LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM041819\
Data File : BM019965.D
Acq On : 18 Apr 2019 22:09
Operator : JU/SJ
Sample : K2461-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-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_M\METHODS\8270-BM041519.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	4.863	313	319	325	rBV2	42195	68388	1.16%	0.211%
2	5.128	358	364	389	rBV	813747	1396673	23.73%	4.300%
3	6.710	627	633	652	rBV	419248	893448	15.18%	2.751%
4	7.045	682	690	705	rBV	1681694	2731010	46.39%	8.409%
5	7.510	763	769	783	rBV	375869	630468	10.71%	1.941%
6	7.822	814	822	839	rVB	1508490	2420426	41.12%	7.452%
7	8.586	948	952	961	rVB2	37120	58987	1.00%	0.182%
8	8.686	961	969	986	rBV	966722	1903847	32.34%	5.862%
9	9.681	1133	1138	1146	rBV2	33179	59828	1.02%	0.184%
10	10.292	1232	1242	1256	rBV	386296	761647	12.94%	2.345%
11	12.022	1528	1536	1547	rBV2	38971	146865	2.49%	0.452%
12	12.780	1659	1665	1680	rBV	2902933	4225742	71.78%	13.011%
13	13.051	1707	1711	1718	rVB2	43504	73971	1.26%	0.228%
14	14.180	1896	1903	1910	rBV2	630813	988670	16.79%	3.044%
15	15.686	2153	2159	2177	rBV	2171888	3426991	58.21%	10.552%
16	16.468	2287	2292	2298	rBV	74901	136006	2.31%	0.419%
17	16.945	2368	2373	2379	rBV2	817812	1147147	19.49%	3.532%
18	17.839	2520	2525	2535	rBV	380109	620403	10.54%	1.910%
19	18.703	2668	2672	2678	rVB	138207	169853	2.89%	0.523%
20	19.133	2741	2745	2759	rVB	256676	381187	6.48%	1.174%
21	19.592	2817	2823	2830	rBV	4905465	5886822	100.00%	18.125%
22	20.856	3035	3038	3045	rVB3	144313	180504	3.07%	0.556%
23	21.162	3085	3090	3099	rVB	977159	1334074	22.66%	4.108%
24	21.709	3180	3183	3187	rBV	144691	143849	2.44%	0.443%
25	21.874	3208	3211	3217	rVB	296159	334483	5.68%	1.030%
26	22.156	3256	3259	3264	rVB	205266	241678	4.11%	0.744%
27	22.639	3338	3341	3349	rVB	264843	347816	5.91%	1.071%
28	23.180	3430	3433	3439	rVB	246423	356375	6.05%	1.097%
29	23.344	3456	3461	3475	rVB	734863	1411303	23.97%	4.345%

Sum of corrected areas: 32478461

LSC Report - Integrated Chromatogram

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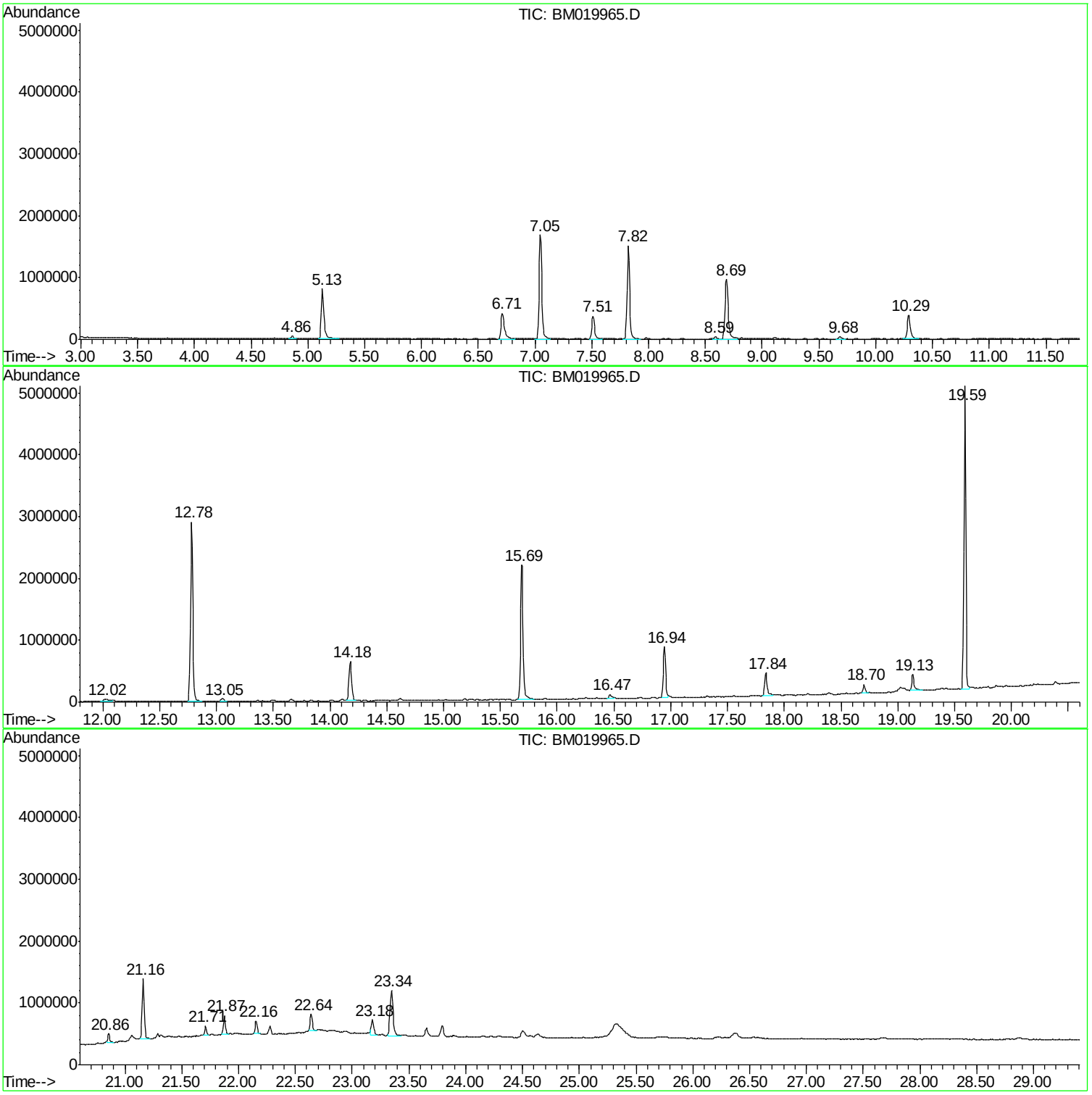
Data File : BM019965.D
Acq On : 18 Apr 2019 22:09
Operator : JU/SJ
Sample : K2461-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
GMW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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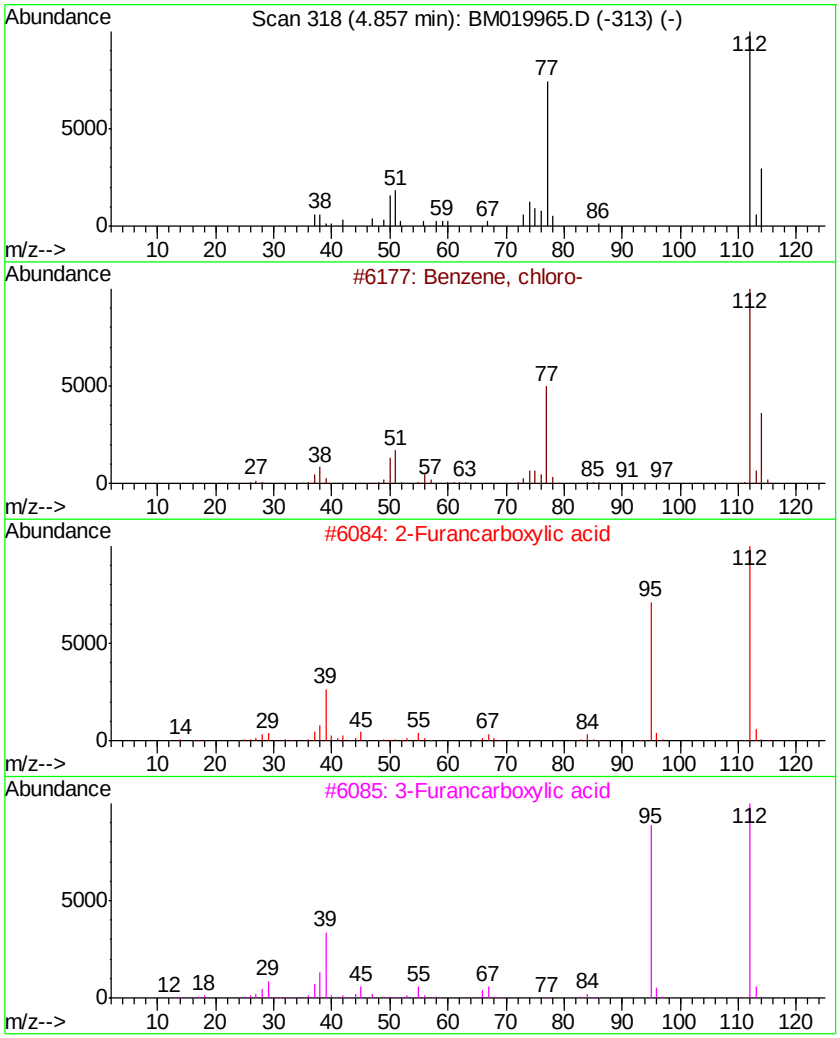
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

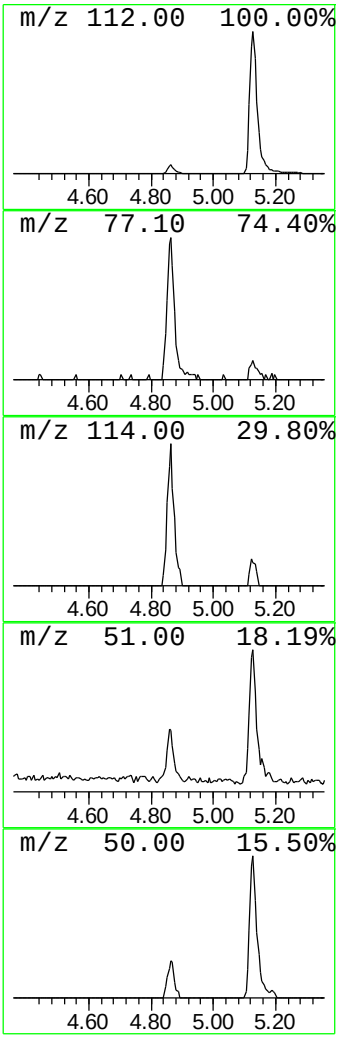
****

Peak Number 1 unknown4.86 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	2.17 ng	68388	1,4-Dichlorobenzene-d4	7.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, chloro-	112	C6H5Cl	000108-90-7	91
2	2-Furancarboxylic acid	112	C5H4O3	000088-14-2	25
3	3-Furancarboxylic acid	112	C5H4O3	000488-93-7	17
4	3-Nitropyrrole	112	C4H4N2O2	005930-94-9	9
5	Phenol, 4-fluoro-	112	C6H5FO	000371-41-5	9





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Operator : JU/SJ
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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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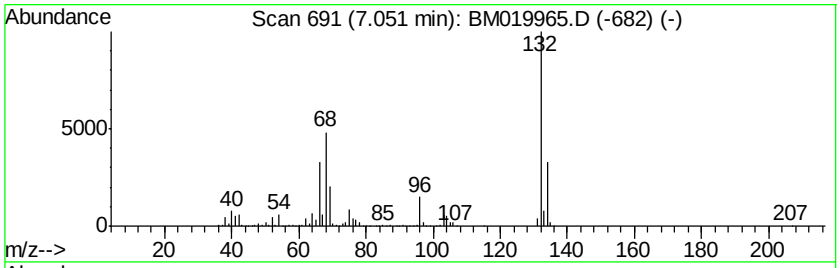
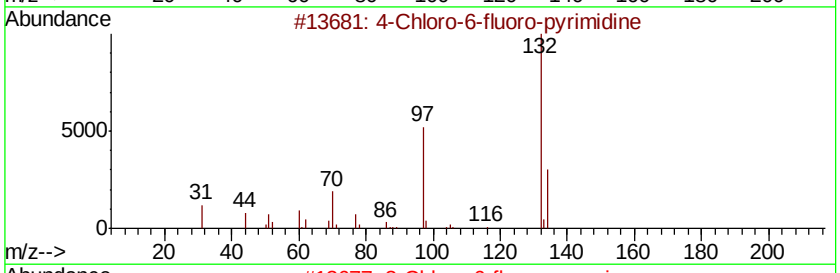
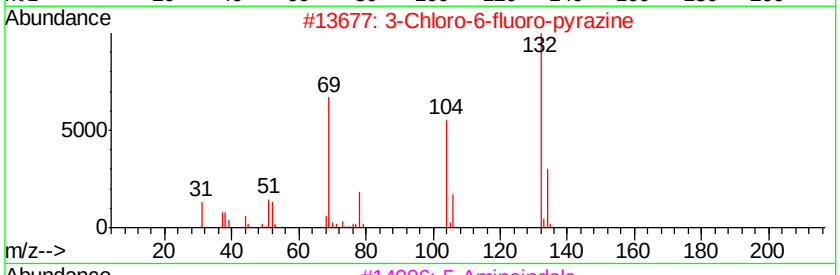
Peak Number 2 unknown7.05 Concentration Rank 1

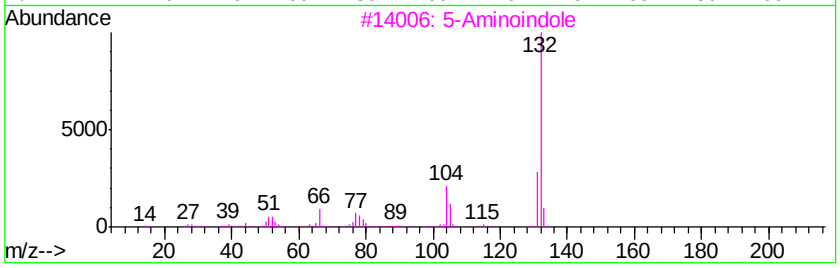
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.05	86.63 ng	2731010	1,4-Dichlorobenzene-d4	7.51

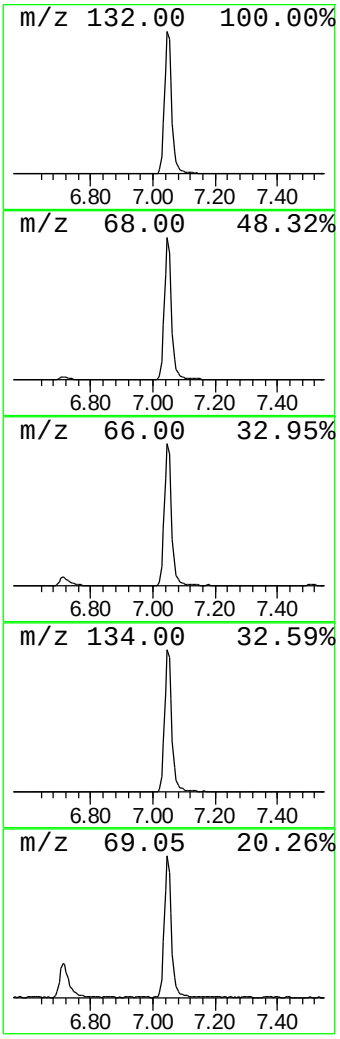
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	5-Aminoindole	132	C8H8N2	005192-03-0	22
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12











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Operator : JU/SJ
Sample : K2461-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

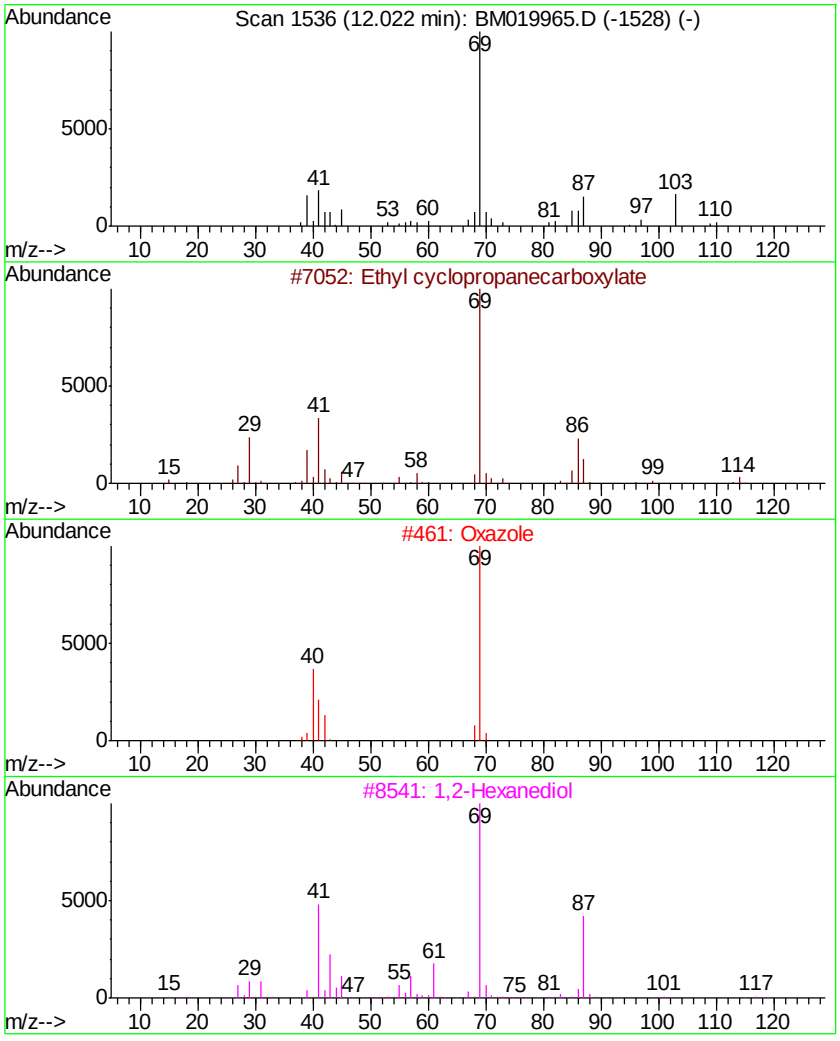
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

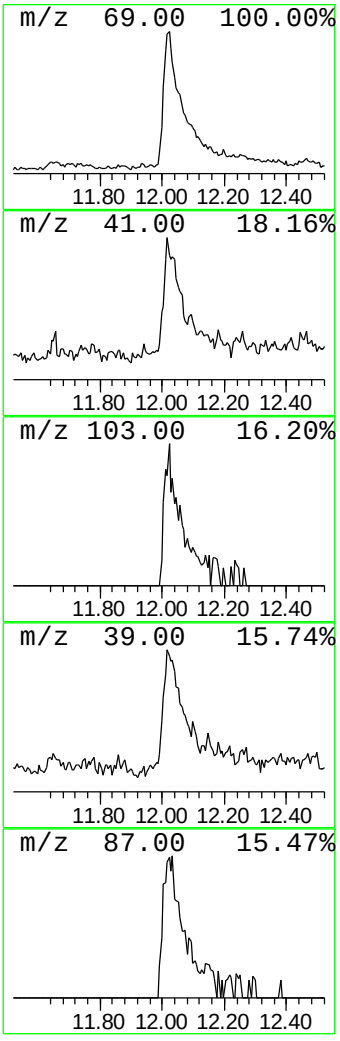
****

Peak Number 4 unknown12.02 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	3.86 ng	146865	Naphthalene-d8	10.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	45
2	Oxazole	69	C3H3NO	000288-42-6	9
3	1,2-Hexanediol	118	C6H14O2	006920-22-5	9
4	meso-5,6-Decanediol	174	C10H22O2	003266-25-9	9
5	Cyclopropanecarboxylic acid,buty...	142	C8H14O2	054947-39-6	9





Library Search Compound Report

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Operator : JU/SJ
Sample : K2461-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.M
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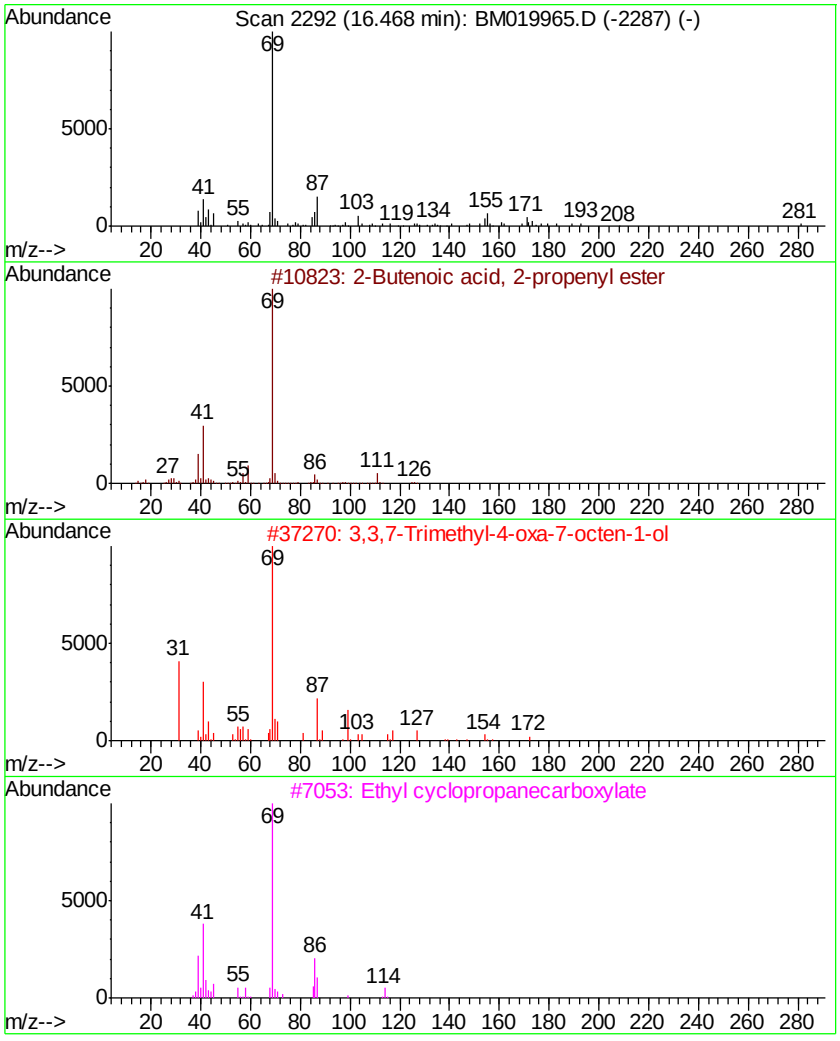
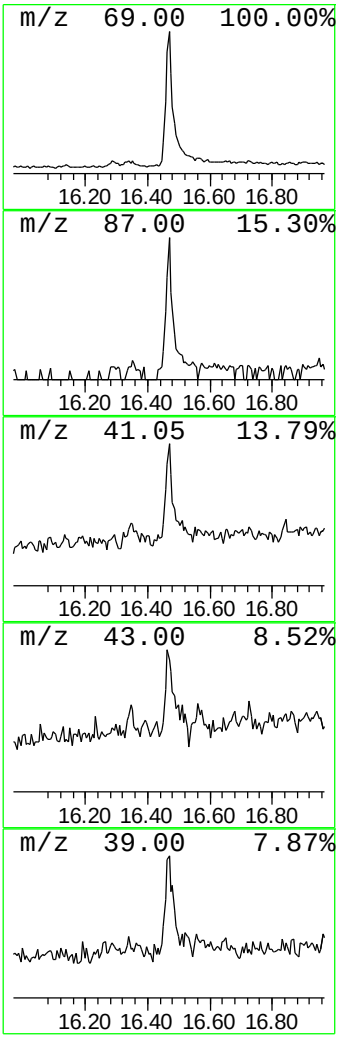
Peak Number 5 unknown16.47 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.47	2.37 ng	136006	Phenanthrene-d10	16.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenoic acid, 2-propenyl ester	126	C7H10O2	020474-93-5	42
2	3,3,7-Trimethyl-4-oxa-7-octen-1-ol	172	C10H20O2	069161-47-3	38
3	Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	36
4	Cyclopentane, bromo-	148	C5H9Br	000137-43-9	9
5	Undecanol-5	172	C11H24O	037493-70-2	9





Library Search Compound Report

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Operator : JU/SJ
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Misc :
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Instrument : BNA_M
ClientSampleId : GMW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.M
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TIC Library : C:\DATABASE\NIST02.L
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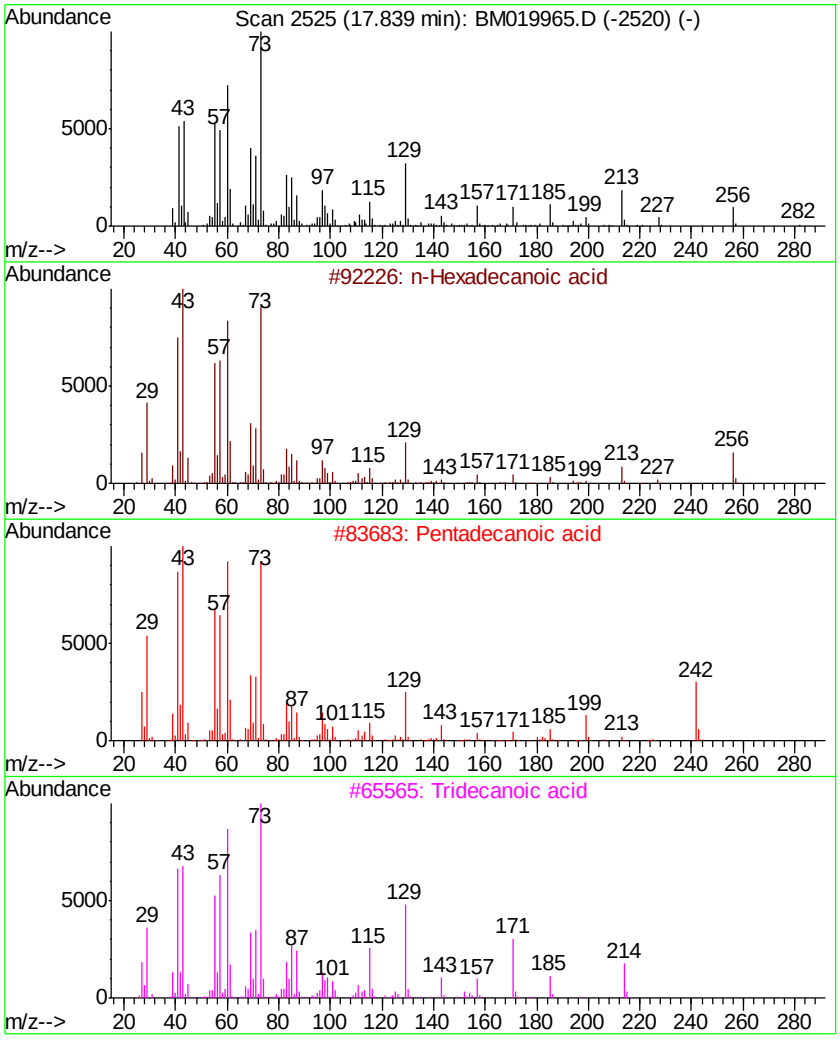
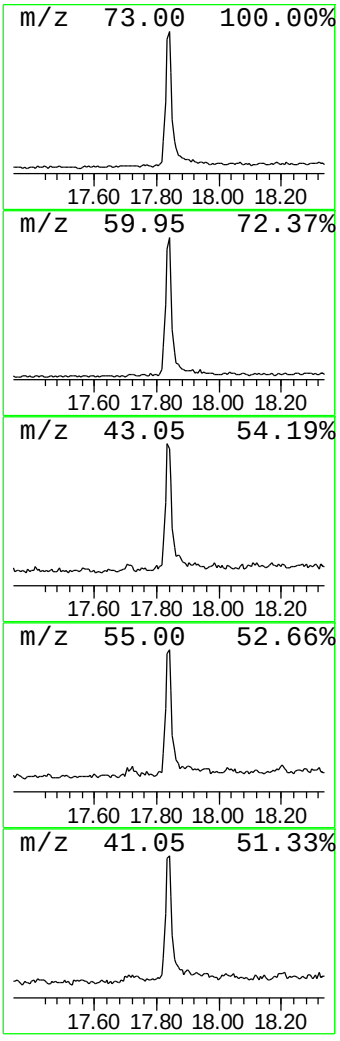
Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.84	10.82 ng	620403	Phenanthrene-d10	16.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	n-Decanoic acid	172	C10H20O2	000334-48-5	47





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Instrument : BNA_M
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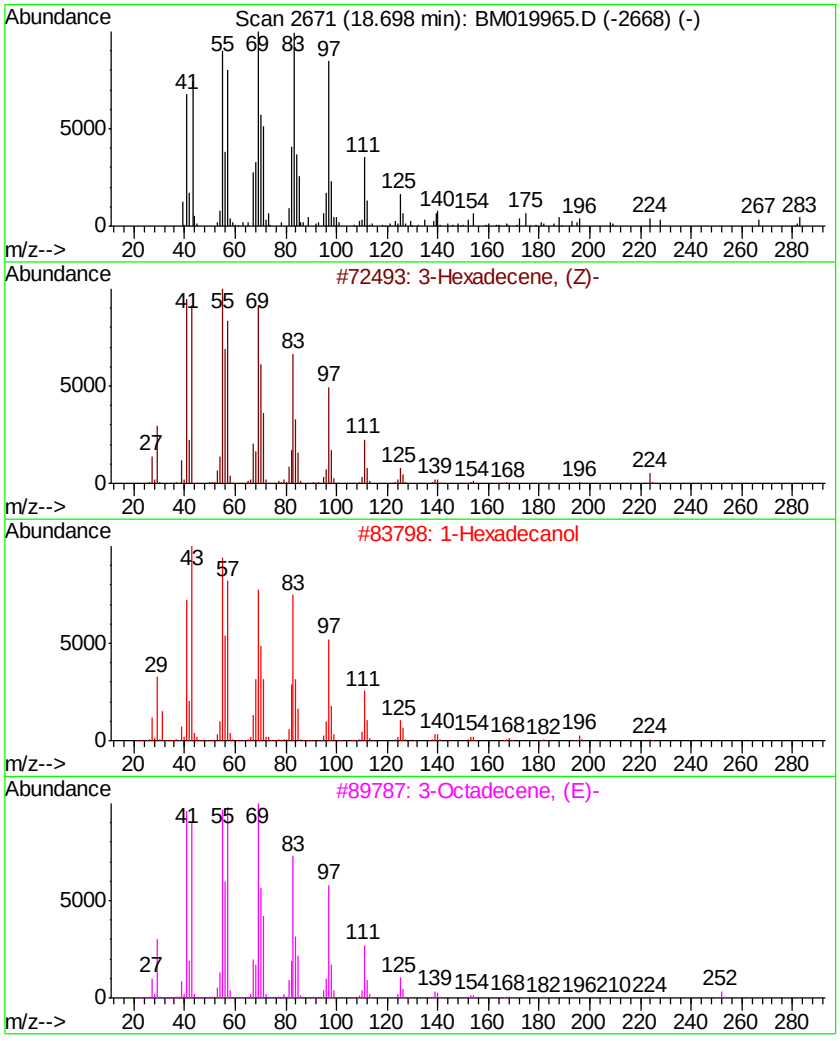
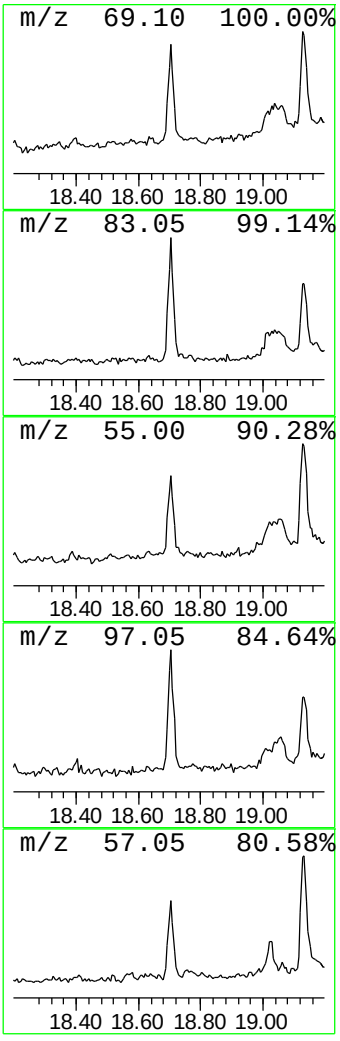
Peak Number 7 3-Hexadecene, (Z)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.70	2.96 ng	169853	Phenanthrene-d10	16.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexadecene, (Z)-	224	C16H32	034303-81-6	96
2	1-Hexadecanol	242	C16H34O	036653-82-4	91
3	3-Octadecene, (E)-	252	C18H36	007206-19-1	91
4	Acetic acid, trifluoro-, tetrade...	310	C16H29F3O2	006222-02-2	91
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	91





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Misc :
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Instrument : BNA_M
ClientSampleId : GMW-1

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TIC Library : C:\DATABASE\NIST02.L
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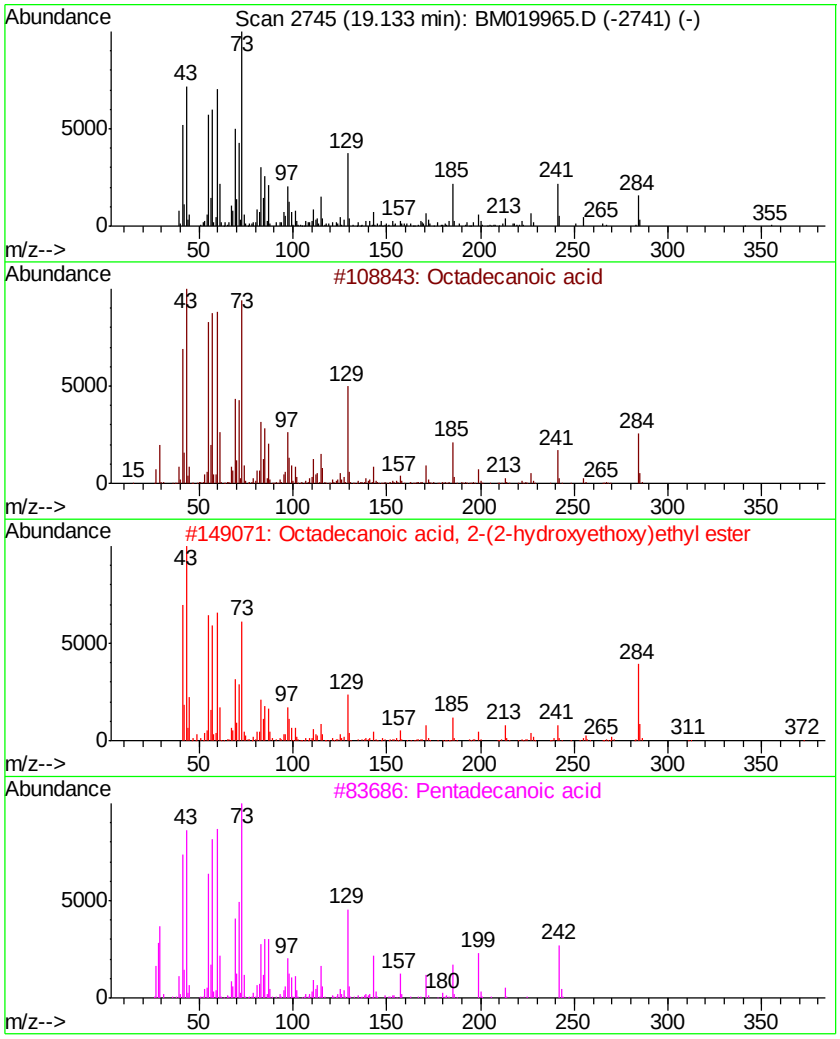
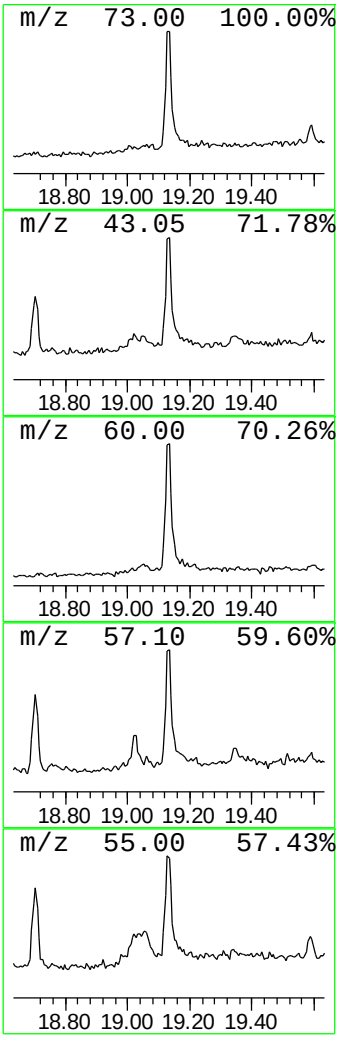
Peak Number 8 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.13	5.71 ng	381187	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Pentadecane	212	C15H32	000629-62-9	25





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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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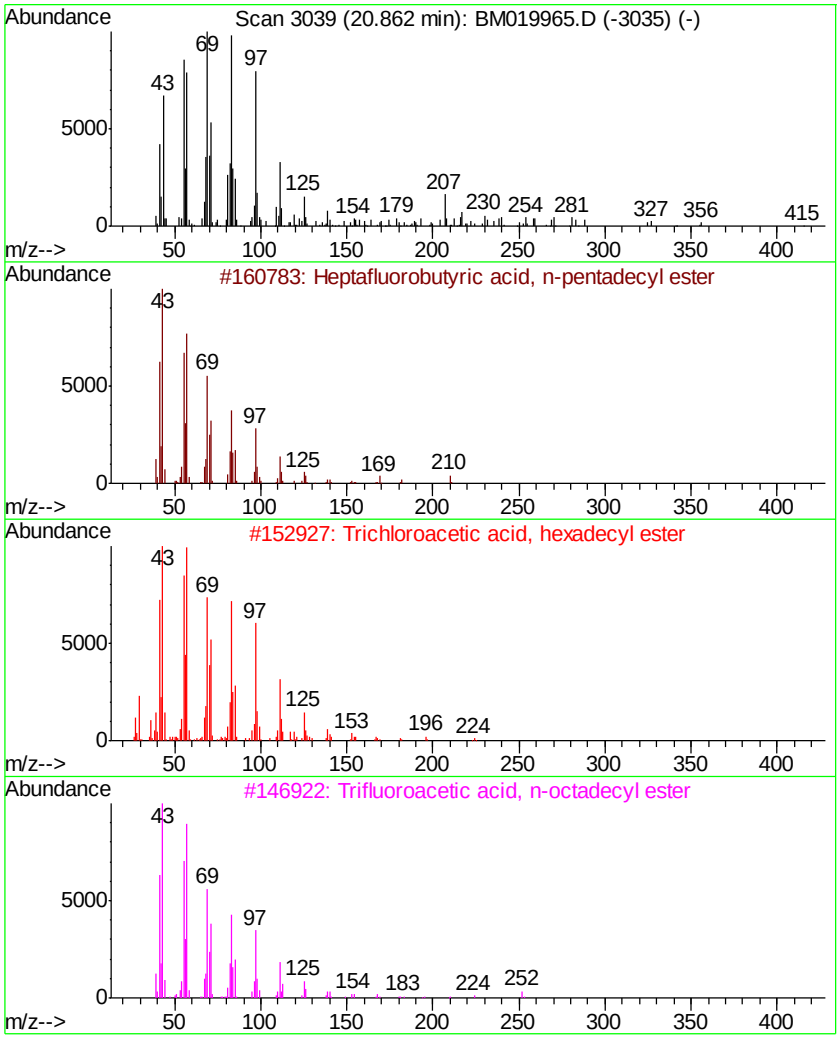
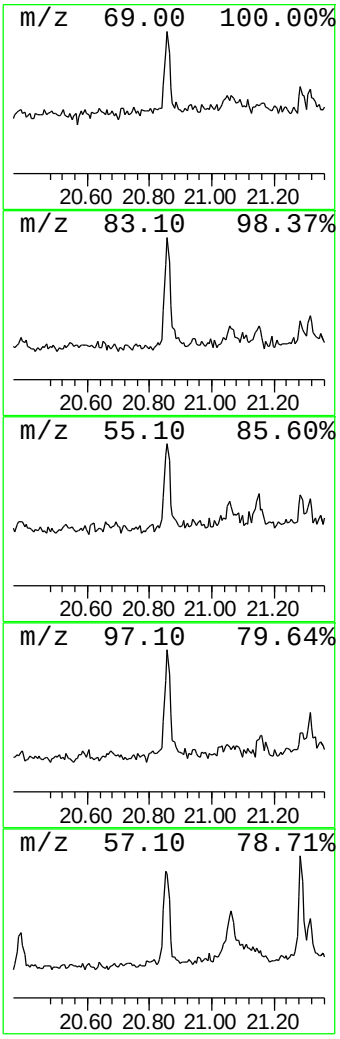
Peak Number 9 Heptafluorobutyric acid, n-... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.86	2.71 ng	180504	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	91
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
4	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	90
5	1-Octadecanethiol	286	C18H38S	002885-00-9	87





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Instrument : BNA_M
ClientSampleId : GMW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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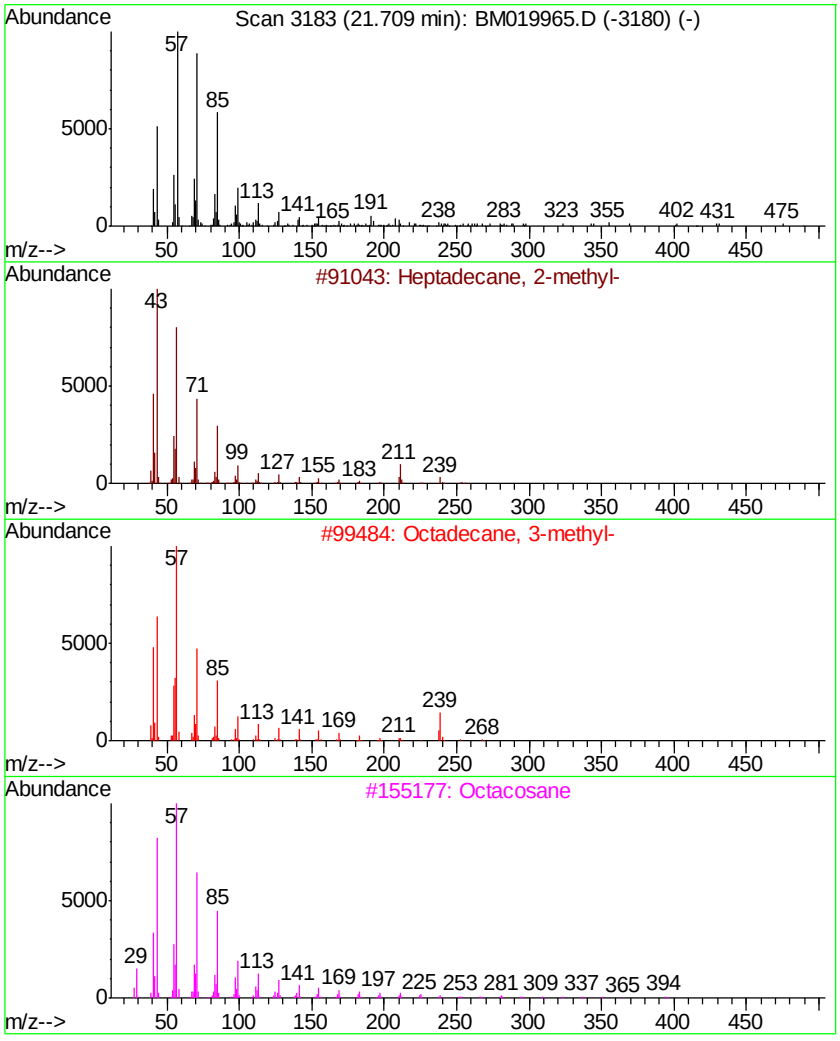
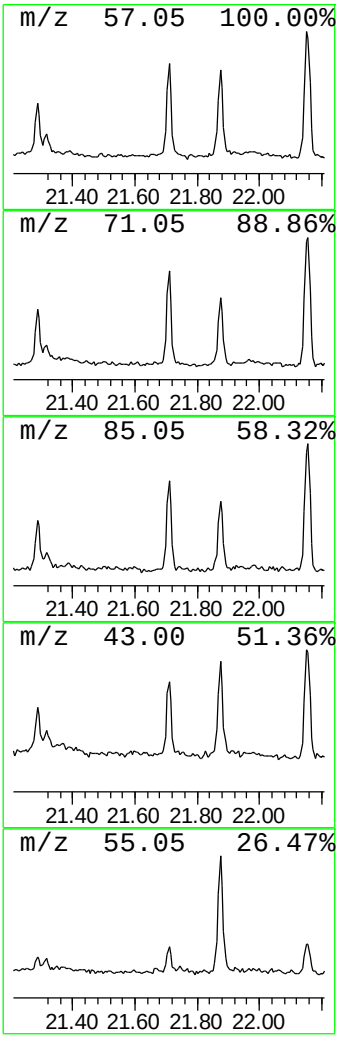
Peak Number 10 Heptadecane, 2-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.71	2.16 ng	143849	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	87
2	Octadecane, 3-methyl-	268	C19H40	006561-44-0	86
3	Octacosane	394	C28H58	000630-02-4	86
4	Heneicosane	296	C21H44	000629-94-7	83
5	Octadecane, 2-methyl-	268	C19H40	001560-88-9	80





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM041819\
Data File : BM019965.D
Acq On : 18 Apr 2019 22:09
Operator : JU/SJ
Sample : K2461-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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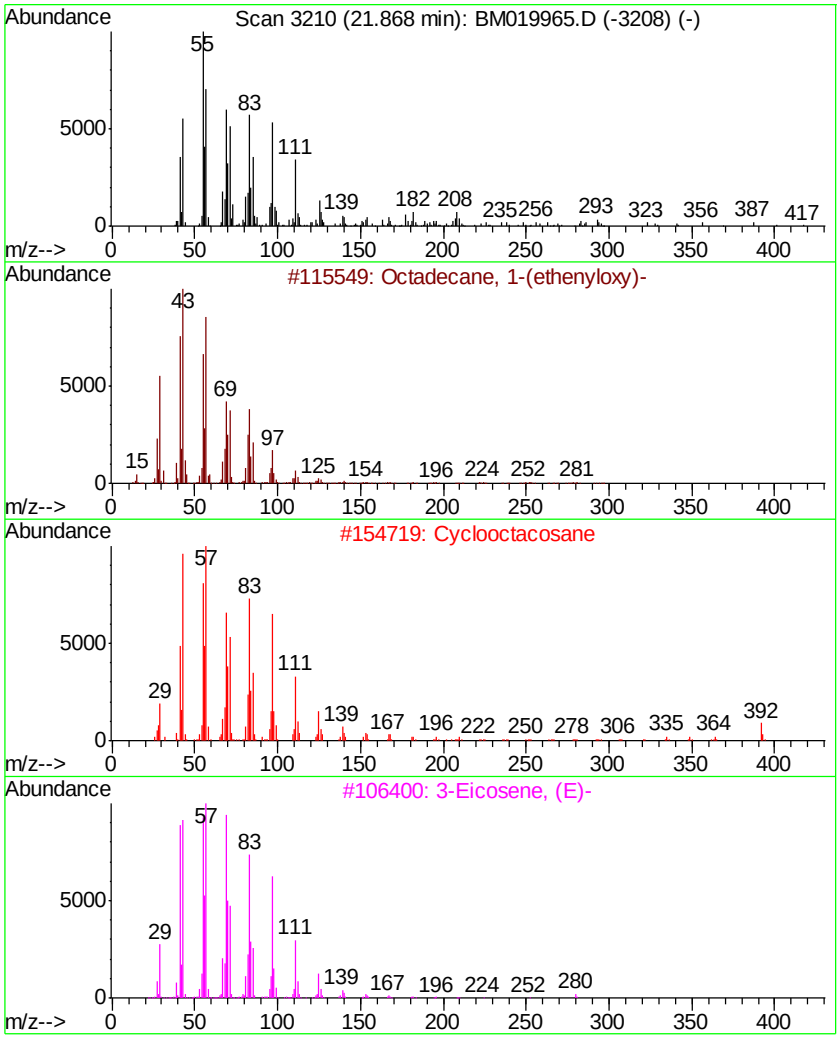
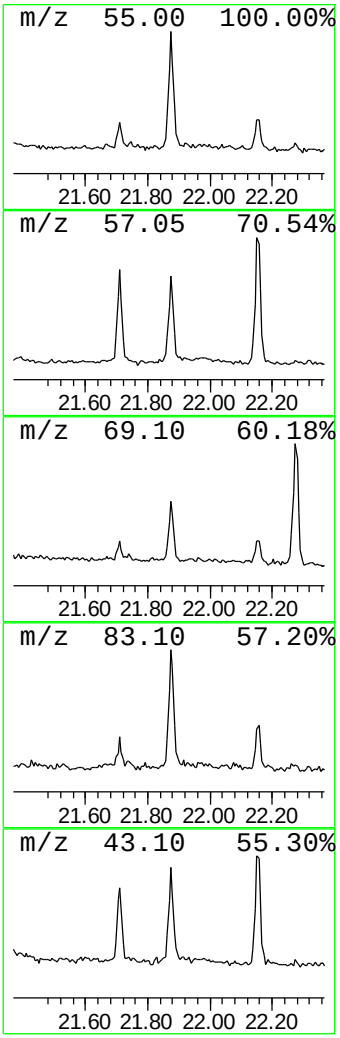
Peak Number 11 Octadecane, 1-(ethenyloxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.87	5.01 ng	334483	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	90
2	Cyclooctacosane	392	C28H56	000297-24-5	83
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	81
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	81
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	81





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Acq On : 18 Apr 2019 22:09
Operator : JU/SJ
Sample : K2461-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.M
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TIC Library : C:\DATABASE\NIST02.L
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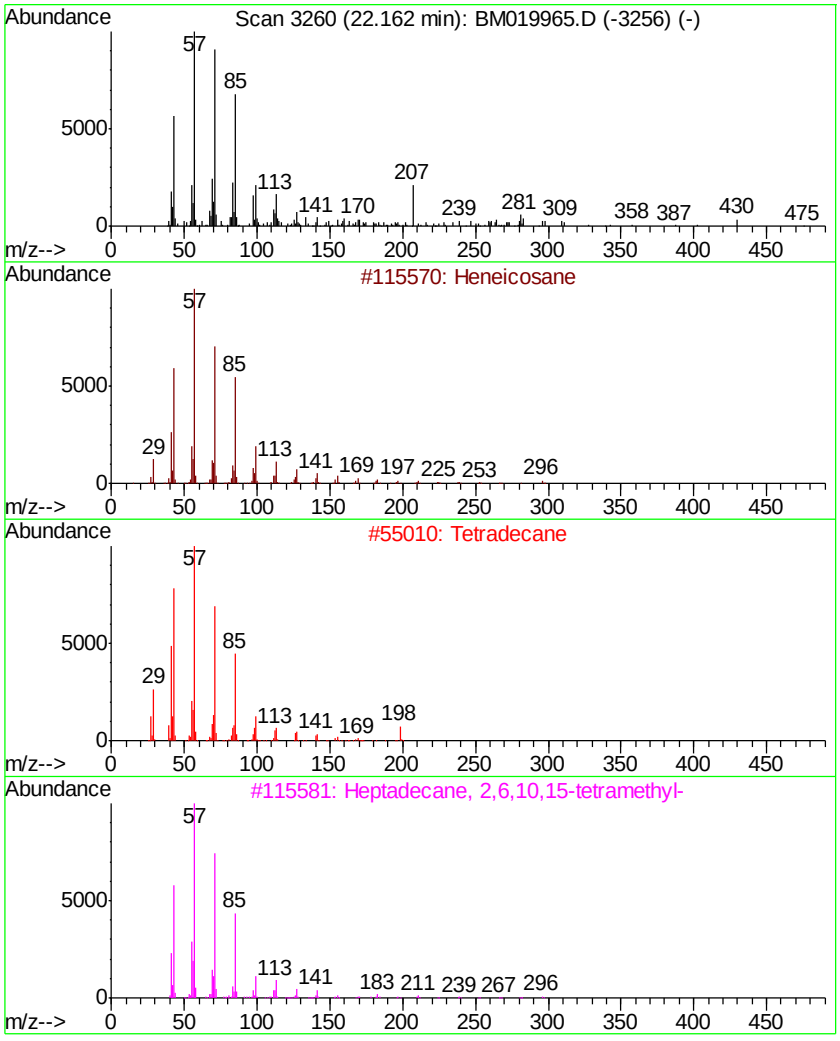
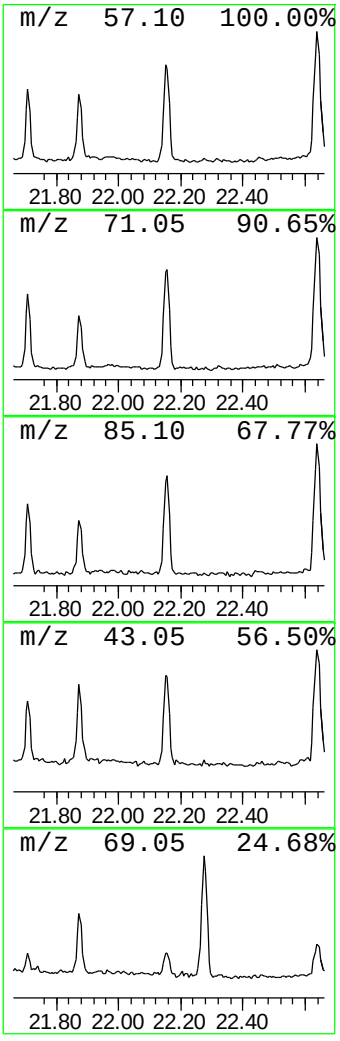
Peak Number 12 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.16	3.62 ng	241678	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	93
2	Tetradecane	198	C14H30	000629-59-4	91
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	89
4	Tetracosane	338	C24H50	000646-31-1	86
5	Tridecane, 7-hexyl-	268	C19H40	007225-66-3	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM041819\
Data File : BM019965.D
Acq On : 18 Apr 2019 22:09
Operator : JU/SJ
Sample : K2461-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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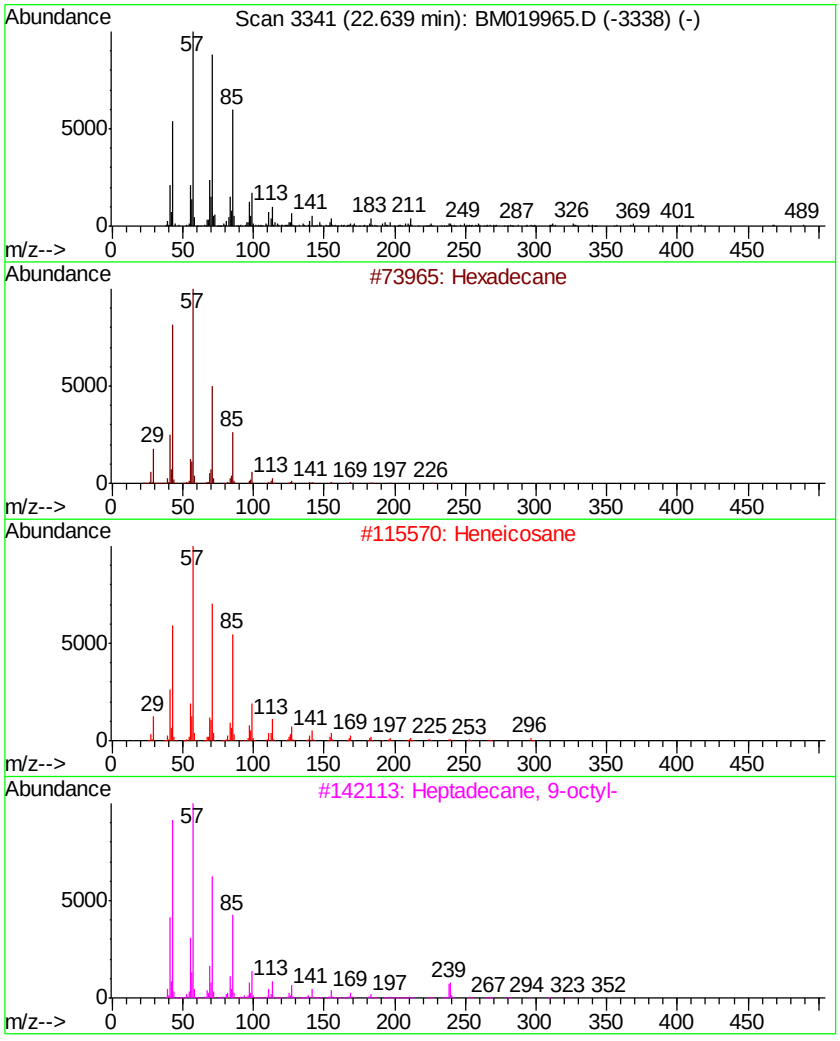
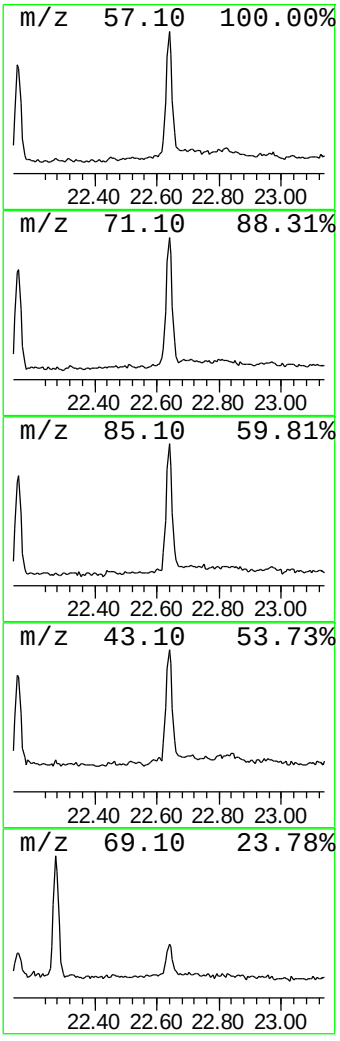
Peak Number 13 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.64	4.93 ng	347816	Perylene-d12	23.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	90
5	Tetracosane	338	C24H50	000646-31-1	90





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Data File : BM019965.D
Acq On : 18 Apr 2019 22:09
Operator : JU/SJ
Sample : K2461-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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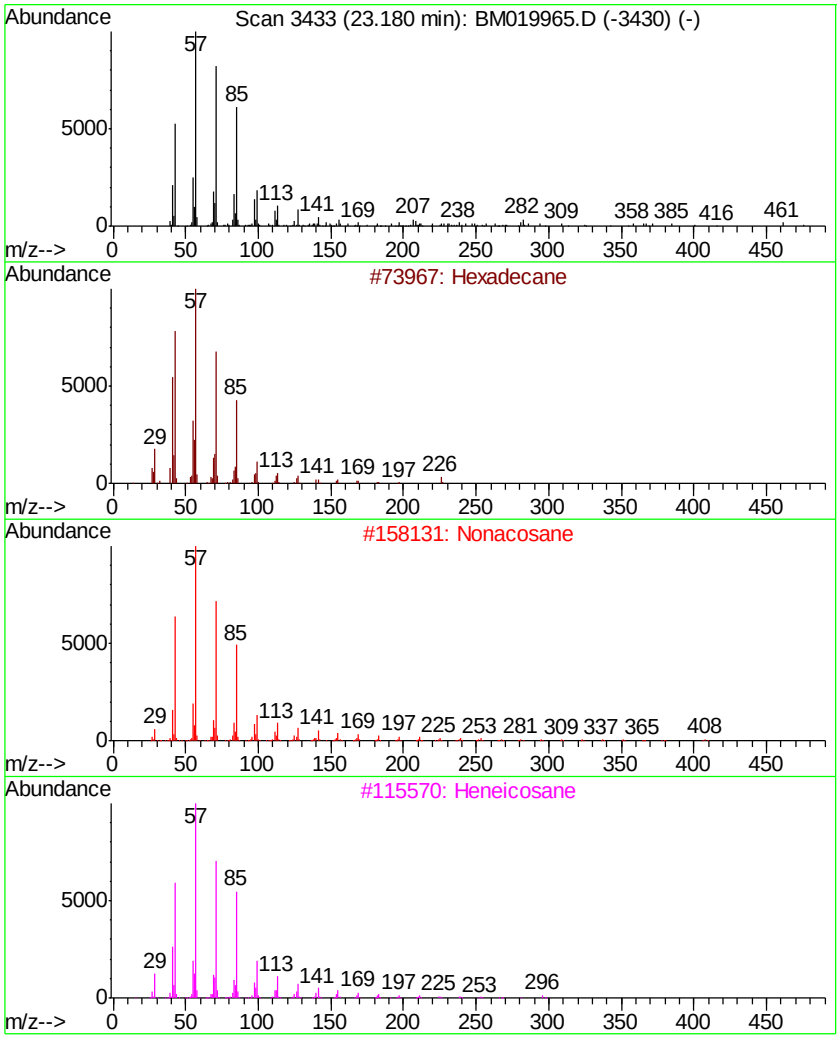
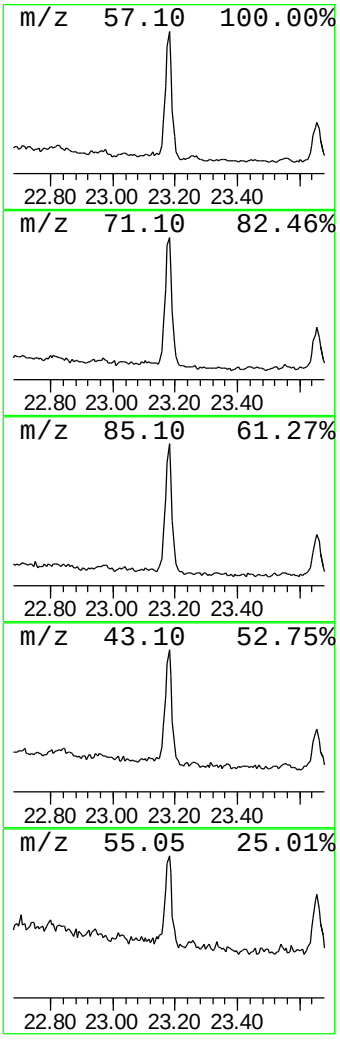
Peak Number 14 Nonacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.18	5.05 ng	356375	Perylene-d12	23.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Nonacosane	408	C29H60	000630-03-5	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	90
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM041819\
Data File : BM019965.D
Acq On : 18 Apr 2019 22:09
Operator : JU/SJ
Sample : K2461-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GMW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown4.86	4.86	2.2	ng	68388	1	7.51	630468	20.0
unknown7.05	7.05	86.6	ng	2731010	1	7.51	630468	20.0
unknown12.02	12.02	3.9	ng	146865	2	10.29	761647	20.0
unknown16.47	16.47	2.4	ng	136006	4	16.94	1147150	20.0
n-Hexadecanoic acid	17.84	10.8	ng	620403	4	16.94	1147150	20.0
3-Hexadecene, (Z)-	18.70	3.0	ng	169853	4	16.94	1147150	20.0
Octadecanoic acid	19.13	5.7	ng	381187	5	21.16	1334070	20.0
Heptafluorobutyri...	20.86	2.7	ng	180504	5	21.16	1334070	20.0
Heptadecane, 2-me...	21.71	2.2	ng	143849	5	21.16	1334070	20.0
Octadecane, 1-(et...	21.87	5.0	ng	334483	5	21.16	1334070	20.0
Heneicosane	22.16	3.6	ng	241678	5	21.16	1334070	20.0
Hexadecane	22.64	4.9	ng	347816	6	23.34	1411300	20.0
Nonacosane	23.18	5.0	ng	356375	6	23.34	1411300	20.0