LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032318\
Data File : BF103882.D
Acq On : 23 Mar 2018 16:06
Operator : JU/SJ
Sample : J1748-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-032218-D

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	2.305	32	37	43	rVB	116824	152833	4.32%	0.381%
2	5.116	508	515	525	rBV	149705	313354	8.86%	0.782%
3	5.222	528	533	542	rVB	163276	190558	5.39%	0.475%
4	5.604	592	598	601	rBV	3239835	3353299	94.77%	8.365%
5	6.604	762	768	777	rBV	2975858	3444704	97.36%	8.593%
6	6.745	787	792	795	rBV	3475565	3437275	97.15%	8.575%
7	6.975	827	831	834	rBV	1100168	886940	25.07%	2.213%
8	7.134	853	858	861	rBV	2922696	2598117	73.43%	6.481%
9	7.539	922	927	930	rBV	2265017	2135676	60.36%	5.328%
10	8.257	1045	1049	1052	rBV	1403604	1144250	32.34%	2.854%
11	8.828	1142	1146	1152	rBV	29404	36686	1.04%	0.092%
12	9.198	1205	1209	1214	rBV	44076	42302	1.20%	0.106%
13	9.328	1227	1231	1235	rBV	3507775	3377975	95.47%	8.427%
14	9.398	1239	1243	1246	rVB	87485	83460	2.36%	0.208%
15	9.439	1246	1250	1254	rBV3	34494	41060	1.16%	0.102%
16	9.663	1285	1288	1292	rVB	387135	339302	9.59%	0.846%
17	9.716	1292	1297	1305	rVB	348122	373935	10.57%	0.933%
18	9.928	1328	1333	1337	rVB	201540	187614	5.30%	0.468%
19	9.980	1337	1342	1344	rBV4	28515	41252	1.17%	0.103%
20	10.016	1344	1348	1361	rVB	1422734	1271562	35.94%	3.172%
21	10.128	1364	1367	1369	rVB	76883	56707	1.60%	0.141%
22	10.163	1369	1373	1376	rBV2	56391	63124	1.78%	0.157%
23	10.251	1385	1388	1392	rBV2	47552	49334	1.39%	0.123%
24	10.428	1415	1418	1421	rVB	195790	157469	4.45%	0.393%
25	10.528	1432	1435	1439	rVB4	70462	59486	1.68%	0.148%
26	10.651	1451	1456	1458	rBV	69202	87885	2.48%	0.219%
27	10.780	1473	1478	1479	rBV2	57371	71662	2.03%	0.179%
28	10.810	1479	1483	1486	rVV	2037732	1899292	53.68%	4.738%
29	10.833	1486	1487	1491	rVB3	49197	38652	1.09%	0.096%
30	10.904	1496	1499	1508	rVB	176554	230791	6.52%	0.576%
31	11.351	1572	1575	1578	rBV	81726	68509	1.94%	0.171%
32	11.510	1598	1602	1605	rBV	1206337	1009080	28.52%	2.517%
33	11.533	1605	1606	1610	rVB	83127	45867	1.30%	0.114%
34	11.880	1662	1665	1669	rBV	1407597	1233568	34.86%	3.077%

LSC Area Percent Report

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Operator : JU/SJ
Sample : J1748-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-032218-D

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	12.016	1685	1688	1691	rBV2	160623	166424	4.70%	0.415%
36	12.192	1715	1718	1720	rBV2	36209	43003	1.22%	0.107%
37	12.574	1779	1783	1785	rBV	3517604	3538241	100.00%	8.827%
38	12.598	1785	1787	1793	rVB2	2832969	2491137	70.41%	6.214%
39	12.680	1797	1801	1804	rVB	630293	530604	15.00%	1.324%
40	12.727	1806	1809	1812	rBV	165213	148363	4.19%	0.370%
41	12.957	1843	1848	1855	rBV	171844	215678	6.10%	0.538%
42	13.098	1867	1872	1875	rBV	2617784	2364299	66.82%	5.898%
43	13.280	1901	1903	1906	rVB2	54003	44972	1.27%	0.112%
44	13.516	1941	1943	1945	rBV2	49298	46003	1.30%	0.115%
45	13.974	2018	2021	2025	rBV	438763	387656	10.96%	0.967%
46	14.074	2036	2038	2041	rBV2	68430	64999	1.84%	0.162%
47	14.163	2049	2053	2056	rBV	901954	873126	24.68%	2.178%
48	15.710	2312	2316	2321	rVB	516045	648296	18.32%	1.617%

Sum of corrected areas: 40086381

LSC Report - Integrated Chromatogram

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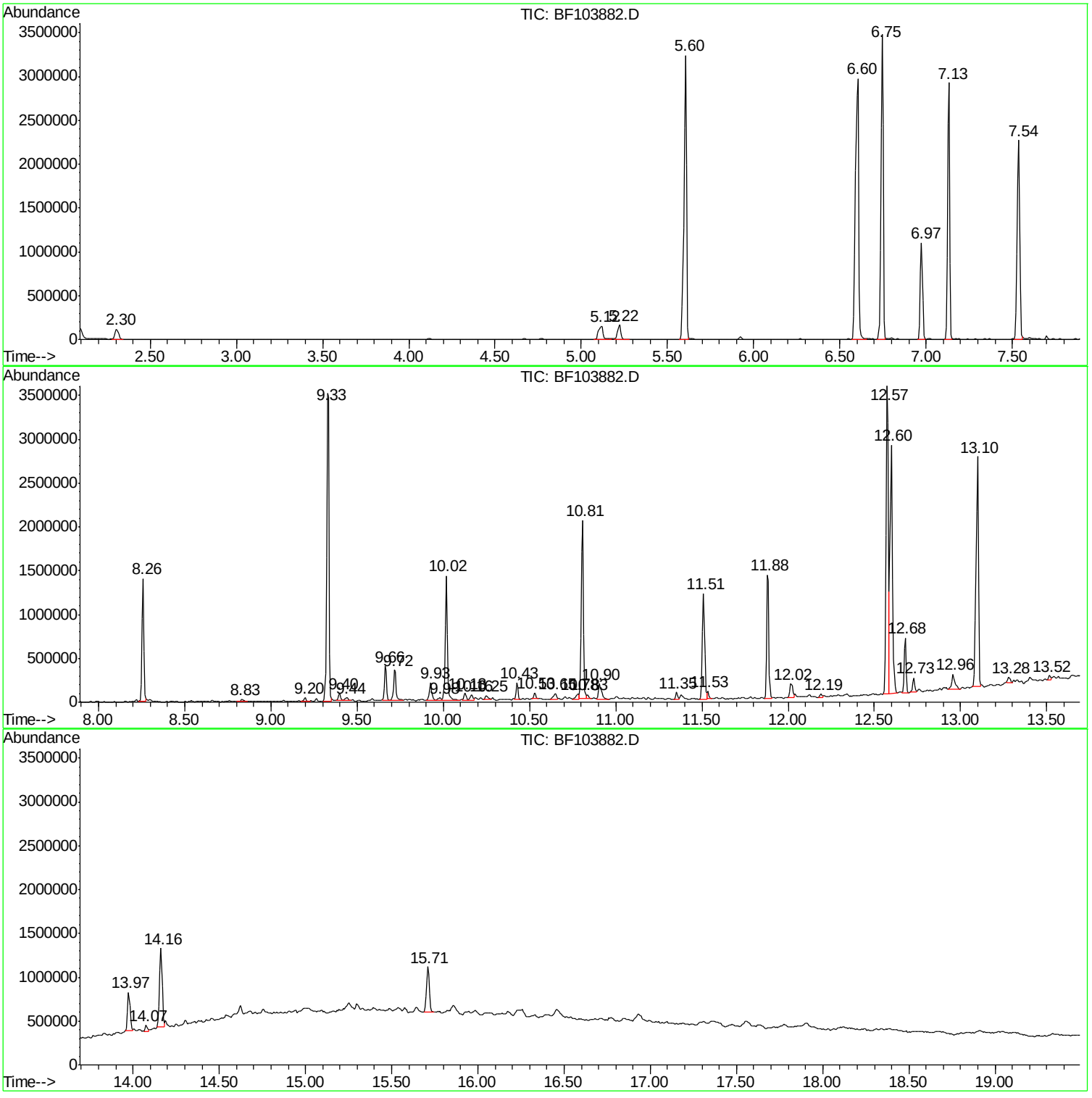
Sample : J1748-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-05-032218-D

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032318\
Data File : BF103882.D
Acq On : 23 Mar 2018 16:06
Operator : JU/SJ
Sample : J1748-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-032218-D

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

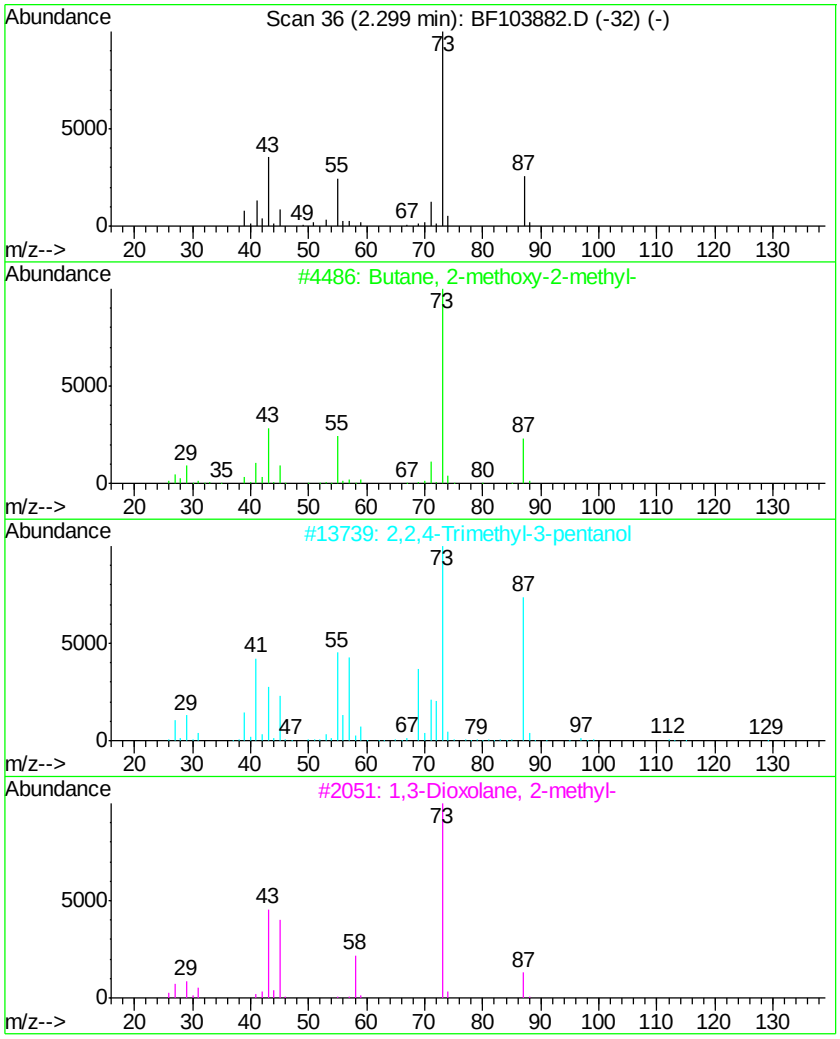
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

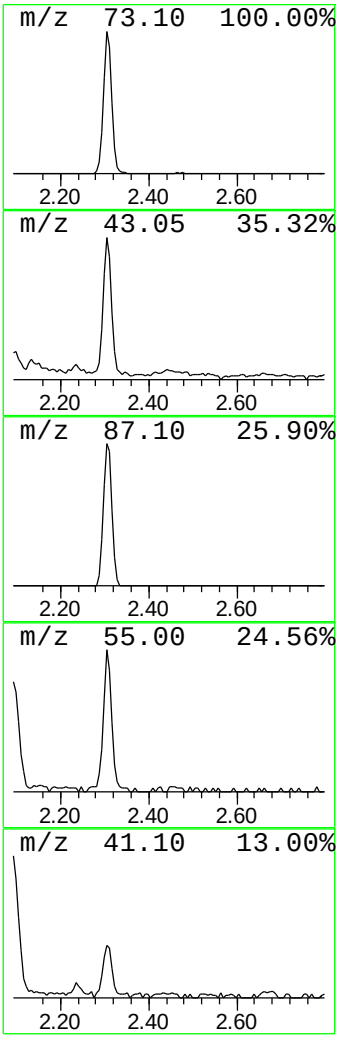
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.30	3.45 ng	152833	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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





Data Path : Z:\HPCHEM1\BNA F\DATA\BF032318\
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Acq On : 23 Mar 2018 16:06
Operator : JU/SJ
Sample : J1748-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-032218-D

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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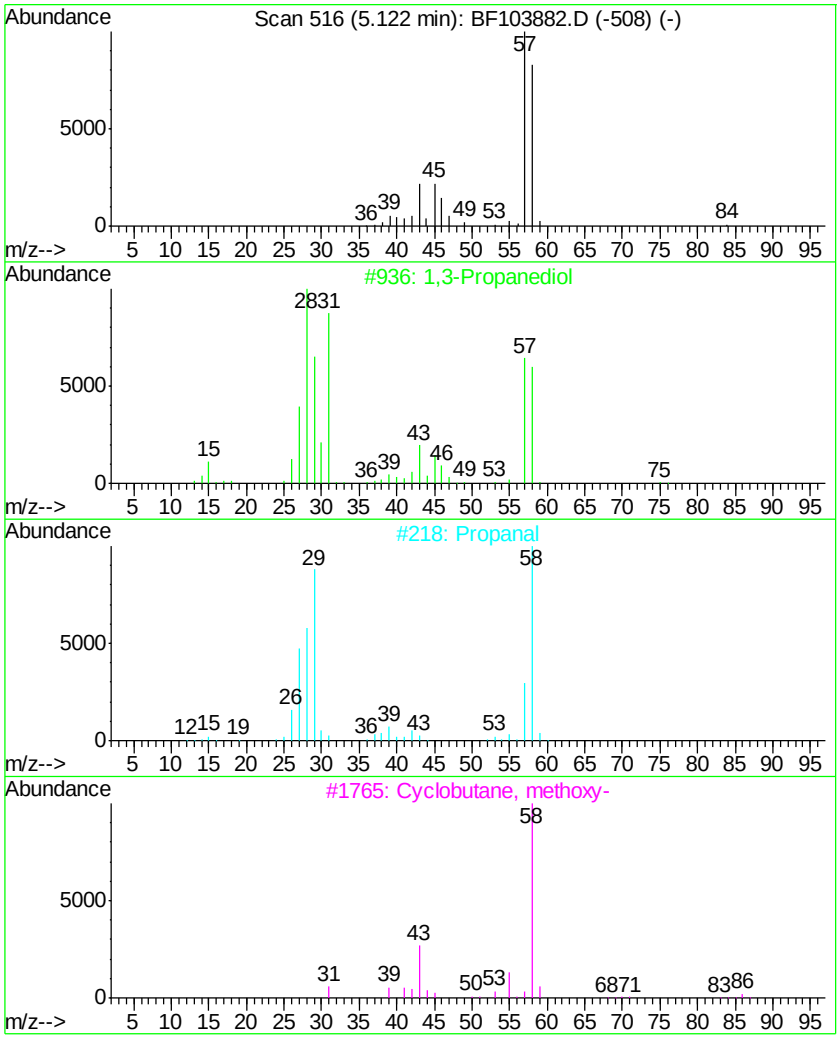
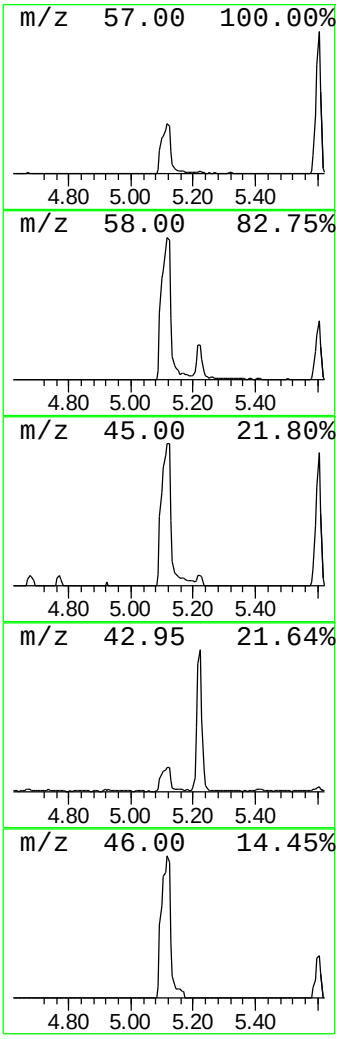
Peak Number 2 1,3-Propanediol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	7.07 ng	313354	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Propanediol	76	C3H8O2	000504-63-2	74
2	Propanal	58	C3H6O	000123-38-6	9
3	Cyclobutane, methoxy-	86	C5H10O	018593-33-4	9
4	1,2-Diaminoethane, N-trifluoroac...	184	C6H11F3N2O	095778-71-5	9
5	Cyclohexanol, 2-[(dimethylamino)...	263	C16H25NO2	002914-77-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032318\
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Acq On : 23 Mar 2018 16:06
Operator : JU/SJ
Sample : J1748-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-032218-D

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

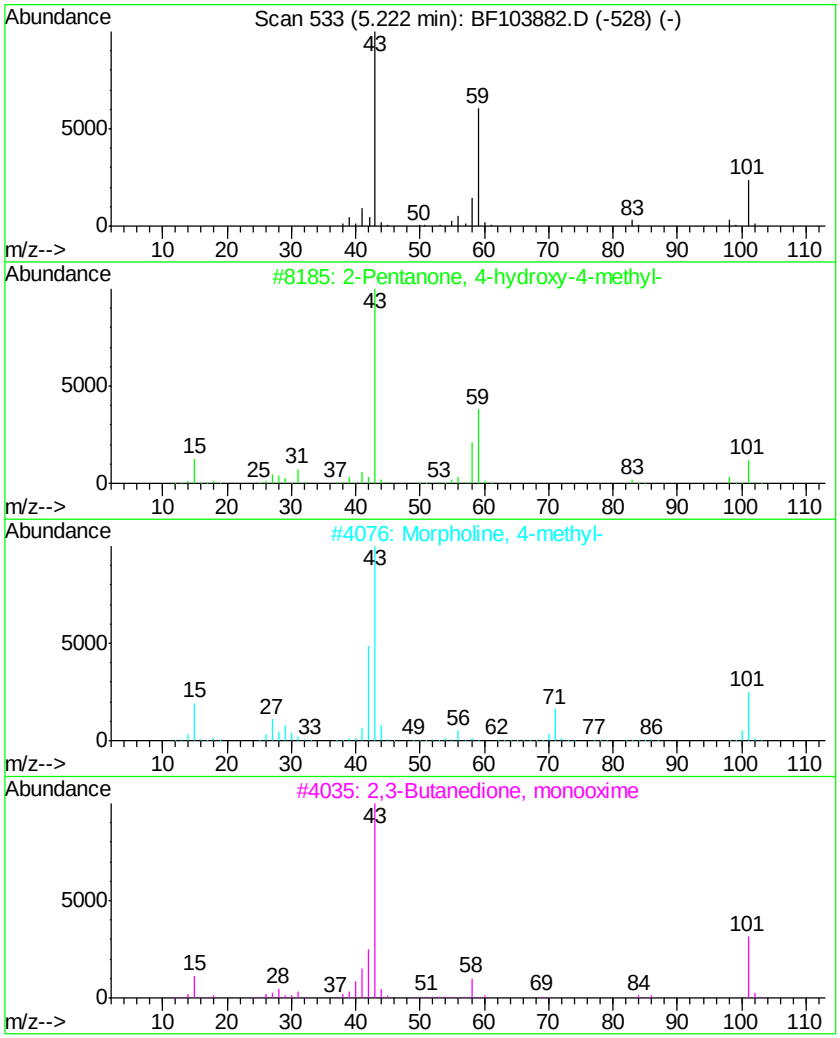
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

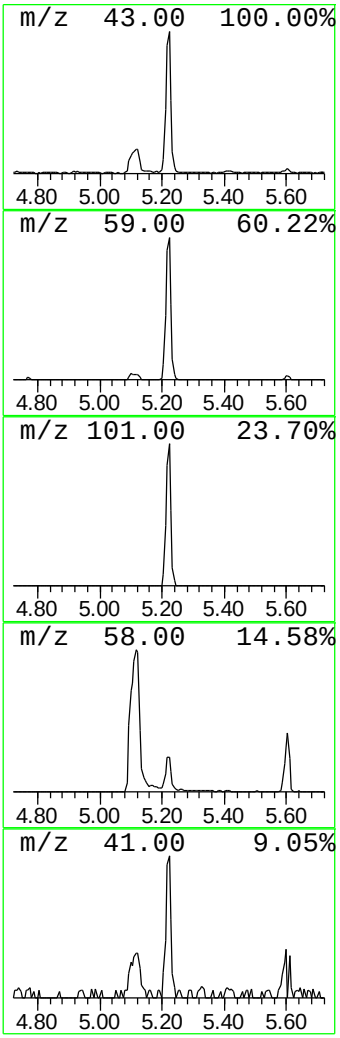
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	4.30 ng	190558	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	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Sample : J1748-13
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ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-032218-D

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

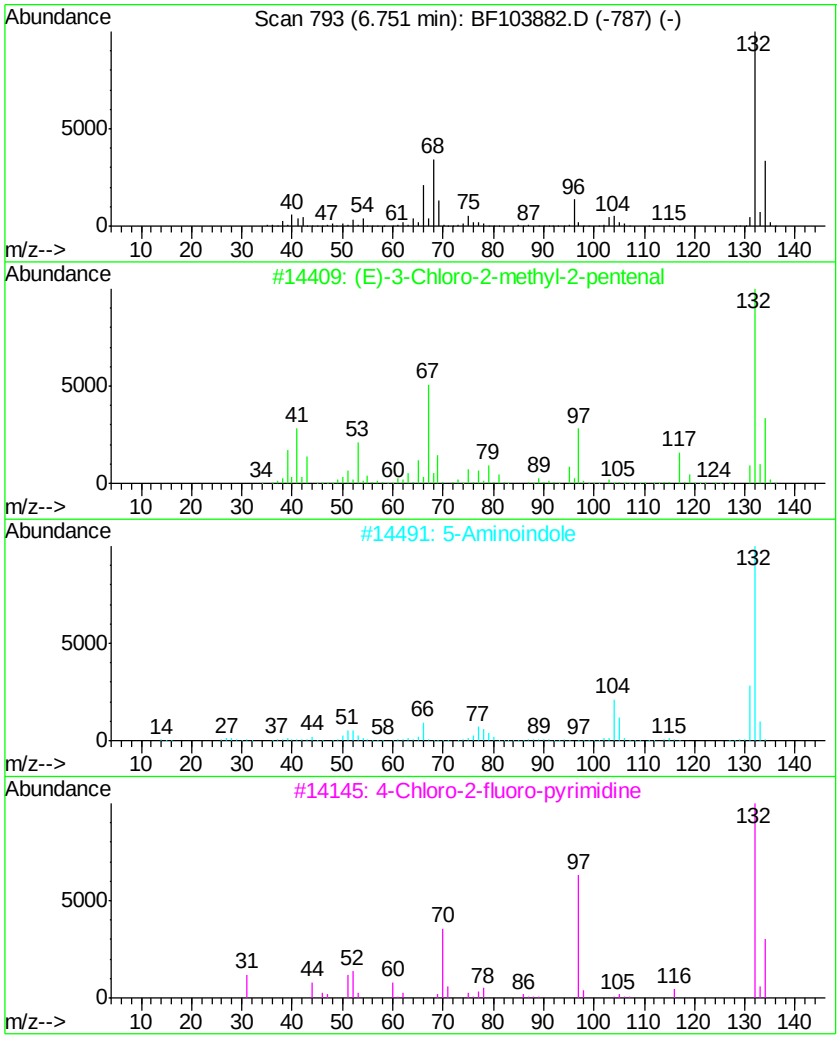
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

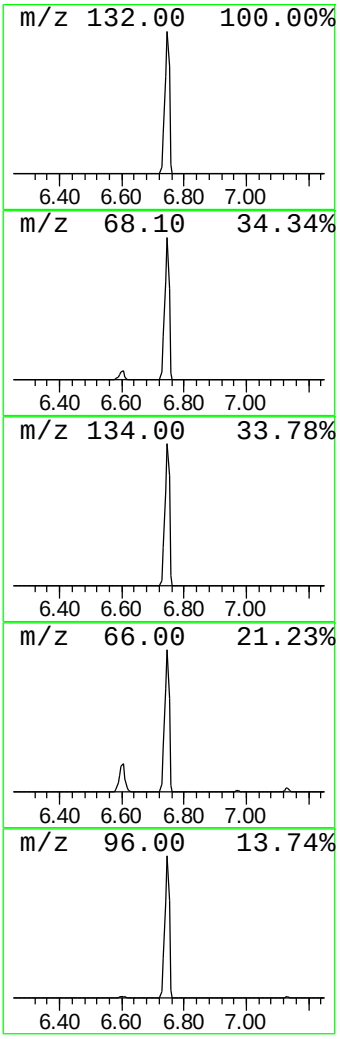
****

Peak Number 4 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	77.51 ng	3437280	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	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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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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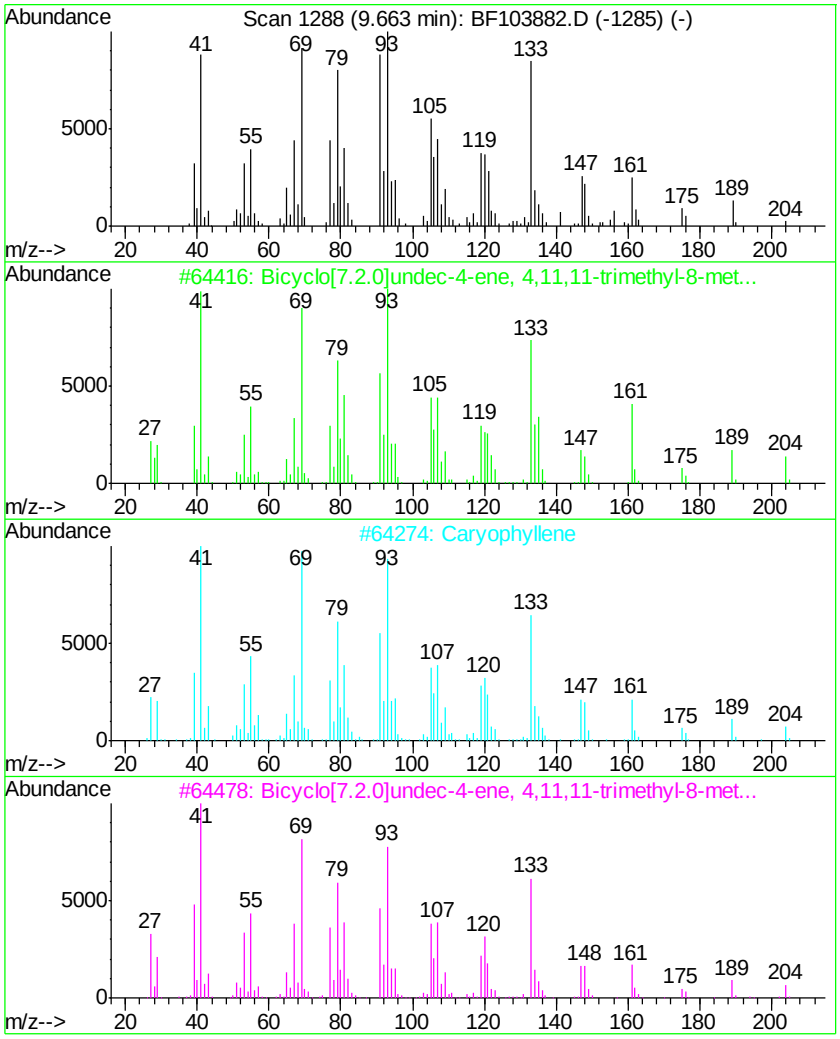
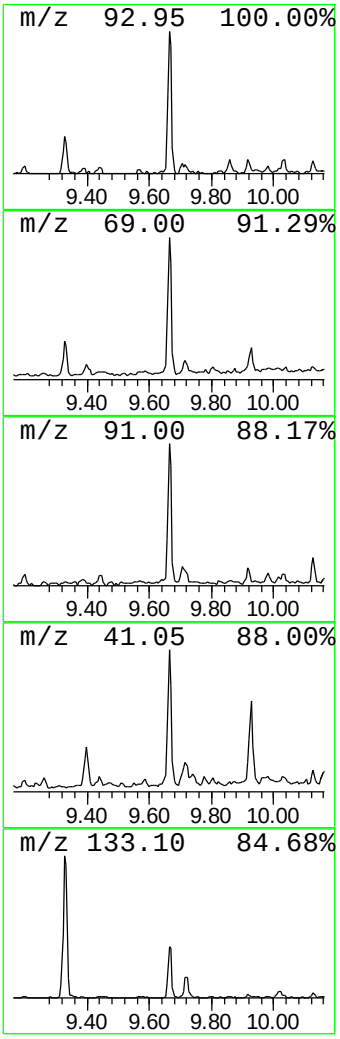
****

Peak Number 6 Bicyclo[7.2.0]undec-4-ene, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.66	5.34 ng	339302	Acenaphthene-d10	10.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	93
2	Caryophyllene	204	C15H24	000087-44-5	91
3	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	91
4	Cyclohexane, 1,5-diethenyl-3-met...	162	C12H18	074742-35-1	58
5	Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-03-6	38





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ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-032218-D

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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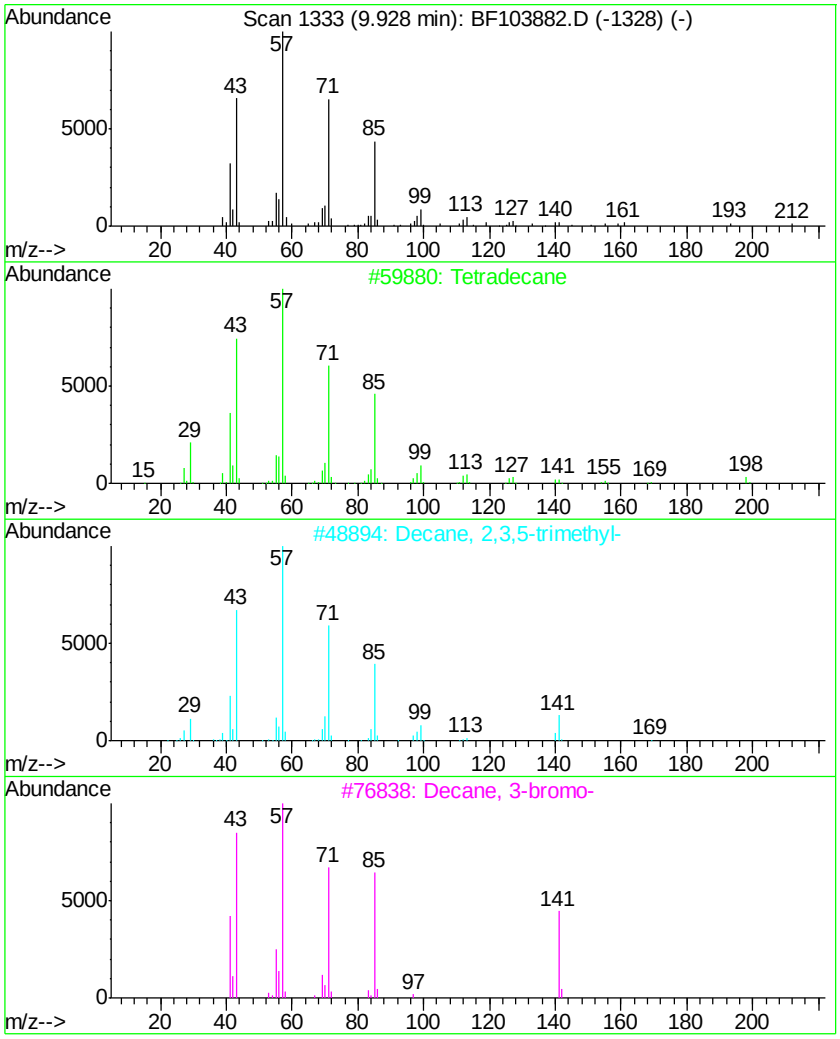
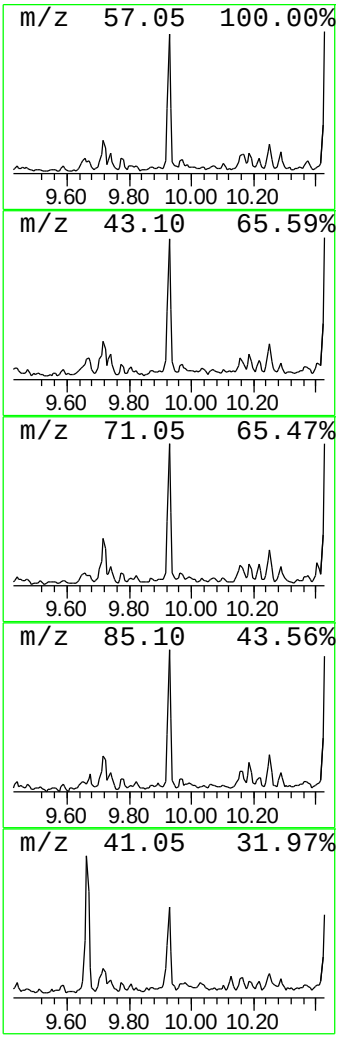
****

Peak Number 7 Tetradecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.93	2.95 ng	187614	Acenaphthene-d10	10.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	91
2	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83
3	Decane, 3-bromo-	220	C10H21Br	030571-71-2	72
4	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	72
5	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	72





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

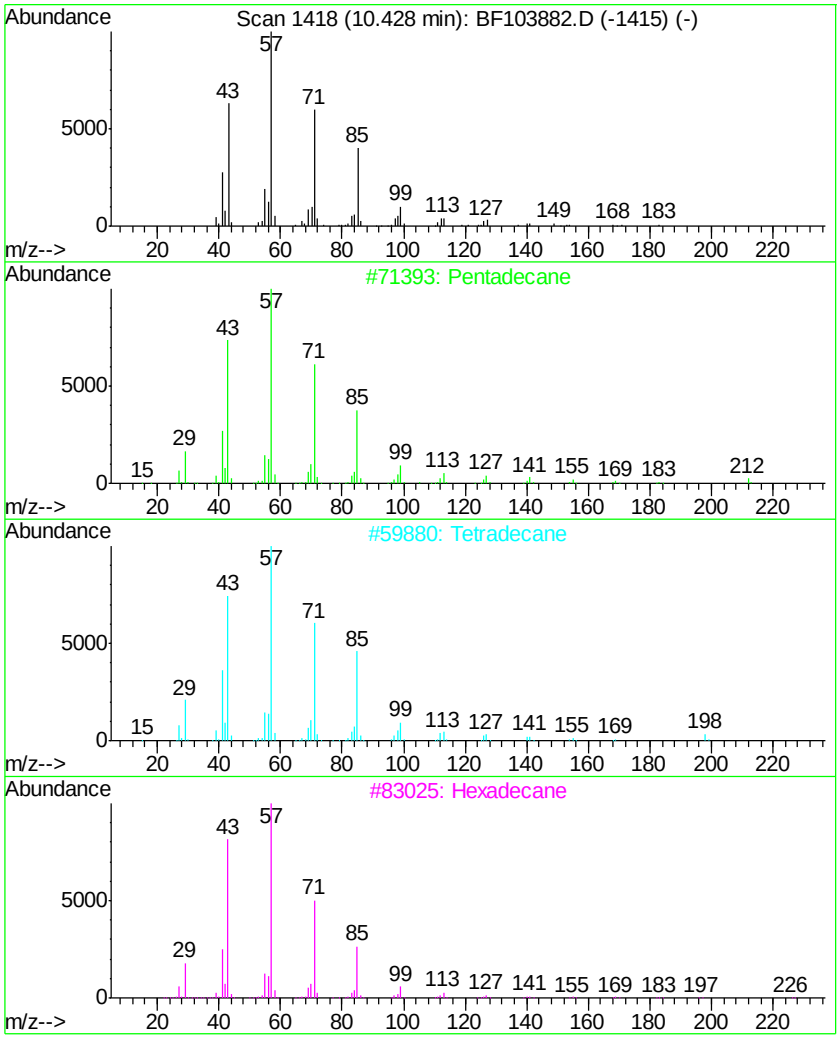
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

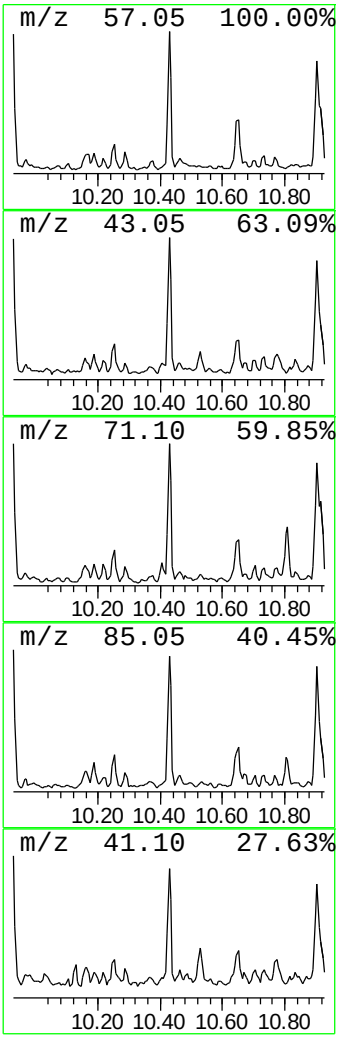
****

Peak Number 8 Pentadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.43	2.48 ng	157469	Acenaphthene-d10	10.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	86
2	Tetradecane	198	C14H30	000629-59-4	86
3	Hexadecane	226	C16H34	000544-76-3	83
4	Heptadecane	240	C17H36	000629-78-7	83
5	Heneicosane	296	C21H44	000629-94-7	83





Library Search Compound Report

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Acq On : 23 Mar 2018 16:06
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Sample : J1748-13
Misc :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

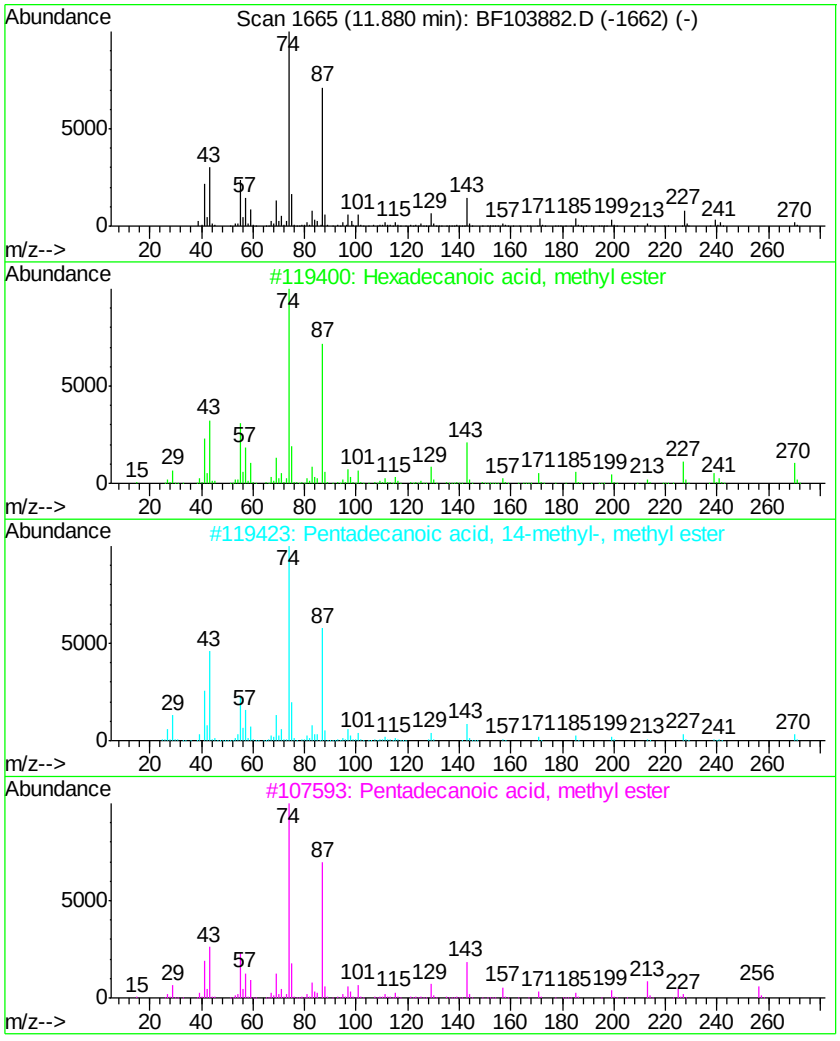
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

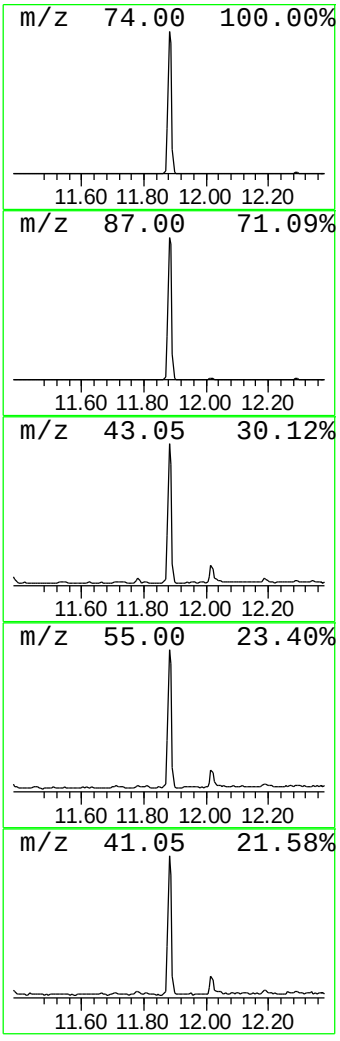
****

Peak Number 10 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	24.45 ng	1233570	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	97
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4	Hexadecanoic acid, 2-methyl-	270	C17H34O2	027147-71-3	90
5	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF032318\
Data File : BF103882.D
Acq On : 23 Mar 2018 16:06
Operator : JU/SJ
Sample : J1748-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-032218-D

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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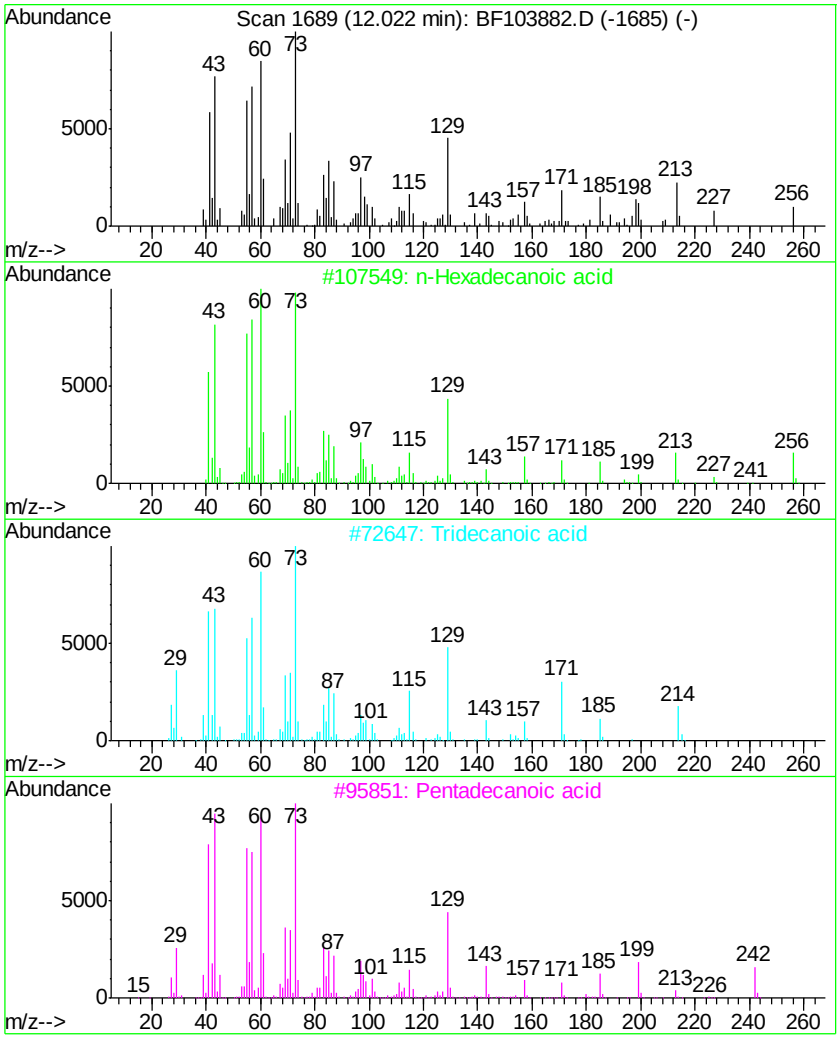
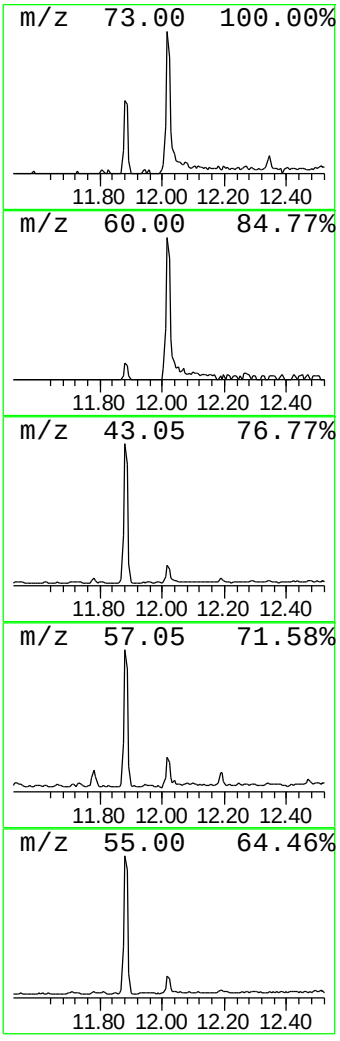
Peak Number 11 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	3.30 ng	166424	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-032218-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
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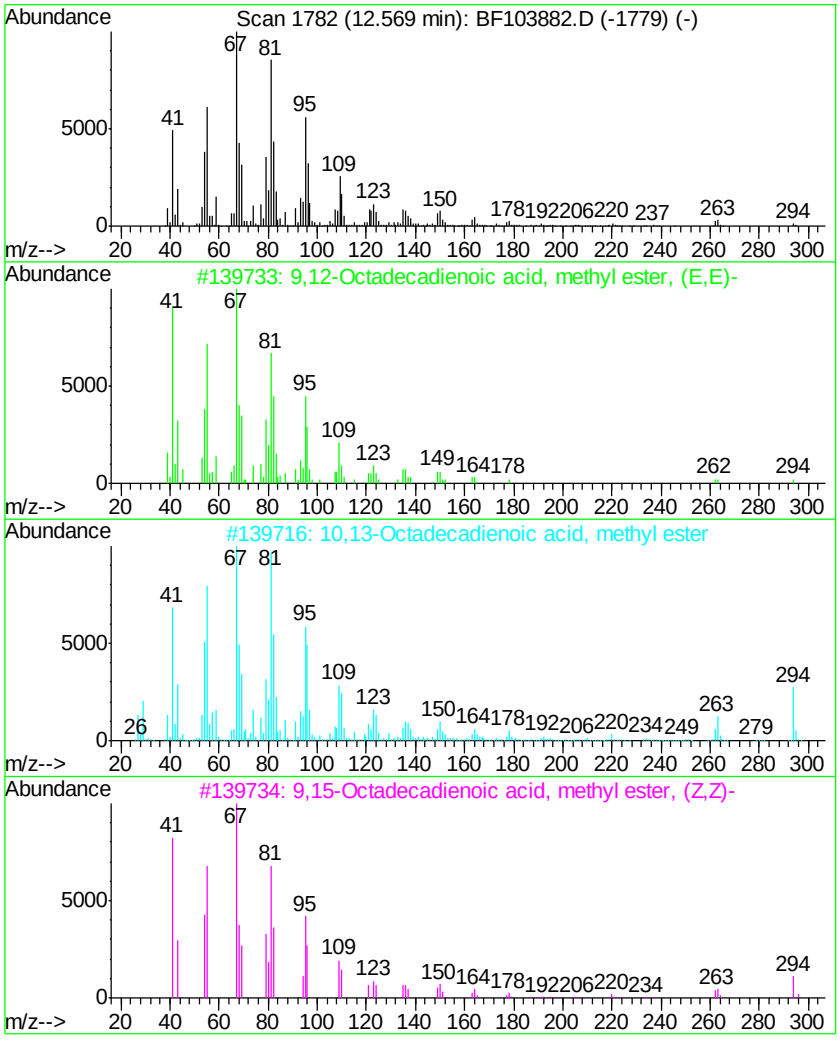
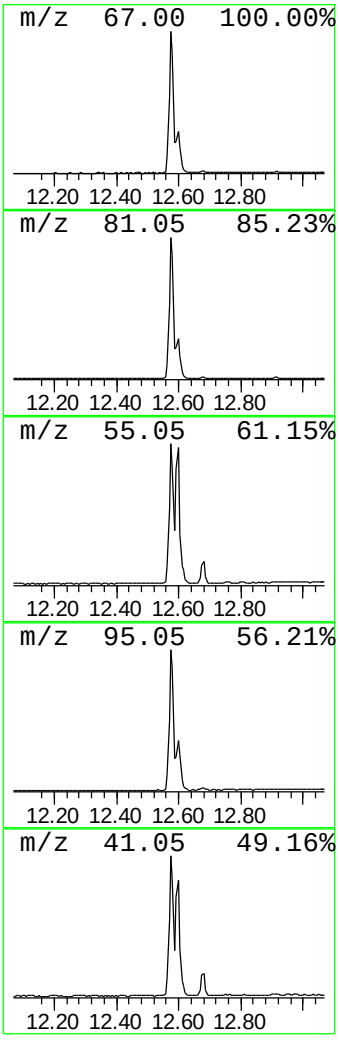
Peak Number 12 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	70.13 ng	3538240	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
4	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99
5	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99





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Operator : JU/SJ
Sample : J1748-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-032218-D

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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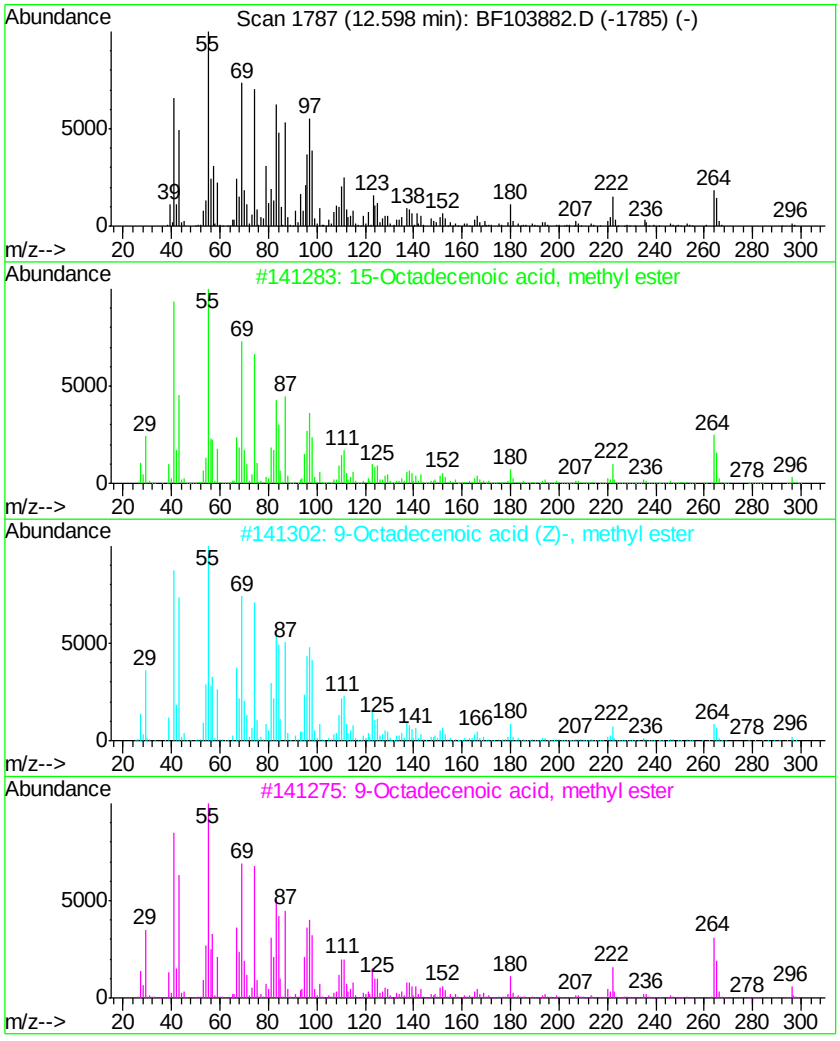
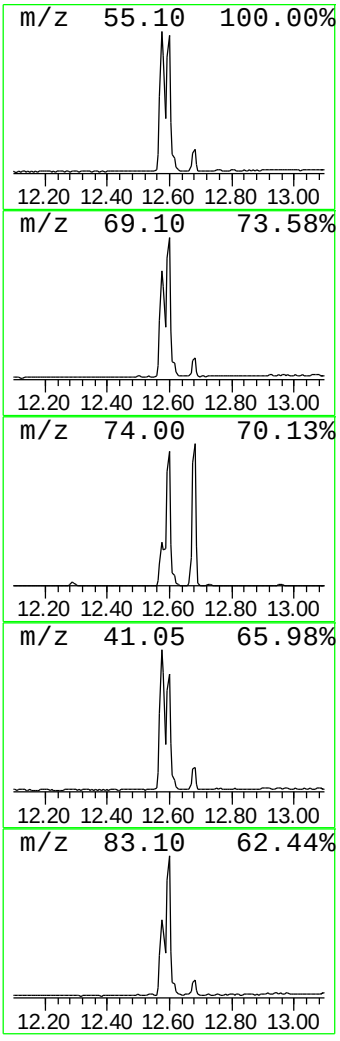
Peak Number 13 15-Octadecenoic acid, methy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.60	49.37 ng	2491140	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	98
3	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	95
4	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	89
5	8-Octadecenoic acid, methyl este...	296	C19H36O2	026528-50-7	89





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Sample : J1748-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-032218-D

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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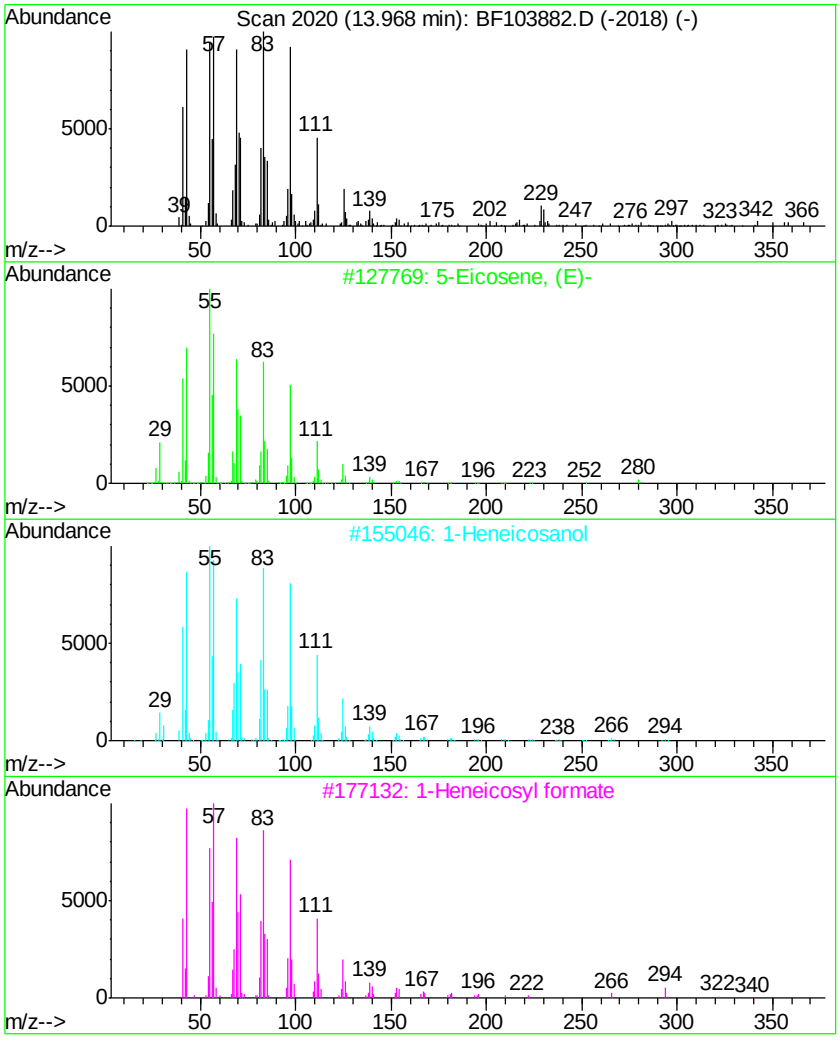
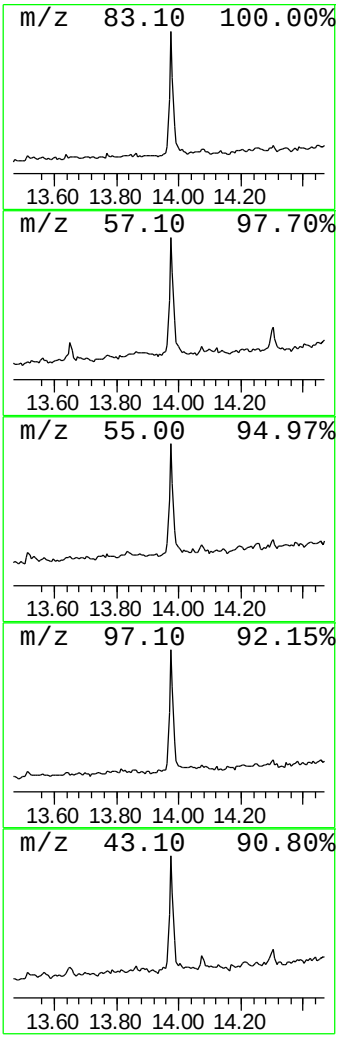
Peak Number 14 5-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	8.88 ng	387656	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	1-Heneicosanol	312	C21H44O	015594-90-8	94
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
5	Behenic alcohol	326	C22H46O	000661-19-8	94





Tentatively Identified Compound (LSC) summary

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Data File : BF103882.D
Acq On : 23 Mar 2018 16:06
Operator : JU/SJ
Sample : J1748-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-032218-D

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	3.5	ng	152833	1	6.97	886940	20.0
1,3-Propanediol	5.12	7.1	ng	313354	1	6.97	886940	20.0
2-Pentanone, 4-hy...	5.22	4.3	ng	190558	1	6.97	886940	20.0
unknown6.75	6.75	77.5	ng	3437280	1	6.97	886940	20.0
Bicyclo[7.2.0]und...	9.66	5.3	ng	339302	3	10.02	1271560	20.0
Tetradecane	9.93	3.0	ng	187614	3	10.02	1271560	20.0
Pentadecane	10.43	2.5	ng	157469	3	10.02	1271560	20.0
Hexadecanoic acid...	11.88	24.4	ng	1233570	4	11.51	1009080	20.0
n-Hexadecanoic acid	12.02	3.3	ng	166424	4	11.51	1009080	20.0
9,12-Octadecadien...	12.57	70.1	ng	3538240	4	11.51	1009080	20.0
15-Octadecenoic a...	12.60	49.4	ng	2491140	4	11.51	1009080	20.0
5-Eicosene, (E)-	13.97	8.9	ng	387656	5	14.16	873126	20.0