LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020420\
Data File : BG044289.D
Acq On : 4 Feb 2020 20:34
Operator : CG/JU
Sample : PB126573BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126573BL

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-BG013020.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	5.021	323	329	340	rVB	40245	70804	1.20%	0.252%
2	5.491	402	409	420	rBV	803185	1354559	22.96%	4.827%
3	7.083	669	680	698	rBV	522082	943421	15.99%	3.362%
4	7.918	813	822	830	rBV	281340	489481	8.30%	1.744%
5	8.241	869	877	886	rBV	987167	1761285	29.86%	6.276%
6	9.069	1010	1018	1036	rBV	763570	1434426	24.32%	5.111%
7	10.714	1290	1298	1310	rBV	373070	686825	11.64%	2.447%
8	13.176	1710	1717	1735	rBV	2210053	3457931	58.62%	12.322%
9	14.005	1852	1858	1868	rBV	97157	156136	2.65%	0.556%
10	14.551	1942	1951	1960	rBV	652146	1023498	17.35%	3.647%
11	16.044	2197	2205	2221	rBV	1879335	2967714	50.31%	10.575%
12	17.295	2411	2418	2430	rBV	844316	1309630	22.20%	4.667%
13	17.418	2430	2439	2447	rVB3	38298	64908	1.10%	0.231%
14	19.915	2857	2864	2878	rBV	4362891	5898718	100.00%	21.020%
15	20.726	2996	3002	3006	rBV2	96738	105369	1.79%	0.375%
16	21.214	3079	3085	3094	rBV2	272436	476419	8.08%	1.698%
17	21.543	3134	3141	3150	rBV2	867708	1474184	24.99%	5.253%
18	21.754	3171	3177	3182	rBV	232189	317903	5.39%	1.133%
19	22.342	3271	3277	3289	rBV	272367	442450	7.50%	1.577%
20	23.012	3385	3391	3400	rVB	267134	488412	8.28%	1.740%
21	23.194	3415	3422	3430	rVB	369364	650618	11.03%	2.318%
22	23.787	3516	3523	3531	rBV2	214019	447332	7.58%	1.594%
23	24.639	3657	3668	3675	rBV	525880	1523032	25.82%	5.427%
24	25.785	3854	3863	3874	rBV	116871	365209	6.19%	1.301%
25	27.084	4078	4084	4093	rVB4	50541	152798	2.59%	0.544%

Sum of corrected areas: 28063062

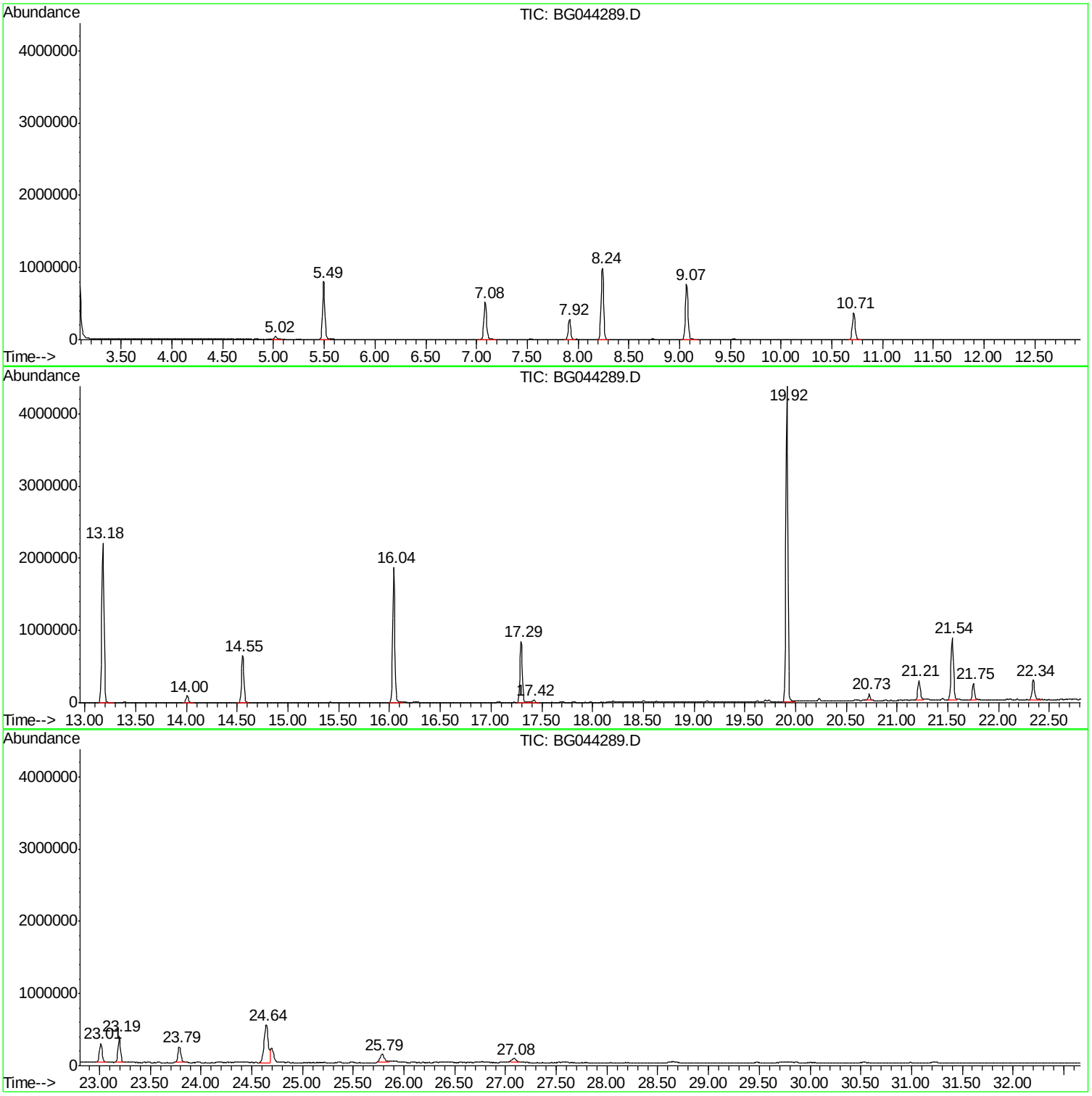
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020420\
Data File : BG044289.D
Acq On : 4 Feb 2020 20:34
Operator : CG/JU
Sample : PB126573BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126573BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020420\
Data File : BG044289.D
Acq On : 4 Feb 2020 20:34
Operator : CG/JU
Sample : PB126573BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126573BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

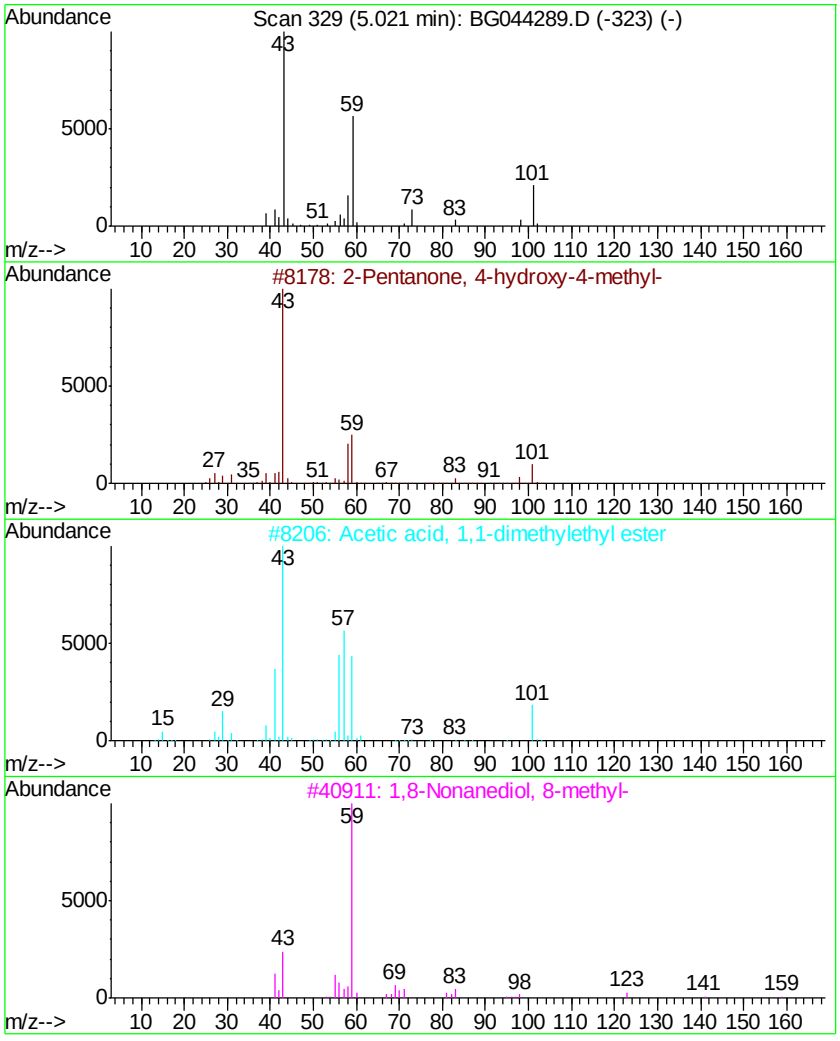
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

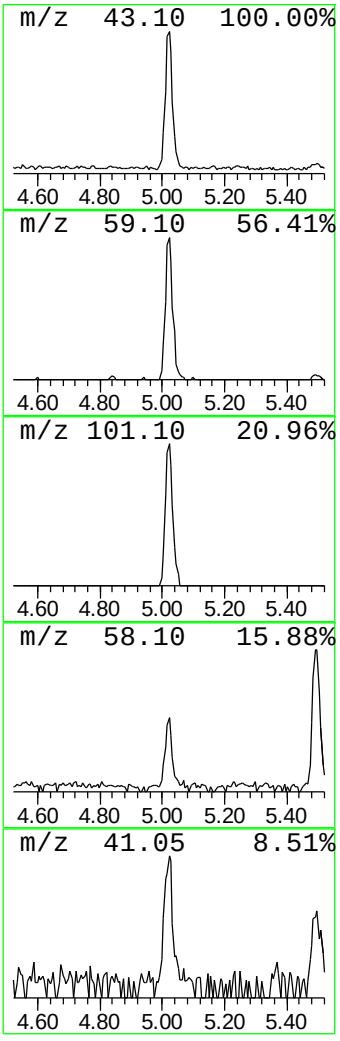
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	2.89 ng	70804	1,4-Dichlorobenzene-d4	7.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	17
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020420\
Data File : BG044289.D
Acq On : 4 Feb 2020 20:34
Operator : CG/JU
Sample : PB126573BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126573BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.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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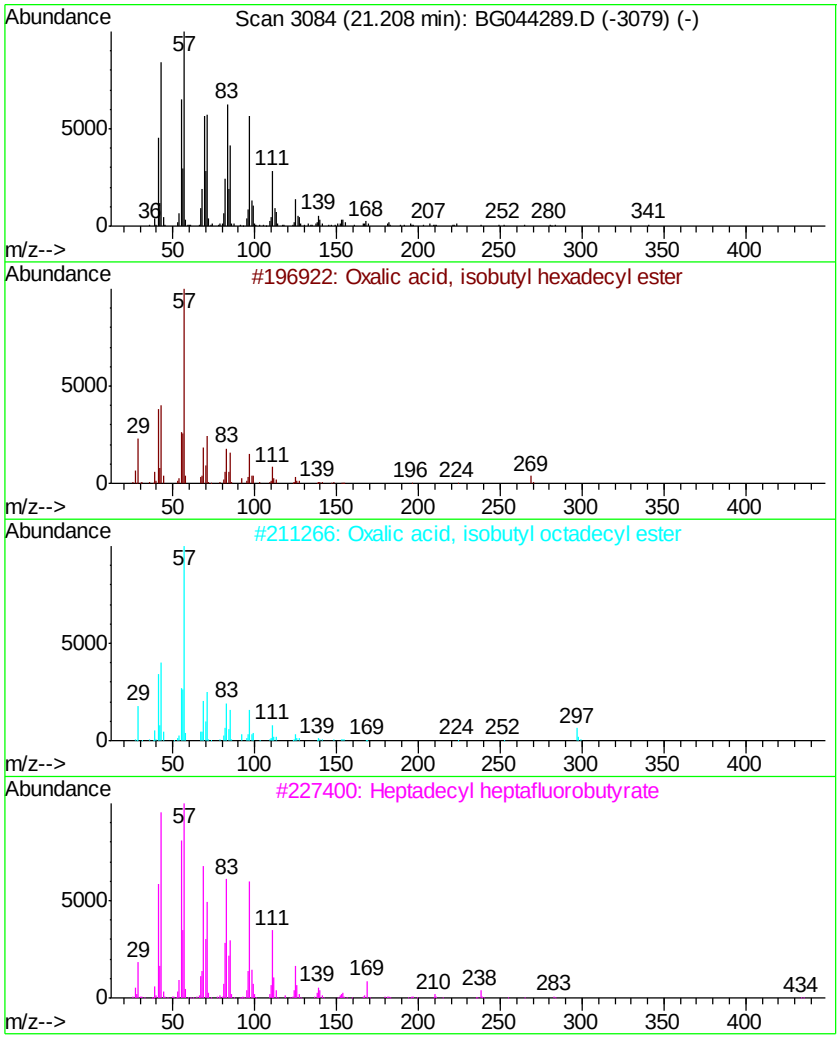
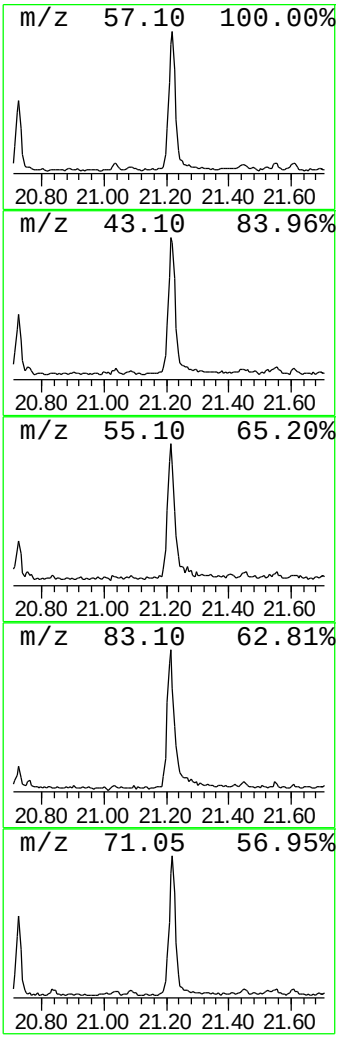
Peak Number 3 Oxalic acid, isobutyl hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.21	6.46 ng	476419	Chrysene-d12	21.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
2	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	91
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	76
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	76
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	76





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020420\
Data File : BG044289.D
Acq On : 4 Feb 2020 20:34
Operator : CG/JU
Sample : PB126573BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126573BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.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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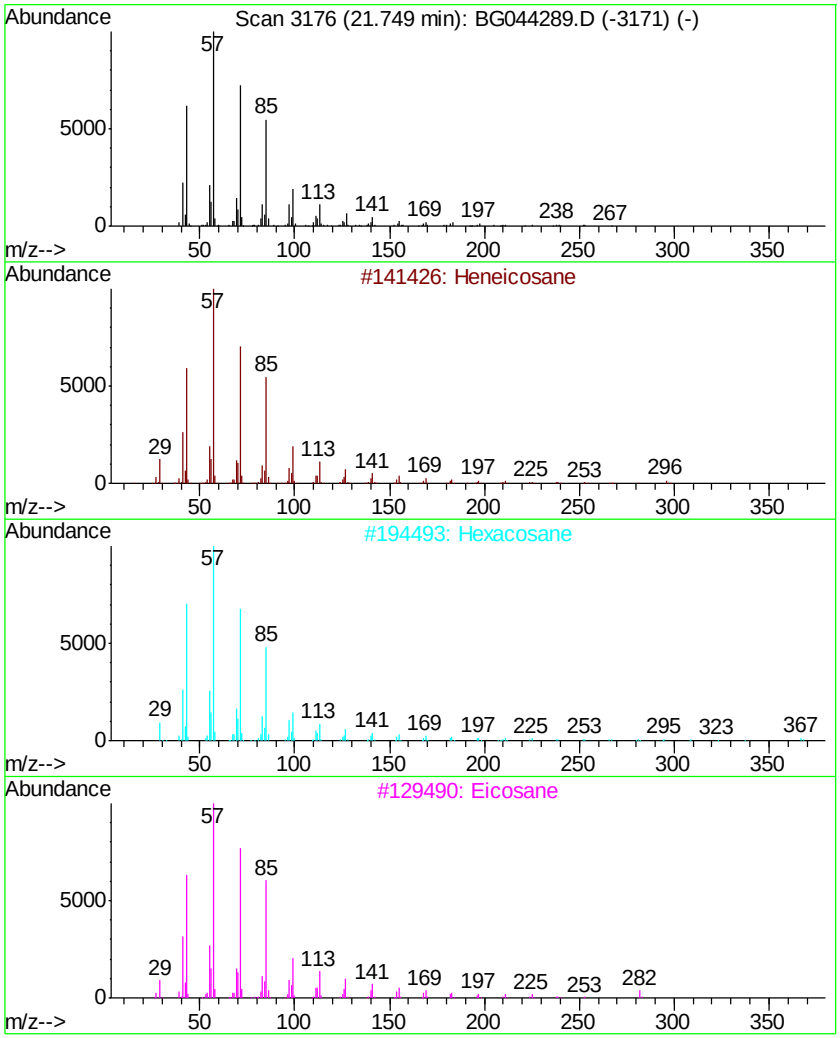
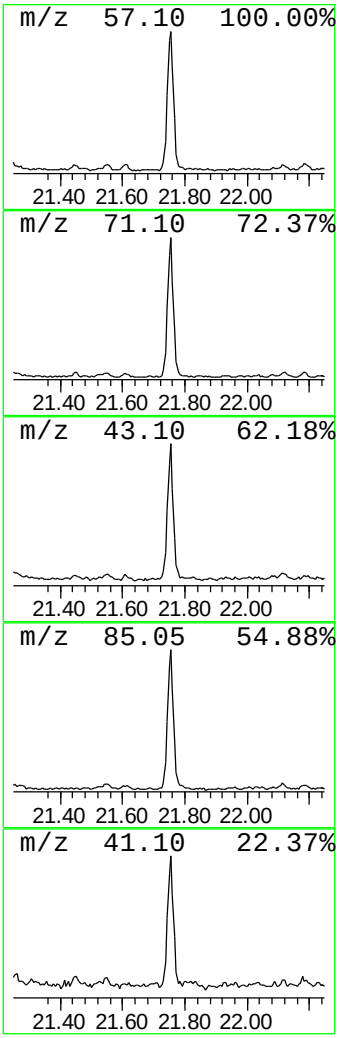
Peak Number 4 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.75	4.31 ng	317903	Chrysene-d12	21.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Eicosane	282	C20H42	000112-95-8	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020420\
Data File : BG044289.D
Acq On : 4 Feb 2020 20:34
Operator : CG/JU
Sample : PB126573BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126573BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.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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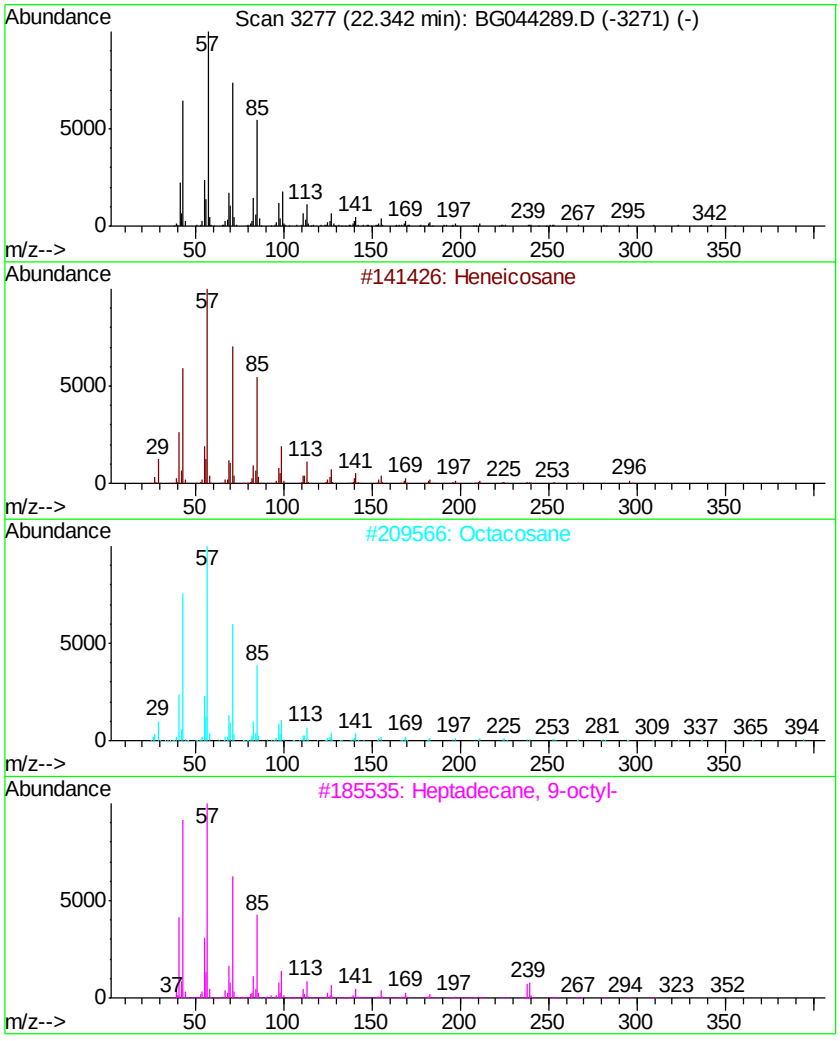
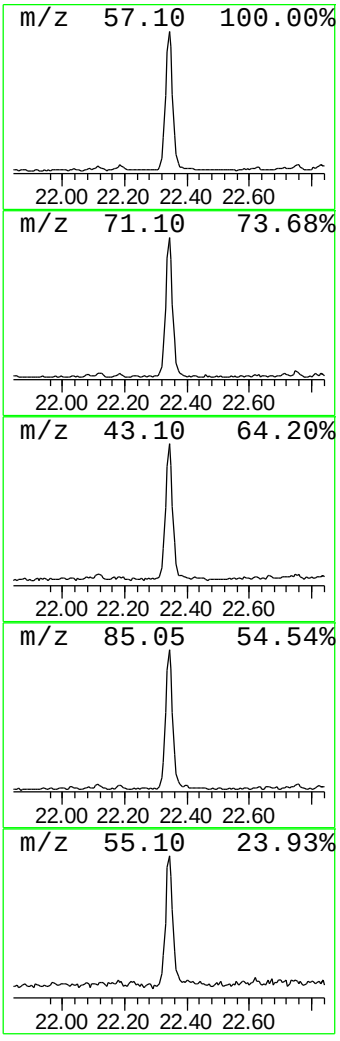
Peak Number 5 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.34	6.00 ng	442450	Chrysene-d12	21.54

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	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5	Heptadecane	240	C17H36	000629-78-7	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020420\
Data File : BG044289.D
Acq On : 4 Feb 2020 20:34
Operator : CG/JU
Sample : PB126573BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126573BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

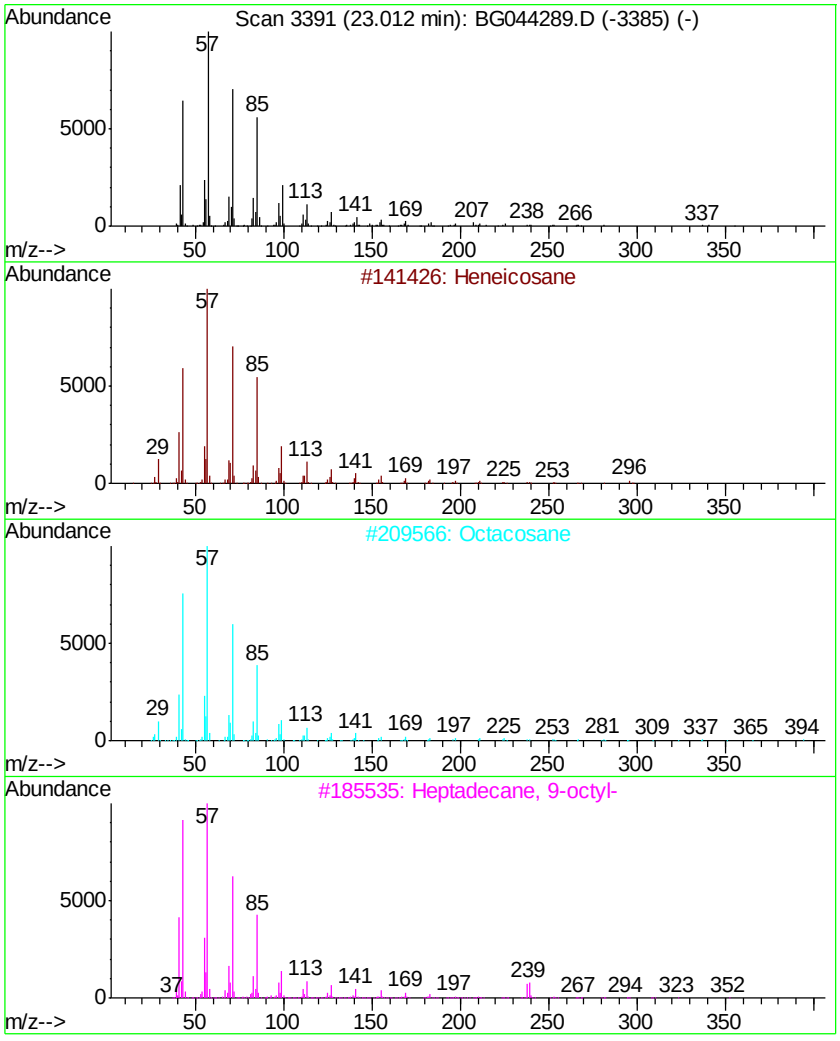
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

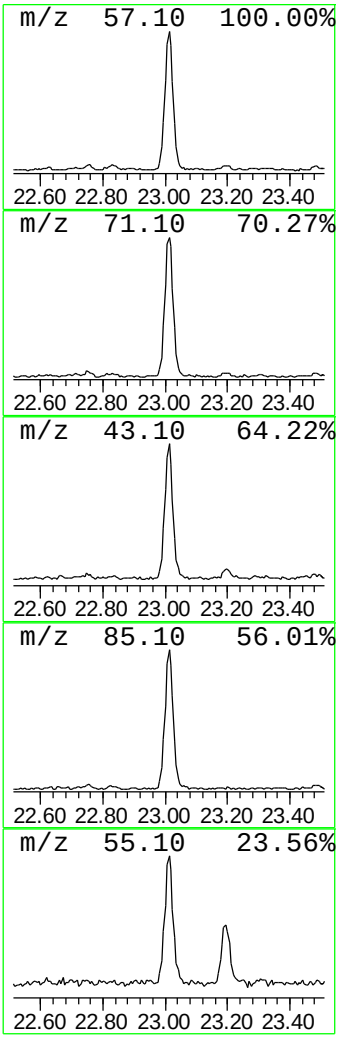
****

Peak Number 6 Heptadecane, 9-octyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.01	6.63 ng	488412	Chrysene-d12	21.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	90
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4	Hexadecane	226	C16H34	000544-76-3	83
5	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	81





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020420\
Data File : BG044289.D
Acq On : 4 Feb 2020 20:34
Operator : CG/JU
Sample : PB126573BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126573BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

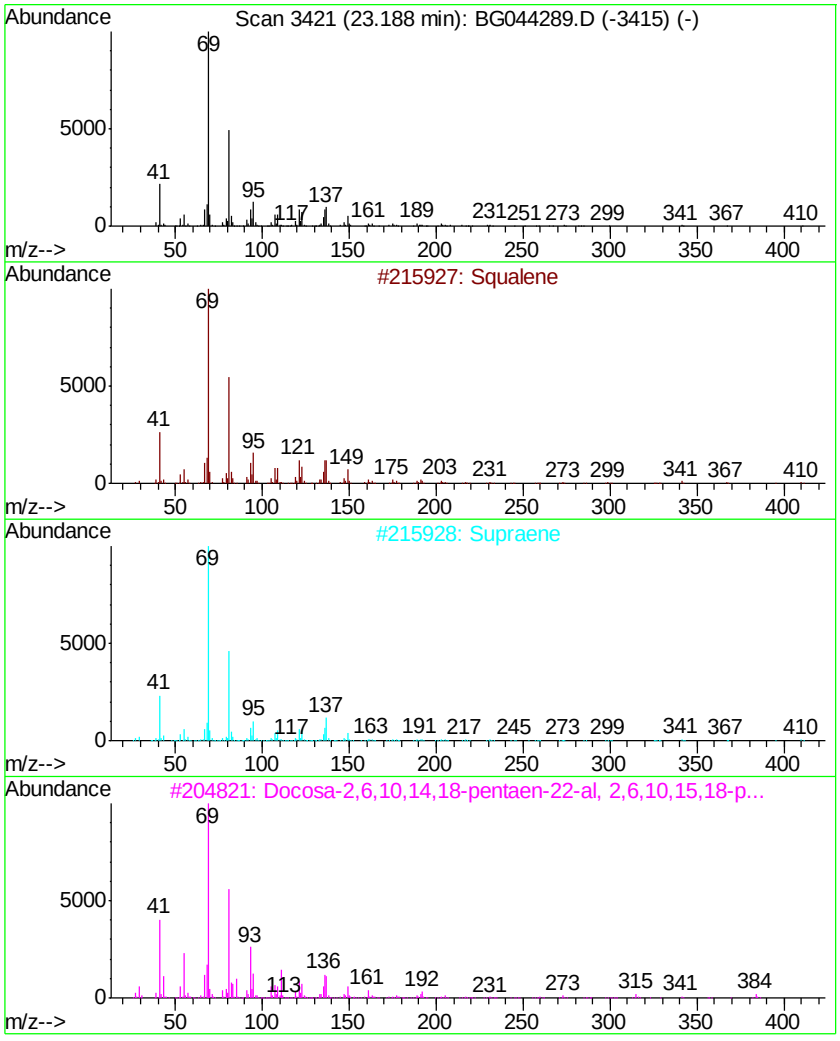
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

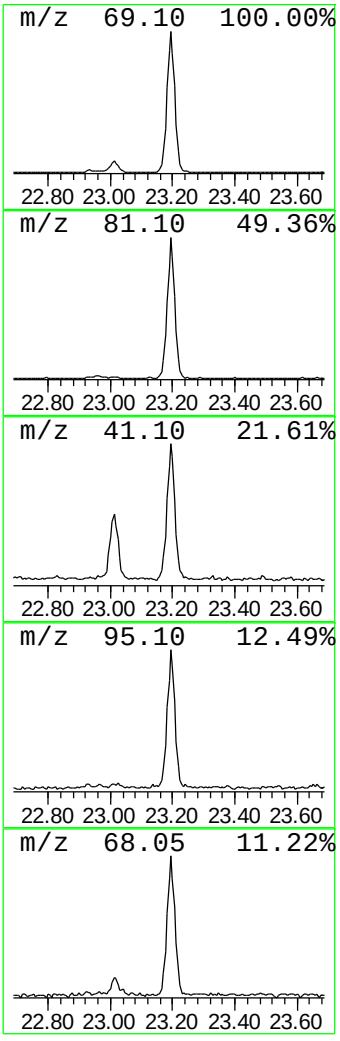
****

Peak Number 7 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.19	8.54 ng	650618	Perylene-d12	24.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
4	Farnesol isomer a	222	C15H26O	1000108-92-4	64
5	Trideca-1,3,7,11-tetraene-1,1-di...	268	C18H24N2	1000159-88-9	53





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020420\
Data File : BG044289.D
Acq On : 4 Feb 2020 20:34
Operator : CG/JU
Sample : PB126573BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126573BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

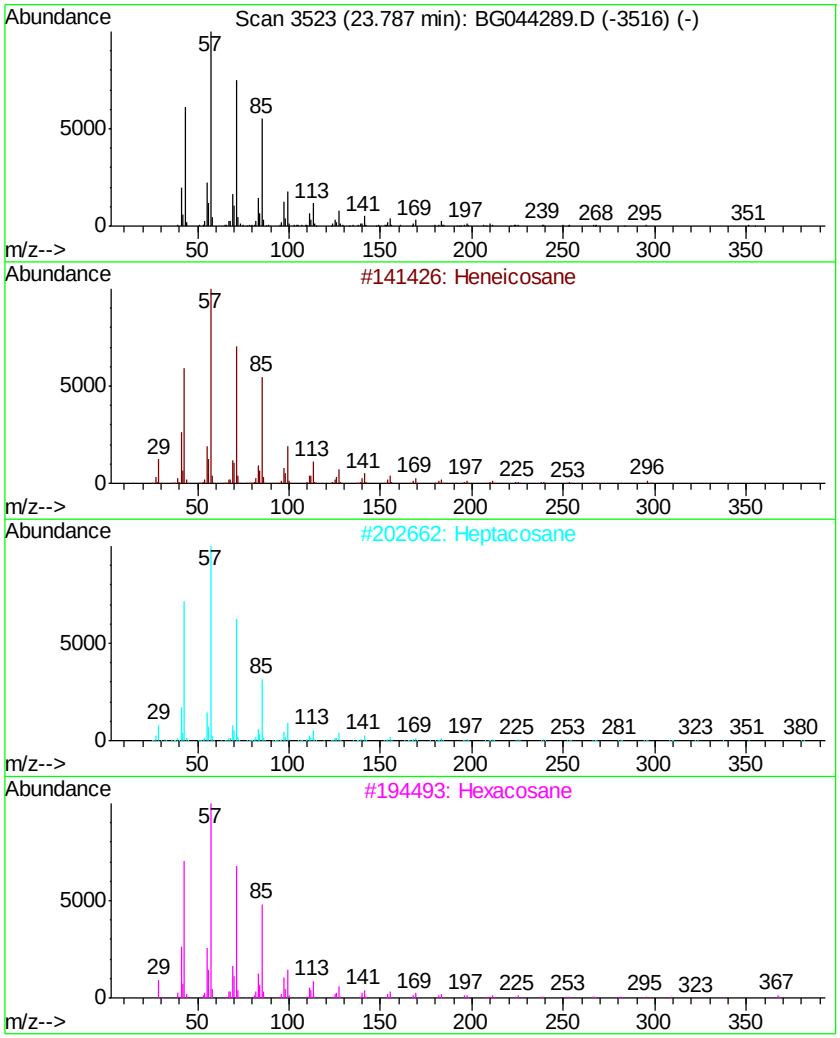
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

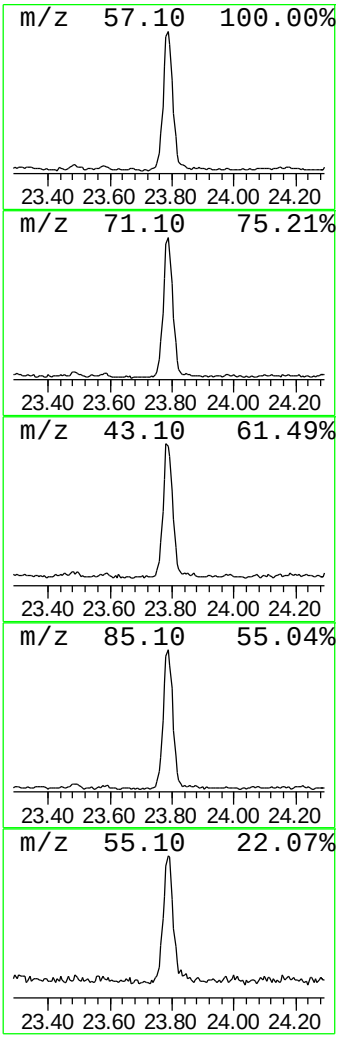
****

Peak Number 8 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.79	5.87 ng	447332	Perylene-d12	24.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Tetracosane	338	C24H50	000646-31-1	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020420\
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Operator : CG/JU
Sample : PB126573BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126573BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.M
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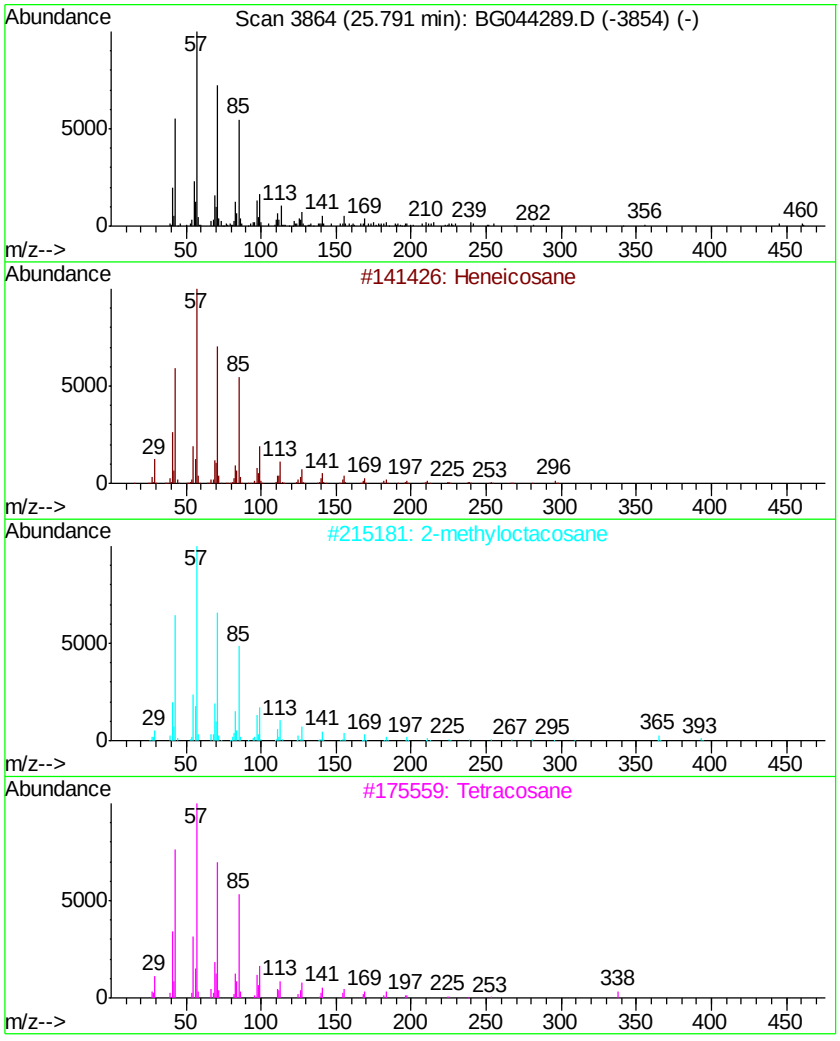
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

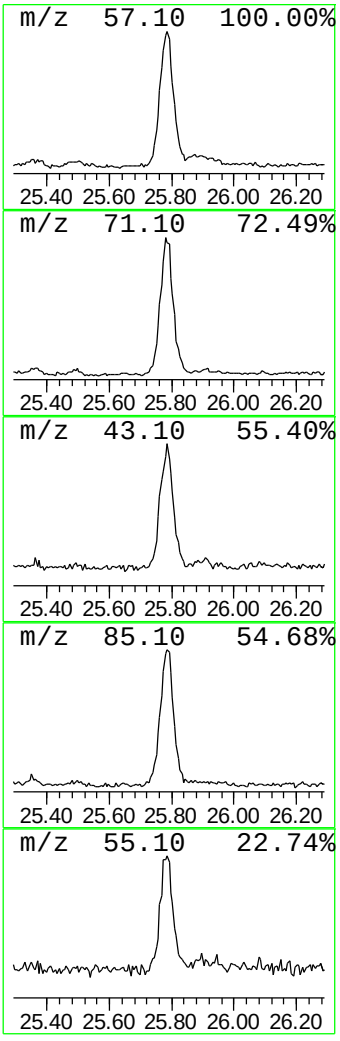
****

Peak Number 9 2-methyloctacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.79	4.80 ng	365209	Perylene-d12	24.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	2-methyloctacosane	408	C29H60	1000376-72-8	87
3	Tetracosane	338	C24H50	000646-31-1	87
4	Octacosane	394	C28H58	000630-02-4	83
5	Hexacosane	366	C26H54	000630-01-3	81





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020420\
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Acq On : 4 Feb 2020 20:34
Operator : CG/JU
Sample : PB126573BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126573BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

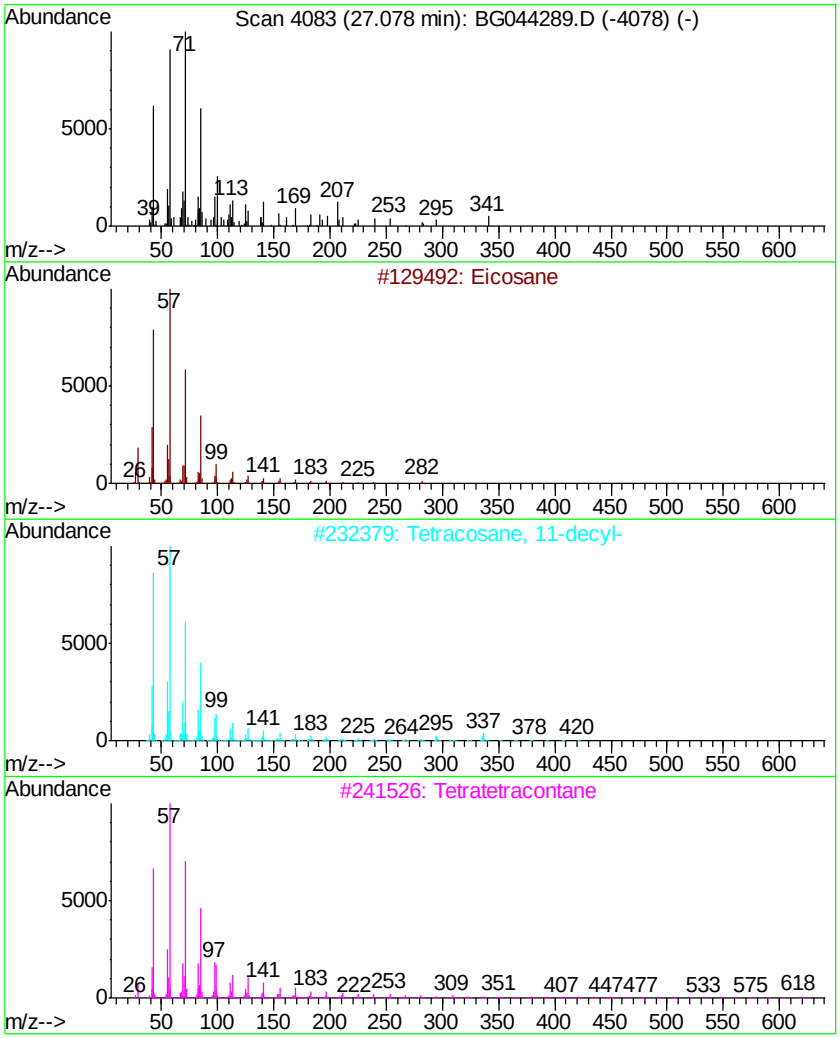
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

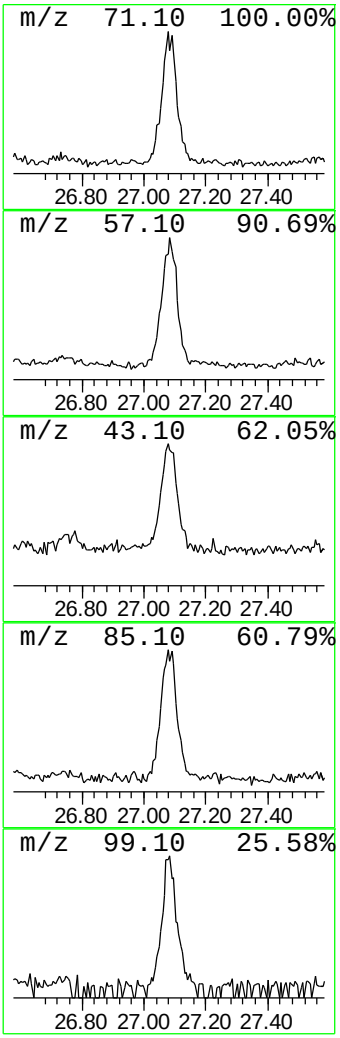
****

Peak Number 10 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.08	2.01 ng	152798	Perylene-d12	24.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	86
2	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	72
3	Tetratetracontane	619	C44H90	007098-22-8	72
4	Octacosane	394	C28H58	000630-02-4	72
5	Hentriacontane	437	C31H64	000630-04-6	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG020420\
Data File : BG044289.D
Acq On : 4 Feb 2020 20:34
Operator : CG/JU
Sample : PB126573BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126573BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.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
2-Pentanone, 4-hy...	5.02	2.9	ng	70804	1	7.92	489481	20.0
Oxalic acid, isob...	21.21	6.5	ng	476419	5	21.54	1474180	20.0
Heneicosane	21.75	4.3	ng	317903	5	21.54	1474180	20.0
Octacosane	22.34	6.0	ng	442450	5	21.54	1474180	20.0
Heptadecane, 9-oc...	23.01	6.6	ng	488412	5	21.54	1474180	20.0
Squalene	23.19	8.5	ng	650618	6	24.64	1523030	20.0
Heptacosane	23.79	5.9	ng	447332	6	24.64	1523030	20.0
2-methyloctacosane	25.79	4.8	ng	365209	6	24.64	1523030	20.0
Eicosane	27.08	2.0	ng	152798	6	24.64	1523030	20.0