LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG072115\
Data File : BG018042.D
Acq On : 22 Jul 2015 4:20
Operator : TP/UM
Sample : G2973-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3D23

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-BG071715.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	2.811	16	21	26	rBV	292156	348227	8.36%	1.230%
2	4.103	237	241	245	rBV2	35991	46321	1.11%	0.164%
3	4.697	335	342	349	rVB	695581	977450	23.47%	3.452%
4	5.155	414	420	427	rBV	1227858	1704208	40.91%	6.018%
5	5.754	517	522	532	rVB	68009	102039	2.45%	0.360%
6	6.741	682	690	700	rVB	1251591	1968361	47.25%	6.951%
7	7.088	741	749	757	rVB	1338113	2109869	50.65%	7.451%
8	7.546	821	827	835	rVB	266159	426729	10.24%	1.507%
9	7.863	874	881	888	rBV	944294	1516641	36.41%	5.356%
10	8.704	1016	1024	1032	rBV	798177	1292167	31.02%	4.563%
11	10.325	1293	1300	1308	rBV	435109	728315	17.48%	2.572%
12	12.828	1718	1726	1734	rBV	2195511	3261018	78.29%	11.516%
13	13.674	1864	1870	1879	rVB	387736	525255	12.61%	1.855%
14	14.209	1955	1961	1969	rBV2	695939	1086591	26.09%	3.837%
15	15.707	2209	2216	2232	rBV	1882284	2682824	64.41%	9.474%
16	16.965	2423	2430	2435	rBV	847804	1240025	29.77%	4.379%
17	17.881	2581	2586	2595	rBV2	80851	135108	3.24%	0.477%
18	19.033	2776	2782	2786	rBV	50286	76218	1.83%	0.269%
19	19.321	2826	2831	2836	rVB	185730	209722	5.03%	0.741%
20	19.397	2836	2844	2848	rBV2	58021	90989	2.18%	0.321%
21	19.438	2848	2851	2855	rVB3	37181	42067	1.01%	0.149%
22	19.614	2875	2881	2888	rBV	3299532	4165431	100.00%	14.710%
23	20.372	3005	3010	3015	rBV	148997	166059	3.99%	0.586%
24	20.431	3016	3020	3024	rVV2	54997	62421	1.50%	0.220%
25	20.895	3095	3099	3104	rBV2	58944	74062	1.78%	0.262%
26	21.166	3139	3145	3149	rBV	1178318	1470042	35.29%	5.191%
27	21.330	3170	3173	3178	rVB	60037	64061	1.54%	0.226%
28	21.759	3242	3246	3252	rBV3	42552	55885	1.34%	0.197%
29	22.211	3320	3323	3328	rVB2	52956	71594	1.72%	0.253%
30	22.335	3340	3344	3349	rVB5	25061	43566	1.05%	0.154%
31	22.705	3405	3407	3412	rVB4	35682	50313	1.21%	0.178%
32	23.263	3499	3502	3509	rVB4	33034	60444	1.45%	0.213%
33	23.369	3512	3520	3527	rVV	766245	1463113	35.13%	5.167%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG072115\
Data File : BG018042.D
Acq On : 22 Jul 2015 4:20
Operator : TP/UM
Sample : G2973-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3D23

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-BG071715.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

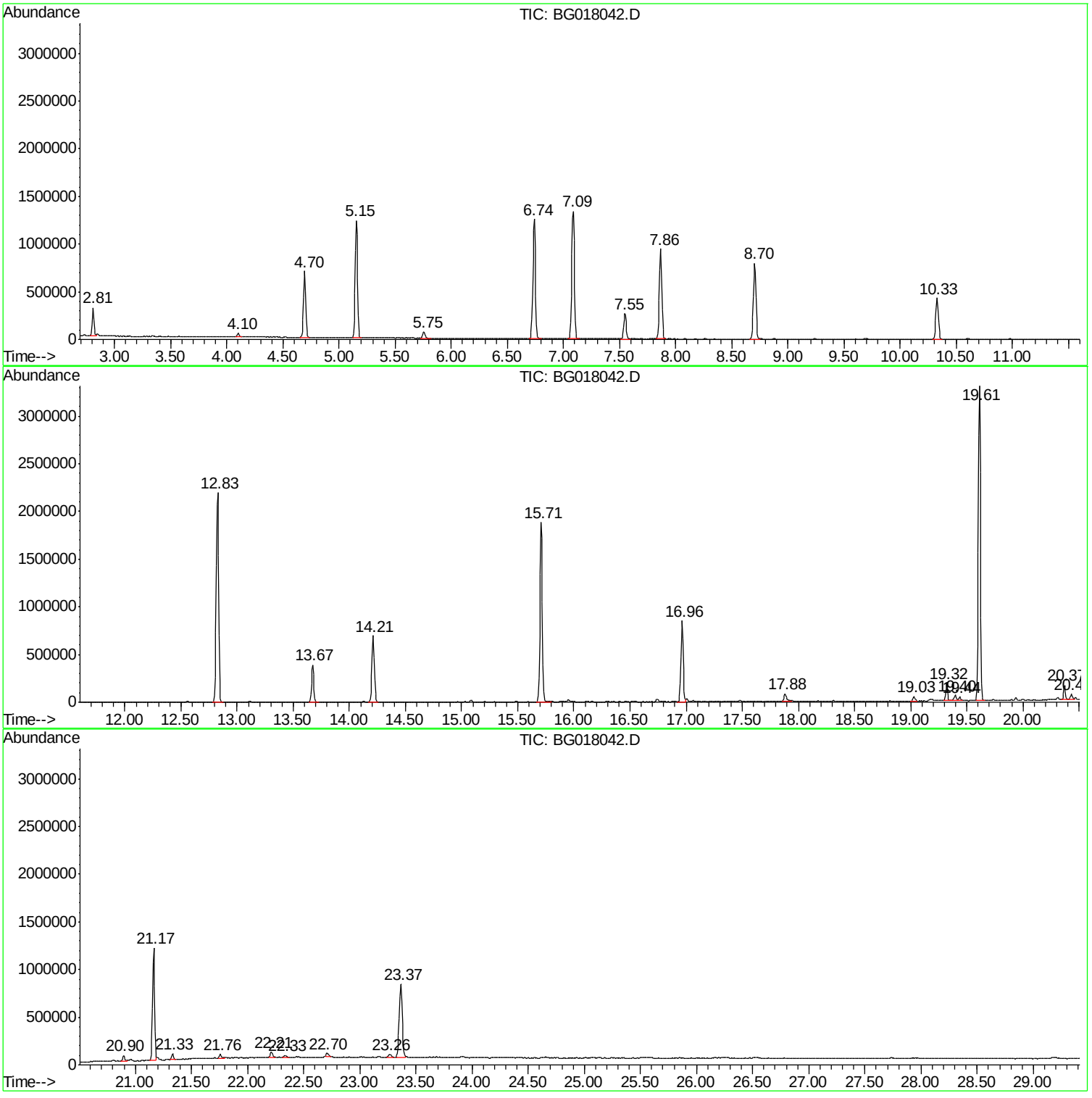
Sum of corrected areas: 28317135

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG072115\
Data File : BG018042.D
Acq On : 22 Jul 2015 4:20
Operator : TP/UM
Sample : G2973-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3D23

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.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\BG072115\
Data File : BG018042.D
Acq On : 22 Jul 2015 4:20
Operator : TP/UM
Sample : G2973-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3D23

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

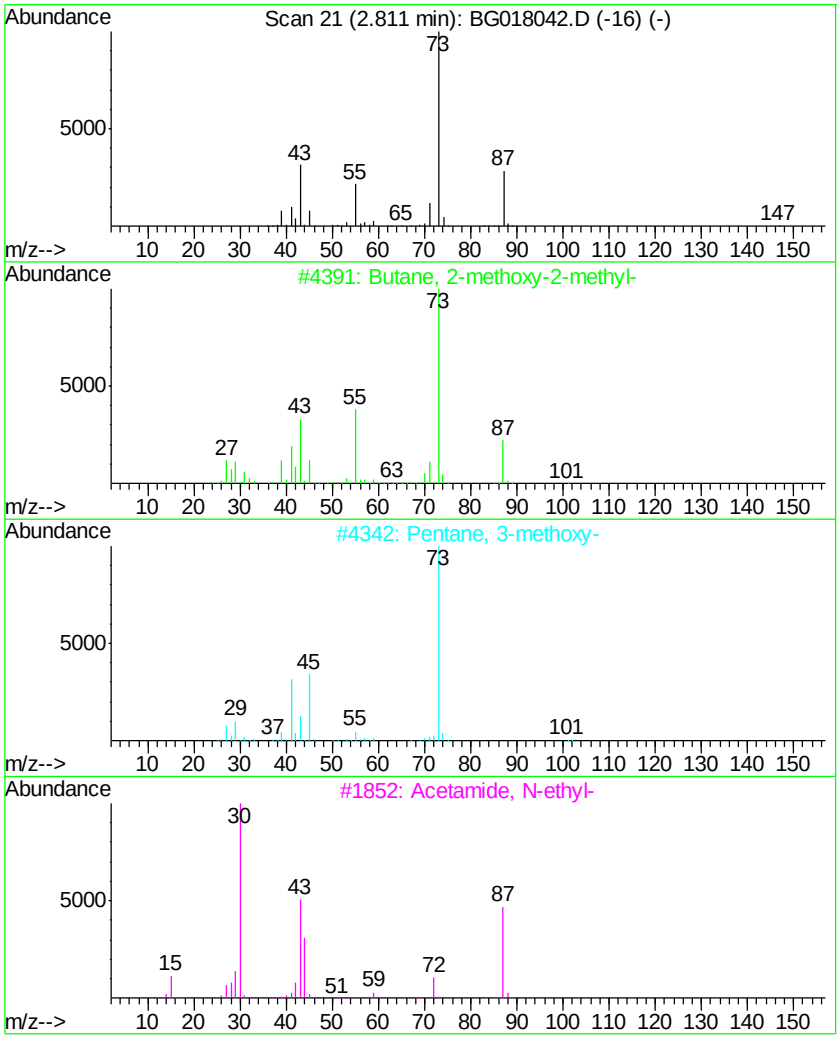
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

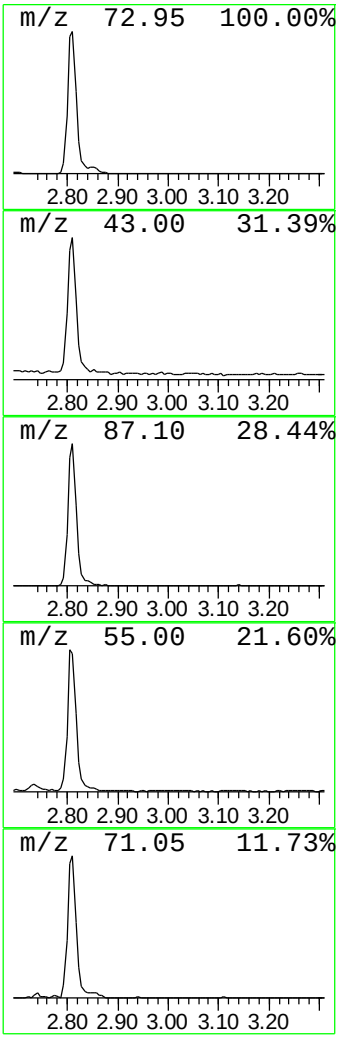
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.81	16.32 ng	348227	1,4-Dichlorobenzene-d4	7.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	25
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG072115\
Data File : BG018042.D
Acq On : 22 Jul 2015 4:20
Operator : TP/UM
Sample : G2973-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3D23

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

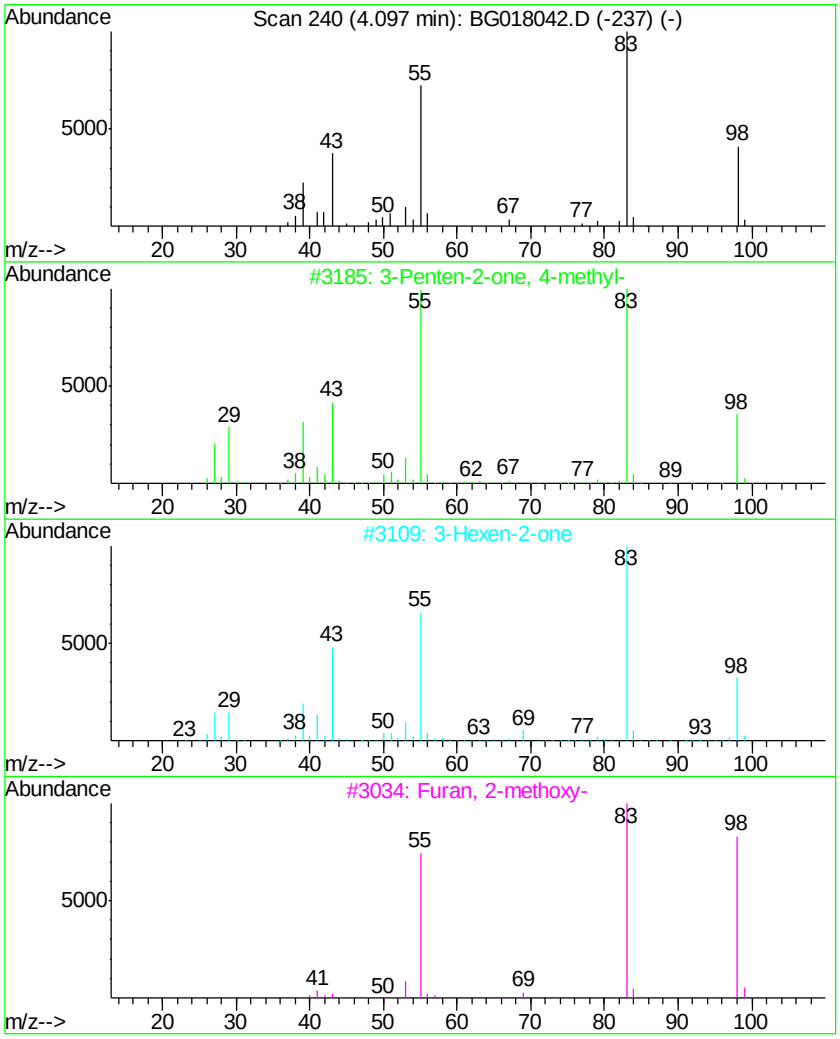
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

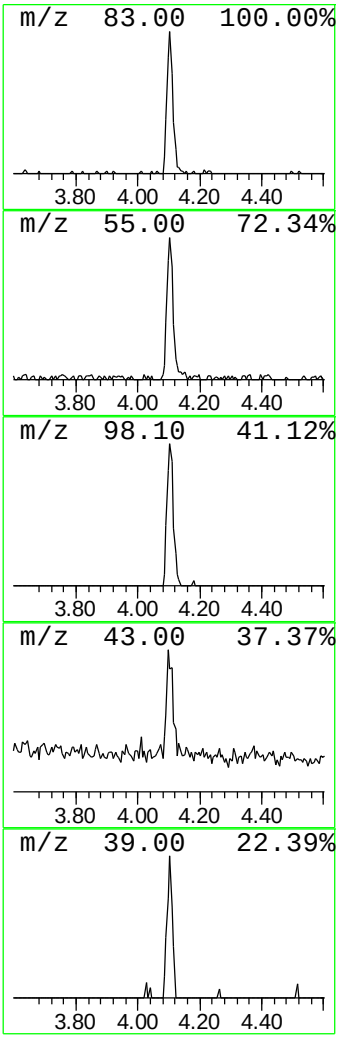
****

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.10	2.17 ng	46321	1,4-Dichlorobenzene-d4	7.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	86
2	3-Hexen-2-one	98	C6H10O	000763-93-9	86
3	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72
5	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	72





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG072115\
Data File : BG018042.D
Acq On : 22 Jul 2015 4:20
Operator : TP/UM
Sample : G2973-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3D23

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

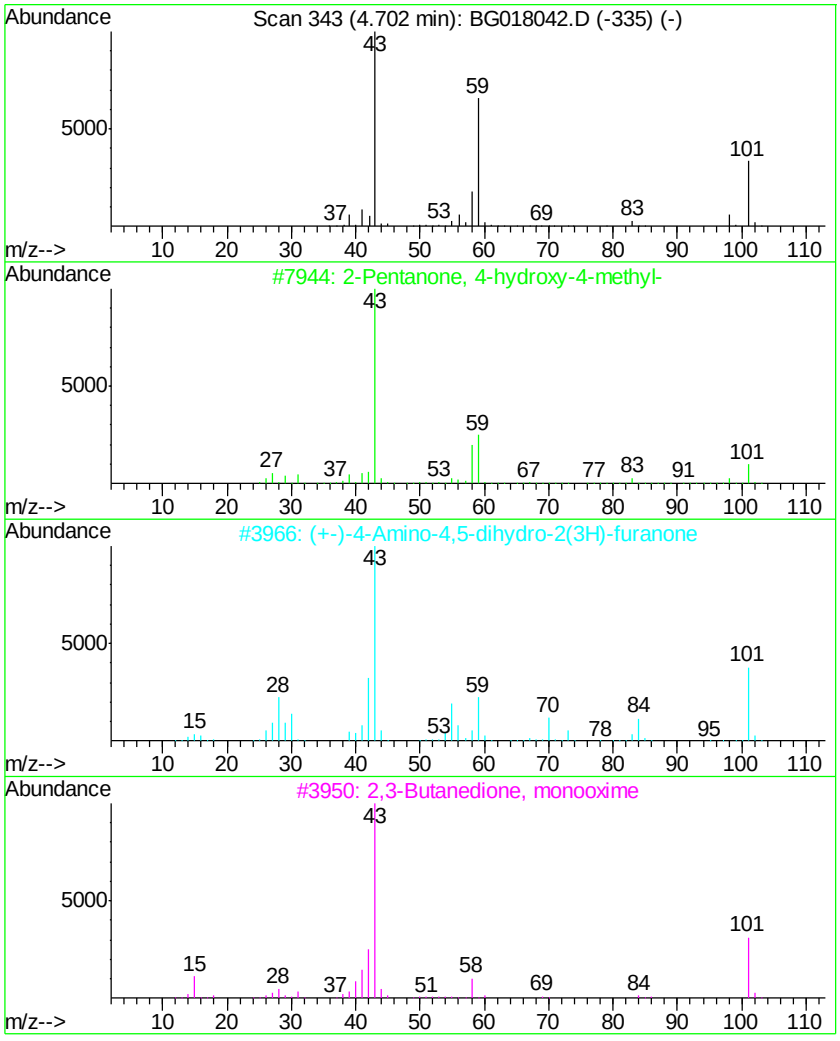
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

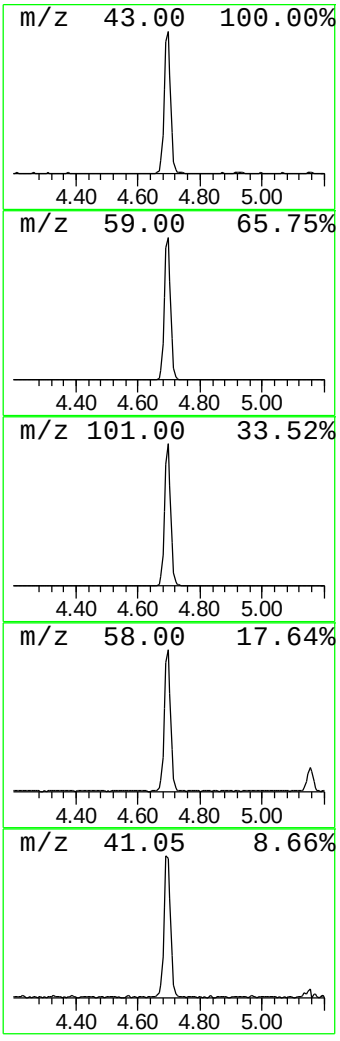
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.70	45.81 ng	977450	1,4-Dichlorobenzene-d4	7.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Acetone	58	C3H6O	000067-64-1	10





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG072115\
Data File : BG018042.D
Acq On : 22 Jul 2015 4:20
Operator : TP/UM
Sample : G2973-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3D23

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

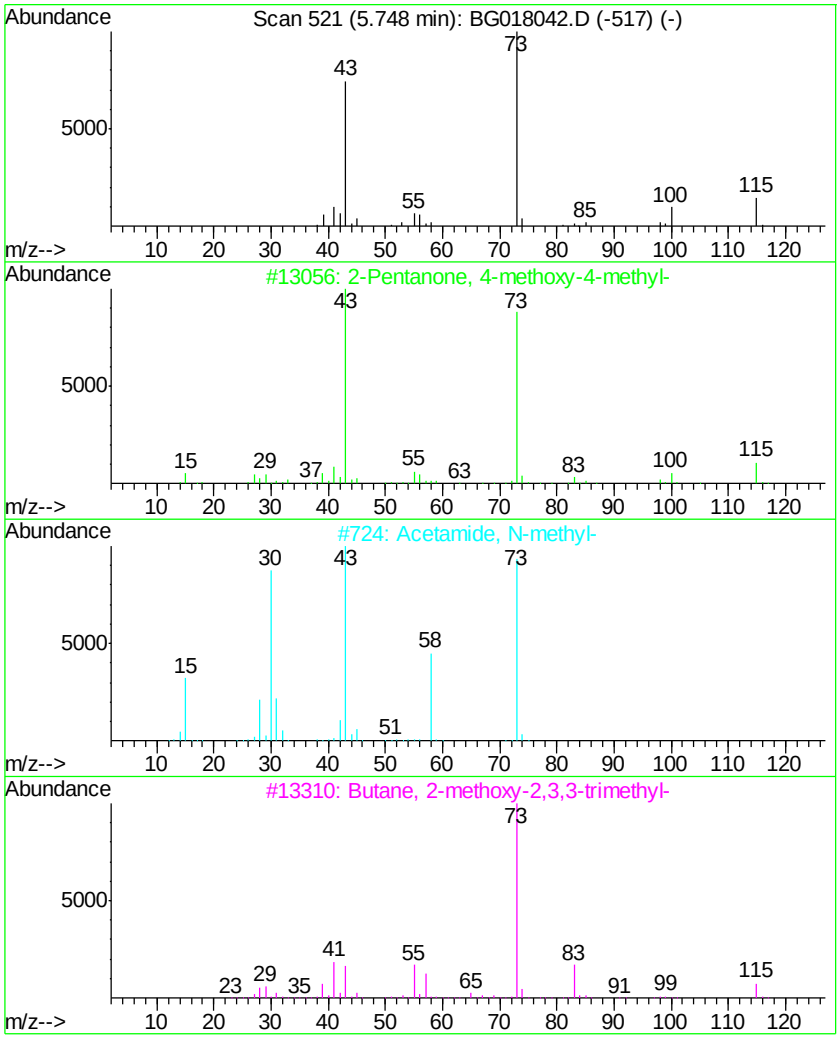
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

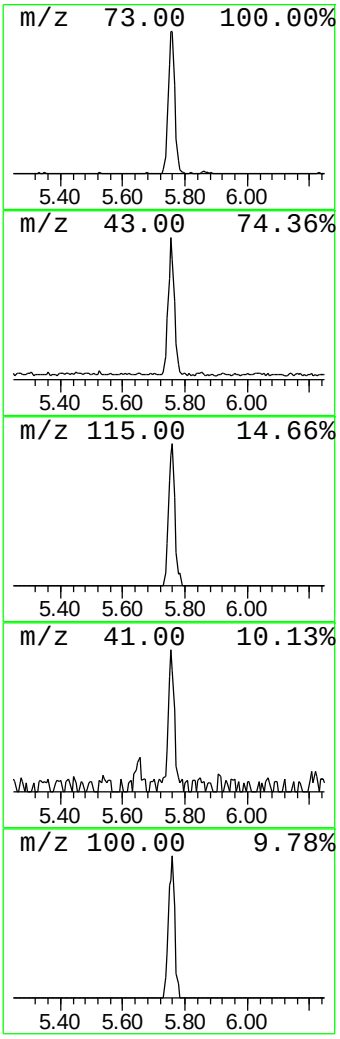
****

Peak Number 4 unknown5.75 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.75	4.78 ng	102039	1,4-Dichlorobenzene-d4	7.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	38
3	Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	23
4	2,3-Pentanedione	100	C5H8O2	000600-14-6	22
5	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	17





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG072115\
Data File : BG018042.D
Acq On : 22 Jul 2015 4:20
Operator : TP/UM
Sample : G2973-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3D23

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

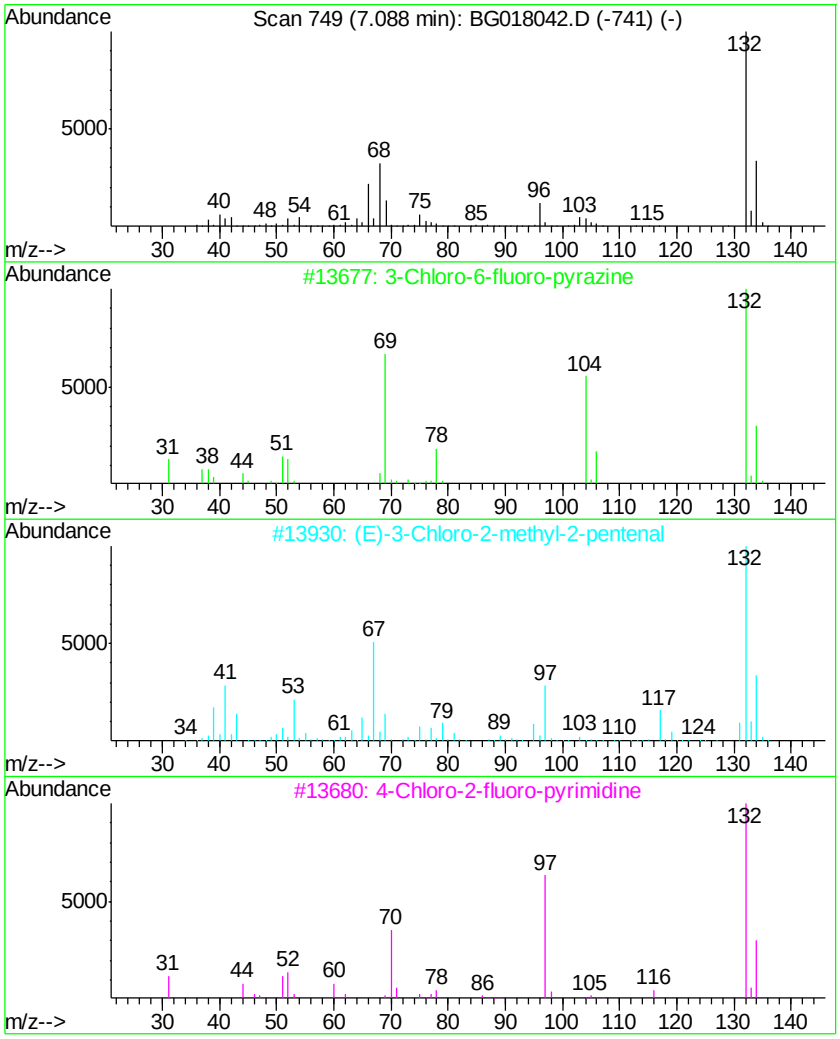
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

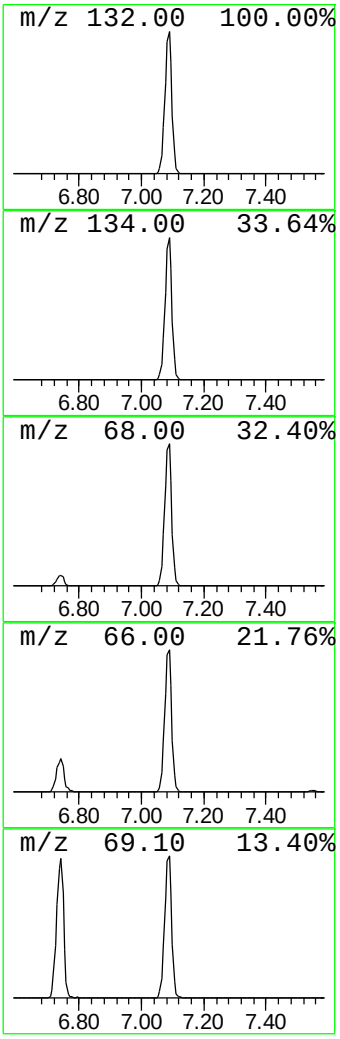
****

Peak Number 5 unknown7.09 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.09	98.89 ng	2109870	1,4-Dichlorobenzene-d4	7.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG072115\
Data File : BG018042.D
Acq On : 22 Jul 2015 4:20
Operator : TP/UM
Sample : G2973-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3D23

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

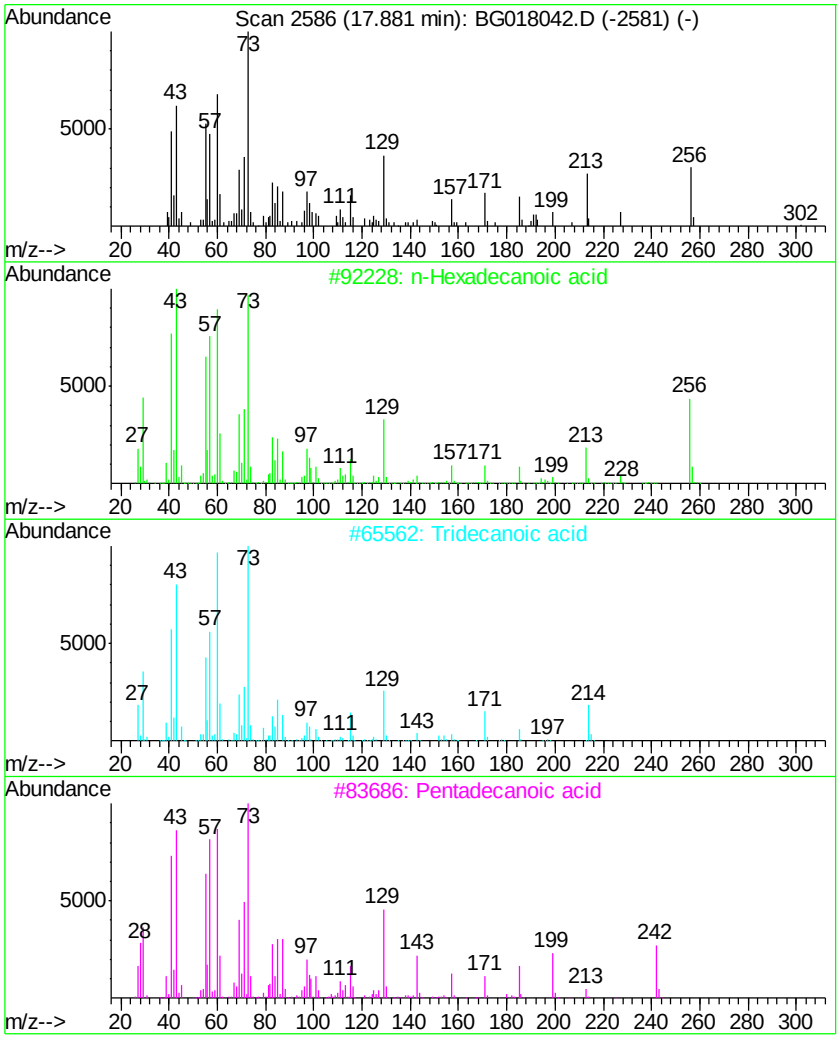
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

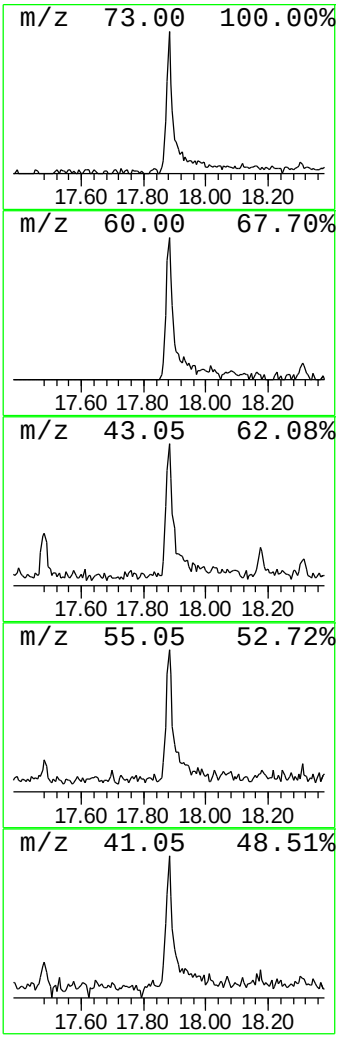
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.88	2.18 ng	135108	Phenanthrene-d10	16.96

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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
5	n-Decanoic acid	172	C10H20O2	000334-48-5	35





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG072115\
Data File : BG018042.D
Acq On : 22 Jul 2015 4:20
Operator : TP/UM
Sample : G2973-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3D23

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

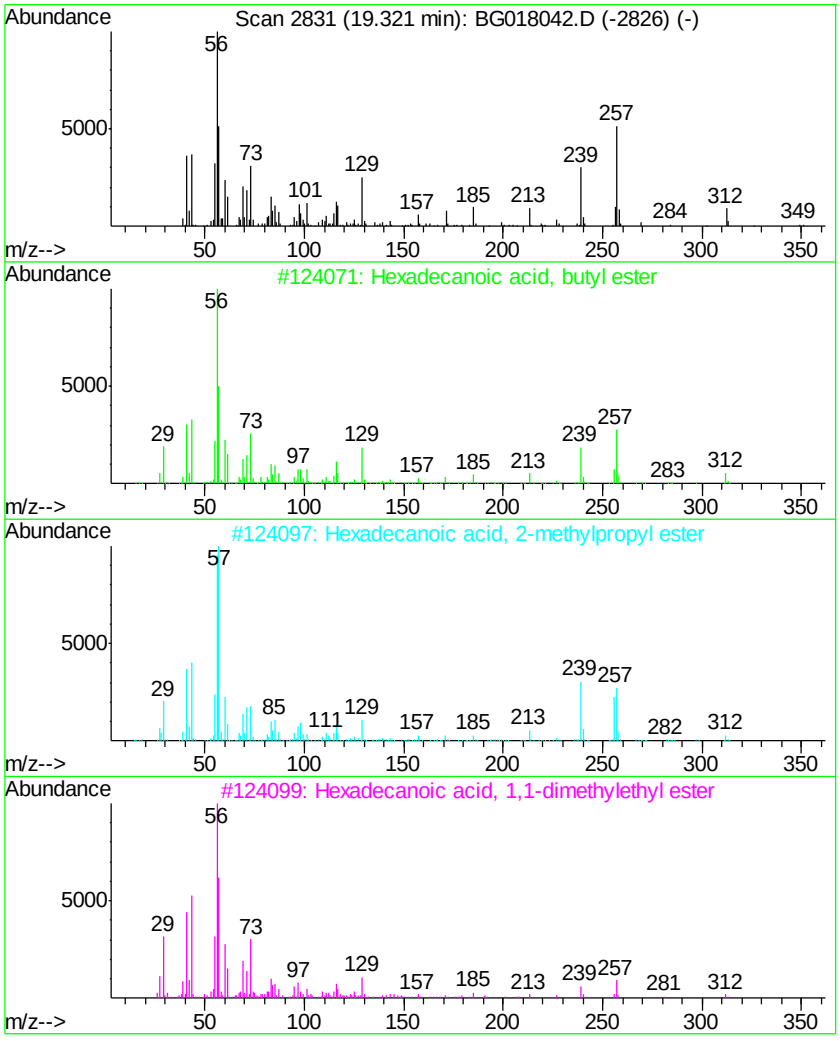
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

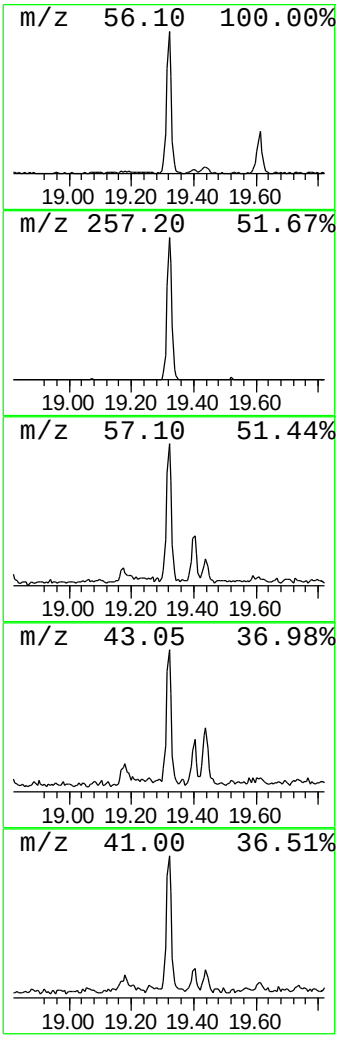
****

Peak Number 8 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.32	2.85 ng	209722	Chrysene-d12	21.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	99
2	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	53
3	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	49
4	Nordextromethorphan	257	C17H23NO	051195-74-5	47
5	Benz[c]acridine, 7,10-dimethyl-	257	C19H15N	002381-40-0	43





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG072115\
Data File : BG018042.D
Acq On : 22 Jul 2015 4:20
Operator : TP/UM
Sample : G2973-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3D23

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

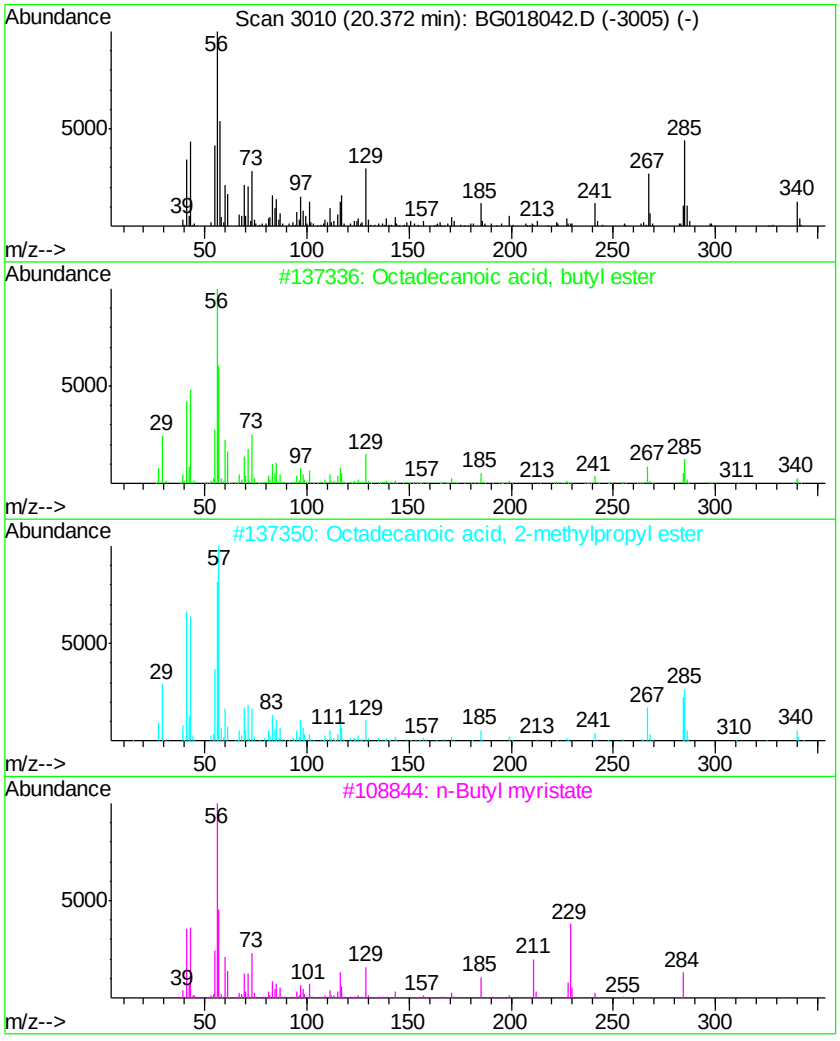
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

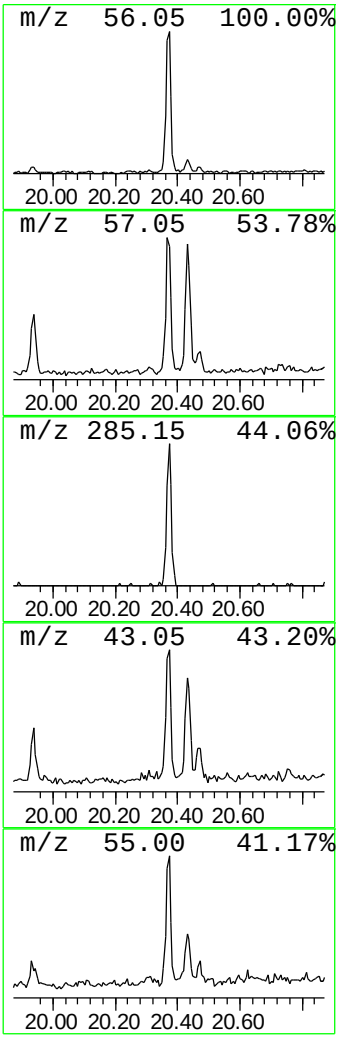
****

Peak Number 9 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.37	2.26 ng	166059	Chrysene-d12	21.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	95
2	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	94
3	n-Butyl myristate	284	C18H36O2	000110-36-1	46
4	Nipecotic acid	129	C6H11NO2	000498-95-3	38
5	2-Methyl-1-octadecene	266	C19H38	061868-20-0	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG072115\
Data File : BG018042.D
Acq On : 22 Jul 2015 4:20
Operator : TP/UM
Sample : G2973-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3D23

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.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
Butane, 2-methoxy...	2.81	16.3	ng	348227	1	7.55	426729	20.0
3-Penten-2-one, 4...	4.10	2.2	ng	46321	1	7.55	426729	20.0
2-Pentanone, 4-hy...	4.70	45.8	ng	977450	1	7.55	426729	20.0
unknown5.75	5.75	4.8	ng	102039	1	7.55	426729	20.0
unknown7.09	7.09	98.9	ng	2109870	1	7.55	426729	20.0
n-Hexadecanoic acid	17.88	2.2	ng	135108	4	16.96	1240030	20.0
Hexadecanoic acid...	19.32	2.9	ng	209722	5	21.17	1470040	20.0
Octadecanoic acid...	20.37	2.3	ng	166059	5	21.17	1470040	20.0