LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080218\
Data File : BF107920.D
Acq On : 2 Aug 2018 20:12
Operator : JU/SJ
Sample : J4285-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KG-PIT-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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.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	5.190	481	485	495	rBV	309143	446867	15.42%	1.580%
2	5.601	551	555	595	rBV	1059689	2531319	87.35%	8.948%
3	6.601	722	725	743	rBV	1128136	2446502	84.43%	8.648%
4	6.731	743	747	773	rVB	1885552	2897833	100.00%	10.243%
5	6.954	782	785	807	rVB	351720	733646	25.32%	2.593%
6	7.107	807	811	839	rVB	1637061	2115678	73.01%	7.479%
7	7.525	878	882	905	rBV	692769	1633986	56.39%	5.776%
8	8.236	999	1003	1023	rBV	552249	948323	32.73%	3.352%
9	9.307	1181	1185	1209	rBV	1800471	2365262	81.62%	8.361%
10	9.701	1246	1252	1262	rBV	255950	306383	10.57%	1.083%
11	9.995	1296	1302	1314	rBV	727606	868640	29.98%	3.071%
12	10.401	1368	1371	1378	rVB	173968	165926	5.73%	0.587%
13	10.554	1389	1397	1401	rBV5	17332	35054	1.21%	0.124%
14	10.789	1433	1437	1449	rBV	890349	1338497	46.19%	4.731%
15	10.871	1449	1451	1461	rVB6	40135	90901	3.14%	0.321%
16	11.489	1552	1556	1559	rBV	537987	684788	23.63%	2.421%
17	11.513	1559	1560	1568	rVV	357636	463958	16.01%	1.640%
18	11.571	1568	1570	1579	rVB	48664	102868	3.55%	0.364%
19	11.995	1638	1642	1645	rBV	94848	126284	4.36%	0.446%
20	12.024	1645	1647	1653	rVV2	62854	108200	3.73%	0.382%
21	12.107	1657	1661	1664	rVV2	61666	100717	3.48%	0.356%
22	12.289	1689	1692	1697	rBV	25533	40727	1.41%	0.144%
23	12.542	1732	1735	1738	rBV2	61775	69973	2.41%	0.247%
24	12.642	1747	1752	1759	rVB7	22345	37954	1.31%	0.134%
25	12.707	1759	1763	1772	rBV	476731	655836	22.63%	2.318%
26	12.807	1778	1780	1785	rVB	23519	32701	1.13%	0.116%
27	12.942	1796	1803	1809	rBV	435699	640006	22.09%	2.262%
28	13.071	1821	1825	1835	rBV	1752547	2031041	70.09%	7.179%
29	13.271	1852	1859	1864	rBV2	77406	115834	4.00%	0.409%
30	13.618	1915	1918	1920	rBV	53513	46932	1.62%	0.166%
31	13.912	1960	1968	1971	rBV4	171796	479549	16.55%	1.695%
32	13.948	1971	1974	1988	rVB5	322795	715659	24.70%	2.530%
33	14.142	2002	2007	2010	rBV2	848483	1174530	40.53%	4.152%
34	14.260	2024	2027	2031	rBV2	60292	68963	2.38%	0.244%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080218\
Data File : BF107920.D
Acq On : 2 Aug 2018 20:12
Operator : JU/SJ
Sample : J4285-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KG-PIT-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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.565	2077	2079	2086	rVB	82557	93468	3.23%	0.330%
36	14.883	2131	2133	2140	rVB	86600	96493	3.33%	0.341%
37	15.230	2186	2192	2202	rBV2	187017	524795	18.11%	1.855%
38	15.542	2242	2245	2253	rVB	68737	111829	3.86%	0.395%
39	15.612	2254	2257	2260	rVV2	100956	175512	6.06%	0.620%
40	15.677	2264	2268	2279	rVB	377008	666146	22.99%	2.355%

Sum of corrected areas: 28289580

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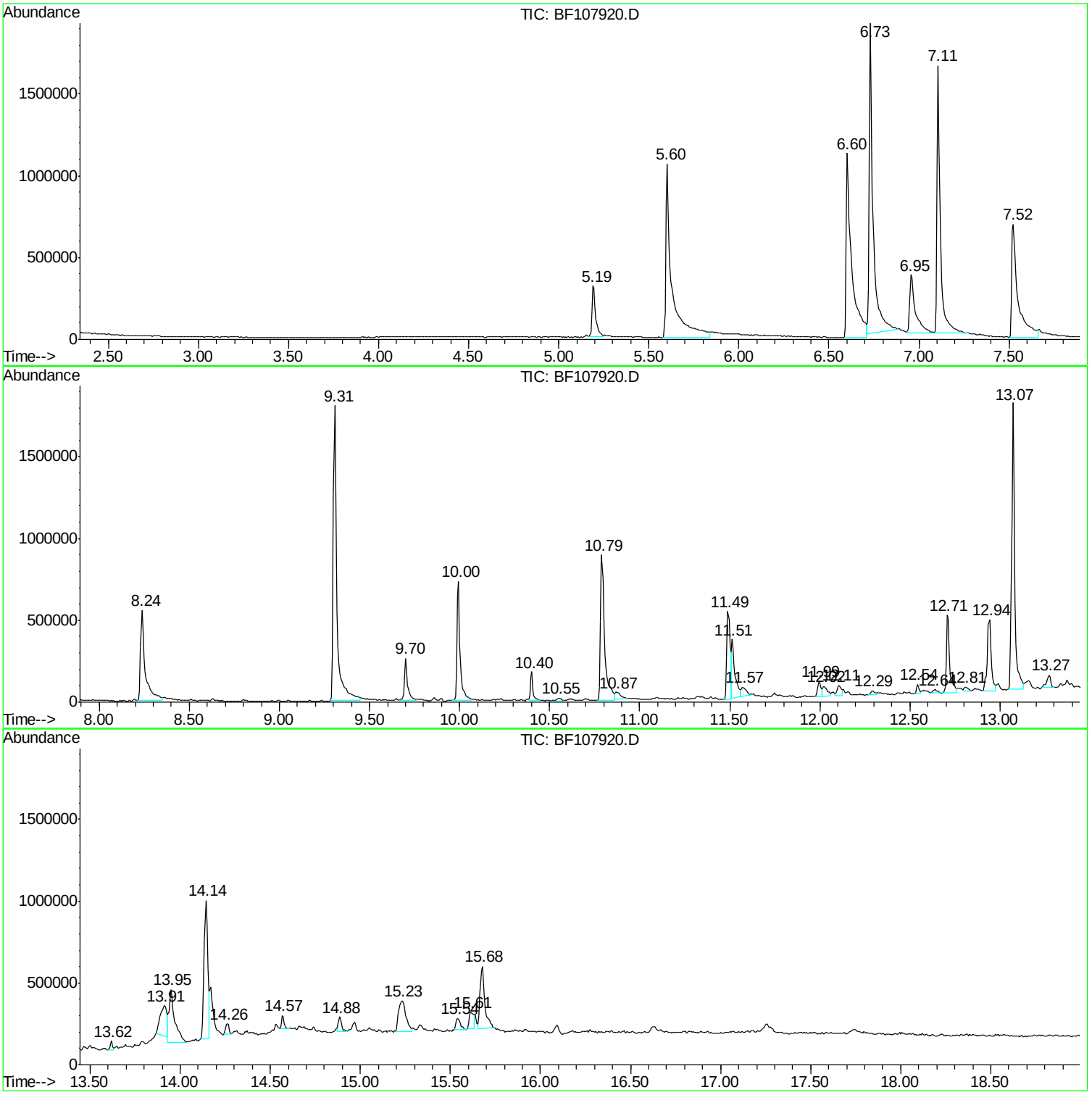
ClientSampleId : KG-PIT-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.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

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Data File : BF107920.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

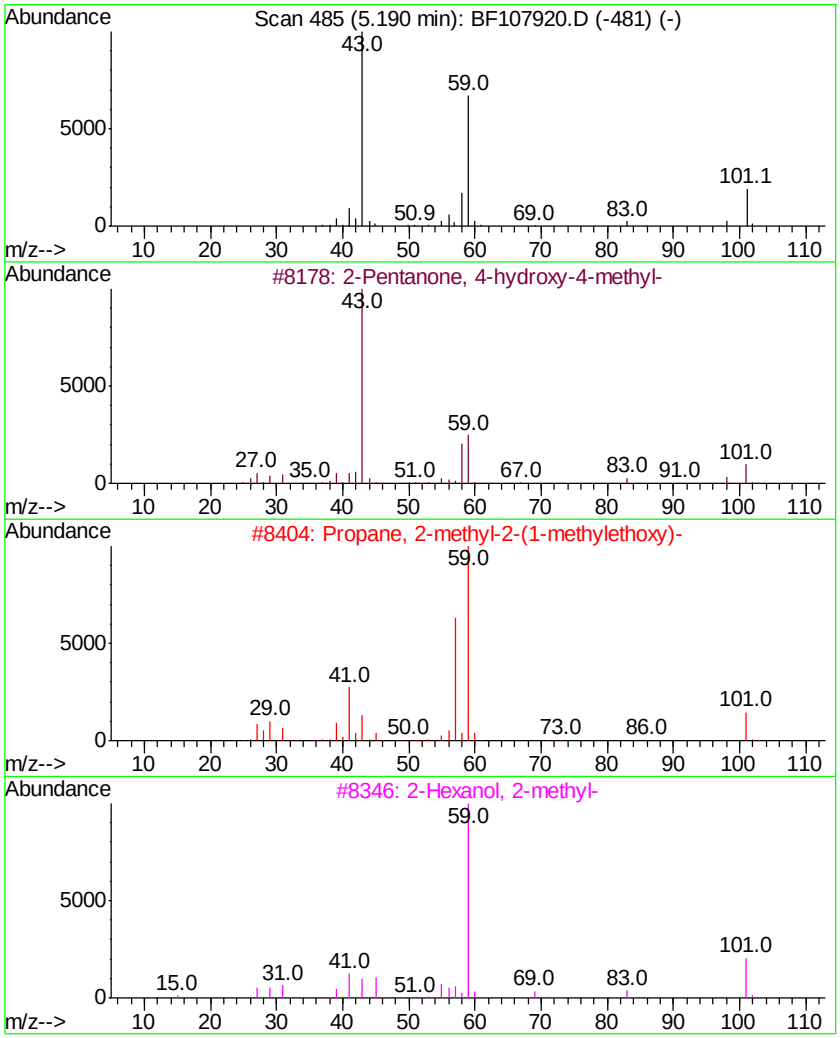
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

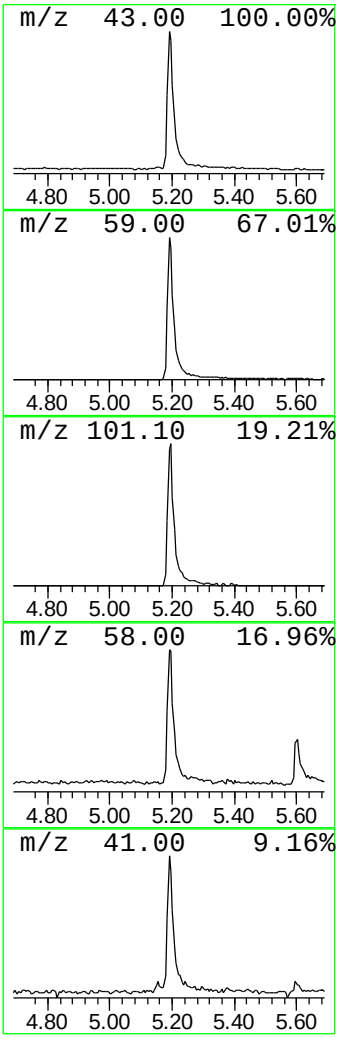
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	12.18 ng	446867	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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Operator : JU/SJ
Sample : J4285-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KG-PIT-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

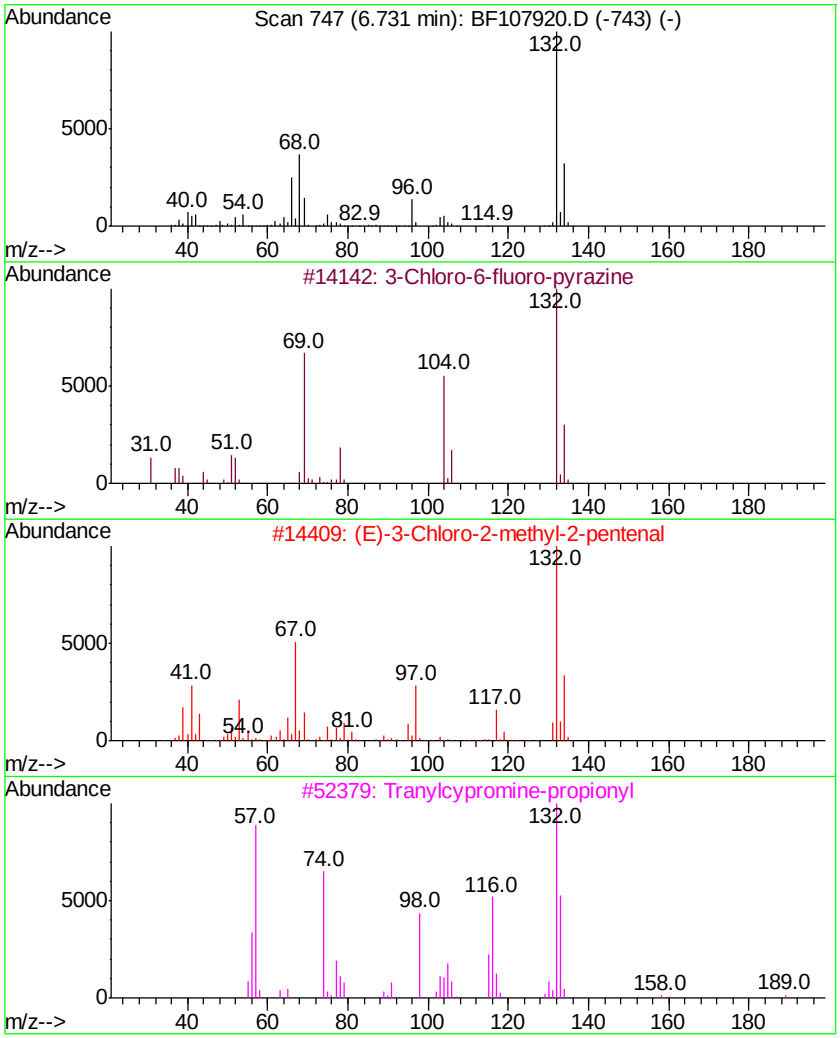
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

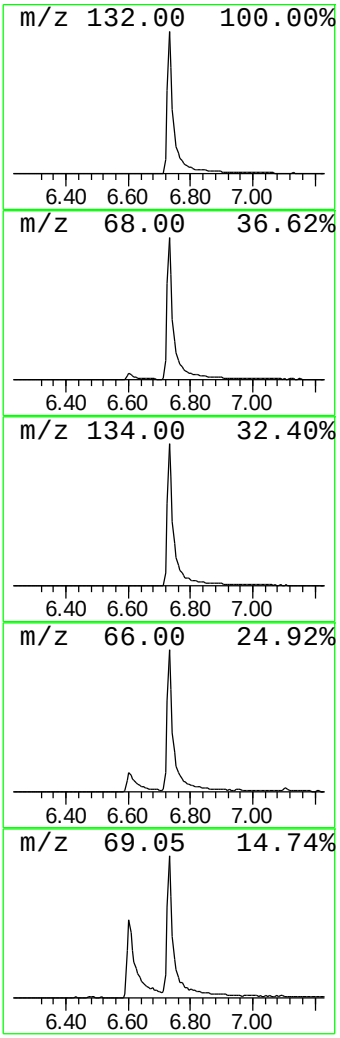
****

Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	79.00 ng	2897830	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Operator : JU/SJ
Sample : J4285-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KG-PIT-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

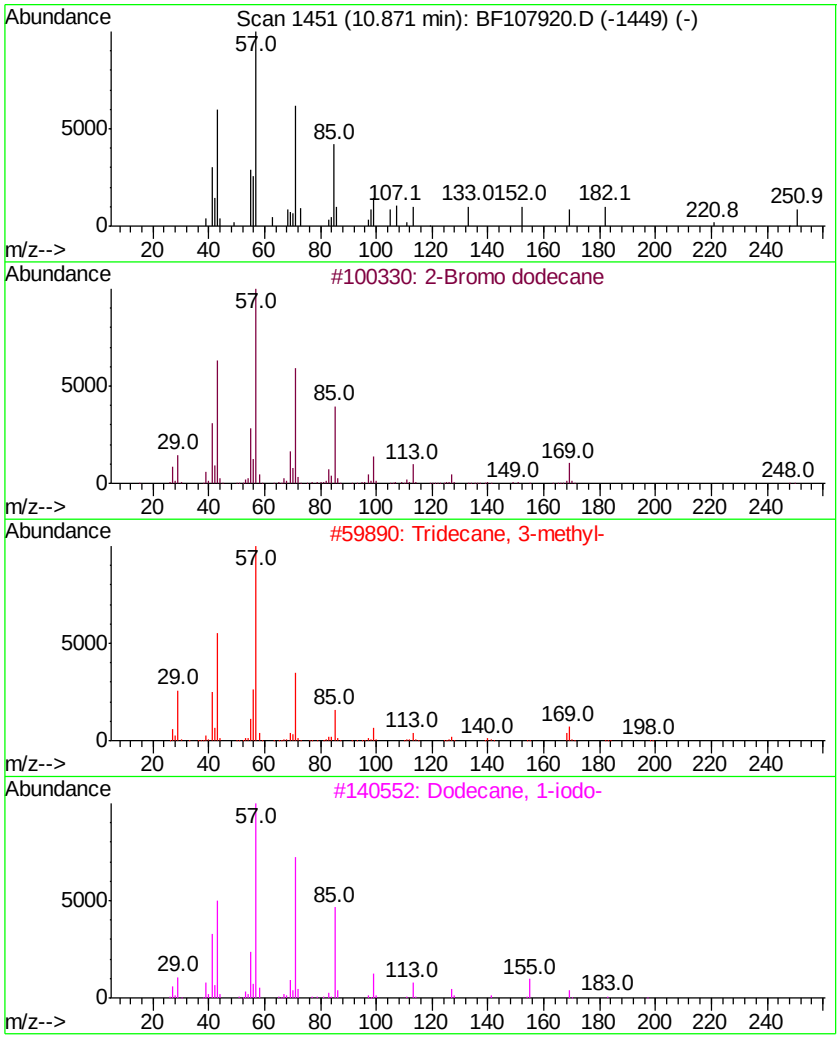
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

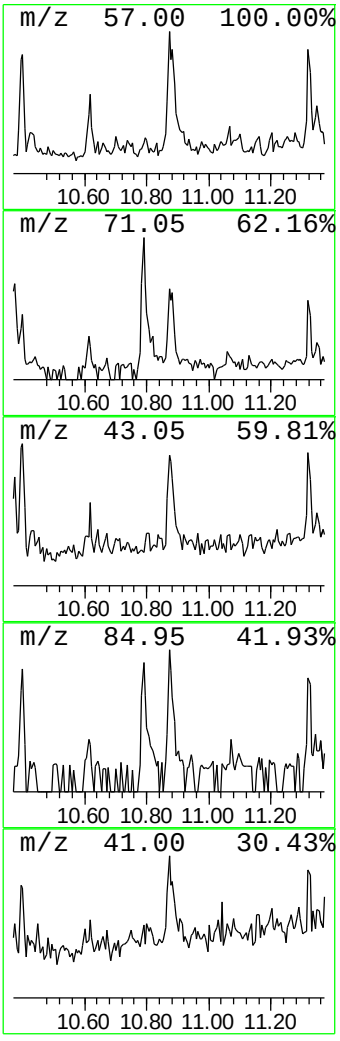
****

Peak Number 4 2-Bromo dodecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.87	2.65 ng	90901	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	64
2	Tridecane, 3-methyl-	198	C14H30	006418-41-3	50
3	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	50
4	Tridecane, 2-methyl-	198	C14H30	001560-96-9	50
5	Octadecane	254	C18H38	000593-45-3	50





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080218\
Data File : BF107920.D
Acq On : 2 Aug 2018 20:12
Operator : JU/SJ
Sample : J4285-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KG-PIT-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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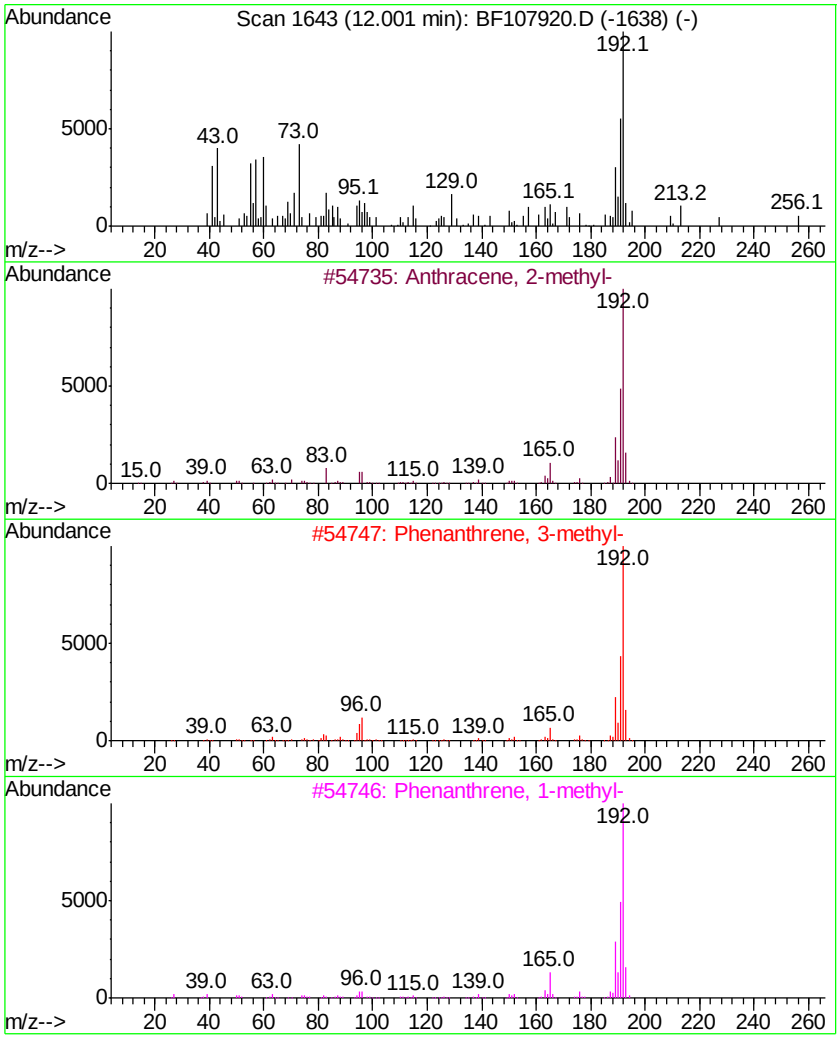
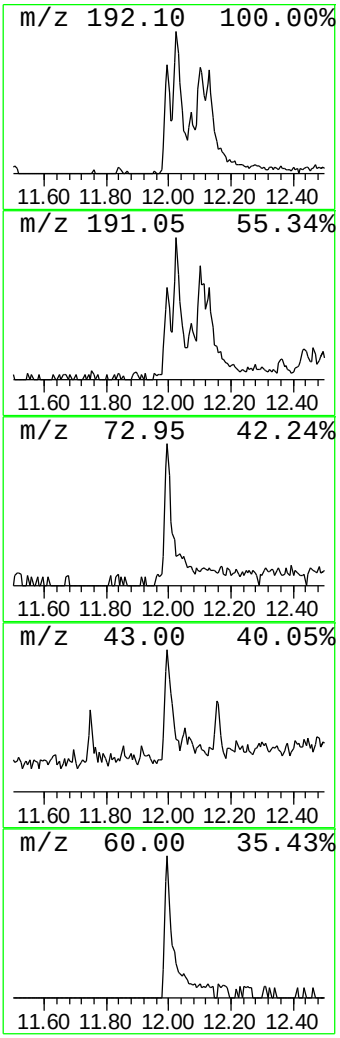
****

Peak Number 5 Anthracene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	3.69 ng	126284	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	92
2	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	78
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	78
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	78
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	70





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080218\
Data File : BF107920.D
Acq On : 2 Aug 2018 20:12
Operator : JU/SJ
Sample : J4285-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KG-PIT-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

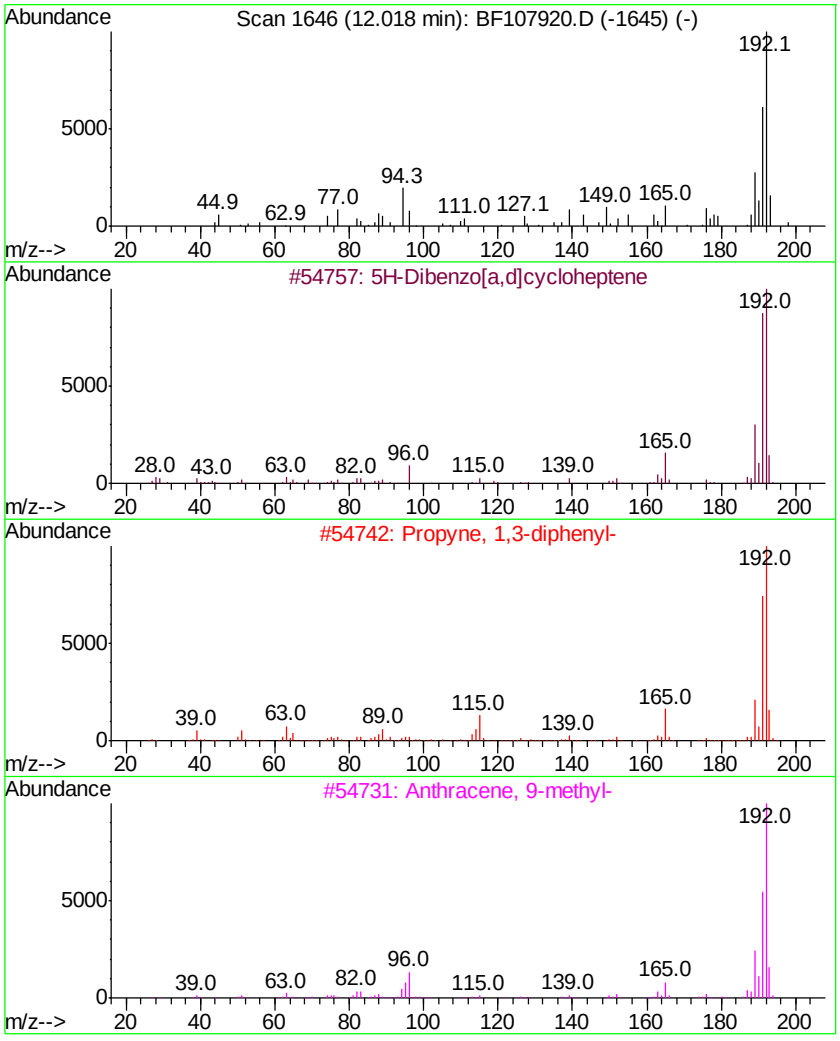
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

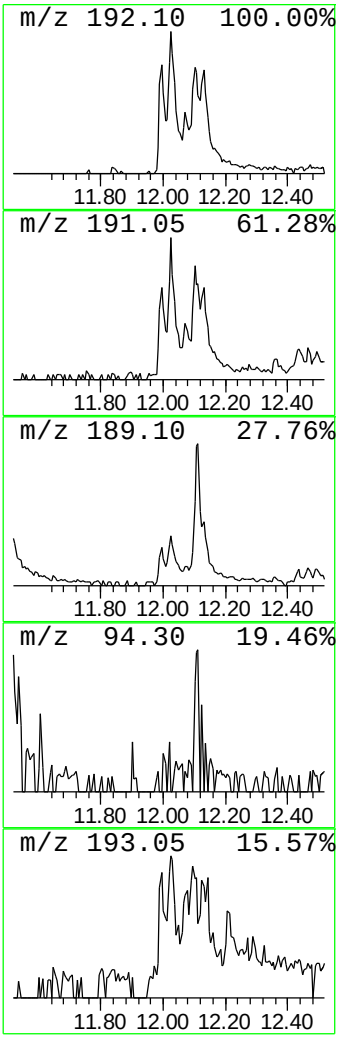
****

Peak Number 6 5H-Dibenzo[a,d]cycloheptene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	3.16 ng	108200	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	64
2	Propyne, 1,3-diphenyl-	192	C15H12	004980-70-5	64
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	59
4	2-Hydroxy-4-methyl-6-(2-thienyl)...	192	C9H8N2OS	026963-45-1	53
5	5-Methyl-2-phenylimino-1,3-thiaz...	192	C10H12N2S	013163-27-4	53





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Sample : J4285-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KG-PIT-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

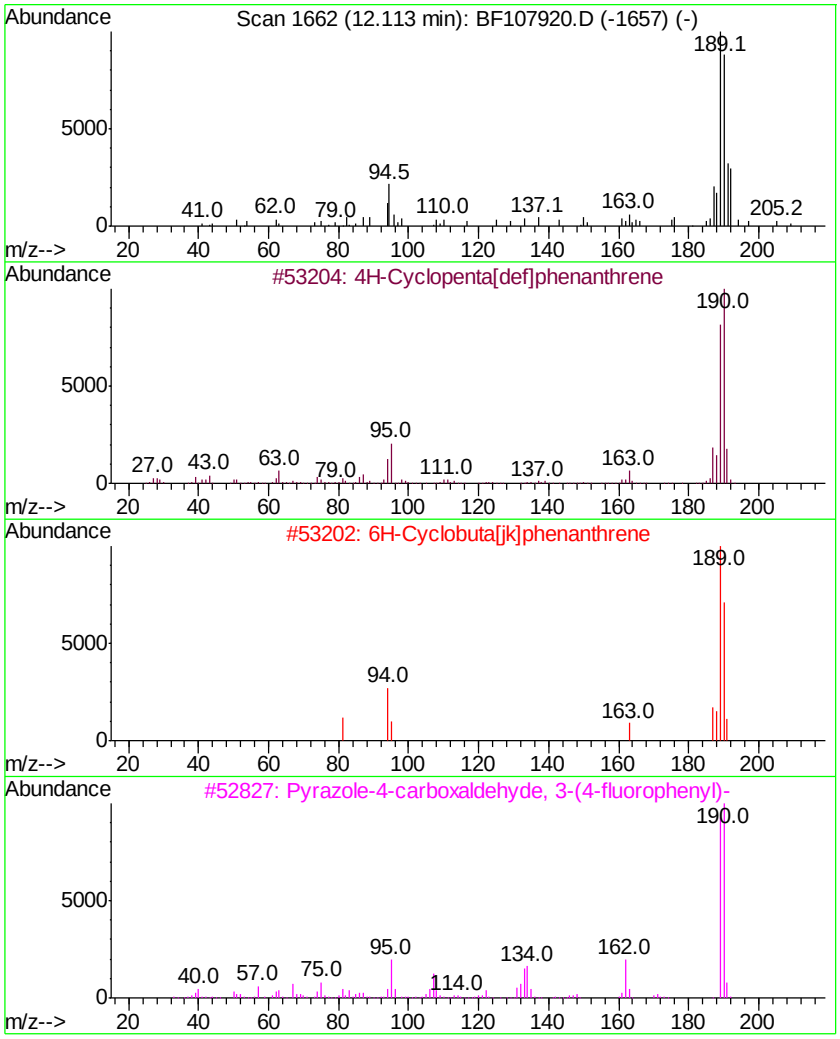
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

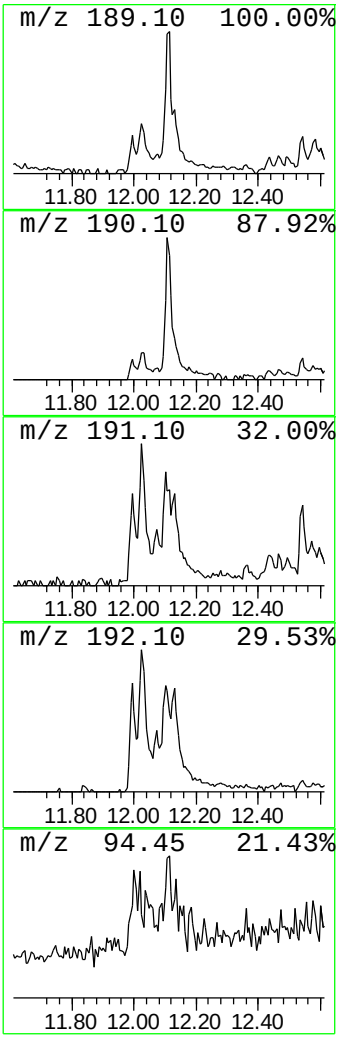
****

Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.11	2.94 ng	100717	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	68
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	59
3	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	49
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	28
5	3,5-Dichlorobenzoic acid	190	C7H4Cl2O2	000051-36-5	27





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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KG-PIT-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

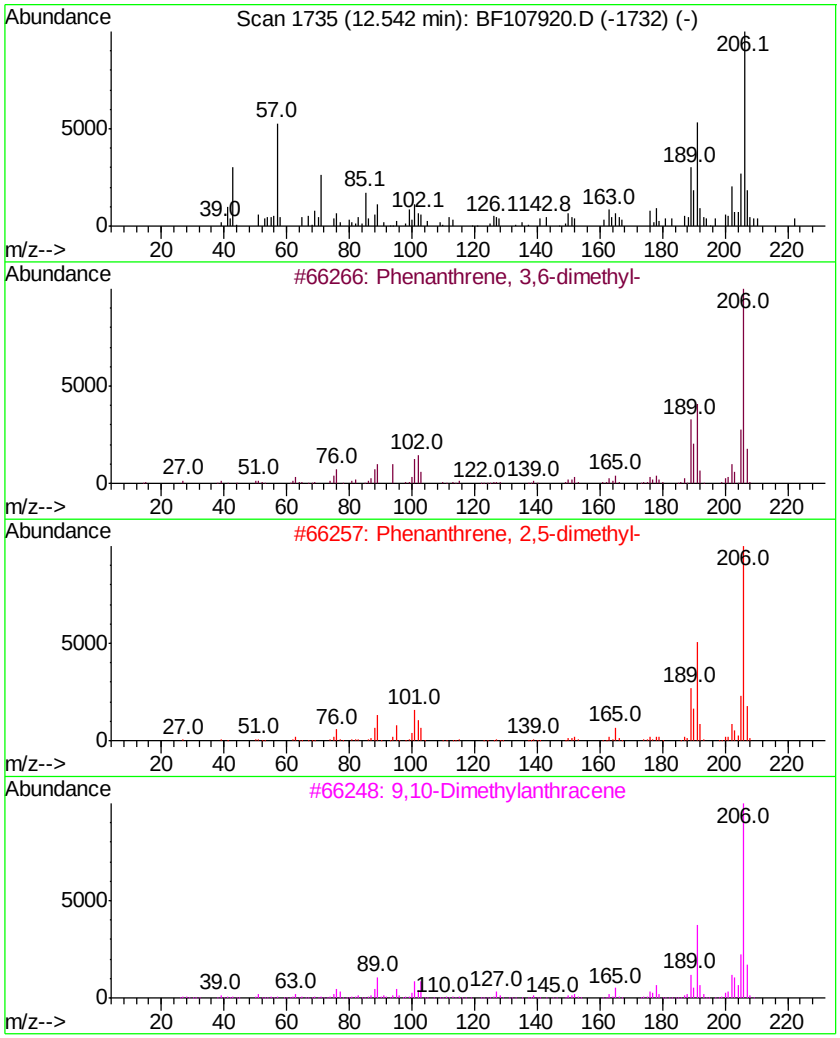
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

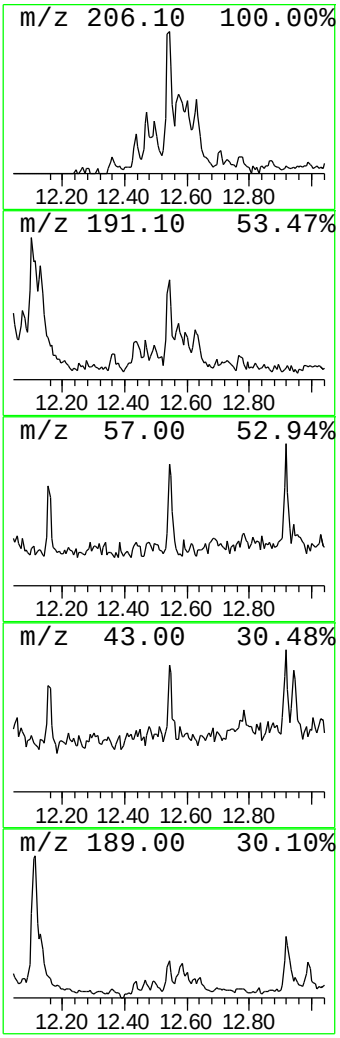
****

Peak Number 8 Phenanthrene, 3,6-dimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.54	2.04 ng	69973	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	93
2	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	91
3	9,10-Dimethylanthracene	206	C16H14	000781-43-1	90
4	1-Methyl-3-phenyl-1H-indene	206	C16H14	022360-62-9	76
5	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	76





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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KG-PIT-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

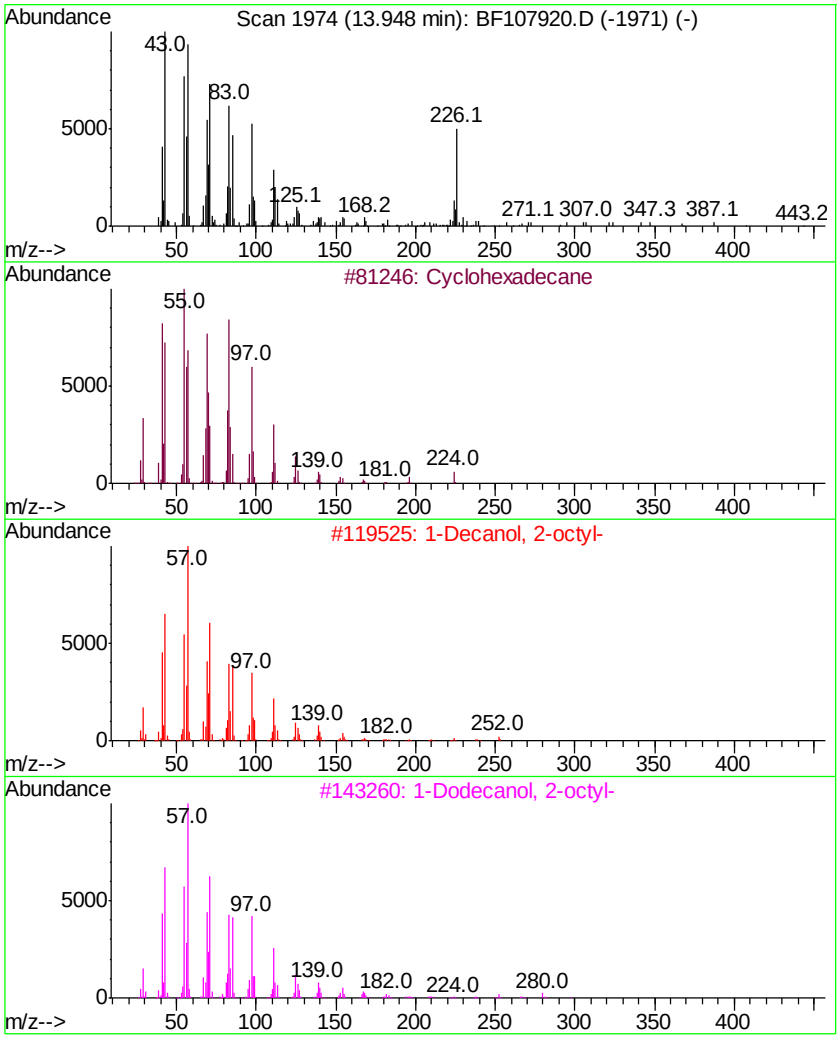
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

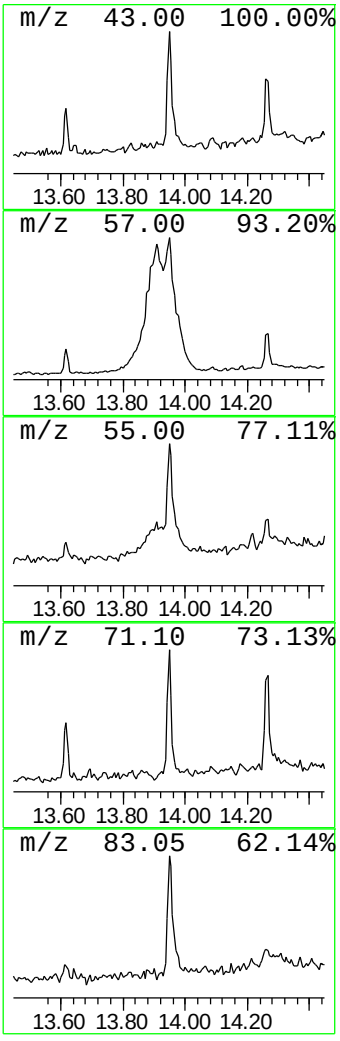
****

Peak Number 10 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	12.19 ng	715659	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	95
2	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	83
3	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	74
4	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	62
5	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	62





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Instrument : BNA_F
ClientSampleId : KG-PIT-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

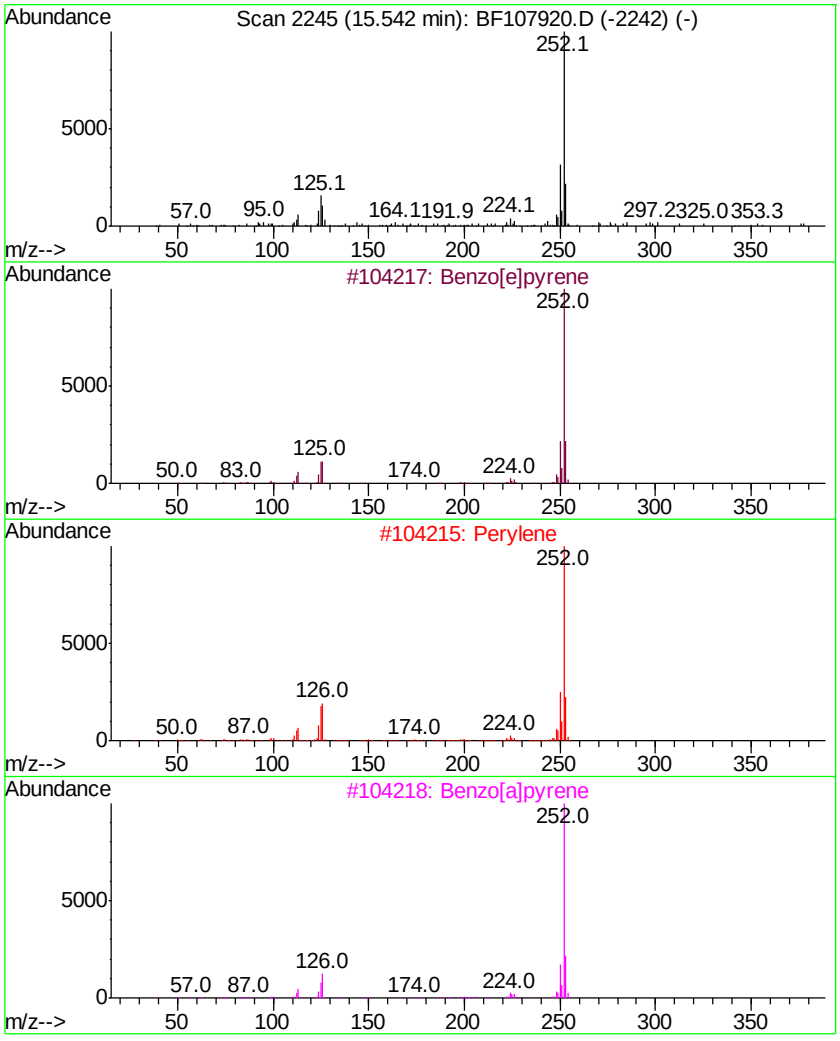
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

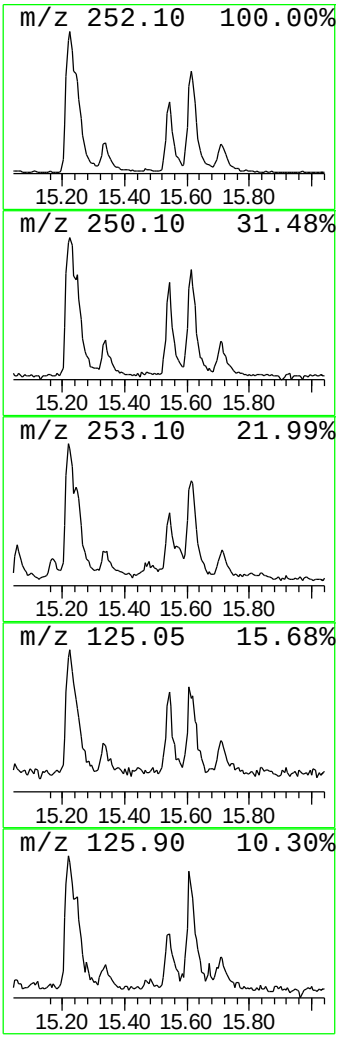
****

Peak Number 11 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.54	3.36 ng	111829	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	90
2	Perylene	252	C20H12	000198-55-0	81
3	Benzo[a]pyrene	252	C20H12	000050-32-8	76
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	76
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF080218\
Data File : BF107920.D
Acq On : 2 Aug 2018 20:12
Operator : JU/SJ
Sample : J4285-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KG-PIT-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.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...	5.19	12.2	ng	446867	1	6.96	733646	20.0
unknown6.73	6.73	79.0	ng	2897830	1	6.96	733646	20.0
2-Bromo dodecane	10.87	2.6	ng	90901	4	11.49	684788	20.0
Anthracene, 2-met...	12.00	3.7	ng	126284	4	11.49	684788	20.0
5H-Dibenzo[a,d]cy...	12.02	3.2	ng	108200	4	11.49	684788	20.0
4H-Cyclopenta[def...	12.11	2.9	ng	100717	4	11.49	684788	20.0
Phenanthrene, 3,6...	12.54	2.0	ng	69973	4	11.49	684788	20.0
Cyclohexadecane	13.95	12.2	ng	715659	5	14.14	1174530	20.0
Benzo[e]pyrene	15.54	3.4	ng	111829	6	15.68	666146	20.0