LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF030618\
Data File : BF103468.D
Acq On : 6 Mar 2018 21:02
Operator : SJ/JU
Sample : J1722-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-7

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-BF022218.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	2.128	3	7	15	rBV	175771	231443	6.56%	0.752%
2	5.110	511	514	523	rBV	50581	82507	2.34%	0.268%
3	5.498	576	580	603	rBV	2432752	3285187	93.15%	10.672%
4	6.510	748	752	771	rBV	2425906	3526755	100.00%	11.456%
5	6.645	771	775	798	rVB	2873535	3283909	93.11%	10.667%
6	6.869	810	813	830	rVB	745295	820539	23.27%	2.665%
7	7.028	836	840	856	rBV	2086282	2370907	67.23%	7.702%
8	7.439	906	910	931	rBV	1576793	2169311	61.51%	7.047%
9	8.157	1028	1032	1051	rBV	764803	1113064	31.56%	3.616%
10	9.227	1210	1214	1223	rBV	2778769	2821864	80.01%	9.167%
11	9.292	1223	1225	1229	rVB	60373	59183	1.68%	0.192%
12	9.622	1275	1281	1287	rBV	197757	243366	6.90%	0.791%
13	9.774	1303	1307	1312	rBV	48418	64823	1.84%	0.211%
14	9.822	1312	1315	1319	rVB	126896	106273	3.01%	0.345%
15	9.910	1327	1330	1335	rBV2	990392	975244	27.65%	3.168%
16	10.116	1362	1365	1368	rBV2	24223	38016	1.08%	0.123%
17	10.145	1368	1370	1374	rVB3	33954	39686	1.13%	0.129%
18	10.322	1397	1400	1404	rVB	163233	125781	3.57%	0.409%
19	10.469	1421	1425	1430	rVB2	26951	37253	1.06%	0.121%
20	10.545	1433	1438	1440	rBV	50492	58870	1.67%	0.191%
21	10.710	1462	1466	1478	rBV	1139248	1393500	39.51%	4.527%
22	10.798	1478	1481	1492	rVB	124650	164681	4.67%	0.535%
23	10.951	1503	1507	1511	rBV	34186	37485	1.06%	0.122%
24	11.245	1555	1557	1560	rBV2	63679	50355	1.43%	0.164%
25	11.404	1581	1584	1587	rBV	784171	825695	23.41%	2.682%
26	11.427	1587	1588	1593	rVV	333702	318453	9.03%	1.034%
27	11.486	1595	1598	1602	rVB	77151	79210	2.25%	0.257%
28	11.916	1667	1671	1673	rBV2	163784	172268	4.88%	0.560%
29	11.939	1673	1675	1679	rVB2	74844	86940	2.47%	0.282%
30	12.021	1686	1689	1692	rBV2	77659	95969	2.72%	0.312%
31	12.204	1717	1720	1723	rBV	41466	46438	1.32%	0.151%
32	12.245	1724	1727	1731	rVB2	33111	44485	1.26%	0.145%
33	12.457	1760	1763	1767	rBV2	42640	63172	1.79%	0.205%
34	12.557	1778	1780	1788	rVB2	42185	70124	1.99%	0.228%

LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF030618\
Data File : BF103468.D
Acq On : 6 Mar 2018 21:02
Operator : SJ/JU
Sample : J1722-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-7

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-BF022218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.627	1788	1792	1800	rBV	629061	663889	18.82%	2.157%
36	12.704	1802	1805	1814	rVV3	124390	182521	5.18%	0.593%
37	12.857	1825	1831	1837	rBV	574964	705175	20.00%	2.291%
38	12.992	1849	1854	1857	rBV	1867579	1786959	50.67%	5.805%
39	13.168	1881	1884	1885	rBV2	67326	68312	1.94%	0.222%
40	13.251	1895	1898	1900	rBV2	45847	54352	1.54%	0.177%
41	13.386	1918	1921	1923	rBV2	45643	45285	1.28%	0.147%
42	13.415	1924	1926	1930	rBV3	40961	51721	1.47%	0.168%
43	13.704	1973	1975	1978	rBV	57120	49250	1.40%	0.160%
44	13.868	2000	2003	2009	rBV4	133718	198292	5.62%	0.644%
45	13.915	2009	2011	2017	rVB2	62444	75823	2.15%	0.246%
46	14.009	2025	2027	2030	rBV	94930	83651	2.37%	0.272%
47	14.062	2031	2036	2039	rVV2	690950	919278	26.07%	2.986%
48	14.092	2039	2041	2044	rVB	233573	208878	5.92%	0.679%
49	15.133	2215	2218	2221	rBV	162513	234974	6.66%	0.763%
50	15.445	2269	2271	2275	rVB	91071	102159	2.90%	0.332%
51	15.515	2280	2283	2286	rVV	112374	126948	3.60%	0.412%
52	15.574	2290	2293	2297	rBV	259325	324229	9.19%	1.053%

Sum of corrected areas: 30784452

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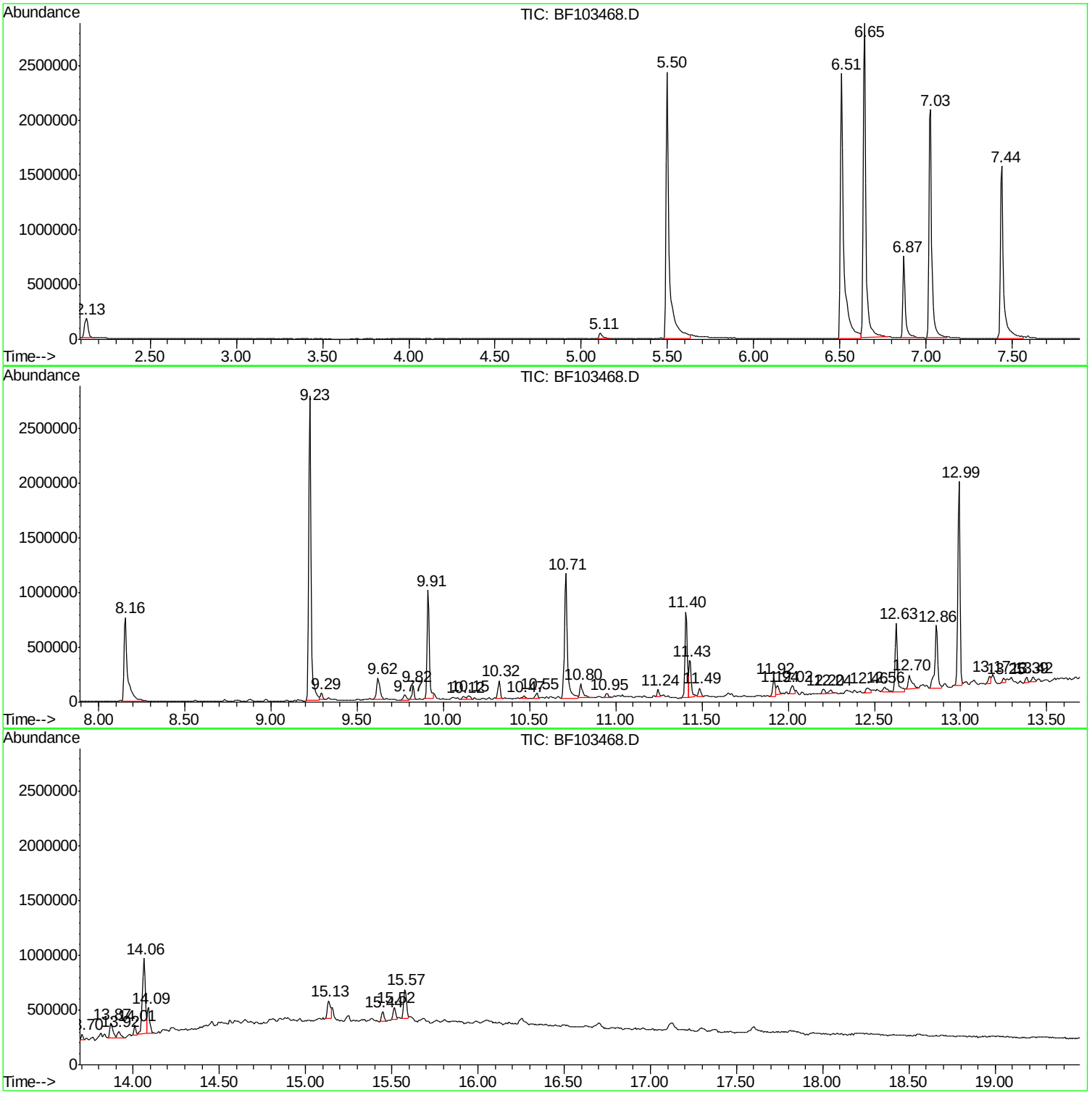
Sample : J1722-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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 : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF030618\
Data File : BF103468.D
Acq On : 6 Mar 2018 21:02
Operator : SJ/JU
Sample : J1722-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

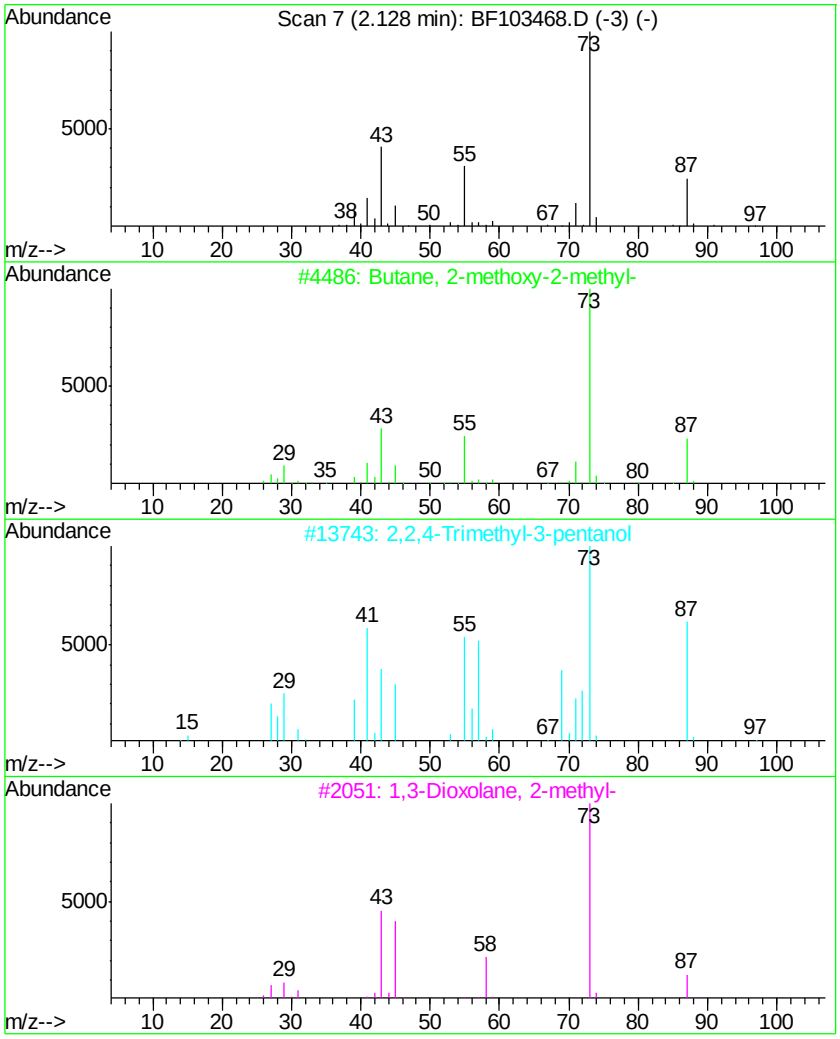
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

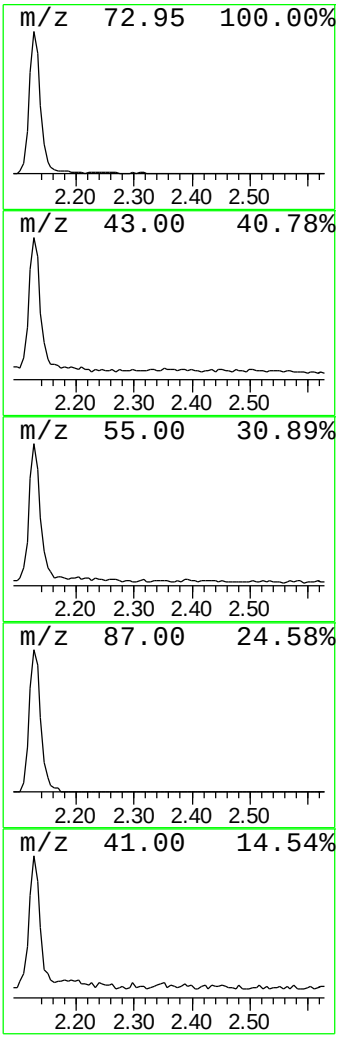
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	5.64 ng	231443	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	38
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	32
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	28





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF030618\
Data File : BF103468.D
Acq On : 6 Mar 2018 21:02
Operator : SJ/JU
Sample : J1722-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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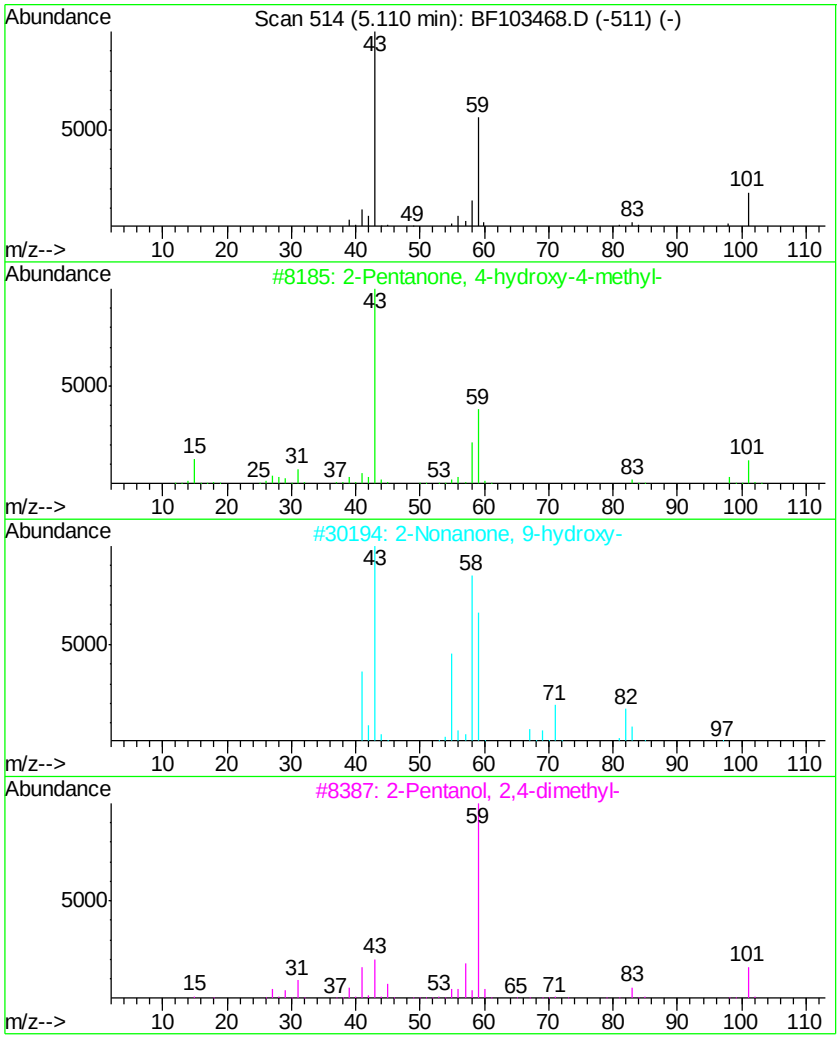
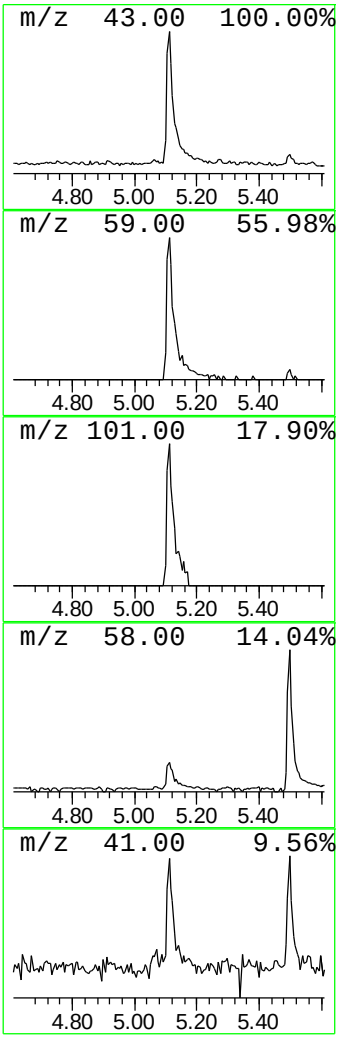
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	2.01 ng	82507	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	36
3	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	28
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF030618\
Data File : BF103468.D
Acq On : 6 Mar 2018 21:02
Operator : SJ/JU
Sample : J1722-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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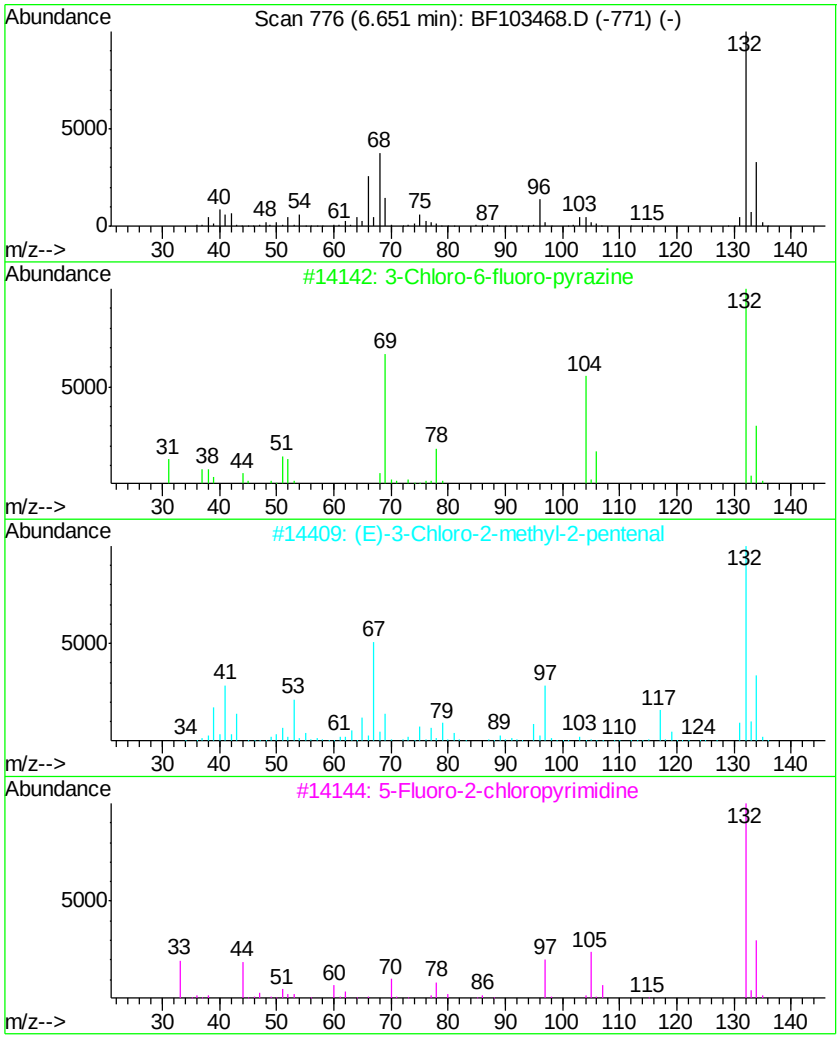
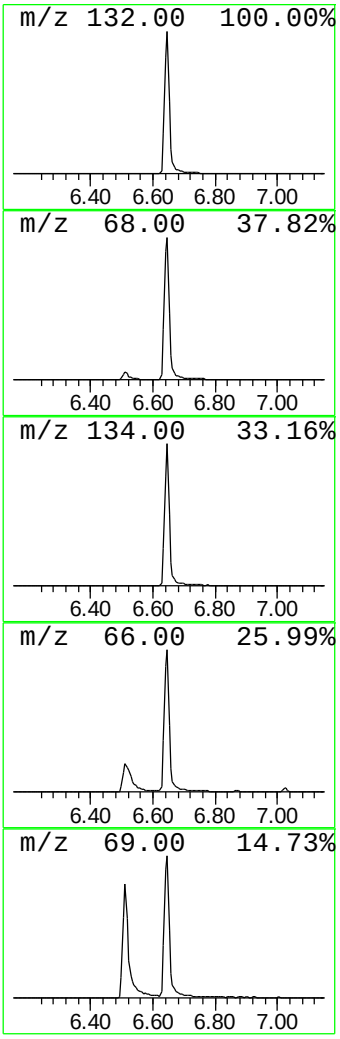
Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	80.04 ng	3283910	1,4-Dichlorobenzene-d4	6.87

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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





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Acq On : 6 Mar 2018 21:02
Operator : SJ/JU
Sample : J1722-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

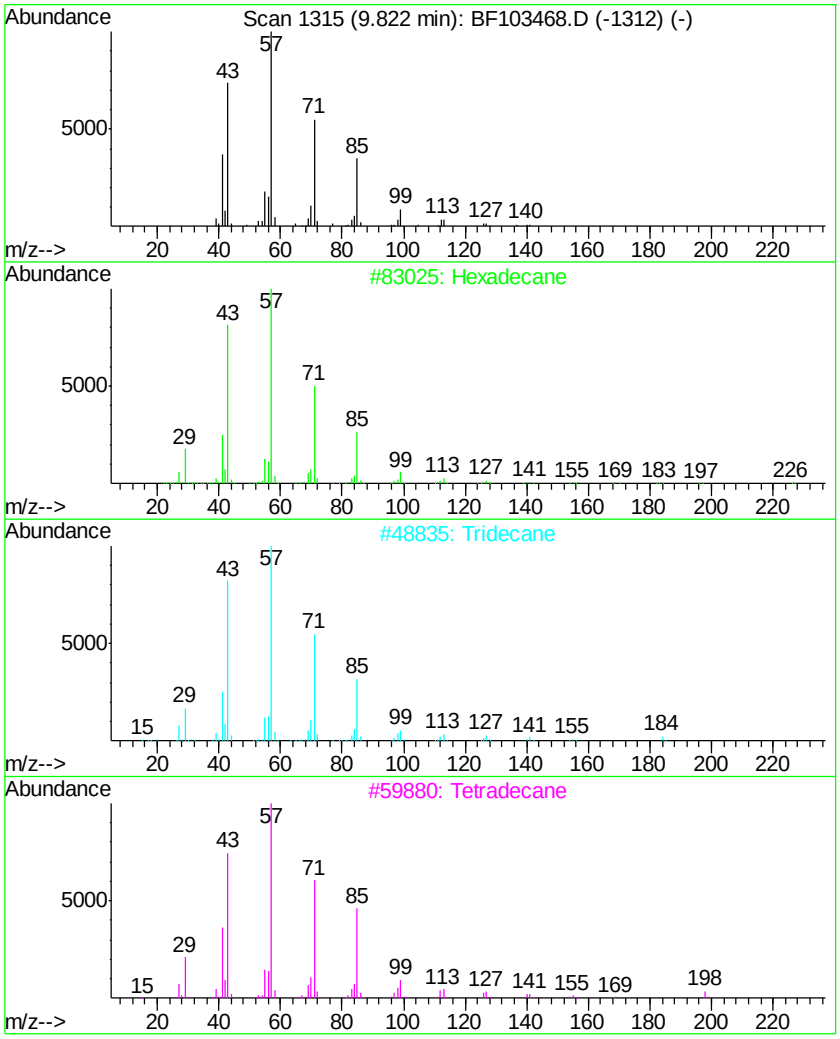
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

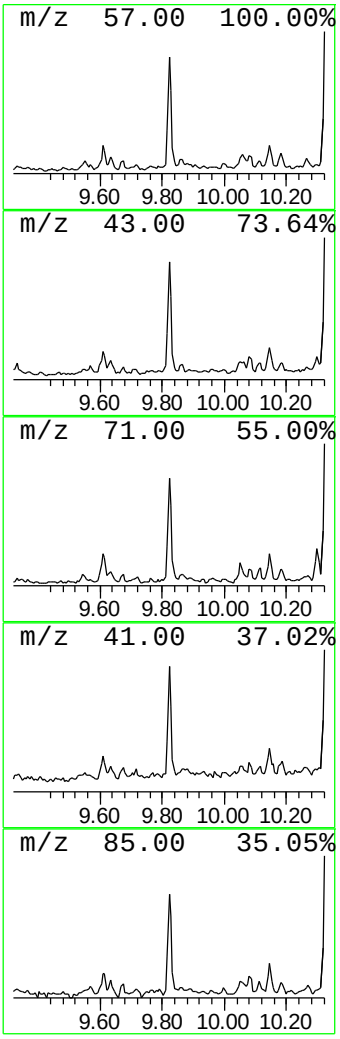
****

Peak Number 5 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.82	2.18 ng	106273	Acenaphthene-d10	9.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Tridecane	184	C13H28	000629-50-5	90
3	Tetradecane	198	C14H30	000629-59-4	90
4	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	78
5	Pentadecane	212	C15H32	000629-62-9	78





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Data File : BF103468.D
Acq On : 6 Mar 2018 21:02
Operator : SJ/JU
Sample : J1722-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

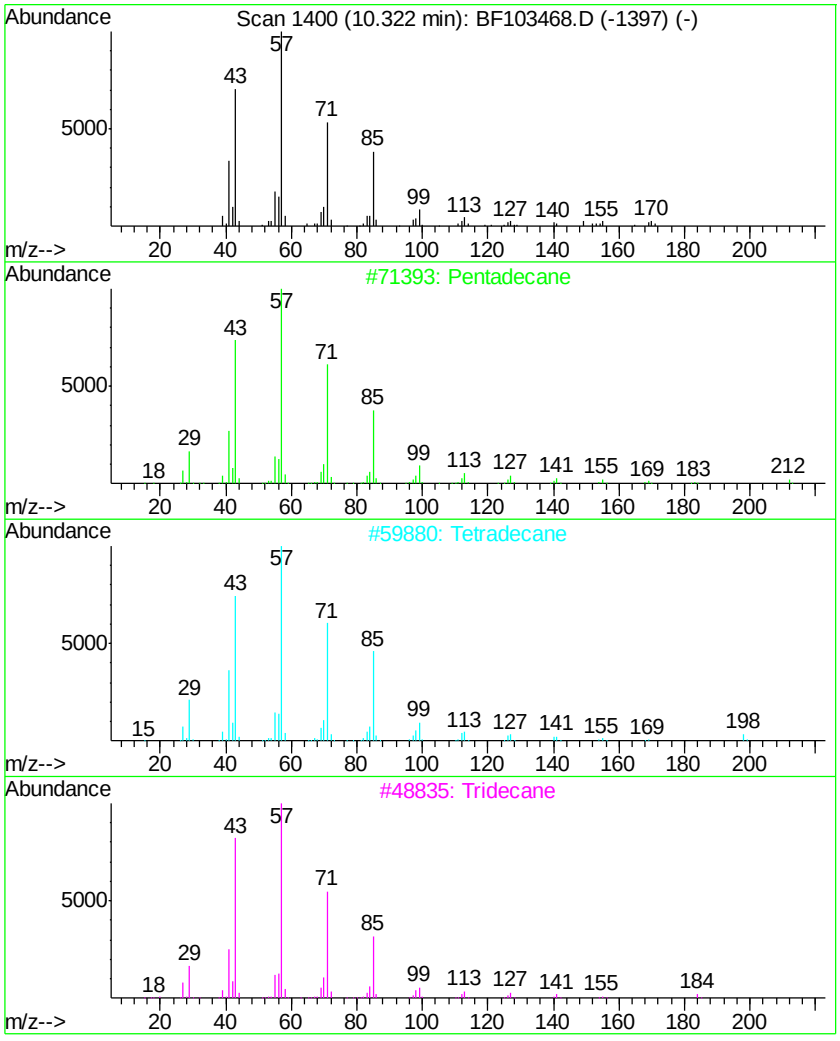
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

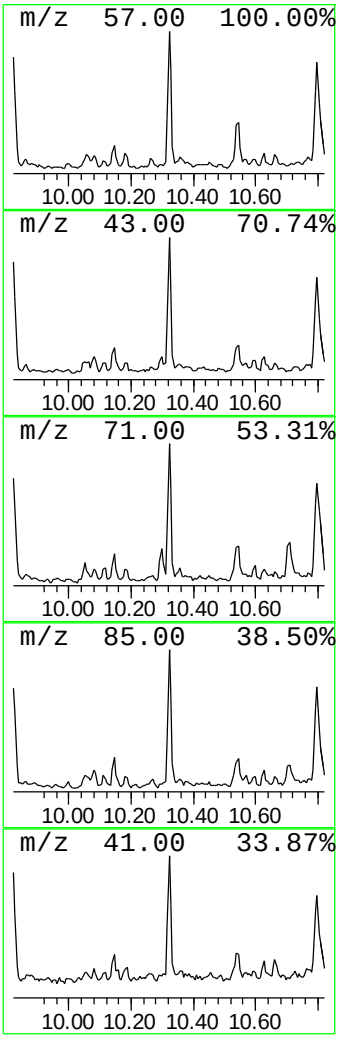
****

Peak Number 6 Pentadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.32	2.58 ng	125781	Acenaphthene-d10	9.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	90
2	Tetradecane	198	C14H30	000629-59-4	86
3	Tridecane	184	C13H28	000629-50-5	86
4	Hexadecane	226	C16H34	000544-76-3	86
5	Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	78





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF030618\
Data File : BF103468.D
Acq On : 6 Mar 2018 21:02
Operator : SJ/JU
Sample : J1722-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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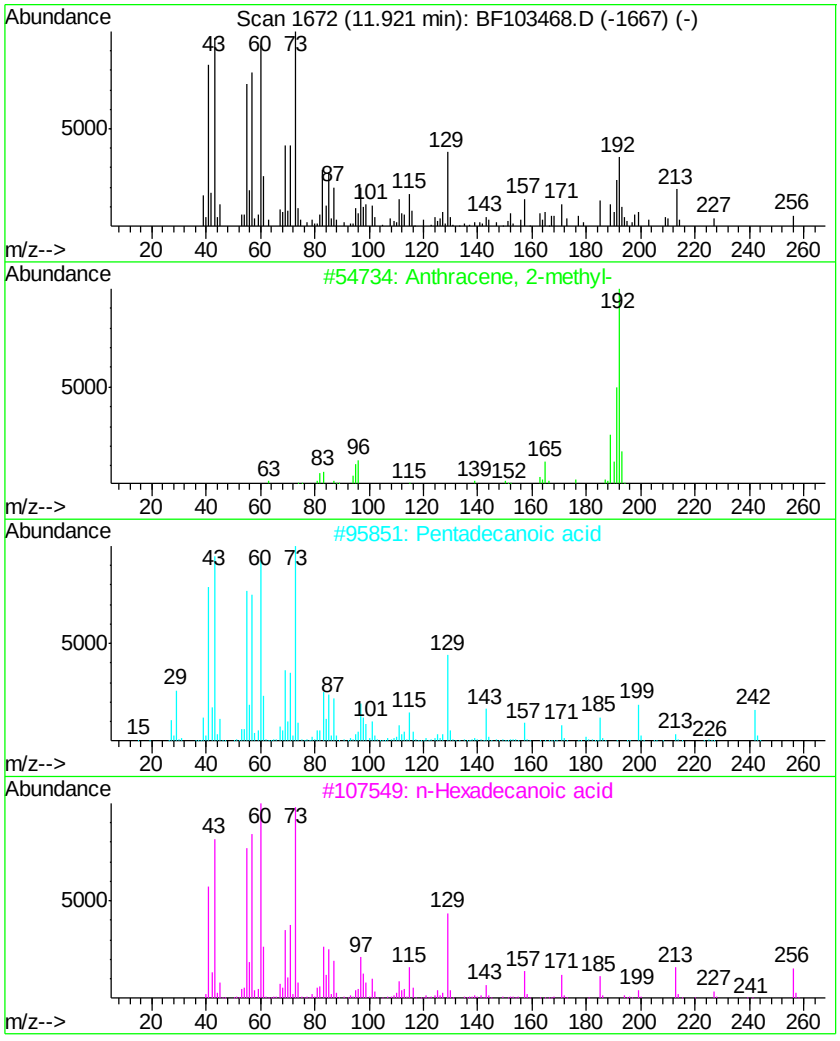
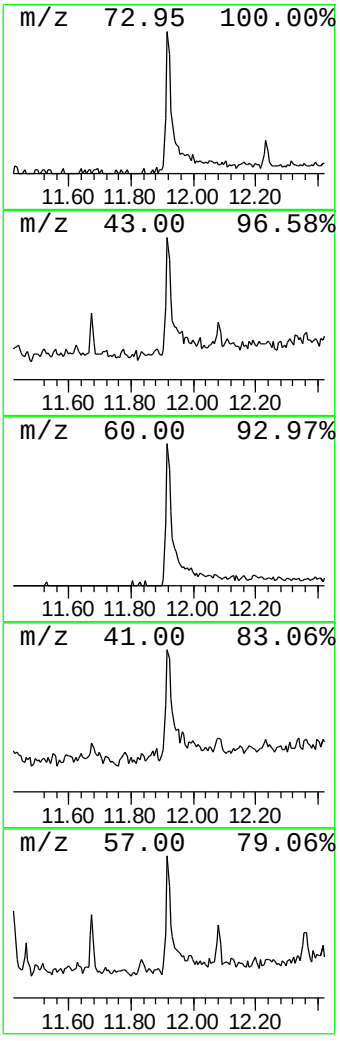
Peak Number 8 Anthracene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	4.17 ng	172268	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	55
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	55
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	55
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	48
5	Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	47





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Operator : SJ/JU
Sample : J1722-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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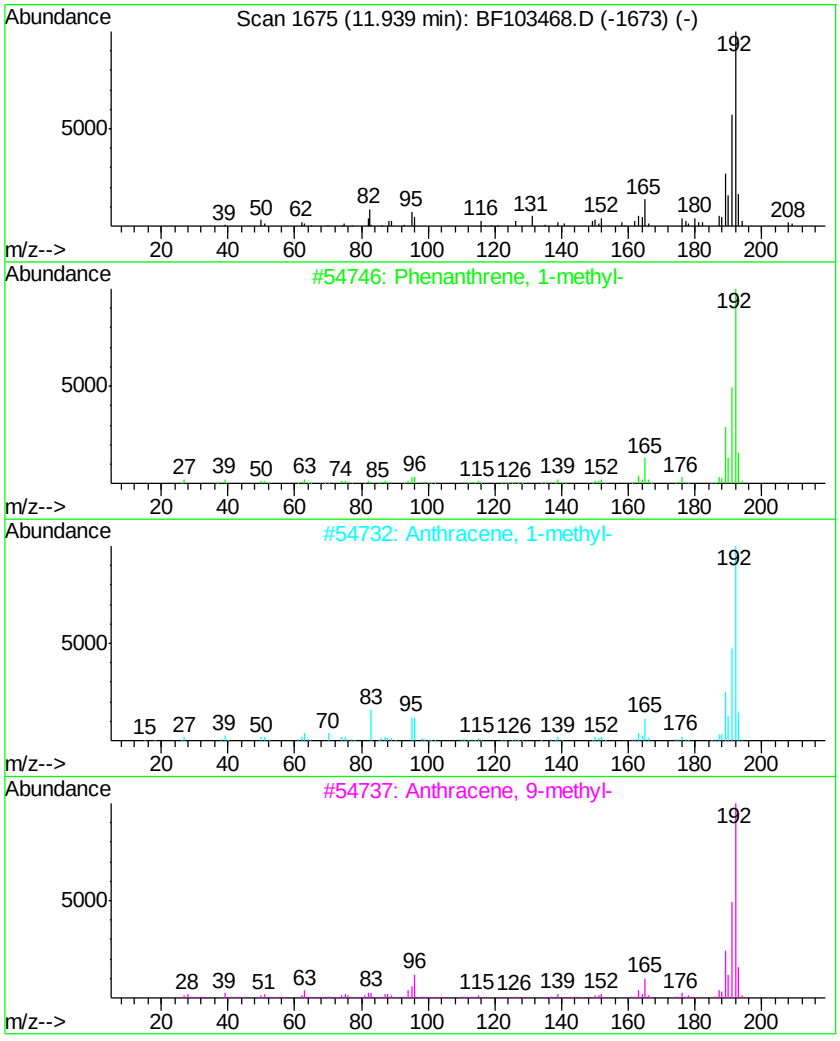
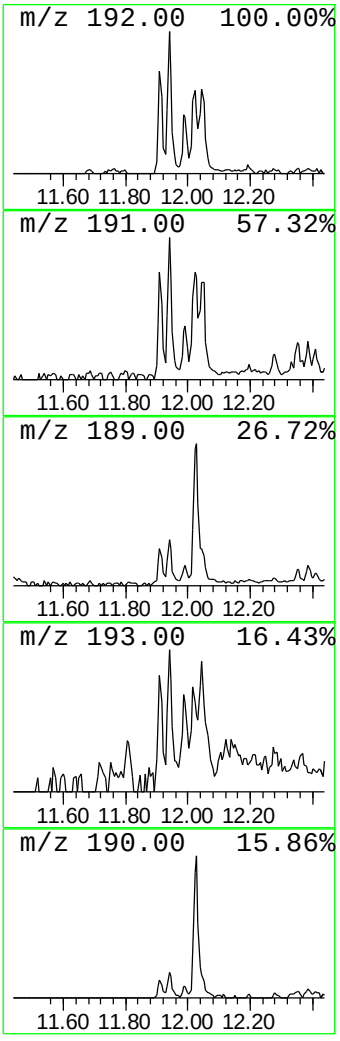
Peak Number 9 Phenanthrene, 1-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	2.11 ng	86940	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	94
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91





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Data File : BF103468.D
Acq On : 6 Mar 2018 21:02
Operator : SJ/JU
Sample : J1722-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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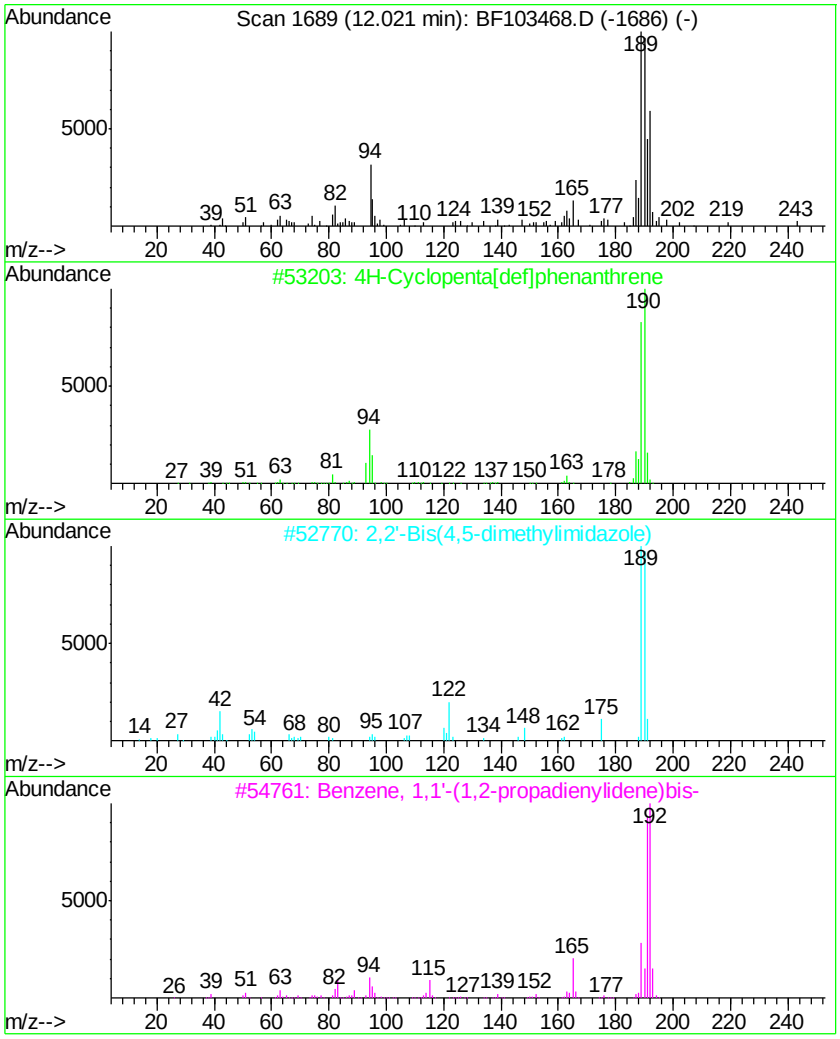
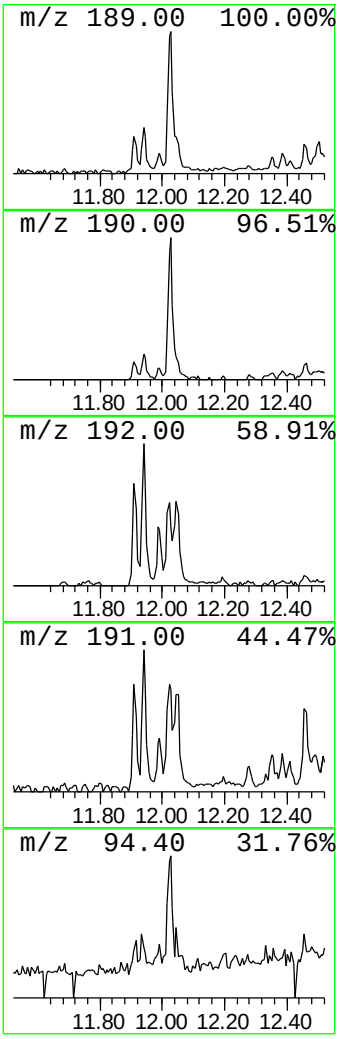
Peak Number 10 4H-Cyclopenta[def]phenanthrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	2.32 ng	95969	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	68
2	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38
3	Benzene, 1,1'-(1,2-propadienylid...	192	C15H12	014251-57-1	22
4	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	18
5	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	14





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Acq On : 6 Mar 2018 21:02
Operator : SJ/JU
Sample : J1722-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-7

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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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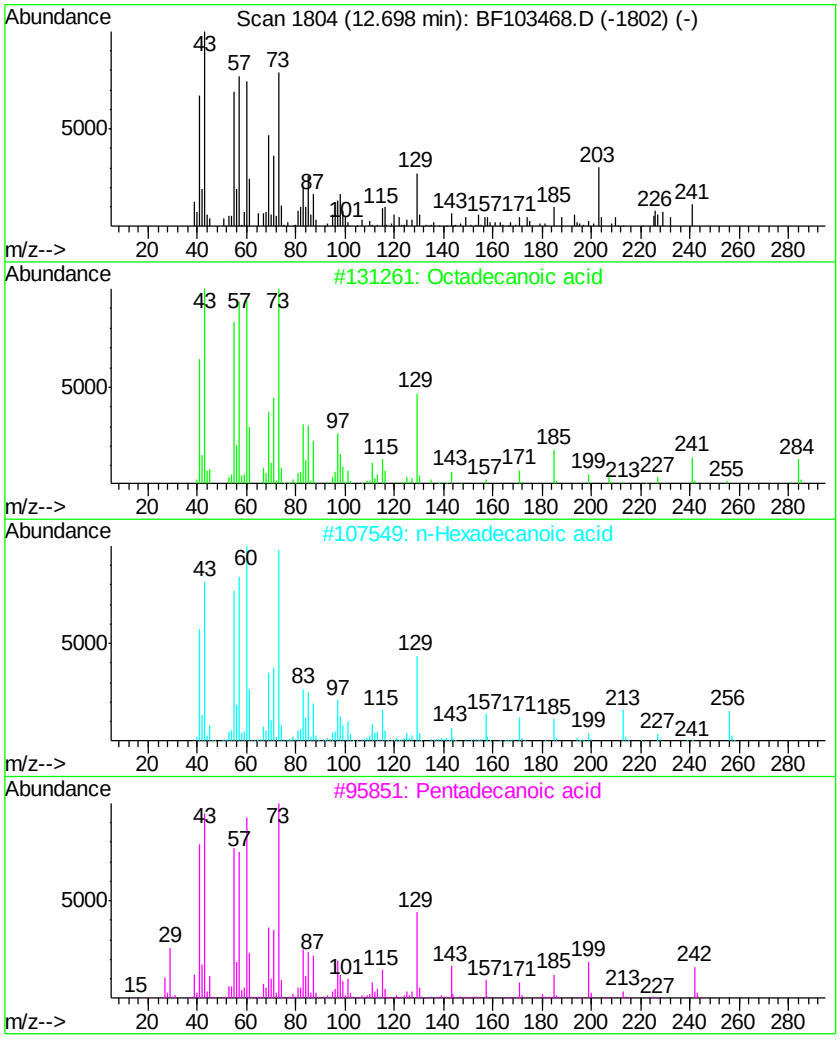
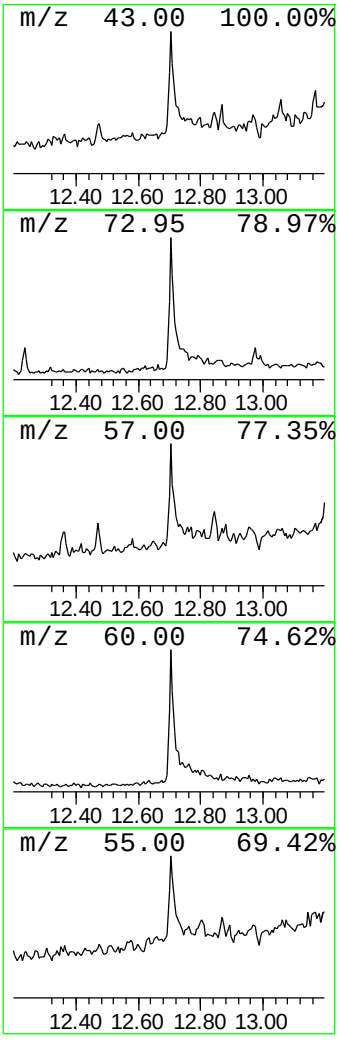
Peak Number 11 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	4.42 ng	182521	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Tridecanoic acid	214	C13H26O2	000638-53-9	72





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Acq On : 6 Mar 2018 21:02
Operator : SJ/JU
Sample : J1722-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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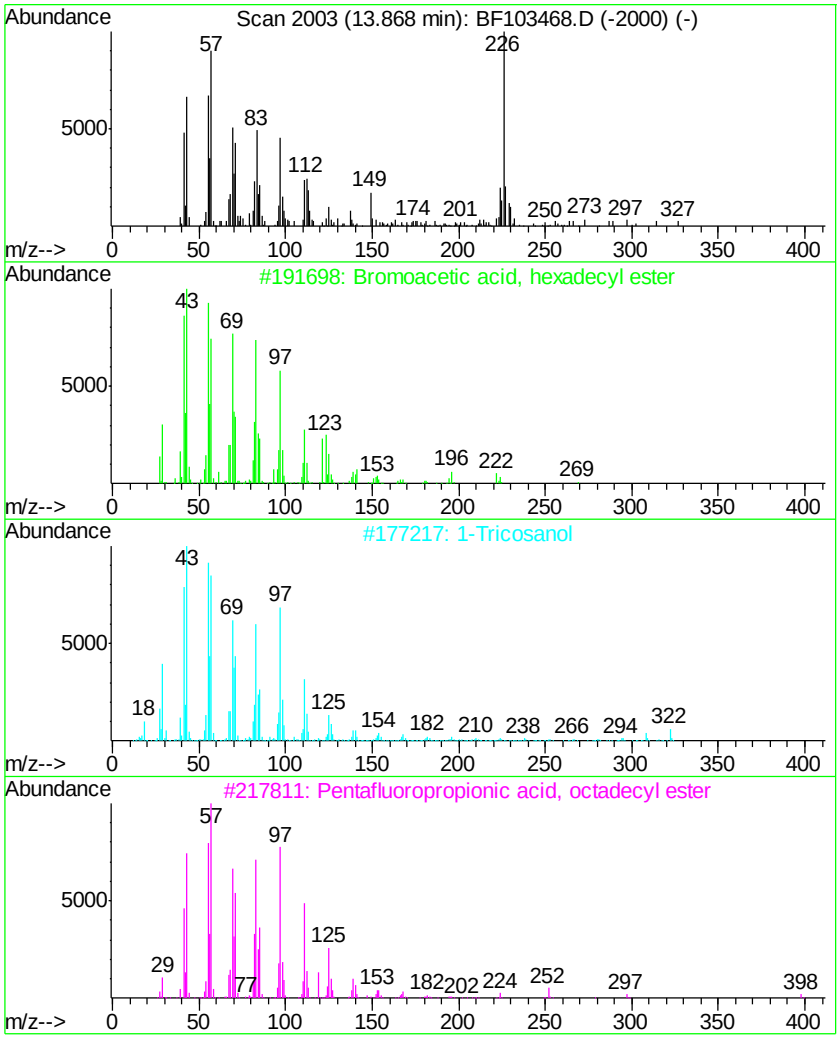
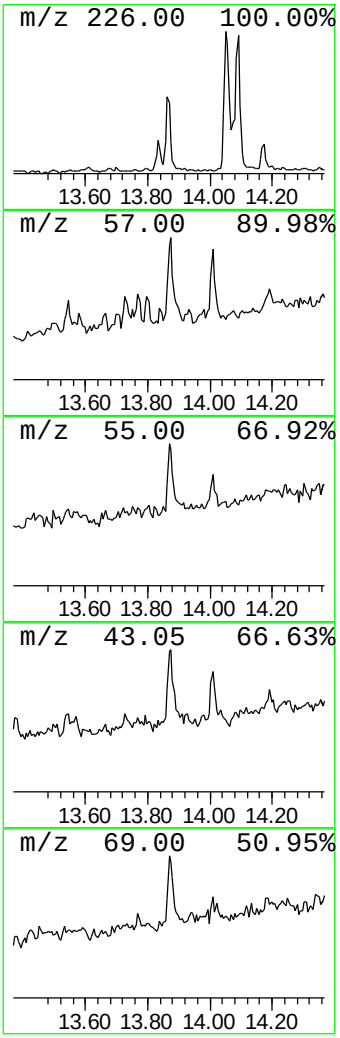
Peak Number 12 Bromoacetic acid, hexadecyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	4.31 ng	198292	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	59
2	1-Tricosanol	340	C23H48O	003133-01-5	55
3	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	45
4	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	45
5	17-Pentatriacontene	491	C35H70	006971-40-0	45





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF030618\
Data File : BF103468.D
Acq On : 6 Mar 2018 21:02
Operator : SJ/JU
Sample : J1722-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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...	2.13	5.6	ng	231443	1	6.87	820539	20.0
2-Pentanone, 4-hy...	5.11	2.0	ng	82507	1	6.87	820539	20.0
unknown6.65	6.65	80.0	ng	3283910	1	6.87	820539	20.0
Hexadecane	9.82	2.2	ng	106273	3	9.91	975244	20.0
Pentadecane	10.32	2.6	ng	125781	3	9.91	975244	20.0
Anthracene, 2-met...	11.92	4.2	ng	172268	4	11.40	825695	20.0
Phenanthrene, 1-m...	11.94	2.1	ng	86940	4	11.40	825695	20.0
4H-Cyclopenta[def...	12.02	2.3	ng	95969	4	11.40	825695	20.0
Octadecanoic acid	12.70	4.4	ng	182521	4	11.40	825695	20.0
Bromoacetic acid,...	13.87	4.3	ng	198292	5	14.06	919278	20.0