LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
Data File : BF103763.D
Acq On : 19 Mar 2018 18:43
Operator : JU/SJ
Sample : J1963-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-4-RO

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-BF031518.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	2.304	31	37	44	rVB	146099	191655	5.02%	0.458%
2	5.216	526	532	539	rBV	151591	196193	5.14%	0.469%
3	5.598	591	597	600	rBV	3116355	3516447	92.15%	8.399%
4	5.916	647	651	660	rVB	72230	67687	1.77%	0.162%
5	6.592	760	766	769	rBV	3050630	3607971	94.55%	8.618%
6	6.739	786	791	795	rBV	3466586	3591490	94.12%	8.578%
7	6.969	827	830	834	rVB	1158878	990049	25.95%	2.365%
8	7.128	853	857	860	rBV	3225308	2780106	72.86%	6.640%
9	7.534	921	926	929	rBV	2439060	2294146	60.12%	5.479%
10	8.251	1045	1048	1052	rBV	1538834	1316832	34.51%	3.145%
11	8.828	1143	1146	1151	rBV	68288	59957	1.57%	0.143%
12	9.328	1226	1231	1234	rBV	4131375	3815880	100.00%	9.114%
13	9.392	1240	1242	1246	rBV	109245	102459	2.69%	0.245%
14	9.663	1281	1288	1291	rBV7	24965	57280	1.50%	0.137%
15	9.716	1294	1297	1300	rBV	491326	372122	9.75%	0.889%
16	9.927	1330	1333	1336	rVB	237040	178290	4.67%	0.426%
17	10.010	1343	1347	1351	rBV	1609029	1459135	38.24%	3.485%
18	10.157	1369	1372	1375	rBV3	30396	42512	1.11%	0.102%
19	10.251	1385	1388	1392	rBV2	53641	62897	1.65%	0.150%
20	10.322	1397	1400	1403	rBV2	39965	47513	1.25%	0.113%
21	10.427	1415	1418	1421	rVB	282793	215242	5.64%	0.514%
22	10.645	1451	1455	1458	rBV	91197	111506	2.92%	0.266%
23	10.804	1478	1482	1485	rBV	2472471	2351693	61.63%	5.617%
24	10.904	1496	1499	1504	rBV	205109	247619	6.49%	0.591%
25	11.057	1522	1525	1528	rVB	47864	39862	1.04%	0.095%
26	11.351	1572	1575	1577	rBV	158487	123878	3.25%	0.296%
27	11.380	1577	1580	1582	rVV	71635	62248	1.63%	0.149%
28	11.504	1597	1601	1603	rBV	1659972	1420281	37.22%	3.392%
29	11.527	1603	1605	1609	rVV	266405	215131	5.64%	0.514%
30	11.574	1611	1613	1617	rVB	47040	44451	1.16%	0.106%
31	11.780	1645	1648	1650	rBV	92801	74982	1.96%	0.179%
32	11.880	1662	1665	1668	rVB	881300	664529	17.41%	1.587%
33	12.016	1684	1688	1697	rBV3	408675	486627	12.75%	1.162%
34	12.186	1714	1717	1720	rBV2	90033	87130	2.28%	0.208%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
ClientSampleId : 1-4-RO

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-BF031518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.574	1779	1783	1784	rBV	1962511	1933002	50.66%	4.617%
36	12.592	1784	1786	1792	rVB2	1847318	1705000	44.68%	4.072%
37	12.674	1797	1800	1803	rBV	359003	273708	7.17%	0.654%
38	12.721	1804	1808	1812	rVV	354030	314939	8.25%	0.752%
39	12.804	1819	1822	1827	rVB2	88129	94120	2.47%	0.225%
40	12.951	1844	1847	1853	rVB	340133	305770	8.01%	0.730%
41	13.092	1866	1871	1874	rBV	3148025	3226644	84.56%	7.707%
42	13.239	1893	1896	1900	rBV5	61171	85277	2.23%	0.204%
43	13.968	2017	2020	2025	rBV	556426	565596	14.82%	1.351%
44	14.151	2047	2051	2054	rBV	1117772	1177693	30.86%	2.813%
45	14.180	2054	2056	2061	rVB	130884	117507	3.08%	0.281%
46	14.610	2127	2129	2133	rVB2	78494	82413	2.16%	0.197%
47	15.227	2231	2234	2238	rBV	108622	166611	4.37%	0.398%
48	15.692	2308	2313	2322	rVB	692736	923835	24.21%	2.207%

Sum of corrected areas: 41867915

LSC Report - Integrated Chromatogram

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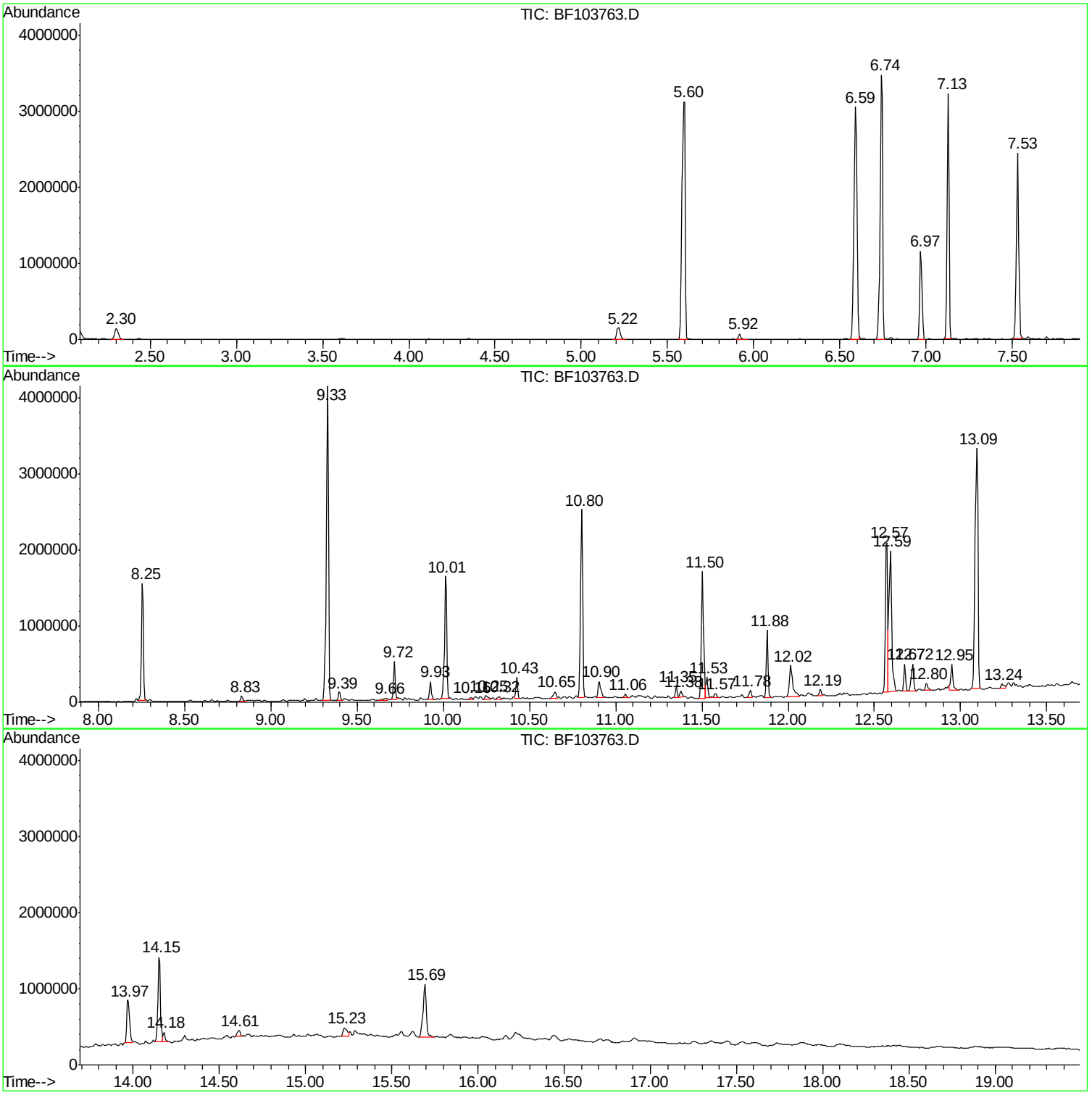
Sample : J1963-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-4-RO

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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\BF031918\
Data File : BF103763.D
Acq On : 19 Mar 2018 18:43
Operator : JU/SJ
Sample : J1963-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-4-RO

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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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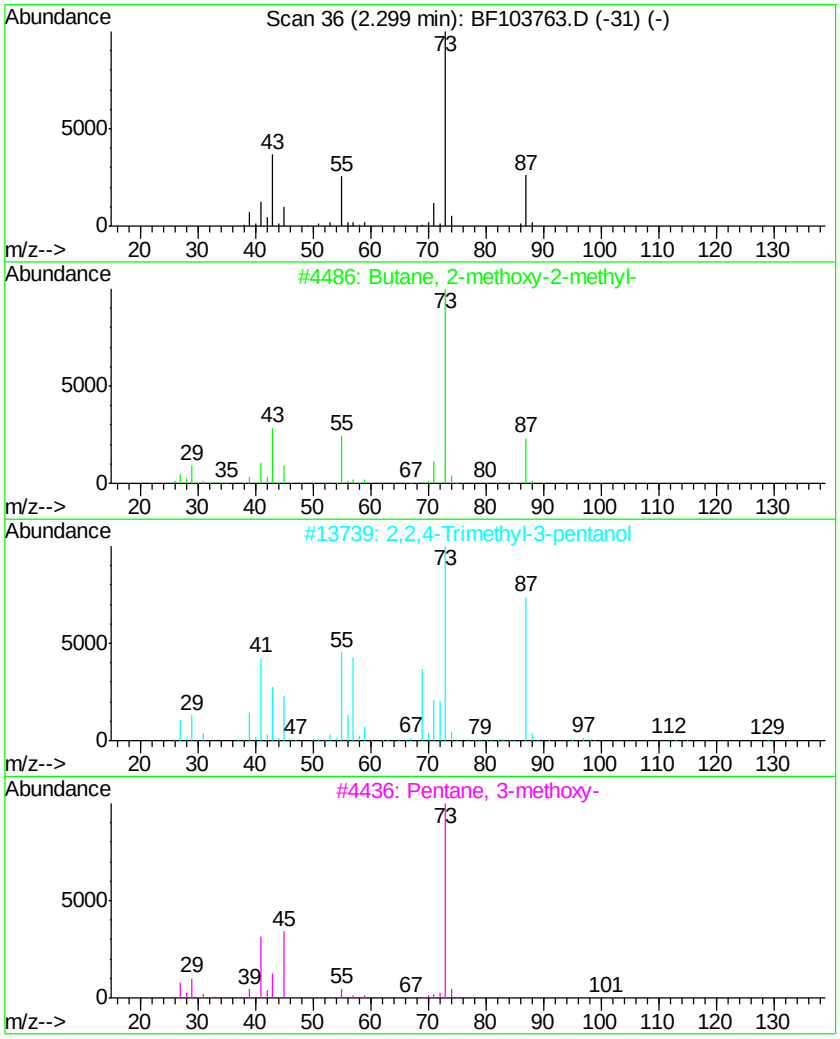
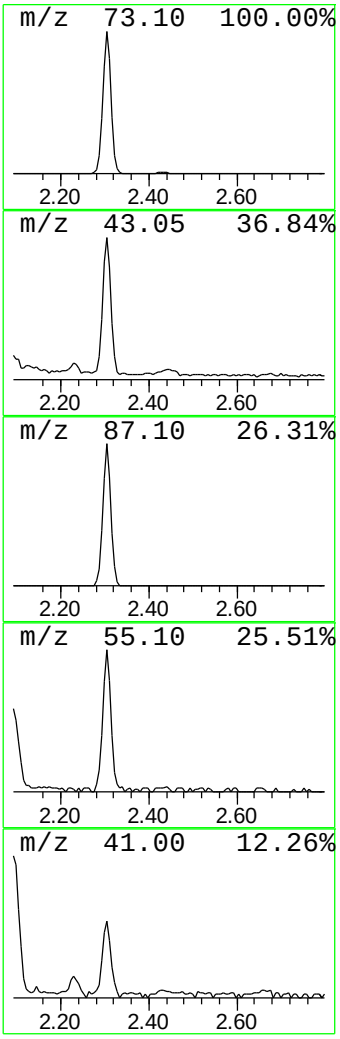
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.30	3.87 ng	191655	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Data File : BF103763.D
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Sample : J1963-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-4-RO

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

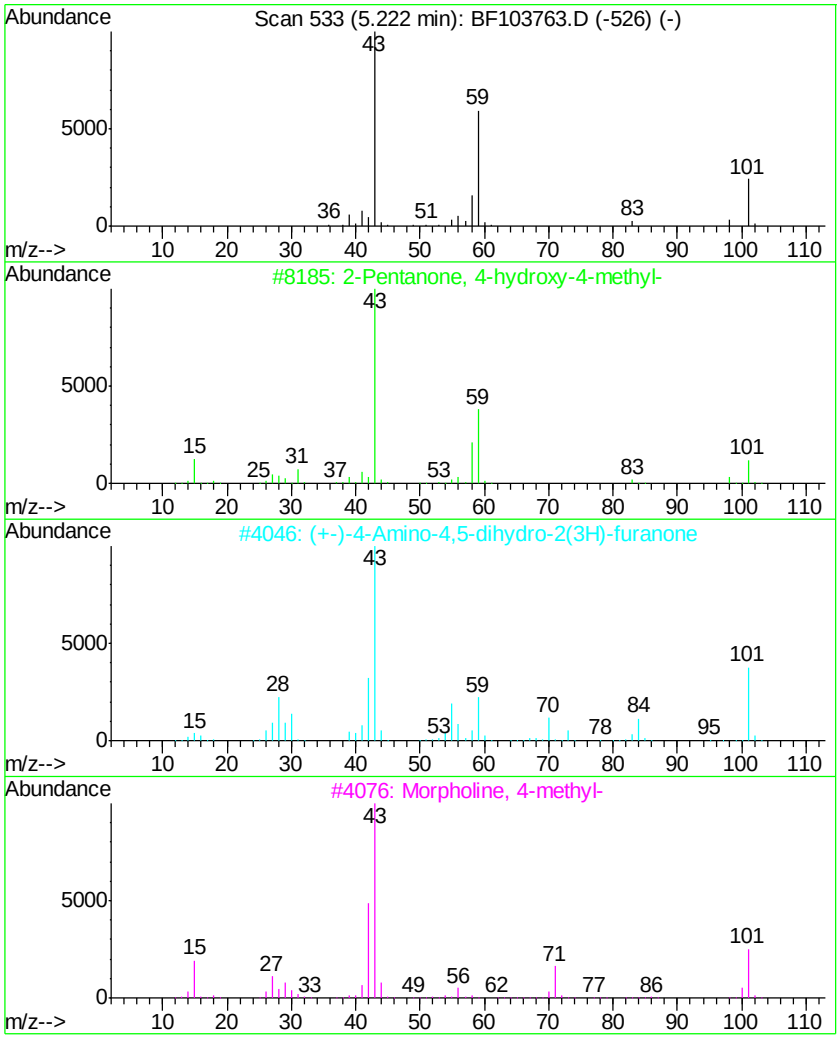
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

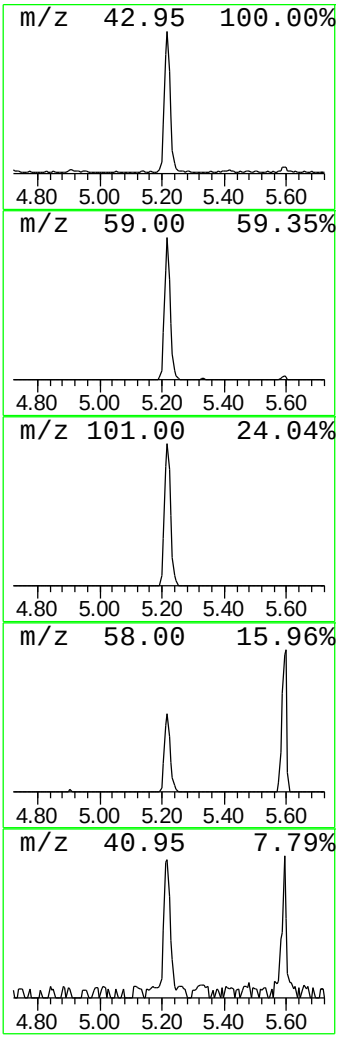
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	3.96 ng	196193	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Guanidine	59	CH5N3	000113-00-8	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
Data File : BF103763.D
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Operator : JU/SJ
Sample : J1963-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-4-RO

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

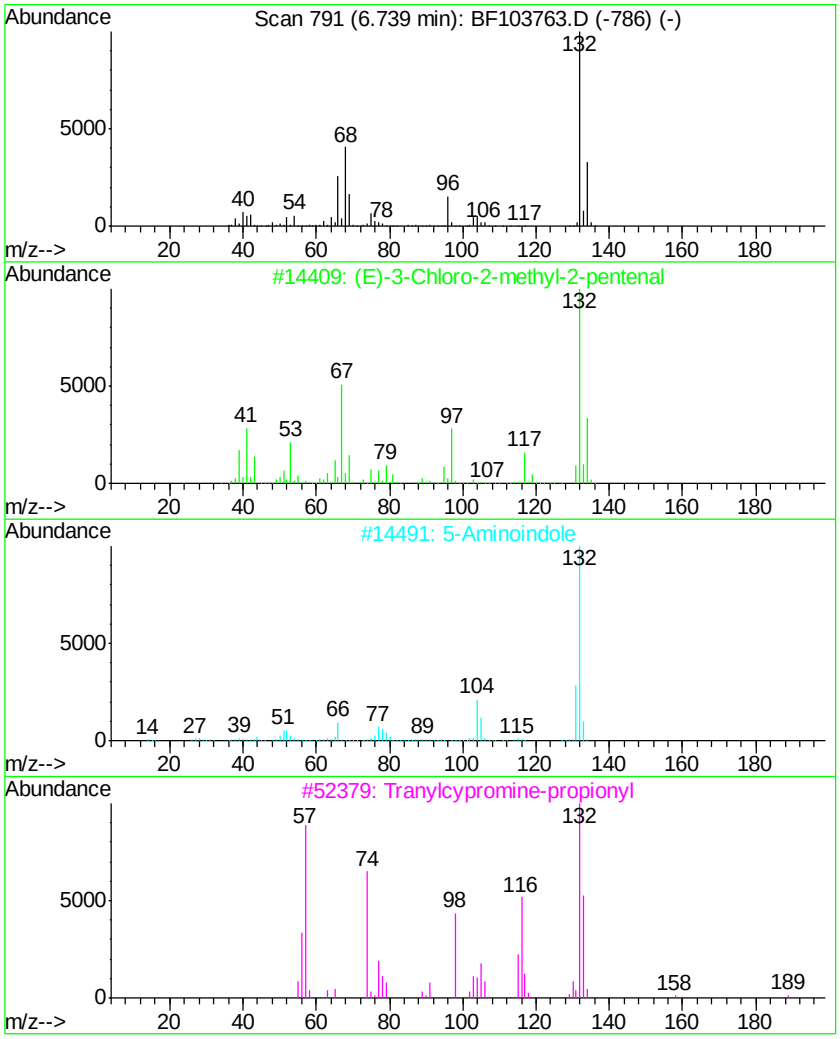
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

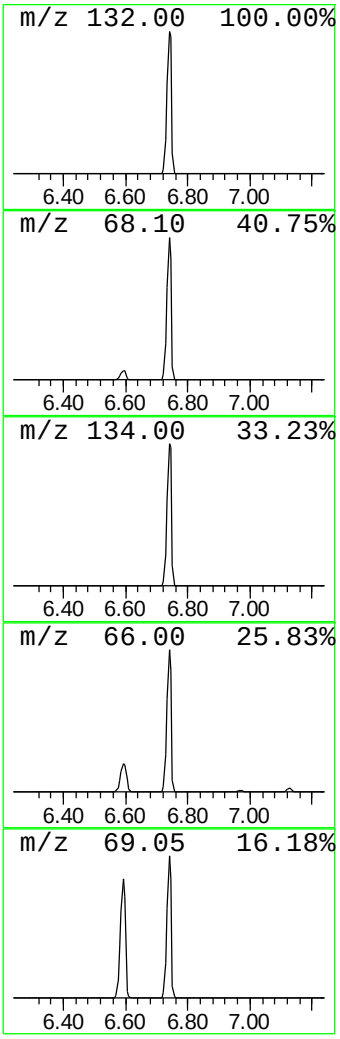
****

Peak Number 3 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	72.55 ng	3591490	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-4-RO

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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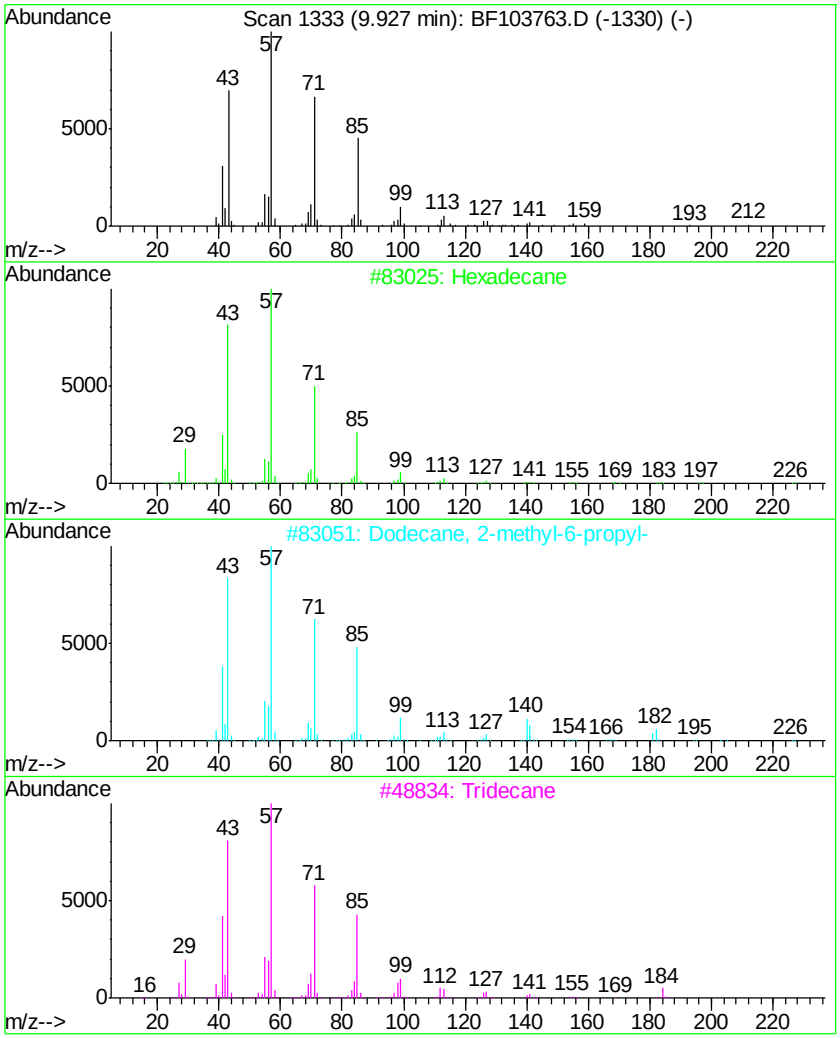
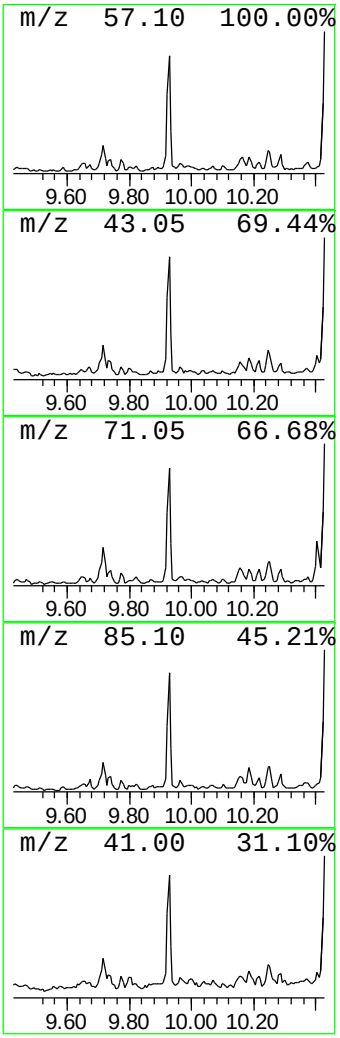
Peak Number 5 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.93	2.44 ng	178290	Acenaphthene-d10	10.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	80
2	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	78
3	Tridecane	184	C13H28	000629-50-5	64
4	Dodecane, 4-methyl-	184	C13H28	006117-97-1	64
5	Nonane, 5-(2-methylpropyl)-	184	C13H28	062185-53-9	64





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Sample : J1963-01
Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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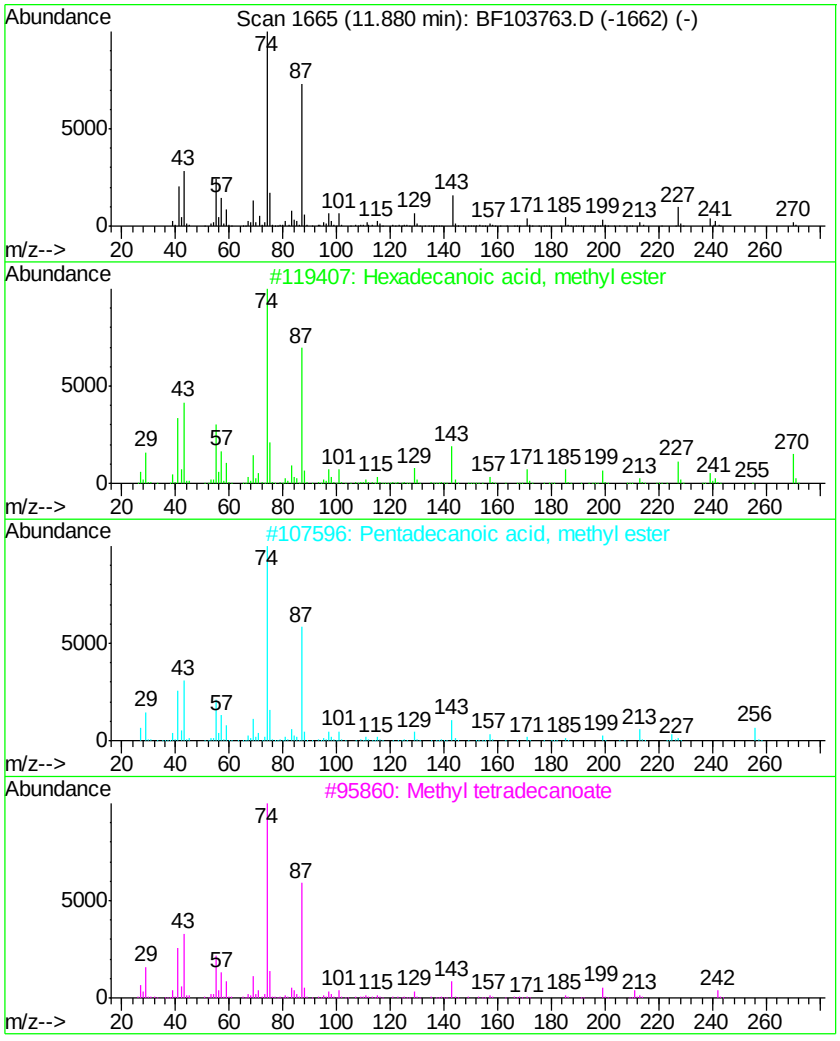
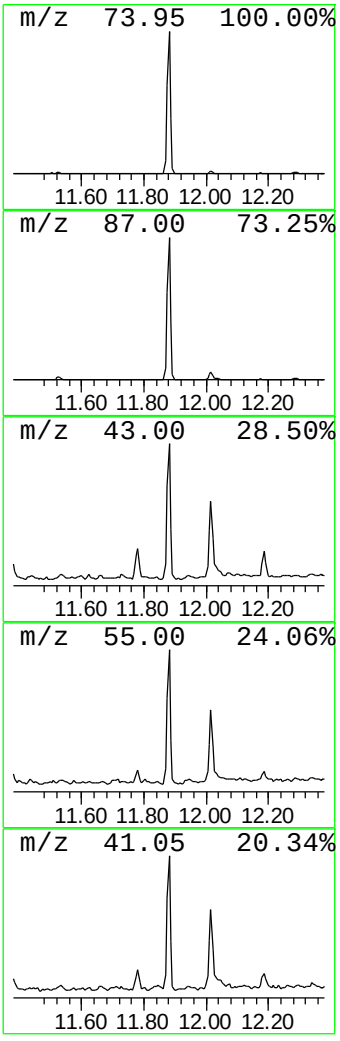
****

Peak Number 8 Hexadecanoic acid, methyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	9.36 ng	664529	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	95
2	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	83
4	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	80
5	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	72





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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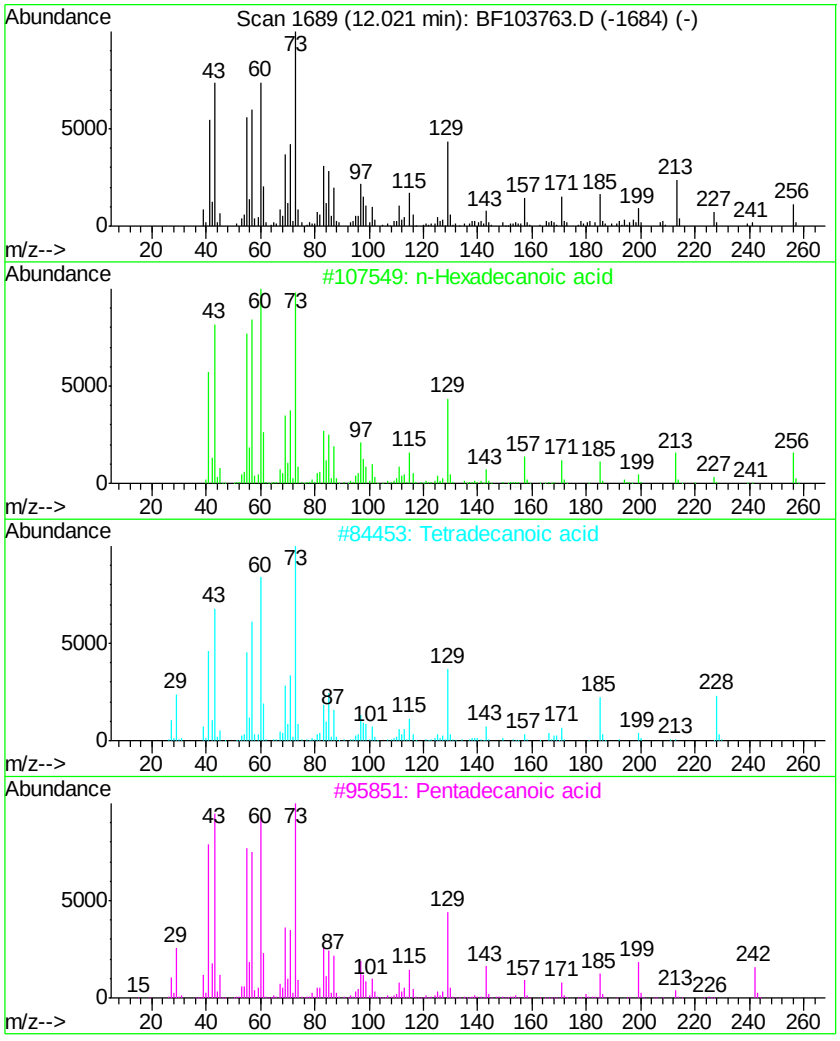
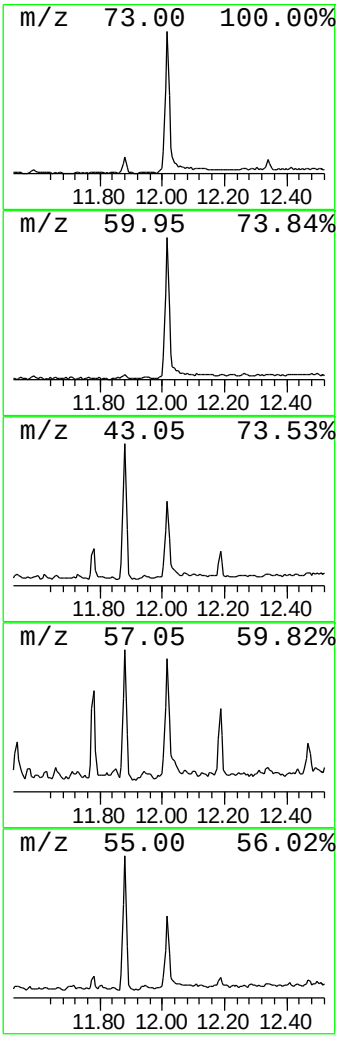
Peak Number 9 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	6.85 ng	486627	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	90
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





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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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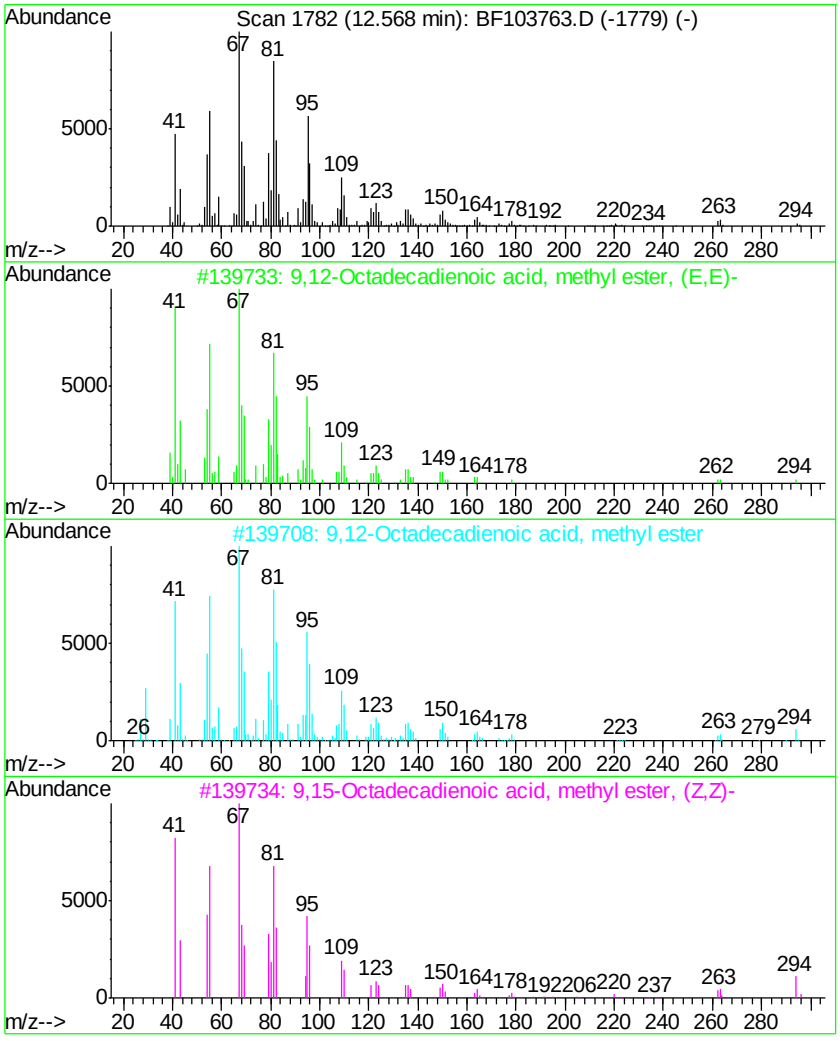
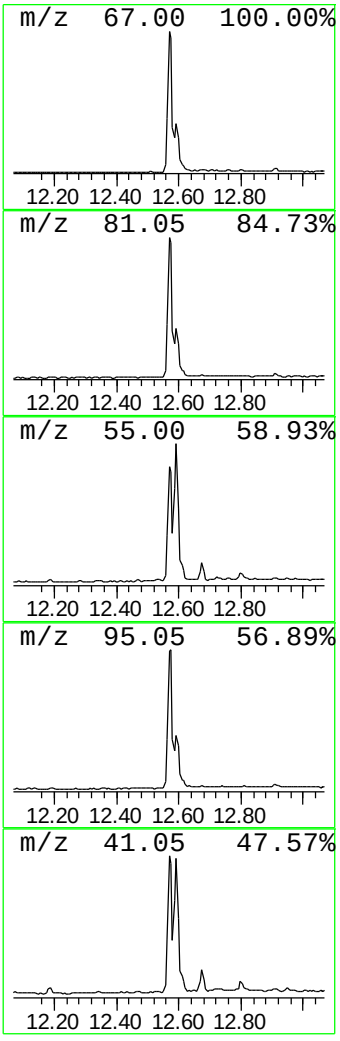
Peak Number 10 9,12-Octadecadienoic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	27.22 ng	1933000	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
4	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
5	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
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Sample : J1963-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-4-RO

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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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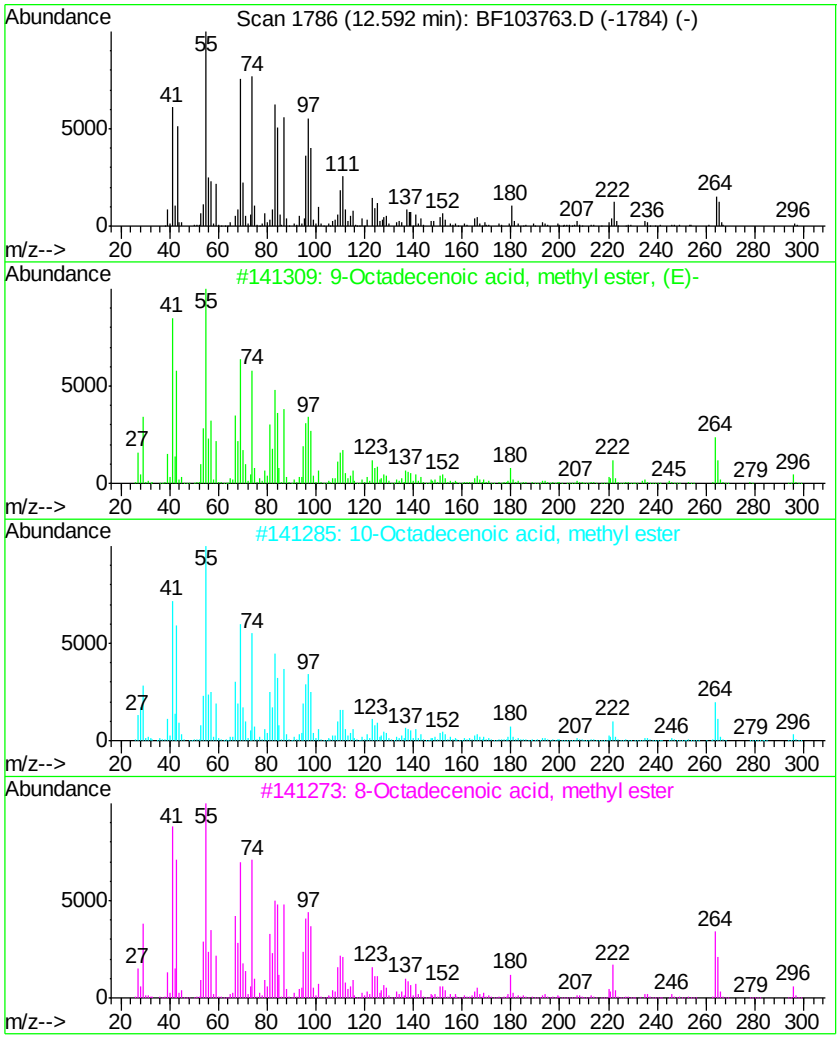
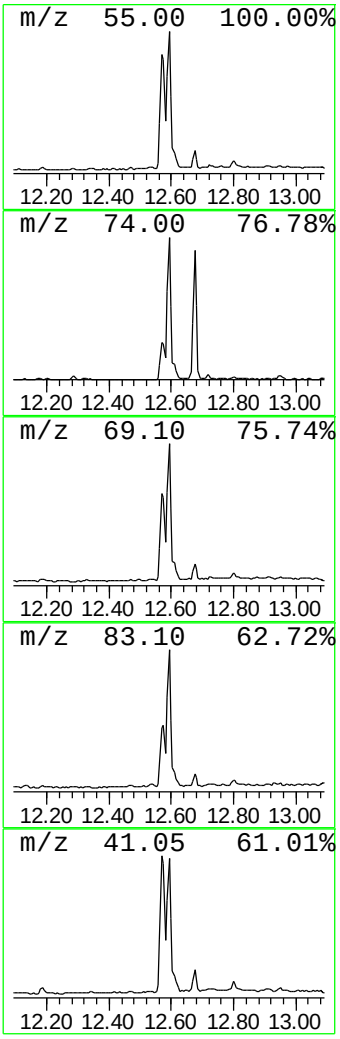
Peak Number 11 9-Octadecenoic acid, methyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.59	24.01 ng	1705000	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	95
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
3	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	93
4	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	90
5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	83





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
Data File : BF103763.D
Acq On : 19 Mar 2018 18:43
Operator : JU/SJ
Sample : J1963-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-4-RO

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

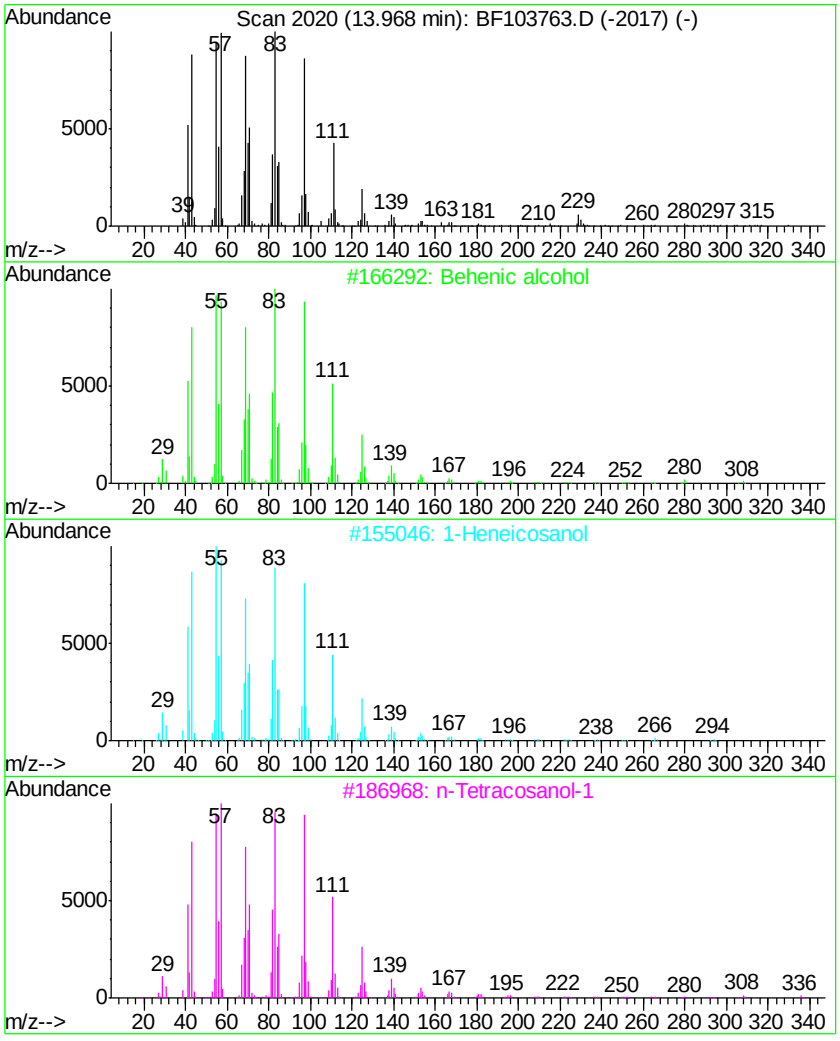
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

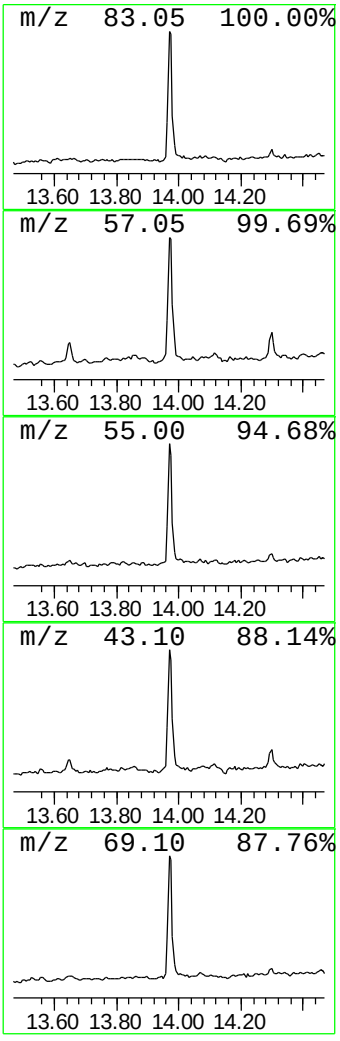
****

Peak Number 12 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	9.61 ng	565596	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	91
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031918\
Data File : BF103763.D
Acq On : 19 Mar 2018 18:43
Operator : JU/SJ
Sample : J1963-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-4-RO

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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...	2.30	3.9	ng	191655	1	6.97	990049	20.0
2-Pentanone, 4-hy...	5.22	4.0	ng	196193	1	6.97	990049	20.0
unknown6.74	6.74	72.5	ng	3591490	1	6.97	990049	20.0
Hexadecane	9.93	2.4	ng	178290	3	10.01	1459140	20.0
Hexadecanoic acid...	11.88	9.4	ng	664529	4	11.50	1420280	20.0
n-Hexadecanoic acid	12.02	6.8	ng	486627	4	11.50	1420280	20.0
9,12-Octadecadien...	12.57	27.2	ng	1933000	4	11.50	1420280	20.0
9-Octadecenoic ac...	12.59	24.0	ng	1705000	4	11.50	1420280	20.0
Behenic alcohol	13.97	9.6	ng	565596	5	14.16	1177690	20.0