LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
Data File : BG044094.D
Acq On : 20 Jan 2020 12:26
Operator : JU
Sample : PB126101BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126101BL

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	5.035	325	331	342	rBV	263030	410619	8.09%	1.375%
2	5.511	404	412	427	rBV	1229760	1974713	38.91%	6.615%
3	7.104	675	683	704	rBV	1322352	2375252	46.80%	7.956%
4	7.468	736	745	757	rBV	1315800	2263052	44.59%	7.581%
5	7.932	817	824	832	rBV	310960	522544	10.30%	1.750%
6	8.255	871	879	888	rBV	940445	1624667	32.01%	5.442%
7	9.090	1013	1021	1031	rBV	743947	1368263	26.96%	4.583%
8	10.735	1292	1301	1313	rBV	444642	811334	15.99%	2.718%
9	13.191	1712	1719	1739	rBV	2195525	3661292	72.14%	12.264%
10	14.025	1855	1861	1866	rBV	38911	63073	1.24%	0.211%
11	14.571	1945	1954	1966	rBV	780126	1249517	24.62%	4.186%
12	16.058	2200	2207	2226	rBV	1707841	2733156	53.85%	9.155%
13	17.315	2413	2421	2433	rBV	850144	1366910	26.93%	4.579%
14	19.930	2859	2866	2879	rBV	3806271	5075271	100.00%	17.001%
15	21.240	3083	3089	3099	rBV2	65515	152952	3.01%	0.512%
16	21.563	3137	3144	3154	rBV2	818002	1375370	27.10%	4.607%
17	22.368	3276	3281	3293	rBV	57904	113970	2.25%	0.382%
18	23.003	3382	3389	3393	rBV2	213237	428244	8.44%	1.435%
19	23.220	3422	3426	3434	rVB2	44268	92250	1.82%	0.309%
20	23.819	3522	3528	3539	rVB2	87059	182109	3.59%	0.610%
21	24.671	3663	3673	3681	rBV2	501451	1447882	28.53%	4.850%
22	25.541	3815	3821	3836	rVB2	22731	80438	1.58%	0.269%
23	25.829	3863	3870	3882	rVB3	66266	199003	3.92%	0.667%
24	27.145	4086	4094	4106	rVB3	60043	203502	4.01%	0.682%
25	28.714	4355	4361	4371	rVB7	23718	77650	1.53%	0.260%

Sum of corrected areas: 29853033

LSC Report - Integrated Chromatogram

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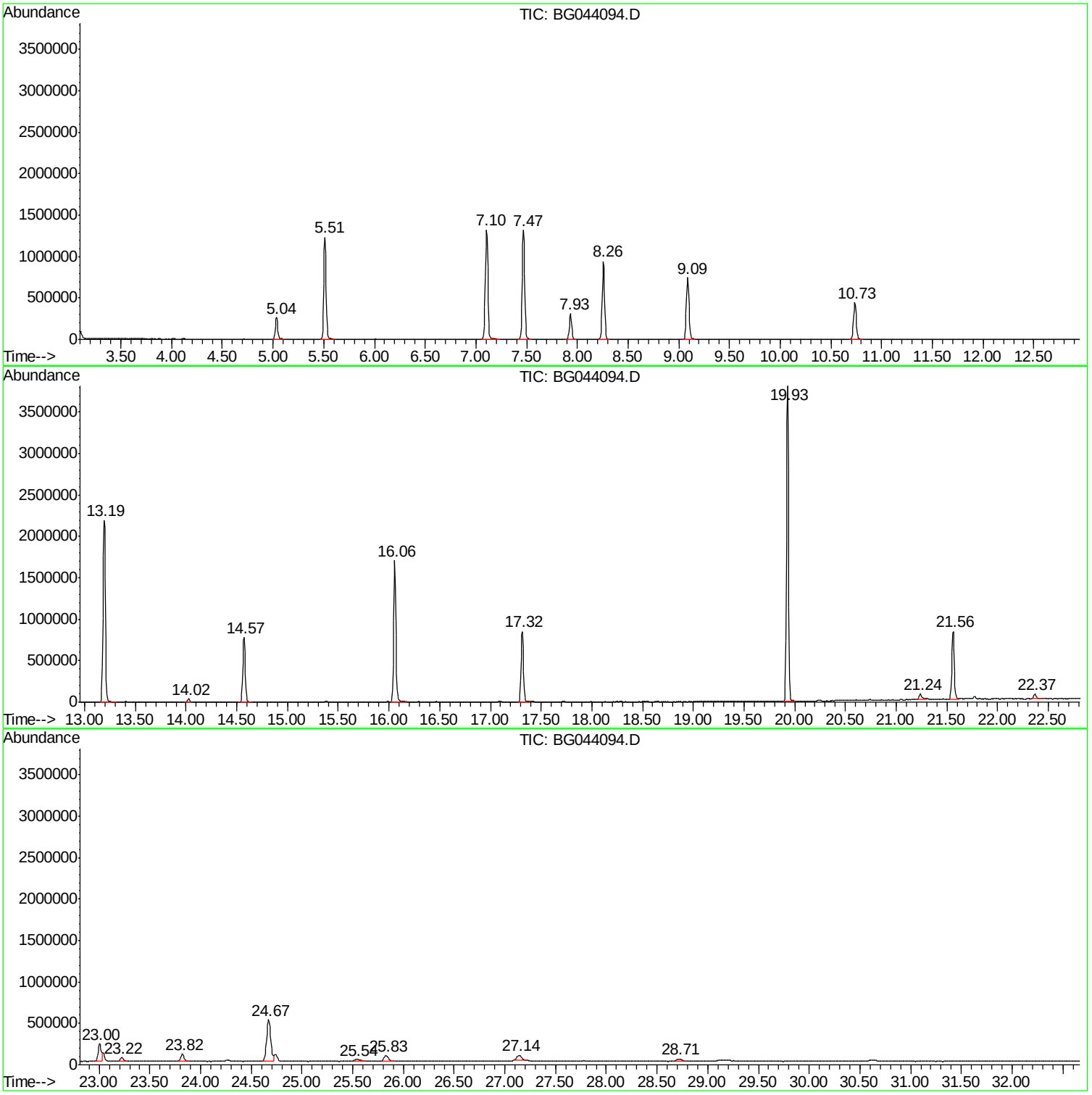
Operator : JU
Sample : PB126101BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126101BL

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



Library Search Compound Report

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Data File : BG044094.D
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Operator : JU
Sample : PB126101BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126101BL

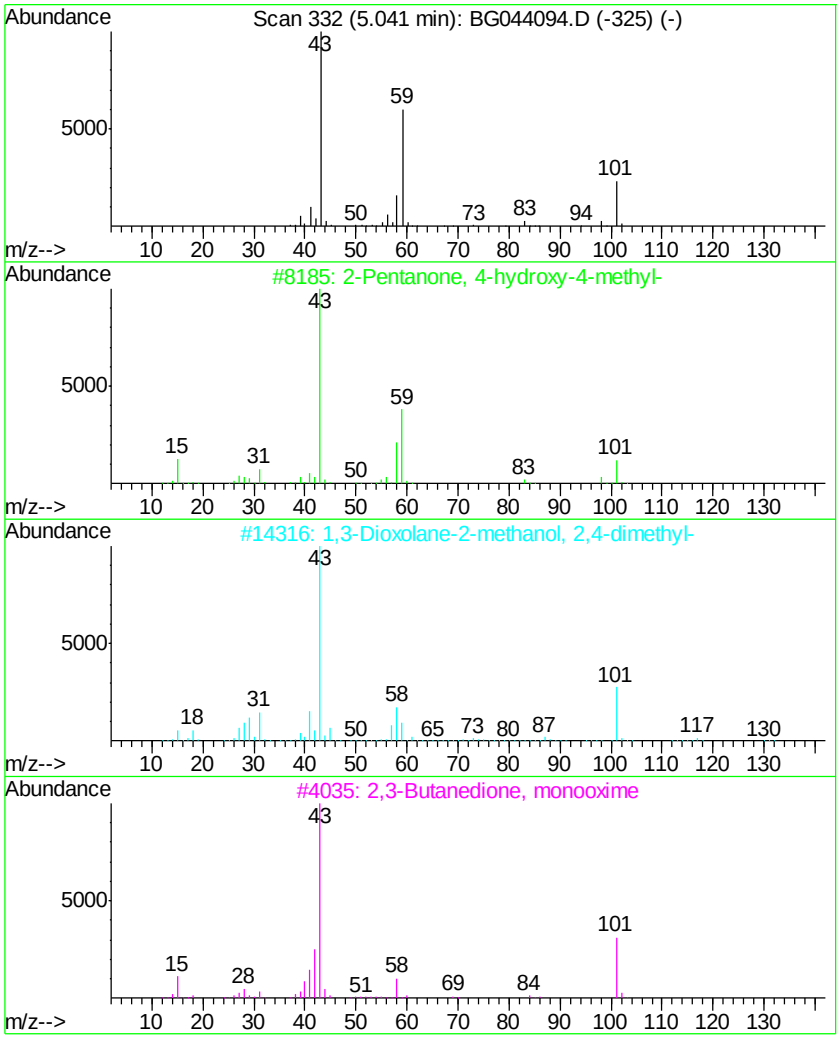
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

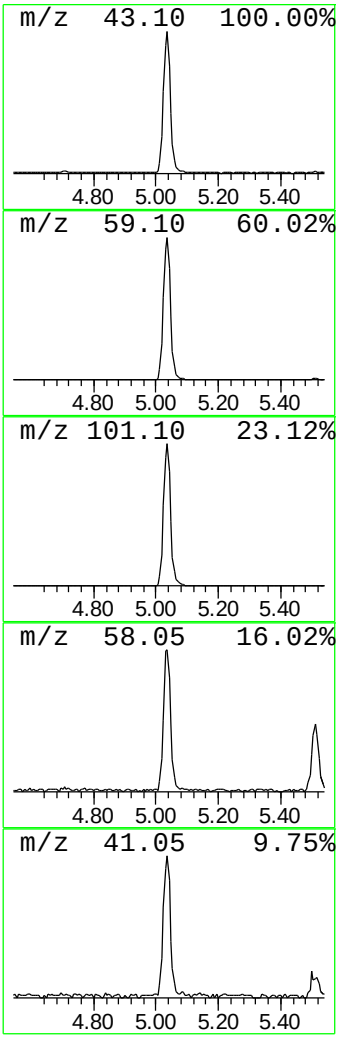
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	15.72 ng	410619	1,4-Dichlorobenzene-d4	7.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47
2	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Data File : BG044094.D
Acq On : 20 Jan 2020 12:26
Operator : JU
Sample : PB126101BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126101BL

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

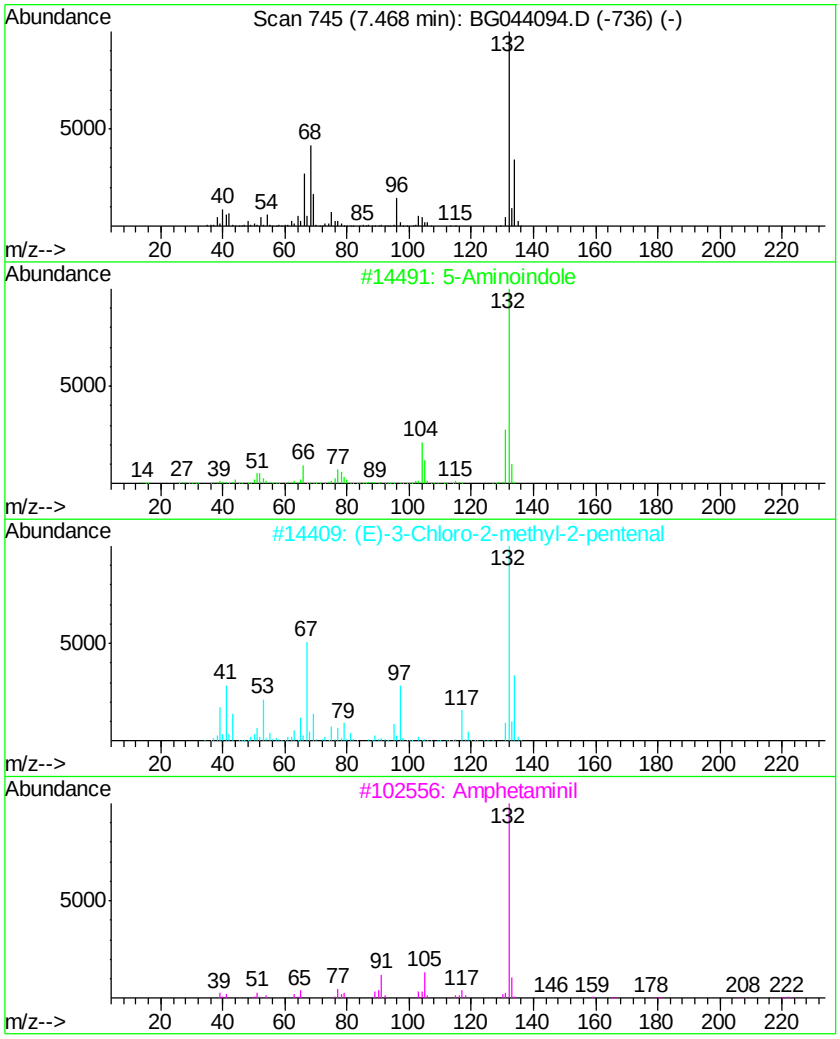
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

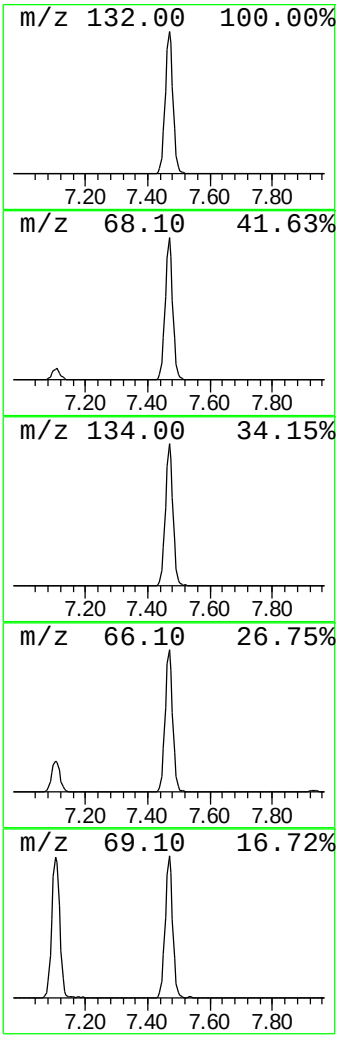
****

Peak Number 2 unknown7.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.47	86.62 ng	2263050	1,4-Dichlorobenzene-d4	7.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	22
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	Amphetaminil	250	C17H18N2	017590-01-1	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	12





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Data File : BG044094.D
Acq On : 20 Jan 2020 12:26
Operator : JU
Sample : PB126101BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126101BL

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

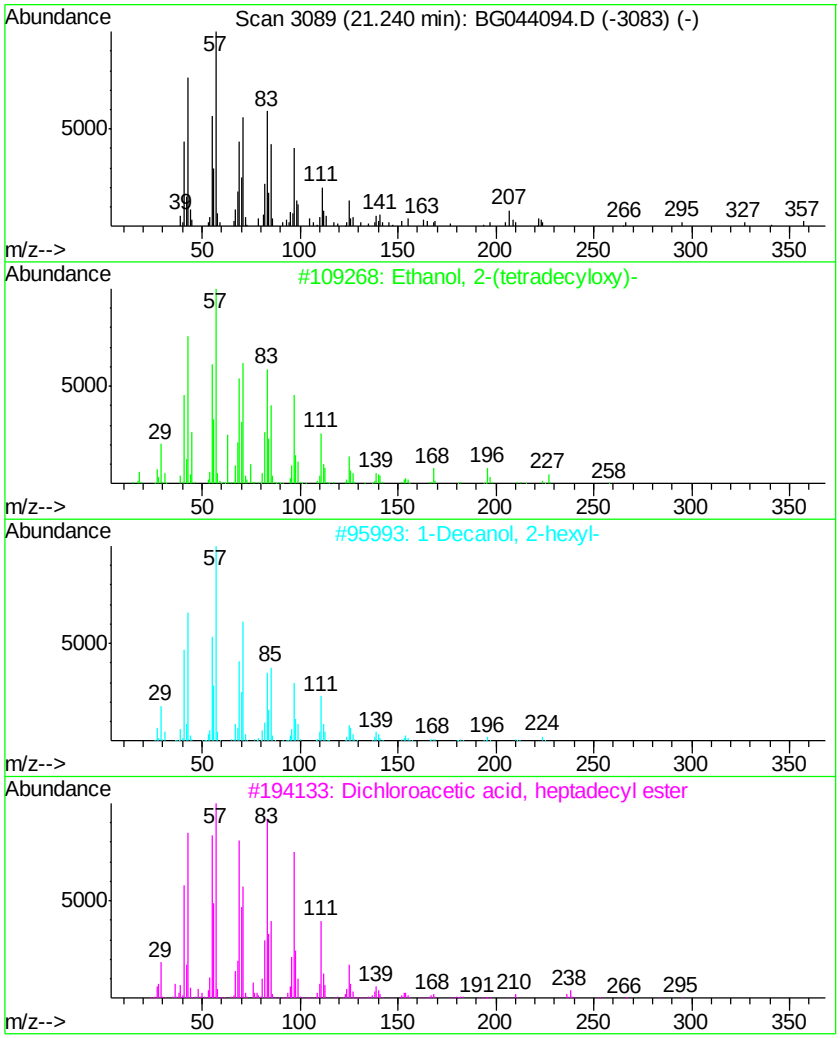
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

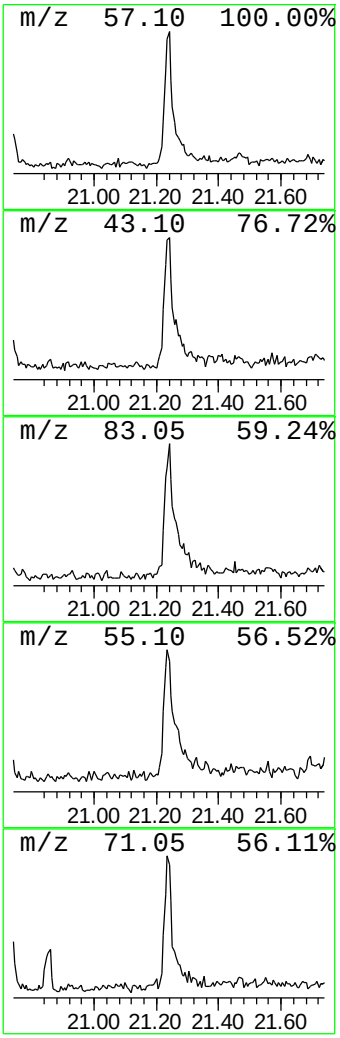
****

Peak Number 4 Ethanol, 2-(tetradecyloxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.24	2.22 ng	152952	Chrysene-d12	21.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	81
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	76
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	70
5	Cyclotetracosane	336	C24H48	000297-03-0	70





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
Data File : BG044094.D
Acq On : 20 Jan 2020 12:26
Operator : JU
Sample : PB126101BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126101BL

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

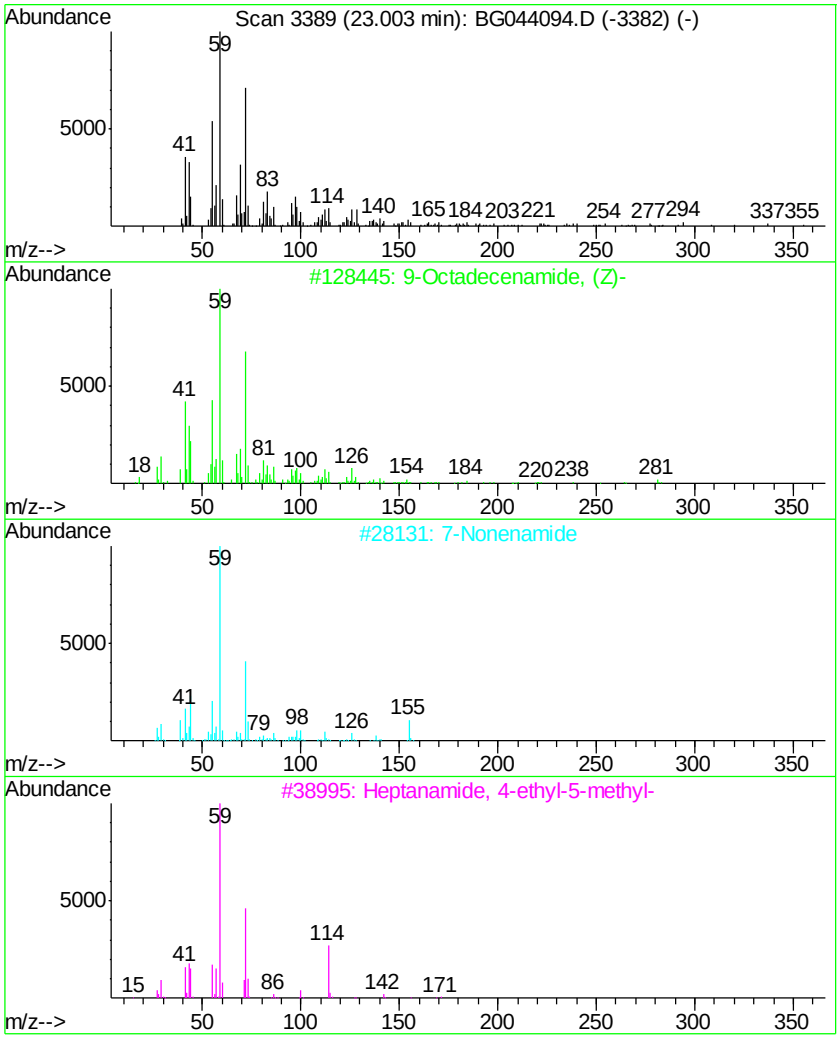
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

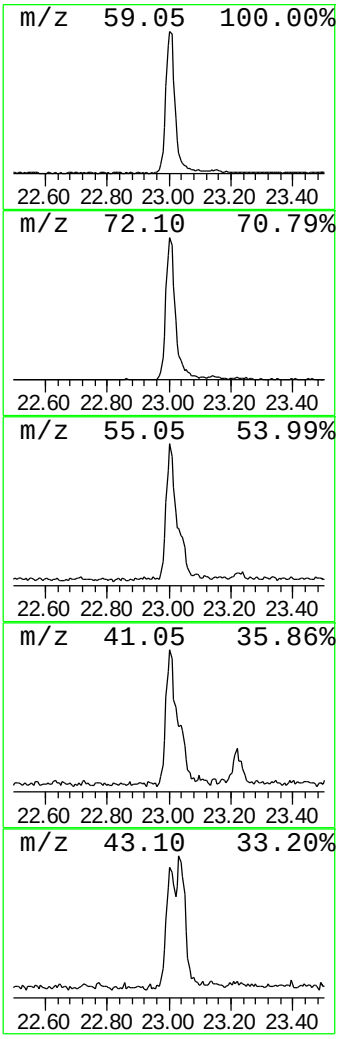
****

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.00	6.23 ng	428244	Chrysene-d12	21.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	7-Nonenamide	155	C9H17NO	090949-53-4	64
3	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	64
4	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	58
5	Hexadecanamide	255	C16H33NO	000629-54-9	53





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
Data File : BG044094.D
Acq On : 20 Jan 2020 12:26
Operator : JU
Sample : PB126101BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126101BL

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

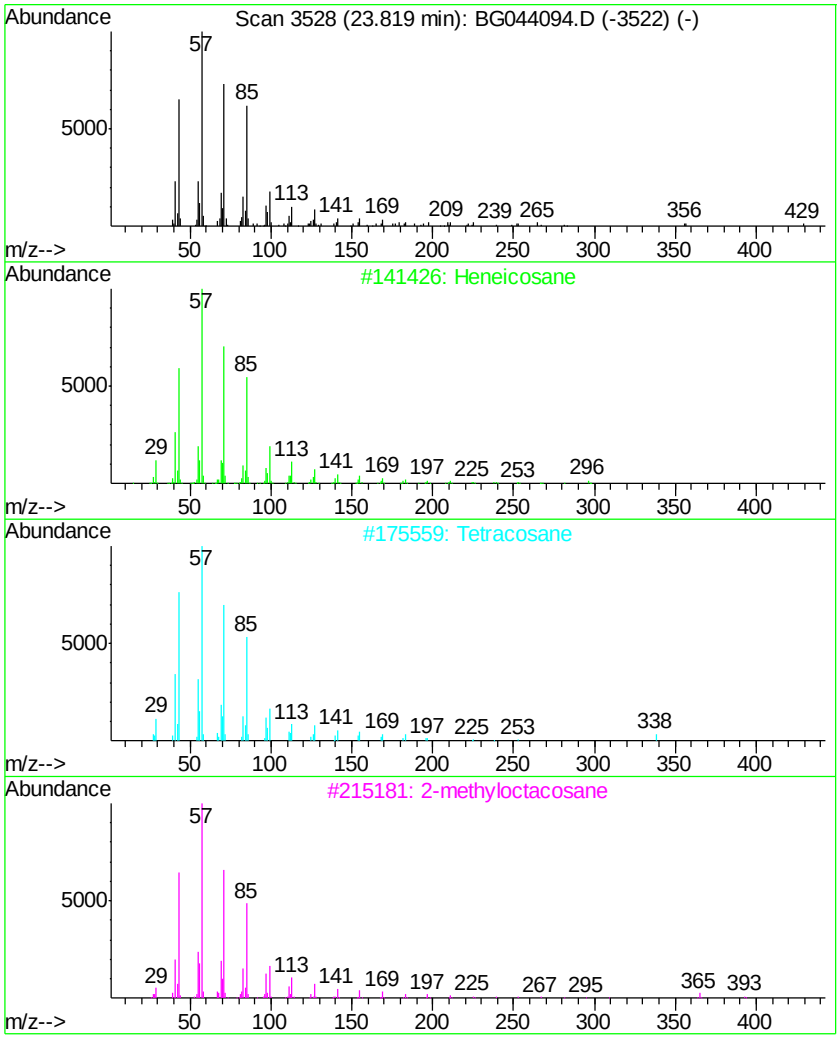
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

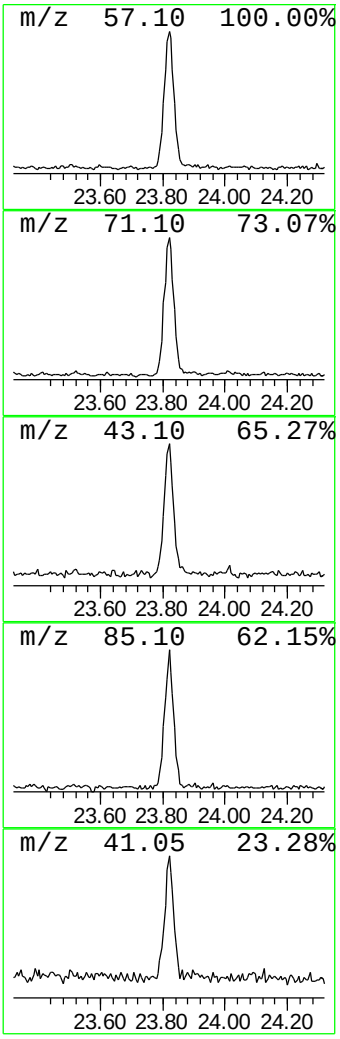
****

Peak Number 6 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.82	2.52 ng	182109	Perylene-d12	24.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Tetracosane	338	C24H50	000646-31-1	90
3	2-methyloctacosane	408	C29H60	1000376-72-8	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Heptadecane	240	C17H36	000629-78-7	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
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Sample : PB126101BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB126101BL

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

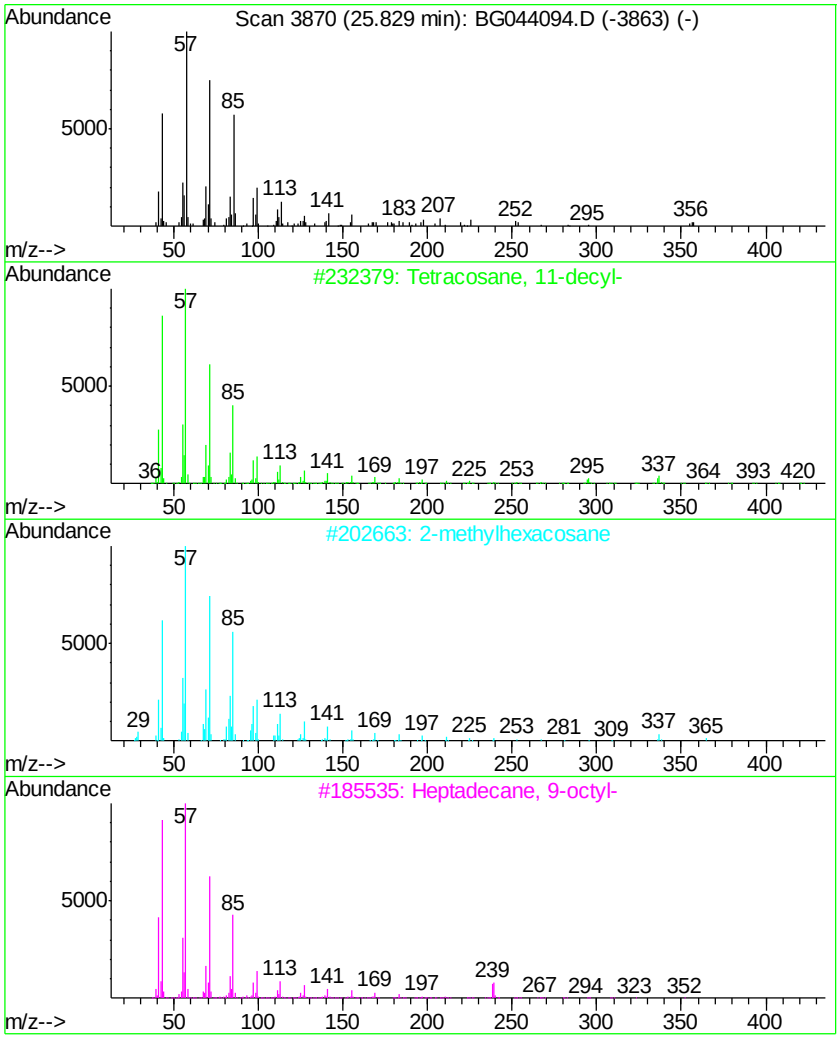
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

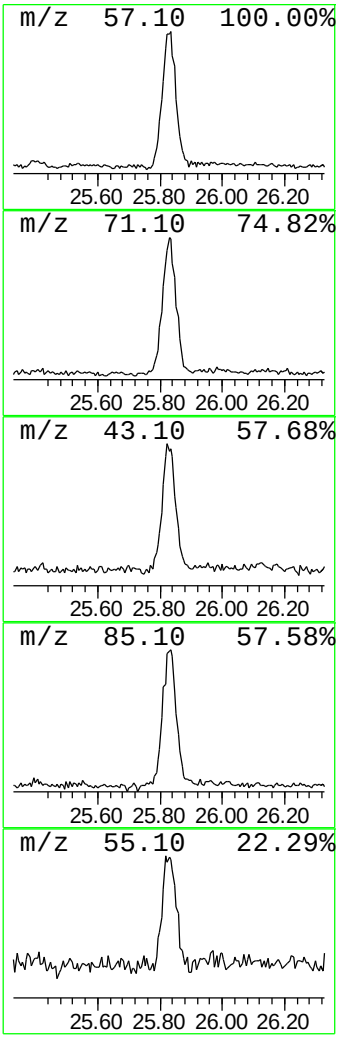
****

Peak Number 7 Tetracosane, 11-decyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.83	2.75 ng	199003	Perylene-d12	24.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	91
2	2-methylhexacosane	380	C27H56	1000376-72-7	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Octacosane	394	C28H58	000630-02-4	91





Library Search Compound Report

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Sample : PB126101BL
Misc :
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Instrument : BNA_G
ClientSampleId : PB126101BL

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

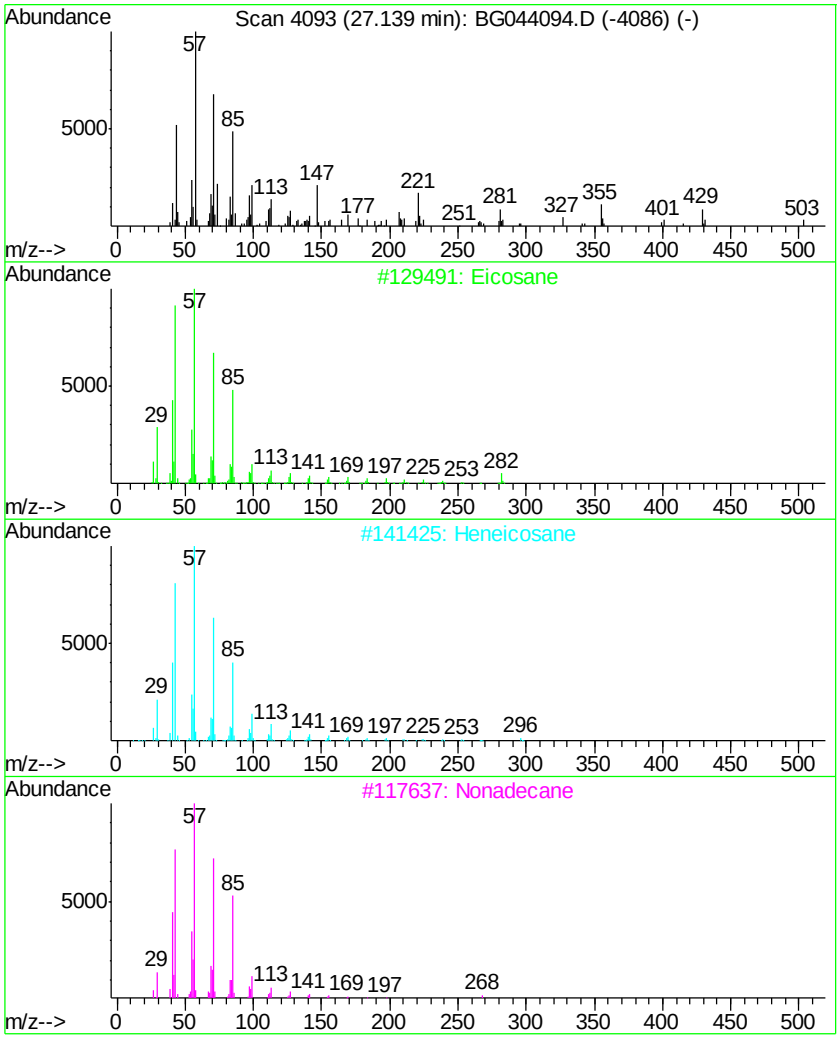
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

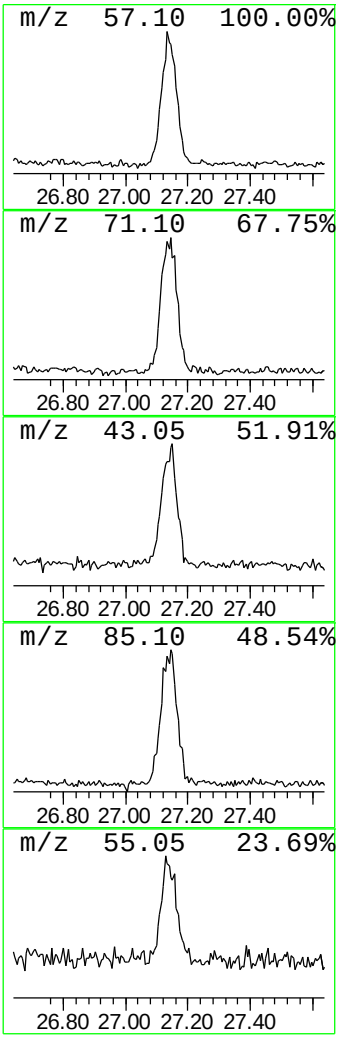
****

Peak Number 8 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.14	2.81 ng	203502	Perylene-d12	24.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Heneicosane	296	C21H44	000629-94-7	83
3	Nonadecane	268	C19H40	000629-92-5	83
4	Hexacosane	366	C26H54	000630-01-3	64
5	Heptacosane	380	C27H56	000593-49-7	62





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG012020\
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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...	5.04	15.7	ng	410619	1	7.93	522544	20.0
unknown7.47	7.47	86.6	ng	2263050	1	7.93	522544	20.0
Ethanol, 2-(tetra...	21.24	2.2	ng	152952	5	21.56	1375370	20.0
9-Octadecenamide,...	23.00	6.2	ng	428244	5	21.56	1375370	20.0
Heneicosane	23.82	2.5	ng	182109	6	24.67	1447880	20.0
Tetracosane, 11-d...	25.83	2.8	ng	199003	6	24.67	1447880	20.0
Eicosane	27.14	2.8	ng	203502	6	24.67	1447880	20.0