LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092217\
Data File : BF098720.D
Acq On : 23 Sep 2017 2:27
Operator : SJ/JU
Sample : I5308-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 220-1-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-BF092117.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	2.246	23	27	38	rVB	72761	125049	3.94%	0.379%
2	2.628	88	92	100	rVB2	28414	40802	1.28%	0.124%
3	3.557	247	250	259	rBV	11391	34174	1.08%	0.104%
4	5.157	518	522	532	rVB	533483	621706	19.57%	1.884%
5	5.545	583	588	591	rBV	2871631	2915597	91.78%	8.834%
6	6.551	753	759	762	rBV	2823130	3137614	98.77%	9.507%
7	6.698	779	784	787	rBV	3219179	3083087	97.05%	9.342%
8	6.928	817	823	827	rVB	1232007	997909	31.41%	3.024%
9	7.086	846	850	853	rVB	2429717	2079517	65.46%	6.301%
10	7.486	913	918	921	rBV	1957687	1972118	62.08%	5.975%
11	8.210	1037	1041	1044	rBV	1608681	1256932	39.57%	3.808%
12	8.792	1137	1140	1144	rVB	49662	37566	1.18%	0.114%
13	9.151	1198	1201	1205	rBV	46531	41714	1.31%	0.126%
14	9.286	1218	1224	1227	rBV	3401290	3176648	100.00%	9.625%
15	9.357	1233	1236	1238	rBV	66195	50210	1.58%	0.152%
16	9.674	1286	1290	1293	rBV	324242	261415	8.23%	0.792%
17	9.886	1322	1326	1329	rVB	82359	62084	1.95%	0.188%
18	9.963	1335	1339	1343	rVB	1390675	1275427	40.15%	3.865%
19	10.151	1368	1371	1377	rBV3	54347	66728	2.10%	0.202%
20	10.363	1404	1407	1409	rBV	33146	40621	1.28%	0.123%
21	10.386	1409	1411	1414	rVB	104628	77503	2.44%	0.235%
22	10.604	1445	1448	1451	rBV2	28460	35199	1.11%	0.107%
23	10.751	1467	1473	1476	rBV	1837266	1565604	49.28%	4.744%
24	10.857	1488	1491	1497	rBV2	126764	151511	4.77%	0.459%
25	11.310	1564	1568	1570	rBV	111641	97797	3.08%	0.296%
26	11.339	1570	1573	1579	rVB3	37985	58645	1.85%	0.178%
27	11.398	1579	1583	1588	rBV2	28677	37844	1.19%	0.115%
28	11.451	1588	1592	1595	rBV	1271017	1095848	34.50%	3.320%
29	11.474	1595	1596	1599	rVB	174305	91230	2.87%	0.276%
30	11.733	1637	1640	1644	rVB	104920	77433	2.44%	0.235%
31	11.898	1664	1668	1671	rBV4	39556	57733	1.82%	0.175%
32	11.968	1674	1680	1688	rVV3	599442	648641	20.42%	1.965%
33	12.063	1693	1696	1698	rBV2	38044	38338	1.21%	0.116%
34	12.139	1707	1709	1714	rVB	93727	81601	2.57%	0.247%

LSC Area Percent Report

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Data File : BF098720.D
Acq On : 23 Sep 2017 2:27
Operator : SJ/JU
Sample : I5308-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 220-1-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-BF092117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.498	1768	1770	1773	rVB2	47790	39875	1.26%	0.121%
36	12.527	1773	1775	1779	rBV	104410	94933	2.99%	0.288%
37	12.663	1794	1798	1804	rBV	278982	332130	10.46%	1.006%
38	12.751	1810	1813	1823	rBV	491338	622855	19.61%	1.887%
39	12.851	1827	1830	1832	rVB2	50818	45520	1.43%	0.138%
40	12.892	1832	1837	1841	rBV2	227000	287017	9.04%	0.870%
41	13.033	1857	1861	1865	rBV	2538725	2372950	74.70%	7.190%
42	13.257	1896	1899	1902	rBV	94159	80537	2.54%	0.244%
43	13.598	1955	1957	1960	rVB2	74915	56962	1.79%	0.173%
44	13.921	2009	2012	2020	rVB3	265995	327076	10.30%	0.991%
45	14.092	2036	2041	2044	rBV	1060628	1082826	34.09%	3.281%
46	14.115	2044	2045	2047	rVB	100774	49661	1.56%	0.150%
47	14.245	2064	2067	2069	rBV	75723	62116	1.96%	0.188%
48	14.551	2116	2119	2125	rBV4	100344	120122	3.78%	0.364%
49	15.145	2217	2220	2228	rVB	95130	169526	5.34%	0.514%
50	15.209	2229	2231	2237	rVB2	97112	111389	3.51%	0.338%
51	15.586	2290	2295	2306	rVB	629346	971892	30.59%	2.945%
52	16.056	2371	2375	2381	rVB	158340	217874	6.86%	0.660%
53	16.580	2461	2464	2470	rVB	110987	168581	5.31%	0.511%
54	17.198	2564	2569	2578	rVB2	100201	209668	6.60%	0.635%
55	17.927	2688	2693	2703	rVB	75460	188111	5.92%	0.570%

Sum of corrected areas: 33003466

LSC Report - Integrated Chromatogram

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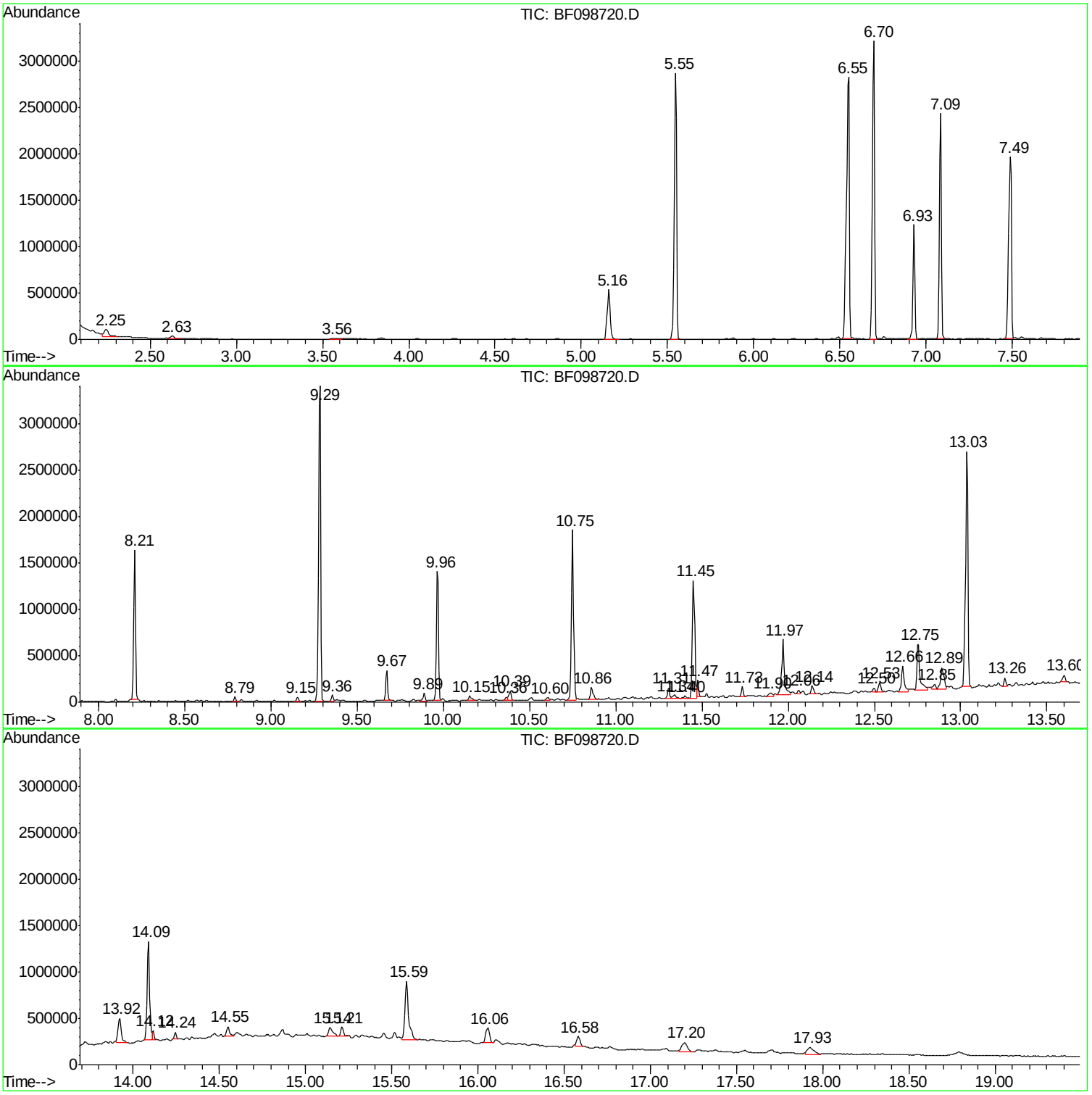
Operator : SJ/JU
Sample : I5308-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 220-1-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.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\BF092217\
Data File : BF098720.D
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Operator : SJ/JU
Sample : I5308-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 220-1-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

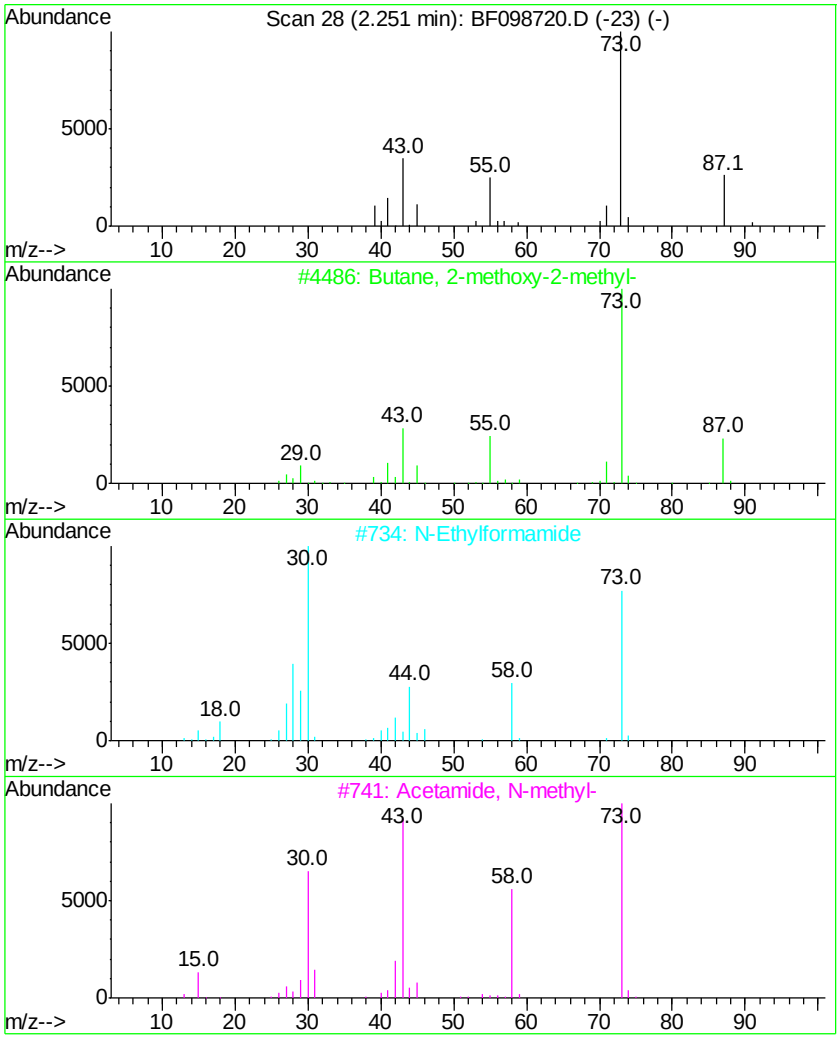
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

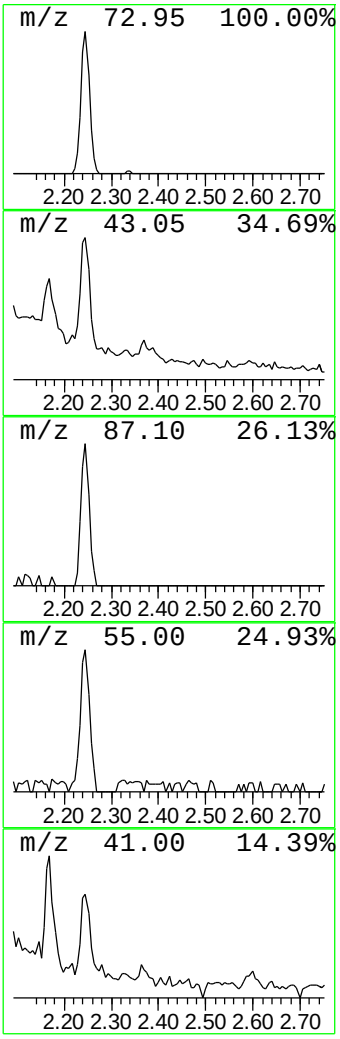
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	2.51 ng	125049	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5	1,4-Butanediamine	88	C4H12N2	000110-60-1	9





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Acq On : 23 Sep 2017 2:27
Operator : SJ/JU
Sample : I5308-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 220-1-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

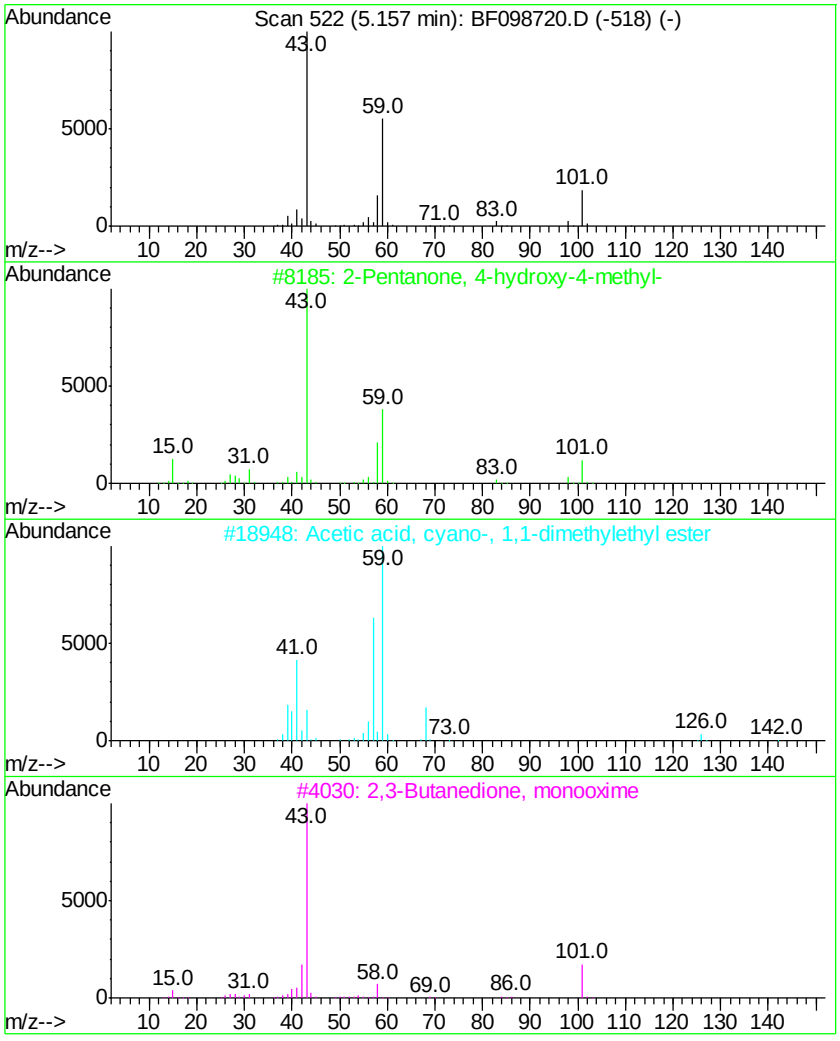
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

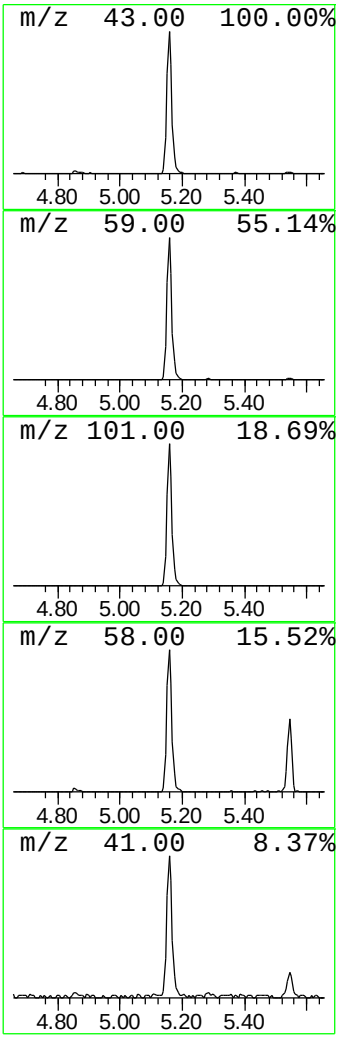
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	12.46 ng	621706	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Data File : BF098720.D
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Operator : SJ/JU
Sample : I5308-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 220-1-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

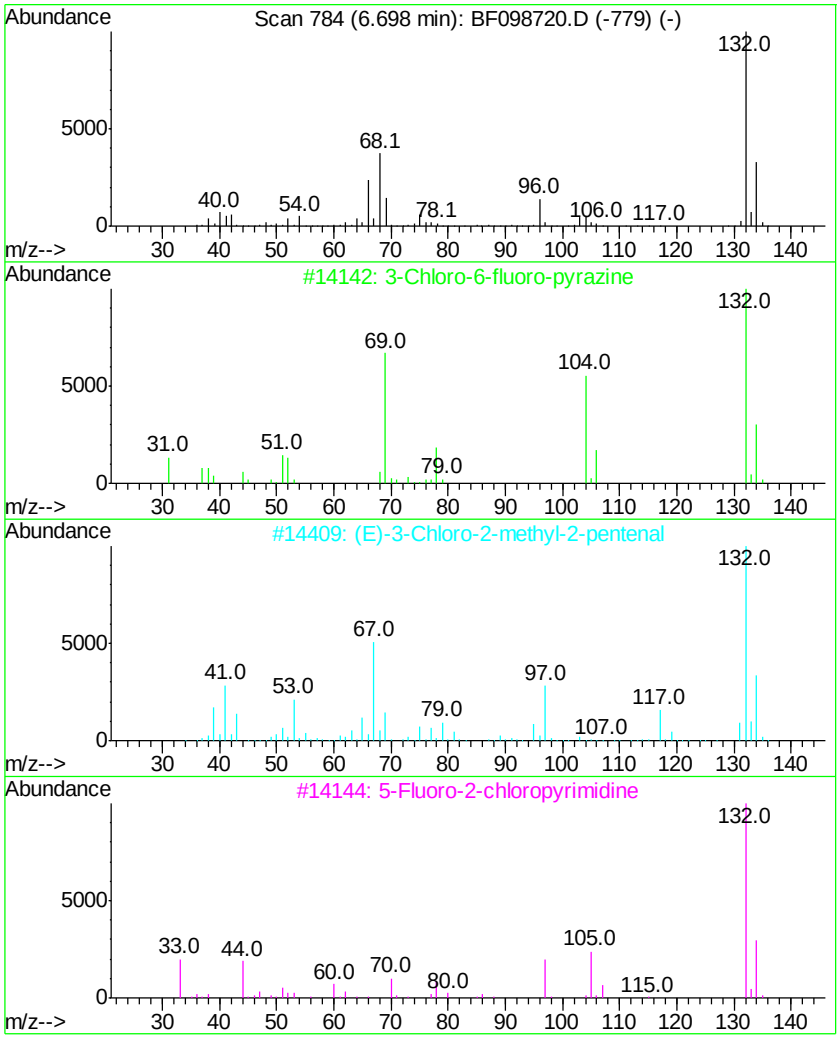
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

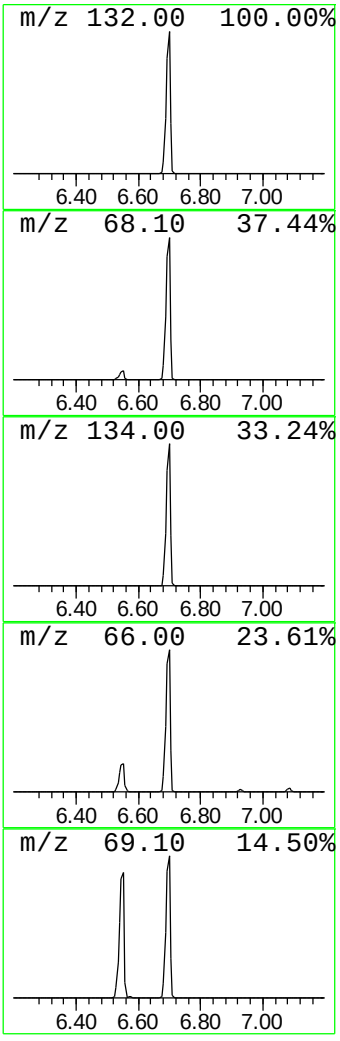
****

Peak Number 3 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	61.79 ng	3083090	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Sample : I5308-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 220-1-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

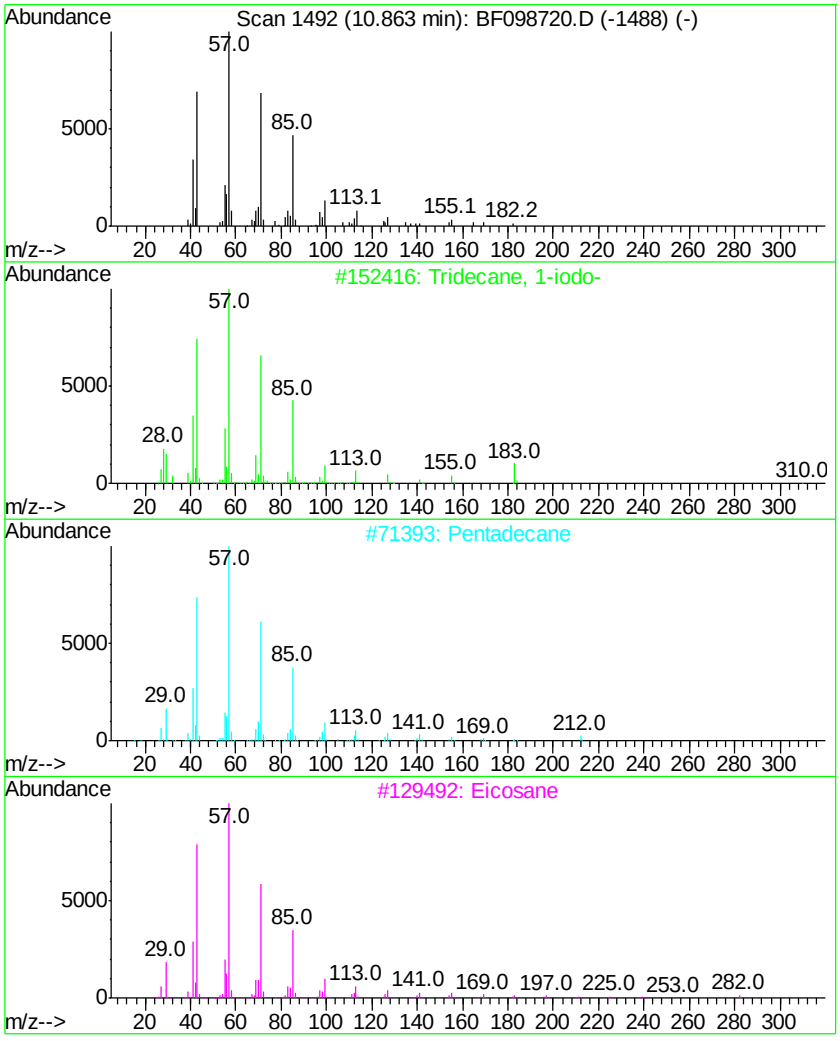
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

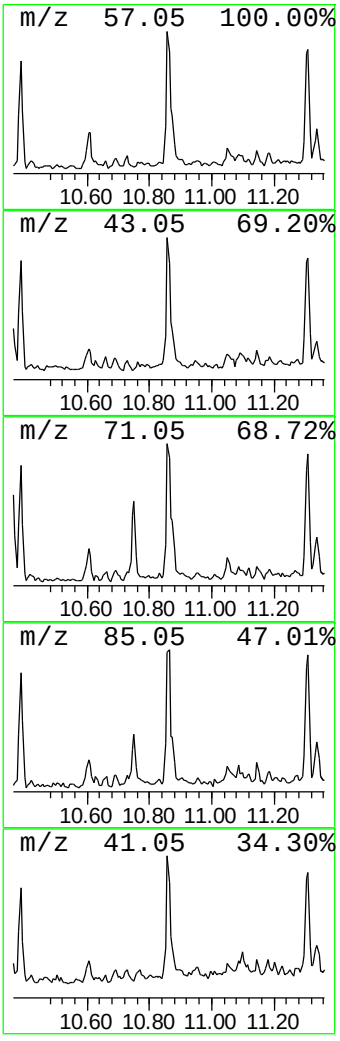
****

Peak Number 5 Tridecane, 1-iodo- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.86	2.77 ng	151511	Phenanthrene-d10	11.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
2	Pentadecane	212	C15H32	000629-62-9	80
3	Eicosane	282	C20H42	000112-95-8	80
4	Heptacosane	380	C27H56	000593-49-7	80
5	Tridecane	184	C13H28	000629-50-5	72





Library Search Compound Report

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Data File : BF098720.D
Acq On : 23 Sep 2017 2:27
Operator : SJ/JU
Sample : I5308-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 220-1-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.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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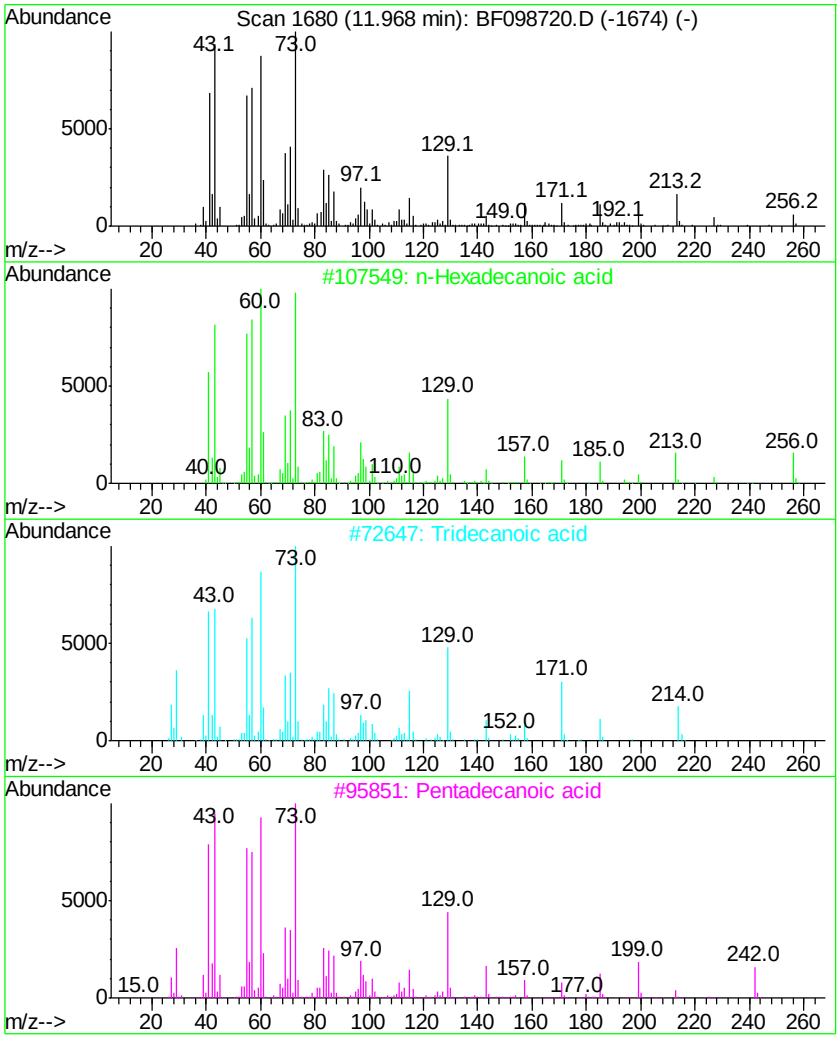
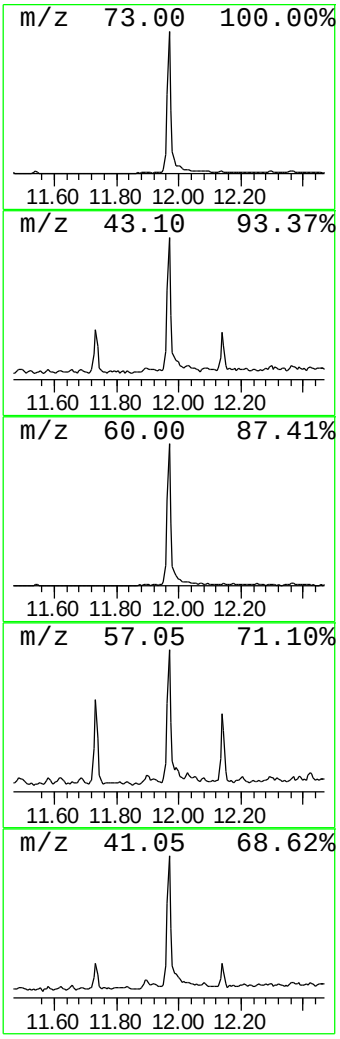
Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.97	11.84 ng	648641	Phenanthrene-d10	11.45

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	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5	d-Gluco-heptulosan	210	C7H14O7	1000126-85-2	38





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Sample : I5308-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 220-1-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.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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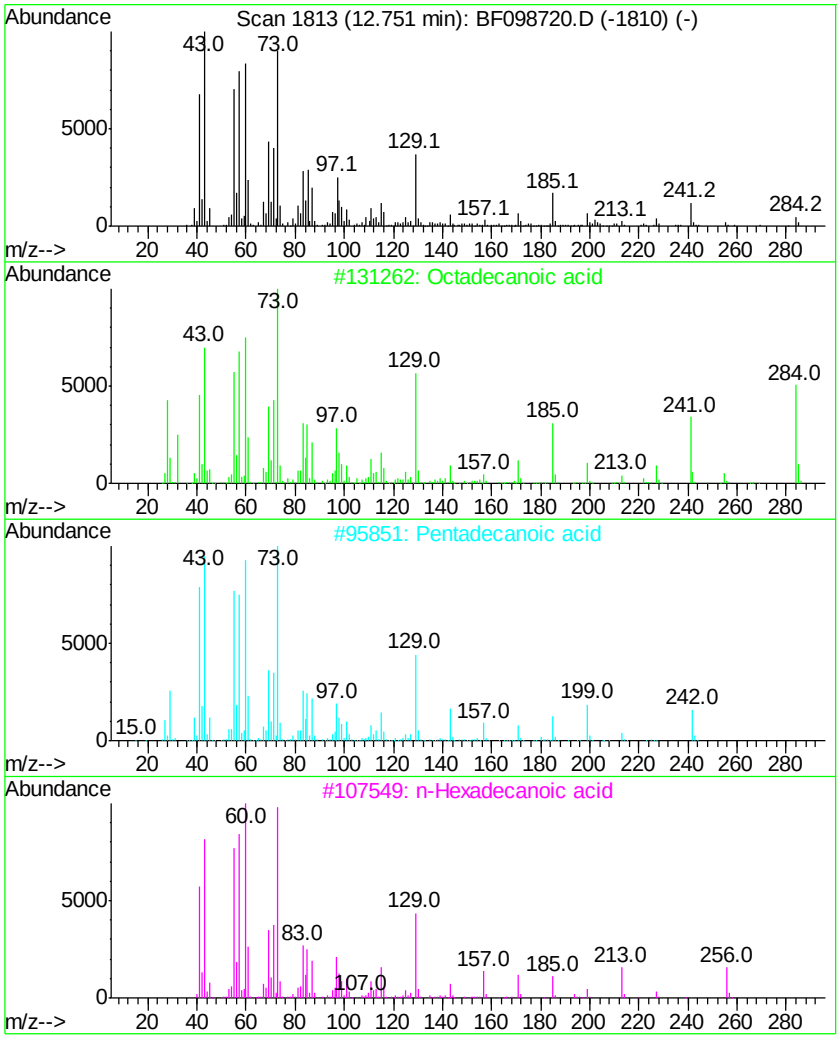
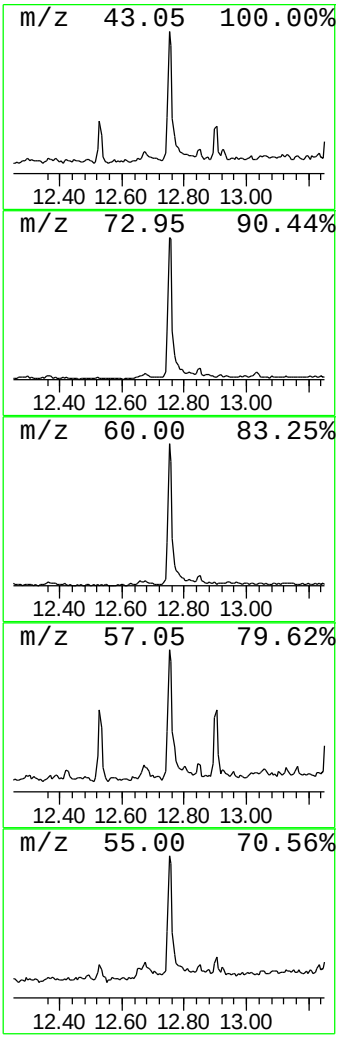
Peak Number 7 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.75	11.37 ng	622855	Phenanthrene-d10	11.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
4	Tridecanoic acid	214	C13H26O2	000638-53-9	91
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91





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Sample : I5308-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 220-1-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.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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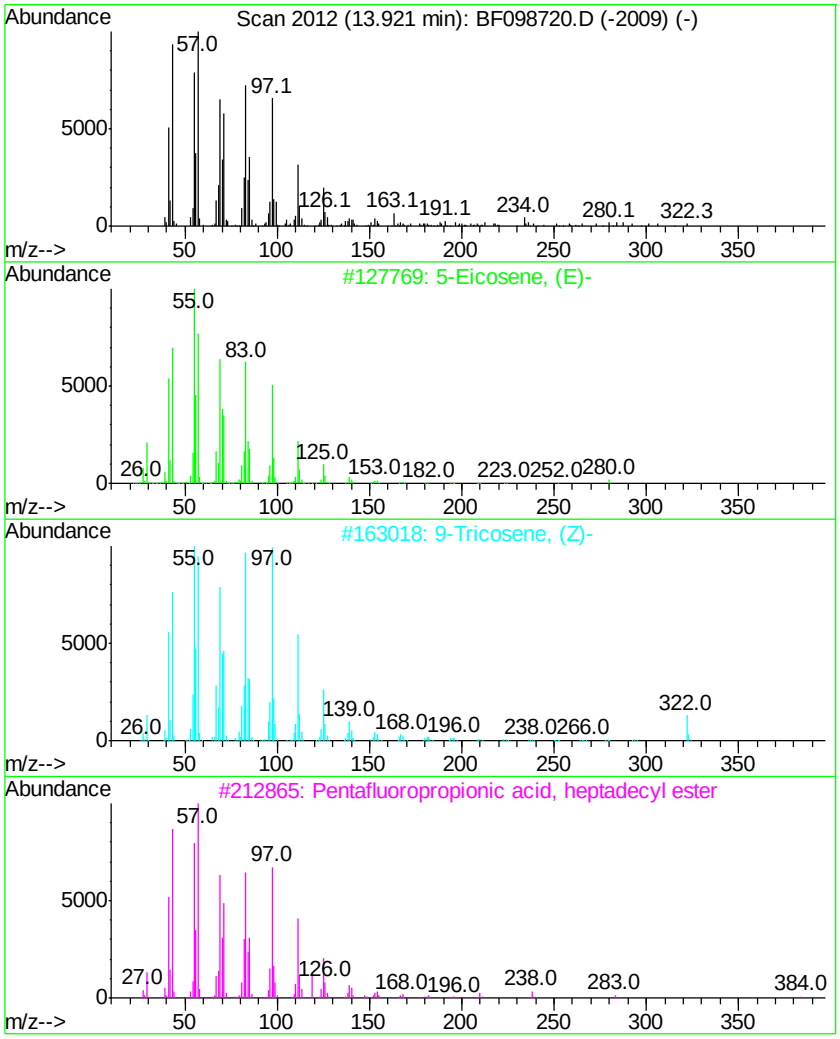
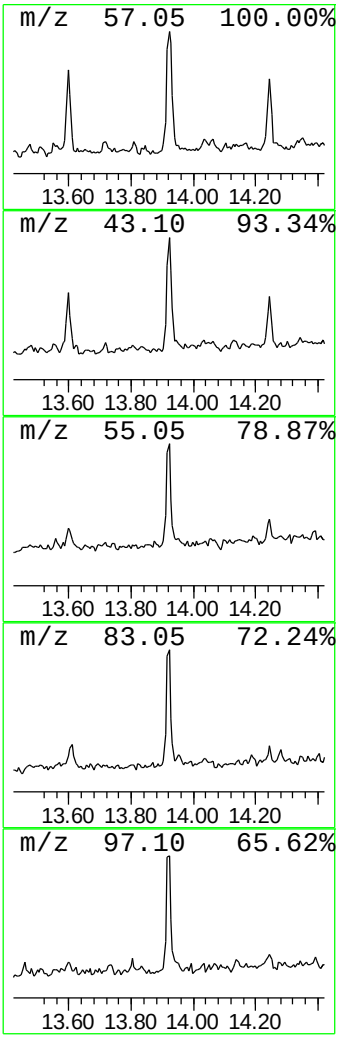
Peak Number 8 5-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	6.04 ng	327076	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	95
2	9-Tricosene, (Z)-	322	C23H46	027519-02-4	93
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	93
4	1-Tricosene	322	C23H46	018835-32-0	93
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	92





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092217\
Data File : BF098720.D
Acq On : 23 Sep 2017 2:27
Operator : SJ/JU
Sample : I5308-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 220-1-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.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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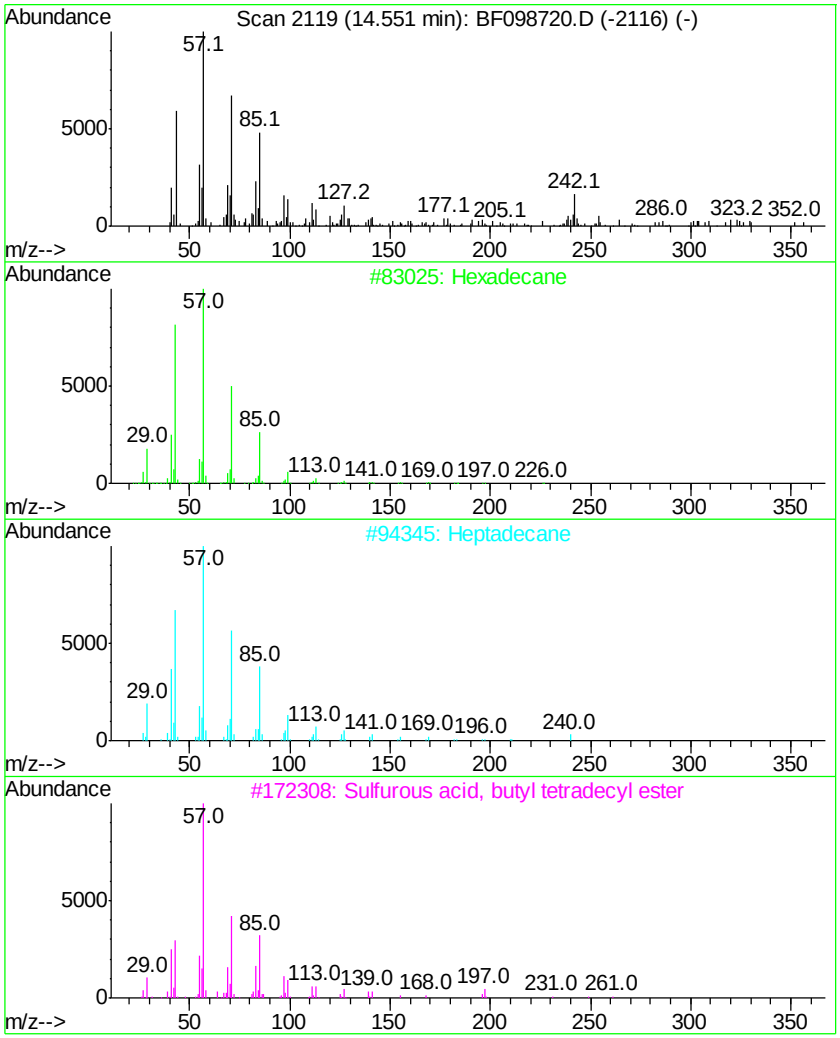
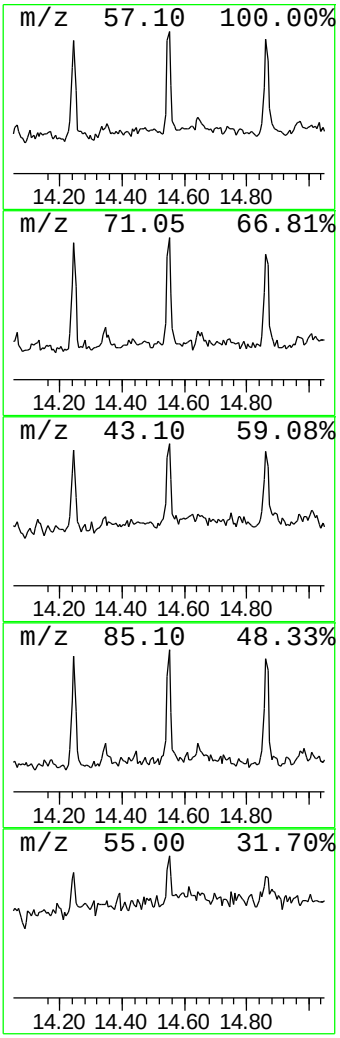
Peak Number 9 Hexadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.55	2.22 ng	120122	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	92
2	Heptadecane	240	C17H36	000629-78-7	92
3	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	87
4	Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	87
5	Tetratetracontane	619	C44H90	007098-22-8	87





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Data File : BF098720.D
Acq On : 23 Sep 2017 2:27
Operator : SJ/JU
Sample : I5308-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 220-1-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.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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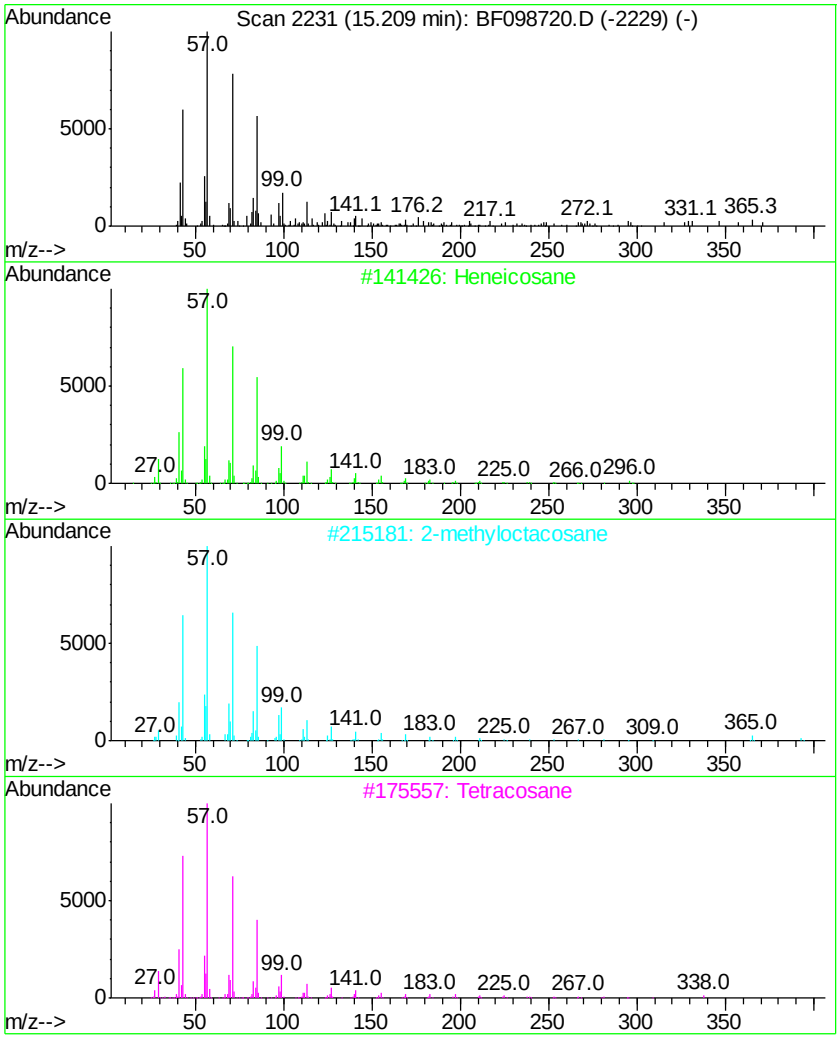
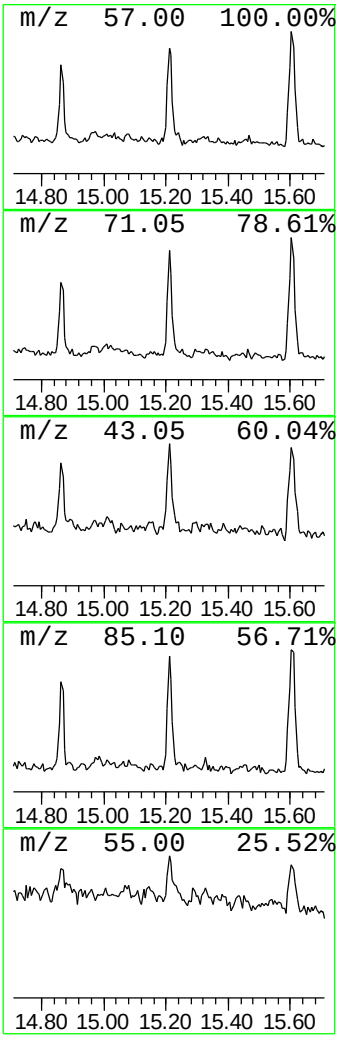
Peak Number 10 Heneicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.21	2.29 ng	111389	Perylene-d12	15.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	95
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Eicosane, 2-methyl-	296	C21H44	001560-84-5	90
5	Eicosane	282	C20H42	000112-95-8	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092217\
Data File : BF098720.D
Acq On : 23 Sep 2017 2:27
Operator : SJ/JU
Sample : I5308-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 220-1-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.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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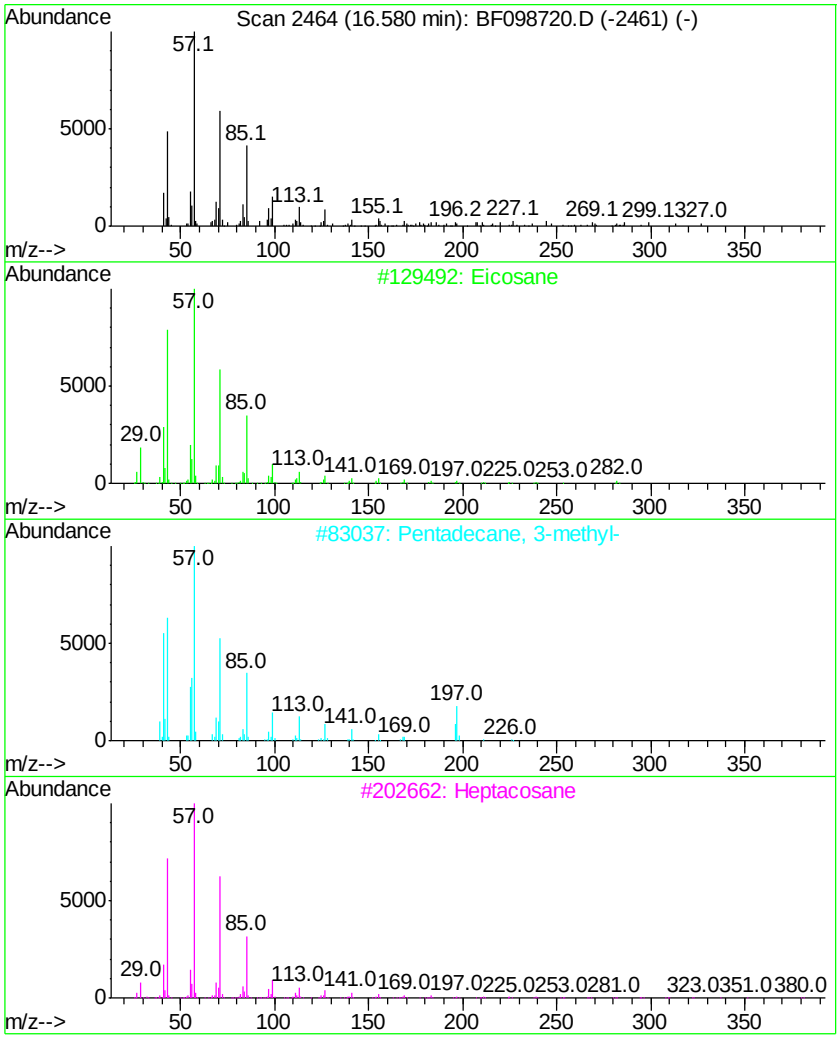
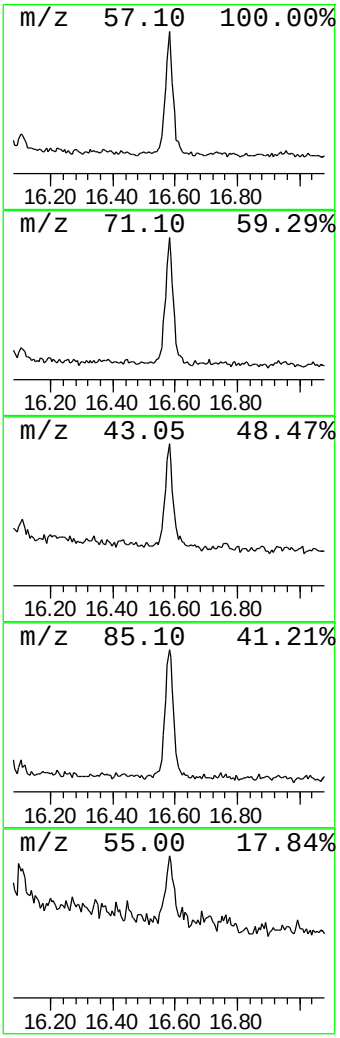
Peak Number 12 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.58	3.47 ng	168581	Perylene-d12	15.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Pentadecane, 3-methyl-	226	C16H34	002882-96-4	90
3	Heptacosane	380	C27H56	000593-49-7	90
4	Tetracosane	338	C24H50	000646-31-1	87
5	Nonadecane	268	C19H40	000629-92-5	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092217\
Data File : BF098720.D
Acq On : 23 Sep 2017 2:27
Operator : SJ/JU
Sample : I5308-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 220-1-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.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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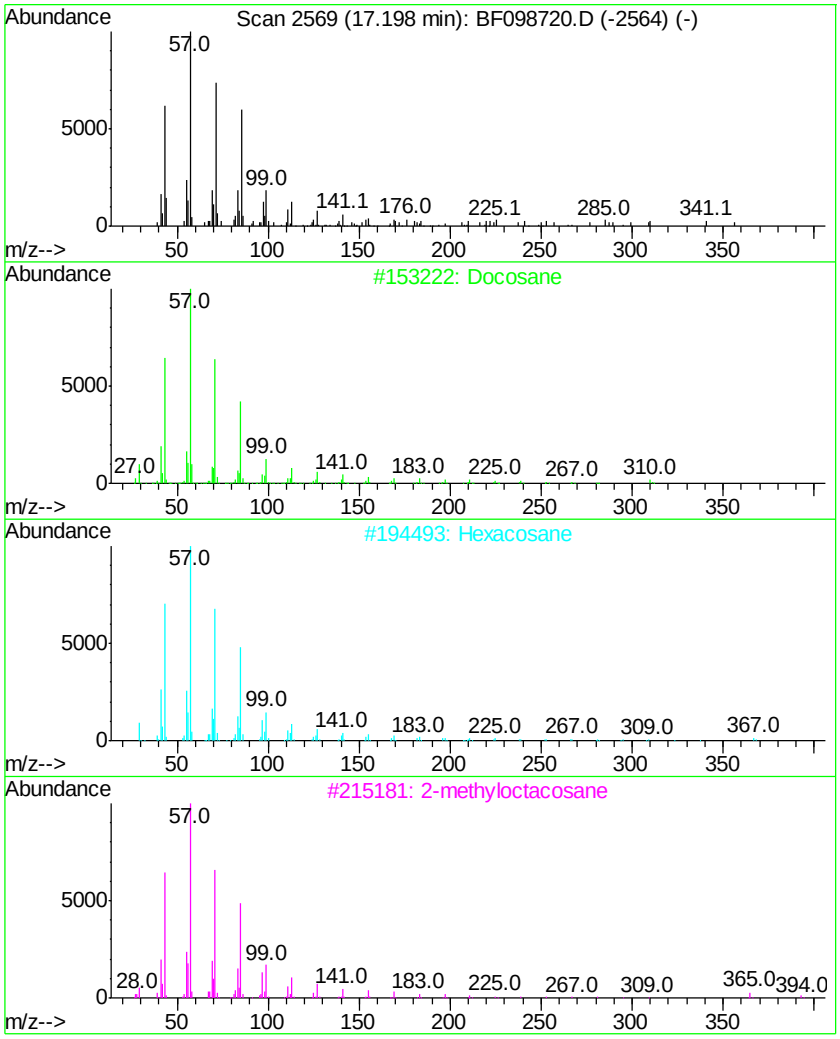
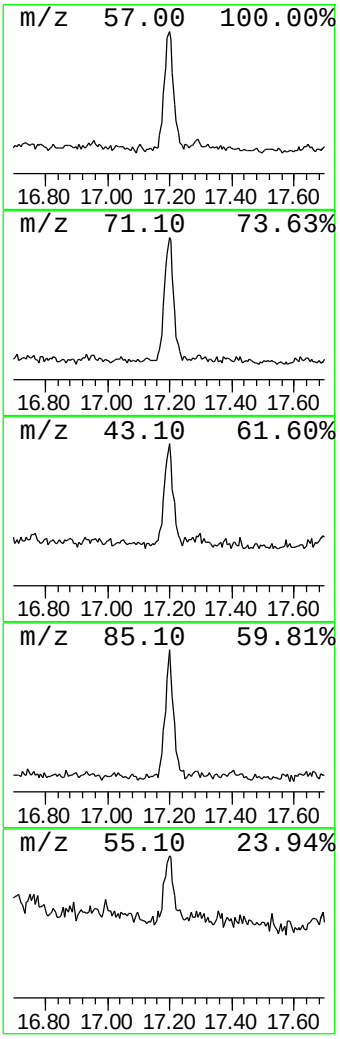
Peak Number 13 Docosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.20	4.31 ng	209668	Perylene-d12	15.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	94
2	Hexacosane	366	C26H54	000630-01-3	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	2-methyltetracosane	352	C25H52	1000376-72-6	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092217\
Data File : BF098720.D
Acq On : 23 Sep 2017 2:27
Operator : SJ/JU
Sample : I5308-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 220-1-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.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
Butane, 2-methoxy...	2.25	2.5	ng	125049	1	6.93	997909	20.0
2-Pentanone, 4-hy...	5.16	12.5	ng	621706	1	6.93	997909	20.0
unknown6.70	6.70	61.8	ng	3083090	1	6.93	997909	20.0
Tridecane, 1-iodo-	10.86	2.8	ng	151511	4	11.45	1095850	20.0
n-Hexadecanoic acid	11.97	11.8	ng	648641	4	11.45	1095850	20.0
Octadecanoic acid	12.75	11.4	ng	622855	4	11.45	1095850	20.0
5-Eicosene, (E)-	13.92	6.0	ng	327076	5	14.09	1082830	20.0
Hexadecane	14.55	2.2	ng	120122	5	14.09	1082830	20.0
Heneicosane	15.21	2.3	ng	111389	6	15.59	971892	20.0
Eicosane	16.58	3.5	ng	168581	6	15.59	971892	20.0
Docosane	17.20	4.3	ng	209668	6	15.59	971892	20.0