LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG092718\
Data File : BG037045.D
Acq On : 28 Sep 2018 11:29
Operator : JU/SJ
Sample : J5090-02
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-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-BG092018.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	5.150	312	317	325	rBV	33691	54380	1.96%	0.405%
2	5.614	391	396	408	rBV	161691	306945	11.04%	2.286%
3	7.207	661	667	683	rBV2	97747	329651	11.85%	2.455%
4	7.571	722	729	743	rBV	295726	587060	21.11%	4.372%
5	8.041	803	809	824	rBV	132377	270685	9.73%	2.016%
6	8.364	856	864	882	rBV	426365	827063	29.73%	6.159%
7	9.198	999	1006	1023	rBV	336478	743273	26.72%	5.535%
8	10.844	1279	1286	1303	rBV	179506	366601	13.18%	2.730%
9	13.288	1695	1702	1718	rBV	955774	1639945	58.96%	12.213%
10	14.110	1837	1842	1851	rBV	91334	152561	5.48%	1.136%
11	14.663	1929	1936	1946	rBV2	296569	537645	19.33%	4.004%
12	16.149	2182	2189	2210	rBV	497828	884997	31.82%	6.591%
13	17.412	2397	2404	2419	rBV	424671	747511	26.87%	5.567%
14	18.294	2549	2554	2565	rBV	109661	197382	7.10%	1.470%
15	19.557	2766	2769	2777	rBV5	20785	38409	1.38%	0.286%
16	20.015	2841	2847	2861	rBV	1952795	2781467	100.00%	20.713%
17	21.314	3064	3068	3081	rBV2	77494	203997	7.33%	1.519%
18	21.678	3123	3130	3142	rBV2	468142	878018	31.57%	6.539%
19	22.465	3259	3264	3268	rBV2	22798	36867	1.33%	0.275%
20	23.147	3371	3380	3390	rBV3	65792	176088	6.33%	1.311%
21	23.341	3406	3413	3426	rVB	244005	481022	17.29%	3.582%
22	23.952	3511	3517	3524	rVB	49091	98938	3.56%	0.737%
23	24.880	3664	3675	3688	rBV2	308243	932012	33.51%	6.941%
24	26.002	3859	3866	3877	rVB3	34641	103594	3.72%	0.771%
25	27.348	4089	4095	4104	rVB5	19723	52248	1.88%	0.389%

Sum of corrected areas: 13428359

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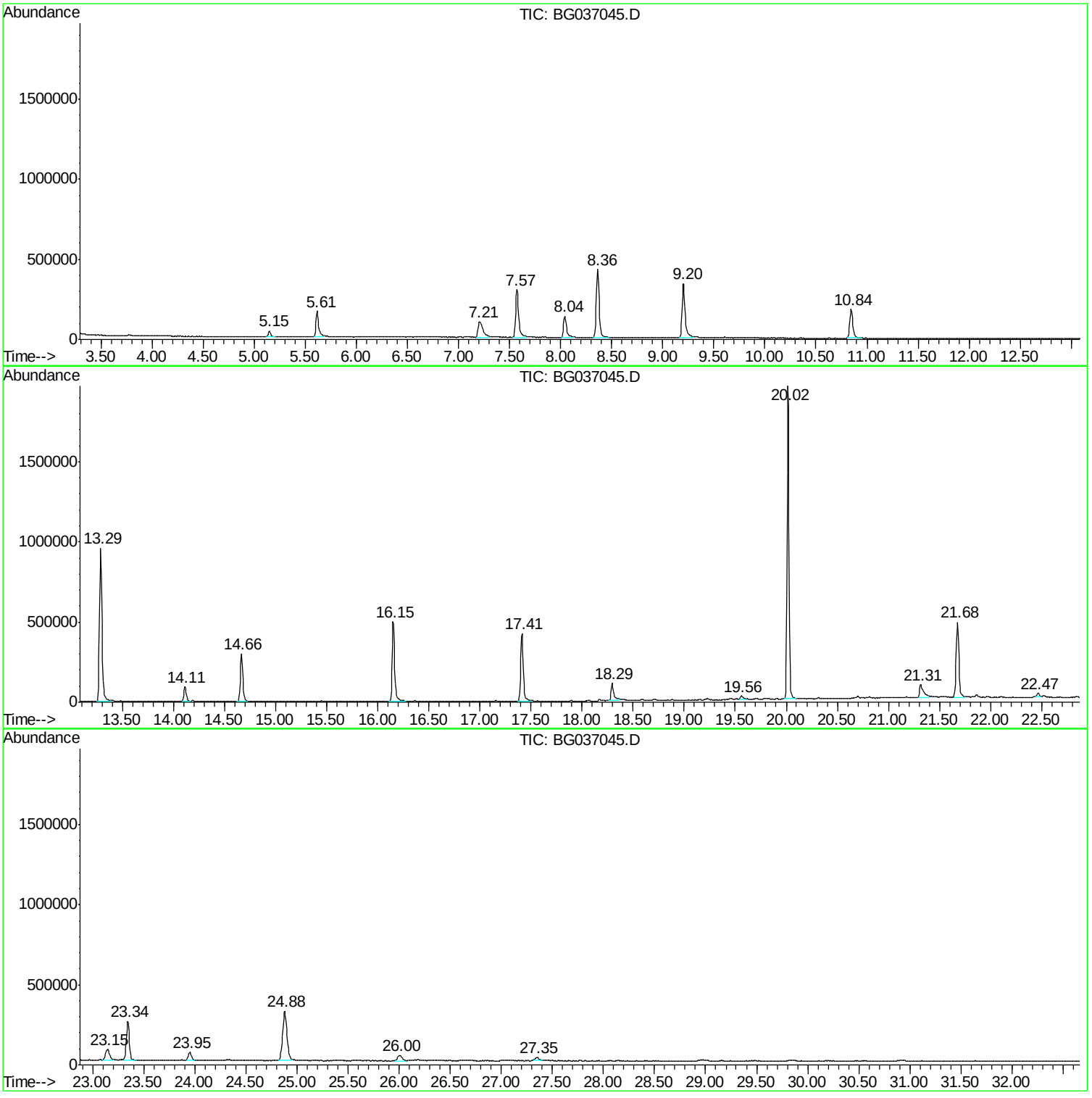
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.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\BG092718\
Data File : BG037045.D
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Operator : JU/SJ
Sample : J5090-02
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-2

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

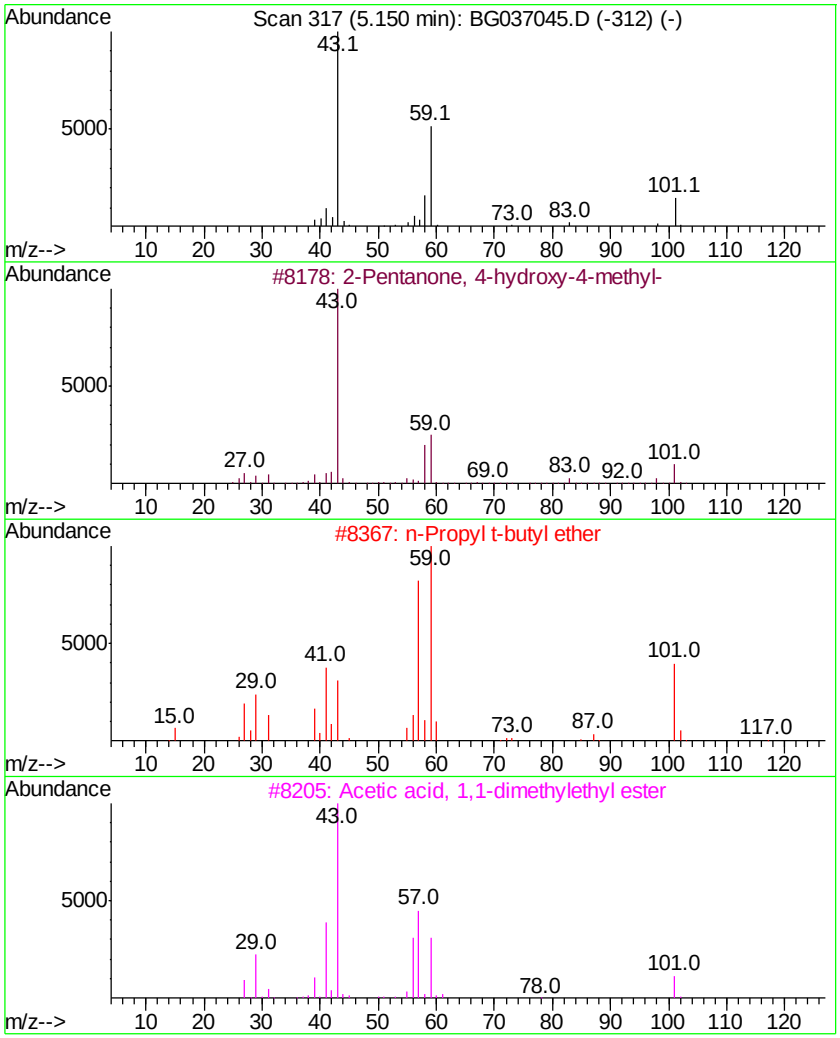
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

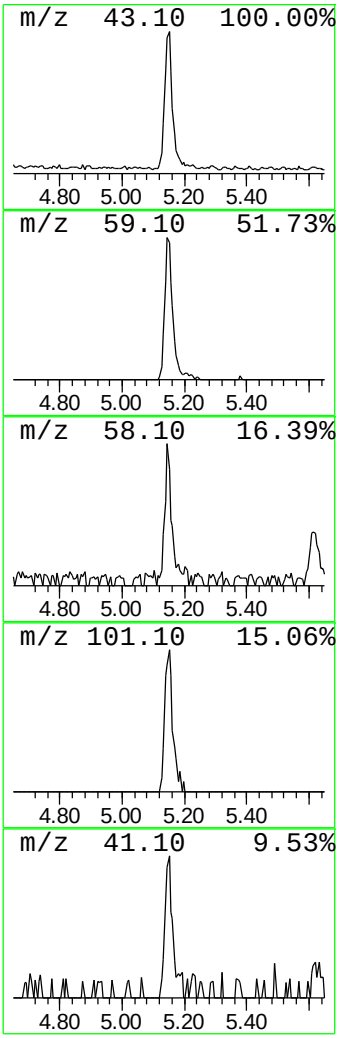
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	4.02 ng	54380	1,4-Dichlorobenzene-d4	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	28
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

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Data File : BG037045.D
Acq On : 28 Sep 2018 11:29
Operator : JU/SJ
Sample : J5090-02
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

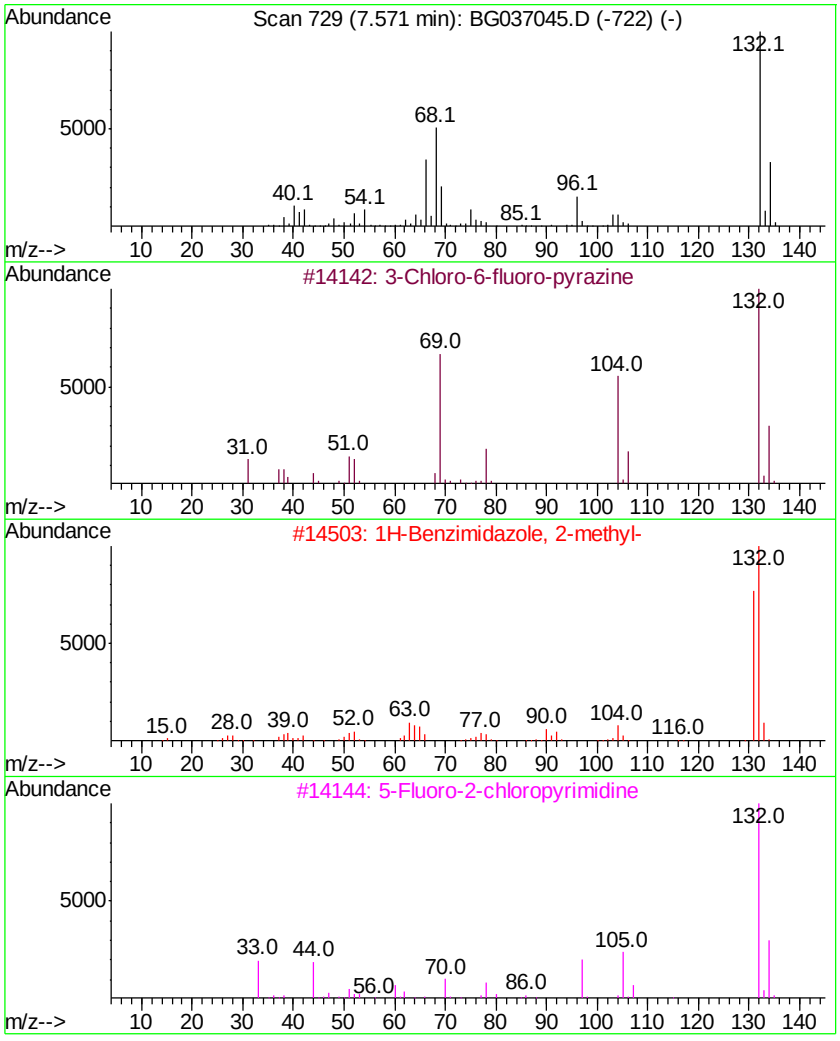
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

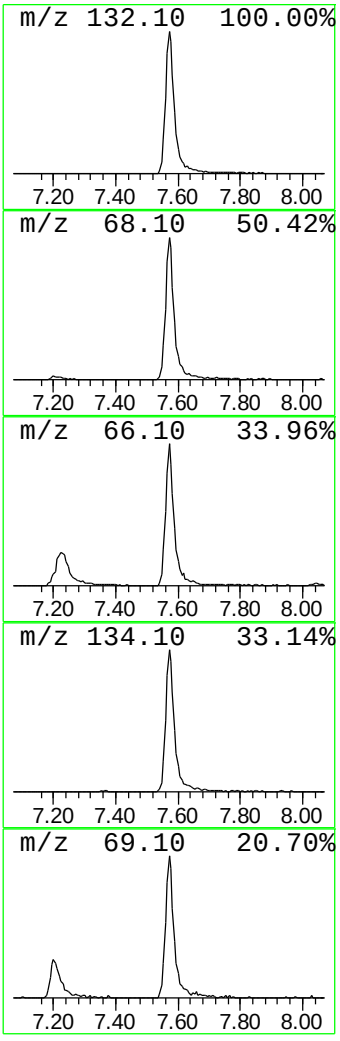
****

Peak Number 2 unknown7.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.57	43.38 ng	587060	1,4-Dichlorobenzene-d4	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





Library Search Compound Report

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Data File : BG037045.D
Acq On : 28 Sep 2018 11:29
Operator : JU/SJ
Sample : J5090-02
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

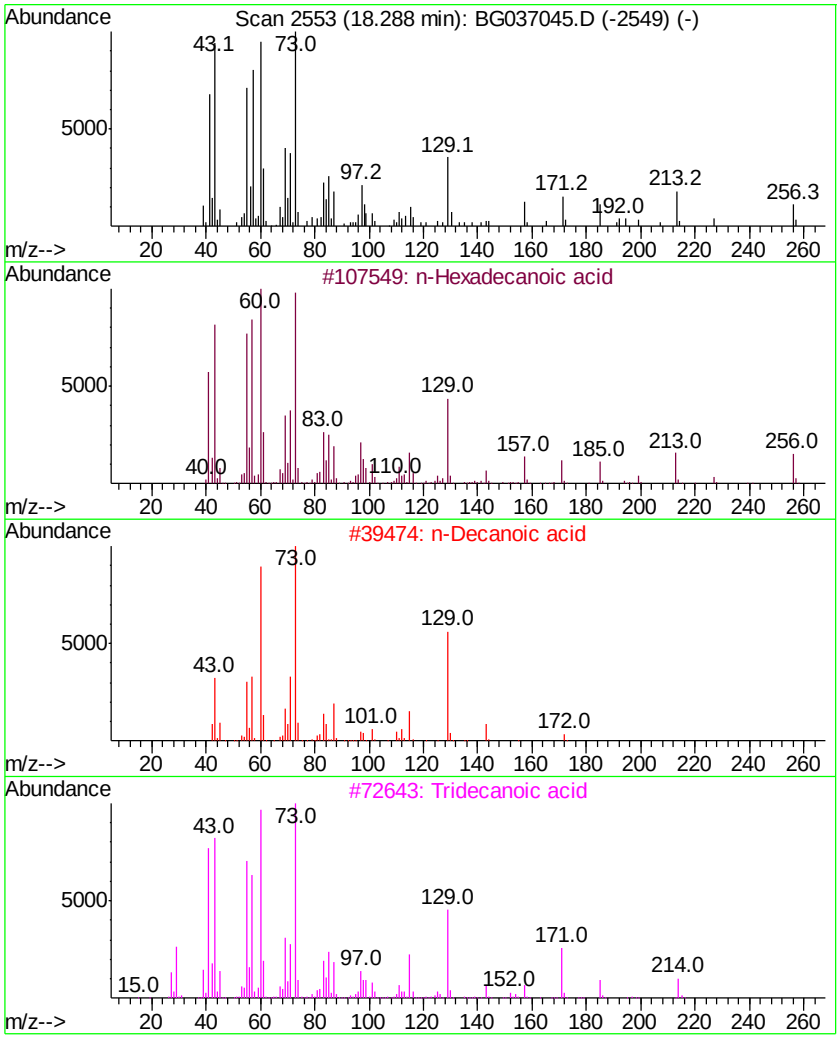
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

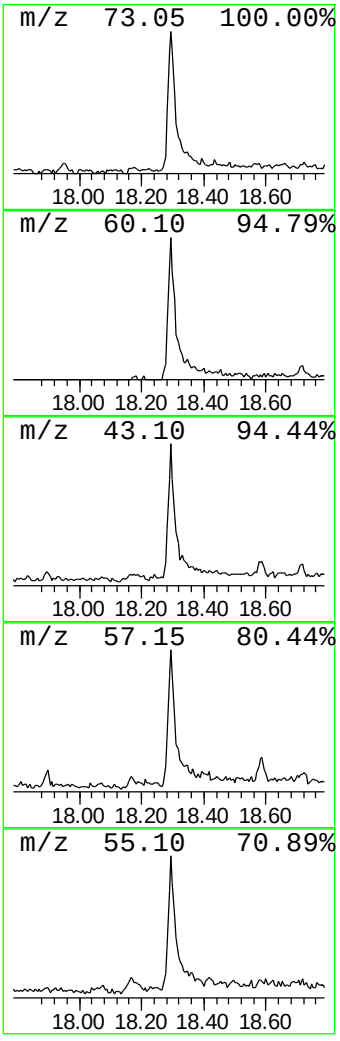
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.29	5.28 ng	197382	Phenanthrene-d10	17.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	n-Decanoic acid	172	C10H20O2	000334-48-5	92
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG092718\
Data File : BG037045.D
Acq On : 28 Sep 2018 11:29
Operator : JU/SJ
Sample : J5090-02
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

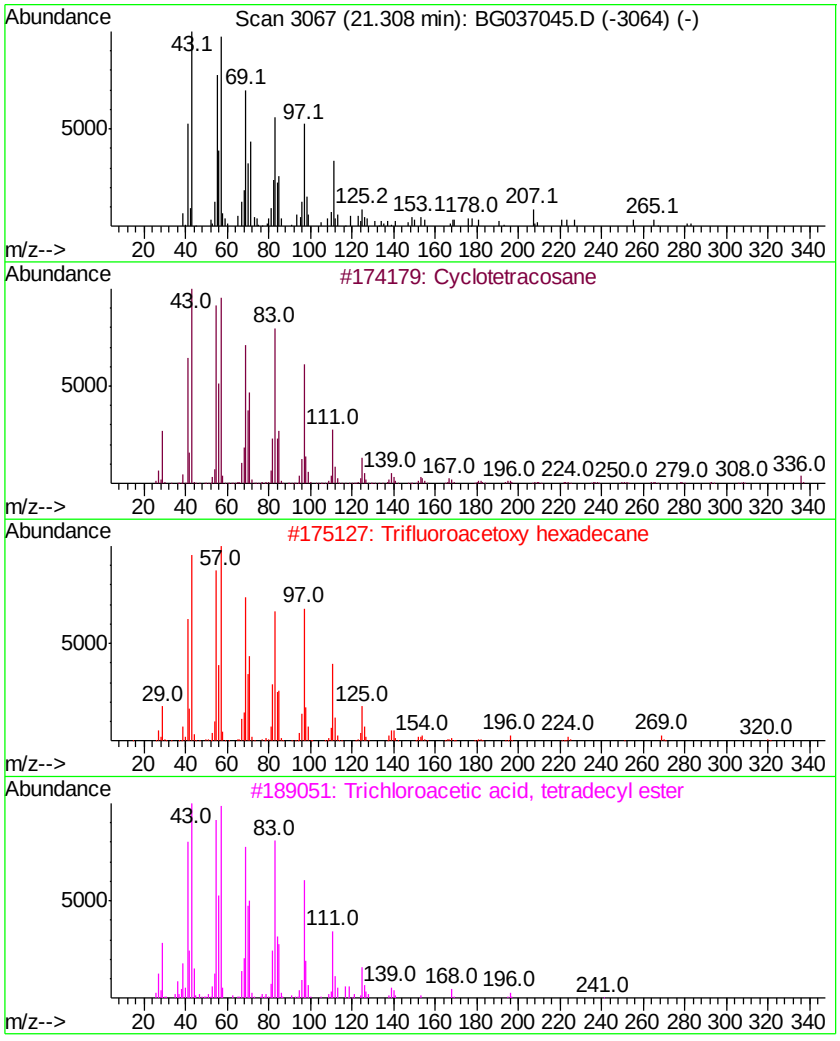
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

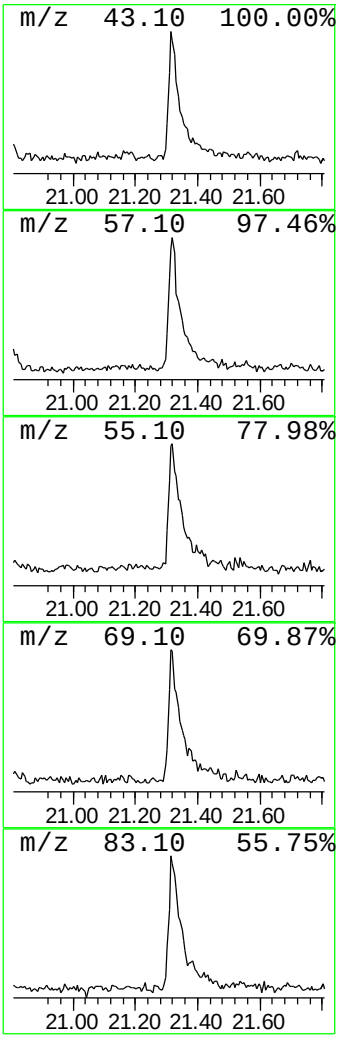
****

Peak Number 5 Cyclotetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	4.65 ng	203997	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	91
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
4	1-Tricosene	322	C23H46	018835-32-0	91
5	1-Nonadecene	266	C19H38	018435-45-5	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG092718\
Data File : BG037045.D
Acq On : 28 Sep 2018 11:29
Operator : JU/SJ
Sample : J5090-02
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

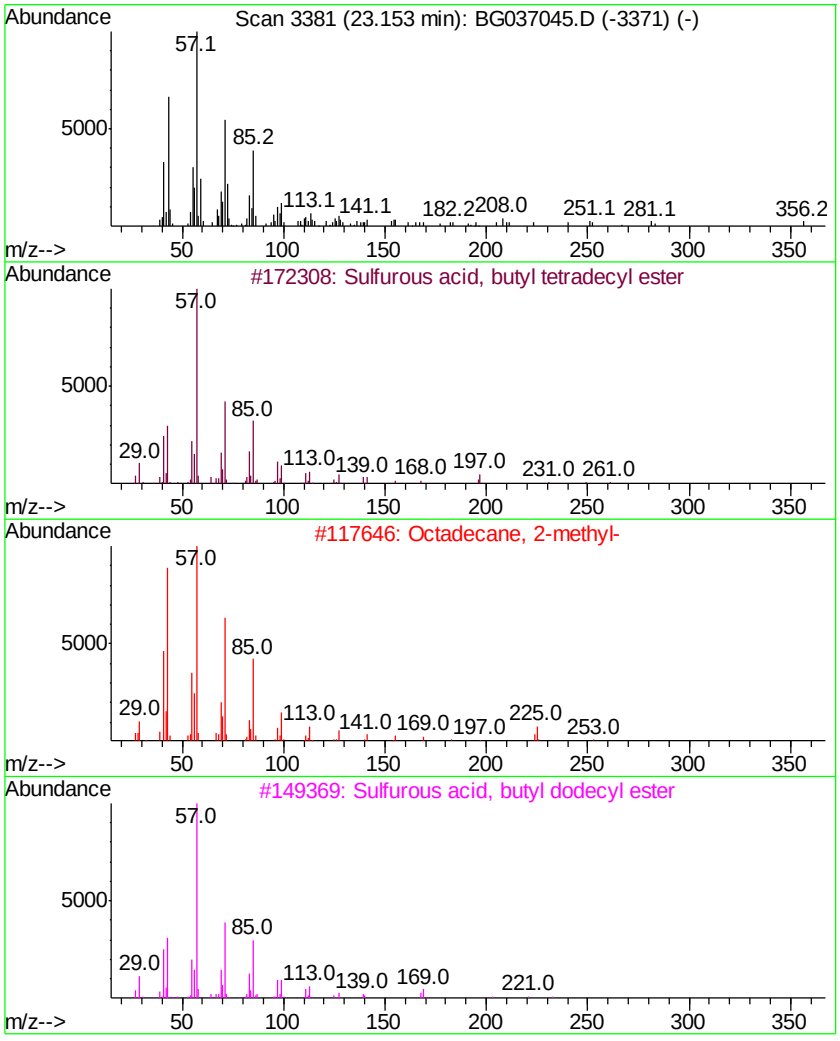
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

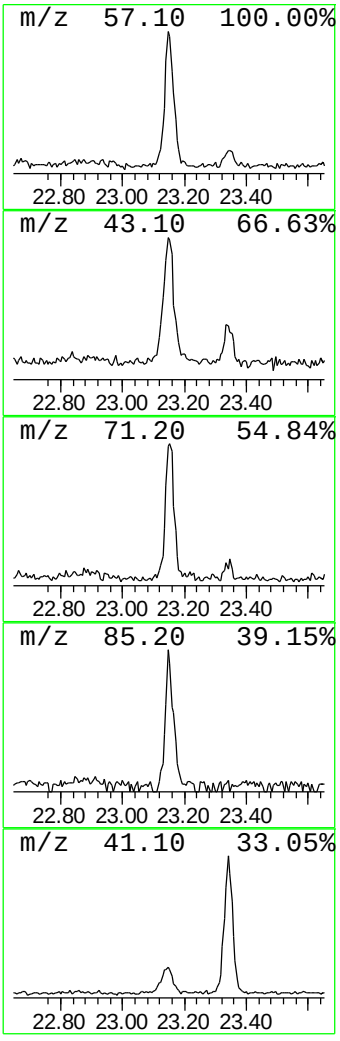
****

Peak Number 6 Sulfurous acid, butyl tetra... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.15	4.01 ng	176088	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	64
2	Octadecane, 2-methyl-	268	C19H40	001560-88-9	64
3	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	64
4	Tetratetracontane	619	C44H90	007098-22-8	62
5	Octacosane	394	C28H58	000630-02-4	62





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Sample : J5090-02
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

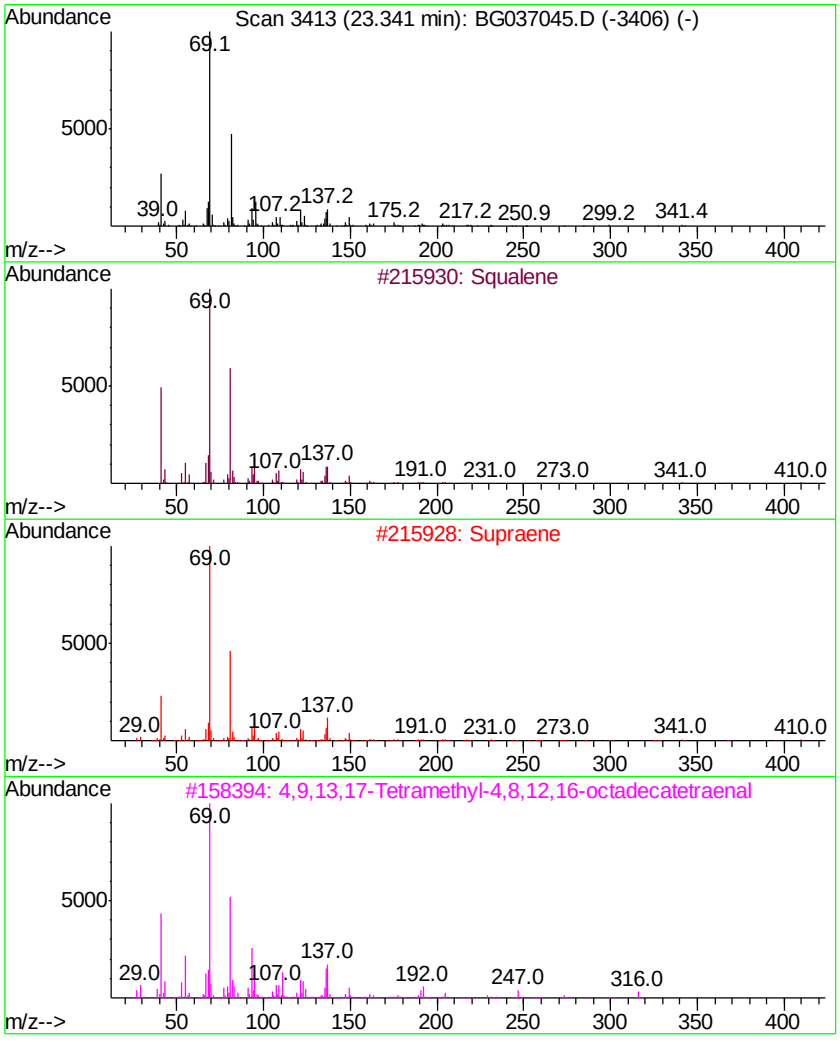
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

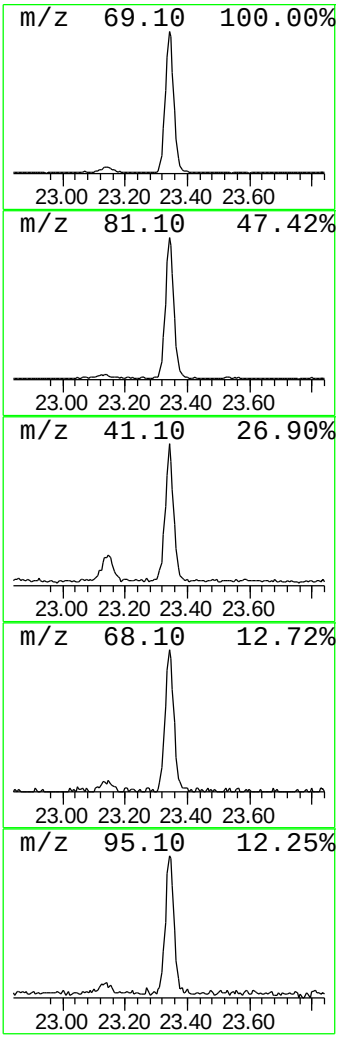
****

Peak Number 7 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.34	10.32 ng	481022	Perylene-d12	24.87

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	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	83
5	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	64





Library Search Compound Report

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Misc :
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Instrument : BNA_G
ClientSampleId : MW-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

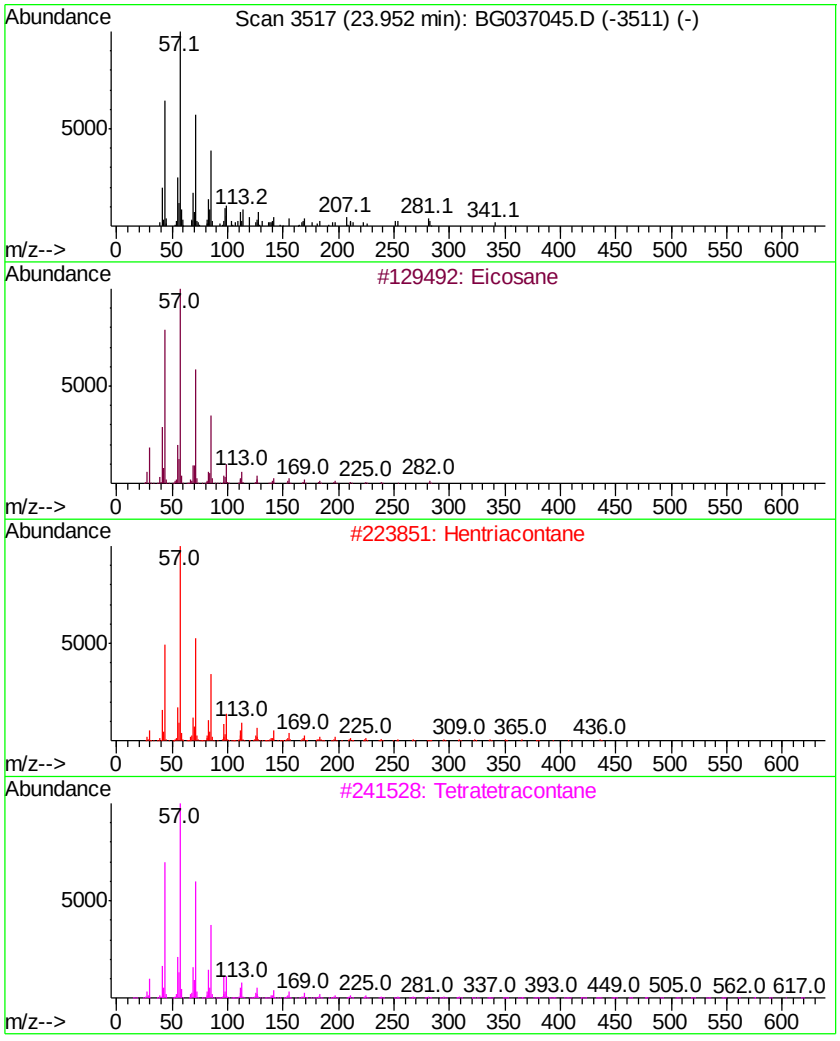
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

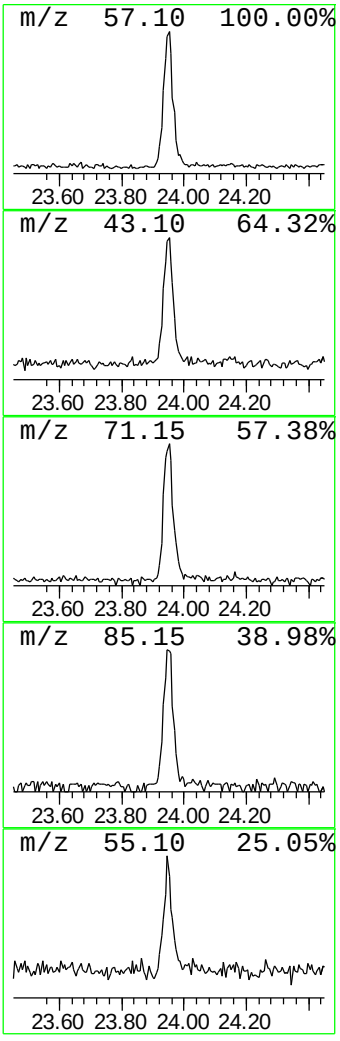
****

Peak Number 8 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.95	2.12 ng	98938	Perylene-d12	24.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Hentriacontane	437	C31H64	000630-04-6	87
3	Tetratetracontane	619	C44H90	007098-22-8	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	87





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Instrument : BNA_G
ClientSampleId : MW-2

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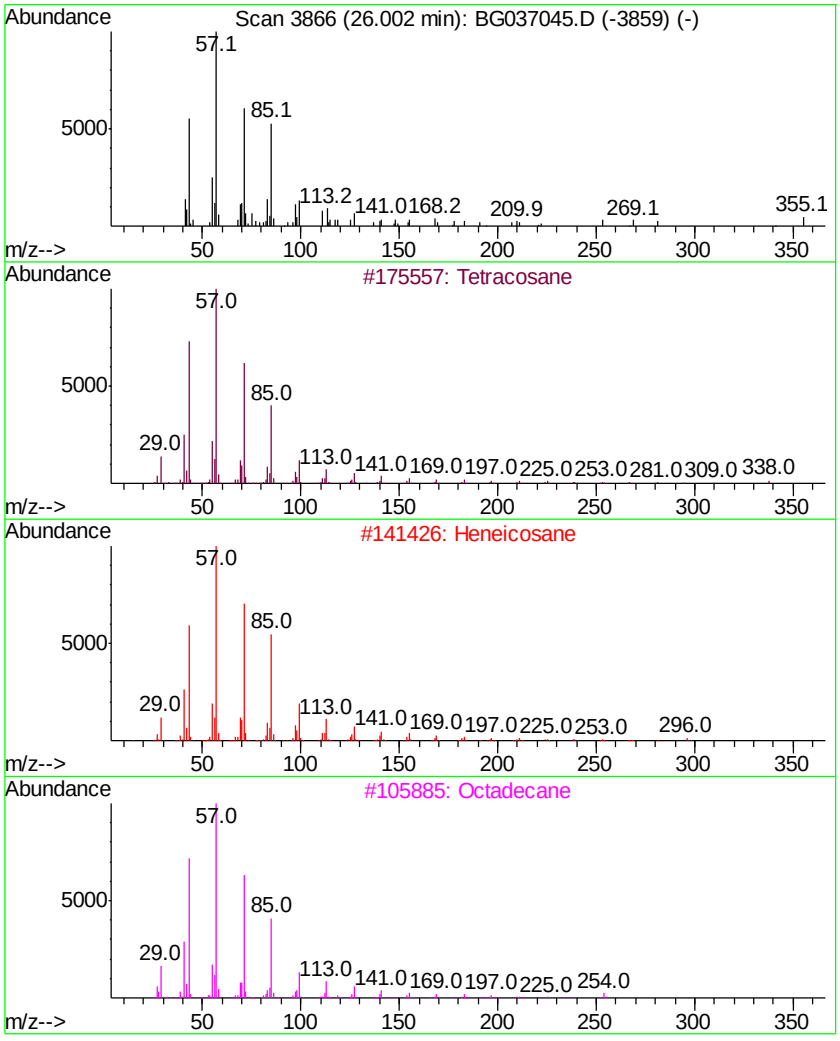
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

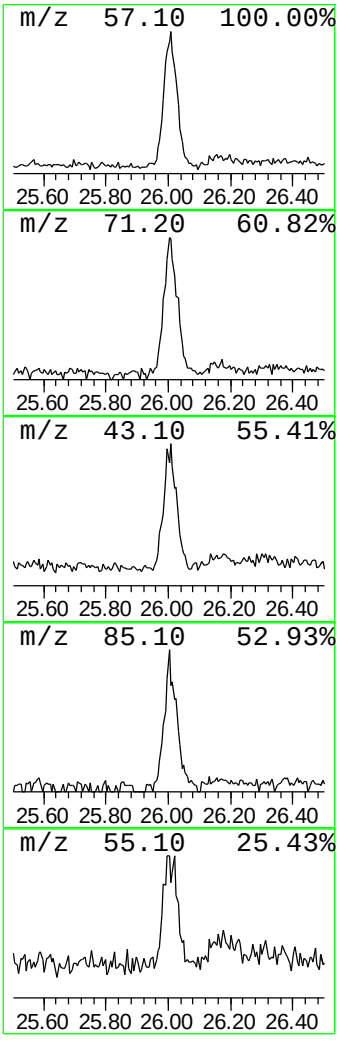
****

Peak Number 9 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.00	2.22 ng	103594	Perylene-d12	24.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	87
2	Heneicosane	296	C21H44	000629-94-7	87
3	Octadecane	254	C18H38	000593-45-3	83
4	Hexadecane	226	C16H34	000544-76-3	83
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.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...	5.15	4.0	ng	54380	1	8.04	270685	20.0
unknown7.57	7.57	43.4	ng	587060	1	8.04	270685	20.0
n-Hexadecanoic acid	18.29	5.3	ng	197382	4	17.41	747511	20.0
Cyclotetracosane	21.31	4.7	ng	203997	5	21.68	878018	20.0
Sulfurous acid, b...	23.15	4.0	ng	176088	5	21.68	878018	20.0
Squalene	23.34	10.3	ng	481022	6	24.87	932012	20.0
Eicosane	23.95	2.1	ng	98938	6	24.87	932012	20.0
Tetracosane	26.00	2.2	ng	103594	6	24.87	932012	20.0