LSC Area Percent Report

Data Path : V:\HPCHEM1\BNA G\DATA\BG070916\
Data File : BG022946.D
Acq On : 9 Jul 2016 1:25
Operator : UM/SJ
Sample : H3900-05
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P-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-BG070816.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	3.044	30	35	42	rVB	153152	214234	2.77%	0.458%
2	5.224	399	406	412	rBV2	92034	152838	1.98%	0.326%
3	5.700	477	487	499	rBV	1375129	2254858	29.14%	4.815%
4	7.309	753	761	772	rBV	1680390	2904588	37.54%	6.203%
5	7.680	817	824	833	rBV	1453391	2650506	34.26%	5.660%
6	8.155	897	905	914	rVB	410231	726099	9.38%	1.551%
7	8.479	951	960	968	rBV	1125494	1924534	24.87%	4.110%
8	9.325	1096	1104	1115	rBV	1060162	1929602	24.94%	4.121%
9	10.982	1378	1386	1394	rBV	661812	1181037	15.26%	2.522%
10	13.420	1793	1801	1813	rVB	3079877	5003316	64.66%	10.685%
11	14.237	1934	1940	1945	rBV	397779	593801	7.67%	1.268%
12	14.795	2028	2035	2043	rBV2	1145853	1947025	25.16%	4.158%
13	16.287	2283	2289	2302	rBV	2921239	4528313	58.53%	9.670%
14	16.481	2318	2322	2325	rBV3	62998	84662	1.09%	0.181%
15	17.274	2452	2457	2463	rBV2	68969	109147	1.41%	0.233%
16	17.550	2498	2504	2509	rBV	1509977	2427147	31.37%	5.183%
17	17.591	2509	2511	2519	rVB	197121	282525	3.65%	0.603%
18	17.909	2561	2565	2571	rBV3	63634	107566	1.39%	0.230%
19	18.420	2648	2652	2659	rBV2	307501	438352	5.67%	0.936%
20	19.272	2793	2797	2802	rBV5	91601	132604	1.71%	0.283%
21	19.601	2848	2853	2860	rVB	323975	481226	6.22%	1.028%
22	19.689	2864	2868	2875	rVV5	106955	151191	1.95%	0.323%
23	19.930	2903	2909	2910	rBV5	60556	109592	1.42%	0.234%
24	19.965	2911	2915	2921	rVB	260979	374192	4.84%	0.799%
25	20.153	2941	2947	2953	rBV	5877168	7737339	100.00%	16.523%
26	20.282	2964	2969	2976	rVB8	35619	102537	1.33%	0.219%
27	20.441	2992	2996	3003	rVB7	72303	125341	1.62%	0.268%
28	21.452	3164	3168	3174	rBV3	220571	318221	4.11%	0.680%
29	21.845	3227	3235	3240	rBV	1773112	3064368	39.60%	6.544%
30	23.349	3484	3491	3500	rBV	957312	1811896	23.42%	3.869%
31	24.131	3618	3624	3630	rBV4	93132	255409	3.30%	0.545%
32	25.200	3796	3806	3817	rBV2	924044	2702929	34.93%	5.772%

LSC Area Percent Report

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Data File : BG022946.D
Acq On : 9 Jul 2016 1:25
Operator : UM/SJ
Sample : H3900-05
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P-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-BG070816.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

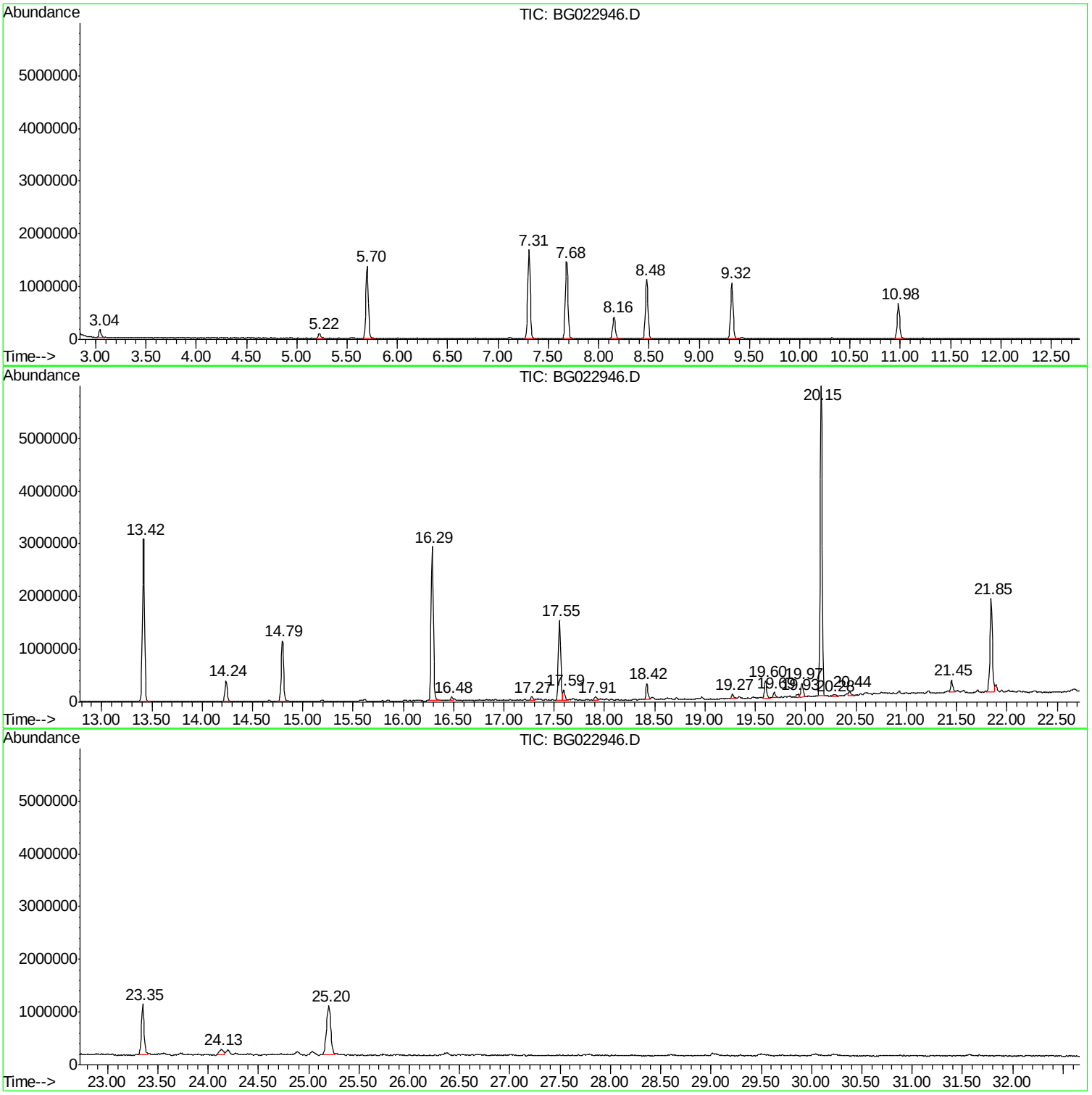
Sum of corrected areas: 46826995

Data Path : V:\HPCHEM1\BNA G\DATA\BG070916\
Data File : BG022946.D
Acq On : 9 Jul 2016 1:25
Operator : UM/SJ
Sample : H3900-05
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : V:\HPCHEM1\BNA G\DATA\BG070916\
Data File : BG022946.D
Acq On : 9 Jul 2016 1:25
Operator : UM/SJ
Sample : H3900-05
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

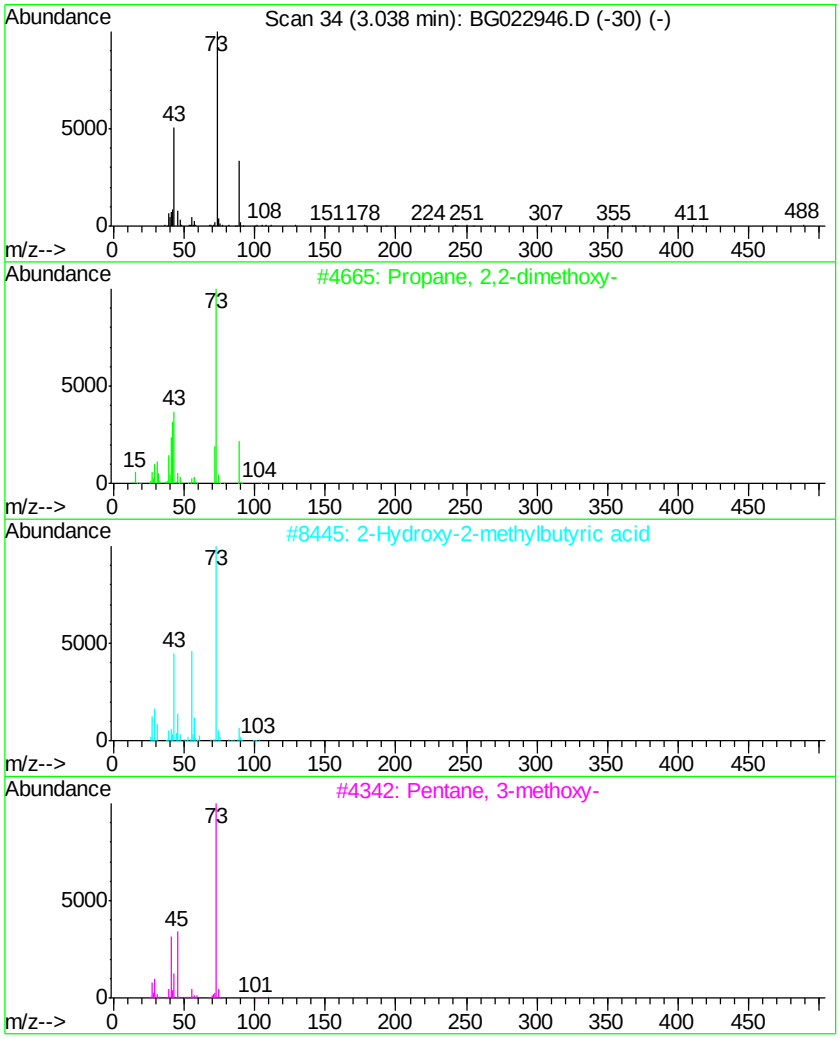
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

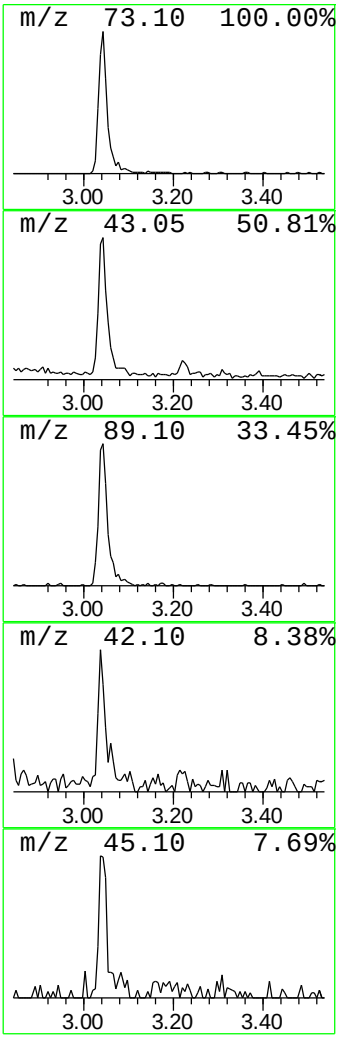
****

Peak Number 1 unknown3.04 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	5.90 ng	214234	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	33
2	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	17
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	14
4	1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9





Library Search Compound Report

Data Path : V:\HPCHEM1\BNA G\DATA\BG070916\
Data File : BG022946.D
Acq On : 9 Jul 2016 1:25
Operator : UM/SJ
Sample : H3900-05
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

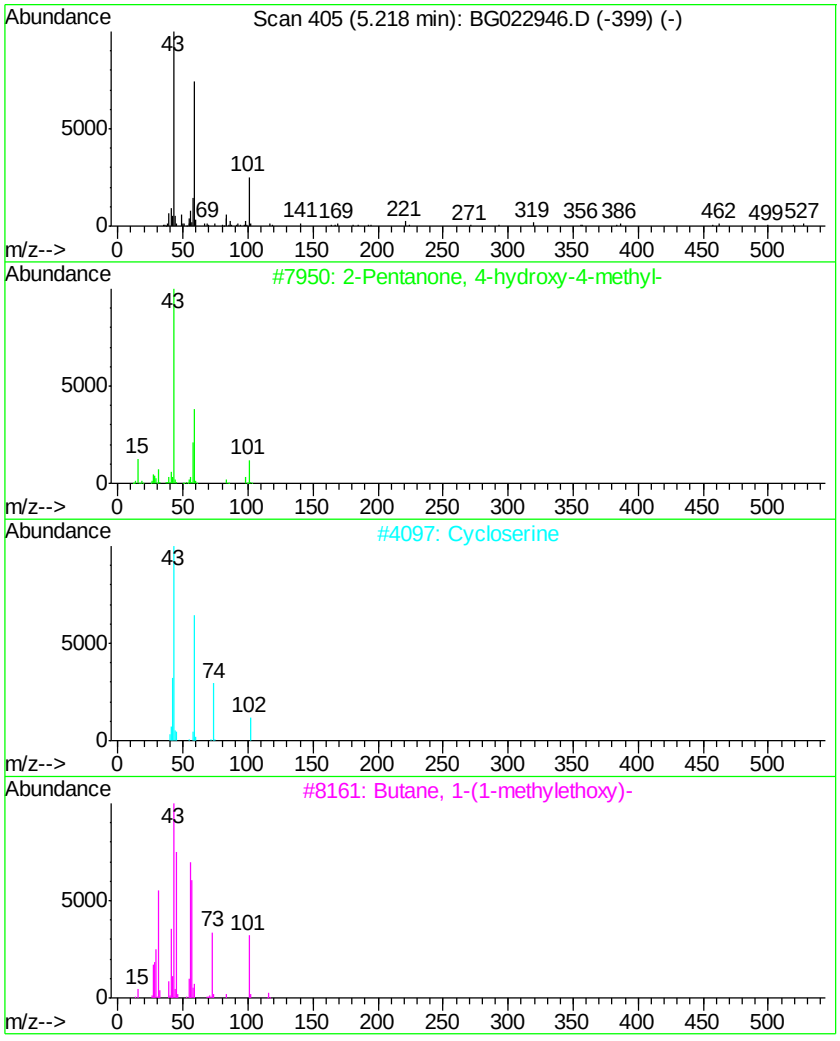
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

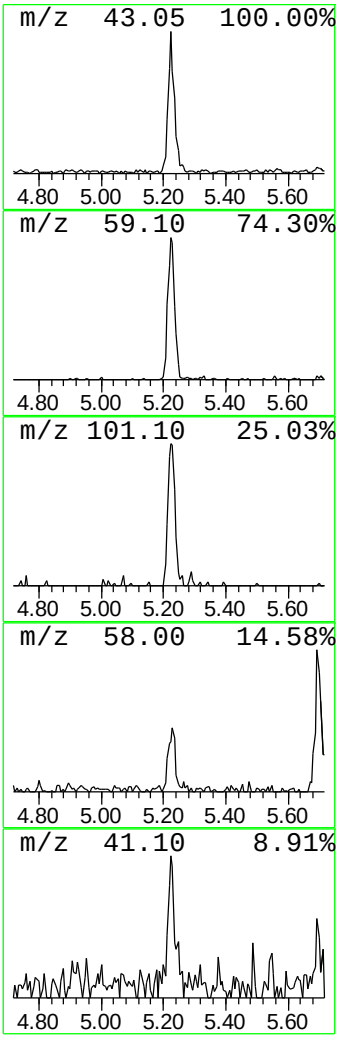
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	4.21 ng	152838	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Cycloserine	102	C3H6N2O2	000068-41-7	33
3	Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	32
4	3-Heptanol	116	C7H16O	000589-82-2	17
5	Butane, 2-methoxy-	88	C5H12O	006795-87-5	16





Data Path : V:\HPCHEM1\BNA G\DATA\BG070916\
Data File : BG022946.D
Acq On : 9 Jul 2016 1:25
Operator : UM/SJ
Sample : H3900-05
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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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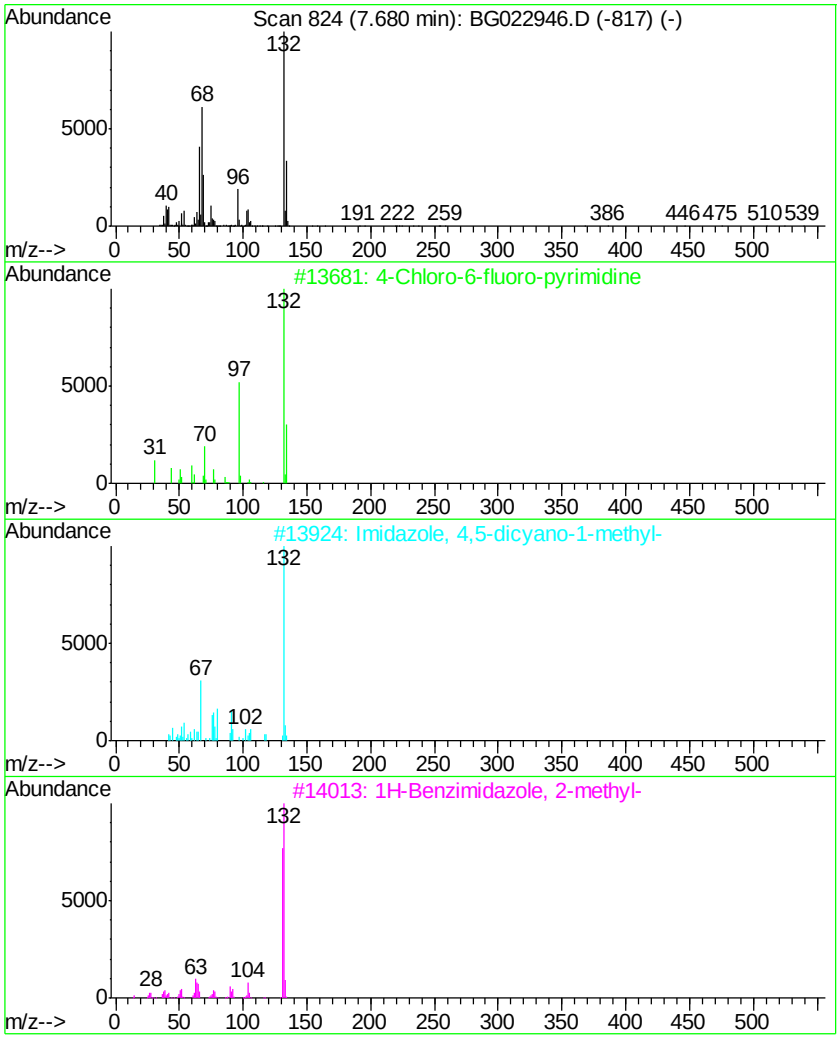
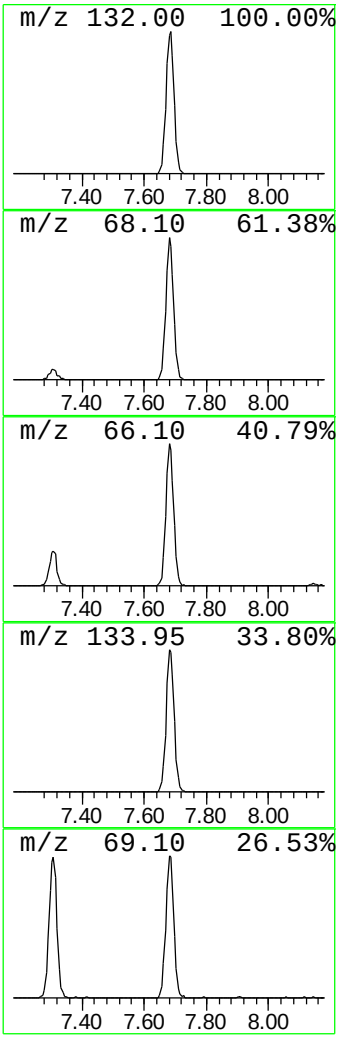
Peak Number 3 unknown7.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	73.01 ng	2650510	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
2	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	11
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4	5-Aminoindole	132	C8H8N2	005192-03-0	10
5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	10





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Operator : UM/SJ
Sample : H3900-05
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

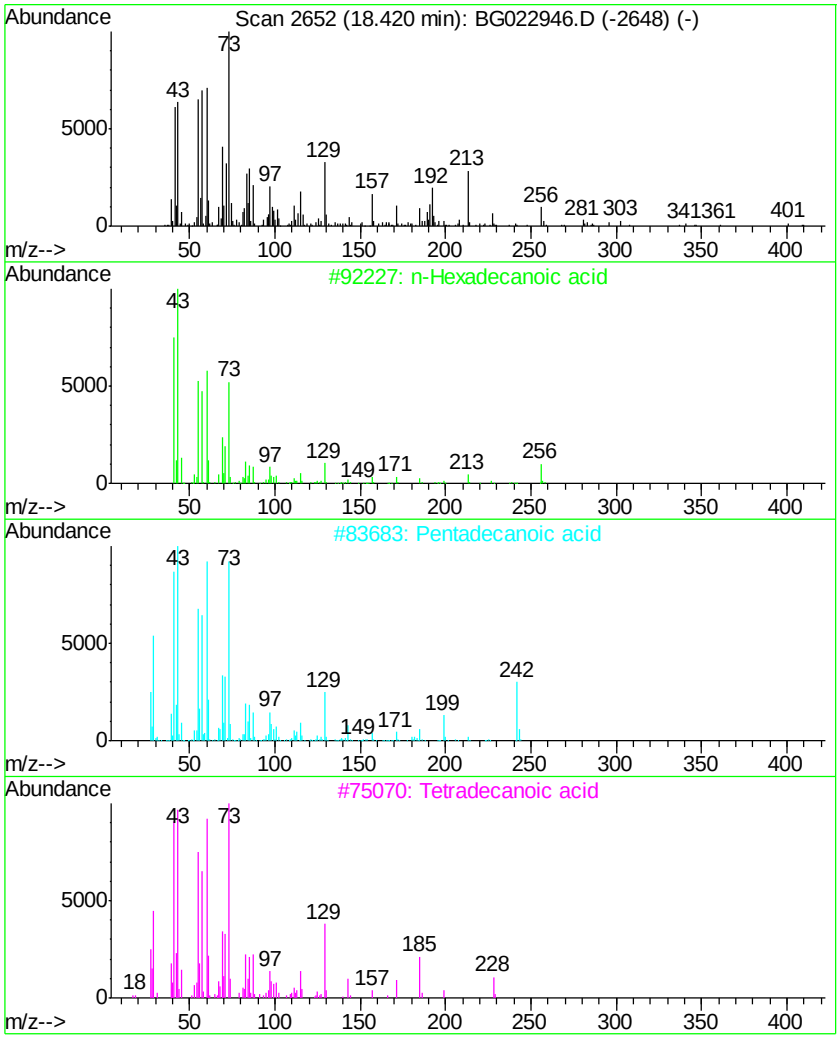
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

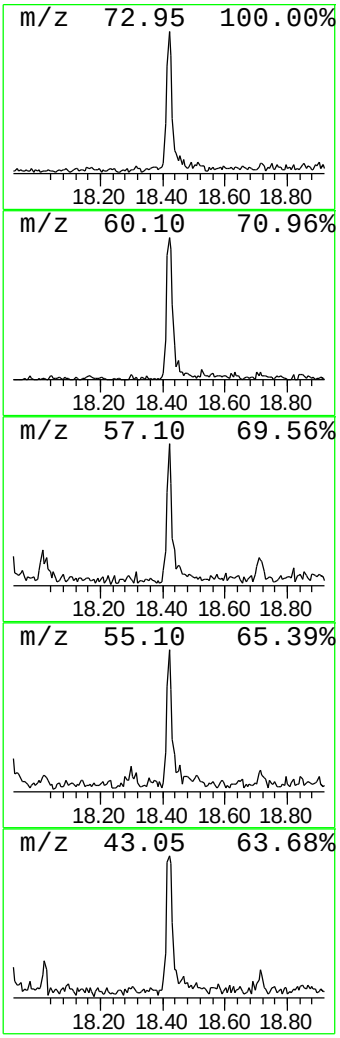
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	3.61 ng	438352	Phenanthrene-d10	17.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
4	Tridecanoic acid	214	C13H26O2	000638-53-9	38
5	Methyl 2,6-anhydro-.alpha.-d-alt...	176	C7H12O5	1000130-02-0	35





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Sample : H3900-05
Misc :
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Instrument : BNA_G
ClientSampleId : P-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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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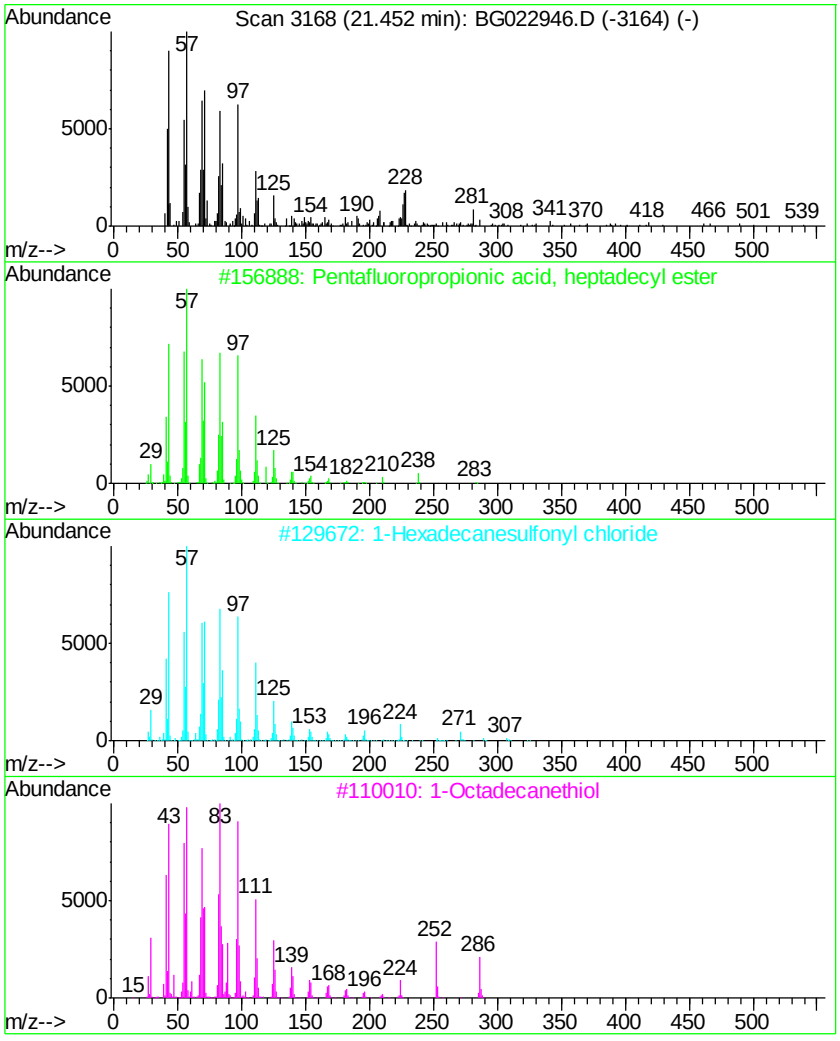
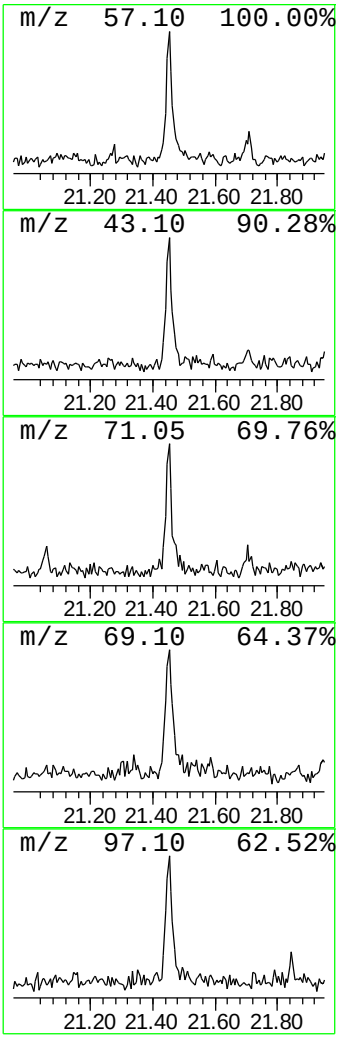
Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.45	2.08 ng	318221	Chrysene-d12	21.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
2	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	90
3	1-Octadecanethiol	286	C18H38S	002885-00-9	89
4	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	83
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	83





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Sample : H3900-05
Misc :
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Instrument : BNA_G
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

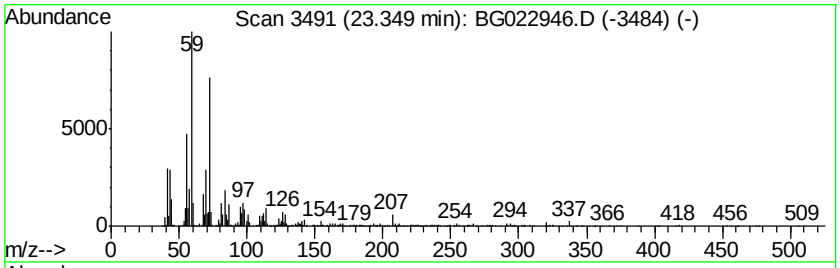
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

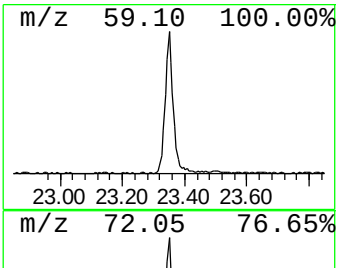
****

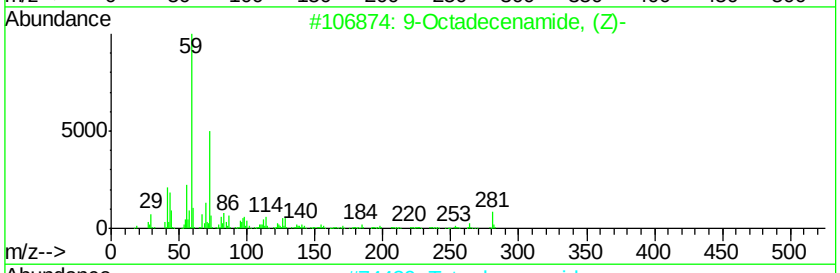
Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 3

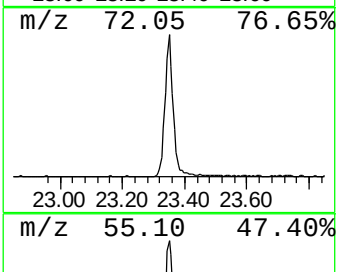
R.T.	EstConc	Area	Relative to ISTD	R.T.
23.35	11.83 ng	1811900	Chrysene-d12	21.85

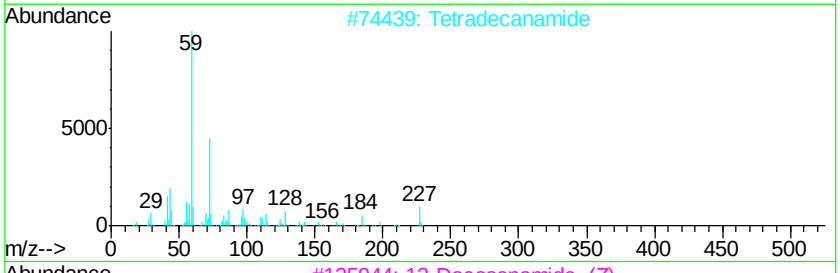
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	58
2	Tetradecanamide	227	C14H29NO	000638-58-4	53
3	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	42
4	2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	30
5	Cyclopentylsilane	100	C5H12Si	080249-74-7	30

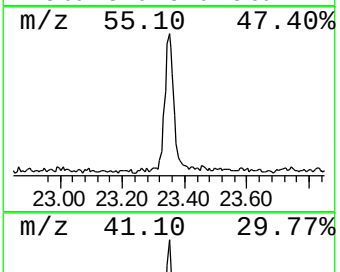


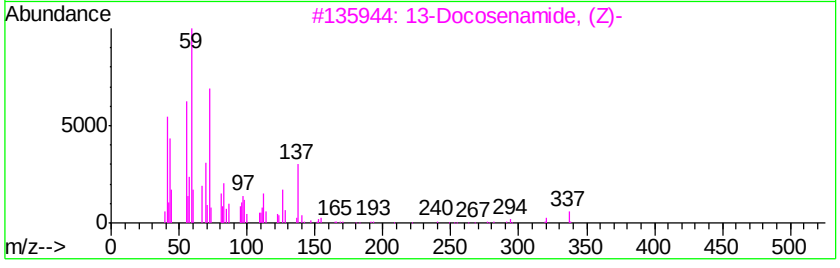


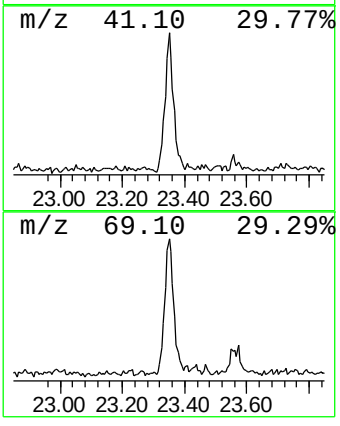












Tentatively Identified Compound (LSC) summary

Data Path : V:\HPCHEM1\BNA_G\DATA\BG070916\
Data File : BG022946.D
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Operator : UM/SJ
Sample : H3900-05
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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
unknown3.04	3.04	5.9	ng	214234	1	8.16	726099	20.0
2-Pentanone, 4-hy...	5.22	4.2	ng	152838	1	8.16	726099	20.0
unknown7.68	7.68	73.0	ng	2650510	1	8.16	726099	20.0
n-Hexadecanoic acid	18.42	3.6	ng	438352	4	17.55	2427150	20.0
Pentafluoropropio...	21.45	2.1	ng	318221	5	21.85	3064370	20.0
9-Octadecenamide,...	23.35	11.8	ng	1811900	5	21.85	3064370	20.0