LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010320\
Data File : BG043905.D
Acq On : 4 Jan 2020 2:27
Operator : JU
Sample : K6449-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : OW-4

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-BG123019.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	3.146	5	10	30	rVB	2176607	3264052	33.68%	5.597%
2	5.073	331	338	347	rBV	311306	486410	5.02%	0.834%
3	5.543	411	418	429	rBV	1567734	2487683	25.67%	4.265%
4	7.130	679	688	703	rVB	1142857	2008493	20.72%	3.444%
5	7.500	740	751	761	rBV	2404342	4203680	43.37%	7.208%
6	7.964	823	830	839	rBV	469852	792673	8.18%	1.359%
7	8.287	877	885	894	rBV	1796780	3140885	32.40%	5.385%
8	9.116	1017	1026	1037	rBV	1508599	2757567	28.45%	4.728%
9	10.767	1296	1307	1314	rBV	656994	1188953	12.27%	2.039%
10	13.223	1716	1725	1732	rBV	3980408	6448429	66.53%	11.056%
11	14.045	1855	1865	1875	rBV	296240	446348	4.61%	0.765%
12	14.597	1948	1959	1966	rBV	1092430	1797940	18.55%	3.083%
13	16.084	2204	2212	2227	rBV	3640845	5667522	58.47%	9.717%
14	17.335	2419	2425	2432	rBV	1404674	2179576	22.49%	3.737%
15	19.956	2864	2871	2881	rBV	6515815	9692644	100.00%	16.619%
16	20.273	2922	2925	2930	rVB	96509	113464	1.17%	0.195%
17	20.767	3006	3009	3013	rVB	179023	190569	1.97%	0.327%
18	21.254	3087	3092	3104	rBV2	1138457	1896629	19.57%	3.252%
19	21.589	3142	3149	3156	rBV	1320749	2175819	22.45%	3.731%
20	21.807	3181	3186	3193	rBV	377343	531571	5.48%	0.911%
21	22.406	3282	3288	3294	rBV	474825	813076	8.39%	1.394%
22	23.087	3398	3404	3411	rBV	473285	876002	9.04%	1.502%
23	23.875	3531	3538	3552	rVB	461388	997092	10.29%	1.710%
24	24.715	3672	3681	3689	rBV	811727	2182038	22.51%	3.741%
25	24.803	3690	3696	3712	rVB	370696	915284	9.44%	1.569%
26	25.914	3876	3885	3895	rBV3	245269	713103	7.36%	1.223%
27	27.236	4102	4110	4120	rBV3	113473	355463	3.67%	0.609%

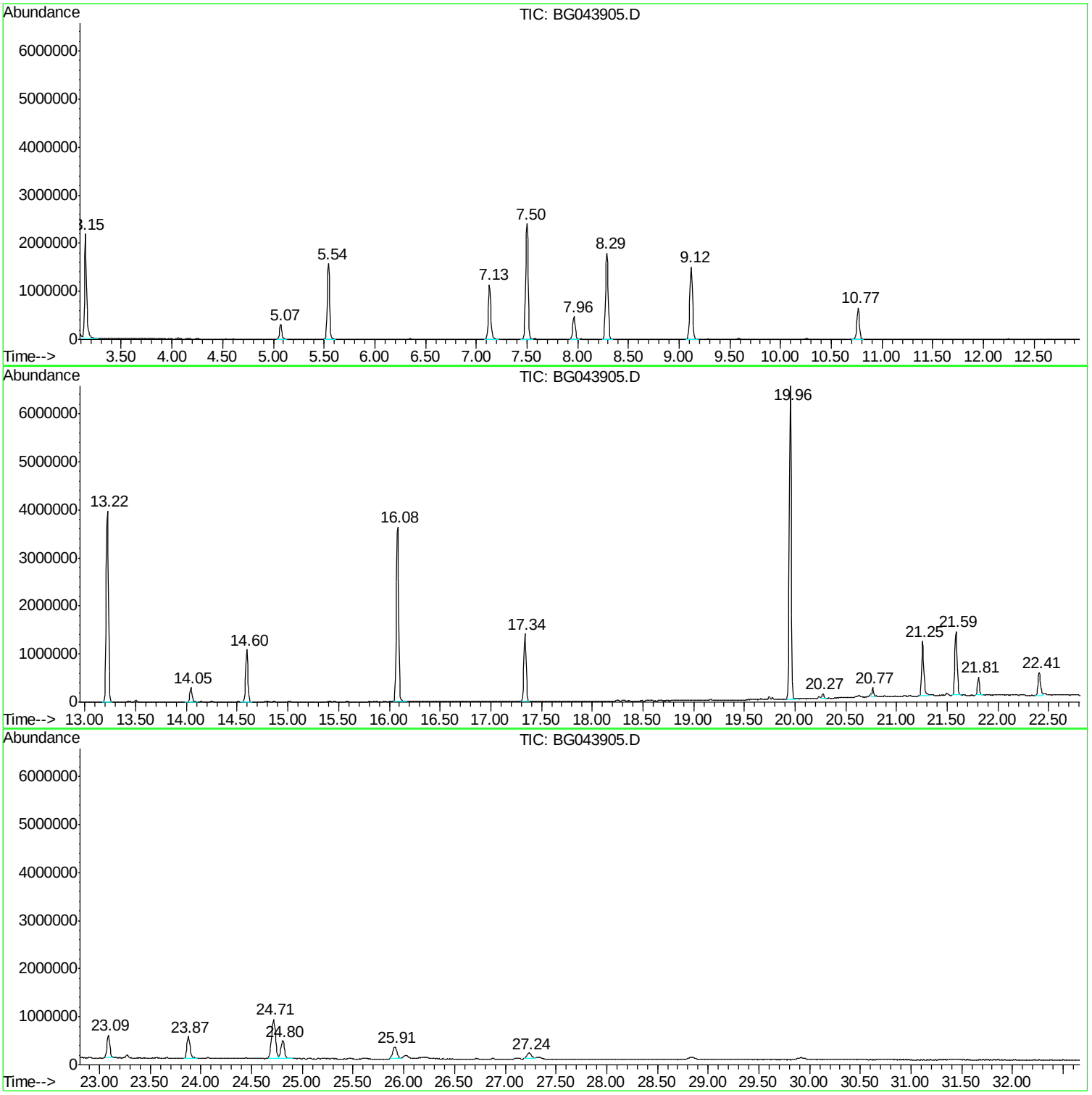
Sum of corrected areas: 58322965

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010320\
Data File : BG043905.D
Acq On : 4 Jan 2020 2:27
Operator : JU
Sample : K6449-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : OW-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.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\BG010320\
Data File : BG043905.D
Acq On : 4 Jan 2020 2:27
Operator : JU
Sample : K6449-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : OW-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

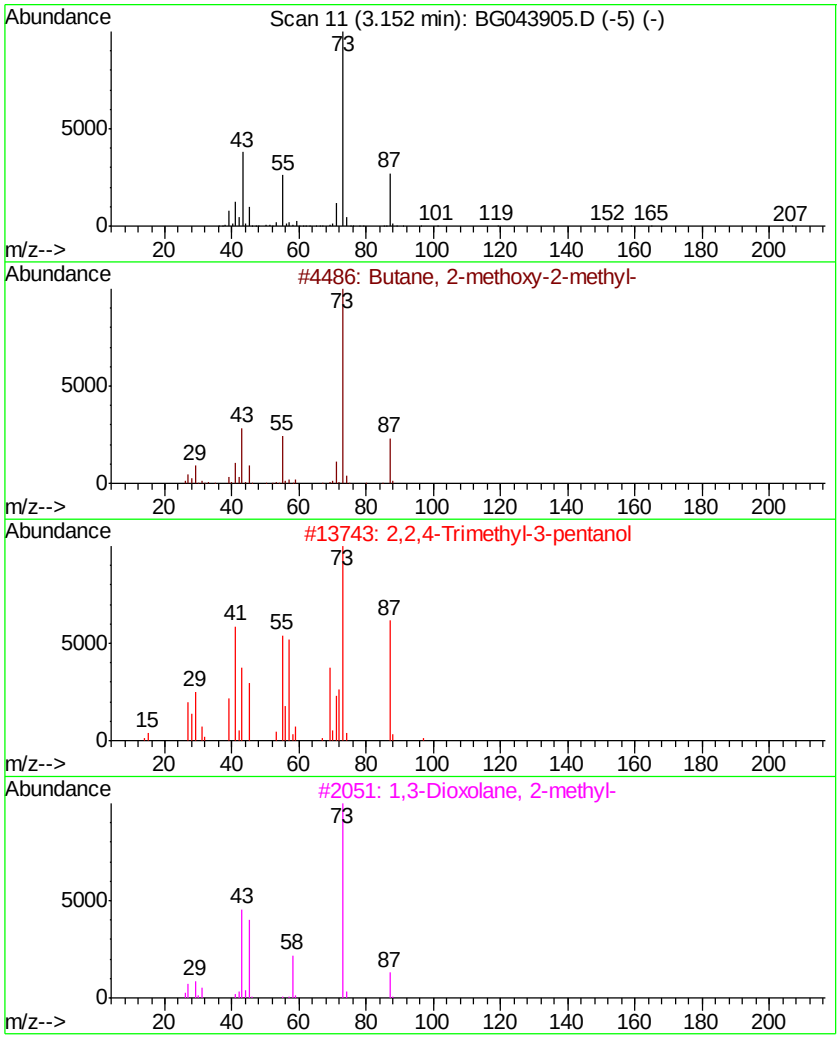
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

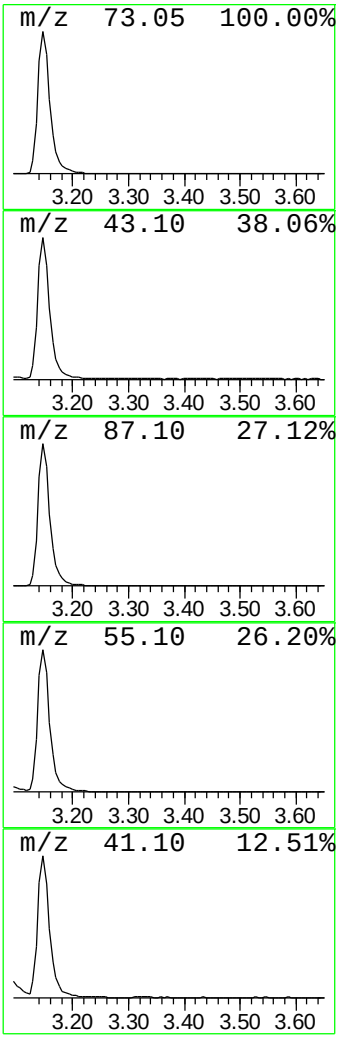
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.15	82.36 ng	3264050	1,4-Dichlorobenzene-d4	7.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	38
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010320\
Data File : BG043905.D
Acq On : 4 Jan 2020 2:27
Operator : JU
Sample : K6449-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : OW-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

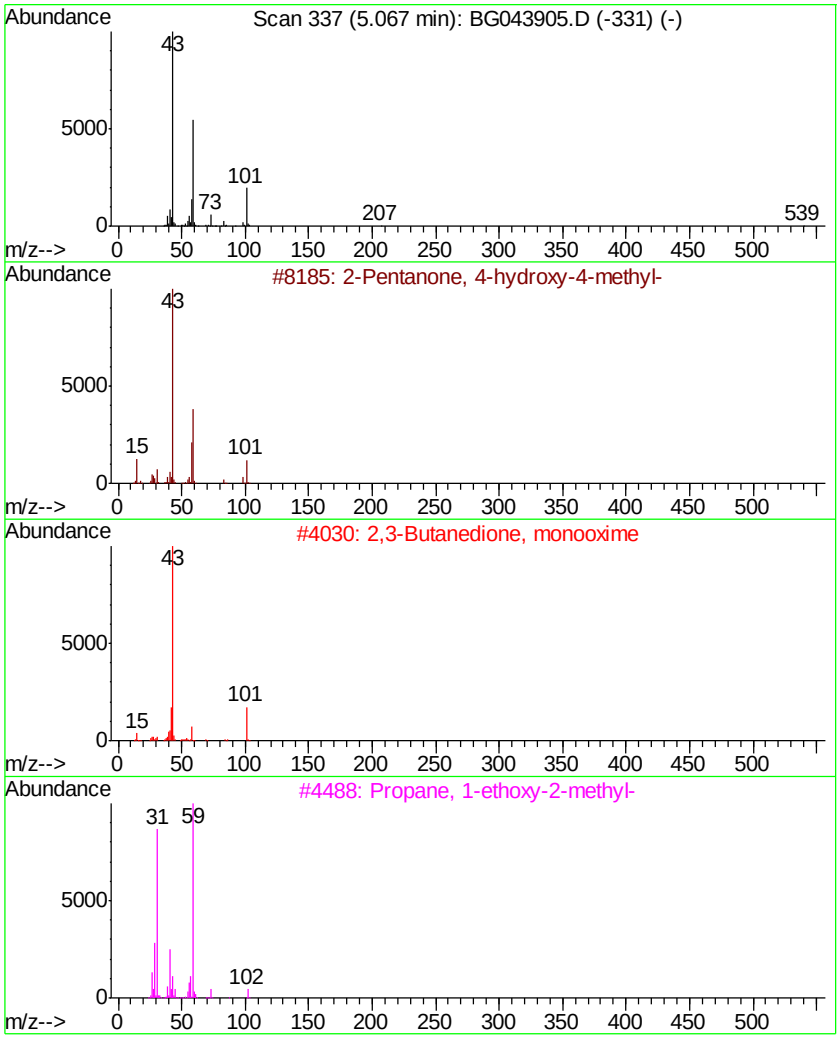
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

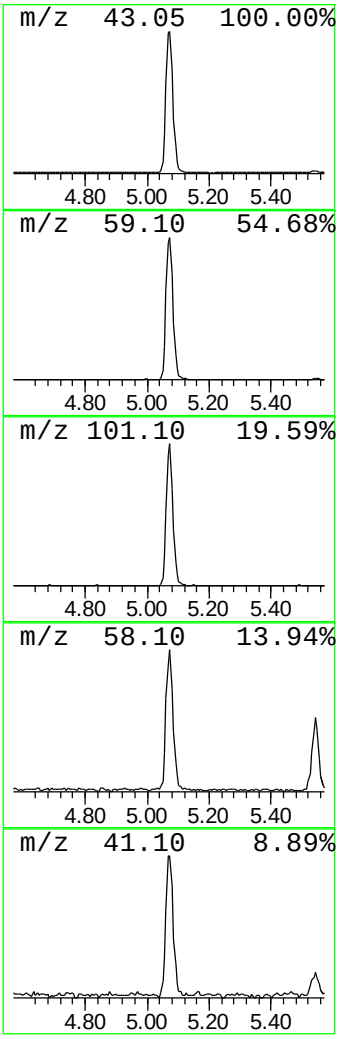
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	12.27 ng	486410	1,4-Dichlorobenzene-d4	7.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	23
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010320\
Data File : BG043905.D
Acq On : 4 Jan 2020 2:27
Operator : JU
Sample : K6449-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : OW-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

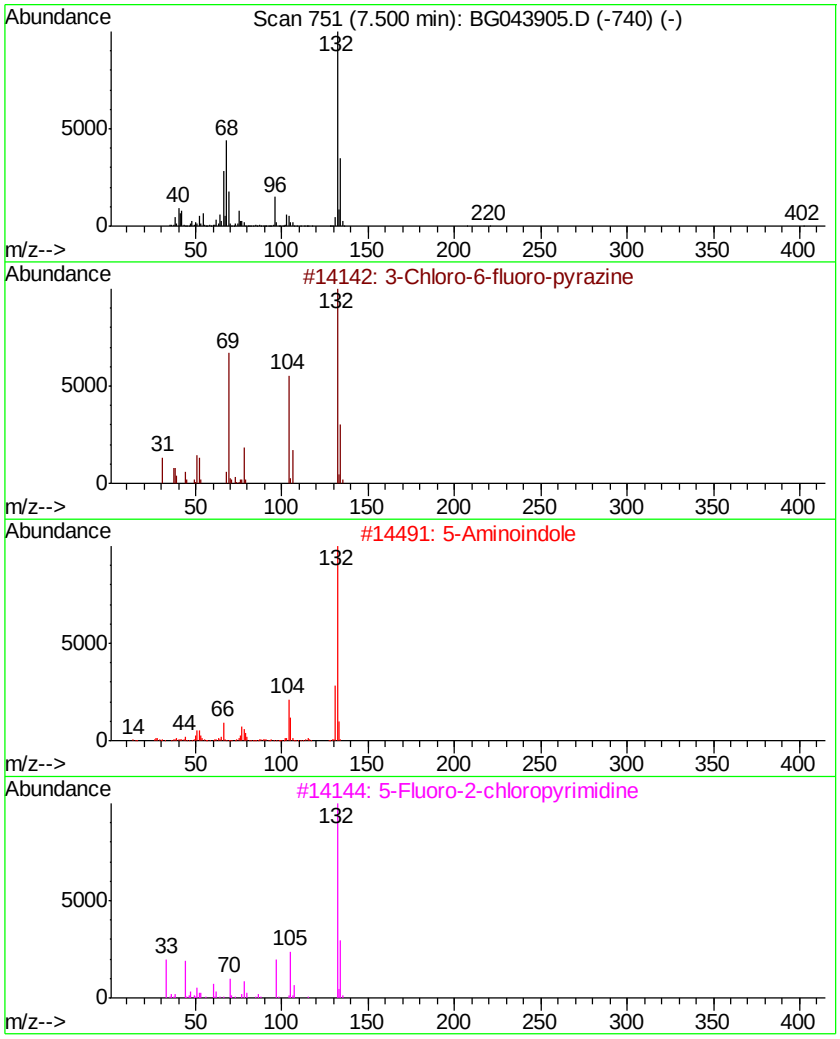
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

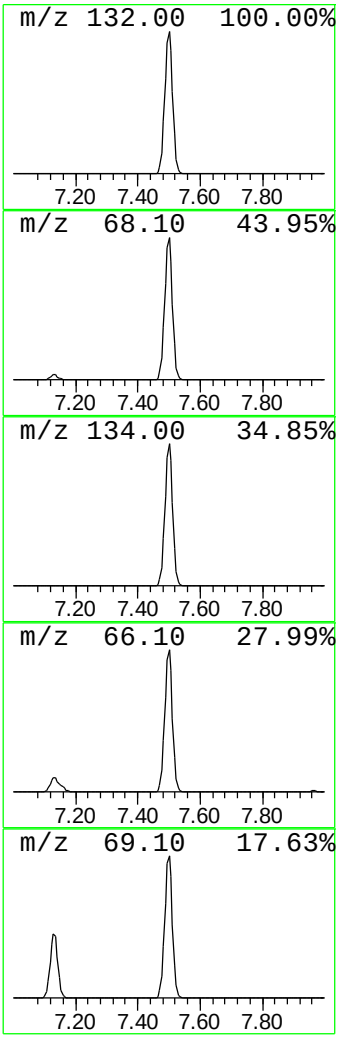
****

Peak Number 3 unknown7.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.50	106.06 ng	4203680	1,4-Dichlorobenzene-d4	7.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010320\
Data File : BG043905.D
Acq On : 4 Jan 2020 2:27
Operator : JU
Sample : K6449-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : OW-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

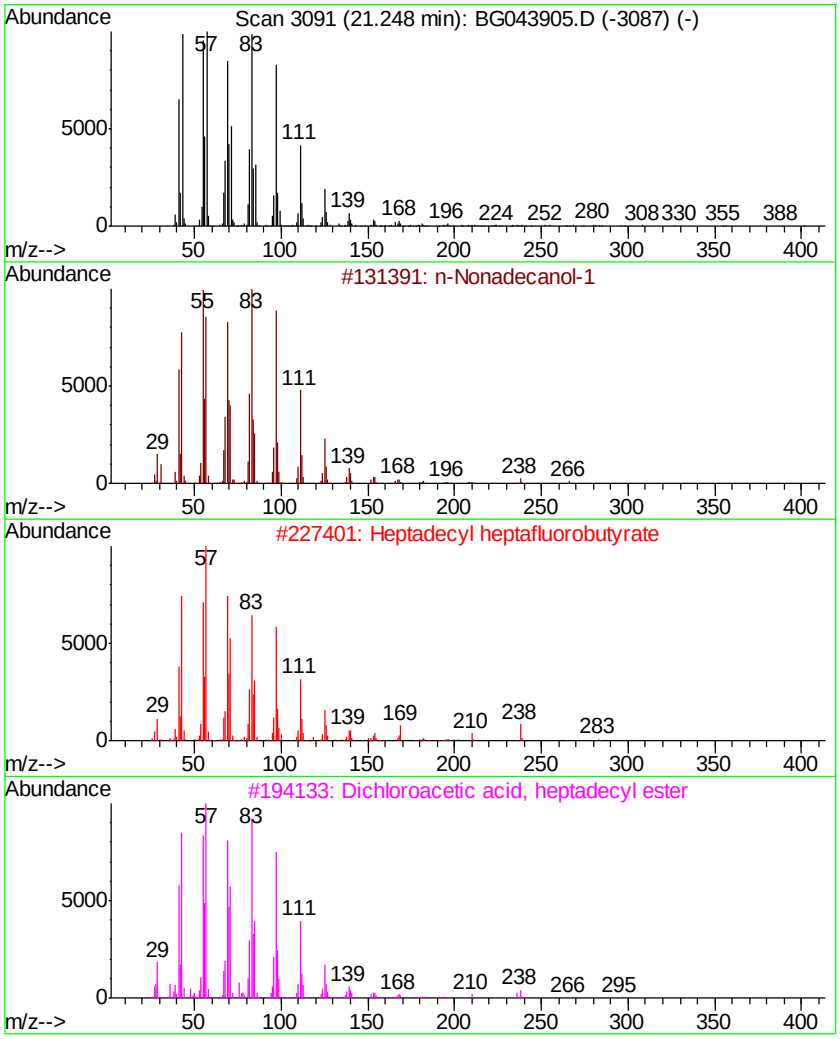
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

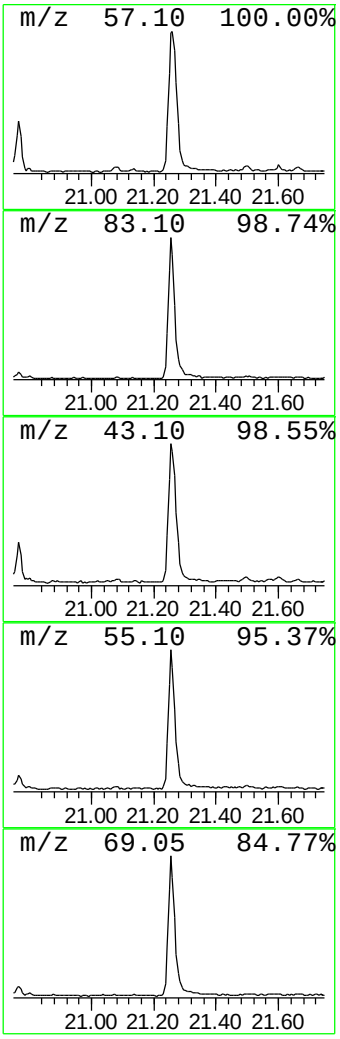
****

Peak Number 5 n-Nonadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.25	17.43 ng	1896630	Chrysene-d12	21.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010320\
Data File : BG043905.D
Acq On : 4 Jan 2020 2:27
Operator : JU
Sample : K6449-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : OW-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

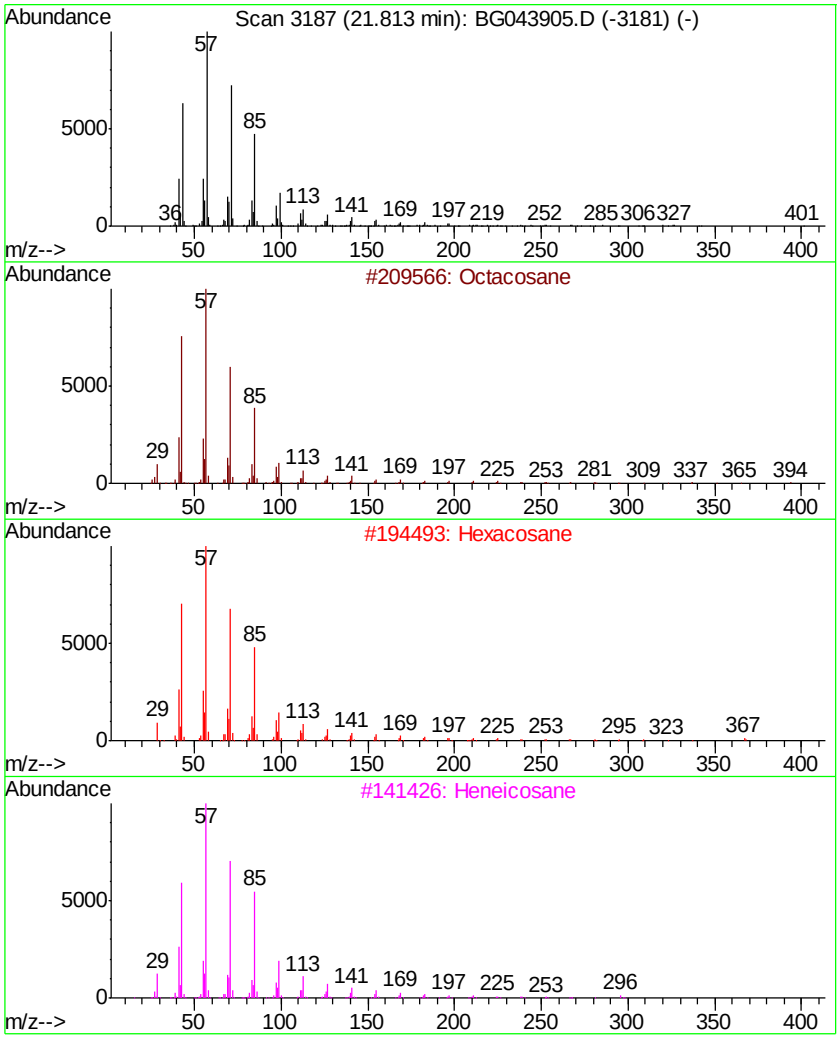
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

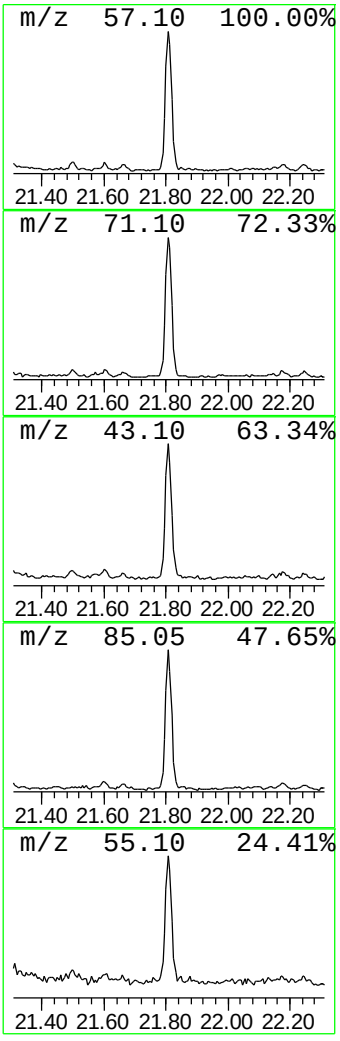
****

Peak Number 6 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.81	4.89 ng	531571	Chrysene-d12	21.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Nonadecane	268	C19H40	000629-92-5	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010320\
Data File : BG043905.D
Acq On : 4 Jan 2020 2:27
Operator : JU
Sample : K6449-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : OW-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

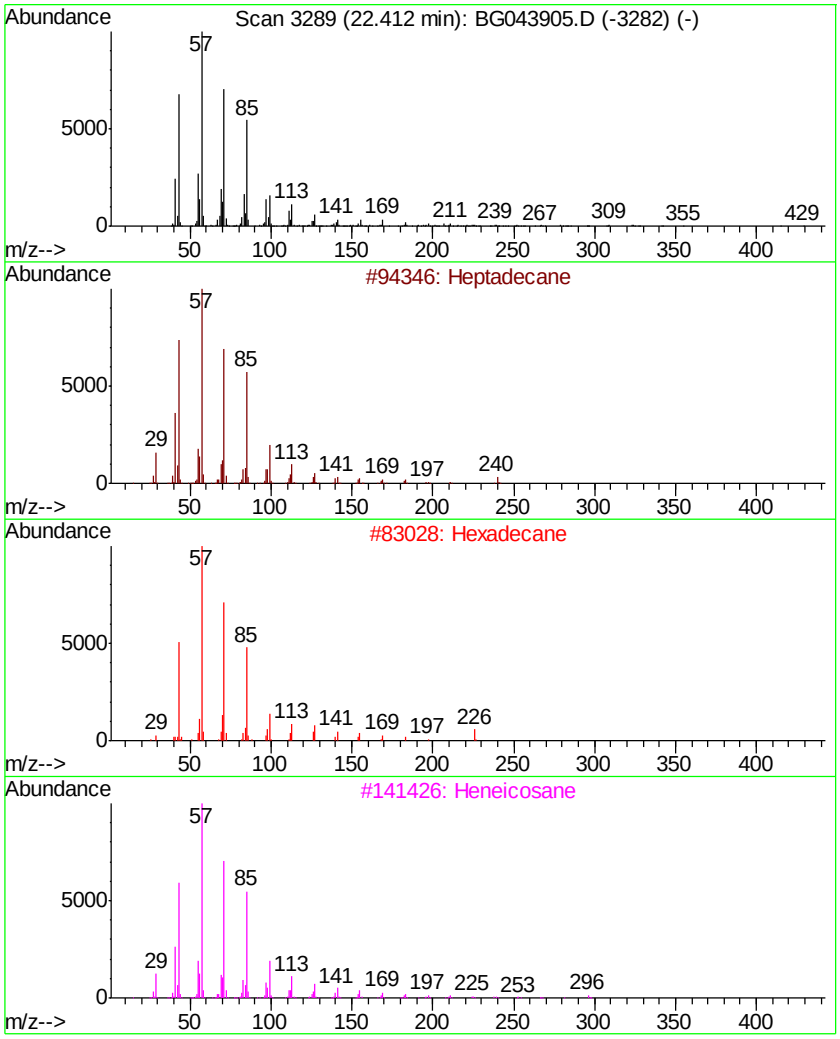
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

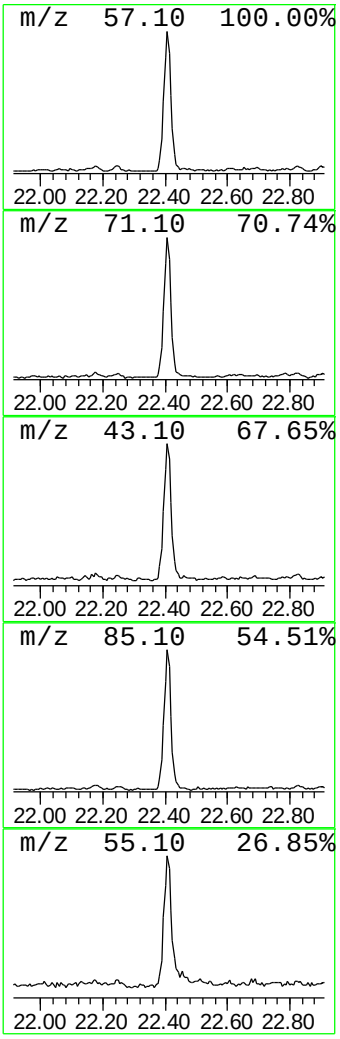
****

Peak Number 7 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.41	7.47 ng	813076	Chrysene-d12	21.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	93
2	Hexadecane	226	C16H34	000544-76-3	93
3	Heneicosane	296	C21H44	000629-94-7	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Tetracosane	338	C24H50	000646-31-1	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010320\
Data File : BG043905.D
Acq On : 4 Jan 2020 2:27
Operator : JU
Sample : K6449-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : OW-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

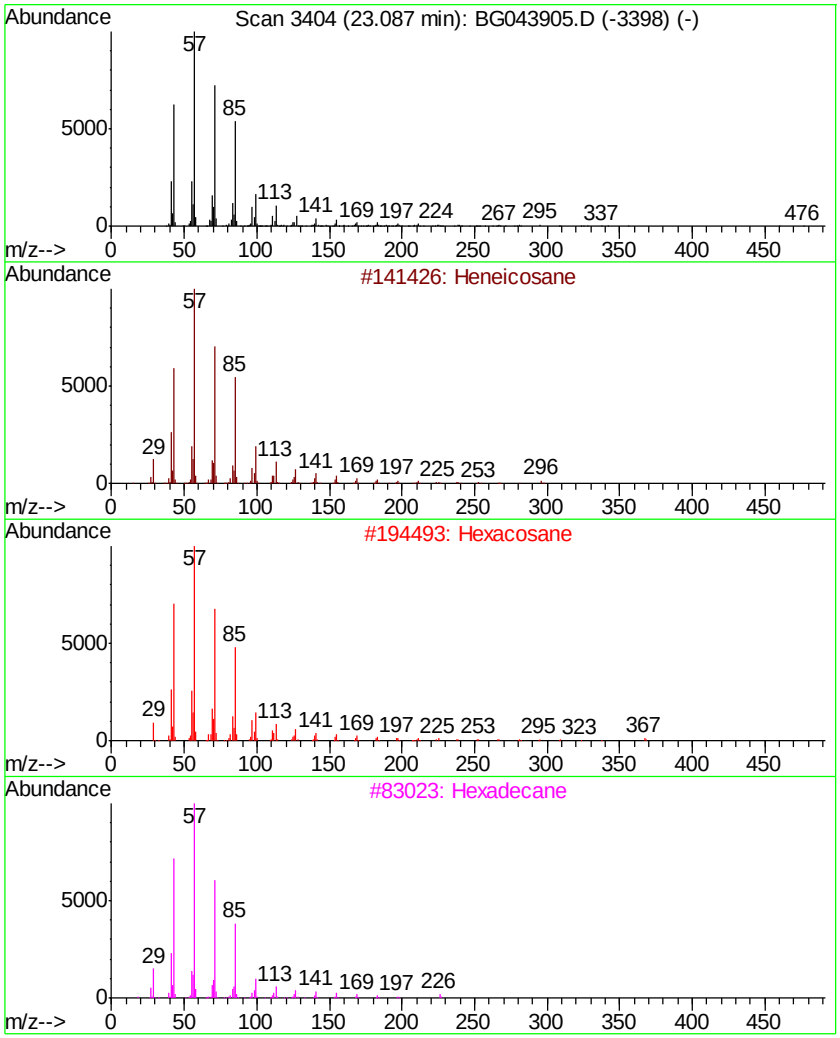
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

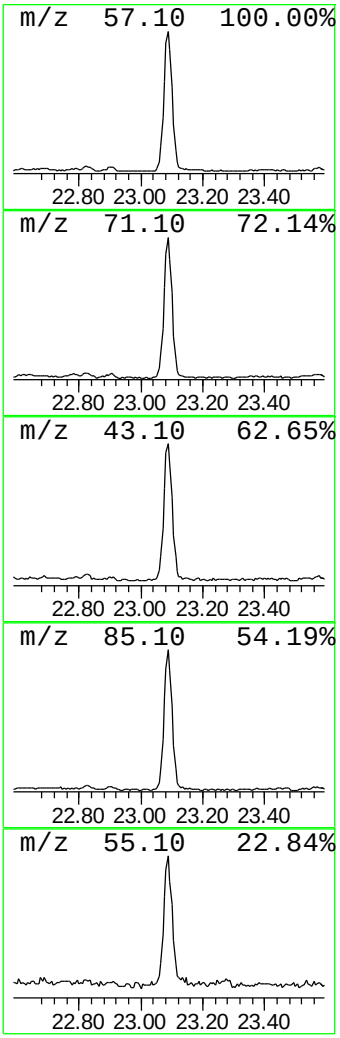
****

Peak Number 8 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.09	8.05 ng	876002	Chrysene-d12	21.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	87
3	Hexadecane	226	C16H34	000544-76-3	86
4	Octadecane	254	C18H38	000593-45-3	86
5	Tetratetracontane	619	C44H90	007098-22-8	83





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010320\
Data File : BG043905.D
Acq On : 4 Jan 2020 2:27
Operator : JU
Sample : K6449-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : OW-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

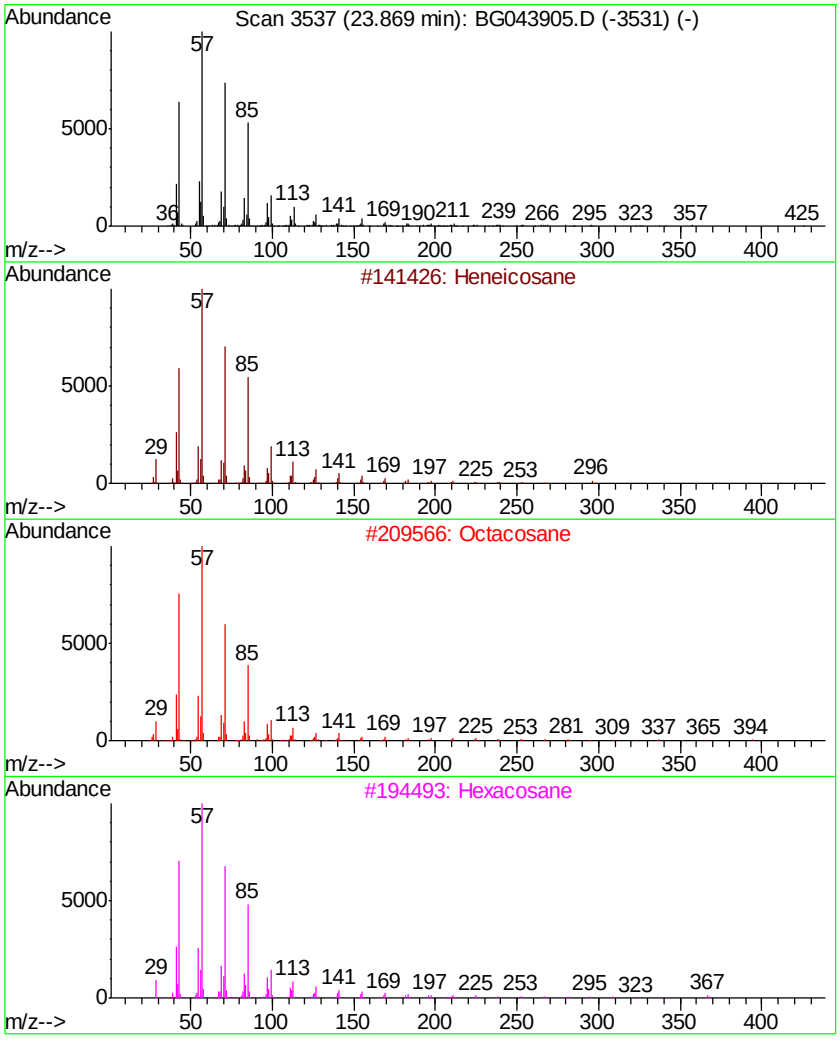
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

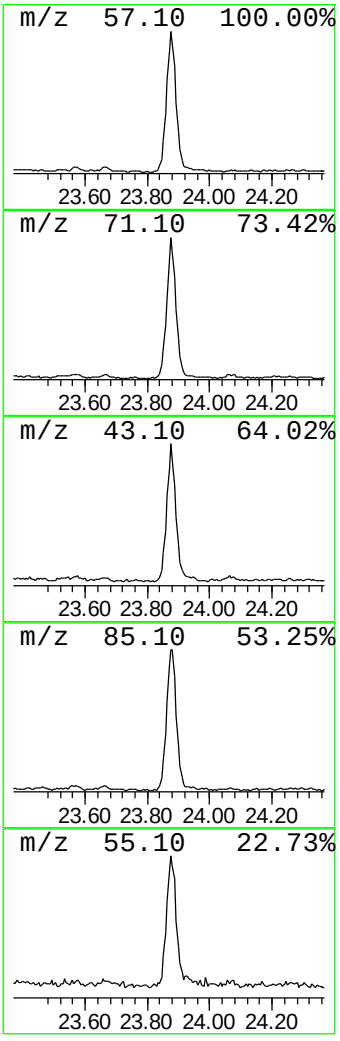
****

Peak Number 9 Eicosane, 7-hexyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.87	9.14 ng	997092	Perylene-d12	24.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
5	Tetracosane	338	C24H50	000646-31-1	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010320\
Data File : BG043905.D
Acq On : 4 Jan 2020 2:27
Operator : JU
Sample : K6449-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : OW-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

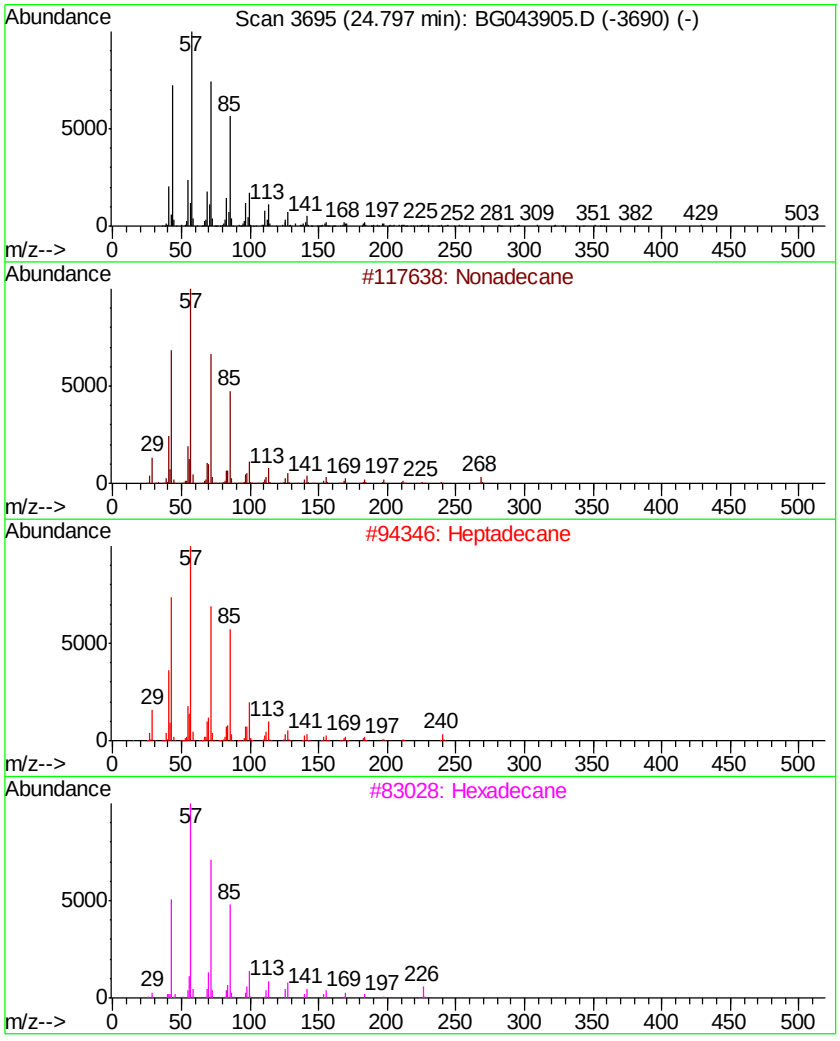
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

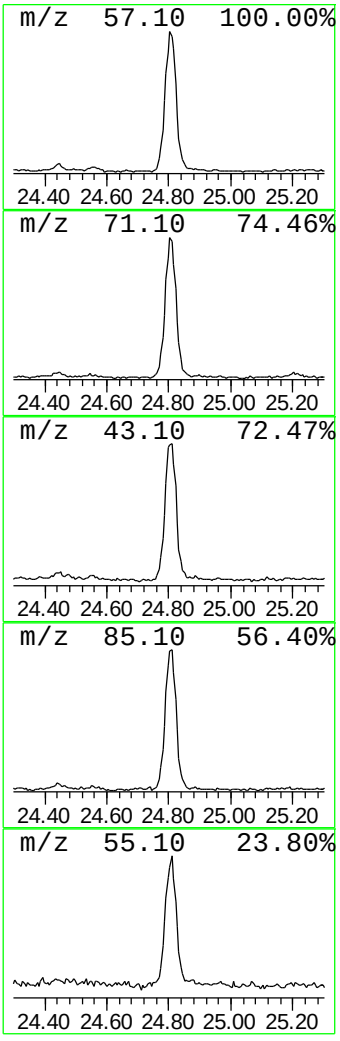
****

Peak Number 10 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.80	8.39 ng	915284	Perylene-d12	24.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	94
2	Heptadecane	240	C17H36	000629-78-7	94
3	Hexadecane	226	C16H34	000544-76-3	93
4	Hexacosane	366	C26H54	000630-01-3	91
5	Heneicosane	296	C21H44	000629-94-7	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010320\
Data File : BG043905.D
Acq On : 4 Jan 2020 2:27
Operator : JU
Sample : K6449-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : OW-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

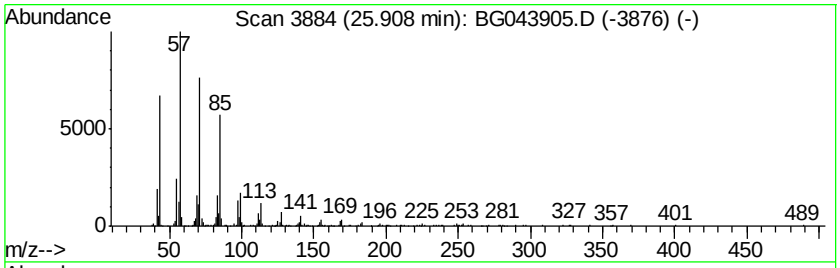
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

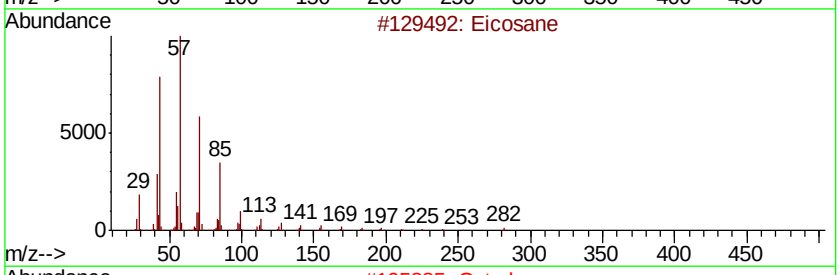
****

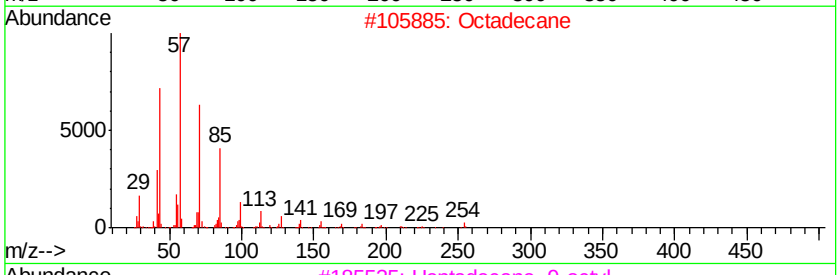
Peak Number 11 Eicosane Concentration Rank 10

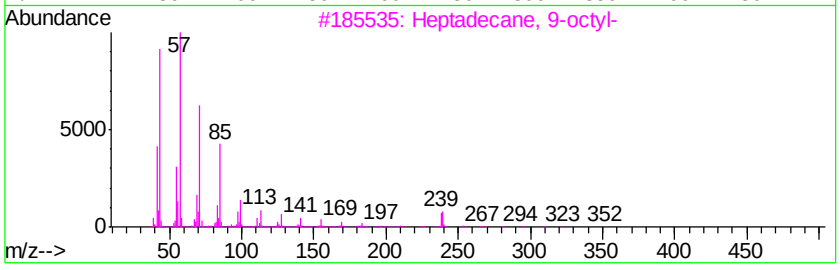
R.T.	EstConc	Area	Relative to ISTD	R.T.
25.91	6.54 ng	713103	Perylene-d12	24.72

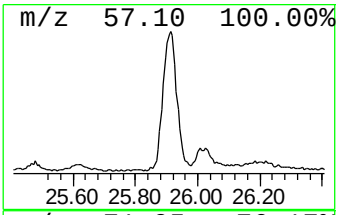
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Octadecane	254	C18H38	000593-45-3	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Tetratetracontane	619	C44H90	007098-22-8	90

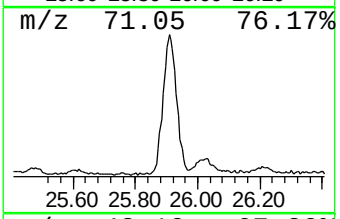


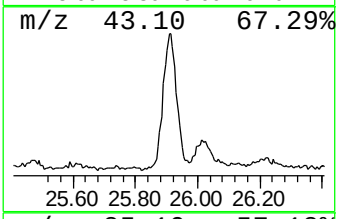


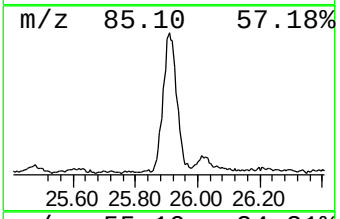


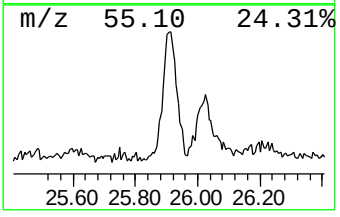












Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010320\
Data File : BG043905.D
Acq On : 4 Jan 2020 2:27
Operator : JU
Sample : K6449-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : OW-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

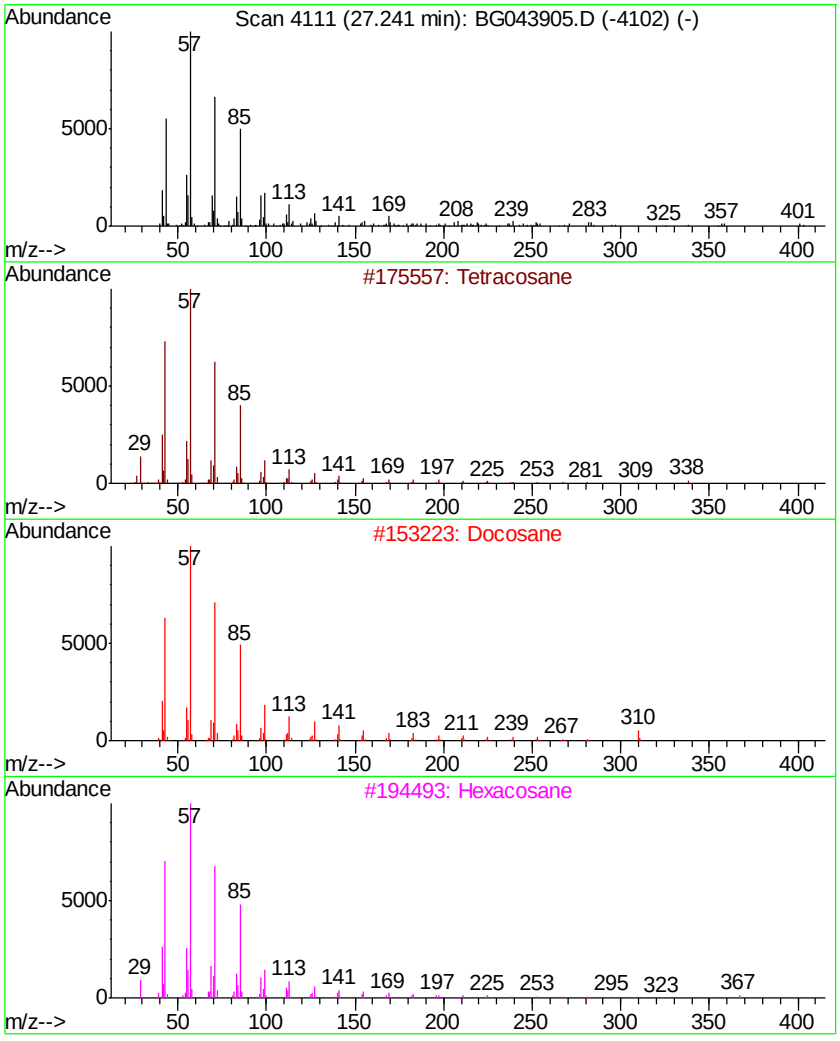
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

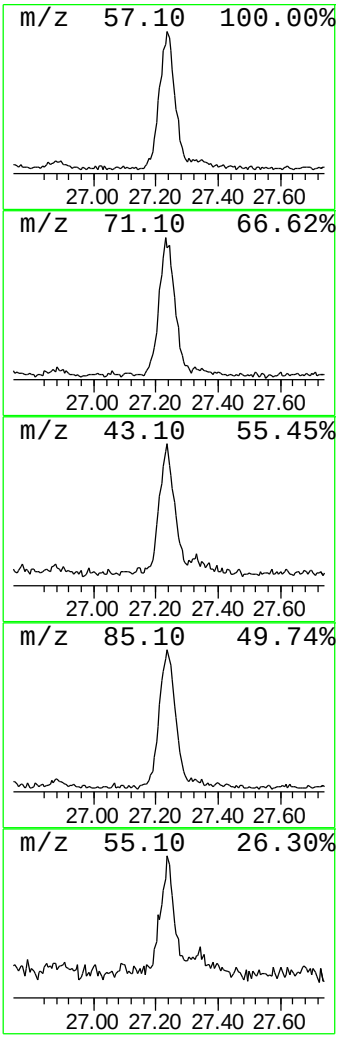
****

Peak Number 12 Tetracosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.24	3.26 ng	355463	Perylene-d12	24.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	87
2	Docosane	310	C22H46	000629-97-0	87
3	Hexacosane	366	C26H54	000630-01-3	83
4	Hexadecane	226	C16H34	000544-76-3	80
5	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG010320\
Data File : BG043905.D
Acq On : 4 Jan 2020 2:27
Operator : JU
Sample : K6449-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : OW-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.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...	3.15	82.4	ng	3264050	1	7.96	792673	20.0
2-Pentanone, 4-hy...	5.07	12.3	ng	486410	1	7.96	792673	20.0
unknown7.50	7.50	106.1	ng	4203680	1	7.96	792673	20.0
n-Nonadecanol-1	21.25	17.4	ng	1896630	5	21.59	2175820	20.0
Octacosane	21.81	4.9	ng	531571	5	21.59	2175820	20.0
Heptadecane	22.41	7.5	ng	813076	5	21.59	2175820	20.0
Heneicosane	23.09	8.1	ng	876002	5	21.59	2175820	20.0
Eicosane, 7-hexyl-	23.87	9.1	ng	997092	6	24.72	2182040	20.0
Nonadecane	24.80	8.4	ng	915284	6	24.72	2182040	20.0
Eicosane	25.91	6.5	ng	713103	6	24.72	2182040	20.0
Tetracosane	27.24	3.3	ng	355463	6	24.72	2182040	20.0