LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020520\
Data File : BG044307.D
Acq On : 5 Feb 2020 16:47
Operator : CG/JU
Sample : L1390-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-2

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	5.015	323	328	337	rBV	34541	57012	1.04%	0.204%
2	5.491	402	409	428	rBV	1257047	2054240	37.49%	7.367%
3	7.083	672	680	693	rBV	1241193	2261272	41.27%	8.110%
4	7.912	812	821	830	rBV	265932	465593	8.50%	1.670%
5	8.241	868	877	886	rBV	984760	1767227	32.25%	6.338%
6	9.069	1009	1018	1037	rBV	750635	1408416	25.71%	5.051%
7	10.714	1291	1298	1310	rBV	348712	656312	11.98%	2.354%
8	13.176	1709	1717	1728	rBV	2107142	3357414	61.28%	12.041%
9	14.005	1851	1858	1865	rBV	119972	195749	3.57%	0.702%
10	14.551	1944	1951	1963	rBV	620318	1020983	18.63%	3.662%
11	16.043	2197	2205	2215	rBV	1842687	2902625	52.98%	10.410%
12	17.295	2412	2418	2430	rBV	838763	1322806	24.14%	4.744%
13	19.915	2857	2864	2878	rBV	4014728	5478972	100.00%	19.650%
14	21.208	3079	3084	3096	rBV2	243177	449646	8.21%	1.613%
15	21.543	3134	3141	3151	rBV	861922	1451189	26.49%	5.204%
16	21.754	3172	3177	3185	rBV	84226	124538	2.27%	0.447%
17	22.342	3271	3277	3286	rBV2	123609	210052	3.83%	0.753%
18	23.012	3384	3391	3401	rVB	130882	254067	4.64%	0.911%
19	23.194	3416	3422	3428	rVB	106519	192549	3.51%	0.691%
20	23.787	3516	3523	3531	rVB2	111162	236561	4.32%	0.848%
21	24.639	3657	3668	3688	rBV2	494795	1724928	31.48%	6.186%
22	25.785	3854	3863	3872	rBV3	63450	216076	3.94%	0.775%
23	27.072	4076	4082	4093	rVB4	26589	75163	1.37%	0.270%

Sum of corrected areas: 27883390

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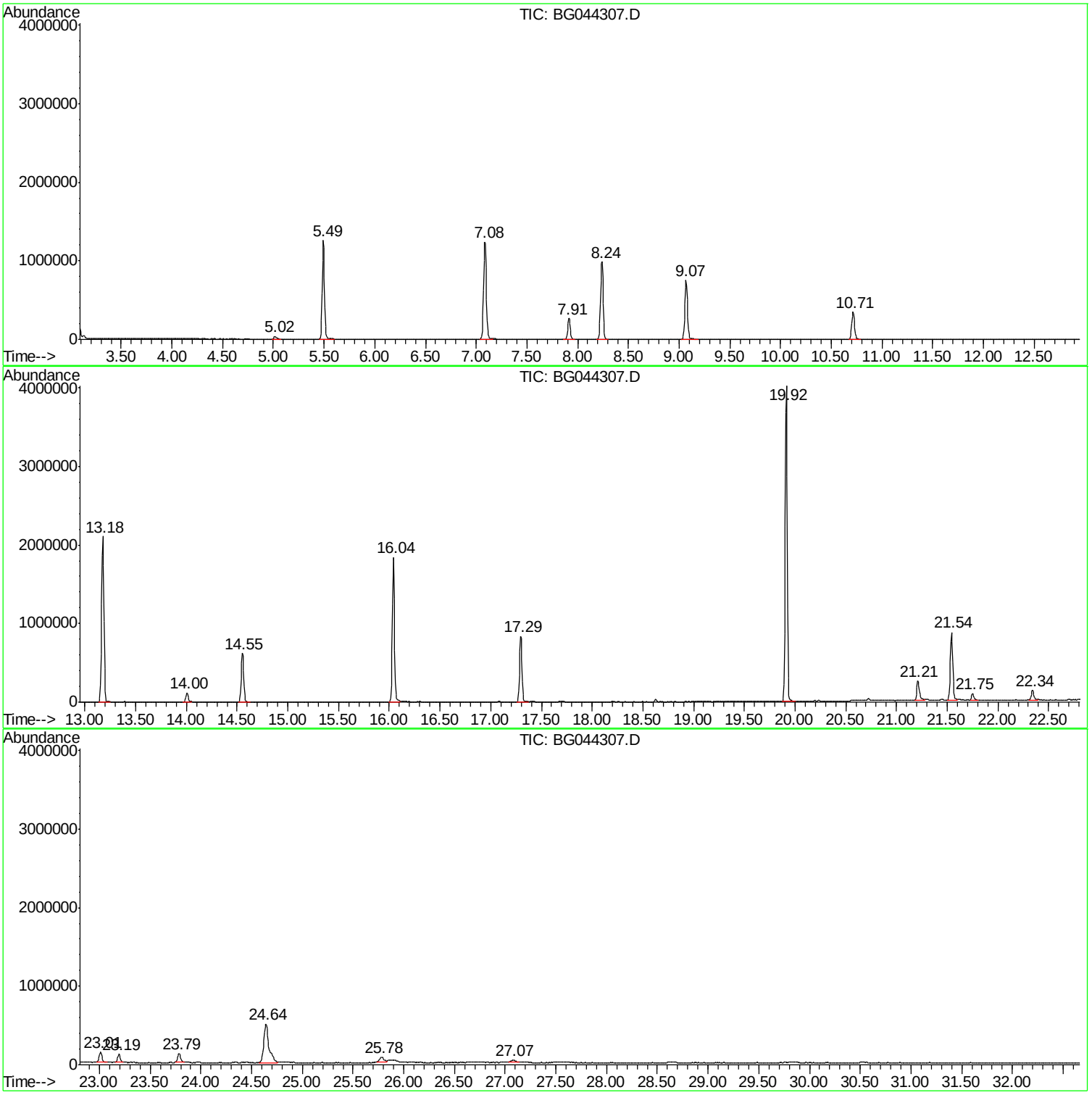
Sample : L1390-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-2

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\BG020520\
Data File : BG044307.D
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Operator : CG/JU
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Misc :
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Instrument : BNA_G
ClientSampleId : SB-2

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

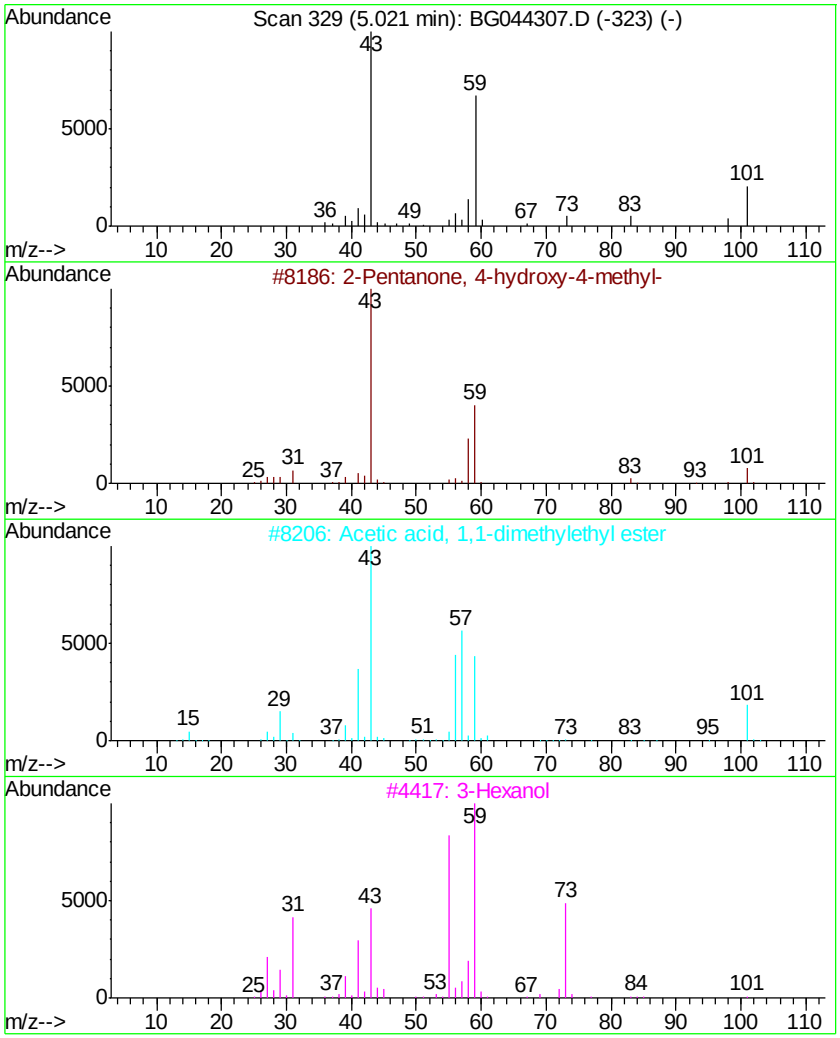
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

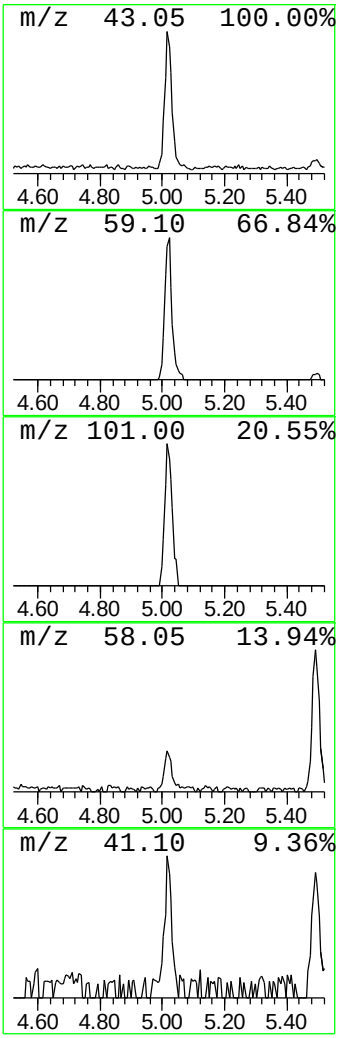
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	2.45 ng	57012	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	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50
3	3-Hexanol	102	C6H14O	000623-37-0	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Hexanamide	115	C6H13NO	000628-02-4	23





Library Search Compound Report

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Data File : BG044307.D
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Operator : CG/JU
Sample : L1390-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-2

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

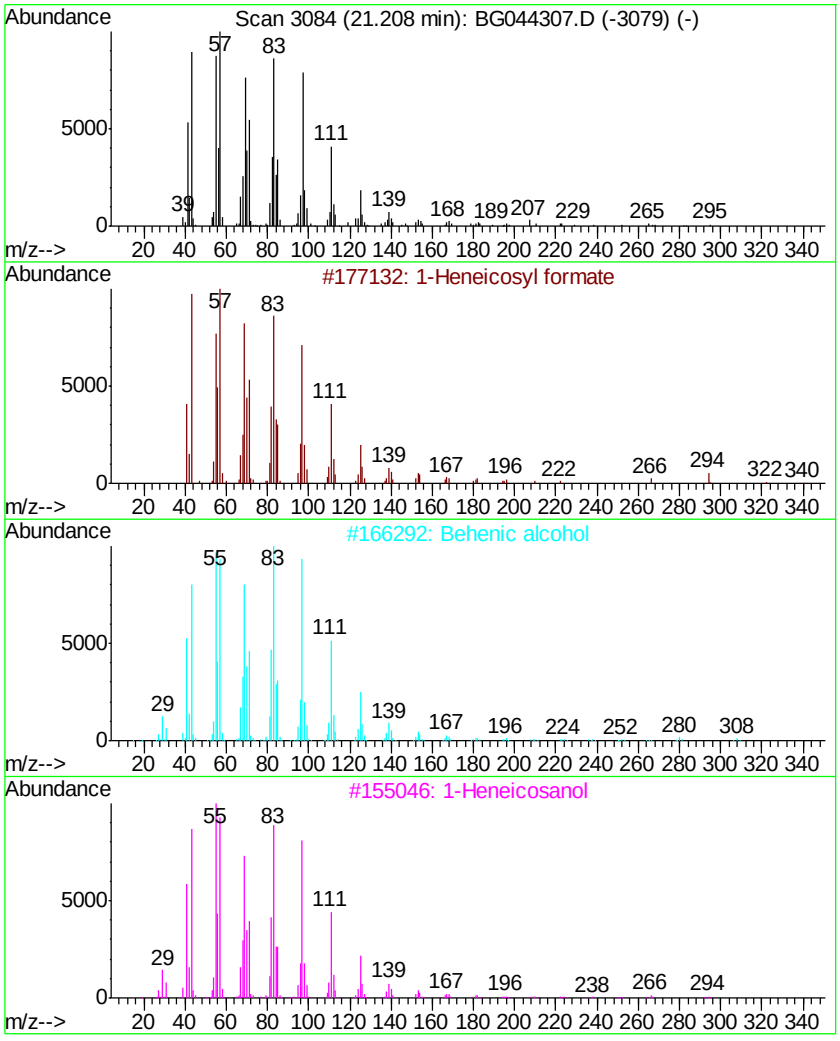
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

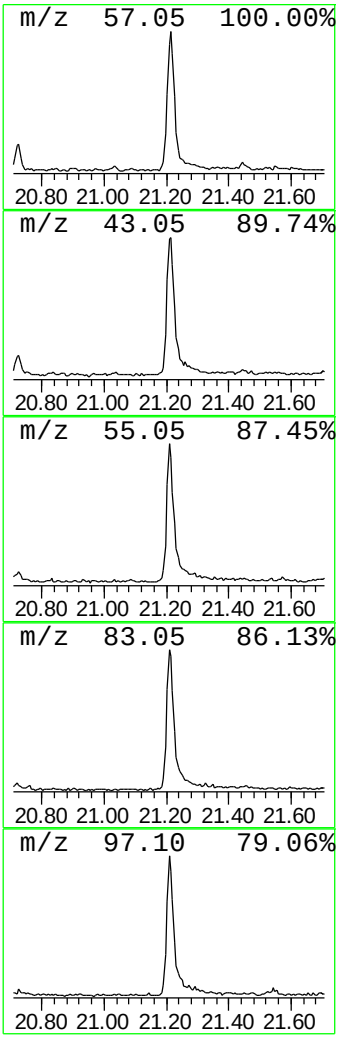
****

Peak Number 3 1-Heneicosyl formate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.21	6.20 ng	449646	Chrysene-d12	21.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020520\
Data File : BG044307.D
Acq On : 5 Feb 2020 16:47
Operator : CG/JU
Sample : L1390-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-2

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

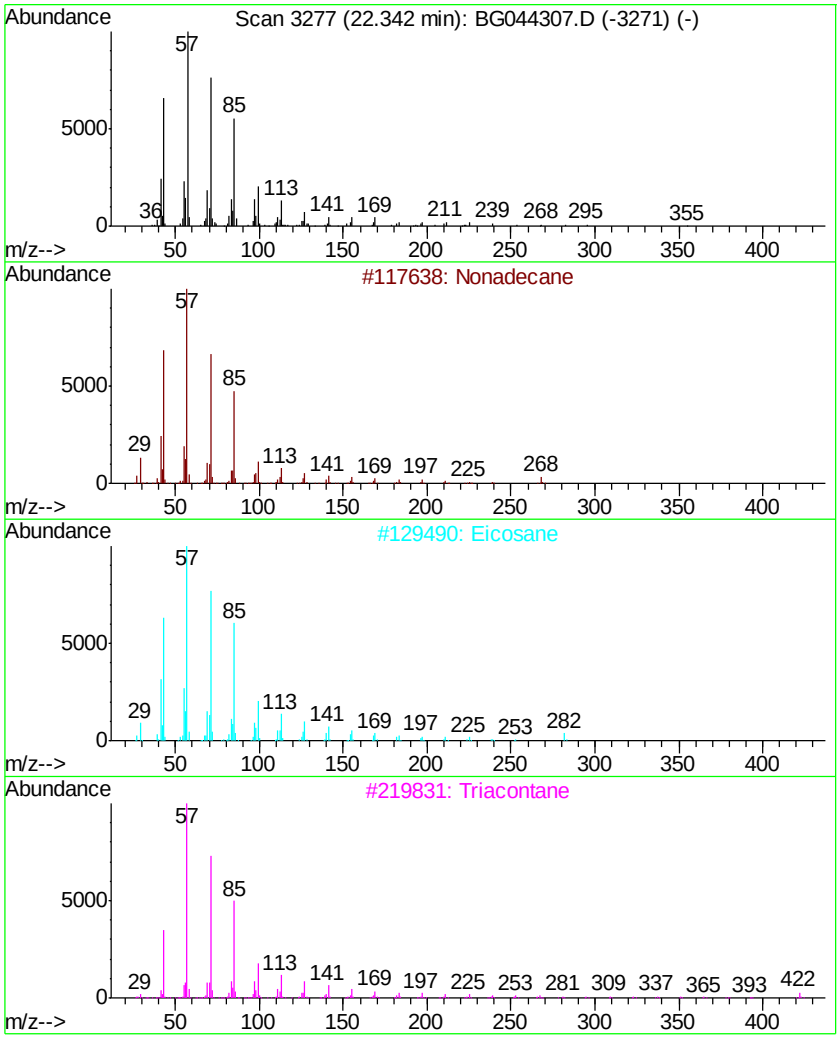
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

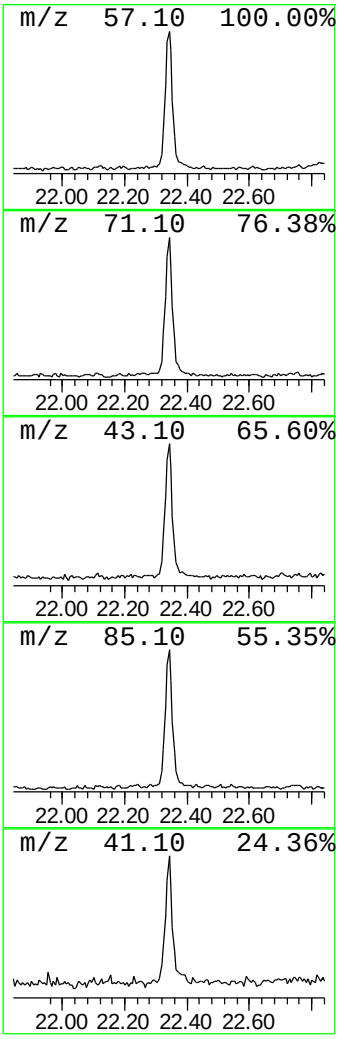
****

Peak Number 4 Nonadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.34	2.89 ng	210052	Chrysene-d12	21.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	94
2	Eicosane	282	C20H42	000112-95-8	94
3	Triacontane	422	C30H62	000638-68-6	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Heneicosane	296	C21H44	000629-94-7	91





Library Search Compound Report

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Data File : BG044307.D
Acq On : 5 Feb 2020 16:47
Operator : CG/JU
Sample : L1390-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-2

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

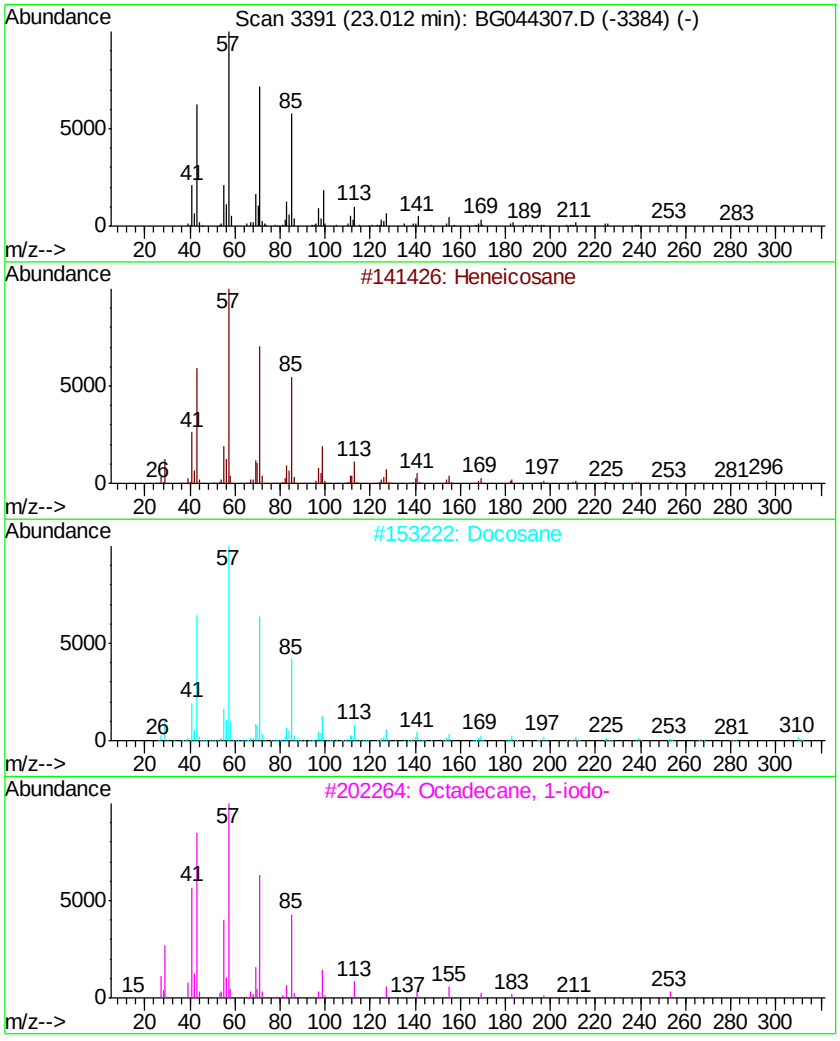
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

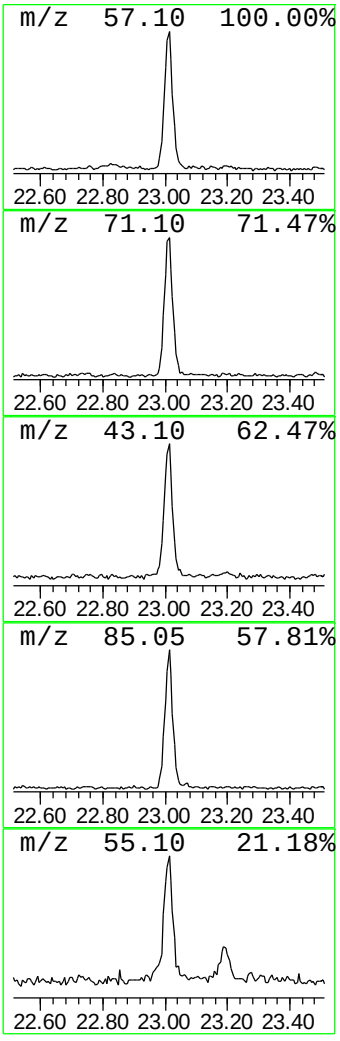
****

Peak Number 5 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.01	3.50 ng	254067	Chrysene-d12	21.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Docosane	310	C22H46	000629-97-0	91
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
4	2-methyloctacosane	408	C29H60	1000376-72-8	86
5	Hentriacontane	437	C31H64	000630-04-6	83





Library Search Compound Report

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Operator : CG/JU
Sample : L1390-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-2

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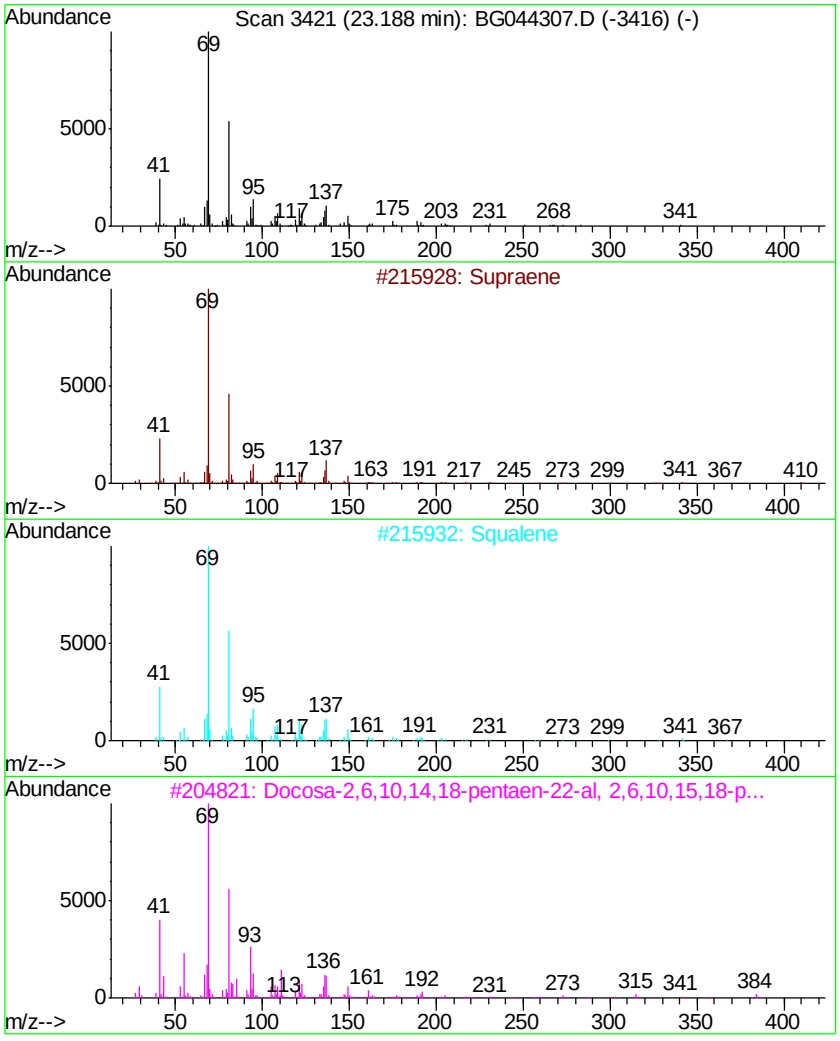
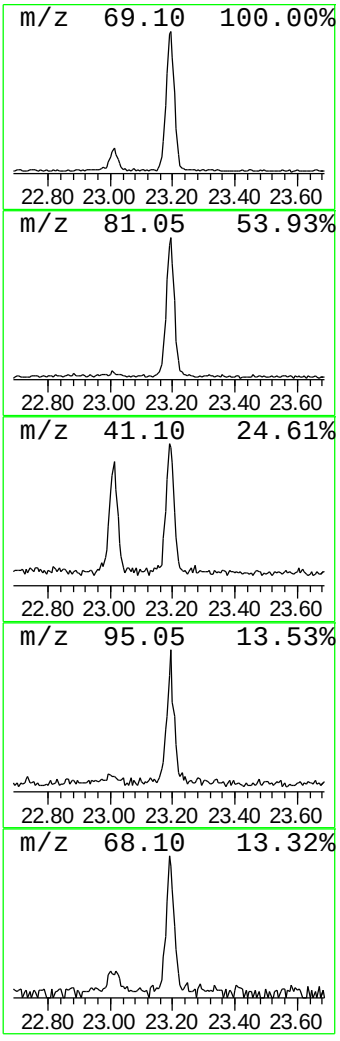
****

Peak Number 6 Supraene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.19	2.23 ng	192549	Perylene-d12	24.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	91
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
4	Farnesol isomer a	222	C15H26O	1000108-92-4	80
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	80





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Instrument : BNA_G
ClientSampleId : SB-2

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

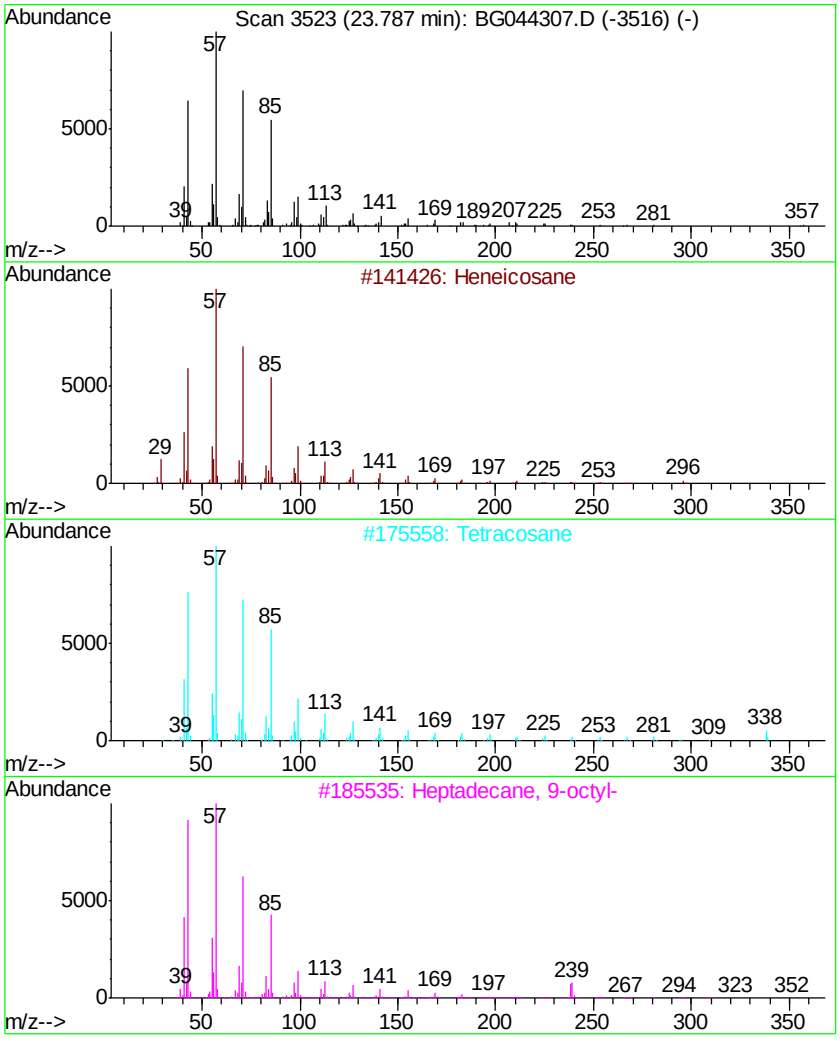
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

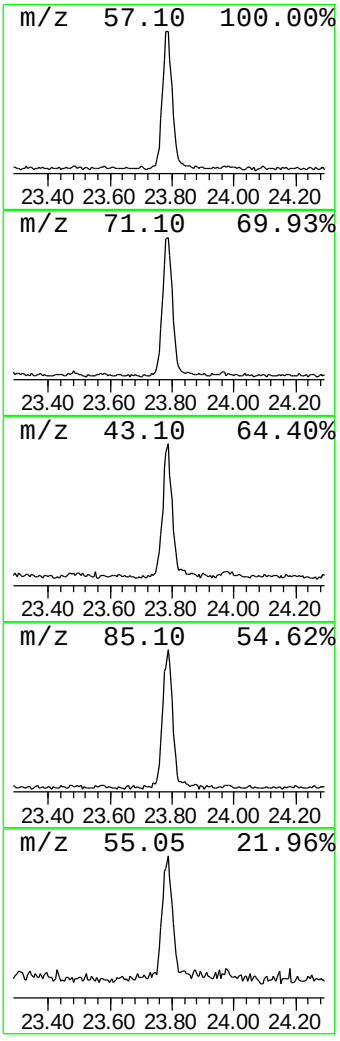
****

Peak Number 7 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.79	2.74 ng	236561	Perylene-d12	24.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Hexacosane	366	C26H54	000630-01-3	90
5	Nonadecane	268	C19H40	000629-92-5	87





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Instrument : BNA_G
ClientSampleId : SB-2

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TIC Library : C:\Database\NIST11.L
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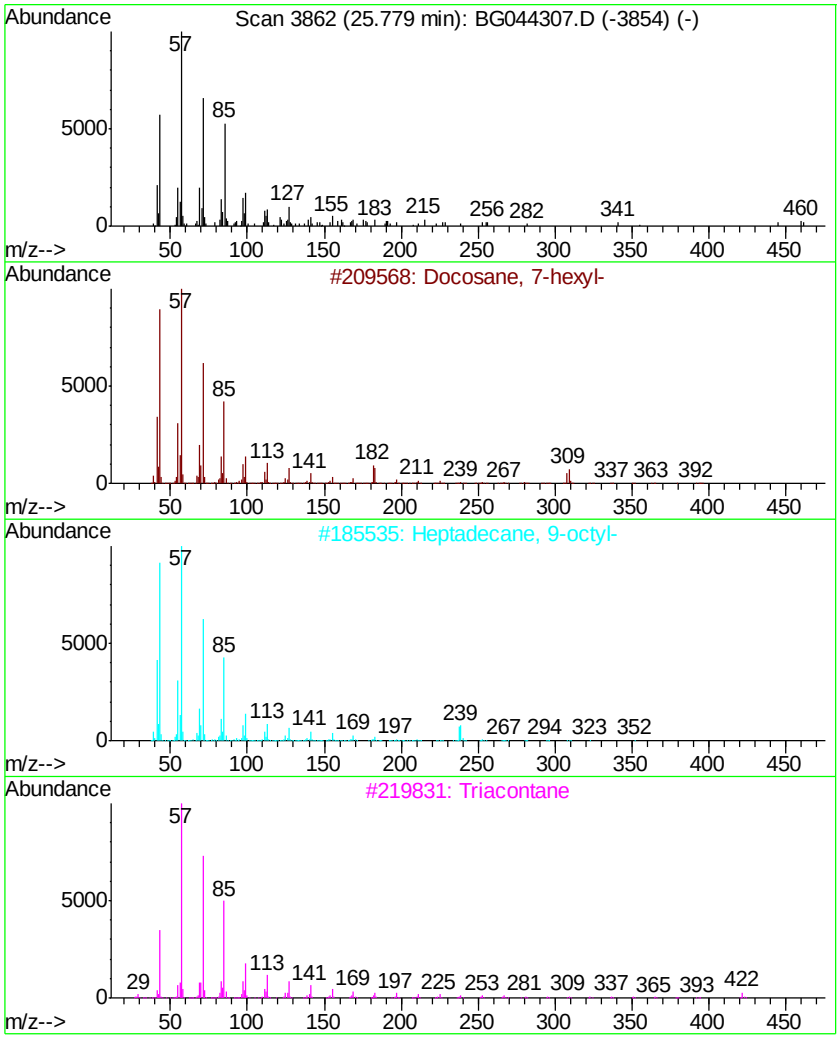
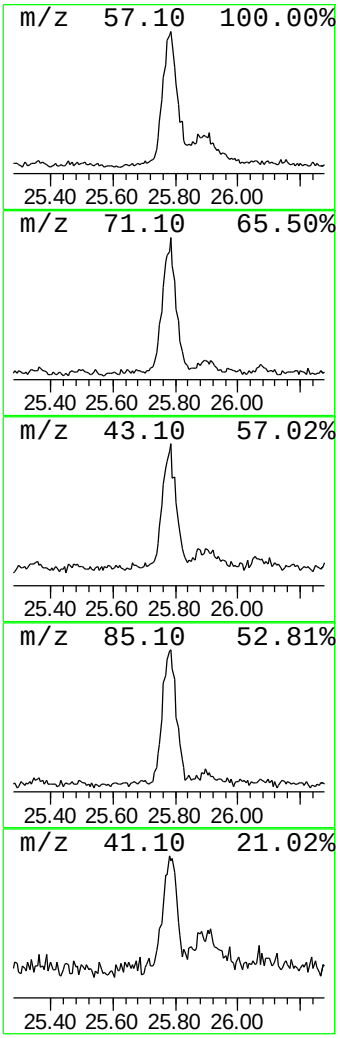
Peak Number 8 Docosane, 7-hexyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.78	2.51 ng	216076	Perylene-d12	24.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 7-hexyl-	394	C28H58	055373-86-9	90
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
3	Triacontane	422	C30H62	000638-68-6	83
4	Heneicosane	296	C21H44	000629-94-7	83
5	Tetratetracontane	619	C44H90	007098-22-8	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG020520\
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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	2.5	ng	57012	1	7.92	465593	20.0
1-Heneicosyl formate	21.21	6.2	ng	449646	5	21.54	1451190	20.0
Nonadecane	22.34	2.9	ng	210052	5	21.54	1451190	20.0
Heneicosane	23.01	3.5	ng	254067	5	21.54	1451190	20.0
Supraene	23.19	2.2	ng	192549	6	24.64	1724930	20.0
Tetracosane	23.79	2.7	ng	236561	6	24.64	1724930	20.0
Docosane, 7-hexyl-	25.78	2.5	ng	216076	6	24.64	1724930	20.0