LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG050919\
Data File : BG040843.D
Acq On : 10 May 2019 9:39
Operator : HP/JU
Sample : K2762-19
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P021-SS004-0002-01

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-BG042319.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	3.153	4	11	19	rBV	124442	232415	5.46%	0.730%
2	3.229	20	24	36	rVB	251978	344054	8.08%	1.081%
3	5.673	433	440	454	rBV	1329382	2080988	48.89%	6.539%
4	7.283	703	714	729	rBV	1434187	2489941	58.49%	7.824%
5	7.665	770	779	790	rBV	1344700	2310339	54.28%	7.260%
6	8.141	854	860	871	rVB	187588	324464	7.62%	1.020%
7	8.464	906	915	930	rVB	984325	1663445	39.08%	5.227%
8	9.322	1051	1061	1070	rBV	852622	1561224	36.68%	4.906%
9	10.967	1332	1341	1349	rBV	245926	463021	10.88%	1.455%
10	13.394	1747	1754	1762	rVB	2140451	3245668	76.25%	10.199%
11	14.211	1888	1893	1899	rBV	354379	511073	12.01%	1.606%
12	14.769	1981	1988	1997	rVB2	434749	701992	16.49%	2.206%
13	16.255	2233	2241	2254	rBV	2022119	3066189	72.03%	9.635%
14	17.513	2447	2455	2468	rBV2	605856	928534	21.81%	2.918%
15	18.370	2595	2601	2609	rBV	403416	605972	14.24%	1.904%
16	19.628	2810	2815	2822	rBV	214156	321166	7.54%	1.009%
17	20.110	2890	2897	2905	rBV	3248612	4256723	100.00%	13.376%
18	21.402	3112	3117	3133	rBV6	88096	285972	6.72%	0.899%
19	21.796	3177	3184	3196	rVB2	573343	997592	23.44%	3.135%
20	21.949	3206	3210	3214	rVB5	30923	52880	1.24%	0.166%
21	22.577	3312	3317	3322	rBV2	73503	118104	2.77%	0.371%
22	22.642	3322	3328	3339	rVV2	44433	136262	3.20%	0.428%
23	23.288	3431	3438	3445	rBV3	83831	180366	4.24%	0.567%
24	23.488	3468	3472	3482	rVB2	49378	109573	2.57%	0.344%
25	23.670	3493	3503	3510	rBV	362729	750907	17.64%	2.360%
26	24.134	3574	3582	3589	rVB2	256146	556178	13.07%	1.748%
27	24.222	3589	3597	3616	rBV3	323301	1305540	30.67%	4.102%
28	25.151	3743	3755	3766	rBV2	289008	941896	22.13%	2.960%
29	25.679	3836	3845	3853	rVB3	126964	366440	8.61%	1.151%
30	26.302	3941	3951	3960	rVB3	193875	581168	13.65%	1.826%
31	28.558	4325	4335	4351	rVB6	85070	333574	7.84%	1.048%

Sum of corrected areas: 31823660

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG050919\
Data File : BG040843.D
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Misc :
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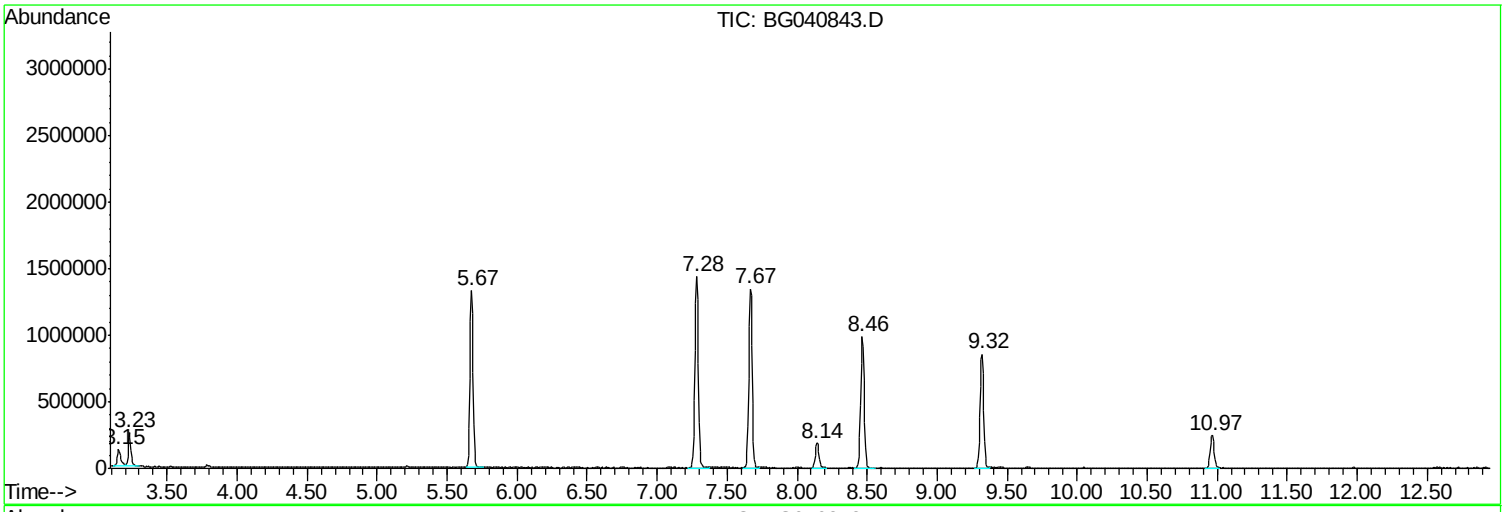
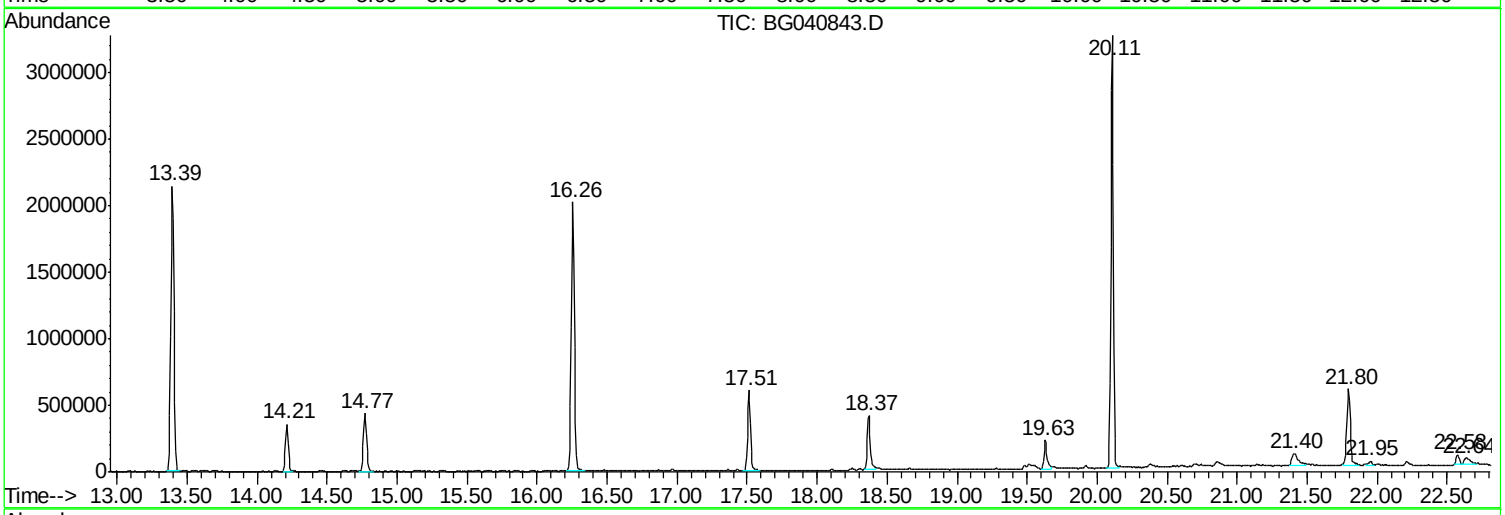
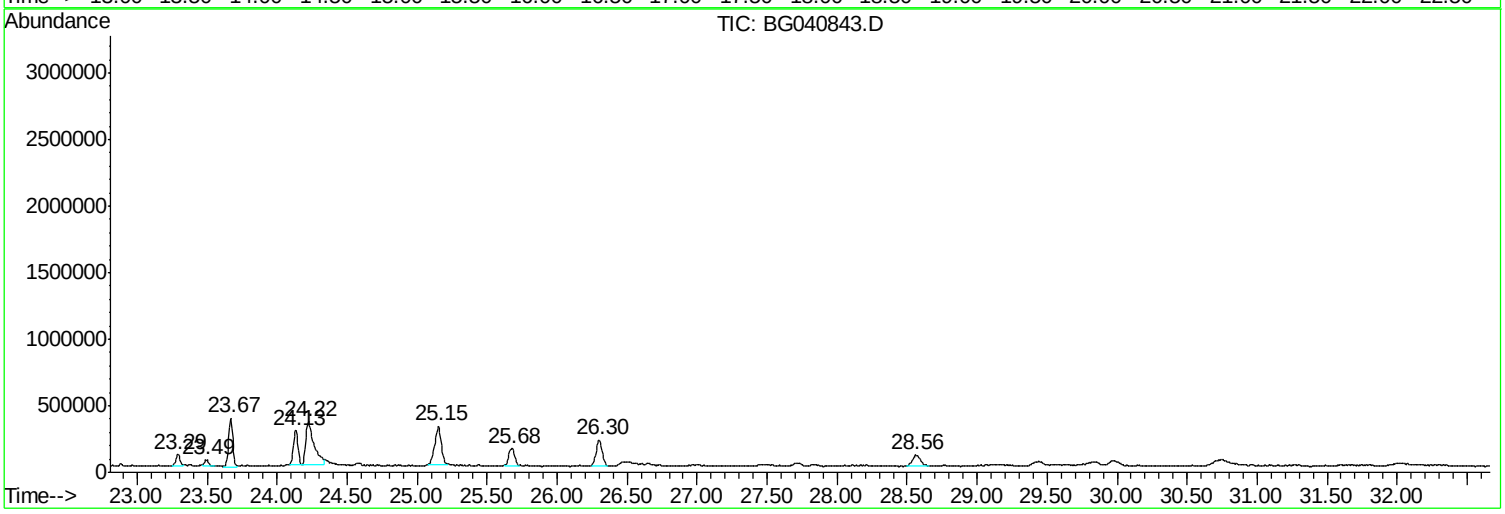
Instrument :
BNA_G
ClientSampleId :
P021-SS004-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

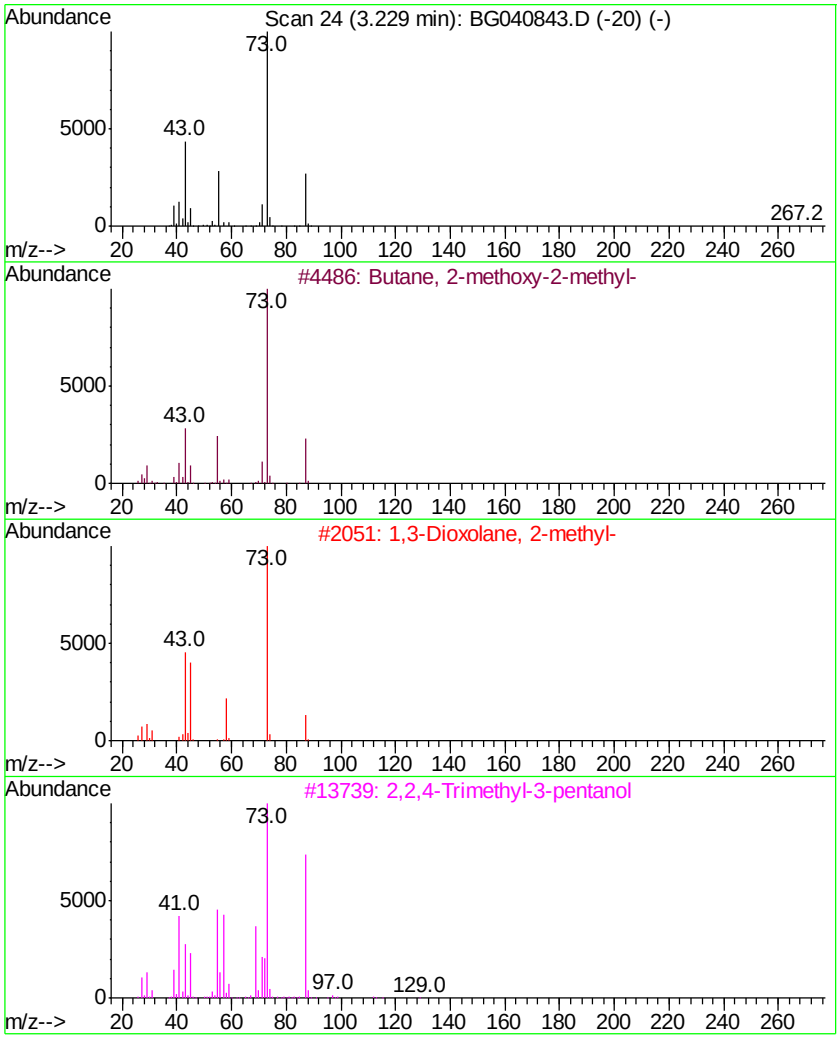
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

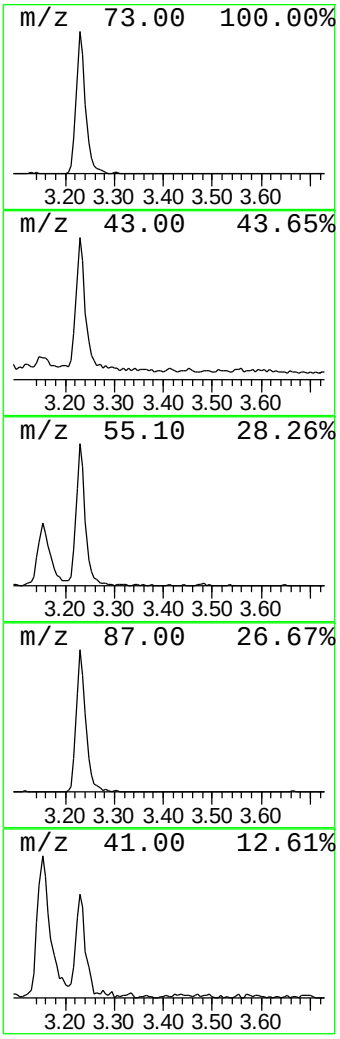
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.23	21.21 ng	344054	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	38
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Operator : HP/JU
Sample : K2762-19
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P021-SS004-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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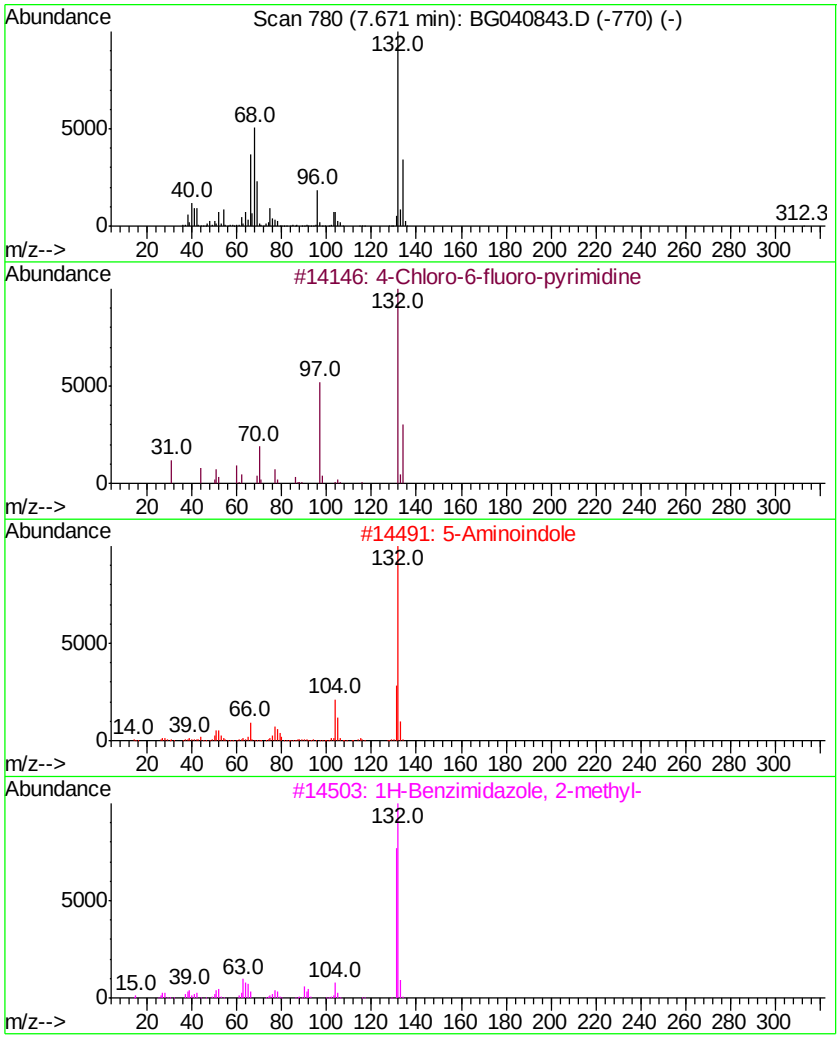
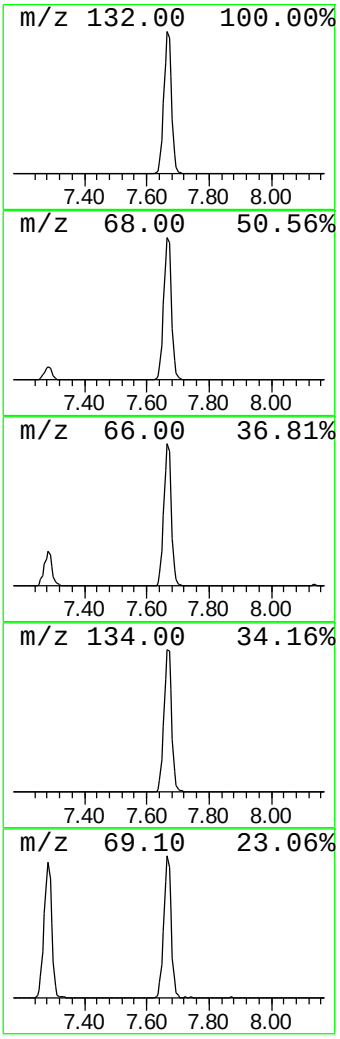
****

Peak Number 3 unknown7.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.67	142.41 ng	2310340	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	22
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	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

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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P021-SS004-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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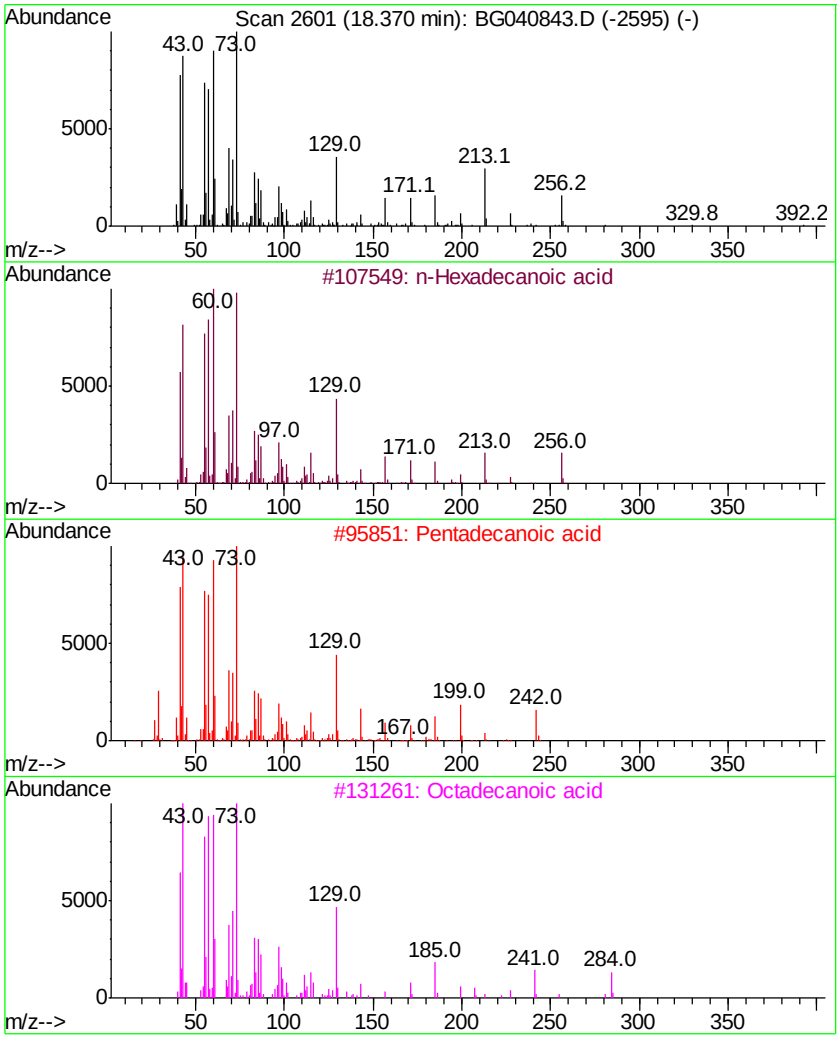
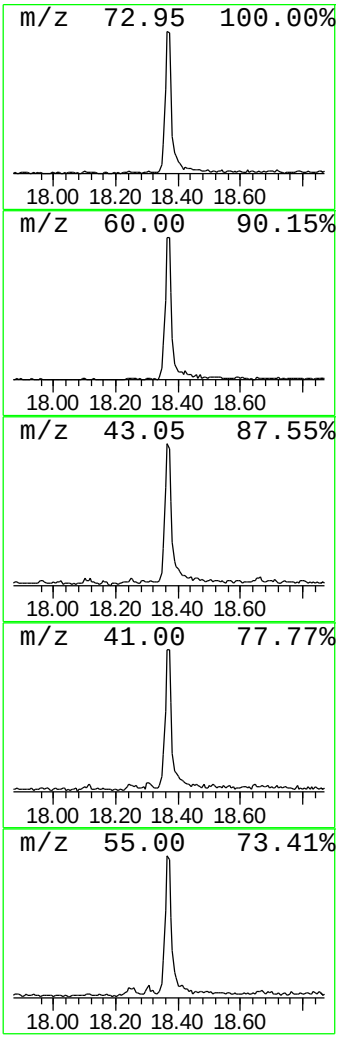
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.37	13.05 ng	605972	Phenanthrene-d10	17.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Octadecanoic acid	284	C18H36O2	000057-11-4	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	70
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





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Instrument :
BNA_G
ClientSampleId :
P021-SS004-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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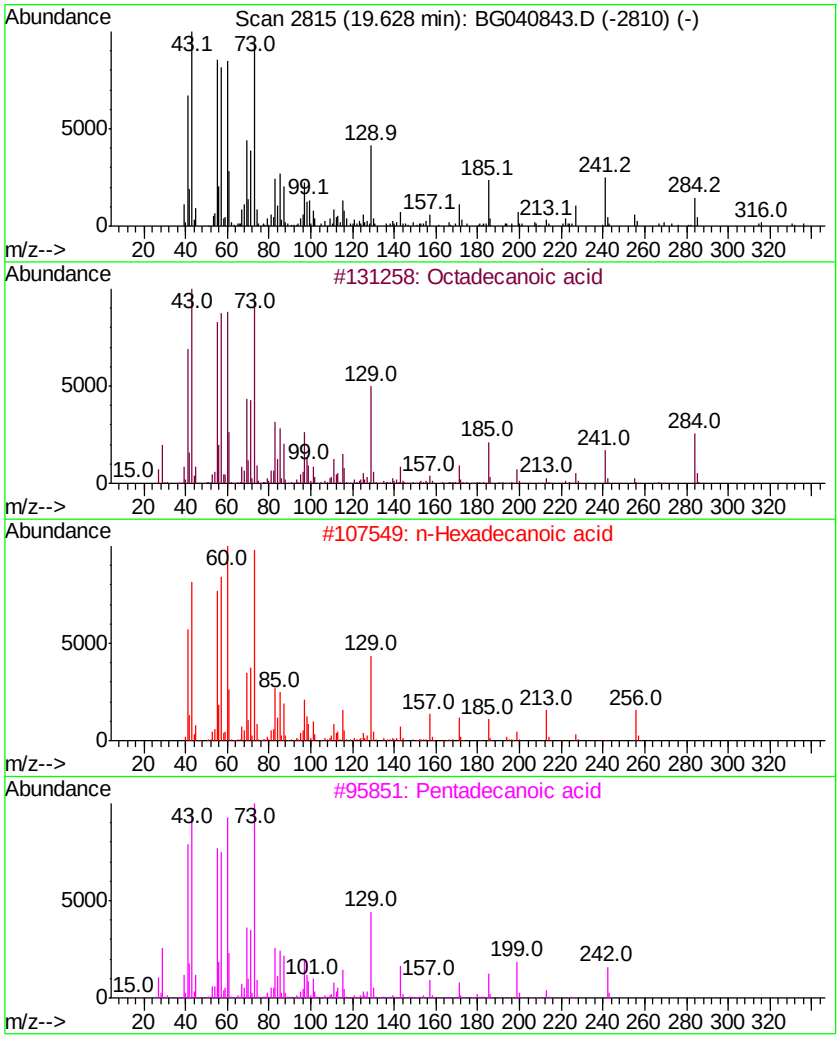
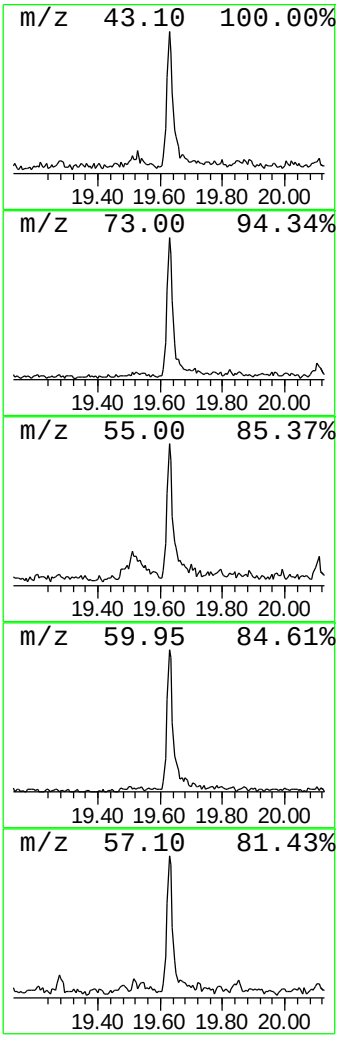
****

Peak Number 6 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.63	6.92 ng	321166	Phenanthrene-d10	17.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Tridecanoic acid	214	C13H26O2	000638-53-9	72





Library Search Compound Report

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Misc :
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Instrument :
BNA_G
ClientSampleId :
P021-SS004-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

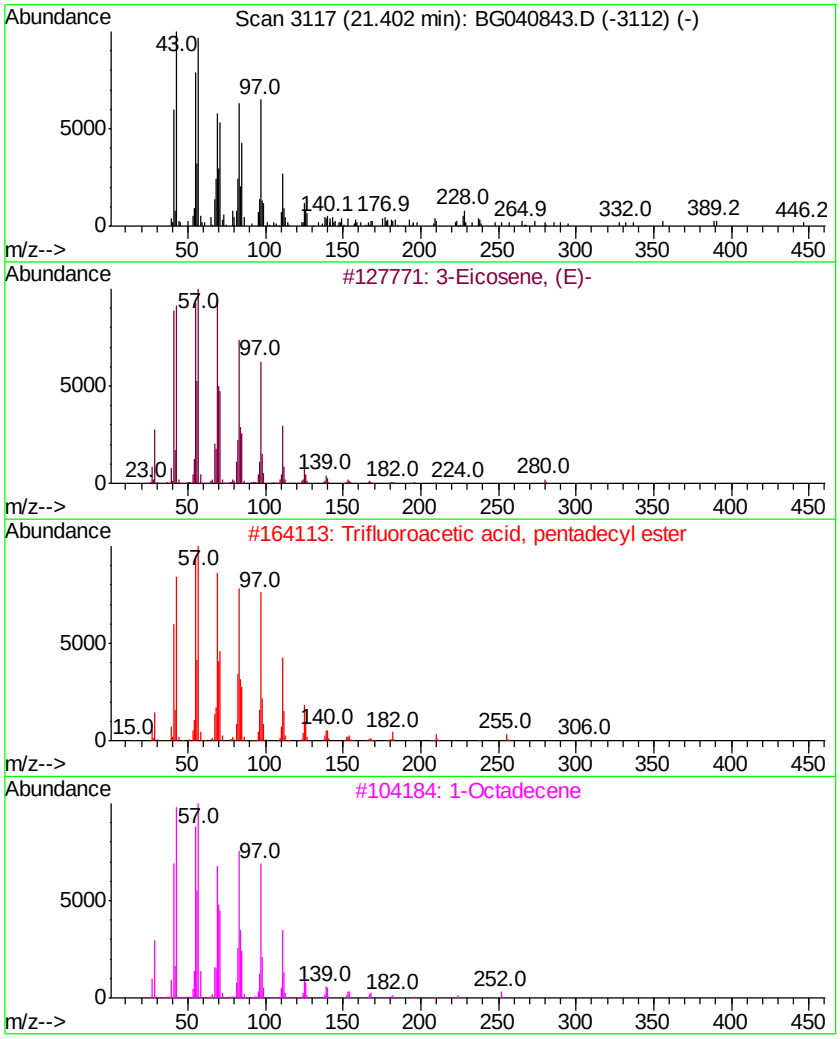
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

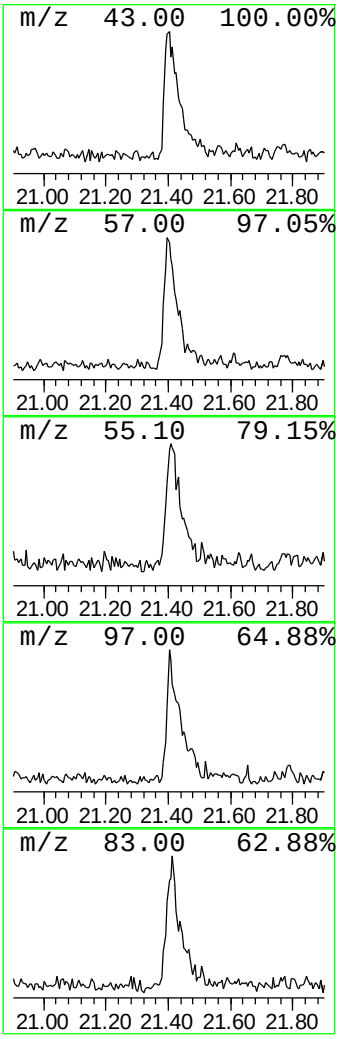
****

Peak Number 7 3-Eicosene, (E)- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.40	5.73 ng	285972	Chrysene-d12	21.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	95
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
3	1-Octadecene	252	C18H36	000112-88-9	93
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5	Cyclopentadecane	210	C15H30	000295-48-7	90





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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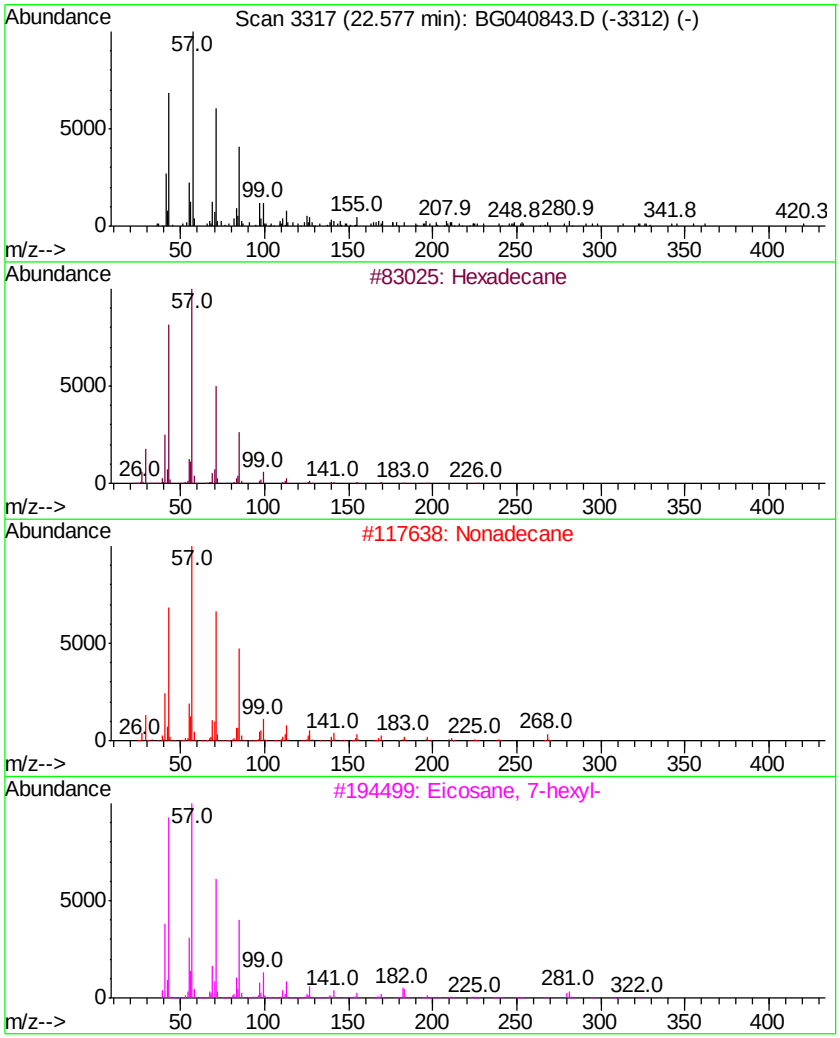
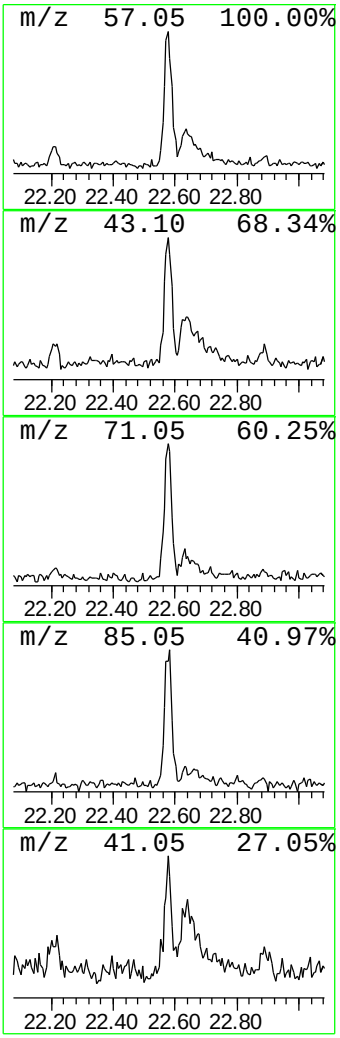
****

Peak Number 8 Hexadecane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.58	2.37 ng	118104	Chrysene-d12	21.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	93
2	Nonadecane	268	C19H40	000629-92-5	91
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Tetracosane	338	C24H50	000646-31-1	87





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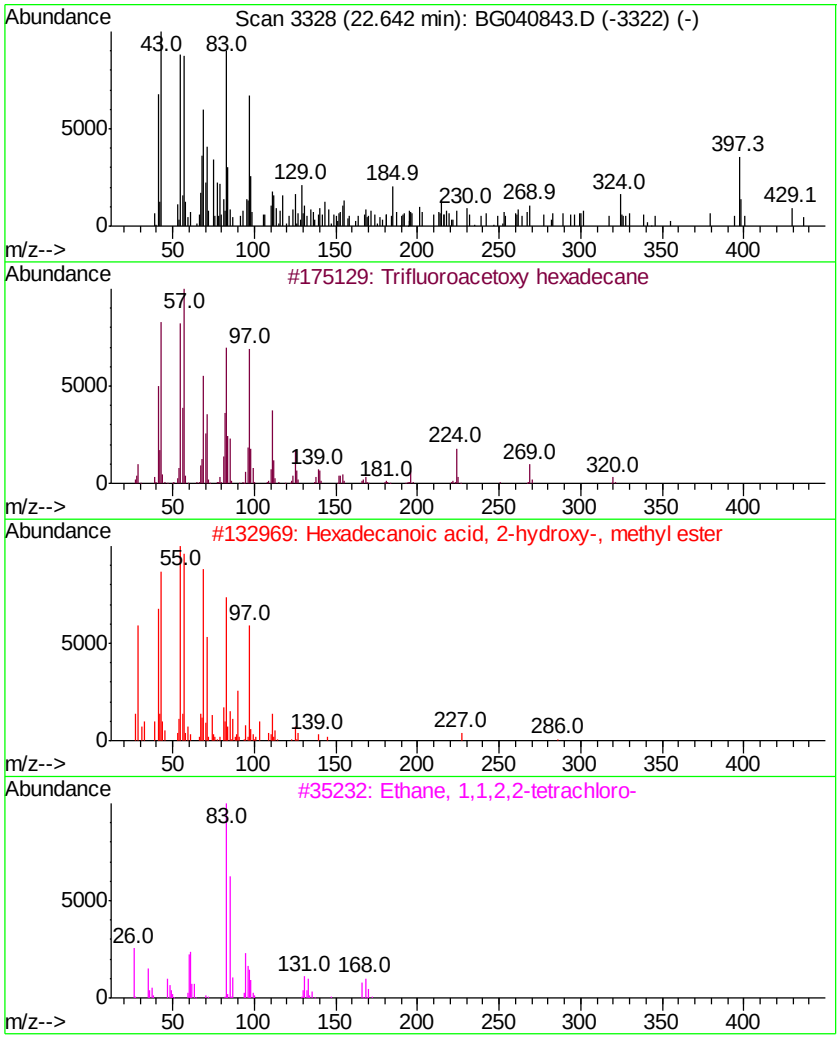
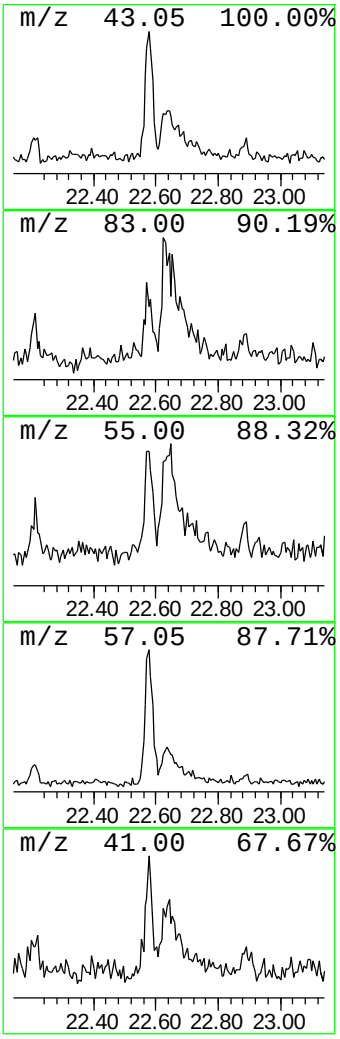
****

Peak Number 9 unknown22.64 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.64	2.73 ng	136262	Chrysene-d12	21.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	49
2	Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	38
3	Ethane, 1,1,2,2-tetrachloro-	166	C2H2Cl4	000079-34-5	27
4	ANHYDRO-4,6-DIMETHYL-3-[3,4-DICH...	324	C13H10Cl2N4O2	1000214-56-5	25
5	Oxalic acid, hexadecyl propyl ester	356	C21H40O4	1000309-26-9	16





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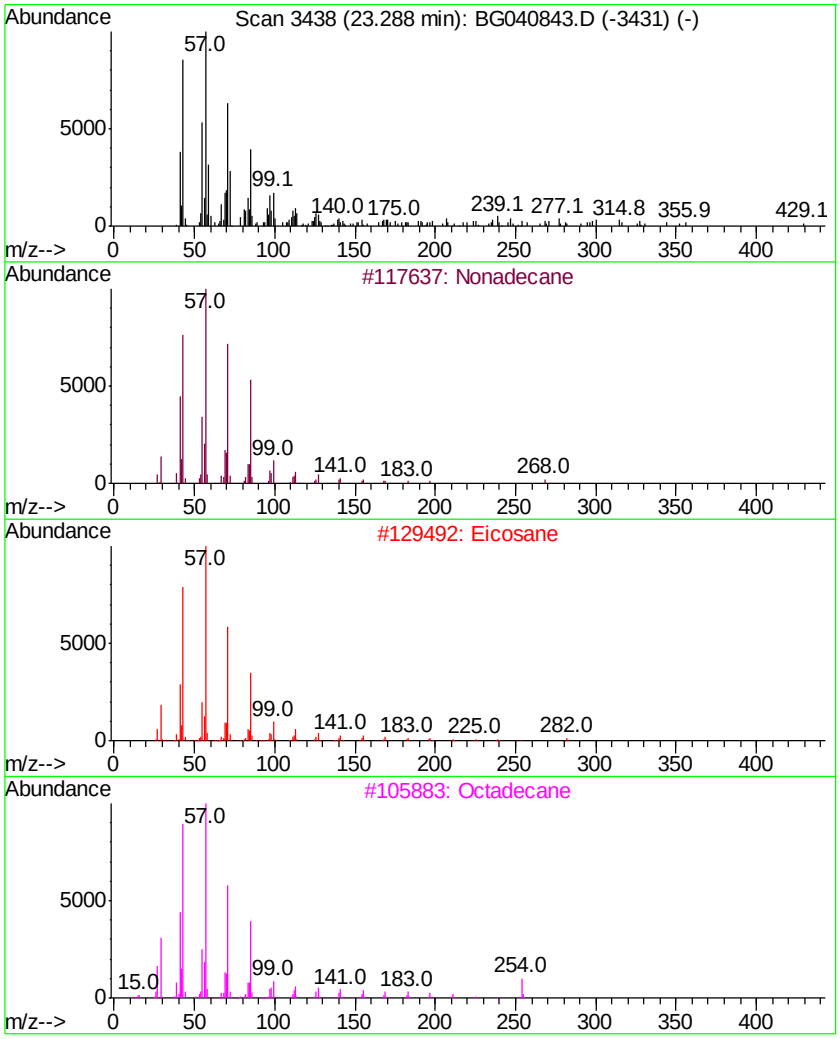
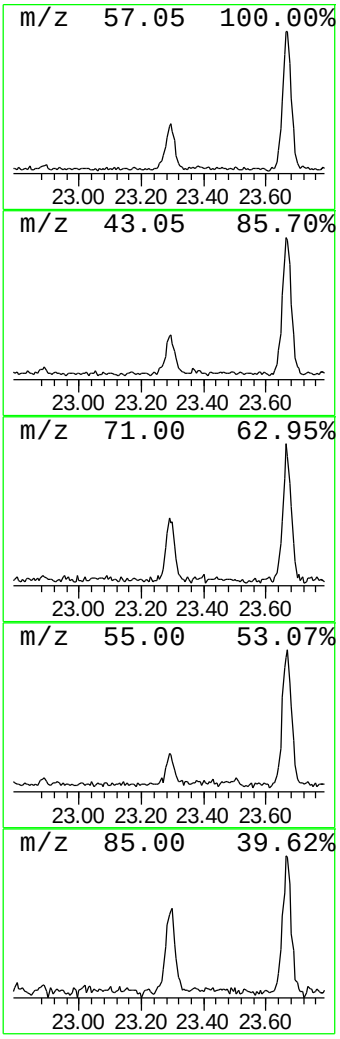
****

Peak Number 10 Nonadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.29	3.62 ng	180366	Chrysene-d12	21.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	92
2	Eicosane	282	C20H42	000112-95-8	90
3	Octadecane	254	C18H38	000593-45-3	78
4	Heneicosane	296	C21H44	000629-94-7	78
5	Heptadecane	240	C17H36	000629-78-7	60





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ALS Vial : 22 Sample Multiplier: 1

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
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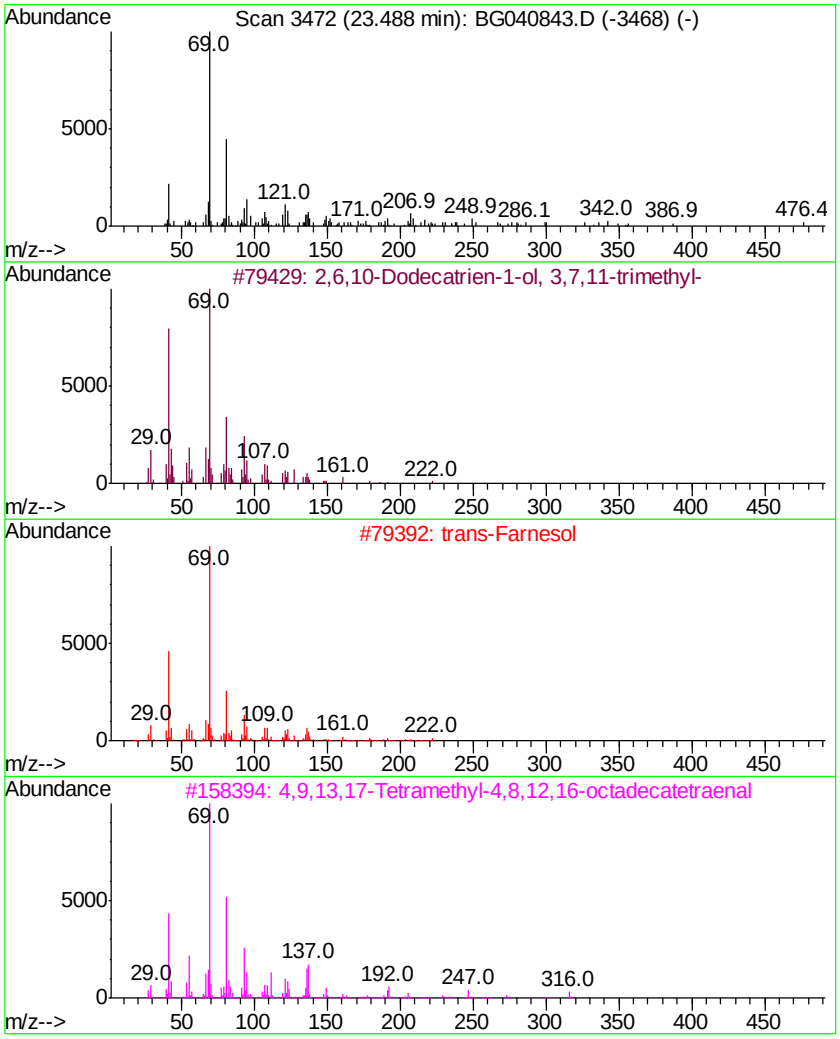
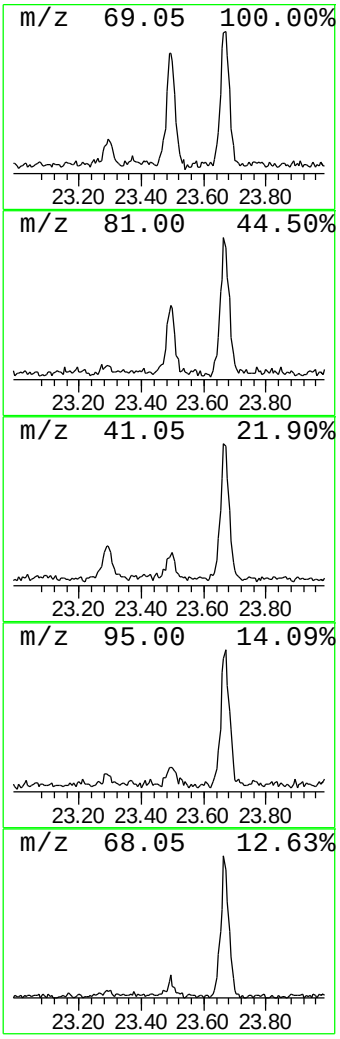
****
Peak Number 11 2,6,10-Dodecatrien-1-ol, 3,... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.49	2.33 ng	109573	Perylene-d12	25.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72
2	trans-Farnesol	222	C15H26O	000106-28-5	72
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	64
4	Squalene	410	C30H50	000111-02-4	50
5	6,10-Dodecadien-1-yn-3-ol, 3,7,1...	220	C15H24O	002387-68-0	50





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG050919\
Data File : BG040843.D
Acq On : 10 May 2019 9:39
Operator : HP/JU
Sample : K2762-19
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P021-SS004-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.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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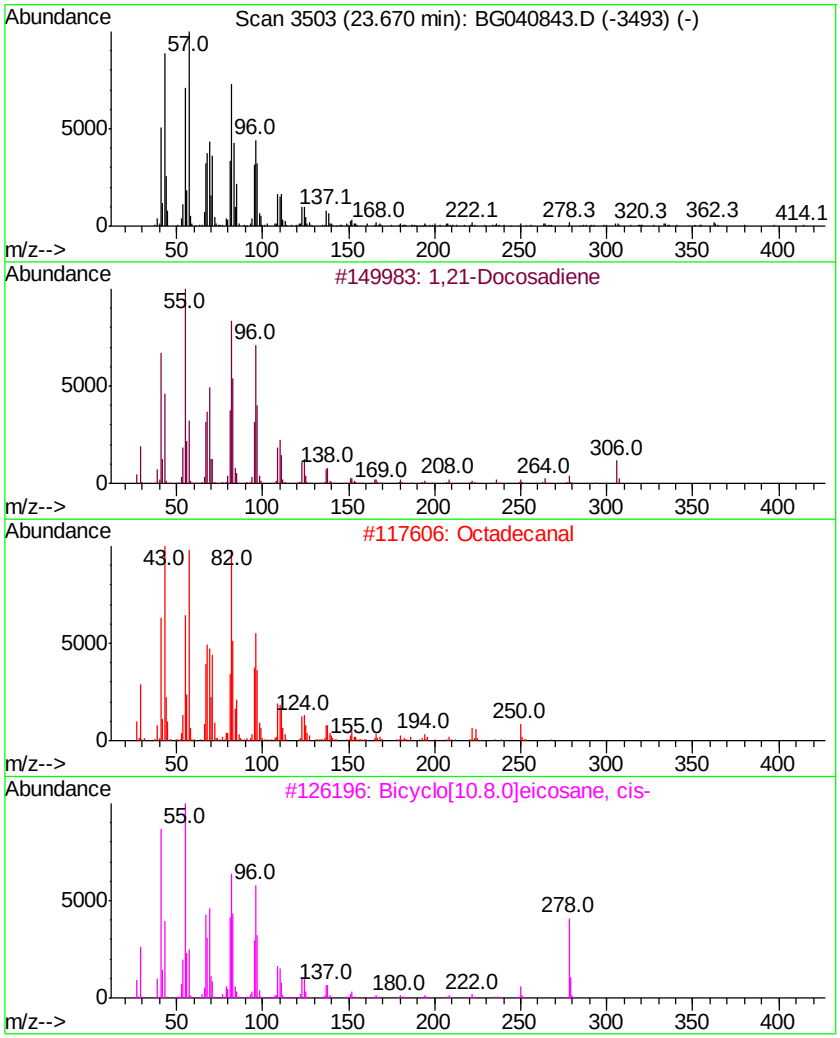
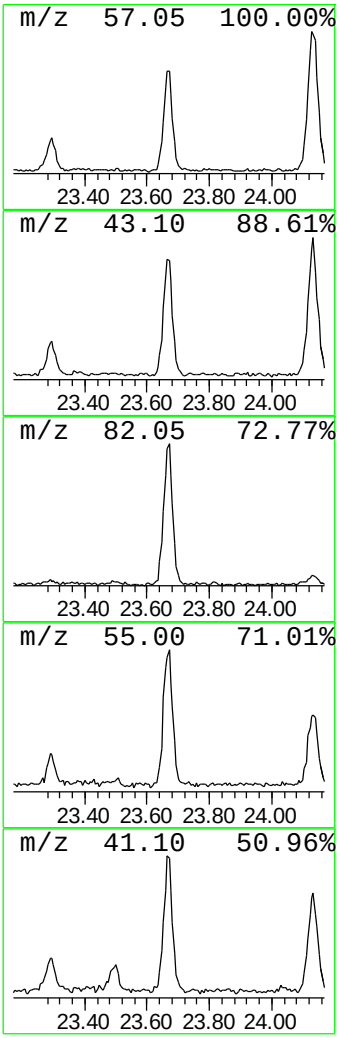
Peak Number 12 1,21-Docosadiene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.67	15.94 ng	750907	Perylene-d12	25.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,21-Docosadiene	306	C22H42	053057-53-7	96
2	Octadecanal	268	C18H36O	000638-66-4	95
3	Bicyclo[10.8.0]eicosane, cis-	278	C20H38	1000155-82-2	93
4	(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	93
5	Oxirane, tetradecyl-	240	C16H32O	007320-37-8	92





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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P021-SS004-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.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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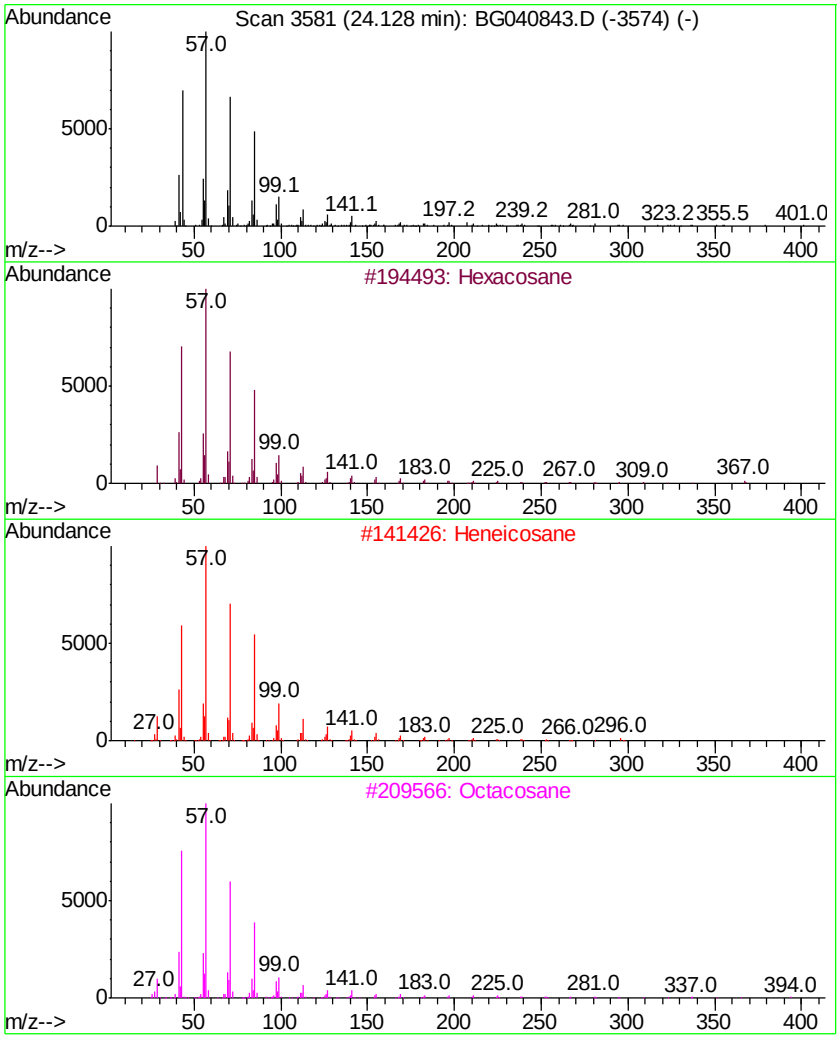
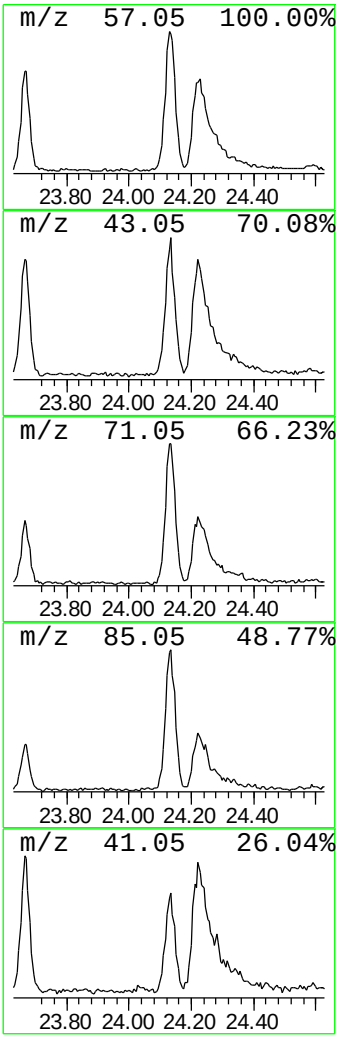
Peak Number 13 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.13	11.81 ng	556178	Perylene-d12	25.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Heneicosane	296	C21H44	000629-94-7	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Tetracosane	338	C24H50	000646-31-1	90
5	Triacontane	422	C30H62	000638-68-6	87





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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P021-SS004-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
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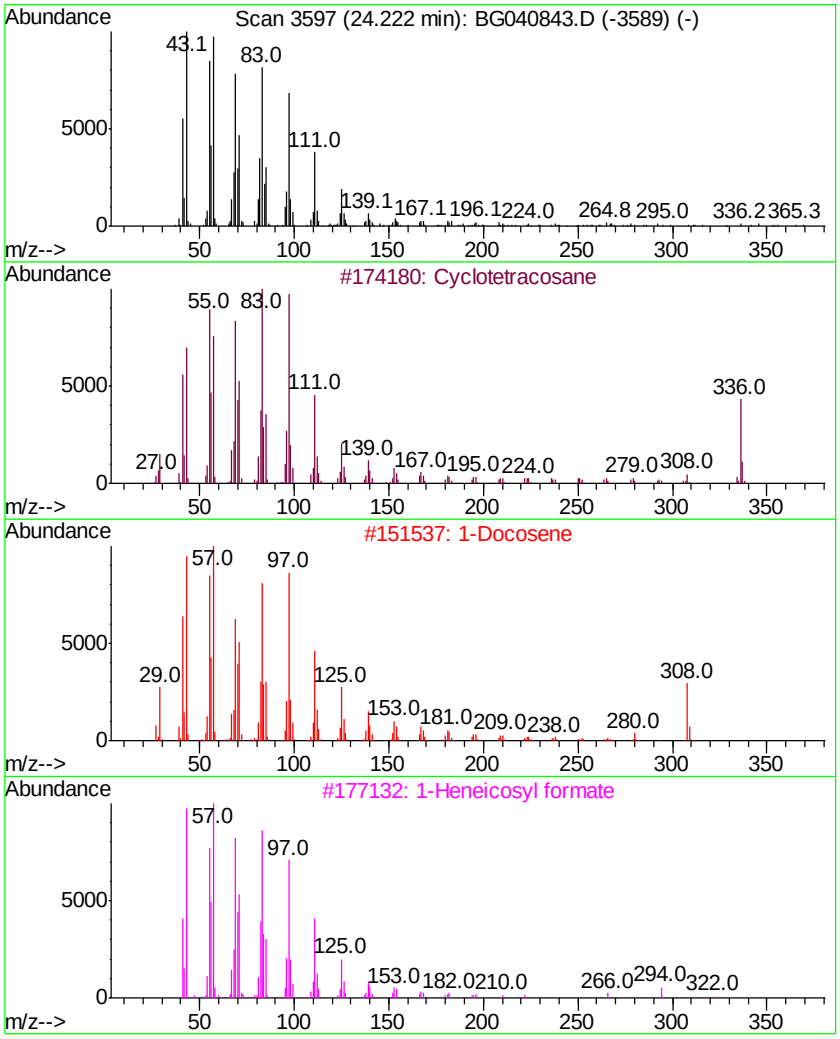
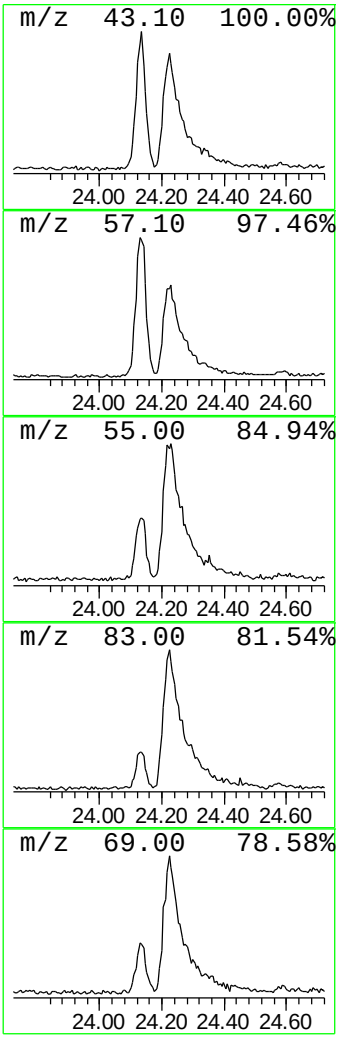
Peak Number 14 Cyclotetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.22	27.72 ng	1305540	Perylene-d12	25.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	99
2	1-Docosene	308	C22H44	001599-67-3	95
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	86





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ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P021-SS004-0002-01

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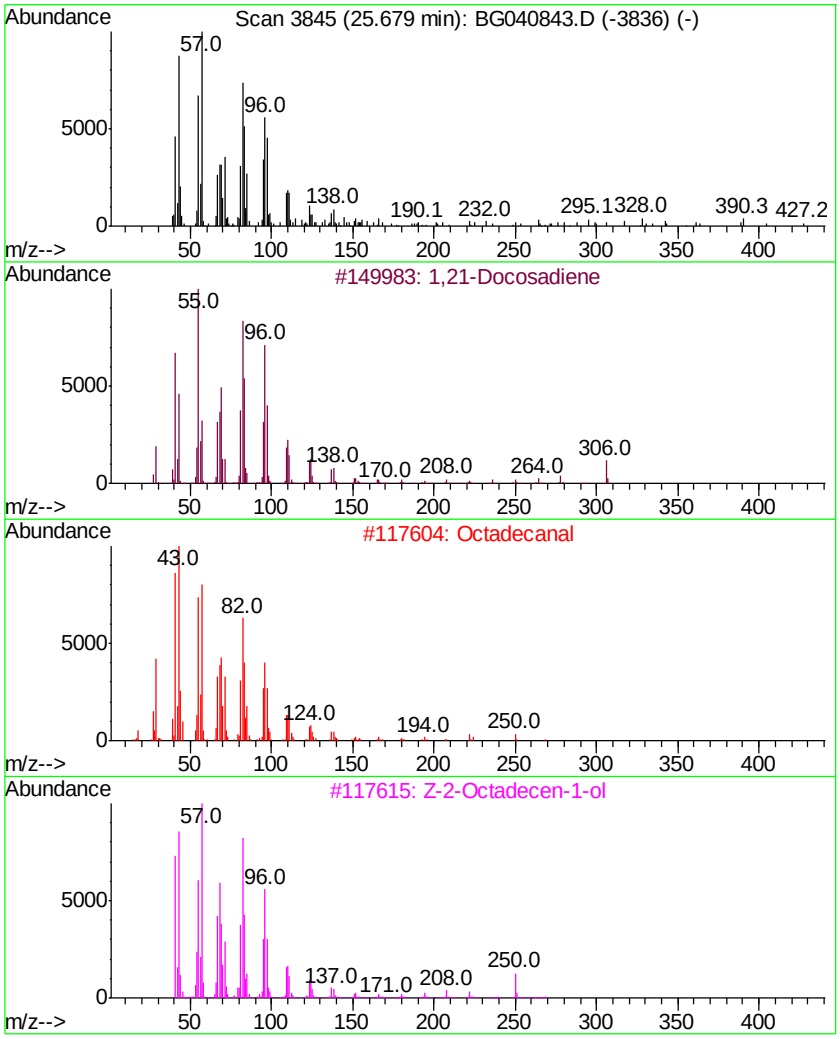
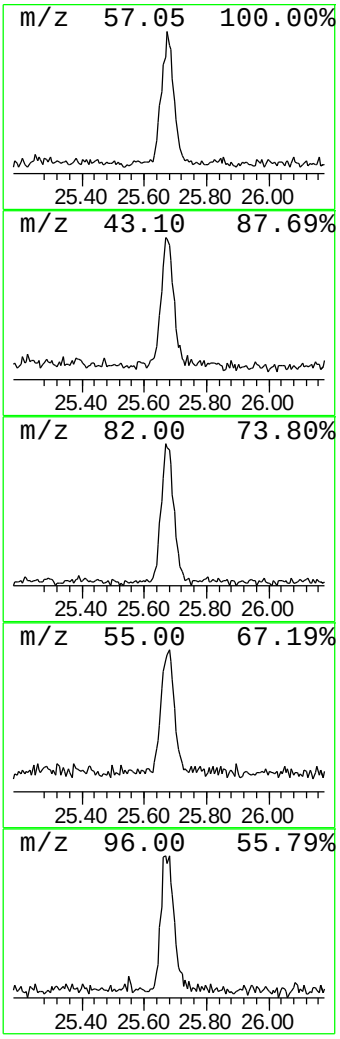
Peak Number 15 Octadecanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.68	7.78 ng	366440	Perylene-d12	25.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,21-Docosadiene	306	C22H42	053057-53-7	93
2	Octadecanal	268	C18H36O	000638-66-4	91
3	Z-2-Octadecen-1-ol	268	C18H36O	1000131-11-0	90
4	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
5	(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	83





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Misc :
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BNA_G
ClientSampleId :
P021-SS004-0002-01

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TIC Integration Parameters: LSCINT.P

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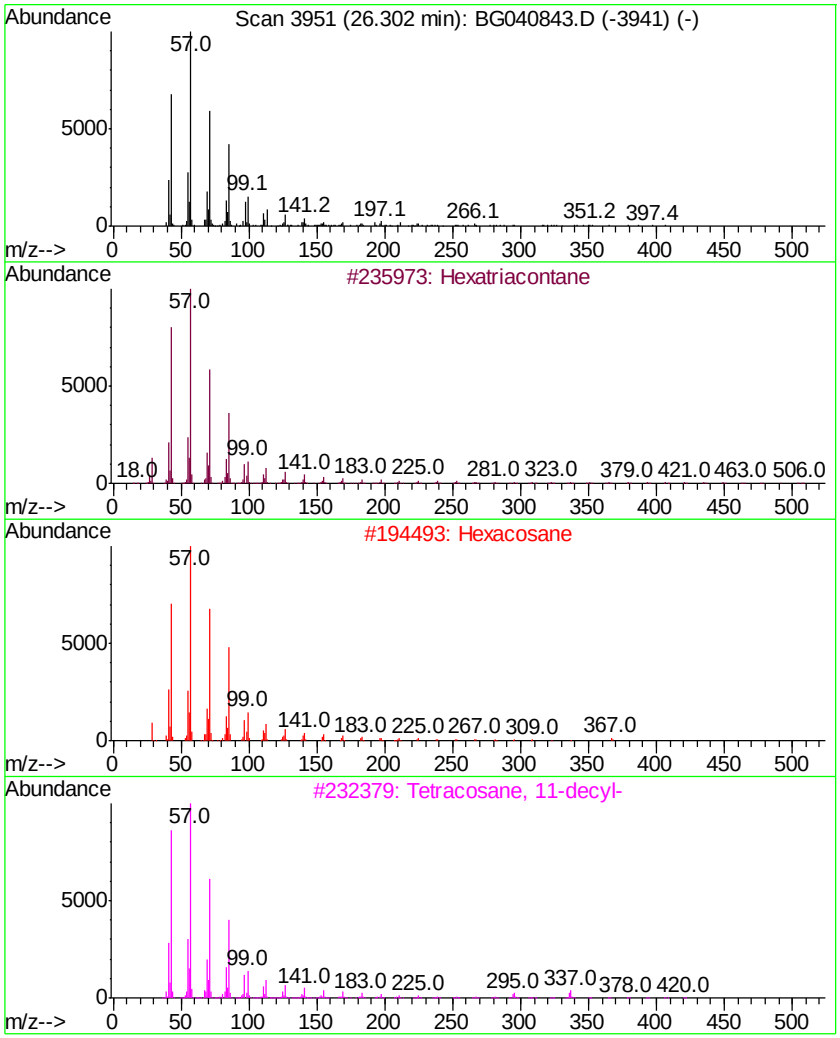
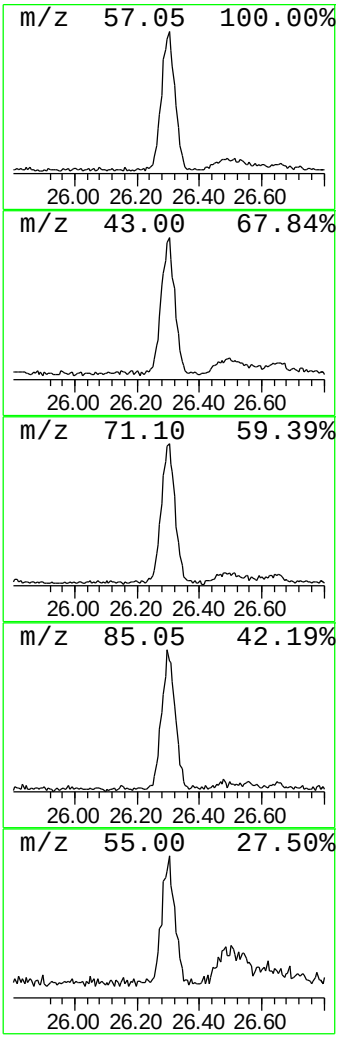
Peak Number 16 Hexatriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.30	12.34 ng	581168	Perylene-d12	25.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexatriacontane	507	C36H74	000630-06-8	91
2	Hexacosane	366	C26H54	000630-01-3	90
3	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	90
4	Heneicosane	296	C21H44	000629-94-7	87
5	Tetratetracontane	619	C44H90	007098-22-8	87





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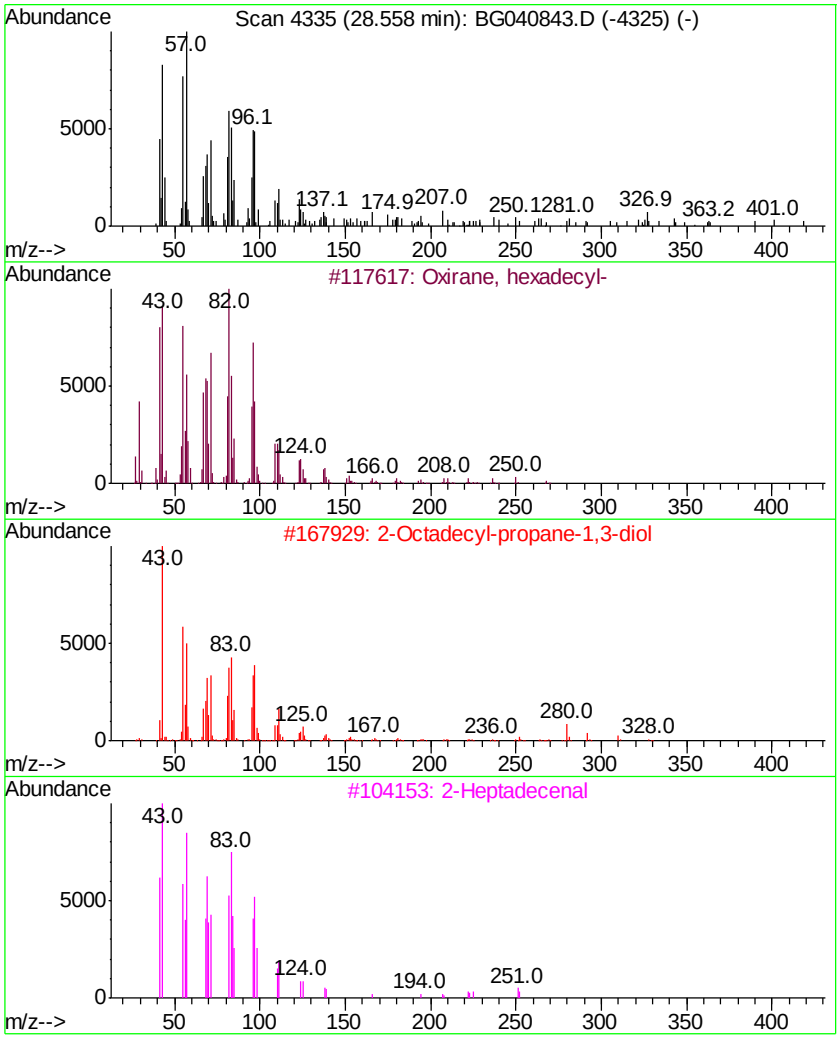
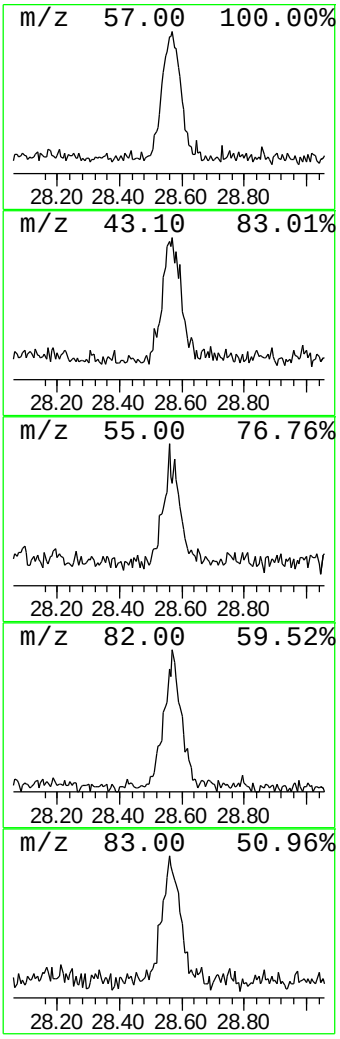
Peak Number 17 Oxirane, hexadecyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.56	7.08 ng	333574	Perylene-d12	25.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	92
2	2-Octadecyl-propane-1,3-diol	328	C21H44O2	005337-61-1	91
3	2-Heptadecenal	252	C17H32O	1000143-48-6	68
4	1-Hexacosene	364	C26H52	018835-33-1	58
5	Cyclohexane, 1-(1,5-dimethylhexy...	280	C20H40	056009-20-2	55





Tentatively Identified Compound (LSC) summary

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Acq On : 10 May 2019 9:39
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Instrument :
BNA_G
ClientSampleId :
P021-SS004-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
Butane, 2-methoxy...	3.23	21.2	ng	344054	1	8.14	324464	20.0
unknown7.67	7.67	142.4	ng	2310340	1	8.14	324464	20.0
n-Hexadecanoic acid	18.37	13.1	ng	605972	4	17.51	928534	20.0
Octadecanoic acid	19.63	6.9	ng	321166	4	17.51	928534	20.0
3-Eicosene, (E)-	21.40	5.7	ng	285972	5	21.80	997592	20.0
Hexadecane	22.58	2.4	ng	118104	5	21.80	997592	20.0
unknown22.64	22.64	2.7	ng	136262	5	21.80	997592	20.0
Nonadecane	23.29	3.6	ng	180366	5	21.80	997592	20.0
2,6,10-Dodecatrie...	23.49	2.3	ng	109573	6	25.15	941896	20.0
1,21-Docosadiene	23.67	15.9	ng	750907	6	25.15	941896	20.0
Hexacosane	24.13	11.8	ng	556178	6	25.15	941896	20.0
Cyclotetracosane	24.22	27.7	ng	1305540	6	25.15	941896	20.0
Octadecanal	25.68	7.8	ng	366440	6	25.15	941896	20.0
Hexatriacontane	26.30	12.3	ng	581168	6	25.15	941896	20.0
Oxirane, hexadecyl-	28.56	7.1	ng	333574	6	25.15	941896	20.0