LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091119\
Data File : BF116970.D
Acq On : 12 Sep 2019 2:01
Operator : HP/JU
Sample : K4814-01 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-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-BF083019.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	5.434	565	569	584	rBV	656905	611027	51.40%	3.964%
2	6.451	738	742	760	rBV	712406	687125	57.80%	4.458%
3	6.592	762	766	769	rBV	770594	693769	58.36%	4.501%
4	6.822	802	805	816	rBV	482782	398439	33.52%	2.585%
5	6.981	828	832	844	rBV	595340	529283	44.52%	3.434%
6	7.381	896	900	919	rBV	414342	420604	35.38%	2.729%
7	8.104	1019	1023	1039	rBV	584908	563071	47.37%	3.653%
8	9.175	1201	1205	1216	rBV	984809	810532	68.18%	5.258%
9	9.563	1268	1271	1276	rBV	125115	110237	9.27%	0.715%
10	9.716	1294	1297	1301	rBV	34915	31838	2.68%	0.207%
11	9.851	1317	1320	1324	rBV	749035	665470	55.98%	4.317%
12	9.886	1324	1326	1329	rVB	23676	22131	1.86%	0.144%
13	10.057	1349	1355	1359	rBV	16471	18082	1.52%	0.117%
14	10.398	1410	1413	1419	rBV2	24715	27175	2.29%	0.176%
15	10.639	1450	1454	1466	rBV	544287	531034	44.67%	3.445%
16	10.769	1472	1476	1479	rBV3	24146	29558	2.49%	0.192%
17	11.075	1525	1528	1530	rBV3	15077	16722	1.41%	0.108%
18	11.139	1537	1539	1543	rBV	30188	32075	2.70%	0.208%
19	11.233	1552	1555	1560	rVB2	44523	48787	4.10%	0.317%
20	11.333	1569	1572	1574	rBV	760024	694829	58.45%	4.508%
21	11.357	1574	1576	1580	rVV	523845	446685	37.58%	2.898%
22	11.410	1582	1585	1589	rVV	87010	83569	7.03%	0.542%
23	11.445	1589	1591	1594	rVB3	13948	15391	1.29%	0.100%
24	11.563	1607	1611	1613	rBV2	45067	50327	4.23%	0.327%
25	11.627	1620	1622	1626	rVB3	26785	24694	2.08%	0.160%
26	11.669	1626	1629	1634	rBV5	19988	26648	2.24%	0.173%
27	11.792	1648	1650	1652	rBV2	16605	14189	1.19%	0.092%
28	11.833	1654	1657	1659	rVV	67732	62559	5.26%	0.406%
29	11.863	1659	1662	1666	rVB	161959	139102	11.70%	0.902%
30	11.910	1668	1670	1673	rBV	29082	22718	1.91%	0.147%
31	11.945	1673	1676	1679	rBV2	106139	129614	10.90%	0.841%
32	12.127	1704	1707	1709	rBV	63849	57640	4.85%	0.374%
33	12.157	1709	1712	1716	rVB2	56439	65125	5.48%	0.423%
34	12.280	1731	1733	1735	rVB2	29039	20692	1.74%	0.134%

LSC Area Percent Report

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Data File : BF116970.D
Acq On : 12 Sep 2019 2:01
Operator : HP/JU
Sample : K4814-01 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-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-BF083019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.316	1736	1739	1741	rBV3	34401	32414	2.73%	0.210%
36	12.386	1748	1751	1754	rBV2	71661	89002	7.49%	0.577%
37	12.469	1762	1765	1770	rBV	64212	67295	5.66%	0.437%
38	12.545	1774	1778	1783	rBV	847911	778472	65.49%	5.050%
39	12.639	1792	1794	1797	rBV2	79272	79441	6.68%	0.515%
40	12.774	1811	1817	1823	rBV	791819	803620	67.60%	5.214%
41	12.822	1823	1825	1830	rVV2	34967	40423	3.40%	0.262%
42	12.916	1837	1841	1849	rVB	987763	910022	76.55%	5.904%
43	12.992	1850	1854	1857	rBV2	69650	114532	9.63%	0.743%
44	13.098	1870	1872	1875	rVB	88564	84653	7.12%	0.549%
45	13.204	1888	1890	1898	rVB2	84903	98418	8.28%	0.639%
46	13.604	1956	1958	1964	rVB	92038	94577	7.96%	0.614%
47	13.745	1980	1982	1984	rVB	58311	44920	3.78%	0.291%
48	13.768	1984	1986	1988	rBV	41215	39168	3.29%	0.254%
49	13.816	1992	1994	2000	rVB4	88430	132849	11.18%	0.862%
50	13.968	2013	2020	2023	rBV3	744525	1188736	100.00%	7.712%
51	13.992	2023	2024	2030	rVB	306571	259472	21.83%	1.683%
52	14.998	2191	2195	2203	rBV	282510	530303	44.61%	3.440%
53	15.068	2204	2207	2210	rVB2	64124	72910	6.13%	0.473%
54	15.104	2211	2213	2216	rVB	54197	45864	3.86%	0.298%
55	15.292	2242	2245	2252	rVB	160769	220529	18.55%	1.431%
56	15.357	2252	2256	2261	rVV	214046	293324	24.68%	1.903%
57	15.415	2262	2266	2278	rVB2	409024	710959	59.81%	4.612%
58	16.527	2451	2455	2467	rVB8	57727	147777	12.43%	0.959%
59	16.845	2504	2509	2517	rVB2	110931	203531	17.12%	1.320%
60	17.086	2544	2550	2556	rBV6	27719	78245	6.58%	0.508%
61	17.274	2578	2582	2592	rVB	76325	151603	12.75%	0.984%

Sum of corrected areas: 15413800

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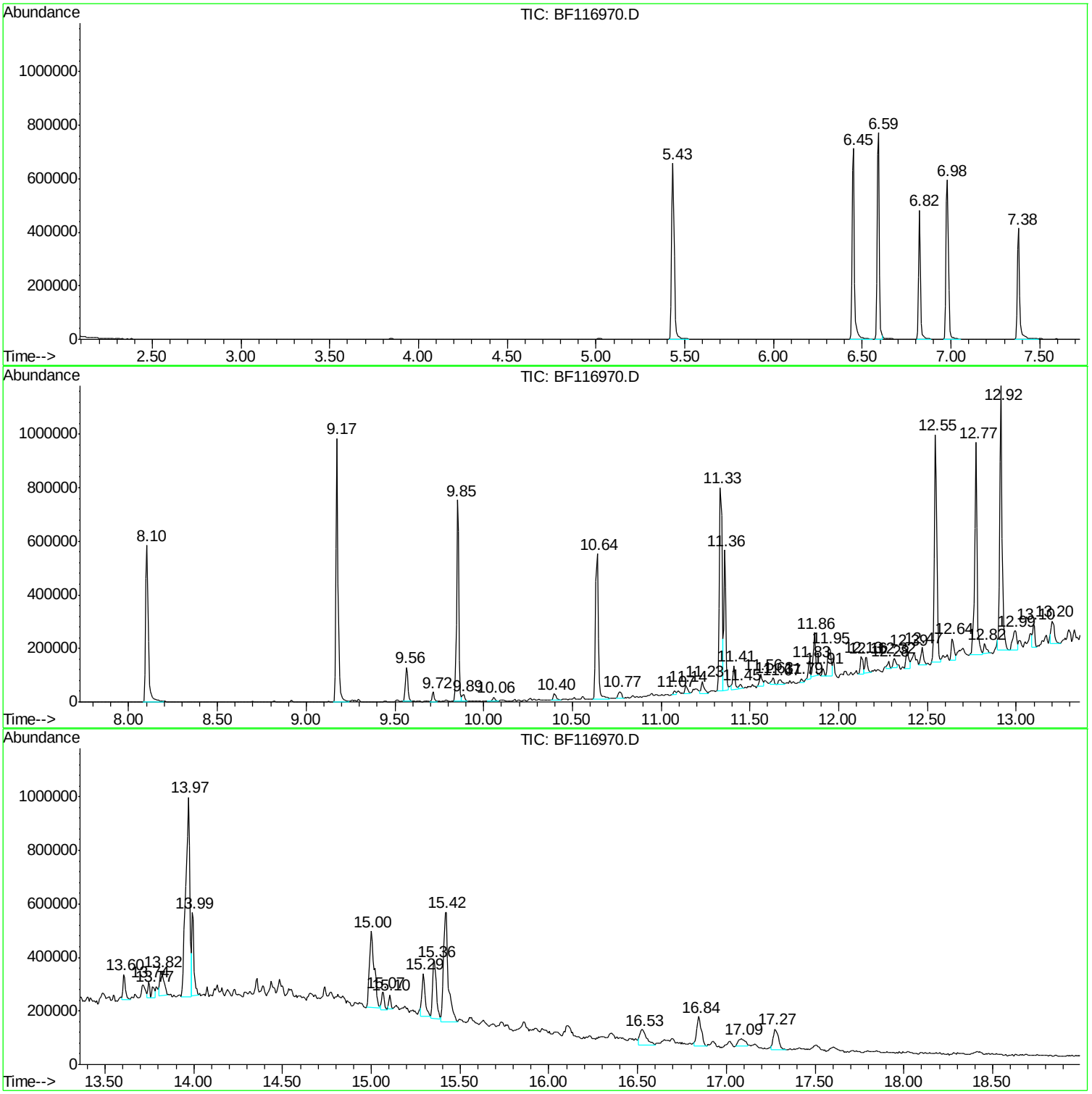
Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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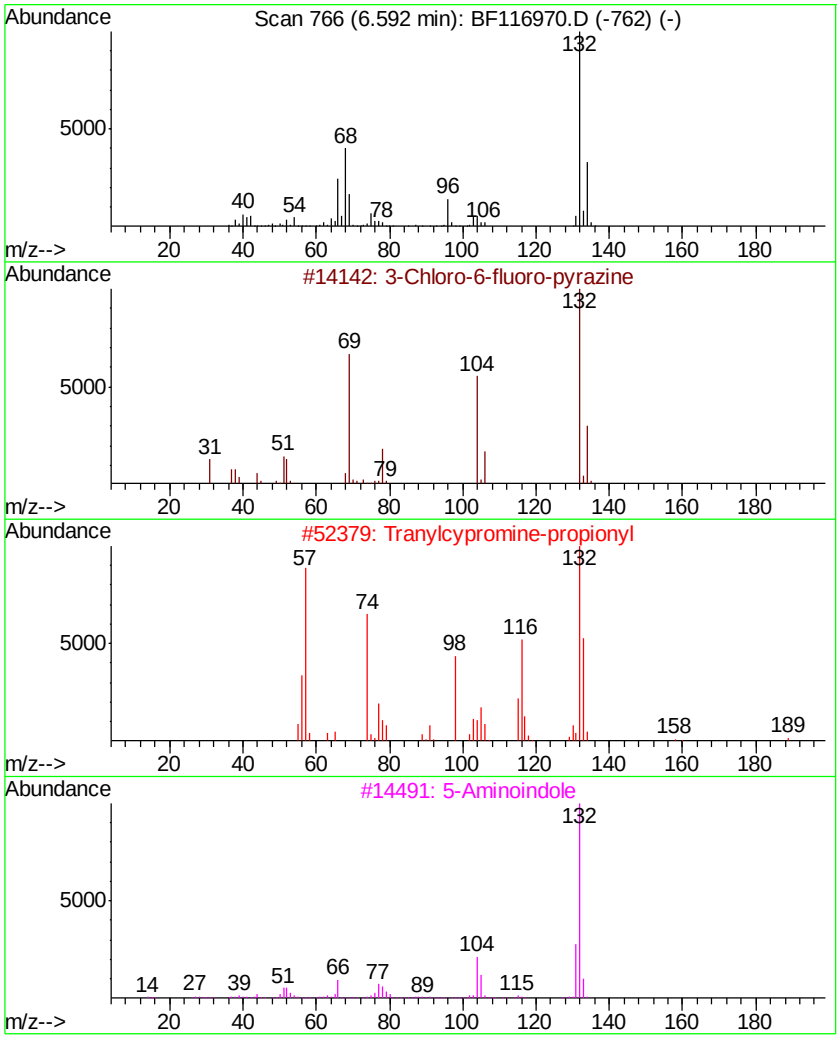
TIC Integration Parameters: LSCINT.P

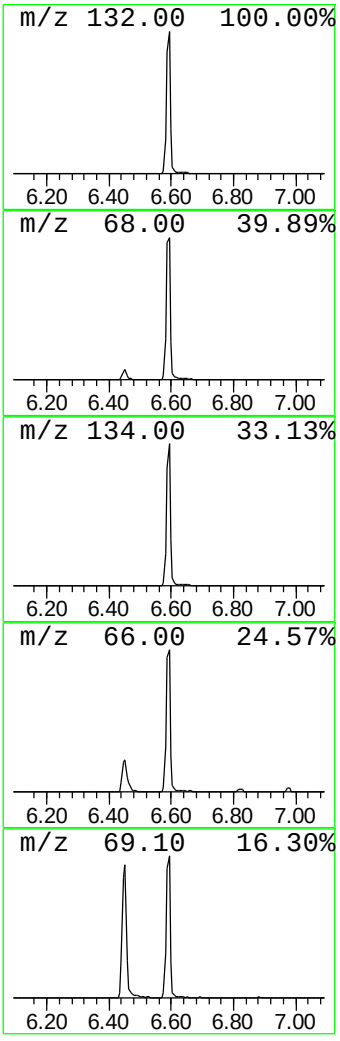
****

Peak Number 1 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	34.82 ng	693769	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

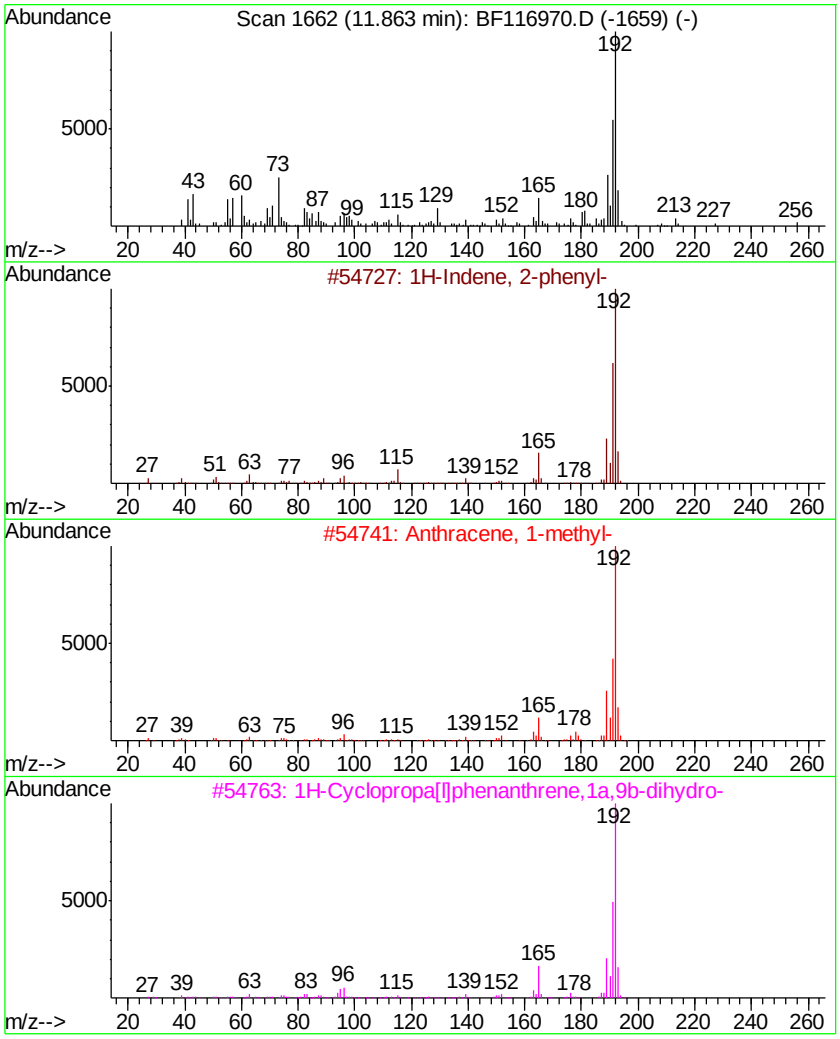
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

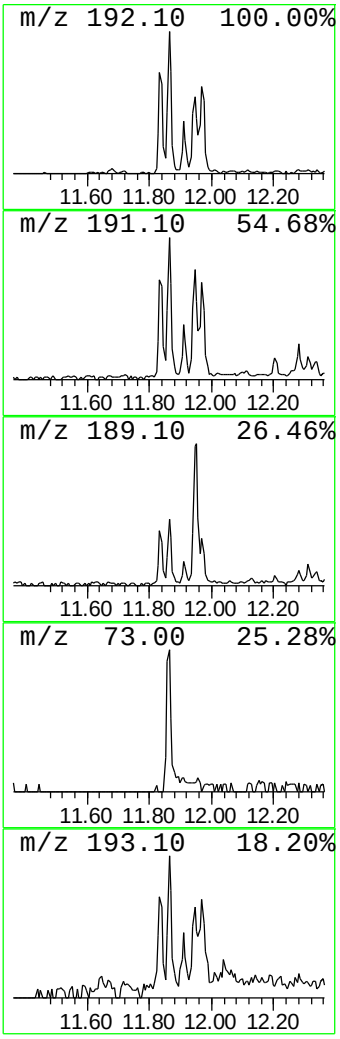
****

Peak Number 3 1H-Indene, 2-phenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	4.00 ng	139102	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	96
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	96
3	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	95
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93





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Sample : K4814-01 2X
Misc :
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Instrument : BNA_F
ClientSampleId : WC-1

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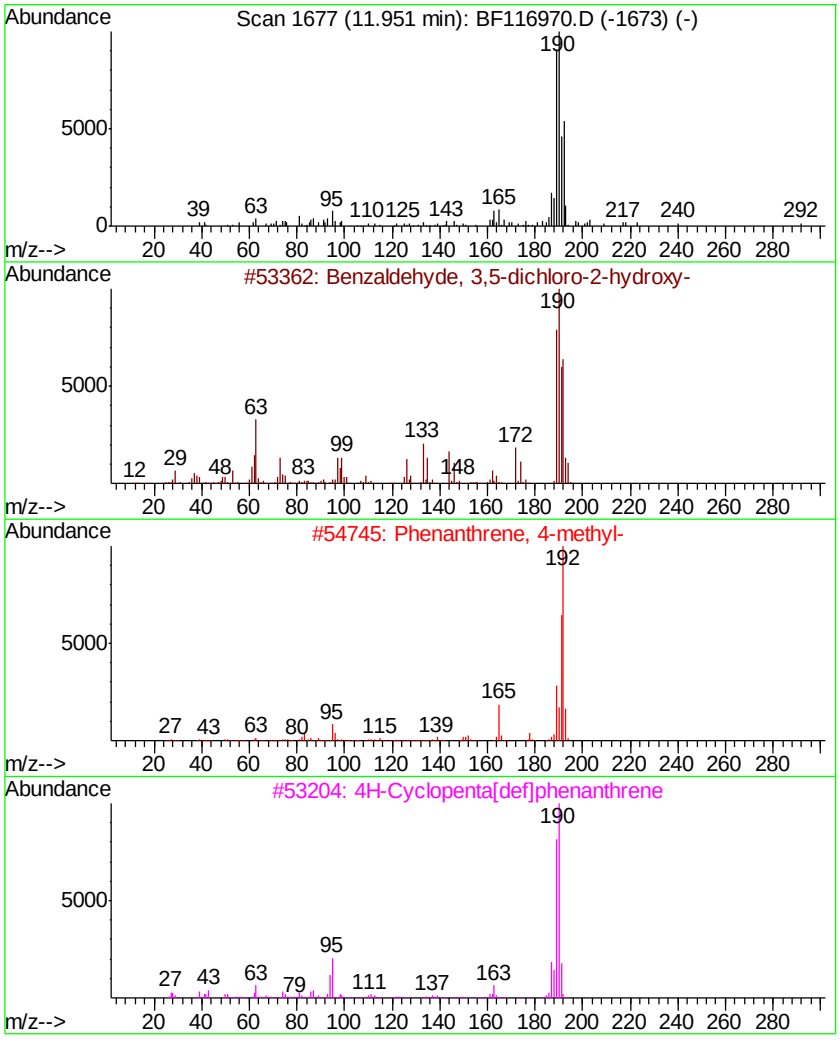
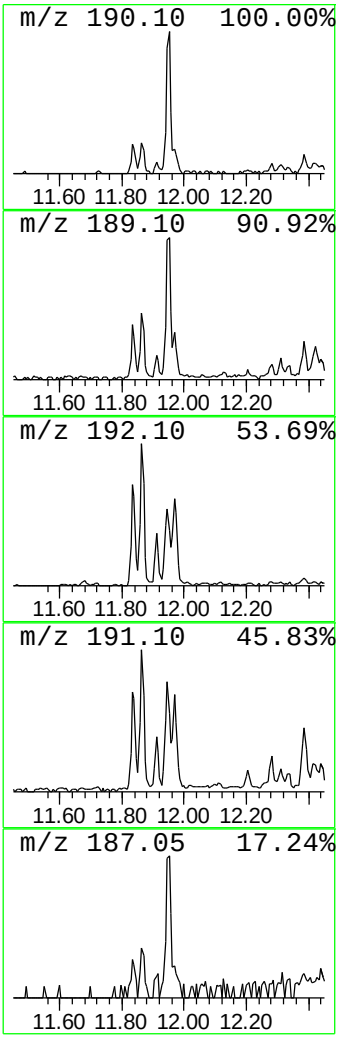
****

Peak Number 4 Benzaldehyde, 3,5-dichloro-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	3.73 ng	129614	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	86
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	50
3	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	45
4	Propyne, 1,3-diphenyl-	192	C15H12	004980-70-5	43
5	Benzene, 1,1'-(1,2-propadienylid...	192	C15H12	014251-57-1	43





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Misc :
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Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

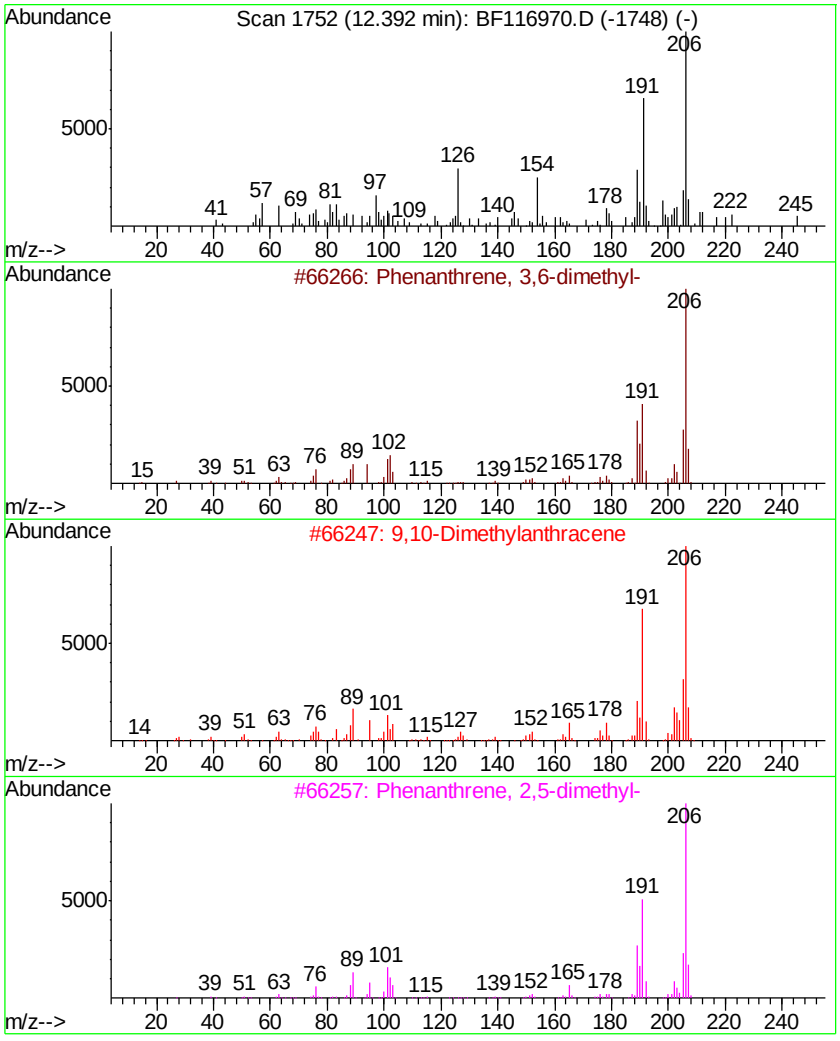
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

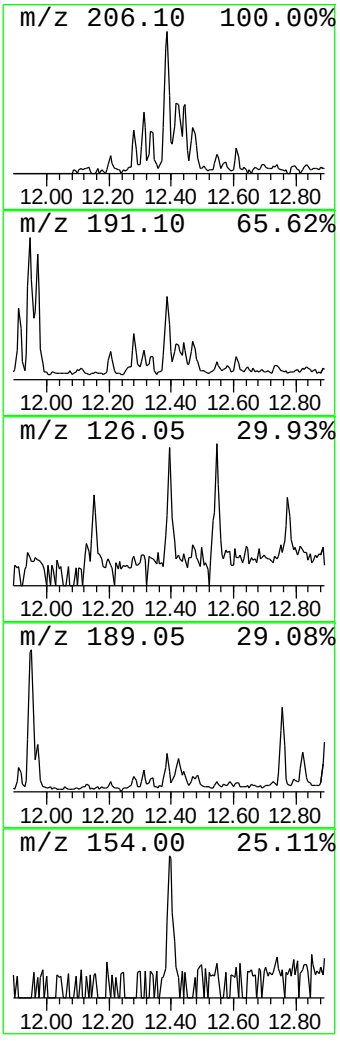
****

Peak Number 5 Phenanthrene, 3,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.39	2.56 ng	89002	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	93
2	9,10-Dimethylanthracene	206	C16H14	000781-43-1	93
3	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	91
4	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	91
5	1,3-Diphenyl-3-methylcyclopropene	206	C16H14	086544-79-8	87





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Misc :
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Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

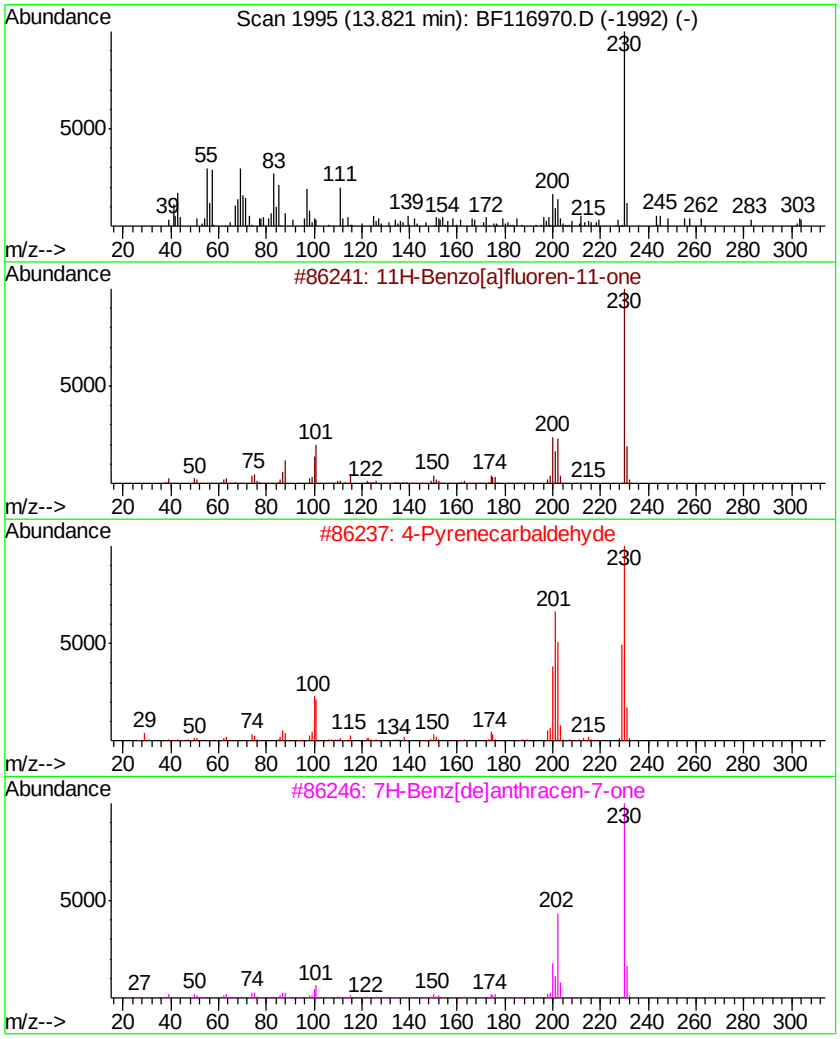
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

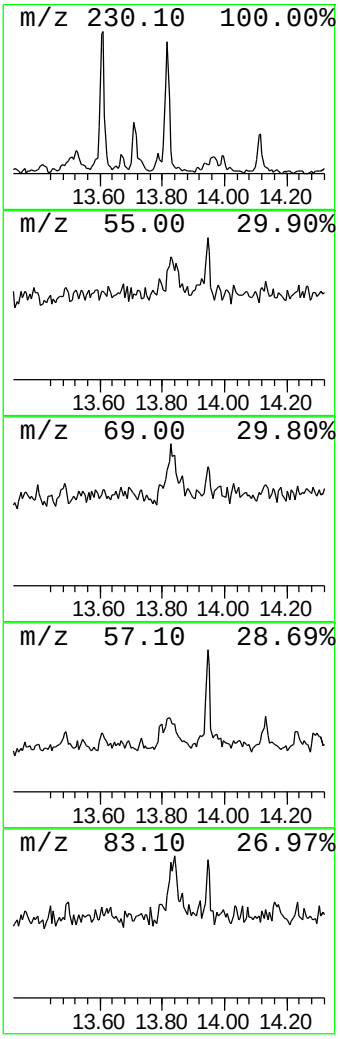
****

Peak Number 7 11H-Benzo[a]fluoren-11-one Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	2.24 ng	132849	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	83
2	4-Pyrenecarbaldehyde	230	C17H10O	022245-51-8	83
3	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	81
4	1-Pyrenecarboxaldehyde	230	C17H10O	003029-19-4	72
5	6H-Benz[de]anthracen-6-one	230	C17H10O	080252-14-8	64





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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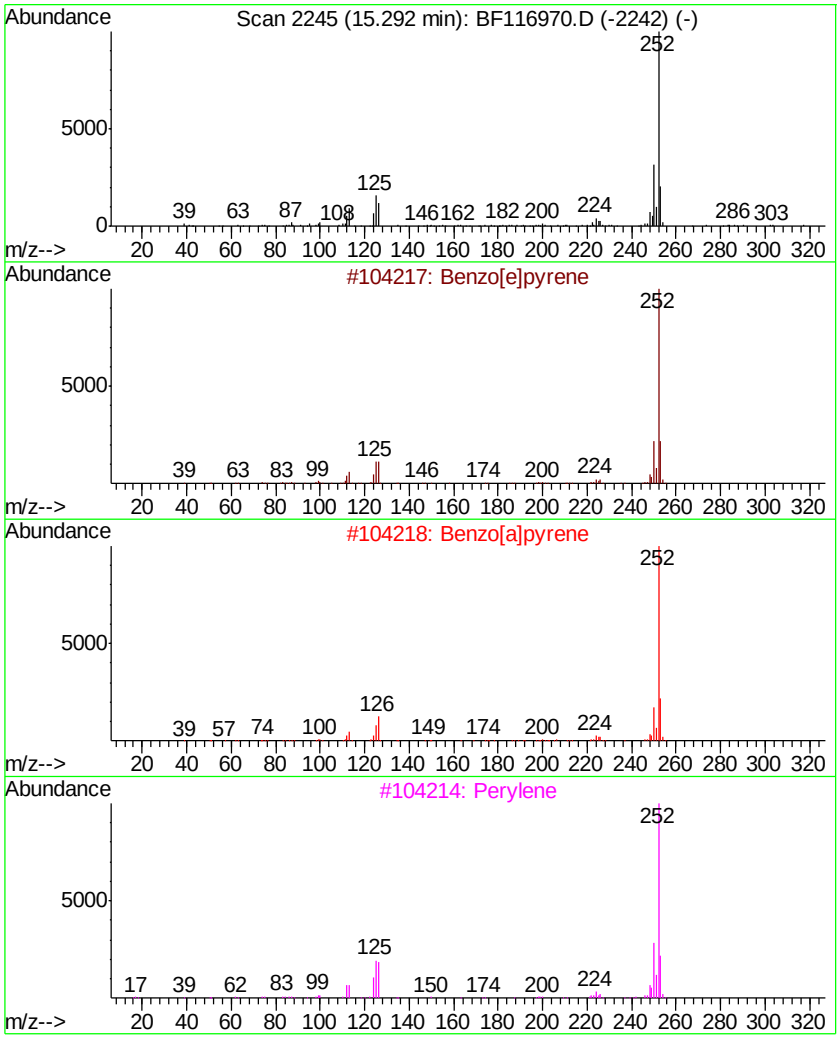
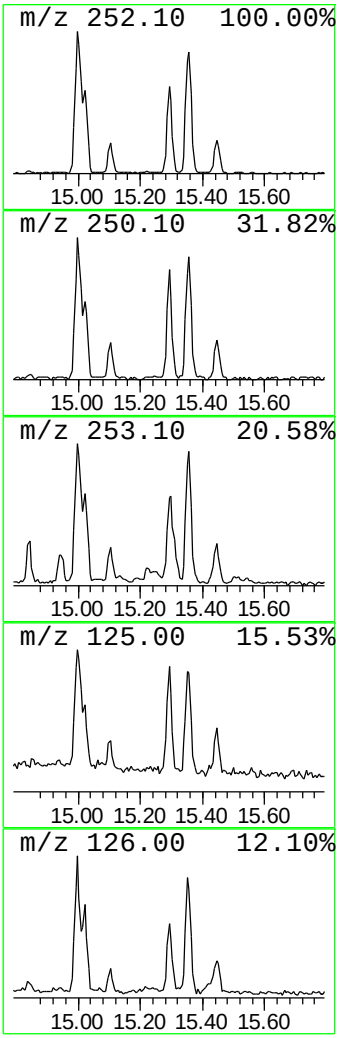
****

Peak Number 8 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.29	6.20 ng	220529	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[a]pyrene	252	C20H12	000050-32-8	94
3	Perylene	252	C20H12	000198-55-0	94
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	94
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93





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Misc :
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Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

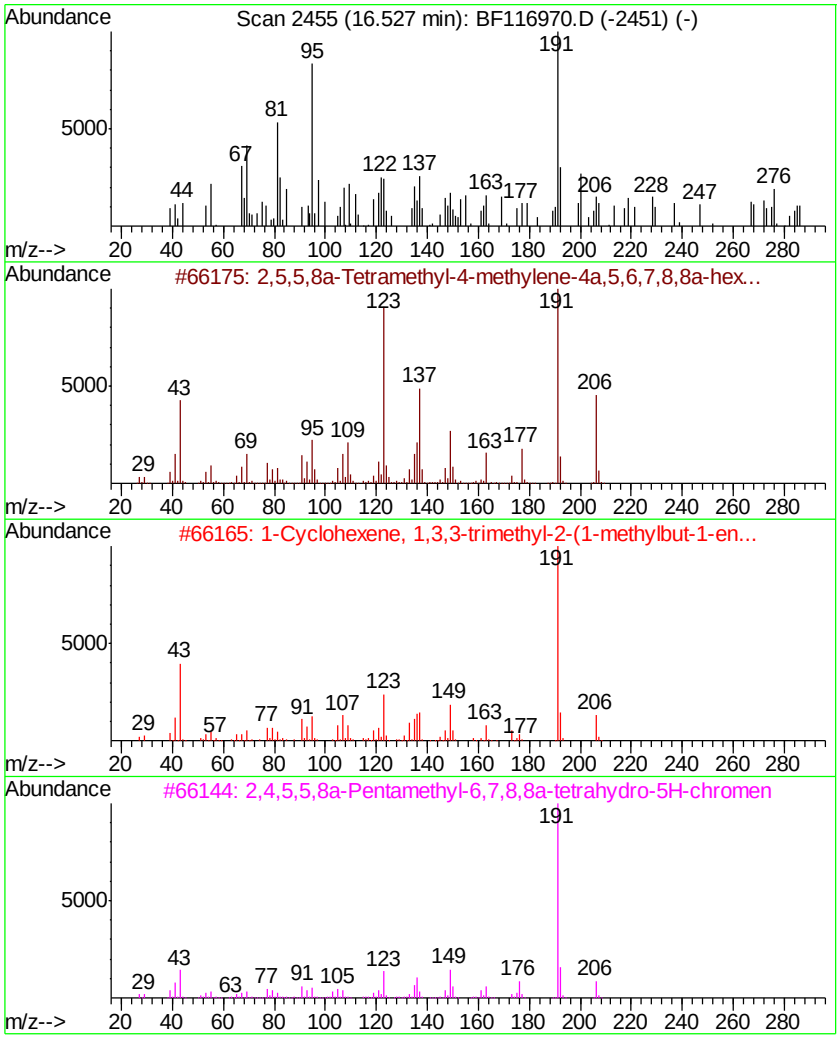
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

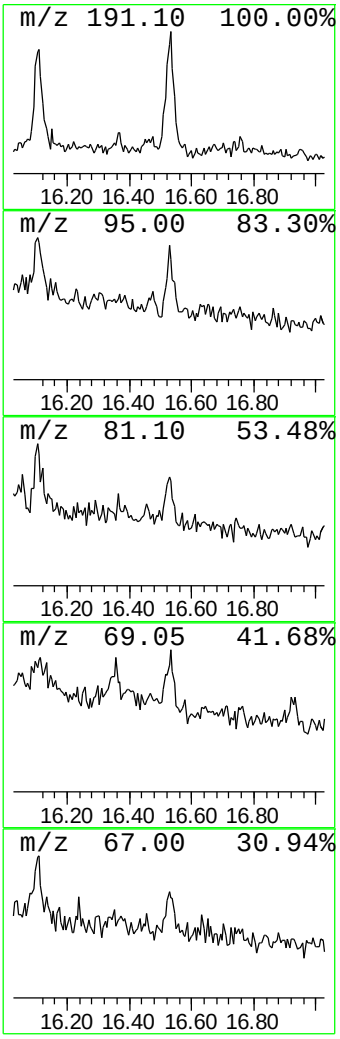
****

Peak Number 9 unknown16.53 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	4.16 ng	147777	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5,5,8a-Tetramethyl-4-methylene...	206	C14H22O	093175-76-9	38
2	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	25
3	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	25
4	N-(3,4,5,6-Tetrahydro-1,3-thiazi...	192	C10H12N2S	003420-40-4	22
5	2-Phenylamino-5,6(4H)dihydro-1,3...	192	C10H12N2S	1000147-35-4	22





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ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

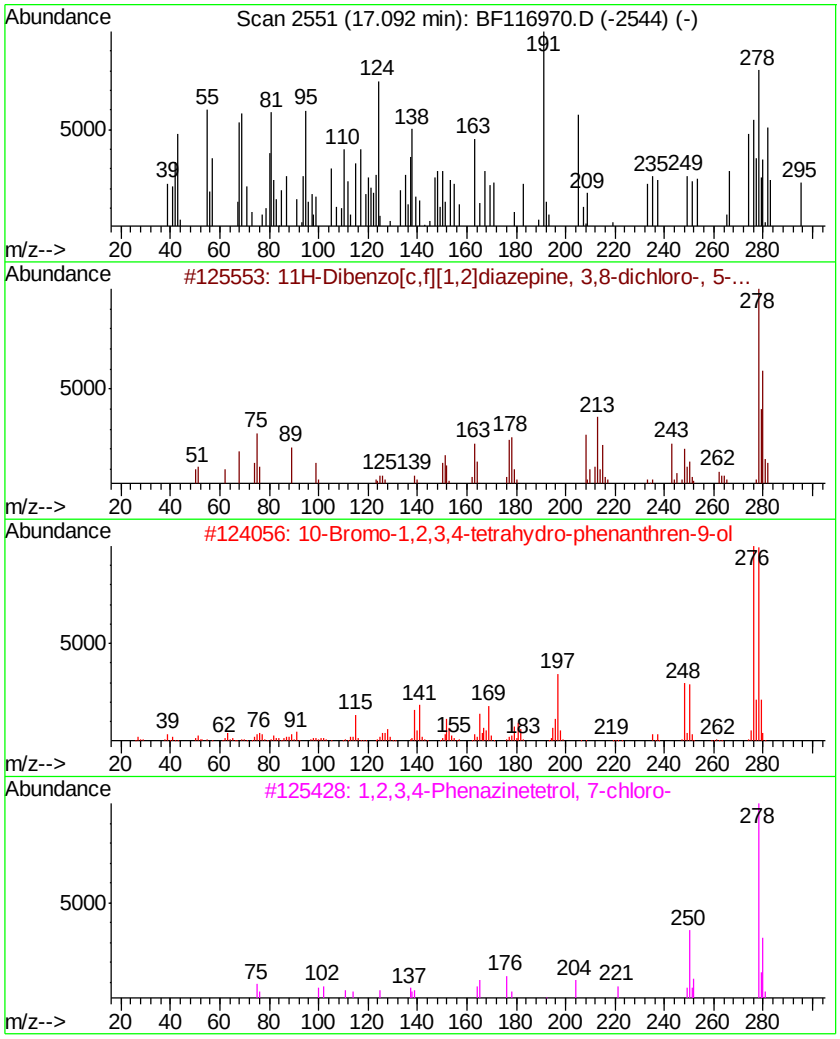
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

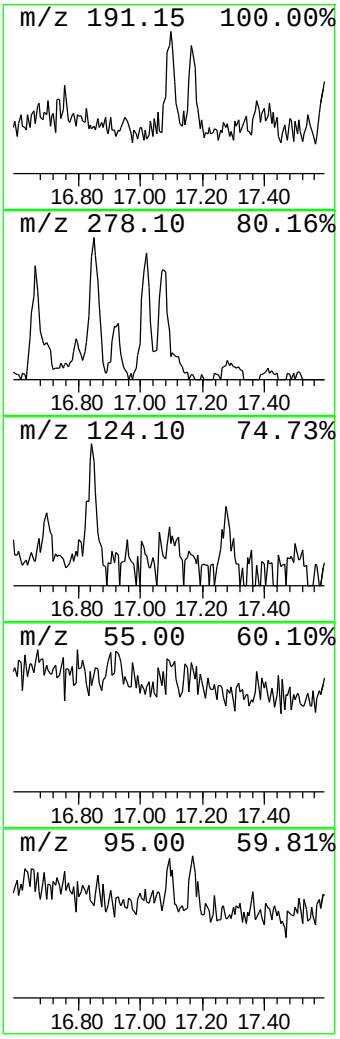
****

Peak Number 10 unknown17.09 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.09	2.20 ng	78245	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Dibenzo[c,f][1,2]diazepine, ...	278	C13H8Cl2N2O	000958-71-4	27
2	10-Bromo-1,2,3,4-tetrahydro-phen...	276	C14H13BrO	1000190-54-9	14
3	1,2,3,4-Phenazinetetrol, 7-chloro-	278	C12H7ClN2O4	023774-10-9	14
4	1-Butaneboronic acid, cyclic dip...	278	C18H19BO2	024371-99-1	14
5	Phenol, 2-[3-[2-(4-hydroxyphenyl...	279	C16H13N3O2	1000362-51-6	12





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091119\
Data File : BF116970.D
Acq On : 12 Sep 2019 2:01
Operator : HP/JU
Sample : K4814-01 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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
unknown6.59	6.59	34.8	ng	693769	1	6.82	398439	20.0
1H-Indene, 2-phenyl-	11.86	4.0	ng	139102	4	11.33	694829	20.0
Benzaldehyde, 3,5...	11.95	3.7	ng	129614	4	11.33	694829	20.0
Phenanthrene, 3,6...	12.39	2.6	ng	89002	4	11.33	694829	20.0
11H-Benzo[a]fluor...	13.82	2.2	ng	132849	5	13.97	1188740	20.0
Benzo[e]pyrene	15.29	6.2	ng	220529	6	15.42	710959	20.0
unknown16.53	16.53	4.2	ng	147777	6	15.42	710959	20.0
unknown17.09	17.09	2.2	ng	78245	6	15.42	710959	20.0