LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023149.D
Acq On : 16 Jul 2016 16:22
Operator : UM/SJ
Sample : H4018-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : D8-B3(0-6)C

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	3.045	29	35	46	rVB	2021944	3179640	42.55%	5.571%
2	5.225	399	406	416	rVB	299167	479193	6.41%	0.840%
3	5.701	480	487	495	rBV	2050421	3355758	44.90%	5.880%
4	7.310	753	761	772	rBV	2352105	4137178	55.36%	7.249%
5	7.681	816	824	833	rBV	2217464	3900890	52.20%	6.835%
6	8.151	895	904	911	rBV2	567541	988431	13.23%	1.732%
7	8.480	950	960	970	rBV	1571566	2842678	38.04%	4.981%
8	9.326	1096	1104	1111	rBV	1489135	2709877	36.26%	4.748%
9	10.977	1378	1385	1394	rBV	803878	1475171	19.74%	2.585%
10	13.415	1792	1800	1813	rBV	3663169	5914790	79.14%	10.363%
11	14.238	1934	1940	1947	rBV	599866	842115	11.27%	1.475%
12	14.796	2027	2035	2042	rBV2	1224274	2083045	27.87%	3.650%
13	16.288	2282	2289	2303	rBV	3006657	4821146	64.51%	8.447%
14	16.482	2318	2322	2330	rVB2	60496	120604	1.61%	0.211%
15	17.275	2453	2457	2461	rBV	81013	106148	1.42%	0.186%
16	17.416	2477	2481	2484	rBV3	82679	112623	1.51%	0.197%
17	17.551	2497	2504	2509	rBV	1532909	2360669	31.59%	4.136%
18	17.592	2509	2511	2518	rVB2	171757	240145	3.21%	0.421%
19	18.015	2579	2583	2589	rVB4	64453	85674	1.15%	0.150%
20	18.303	2627	2632	2638	rVB10	44589	79505	1.06%	0.139%
21	18.415	2647	2651	2658	rBV3	327171	495822	6.63%	0.869%
22	18.709	2697	2701	2706	rBV3	77044	130074	1.74%	0.228%
23	19.596	2847	2852	2859	rVB	476567	685723	9.18%	1.201%
24	19.684	2863	2867	2873	rBV7	114415	184199	2.46%	0.323%
25	19.825	2888	2891	2900	rVB10	50357	89871	1.20%	0.157%
26	19.960	2907	2914	2922	rVB	391659	659860	8.83%	1.156%
27	20.154	2941	2947	2953	rVB	5400424	7473505	100.00%	13.094%
28	21.464	3165	3170	3175	rBV5	191832	360108	4.82%	0.631%
29	21.711	3209	3212	3216	rVB	151044	196634	2.63%	0.345%
30	21.858	3229	3237	3242	rBV	1535655	2940998	39.35%	5.153%
31	22.657	3370	3373	3376	rBV4	86960	116357	1.56%	0.204%
32	23.750	3553	3559	3567	rVB5	235604	520132	6.96%	0.911%
33	24.149	3623	3627	3632	rBV2	126528	301079	4.03%	0.528%
34	24.220	3636	3639	3648	rVB4	314639	607691	8.13%	1.065%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023149.D
Acq On : 16 Jul 2016 16:22
Operator : UM/SJ
Sample : H4018-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : D8-B3(0-6)C

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	25.231	3801	3811	3820	rBV2	805507	2477231	33.15%	4.340%

Sum of corrected areas: 57074564

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
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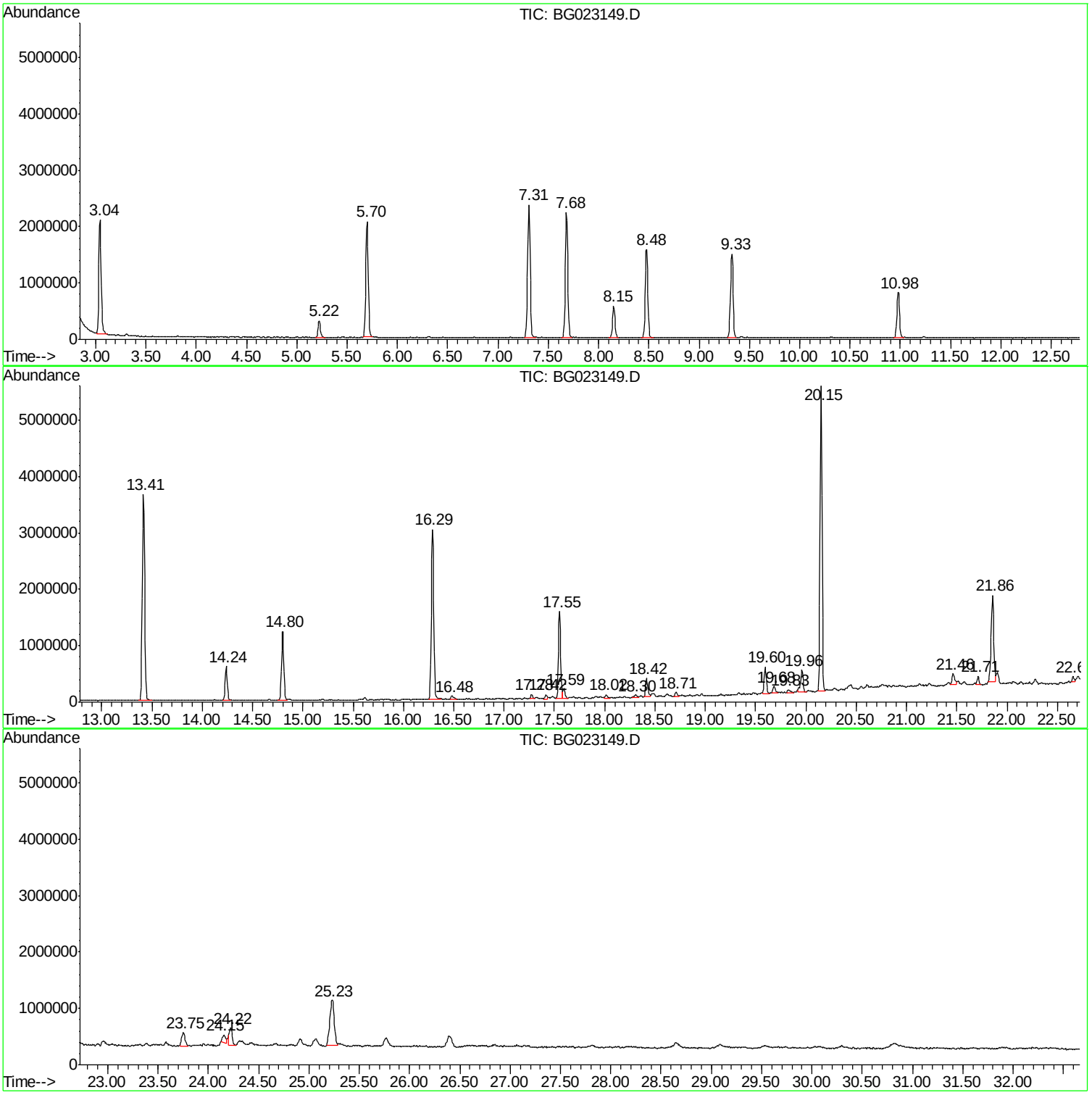
Acq On : 16 Jul 2016 16:22
Operator : UM/SJ
Sample : H4018-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
D8-B3(0-6)C

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

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



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023149.D
Acq On : 16 Jul 2016 16:22
Operator : UM/SJ
Sample : H4018-02
Misc :
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Instrument : BNA_G
ClientSampleId : D8-B3(0-6)C

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

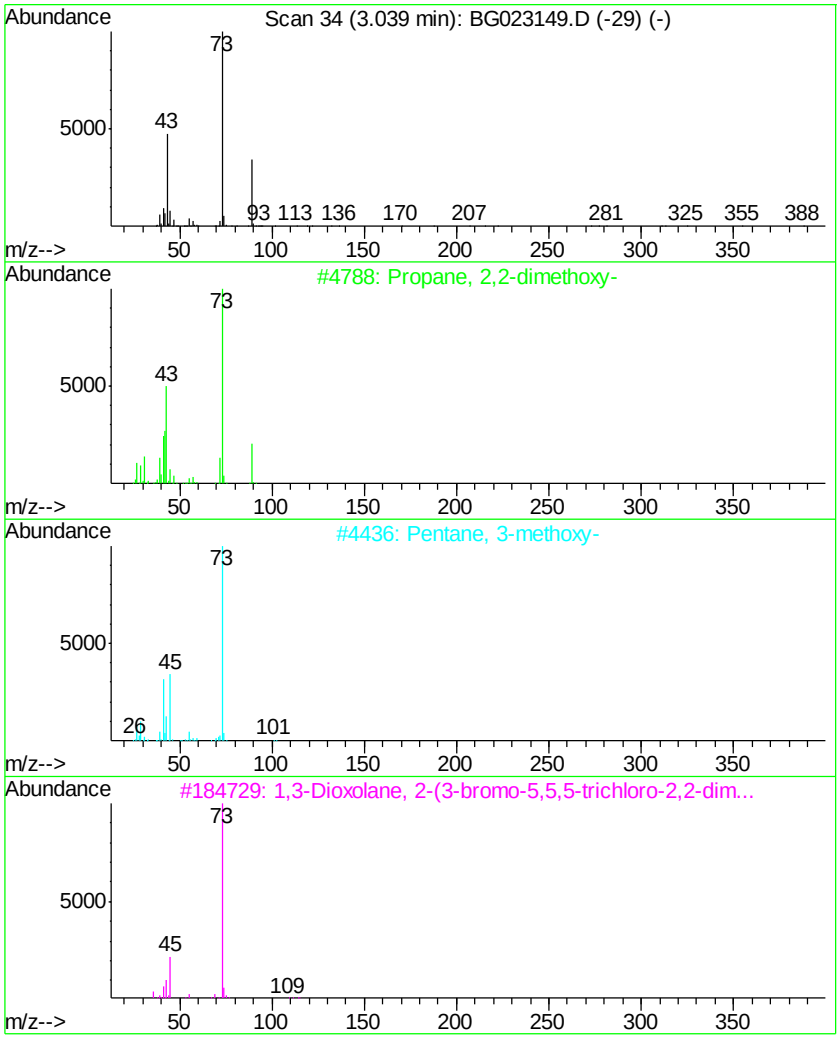
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

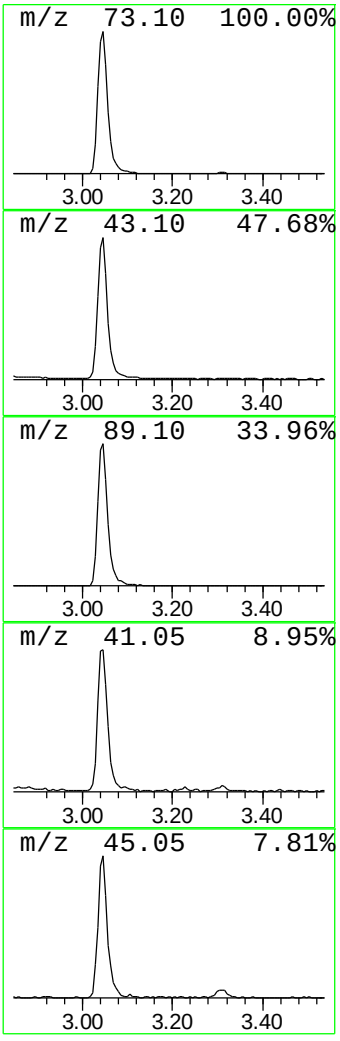
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	64.34 ng	3179640	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	56
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
3	1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	5





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023149.D
Acq On : 16 Jul 2016 16:22
Operator : UM/SJ
Sample : H4018-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : D8-B3(0-6)C

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

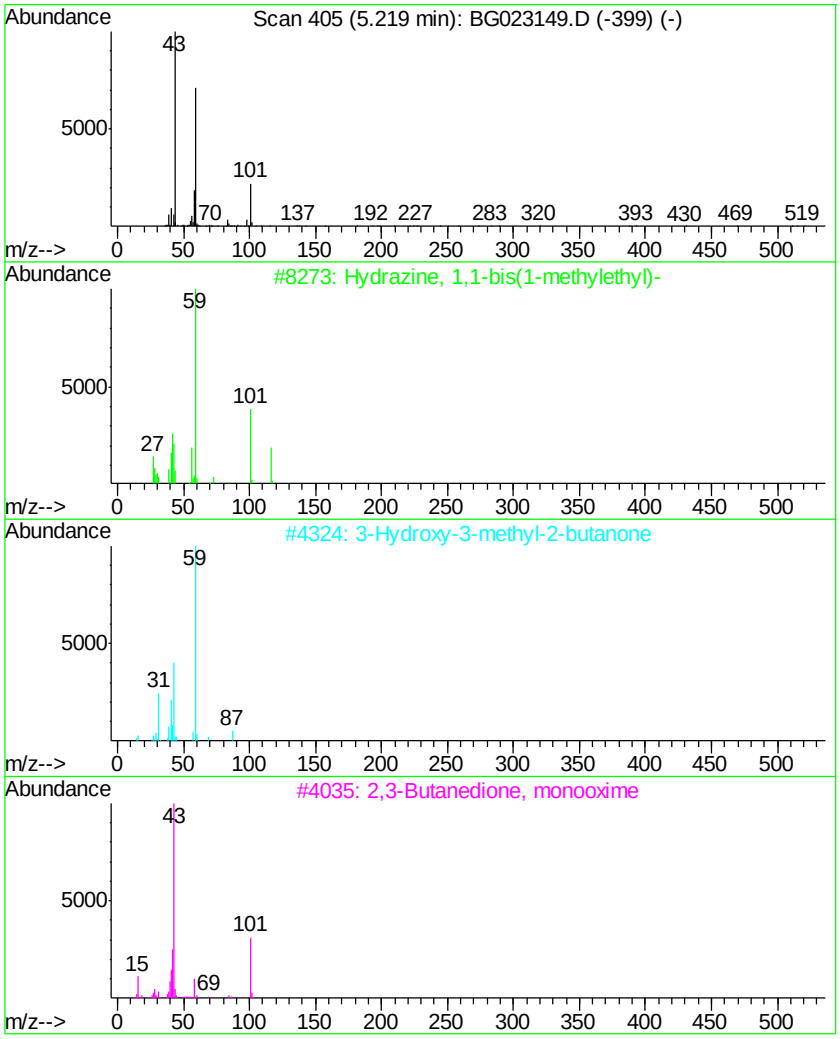
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

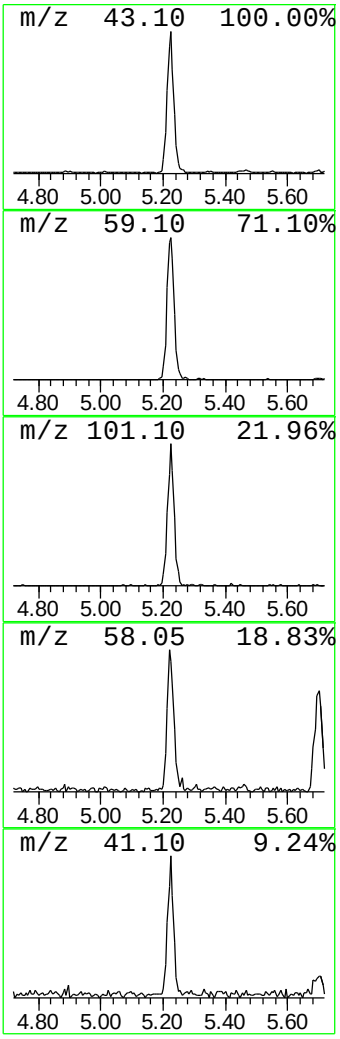
****

Peak Number 2 unknown5.22 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	9.70 ng	479193	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	27
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Acetone	58	C3H6O	000067-64-1	9
5	Guanidine	59	CH5N3	000113-00-8	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023149.D
Acq On : 16 Jul 2016 16:22
Operator : UM/SJ
Sample : H4018-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : D8-B3(0-6)C

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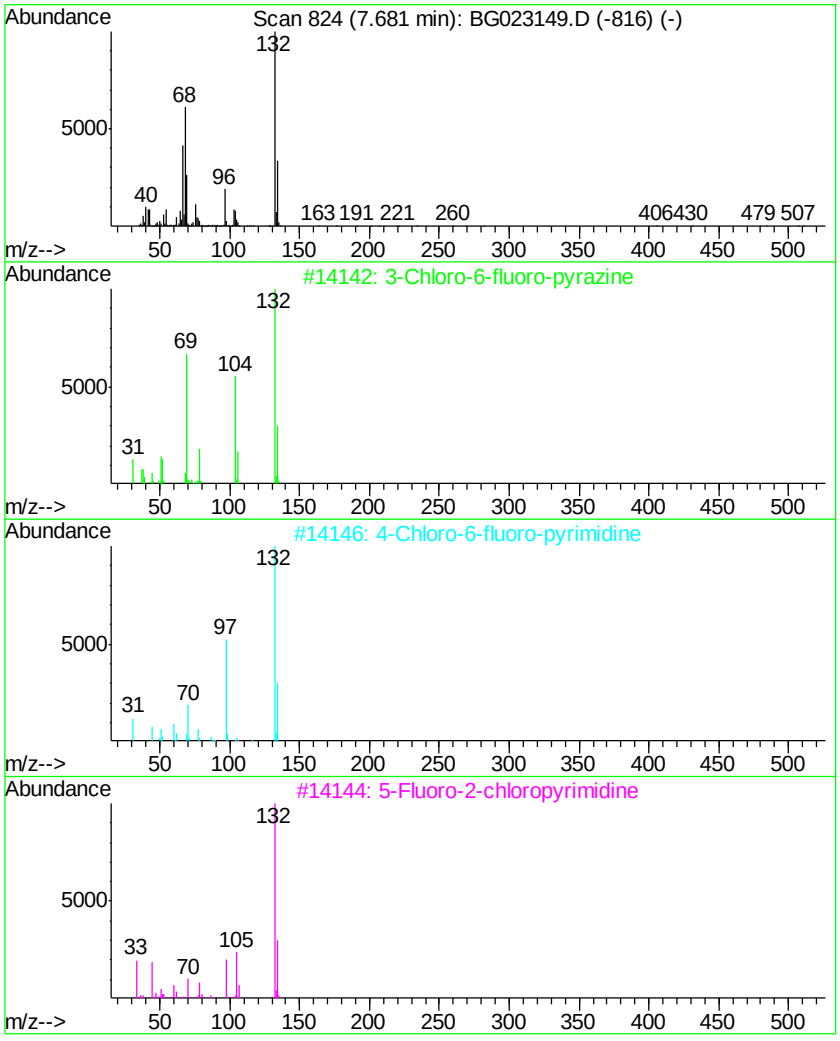
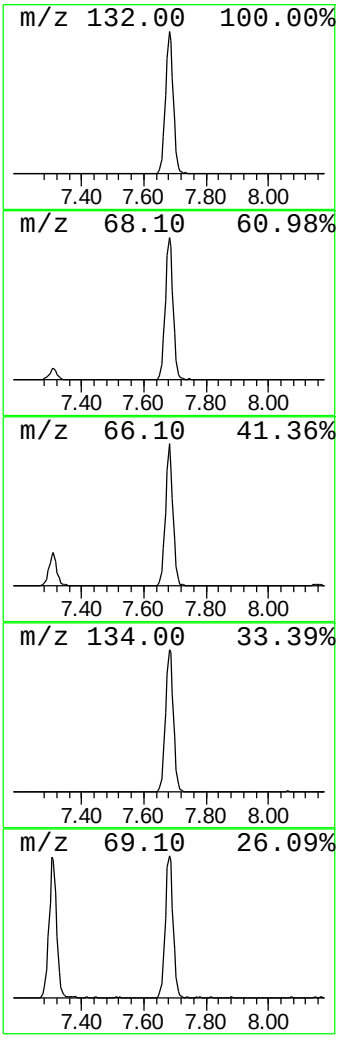
Peak Number 3 unknown7.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	78.93 ng	3900890	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	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	10
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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Data File : BG023149.D
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Operator : UM/SJ
Sample : H4018-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : D8-B3(0-6)C

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

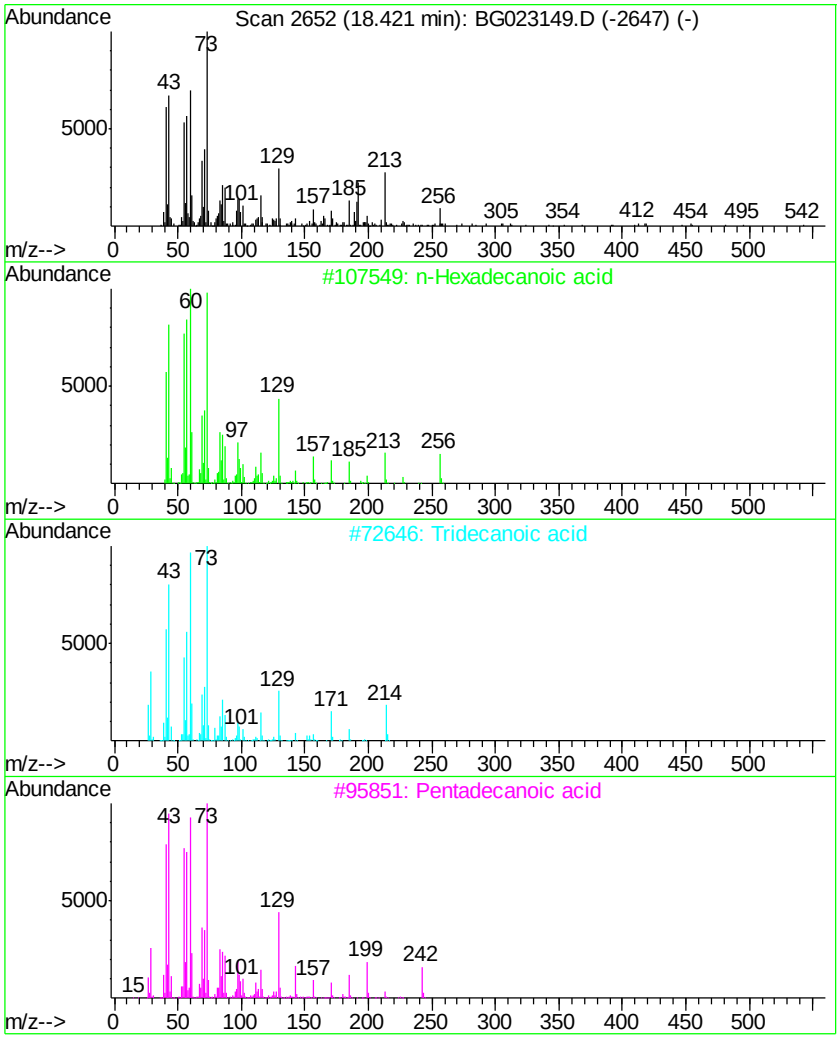
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

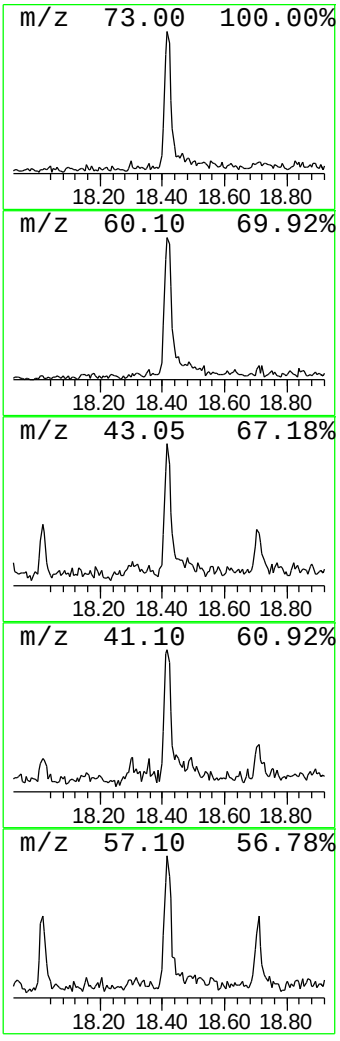
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	4.20 ng	495822	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	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
5	Octadecanoic acid	284	C18H36O2	000057-11-4	43





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Sample : H4018-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : D8-B3(0-6)C

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

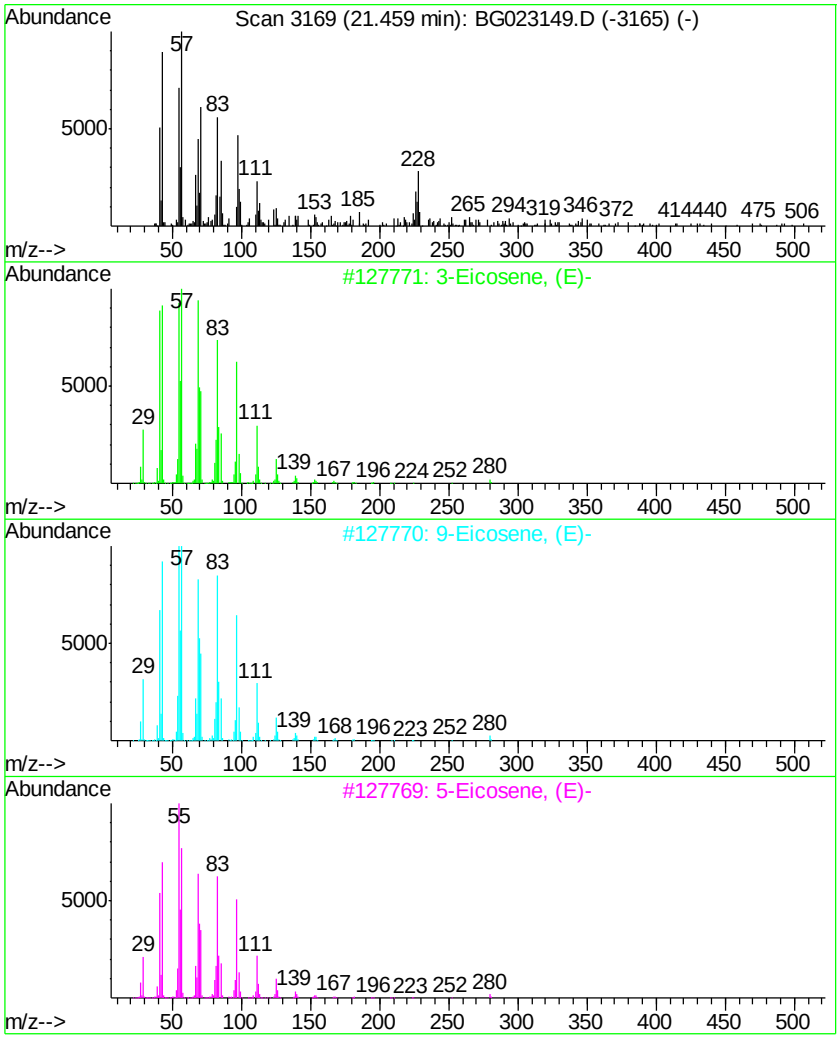
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

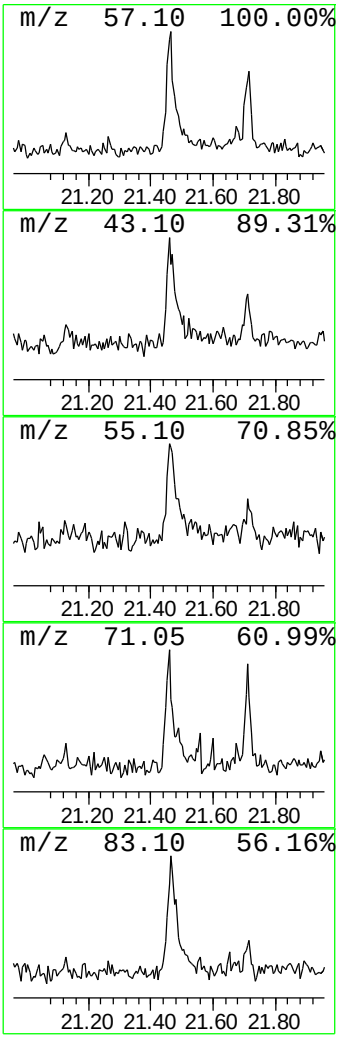
****

Peak Number 6 3-Eicosene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.46	2.45 ng	360108	Chrysene-d12	21.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	90
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	81
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	80
4	E-14-Hexadecenal	238	C16H30O	330207-53-9	56
5	Cyclohexadecane	224	C16H32	000295-65-8	52





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Misc :
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Instrument : BNA_G
ClientSampleId : D8-B3(0-6)C

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

TIC Library : C:\DATABASE\NIST11.L
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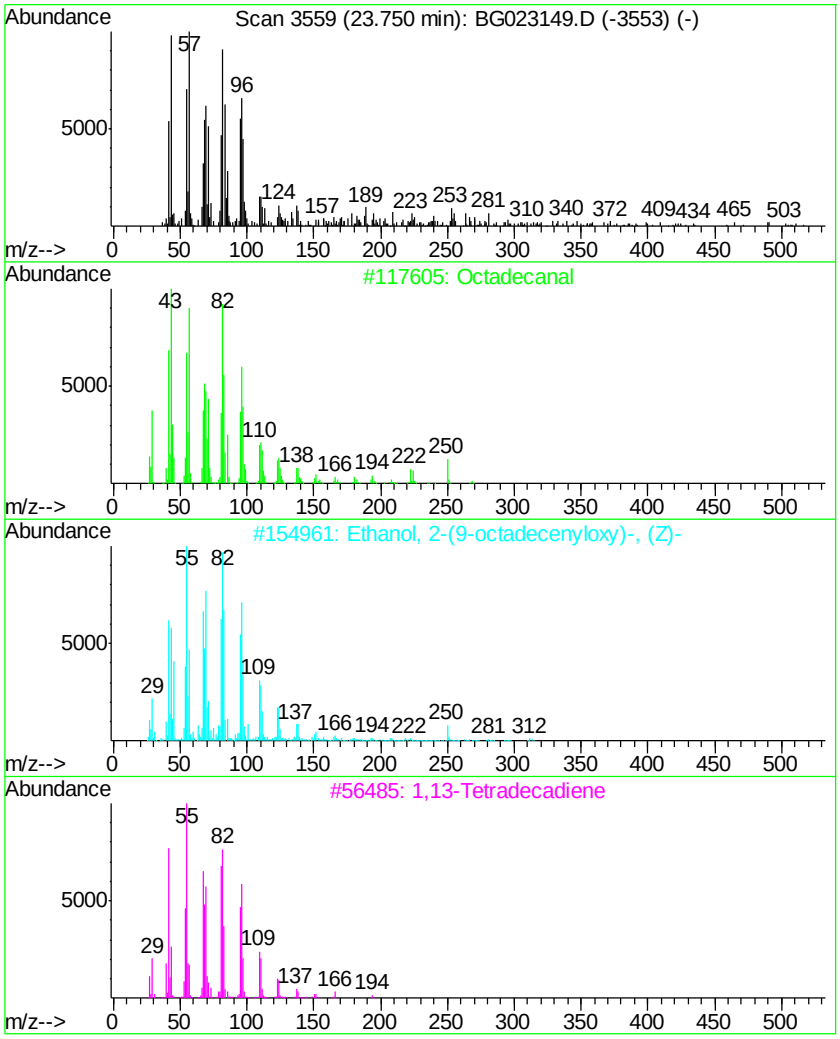
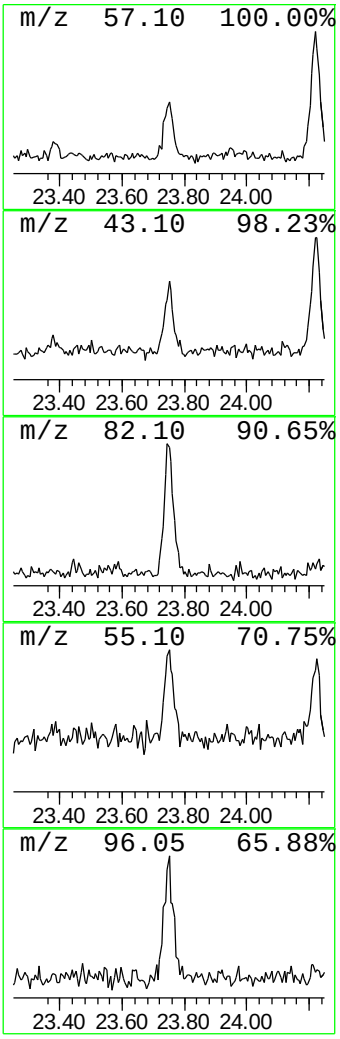
Peak Number 7 Octadecanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.75	4.20 ng	520132	Perylene-d12	25.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	87
2	Ethanol, 2-(9-octadecenyloxy)-, ...	312	C20H40O2	005353-25-3	72
3	1,13-Tetradecadiene	194	C14H26	021964-49-8	62
4	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	58
5	2-Heptadecenal	252	C17H32O	1000143-48-6	58





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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : D8-B3(0-6)C

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

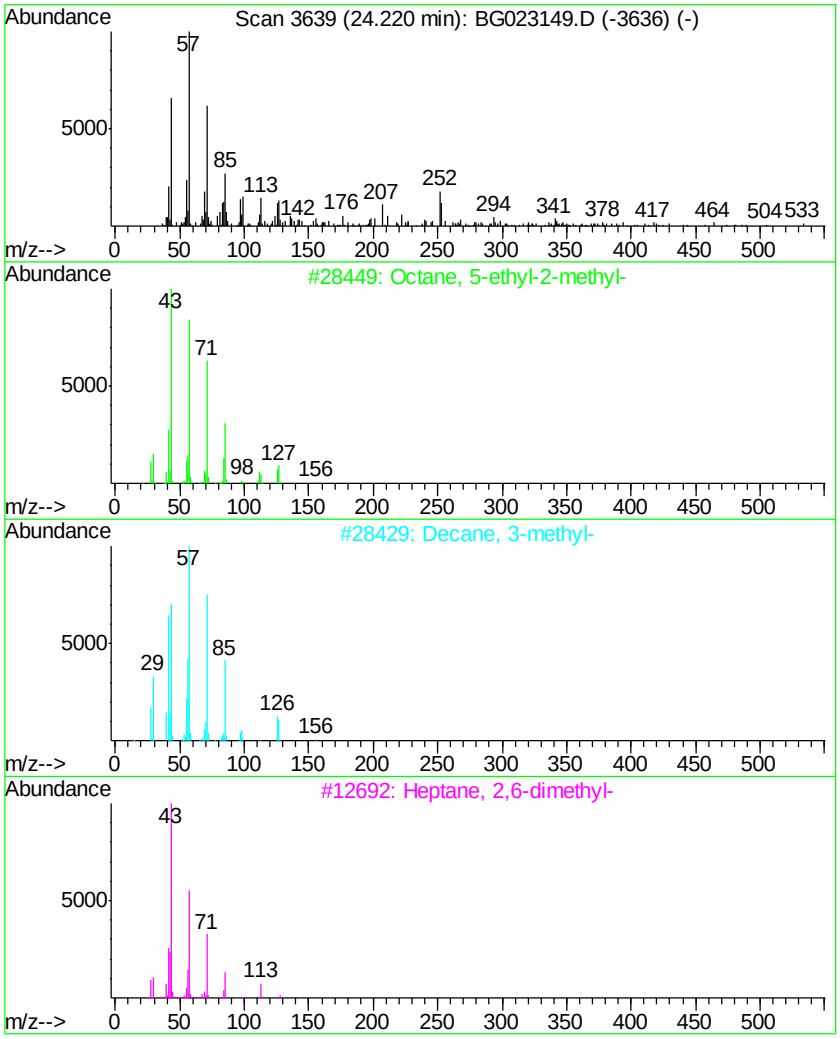
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

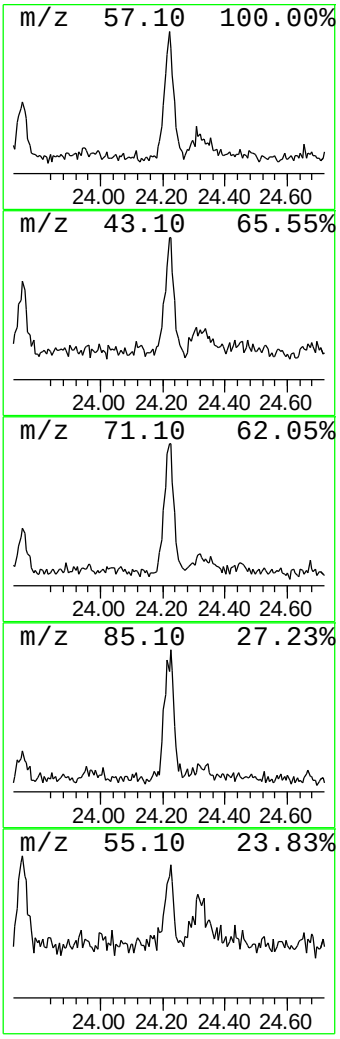
****

Peak Number 8 Octane, 5-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.22	4.91 ng	607691	Perylene-d12	25.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 5-ethyl-2-methyl-	156	C11H24	062016-18-6	58
2	Decane, 3-methyl-	156	C11H24	013151-34-3	52
3	Heptane, 2,6-dimethyl-	128	C9H20	001072-05-5	52
4	Tetradecane	198	C14H30	000629-59-4	52
5	1-Chloroeicosane	316	C20H41Cl	042217-02-7	50





Tentatively Identified Compound (LSC) summary

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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\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 2,2-dime...	3.04	64.3	ng	3179640	1	8.15	988431	20.0
unknown5.22	5.22	9.7	ng	479193	1	8.15	988431	20.0
unknown7.68	7.68	78.9	ng	3900890	1	8.15	988431	20.0
n-Hexadecanoic acid	18.42	4.2	ng	495822	4	17.55	2360670	20.0
3-Eicosene, (E)-	21.46	2.5	ng	360108	5	21.86	2941000	20.0
Octadecanal	23.75	4.2	ng	520132	6	25.22	2477230	20.0
Octane, 5-ethyl-2...	24.22	4.9	ng	607691	6	25.22	2477230	20.0