LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104892.D
Acq On : 27 Apr 2018 20:12
Operator : JU/SJ
Sample : J2564-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

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-BF040618.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	3.834	292	297	303	rBV	18187	26198	1.06%	0.115%
2	5.016	493	498	504	rBV	63983	83188	3.36%	0.366%
3	5.428	564	568	584	rBV	1874175	1982538	80.10%	8.721%
4	6.445	737	741	759	rBV	1715660	2053867	82.99%	9.035%
5	6.575	759	763	766	rBV	2350265	2042472	82.53%	8.984%
6	6.798	797	801	808	rVB	695302	565968	22.87%	2.490%
7	6.951	823	827	831	rBV	1755600	1675048	67.68%	7.368%
8	7.216	868	872	893	rBV	796183	989507	39.98%	4.353%
9	7.363	893	897	901	rBV	1200063	1221559	49.36%	5.373%
10	7.533	923	926	929	rVB	32538	25064	1.01%	0.110%
11	8.080	1016	1019	1036	rVB	803575	773253	31.24%	3.401%
12	8.739	1128	1131	1139	rVB	16297	25012	1.01%	0.110%
13	8.998	1171	1175	1178	rBV2	26109	30364	1.23%	0.134%
14	9.157	1197	1202	1211	rBV	2608502	2474957	100.00%	10.887%
15	9.233	1211	1215	1217	rVV	35228	37045	1.50%	0.163%
16	9.280	1220	1223	1231	rVB	34549	50124	2.03%	0.220%
17	9.551	1264	1269	1276	rBV	179198	175082	7.07%	0.770%
18	9.757	1300	1304	1309	rBV2	136574	147270	5.95%	0.648%
19	9.839	1313	1318	1326	rVB2	979742	872136	35.24%	3.836%
20	10.045	1350	1353	1357	rBV	51017	48717	1.97%	0.214%
21	10.233	1381	1385	1387	rBV2	40949	47124	1.90%	0.207%
22	10.263	1387	1390	1392	rVB	89440	78491	3.17%	0.345%
23	10.480	1421	1427	1429	rBV	29290	37265	1.51%	0.164%
24	10.633	1449	1453	1462	rBV	1475826	1362298	55.04%	5.992%
25	10.733	1467	1470	1475	rBV	79693	78684	3.18%	0.346%
26	10.986	1511	1513	1518	rBV	82492	79350	3.21%	0.349%
27	11.180	1544	1546	1549	rBV	37181	34590	1.40%	0.152%
28	11.333	1568	1572	1581	rBV	747401	756787	30.58%	3.329%
29	11.780	1645	1648	1651	rBV4	17563	26024	1.05%	0.114%
30	11.857	1656	1661	1669	rVV	701584	687385	27.77%	3.024%
31	12.563	1774	1781	1791	rBV2	431324	715139	28.90%	3.146%
32	12.639	1791	1794	1804	rVB	122736	153933	6.22%	0.677%
33	12.921	1837	1842	1845	rBV	2003949	1919183	77.54%	8.442%
34	13.804	1989	1992	1995	rBV	165606	164937	6.66%	0.726%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104892.D
Acq On : 27 Apr 2018 20:12
Operator : JU/SJ
Sample : J2564-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

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-BF040618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.839	1996	1998	2003	rVB	96432	111637	4.51%	0.491%
36	13.980	2018	2022	2030	rBV	666105	621913	25.13%	2.736%
37	15.451	2268	2272	2283	rVB	359549	559378	22.60%	2.461%

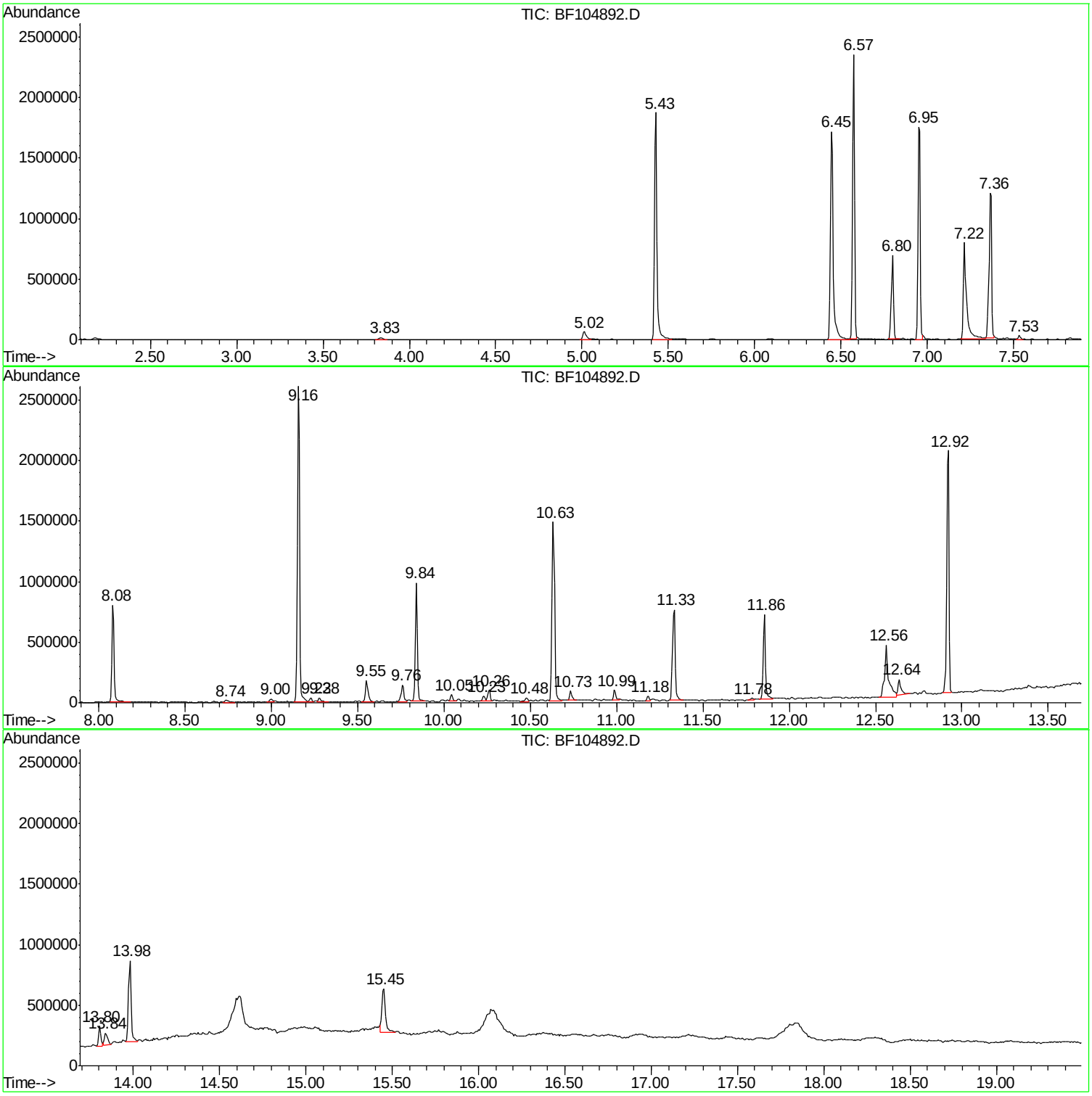
Sum of corrected areas: 22733487

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104892.D
Acq On : 27 Apr 2018 20:12
Operator : JU/SJ
Sample : J2564-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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\BF042718\
Data File : BF104892.D
Acq On : 27 Apr 2018 20:12
Operator : JU/SJ
Sample : J2564-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

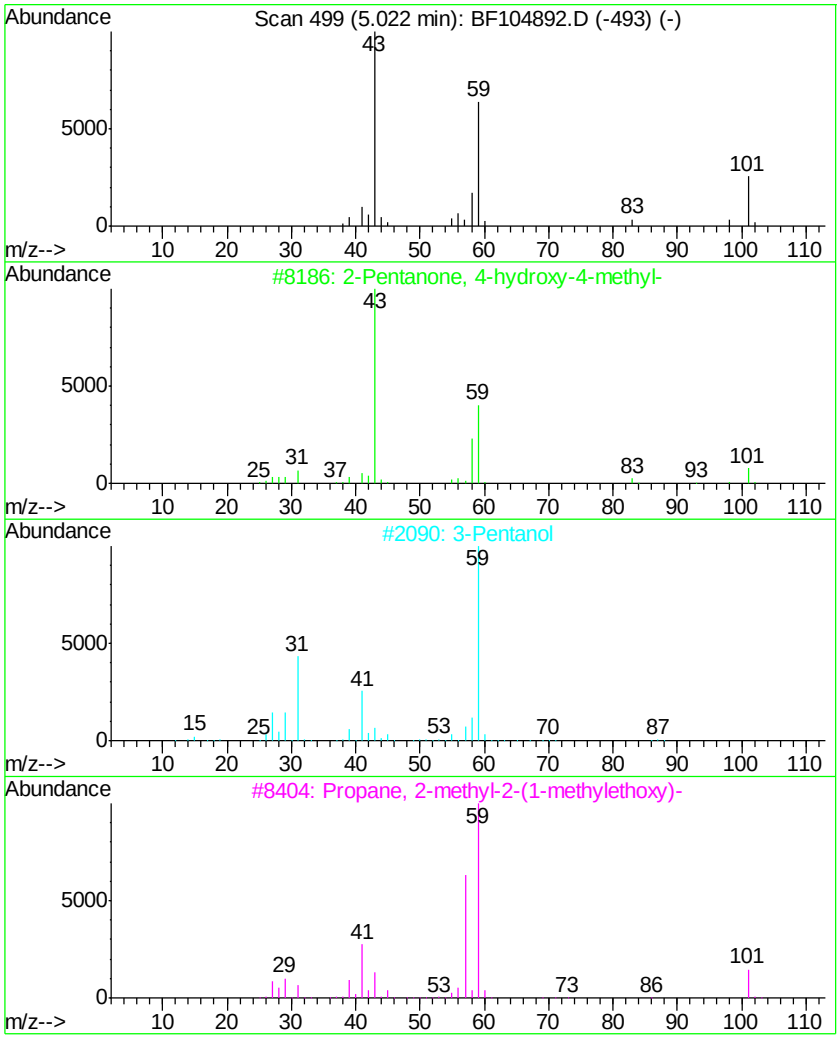
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

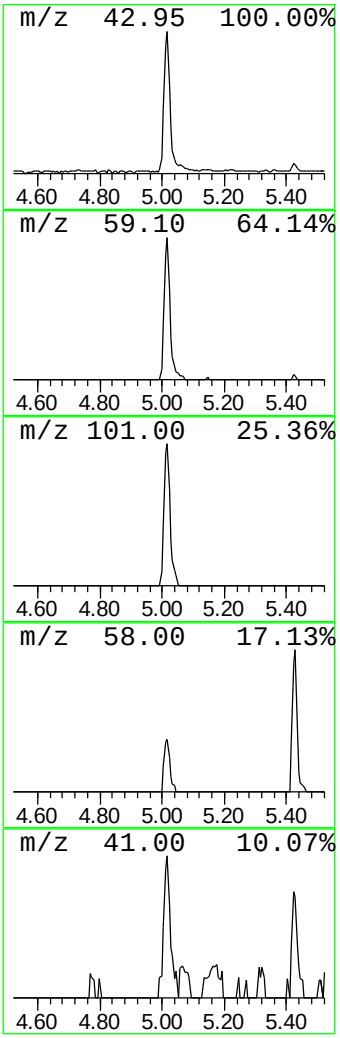
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	2.94 ng	83188	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	3-Pentanol	88	C5H12O	000584-02-1	25
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23
4	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	23
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104892.D
Acq On : 27 Apr 2018 20:12
Operator : JU/SJ
Sample : J2564-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

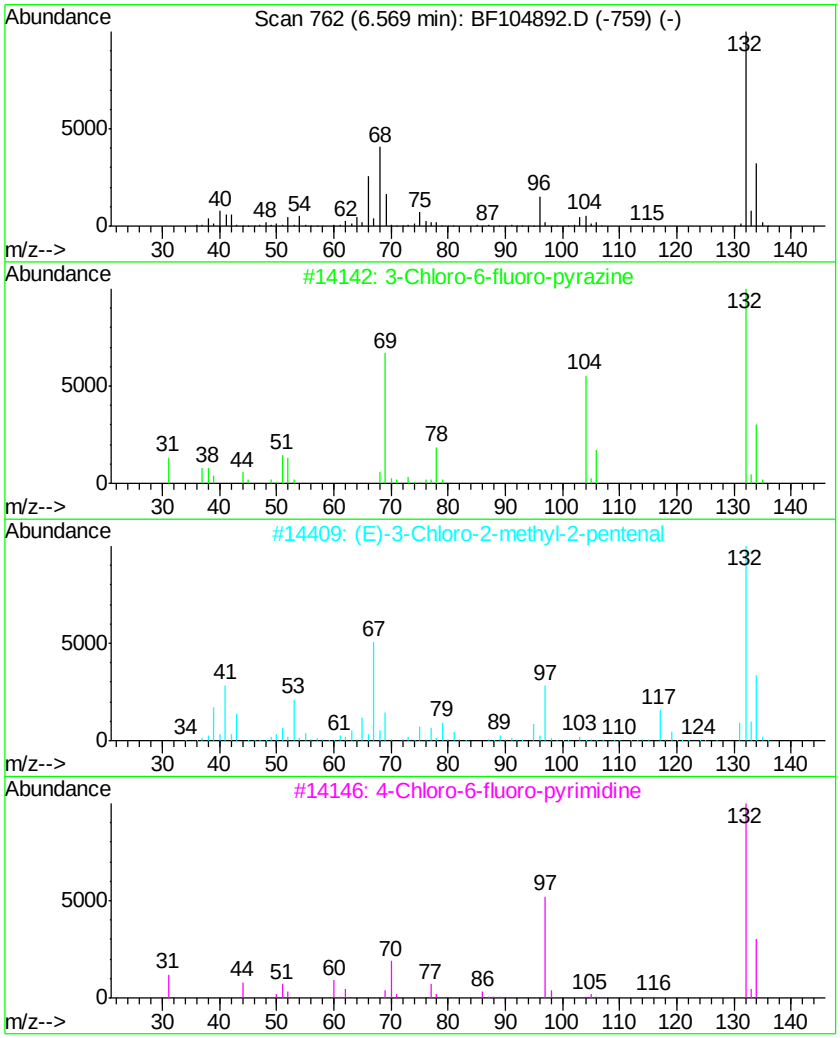
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

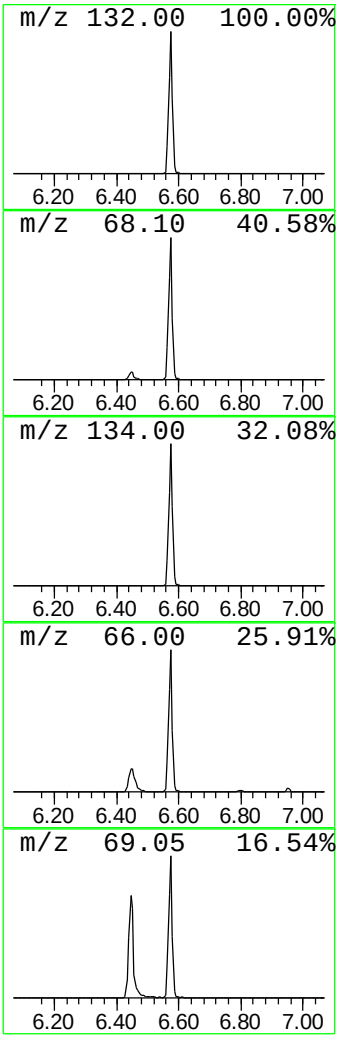
****

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	72.18 ng	2042470	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	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104892.D
Acq On : 27 Apr 2018 20:12
Operator : JU/SJ
Sample : J2564-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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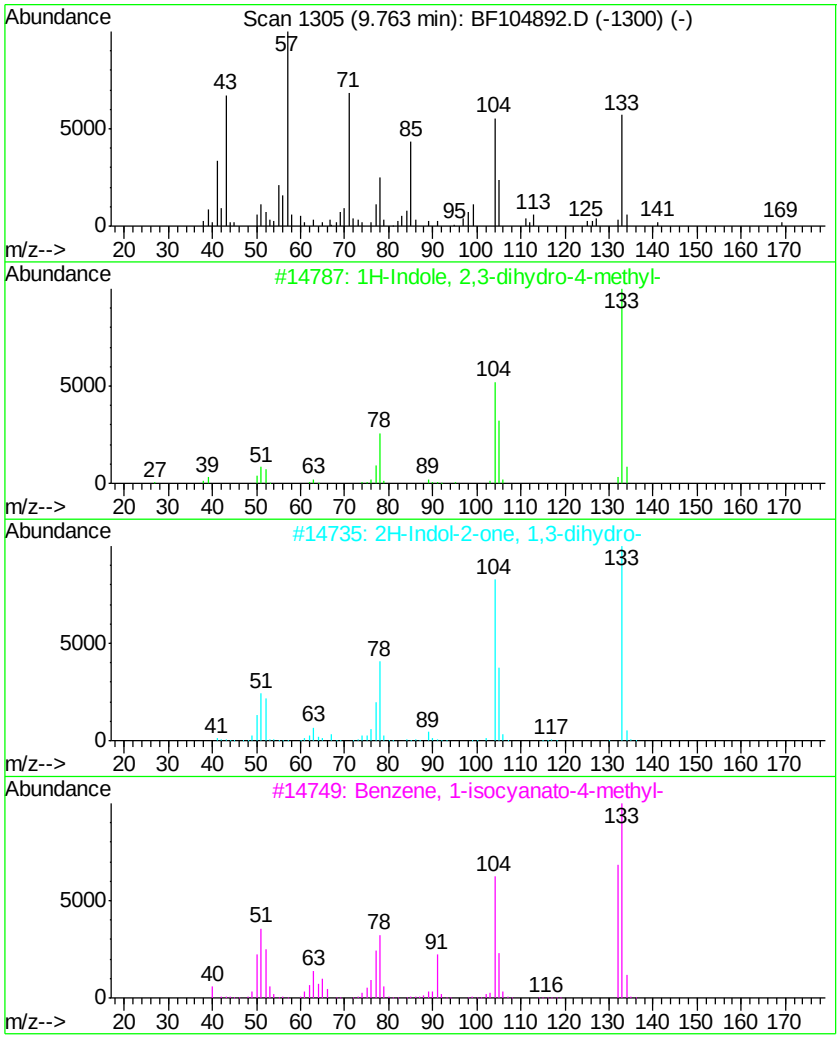
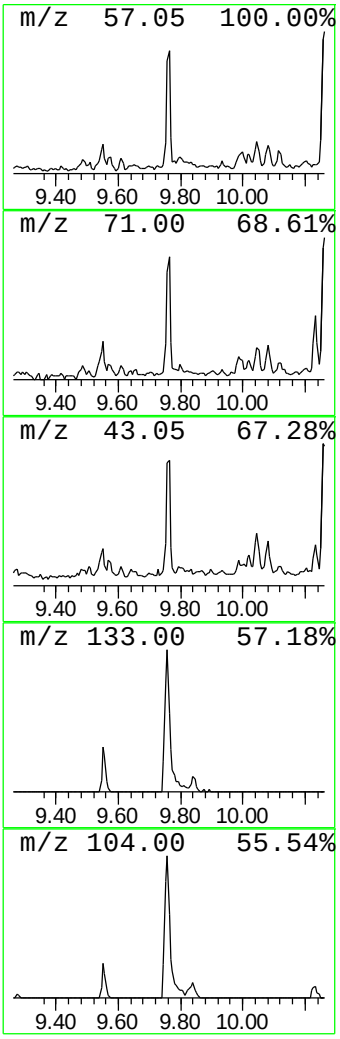
Peak Number 4 1H-Indole, 2,3-dihydro-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.76	3.38 ng	147270	Acenaphthene-d10	9.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indole, 2,3-dihydro-4-methyl-	133	C9H11N	062108-16-1	93
2	2H-Indol-2-one, 1,3-dihydro-	133	C8H7NO	000059-48-3	70
3	Benzene, 1-isocyanato-4-methyl-	133	C8H7NO	000622-58-2	62
4	1H-Indol-5-ol	133	C8H7NO	001953-54-4	58
5	1H-Benzotriazole, 4-methyl-	133	C7H7N3	029878-31-7	58





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104892.D
Acq On : 27 Apr 2018 20:12
Operator : JU/SJ
Sample : J2564-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

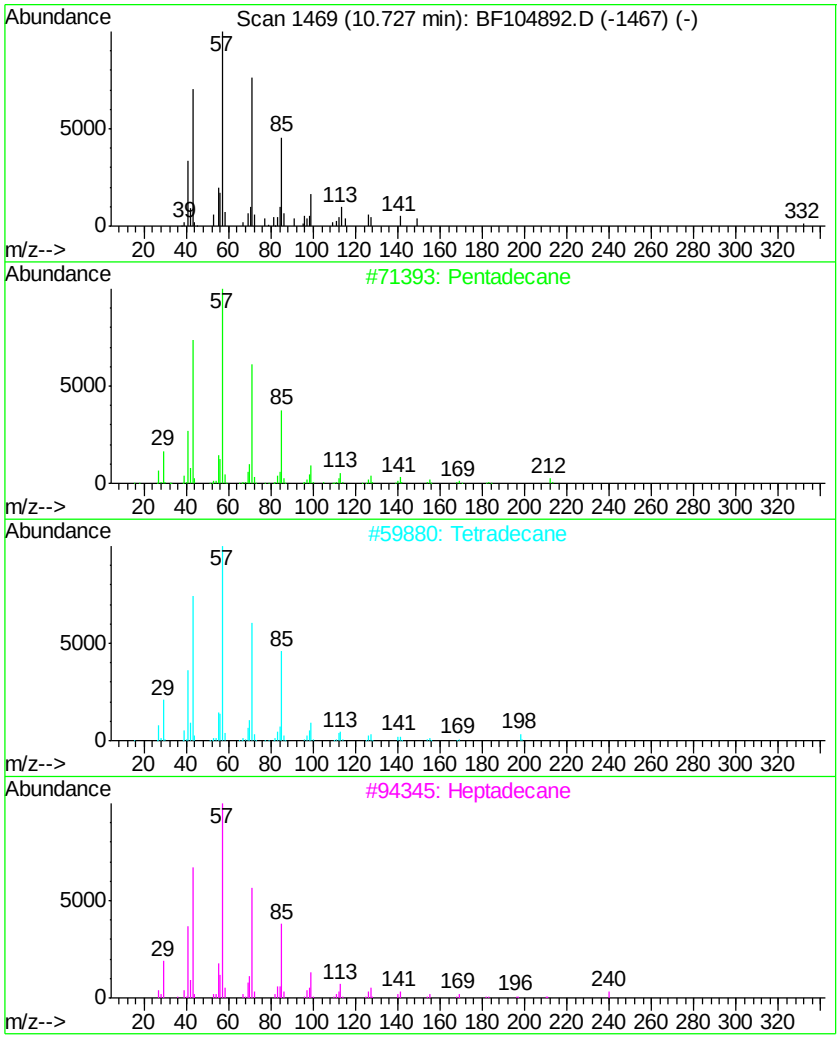
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

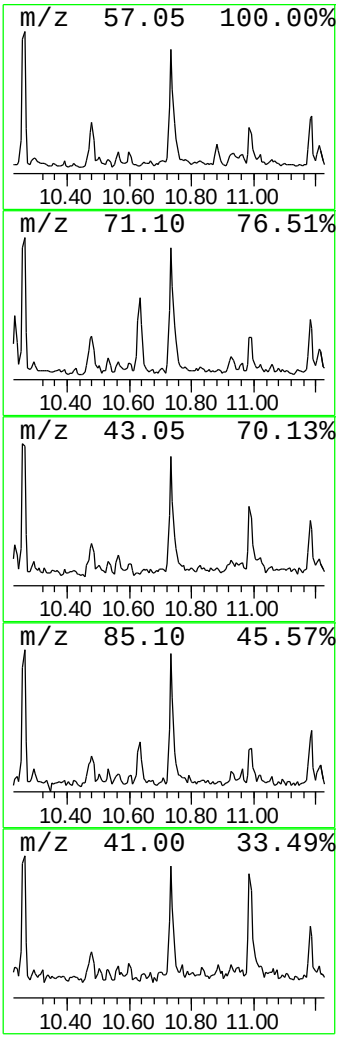
****

Peak Number 5 Pentadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.73	2.08 ng	78684	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	91
2	Tetradecane	198	C14H30	000629-59-4	91
3	Heptadecane	240	C17H36	000629-78-7	90
4	Hexadecane	226	C16H34	000544-76-3	90
5	Heptacosane	380	C27H56	000593-49-7	83





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104892.D
Acq On : 27 Apr 2018 20:12
Operator : JU/SJ
Sample : J2564-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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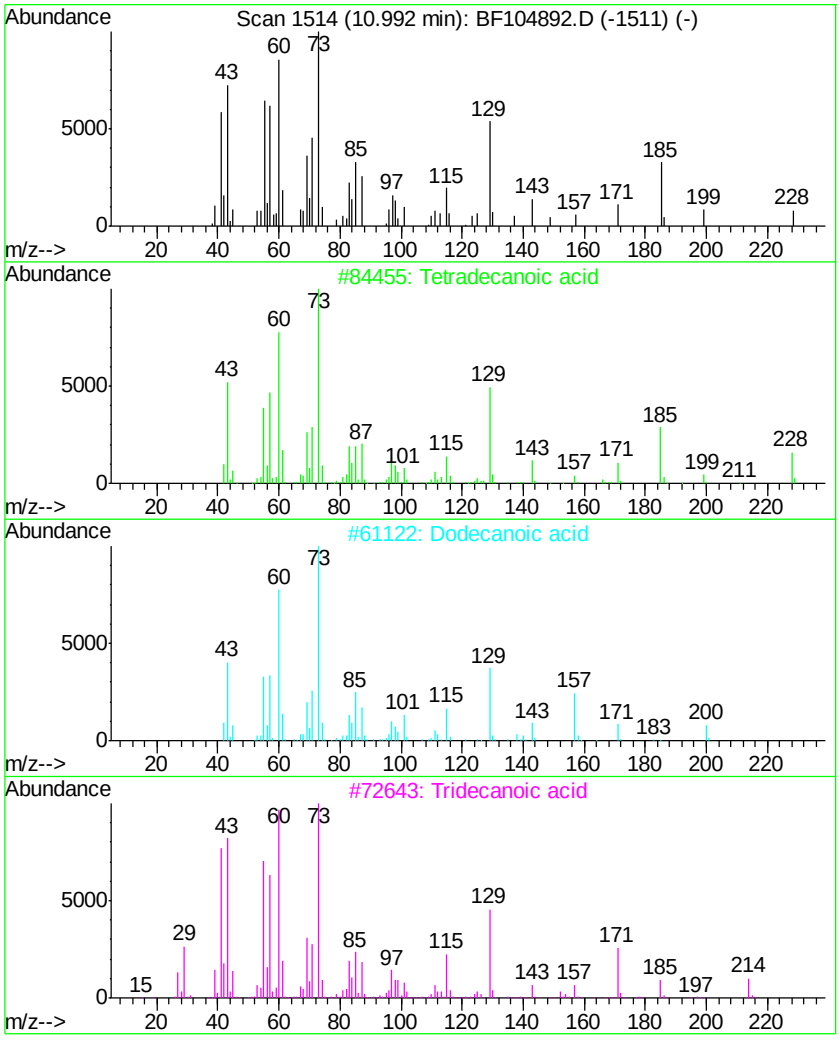
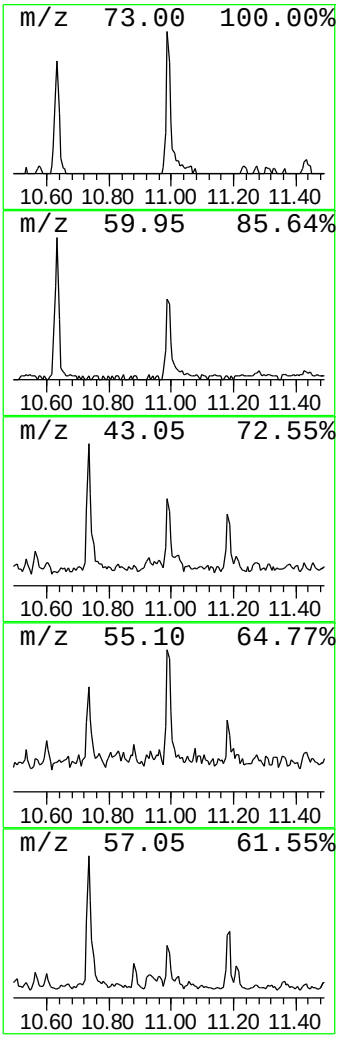
Peak Number 6 Tetradecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.99	2.10 ng	79350	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
2	Dodecanoic acid	200	C12H24O2	000143-07-7	64
3	Tridecanoic acid	214	C13H26O2	000638-53-9	59
4	n-Decanoic acid	172	C10H20O2	000334-48-5	49
5	Undecanoic acid	186	C11H22O2	000112-37-8	41





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104892.D
Acq On : 27 Apr 2018 20:12
Operator : JU/SJ
Sample : J2564-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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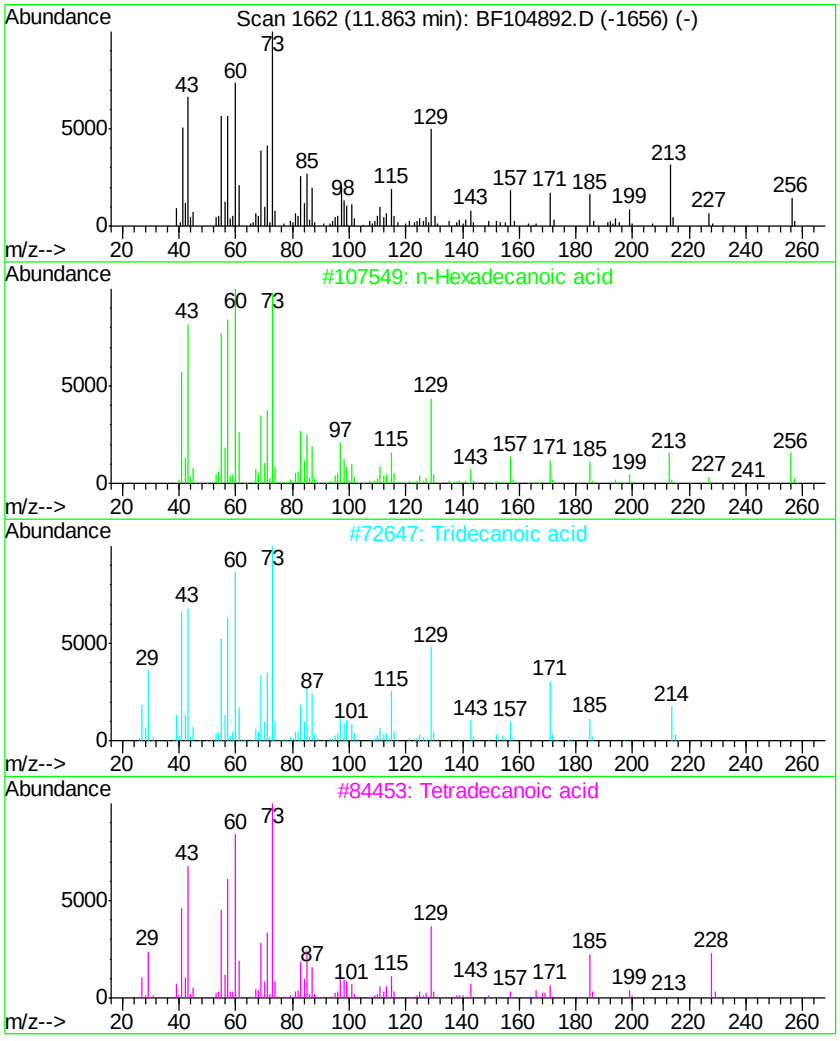
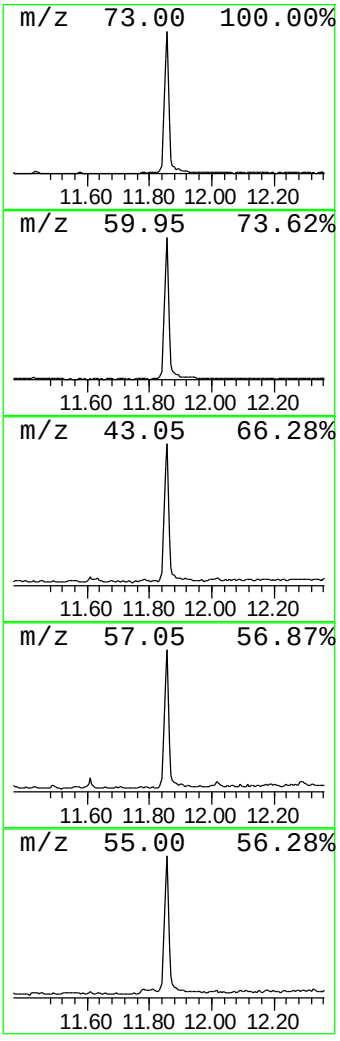
Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	18.17 ng	687385	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	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	Undecanoic acid	186	C11H22O2	000112-37-8	83





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104892.D
Acq On : 27 Apr 2018 20:12
Operator : JU/SJ
Sample : J2564-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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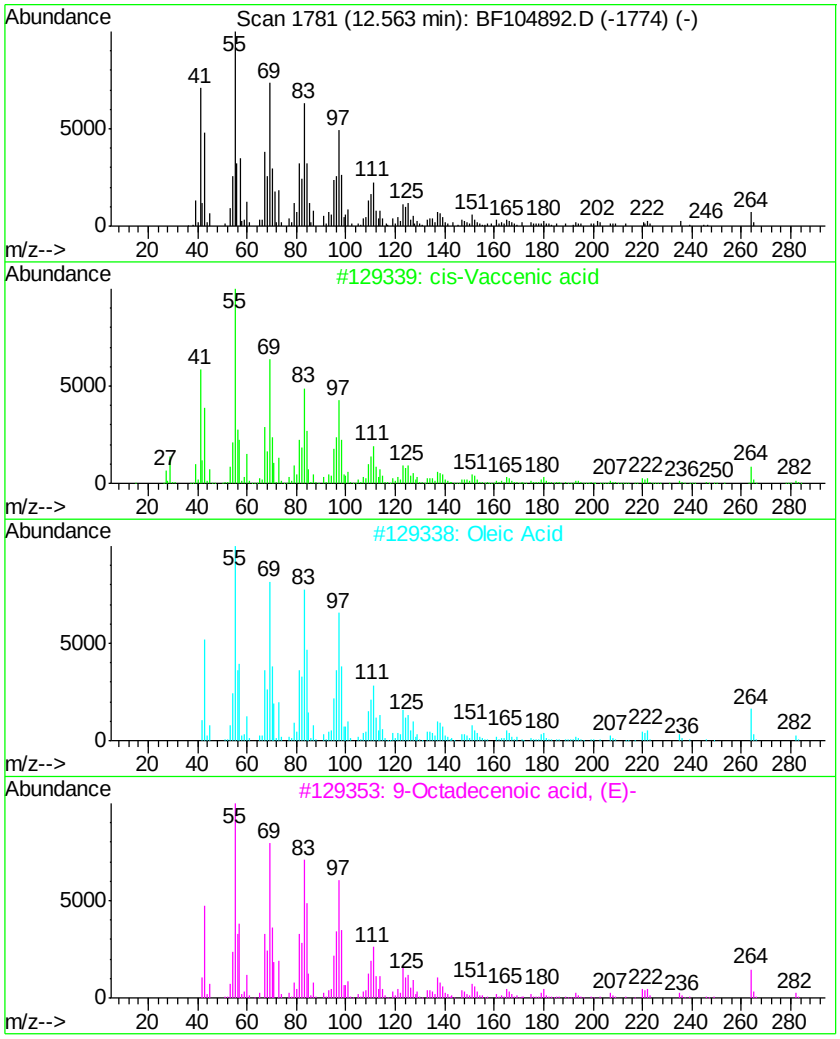
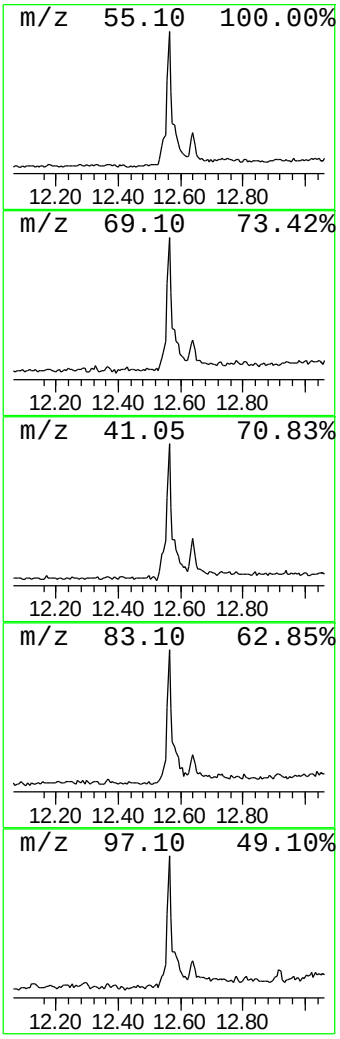
Peak Number 8 cis-Vaccenic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	18.90 ng	715139	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-Vaccenic acid	282	C18H34O2	000506-17-2	86
2	Oleic Acid	282	C18H34O2	000112-80-1	81
3	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	81
4	1-Hexadecanol	242	C16H34O	036653-82-4	70
5	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	70





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104892.D
Acq On : 27 Apr 2018 20:12
Operator : JU/SJ
Sample : J2564-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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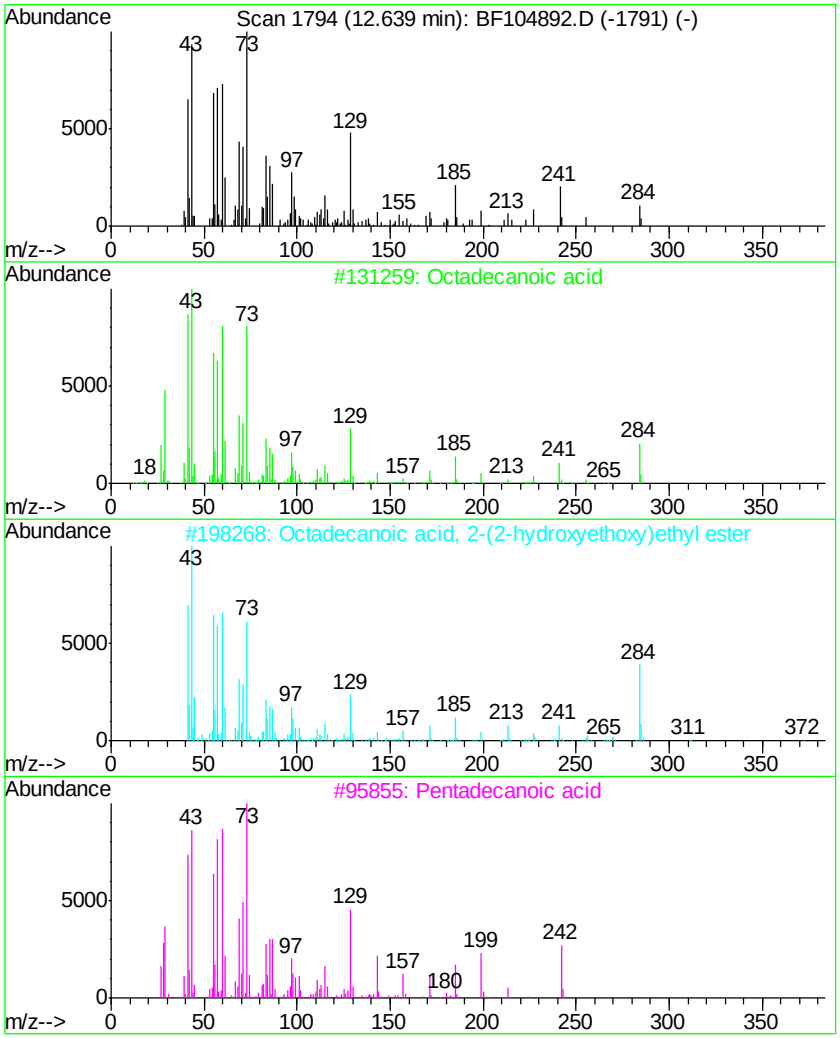
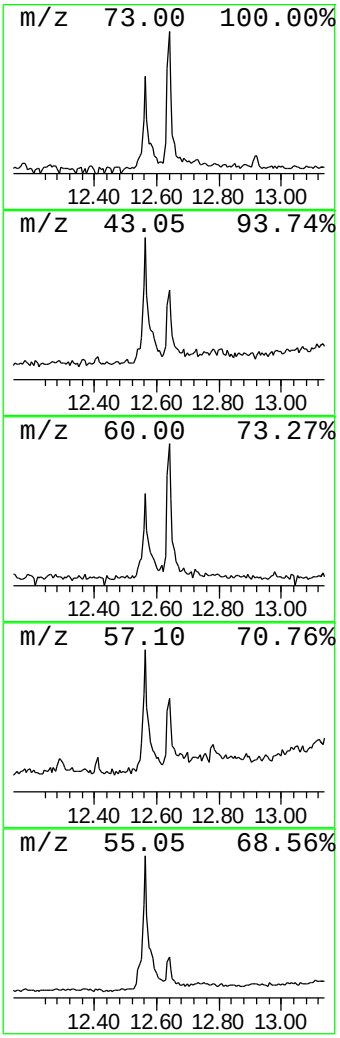
Peak Number 9 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	4.07 ng	153933	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104892.D
Acq On : 27 Apr 2018 20:12
Operator : JU/SJ
Sample : J2564-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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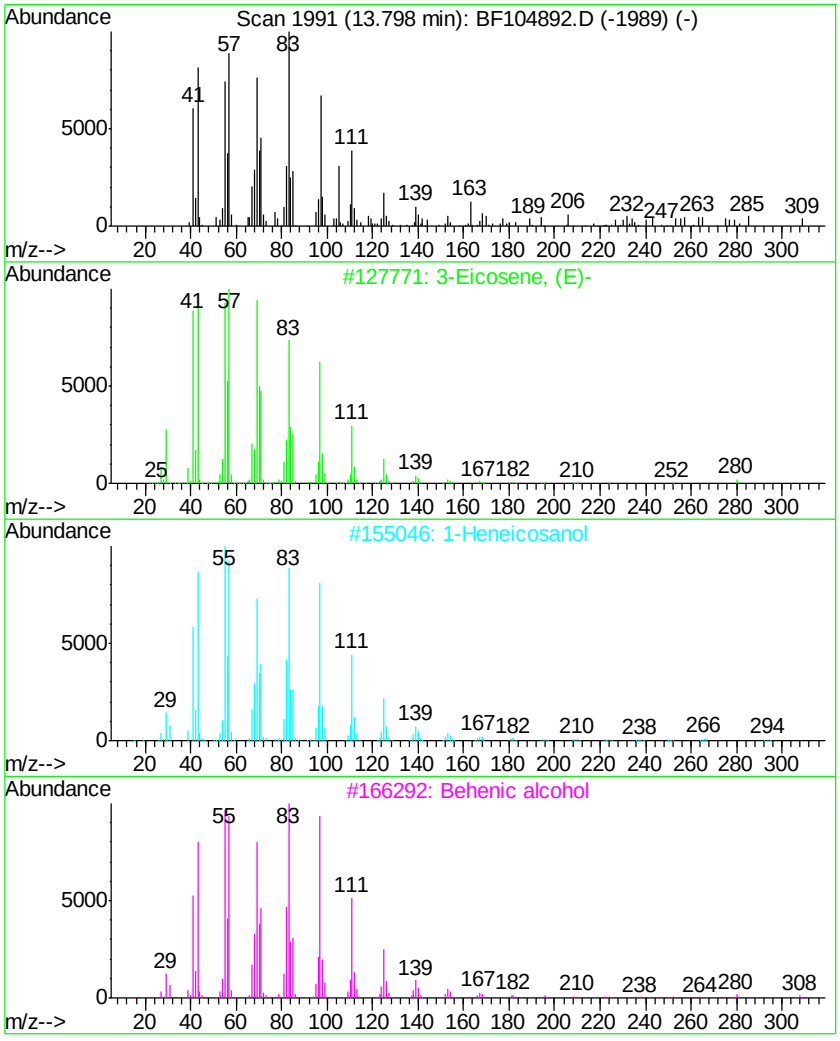
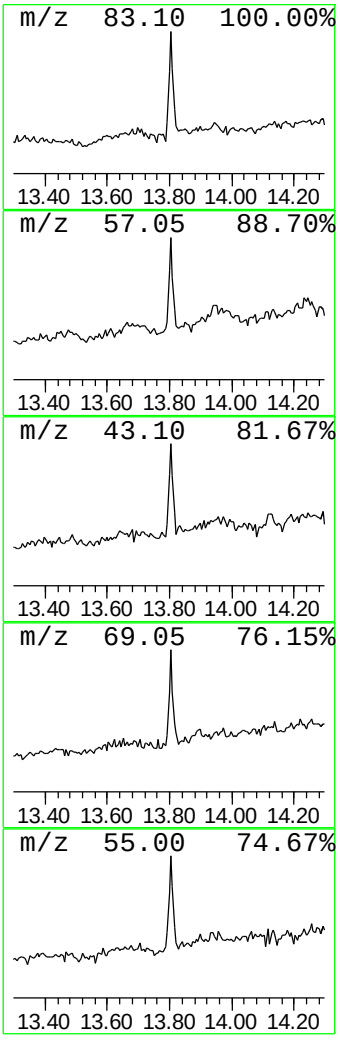
Peak Number 10 3-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	5.30 ng	164937	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	96
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Behenic alcohol	326	C22H46O	000661-19-8	95
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	93





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104892.D
Acq On : 27 Apr 2018 20:12
Operator : JU/SJ
Sample : J2564-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

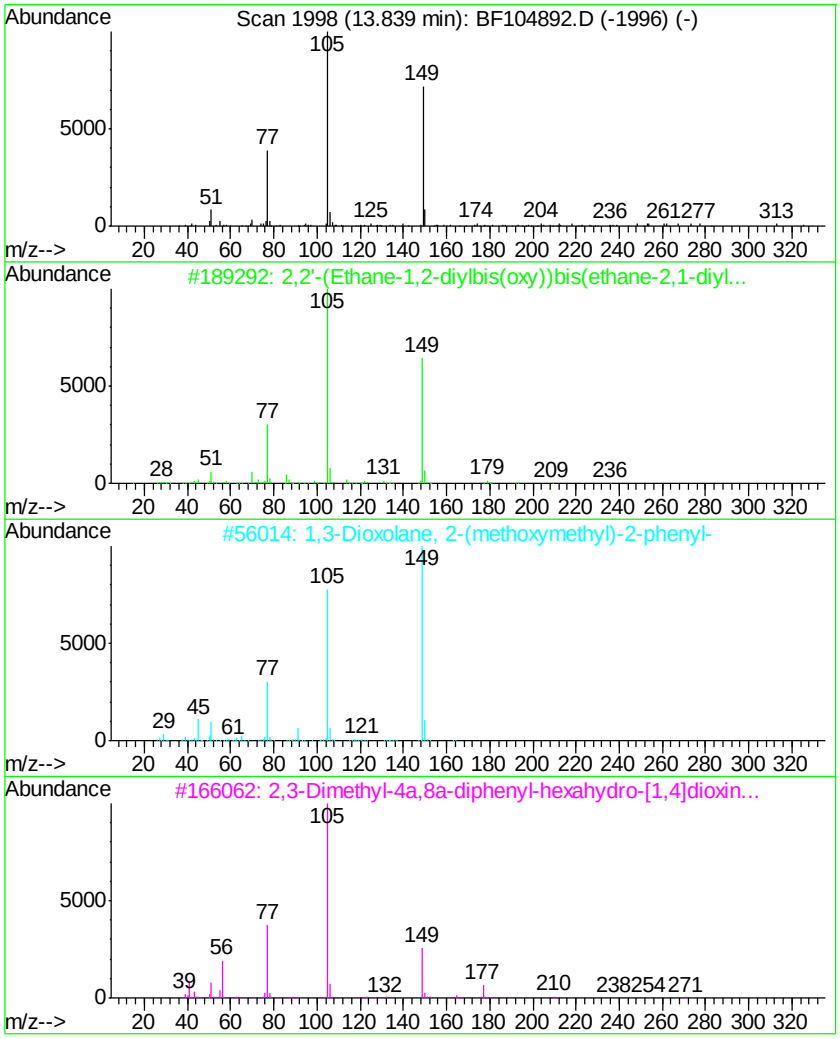
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

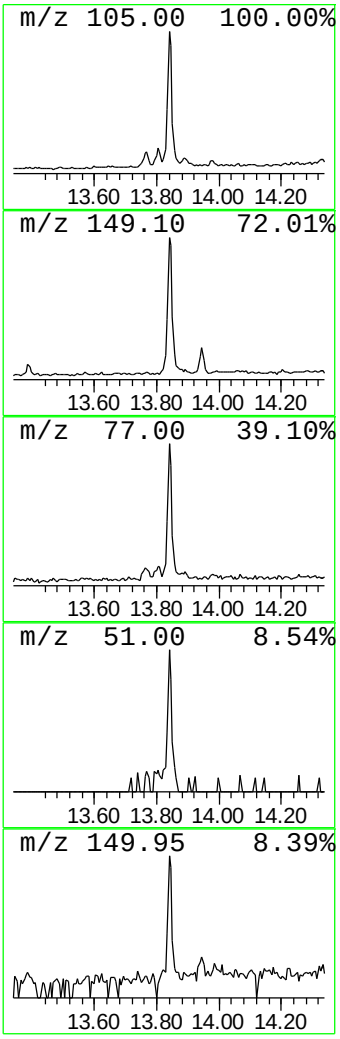
****

Peak Number 11 2,2'-(Ethane-1,2-diylbis(ox... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	3.59 ng	111637	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2'-(Ethane-1,2-divlbis(oxy))bi...	358	C20H22O6	1000366-99-4	72
2	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	47
3	2,3-Dimethyl-4a,8a-diphenyl-hexa...	326	C20H22O4	1000297-07-0	47
4	2-Phenyl-4-(4-phenylbenzylidene)...	325	C22H15NO2	066404-26-0	38
5	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042718\
Data File : BF104892.D
Acq On : 27 Apr 2018 20:12
Operator : JU/SJ
Sample : J2564-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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...	5.02	2.9	ng	83188	1	6.80	565968	20.0
unknown6.57	6.57	72.2	ng	2042470	1	6.80	565968	20.0
1H-Indole, 2,3-di...	9.76	3.4	ng	147270	3	9.84	872136	20.0
Pentadecane	10.73	2.1	ng	78684	4	11.33	756787	20.0
Tetradecanoic acid	10.99	2.1	ng	79350	4	11.33	756787	20.0
n-Hexadecanoic acid	11.86	18.2	ng	687385	4	11.33	756787	20.0
cis-Vaccenic acid	12.56	18.9	ng	715139	4	11.33	756787	20.0
Octadecanoic acid	12.64	4.1	ng	153933	4	11.33	756787	20.0
3-Eicosene, (E)-	13.80	5.3	ng	164937	5	13.98	621913	20.0
2,2'-(Ethane-1,2-...	13.84	3.6	ng	111637	5	13.98	621913	20.0