LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG032019\
Data File : BG040046.D
Acq On : 20 Mar 2019 21:44
Operator : JU/SJ
Sample : K1935-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-18(14-15)

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-BG030419.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	3.196	14	18	26	rVV2	65254	103721	4.83%	0.557%
2	3.267	26	30	36	rVB	121065	153693	7.15%	0.825%
3	5.687	435	442	460	rVB	870233	1385821	64.50%	7.442%
4	7.290	706	715	728	rBV	891170	1606611	74.77%	8.628%
5	7.672	772	780	792	rBV	848235	1494994	69.58%	8.028%
6	8.142	852	860	870	rBV	164409	289073	13.45%	1.552%
7	8.465	907	915	922	rBV	610933	1040886	48.44%	5.590%
8	9.317	1052	1060	1073	rVB	539743	988117	45.99%	5.306%
9	10.962	1332	1340	1347	rBV	231602	416531	19.39%	2.237%
10	13.388	1746	1753	1761	rBV	1203086	1899957	88.42%	10.203%
11	14.211	1886	1893	1899	rBV	119318	173066	8.05%	0.929%
12	14.769	1981	1988	1996	rVB2	378008	613037	28.53%	3.292%
13	16.255	2234	2241	2252	rBV	1212761	1829527	85.15%	9.825%
14	17.512	2449	2455	2461	rBV2	491361	753530	35.07%	4.047%
15	18.364	2593	2600	2609	rBV2	69349	120043	5.59%	0.645%
16	19.621	2811	2814	2821	rBV6	20325	35091	1.63%	0.188%
17	20.020	2878	2882	2888	rVB	47389	53484	2.49%	0.287%
18	20.103	2890	2896	2902	rBV	1645264	2148687	100.00%	11.539%
19	20.373	2938	2942	2945	rBV2	15772	22057	1.03%	0.118%
20	21.060	3054	3059	3066	rVB	154562	188420	8.77%	1.012%
21	21.389	3110	3115	3126	rBV2	133641	351669	16.37%	1.889%
22	21.794	3178	3184	3192	rVB	454225	780089	36.31%	4.189%
23	21.941	3205	3209	3212	rVB2	30031	41291	1.92%	0.222%
24	22.200	3247	3253	3258	rBV	106248	166230	7.74%	0.893%
25	22.564	3309	3315	3318	rBV	70274	119817	5.58%	0.643%
26	22.611	3318	3323	3337	rVB3	126727	381648	17.76%	2.050%
27	23.275	3430	3436	3443	rVB2	78017	143141	6.66%	0.769%
28	23.645	3493	3499	3509	rVB2	22935	49954	2.32%	0.268%
29	24.103	3571	3577	3586	rVB	84021	179946	8.37%	0.966%
30	24.203	3588	3594	3605	rBV5	39545	133480	6.21%	0.717%
31	25.090	3738	3745	3748	rBV2	37939	91810	4.27%	0.493%
32	25.155	3748	3756	3768	rVB2	254413	707399	32.92%	3.799%
33	26.253	3934	3943	3952	rBV3	39694	122229	5.69%	0.656%
34	27.663	4176	4183	4190	rBV6	13618	36422	1.70%	0.196%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG032019\
Data File : BG040046.D
Acq On : 20 Mar 2019 21:44
Operator : JU/SJ
Sample : K1935-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-18(14-15)

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-BG030419.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 18621471

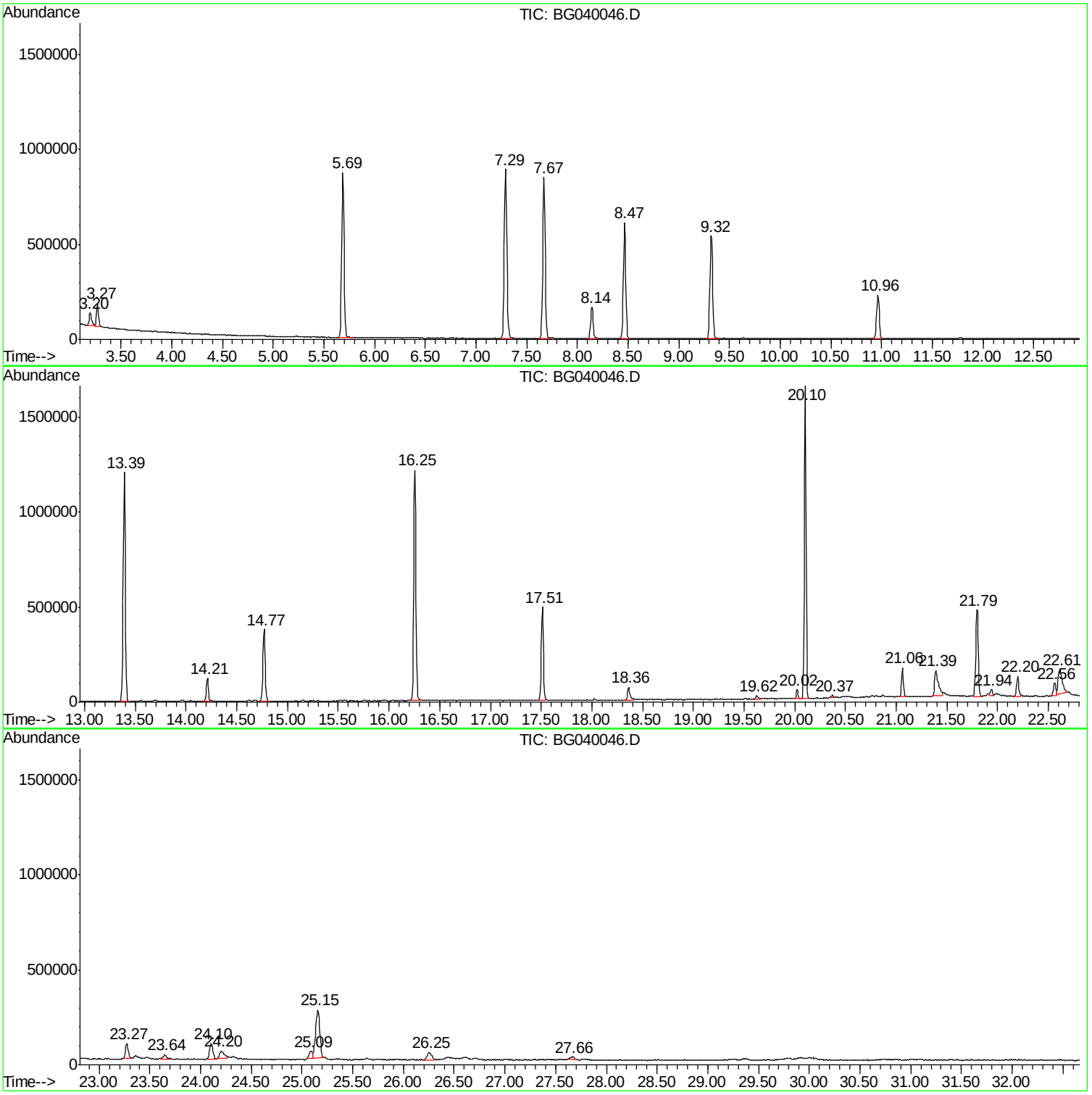
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG032019\
Data File : BG040046.D
Acq On : 20 Mar 2019 21:44
Operator : JU/SJ
Sample : K1935-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-18(14-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG032019\
Data File : BG040046.D
Acq On : 20 Mar 2019 21:44
Operator : JU/SJ
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Instrument : BNA_G
ClientSampleId : SB-18(14-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

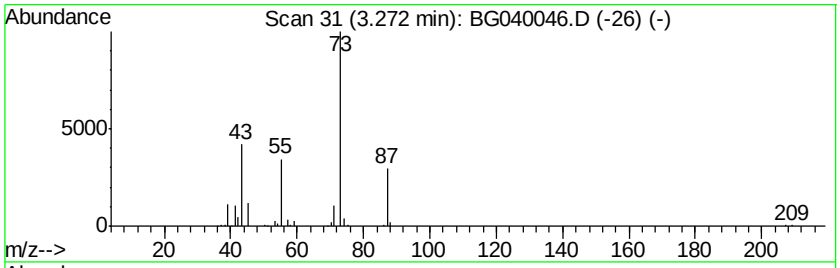
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

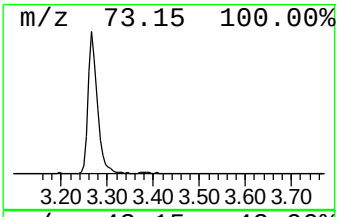
****

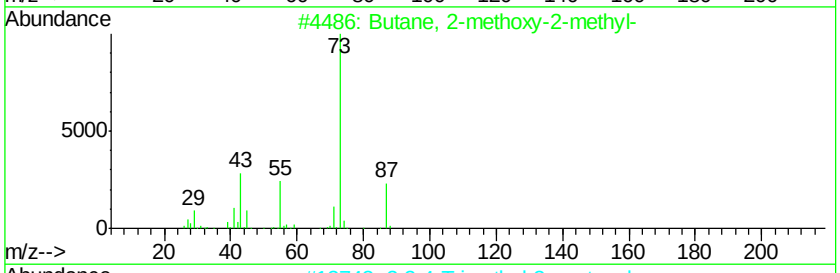
Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

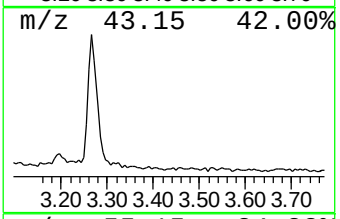
R.T.	EstConc	Area	Relative to ISTD	R.T.
3.27	10.63 ng	153693	1,4-Dichlorobenzene-d4	8.14

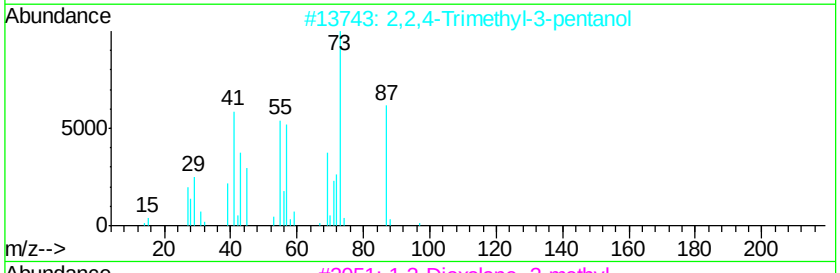
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	74
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9

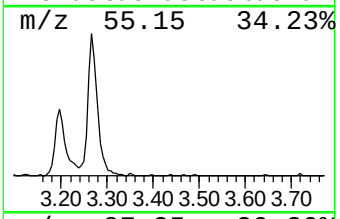


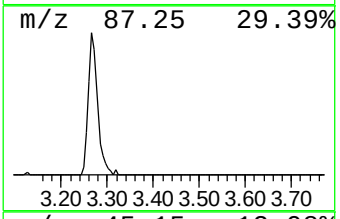


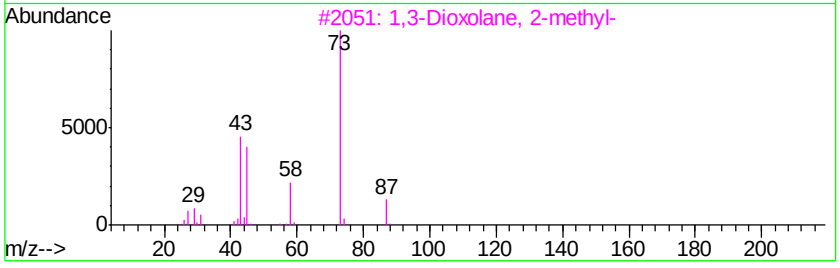


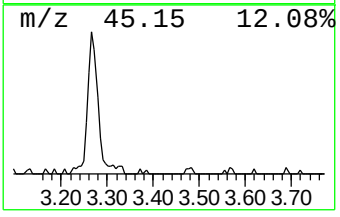












Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG032019\
Data File : BG040046.D
Acq On : 20 Mar 2019 21:44
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Sample : K1935-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-18(14-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

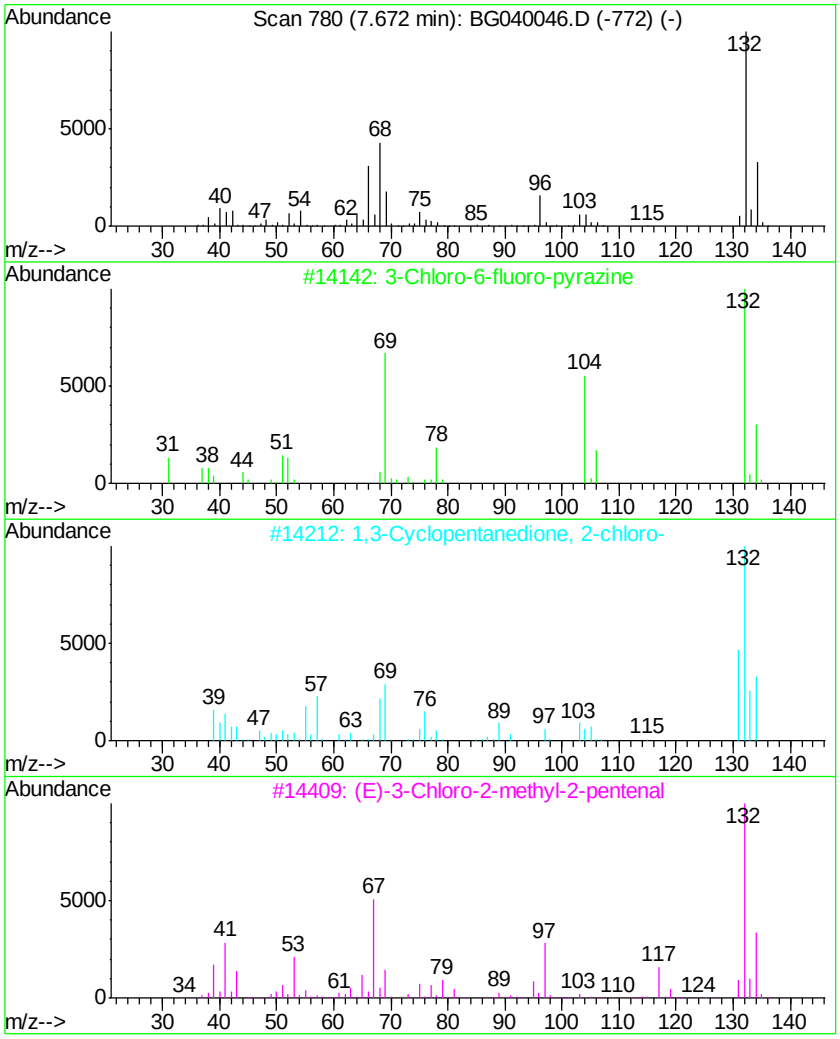
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

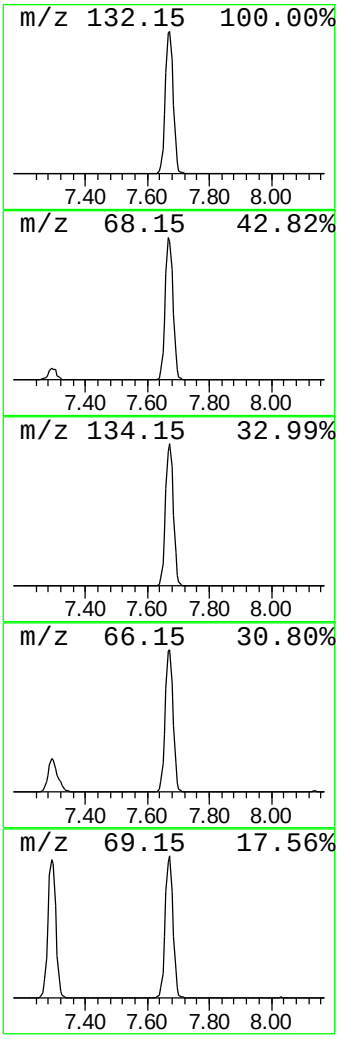
****

Peak Number 3 unknown7.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.67	103.43 ng	1494990	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12





Library Search Compound Report

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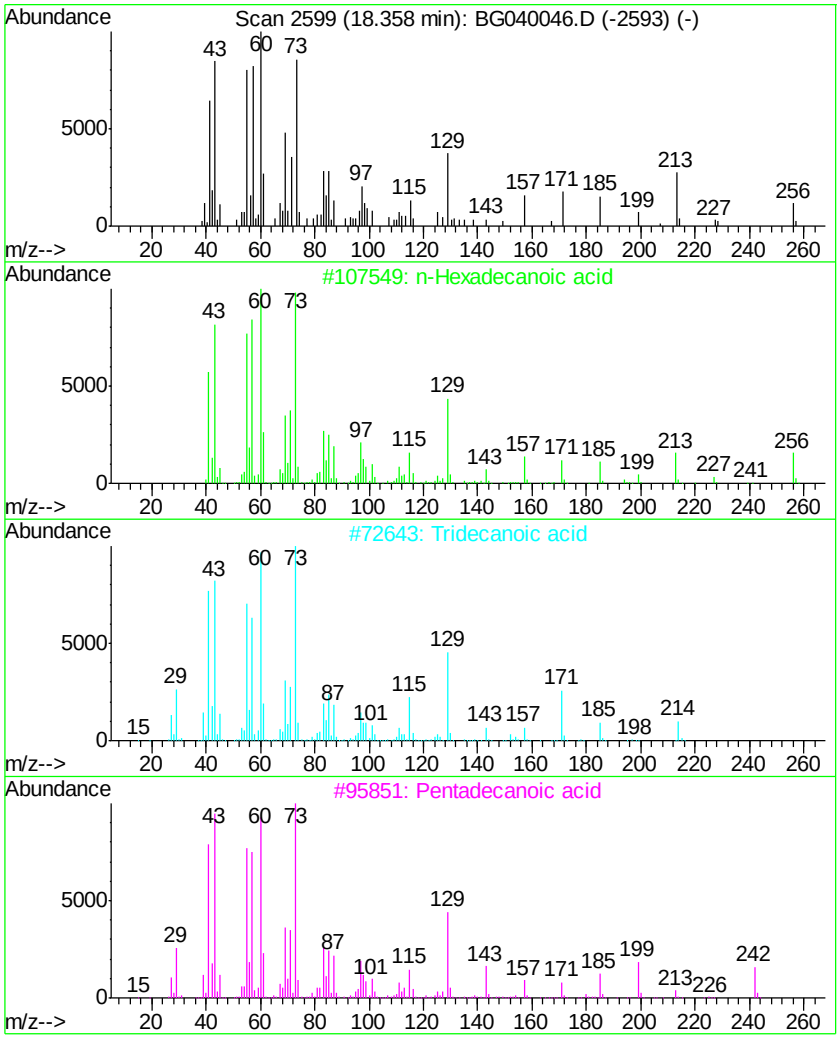
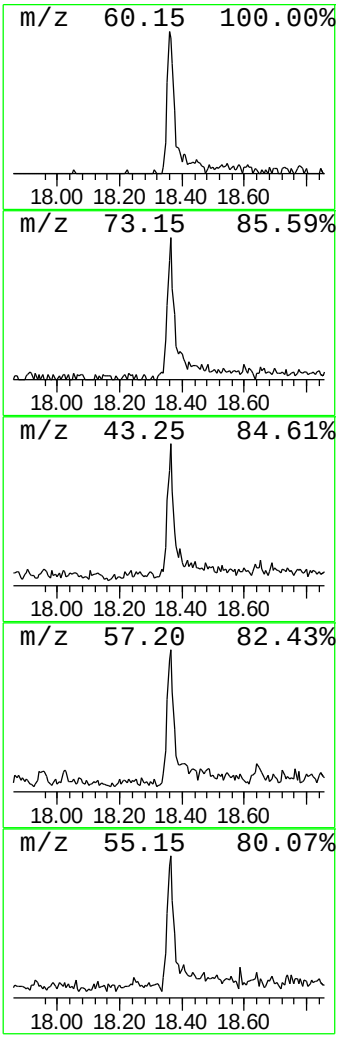
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	3.19 ng	120043	Phenanthrene-d10	17.51

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	76
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





Library Search Compound Report

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Sample : K1935-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-18(14-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

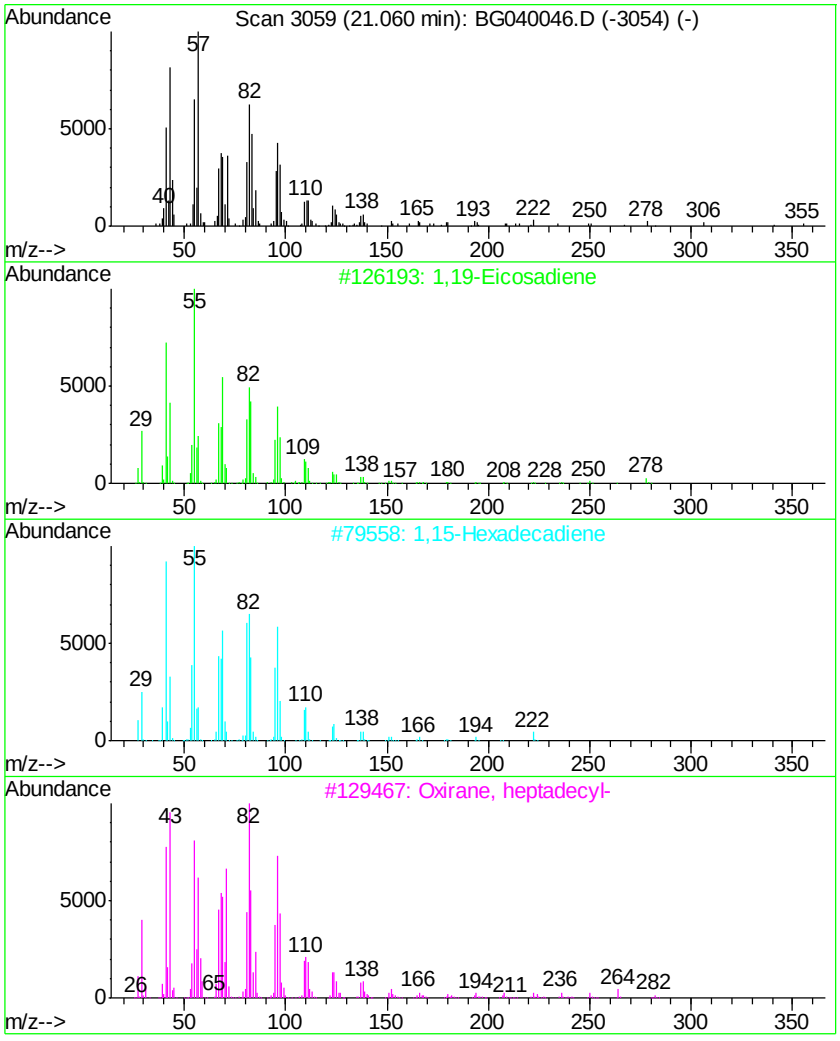
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

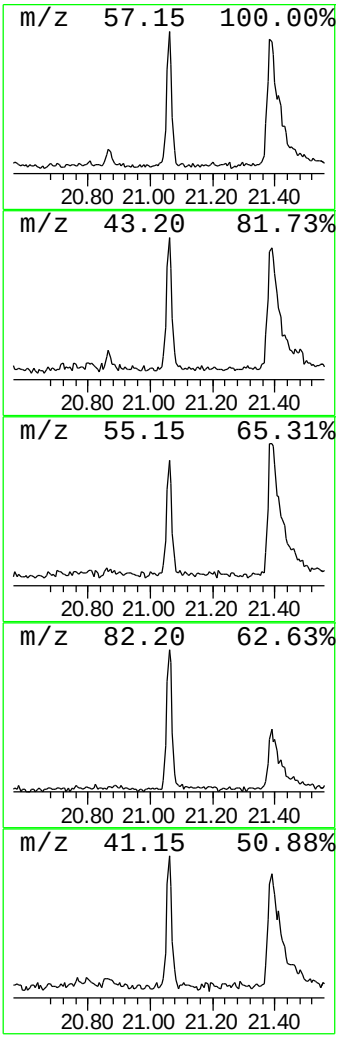
****

Peak Number 6 1,19-Eicosadiene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.06	4.83 ng	188420	Chrysene-d12	21.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	94
2	1,15-Hexadecadiene	222	C16H30	021964-51-2	93
3	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	93
4	Octadecanal	268	C18H36O	000638-66-4	91
5	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	91





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Instrument :
BNA_G
ClientSampleId :
SB-18(14-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

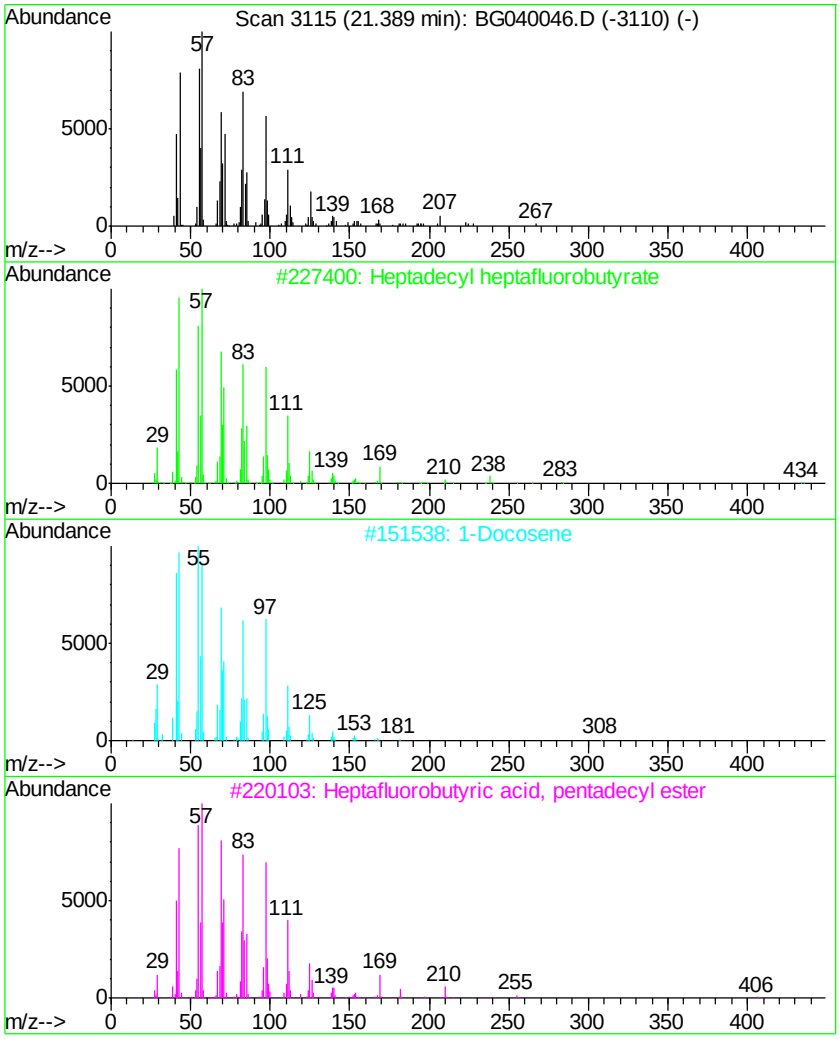
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

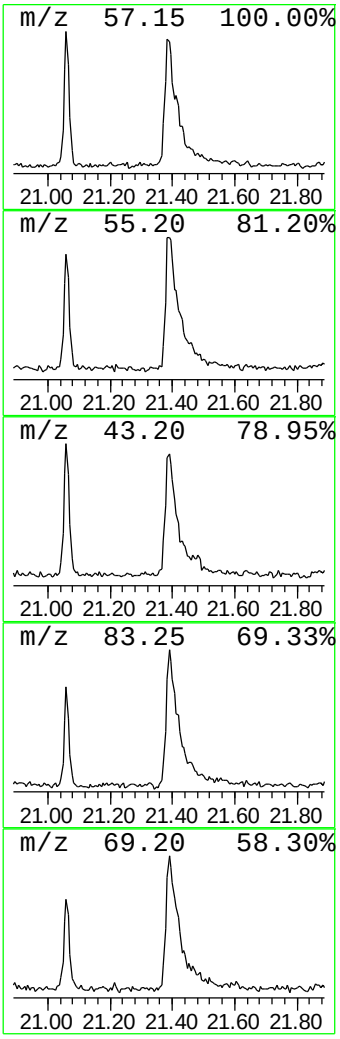
****

Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.39	9.02 ng	351669	Chrysene-d12	21.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	1-Docosene	308	C22H44	001599-67-3	94
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4	Octacosanol	410	C28H58O	000557-61-9	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





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Instrument : BNA_G
ClientSampleId : SB-18(14-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

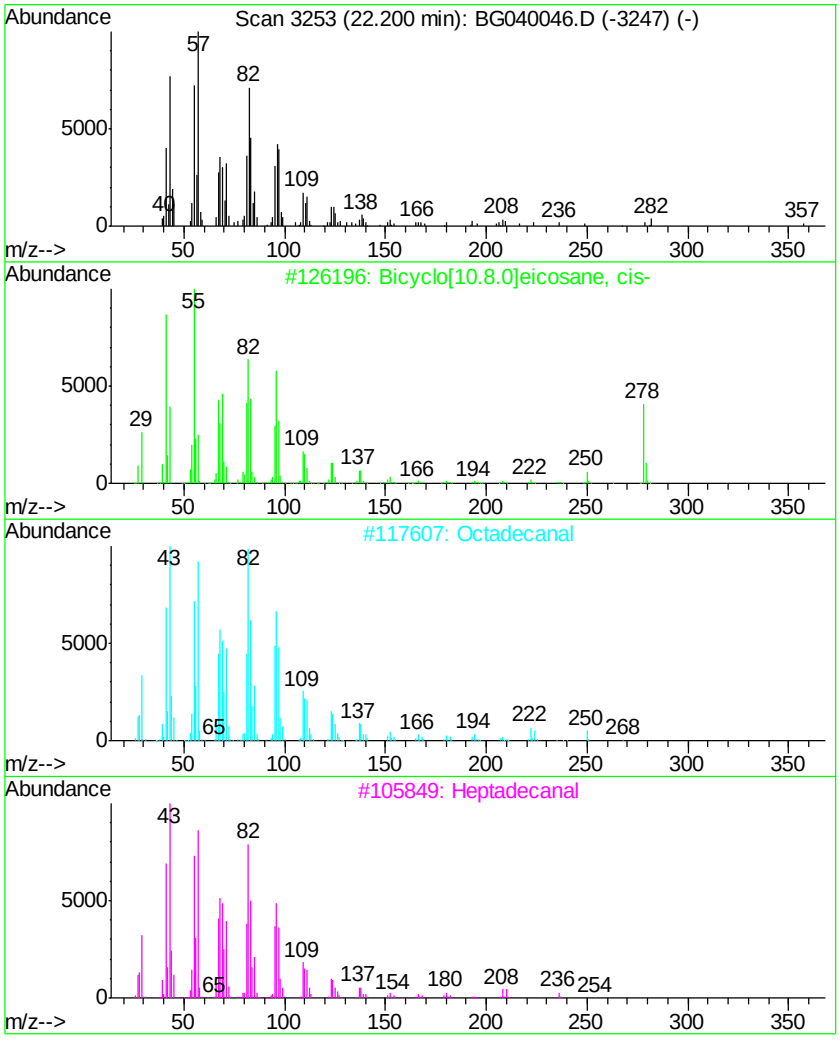
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

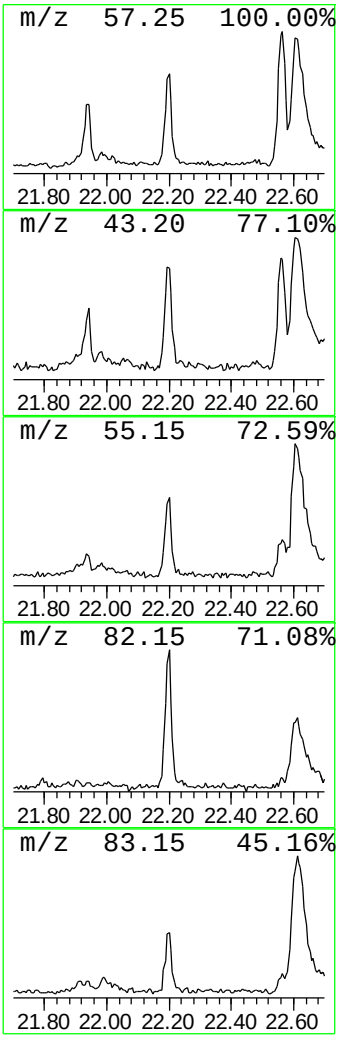
****

Peak Number 8 Bicyclo[10.8.0]eicosane, cis- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.20	4.26 ng	166230	Chrysene-d12	21.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[10.8.0]eicosane, cis-	278	C20H38	1000155-82-2	91
2	Octadecanal	268	C18H36O	000638-66-4	90
3	Heptadecanal	254	C17H34O	1000376-70-0	87
4	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	87
5	Hexadecanal	240	C16H32O	000629-80-1	87





Library Search Compound Report

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Instrument : BNA_G
ClientSampleId : SB-18(14-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

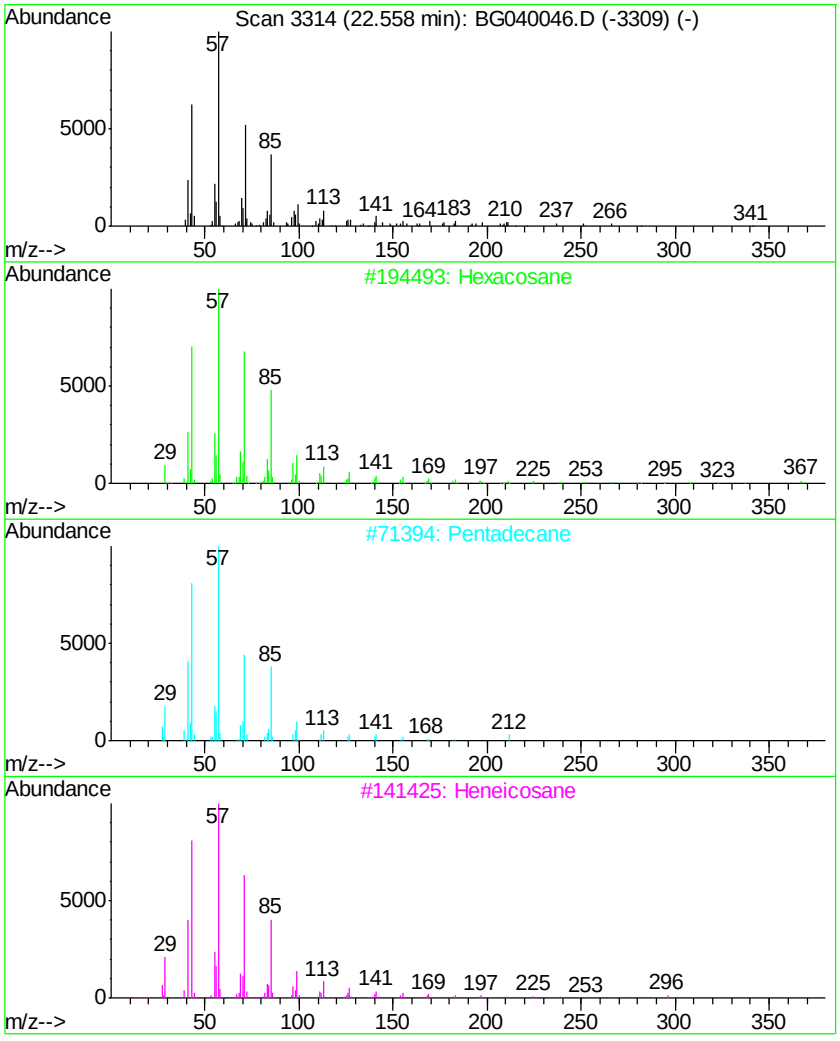
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

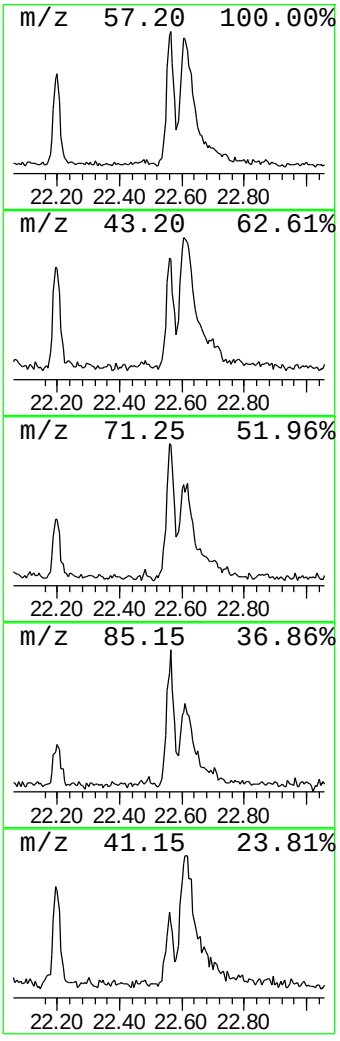
****

Peak Number 9 Hexacosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.56	3.07 ng	119817	Chrysene-d12	21.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	87
2	Pentadecane	212	C15H32	000629-62-9	87
3	Heneicosane	296	C21H44	000629-94-7	86
4	Hexadecane	226	C16H34	000544-76-3	83
5	Octadecane	254	C18H38	000593-45-3	80





Library Search Compound Report

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Instrument : BNA_G
ClientSampleId : SB-18(14-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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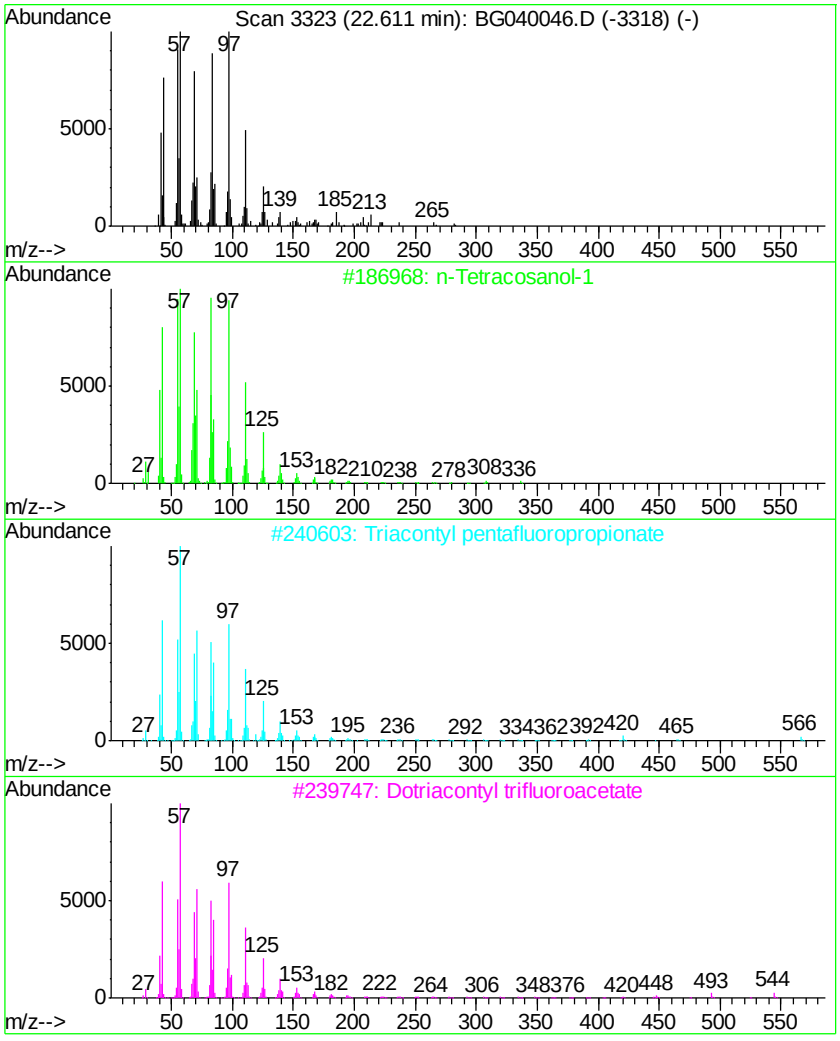
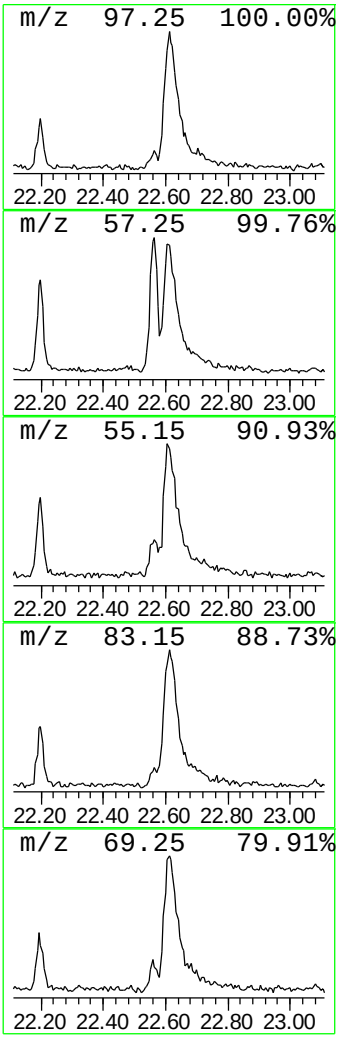
****

Peak Number 10 unknown22.61 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.61	9.78 ng	381648	Chrysene-d12	21.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	43
2	Triacontyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	38
3	Dotriacontyl trifluoroacetate	562	C34H65F3O2	1000351-75-4	38
4	Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	38
5	Triacontyl trifluoroacetate	534	C32H61F3O2	1000351-75-7	38





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Data File : BG040046.D
Acq On : 20 Mar 2019 21:44
Operator : JU/SJ
Sample : K1935-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-18(14-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.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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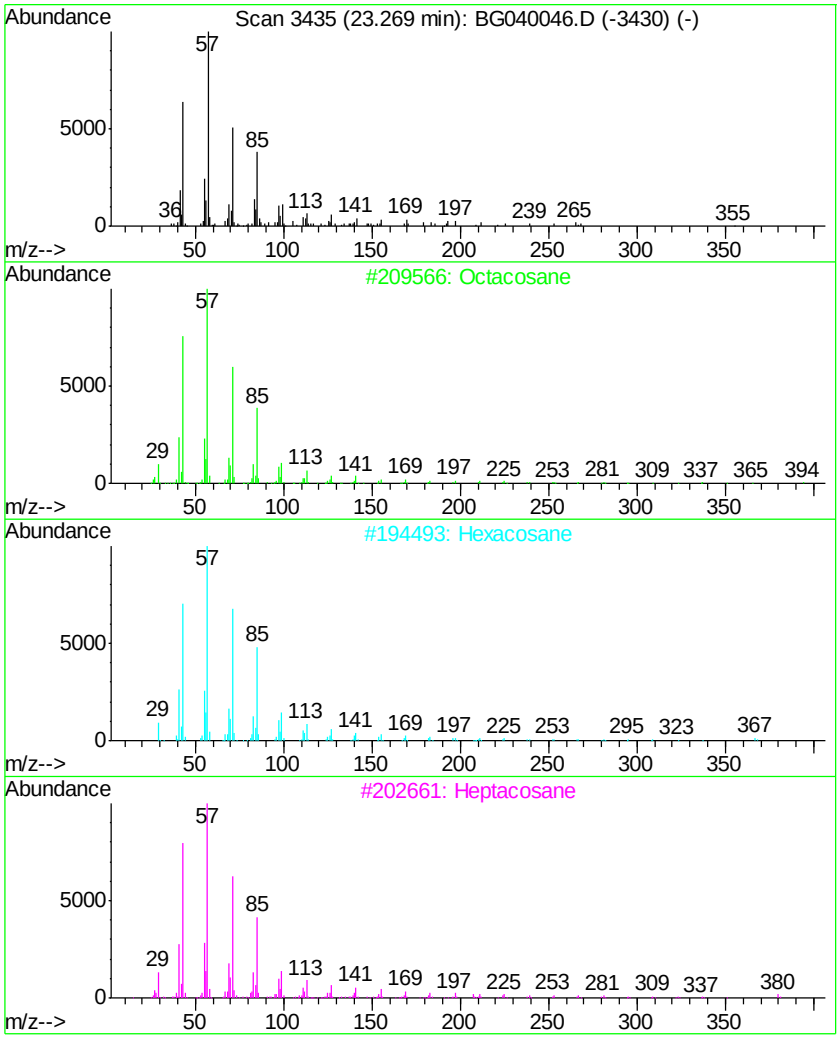
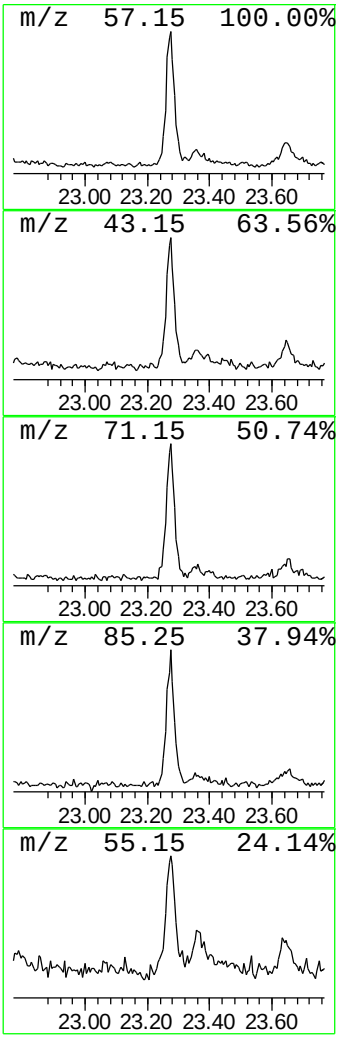
Peak Number 11 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.27	3.67 ng	143141	Chrysene-d12	21.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	87
2	Hexacosane	366	C26H54	000630-01-3	87
3	Heptacosane	380	C27H56	000593-49-7	86
4	5-Ethylnonadecane	296	C21H44	1000360-43-1	86
5	Pentadecane	212	C15H32	000629-62-9	83





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Sample : K1935-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-18(14-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
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TIC Library : C:\Database\NIST11.L
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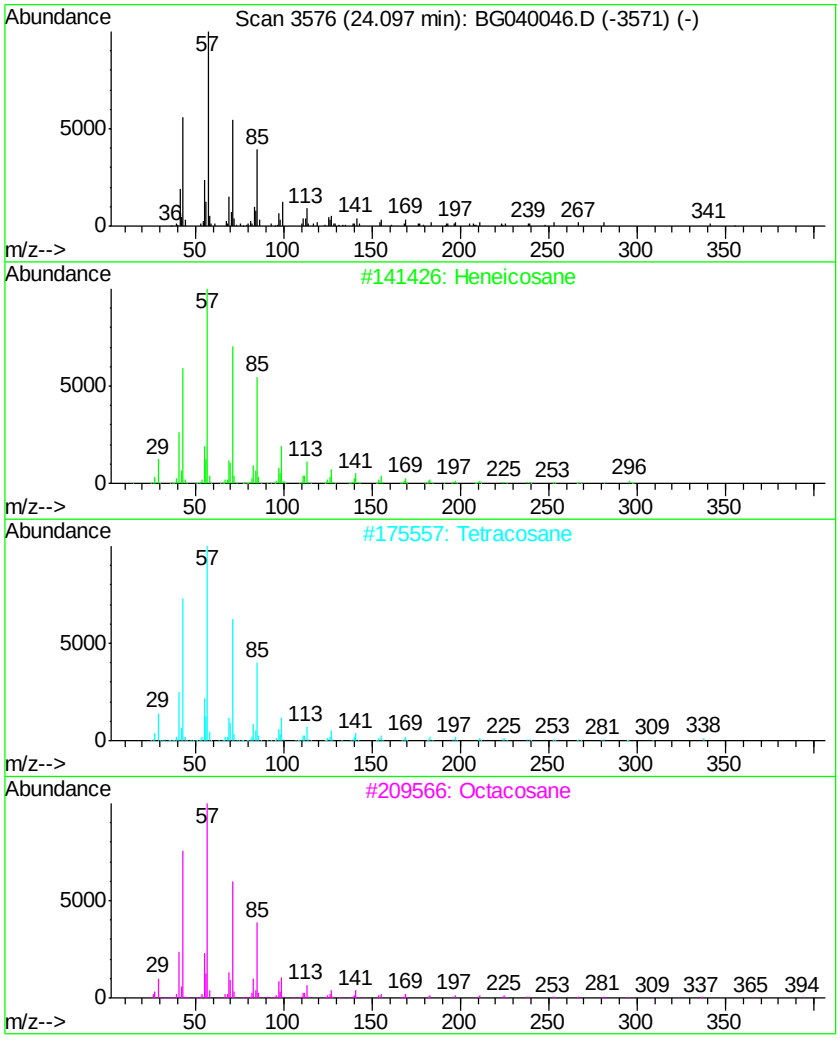
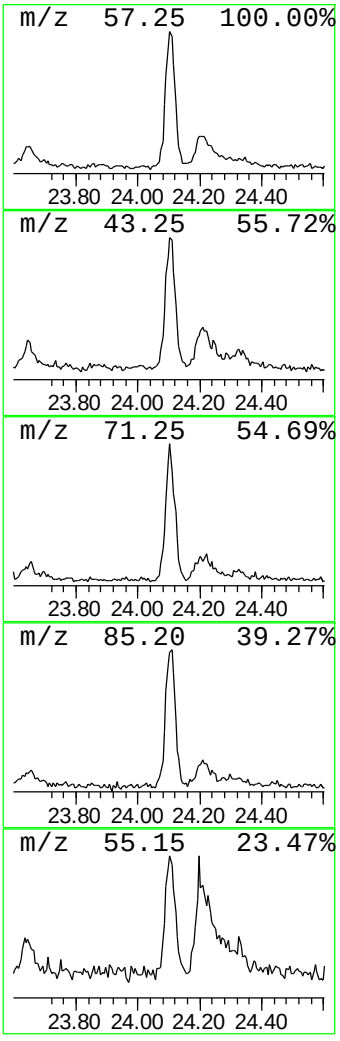
Peak Number 12 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.10	5.09 ng	179946	Perylene-d12	25.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Hexacosane	366	C26H54	000630-01-3	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG032019\
Data File : BG040046.D
Acq On : 20 Mar 2019 21:44
Operator : JU/SJ
Sample : K1935-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-18(14-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
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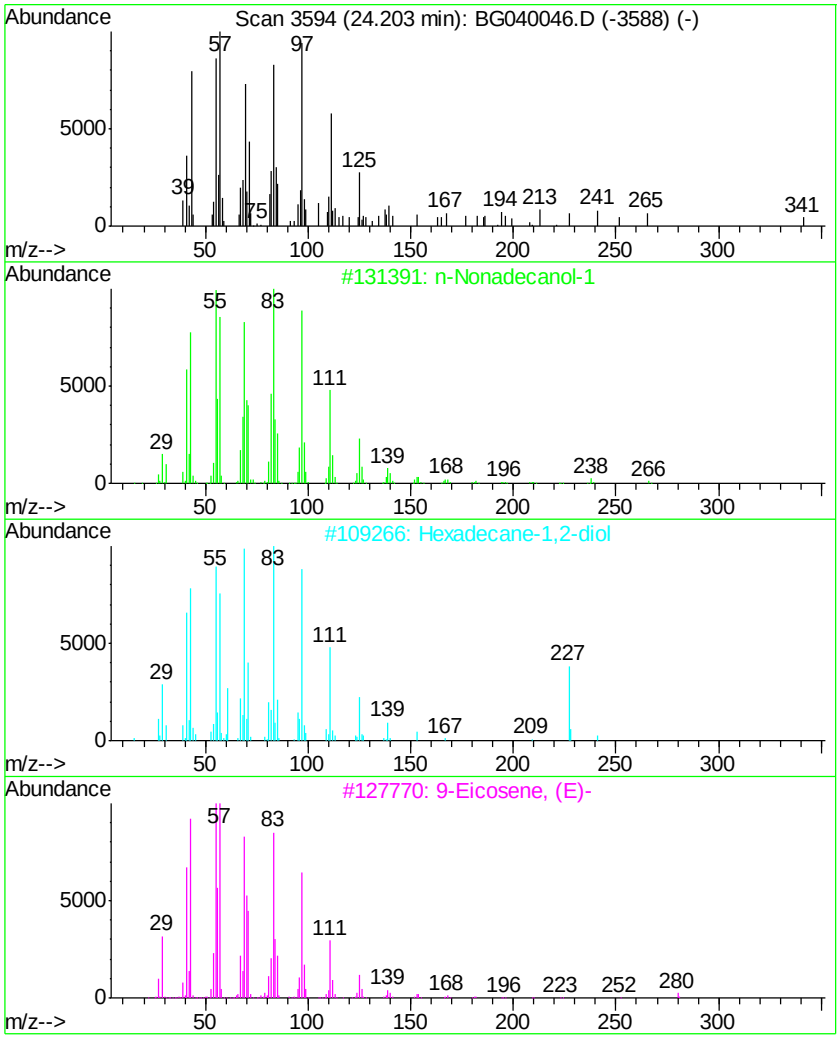
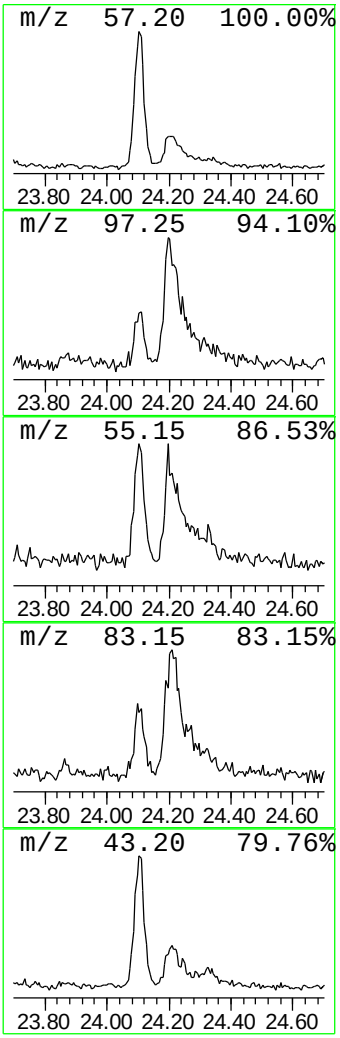
Peak Number 13 n-Nonadecanol-1 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.20	3.77 ng	133480	Perylene-d12	25.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	90
2	Hexadecane-1,2-diol	258	C16H34O2	006920-24-7	80
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	72
4	Cyclotetradecane	196	C14H28	000295-17-0	70
5	9-Octadecene, (E)-	252	C18H36	007206-25-9	64





Library Search Compound Report

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Data File : BG040046.D
Acq On : 20 Mar 2019 21:44
Operator : JU/SJ
Sample : K1935-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-18(14-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
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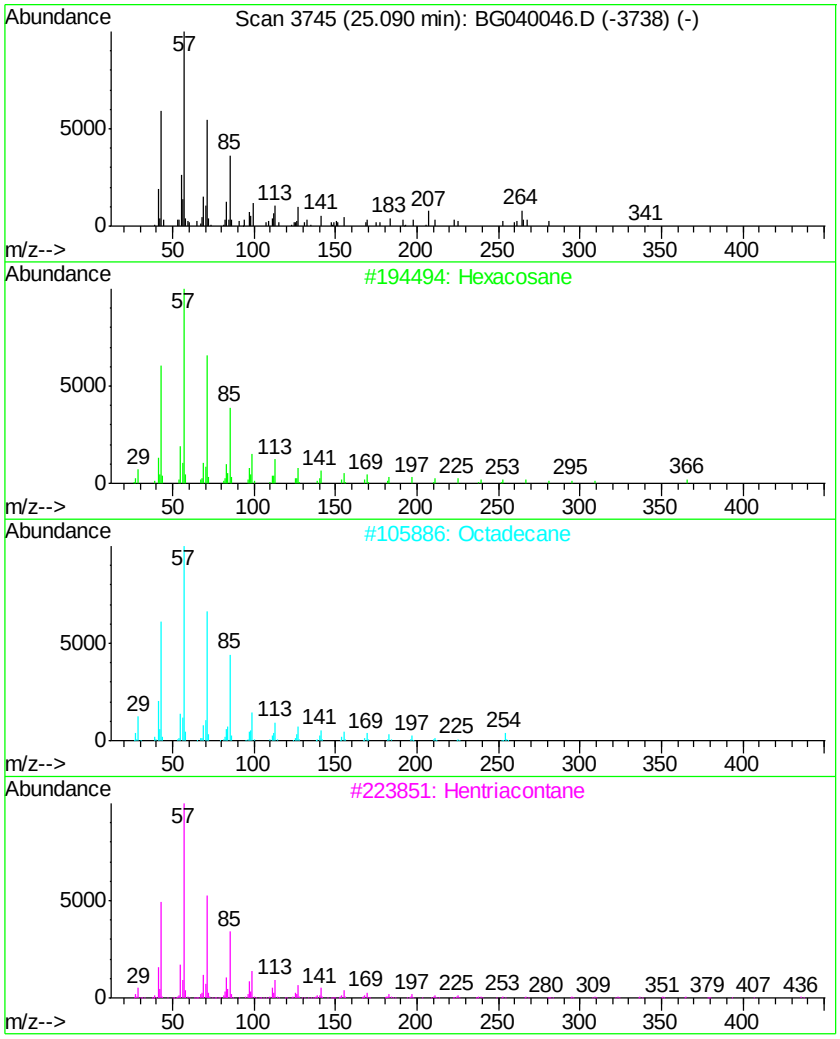
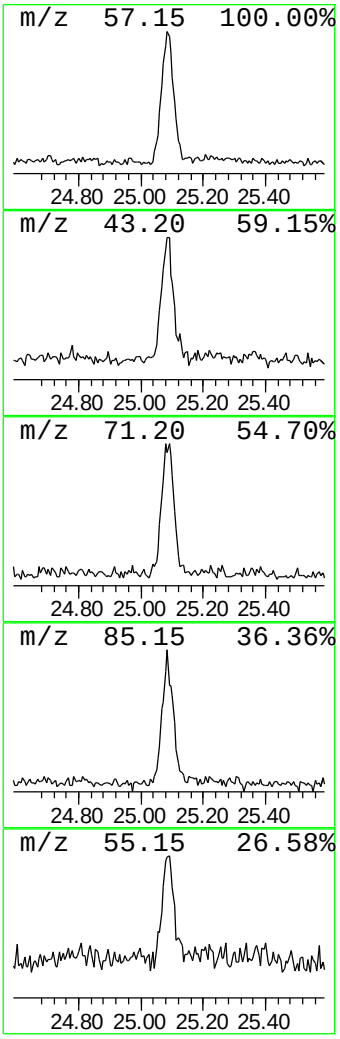
Peak Number 14 Hentriacontane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.09	2.60 ng	91810	Perylene-d12	25.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	87
2	Octadecane	254	C18H38	000593-45-3	83
3	Hentriacontane	437	C31H64	000630-04-6	83
4	Heptadecane, 3-methyl-	254	C18H38	006418-44-6	83
5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	83





Library Search Compound Report

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Acq On : 20 Mar 2019 21:44
Operator : JU/SJ
Sample : K1935-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-18(14-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.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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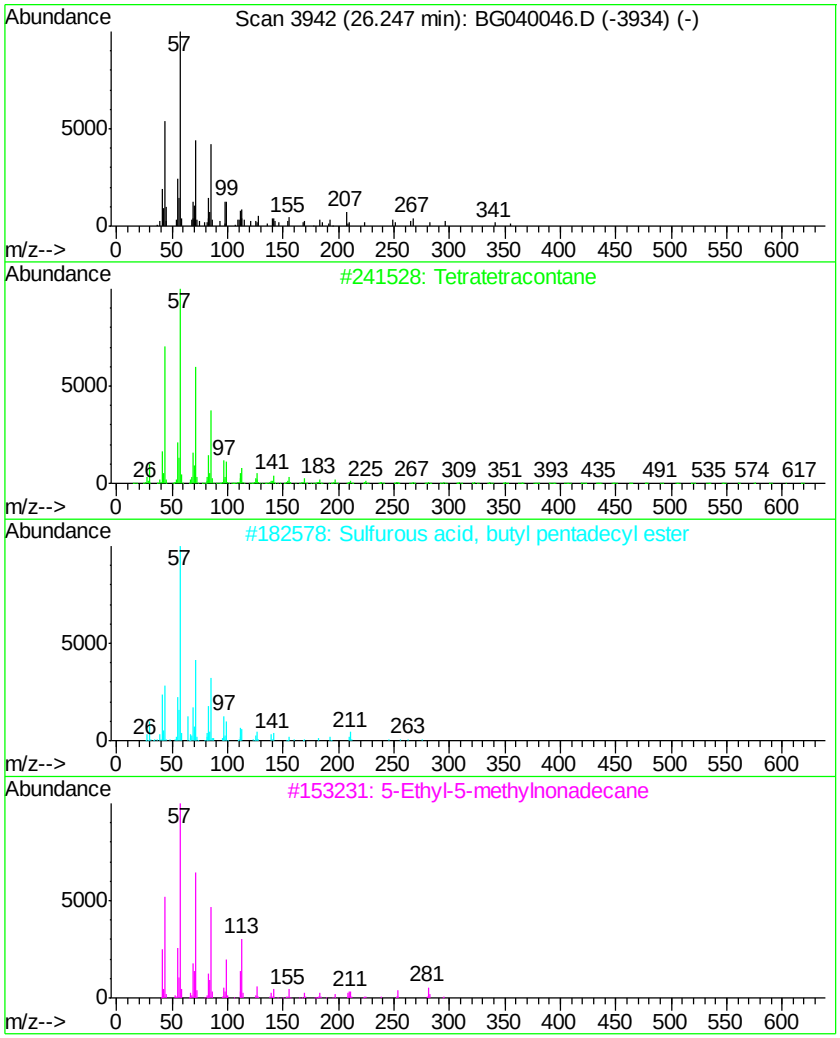
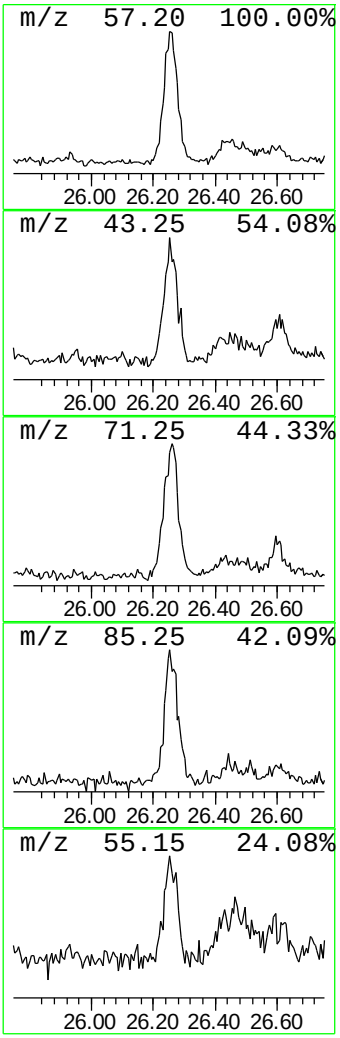
Peak Number 15 Tetratetracontane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.25	3.46 ng	122229	Perylene-d12	25.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	87
2	Sulfurous acid, butyl pentadecyl...	348	C19H40O3S	1000309-18-2	86
3	5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	86
4	Eicosane, 9-octyl-	394	C28H58	013475-77-9	83
5	Eicosane	282	C20H42	000112-95-8	81





Tentatively Identified Compound (LSC) summary

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Data File : BG040046.D
Acq On : 20 Mar 2019 21:44
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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
Butane, 2-methoxy...	3.27	10.6	ng	153693	1	8.14	289073	20.0
unknown7.67	7.67	103.4	ng	1494990	1	8.14	289073	20.0
n-Hexadecanoic acid	18.36	3.2	ng	120043	4	17.51	753530	20.0
1,19-Eicosadiene	21.06	4.8	ng	188420	5	21.79	780089	20.0
Heptadecyl heptaf...	21.39	9.0	ng	351669	5	21.79	780089	20.0
Bicyclo[10.8.0]ei...	22.20	4.3	ng	166230	5	21.79	780089	20.0
Hexacosane	22.56	3.1	ng	119817	5	21.79	780089	20.0
unknown22.61	22.61	9.8	ng	381648	5	21.79	780089	20.0
Octacosane	23.27	3.7	ng	143141	5	21.79	780089	20.0
Heneicosane	24.10	5.1	ng	179946	6	25.15	707399	20.0
n-Nonadecanol-1	24.20	3.8	ng	133480	6	25.15	707399	20.0
Hentriacontane	25.09	2.6	ng	91810	6	25.15	707399	20.0
Tetratetracontane	26.25	3.5	ng	122229	6	25.15	707399	20.0