LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022978.D
Acq On : 9 Jul 2016 23:29
Operator : UM/SJ
Sample : H3935-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C3-5

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	2.896	6	10	29	rVB	333254	750538	7.33%	1.227%
2	3.037	29	34	53	rVB	4318622	6423304	62.77%	10.497%
3	3.190	54	60	71	rVB	326007	579085	5.66%	0.946%
4	5.223	401	406	414	rBV	257642	402778	3.94%	0.658%
5	5.699	480	487	497	rBV	2044958	3331606	32.56%	5.445%
6	7.309	753	761	771	rBV	2395476	4209877	41.14%	6.880%
7	7.679	817	824	833	rBV	2190639	3758615	36.73%	6.142%
8	8.149	898	904	911	rBV	358689	619645	6.05%	1.013%
9	8.478	952	960	968	rBV	1525571	2673637	26.13%	4.369%
10	9.324	1095	1104	1112	rBV	1434334	2631138	25.71%	4.300%
11	10.975	1377	1385	1394	rBV	549997	1012212	9.89%	1.654%
12	13.413	1792	1800	1809	rBV	4230547	6695409	65.43%	10.942%
13	14.236	1933	1940	1946	rBV	649264	953168	9.31%	1.558%
14	14.794	2027	2035	2042	rBV2	1006186	1688278	16.50%	2.759%
15	16.286	2283	2289	2301	rBV	3978960	6296162	61.52%	10.289%
16	17.279	2454	2458	2462	rBV	145686	185709	1.81%	0.303%
17	17.556	2498	2505	2513	rBV	1380370	2146133	20.97%	3.507%
18	18.419	2647	2652	2663	rBV2	352844	509177	4.98%	0.832%
19	19.688	2863	2868	2876	rBV3	171865	257632	2.52%	0.421%
20	20.153	2941	2947	2954	rVB	7186773	10233707	100.00%	16.724%
21	21.422	3156	3163	3164	rBV6	48676	106928	1.04%	0.175%
22	21.457	3164	3169	3182	rVB3	321428	708690	6.93%	1.158%
23	21.704	3207	3211	3216	rBV	101950	146766	1.43%	0.240%
24	21.845	3228	3235	3242	rBV	1414039	2493750	24.37%	4.075%
25	25.200	3795	3806	3818	rVB	817517	2377523	23.23%	3.885%

Sum of corrected areas: 61191467

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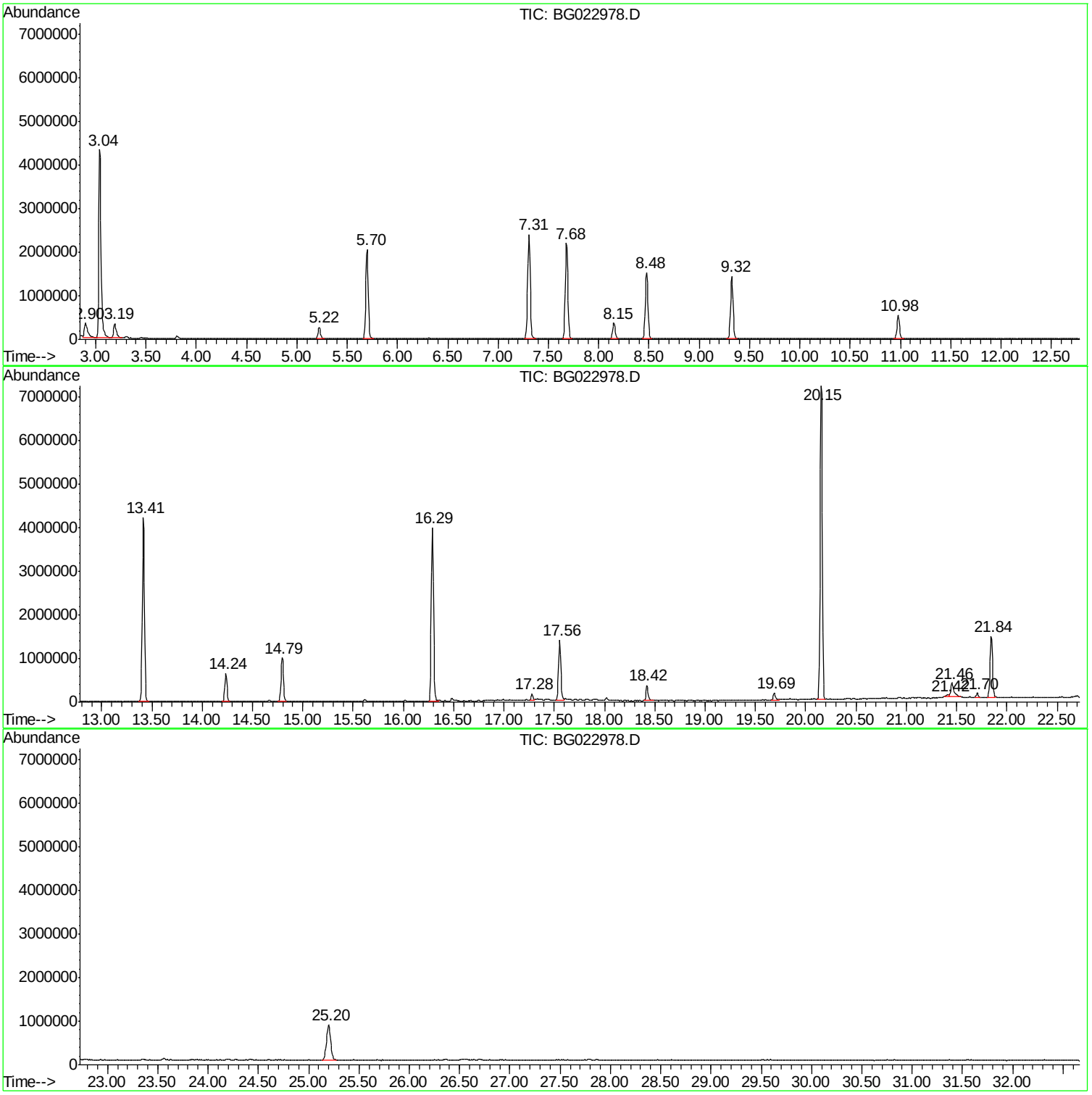
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022978.D
Acq On : 9 Jul 2016 23:29
Operator : UM/SJ
Sample : H3935-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C3-5

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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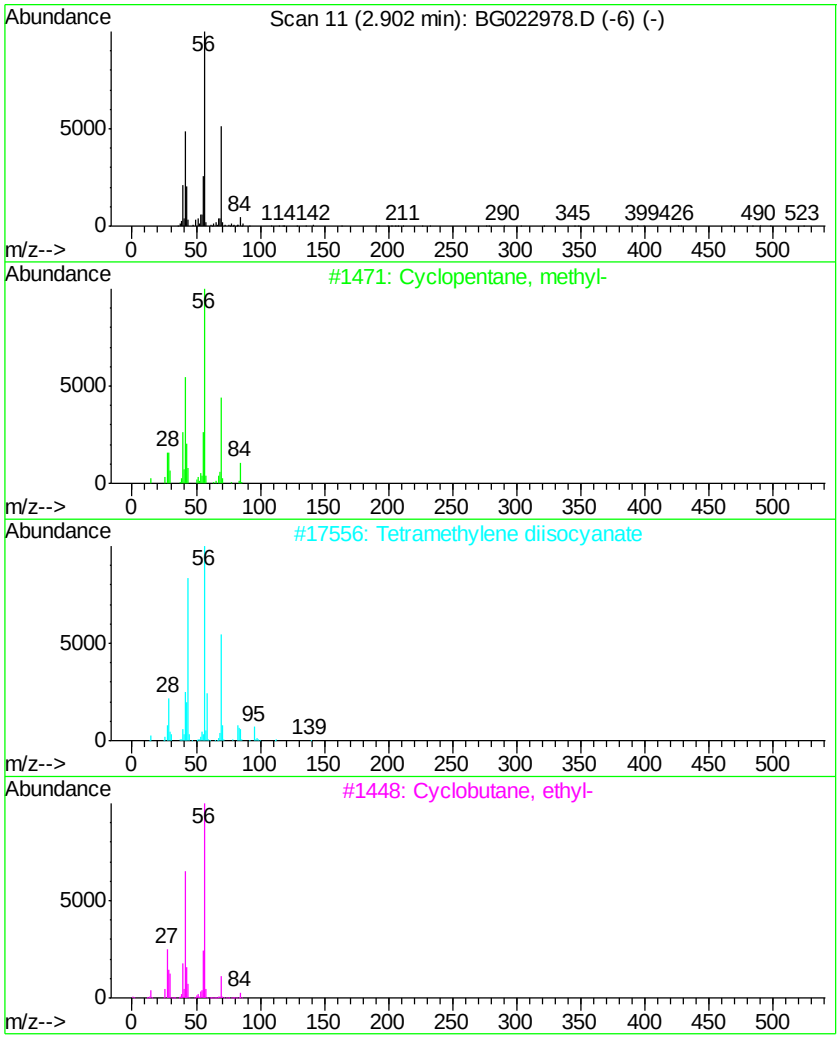
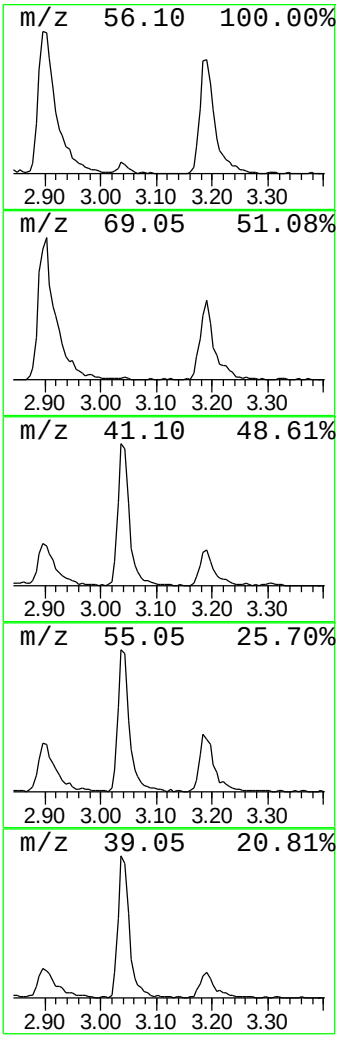
Peak Number 1 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.90	24.22 ng	750538	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	83
2	Tetramethylene diisocyanate	140	C6H8N2O2	004538-37-8	72
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	64
5	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	56





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Data File : BG022978.D
Acq On : 9 Jul 2016 23:29
Operator : UM/SJ
Sample : H3935-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C3-5

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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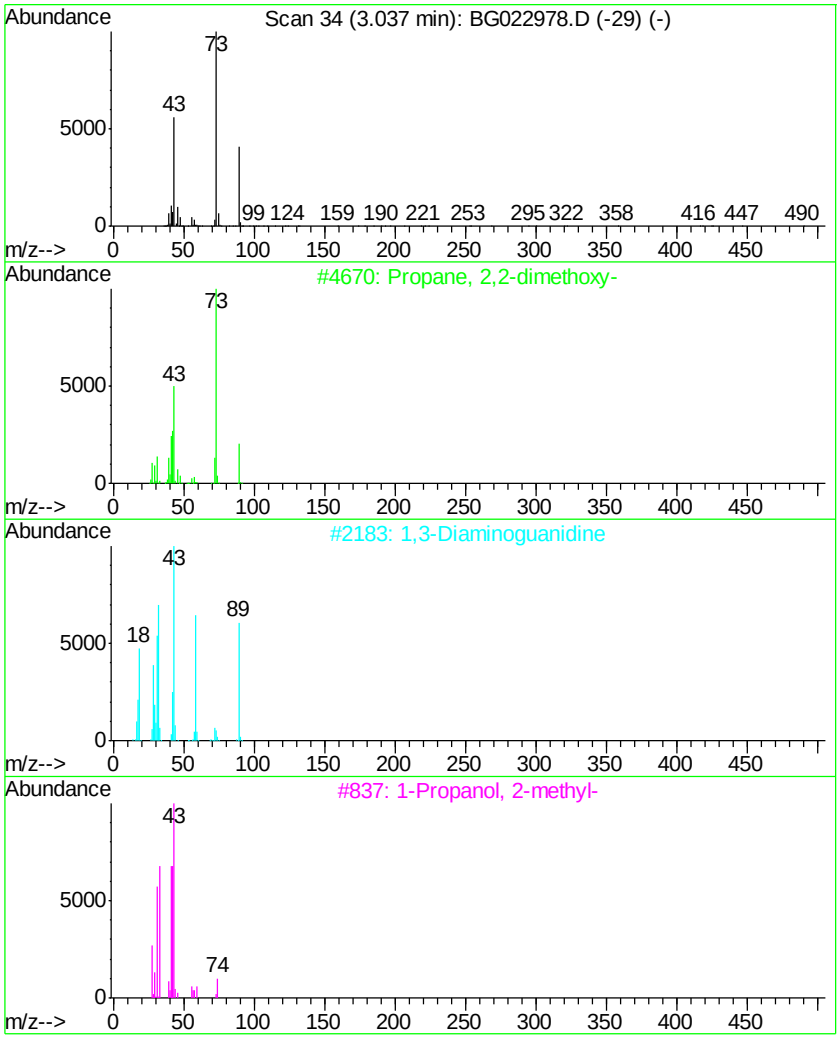
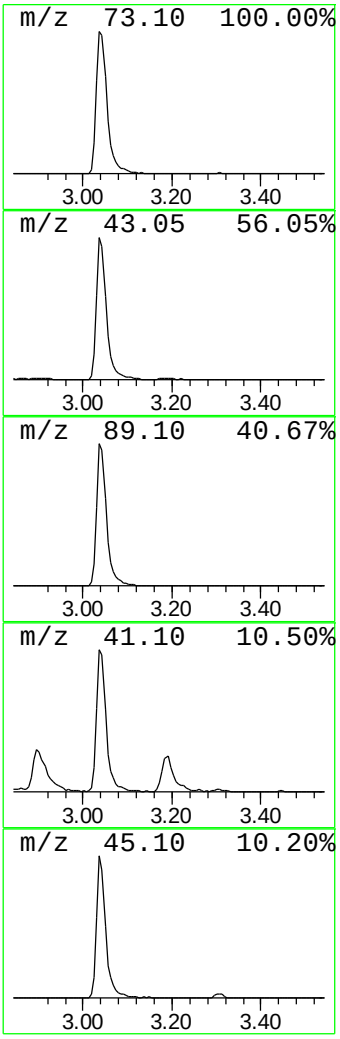
Peak Number 2 unknown3.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	207.32 ng	6423300	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	42
2	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	25
3	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5	1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022978.D
Acq On : 9 Jul 2016 23:29
Operator : UM/SJ
Sample : H3935-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C3-5

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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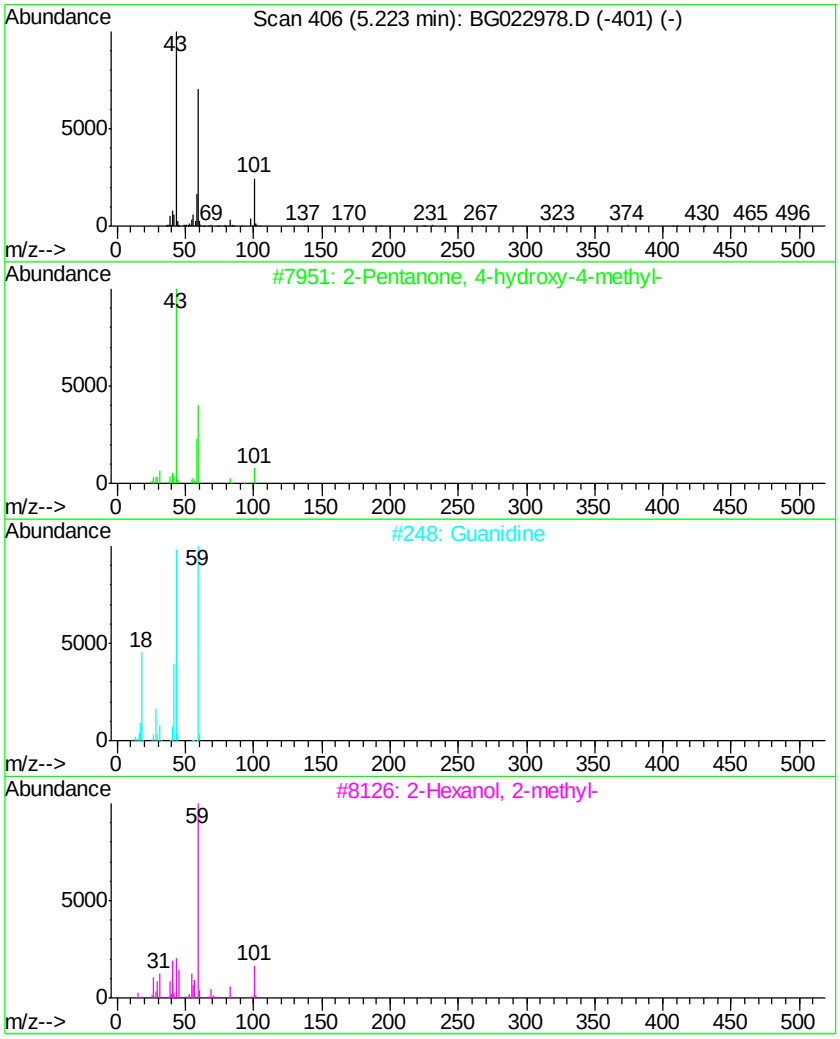
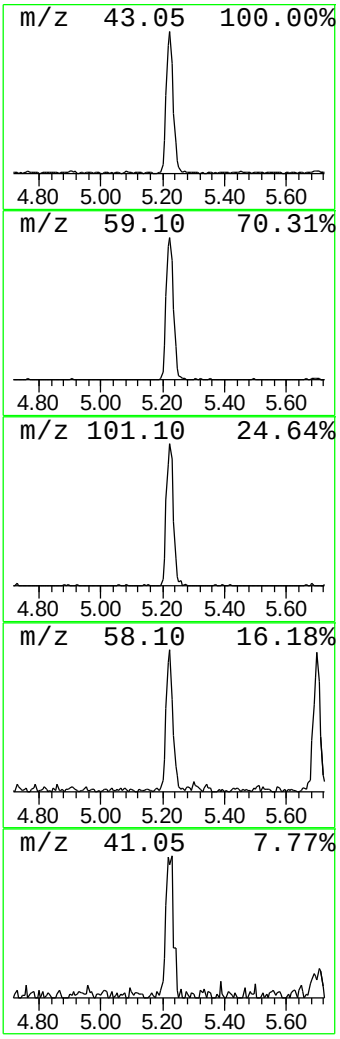
Peak Number 4 unknown5.22 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	13.00 ng	402778	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Guanidine	59	CH5N3	000113-00-8	43
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
4	Acetic acid, 10,11-dihydroxy-3,7...	298	C17H30O4	1000194-28-5	25
5	2,5,8,11,14-Pentaoxapentadecane	222	C10H22O5	000143-24-8	23





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Data File : BG022978.D
Acq On : 9 Jul 2016 23:29
Operator : UM/SJ
Sample : H3935-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C3-5

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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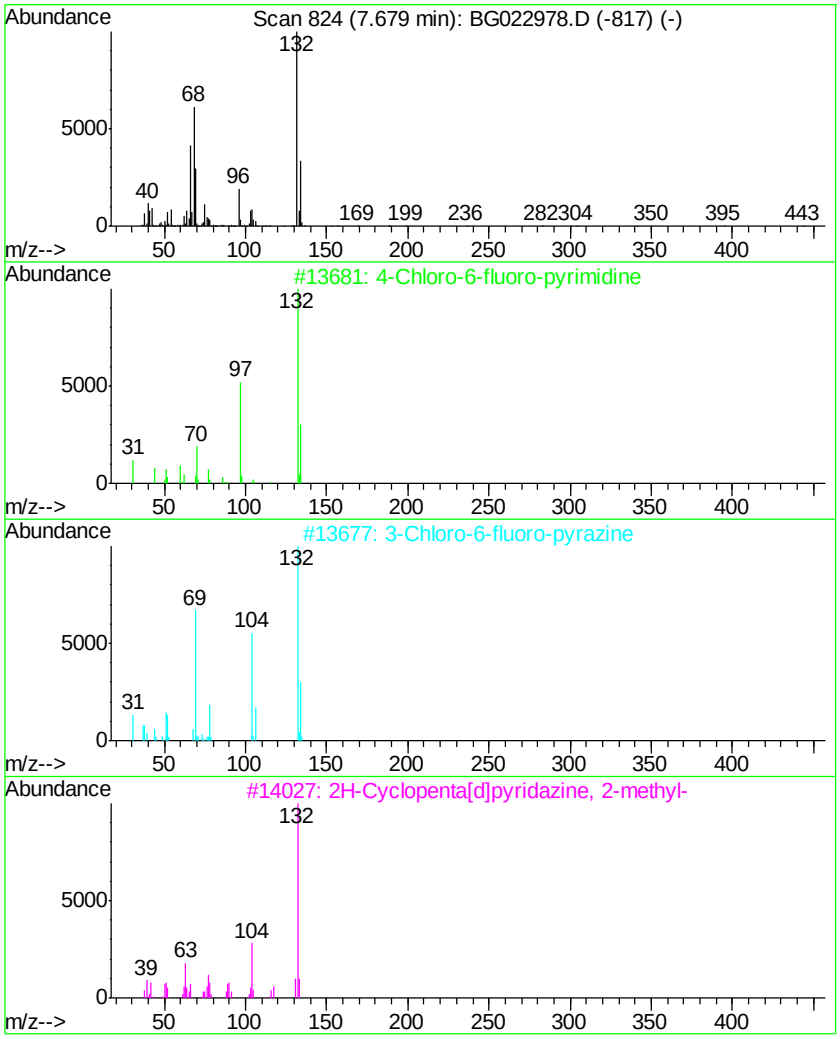
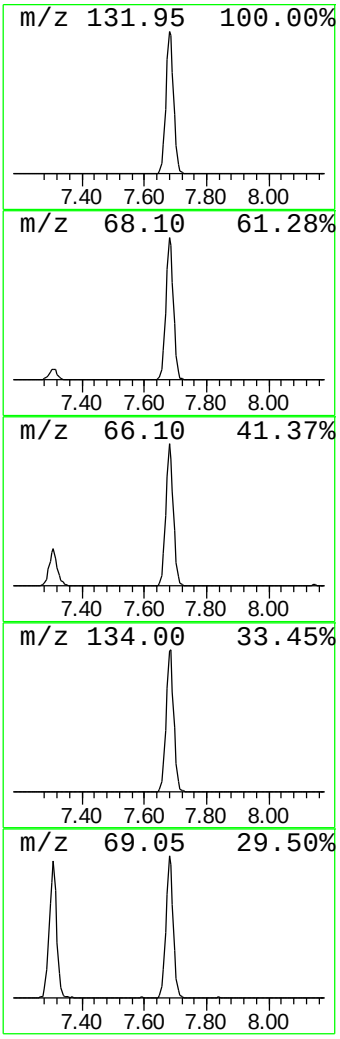
Peak Number 5 unknown7.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	121.32 ng	3758620	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	10
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	10
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022978.D
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Operator : UM/SJ
Sample : H3935-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C3-5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
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TIC Library : C:\DATABASE\NIST02.L
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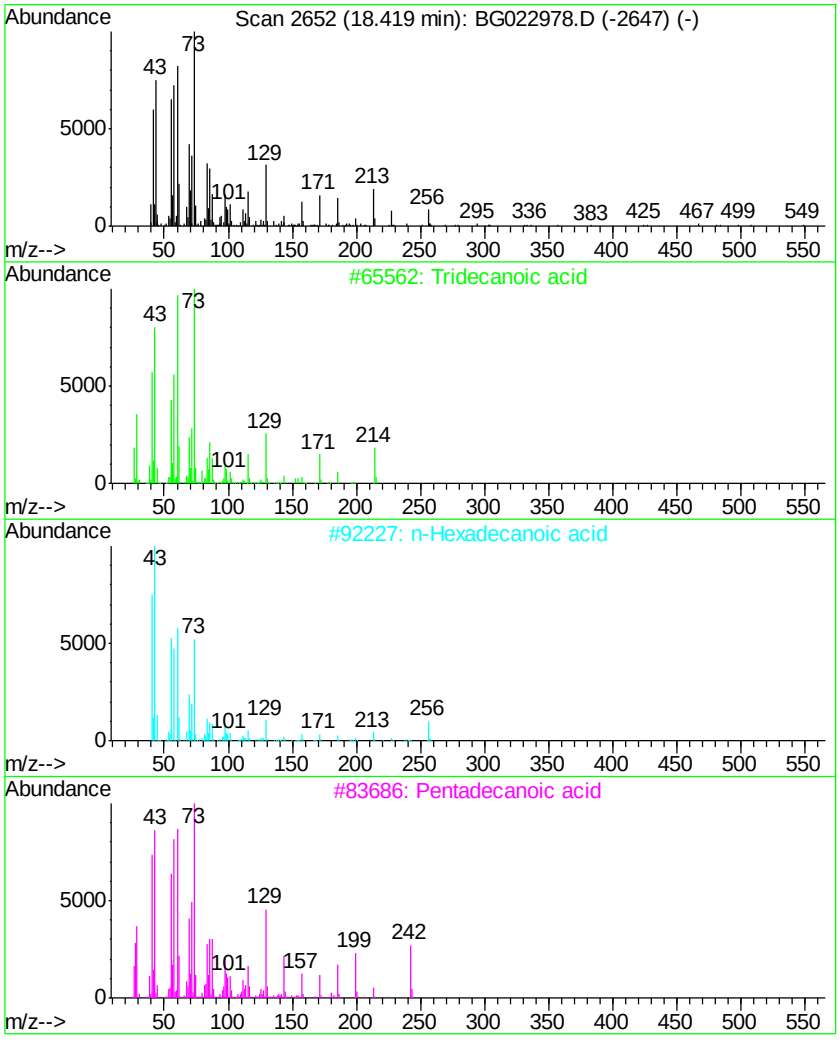
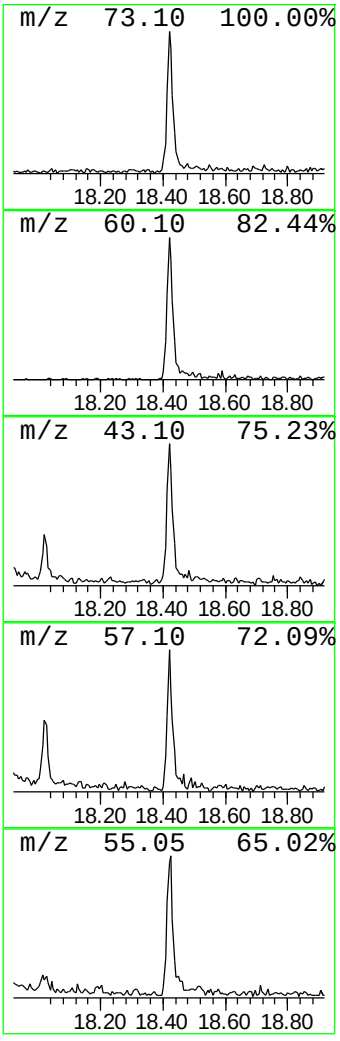
Peak Number 7 Tridecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	4.75 ng	509177	Phenanthrene-d10	17.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	95
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Dodecanoic acid	200	C12H24O2	000143-07-7	59
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	59





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Misc :
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Instrument : BNA_G
ClientSampleId : C3-5

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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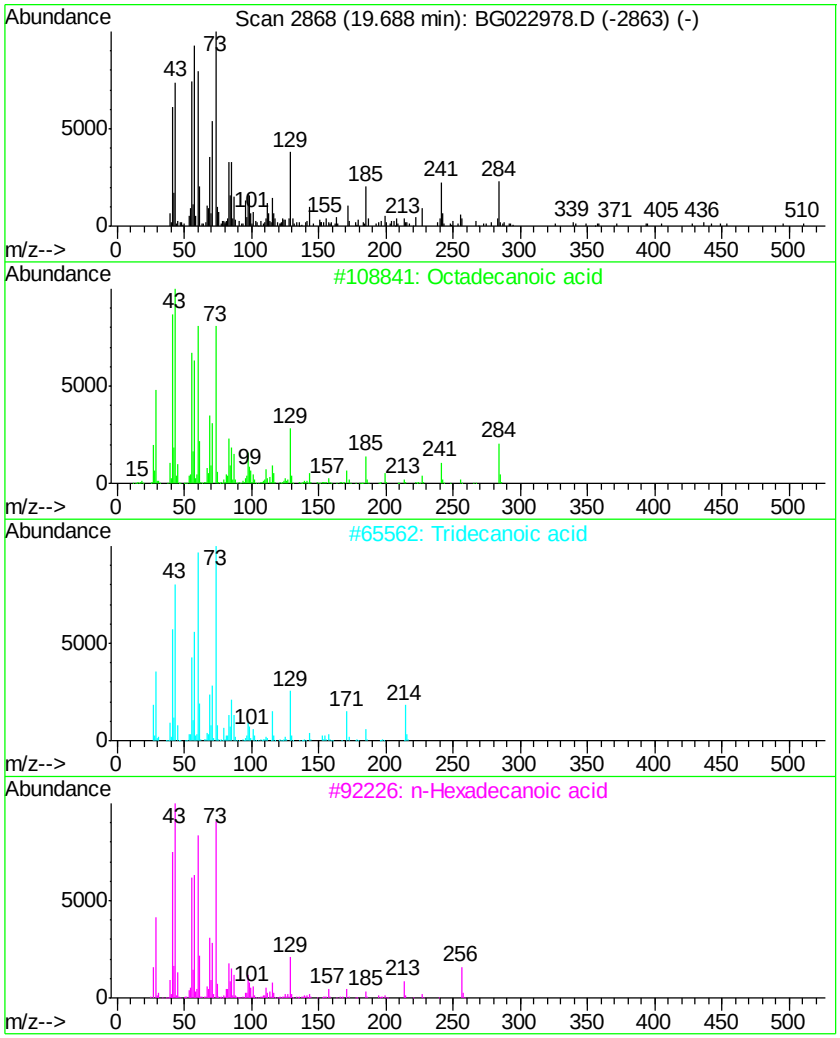
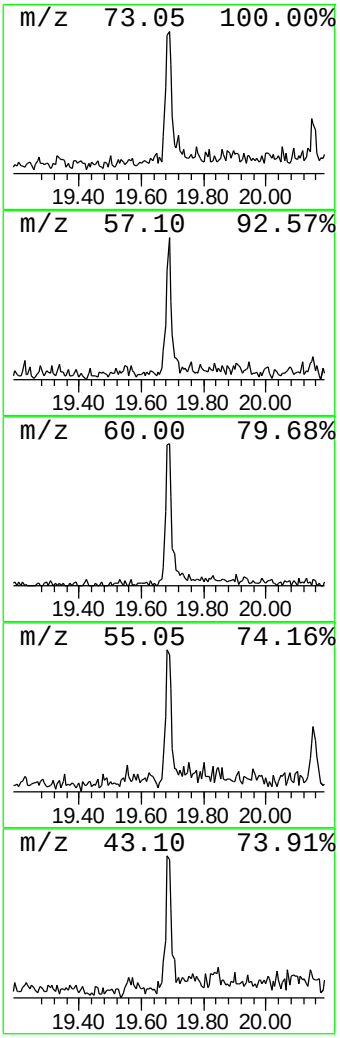
Peak Number 8 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.69	2.40 ng	257632	Phenanthrene-d10	17.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	90
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	68





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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

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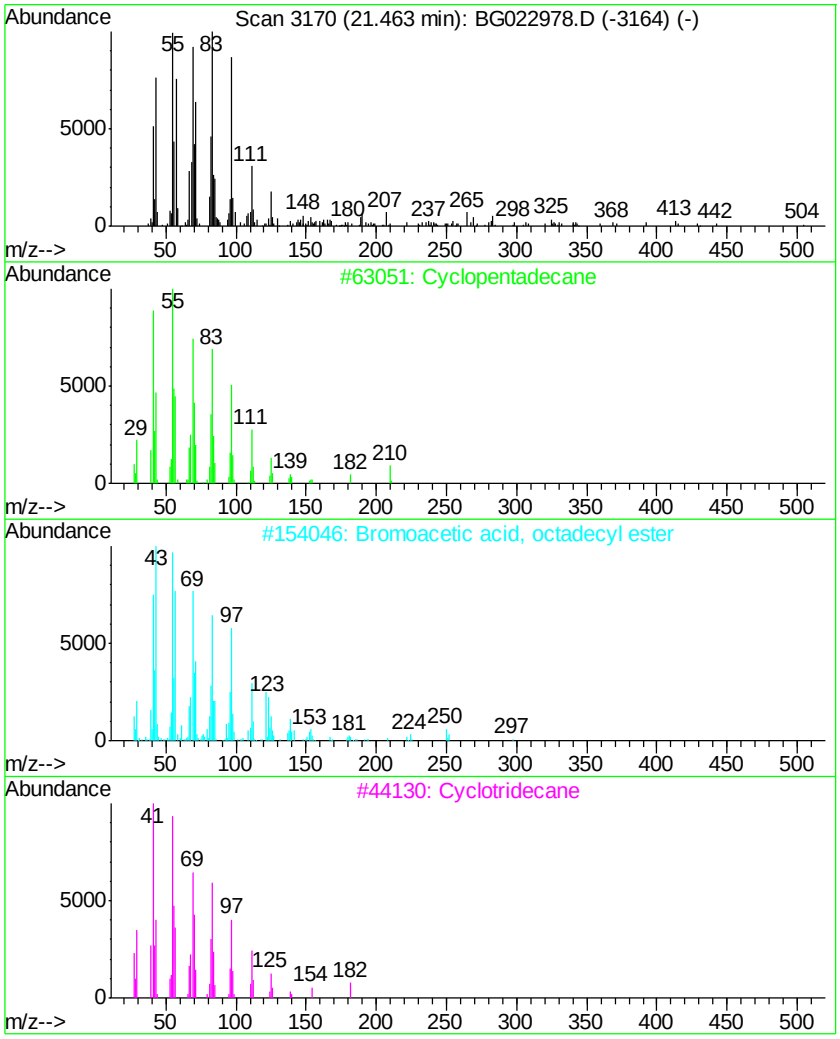
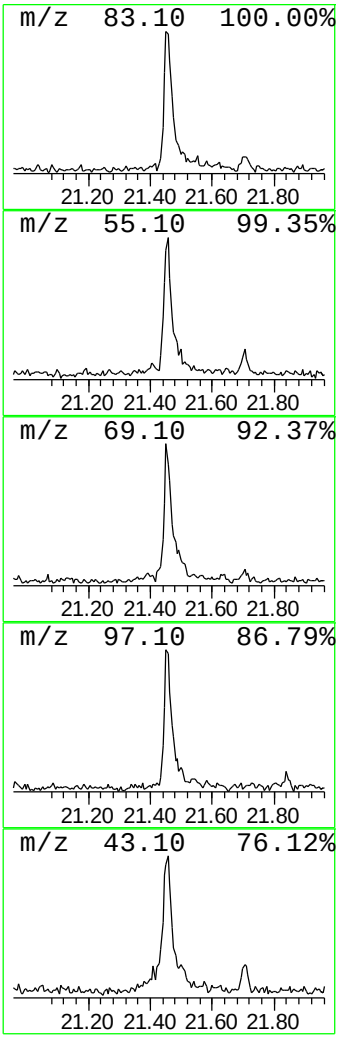
Peak Number 9 Cyclopentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.46	5.68 ng	708690	Chrysene-d12	21.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	95
2	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
3	Cyclotridecane	182	C13H26	000295-02-3	90
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	87
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
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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
Cyclopentane, met...	2.90	24.2	ng	750538	1	8.15	619645	20.0
unknown3.04	3.04	207.3	ng	6423300	1	8.15	619645	20.0
unknown5.22	5.22	13.0	ng	402778	1	8.15	619645	20.0
unknown7.68	7.68	121.3	ng	3758620	1	8.15	619645	20.0
Tridecanoic acid	18.42	4.8	ng	509177	4	17.56	2146130	20.0
Octadecanoic acid	19.69	2.4	ng	257632	4	17.56	2146130	20.0
Cyclopentadecane	21.46	5.7	ng	708690	5	21.84	2493750	20.0