LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG052620\
Data File : BG045461.D
Acq On : 26 May 2020 17:34
Operator : CG/JU
Sample : L2744-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM66-COMP-2020-0-6

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-BG051520.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	3.118	3	5	17	rVB	157419	223229	4.80%	0.879%
2	5.561	414	421	435	rBV	804185	1377603	29.63%	5.424%
3	7.177	688	696	709	rBV	906256	1639742	35.27%	6.456%
4	7.964	822	830	838	rBV	252565	456011	9.81%	1.795%
5	8.287	876	885	893	rBV	790859	1405231	30.23%	5.533%
6	9.121	1017	1027	1037	rBV	631821	1162502	25.01%	4.577%
7	10.766	1300	1307	1325	rBV	339903	662057	14.24%	2.607%
8	13.228	1718	1726	1738	rBV	1852861	3042242	65.44%	11.978%
9	14.056	1860	1867	1875	rBV	298266	470318	10.12%	1.852%
10	14.602	1953	1960	1967	rBV	594235	974795	20.97%	3.838%
11	16.100	2207	2215	2229	rBV	1568921	2480589	53.36%	9.767%
12	16.300	2242	2249	2258	rBV2	31392	62687	1.35%	0.247%
13	17.351	2421	2428	2433	rBV	801611	1256166	27.02%	4.946%
14	17.393	2433	2435	2442	rVV2	108372	141802	3.05%	0.558%
15	19.402	2772	2777	2785	rBV	158688	219102	4.71%	0.863%
16	19.766	2829	2839	2848	rBV	119072	240265	5.17%	0.946%
17	19.966	2867	2873	2887	rBV	3461046	4648893	100.00%	18.304%
18	20.259	2918	2923	2930	rVB6	23907	54391	1.17%	0.214%
19	21.270	3091	3095	3104	rBV5	114991	225179	4.84%	0.887%
20	21.604	3144	3152	3158	rBV2	785186	1392183	29.95%	5.481%
21	21.810	3182	3187	3193	rVB3	87693	130492	2.81%	0.514%
22	22.409	3284	3289	3294	rVB	115914	188013	4.04%	0.740%
23	23.091	3398	3405	3412	rVB	163439	306325	6.59%	1.206%
24	23.766	3511	3520	3527	rBV	40996	133435	2.87%	0.525%
25	23.878	3532	3539	3547	rVB2	155802	352698	7.59%	1.389%
26	24.759	3679	3689	3706	rBV2	454643	1651024	35.51%	6.501%
27	25.910	3874	3885	3895	rVB4	102152	325375	7.00%	1.281%
28	27.220	4099	4108	4121	rVB6	47952	175699	3.78%	0.692%

Sum of corrected areas: 25398048

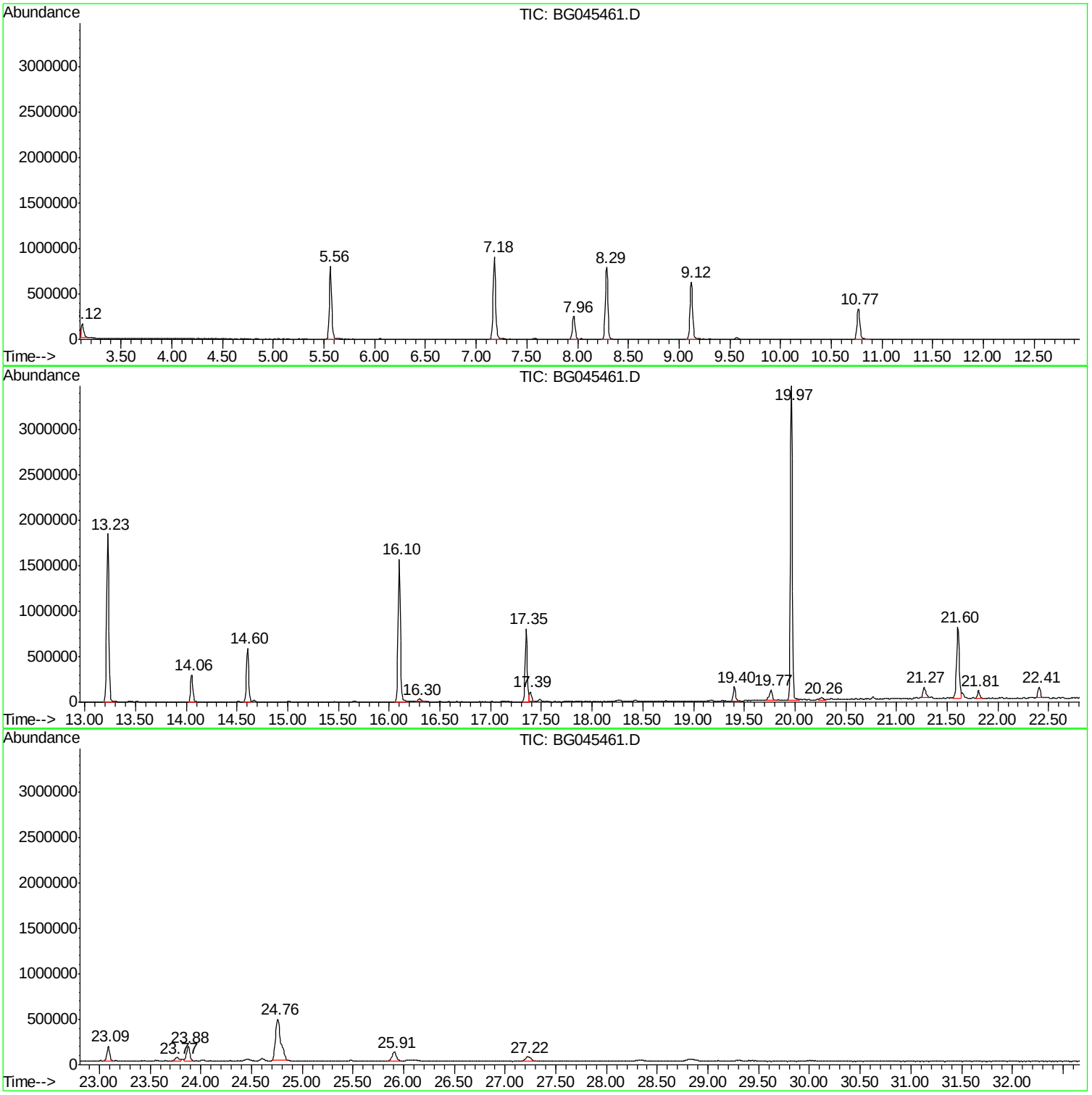
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG052620\
Data File : BG045461.D
Acq On : 26 May 2020 17:34
Operator : CG/JU
Sample : L2744-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM66-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.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\BG052620\
Data File : BG045461.D
Acq On : 26 May 2020 17:34
Operator : CG/JU
Sample : L2744-05
Misc :
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Instrument : BNA_G
ClientSampleId : NM66-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

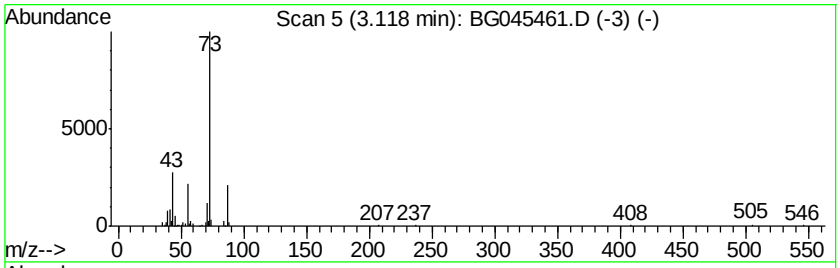
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

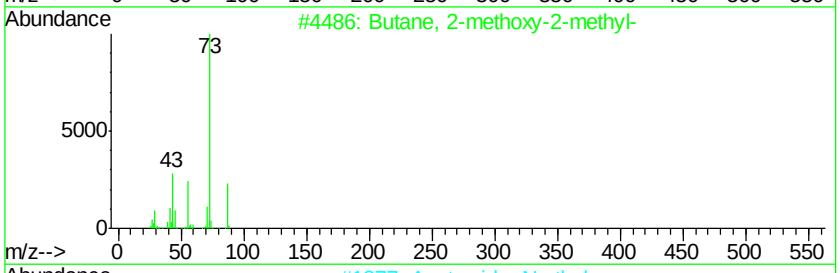
****

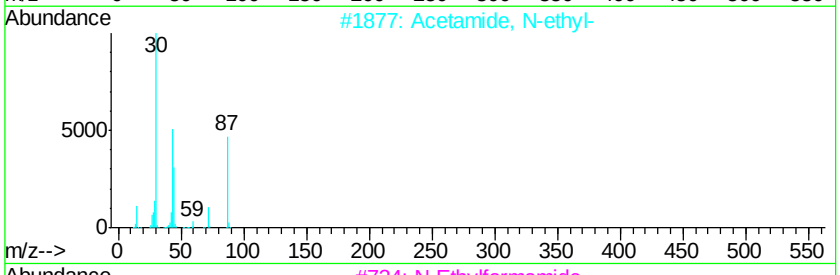
Peak Number 1 unknown3.12 Concentration Rank 2

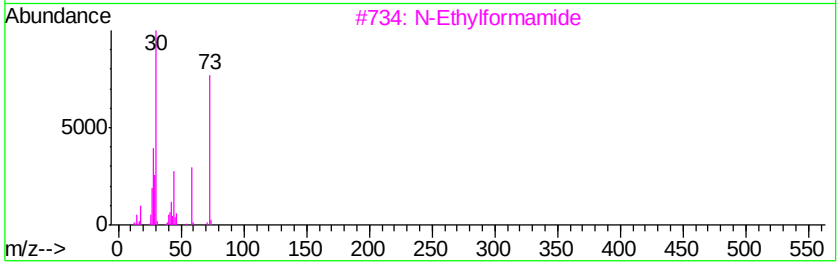
R.T.	EstConc	Area	Relative to ISTD	R.T.
3.12	9.79 ng	223229	1,4-Dichlorobenzene-d4	7.96

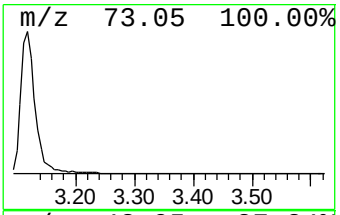
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	45
2	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	D-Epi-Inositol, 4-C-methyl-	194	C7H14O6	040788-89-4	9
5	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	9

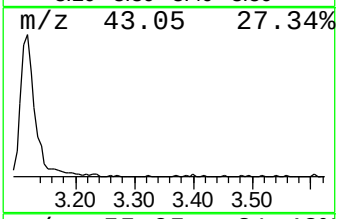


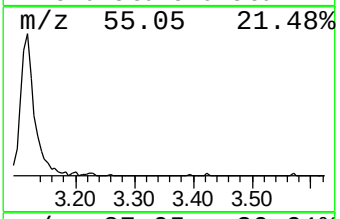


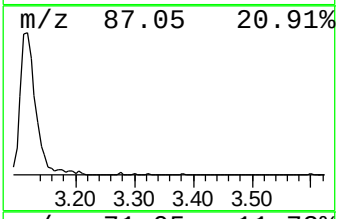


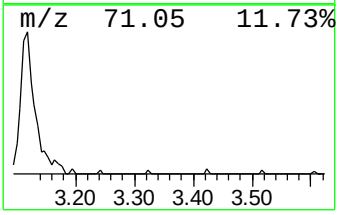












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Data File : BG045461.D
Acq On : 26 May 2020 17:34
Operator : CG/JU
Sample : L2744-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM66-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

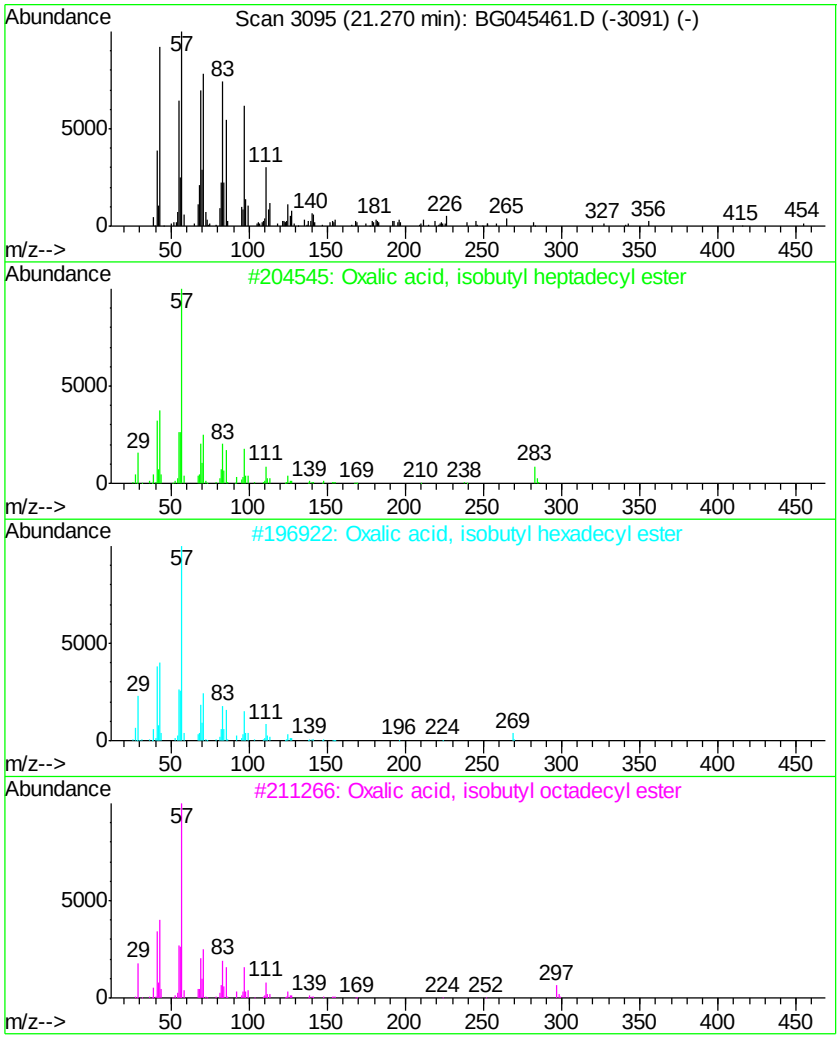
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

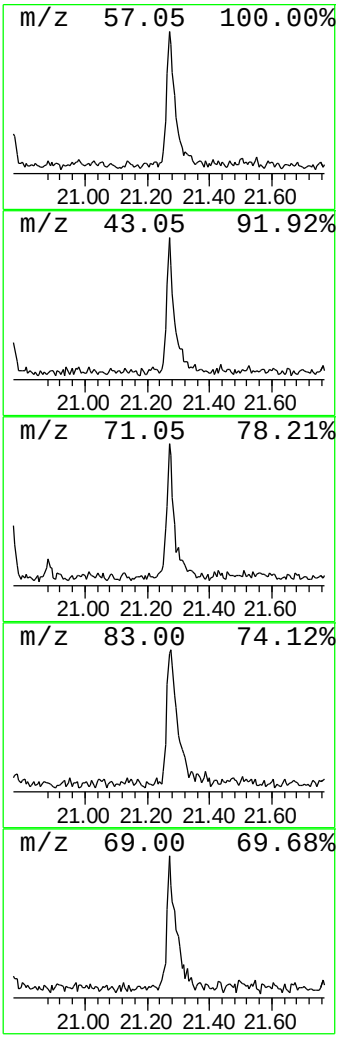
****

Peak Number 3 Oxalic acid, isobutyl hepta... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.27	3.23 ng	225179	Chrysene-d12	21.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	91
2	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
3	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	90
4	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	64
5	Cyclotetradecane	196	C14H28	000295-17-0	55





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG052620\
Data File : BG045461.D
Acq On : 26 May 2020 17:34
Operator : CG/JU
Sample : L2744-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM66-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.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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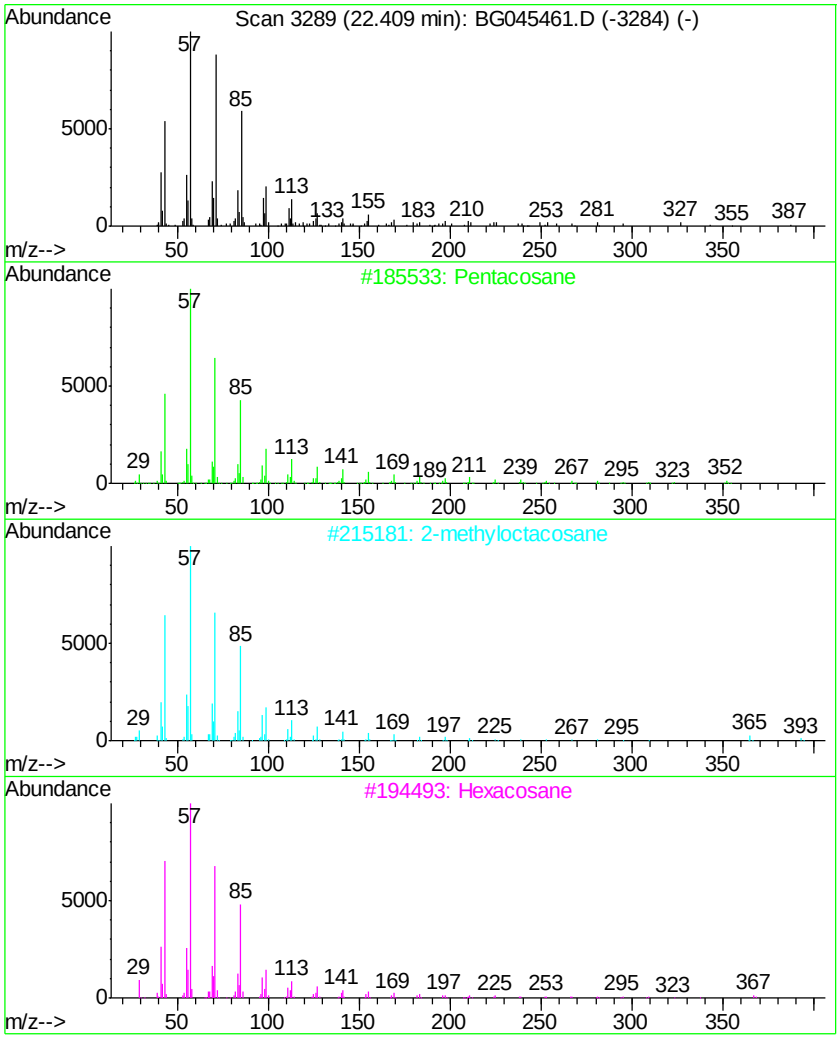
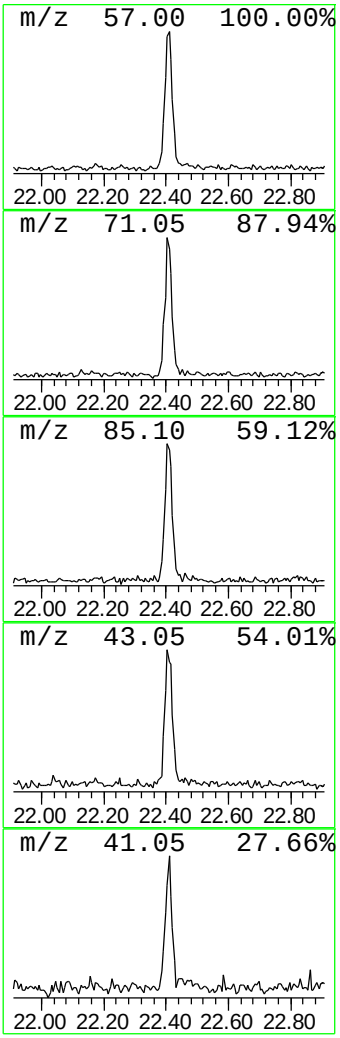
Peak Number 4 Pentacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.41	2.70 ng	188013	Chrysene-d12	21.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Hexacosane	366	C26H54	000630-01-3	90
4	Tetracosane	338	C24H50	000646-31-1	87
5	Heneicosane	296	C21H44	000629-94-7	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG052620\
Data File : BG045461.D
Acq On : 26 May 2020 17:34
Operator : CG/JU
Sample : L2744-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM66-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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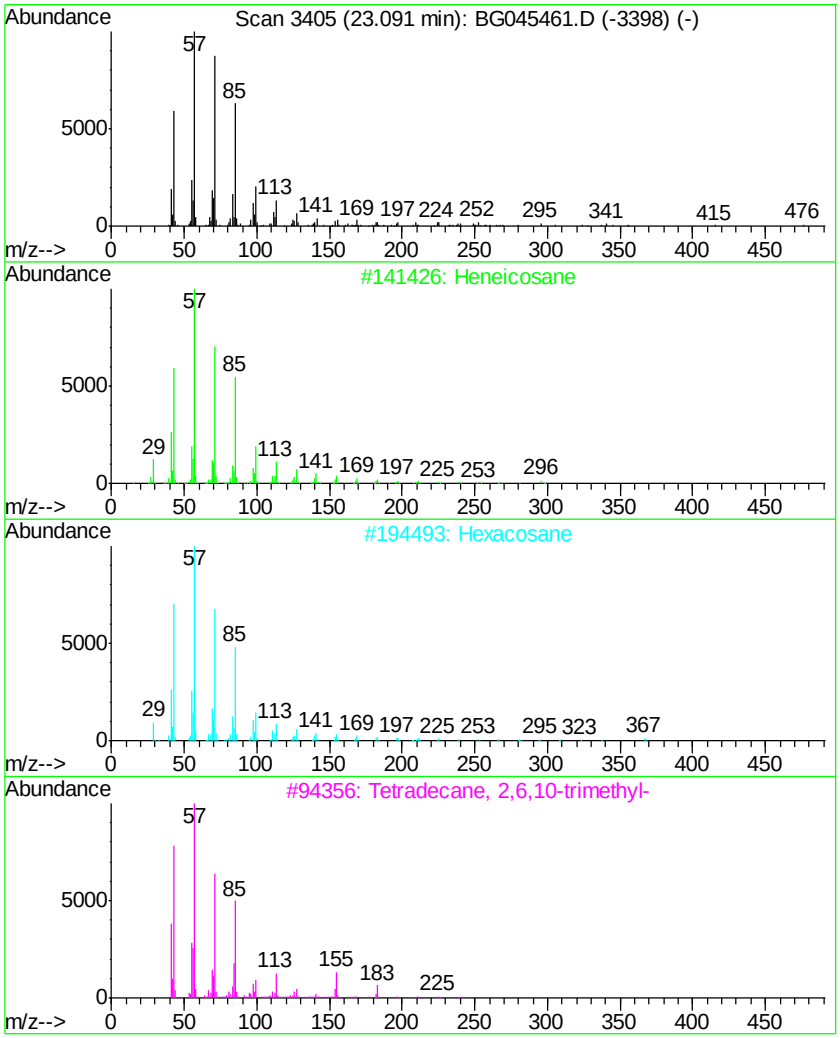
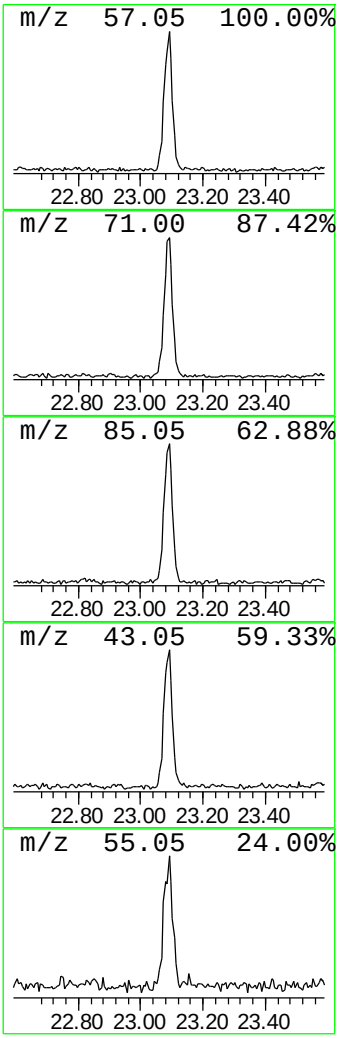
Peak Number 5 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.09	4.40 ng	306325	Chrysene-d12	21.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	90
3	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	83
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80
5	Heptacosane	380	C27H56	000593-49-7	68





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Data File : BG045461.D
Acq On : 26 May 2020 17:34
Operator : CG/JU
Sample : L2744-05
Misc :
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Instrument : BNA_G
ClientSampleId : NM66-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
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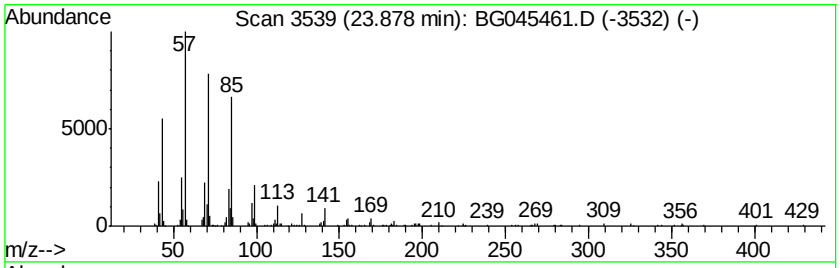
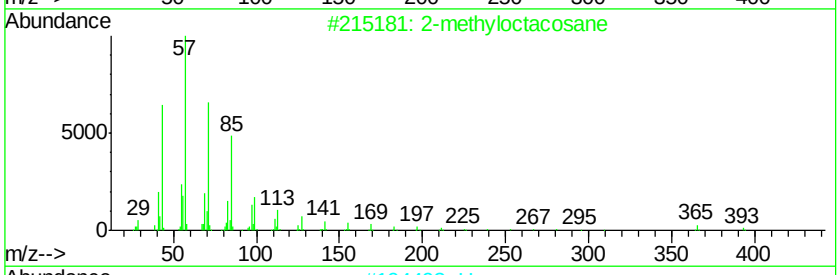
****

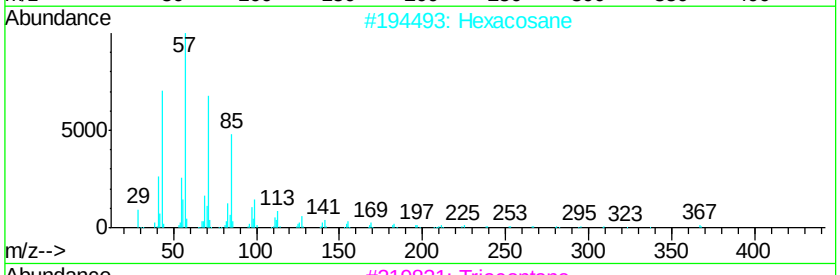
Peak Number 6 2-methyloctacosane Concentration Rank 4

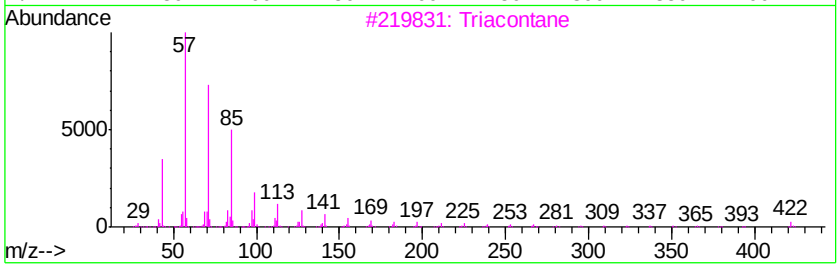
R.T.	EstConc	Area	Relative to ISTD	R.T.
23.88	4.27 ng	352698	Perylene-d12	24.76

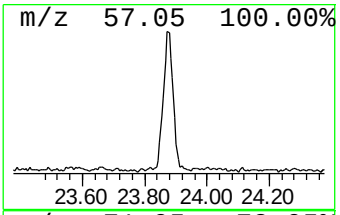
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	90
2	Hexacosane	366	C26H54	000630-01-3	86
3	Triacontane	422	C30H62	000638-68-6	78
4	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	76
5	Heptadecane	240	C17H36	000629-78-7	72

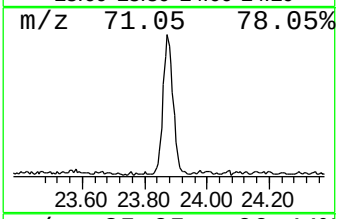


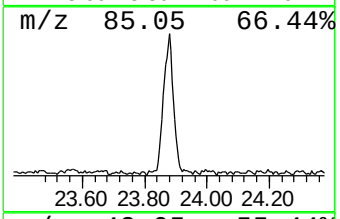


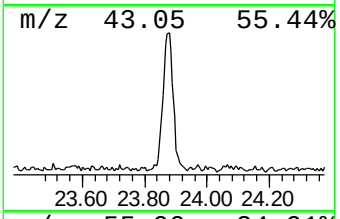


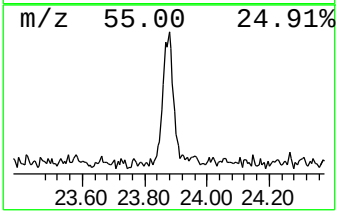












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

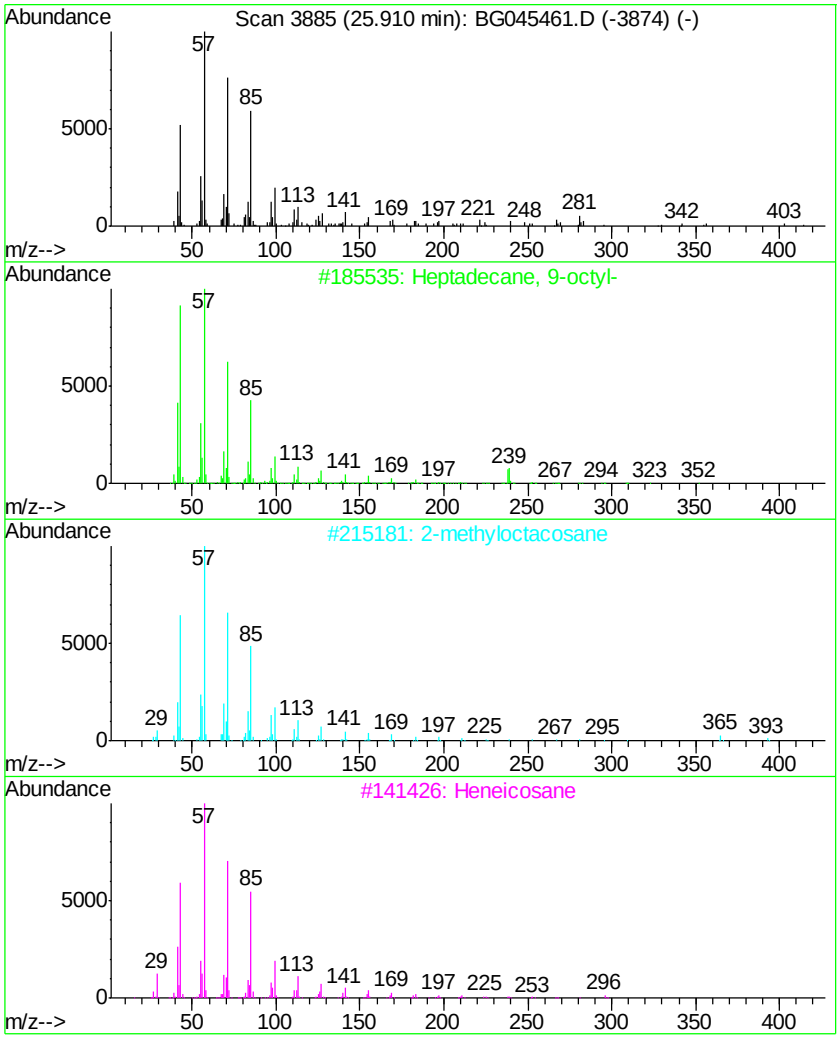
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

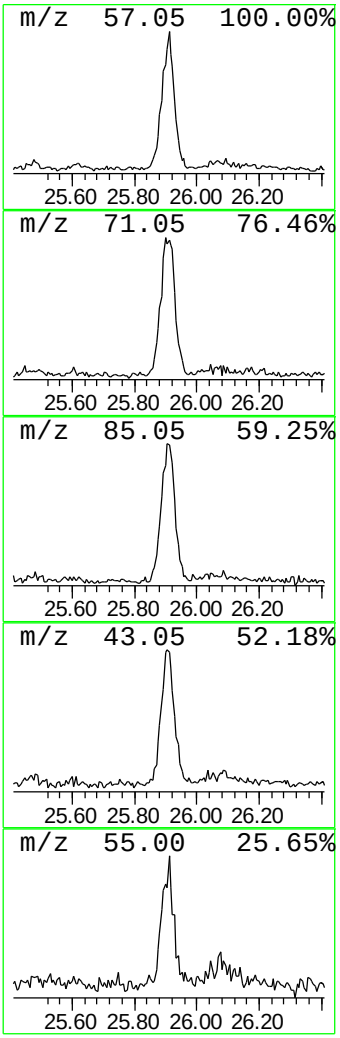
****

Peak Number 7 Heptadecane, 9-octyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.91	3.94 ng	325375	Perylene-d12	24.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
2	2-methyloctacosane	408	C29H60	1000376-72-8	87
3	Heneicosane	296	C21H44	000629-94-7	87
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
5	Octacosane	394	C28H58	000630-02-4	83





Library Search Compound Report

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Instrument : BNA_G
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

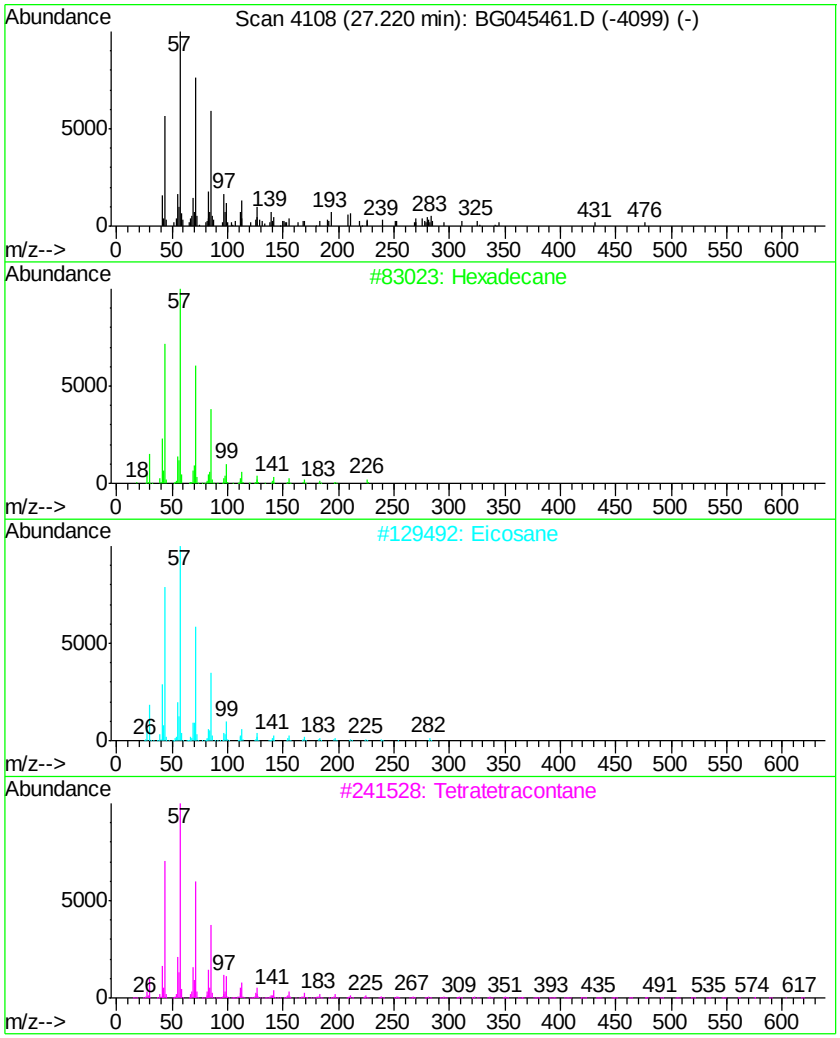
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

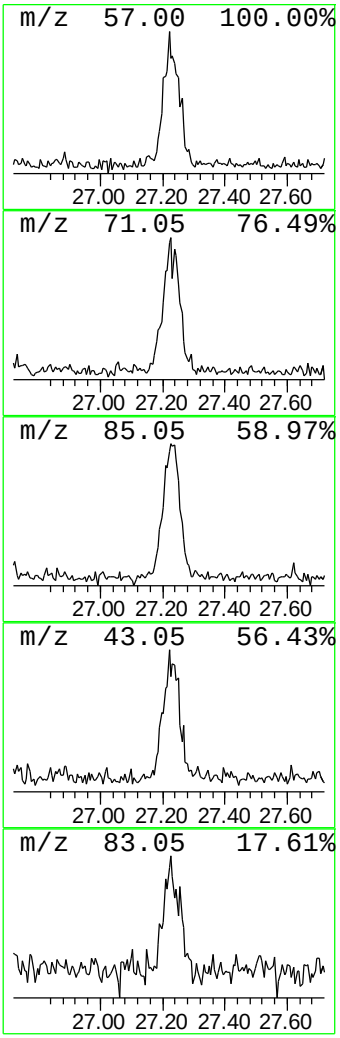
****

Peak Number 8 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.22	2.13 ng	175699	Perylene-d12	24.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	95
2	Eicosane	282	C20H42	000112-95-8	93
3	Tetratetracontane	619	C44H90	007098-22-8	86
4	Nonadecane	268	C19H40	000629-92-5	81
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG052620\
Data File : BG045461.D
Acq On : 26 May 2020 17:34
Operator : CG/JU
Sample : L2744-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM66-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.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
unknown3.12	3.12	9.8	ng	223229	1	7.96	456011	20.0
Oxalic acid, isob...	21.27	3.2	ng	225179	5	21.60	1392180	20.0
Pentacosane	22.41	2.7	ng	188013	5	21.60	1392180	20.0
Heneicosane	23.09	4.4	ng	306325	5	21.60	1392180	20.0
2-methyloctacosane	23.88	4.3	ng	352698	6	24.76	1651020	20.0
Heptadecane, 9-oc...	25.91	3.9	ng	325375	6	24.76	1651020	20.0
Hexadecane	27.22	2.1	ng	175699	6	24.76	1651020	20.0