LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG016967.D
Acq On : 8 May 2015 21:13
Operator : TP/IZ
Sample : G2058-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MPE-1

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	2.917	34	39	47	rBV	318069	497141	11.51%	1.641%
2	2.993	47	52	58	rBV	666734	776797	17.98%	2.565%
3	4.908	373	378	385	rBV2	67509	99919	2.31%	0.330%
4	5.372	451	457	467	rVB	690647	967326	22.39%	3.194%
5	6.959	716	727	737	rBV	517451	795376	18.41%	2.626%
6	7.323	782	789	799	rVB	1286984	1965365	45.50%	6.489%
7	7.793	861	869	877	rBV	343637	560435	12.97%	1.850%
8	8.110	916	923	930	rBV	956128	1500220	34.73%	4.953%
9	8.951	1058	1066	1074	rBV	962490	1603197	37.11%	5.293%
10	10.584	1335	1344	1351	rBV	546029	919033	21.27%	3.034%
11	12.787	1712	1719	1724	rBV	196657	293020	6.78%	0.967%
12	13.052	1756	1764	1772	rBV	2514459	3956039	91.58%	13.061%
13	13.886	1901	1906	1910	rBV	35491	50876	1.18%	0.168%
14	14.432	1992	1999	2005	rVB2	872805	1338324	30.98%	4.418%
15	15.249	2133	2138	2146	rVB	272682	352571	8.16%	1.164%
16	15.790	2226	2230	2236	rVB2	59183	99235	2.30%	0.328%
17	15.919	2245	2252	2263	rBV	2412572	3299580	76.38%	10.893%
18	17.170	2460	2465	2474	rVB2	1130506	1644432	38.07%	5.429%
19	18.075	2614	2619	2627	rBV	317778	476120	11.02%	1.572%
20	19.350	2833	2836	2842	rBV	240742	312798	7.24%	1.033%
21	19.803	2907	2913	2921	rBV	3438837	4319860	100.00%	14.262%
22	21.060	3123	3127	3136	rBV	346253	445410	10.31%	1.471%
23	21.348	3171	3176	3181	rBV	1321619	1646356	38.11%	5.435%
24	22.505	3368	3373	3378	rBV2	568706	791079	18.31%	2.612%
25	23.645	3561	3567	3575	rVB2	846624	1579005	36.55%	5.213%

Sum of corrected areas: 30289514

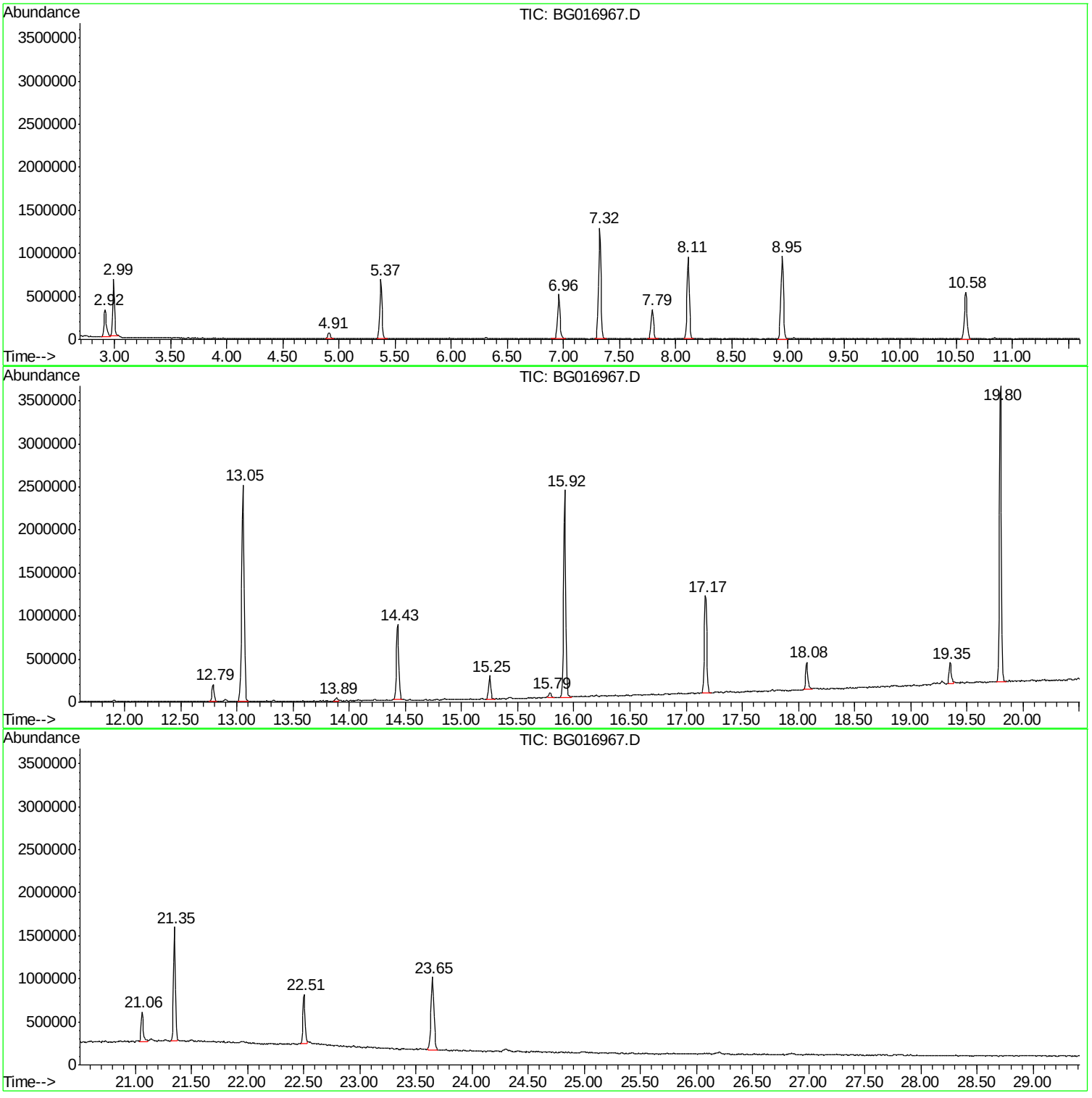
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG016967.D
Acq On : 8 May 2015 21:13
Operator : TP/IZ
Sample : G2058-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MPE-1

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG016967.D
Acq On : 8 May 2015 21:13
Operator : TP/IZ
Sample : G2058-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MPE-1

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

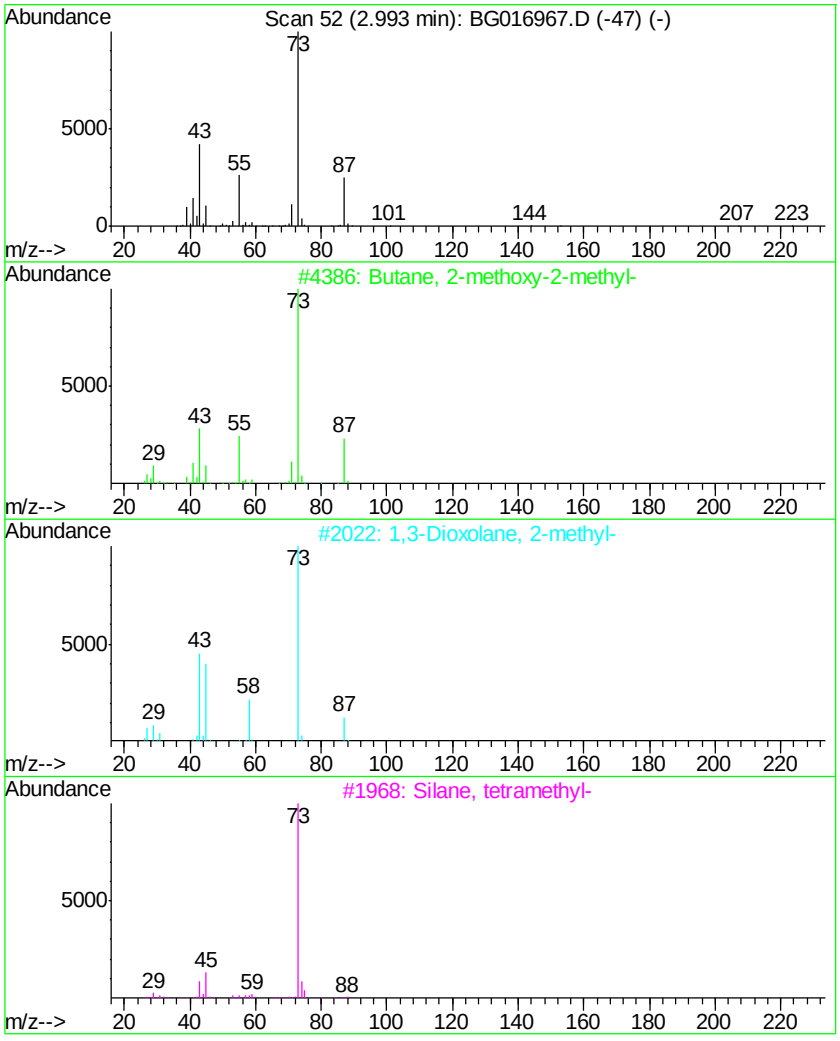
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

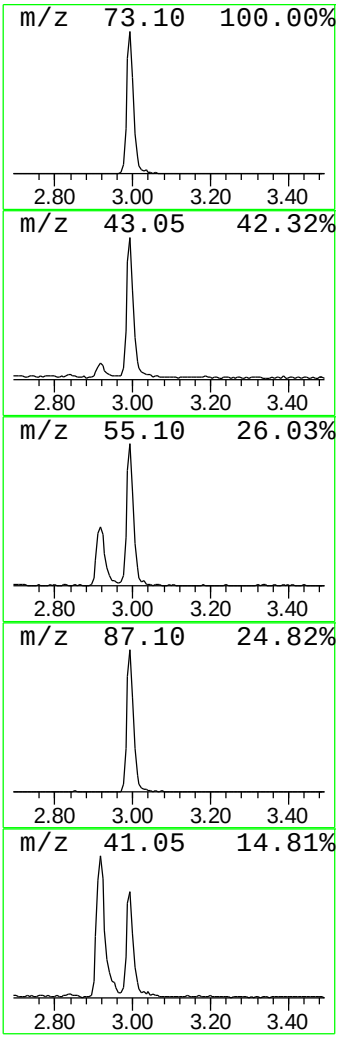
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	27.72 ng	776797	1,4-Dichlorobenzene-d4	7.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	74
2	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG016967.D
Acq On : 8 May 2015 21:13
Operator : TP/IZ
Sample : G2058-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MPE-1

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

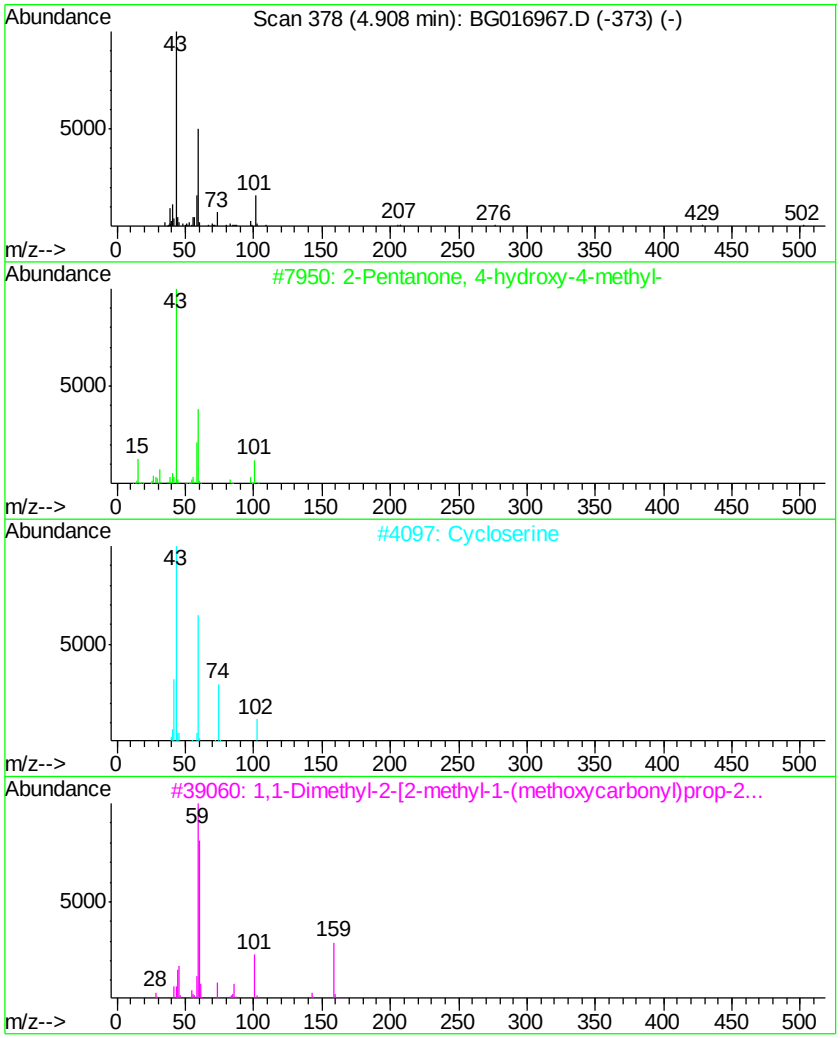
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

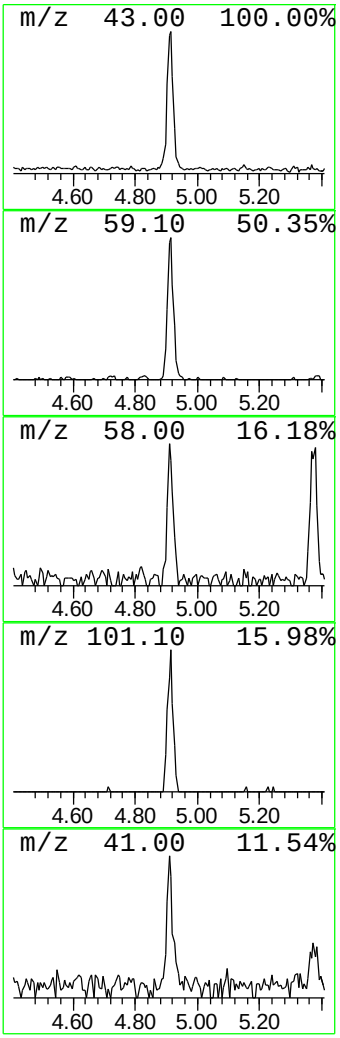
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	3.57 ng	99919	1,4-Dichlorobenzene-d4	7.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	Cycloserine	102	C3H6N2O2	000068-41-7	40
3	1,1-Dimethyl-2-[2-methyl-1-(meth...	174	C8H18N2O2	097812-29-8	28
4	3-Octanol	130	C8H18O	000589-98-0	25
5	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	25





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG016967.D
Acq On : 8 May 2015 21:13
Operator : TP/IZ
Sample : G2058-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MPE-1

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

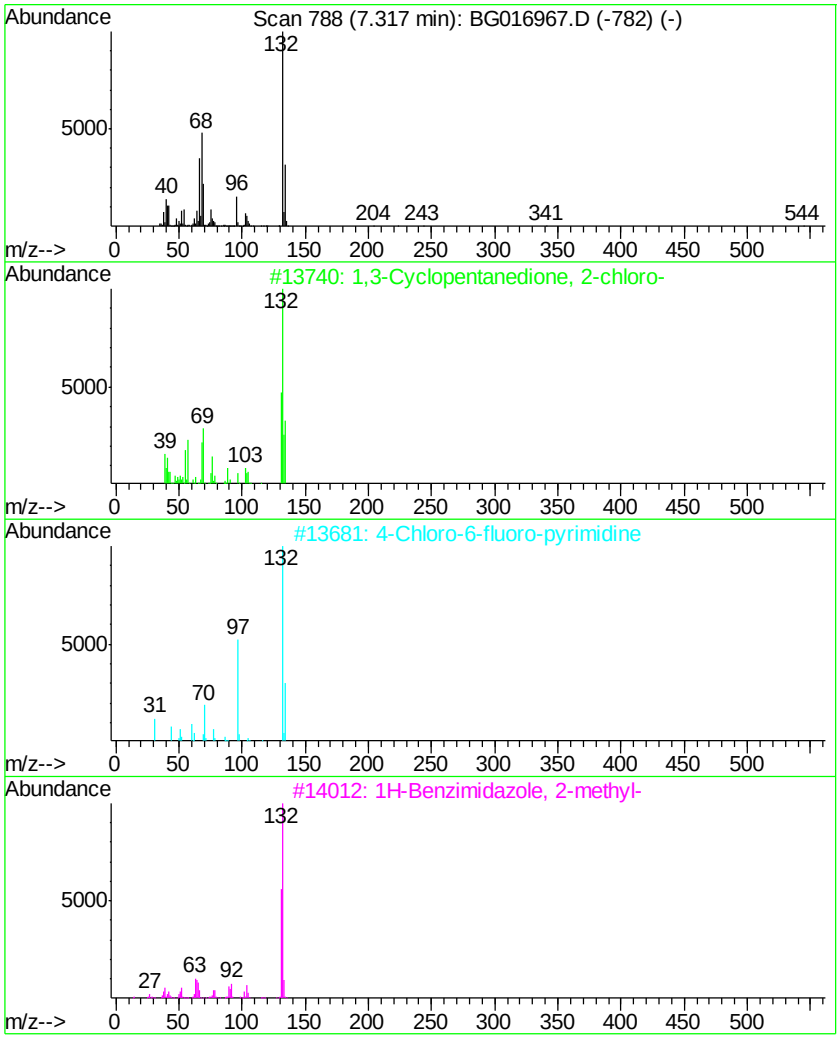
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

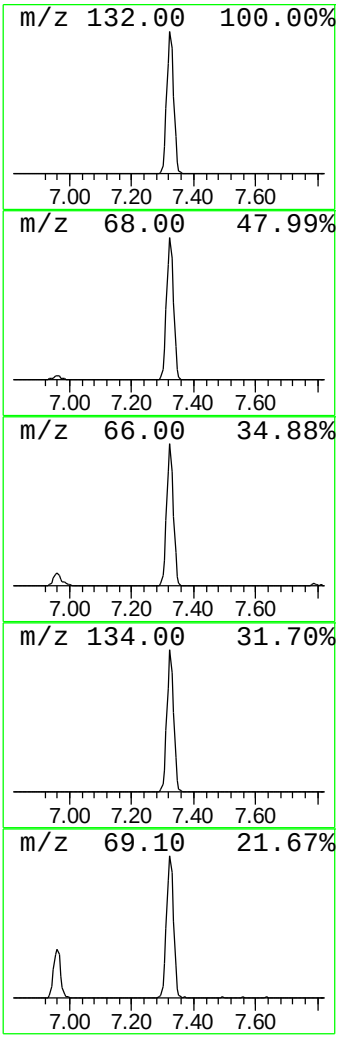
****

Peak Number 4 unknown7.32 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.32	70.14 ng	1965370	1,4-Dichlorobenzene-d4	7.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	35
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	12





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG016967.D
Acq On : 8 May 2015 21:13
Operator : TP/IZ
Sample : G2058-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MPE-1

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

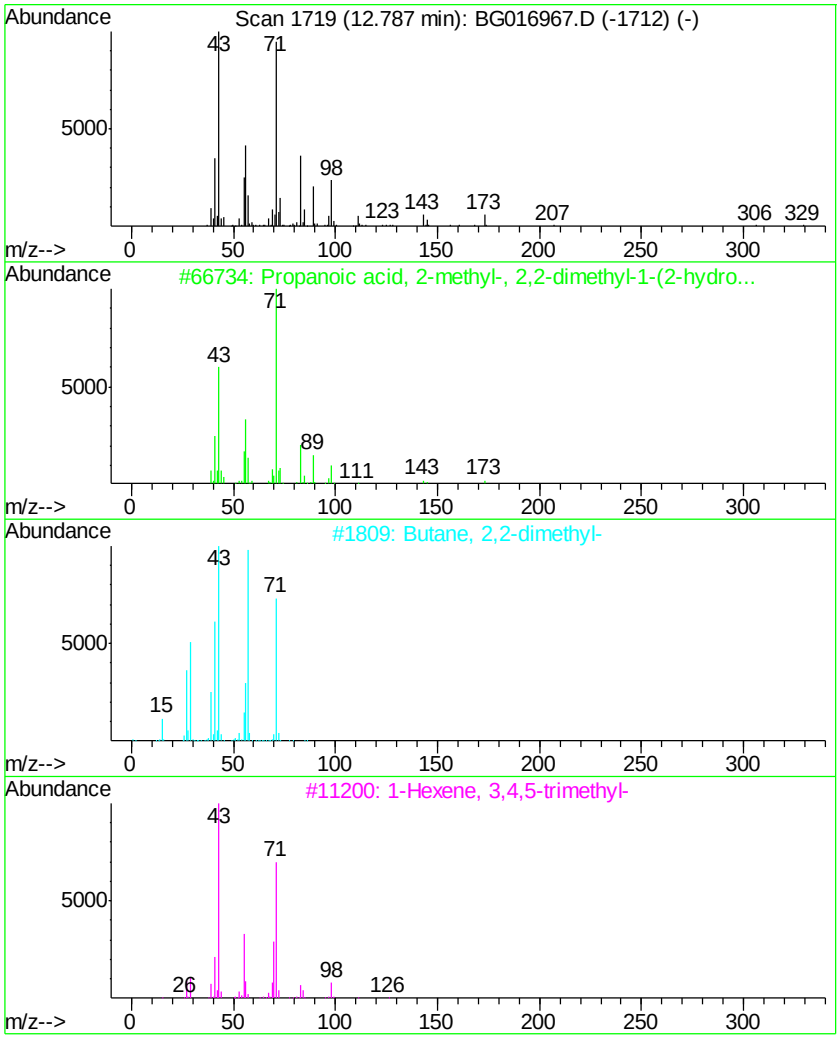
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

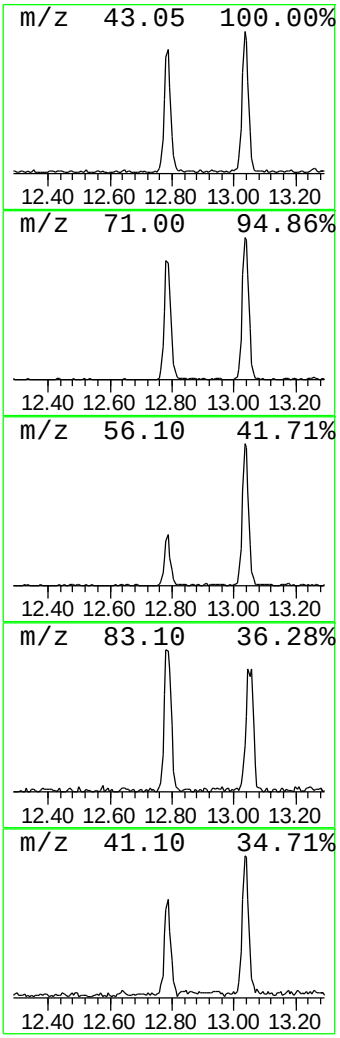
****

Peak Number 6 Propanoic acid, 2-methyl-, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	4.38 ng	293020	Acenaphthene-d10	14.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 2,2-d...	216	C12H24O3	074367-33-2	72
2	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	43
3	1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	43
4	Propanoic acid, 2-methyl-, 3-hyd...	216	C12H24O3	074367-34-3	43
5	Propanoic acid, 2-methyl-, 2-eth...	216	C12H24O3	074367-31-0	40





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG016967.D
Acq On : 8 May 2015 21:13
Operator : TP/IZ
Sample : G2058-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MPE-1

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

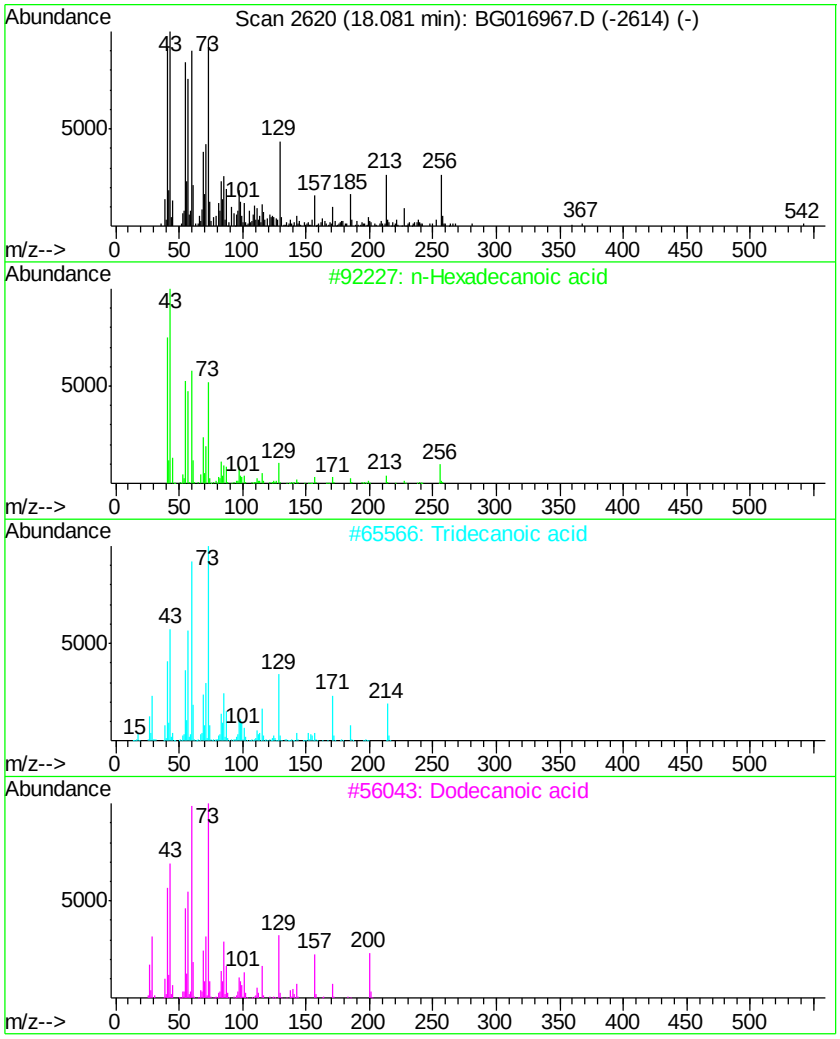
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

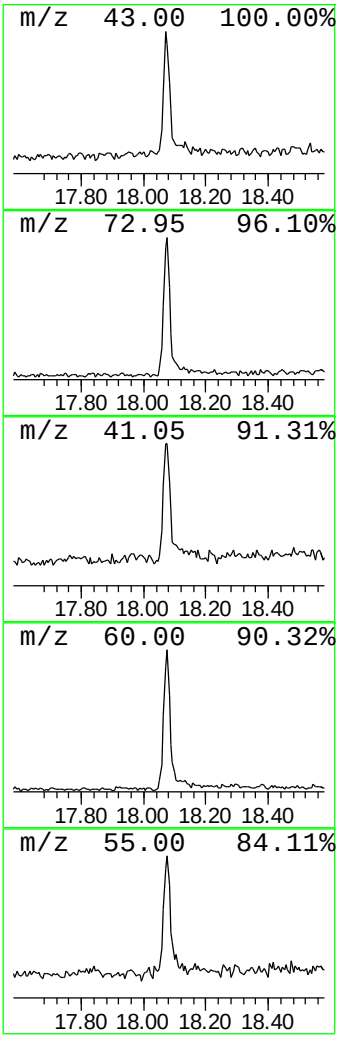
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.08	5.79 ng	476120	Phenanthrene-d10	17.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	76
3	Dodecanoic acid	200	C12H24O2	000143-07-7	68
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	58





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Sample : G2058-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MPE-1

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

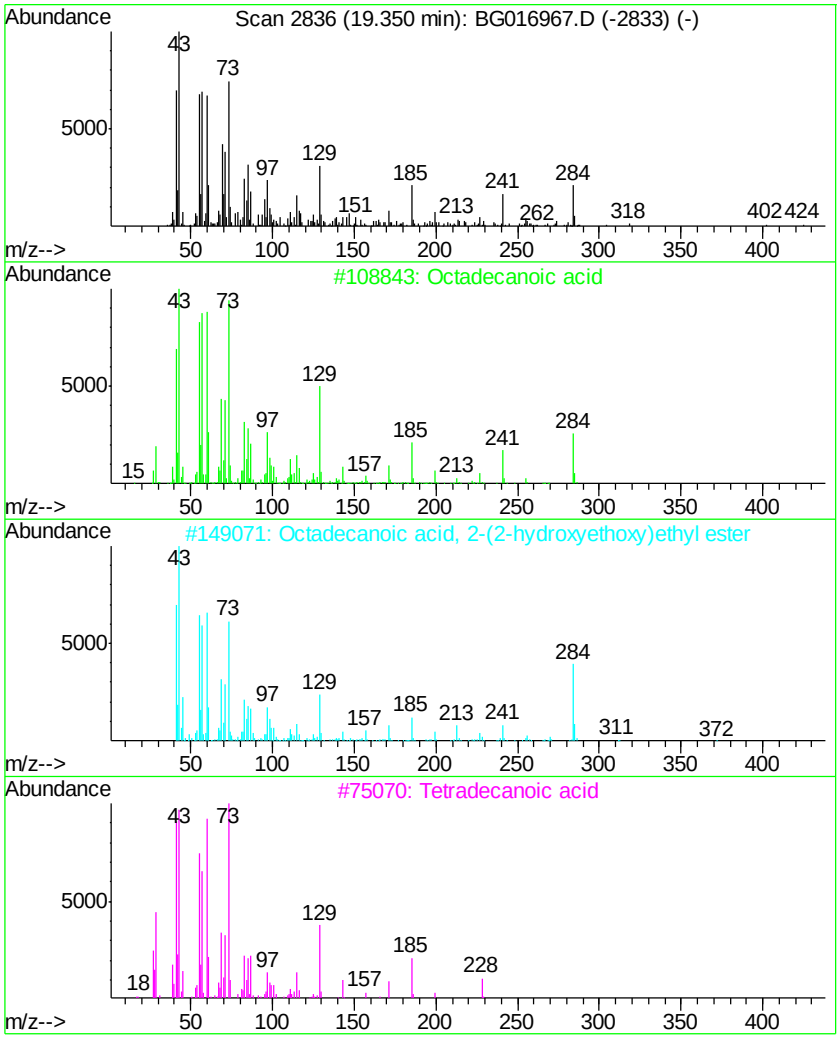
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

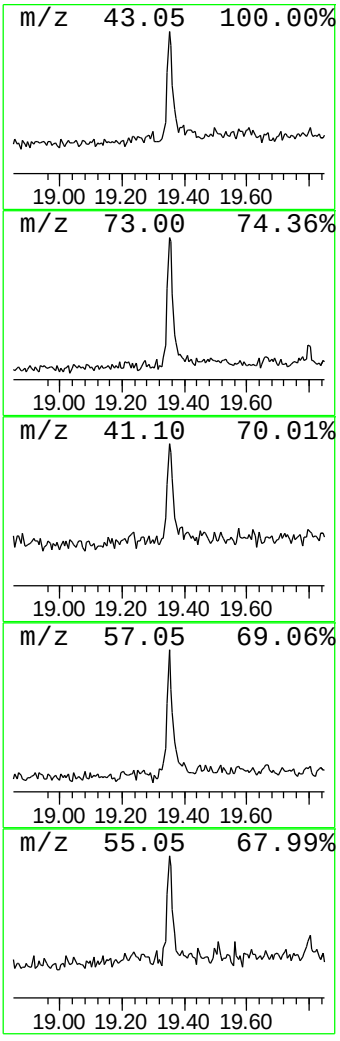
****

Peak Number 8 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.35	3.80 ng	312798	Chrysene-d12	21.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49
5	Tridecanoic acid	214	C13H26O2	000638-53-9	43





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Operator : TP/IZ
Sample : G2058-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MPE-1

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

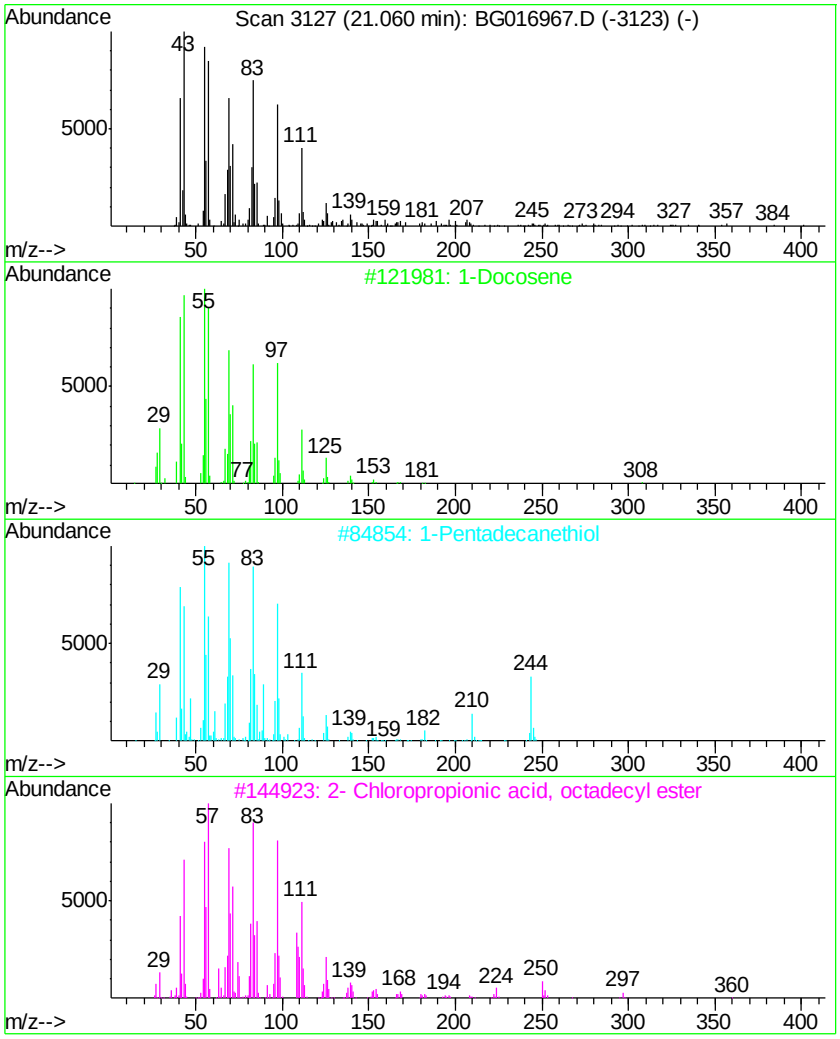
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

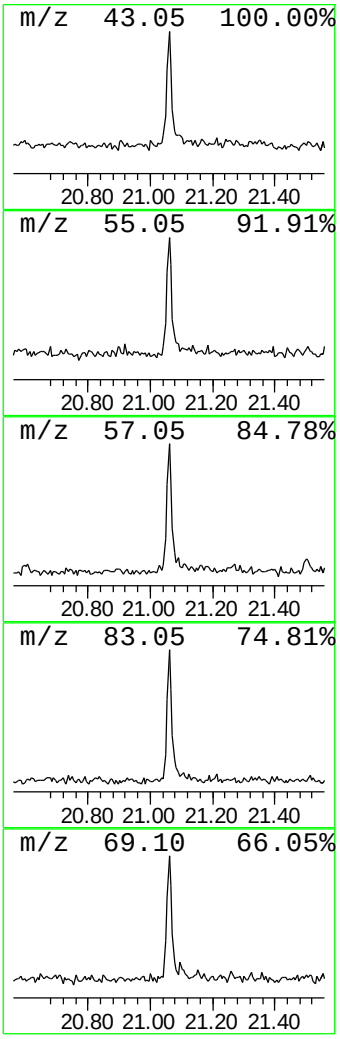
****

Peak Number 9 1-Docosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.06	5.41 ng	445410	Chrysene-d12	21.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	99
2	1-Pentadecanethiol	244	C15H32S	025276-70-4	90
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	87
4	1-Eicosanol	298	C20H42O	000629-96-9	87
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	87





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

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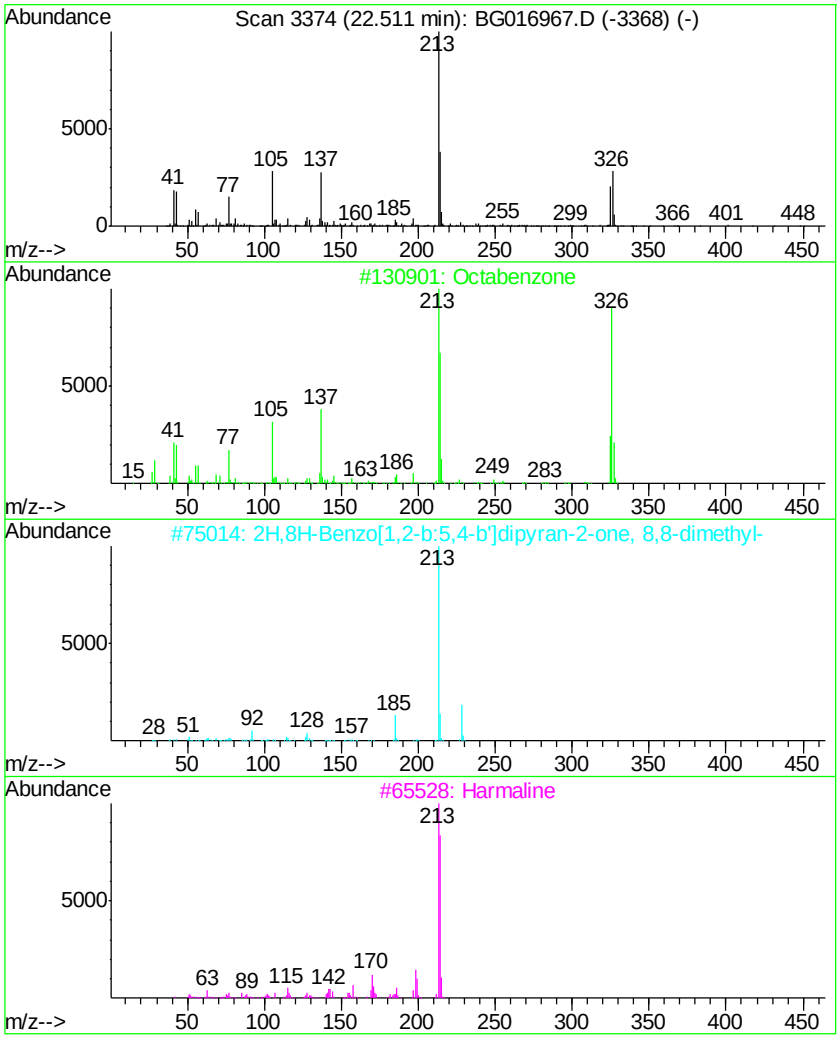
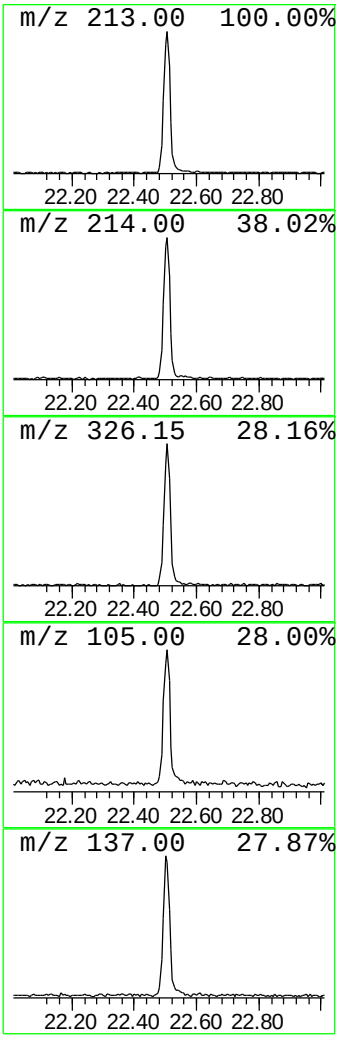
Peak Number 10 Octabenzone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.51	10.02 ng	791079	Perylene-d12	23.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octabenzone	326	C21H26O3	001843-05-6	95
2	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	17
3	Harmaline	214	C13H14N2O	000304-21-2	16
4	10H-Phenothiazine, 10-methyl-	213	C13H11NS	001207-72-3	12
5	Propenenitrile, 3-(4-morpholyl)-...	214	C13H14N2O	020842-95-9	9





Tentatively Identified Compound (LSC) summary

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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
Butane, 2-methoxy...	2.99	27.7	ng	776797	1	7.79	560435	20.0
2-Pentanone, 4-hy...	4.91	3.6	ng	99919	1	7.79	560435	20.0
unknown7.32	7.32	70.1	ng	1965370	1	7.79	560435	20.0
Propanoic acid, 2...	12.79	4.4	ng	293020	3	14.43	1338320	20.0
n-Hexadecanoic acid	18.08	5.8	ng	476120	4	17.17	1644430	20.0
Octadecanoic acid	19.35	3.8	ng	312798	5	21.35	1646360	20.0
1-Docosene	21.06	5.4	ng	445410	5	21.35	1646360	20.0
Octabenzone	22.51	10.0	ng	791079	6	23.65	1579010	20.0