LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022620\
Data File : BG044607.D
Acq On : 26 Feb 2020 17:25
Operator : CG/JU
Sample : L1681-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SH-BORING-1

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-BG022420.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	5.451	395	402	415	rBV	972349	1603537	39.85%	6.078%
2	6.561	585	591	599	rVB	37590	60869	1.51%	0.231%
3	7.049	665	674	691	rBV	975662	1735917	43.14%	6.580%
4	7.871	807	814	824	rBV	223826	379893	9.44%	1.440%
5	8.194	861	869	879	rBV	794643	1366181	33.95%	5.179%
6	9.029	1003	1011	1030	rBV	565282	1074119	26.70%	4.072%
7	10.674	1283	1291	1305	rBV	283600	548390	13.63%	2.079%
8	13.136	1702	1710	1723	rBV	1627417	2625222	65.25%	9.951%
9	13.970	1848	1852	1864	rVB	42897	75955	1.89%	0.288%
10	14.481	1931	1939	1941	rBV	356712	516479	12.84%	1.958%
11	14.516	1941	1945	1954	rVB	481392	788986	19.61%	2.991%
12	16.003	2188	2198	2209	rBV	1416314	2212304	54.98%	8.386%
13	17.260	2405	2412	2418	rBV	618273	1017674	25.29%	3.858%
14	18.165	2556	2566	2573	rBV4	20576	47833	1.19%	0.181%
15	18.418	2603	2609	2632	rBV	85535	198040	4.92%	0.751%
16	19.311	2757	2761	2769	rBV	34857	64265	1.60%	0.244%
17	19.669	2814	2822	2825	rBV2	32206	61058	1.52%	0.231%
18	19.875	2850	2857	2866	rBV	3034488	4023533	100.00%	15.251%
19	20.192	2898	2911	2918	rBV6	39670	104209	2.59%	0.395%
20	20.686	2989	2995	2998	rBV2	54934	70581	1.75%	0.268%
21	20.985	3040	3046	3054	rBV	765729	957839	23.81%	3.631%
22	21.167	3068	3077	3087	rBV	461565	764796	19.01%	2.899%
23	21.496	3126	3133	3148	rBV	705977	1206739	29.99%	4.574%
24	21.702	3163	3168	3175	rBV	135595	192641	4.79%	0.730%
25	21.931	3203	3207	3215	rVB6	28939	43637	1.08%	0.165%
26	22.072	3226	3231	3237	rVB2	21450	45764	1.14%	0.173%
27	22.290	3261	3268	3284	rBV3	233213	591670	14.71%	2.243%
28	22.942	3373	3379	3392	rVB	144691	286729	7.13%	1.087%
29	23.124	3406	3410	3425	rVB7	24686	83337	2.07%	0.316%
30	23.271	3429	3435	3449	rVV4	82591	198498	4.93%	0.752%
31	23.706	3502	3509	3515	rBV	168785	343641	8.54%	1.303%
32	24.563	3645	3655	3674	rBV3	431406	1415120	35.17%	5.364%
33	25.092	3737	3745	3754	rVB2	121101	314310	7.81%	1.191%
34	25.674	3834	3844	3852	rBV2	100626	300949	7.48%	1.141%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022620\
Data File : BG044607.D
Acq On : 26 Feb 2020 17:25
Operator : CG/JU
Sample : L1681-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SH-BORING-1

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-BG022420.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	25.780	3856	3862	3872	rVV7	28352	89543	2.23%	0.339%
36	27.683	4177	4186	4200	rVB5	60454	220191	5.47%	0.835%
37	29.581	4499	4509	4510	rBV9	44766	105740	2.63%	0.401%
38	30.104	4591	4598	4608	rVB10	25206	93210	2.32%	0.353%
39	30.697	4688	4699	4722	rVB5	108002	551894	13.72%	2.092%

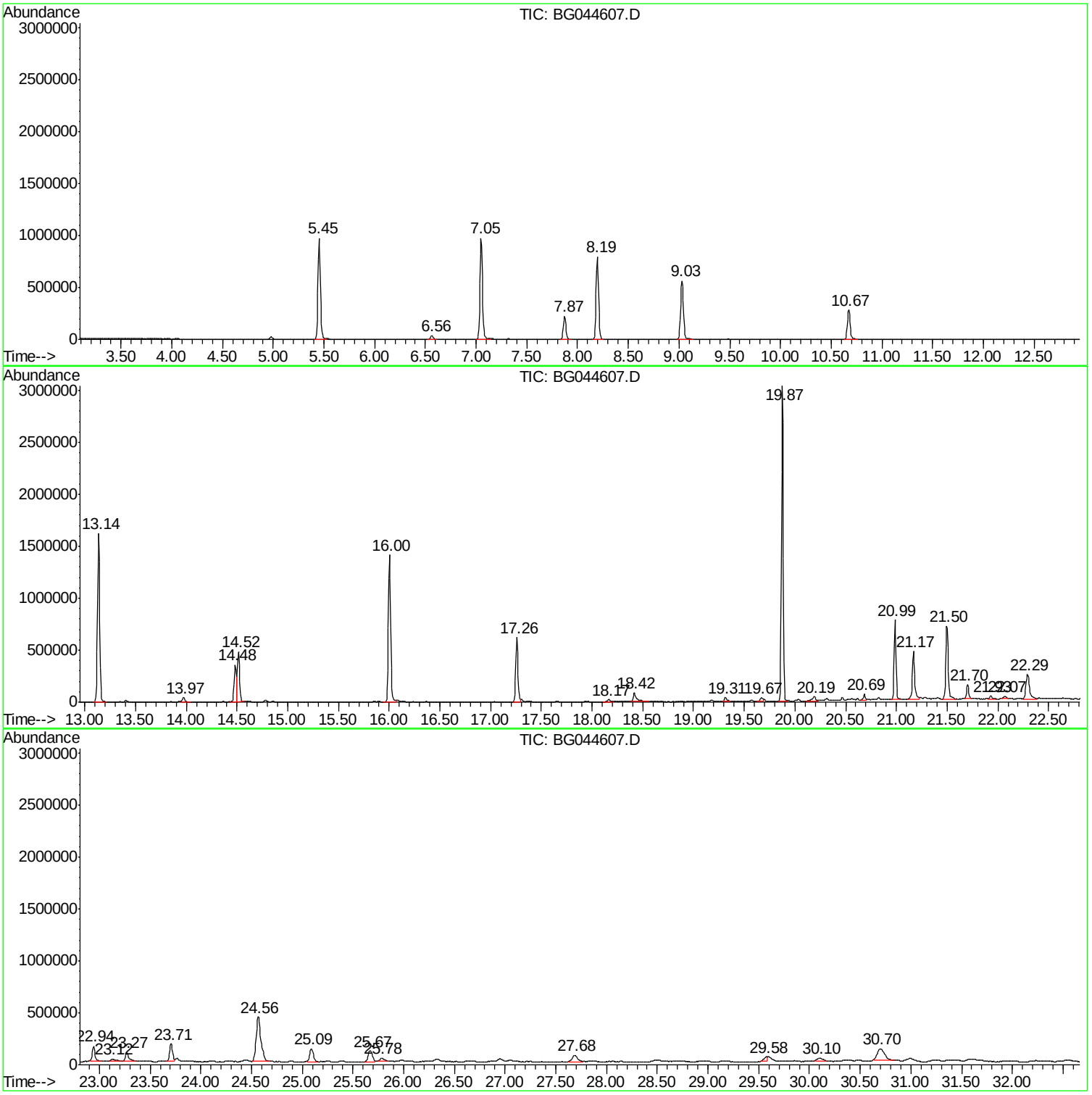
Sum of corrected areas: 26381293

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022620\
Data File : BG044607.D
Acq On : 26 Feb 2020 17:25
Operator : CG/JU
Sample : L1681-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SH-BORING-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG022420.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\BG022620\
Data File : BG044607.D
Acq On : 26 Feb 2020 17:25
Operator : CG/JU
Sample : L1681-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SH-BORING-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG022420.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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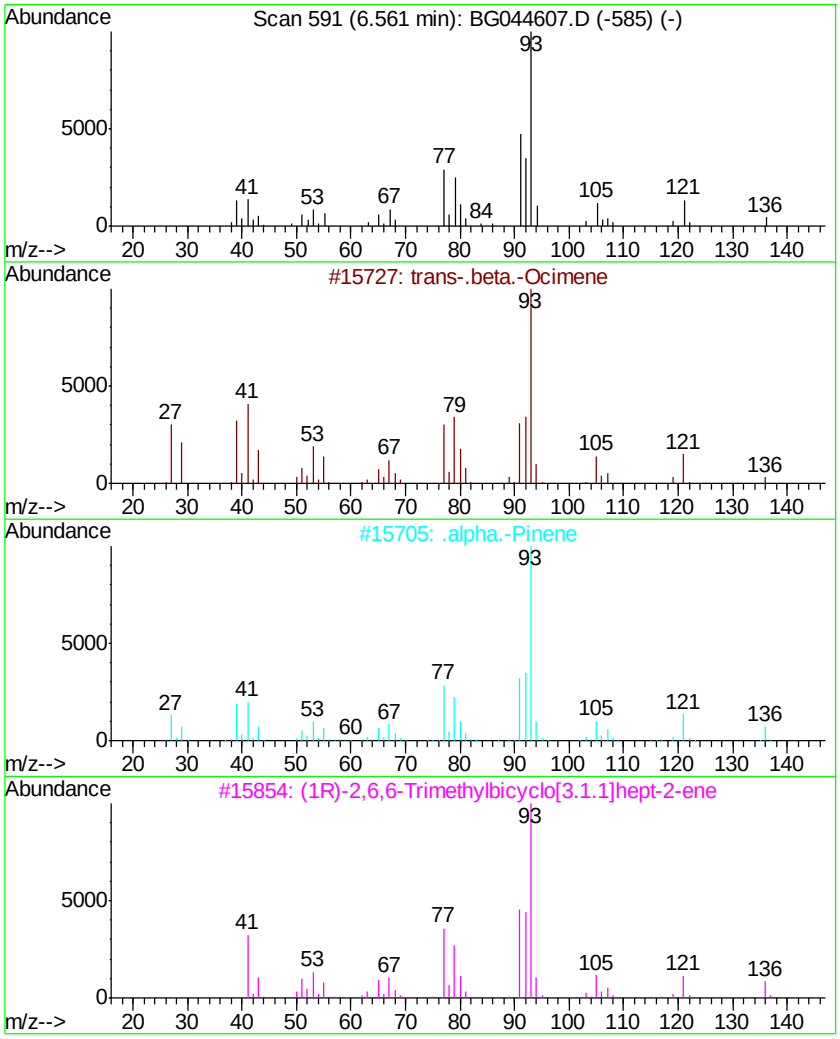
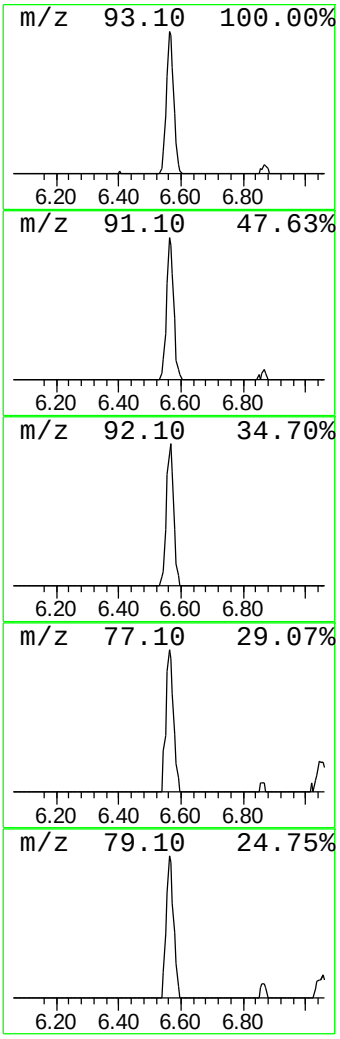
Peak Number 1 trans-.beta.-Ocimene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	3.20 ng	60869	1,4-Dichlorobenzene-d4	7.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-.beta.-Ocimene	136	C10H16	003779-61-1	94
2	.alpha.-Pinene	136	C10H16	000080-56-8	94
3	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	92
4	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	91
5	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022620\
Data File : BG044607.D
Acq On : 26 Feb 2020 17:25
Operator : CG/JU
Sample : L1681-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SH-BORING-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG022420.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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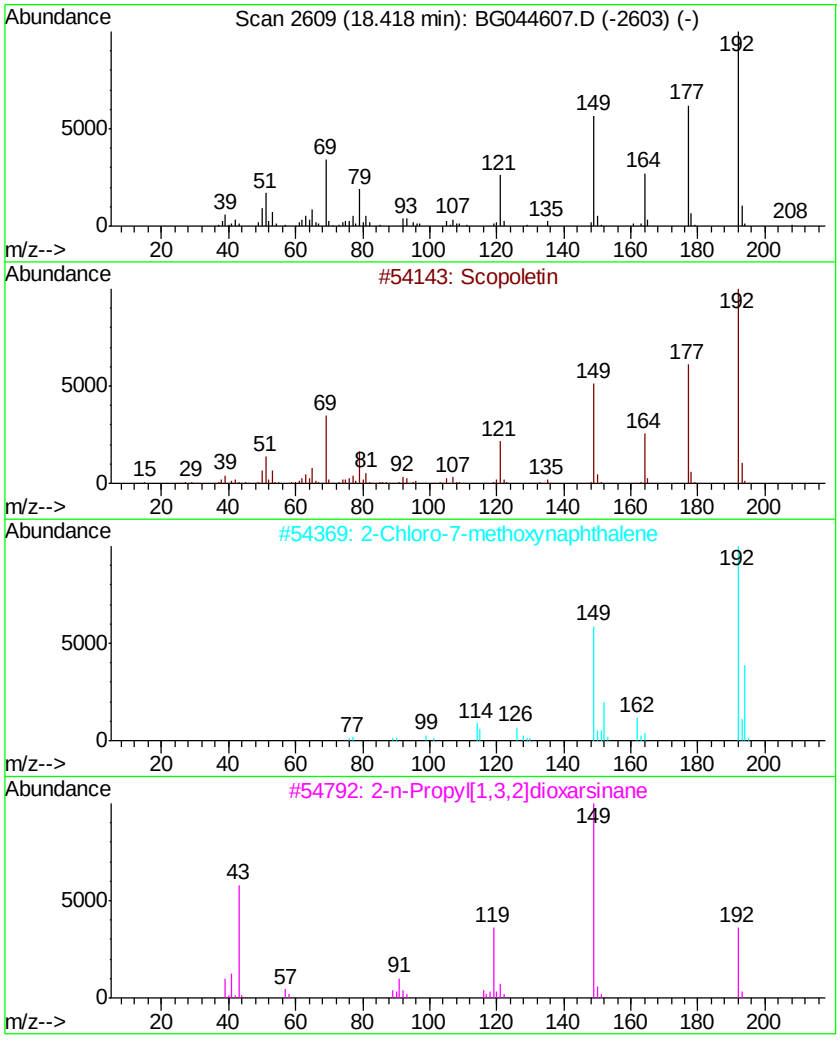
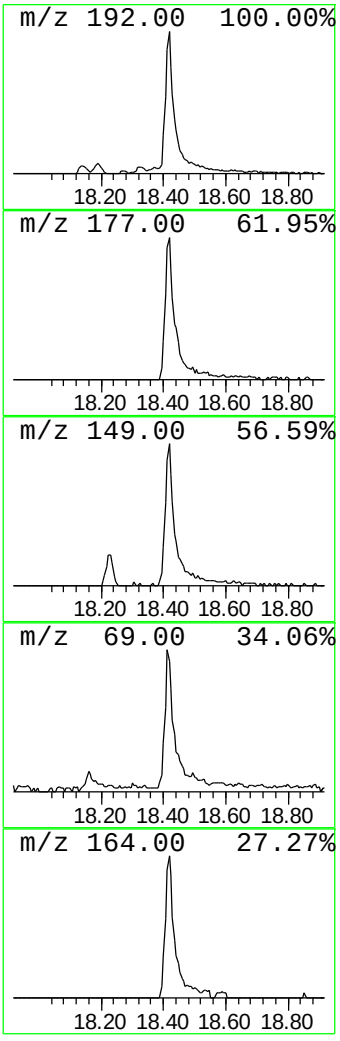
Peak Number 3 Scopoletin Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	3.89 ng	198040	Phenanthrene-d10	17.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Scopoletin	192	C10H8O4	000092-61-5	98
2	2-Chloro-7-methoxynaphthalene	192	C11H9ClO	067061-67-0	50
3	2-n-Propyl[1,3,2]dioxarsinane	192	C6H13AsO2	1000322-39-7	49
4	6-Isopropyl-benzothiazol-2-ylamine	192	C10H12N2S	032895-14-0	47
5	2,3-Diketo-6-methoxybenzo[b]pyran	192	C10H8O4	1000071-89-6	43





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022620\
Data File : BG044607.D
Acq On : 26 Feb 2020 17:25
Operator : CG/JU
Sample : L1681-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SH-BORING-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG022420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

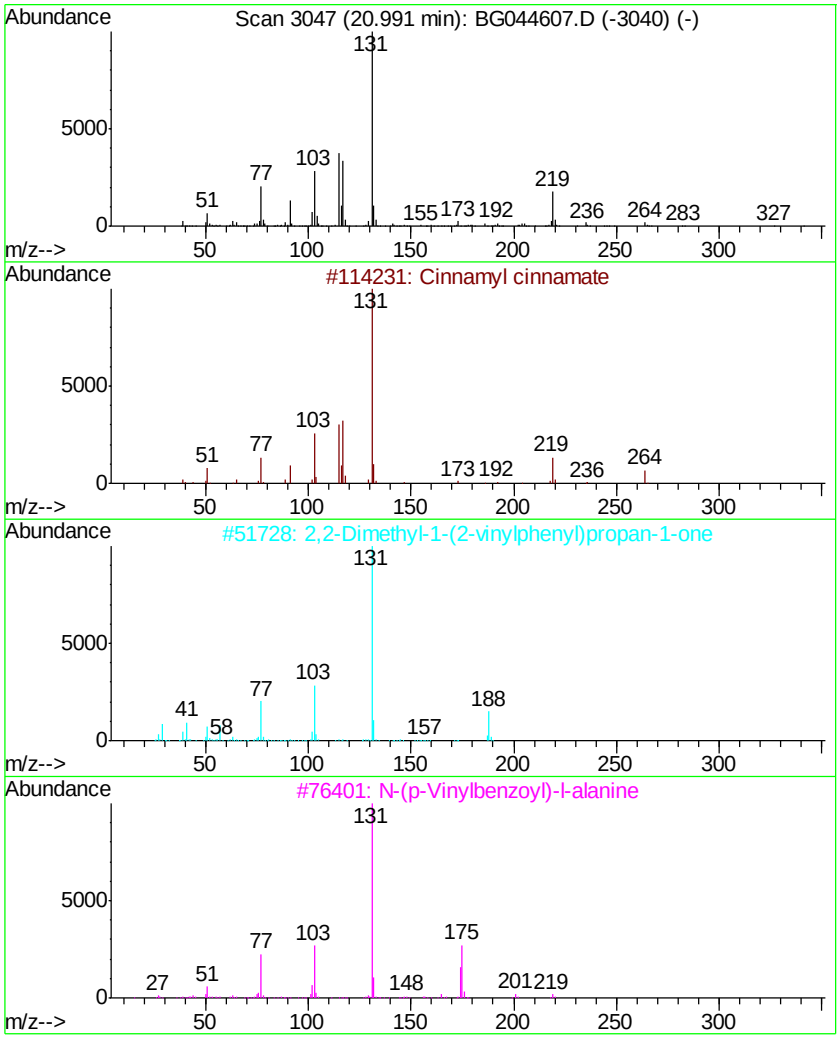
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

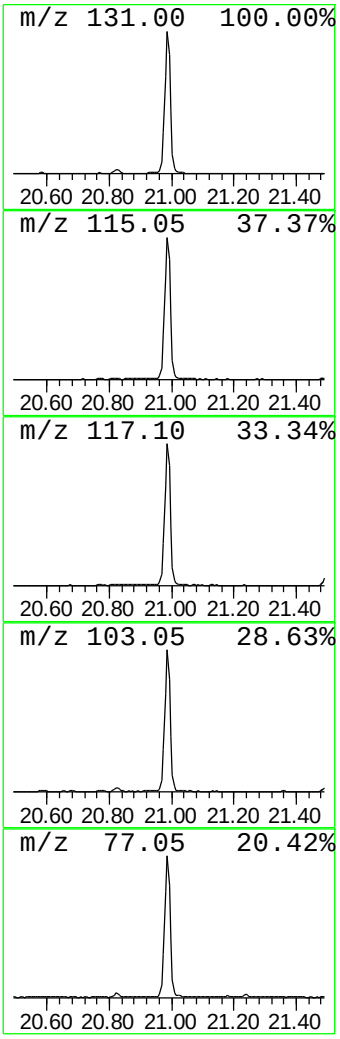
****

Peak Number 4 Cinnamyl cinnamate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.99	15.87 ng	957839	Chrysene-d12	21.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	87
2	2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	52
3	N-(p-Vinylbenzoyl)-l-alanine	219	C12H13NO3	139184-60-4	50
4	trans-1-Cinnamoylimidazole	198	C12H10N2O	001138-15-4	50
5	p-Vinylbenzohydrazide	162	C9H10N2O	1000244-74-9	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022620\
Data File : BG044607.D
Acq On : 26 Feb 2020 17:25
Operator : CG/JU
Sample : L1681-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SH-BORING-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG022420.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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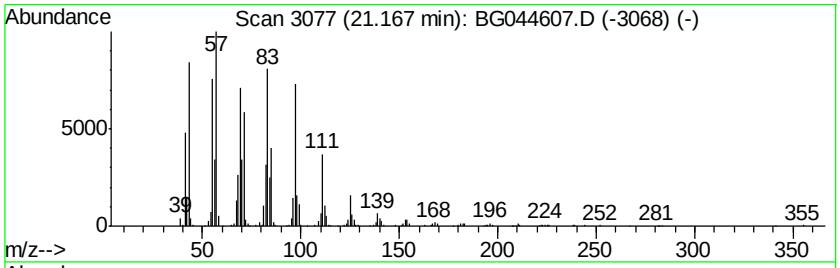
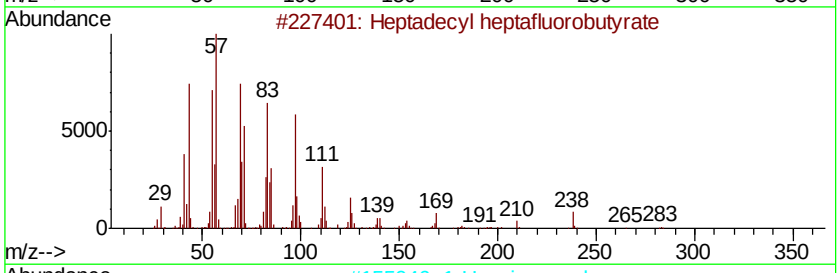
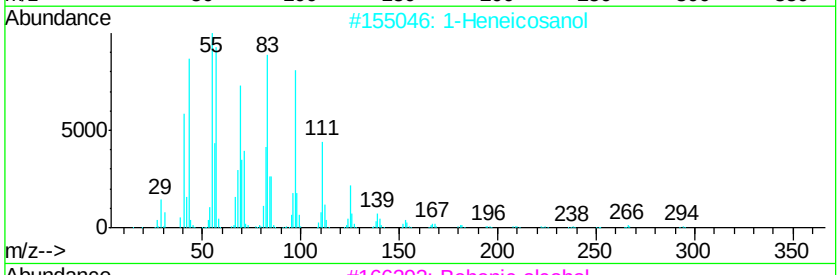
Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 3

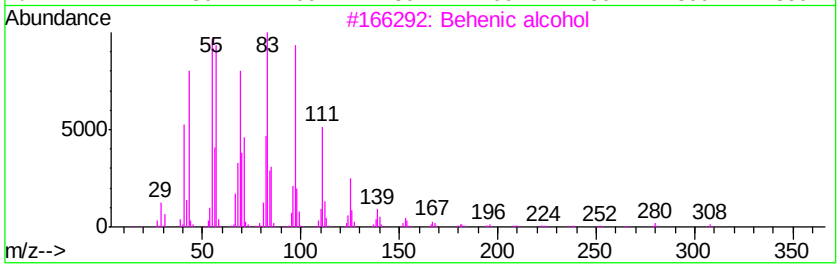
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.17	12.68 ng	764796	Chrysene-d12	21.50

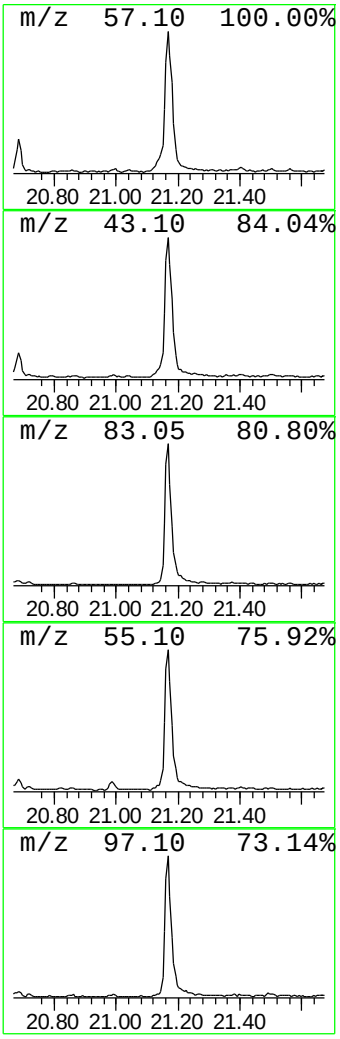
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Behenic alcohol	326	C22H46O	000661-19-8	93
4	Cyclohexadecane	224	C16H32	000295-65-8	93
5	1-Octadecene	252	C18H36	000112-88-9	92











Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022620\
Data File : BG044607.D
Acq On : 26 Feb 2020 17:25
Operator : CG/JU
Sample : L1681-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SH-BORING-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG022420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

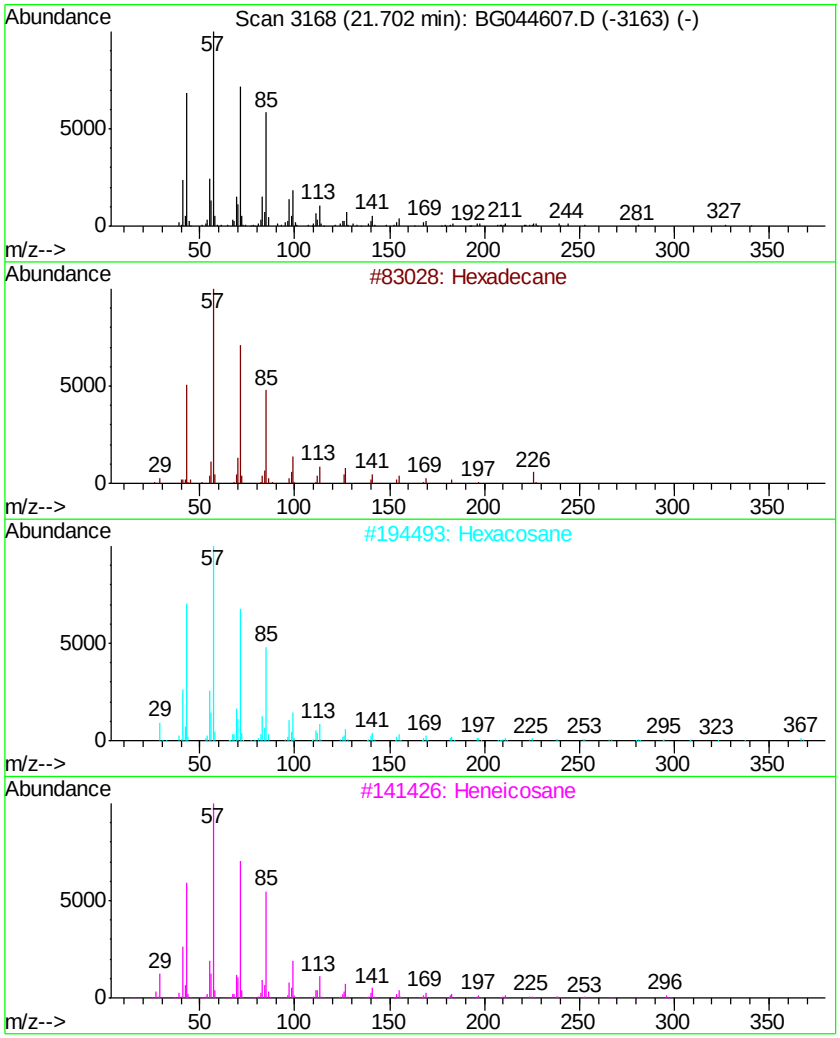
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

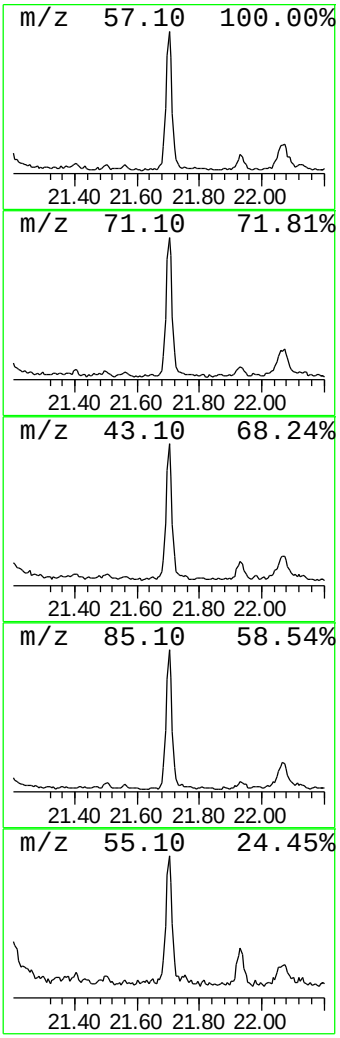
****

Peak Number 6 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.70	3.19 ng	192641	Chrysene-d12	21.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	93
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022620\
Data File : BG044607.D
Acq On : 26 Feb 2020 17:25
Operator : CG/JU
Sample : L1681-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SH-BORING-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG022420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

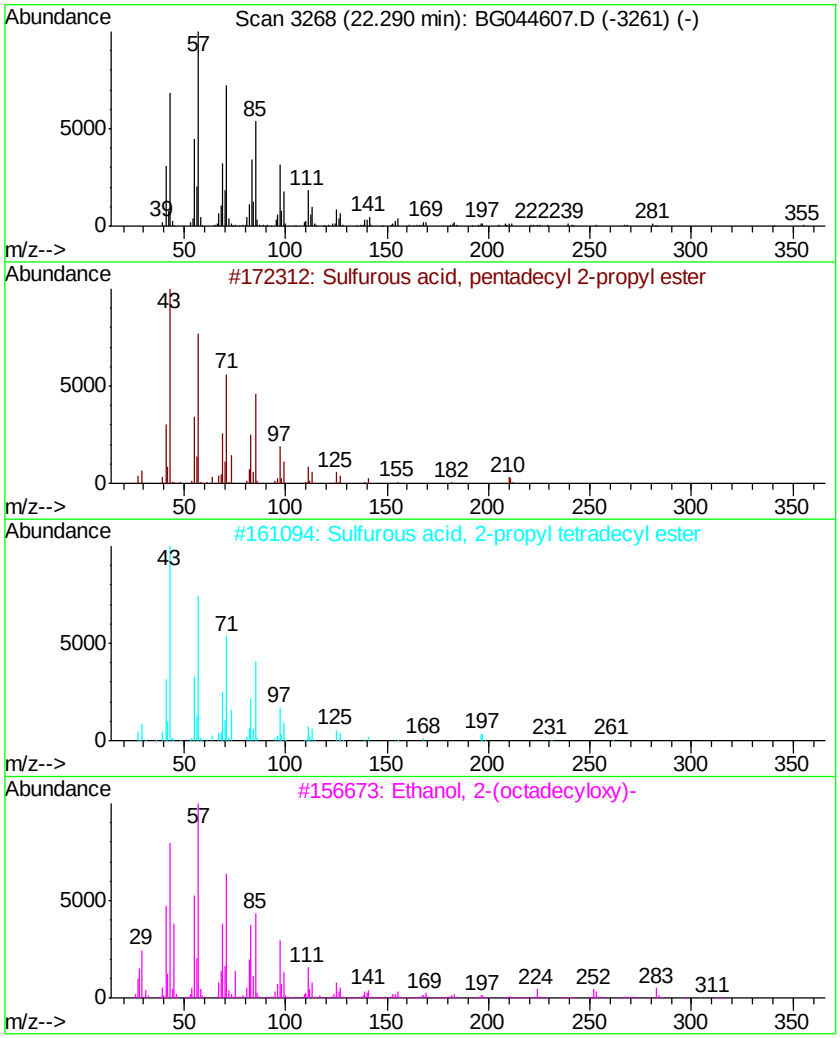
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

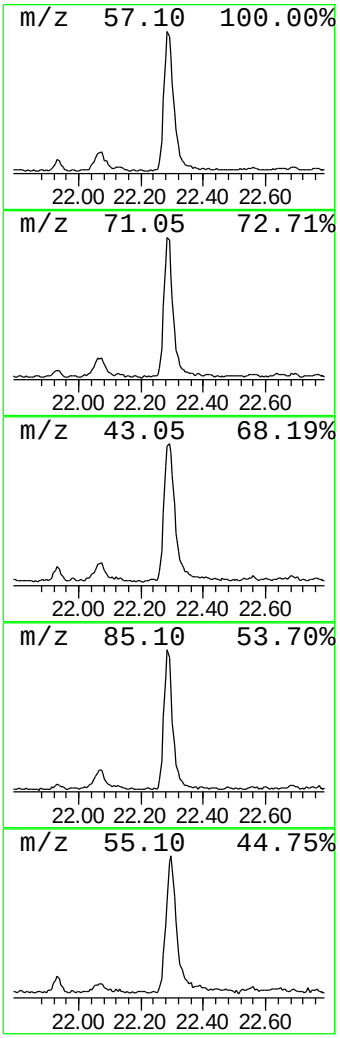
****

Peak Number 7 Sulfurous acid, pentadecyl ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.29	9.81 ng	591670	Chrysene-d12	21.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	91
2	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	91
3	Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	91
4	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	87
5	Nonadecane	268	C19H40	000629-92-5	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022620\
Data File : BG044607.D
Acq On : 26 Feb 2020 17:25
Operator : CG/JU
Sample : L1681-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SH-BORING-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG022420.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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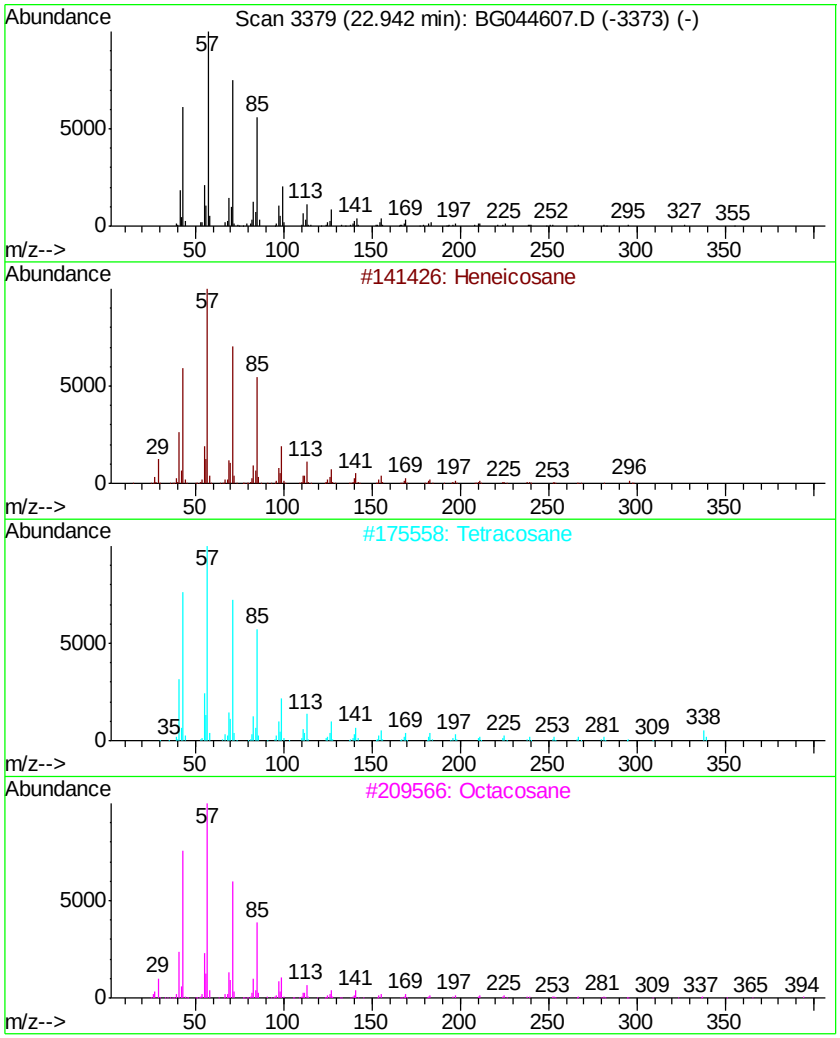
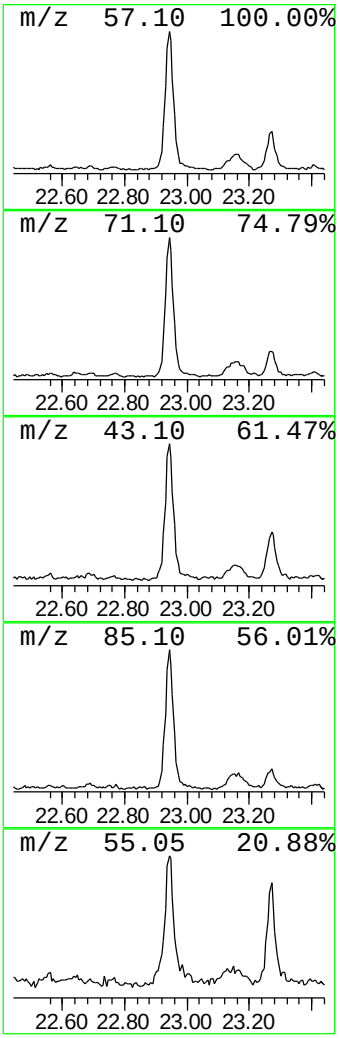
Peak Number 8 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.94	4.75 ng	286729	Chrysene-d12	21.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tetracosane	338	C24H50	000646-31-1	90
3	Octacosane	394	C28H58	000630-02-4	87
4	Pentacosane	352	C25H52	000629-99-2	86
5	Hexadecane	226	C16H34	000544-76-3	83





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022620\
Data File : BG044607.D
Acq On : 26 Feb 2020 17:25
Operator : CG/JU
Sample : L1681-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SH-BORING-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG022420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

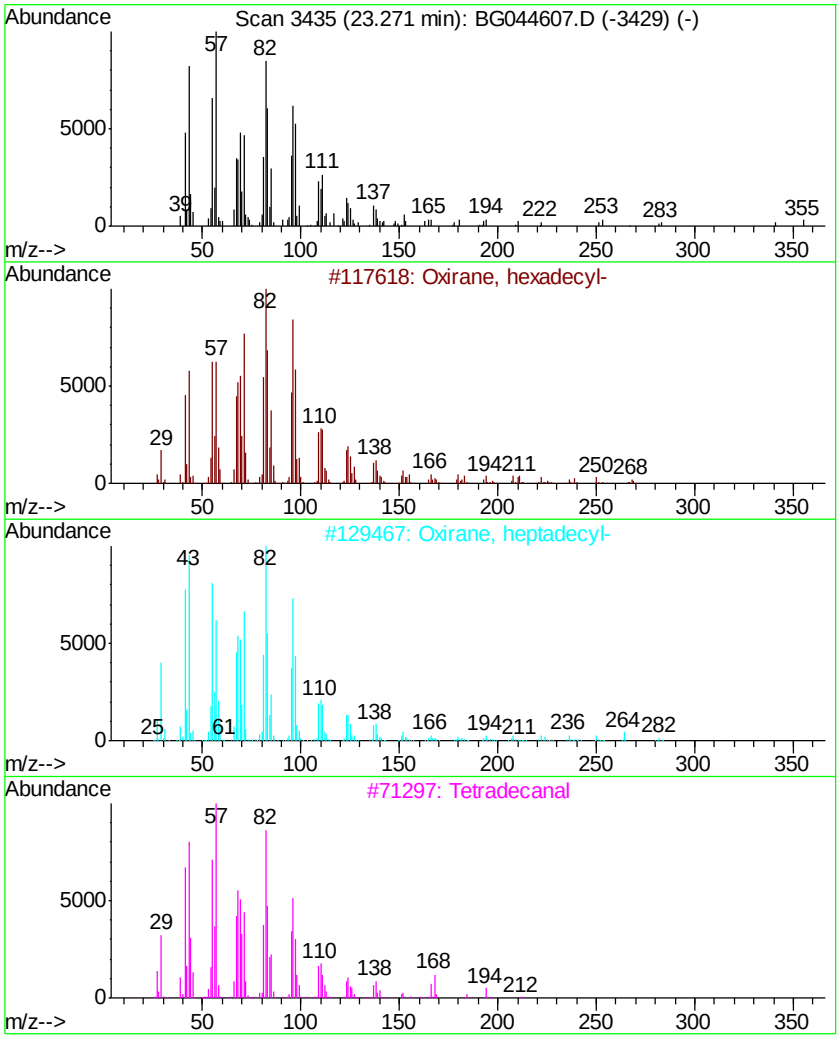
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

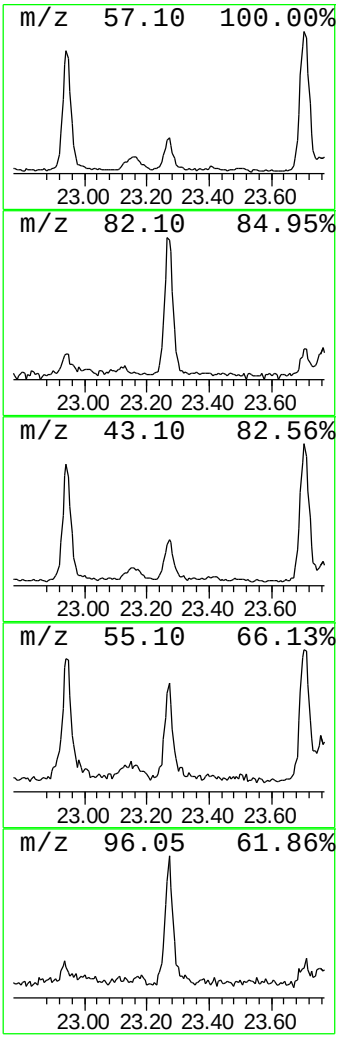
****

Peak Number 9 Oxirane, hexadecyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.27	2.81 ng	198498	Perylene-d12	24.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	95
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	93
3	Tetradecanal	212	C14H28O	000124-25-4	86
4	Octadecanal	268	C18H36O	000638-66-4	80
5	1,19-Eicosadiene	278	C20H38	014811-95-1	68





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Data File : BG044607.D
Acq On : 26 Feb 2020 17:25
Operator : CG/JU
Sample : L1681-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SH-BORING-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG022420.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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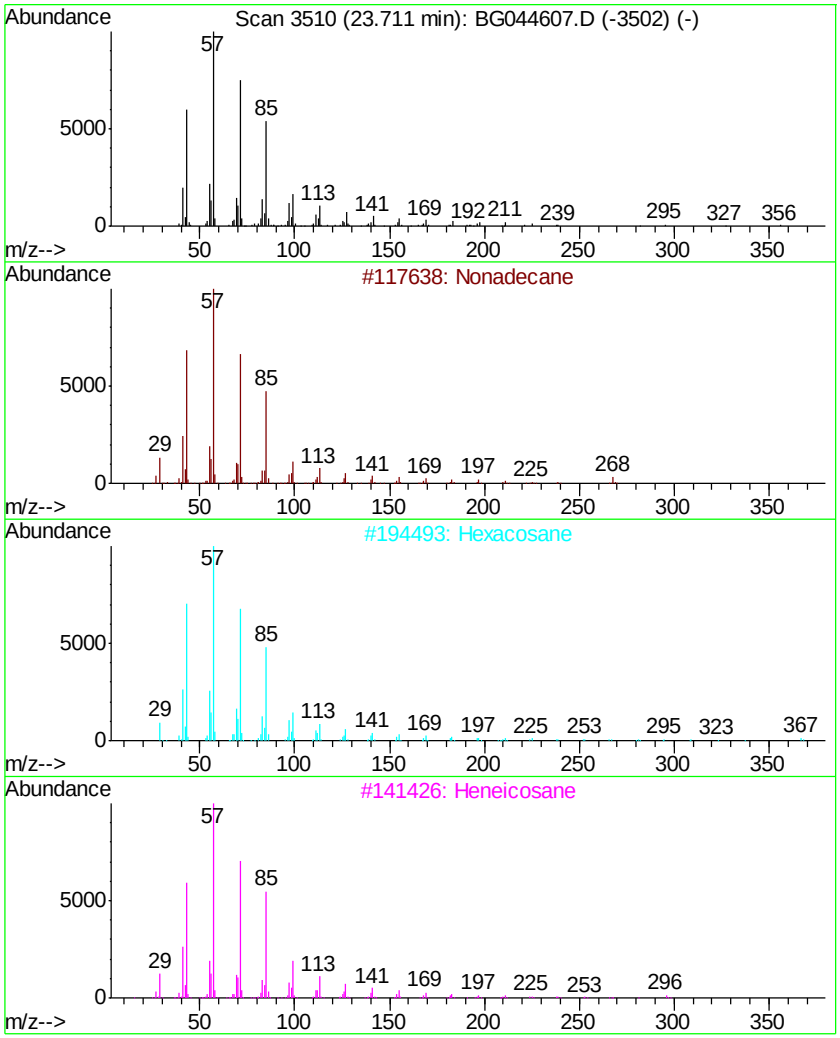
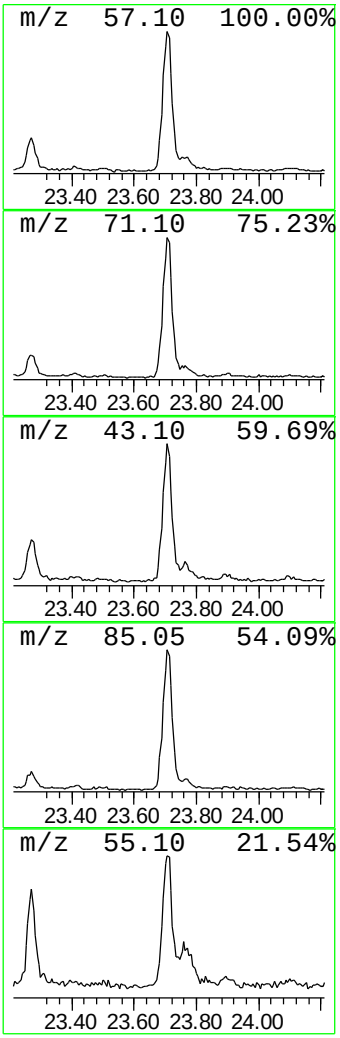
Peak Number 10 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.71	4.86 ng	343641	Perylene-d12	24.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	95
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Octadecane	254	C18H38	000593-45-3	91





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Operator : CG/JU
Sample : L1681-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SH-BORING-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG022420.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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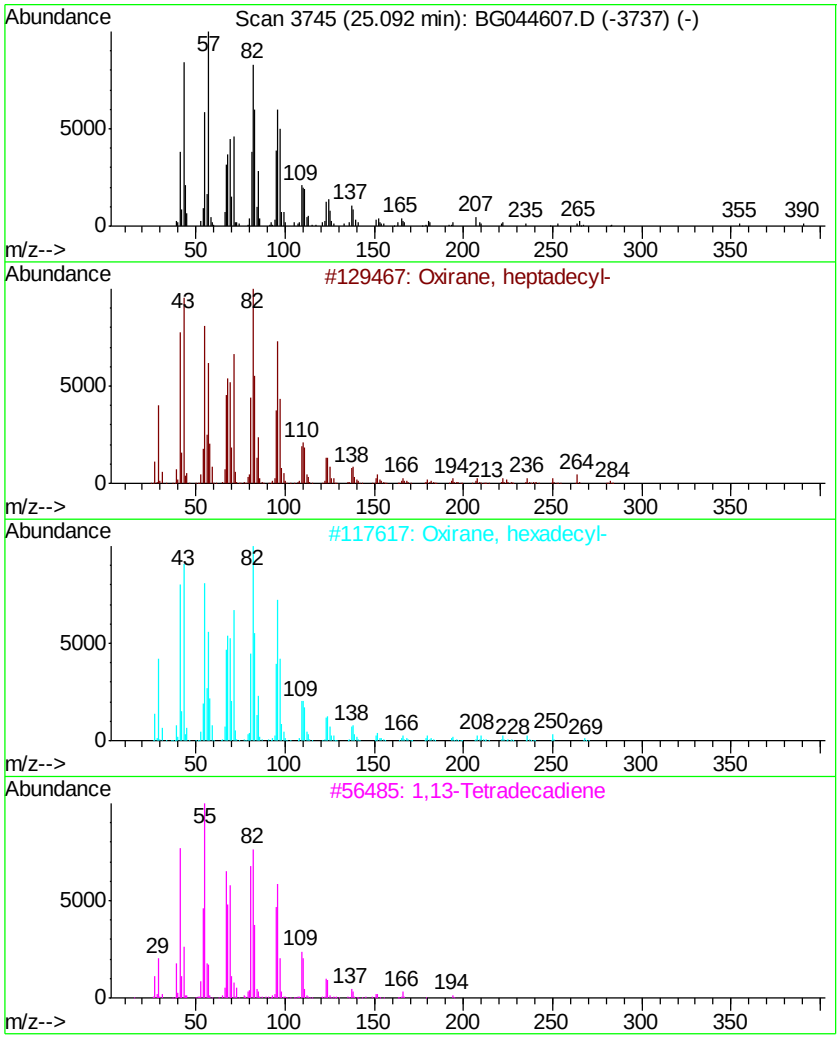
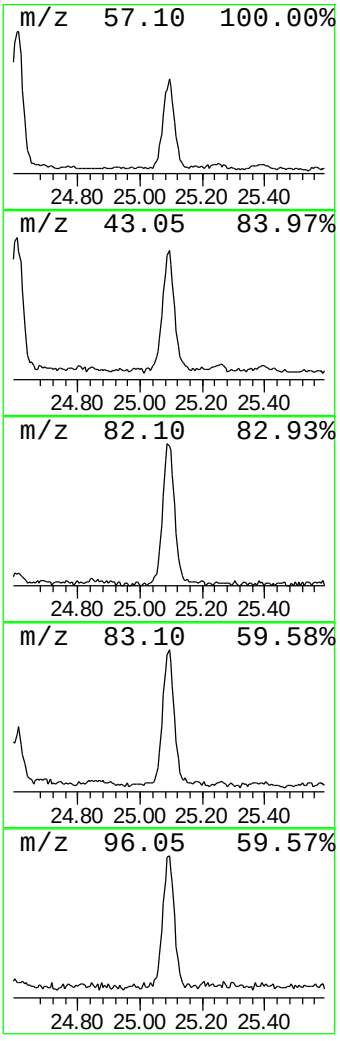
Peak Number 11 Oxirane, heptadecyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.09	4.44 ng	314310	Perylene-d12	24.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	96
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3	1,13-Tetradecadiene	194	C14H26	021964-49-8	83
4	16-Octadecenal	266	C18H34O	056554-87-1	83
5	(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	81





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Data File : BG044607.D
Acq On : 26 Feb 2020 17:25
Operator : CG/JU
Sample : L1681-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SH-BORING-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG022420.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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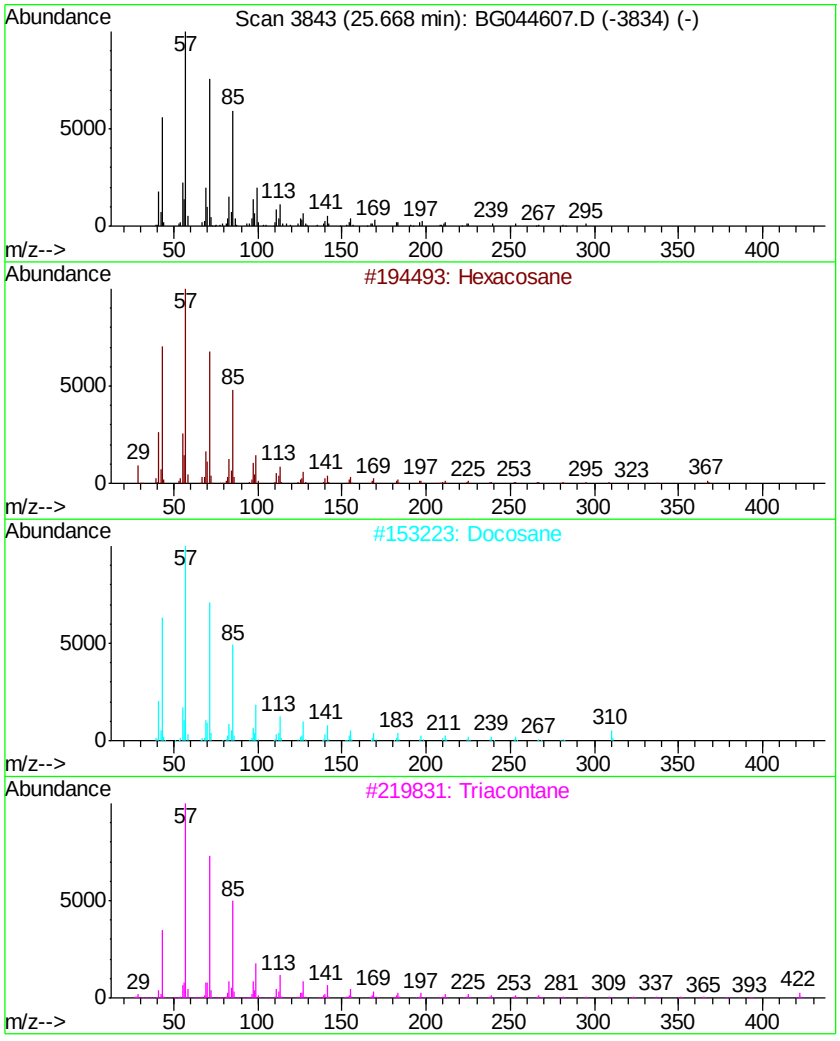
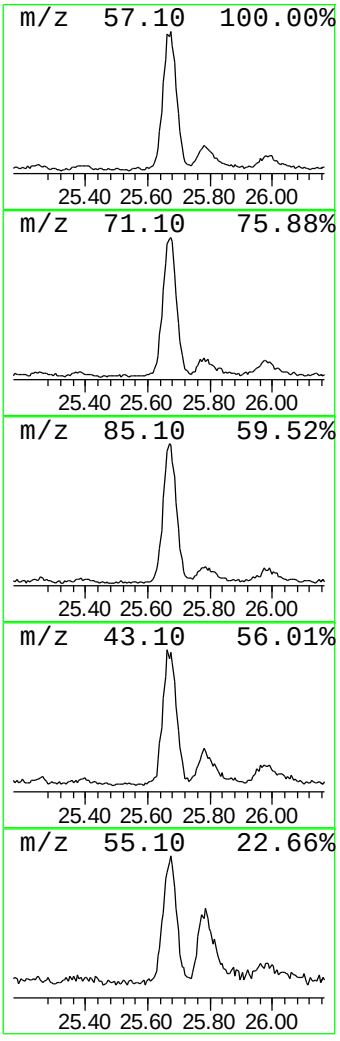
Peak Number 12 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.67	4.25 ng	300949	Perylene-d12	24.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	94
2	Docosane	310	C22H46	000629-97-0	91
3	Triacontane	422	C30H62	000638-68-6	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Octacosane	394	C28H58	000630-02-4	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022620\
Data File : BG044607.D
Acq On : 26 Feb 2020 17:25
Operator : CG/JU
Sample : L1681-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SH-BORING-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG022420.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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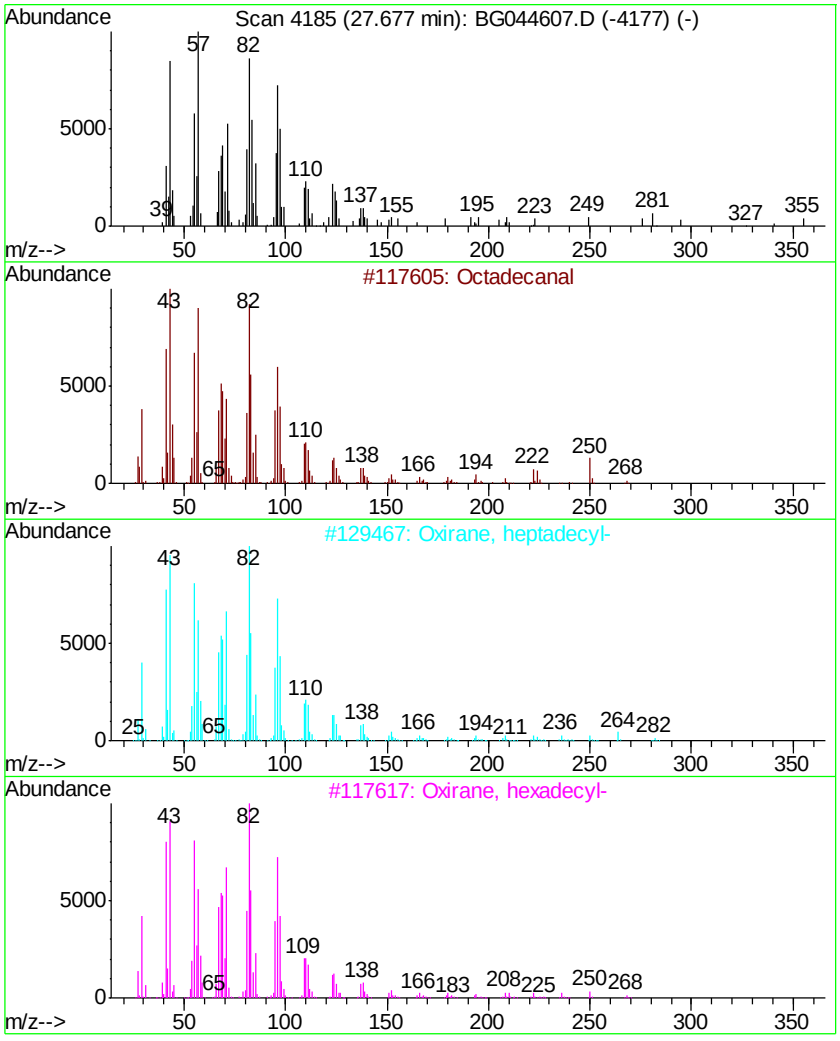
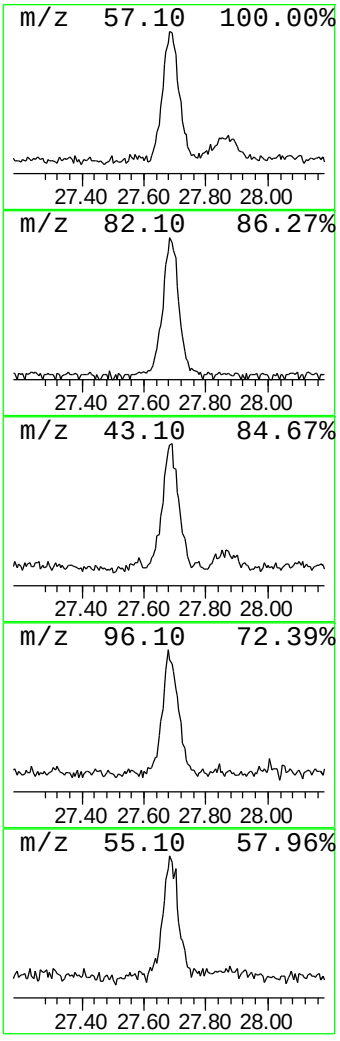
Peak Number 13 Octadecanal Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.68	3.11 ng	220191	Perylene-d12	24.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	91
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
4	Tetradecanal	212	C14H28O	000124-25-4	87
5	12-Octadecenal	266	C18H34O	056554-91-7	80





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022620\
Data File : BG044607.D
Acq On : 26 Feb 2020 17:25
Operator : CG/JU
Sample : L1681-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SH-BORING-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG022420.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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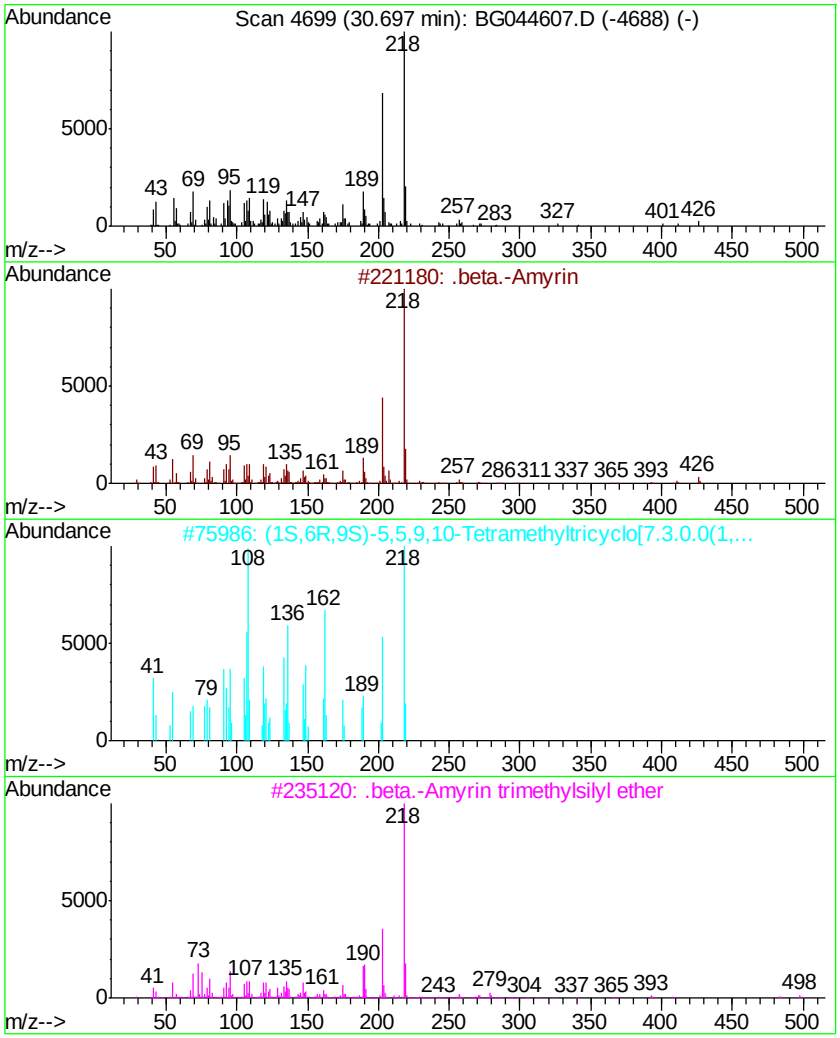
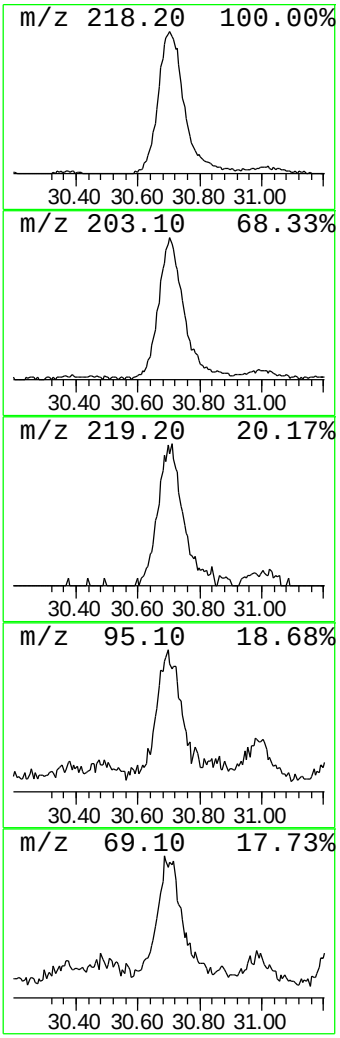
Peak Number 14 .beta.-Amyrin Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.70	7.80 ng	551894	Perylene-d12	24.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Amyrin	426	C30H50O	000559-70-6	89
2	(1S,6R,9S)-5,5,9,10-Tetramethylt...	218	C16H26	1000298-97-8	87
3	.beta.-Amyrin trimethylsilyl ether	498	C33H58OSi	001721-67-1	74
4	8-Amino-6,7-dimethoxy-4-methylqu...	218	C12H14N2O2	1000213-07-2	74
5	Pyrene, hexadecahydro-	218	C16H26	002435-85-0	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG022620\
Data File : BG044607.D
Acq On : 26 Feb 2020 17:25
Operator : CG/JU
Sample : L1681-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SH-BORING-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG022420.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
trans-.beta.-Ocimene	6.56	3.2	ng	60869	1	7.87	379893	20.0
Scopoletin	18.42	3.9	ng	198040	4	17.26	1017670	20.0
Cinnamyl cinnamate	20.99	15.9	ng	957839	5	21.50	1206740	20.0
Heptadecyl heptaf...	21.17	12.7	ng	764796	5	21.50	1206740	20.0
Hexadecane	21.70	3.2	ng	192641	5	21.50	1206740	20.0
Sulfurous acid, p...	22.29	9.8	ng	591670	5	21.50	1206740	20.0
Heneicosane	22.94	4.8	ng	286729	5	21.50	1206740	20.0
Oxirane, hexadecyl-	23.27	2.8	ng	198498	6	24.56	1415120	20.0
Nonadecane	23.71	4.9	ng	343641	6	24.56	1415120	20.0
Oxirane, heptadecyl-	25.09	4.4	ng	314310	6	24.56	1415120	20.0
Hexacosane	25.67	4.3	ng	300949	6	24.56	1415120	20.0
Octadecanal	27.68	3.1	ng	220191	6	24.56	1415120	20.0
.beta.-Amyrin	30.70	7.8	ng	551894	6	24.56	1415120	20.0