LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG072618\
Data File : BG035928.D
Acq On : 27 Jul 2018 3:40
Operator : JU/SJ
Sample : J4160-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 072418-TIPC-F-U-S

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	5.605	388	394	409	rBV	215361	378773	10.12%	2.413%
2	7.191	654	664	679	rBV2	150204	297164	7.94%	1.893%
3	7.561	719	727	743	rBV	403367	725276	19.38%	4.621%
4	8.025	800	806	816	rBV	131470	221859	5.93%	1.413%
5	8.348	852	861	875	rBV	574538	994997	26.58%	6.339%
6	9.188	996	1004	1014	rBV	452907	858463	22.93%	5.469%
7	10.827	1276	1283	1295	rBV	145978	300569	8.03%	1.915%
8	13.271	1692	1699	1712	rBV	1465912	2276167	60.81%	14.501%
9	14.099	1833	1840	1856	rBV	88845	162044	4.33%	1.032%
10	14.646	1926	1933	1944	rBV3	304010	531490	14.20%	3.386%
11	15.938	2148	2153	2158	rBV	40440	54715	1.46%	0.349%
12	16.138	2180	2187	2203	rBV	791719	1295093	34.60%	8.251%
13	17.389	2394	2400	2409	rBV2	461918	753899	20.14%	4.803%
14	19.997	2838	2844	2855	rBV	2772587	3743061	100.00%	23.846%
15	20.297	2889	2895	2899	rBV2	49988	60401	1.61%	0.385%
16	20.790	2975	2979	2982	rBV	83635	88627	2.37%	0.565%
17	21.290	3060	3064	3069	rBV	97045	132990	3.55%	0.847%
18	21.654	3119	3126	3136	rBV	535880	897547	23.98%	5.718%
19	21.836	3150	3157	3168	rBV	108247	169060	4.52%	1.077%
20	22.441	3254	3260	3265	rBV2	100741	166228	4.44%	1.059%
21	23.122	3370	3376	3383	rBV2	102807	188068	5.02%	1.198%
22	23.916	3504	3511	3518	rBV2	88432	180288	4.82%	1.149%
23	24.850	3660	3670	3689	rVB2	349697	985611	26.33%	6.279%
24	25.966	3850	3860	3871	rBV4	51867	150094	4.01%	0.956%
25	27.311	4081	4089	4098	rVB9	27992	84116	2.25%	0.536%

Sum of corrected areas: 15696600

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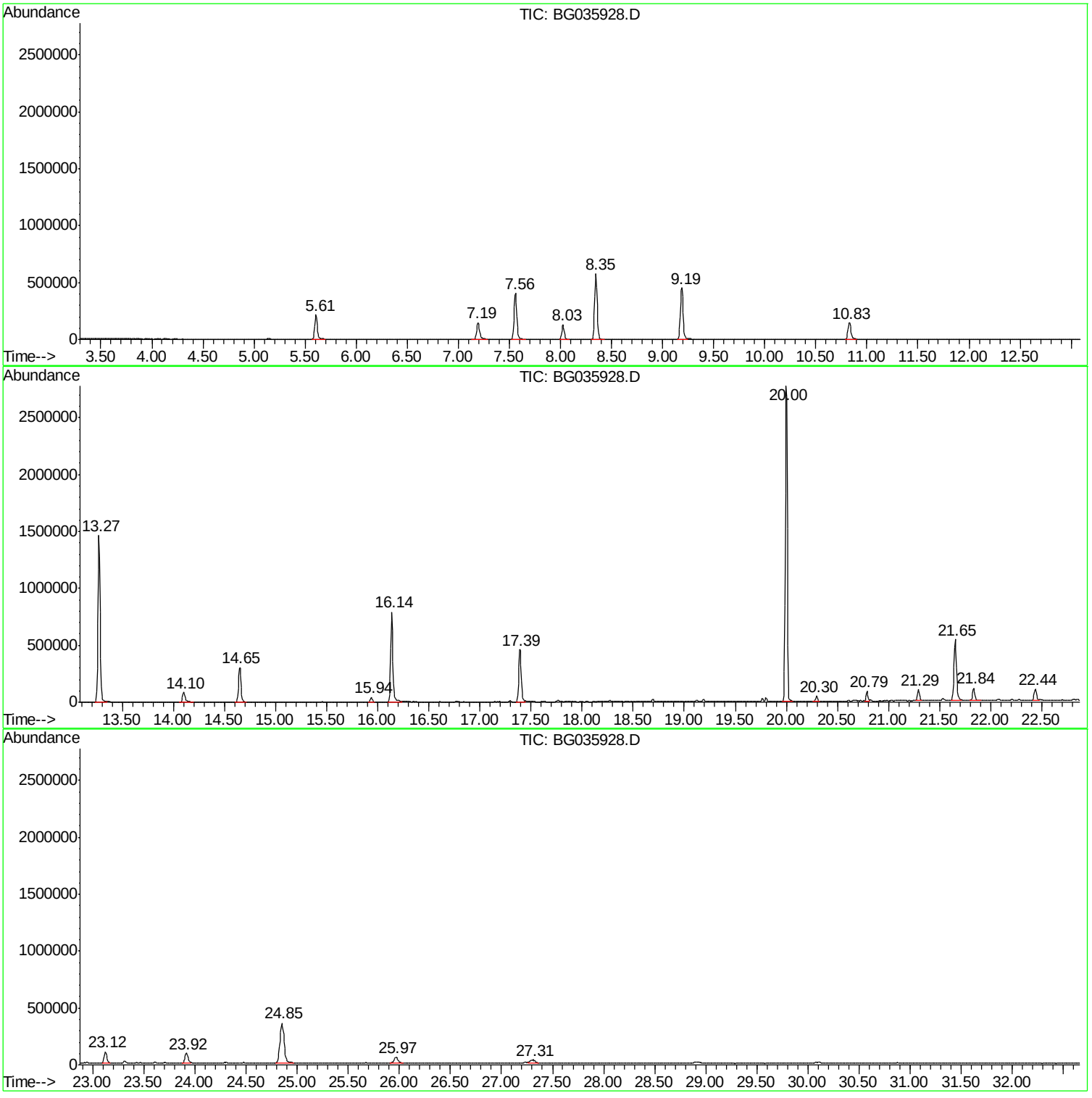
Sample : J4160-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
072418-TIPC-F-U-S

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\BG072618\
Data File : BG035928.D
Acq On : 27 Jul 2018 3:40
Operator : JU/SJ
Sample : J4160-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 072418-TIPC-F-U-S

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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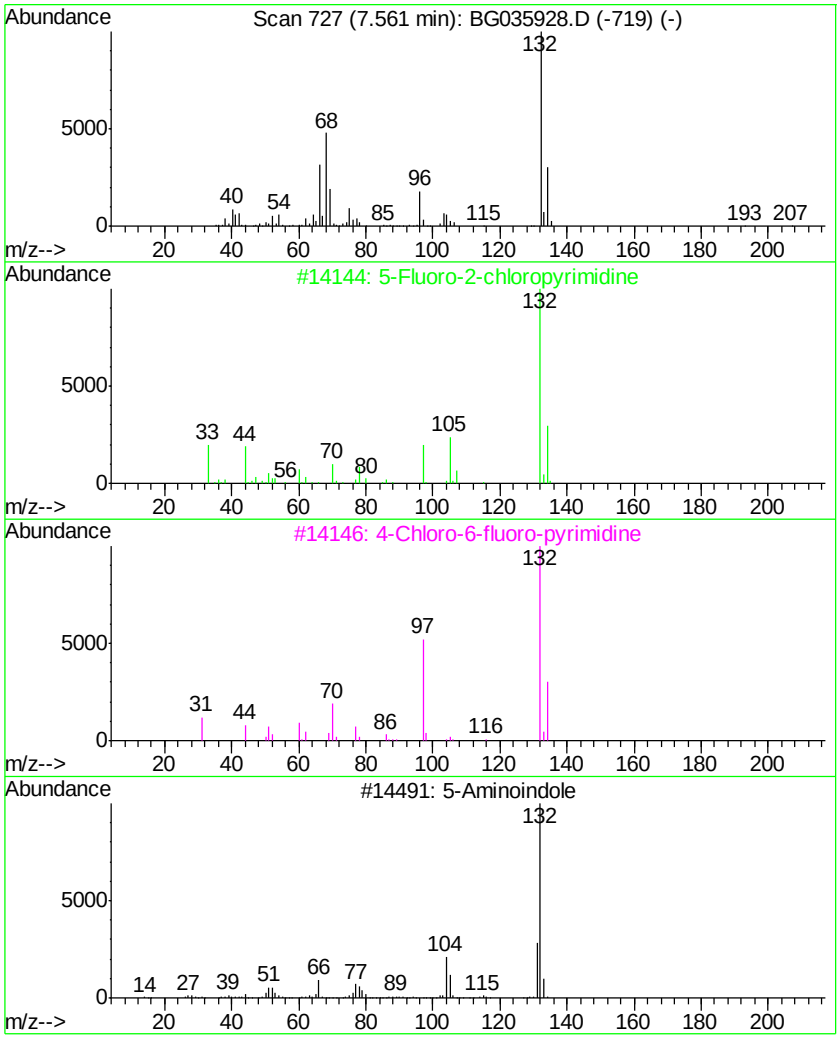
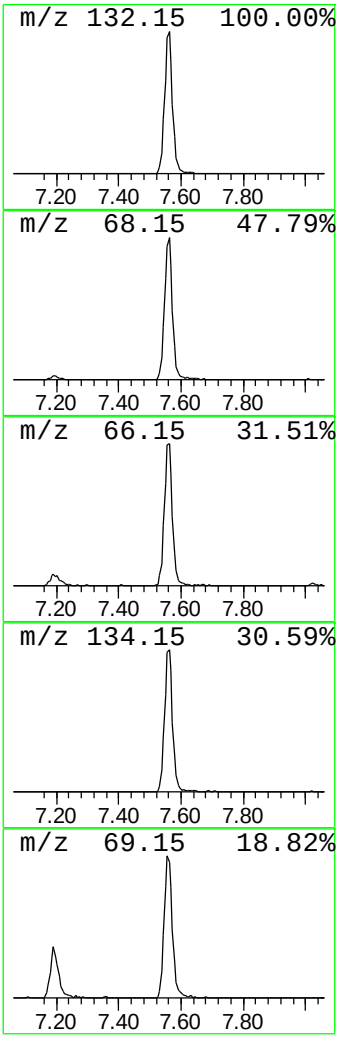
Peak Number 1 unknown7.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	65.38 ng	725276	1,4-Dichlorobenzene-d4	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	5-Aminoindole	132	C8H8N2	005192-03-0	22
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	22





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG072618\
Data File : BG035928.D
Acq On : 27 Jul 2018 3:40
Operator : JU/SJ
Sample : J4160-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 072418-TIPC-F-U-S

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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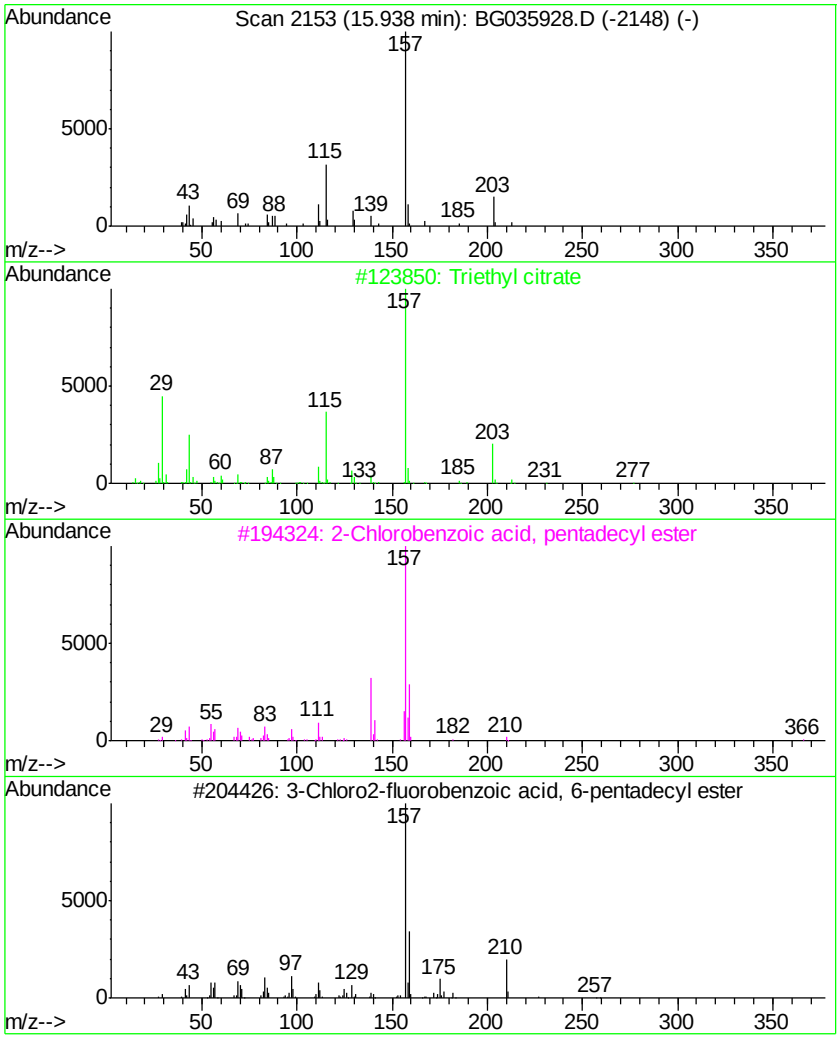
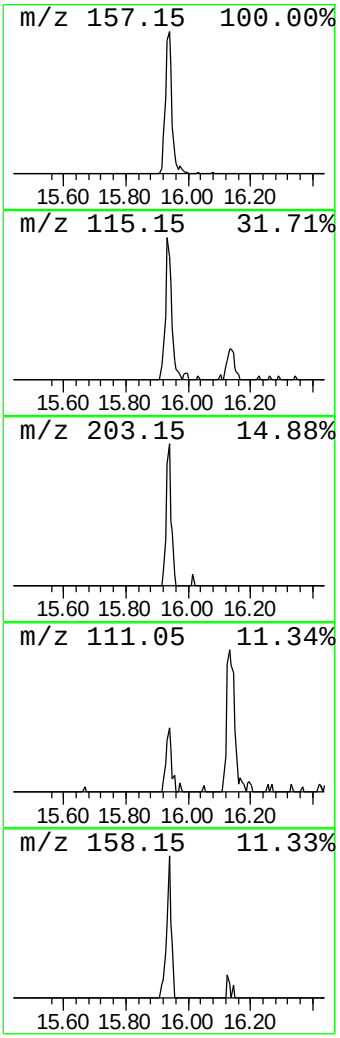
Peak Number 3 Triethyl citrate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	2.06 ng	54715	Acenaphthene-d10	14.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	83
2	2-Chlorobenzoic acid, pentadecyl...	366	C22H35ClO2	1000292-43-0	50
3	3-Chloro2-fluorobenzoic acid, 6-...	384	C22H34ClFO2	1000338-65-3	42
4	3-Chloro2-fluorobenzoic acid, 3-...	370	C21H32ClFO2	1000338-64-6	42
5	Adipic acid, ethyl 4-heptyl ester	272	C15H28O4	1000349-73-4	42





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG072618\
Data File : BG035928.D
Acq On : 27 Jul 2018 3:40
Operator : JU/SJ
Sample : J4160-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 072418-TIPC-F-U-S

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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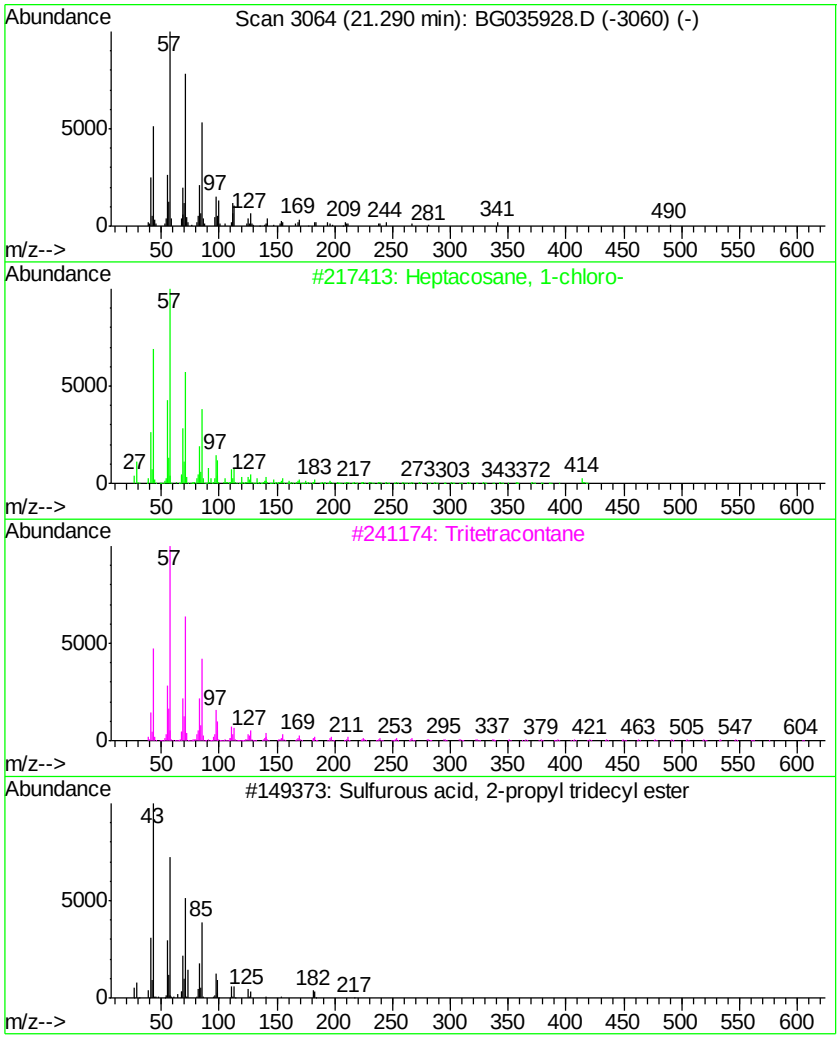
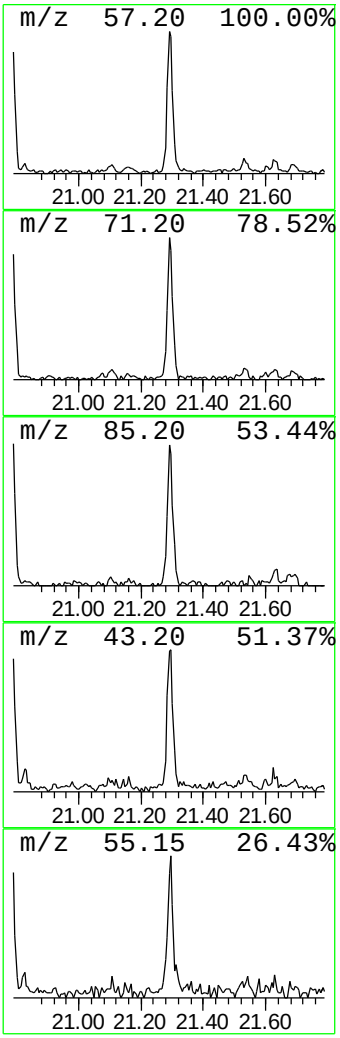
Peak Number 4 Heptacosane, 1-chloro- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.29	2.96 ng	132990	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	91
2	Tritetracontane	605	C43H88	007098-21-7	91
3	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	91
4	Hexacosane	366	C26H54	000630-01-3	90
5	Tetratetracontane	619	C44H90	007098-22-8	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG072618\
Data File : BG035928.D
Acq On : 27 Jul 2018 3:40
Operator : JU/SJ
Sample : J4160-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 072418-TIPC-F-U-S

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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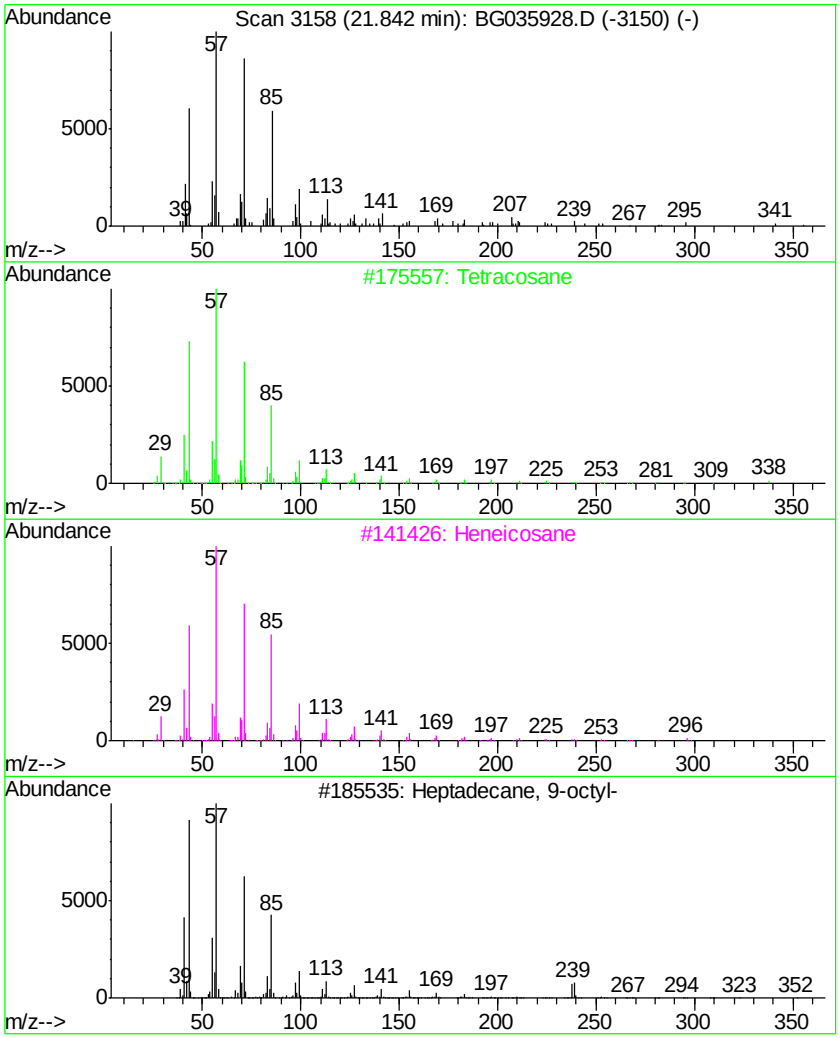
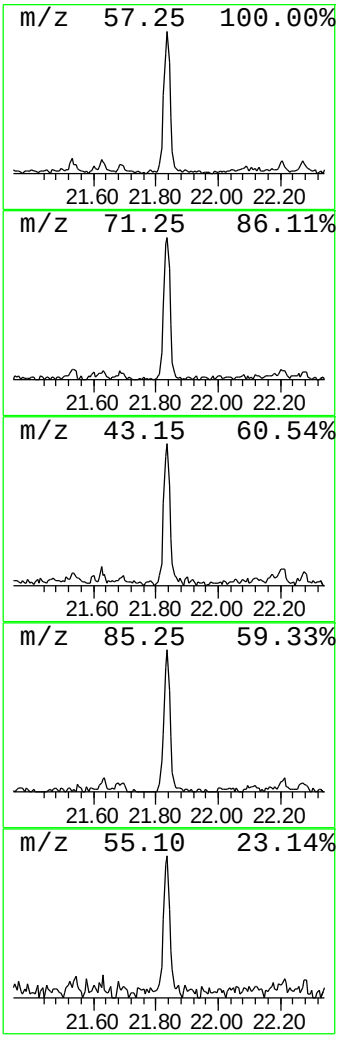
Peak Number 5 Tetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.84	3.77 ng	169060	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	94
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Hexacosane	366	C26H54	000630-01-3	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG072618\
Data File : BG035928.D
Acq On : 27 Jul 2018 3:40
Operator : JU/SJ
Sample : J4160-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 072418-TIPC-F-U-S

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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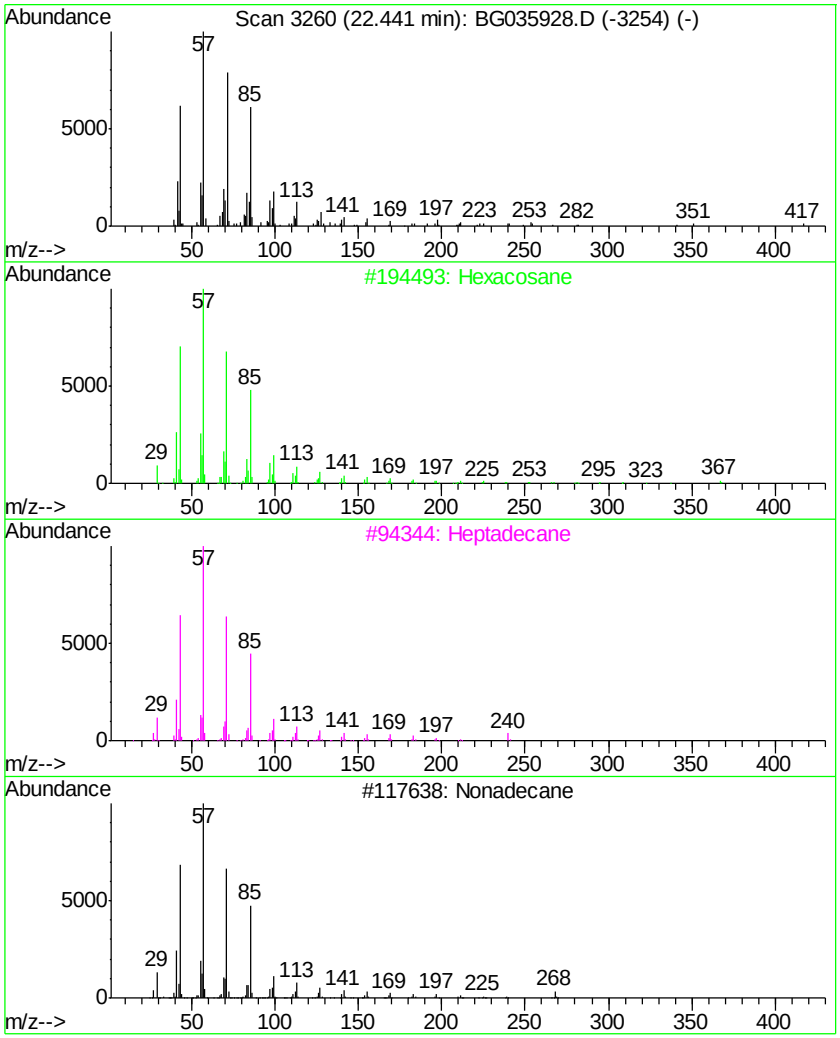
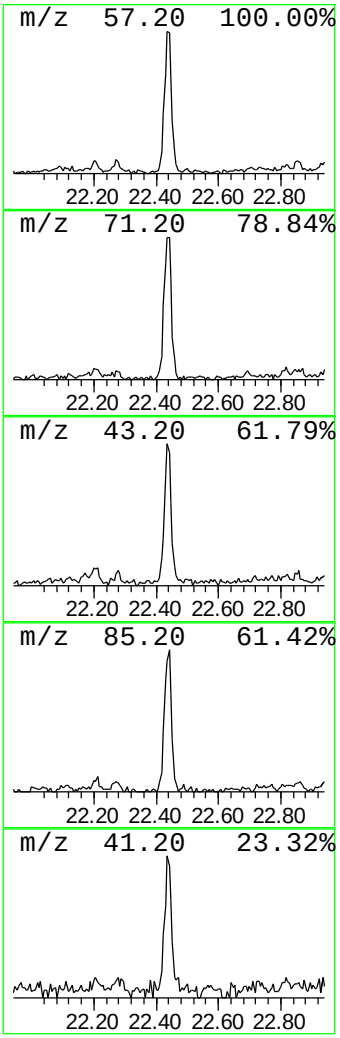
Peak Number 6 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.44	3.70 ng	166228	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heptadecane	240	C17H36	000629-78-7	90
3	Nonadecane	268	C19H40	000629-92-5	90
4	Heneicosane	296	C21H44	000629-94-7	87
5	Eicosane, 9-octyl-	394	C28H58	013475-77-9	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG072618\
Data File : BG035928.D
Acq On : 27 Jul 2018 3:40
Operator : JU/SJ
Sample : J4160-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 072418-TIPC-F-U-S

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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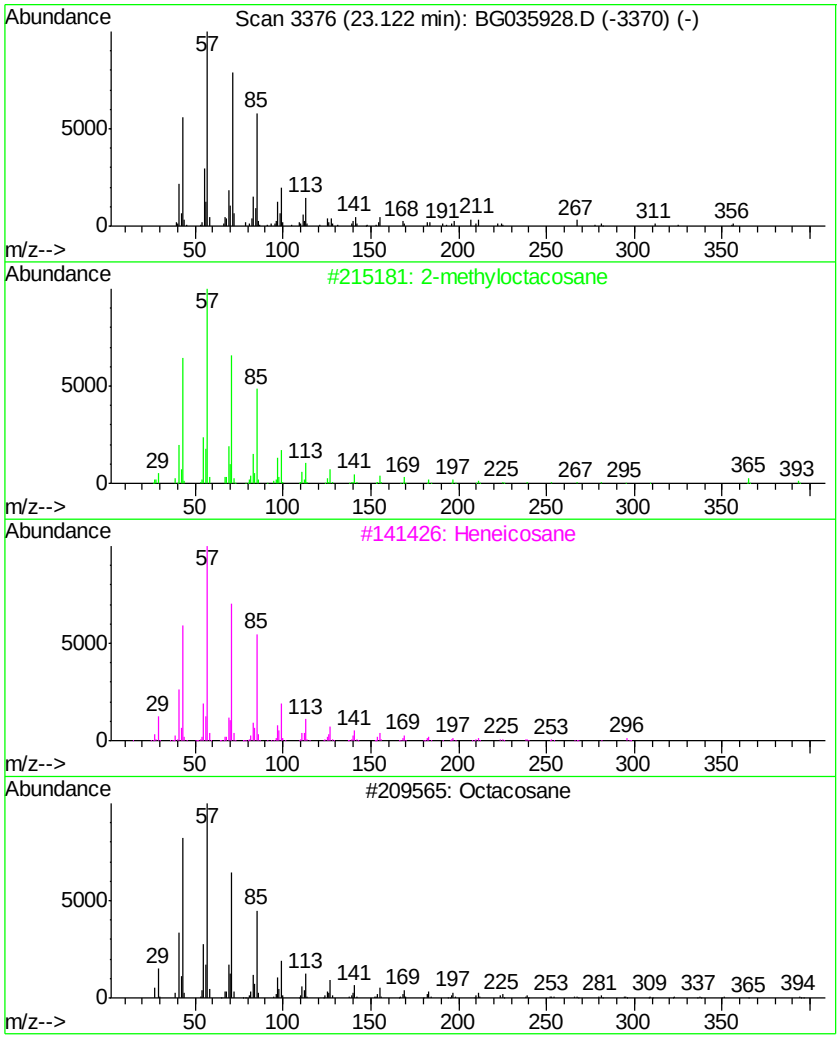
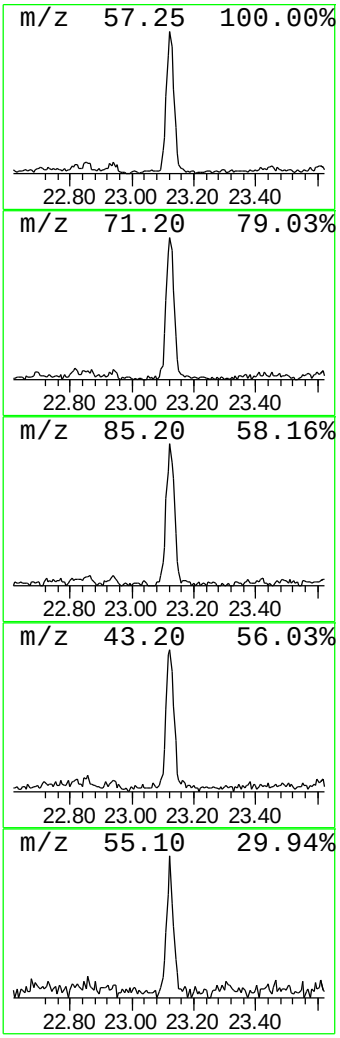
Peak Number 7 2-methyloctacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.12	4.19 ng	188068	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Triacontane	422	C30H62	000638-68-6	90
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	90





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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 072418-TIPC-F-U-S

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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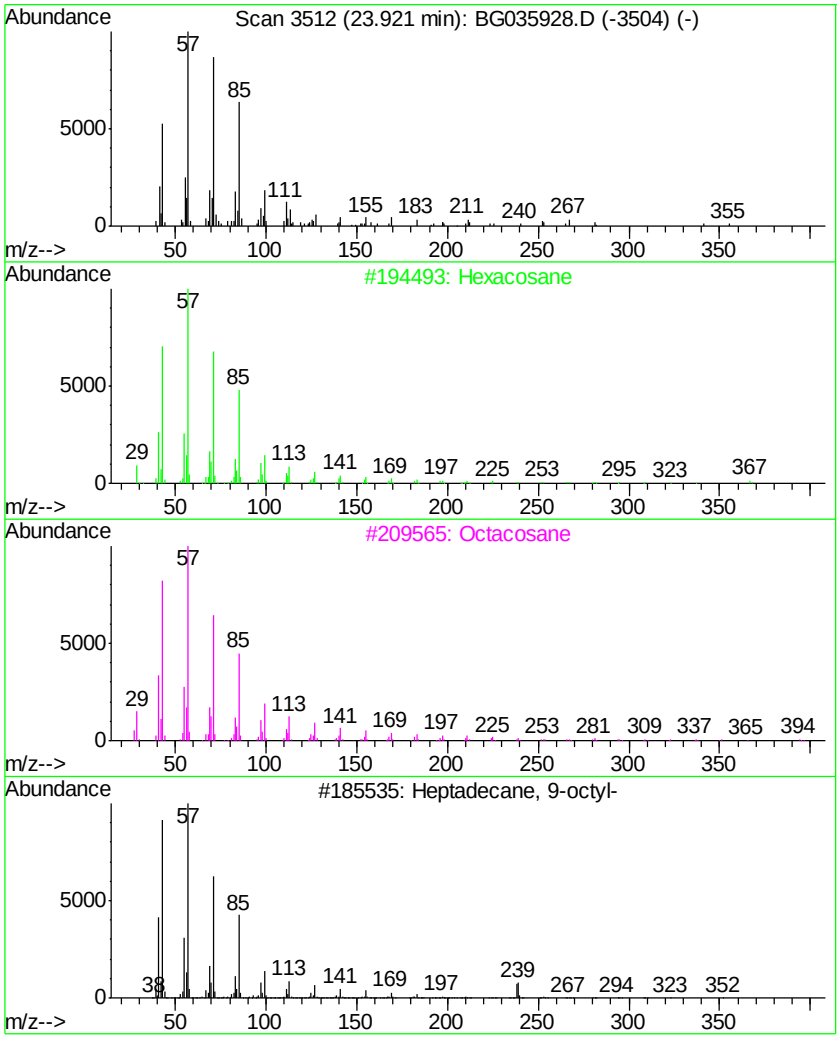
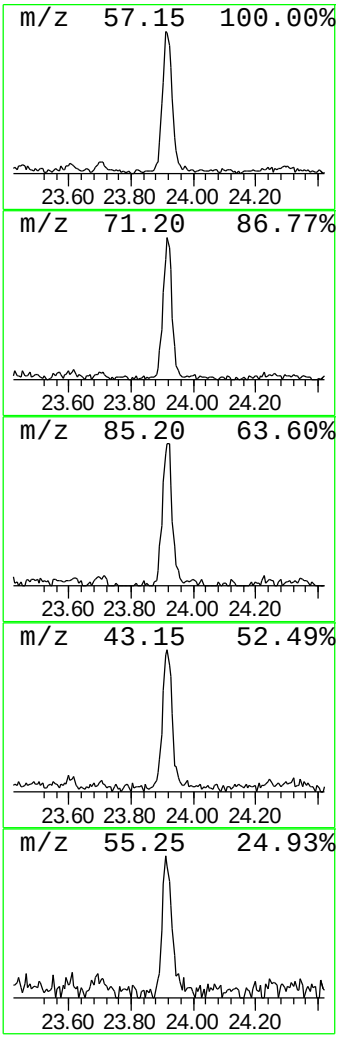
Peak Number 8 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.92	3.66 ng	180288	Perylene-d12	24.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Octacosane	394	C28H58	000630-02-4	87
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4	2-methyloctacosane	408	C29H60	1000376-72-8	87
5	Hentriacontane	437	C31H64	000630-04-6	87





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Misc :
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Instrument : BNA_G
ClientSampleId : 072418-TIPC-F-U-S

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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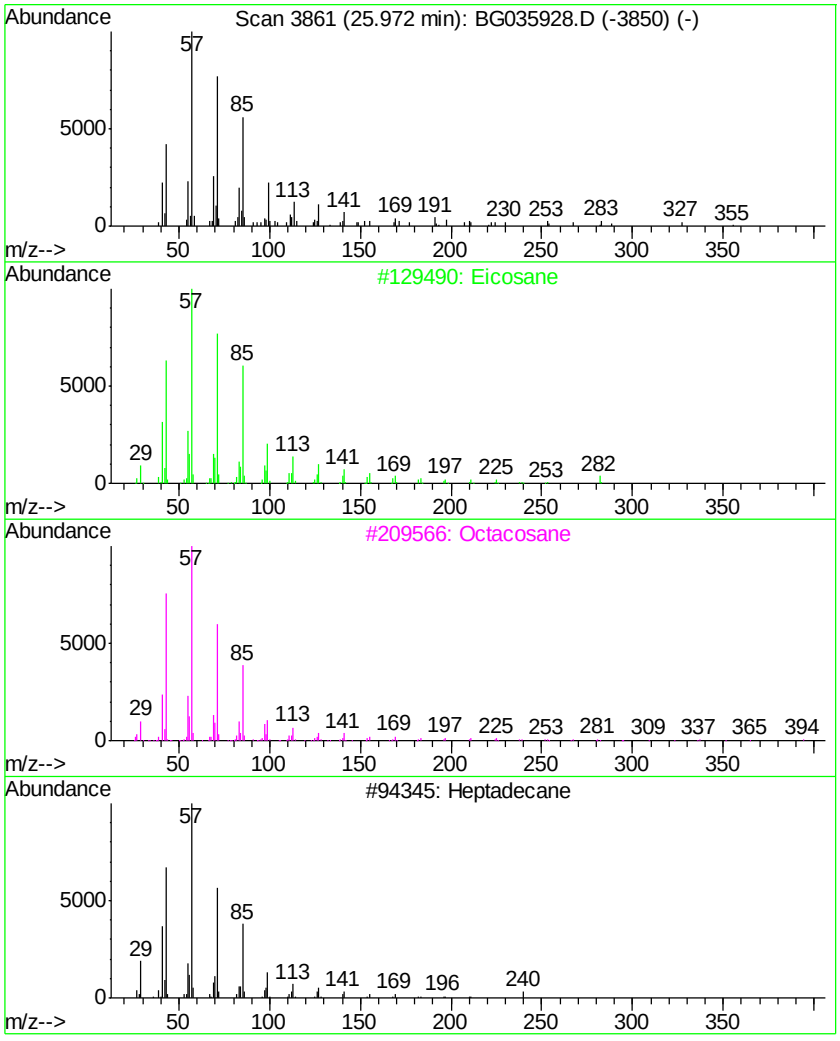
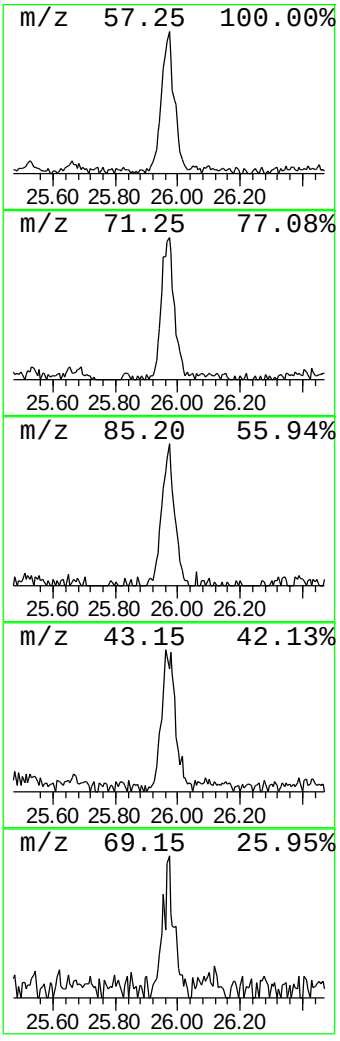
Peak Number 9 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.97	3.05 ng	150094	Perylene-d12	24.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	87
2	Octacosane	394	C28H58	000630-02-4	80
3	Heptadecane	240	C17H36	000629-78-7	80
4	2-Thiopheneacetic acid, 4-tetrad...	338	C20H34O2S	1000280-67-0	72
5	Hexadecane	226	C16H34	000544-76-3	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG072618\
Data File : BG035928.D
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Misc :
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Instrument : BNA_G
ClientSampleId : 072418-TIPC-F-U-S

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
unknown7.56	7.56	65.4	ng	725276	1	8.03	221859	20.0
Triethyl citrate	15.94	2.1	ng	54715	3	14.65	531490	20.0
Heptacosane, 1-ch...	21.29	3.0	ng	132990	5	21.65	897547	20.0
Tetracosane	21.84	3.8	ng	169060	5	21.65	897547	20.0
Hexacosane	22.44	3.7	ng	166228	5	21.65	897547	20.0
2-methyloctacosane	23.12	4.2	ng	188068	5	21.65	897547	20.0
Octacosane	23.92	3.7	ng	180288	6	24.85	985611	20.0
Eicosane	25.97	3.0	ng	150094	6	24.85	985611	20.0