LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM041719\
Data File : BM019942.D
Acq On : 17 Apr 2019 17:25
Operator : JU/SJ
Sample : K2423-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP4-A

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	5.140	360	366	390	rBV	2601680	3846455	70.62%	8.589%
2	6.722	629	635	656	rBV	2464536	4154543	76.28%	9.277%
3	7.063	687	693	712	rBV	2801326	4376327	80.35%	9.772%
4	7.528	766	772	781	rBV	650707	1017951	18.69%	2.273%
5	7.840	818	825	838	rBV	1935685	3064870	56.27%	6.844%
6	8.704	965	972	990	rBV	1238552	2402764	44.11%	5.365%
7	10.304	1237	1244	1265	rBV	719030	1391107	25.54%	3.106%
8	12.798	1661	1668	1695	rBV	3541914	5358400	98.38%	11.965%
9	13.669	1810	1816	1829	rBV	306848	539975	9.91%	1.206%
10	14.192	1899	1905	1920	rVB2	1133260	1716409	31.51%	3.833%
11	15.704	2156	2162	2182	rBV	2086729	3312032	60.81%	7.396%
12	16.957	2369	2375	2394	rBV2	1093446	1776397	32.61%	3.967%
13	17.851	2522	2527	2537	rBV	158609	316409	5.81%	0.707%
14	19.151	2743	2748	2759	rBV3	50766	122165	2.24%	0.273%
15	19.603	2819	2825	2836	rBV	4837227	5446741	100.00%	12.163%
16	19.898	2869	2875	2884	rBV6	38242	76351	1.40%	0.170%
17	20.398	2956	2960	2966	rBV3	54716	78344	1.44%	0.175%
18	20.874	3036	3041	3049	rBV	529547	796460	14.62%	1.779%
19	21.174	3087	3092	3104	rBV	1221446	1709687	31.39%	3.818%
20	21.303	3111	3114	3117	rBV	98076	100274	1.84%	0.224%
21	21.727	3182	3186	3188	rBV	138433	157115	2.88%	0.351%
22	22.168	3258	3261	3268	rVB	169965	210899	3.87%	0.471%
23	22.292	3279	3282	3286	rVB	186055	223483	4.10%	0.499%
24	22.656	3341	3344	3349	rVB2	171007	233775	4.29%	0.522%
25	23.197	3433	3436	3444	rVB	160610	252786	4.64%	0.564%
26	23.368	3459	3465	3478	rVB	940731	1872602	34.38%	4.182%
27	23.815	3538	3541	3549	rVB3	137576	228328	4.19%	0.510%

Sum of corrected areas: 44782649

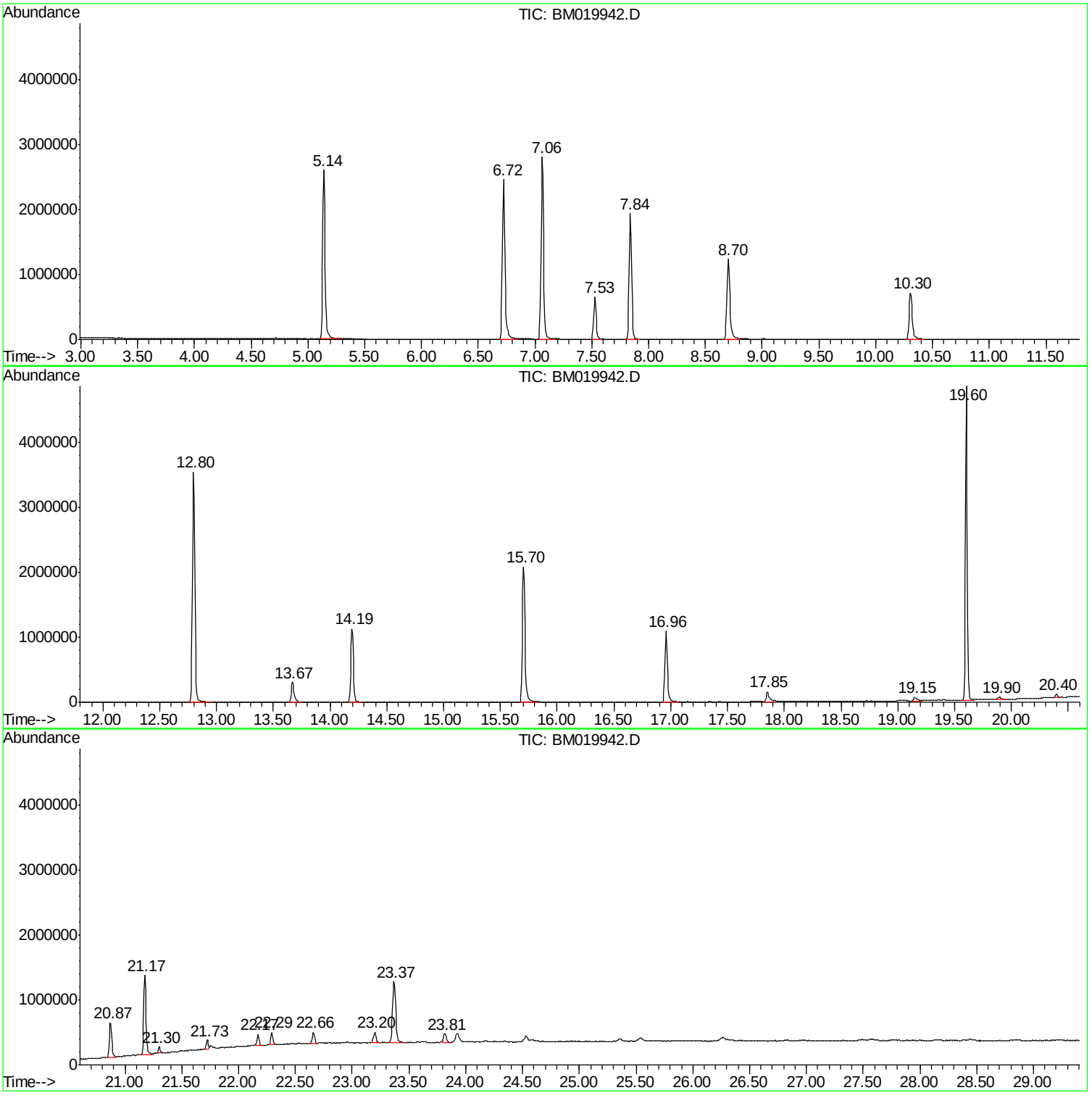
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM041719\
Data File : BM019942.D
Acq On : 17 Apr 2019 17:25
Operator : JU/SJ
Sample : K2423-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP4-A

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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Data File : BM019942.D
Acq On : 17 Apr 2019 17:25
Operator : JU/SJ
Sample : K2423-13
Misc :
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Instrument : BNA_M
ClientSampleId : TP4-A

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

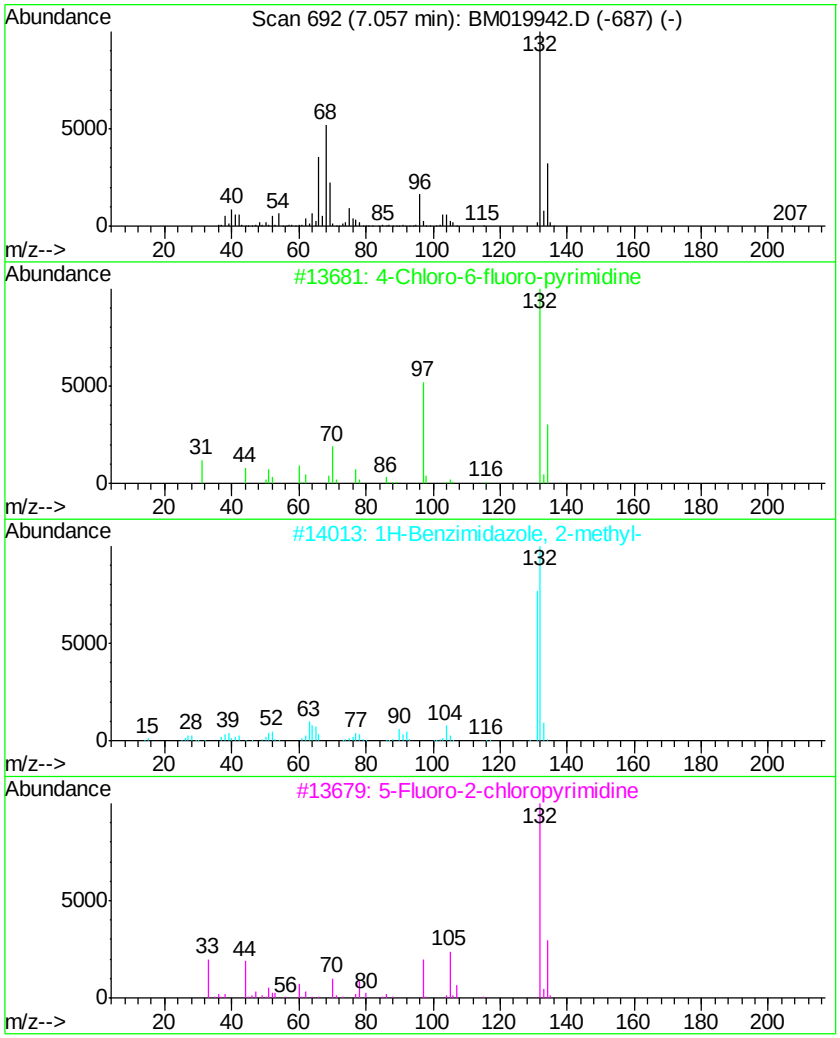
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

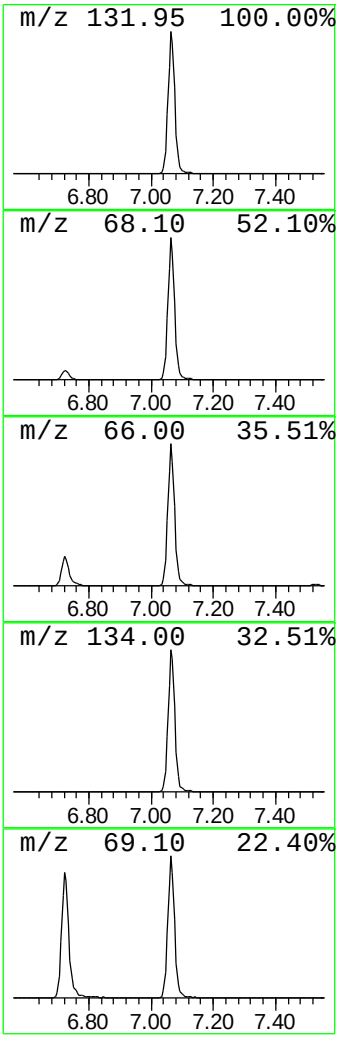
****

Peak Number 1 unknown7.06 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.06	85.98 ng	4376330	1,4-Dichlorobenzene-d4	7.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	10
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM041719\
Data File : BM019942.D
Acq On : 17 Apr 2019 17:25
Operator : JU/SJ
Sample : K2423-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP4-A

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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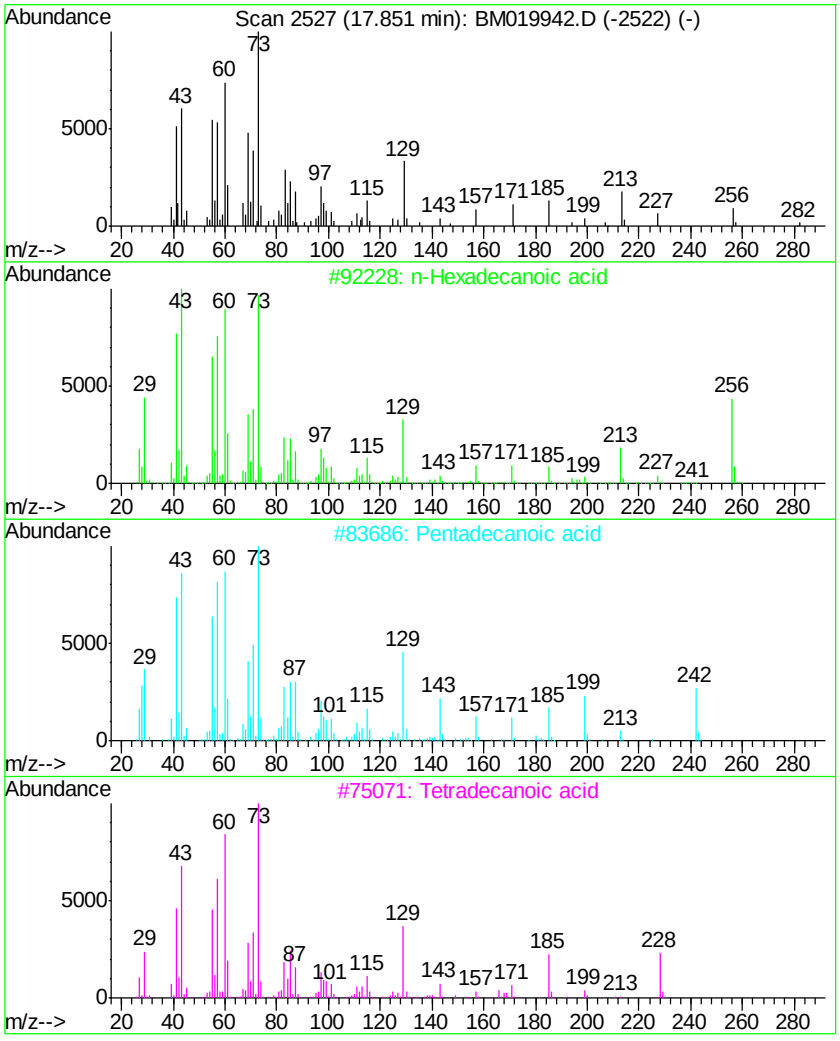
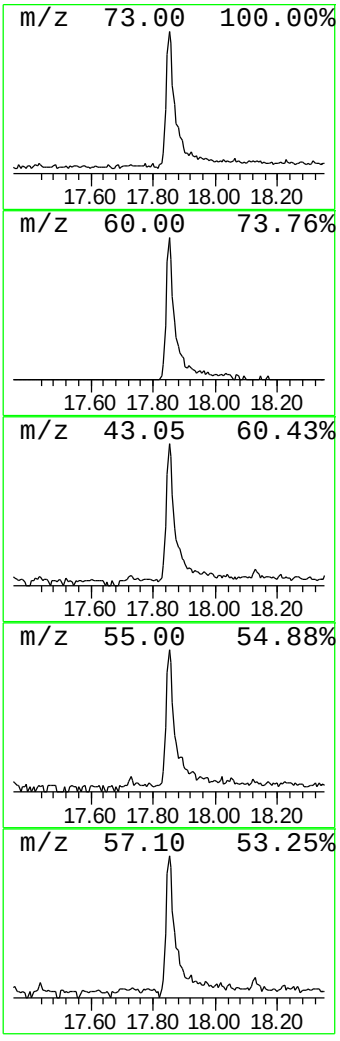
Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.85	3.56 ng	316409	Phenanthrene-d10	16.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Tridecane	184	C13H28	000629-50-5	11





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM041719\
Data File : BM019942.D
Acq On : 17 Apr 2019 17:25
Operator : JU/SJ
Sample : K2423-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP4-A

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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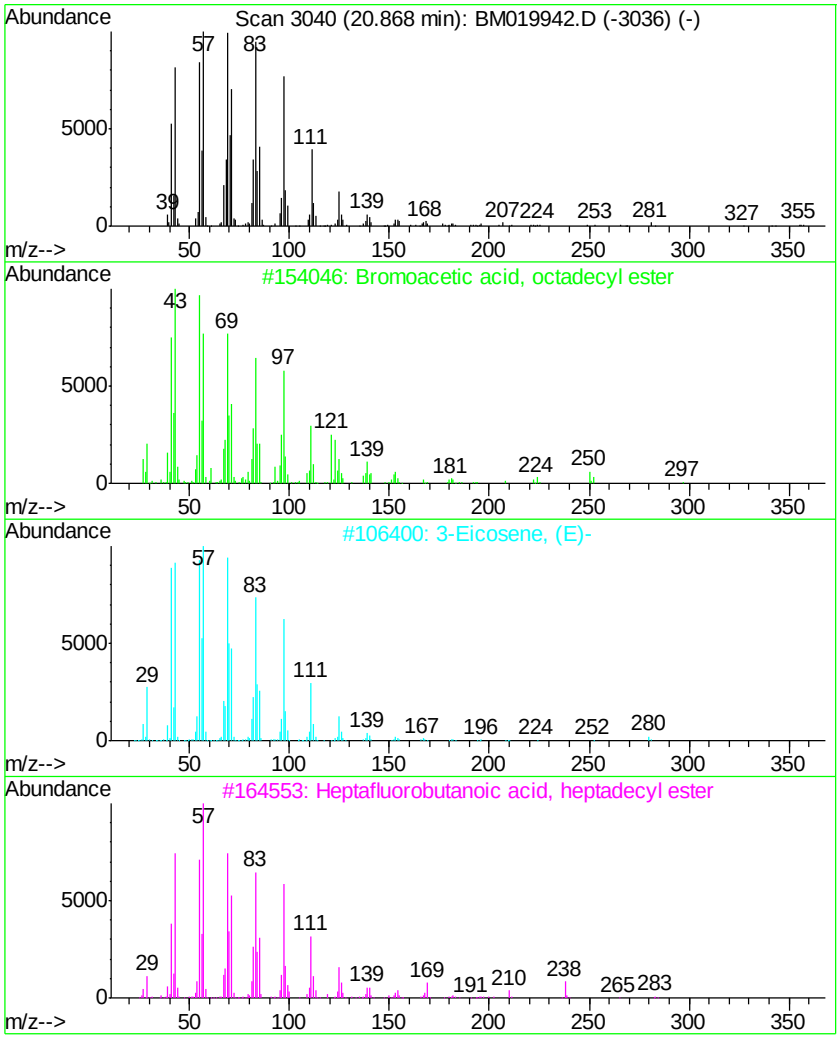
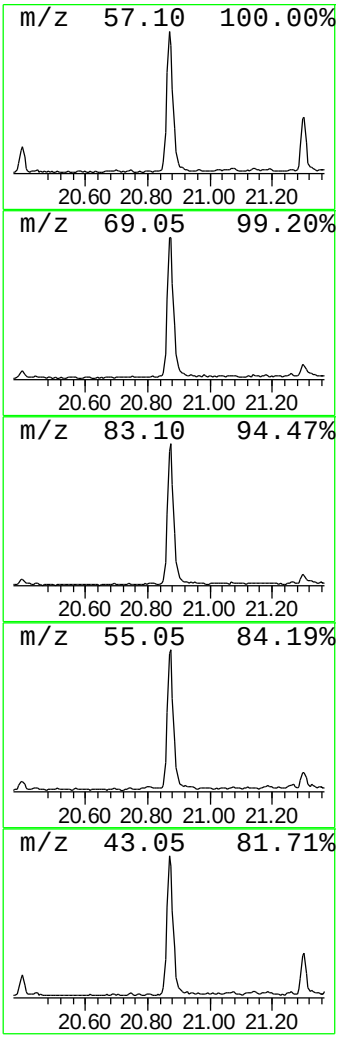
Peak Number 4 Bromoacetic acid, octadecyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.87	9.32 ng	796460	Chrysene-d12	21.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	91
4	Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	91
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM041719\
Data File : BM019942.D
Acq On : 17 Apr 2019 17:25
Operator : JU/SJ
Sample : K2423-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP4-A

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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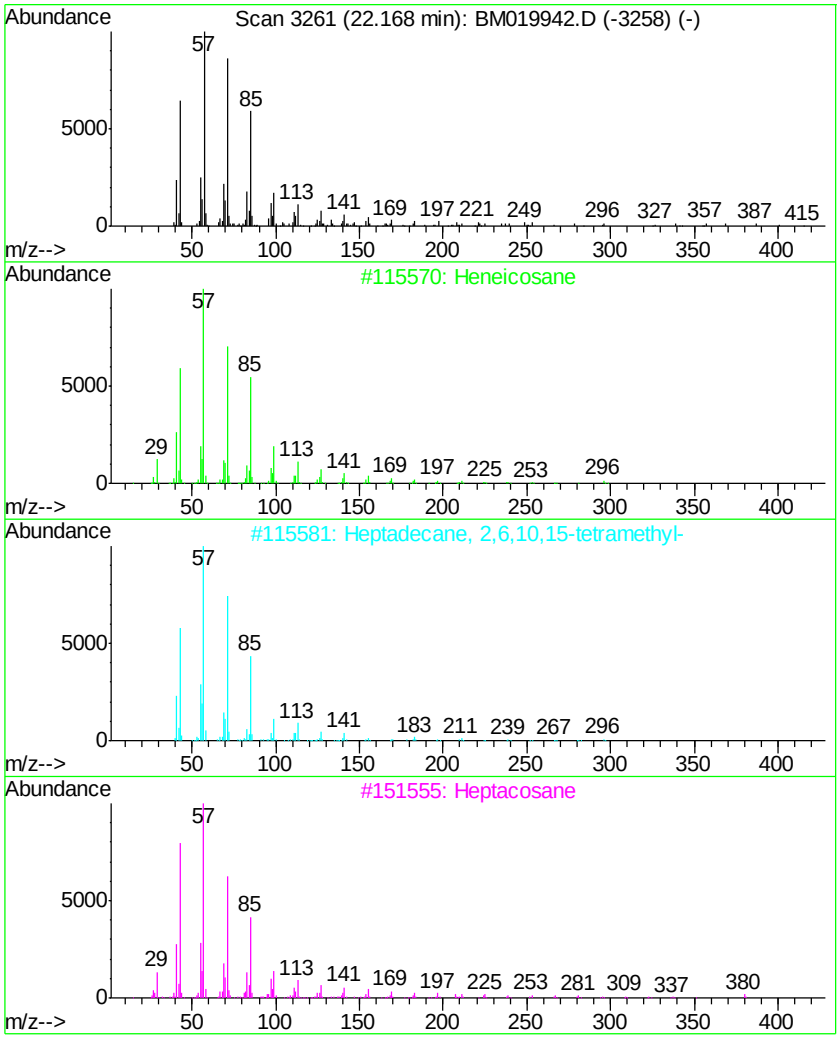
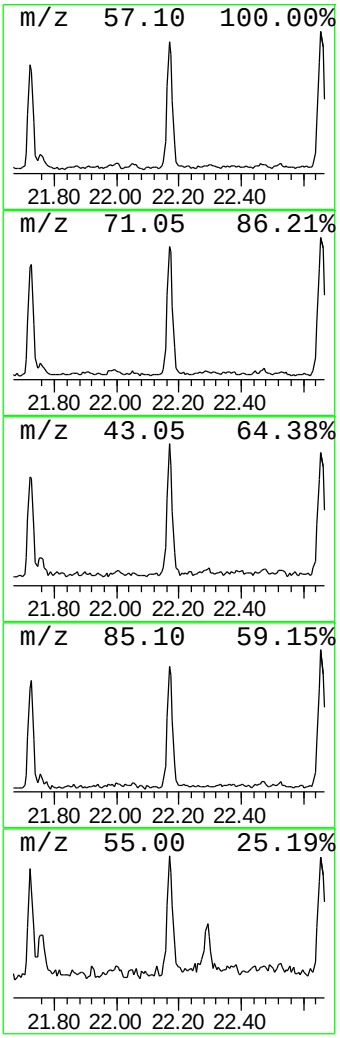
Peak Number 5 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.17	2.47 ng	210899	Chrysene-d12	21.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	98
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
3	Heptacosane	380	C27H56	000593-49-7	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM041719\
Data File : BM019942.D
Acq On : 17 Apr 2019 17:25
Operator : JU/SJ
Sample : K2423-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP4-A

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

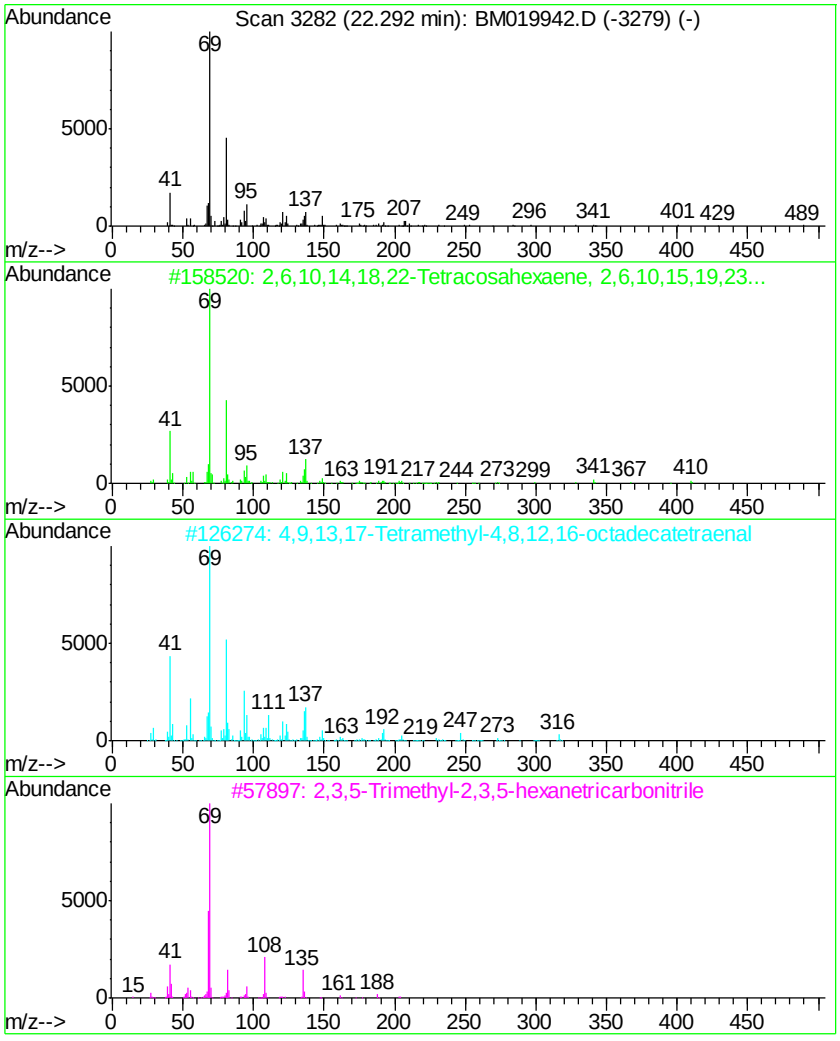
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

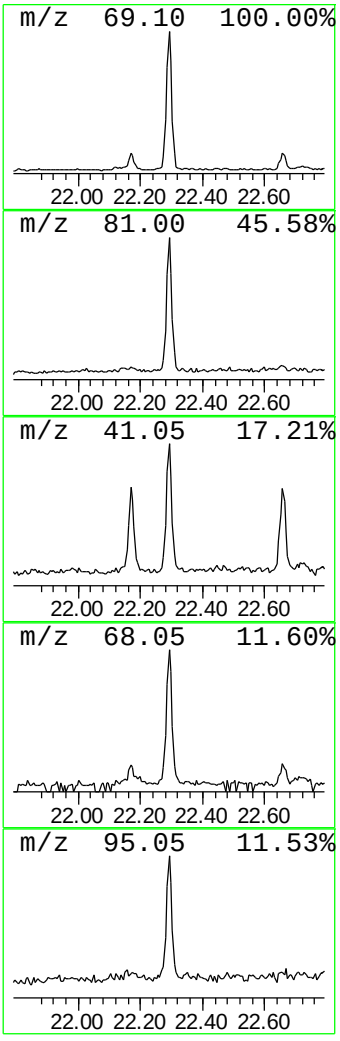
****

Peak Number 6 2,6,10,14,18,22-Tetracosahe... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.29	2.39 ng	223483	Perylene-d12	23.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	80
2	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	72
3	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	64
4	4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	64
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64





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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP4-A

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

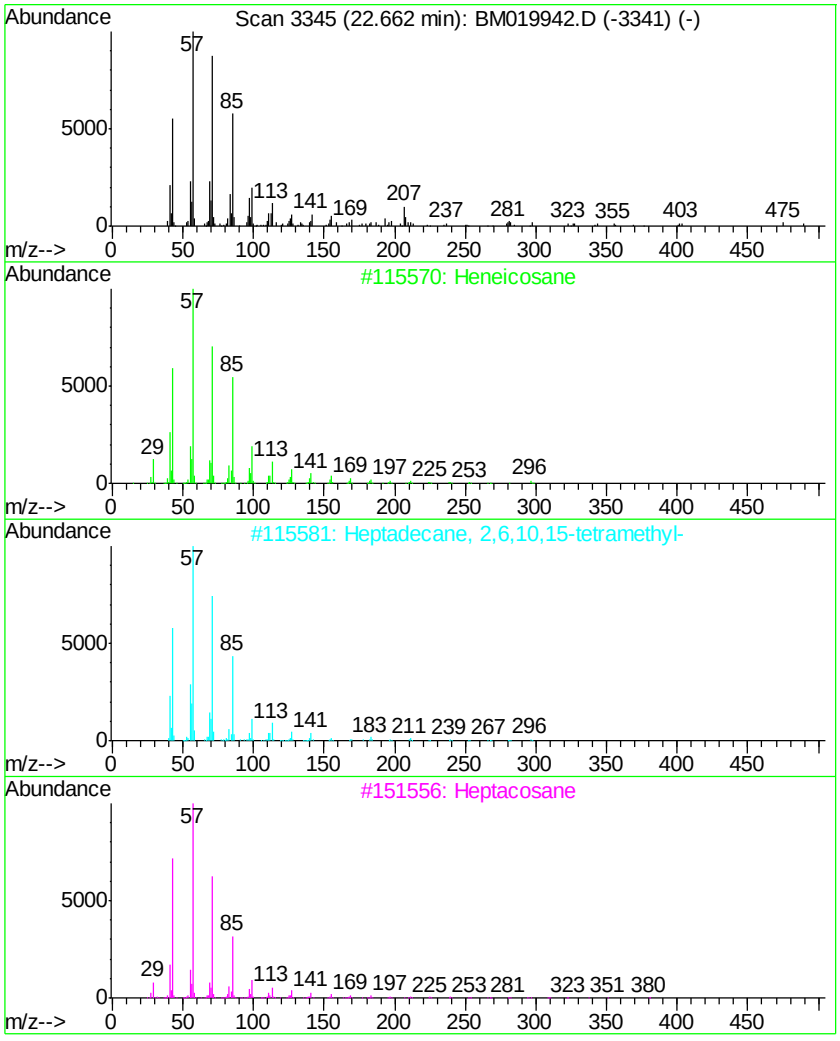
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

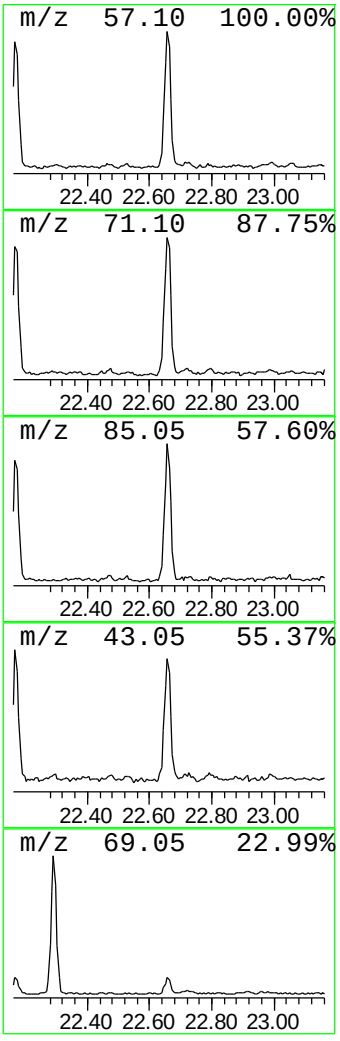
****

Peak Number 7 Heptadecane, 2,6,10,15-tetr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.66	2.50 ng	233775	Perylene-d12	23.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	94
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
3	Heptacosane	380	C27H56	000593-49-7	87
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5	Heptadecane	240	C17H36	000629-78-7	87





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Data File : BM019942.D
Acq On : 17 Apr 2019 17:25
Operator : JU/SJ
Sample : K2423-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP4-A

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

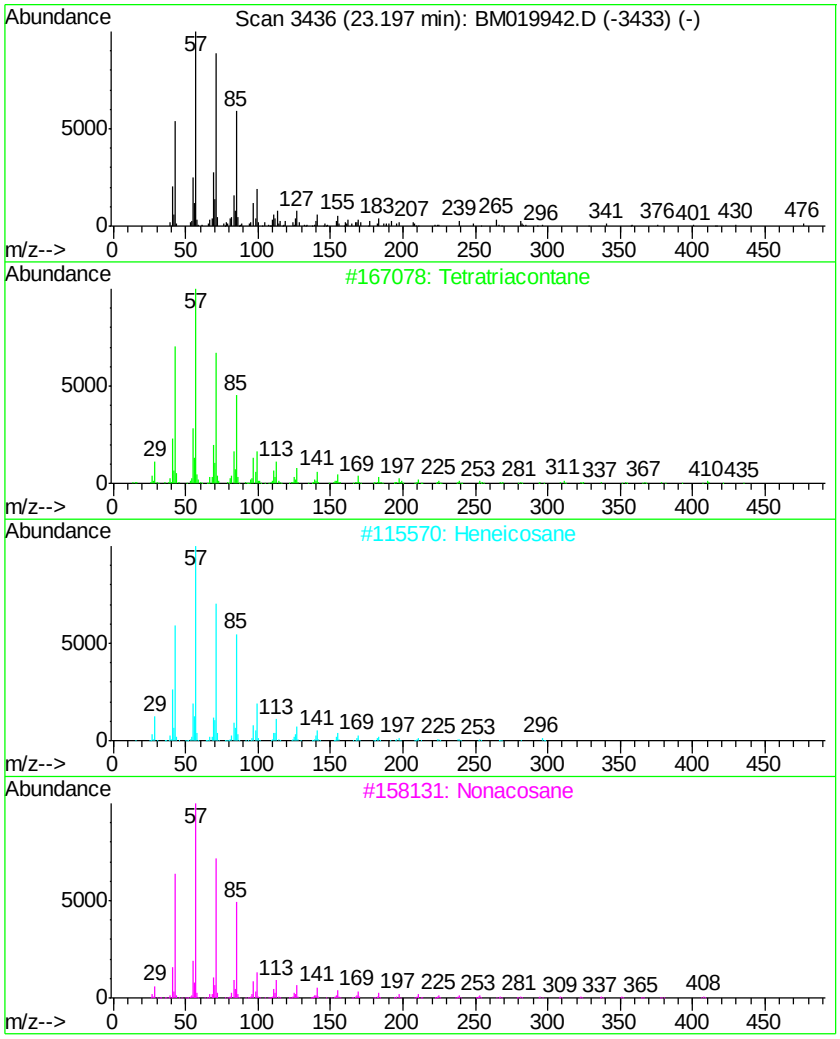
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

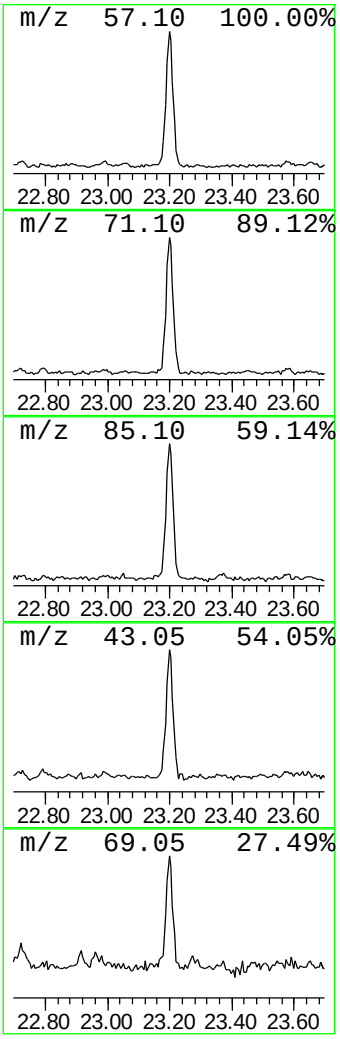
****

Peak Number 8 Tetratriacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.20	2.70 ng	252786	Perylene-d12	23.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratriacontane	479	C34H70	014167-59-0	87
2	Heneicosane	296	C21H44	000629-94-7	87
3	Nonacosane	408	C29H60	000630-03-5	86
4	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	86
5	Heptadecane	240	C17H36	000629-78-7	86





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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP4-A

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

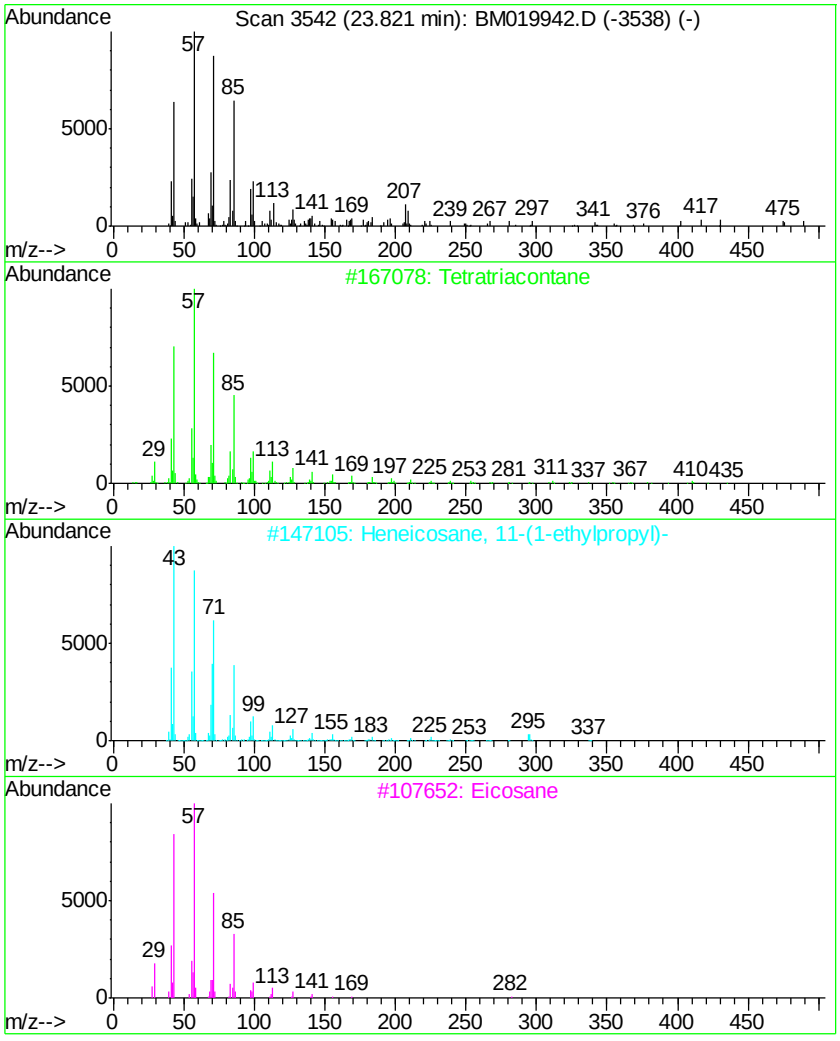
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

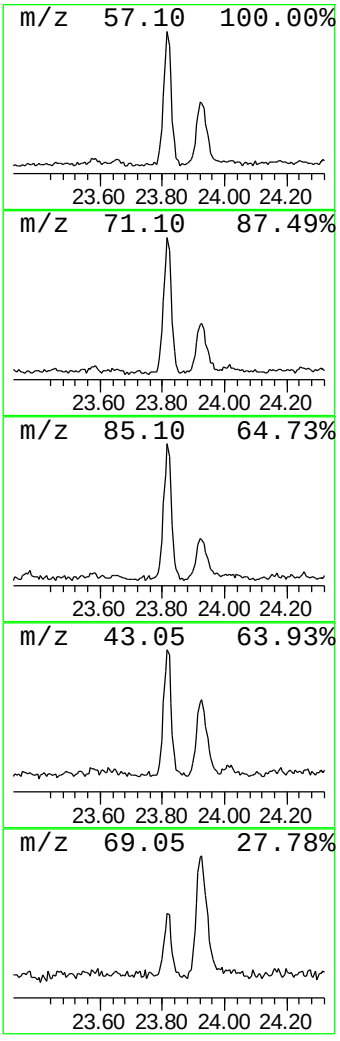
****

Peak Number 9 Heneicosane, 11-(1-ethylpro... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.82	2.44 ng	228328	Perylene-d12	23.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratriacontane	479	C34H70	014167-59-0	91
2	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
3	Eicosane	282	C20H42	000112-95-8	87
4	Heneicosane	296	C21H44	000629-94-7	87
5	10-Methylnonadecane	282	C20H42	056862-62-5	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM041719\
Data File : BM019942.D
Acq On : 17 Apr 2019 17:25
Operator : JU/SJ
Sample : K2423-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP4-A

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
unknown7.06	7.06	86.0	ng	4376330	1	7.53	1017950	20.0
n-Hexadecanoic acid	17.85	3.6	ng	316409	4	16.96	1776400	20.0
Bromoacetic acid,...	20.87	9.3	ng	796460	5	21.17	1709690	20.0
Heneicosane	22.17	2.5	ng	210899	5	21.17	1709690	20.0
2,6,10,14,18,22-T...	22.29	2.4	ng	223483	6	23.37	1872600	20.0
Heptadecane, 2,6,...	22.66	2.5	ng	233775	6	23.37	1872600	20.0
Tetratriacontane	23.20	2.7	ng	252786	6	23.37	1872600	20.0
Heneicosane, 11-(...	23.82	2.4	ng	228328	6	23.37	1872600	20.0