LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF082917\
Data File : BF098117.D
Acq On : 29 Aug 2017 18:11
Operator : SJ/JU
Sample : I4988-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FF5-COMP

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:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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	4.934	481	484	499	rVB	203189	308831	8.21%	0.946%
2	5.346	548	554	557	rBV	3125895	3384812	89.95%	10.363%
3	6.375	720	729	732	rBV	3132548	3700147	98.33%	11.329%
4	6.504	746	751	754	rBV	3304905	3426982	91.07%	10.492%
5	6.734	786	790	793	rBV	925468	809049	21.50%	2.477%
6	6.887	812	816	820	rBV	2519917	2586487	68.74%	7.919%
7	7.298	880	886	889	rBV	2174031	2279307	60.57%	6.979%
8	7.392	897	902	908	rBV	36640	42406	1.13%	0.130%
9	8.016	1003	1008	1011	rBV	1195132	1052793	27.98%	3.223%
10	9.092	1185	1191	1201	rBV	3589906	3762962	100.00%	11.521%
11	9.486	1254	1258	1266	rBV	724068	596228	15.84%	1.825%
12	9.769	1300	1306	1315	rVB	1353510	1176360	31.26%	3.602%
13	10.204	1377	1380	1383	rVB	72948	57007	1.51%	0.175%
14	10.557	1435	1440	1443	rBV	2147976	2198331	58.42%	6.731%
15	10.675	1457	1460	1469	rBV	99676	102156	2.71%	0.313%
16	11.122	1533	1536	1539	rBV2	57141	51901	1.38%	0.159%
17	11.251	1554	1558	1561	rBV	1323613	1156713	30.74%	3.542%
18	11.480	1591	1597	1603	rBV2	106593	114130	3.03%	0.349%
19	11.651	1622	1626	1630	rVB	63755	50825	1.35%	0.156%
20	12.298	1733	1736	1739	rBV	55281	55409	1.47%	0.170%
21	12.357	1742	1746	1753	rVB2	127387	135291	3.60%	0.414%
22	12.839	1823	1828	1831	rBV	3045685	2966193	78.83%	9.082%
23	13.733	1976	1980	1990	rBV	220278	245409	6.52%	0.751%
24	13.880	2001	2005	2009	rBV	765485	726800	19.31%	2.225%
25	14.368	2081	2088	2095	rBV5	40496	66184	1.76%	0.203%
26	14.980	2188	2192	2195	rBV	37927	42388	1.13%	0.130%
27	15.304	2242	2247	2250	rVV	509336	631481	16.78%	1.933%
28	15.333	2250	2252	2258	rVB	63093	79838	2.12%	0.244%
29	15.745	2317	2322	2327	rBV	78314	113613	3.02%	0.348%
30	16.215	2396	2402	2410	rBV	87867	162440	4.32%	0.497%
31	16.774	2490	2497	2506	rBV	74934	149907	3.98%	0.459%
32	17.421	2600	2607	2618	rVB2	71976	163791	4.35%	0.501%
33	18.192	2731	2738	2748	rVB2	46403	127565	3.39%	0.391%
34	19.121	2886	2896	2910	rBV4	38405	137613	3.66%	0.421%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF082917\
Data File : BF098117.D
Acq On : 29 Aug 2017 18:11
Operator : SJ/JU
Sample : I4988-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FF5-COMP

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:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 32661349

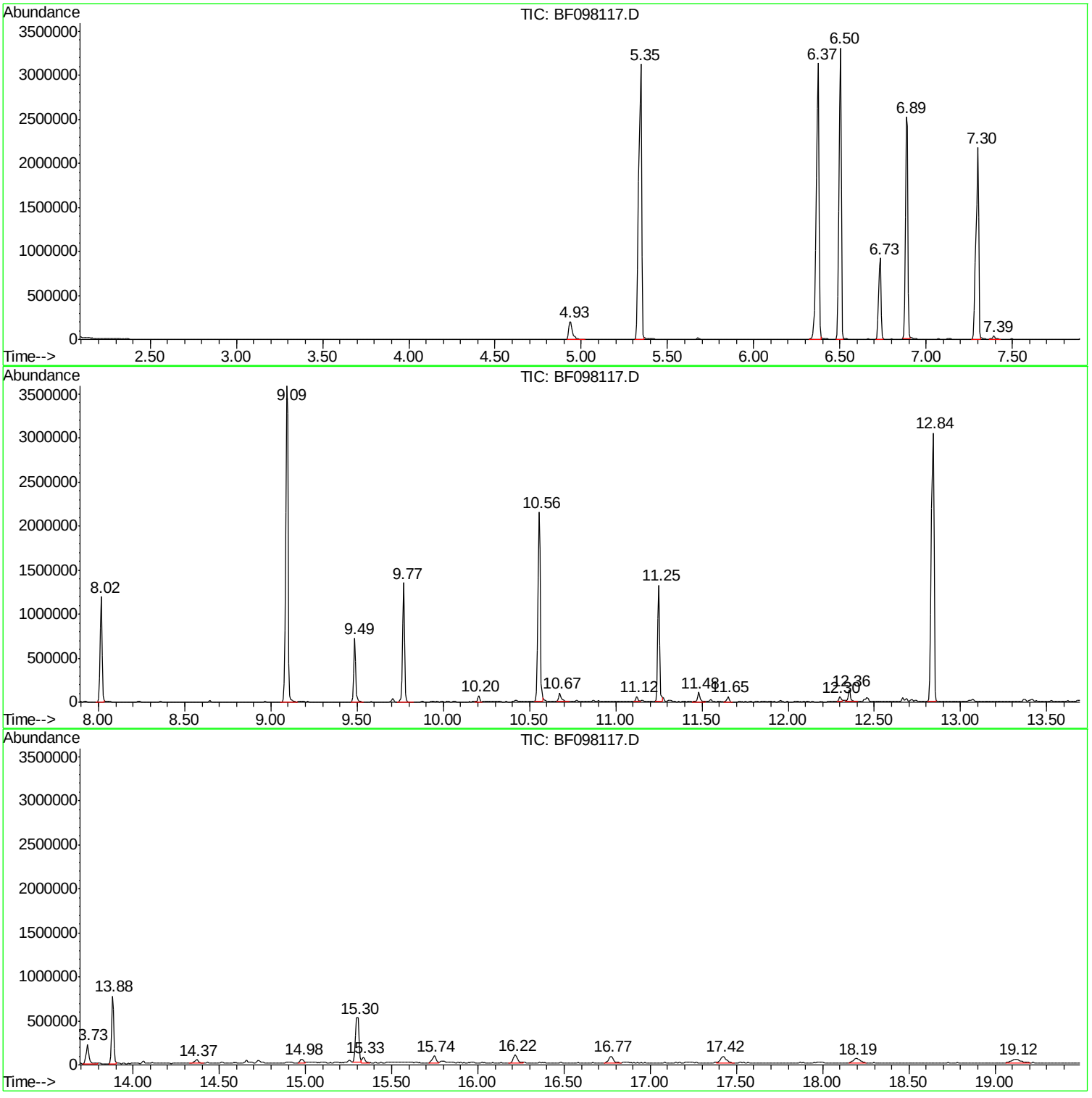
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF082917\
Data File : BF098117.D
Acq On : 29 Aug 2017 18:11
Operator : SJ/JU
Sample : I4988-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FF5-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF082917\
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Acq On : 29 Aug 2017 18:11
Operator : SJ/JU
Sample : I4988-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FF5-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

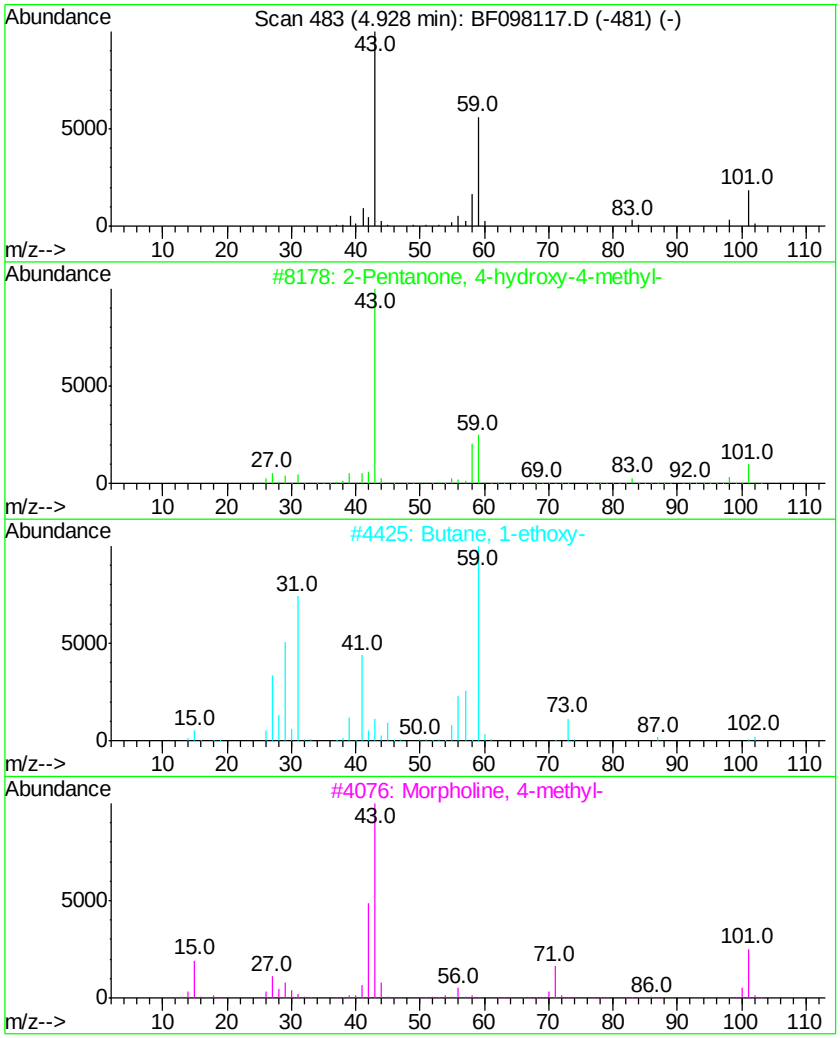
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

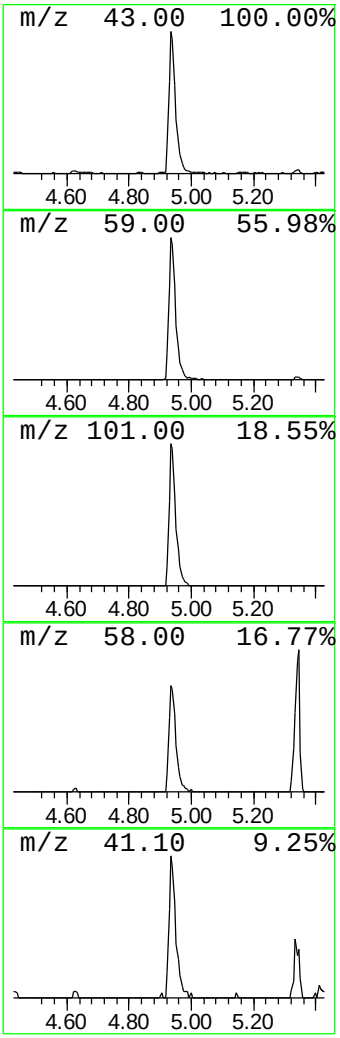
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	7.63 ng	308831	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF082917\
Data File : BF098117.D
Acq On : 29 Aug 2017 18:11
Operator : SJ/JU
Sample : I4988-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FF5-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

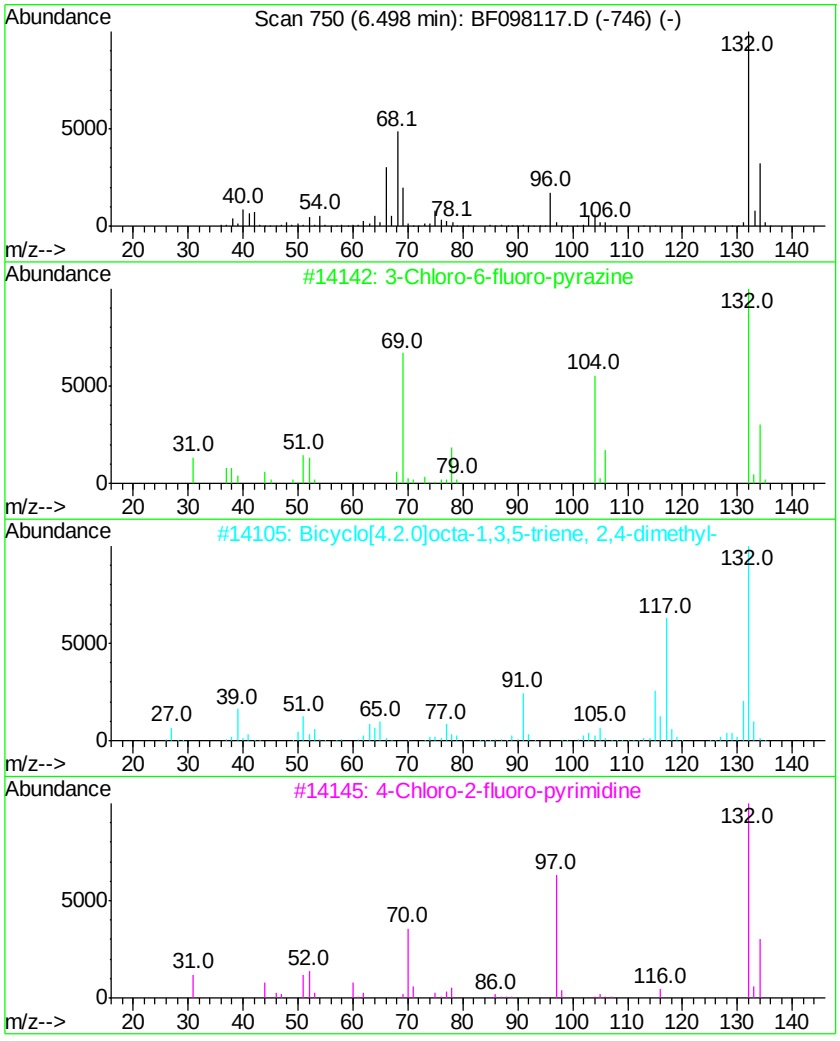
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

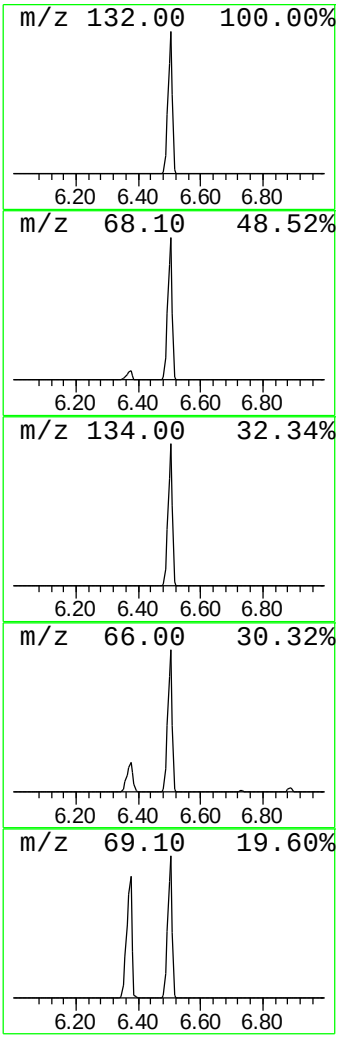
****

Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	84.72 ng	3426980	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	Xenon	132	Xe	007440-63-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF082917\
Data File : BF098117.D
Acq On : 29 Aug 2017 18:11
Operator : SJ/JU
Sample : I4988-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FF5-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

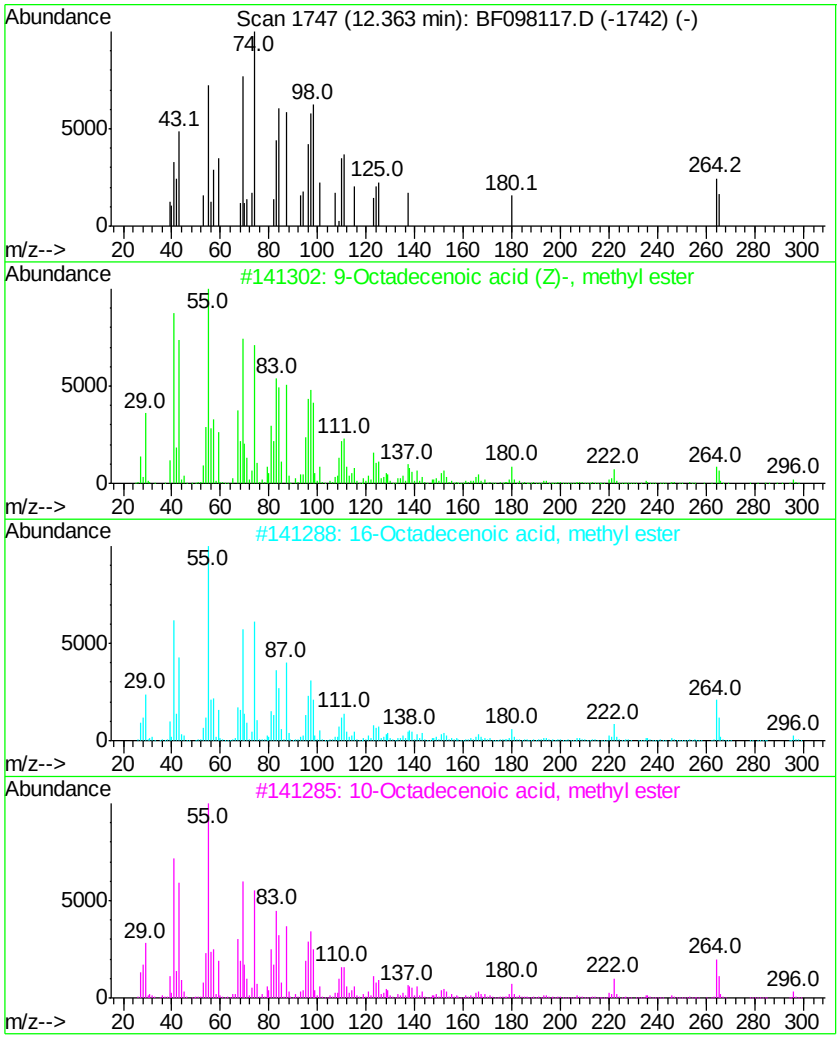
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

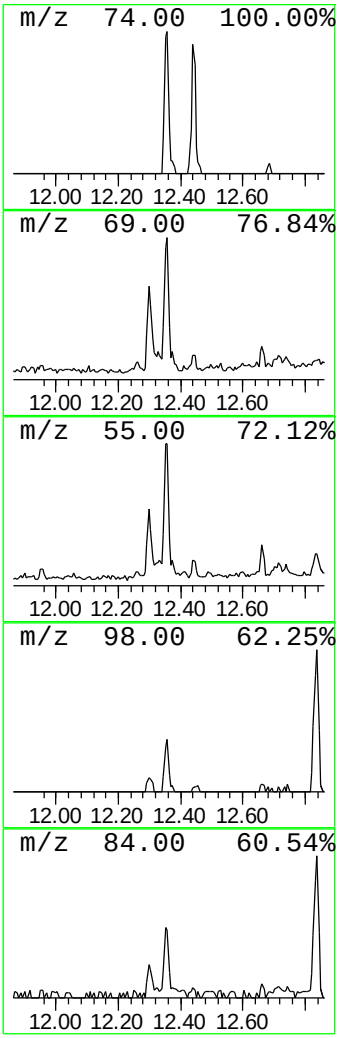
****

Peak Number 4 9-Octadecenoic acid (Z)-, m... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.36	2.34 ng	135291	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	81
3	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	81
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	81
5	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	81





Data Path : Z:\HPCHEM1\BNA F\DATA\BF082917\
Data File : BF098117.D
Acq On : 29 Aug 2017 18:11
Operator : SJ/JU
Sample : I4988-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FF5-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

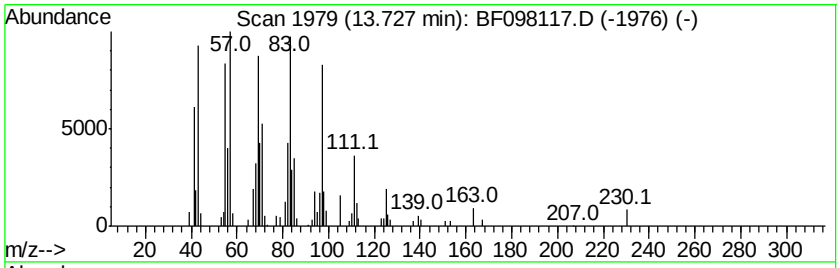
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

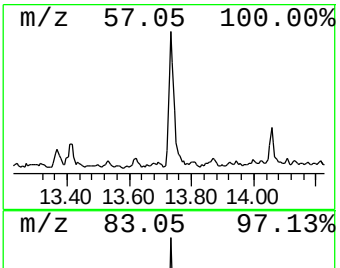
****

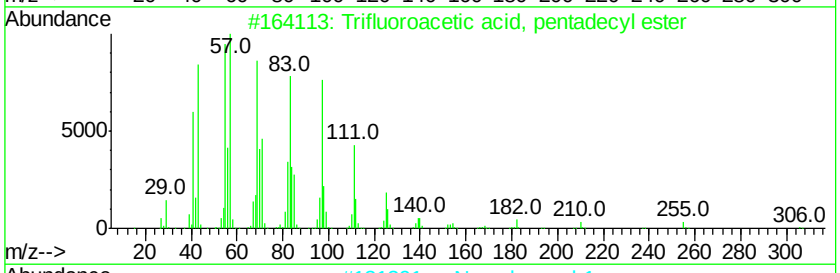
Peak Number 5 Trifluoroacetic acid, penta... Concentration Rank 4

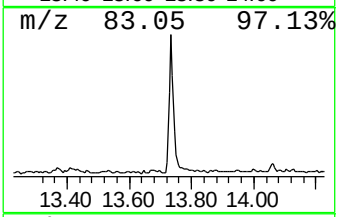
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	6.75 ng	245409	Chrysene-d12	13.88

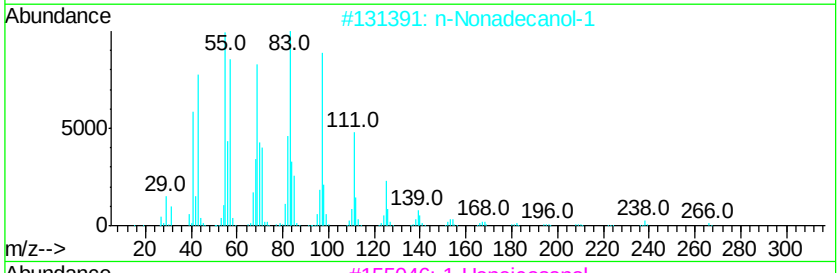
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	90
5	1-Nonadecene	266	C19H38	018435-45-5	87

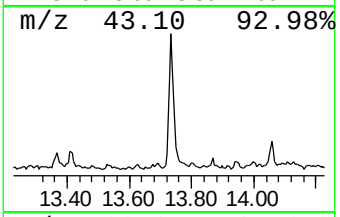


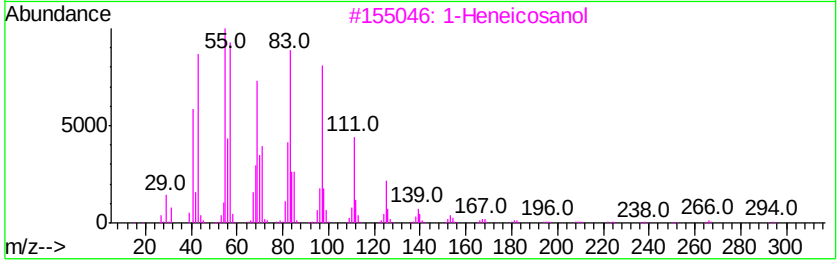


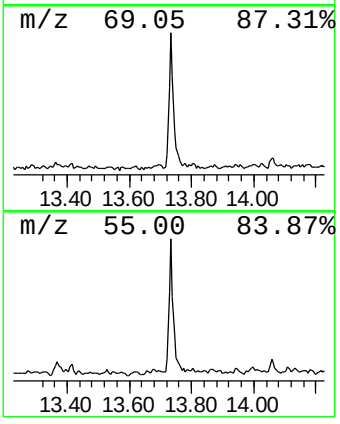












Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF082917\
Data File : BF098117.D
Acq On : 29 Aug 2017 18:11
Operator : SJ/JU
Sample : I4988-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FF5-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

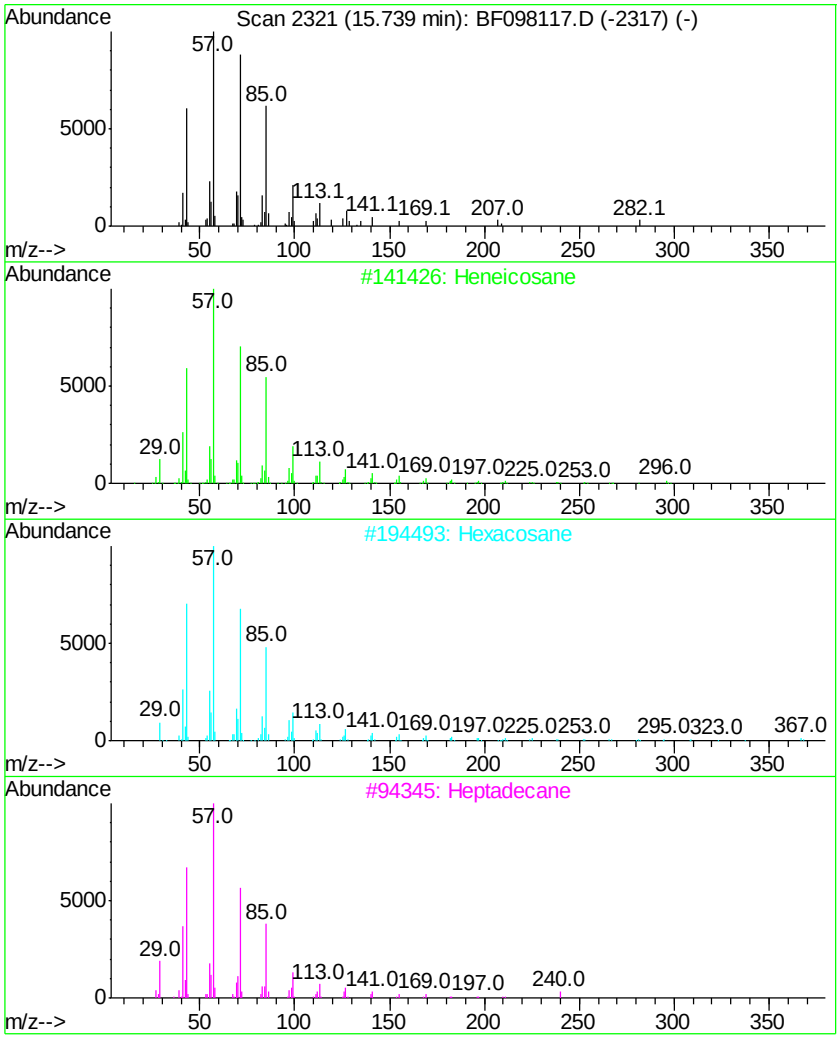
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

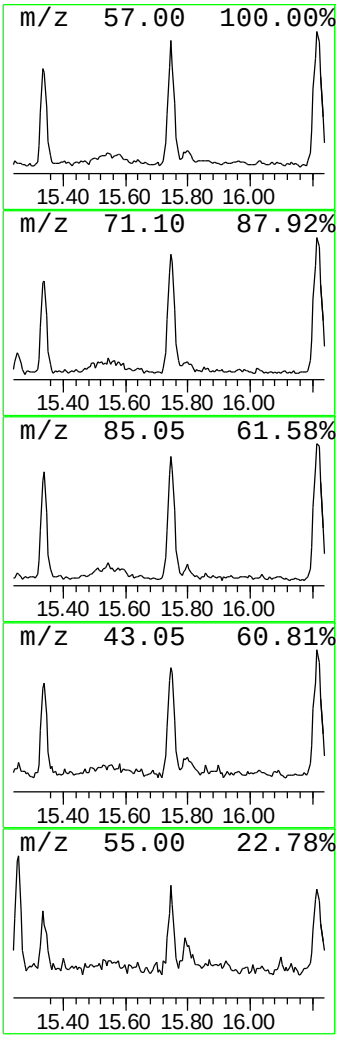
****

Peak Number 6 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	3.60 ng	113613	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heptadecane	240	C17H36	000629-78-7	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Octadecane	254	C18H38	000593-45-3	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF082917\
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ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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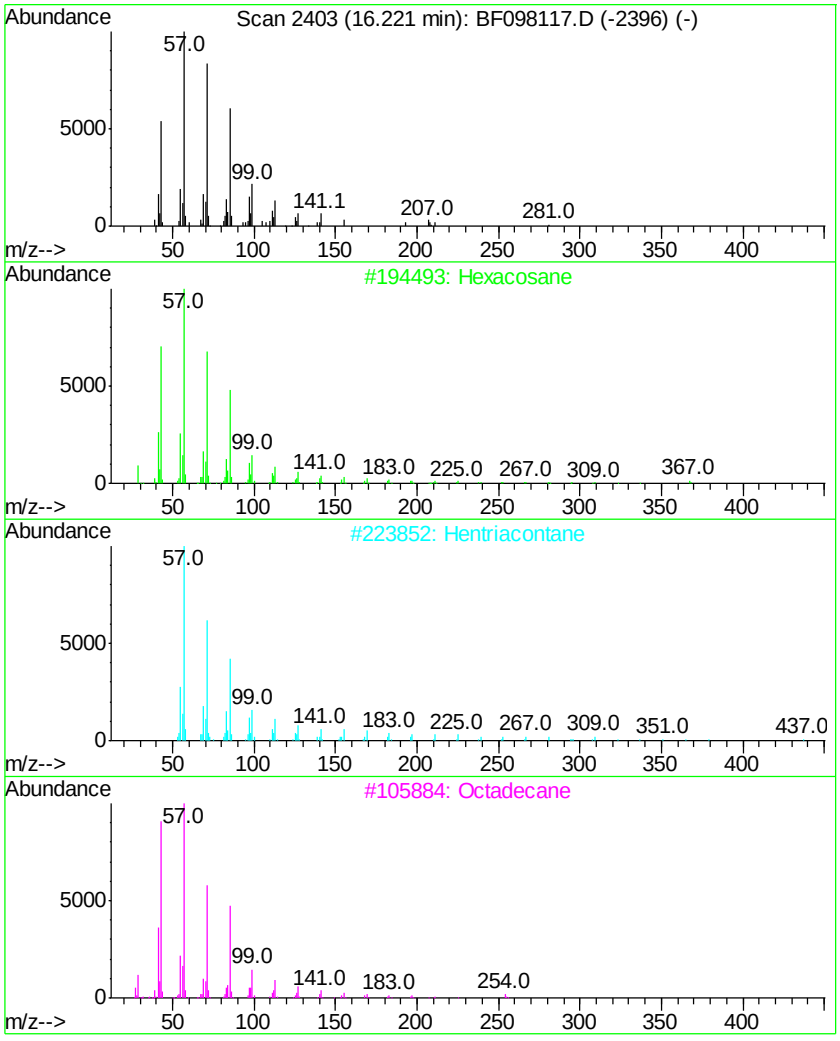
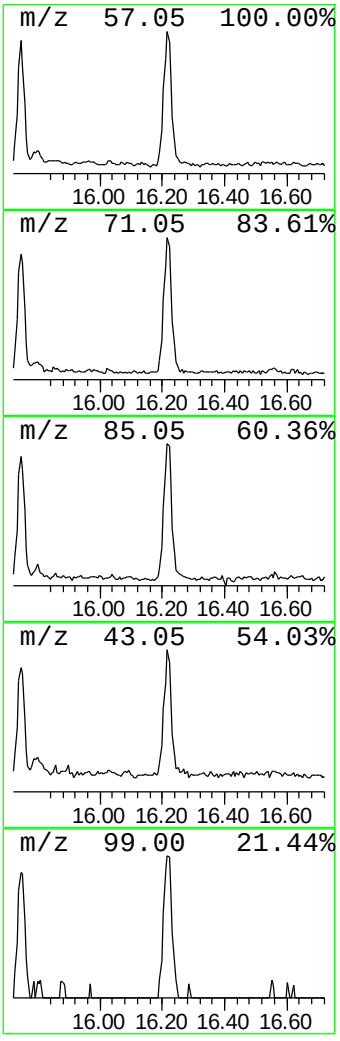
Peak Number 7 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.22	5.14 ng	162440	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Hentriacontane	437	C31H64	000630-04-6	91
3	Octadecane	254	C18H38	000593-45-3	90
4	Octacosane	394	C28H58	000630-02-4	87
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF082917\
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Acq On : 29 Aug 2017 18:11
Operator : SJ/JU
Sample : I4988-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FF5-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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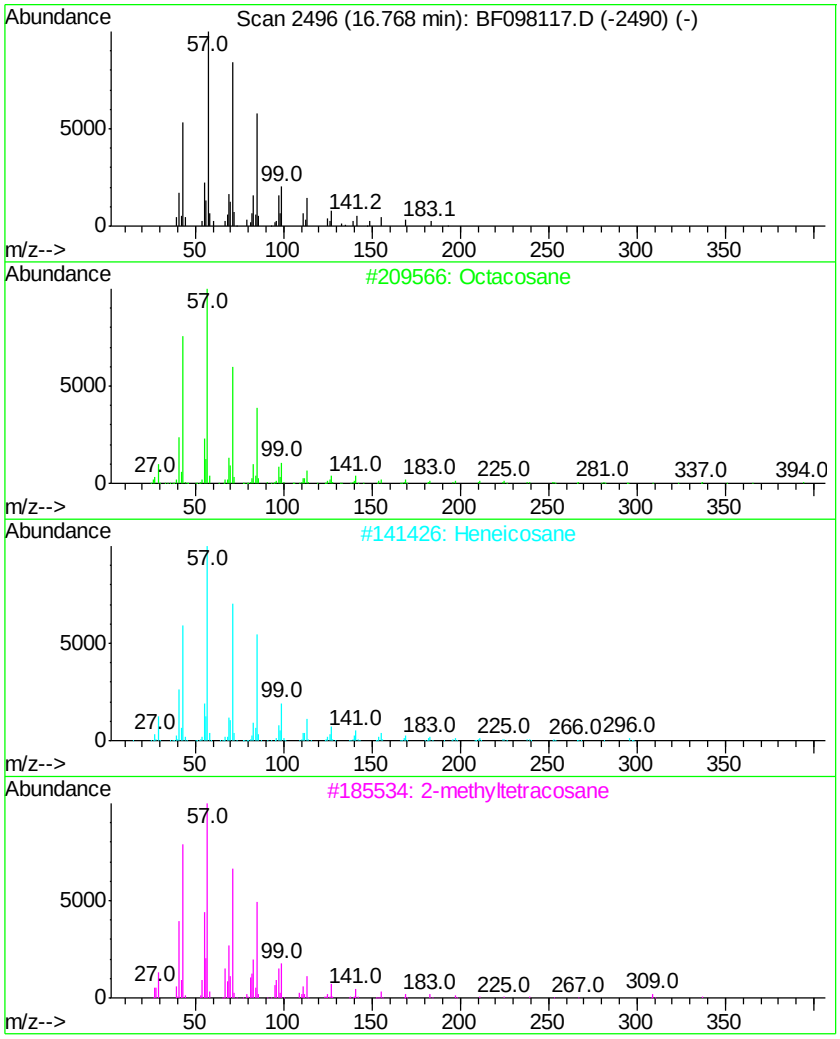
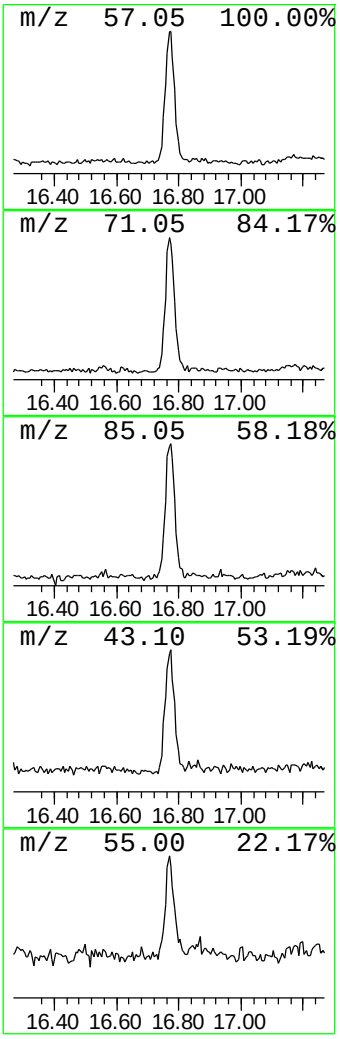
Peak Number 8 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.77	4.75 ng	149907	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	2-methyltetracosane	352	C25H52	1000376-72-6	90
4	Heptadecane	240	C17H36	000629-78-7	87
5	Triacontane	422	C30H62	000638-68-6	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF082917\
Data File : BF098117.D
Acq On : 29 Aug 2017 18:11
Operator : SJ/JU
Sample : I4988-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FF5-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

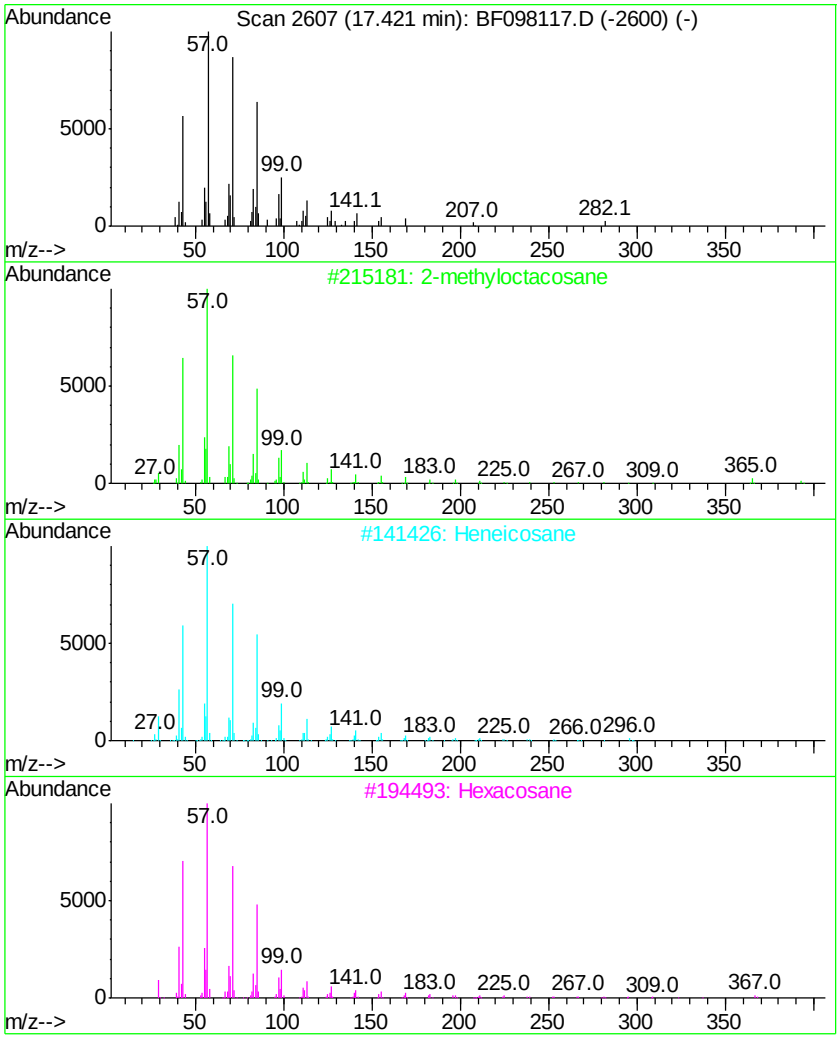
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

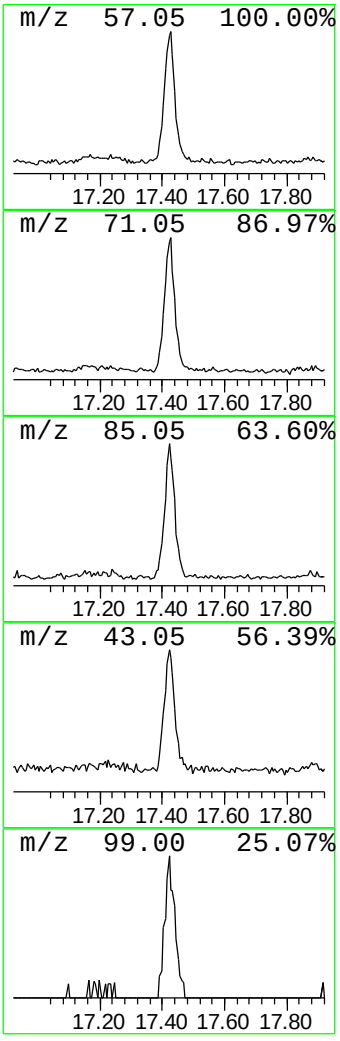
****

Peak Number 9 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.42	5.19 ng	163791	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Heneicosane	296	C21H44	000629-94-7	87
3	Hexacosane	366	C26H54	000630-01-3	83
4	Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	80
5	Heptadecane	240	C17H36	000629-78-7	80





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Data File : BF098117.D
Acq On : 29 Aug 2017 18:11
Operator : SJ/JU
Sample : I4988-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FF5-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

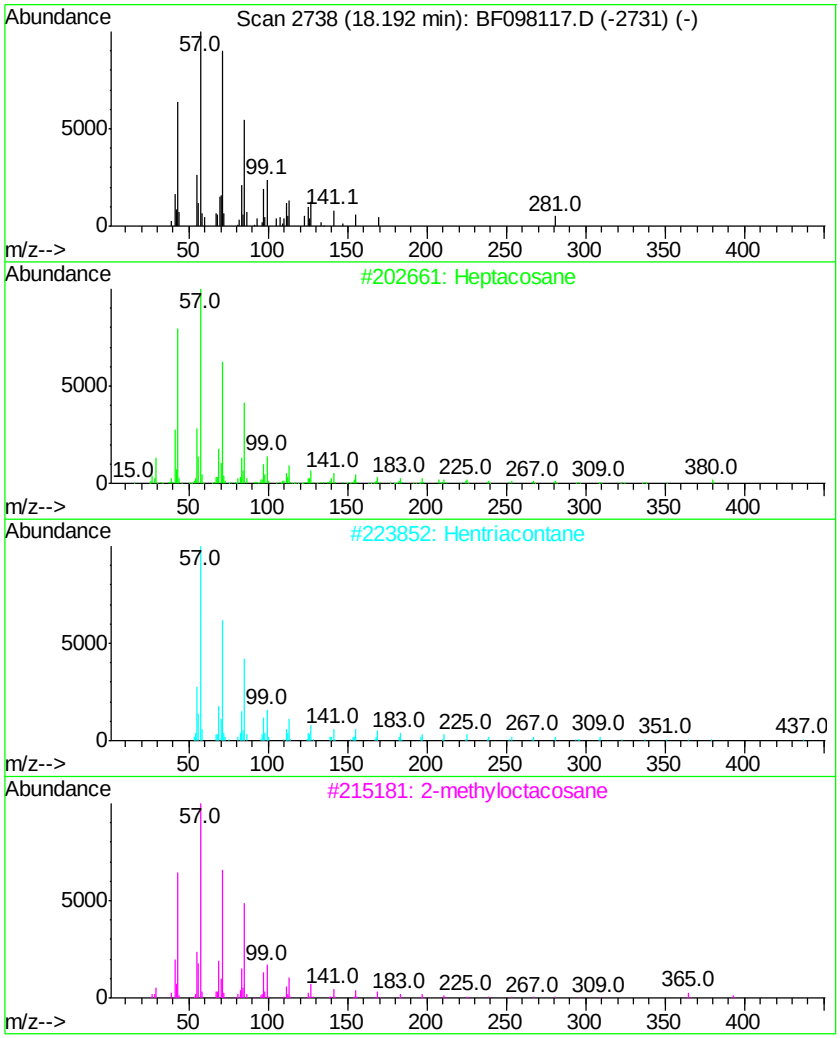
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

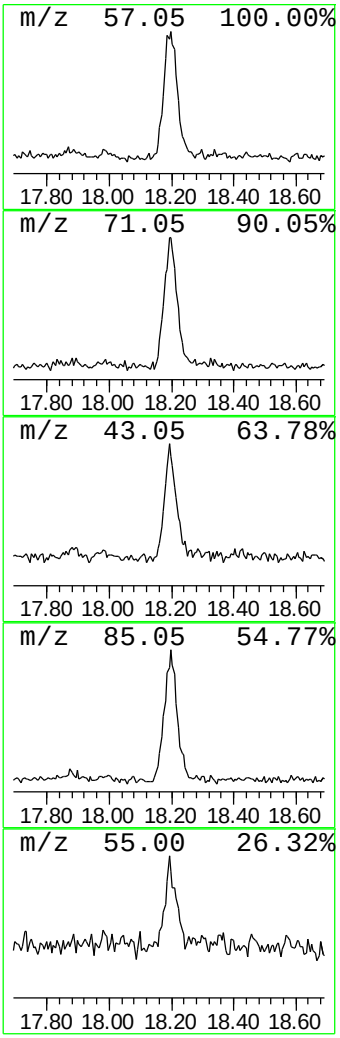
****

Peak Number 10 Heptacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.19	4.04 ng	127565	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	90
2	Hentriacontane	437	C31H64	000630-04-6	90
3	2-methyloctacosane	408	C29H60	1000376-72-8	86
4	Octacosane	394	C28H58	000630-02-4	83
5	Pentacosane	352	C25H52	000629-99-2	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082917\
Data File : BF098117.D
Acq On : 29 Aug 2017 18:11
Operator : SJ/JU
Sample : I4988-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FF5-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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
2-Pentanone, 4-hy...	4.93	7.6	ng	308831	1	6.73	809049	20.0
unknown6.50	6.50	84.7	ng	3426980	1	6.73	809049	20.0
9-Octadecenoic ac...	12.36	2.3	ng	135291	4	11.25	1156710	20.0
Trifluoroacetic a...	13.73	6.8	ng	245409	5	13.88	726800	20.0
Heneicosane	15.74	3.6	ng	113613	6	15.30	631481	20.0
Hexacosane	16.22	5.1	ng	162440	6	15.30	631481	20.0
Octacosane	16.77	4.8	ng	149907	6	15.30	631481	20.0
2-methyloctacosane	17.42	5.2	ng	163791	6	15.30	631481	20.0
Heptacosane	18.19	4.0	ng	127565	6	15.30	631481	20.0