LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091619\
Data File : BG042856.D
Acq On : 16 Sep 2019 19:50
Operator : HP/JU
Sample : K4866-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : N48987

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-BG091219.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	3.217	16	22	30	rBV	660364	1337123	18.32%	3.162%
2	3.294	30	35	56	rVB	2018840	3231194	44.27%	7.641%
3	5.685	433	442	453	rVB	904912	1475528	20.21%	3.489%
4	7.266	704	711	724	rVB	609816	1083104	14.84%	2.561%
5	7.647	766	776	786	rBV	1590114	2878647	39.44%	6.807%
6	8.117	848	856	864	rBV	363044	635455	8.71%	1.503%
7	8.446	903	912	920	rBV	1425603	2578890	35.33%	6.098%
8	9.275	1044	1053	1063	rVB	1318411	2369144	32.46%	5.602%
9	10.926	1326	1334	1342	rBV	481897	862094	11.81%	2.039%
10	13.364	1741	1749	1758	rBV	3168958	5024618	68.84%	11.882%
11	14.181	1880	1888	1892	rBV	110722	171275	2.35%	0.405%
12	14.733	1971	1982	1989	rBV2	742133	1208980	16.56%	2.859%
13	16.220	2227	2235	2246	rBV	2642173	4209125	57.67%	9.953%
14	17.477	2443	2449	2459	rVB2	928378	1432197	19.62%	3.387%
15	17.841	2505	2511	2516	rBV	196486	262701	3.60%	0.621%
16	18.364	2595	2600	2606	rBV2	147855	221890	3.04%	0.525%
17	20.086	2886	2893	2899	rBV	5459718	7299239	100.00%	17.261%
18	21.402	3113	3117	3124	rBV2	183491	308344	4.22%	0.729%
19	21.754	3167	3177	3185	rVB	947112	1598535	21.90%	3.780%
20	21.972	3210	3214	3220	rVB	93449	135305	1.85%	0.320%
21	22.600	3315	3321	3330	rVB2	155929	298687	4.09%	0.706%
22	23.311	3436	3442	3449	rVB	194475	366341	5.02%	0.866%
23	24.146	3576	3584	3592	rBV2	222411	477407	6.54%	1.129%
24	25.027	3723	3734	3744	rBV2	536377	1587743	21.75%	3.755%
25	25.127	3744	3751	3759	rVB	187893	479683	6.57%	1.134%
26	26.302	3941	3951	3959	rVB4	129157	384487	5.27%	0.909%
27	27.706	4182	4190	4200	rVB4	61359	196585	2.69%	0.465%
28	29.398	4469	4478	4487	rBV4	52255	173929	2.38%	0.411%

Sum of corrected areas: 42288250

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091619\
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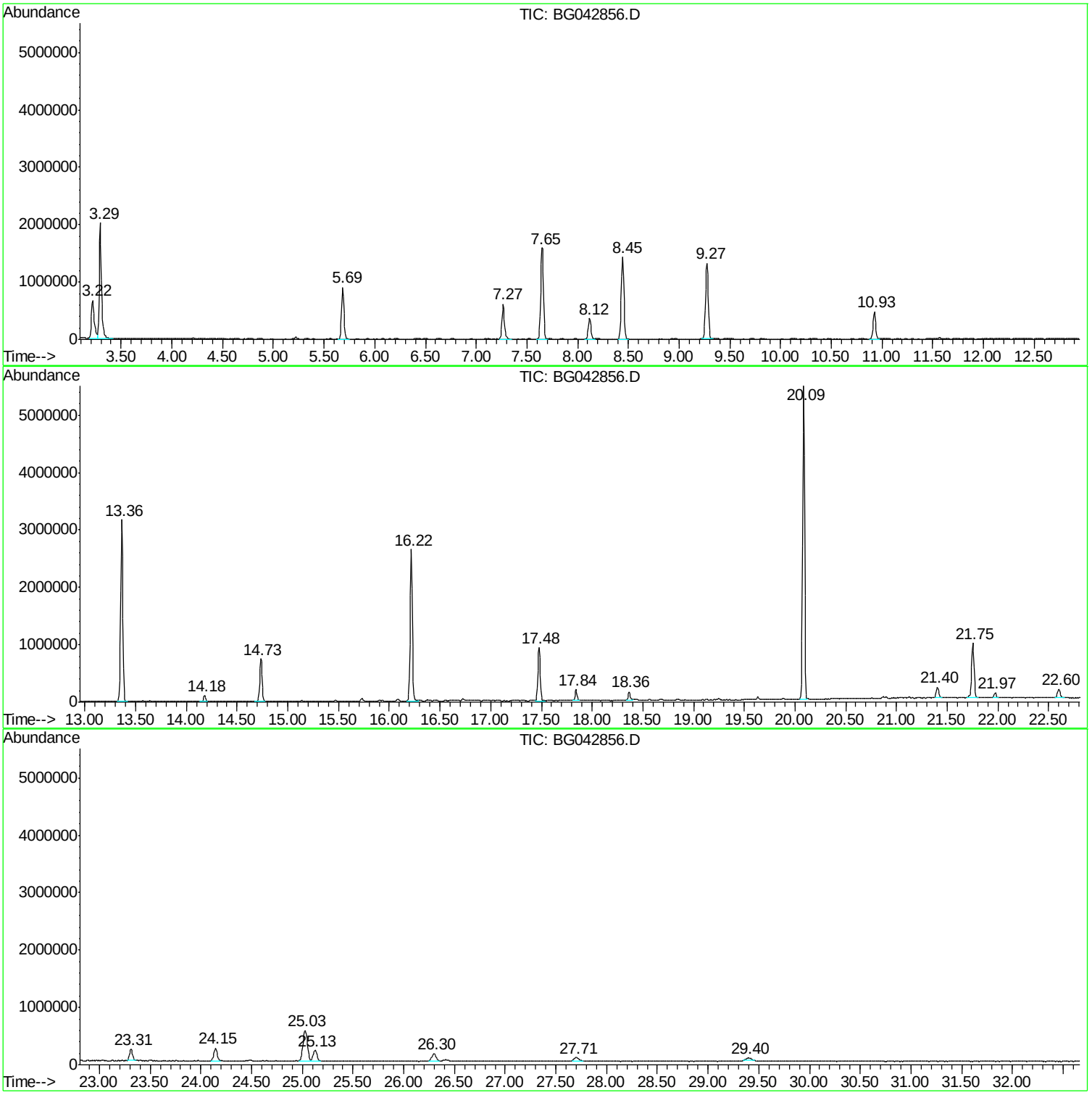
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : N48987

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG091219.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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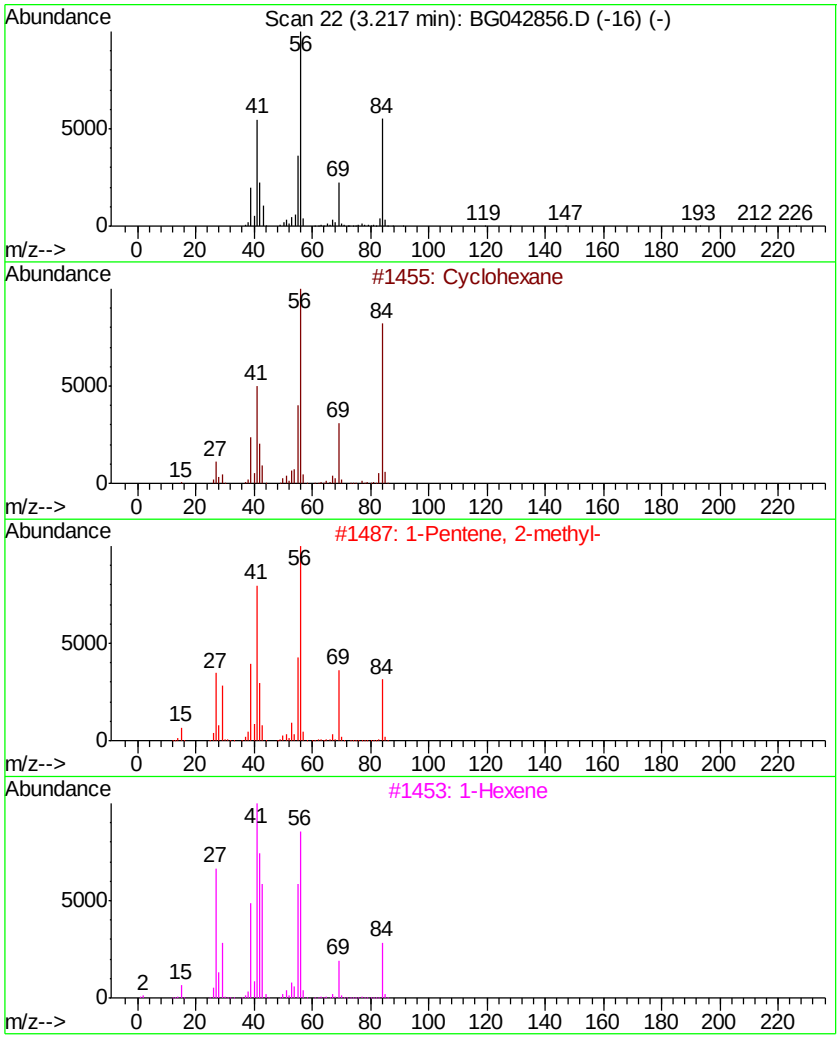
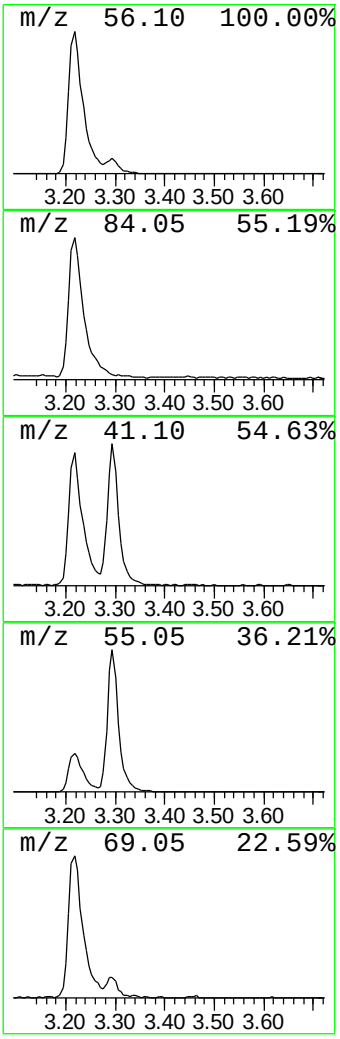
****

Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.22	42.08 ng	1337120	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	91
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	56
3	1-Hexene	84	C6H12	000592-41-6	53
4	2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	50
5	2,2-Dimethylglutaric anhydride	142	C7H10O3	002938-48-9	47





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Operator : HP/JU
Sample : K4866-01
Misc :
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Instrument : BNA_G
ClientSampleId : N48987

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG091219.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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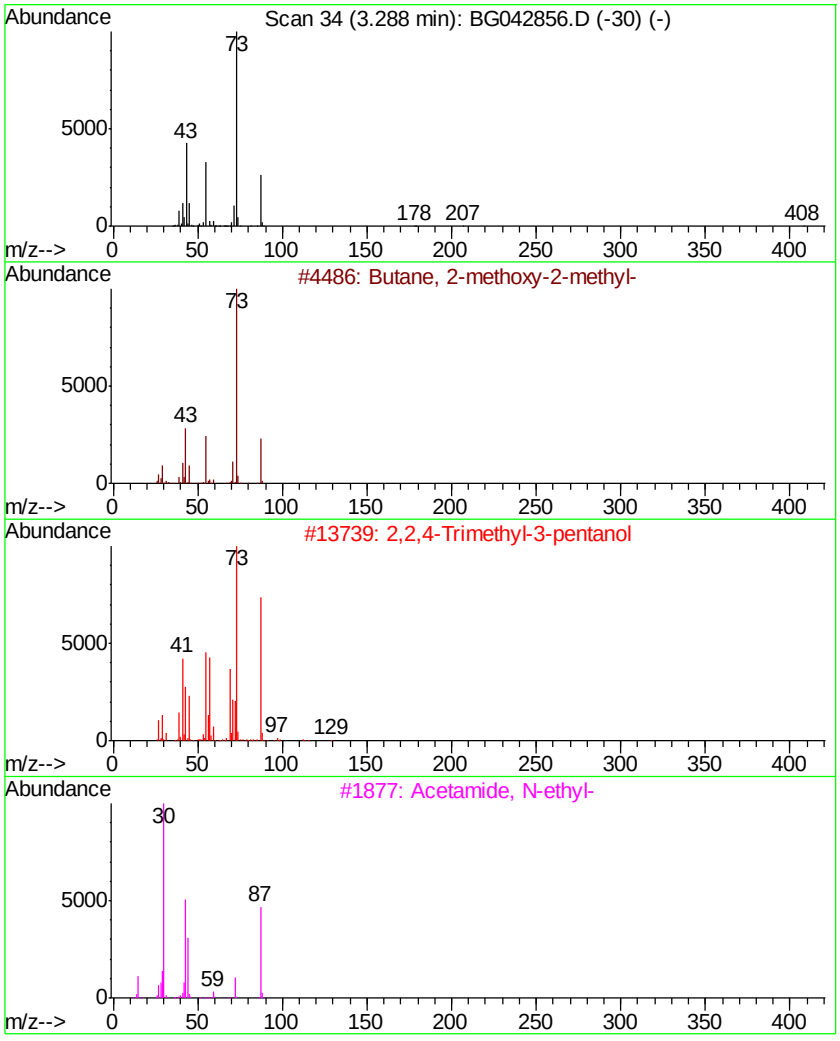
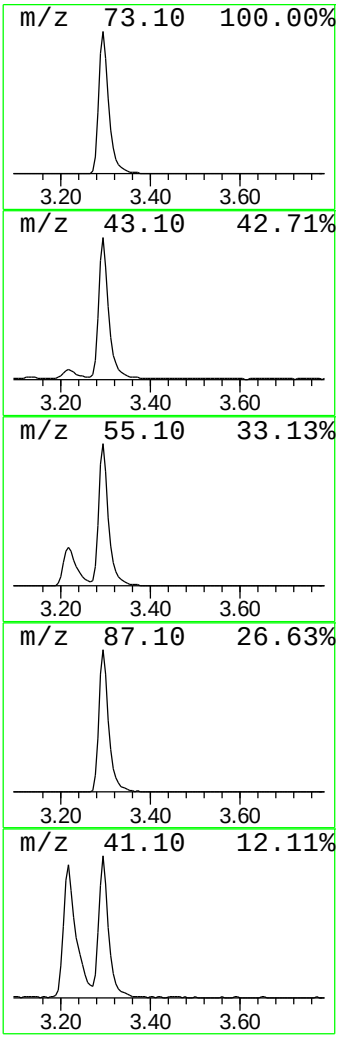
Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.29	101.70 ng	3231190	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	35
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Library Search Compound Report

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Misc :
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Instrument : BNA_G
ClientSampleId : N48987

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG091219.M
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TIC Library : C:\Database\NIST11.L
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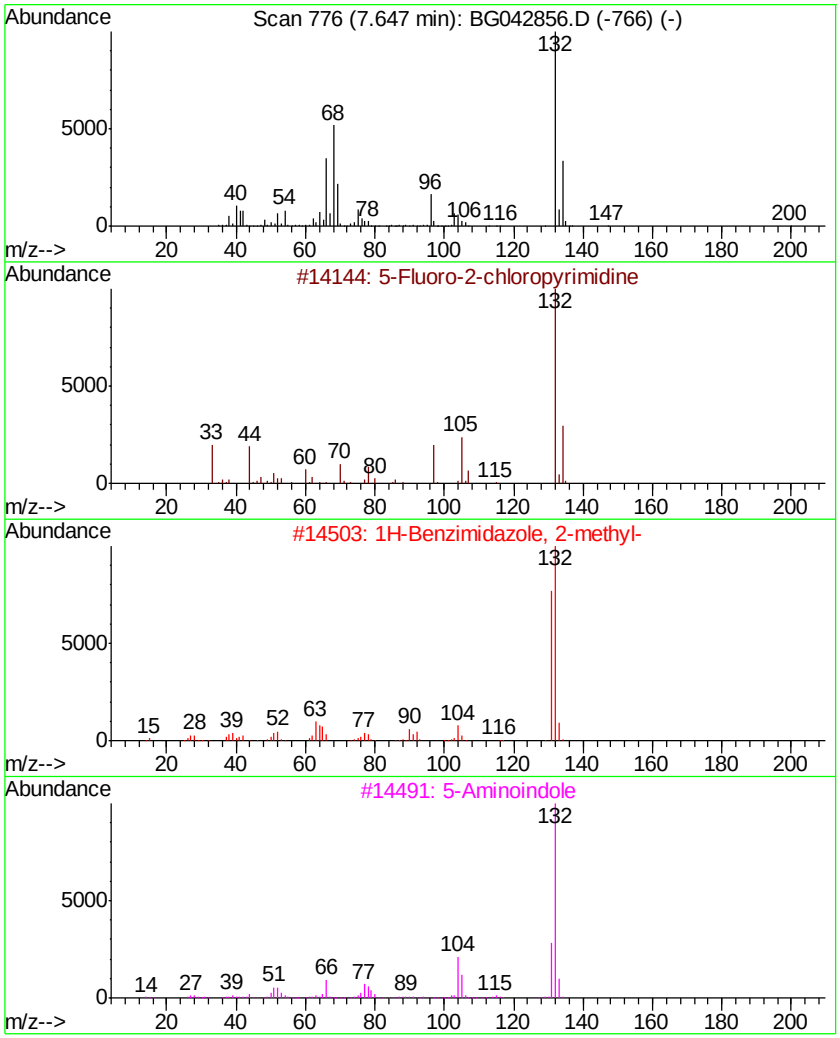
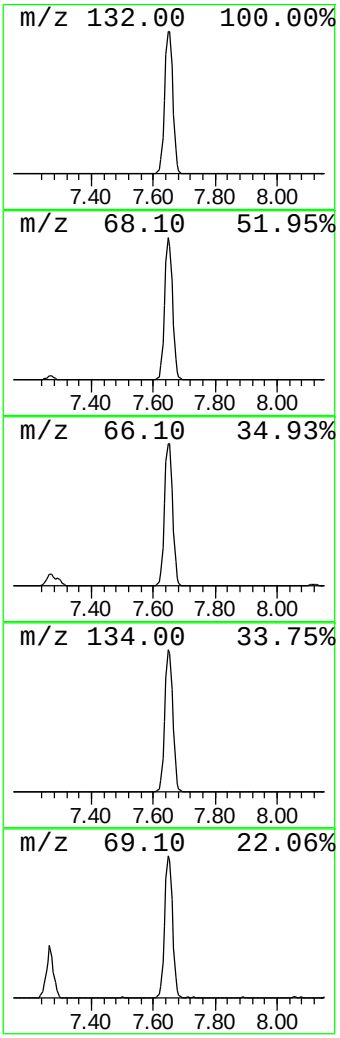
****

Peak Number 3 unknown7.65 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	90.60 ng	2878650	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Aminoindole	132	C8H8N2	005192-03-0	22
4	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091619\
Data File : BG042856.D
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Operator : HP/JU
Sample : K4866-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : N48987

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG091219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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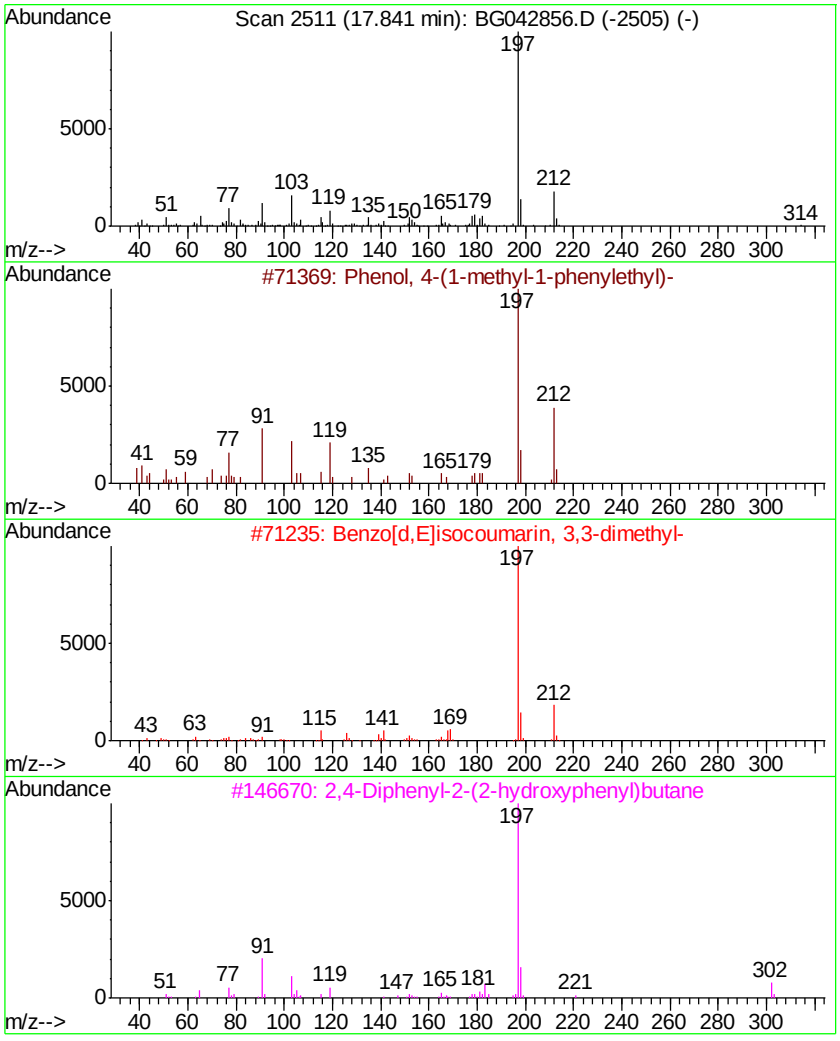
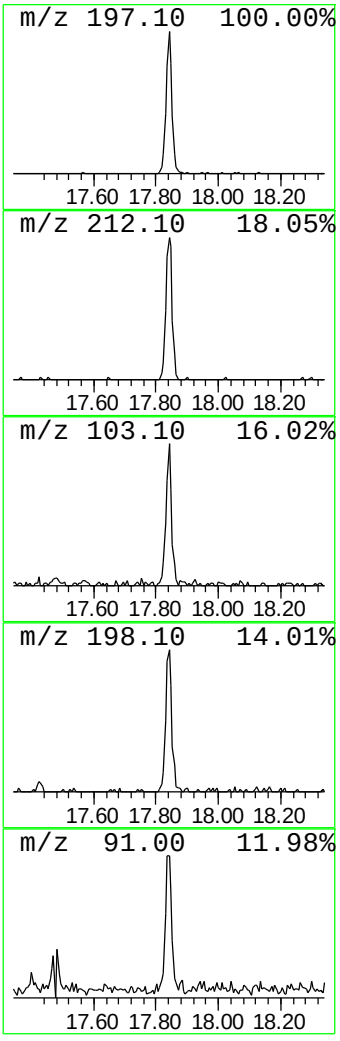
****

Peak Number 5 unknown17.84 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.84	3.67 ng	262701	Phenanthrene-d10	17.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1-methyl-1-phenylethyl)-	212	C15H16O	000599-64-4	64
2	Benzo[d,E]isocoumarin, 3,3-dimet...	212	C14H12O2	005723-17-1	64
3	2,4-Diphenyl-2-(2-hydroxyphenyl)...	302	C22H22O	1000280-74-0	64
4	Dimethyl diphenylsilane	212	C14H16Si	000778-24-5	64
5	2,3-Dimethyl-4-biphenylamine	197	C14H15N	022750-87-4	58





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091619\
Data File : BG042856.D
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Operator : HP/JU
Sample : K4866-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : N48987

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG091219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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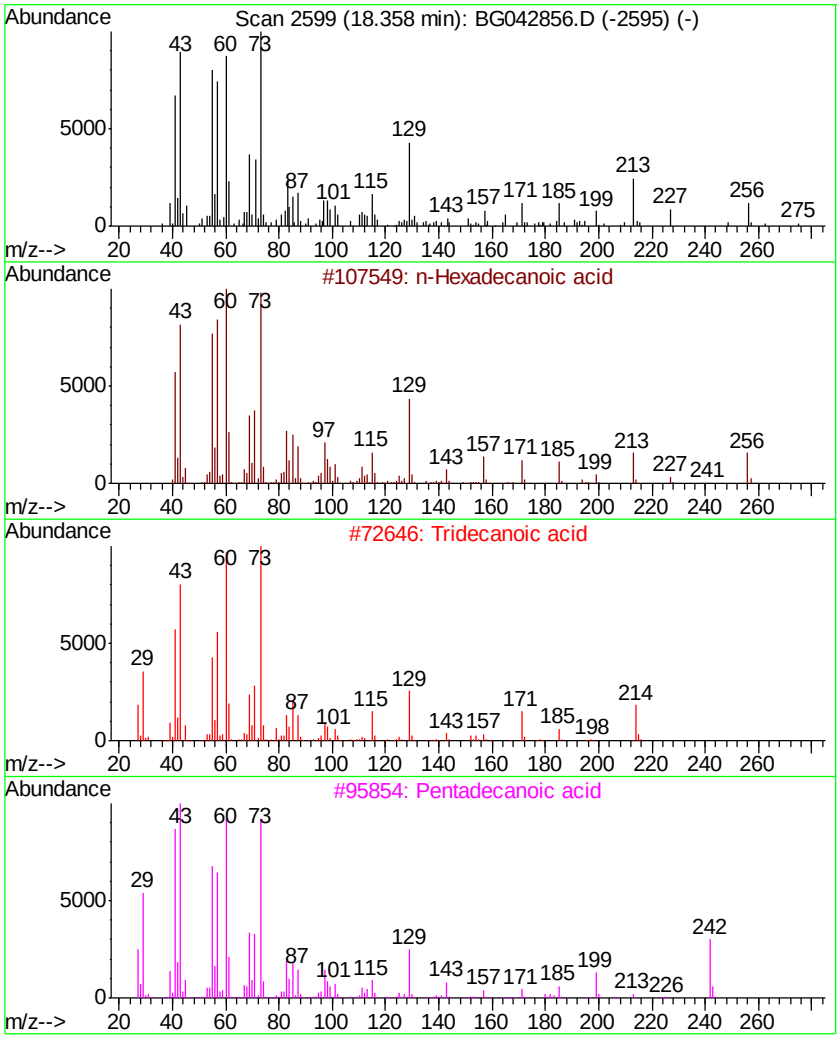
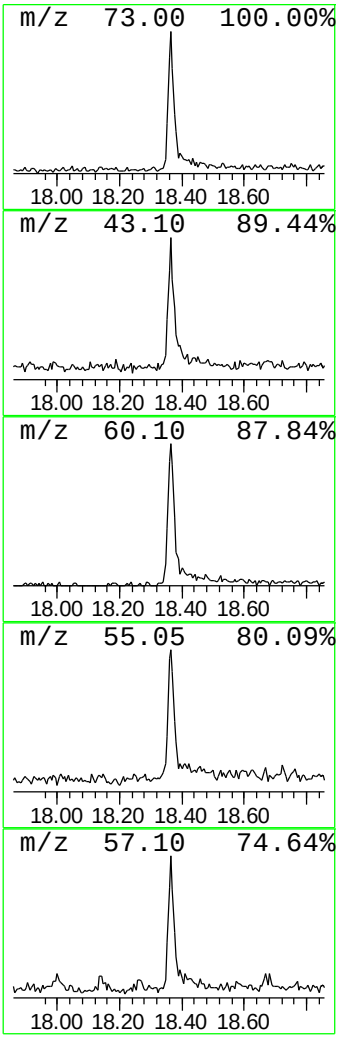
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	3.10 ng	221890	Phenanthrene-d10	17.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	14
5	Nonanoic acid	158	C9H18O2	000112-05-0	14





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091619\
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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : N48987

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG091219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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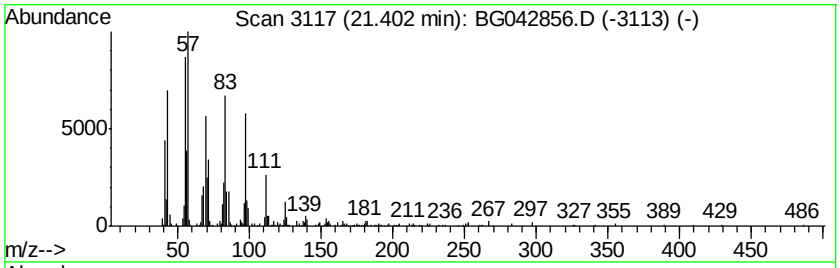
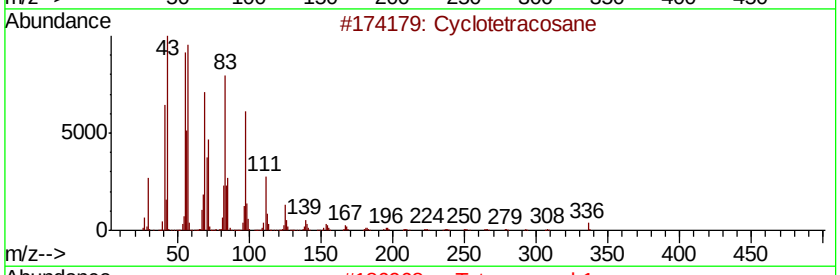
****

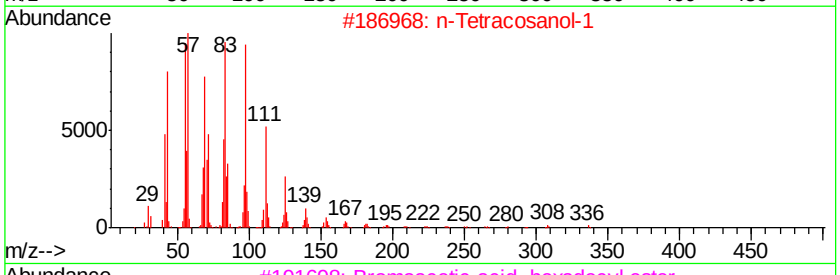
Peak Number 7 Cyclotetracosane Concentration Rank 9

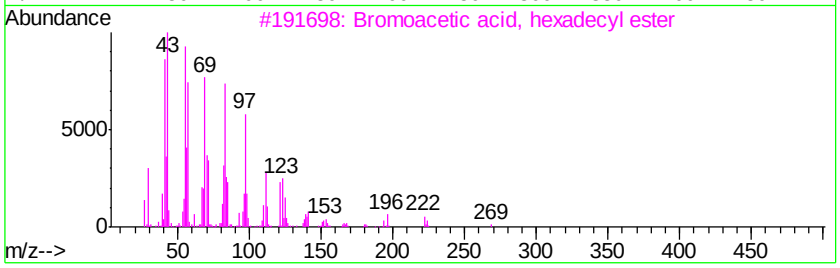
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.40	3.86 ng	308344	Chrysene-d12	21.75

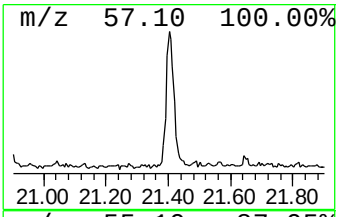
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
4	1-Heneicosanol	312	C21H44O	015594-90-8	91
5	1-Docosene	308	C22H44	001599-67-3	91

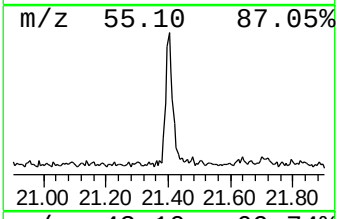


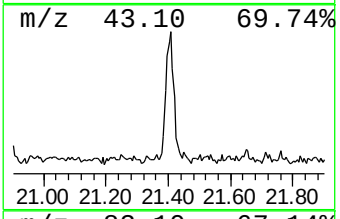


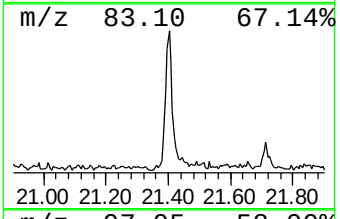


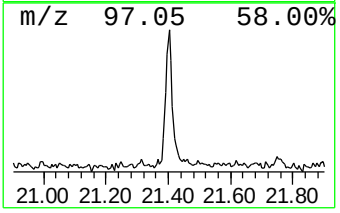












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

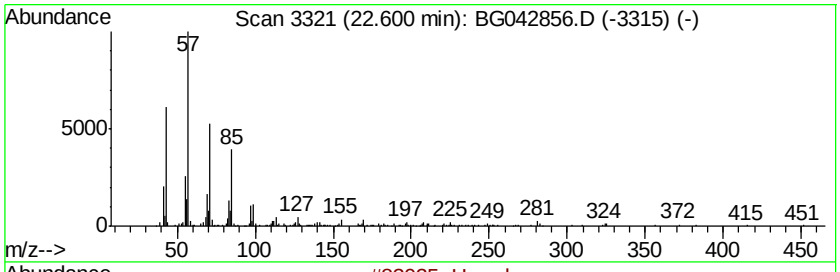
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

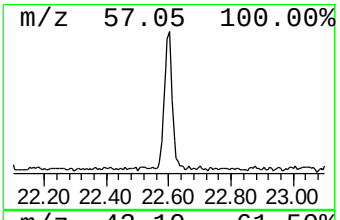
****

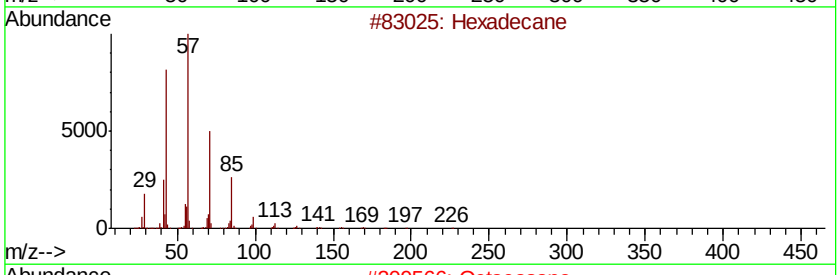
Peak Number 8 Hexadecane Concentration Rank 10

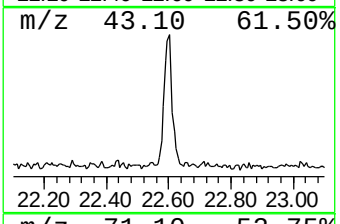
R.T.	EstConc	Area	Relative to ISTD	R.T.
22.60	3.74 ng	298687	Chrysene-d12	21.75

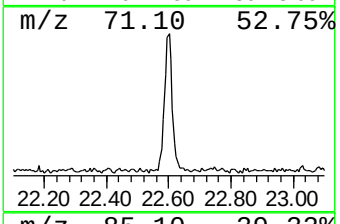
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	87
2	Octacosane	394	C28H58	000630-02-4	87
3	Tricosane	324	C23H48	000638-67-5	87
4	Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	86
5	Tetratetracontane	619	C44H90	007098-22-8	86

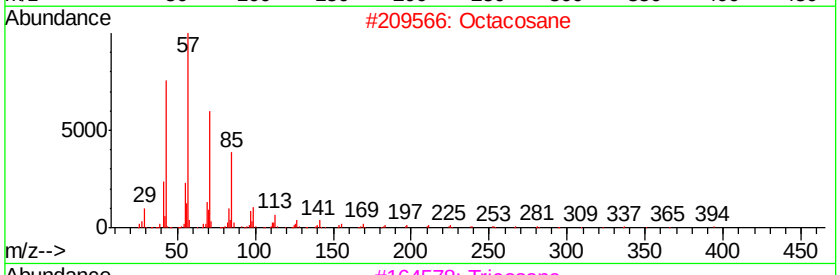


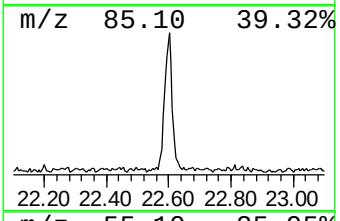


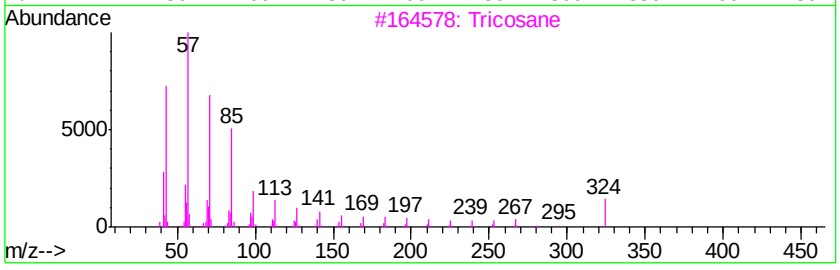


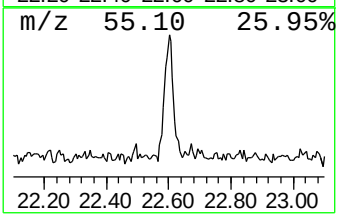












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091619\
Data File : BG042856.D
Acq On : 16 Sep 2019 19:50
Operator : HP/JU
Sample : K4866-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : N48987

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG091219.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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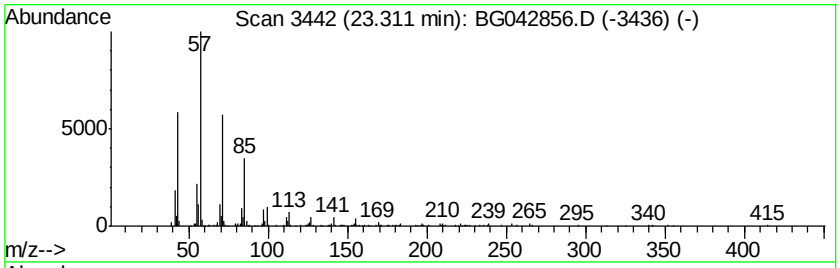
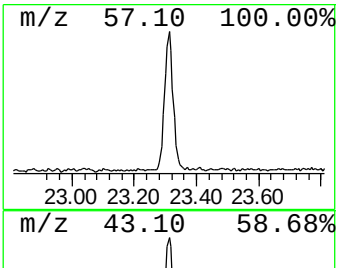
Peak Number 9 Hentriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.31	4.58 ng	366341	Chrysene-d12	21.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	87
2	Heptacosane	380	C27H56	000593-49-7	87
3	Pentacosane	352	C25H52	000629-99-2	87
4	Hexadecane	226	C16H34	000544-76-3	86
5	Undecane, 3,8-dimethyl-	184	C13H28	017301-30-3	86





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Acq On : 16 Sep 2019 19:50
Operator : HP/JU
Sample : K4866-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : N48987

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG091219.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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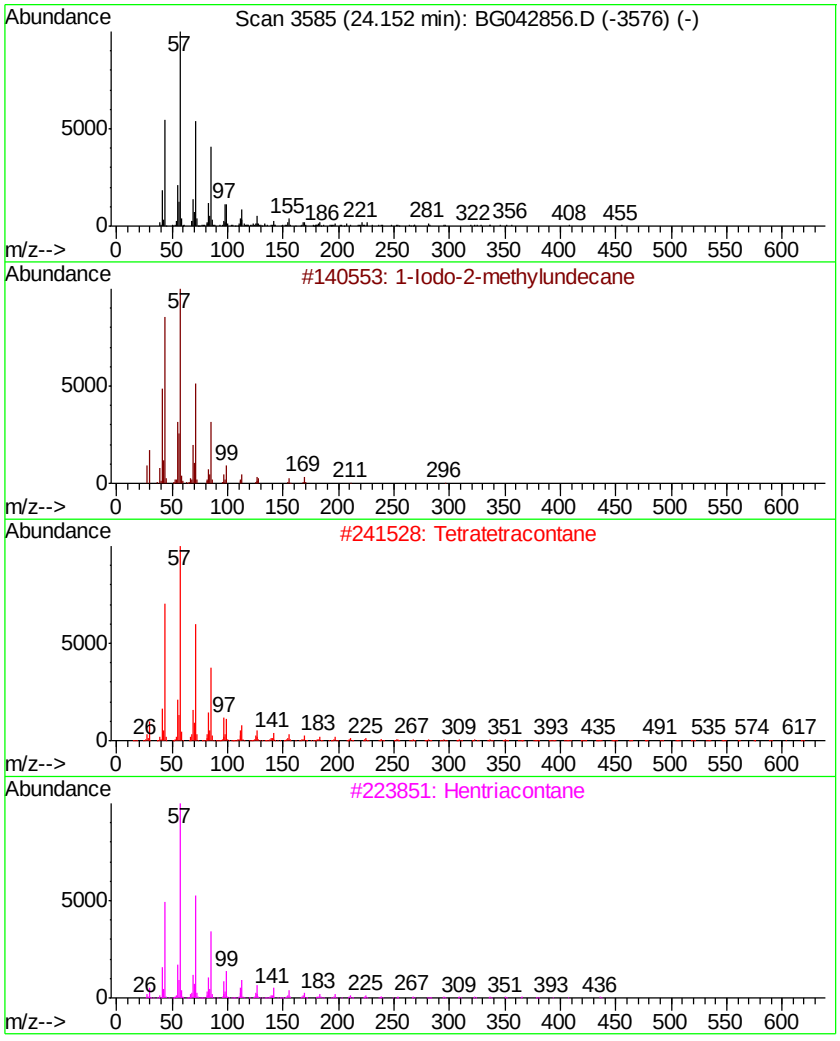
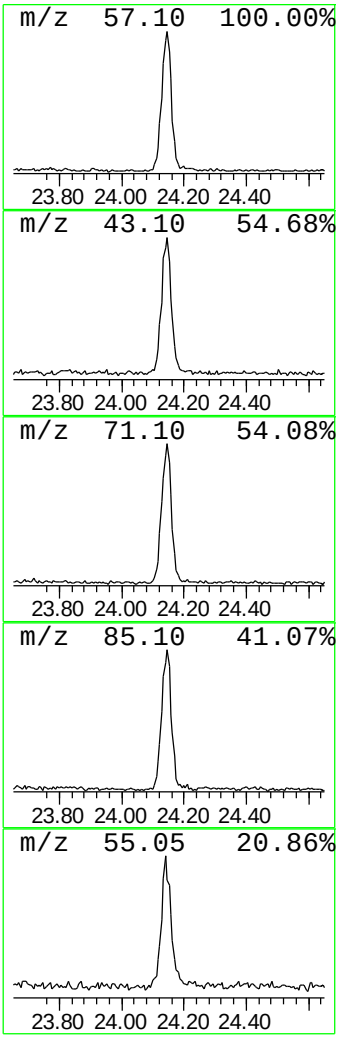
Peak Number 10 1-Iodo-2-methylundecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.15	6.01 ng	477407	Perylene-d12	25.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	93
2	Tetratetracontane	619	C44H90	007098-22-8	90
3	Hentriacontane	437	C31H64	000630-04-6	89
4	Eicosane	282	C20H42	000112-95-8	87
5	Tridecane, 2-methyl-	198	C14H30	001560-96-9	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091619\
Data File : BG042856.D
Acq On : 16 Sep 2019 19:50
Operator : HP/JU
Sample : K4866-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : N48987

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG091219.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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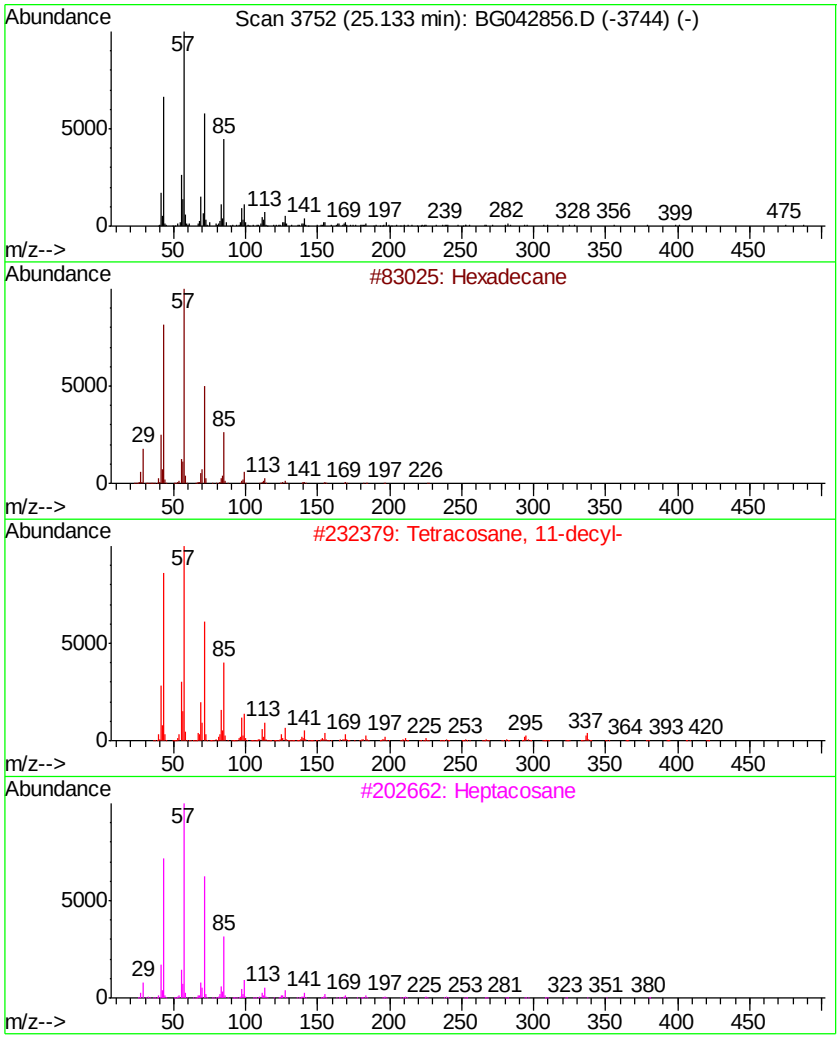
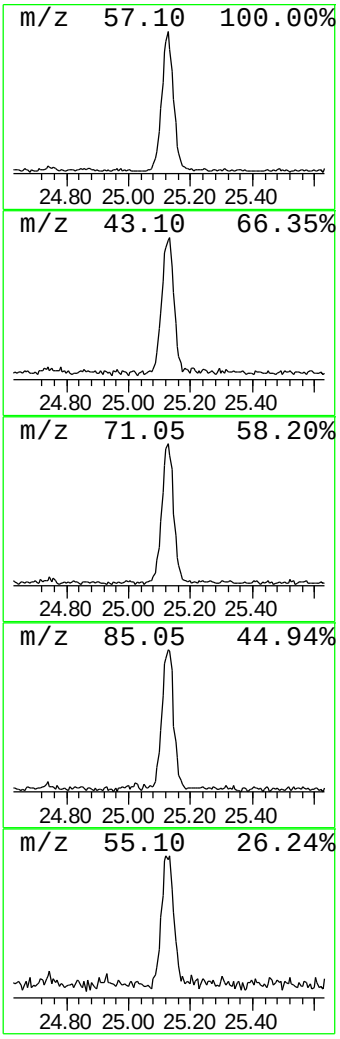
Peak Number 11 Tetracosane, 11-decyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.13	6.04 ng	479683	Perylene-d12	25.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	87
2	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	86
3	Heptacosane	380	C27H56	000593-49-7	83
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	80
5	1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	72





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Acq On : 16 Sep 2019 19:50
Operator : HP/JU
Sample : K4866-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : N48987

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG091219.M
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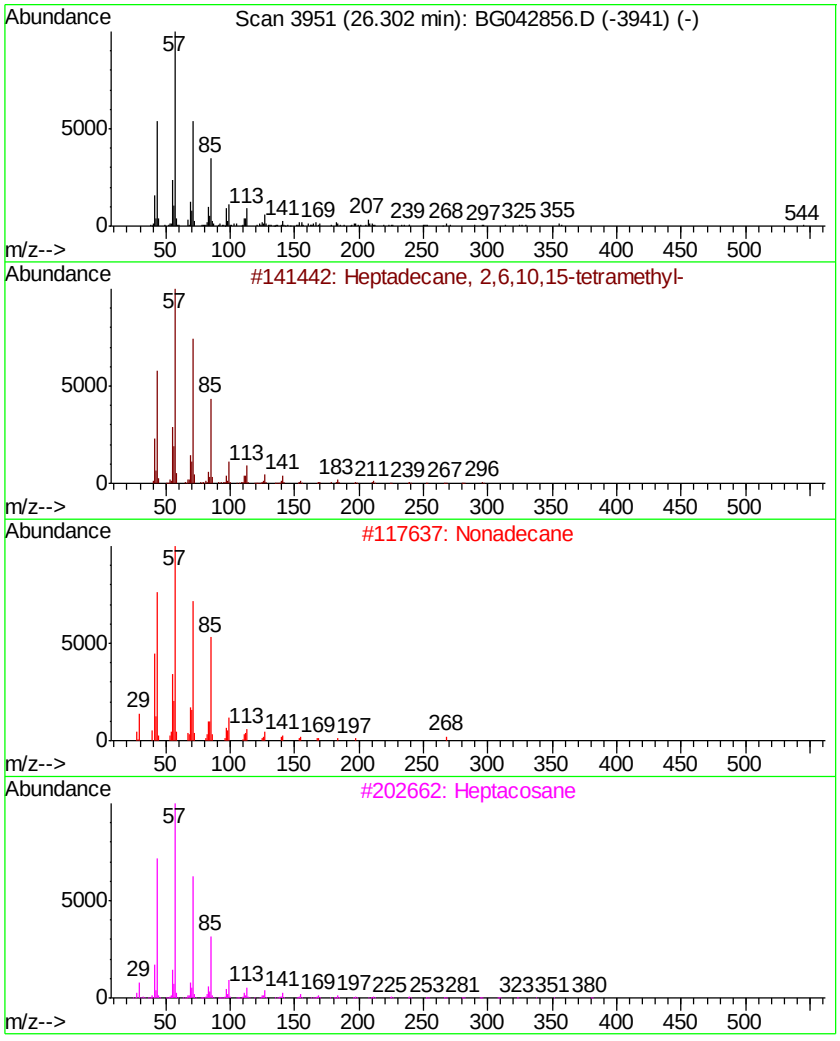
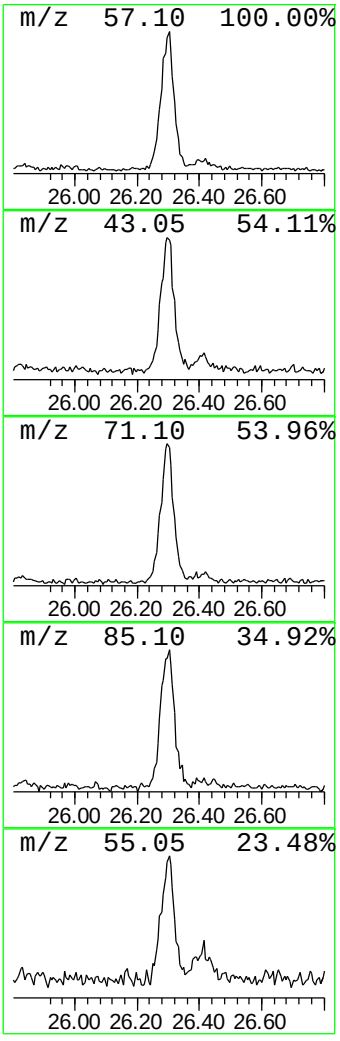
Peak Number 12 Heptadecane, 2,6,10,15-tetr... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.30	4.84 ng	384487	Perylene-d12	25.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	95
2	Nonadecane	268	C19H40	000629-92-5	89
3	Heptacosane	380	C27H56	000593-49-7	87
4	Hentriacontane	437	C31H64	000630-04-6	87
5	Octacosane	394	C28H58	000630-02-4	86





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Data File : BG042856.D
Acq On : 16 Sep 2019 19:50
Operator : HP/JU
Sample : K4866-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : N48987

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG091219.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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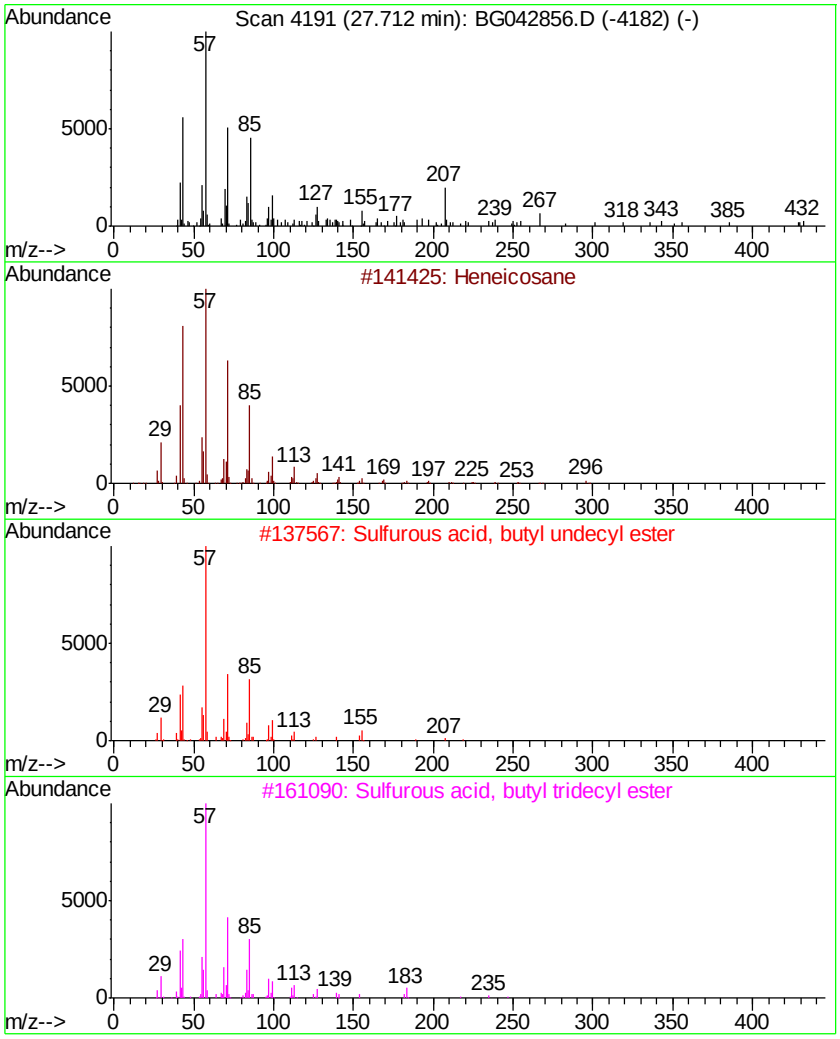
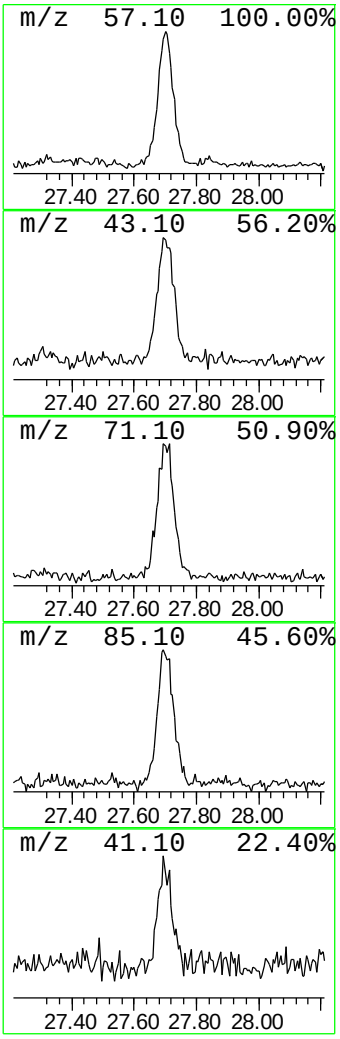
Peak Number 13 Sulfurous acid, butyl undec... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.71	2.48 ng	196585	Perylene-d12	25.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	72
3	Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	72
4	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	72
5	Eicosane, 2-methyl-	296	C21H44	001560-84-5	70





Library Search Compound Report

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Acq On : 16 Sep 2019 19:50
Operator : HP/JU
Sample : K4866-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : N48987

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG091219.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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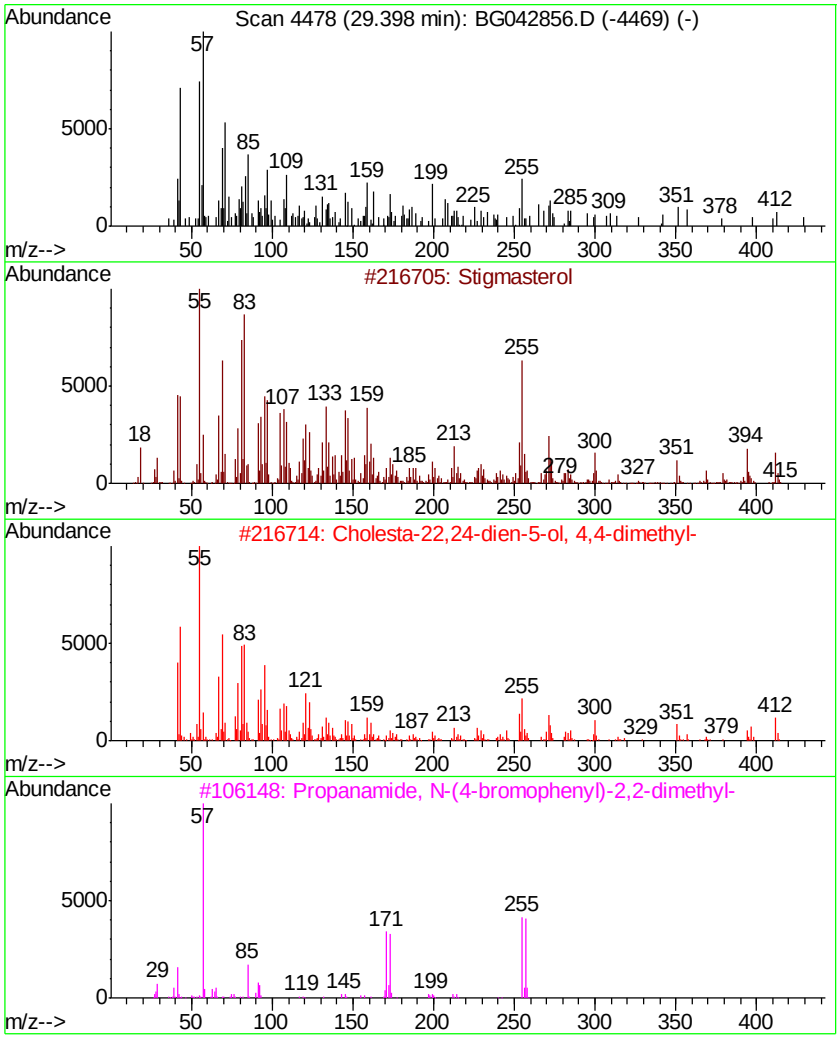
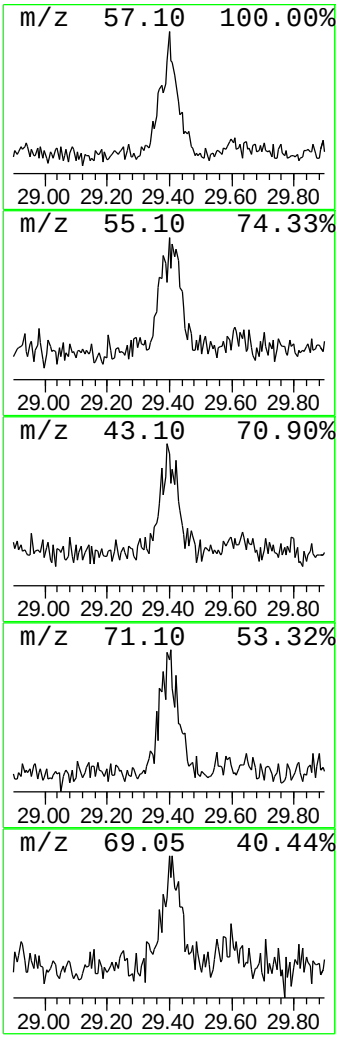
Peak Number 14 unknown29.40 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.40	2.19 ng	173929	Perylene-d12	25.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Stigmasterol	412	C29H48O	000083-48-7	49
2	Cholesta-22,24-dien-5-ol, 4,4-di...	412	C29H48O	1000128-66-1	10
3	Propanamide, N-(4-bromophenyl)-2...	255	C11H14BrNO	024109-06-6	9
4	(Tetra-t-butoxycyclopentadienone...	508	C24H36FeO8	117696-74-9	9
5	1,6-Bis[methyl(tetramethylene)si...	314	C16H34O2Si2	1000217-00-0	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG091619\
Data File : BG042856.D
Acq On : 16 Sep 2019 19:50
Operator : HP/JU
Sample : K4866-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : N48987

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG091219.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
1-Pentene, 2-methyl-	3.22	42.1	ng	1337120	1	8.12	635455	20.0
Butane, 2-methoxy...	3.29	101.7	ng	3231190	1	8.12	635455	20.0
unknown7.65	7.65	90.6	ng	2878650	1	8.12	635455	20.0
unknown17.84	17.84	3.7	ng	262701	4	17.48	1432200	20.0
n-Hexadecanoic acid	18.36	3.1	ng	221890	4	17.48	1432200	20.0
Cyclotetracosane	21.40	3.9	ng	308344	5	21.75	1598540	20.0
Hexadecane	22.60	3.7	ng	298687	5	21.75	1598540	20.0
Hentriacontane	23.31	4.6	ng	366341	5	21.75	1598540	20.0
1-Iodo-2-methylun...	24.15	6.0	ng	477407	6	25.03	1587740	20.0
Tetracosane, 11-d...	25.13	6.0	ng	479683	6	25.03	1587740	20.0
Heptadecane, 2,6,...	26.30	4.8	ng	384487	6	25.03	1587740	20.0
Sulfurous acid, b...	27.71	2.5	ng	196585	6	25.03	1587740	20.0
unknown29.40	29.40	2.2	ng	173929	6	25.03	1587740	20.0