LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG071216\
Data File : BG023064.D
Acq On : 13 Jul 2016 10:08
Operator : UM/SJ
Sample : H3936-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-3(5-6)

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	3.041	29	34	53	rVB	5690572	8723928	93.26%	13.186%
2	3.804	159	164	172	rBV	212047	338817	3.62%	0.512%
3	5.220	399	405	415	rVB	124379	197326	2.11%	0.298%
4	5.696	479	486	495	rBV	2183645	3480655	37.21%	5.261%
5	7.306	751	760	774	rBV	2571347	4541869	48.55%	6.865%
6	7.682	816	824	831	rBV	2325551	4010758	42.88%	6.062%
7	8.152	897	904	915	rVB	382209	656026	7.01%	0.992%
8	8.475	953	959	968	rVB	1527264	2671498	28.56%	4.038%
9	9.327	1095	1104	1113	rBV	1569902	2899515	31.00%	4.383%
10	10.978	1377	1385	1394	rBV	585260	1064592	11.38%	1.609%
11	13.417	1792	1800	1814	rBV	4101622	6720181	71.84%	10.158%
12	13.675	1838	1844	1851	rVB3	60054	95340	1.02%	0.144%
13	14.239	1933	1940	1946	rBV	1240593	1832460	19.59%	2.770%
14	14.797	2029	2035	2044	rBV2	1124010	1866204	19.95%	2.821%
15	16.290	2279	2289	2302	rBV	4342136	6869365	73.43%	10.383%
16	16.484	2318	2322	2329	rBV2	150289	263961	2.82%	0.399%
17	17.277	2453	2457	2462	rBV	131845	175147	1.87%	0.265%
18	17.553	2497	2504	2512	rBV2	1435046	2316148	24.76%	3.501%
19	18.023	2580	2584	2591	rVB	159079	200250	2.14%	0.303%
20	18.423	2647	2652	2657	rBV2	382253	507133	5.42%	0.767%
21	19.692	2862	2868	2873	rBV4	110897	189613	2.03%	0.287%
22	19.833	2889	2892	2897	rVB4	105401	129258	1.38%	0.195%
23	20.109	2931	2939	2942	rBV8	53586	107807	1.15%	0.163%
24	20.162	2942	2948	2954	rVB	6888822	9354449	100.00%	14.139%
25	20.438	2988	2995	2999	rBV4	87396	190819	2.04%	0.288%
26	20.779	3048	3053	3057	rVB4	146528	238880	2.55%	0.361%
27	20.943	3077	3081	3085	rVB2	91037	115346	1.23%	0.174%
28	21.472	3166	3171	3182	rBV5	215988	471001	5.04%	0.712%
29	21.866	3231	3238	3247	rVB2	1528008	2599899	27.79%	3.930%
30	22.036	3262	3267	3274	rVB2	113230	179557	1.92%	0.271%
31	22.671	3371	3375	3381	rVB3	88117	135880	1.45%	0.205%
32	23.393	3494	3498	3506	rVB4	88943	168624	1.80%	0.255%
33	23.605	3529	3534	3538	rVB2	61105	107519	1.15%	0.163%
34	24.245	3638	3643	3650	rVB7	67352	139236	1.49%	0.210%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG071216\
Data File : BG023064.D
Acq On : 13 Jul 2016 10:08
Operator : UM/SJ
Sample : H3936-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-3(5-6)

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

35	25.250	3804	3814	3829	rBV2	848947	2599277	27.79%	3.929%

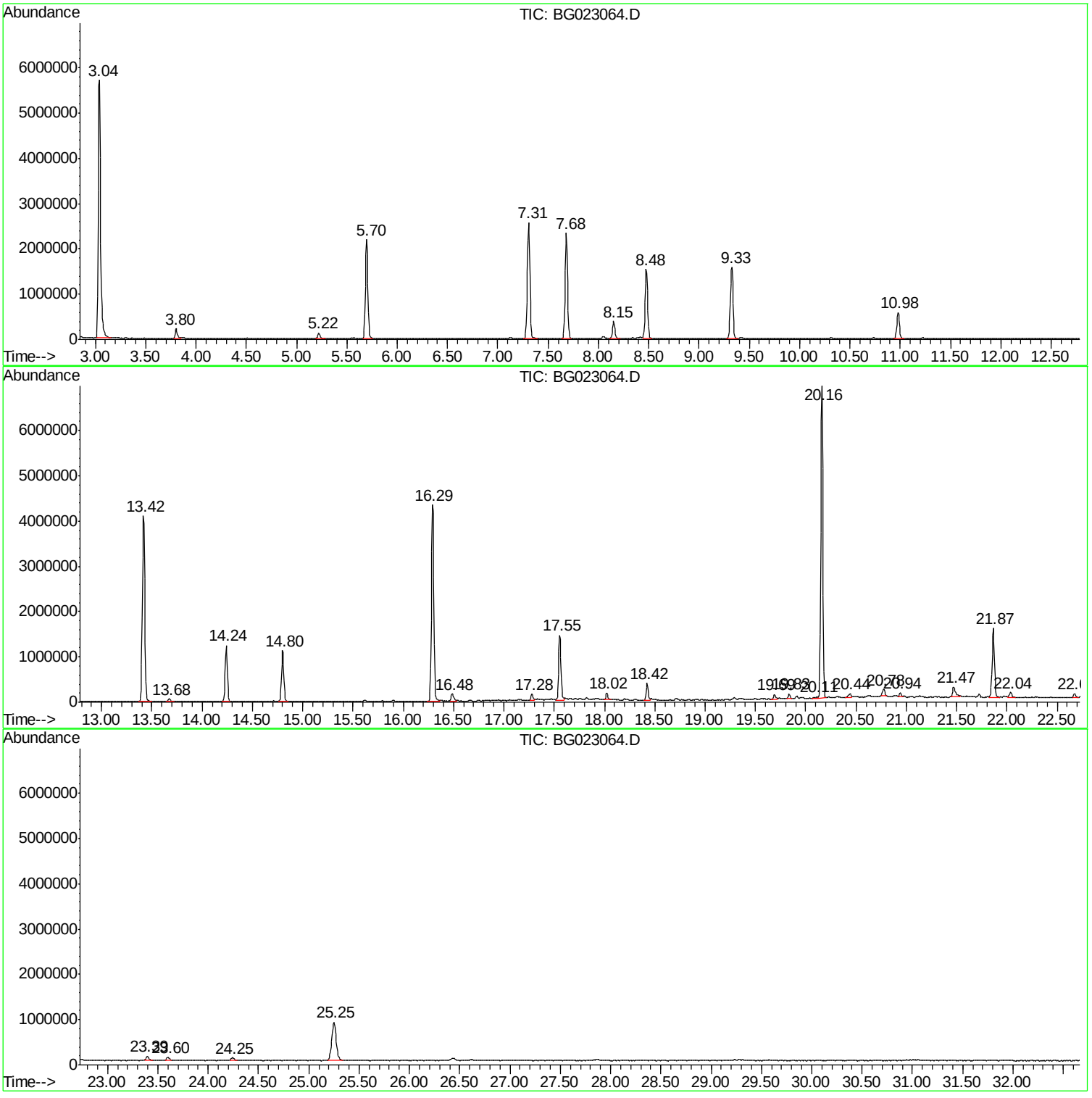
Sum of corrected areas: 66158338

Data Path : Z:\HPCHEM1\BNA G\DATA\BG071216\
Data File : BG023064.D
Acq On : 13 Jul 2016 10:08
Operator : UM/SJ
Sample : H3936-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-3(5-6)

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\BG071216\
Data File : BG023064.D
Acq On : 13 Jul 2016 10:08
Operator : UM/SJ
Sample : H3936-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-3(5-6)

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

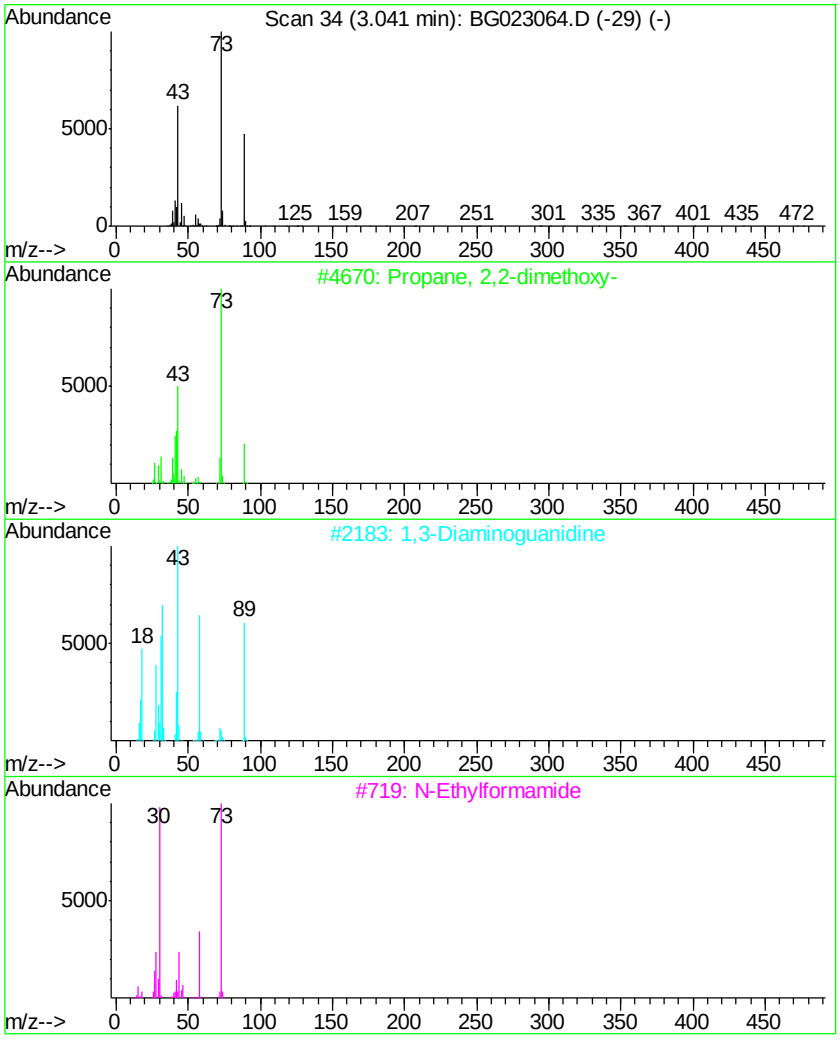
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

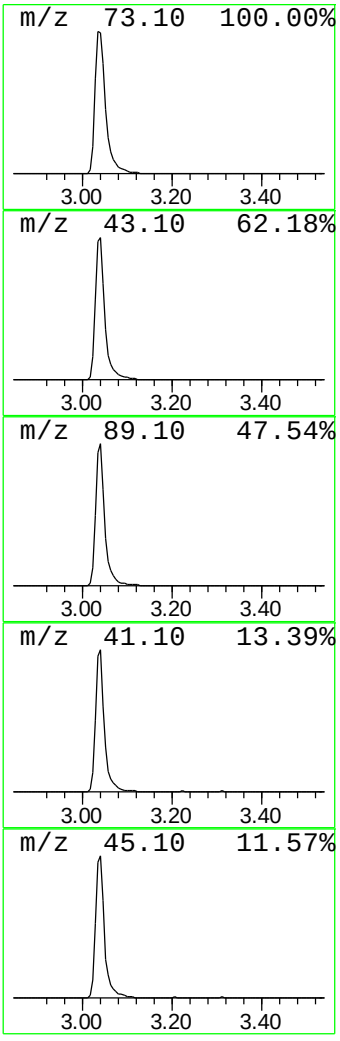
****

Peak Number 1 unknown3.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	265.96 ng	8723930	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	38
2	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	25
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG071216\
Data File : BG023064.D
Acq On : 13 Jul 2016 10:08
Operator : UM/SJ
Sample : H3936-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-3(5-6)

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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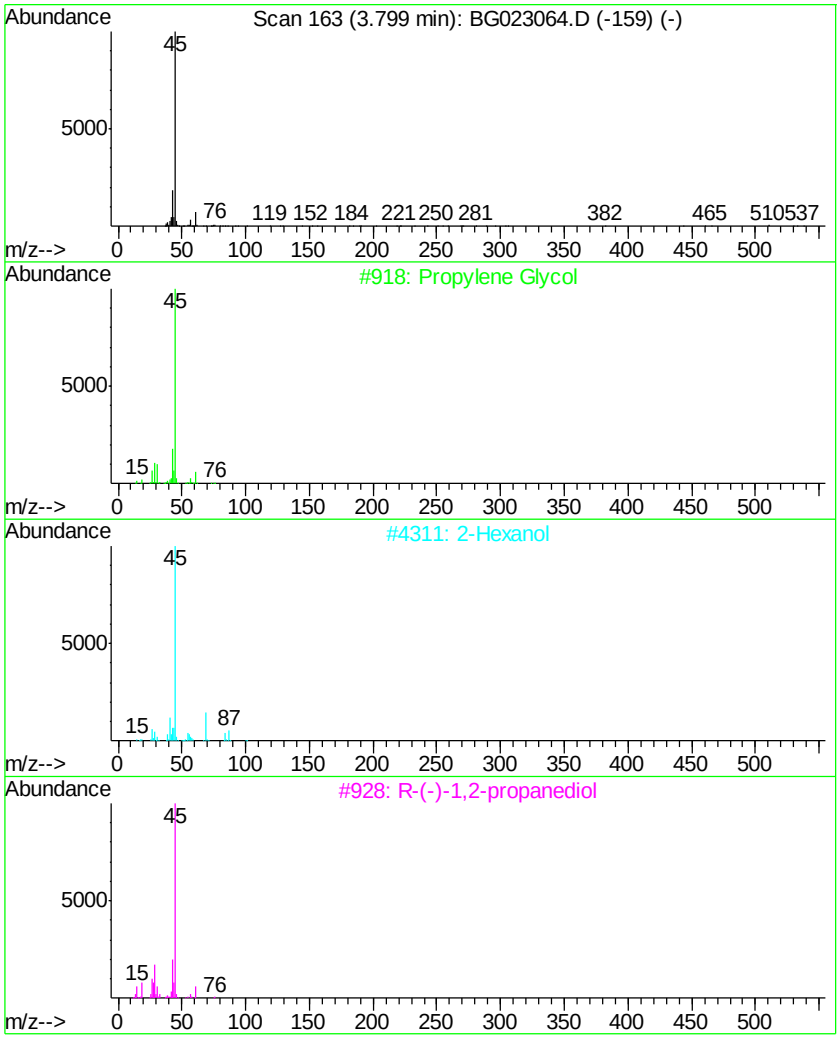
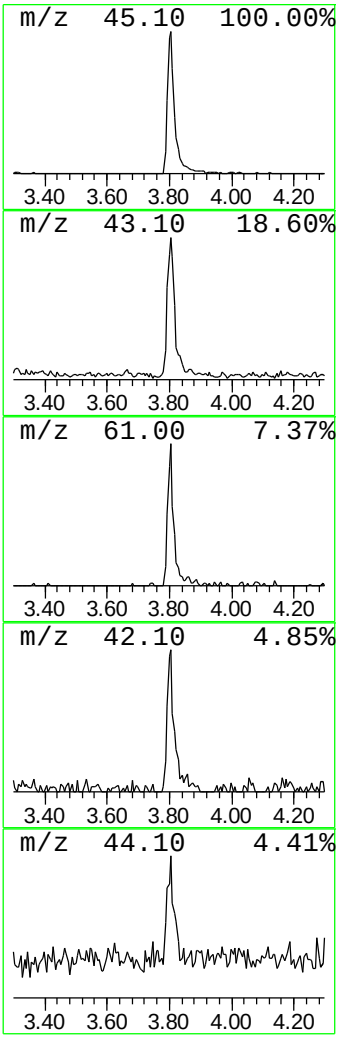
Peak Number 2 Propylene Glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.80	10.33 ng	338817	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	78
2	2-Hexanol	102	C6H14O	000626-93-7	9
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	2-Heptanol, (S)-	116	C7H16O	006033-23-4	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG071216\
Data File : BG023064.D
Acq On : 13 Jul 2016 10:08
Operator : UM/SJ
Sample : H3936-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-3(5-6)

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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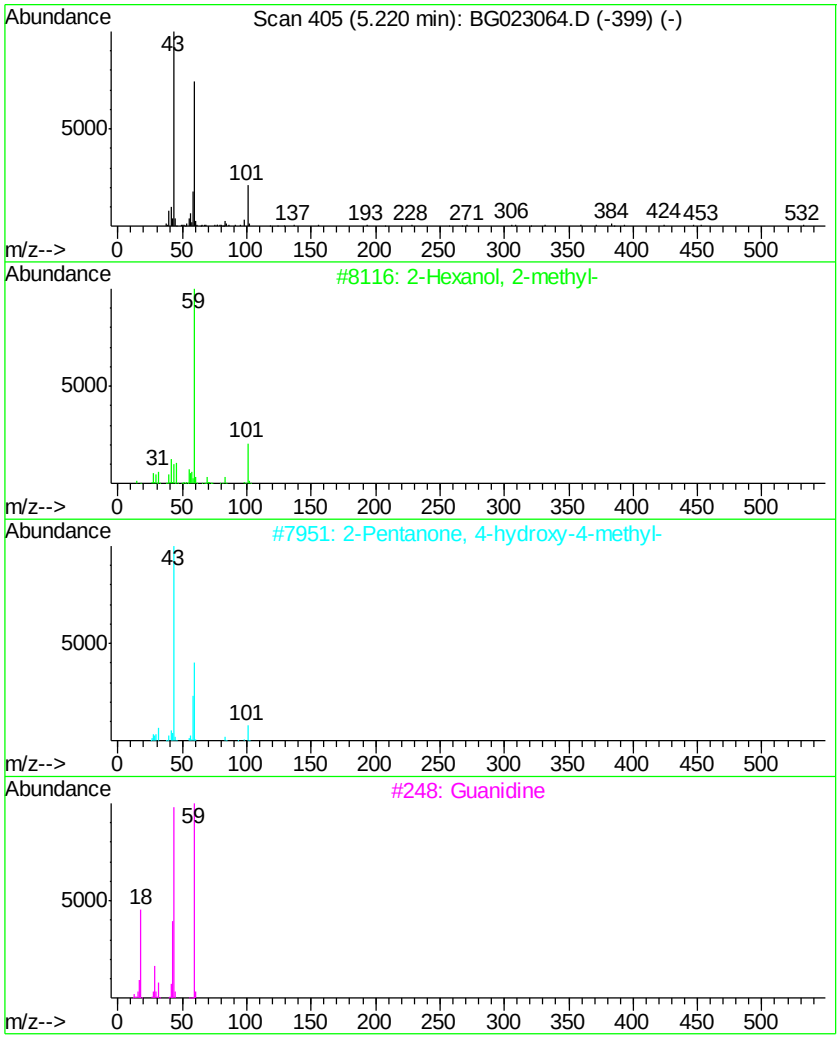
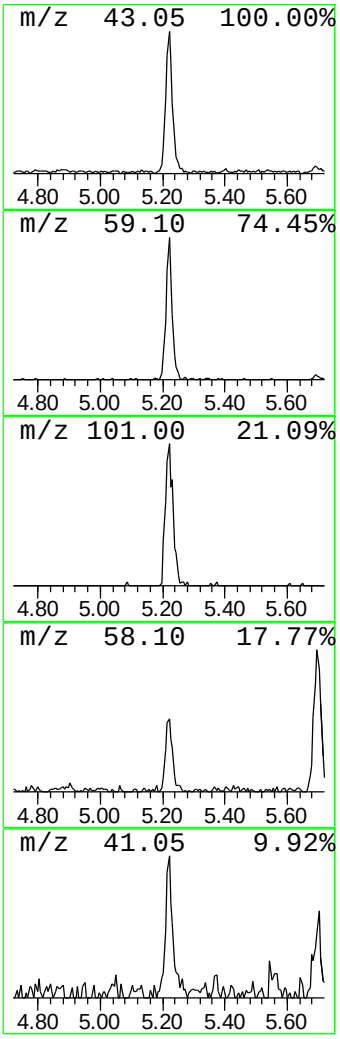
Peak Number 3 2-Hexanol, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	6.02 ng	197326	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	53
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3	Guanidine	59	CH5N3	000113-00-8	50
4	3-Hexanol	102	C6H14O	000623-37-0	33
5	3-Octanol	130	C8H18O	000589-98-0	28





Data Path : Z:\HPCHEM1\BNA G\DATA\BG071216\
Data File : BG023064.D
Acq On : 13 Jul 2016 10:08
Operator : UM/SJ
Sample : H3936-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-3(5-6)

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

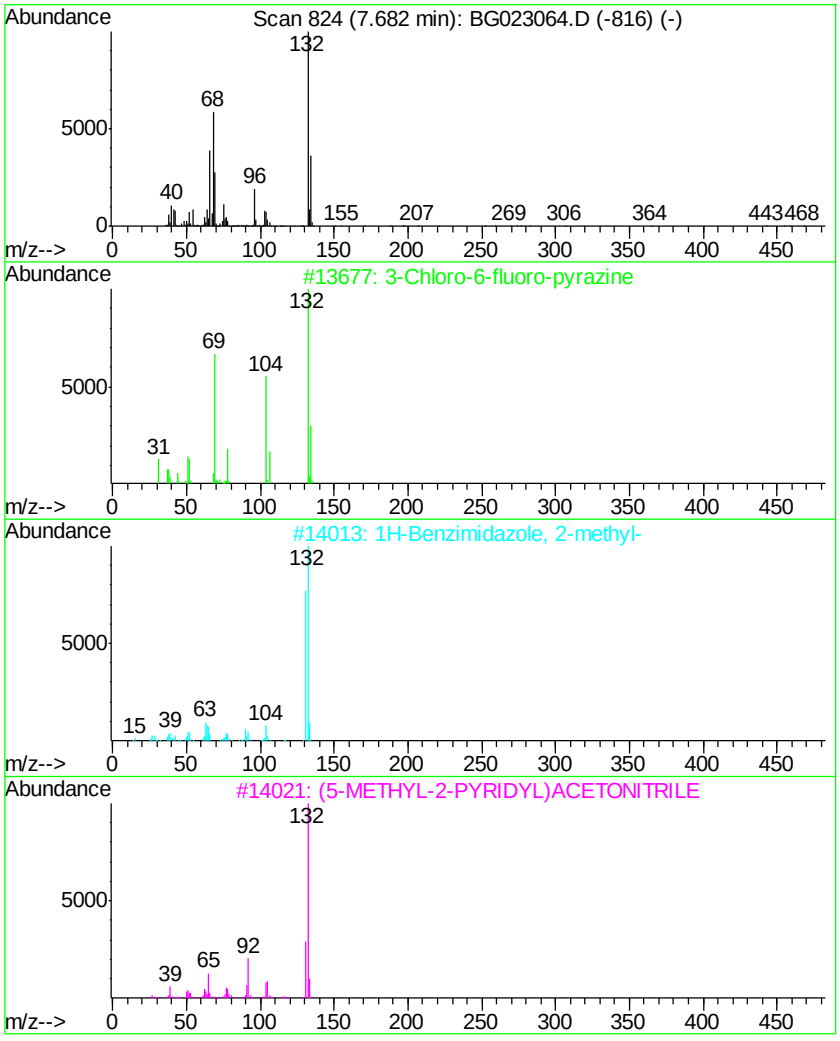
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

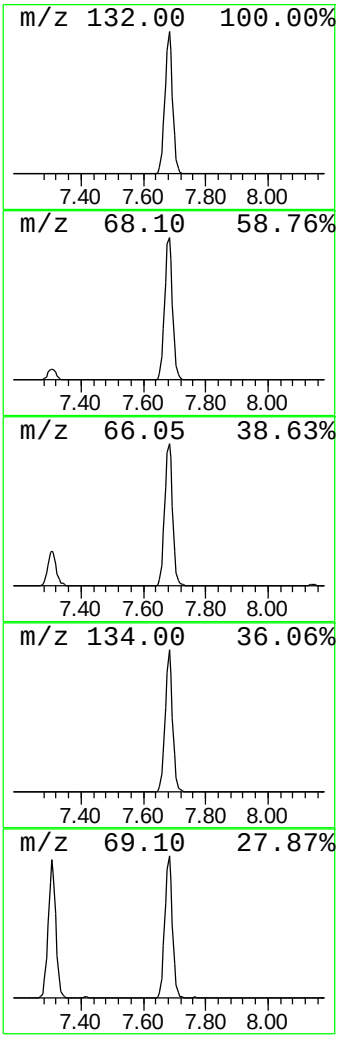
****

Peak Number 4 unknown7.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	122.27 ng	4010760	1,4-Dichlorobenzene-d4	8.15

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	10
3	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4	5-Aminoindole	132	C8H8N2	005192-03-0	10
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





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Operator : UM/SJ
Sample : H3936-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-3(5-6)

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

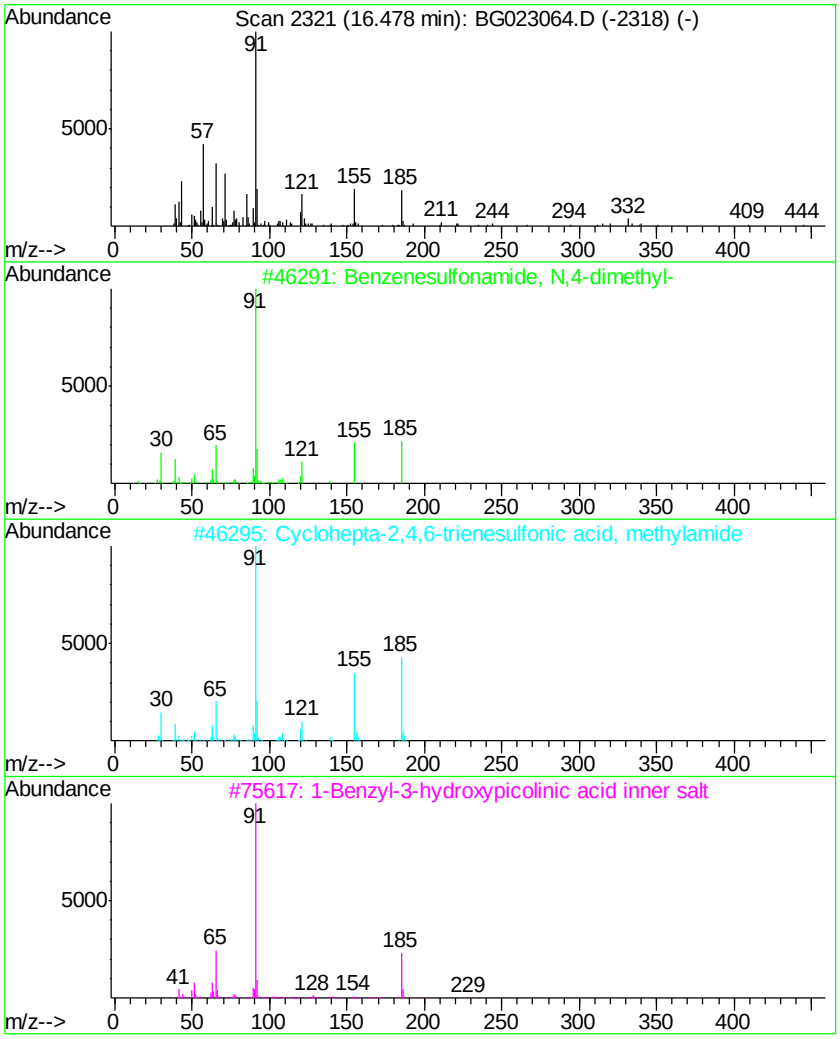
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

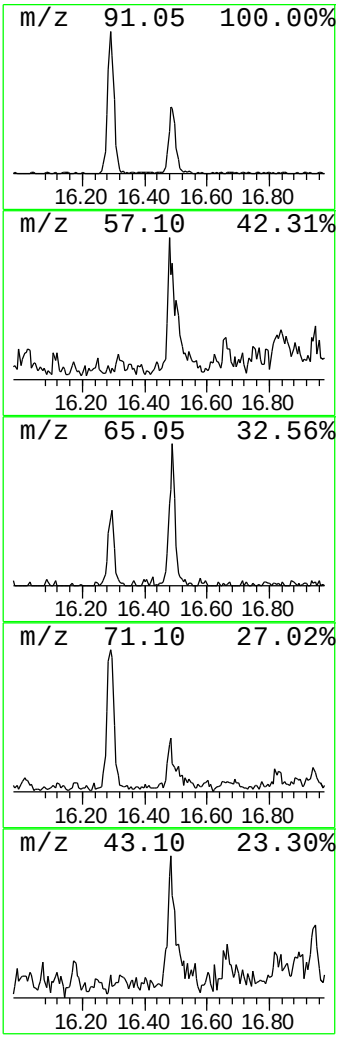
****

Peak Number 6 Benzenesulfonamide, N,4-dim... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.48	2.28 ng	263961	Phenanthrene-d10	17.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	64
2	Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	43
3	1-Benzyl-3-hydroxypicolinic acid...	229	C13H11NO3	1000212-09-1	38
4	Benzene, 1-methyl-2-nitroso-	121	C7H7NO	000611-23-4	30
5	(O-p-Tosylisonitroso)malononitrile	249	C10H7N3O3S	020893-01-0	22





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Instrument : BNA_G
ClientSampleId : SB-3(5-6)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
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TIC Library : C:\DATABASE\NIST02.L
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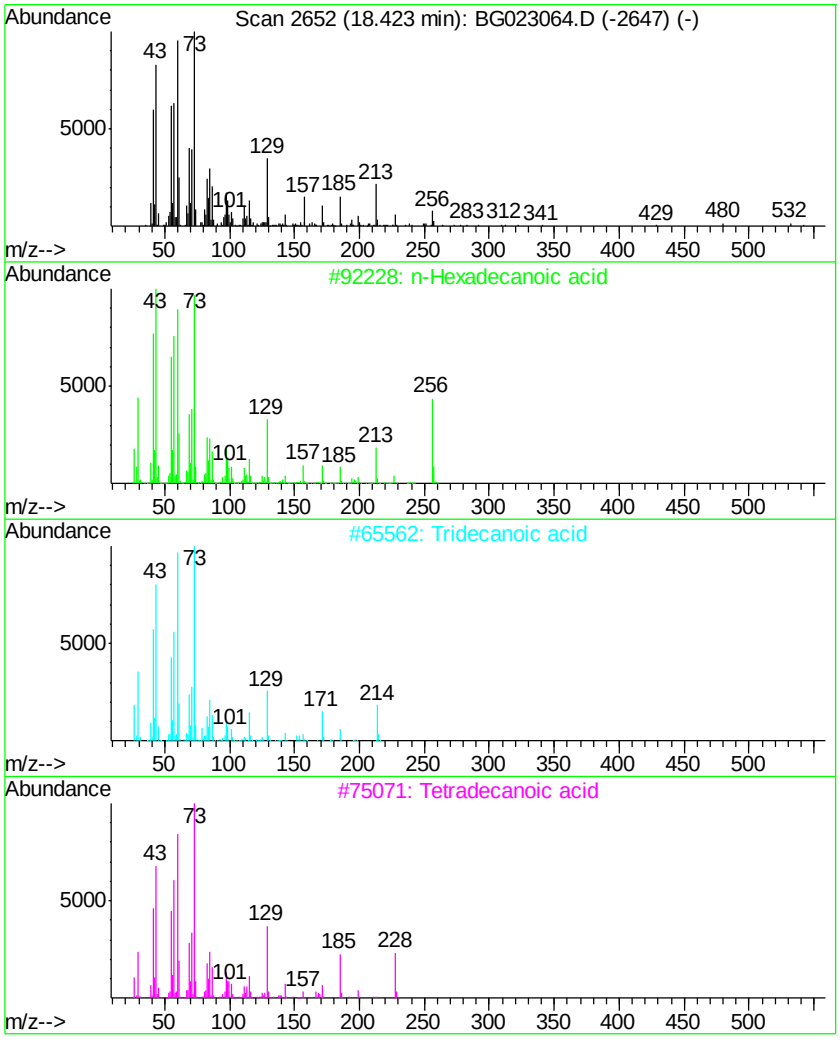
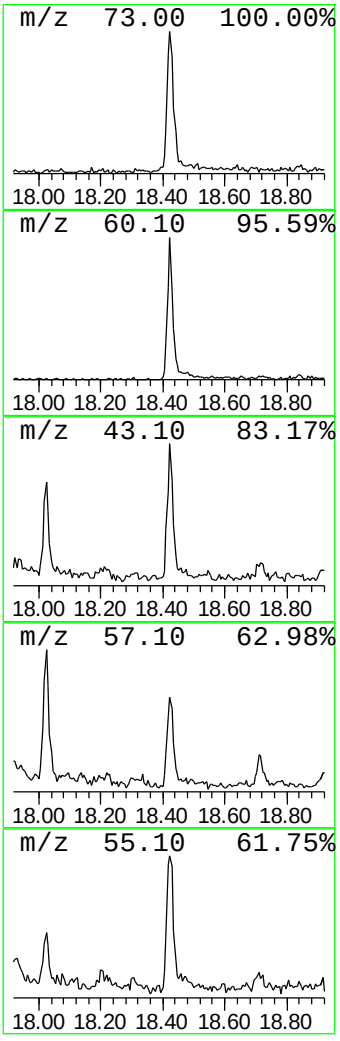
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	4.38 ng	507133	Phenanthrene-d10	17.55

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	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	Undecanoic acid	186	C11H22O2	000112-37-8	83
5	Nonanoic acid	158	C9H18O2	000112-05-0	43





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Instrument : BNA_G
ClientSampleId : SB-3(5-6)

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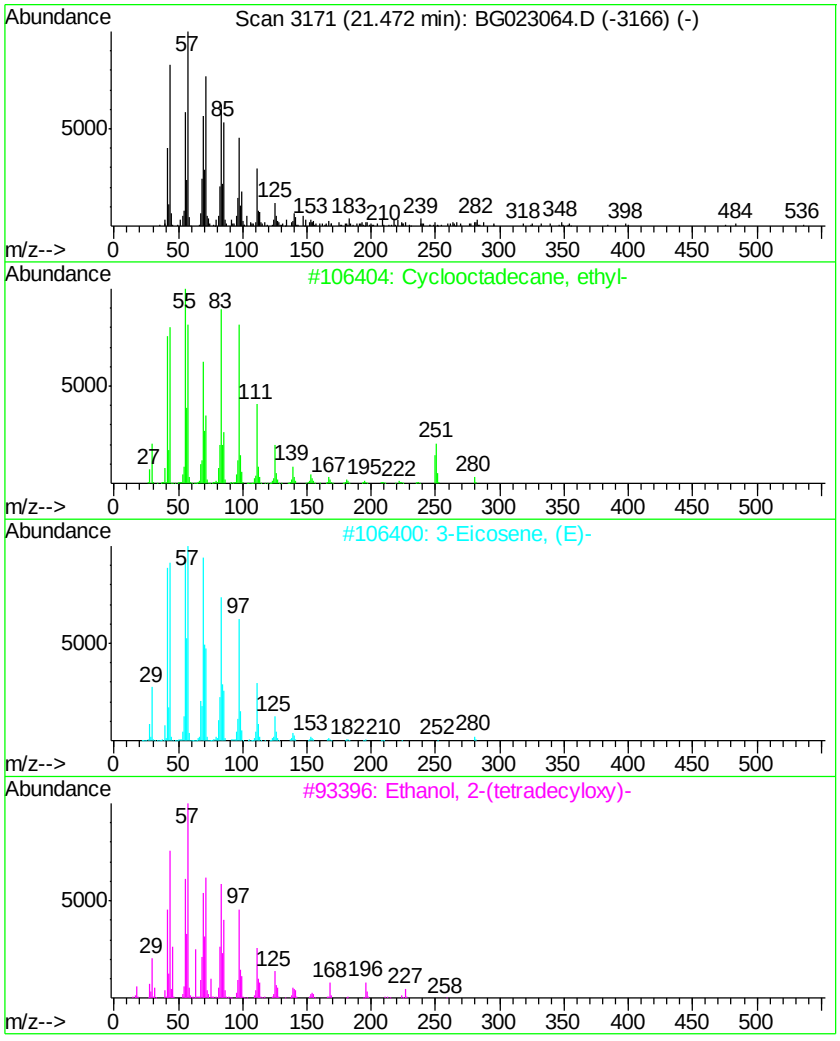
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

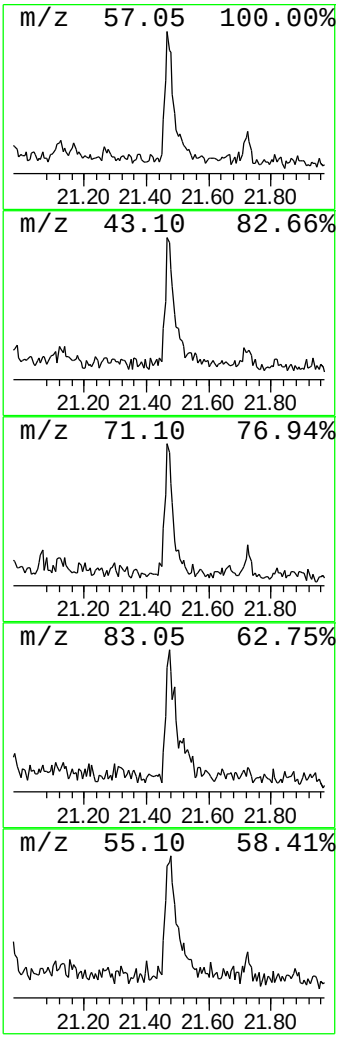
****

Peak Number 8 Cyclooctadecane, ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.47	3.62 ng	471001	Chrysene-d12	21.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclooctadecane, ethyl-	280	C20H40	1000151-22-5	87
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	70
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	62
4	Cyclotetradecane	196	C14H28	000295-17-0	60
5	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071216\
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Operator : UM/SJ
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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	266.0	ng	8723930	1	8.15	656026	20.0
Propylene Glycol	3.80	10.3	ng	338817	1	8.15	656026	20.0
2-Hexanol, 2-methyl-	5.22	6.0	ng	197326	1	8.15	656026	20.0
unknown7.68	7.68	122.3	ng	4010760	1	8.15	656026	20.0
Benzenesulfonamid...	16.48	2.3	ng	263961	4	17.55	2316150	20.0
n-Hexadecanoic acid	18.42	4.4	ng	507133	4	17.55	2316150	20.0
Cyclooctadecane, ...	21.47	3.6	ng	471001	5	21.87	2599900	20.0