LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024614.D
Acq On : 2 Nov 2016 5:43
Operator : UM/SJ
Sample : H5489-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-72-9.5-10.0

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	2.979	18	24	44	rVB	7202983	21791989	100.00%	18.305%
2	3.126	44	49	67	rVB	9027023	17687518	81.17%	14.858%
3	3.273	67	74	97	rVB	6266008	15954358	73.21%	13.402%
4	3.531	113	118	130	rVB3	176474	340141	1.56%	0.286%
5	5.329	417	424	435	rBV	640777	1058162	4.86%	0.889%
6	5.799	494	504	515	rBV	2841925	4745998	21.78%	3.987%
7	7.403	768	777	788	rBV	2865941	5230849	24.00%	4.394%
8	7.791	834	843	853	rBV	2720192	4988745	22.89%	4.191%
9	8.267	917	924	935	rBV	454792	838153	3.85%	0.704%
10	8.596	971	980	989	rBV	2071583	3786547	17.38%	3.181%
11	9.442	1116	1124	1134	rBV	1782133	3300846	15.15%	2.773%
12	11.099	1399	1406	1413	rBV	572953	1058108	4.86%	0.889%
13	13.508	1809	1816	1823	rVB	4584357	7257516	33.30%	6.096%
14	14.319	1946	1954	1961	rBV	1061671	1544535	7.09%	1.297%
15	14.883	2042	2050	2057	rBV3	961945	1560147	7.16%	1.311%
16	16.363	2295	2302	2313	rBV	4245209	6706837	30.78%	5.634%
17	17.626	2508	2517	2529	rBV	1252321	2014894	9.25%	1.693%
18	18.473	2656	2661	2670	rBV4	186421	295870	1.36%	0.249%
19	20.206	2949	2956	2964	rBV	8922877	12377930	56.80%	10.397%
20	21.498	3171	3176	3184	rBV2	297159	527029	2.42%	0.443%
21	21.916	3240	3247	3255	rBV	1598204	2828910	12.98%	2.376%
22	23.643	3535	3541	3547	rVB2	192421	386810	1.78%	0.325%
23	25.347	3819	3831	3842	rVB2	886125	2765400	12.69%	2.323%

Sum of corrected areas: 119047292

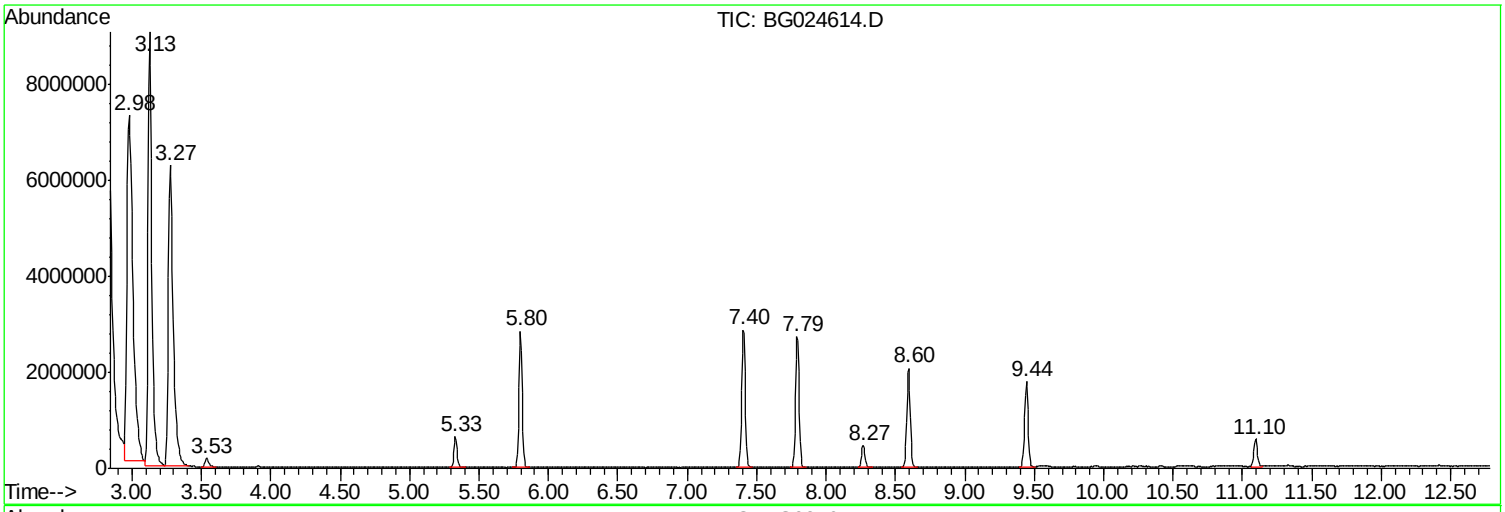
LSC Report - Integrated Chromatogram

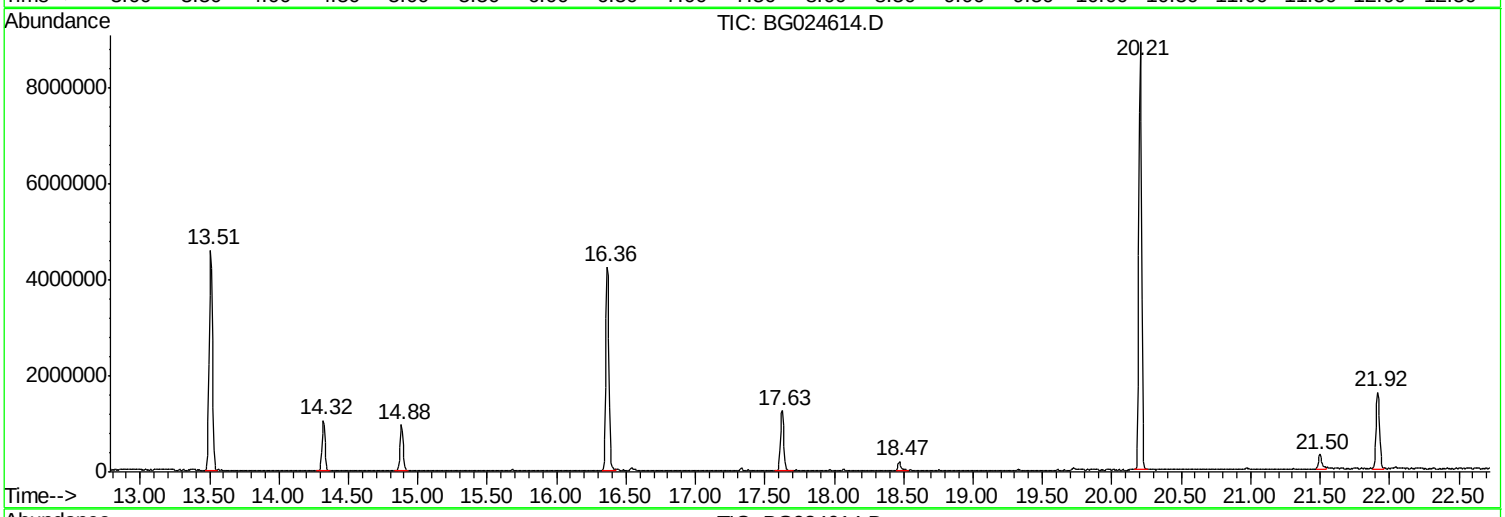
Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024614.D
Acq On : 2 Nov 2016 5:43
Operator : UM/SJ
Sample : H5489-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

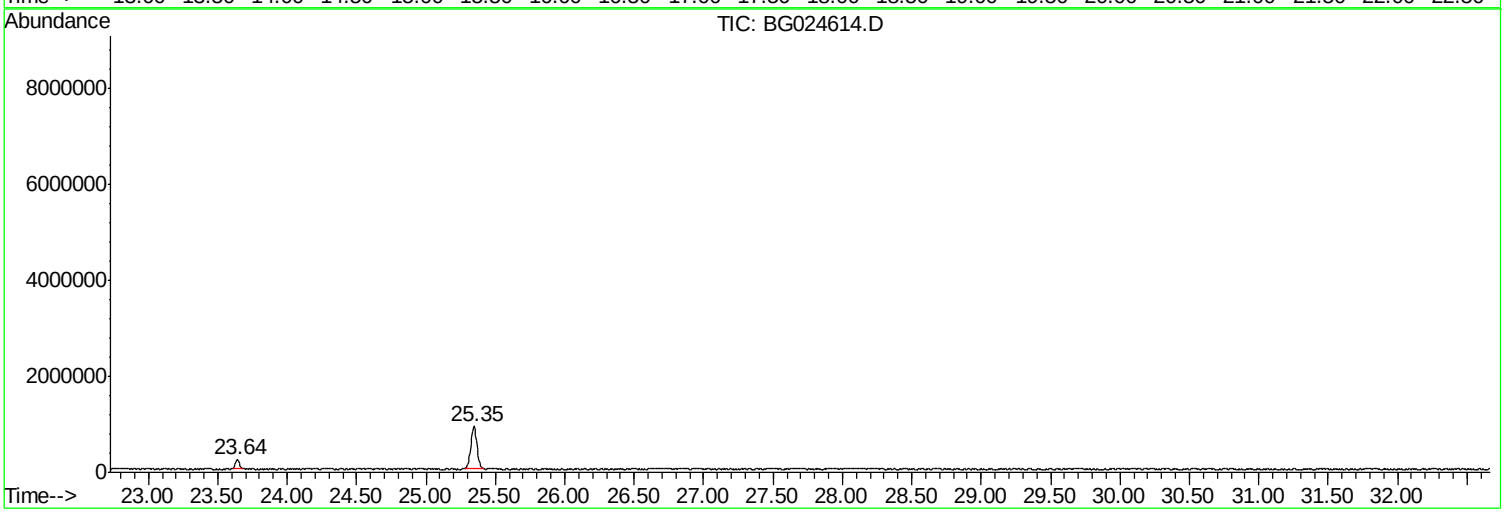
Instrument :
BNA_G
ClientSampleId :
SB-72-9.5-10.0

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

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Data File : BG024614.D
Acq On : 2 Nov 2016 5:43
Operator : UM/SJ
Sample : H5489-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-72-9.5-10.0

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

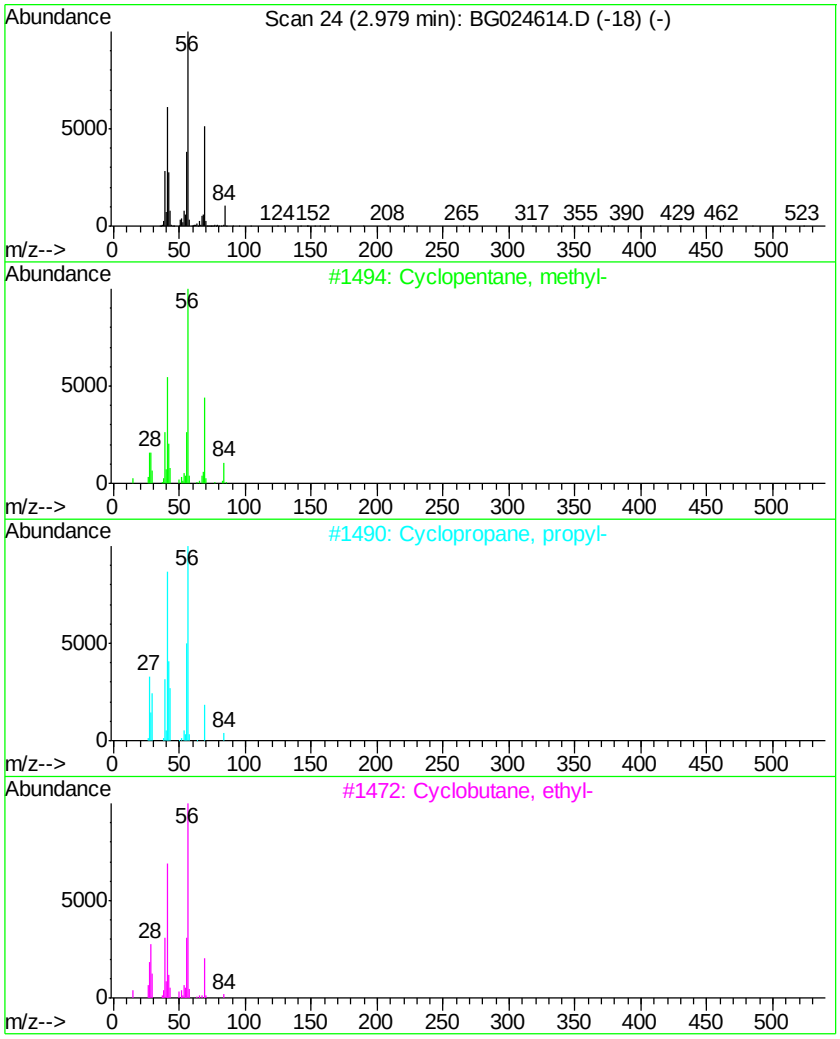
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

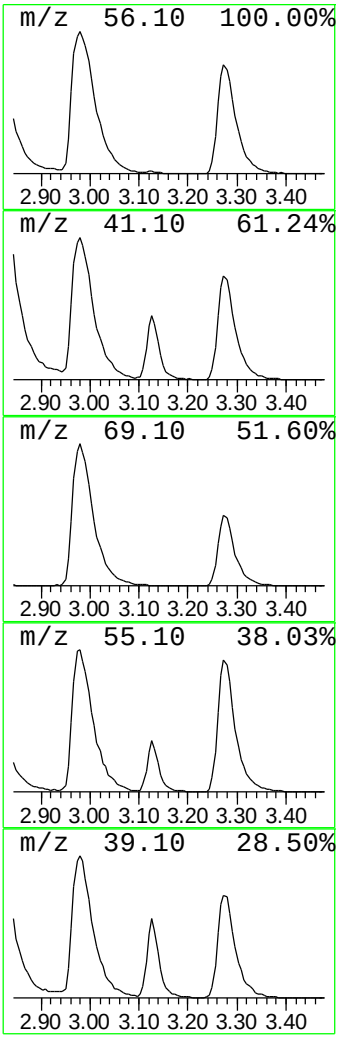
****

Peak Number 1 Cyclopentane, methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.98	520.00 ng	21792000	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclopropane, propyl-	84	C6H12	002415-72-7	64
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	59
4	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	53
5	1-Hexene, 3,4-dimethyl-	112	C8H16	016745-94-1	50





Library Search Compound Report

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Data File : BG024614.D
Acq On : 2 Nov 2016 5:43
Operator : UM/SJ
Sample : H5489-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-72-9.5-10.0

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

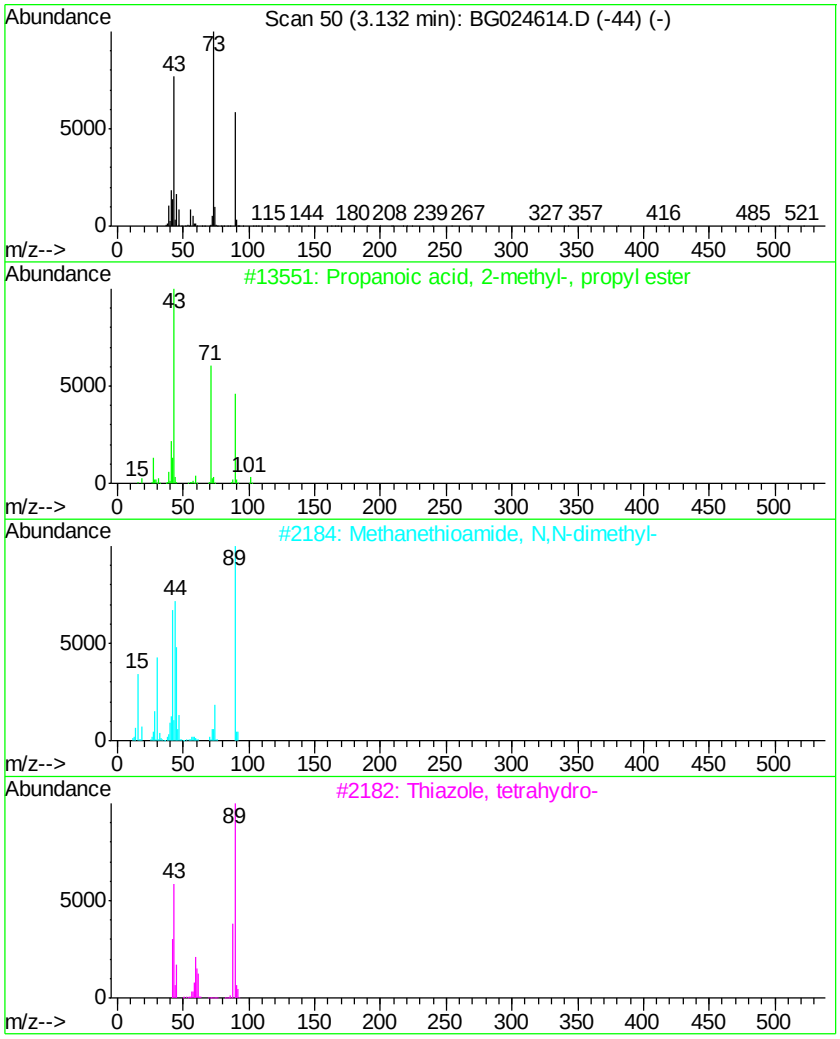
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

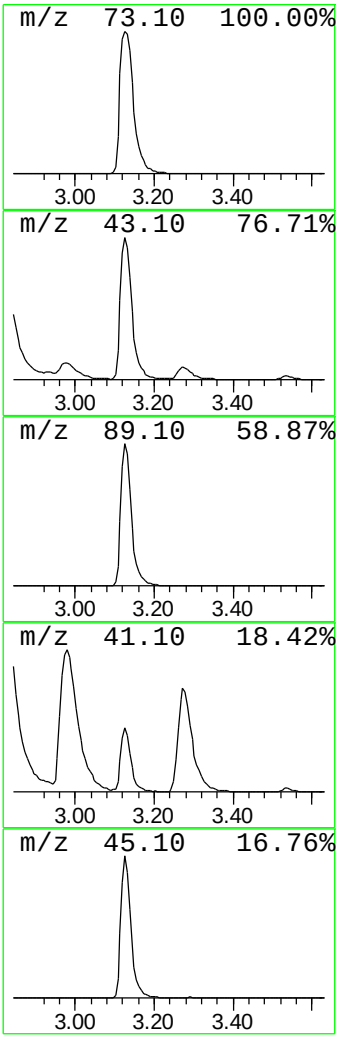
****

Peak Number 2 unknown3.13 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	422.06 ng	17687500	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	43
2	Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	37
3	Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	32
4	N-Methoxydiacetamide	131	C5H9NO3	128459-09-6	23
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	23





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024614.D
Acq On : 2 Nov 2016 5:43
Operator : UM/SJ
Sample : H5489-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-72-9.5-10.0

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

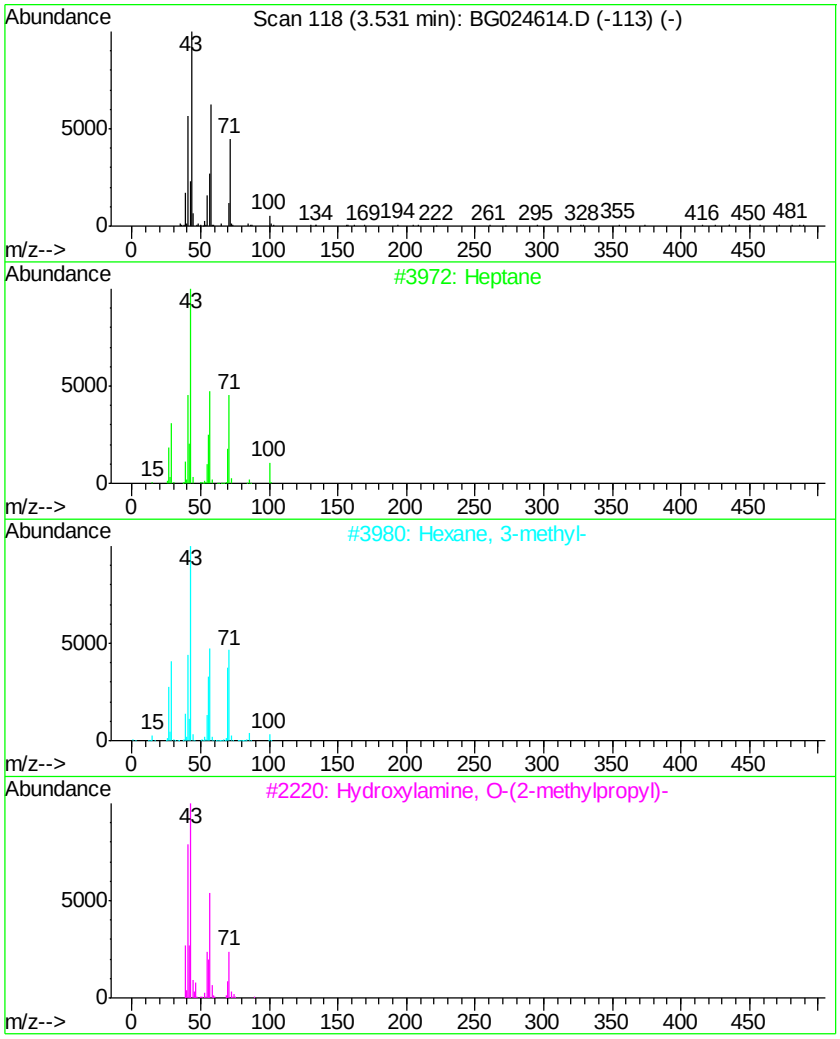
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

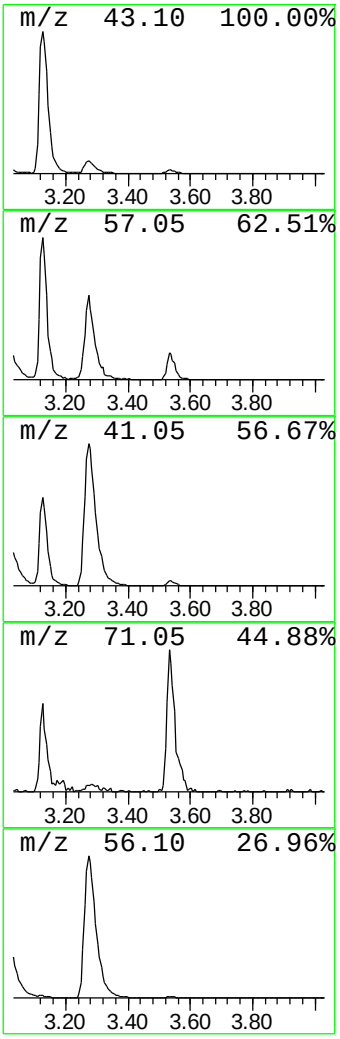
****

Peak Number 4 Heptane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.53	8.12 ng	340141	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	50
2	Hexane, 3-methyl-	100	C7H16	000589-34-4	40
3	Hydroxylamine, O-(2-methylpropyl)-	89	C4H11NO	005618-62-2	40
4	1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	39
5	1-Butanol, 4-butoxy-	146	C8H18O2	004161-24-4	39





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024614.D
Acq On : 2 Nov 2016 5:43
Operator : UM/SJ
Sample : H5489-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-72-9.5-10.0

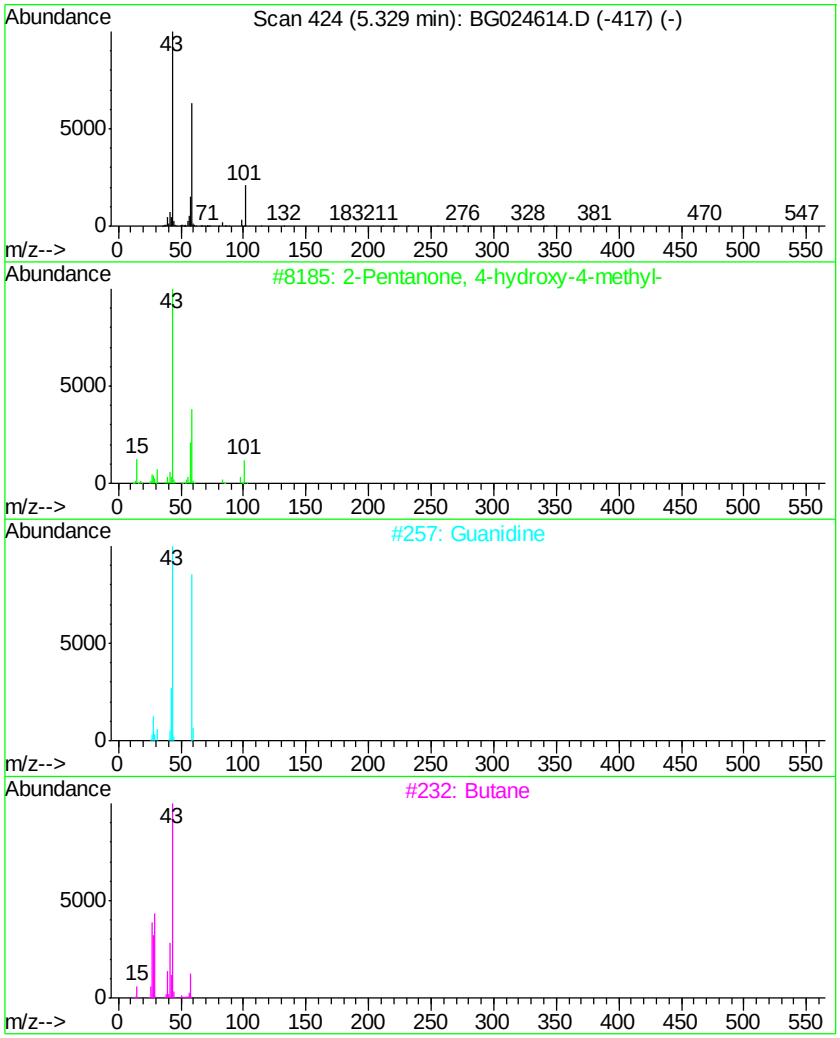
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

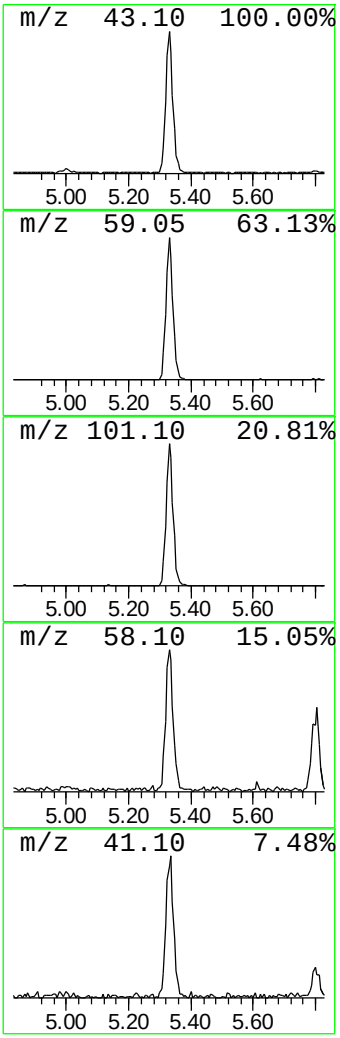
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	25.25 ng	1058160	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	Guanidine	59	CH5N3	000113-00-8	9
3	Butane	58	C4H10	000106-97-8	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9





Library Search Compound Report

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Operator : UM/SJ
Sample : H5489-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-72-9.5-10.0

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

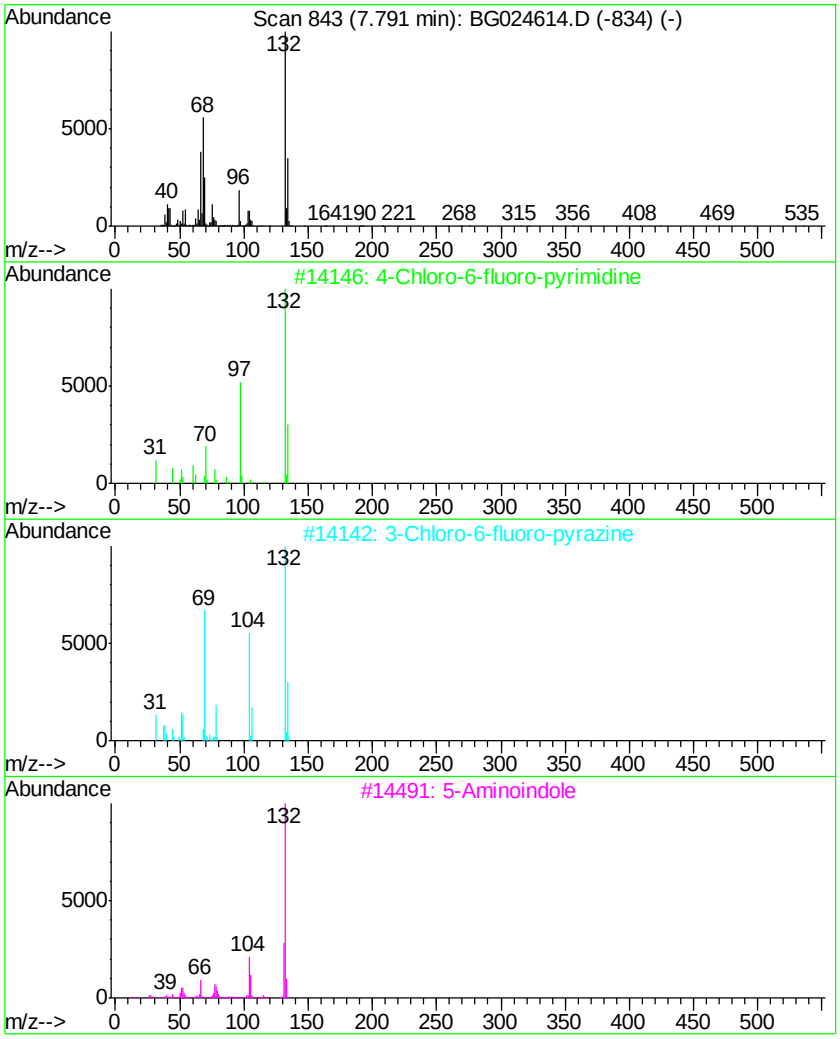
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

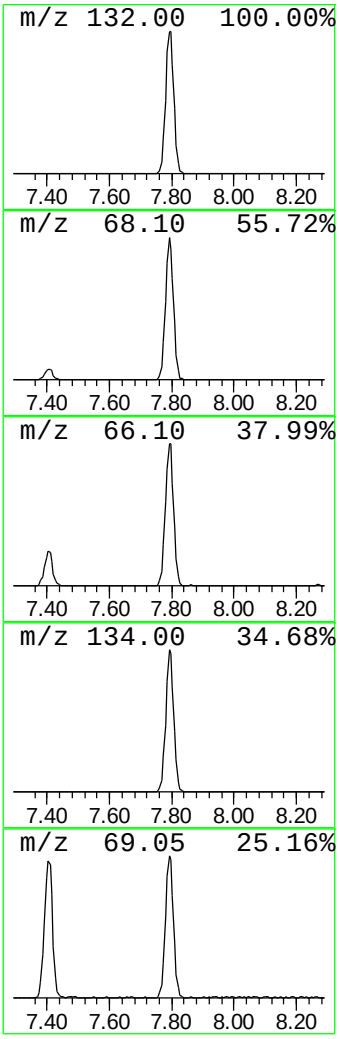
****

Peak Number 6 unknown7.79 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	119.04 ng	4988750	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	5-Aminoindole	132	C8H8N2	005192-03-0	22
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	22
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22





Library Search Compound Report

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Instrument :
BNA_G
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SB-72-9.5-10.0

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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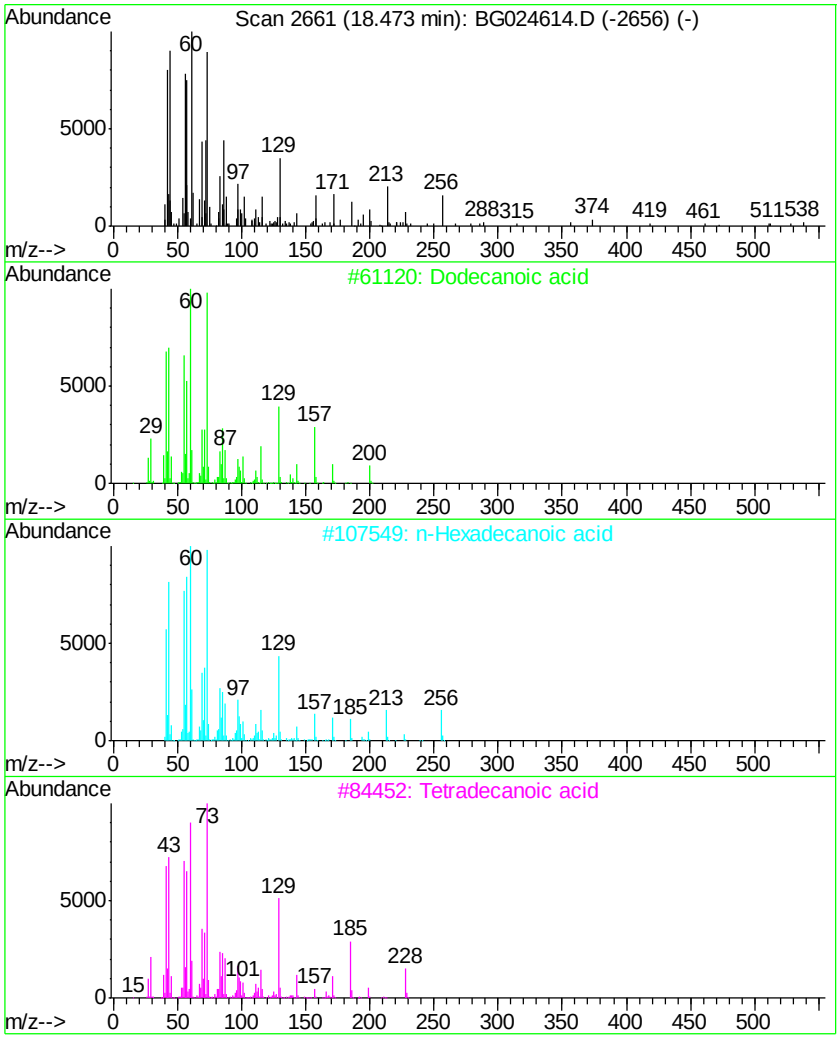
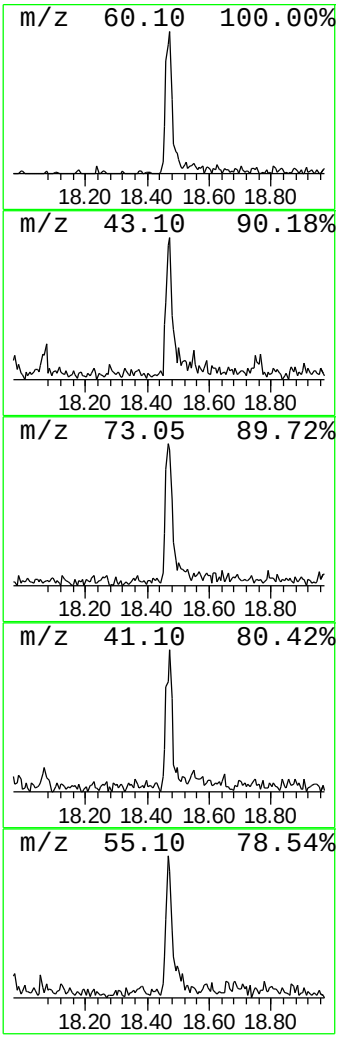
****

Peak Number 8 Dodecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.47	2.94 ng	295870	Phenanthrene-d10	17.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	86
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
4	Nonanoic acid	158	C9H18O2	000112-05-0	49
5	Heptanoic acid	130	C7H14O2	000111-14-8	38





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Operator : UM/SJ
Sample : H5489-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-72-9.5-10.0

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

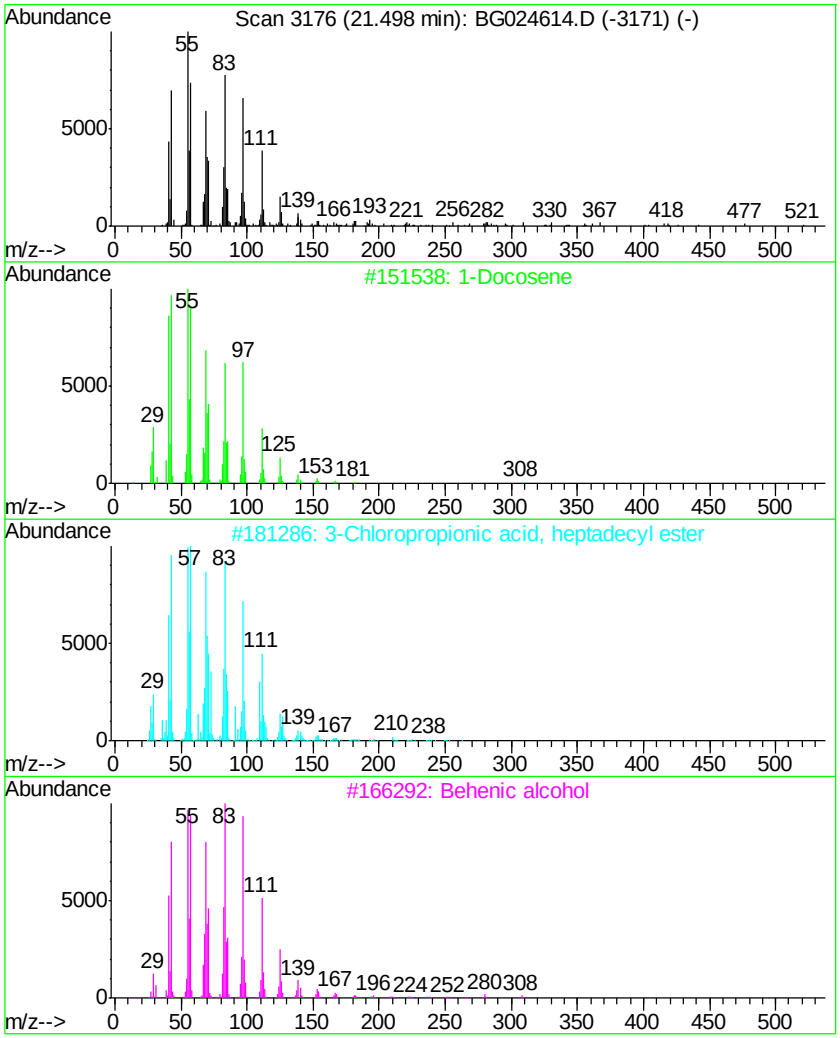
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

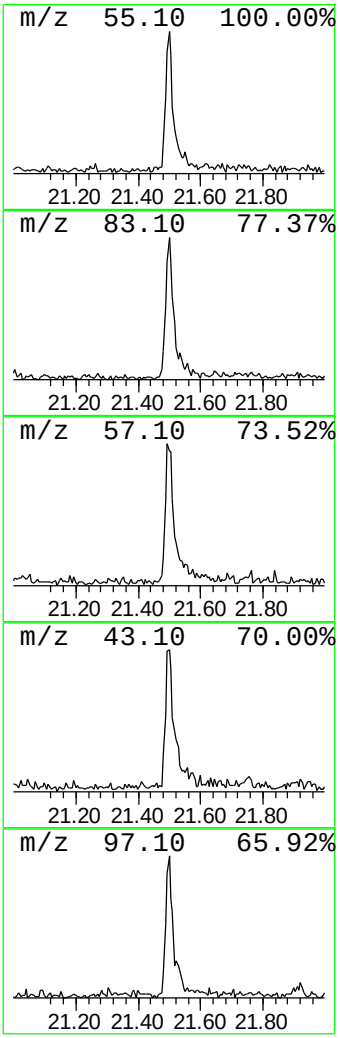
****

Peak Number 9 1-Docosene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.50	3.73 ng	527029	Chrysene-d12	21.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	97
2	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91





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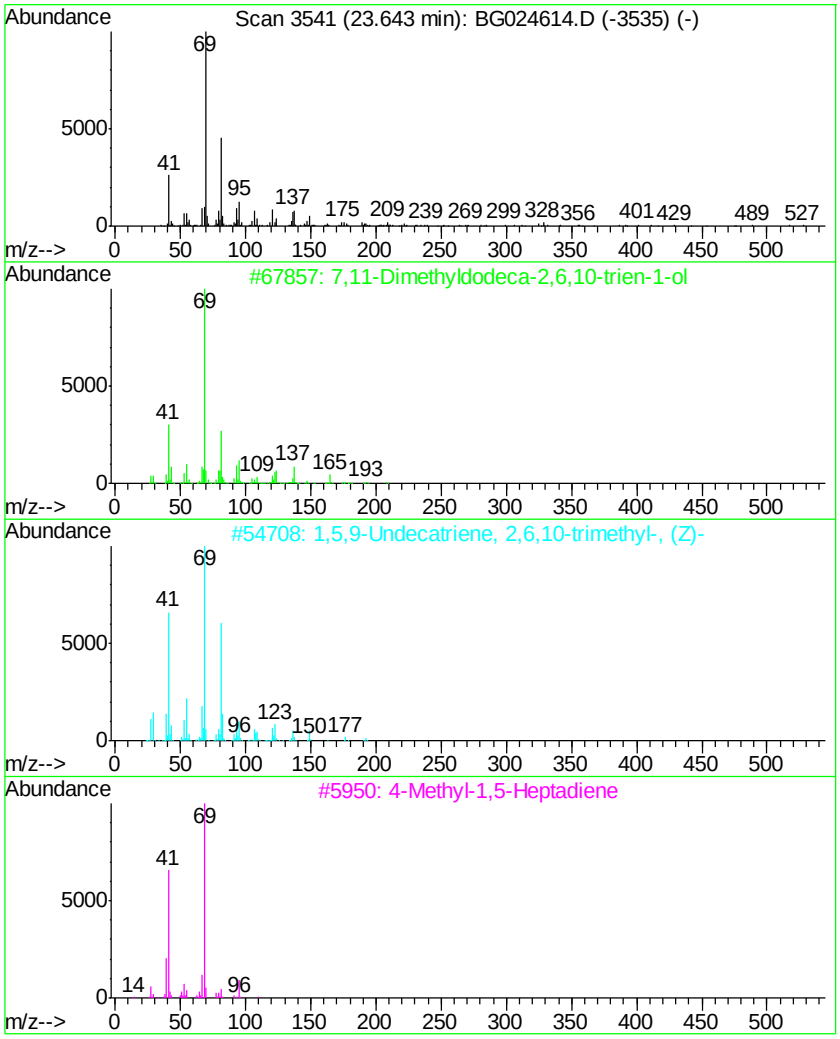
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

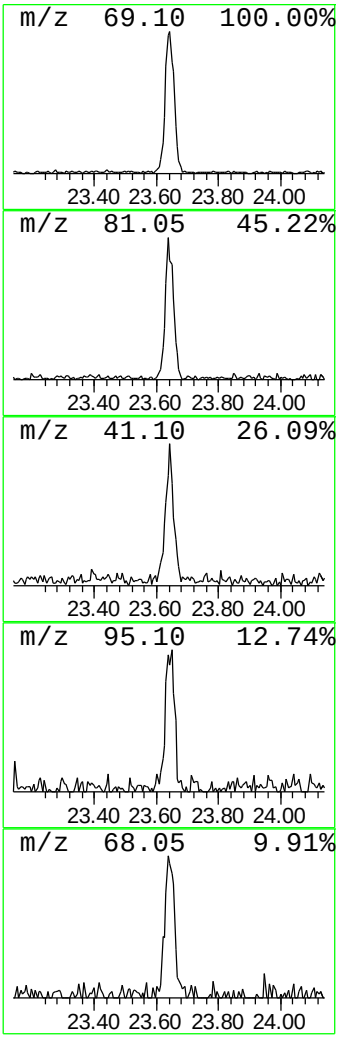
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 7,11-Dimethyldodeca-2,6,10-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.64	2.80 ng	386810	Perylene-d12	25.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
2	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72
3	4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	64
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64
5	Squalene	410	C30H50	000111-02-4	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110116\
Data File : BG024614.D
Acq On : 2 Nov 2016 5:43
Operator : UM/SJ
Sample : H5489-11
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Instrument :
BNA_G
ClientSampleId :
SB-72-9.5-10.0

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
Cyclopentane, met...	2.98	520.0	ng	21792000	1	8.27	838153	20.0
unknown3.13	3.13	422.1	ng	17687500	1	8.27	838153	20.0
Heptane	3.53	8.1	ng	340141	1	8.27	838153	20.0
2-Pentanone, 4-hy...	5.33	25.3	ng	1058160	1	8.27	838153	20.0
unknown7.79	7.79	119.0	ng	4988750	1	8.27	838153	20.0
Dodecanoic acid	18.47	2.9	ng	295870	4	17.63	2014890	20.0
1-Docosene	21.50	3.7	ng	527029	5	21.92	2828910	20.0
7,11-Dimethyldode...	23.64	2.8	ng	386810	6	25.35	2765400	20.0