LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG081018\
Data File : BG036290.D
Acq On : 11 Aug 2018 6:33
Operator : JU/SJ
Sample : J4412-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 080718-TIPC-E-D-M

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-BG071218.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	5.598	387	393	410	rBV	146994	284802	11.36%	2.904%
2	7.184	657	663	674	rBV	88458	193940	7.73%	1.977%
3	7.543	712	724	739	rBV	283279	528470	21.07%	5.388%
4	8.007	797	803	811	rBV2	88860	156284	6.23%	1.593%
5	8.330	849	858	868	rBV	388580	699079	27.87%	7.128%
6	9.170	992	1001	1017	rBV	303121	624822	24.91%	6.371%
7	10.809	1274	1280	1293	rBV	85014	182752	7.29%	1.863%
8	13.253	1688	1696	1709	rBV	877982	1450012	57.81%	14.784%
9	14.099	1833	1840	1850	rBV3	13648	33520	1.34%	0.342%
10	14.633	1925	1931	1946	rVB2	173160	315447	12.58%	3.216%
11	15.920	2143	2150	2156	rBV	75298	106098	4.23%	1.082%
12	16.119	2177	2184	2198	rBV	456444	811935	32.37%	8.278%
13	17.377	2391	2398	2413	rBV	245605	425183	16.95%	4.335%
14	19.985	2835	2842	2854	rBV	1845102	2508059	100.00%	25.572%
15	20.772	2972	2976	2980	rBV3	21900	25307	1.01%	0.258%
16	21.271	3057	3061	3066	rBV3	27686	33238	1.33%	0.339%
17	21.635	3116	3123	3132	rBV	247824	475274	18.95%	4.846%
18	21.812	3149	3153	3157	rVB3	33242	49766	1.98%	0.507%
19	22.411	3249	3255	3260	rBV3	32126	55893	2.23%	0.570%
20	23.086	3365	3370	3379	rVB3	37050	63989	2.55%	0.652%
21	23.280	3397	3403	3408	rVB	36388	66540	2.65%	0.678%
22	23.874	3496	3504	3511	rBV4	36746	81749	3.26%	0.834%
23	24.819	3653	3665	3684	rBV2	138593	524837	20.93%	5.351%
24	25.912	3844	3851	3859	rVB5	23937	64591	2.58%	0.659%
25	27.234	4068	4076	4083	rBV6	15361	46324	1.85%	0.472%

Sum of corrected areas: 9807911

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG081018\
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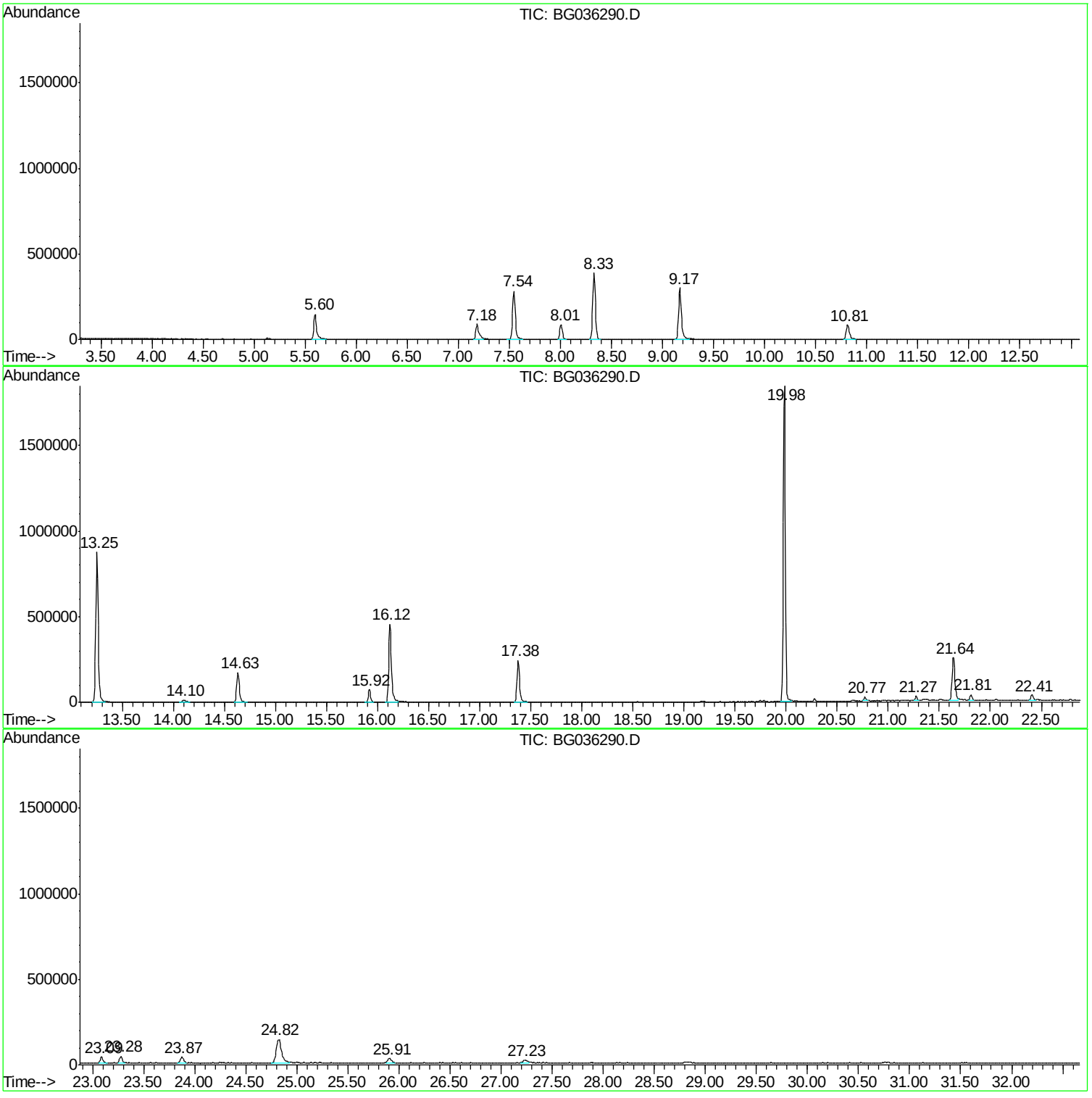
Sample : J4412-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
080718-TIPC-E-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.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\BG081018\
Data File : BG036290.D
Acq On : 11 Aug 2018 6:33
Operator : JU/SJ
Sample : J4412-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 080718-TIPC-E-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

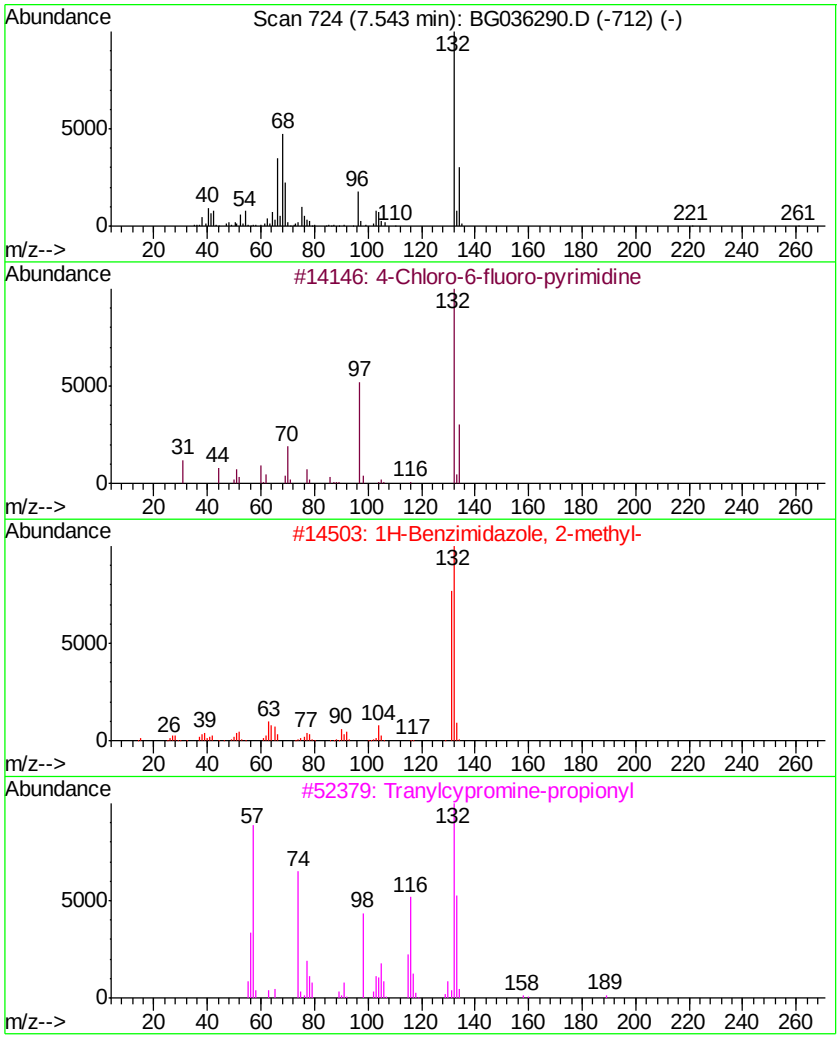
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

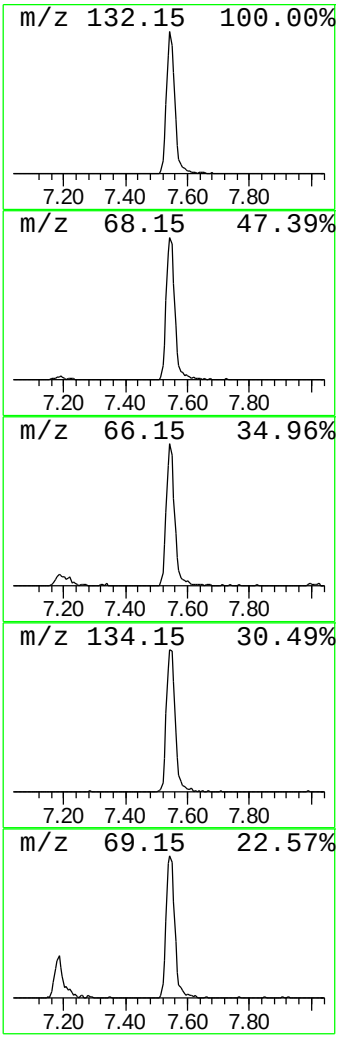
****

Peak Number 1 unknown7.54 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.54	67.63 ng	528470	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG081018\
Data File : BG036290.D
Acq On : 11 Aug 2018 6:33
Operator : JU/SJ
Sample : J4412-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 080718-TIPC-E-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.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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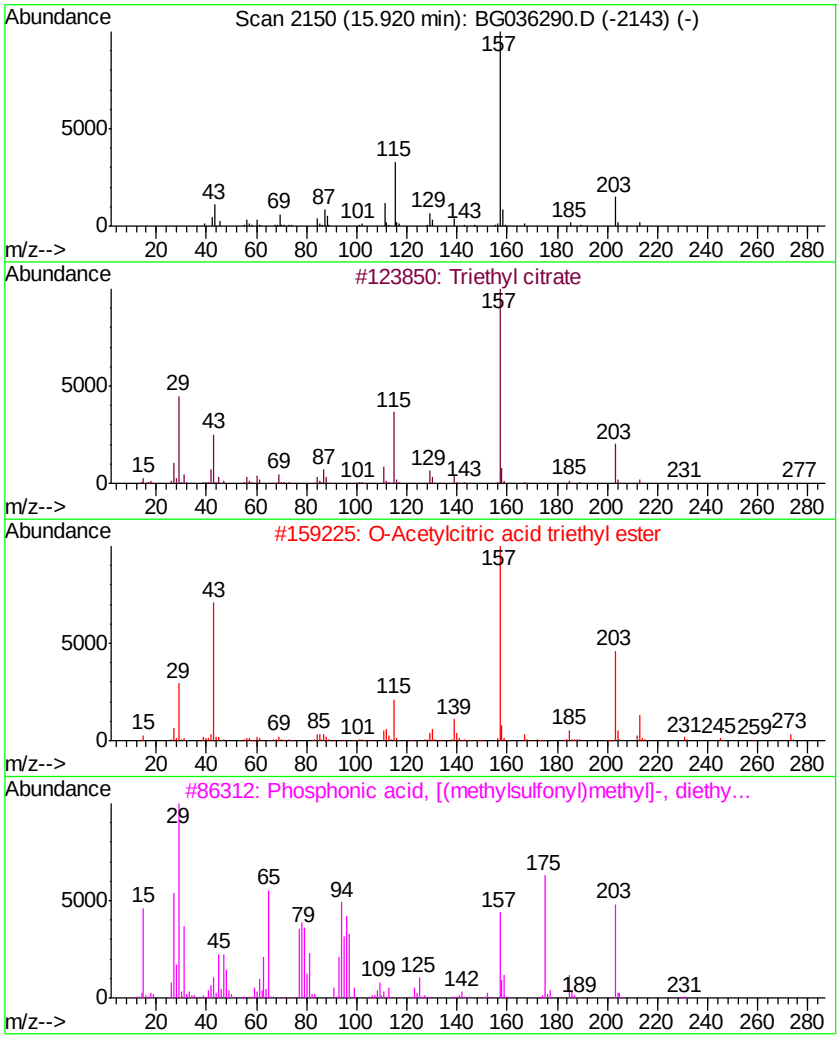
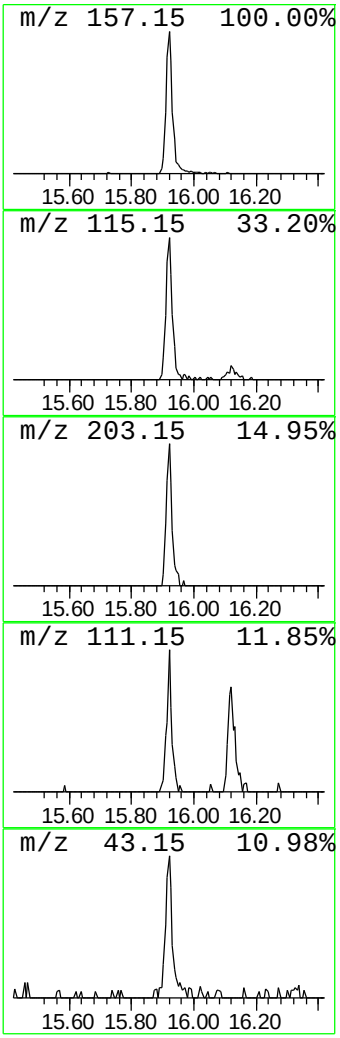
Peak Number 3 Triethyl citrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.92	6.73 ng	106098	Acenaphthene-d10	14.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	86
2	O-Acetylcitric acid triethyl ester	318	C14H22O8	000077-89-4	64
3	Phosphonic acid, [(methylsulfony...	230	C6H15O5PS	040137-11-9	47
4	1-Amino-2-methylnaphthalene	157	C11H11N	002246-44-8	40
5	2-Chlorobenzoic acid, pentadecyl...	366	C22H35ClO2	1000292-43-0	40





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG081018\
Data File : BG036290.D
Acq On : 11 Aug 2018 6:33
Operator : JU/SJ
Sample : J4412-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 080718-TIPC-E-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.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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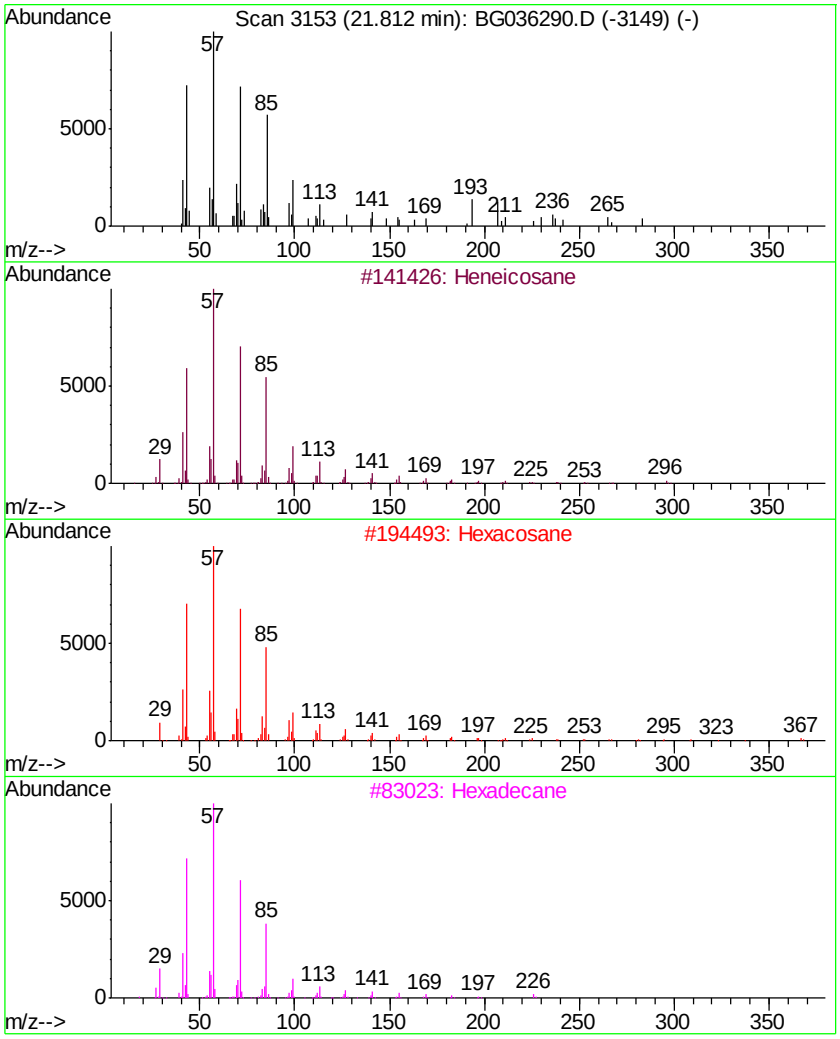
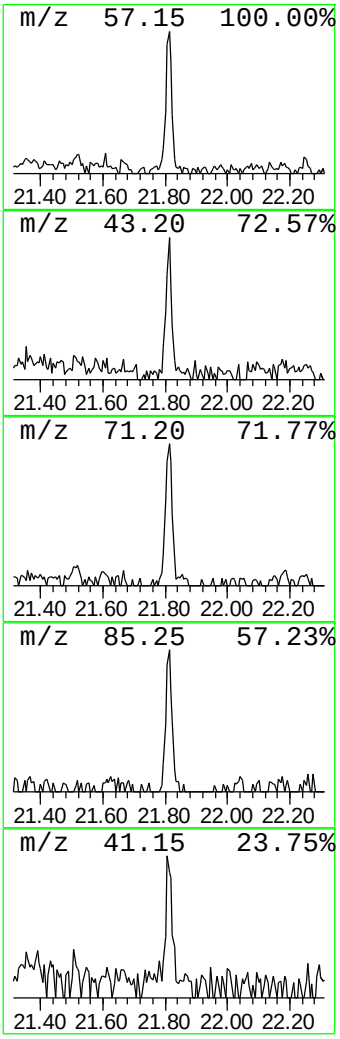
Peak Number 4 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.81	2.09 ng	49766	Chrysene-d12	21.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	70
2	Hexacosane	366	C26H54	000630-01-3	64
3	Hexadecane	226	C16H34	000544-76-3	64
4	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	58
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	58





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG081018\
Data File : BG036290.D
Acq On : 11 Aug 2018 6:33
Operator : JU/SJ
Sample : J4412-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 080718-TIPC-E-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.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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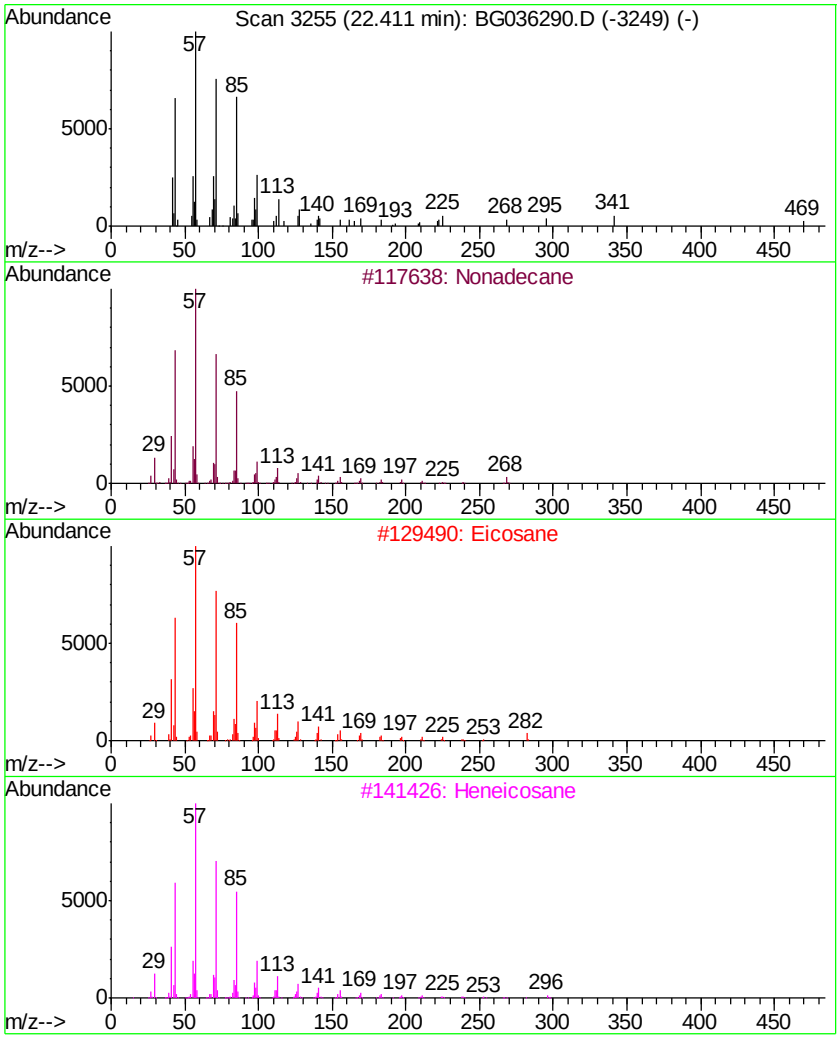
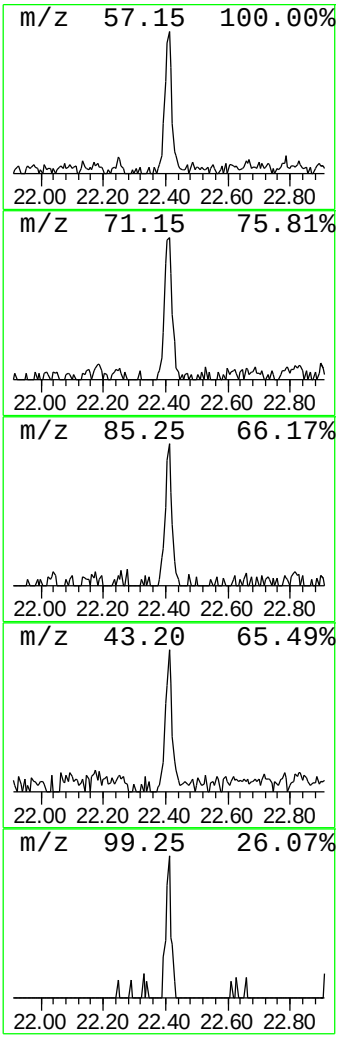
Peak Number 5 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.41	2.35 ng	55893	Chrysene-d12	21.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	87
2	Eicosane	282	C20H42	000112-95-8	86
3	Heneicosane	296	C21H44	000629-94-7	86
4	Heptadecane	240	C17H36	000629-78-7	86
5	Tetracosane	338	C24H50	000646-31-1	72





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG081018\
Data File : BG036290.D
Acq On : 11 Aug 2018 6:33
Operator : JU/SJ
Sample : J4412-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
080718-TIPC-E-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.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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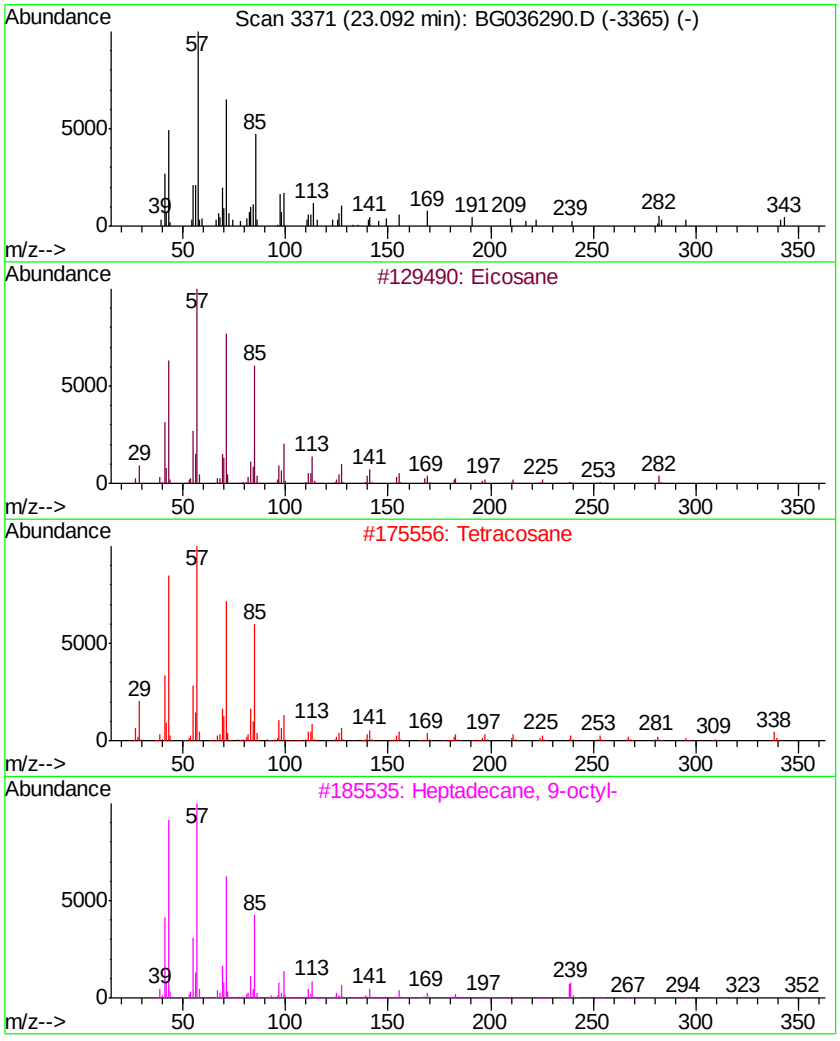
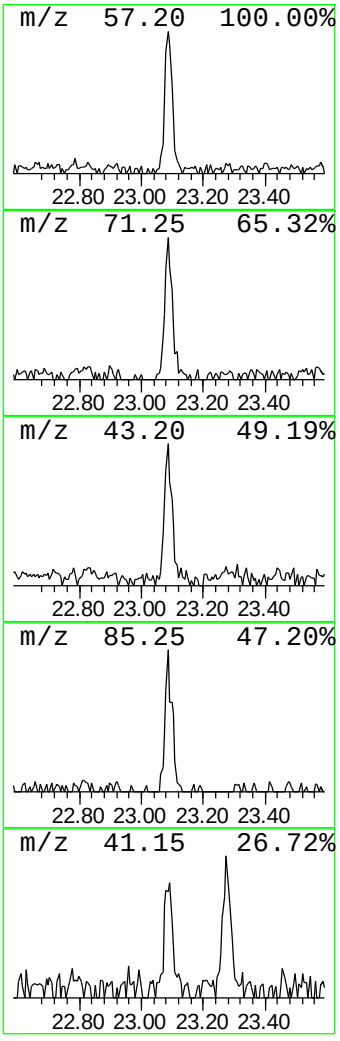
Peak Number 6 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.09	2.69 ng	63989	Chrysene-d12	21.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Tetracosane	338	C24H50	000646-31-1	80
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	80
5	Hexacosane	366	C26H54	000630-01-3	80





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG081018\
Data File : BG036290.D
Acq On : 11 Aug 2018 6:33
Operator : JU/SJ
Sample : J4412-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 080718-TIPC-E-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.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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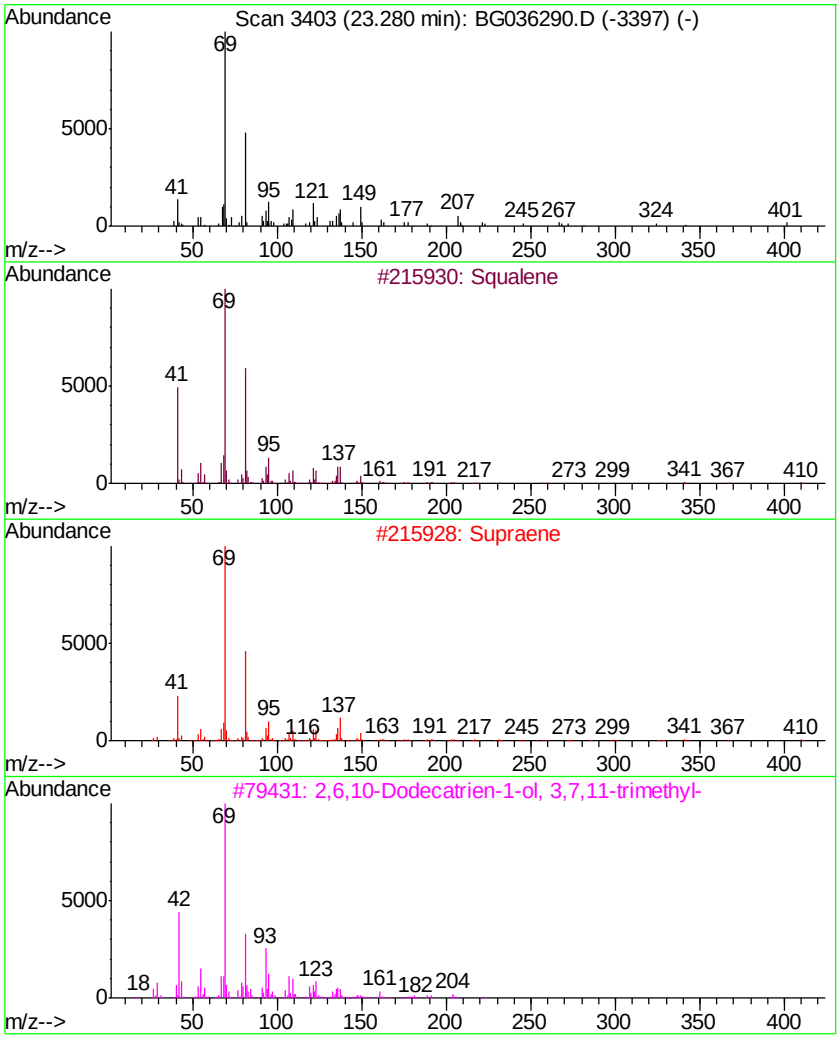
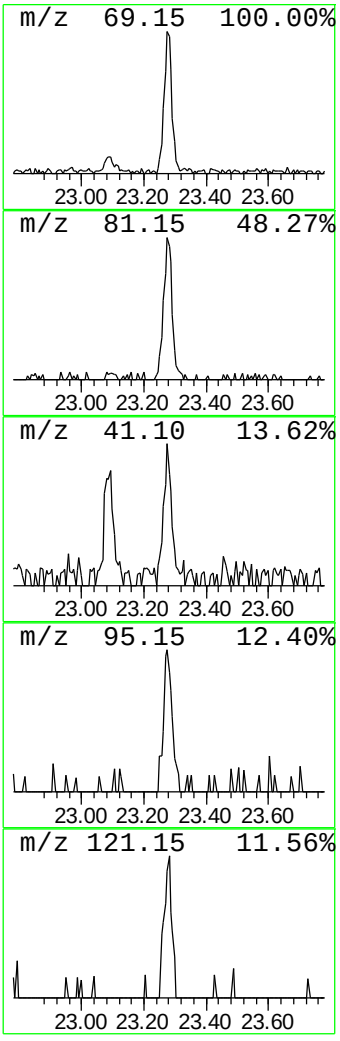
Peak Number 7 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.28	2.54 ng	66540	Perylene-d12	24.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	74
2	Supraene	410	C30H50	007683-64-9	72
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	59
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	59
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	59





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG081018\
Data File : BG036290.D
Acq On : 11 Aug 2018 6:33
Operator : JU/SJ
Sample : J4412-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
080718-TIPC-E-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.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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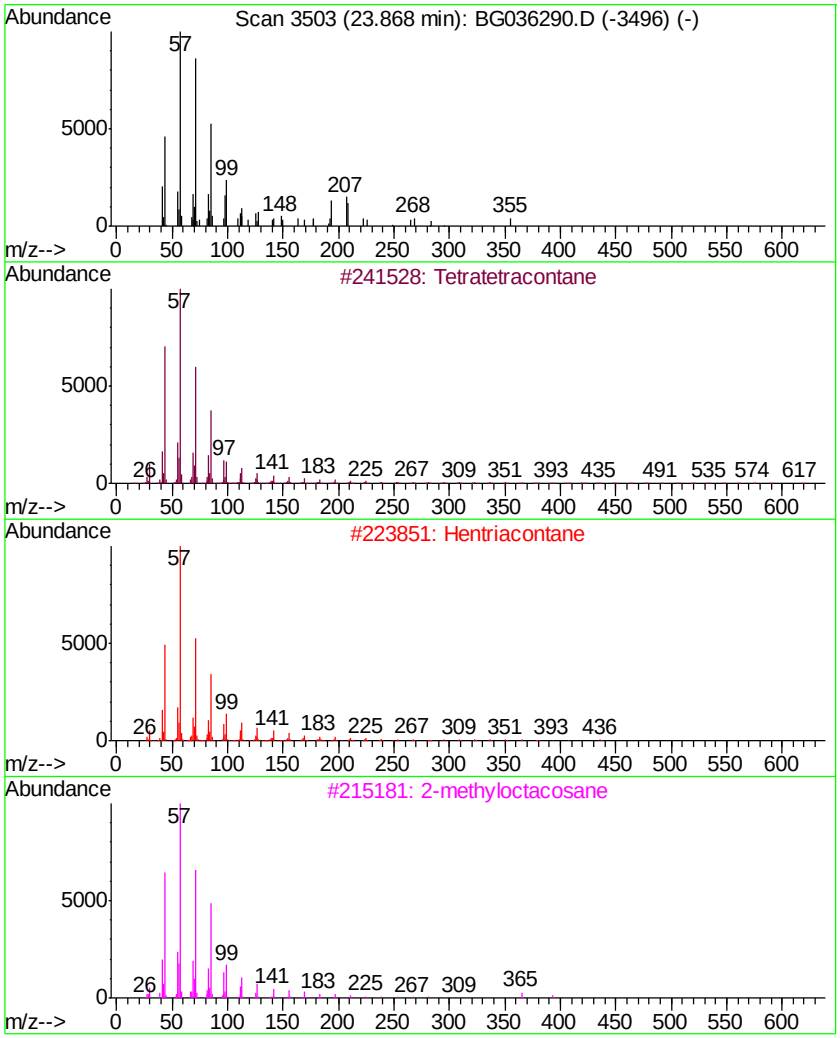
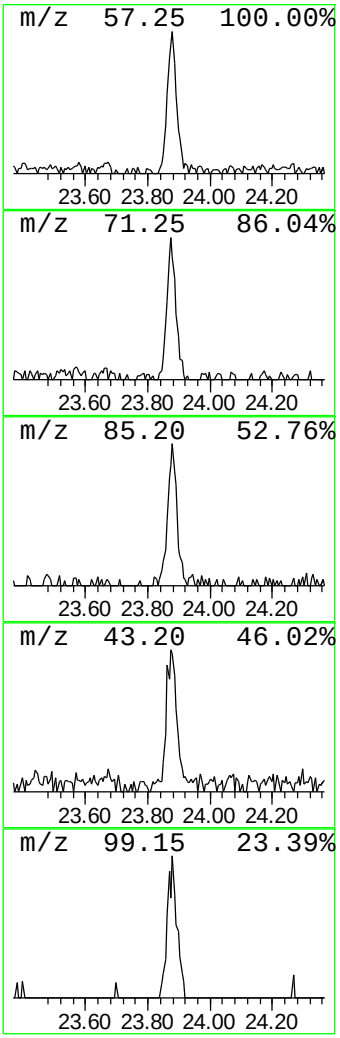
Peak Number 8 Tetratetracontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.87	3.12 ng	81749	Perylene-d12	24.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	87
2	Hentriacontane	437	C31H64	000630-04-6	86
3	2-methyloctacosane	408	C29H60	1000376-72-8	86
4	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	80
5	5,5-Diethylpentadecane	268	C19H40	1000360-41-0	72





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Sample : J4412-01
Misc :
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Instrument : BNA_G
ClientSampleId : 080718-TIPC-E-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

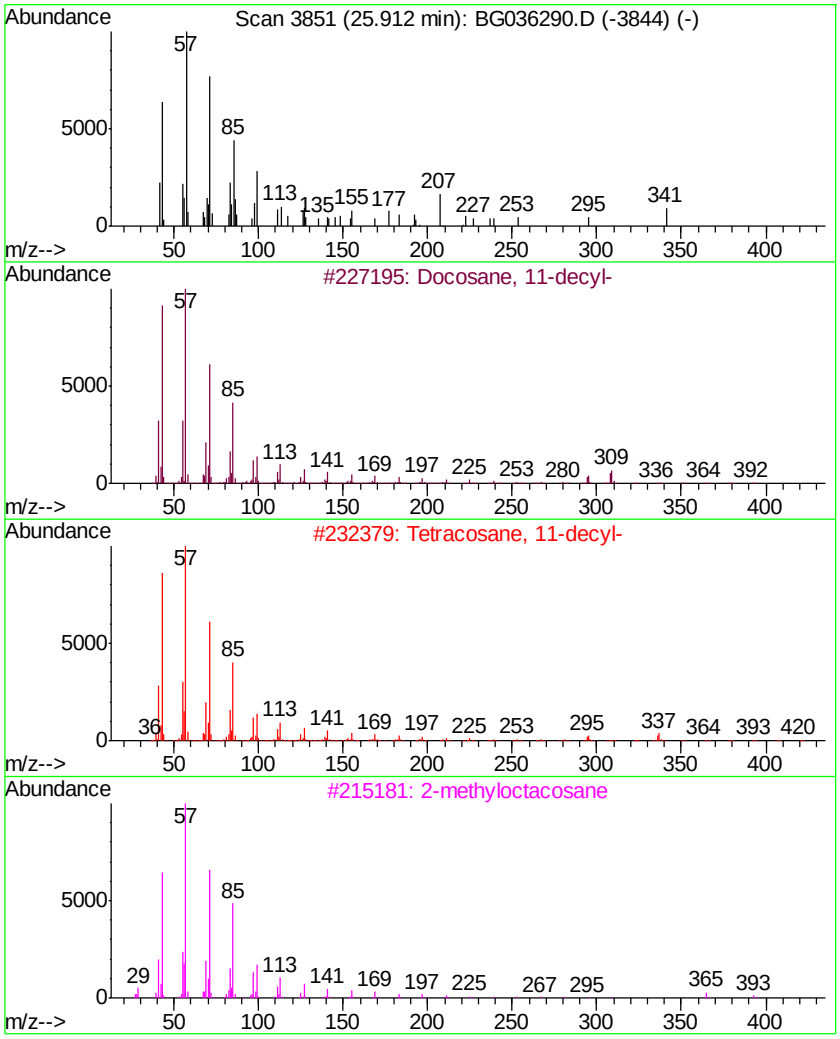
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

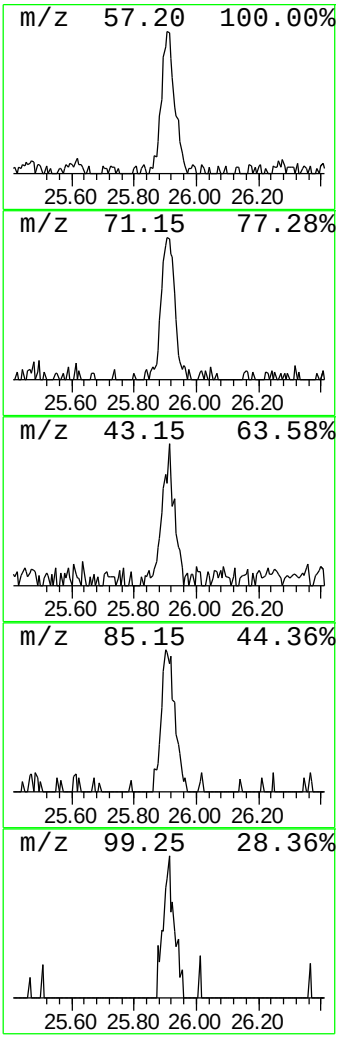
****

Peak Number 9 Docosane, 11-decyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.91	2.46 ng	64591	Perylene-d12	24.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 11-decyl-	451	C32H66	055401-55-3	64
2	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	64
3	2-methyloctacosane	408	C29H60	1000376-72-8	58
4	Tricosane	324	C23H48	000638-67-5	58
5	Tetracosane	338	C24H50	000646-31-1	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG081018\
Data File : BG036290.D
Acq On : 11 Aug 2018 6:33
Operator : JU/SJ
Sample : J4412-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 080718-TIPC-E-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.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
unknown7.54	7.54	67.6	ng	528470	1	8.01	156284	20.0
Triethyl citrate	15.92	6.7	ng	106098	3	14.63	315447	20.0
Heneicosane	21.81	2.1	ng	49766	5	21.64	475274	20.0
Nonadecane	22.41	2.4	ng	55893	5	21.64	475274	20.0
Eicosane	23.09	2.7	ng	63989	5	21.64	475274	20.0
Squalene	23.28	2.5	ng	66540	6	24.83	524837	20.0
Tetratetracontane	23.87	3.1	ng	81749	6	24.83	524837	20.0
Docosane, 11-decyl-	25.91	2.5	ng	64591	6	24.83	524837	20.0