LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110419\
Data File : BG043486.D
Acq On : 4 Nov 2019 18:29
Operator : JU
Sample : K5628-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR200055-RBR200034-RT1868

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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	3.177	10	15	26	rVB2	81789	153438	9.46%	0.958%
2	5.116	339	345	353	rBV	142378	220841	13.62%	1.379%
3	5.598	420	427	443	rBV	511927	919350	56.71%	5.742%
4	7.196	692	699	717	rBV	531446	1016210	62.68%	6.347%
5	7.554	751	760	772	rBV	579412	1045717	64.50%	6.531%
6	8.012	830	838	847	rBV	178696	320146	19.75%	2.000%
7	8.336	885	893	902	rBV	397408	723632	44.64%	4.520%
8	9.176	1027	1036	1051	rBV	298158	615597	37.97%	3.845%
9	10.815	1307	1315	1333	rBV	205060	425774	26.26%	2.659%
10	13.265	1724	1732	1745	rBV	624905	1074089	66.25%	6.709%
11	14.088	1864	1872	1884	rBV	121578	209432	12.92%	1.308%
12	14.640	1959	1966	1981	rBV	362043	620794	38.29%	3.877%
13	16.132	2213	2220	2239	rBV	727639	1253145	77.30%	7.827%
14	16.790	2328	2332	2339	rBV3	7798	16843	1.04%	0.105%
15	17.390	2427	2434	2438	rBV	426799	706394	43.57%	4.412%
16	17.431	2438	2441	2449	rVV2	68772	115895	7.15%	0.724%
17	17.507	2449	2454	2461	rVB5	20318	44547	2.75%	0.278%
18	18.283	2579	2586	2601	rBV	379893	594973	36.70%	3.716%
19	18.459	2612	2616	2620	rBV6	11894	20370	1.26%	0.127%
20	19.129	2726	2730	2736	rBV3	36844	61675	3.80%	0.385%
21	19.440	2777	2783	2795	rVV	128993	241142	14.87%	1.506%
22	19.546	2798	2801	2809	rVB9	23150	33466	2.06%	0.209%
23	19.769	2835	2839	2840	rBV3	25802	28605	1.76%	0.179%
24	19.799	2840	2844	2853	rVB	89834	148965	9.19%	0.930%
25	19.998	2871	2878	2886	rBV	1154348	1621193	100.00%	10.126%
26	20.298	2926	2929	2932	rVB3	26138	33669	2.08%	0.210%
27	20.792	3010	3013	3018	rVB4	21309	29948	1.85%	0.187%
28	21.250	3085	3091	3094	rBV7	21732	50800	3.13%	0.317%
29	21.291	3094	3098	3108	rVV4	132429	267430	16.50%	1.670%
30	21.373	3109	3112	3121	rVB2	36010	73834	4.55%	0.461%
31	21.655	3152	3160	3166	rBV	506925	960077	59.22%	5.997%
32	21.837	3188	3191	3199	rVB3	39802	55256	3.41%	0.345%
33	22.437	3291	3293	3300	rVB3	34235	49069	3.03%	0.306%
34	23.124	3406	3410	3416	rVB3	33890	58852	3.63%	0.368%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110419\
Data File : BG043486.D
Acq On : 4 Nov 2019 18:29
Operator : JU
Sample : K5628-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR200055-RBR200034-RT1868

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	23.835	3526	3531	3532	rBV3	21750	36415	2.25%	0.227%
36	24.317	3608	3613	3623	rVB4	64827	166879	10.29%	1.042%
37	24.852	3694	3704	3714	rBV	344224	998777	61.61%	6.238%
38	25.586	3822	3829	3839	rVB5	83311	260434	16.06%	1.627%
39	27.172	4090	4099	4114	rVB5	83507	351586	21.69%	2.196%
40	29.176	4433	4440	4457	rVB7	82337	385196	23.76%	2.406%

Sum of corrected areas: 16010455

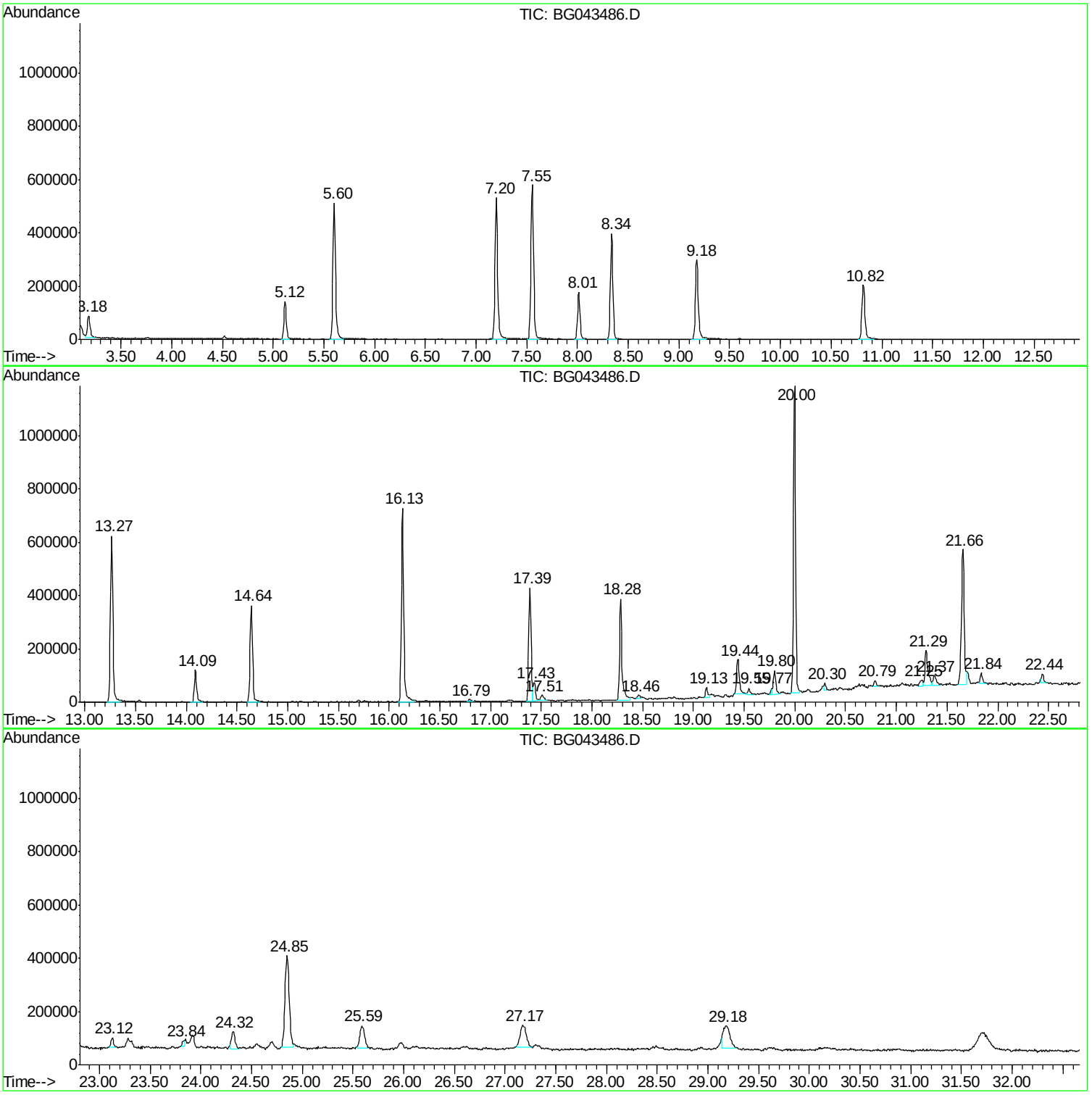
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110419\
Data File : BG043486.D
Acq On : 4 Nov 2019 18:29
Operator : JU
Sample : K5628-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR200055-RBR200034-RT1868

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110419\
Data File : BG043486.D
Acq On : 4 Nov 2019 18:29
Operator : JU
Sample : K5628-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR200055-RBR200034-RT1868

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

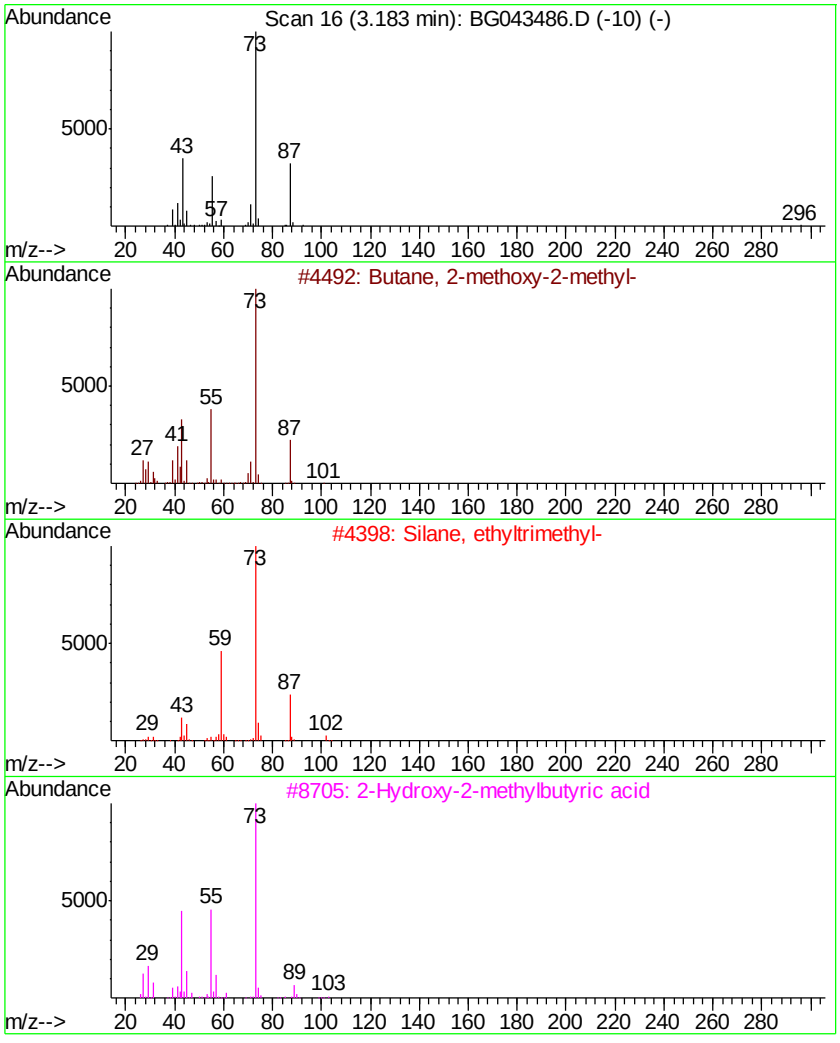
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

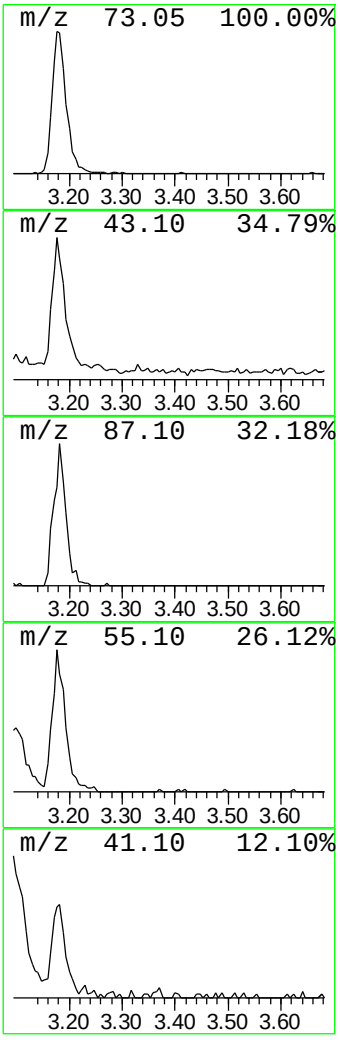
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	9.59 ng	153438	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	33
3	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	32
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110419\
Data File : BG043486.D
Acq On : 4 Nov 2019 18:29
Operator : JU
Sample : K5628-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR200055-RBR200034-RT1868

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

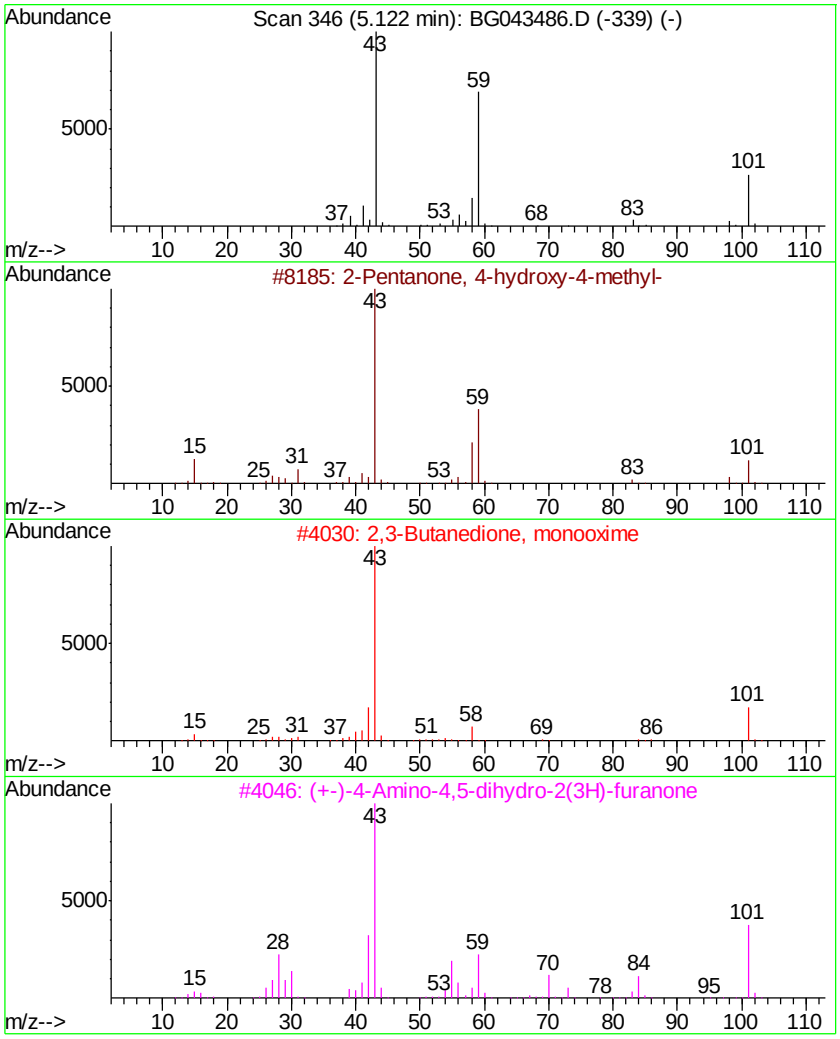
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

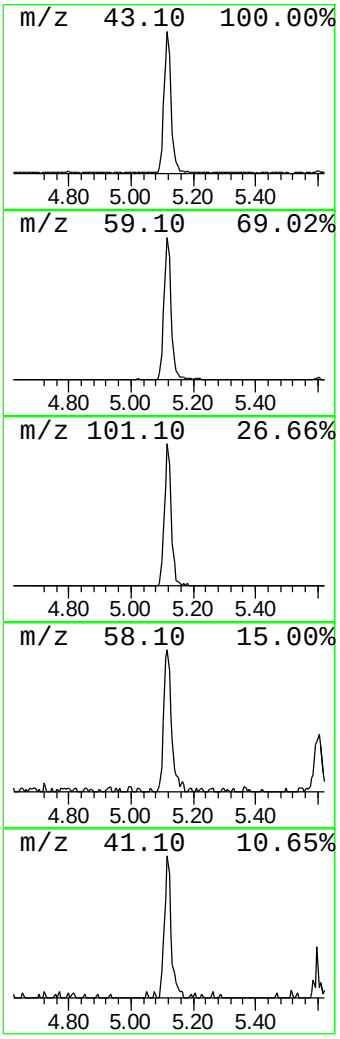
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	13.80 ng	220841	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110419\
Data File : BG043486.D
Acq On : 4 Nov 2019 18:29
Operator : JU
Sample : K5628-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR200055-RBR200034-RT1868

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

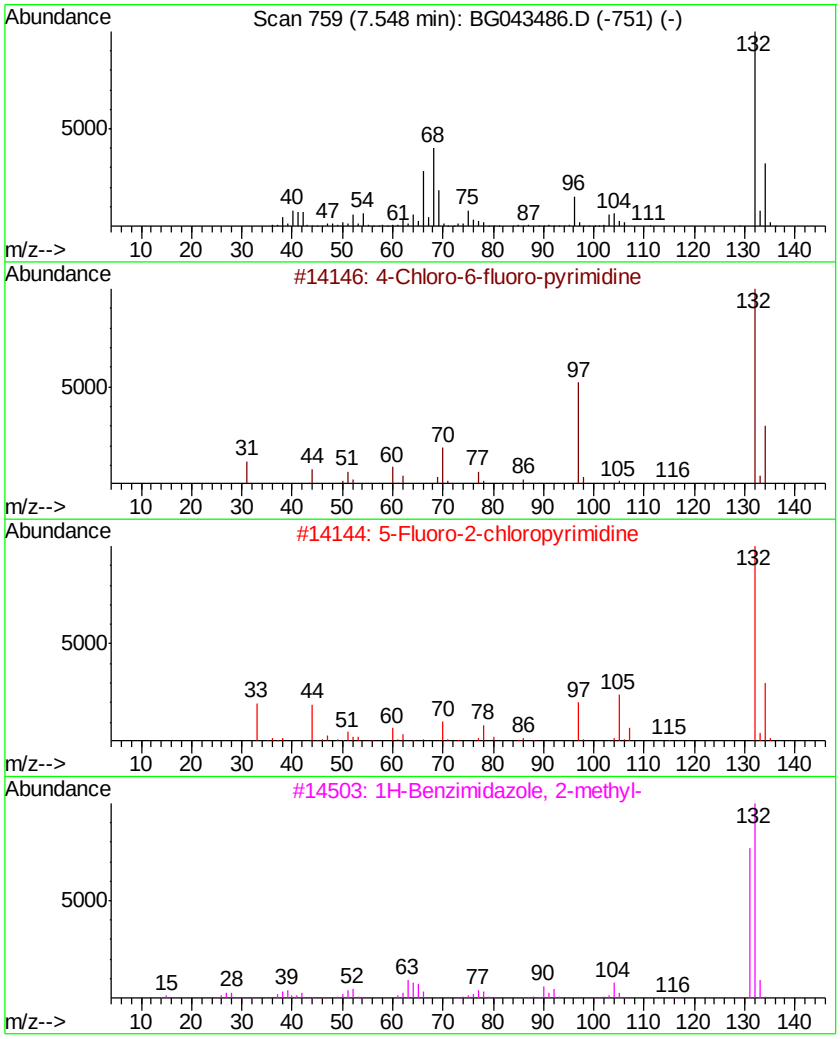
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

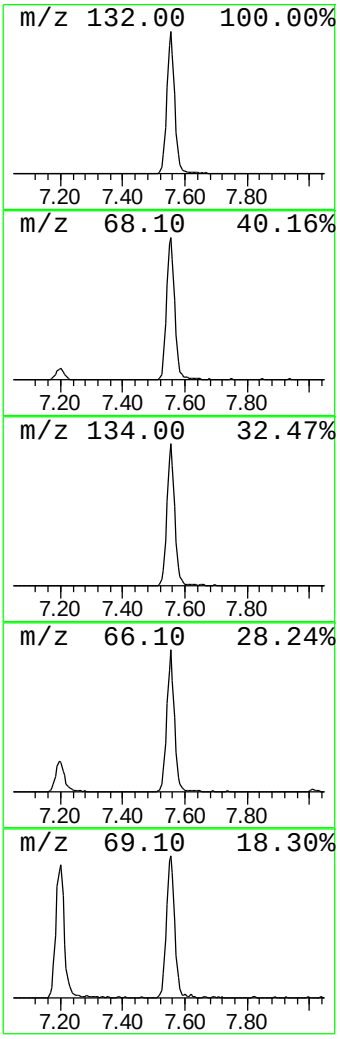
****

Peak Number 3 unknown7.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.55	65.33 ng	1045720	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	12
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110419\
Data File : BG043486.D
Acq On : 4 Nov 2019 18:29
Operator : JU
Sample : K5628-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR200055-RBR200034-RT1868

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

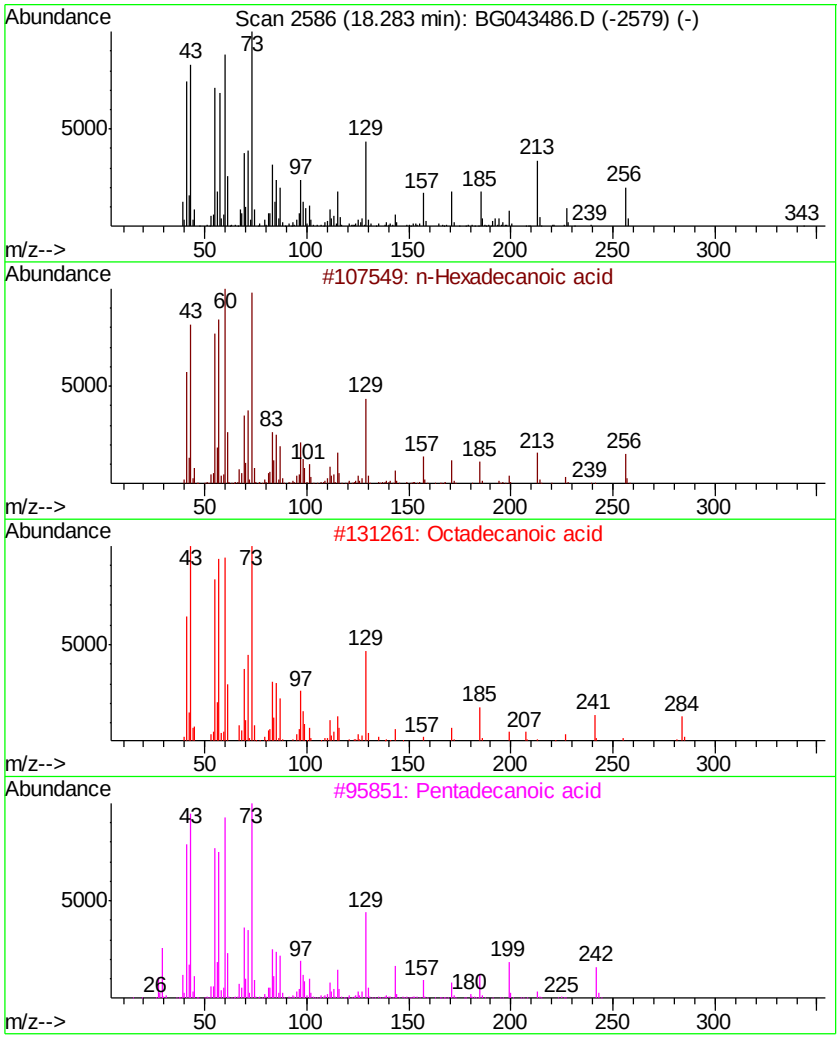
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

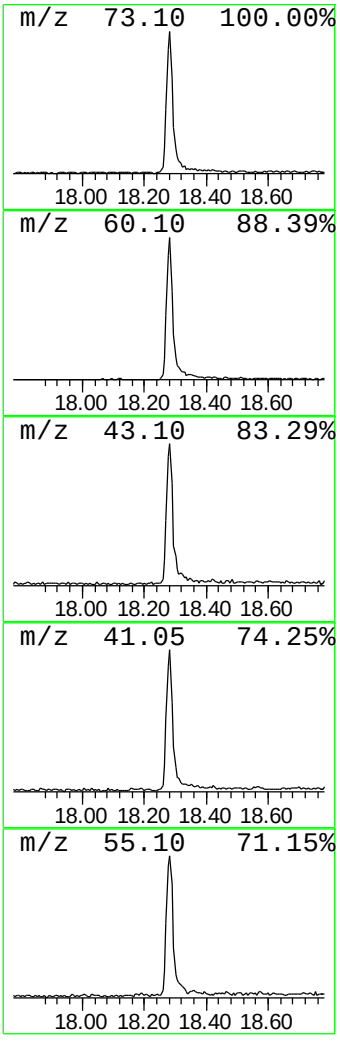
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.28	16.85 ng	594973	Phenanthrene-d10	17.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	86
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110419\
Data File : BG043486.D
Acq On : 4 Nov 2019 18:29
Operator : JU
Sample : K5628-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR200055-RBR200034-RT1868

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

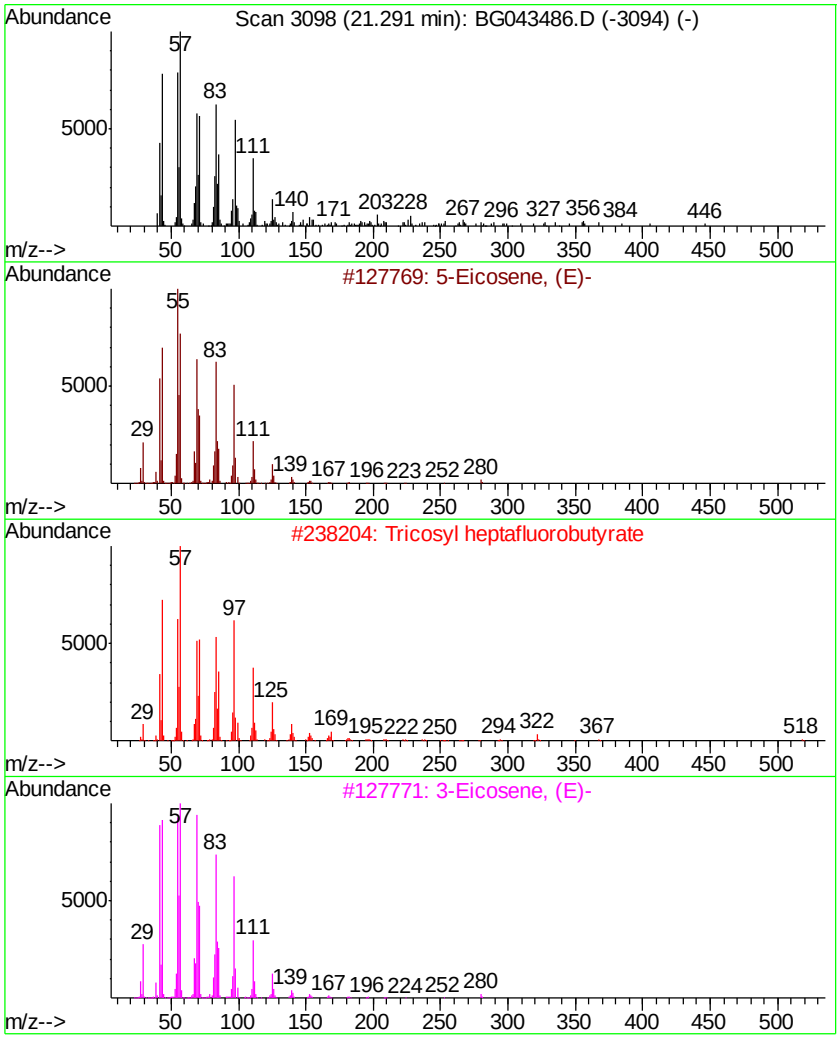
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

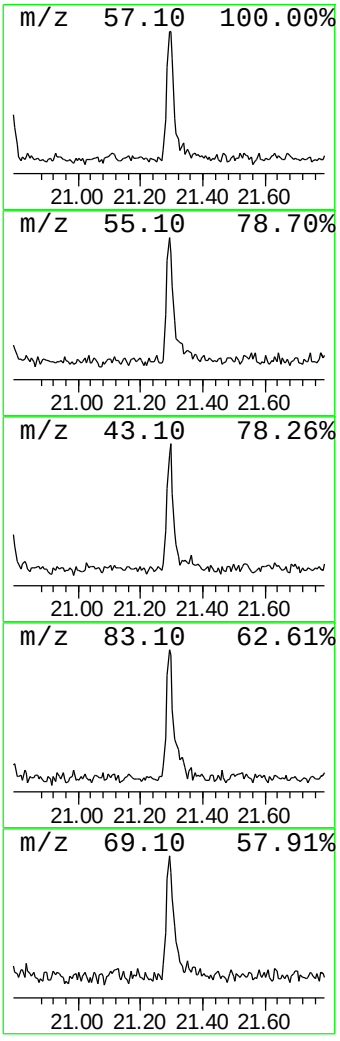
****

Peak Number 6 5-Eicosene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.29	5.57 ng	267430	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
2	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	90
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	90
4	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	89
5	17-Pentatriacontene	491	C35H70	006971-40-0	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110419\
Data File : BG043486.D
Acq On : 4 Nov 2019 18:29
Operator : JU
Sample : K5628-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR200055-RBR200034-RT1868

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

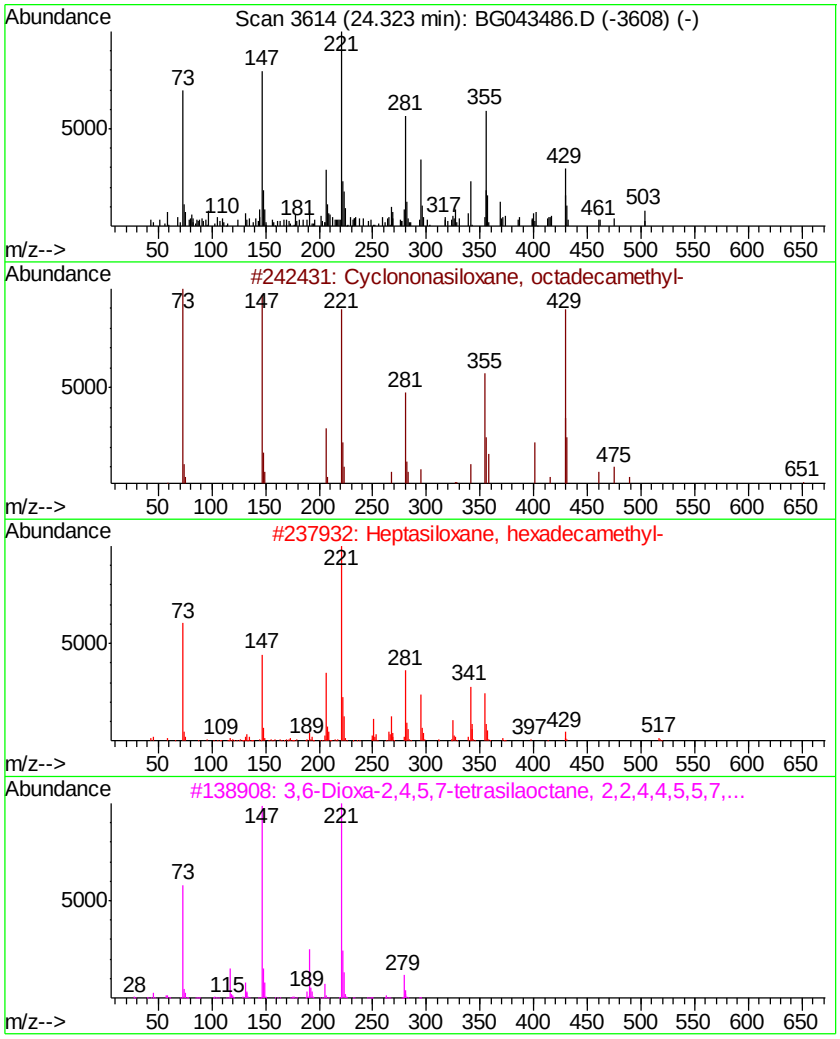
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

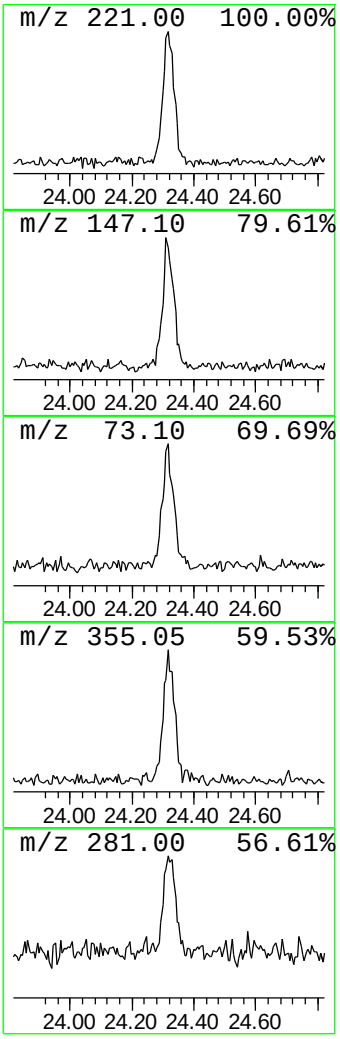
****

Peak Number 7 Cyclononasiloxane, octadeca... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.32	3.34 ng	166879	Perylene-d12	24.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	56
2	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	45
3	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	38
4	Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	27
5	N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	27





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110419\
Data File : BG043486.D
Acq On : 4 Nov 2019 18:29
Operator : JU
Sample : K5628-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR200055-RBR200034-RT1868

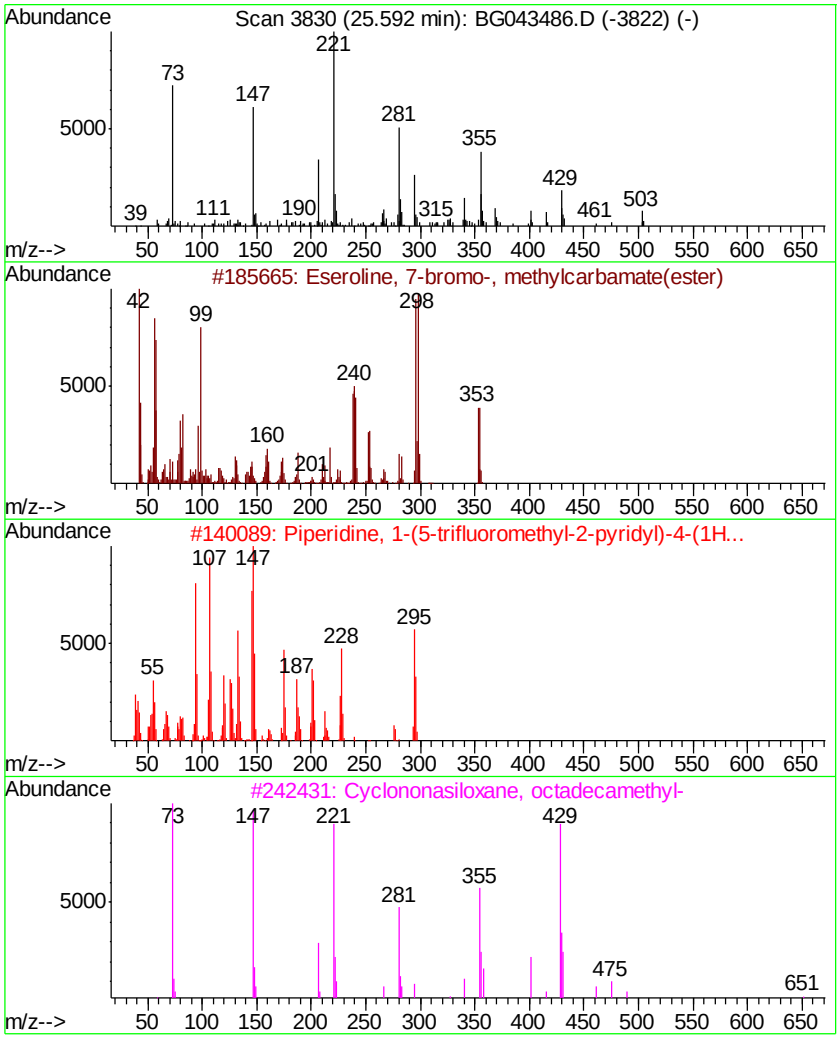
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

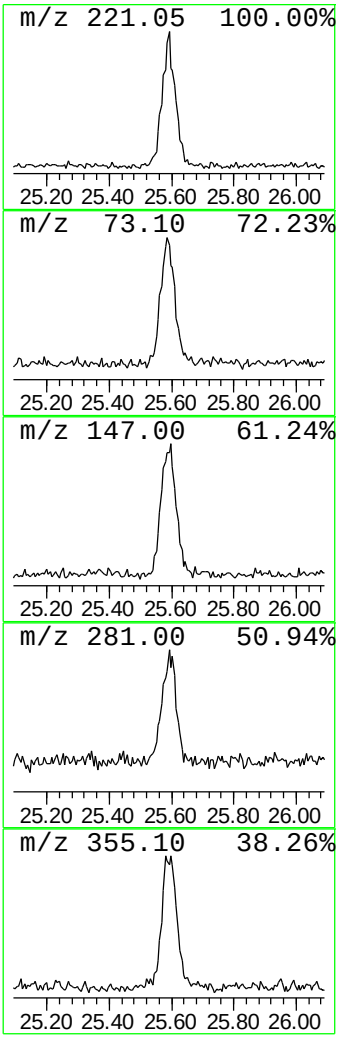
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Eseroline, 7-bromo-, methyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.59	5.22 ng	260434	Perylene-d12	24.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eseroline, 7-bromo-, methylcarba...	353	C15H20BrN3O2	114546-23-5	92
2	Piperidine, 1-(5-trifluoromethyl...	295	C15H16F3N3	1000268-74-7	90
3	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	47
4	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	47
5	4-Hydroxybenzyl alcohol, bis(ter...	352	C19H36O2Si2	1000364-43-9	16





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110419\
Data File : BG043486.D
Acq On : 4 Nov 2019 18:29
Operator : JU
Sample : K5628-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR200055-RBR200034-RT1868

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

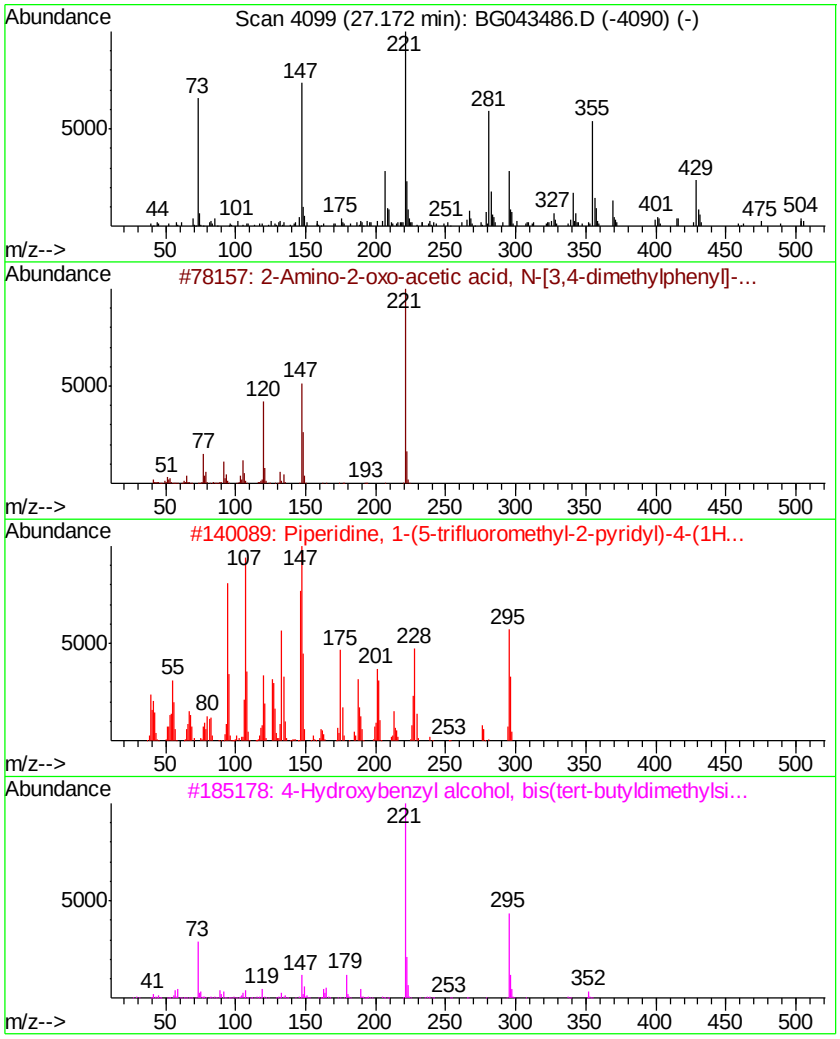
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

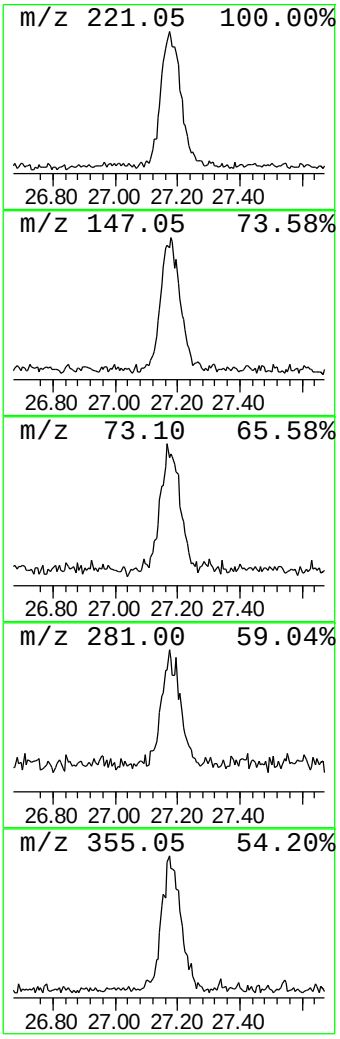
****

Peak Number 9 unknown27.17 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.17	7.04 ng	351586	Perylene-d12	24.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	37
2	Piperidine, 1-(5-trifluoromethyl...	295	C15H16F3N3	1000268-74-7	35
3	4-Hydroxybenzyl alcohol, bis(ter...	352	C19H36O2Si2	1000364-43-9	27
4	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	27
5	1H-Indole-2-carboxylic acid, 6-(...	369	C22H27NO4	1000316-17-3	22





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110419\
Data File : BG043486.D
Acq On : 4 Nov 2019 18:29
Operator : JU
Sample : K5628-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR200055-RBR200034-RT1868

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

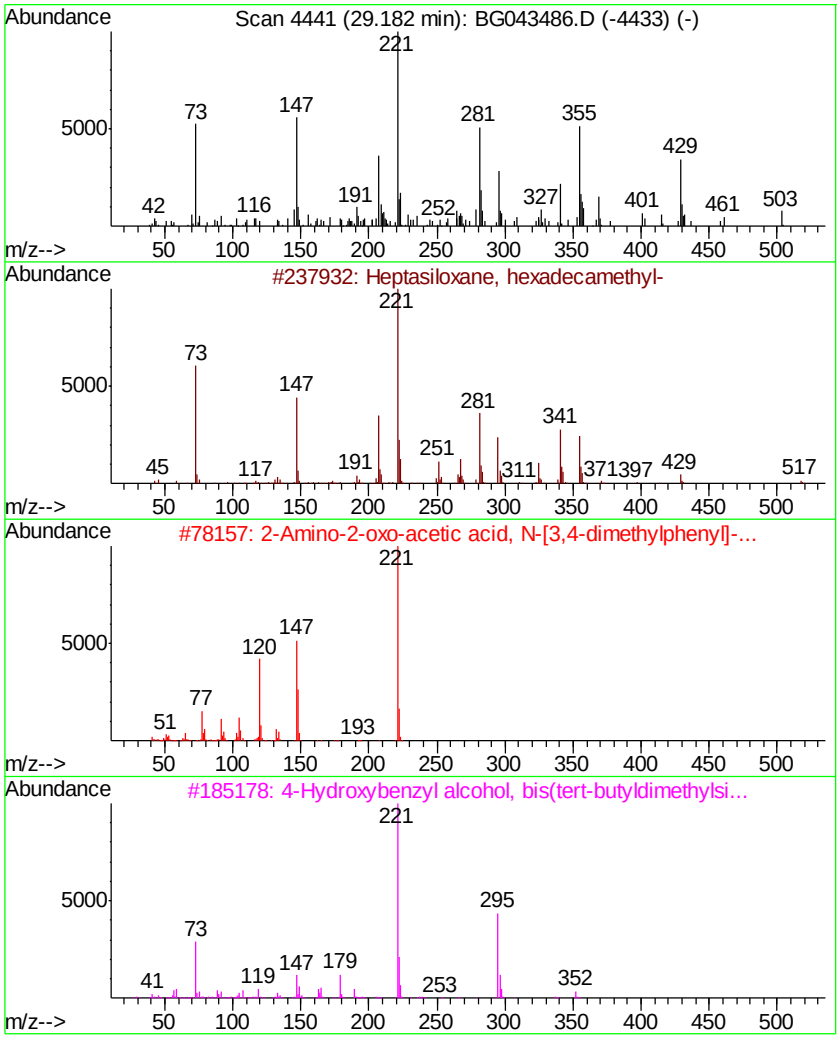
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

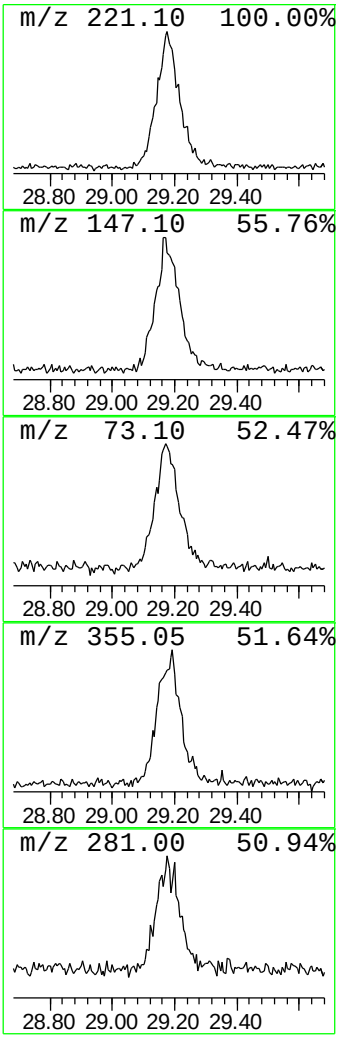
****

Peak Number 10 unknown29.18 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.18	7.71 ng	385196	Perylene-d12	24.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	38
2	2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	27
3	4-Hydroxybenzyl alcohol, bis(ter...	352	C19H36O2Si2	1000364-43-9	16
4	3-Benzylidene-2-indolinone	221	C15H11NO	003359-49-7	11
5	1,3(2H,4H)-Isoquinolinedione, 6,...	369	C20H19NO6	1000115-82-7	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG110419\
Data File : BG043486.D
Acq On : 4 Nov 2019 18:29
Operator : JU
Sample : K5628-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR200055-RBR200034-RT1868

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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
Butane, 2-methoxy...	3.18	9.6	ng	153438	1	8.01	320146	20.0
2-Pentanone, 4-hy...	5.12	13.8	ng	220841	1	8.01	320146	20.0
unknown7.55	7.55	65.3	ng	1045720	1	8.01	320146	20.0
n-Hexadecanoic acid	18.28	16.9	ng	594973	4	17.39	706394	20.0
5-Eicosene, (E)-	21.29	5.6	ng	267430	5	21.66	960077	20.0
Cyclononasiloxane...	24.32	3.3	ng	166879	6	24.85	998777	20.0
Eseroline, 7-brom...	25.59	5.2	ng	260434	6	24.85	998777	20.0
unknown27.17	27.17	7.0	ng	351586	6	24.85	998777	20.0
unknown29.18	29.18	7.7	ng	385196	6	24.85	998777	20.0