LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110416\
Data File : BG024707.D
Acq On : 5 Nov 2016 11:26
Operator : UM/SJ
Sample : H5526-16
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-105-29.5-30.0

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-BG102516.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	3.125	43	49	70	rVB	8074814	14607592	100.00%	21.884%
2	5.329	417	424	434	rBV	483369	799495	5.47%	1.198%
3	5.799	497	504	513	rBV	2293176	3811969	26.10%	5.711%
4	7.409	769	778	788	rBV	2336645	4273119	29.25%	6.402%
5	7.791	834	843	851	rBV	2264341	4018817	27.51%	6.021%
6	8.266	916	924	933	rBV	367616	680991	4.66%	1.020%
7	8.590	971	979	990	rVB	1605148	2904340	19.88%	4.351%
8	9.442	1116	1124	1131	rBV	1477187	2691153	18.42%	4.032%
9	9.518	1132	1137	1150	rVB2	73542	163860	1.12%	0.245%
10	11.093	1397	1405	1412	rBV	476735	885861	6.06%	1.327%
11	13.507	1806	1816	1825	rBV	3459722	5406522	37.01%	8.100%
12	14.318	1945	1954	1961	rBV	1011852	1504554	10.30%	2.254%
13	14.882	2043	2050	2060	rVB	805548	1267989	8.68%	1.900%
14	16.363	2294	2302	2316	rBV	3678720	5923760	40.55%	8.875%
15	17.626	2509	2517	2523	rBV2	1083127	1767538	12.10%	2.648%
16	17.955	2567	2573	2583	rBV2	430469	657132	4.50%	0.984%
17	18.466	2655	2660	2664	rBV2	135713	190268	1.30%	0.285%
18	19.312	2798	2804	2811	rBV2	208827	317678	2.17%	0.476%
19	20.205	2950	2956	2962	rVB	6775076	9279542	63.53%	13.902%
20	21.492	3170	3175	3185	rBV3	148795	265002	1.81%	0.397%
21	21.915	3240	3247	3256	rBV	1409355	2558248	17.51%	3.833%
22	24.277	3645	3649	3656	rVB6	72352	155144	1.06%	0.232%
23	25.346	3815	3831	3845	rBV2	790884	2618257	17.92%	3.923%

Sum of corrected areas: 66748831

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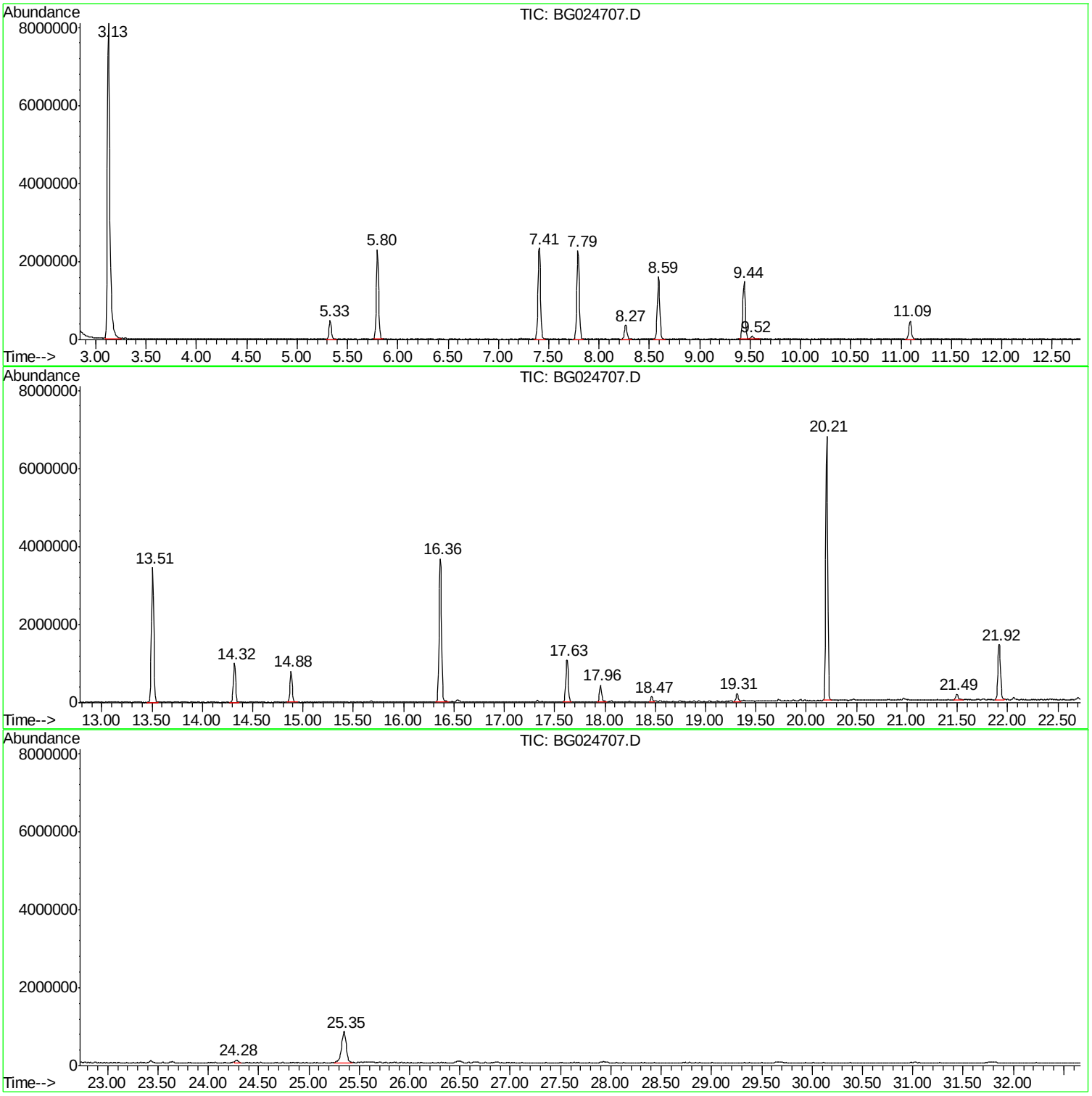
Instrument : BNA_G
ClientSampleId : SB-105-29.5-30.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110416\
Data File : BG024707.D
Acq On : 5 Nov 2016 11:26
Operator : UM/SJ
Sample : H5526-16
Misc :
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Instrument : BNA_G
ClientSampleId : SB-105-29.5-30.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
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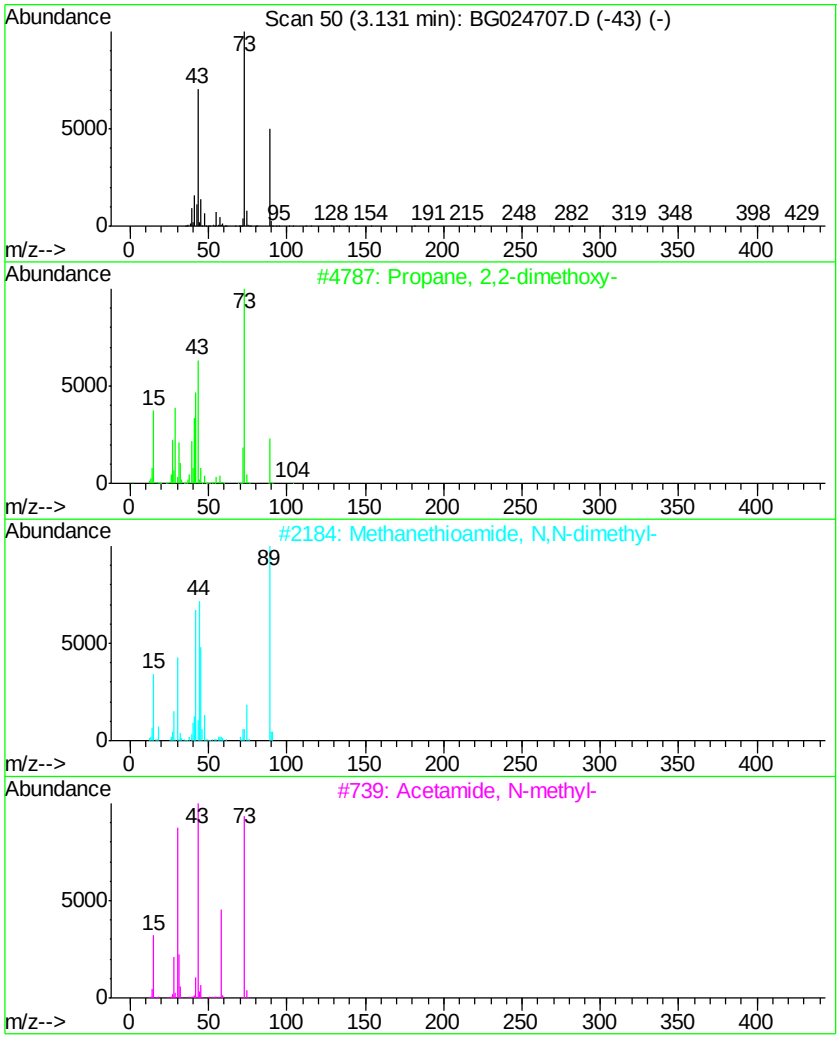
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

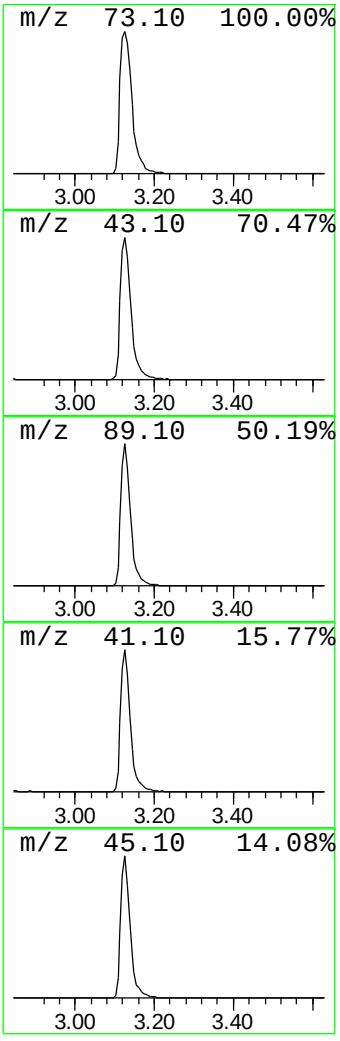
****

Peak Number 1 unknown3.13 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	429.01 ng	14607600	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	33
2	Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	32
3	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
4	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	17
5	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	10





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Data File : BG024707.D
Acq On : 5 Nov 2016 11:26
Operator : UM/SJ
Sample : H5526-16
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-105-29.5-30.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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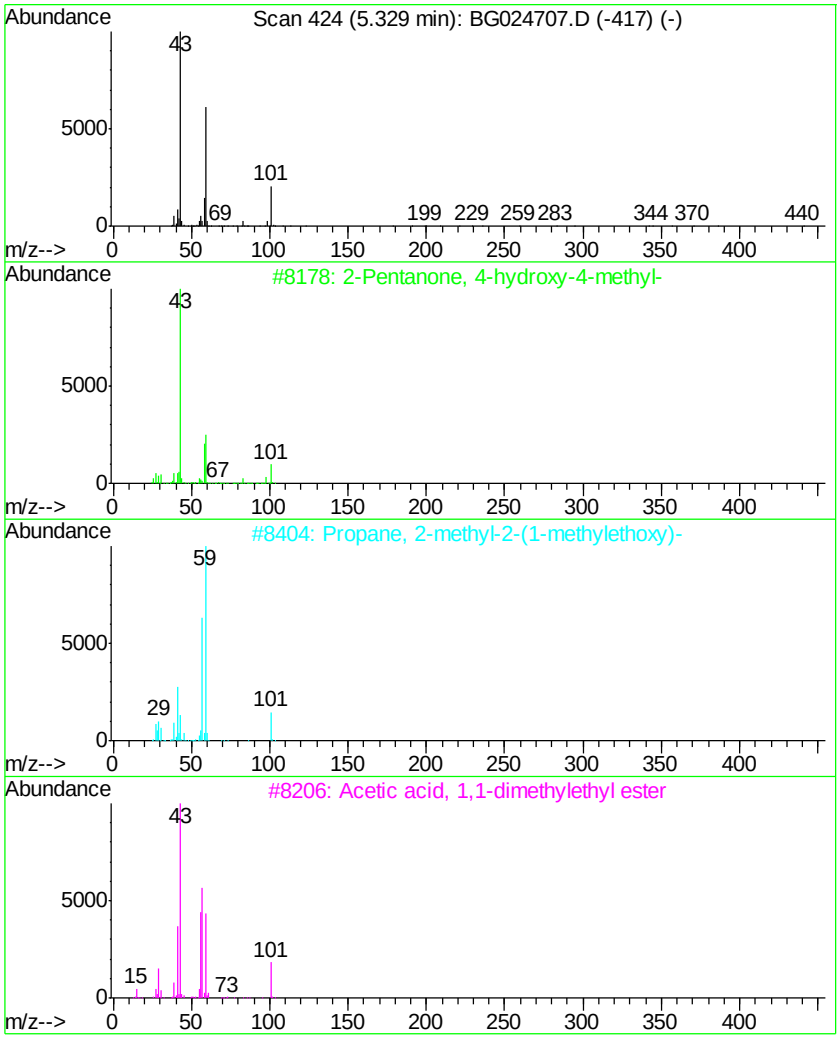
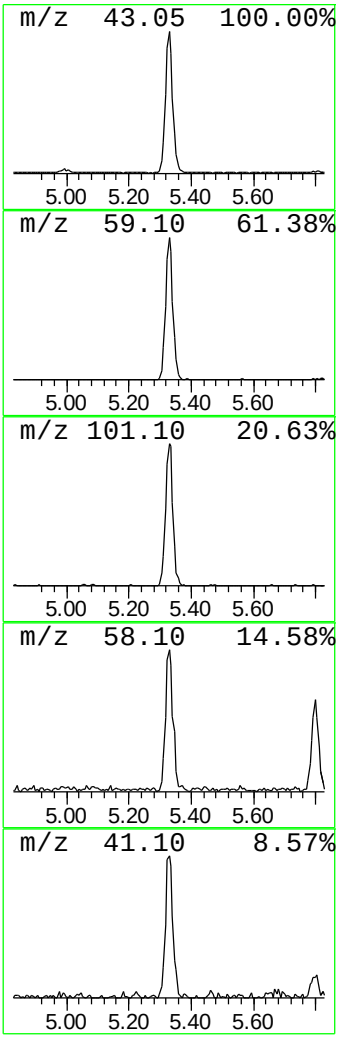
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	23.48 ng	799495	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110416\
Data File : BG024707.D
Acq On : 5 Nov 2016 11:26
Operator : UM/SJ
Sample : H5526-16
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-105-29.5-30.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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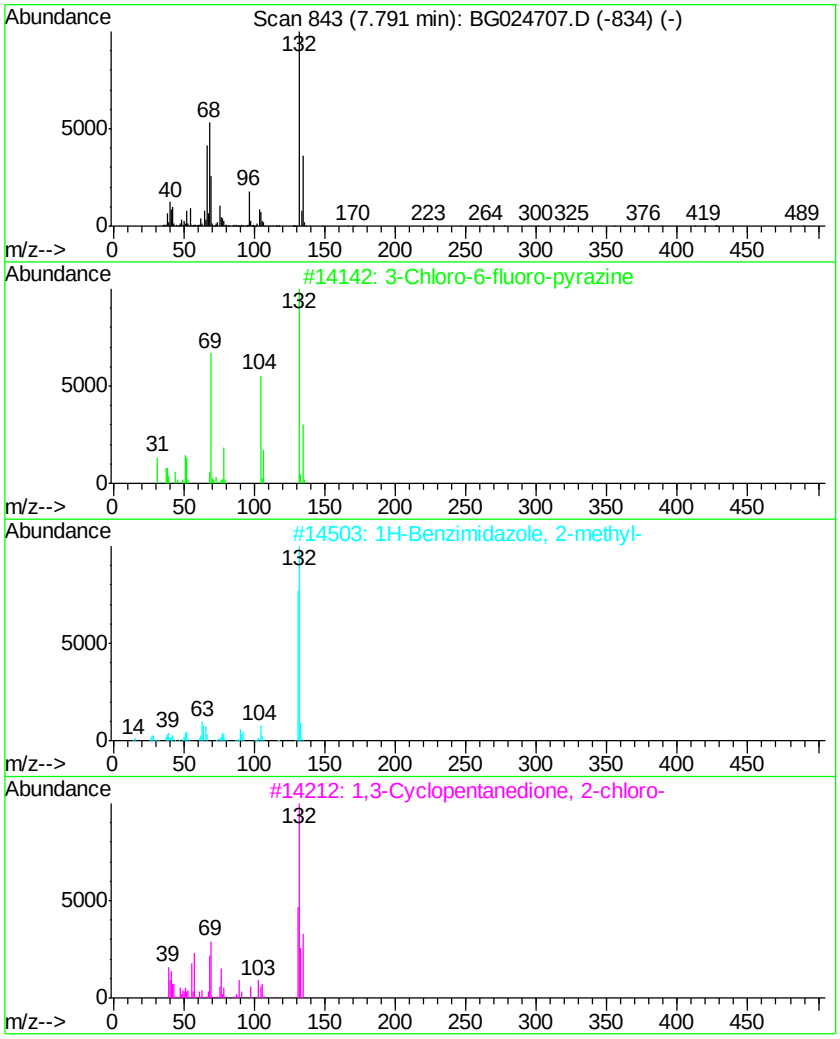
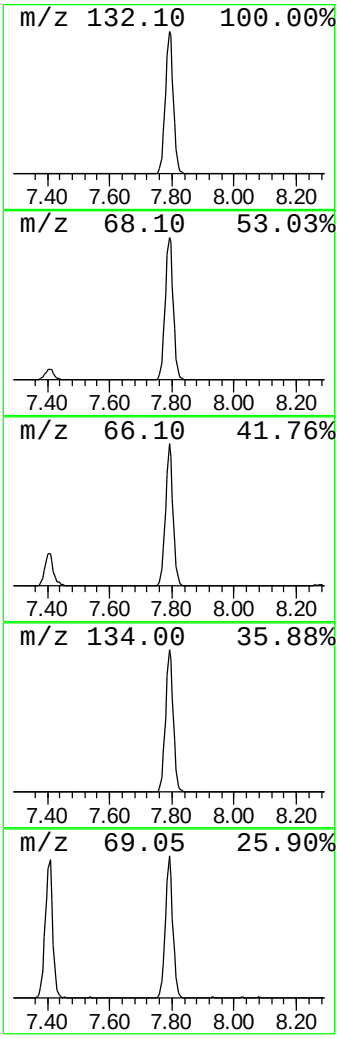
Peak Number 3 unknown7.79 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	118.03 ng	4018820	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
3	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	10
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10





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Data File : BG024707.D
Acq On : 5 Nov 2016 11:26
Operator : UM/SJ
Sample : H5526-16
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-105-29.5-30.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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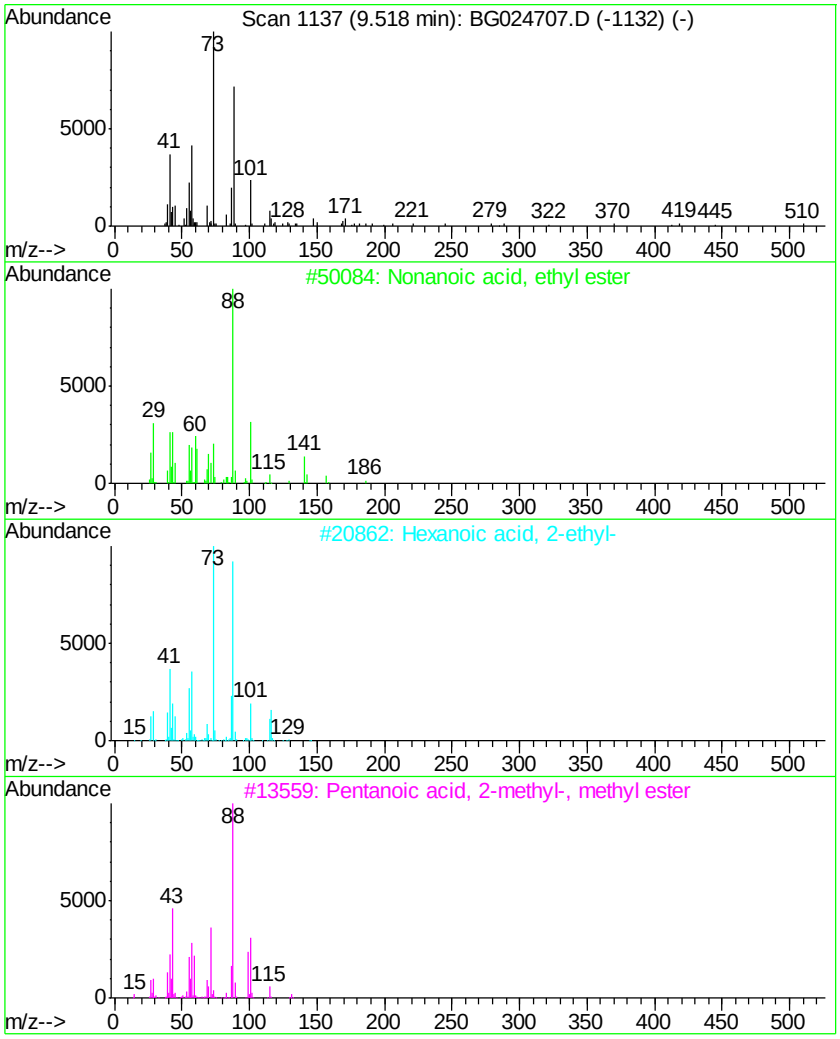
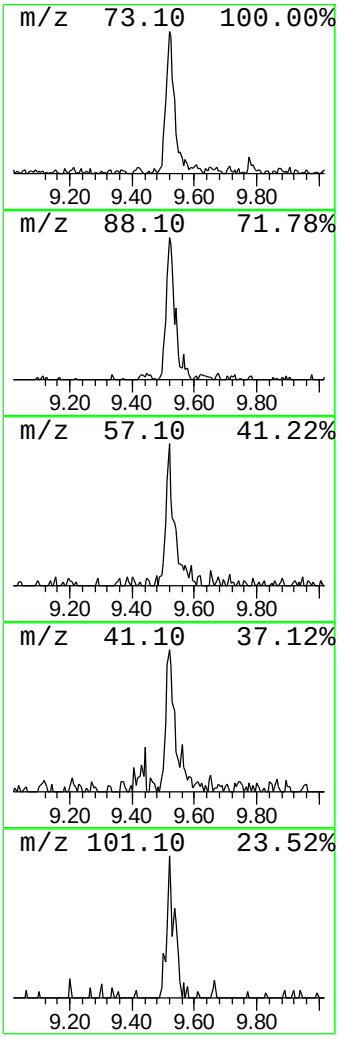
****

Peak Number 5 unknown9.52 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.52	4.81 ng	163860	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid, ethyl ester	186	C11H22O2	000123-29-5	47
2	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	45
3	Pentanoic acid, 2-methyl-, methy...	130	C7H14O2	002177-77-7	38
4	Undecanoic acid, 2-methyl-, meth...	214	C13H26O2	055955-69-6	36
5	Hexanoic acid, 2,4-dimethyl-, me...	158	C9H18O2	014251-44-6	33





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Operator : UM/SJ
Sample : H5526-16
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-105-29.5-30.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

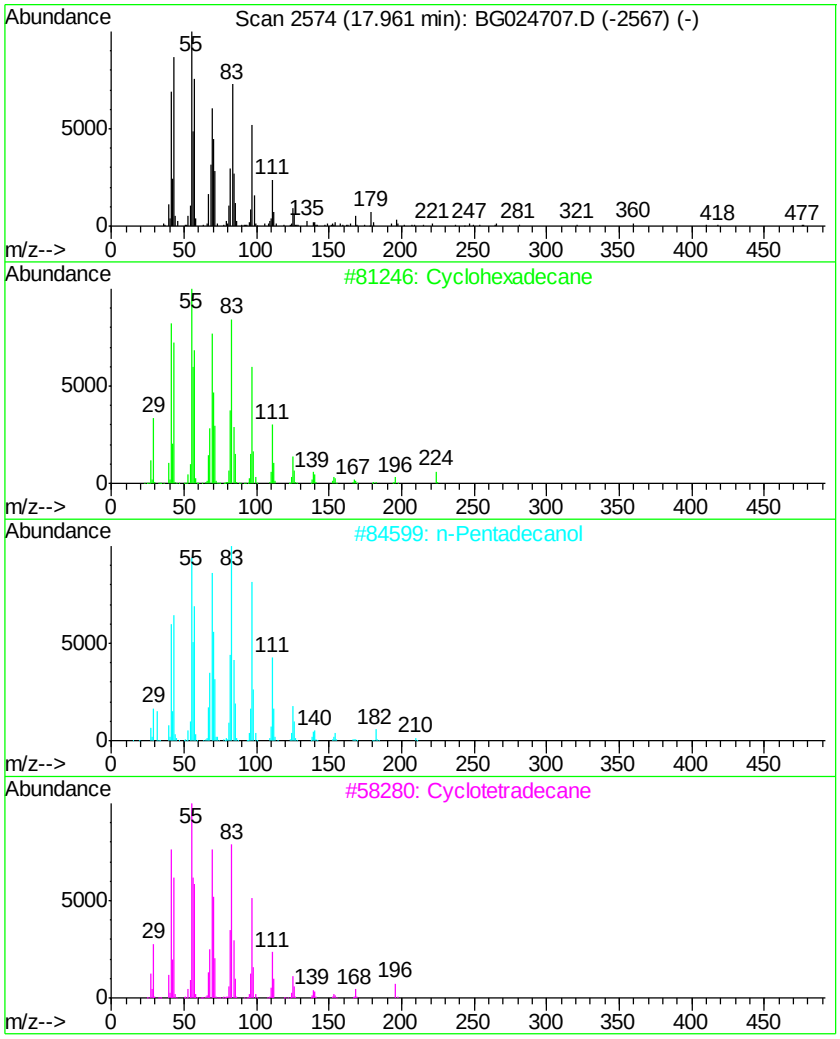
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

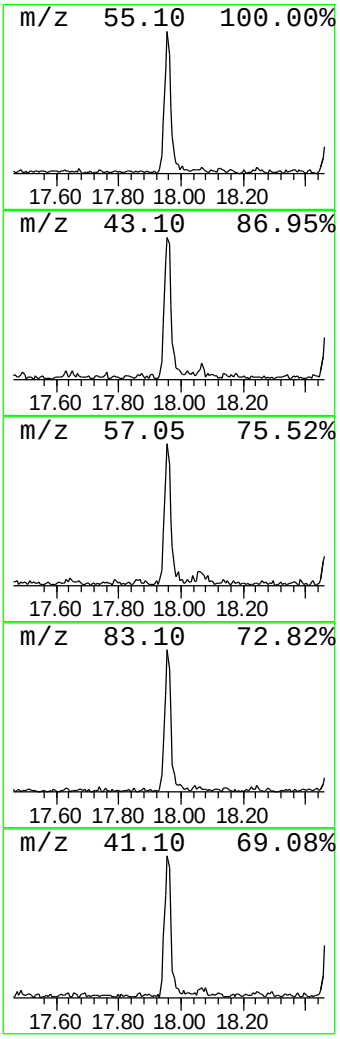
****

Peak Number 6 Cyclohexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.96	7.44 ng	657132	Phenanthrene-d10	17.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	94
2	n-Pentadecanol	228	C15H32O	000629-76-5	91
3	Cyclotetradecane	196	C14H28	000295-17-0	91
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
5	Cyclotetracosane	336	C24H48	000297-03-0	91





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Instrument : BNA_G
ClientSampleId : SB-105-29.5-30.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

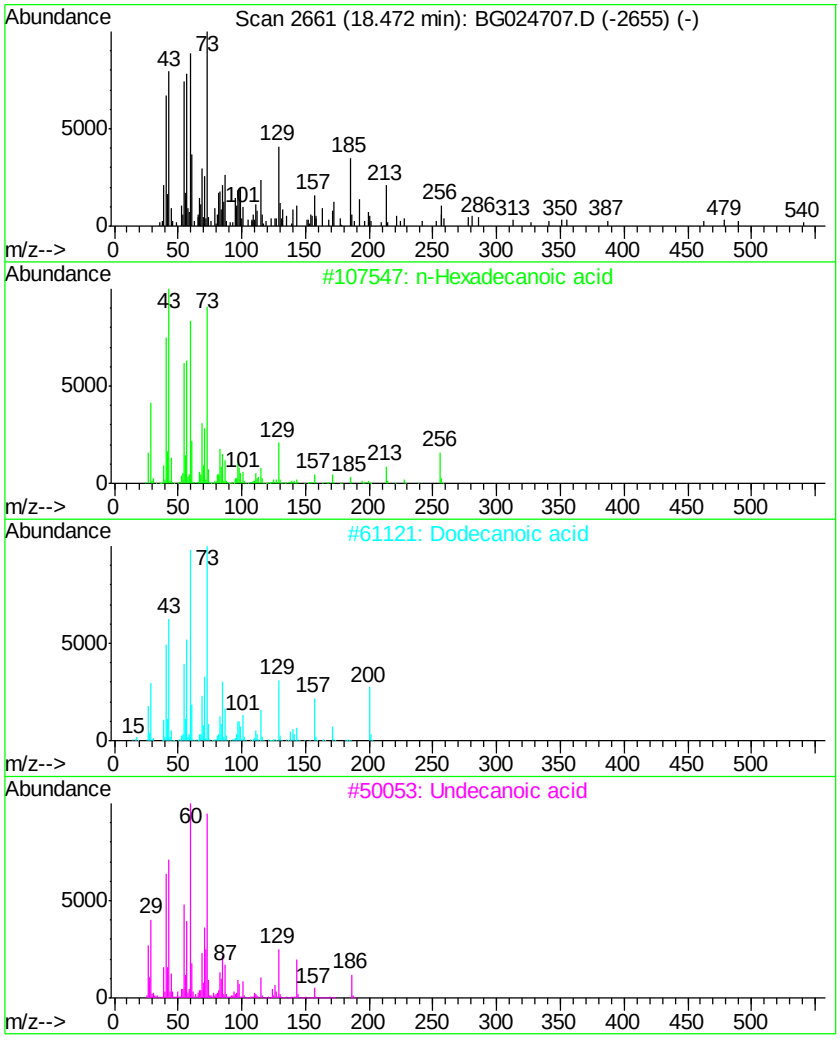
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

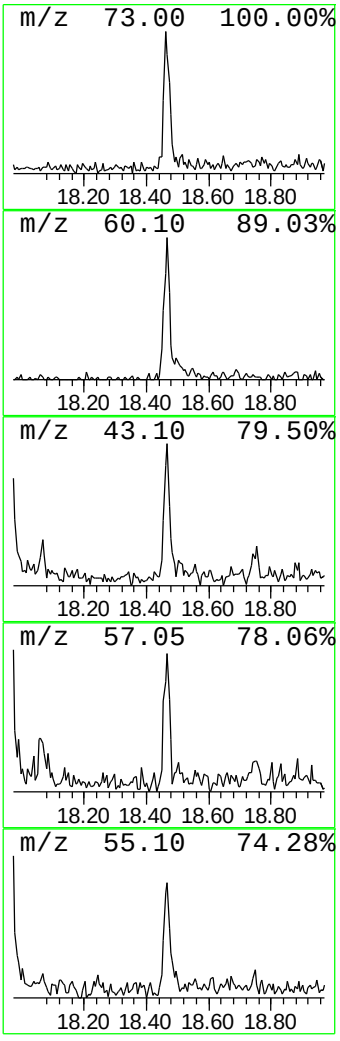
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.47	2.15 ng	190268	Phenanthrene-d10	17.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Dodecanoic acid	200	C12H24O2	000143-07-7	70
3	Undecanoic acid	186	C11H22O2	000112-37-8	50
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	50
5	Tridecanoic acid	214	C13H26O2	000638-53-9	50





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Instrument : BNA_G
ClientSampleId : SB-105-29.5-30.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

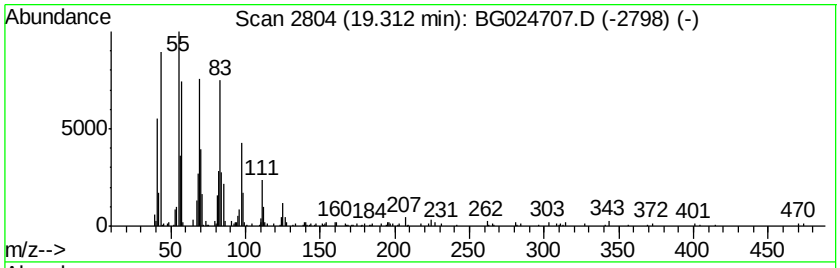
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

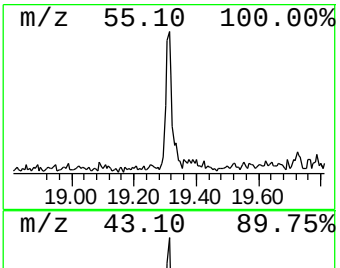
****

Peak Number 8 Pentafluoropropionic acid, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.31	3.59 ng	317678	Phenanthrene-d10	17.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, 4-hex...	388	C19H33F5O2	1000283-04-1	91
2	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	87
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	87





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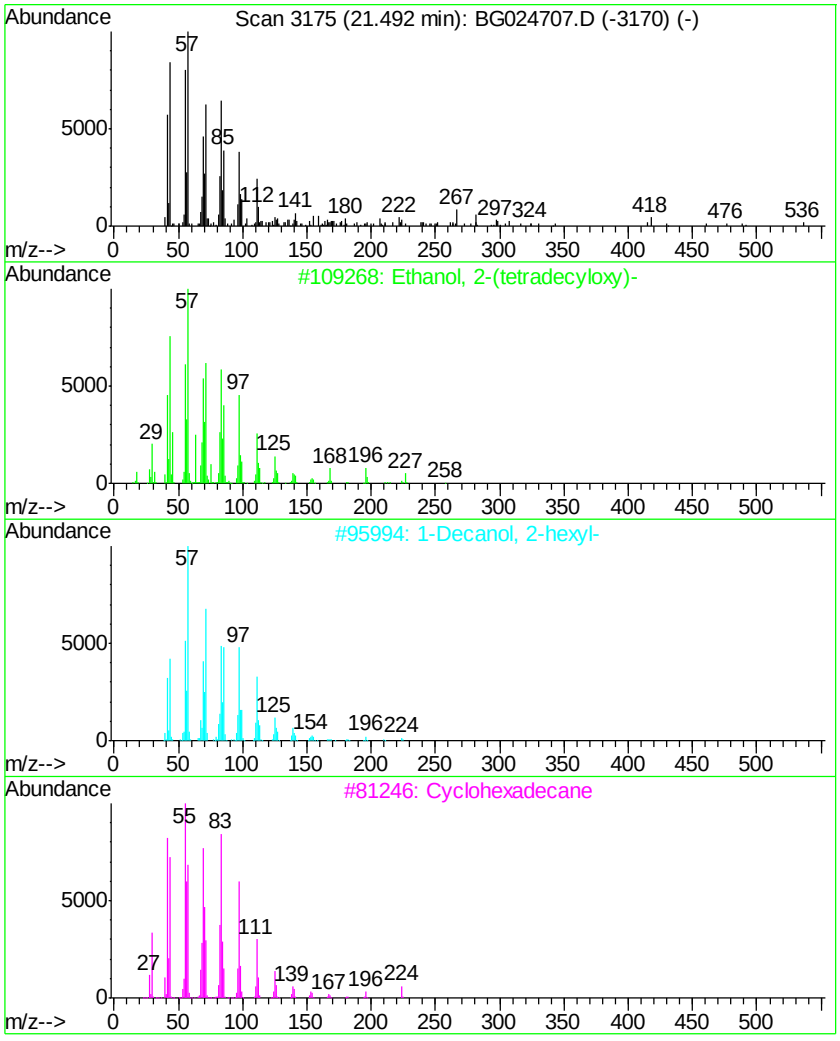
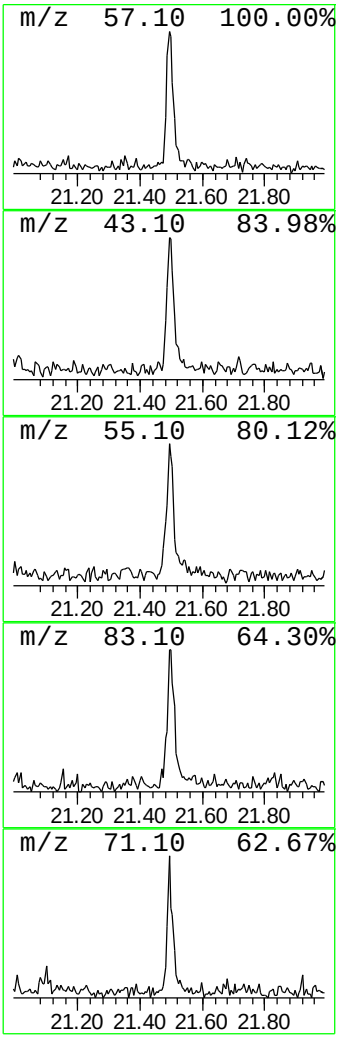
****

Peak Number 9 Ethanol, 2-(tetradecyloxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.49	2.07 ng	265002	Chrysene-d12	21.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
2	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	81
3	Cyclohexadecane	224	C16H32	000295-65-8	70
4	Cyclopentadecane	210	C15H30	000295-48-7	64
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	62





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown3.13	3.13	429.0	ng	14607600	1	8.27	680991	20.0
2-Pentanone, 4-hy...	5.33	23.5	ng	799495	1	8.27	680991	20.0
unknown7.79	7.79	118.0	ng	4018820	1	8.27	680991	20.0
unknown9.52	9.52	4.8	ng	163860	1	8.27	680991	20.0
Cyclohexadecane	17.96	7.4	ng	657132	4	17.63	1767540	20.0
n-Hexadecanoic acid	18.47	2.1	ng	190268	4	17.63	1767540	20.0
Pentafluoropropio...	19.31	3.6	ng	317678	4	17.63	1767540	20.0
Ethanol, 2-(tetra...	21.49	2.1	ng	265002	5	21.92	2558250	20.0