LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102899.D
Acq On : 9 Feb 2018 19:59
Operator : SJ/JU
Sample : J1512-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-3091

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-BF020318.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	2.169	7	14	22	rVB	448494	613390	15.54%	1.654%
2	5.116	511	515	523	rVB	146466	186233	4.72%	0.502%
3	5.504	576	581	584	rBV	3878440	3946558	100.00%	10.643%
4	6.334	717	722	725	rBV	59645	47189	1.20%	0.127%
5	6.510	747	752	762	rBV	3513302	3914997	99.20%	10.558%
6	6.657	772	777	780	rBV	3644932	3764530	95.39%	10.152%
7	6.887	812	816	819	rBV	1173824	1052798	26.68%	2.839%
8	7.040	838	842	846	rBV	3144165	2942817	74.57%	7.936%
9	7.445	906	911	914	rBV	2558623	2471077	62.61%	6.664%
10	7.622	938	941	946	rVB	56297	48774	1.24%	0.132%
11	8.169	1030	1034	1037	rBV	1416520	1310680	33.21%	3.535%
12	9.239	1212	1216	1220	rBV	3484022	3414506	86.52%	9.208%
13	9.316	1226	1229	1232	rVB	62195	47469	1.20%	0.128%
14	9.551	1266	1269	1272	rBV	49638	67487	1.71%	0.182%
15	9.633	1279	1283	1286	rBV	276126	250585	6.35%	0.676%
16	9.845	1315	1319	1322	rBV	180712	139589	3.54%	0.376%
17	9.922	1328	1332	1336	rBV	1363361	1184890	30.02%	3.195%
18	10.169	1370	1374	1378	rBV3	36212	39884	1.01%	0.108%
19	10.345	1401	1404	1407	rVB	206380	154627	3.92%	0.417%
20	10.563	1437	1441	1444	rBV	48003	63745	1.62%	0.172%
21	10.710	1463	1466	1477	rVB	1742904	1717086	43.51%	4.631%
22	10.816	1481	1484	1493	rVB	149149	184637	4.68%	0.498%
23	11.269	1557	1561	1563	rBV	73736	65980	1.67%	0.178%
24	11.298	1563	1566	1572	rVB3	32097	53970	1.37%	0.146%
25	11.410	1581	1585	1588	rBV	1153197	1076801	27.28%	2.904%
26	11.433	1588	1589	1595	rVV	338527	253075	6.41%	0.682%
27	11.486	1595	1598	1601	rVB	61994	56439	1.43%	0.152%
28	11.910	1667	1670	1672	rBV	51239	54694	1.39%	0.147%
29	11.939	1673	1675	1678	rVB	71039	56362	1.43%	0.152%
30	12.022	1686	1689	1692	rBV2	69906	80010	2.03%	0.216%
31	12.233	1722	1725	1731	rVB4	38494	47398	1.20%	0.128%
32	12.463	1760	1764	1766	rBV	42802	45875	1.16%	0.124%
33	12.545	1776	1778	1782	rBV3	36099	40111	1.02%	0.108%
34	12.622	1788	1791	1795	rBV	387029	360025	9.12%	0.971%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102899.D
Acq On : 9 Feb 2018 19:59
Operator : SJ/JU
Sample : J1512-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-3091

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-BF020318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.857	1825	1831	1834	rBV	372776	428870	10.87%	1.157%
36	12.998	1850	1855	1858	rBV	2880234	2683197	67.99%	7.236%
37	13.069	1863	1867	1872	rBV4	37550	59331	1.50%	0.160%
38	13.180	1884	1886	1890	rVB	55948	54992	1.39%	0.148%
39	13.286	1900	1904	1907	rBV2	50086	48874	1.24%	0.132%
40	13.586	1952	1955	1961	rVB6	29269	40381	1.02%	0.109%
41	13.686	1966	1972	1977	rVB	43982	63995	1.62%	0.173%
42	13.804	1987	1992	1994	rBV2	42886	60420	1.53%	0.163%
43	13.880	2002	2005	2011	rVB2	265715	285190	7.23%	0.769%
44	14.021	2026	2029	2031	rBV	209304	200471	5.08%	0.541%
45	14.051	2031	2034	2037	rVV	1178214	1230474	31.18%	3.318%
46	14.074	2037	2038	2046	rVB	194960	170274	4.31%	0.459%
47	14.157	2046	2052	2056	rBV4	33319	59466	1.51%	0.160%
48	14.198	2056	2059	2064	rBV6	22220	47694	1.21%	0.129%
49	14.439	2097	2100	2103	rVB	49810	41009	1.04%	0.111%
50	14.510	2109	2112	2118	rBV6	42812	67427	1.71%	0.182%
51	15.098	2208	2212	2215	rBV	158528	235283	5.96%	0.635%
52	15.163	2220	2223	2226	rVV2	45591	52028	1.32%	0.140%
53	15.410	2261	2265	2271	rVB	93241	126949	3.22%	0.342%
54	15.468	2271	2275	2282	rBV	108832	153538	3.89%	0.414%
55	15.539	2282	2287	2299	rVV	748763	1019647	25.84%	2.750%
56	15.992	2360	2364	2369	rBV	51545	75975	1.93%	0.205%
57	16.051	2370	2374	2381	rVV7	41820	73874	1.87%	0.199%
58	17.492	2614	2619	2625	rBV2	23029	47203	1.20%	0.127%

Sum of corrected areas: 37080850

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Data File : BF102899.D
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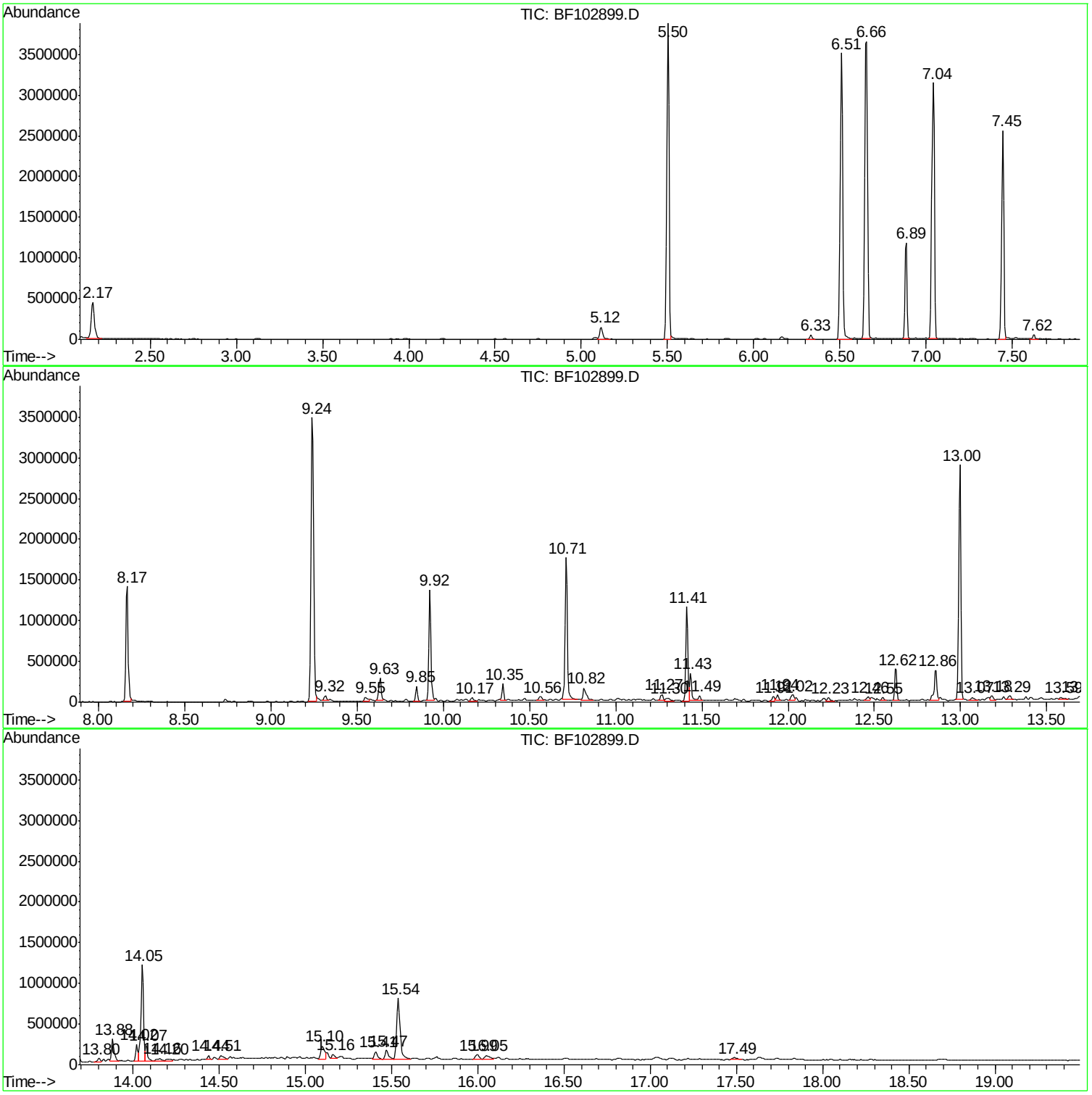
Operator : SJ/JU
Sample : J1512-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-3091

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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\BF020918\
Data File : BF102899.D
Acq On : 9 Feb 2018 19:59
Operator : SJ/JU
Sample : J1512-04
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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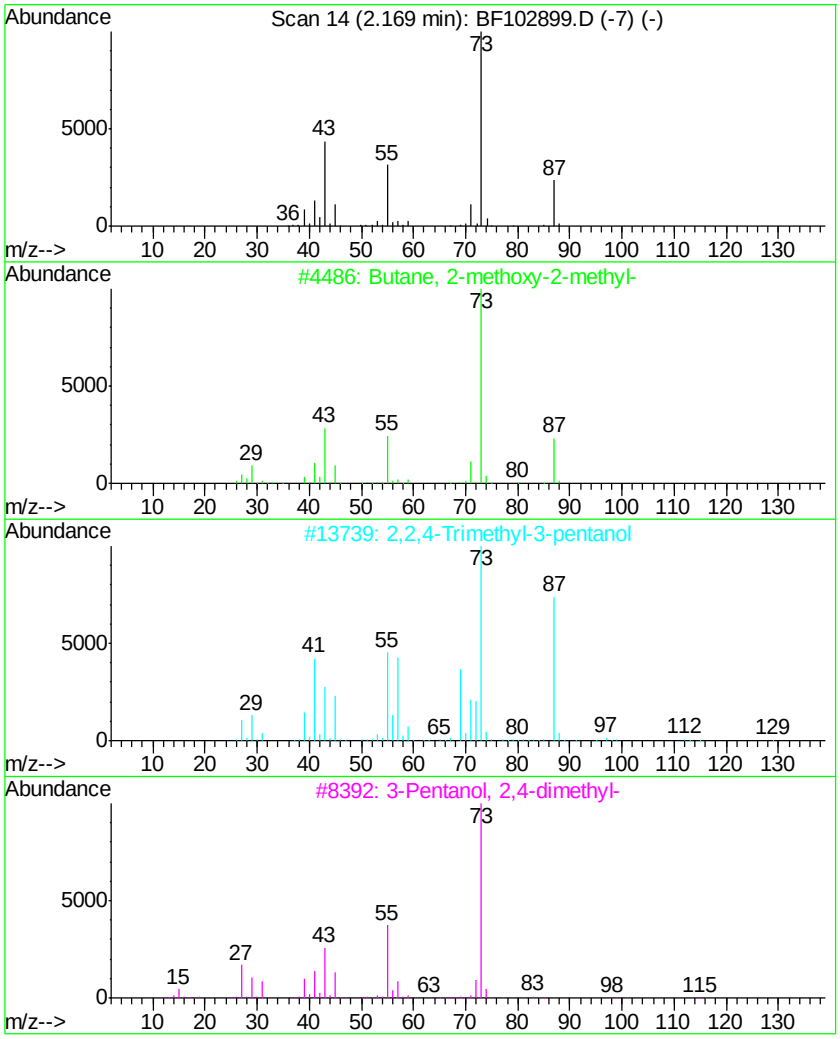
TIC Integration Parameters: LSCINT.P

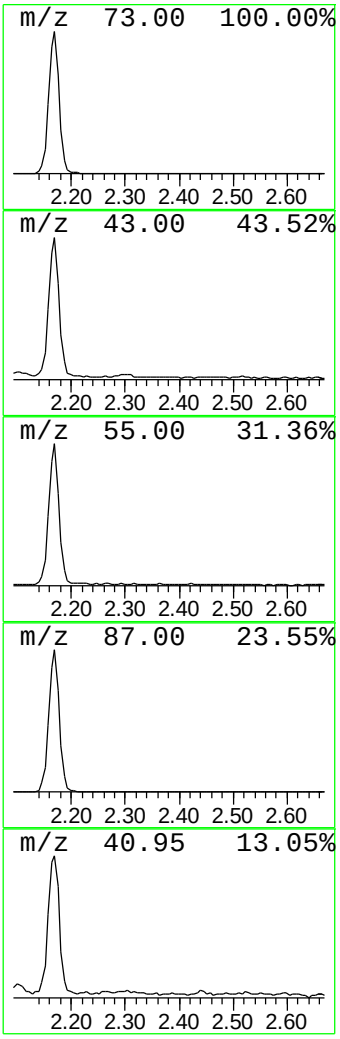
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	11.65 ng	613390	1,4-Dichlorobenzene-d4	6.89

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	40
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102899.D
Acq On : 9 Feb 2018 19:59
Operator : SJ/JU
Sample : J1512-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-3091

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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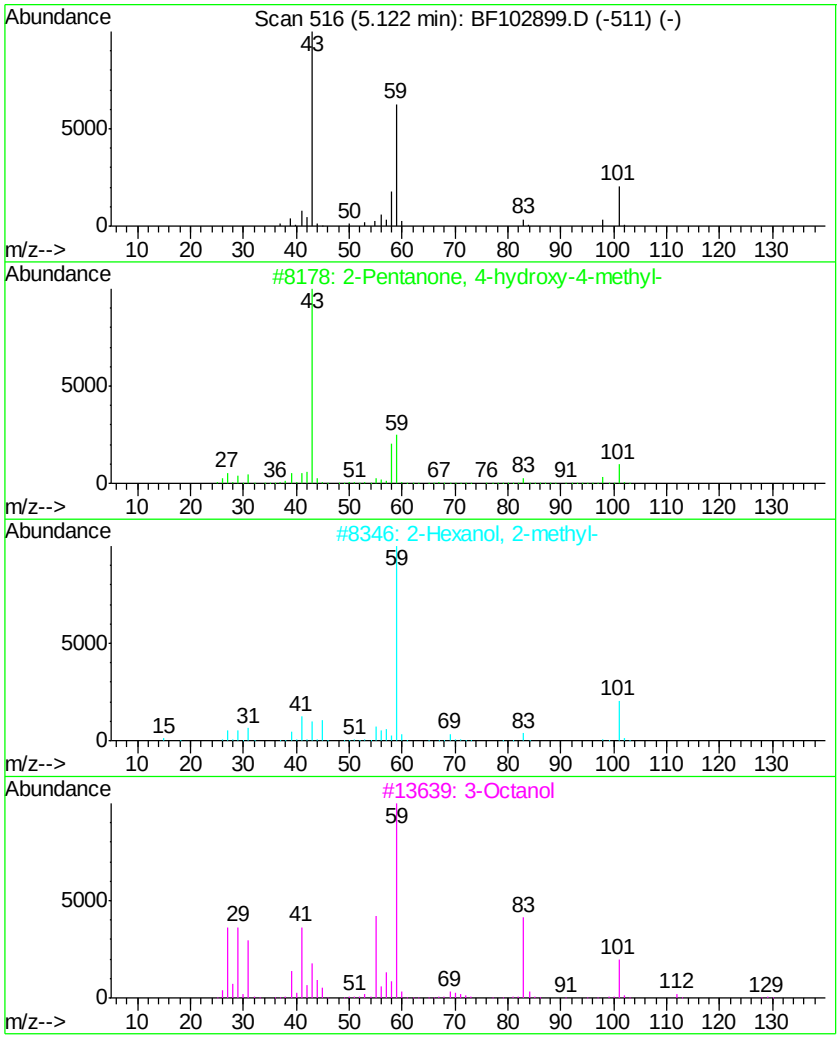
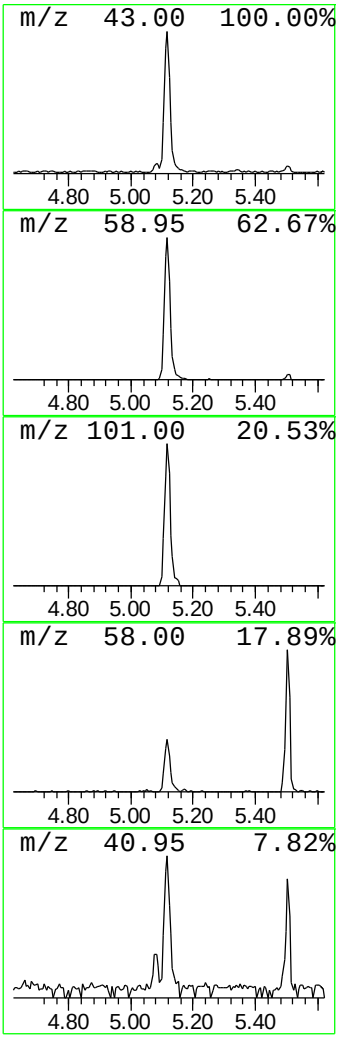
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	3.54 ng	186233	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
3	3-Octanol	130	C8H18O	000589-98-0	33
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102899.D
Acq On : 9 Feb 2018 19:59
Operator : SJ/JU
Sample : J1512-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-3091

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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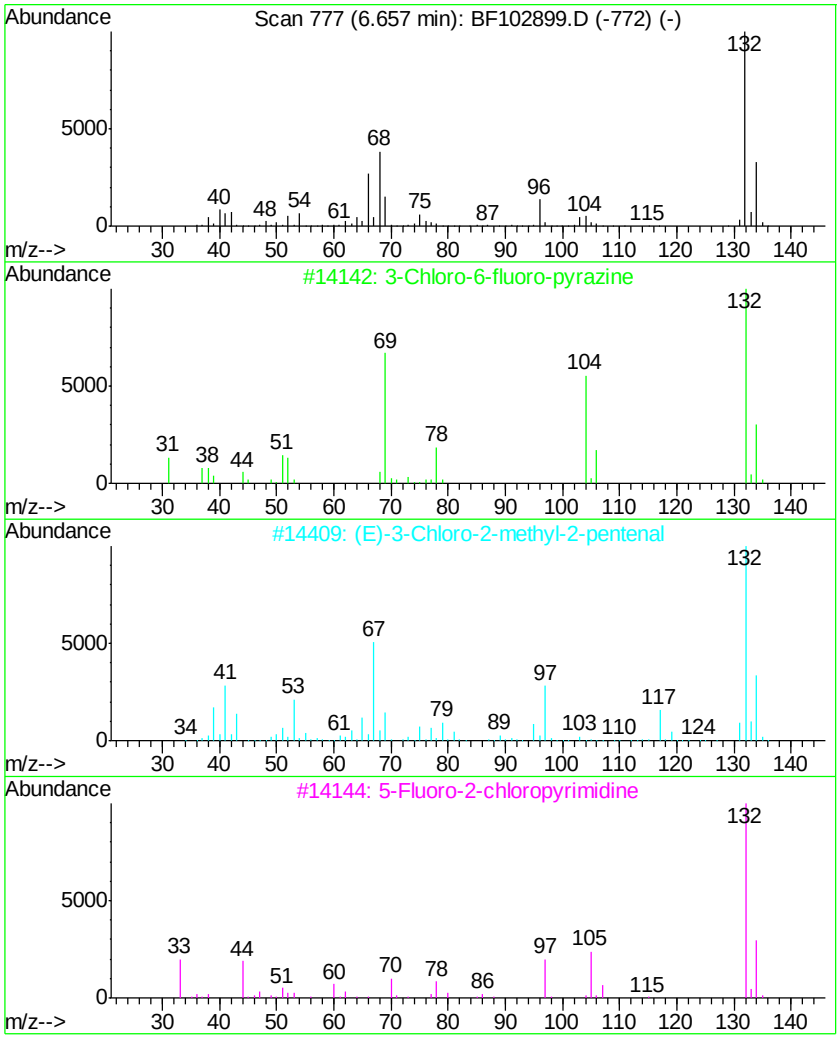
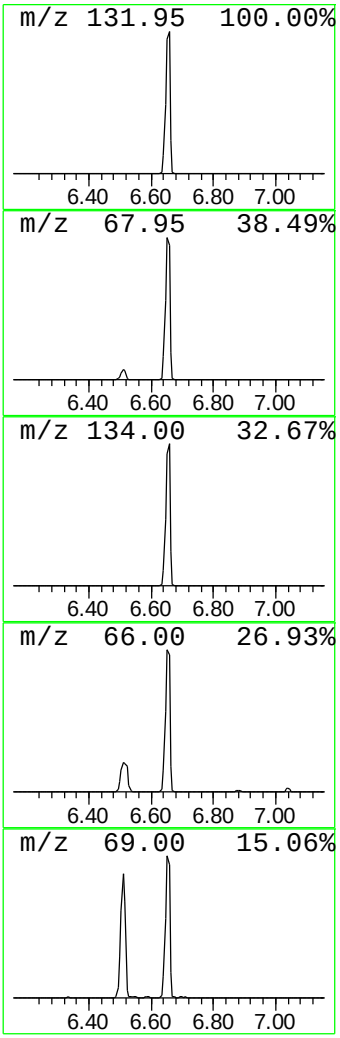
Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	71.51 ng	3764530	1,4-Dichlorobenzene-d4	6.89

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





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102899.D
Acq On : 9 Feb 2018 19:59
Operator : SJ/JU
Sample : J1512-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-3091

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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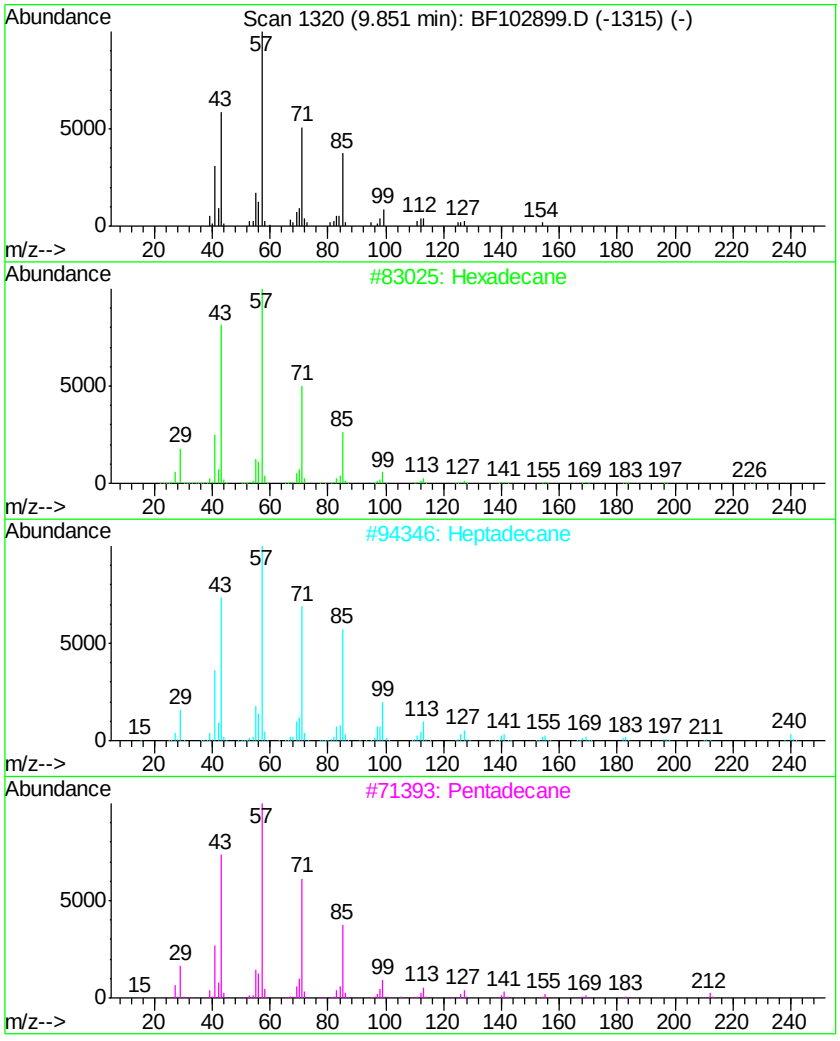
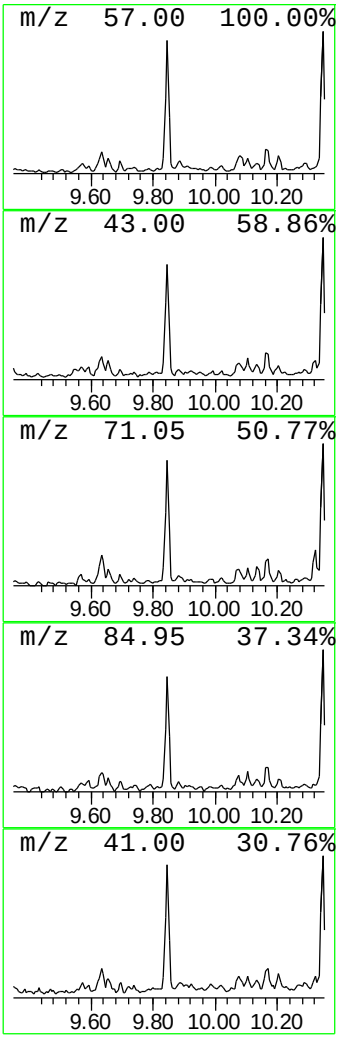
Peak Number 5 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.85	2.36 ng	139589	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Heptadecane	240	C17H36	000629-78-7	83
3	Pentadecane	212	C15H32	000629-62-9	78
4	Tridecane	184	C13H28	000629-50-5	78
5	Dodecane, 3-methyl-	184	C13H28	017312-57-1	64





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Data File : BF102899.D
Acq On : 9 Feb 2018 19:59
Operator : SJ/JU
Sample : J1512-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-3091

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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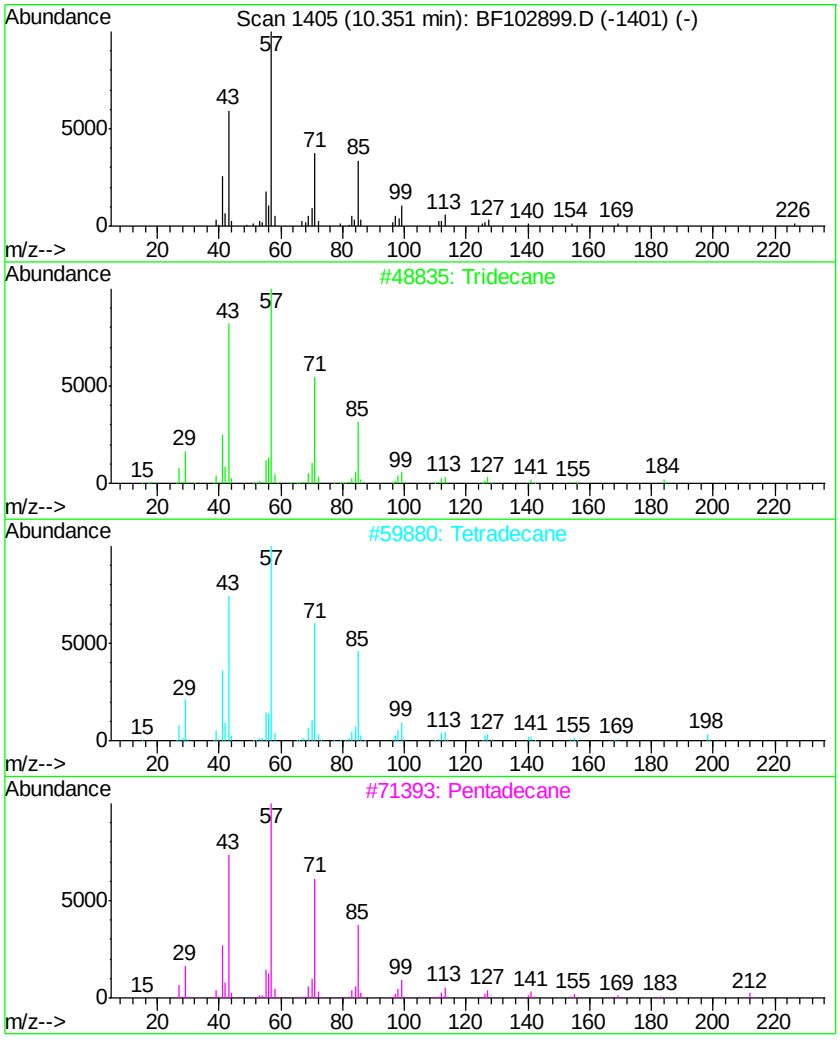
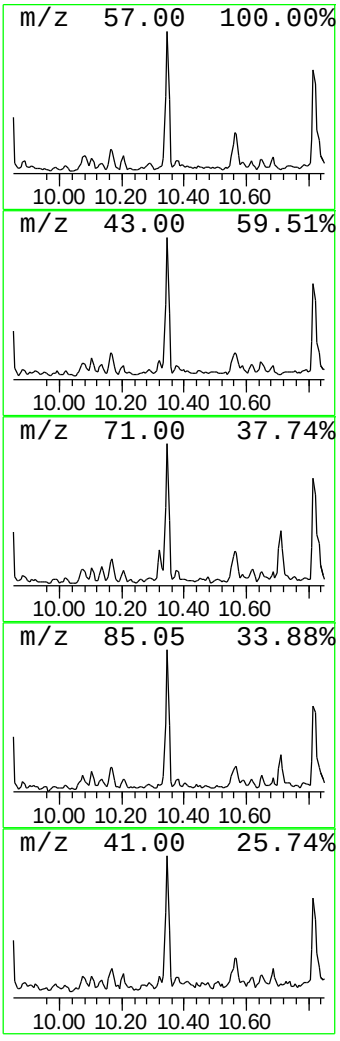
****

Peak Number 6 Tridecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.35	2.61 ng	154627	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	90
2	Tetradecane	198	C14H30	000629-59-4	86
3	Pentadecane	212	C15H32	000629-62-9	80
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78
5	Hexadecane	226	C16H34	000544-76-3	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
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Sample : J1512-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-3091

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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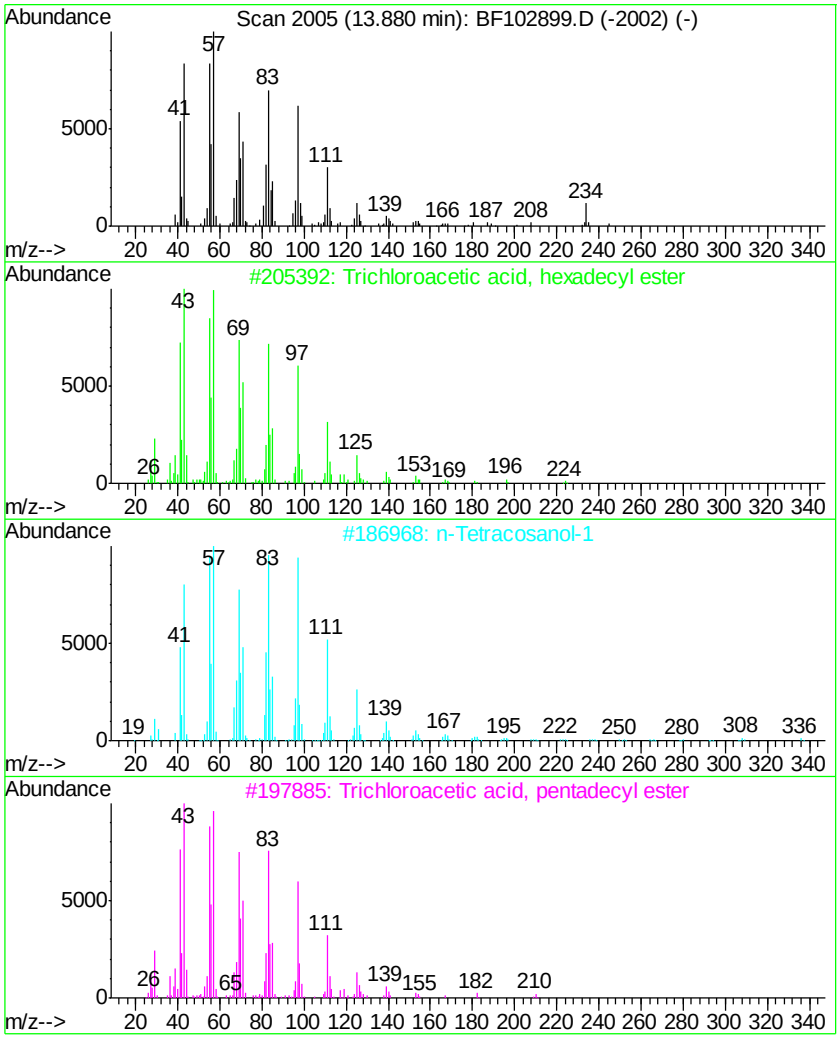
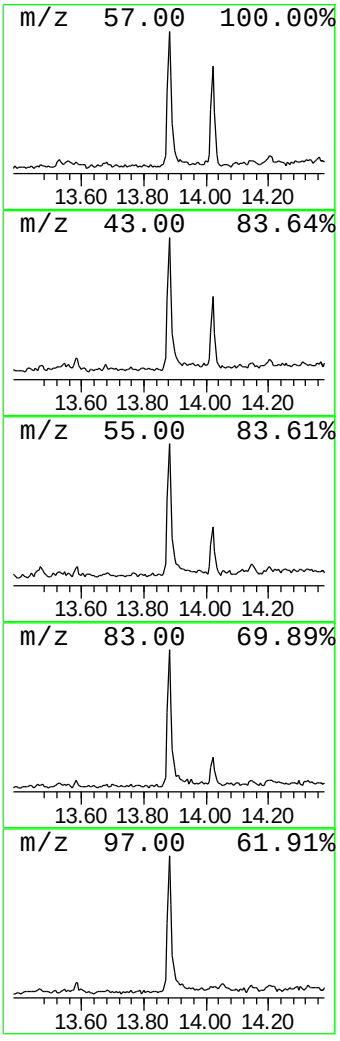
Peak Number 8 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	4.64 ng	285190	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4	Octacosanol	410	C28H58O	000557-61-9	91
5	Behenic alcohol	326	C22H46O	000661-19-8	91





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Operator : SJ/JU
Sample : J1512-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-3091

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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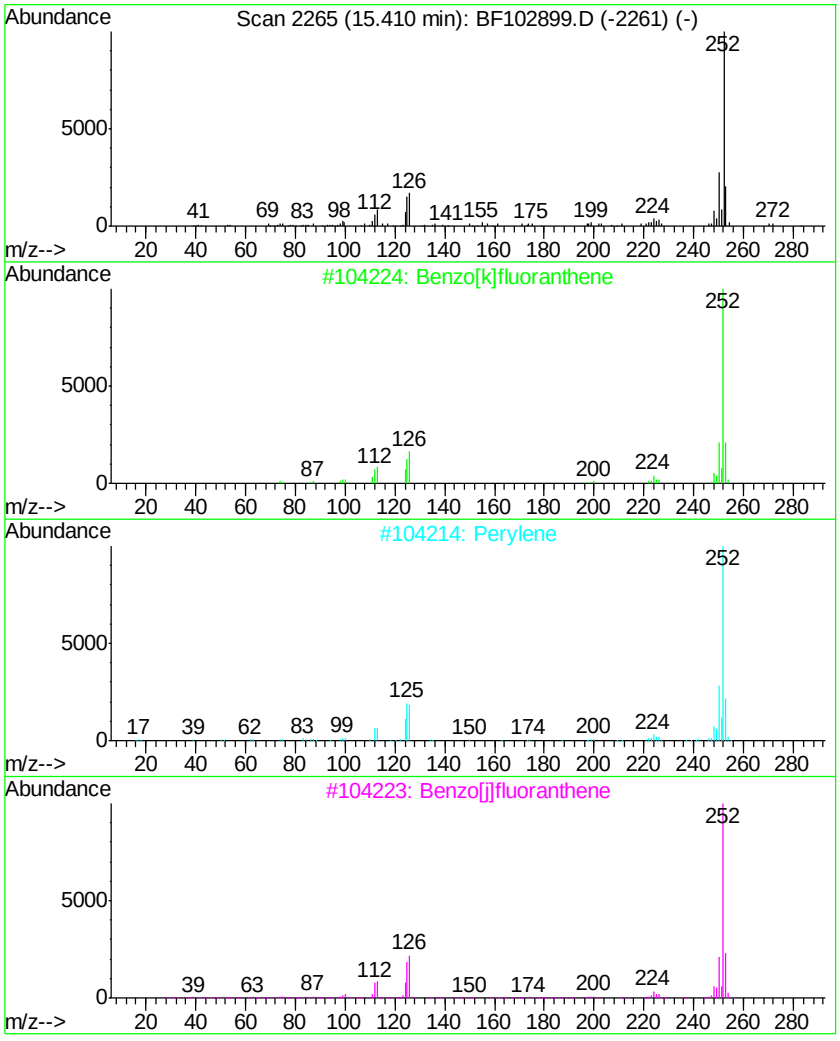
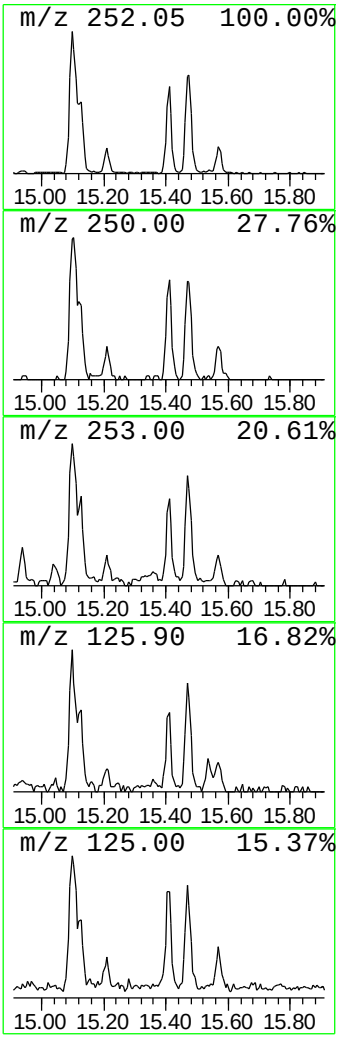
Peak Number 9 Benzo[k]fluoranthene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.41	2.49 ng	126949	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
2	Perylene	252	C20H12	000198-55-0	97
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	97
4	Benzo[e]pyrene	252	C20H12	000192-97-2	97
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020918\
Data File : BF102899.D
Acq On : 9 Feb 2018 19:59
Operator : SJ/JU
Sample : J1512-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-3091

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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...	2.17	11.7	ng	613390	1	6.89	1052800	20.0
2-Pentanone, 4-hy...	5.12	3.5	ng	186233	1	6.89	1052800	20.0
unknown6.66	6.66	71.5	ng	3764530	1	6.89	1052800	20.0
Hexadecane	9.85	2.4	ng	139589	3	9.92	1184890	20.0
Tridecane	10.35	2.6	ng	154627	3	9.92	1184890	20.0
Trichloroacetic a...	13.88	4.6	ng	285190	5	14.05	1230470	20.0
Benzo[k]fluoranthene	15.41	2.5	ng	126949	6	15.54	1019650	20.0