LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102417\
Data File : BF099796.D
Acq On : 24 Oct 2017 18:59
Operator : SJ/JU
Sample : I6025-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-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:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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	5.028	497	500	518	rBV	219751	365082	15.12%	1.745%
2	5.434	565	569	586	rBV	2064794	2183536	90.44%	10.439%
3	6.451	737	742	745	rBV	1931809	2144962	88.85%	10.255%
4	6.581	760	764	767	rBV	2383402	2271627	94.09%	10.861%
5	6.804	799	802	811	rBV	646535	539464	22.35%	2.579%
6	6.963	824	829	832	rBV	1804416	1791226	74.19%	8.564%
7	7.375	895	899	902	rBV	1410824	1355499	56.15%	6.481%
8	8.086	1016	1020	1030	rBV	891296	744536	30.84%	3.560%
9	8.645	1112	1115	1125	rBB	96800	82830	3.43%	0.396%
10	9.163	1198	1203	1206	rBV	2725688	2414233	100.00%	11.542%
11	9.557	1266	1270	1277	rBB	45473	38343	1.59%	0.183%
12	9.839	1315	1318	1331	rVB	849492	795516	32.95%	3.803%
13	10.557	1436	1440	1444	rBV	420920	328715	13.62%	1.572%
14	10.639	1450	1454	1457	rBV	1391319	1279198	52.99%	6.116%
15	11.333	1568	1572	1576	rBV	842063	704207	29.17%	3.367%
16	11.851	1654	1660	1668	rBV3	76644	96648	4.00%	0.462%
17	12.386	1748	1751	1753	rBV	33067	32062	1.33%	0.153%
18	12.551	1774	1779	1782	rBV	50494	48542	2.01%	0.232%
19	12.633	1791	1793	1801	rVB4	29993	35252	1.46%	0.169%
20	12.780	1812	1818	1824	rVB	78310	92089	3.81%	0.440%
21	12.916	1837	1841	1845	rBV	1904549	1788061	74.06%	8.549%
22	13.004	1851	1856	1862	rVB3	16439	29325	1.21%	0.140%
23	13.104	1867	1873	1880	rVB7	19343	43089	1.78%	0.206%
24	13.216	1887	1892	1895	rBV2	25991	31090	1.29%	0.149%
25	13.798	1987	1991	1996	rBV2	119293	145195	6.01%	0.694%
26	13.980	2017	2022	2025	rBV	605295	576988	23.90%	2.759%
27	14.004	2025	2026	2031	rVB	61405	57445	2.38%	0.275%
28	14.374	2083	2089	2090	rBV2	55691	75403	3.12%	0.360%
29	14.404	2091	2094	2096	rVV	30285	34281	1.42%	0.164%
30	14.715	2142	2147	2152	rBV9	13772	26937	1.12%	0.129%
31	15.027	2196	2200	2202	rBV	31750	46074	1.91%	0.220%
32	15.327	2247	2251	2258	rVB	33462	43059	1.78%	0.206%
33	15.386	2258	2261	2264	rBV	34106	39393	1.63%	0.188%
34	15.451	2267	2272	2277	rVV	356652	449517	18.62%	2.149%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102417\
Data File : BF099796.D
Acq On : 24 Oct 2017 18:59
Operator : SJ/JU
Sample : I6025-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-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:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.845	2330	2339	2343	rBV3	52481	134845	5.59%	0.645%
36	16.915	2516	2521	2531	rVB7	19070	52068	2.16%	0.249%

Sum of corrected areas: 20916337

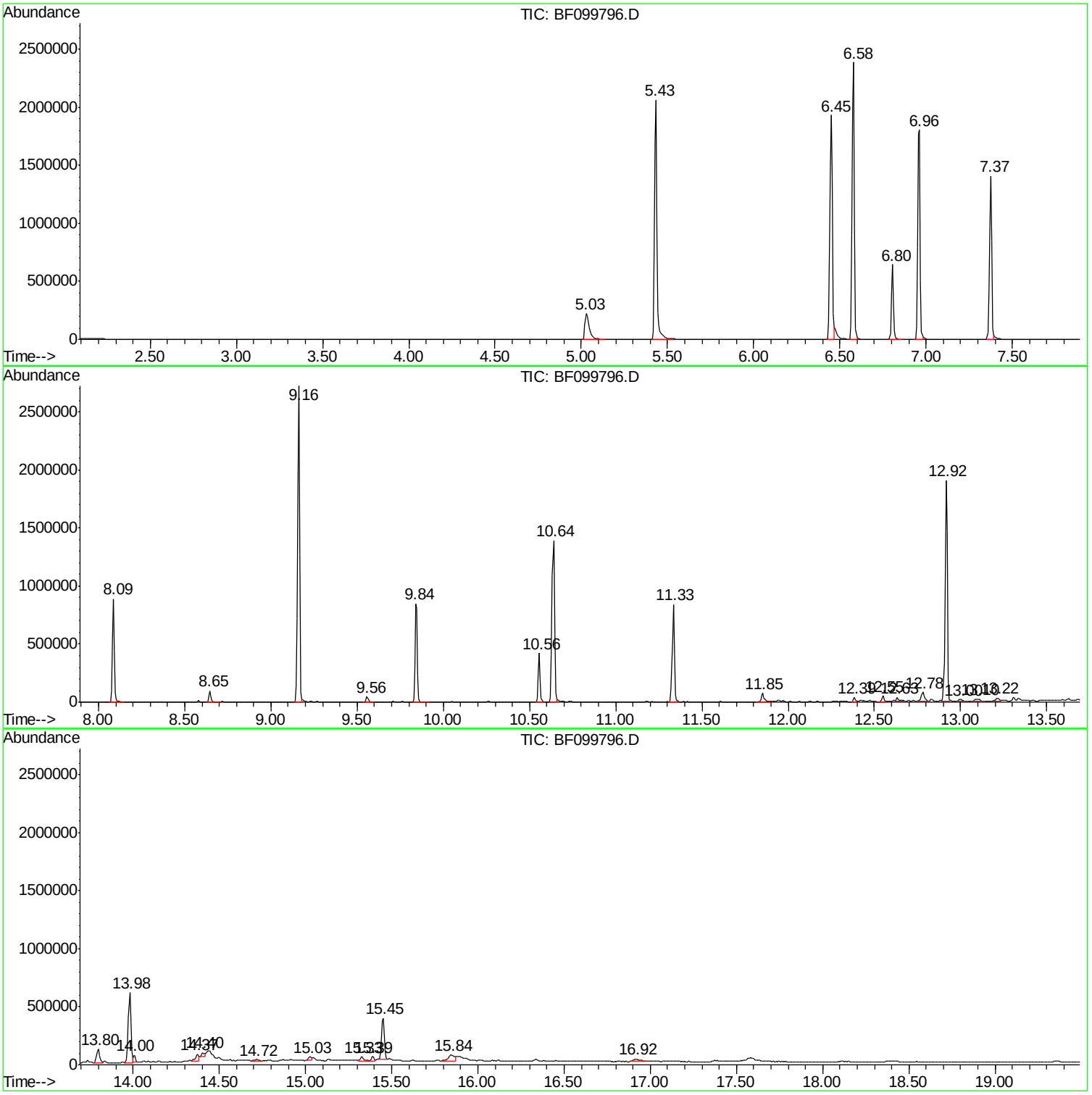
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102417\
Data File : BF099796.D
Acq On : 24 Oct 2017 18:59
Operator : SJ/JU
Sample : I6025-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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\BF102417\
Data File : BF099796.D
Acq On : 24 Oct 2017 18:59
Operator : SJ/JU
Sample : I6025-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

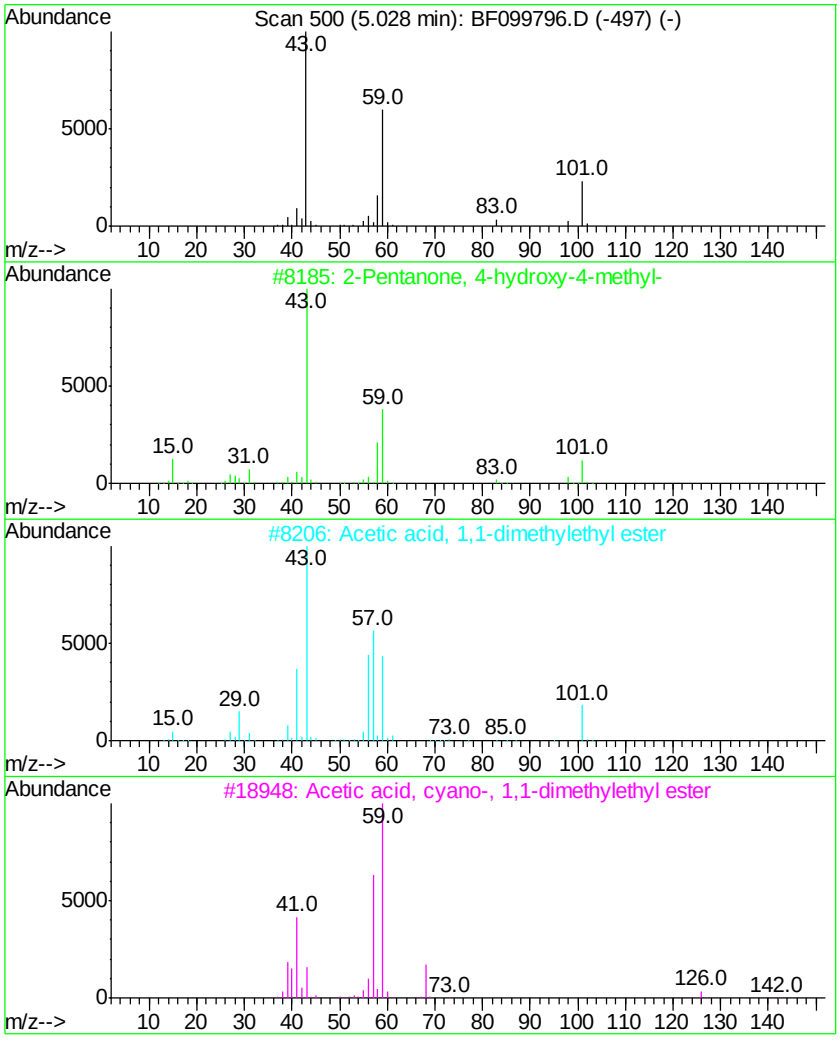
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

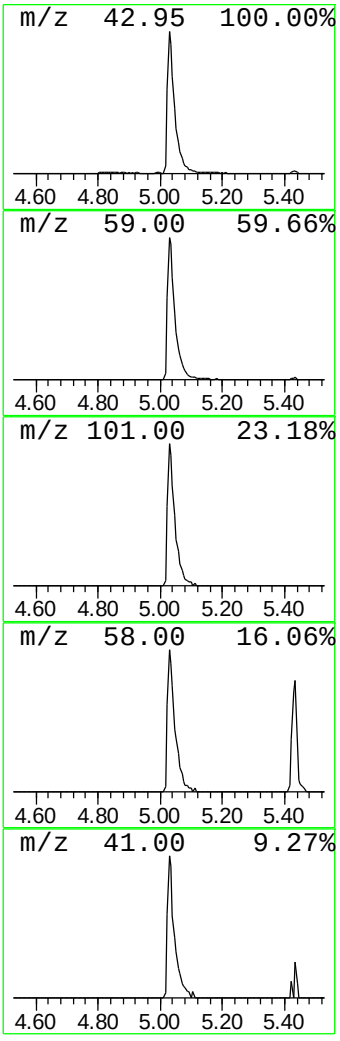
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	13.54 ng	365082	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102417\
Data File : BF099796.D
Acq On : 24 Oct 2017 18:59
Operator : SJ/JU
Sample : I6025-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

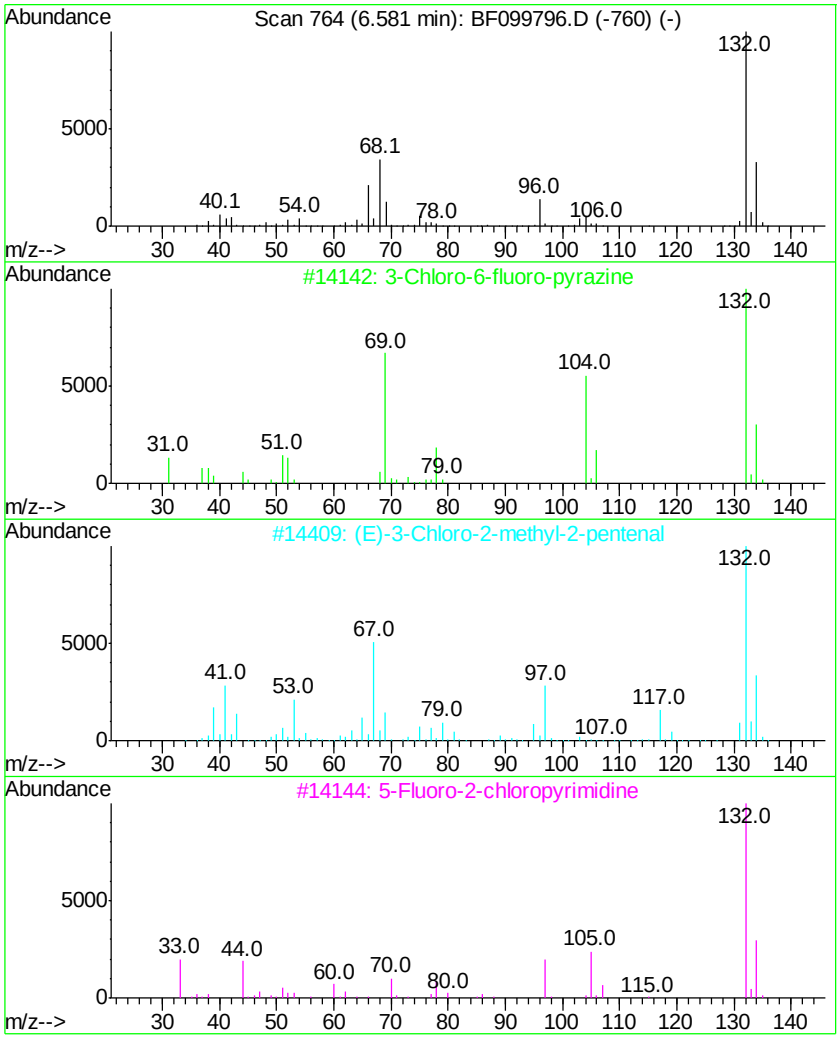
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

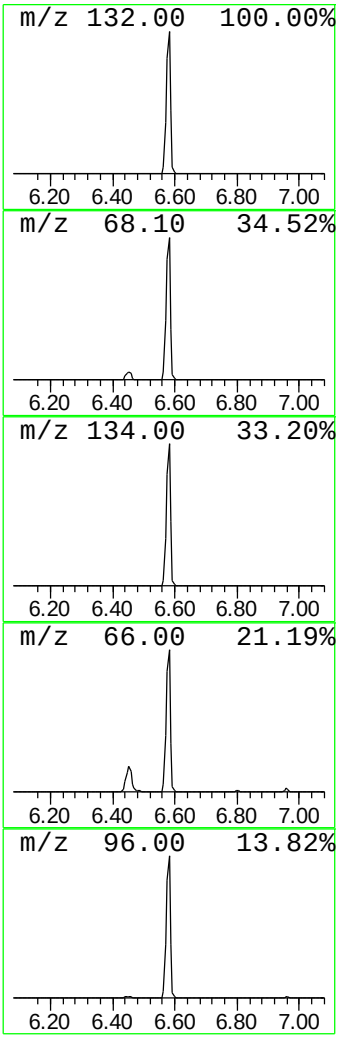
****

Peak Number 2 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	84.22 ng	2271630	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102417\
Data File : BF099796.D
Acq On : 24 Oct 2017 18:59
Operator : SJ/JU
Sample : I6025-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

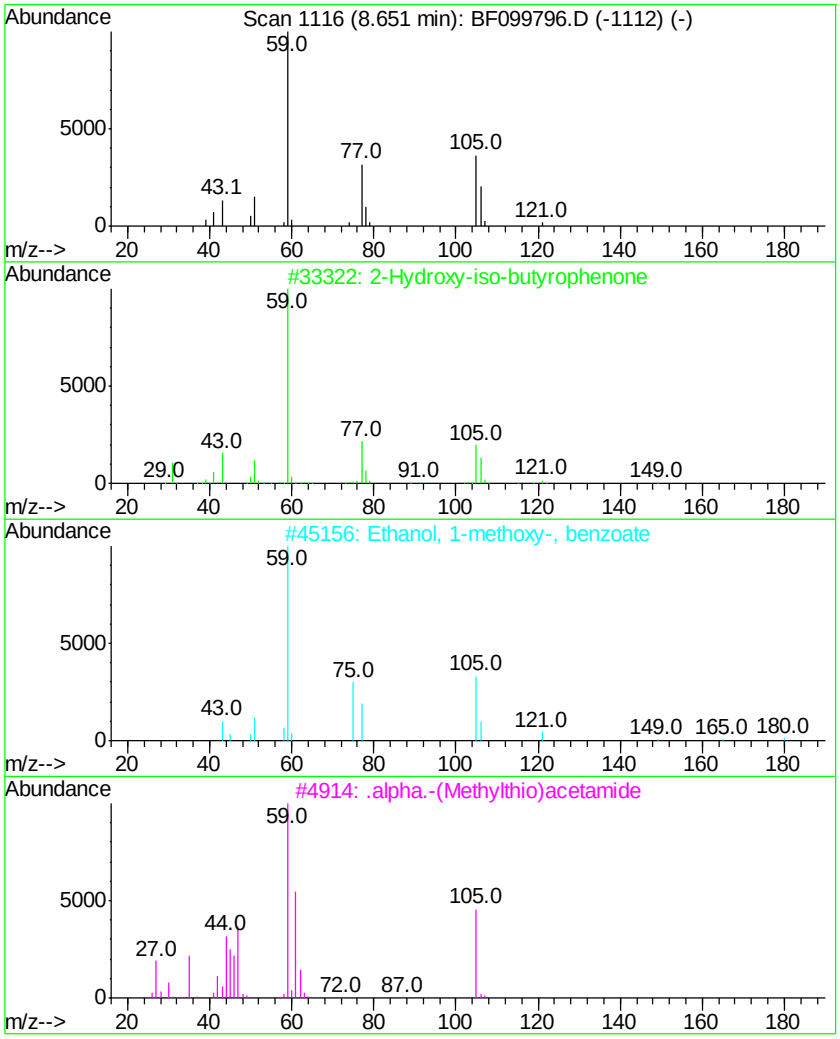
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

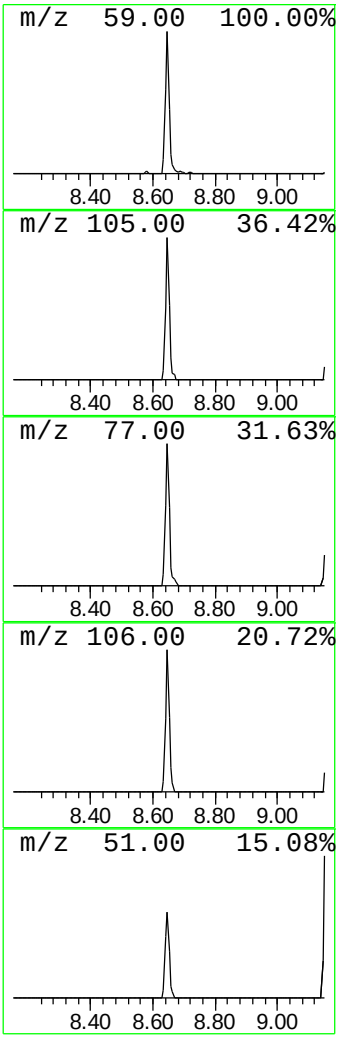
****

Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.65	2.23 ng	82830	Naphthalene-d8	8.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	83
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	56
3	.alpha.-(Methylthio)acetamide	105	C3H7NOS	022551-24-2	7
4	Guanidine	59	CH5N3	000113-00-8	7
5	Acetamide	59	C2H5NO	000060-35-5	5





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102417\
Data File : BF099796.D
Acq On : 24 Oct 2017 18:59
Operator : SJ/JU
Sample : I6025-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

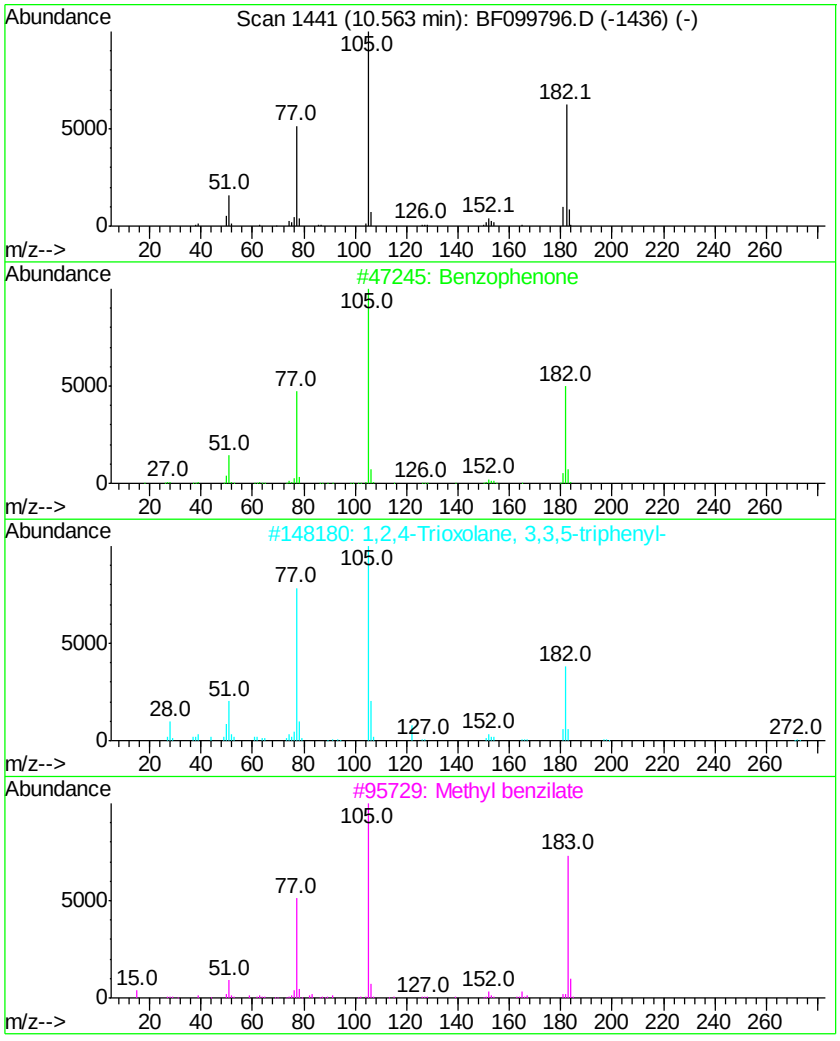
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

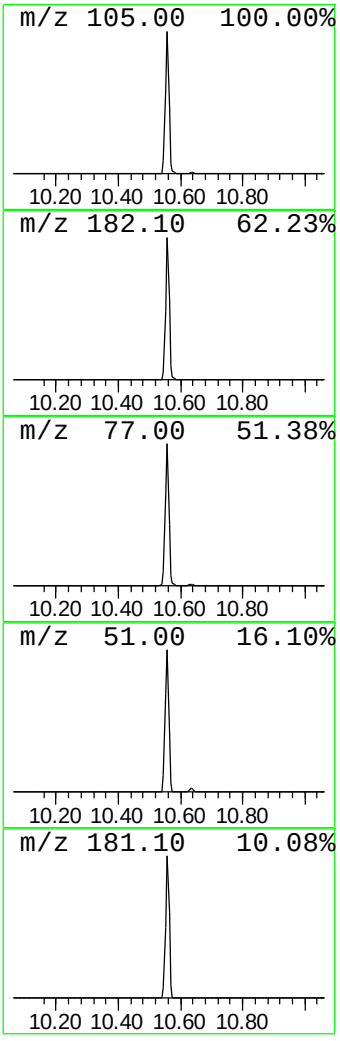
****

Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.56	8.26 ng	328715	Acenaphthene-d10	9.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	64
3	Methyl benzilate	242	C15H14O3	000076-89-1	50
4	Benzopinacol	366	C26H22O2	000464-72-2	50
5	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102417\
Data File : BF099796.D
Acq On : 24 Oct 2017 18:59
Operator : SJ/JU
Sample : I6025-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

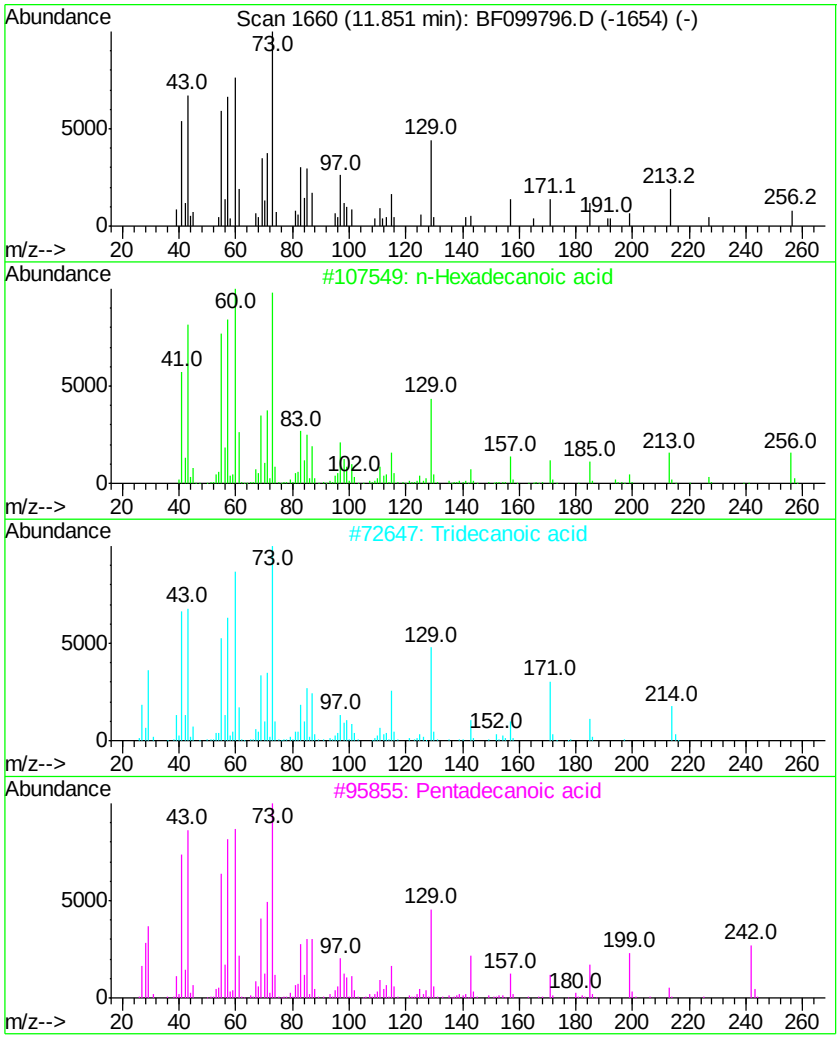
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

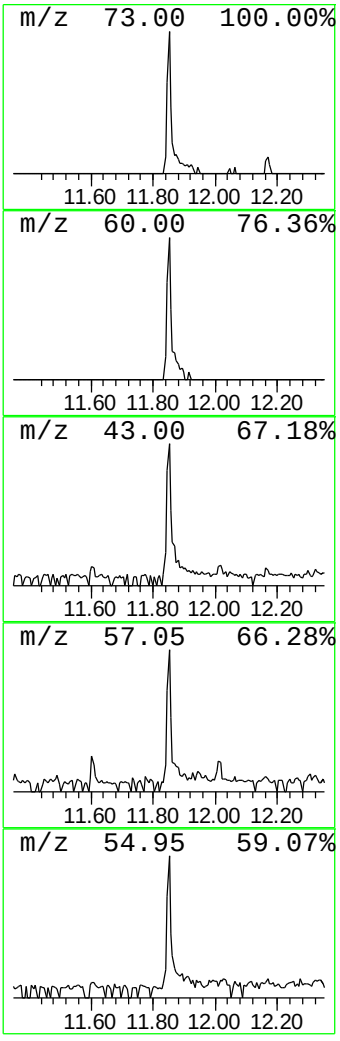
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	2.74 ng	96648	Phenanthrene-d10	11.33

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	72
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





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Data File : BF099796.D
Acq On : 24 Oct 2017 18:59
Operator : SJ/JU
Sample : I6025-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

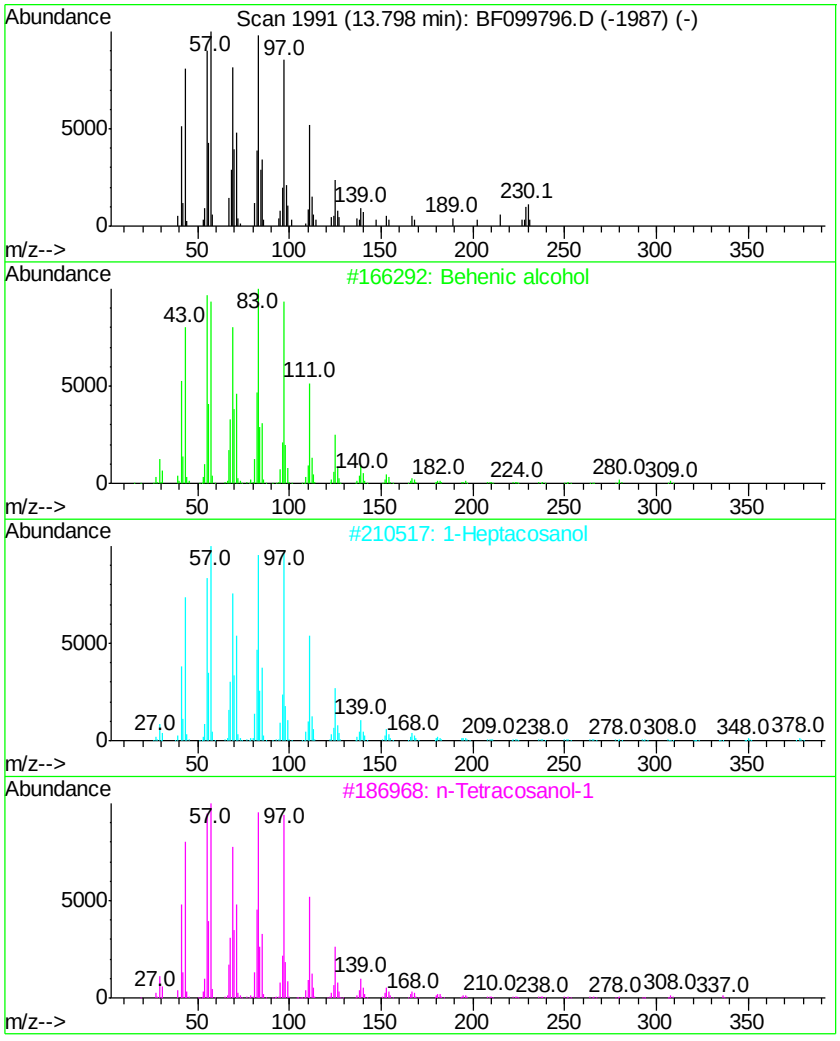
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

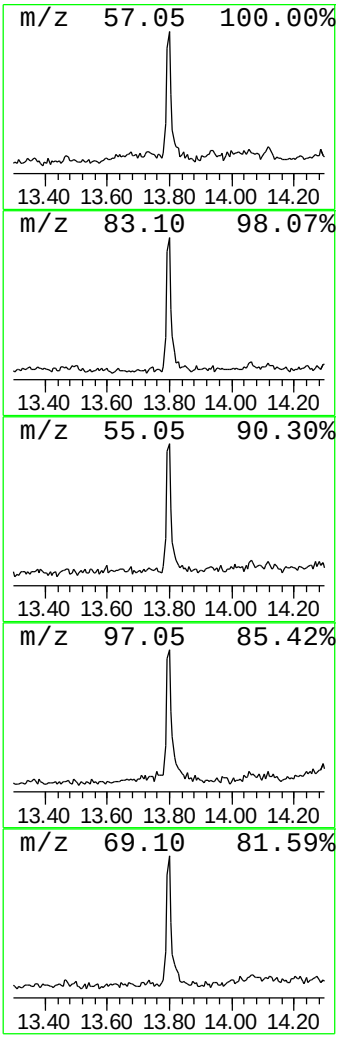
****

Peak Number 7 Behenic alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	5.03 ng	145195	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	1-Heptacosanol	396	C27H56O	002004-39-9	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
5	1-Heneicosanol	312	C21H44O	015594-90-8	95





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102417\
Data File : BF099796.D
Acq On : 24 Oct 2017 18:59
Operator : SJ/JU
Sample : I6025-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

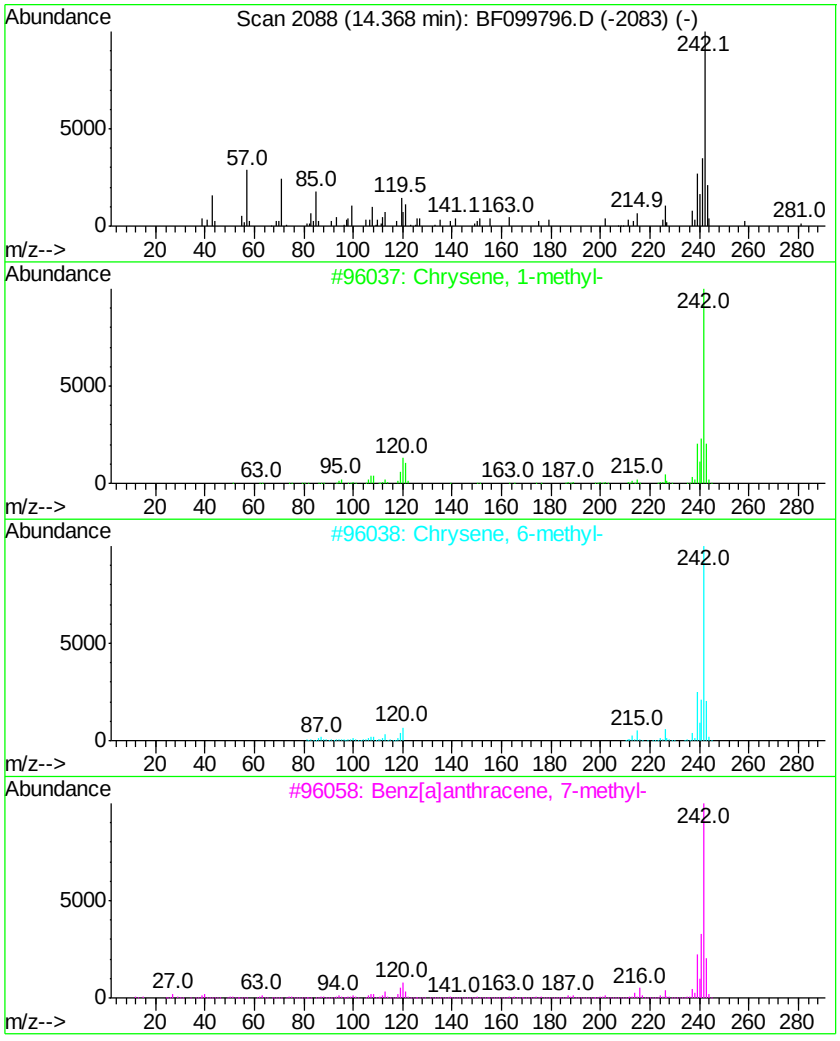
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

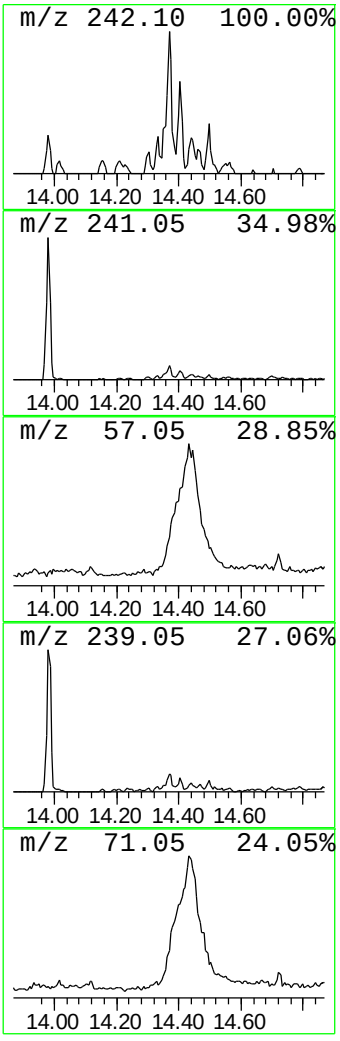
****

Peak Number 8 Chrysene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.37	2.61 ng	75403	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Chrysene, 1-methyl-	242	C19H14	003351-28-8	81
2	Chrysene, 6-methyl-	242	C19H14	001705-85-7	62
3	Benz[a]anthracene, 7-methyl-	242	C19H14	002541-69-7	55
4	2-Methylchrysene	242	C19H14	003351-32-4	49
5	Benz[a]anthracene, 8-methyl-	242	C19H14	002381-31-9	49





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Acq On : 24 Oct 2017 18:59
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Sample : I6025-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

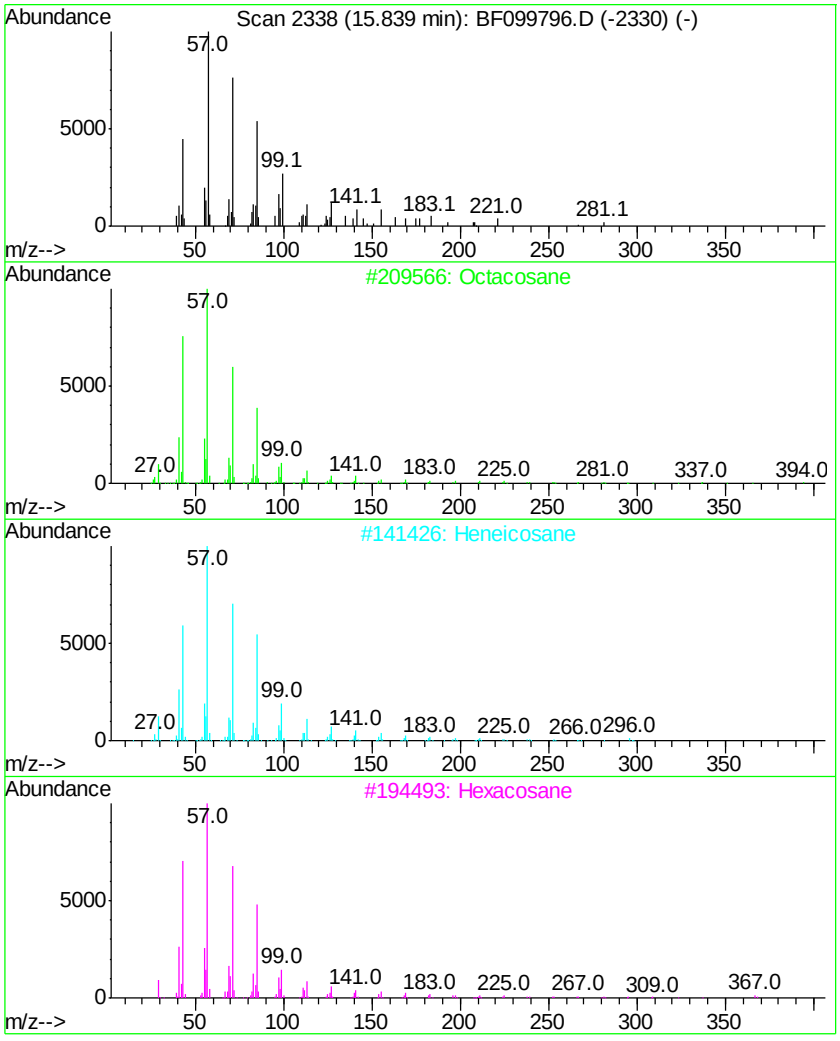
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

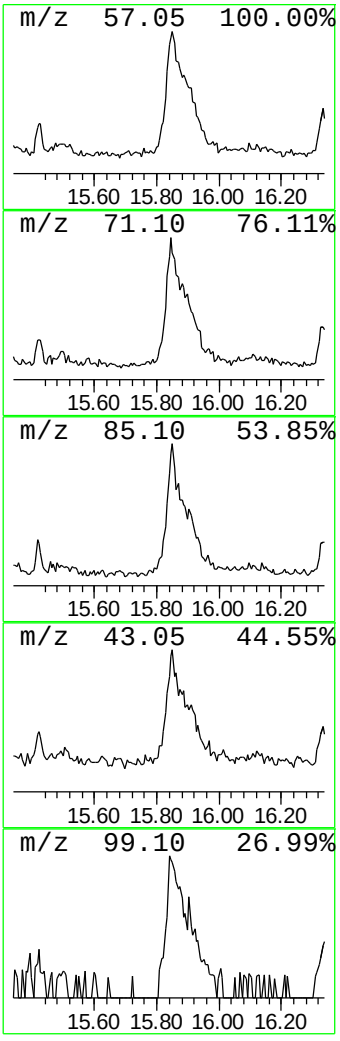
****

Peak Number 10 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.84	6.00 ng	134845	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Triacontane	422	C30H62	000638-68-6	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102417\
Data File : BF099796.D
Acq On : 24 Oct 2017 18:59
Operator : SJ/JU
Sample : I6025-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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...	5.03	13.5	ng	365082	1	6.80	539464	20.0
unknown6.58	6.58	84.2	ng	2271630	1	6.80	539464	20.0
2-Hydroxy-iso-but...	8.65	2.2	ng	82830	2	8.09	744536	20.0
Benzophenone	10.56	8.3	ng	328715	3	9.84	795516	20.0
n-Hexadecanoic acid	11.85	2.7	ng	96648	4	11.33	704207	20.0
Behenic alcohol	13.80	5.0	ng	145195	5	13.98	576988	20.0
Chrysene, 1-methyl-	14.37	2.6	ng	75403	5	13.98	576988	20.0
Octacosane	15.84	6.0	ng	134845	6	15.45	449517	20.0