1075	rBV	765285	1229331	15.10%	3.699%
11	10.597	1339	1346	1353	rVB	432455	734848	9.03%	2.211%
12	12.800	1715	1721	1726	rVB2	100024	145486	1.79%	0.438%
13	13.064	1757	1766	1772	rBV	1701156	2589983	31.81%	7.794%
14	13.899	1903	1908	1914	rVB2	80196	111616	1.37%	0.336%
15	14.439	1990	2000	2007	rBV2	658285	1004167	12.33%	3.022%
16	15.802	2226	2232	2238	rVB	200133	270730	3.33%	0.815%
17	15.926	2245	2253	2261	rBV	1530293	2117030	26.00%	6.371%
18	17.183	2460	2467	2472	rBV	928195	1270079	15.60%	3.822%
19	18.082	2612	2620	2631	rBV2	145046	280390	3.44%	0.844%
20	19.239	2811	2817	2824	rBV2	38749	83554	1.03%	0.251%
21	19.615	2876	2881	2888	rVB5	40255	101355	1.24%	0.305%
22	19.815	2908	2915	2921	rBV	2844232	3456719	42.46%	10.402%
23	21.078	3126	3130	3138	rBV	384722	484478	5.95%	1.458%
24	21.360	3172	3178	3188	rBV	1147629	1436866	17.65%	4.324%
25	22.442	3357	3362	3367	rBV5	59122	104847	1.29%	0.316%
26	23.669	3563	3571	3581	rVB	681241	1324012	16.26%	3.984%

Sum of corrected areas: 33230451

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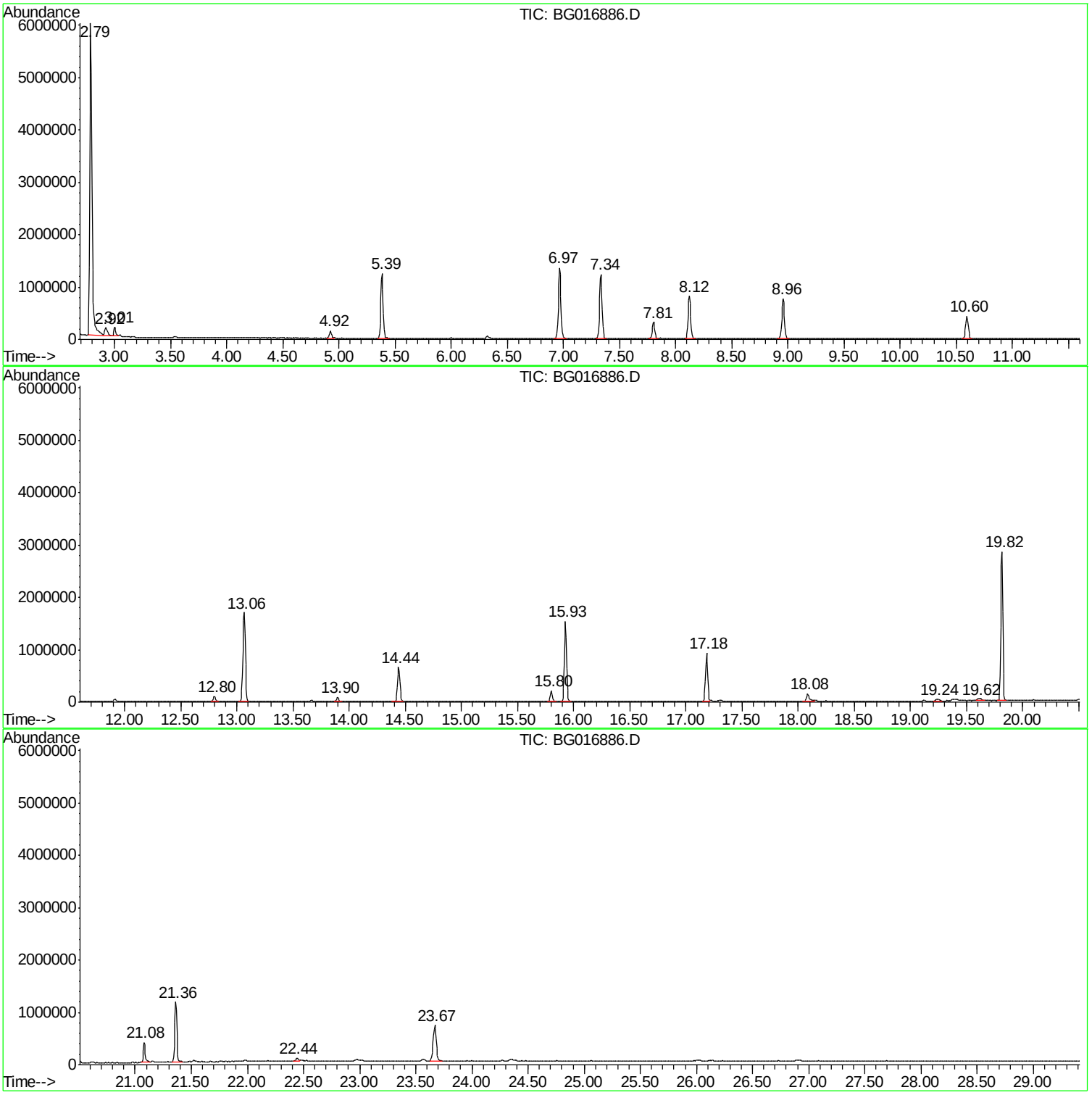
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GRID-3(12-23)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.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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Data File : BG016886.D
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ClientSampleId : GRID-3(12-23)

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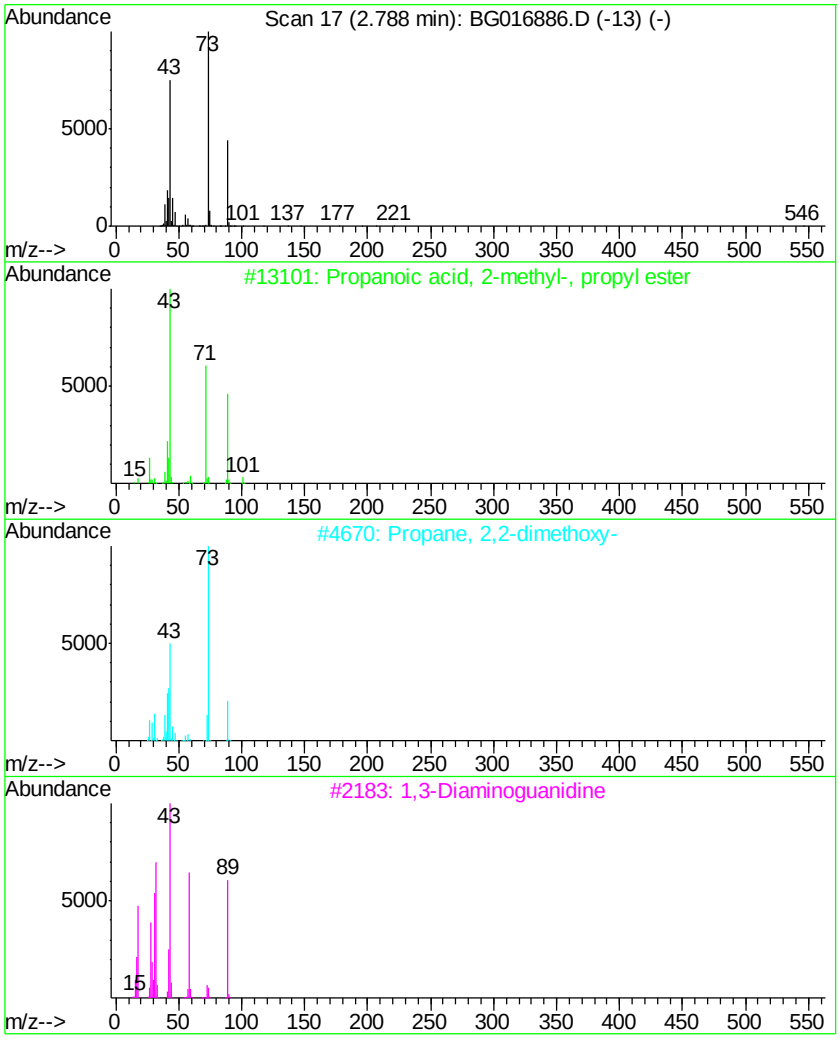
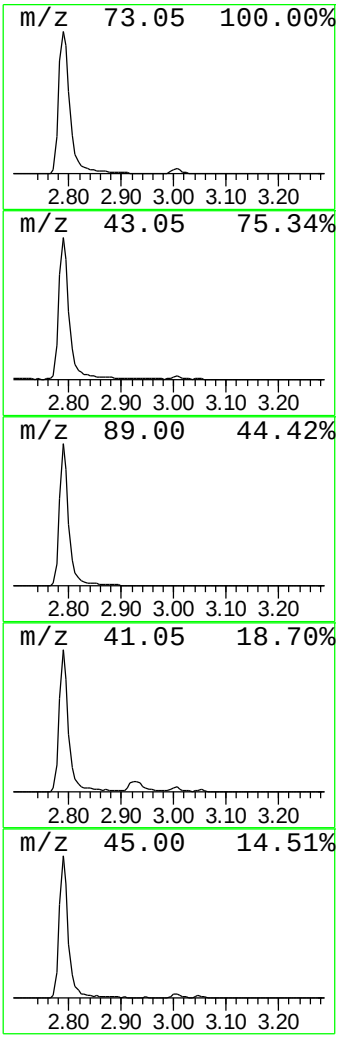
****

Peak Number 1 unknown2.79 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.79	324.20 ng	8142000	1,4-Dichlorobenzene-d4	7.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	47
2	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	42
3	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	40
4	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	12





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Sample : G2114-09
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GRID-3(12-23)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

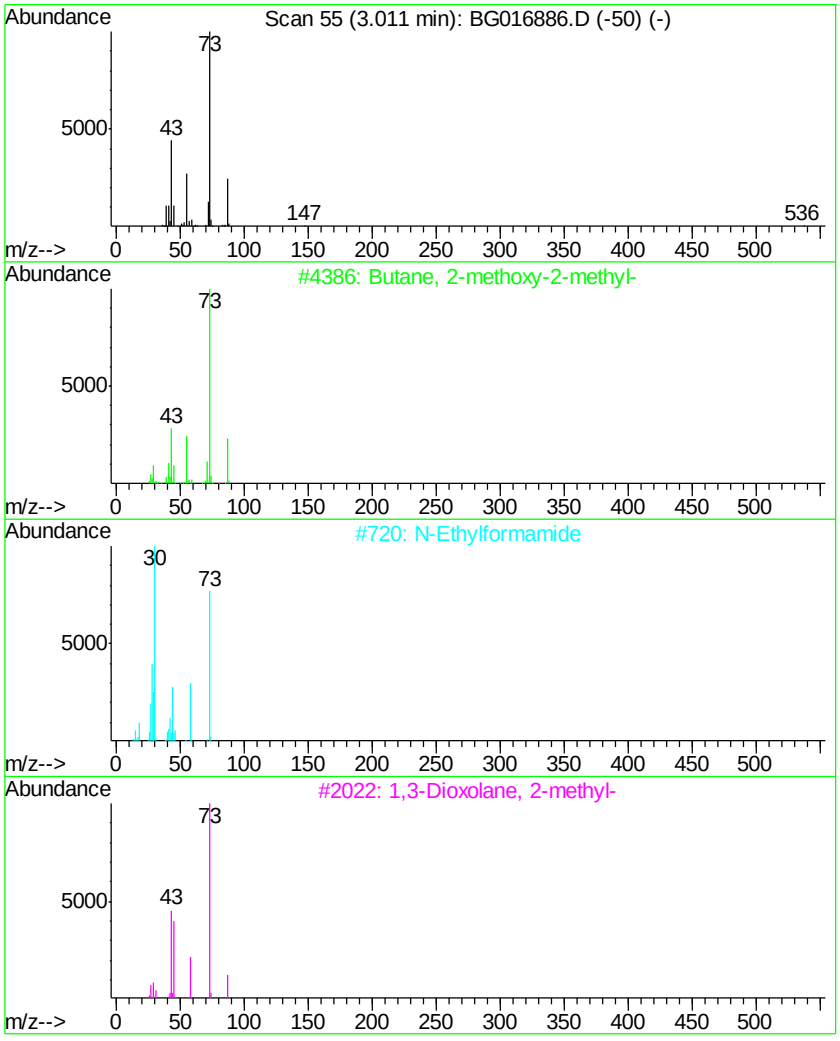
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

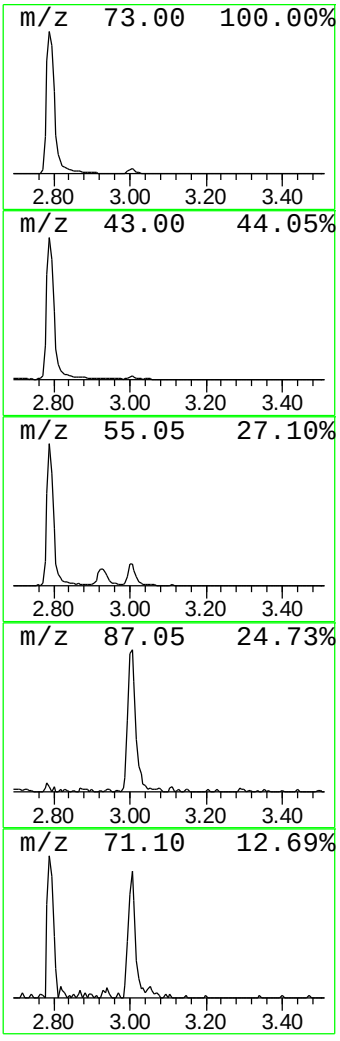
****

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.01	8.34 ng	209523	1,4-Dichlorobenzene-d4	7.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9





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Sample : G2114-09
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GRID-3(12-23)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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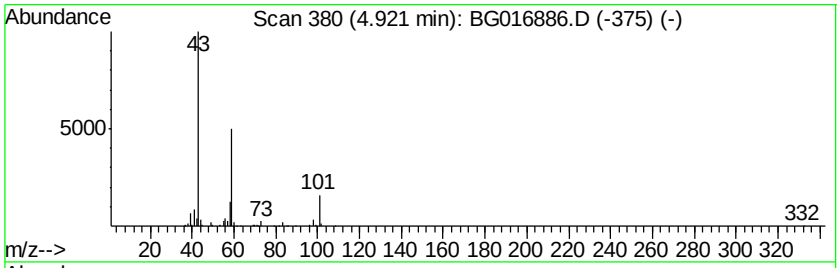
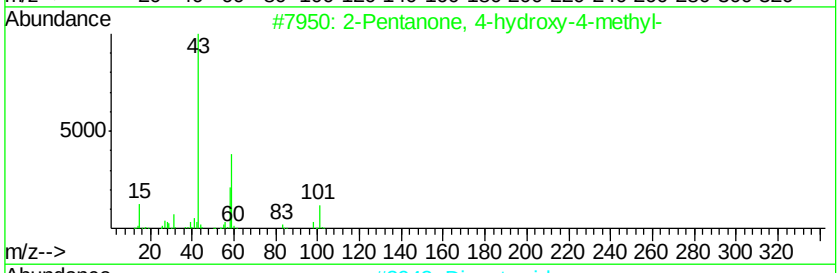
****

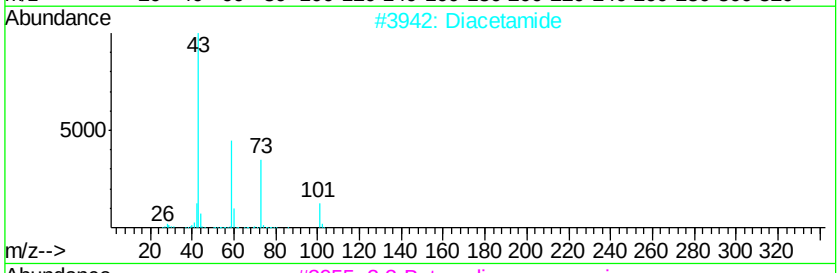
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

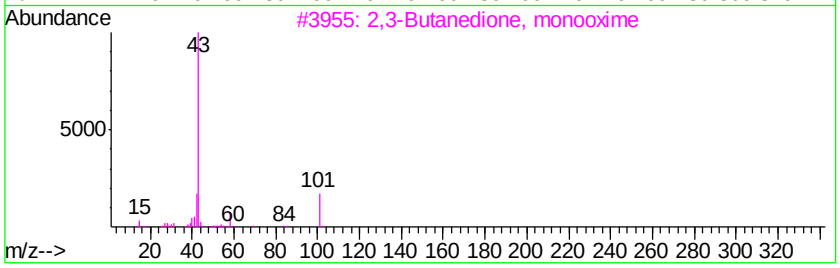
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	7.93 ng	199227	1,4-Dichlorobenzene-d4	7.81

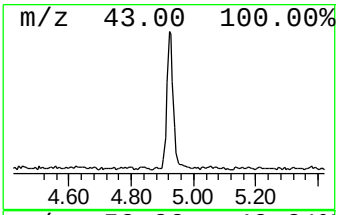
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Diacetamide	101	C4H7NO2	000625-77-4	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9

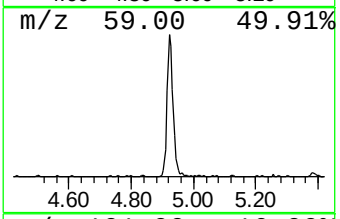


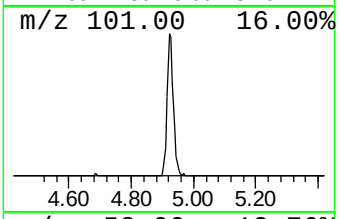


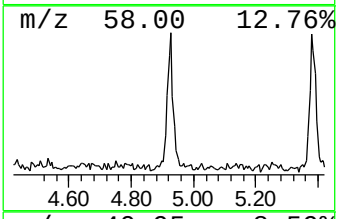


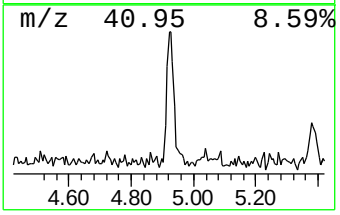












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Instrument : BNA_G
ClientSampleId : GRID-3(12-23)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

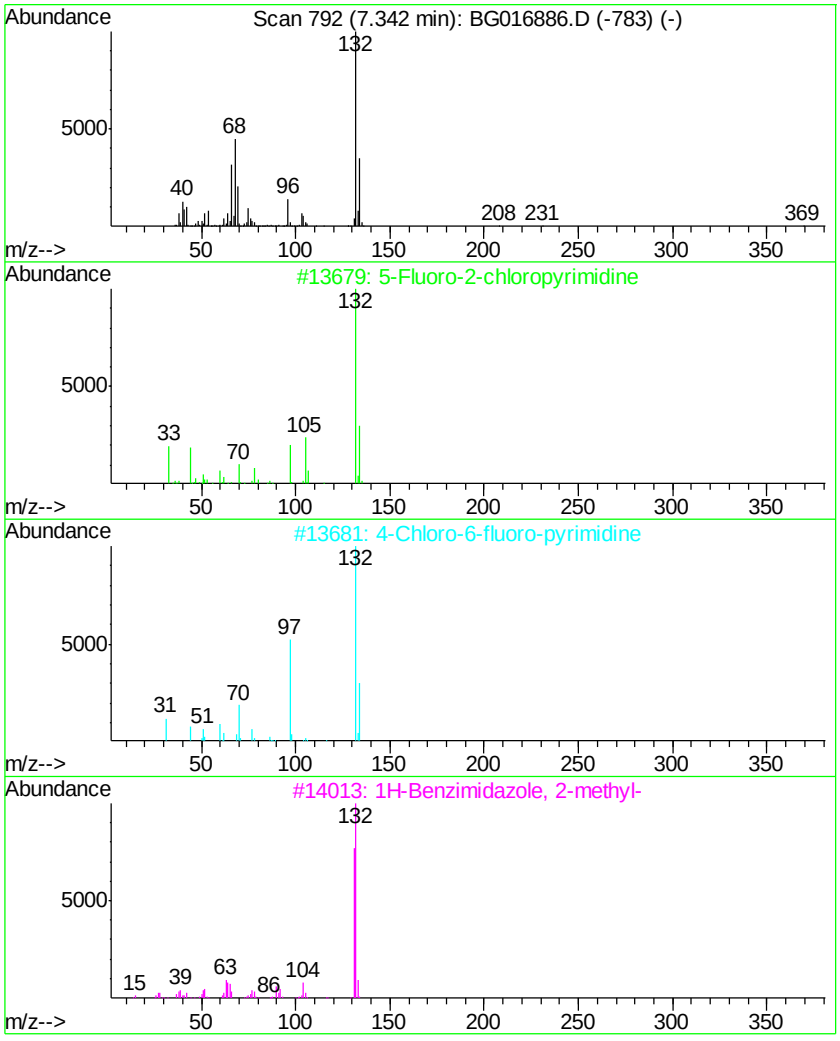
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

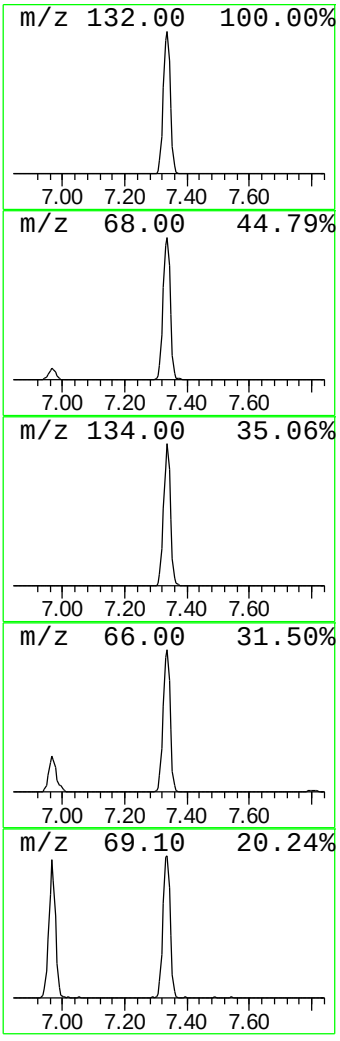
****

Peak Number 5 unknown7.34 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.34	77.24 ng	1939720	1,4-Dichlorobenzene-d4	7.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	Xenon	132	Xe	007440-63-3	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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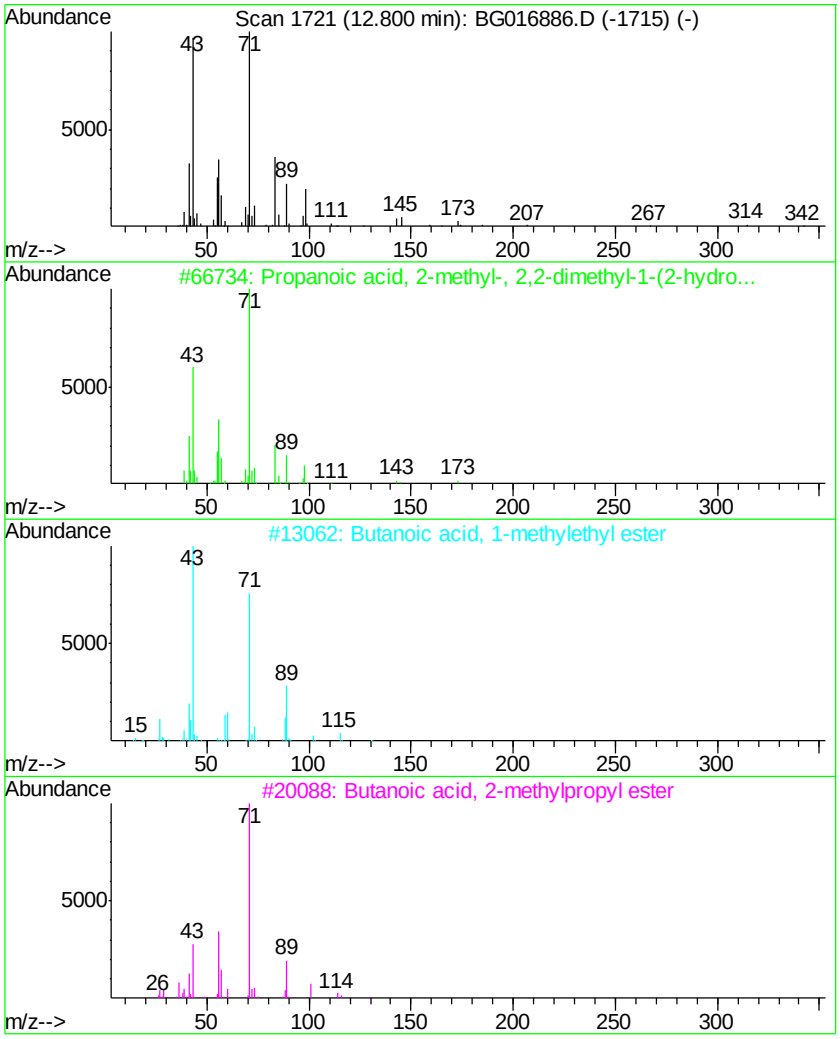
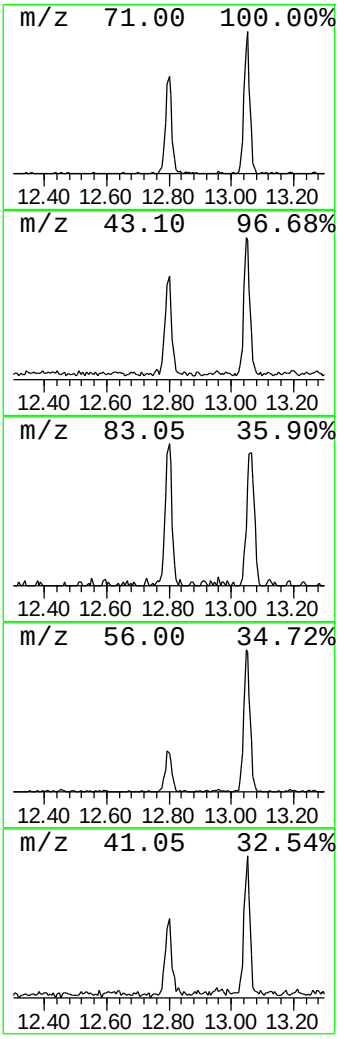
****

Peak Number 7 Propanoic acid, 2-methyl-, ... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	2.90 ng	145486	Acenaphthene-d10	14.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 2,2-d...	216	C12H24O3	074367-33-2	78
2	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	43
3	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	42
4	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	40
5	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	38





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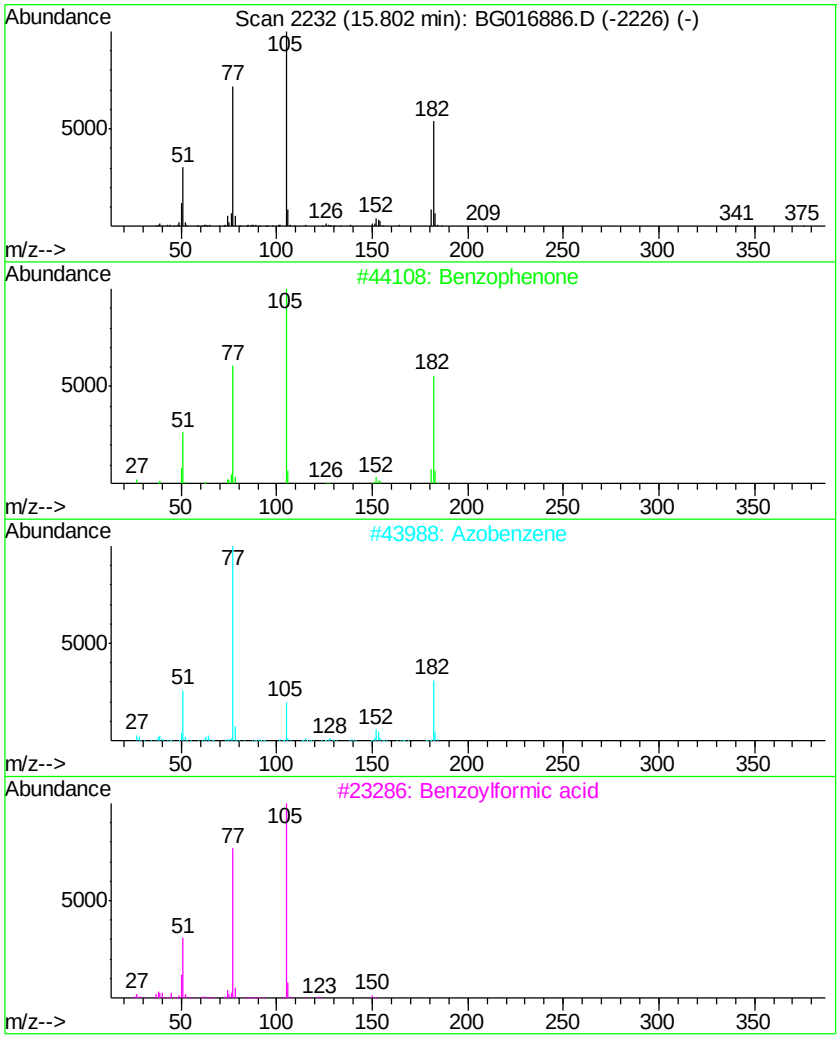
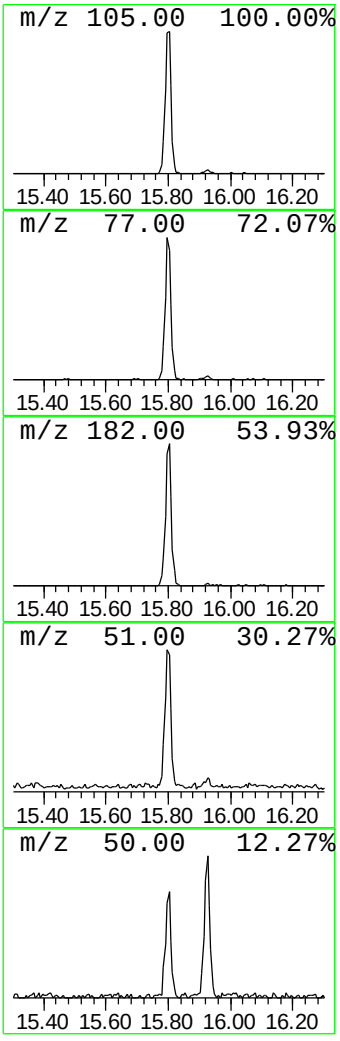
****

Peak Number 8 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.80	5.39 ng	270730	Acenaphthene-d10	14.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	74
3	Benzoylformic acid	150	C8H6O3	000611-73-4	55
4	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
5	2-Pyrazoline-5-carbonitrile, 2-b...	199	C11H9N3O	067872-68-8	47





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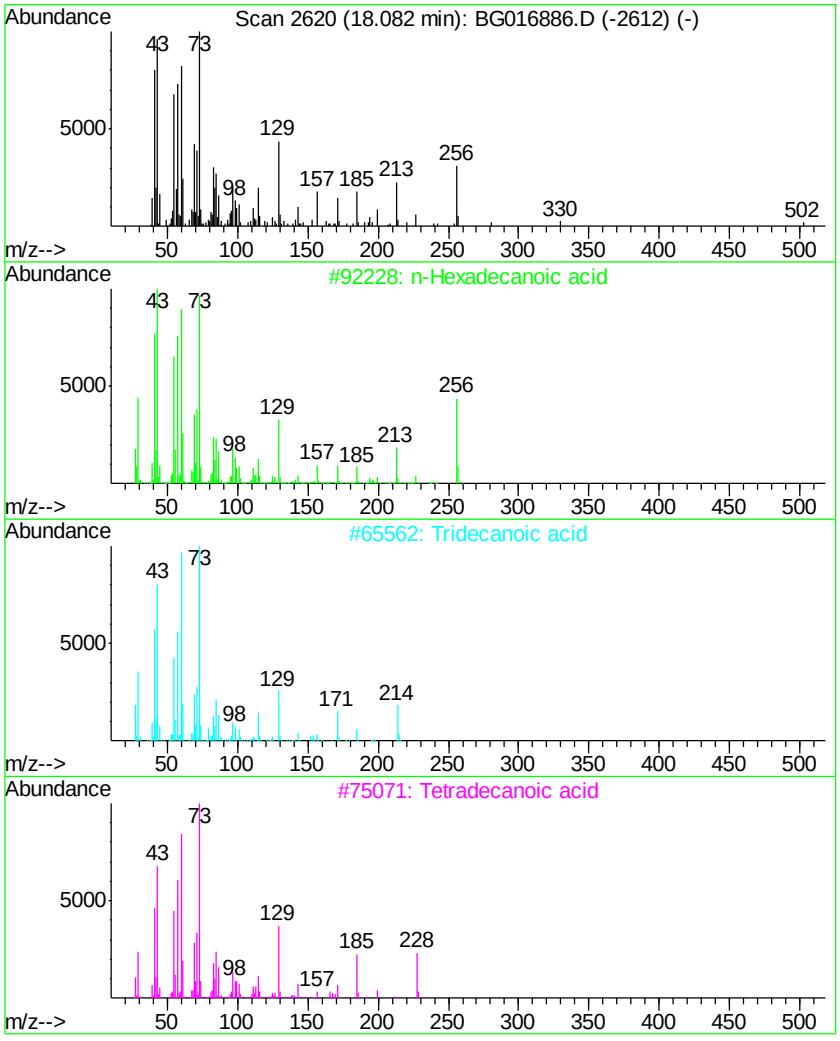
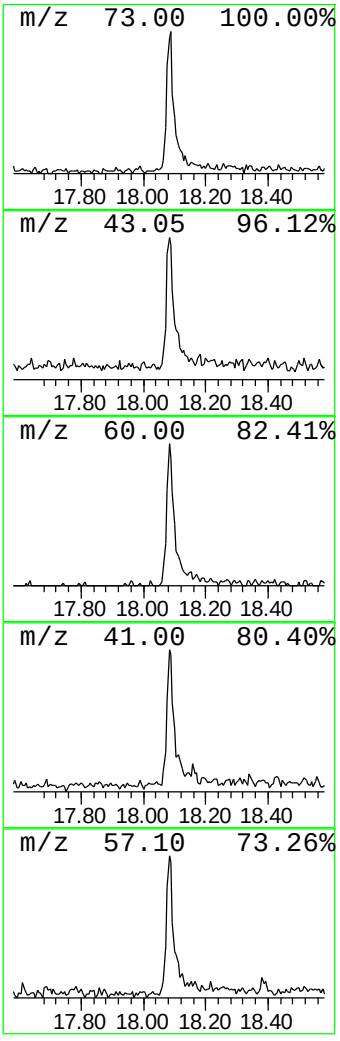
****

Peak Number 9 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.08	4.42 ng	280390	Phenanthrene-d10	17.18

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	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	n-Decanoic acid	172	C10H20O2	000334-48-5	52
5	Dodecanoic acid	200	C12H24O2	000143-07-7	52





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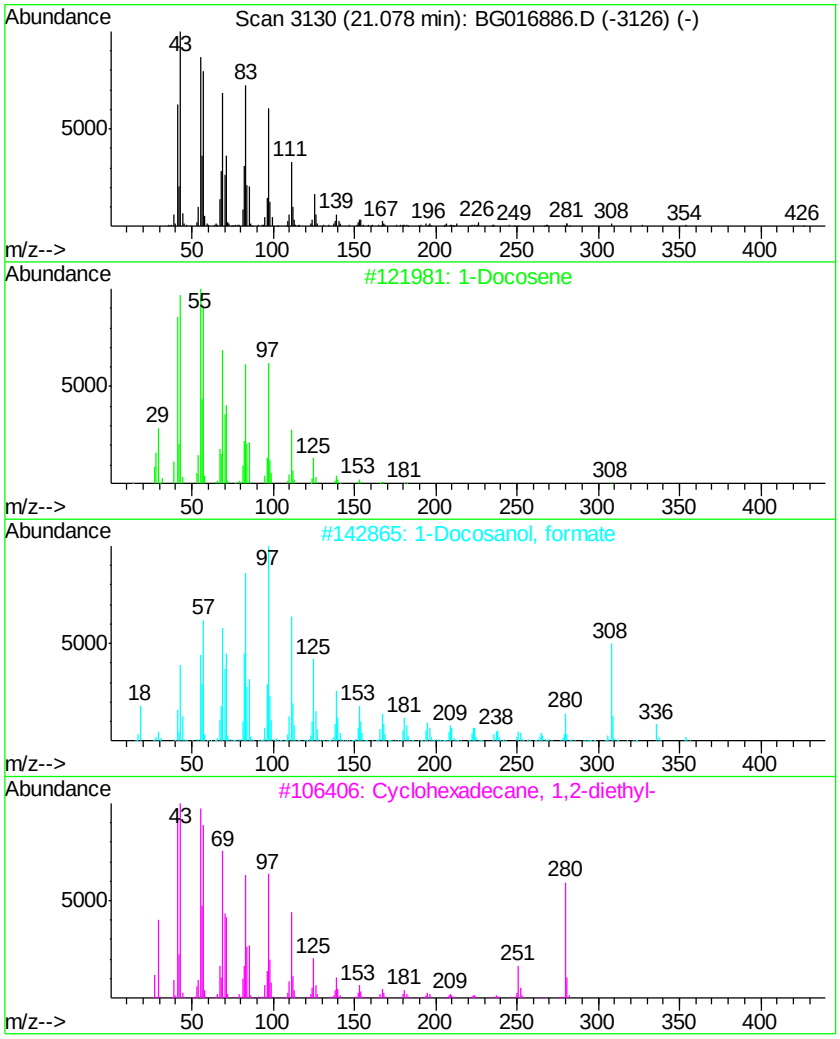
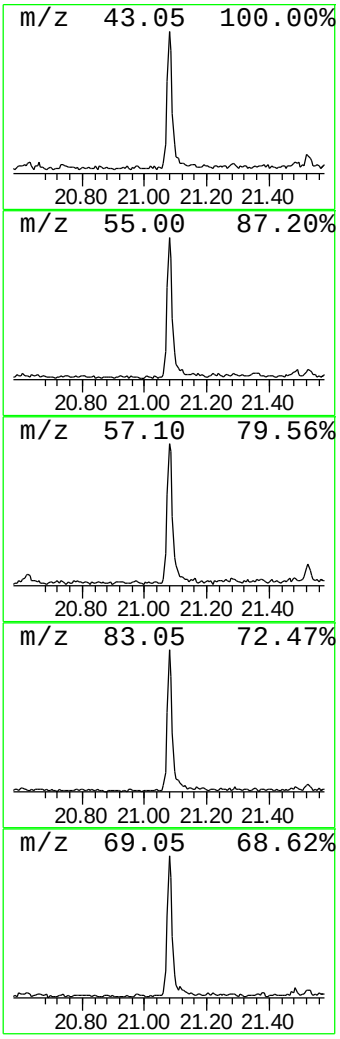
Peak Number 10 1-Docosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.08	6.74 ng	484478	Chrysene-d12	21.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	99
2	1-Docosanol, formate	354	C23H46O2	015155-62-1	97
3	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	97
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
5	1-Eicosene	280	C20H40	003452-07-1	94





Tentatively Identified Compound (LSC) summary

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ClientSampleId : GRID-3(12-23)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.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
unknown2.79	2.79	324.2	ng	8142000	1	7.81	502290	20.0
Butane, 2-methoxy...	3.01	8.3	ng	209523	1	7.81	502290	20.0
2-Pentanone, 4-hy...	4.92	7.9	ng	199227	1	7.81	502290	20.0
unknown7.34	7.34	77.2	ng	1939720	1	7.81	502290	20.0
Propanoic acid, 2...	12.80	2.9	ng	145486	3	14.44	1004170	20.0
Benzophenone	15.80	5.4	ng	270730	3	14.44	1004170	20.0
n-Hexadecanoic acid	18.08	4.4	ng	280390	4	17.18	1270080	20.0
1-Docosene	21.08	6.7	ng	484478	5	21.36	1436870	20.0