LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042123\
Data File : BF132982.D
Acq On : 21 Apr 2023 22:05
Operator : CG\JU
Sample : 02389-27 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPB-7WC-23-04-17

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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132982.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.746	275	282	288	rBV	44151	66823	3.42%	0.244%
2	4.934	480	484	490	rVB	80167	86572	4.43%	0.316%
3	5.351	552	555	559	rVB	1763221	1621439	82.91%	5.918%
4	6.381	726	730	733	rBV	2099068	1597635	81.69%	5.831%
5	6.575	761	763	765	rBV	41113	40299	2.06%	0.147%
6	6.751	789	793	796	rBV	1642381	1265262	64.70%	4.618%
7	7.157	858	862	865	rBV2	36968	43089	2.20%	0.157%
8	7.310	880	888	891	rBV	1329190	1059504	54.18%	3.867%
9	7.975	998	1001	1004	rBV2	45727	39213	2.01%	0.143%
10	8.034	1007	1011	1013	rVV	2136532	1629507	83.32%	5.947%
11	8.057	1013	1015	1018	rVB	205494	154680	7.91%	0.565%
12	8.745	1130	1132	1136	rVB	113251	83653	4.28%	0.305%
13	8.792	1136	1140	1146	rBV	41875	65945	3.37%	0.241%
14	8.845	1146	1149	1152	rVV2	63476	55683	2.85%	0.203%
15	9.110	1190	1194	1197	rBV	2288797	1682406	86.03%	6.140%
16	9.198	1204	1209	1214	rBV3	97910	161887	8.28%	0.591%
17	9.369	1235	1238	1242	rBV	38812	53163	2.72%	0.194%
18	9.445	1249	1251	1254	rBV3	55412	46964	2.40%	0.171%
19	9.498	1258	1260	1262	rBV2	48070	42306	2.16%	0.154%
20	9.645	1283	1285	1287	rBV	37589	43633	2.23%	0.159%
21	9.728	1297	1299	1301	rBV	59173	51845	2.65%	0.189%
22	9.786	1304	1309	1312	rVV	1993849	1622292	82.95%	5.921%
23	9.816	1312	1314	1322	rVB	208595	238497	12.20%	0.870%
24	9.986	1341	1343	1347	rVB	121324	99016	5.06%	0.361%
25	10.198	1376	1379	1382	rBV2	69744	67855	3.47%	0.248%
26	10.333	1399	1402	1406	rBV	112646	97021	4.96%	0.354%
27	10.422	1414	1417	1427	rBV2	301750	635143	32.48%	2.318%
28	10.498	1427	1430	1433	rVB2	131705	149781	7.66%	0.547%
29	10.569	1439	1442	1447	rBV	893084	795970	40.70%	2.905%
30	10.616	1448	1450	1452	rVV2	63149	51166	2.62%	0.187%
31	10.710	1462	1466	1471	rBV6	87638	150052	7.67%	0.548%
32	10.880	1492	1495	1498	rBV	195257	169191	8.65%	0.617%
33	11.069	1525	1527	1531	rBV	87643	81281	4.16%	0.297%
34	11.269	1558	1561	1563	rBV	1532586	1280697	65.49%	4.674%
35	11.292	1563	1565	1568	rVV	1447293	1081439	55.30%	3.947%
36	11.339	1571	1573	1576	rVV	272481	243497	12.45%	0.889%

LSC Area Percent Report

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Misc :
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Instrument :
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ClientSampleId :
SPB-7WC-23-04-17

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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.810	1649	1653	1657	rBV3	324087	540819	27.65%	1.974%
38	11.886	1662	1666	1668	rBV3	241836	349461	17.87%	1.275%
39	12.086	1698	1700	1702	rBV	301814	198212	10.14%	0.723%
40	12.480	1764	1767	1771	rVB	1630579	1451828	74.24%	5.299%
41	12.710	1803	1806	1809	rVB	1303178	1200301	61.37%	4.381%
42	12.857	1828	1831	1835	rBV	1307563	1168970	59.77%	4.266%
43	13.910	2006	2010	2013	rBV3	1640668	1955691	100.00%	7.138%
44	14.057	2032	2035	2038	rVB	1349256	1117161	57.12%	4.077%
45	14.121	2044	2046	2053	rVB	1247952	1337732	68.40%	4.882%
46	15.227	2231	2234	2240	rVB	642496	869521	44.46%	3.173%
47	15.345	2252	2254	2257	rVB2	589438	555563	28.41%	2.028%

Sum of corrected areas: 27399665

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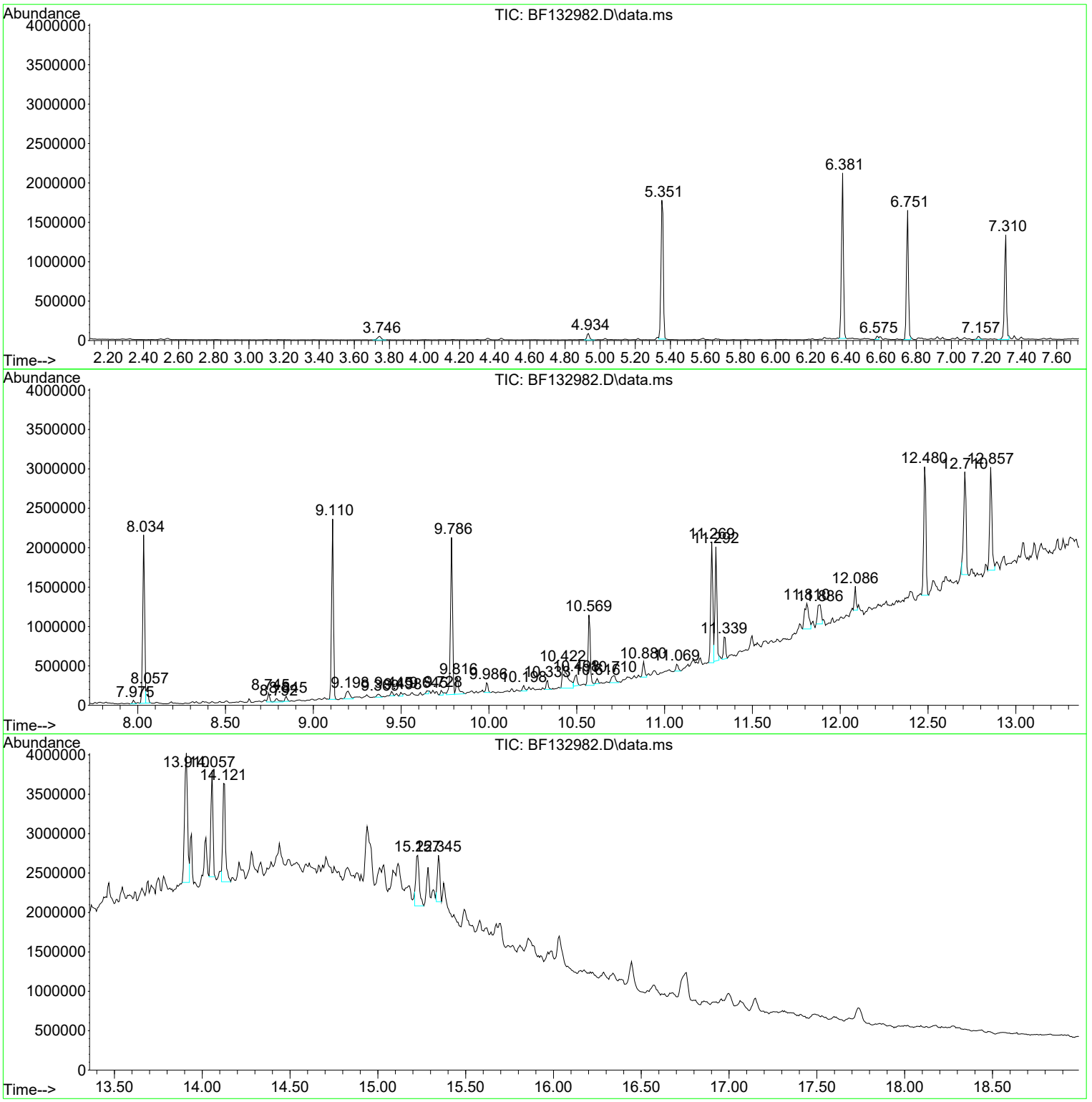
Instrument :
BNA_F
ClientSampleId :
SPB-7WC-23-04-17

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042123\
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Instrument :
BNA_F
ClientSampleId :
SPB-7WC-23-04-17

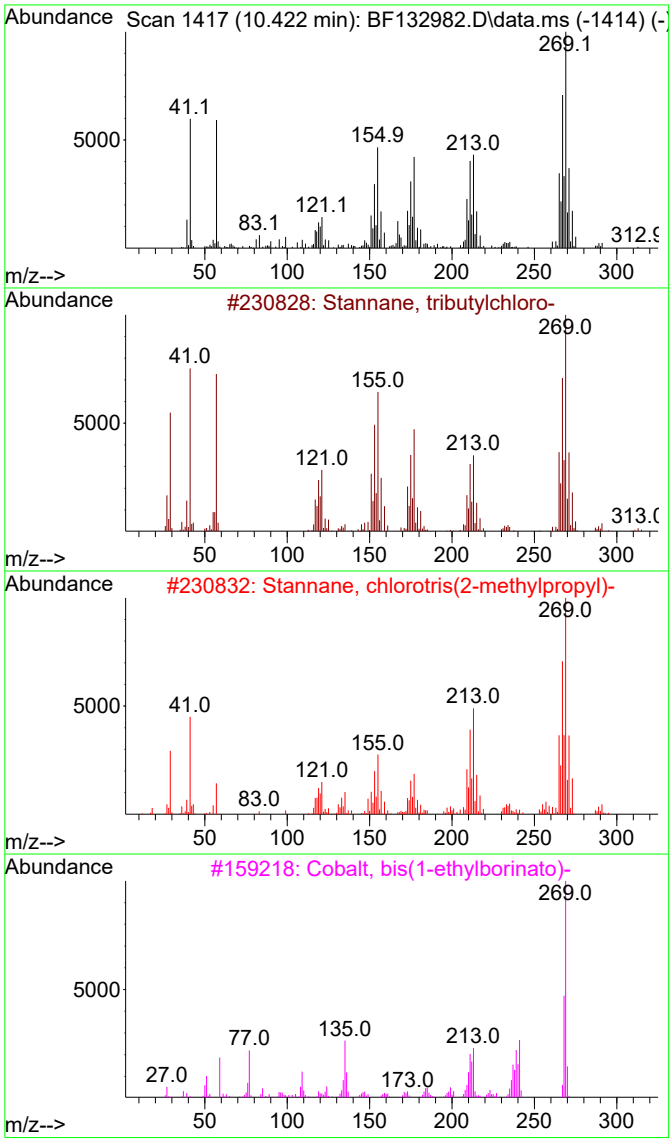
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

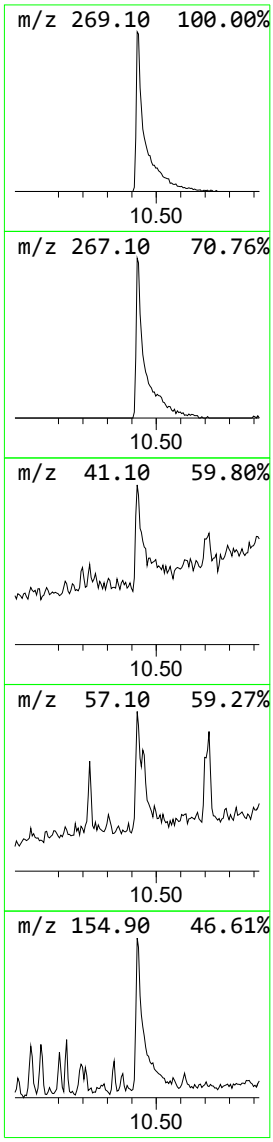
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Stannane, tributylchloro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.422	7.83 ng	635143	Acenaphthene-d10	9.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Stannane, tributylchloro-	326	C12H27ClSn	001461-22-9	91
2	Stannane, chlorotris(2-methylpro...	326	C12H27ClSn	007342-38-3	87
3	Cobalt, bis(1-ethylborinato)-	269	C14H20B2Co	1000151-48-2	22
4	N-Methyl-2-(4-chlorophenyl)eth-2...	268	C16H13ClN2	002562-96-1	15
5	1,2-Diphenyl-1H-indole	269	C20H15N	018434-12-3	14





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

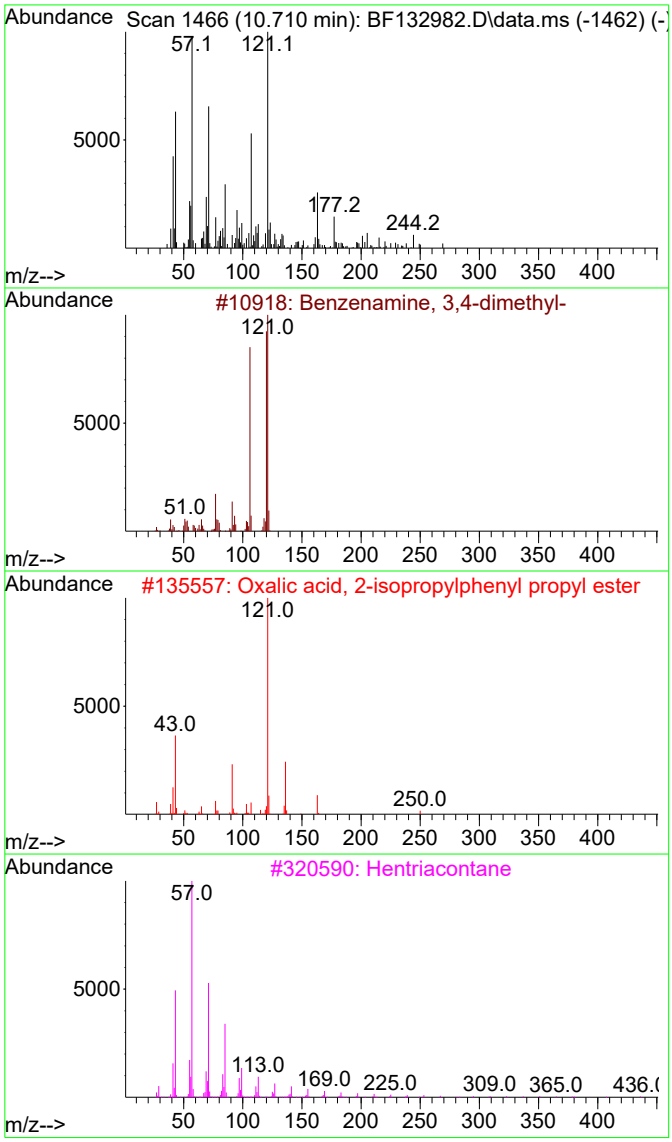
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

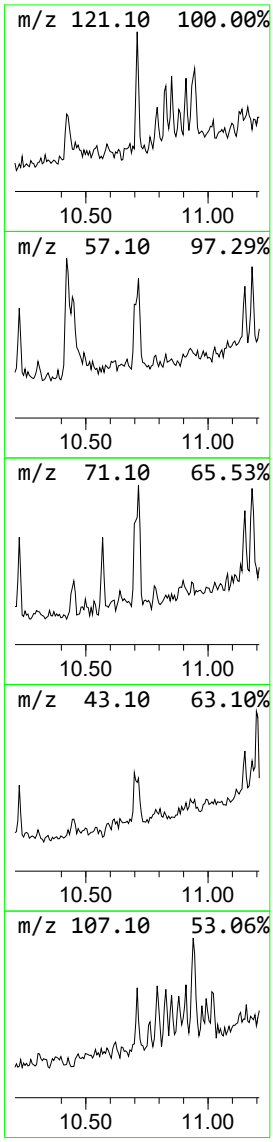
****

Peak Number 2 Benzenamine, 3,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.710	2.34 ng	150052	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 3,4-dimethyl-	121	C8H11N	000095-64-7	25
2	Oxalic acid, 2-isopropylphenyl p...	250	C14H18O4	1000309-56-1	22
3	Hentriacontane	437	C31H64	000630-04-6	18
4	Benzenemethanol, .alpha.-butyl-....	178	C12H18O	004396-98-9	18
5	1H-1,2,3,4-Tetrazole-1,5-diamine...	220	C9H12N6O	1000349-95-8	18





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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPB-7WC-23-04-17

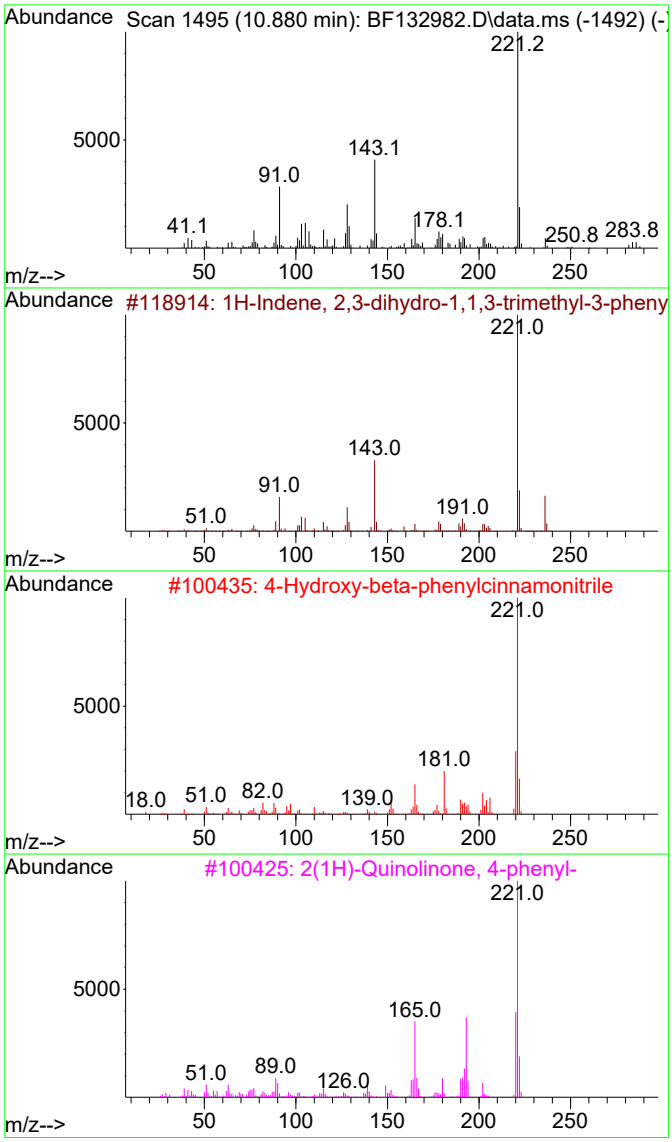
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

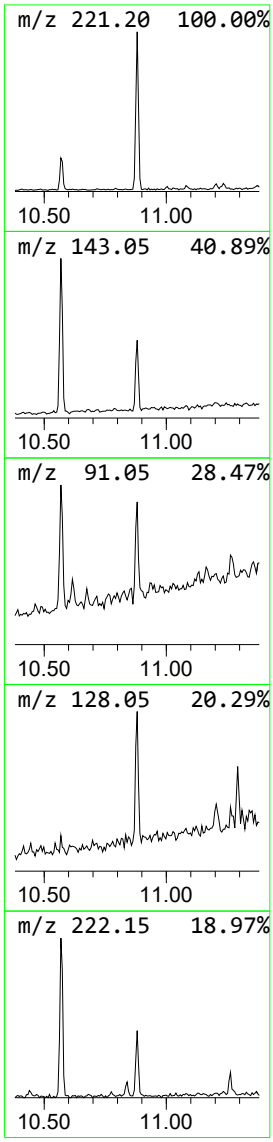
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1H-Indene, 2,3-dihydro-1,1,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.880	2.64 ng	169191	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	64
2	4-Hydroxy-beta-phenylcinnamonitrile	221	C15H11NO	016281-90-6	46
3	2(1H)-Quinolinone, 4-phenyl-	221	C15H11NO	005855-57-2	43
4	Boron, diethyl(5-ethyl-4,6-nonan...	250	C15H31BN2	136705-03-8	38
5	4-Quinolinol, 2-phenyl-	221	C15H11NO	001144-20-3	38





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Instrument :
BNA_F
ClientSampleId :
SPB-7WC-23-04-17

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

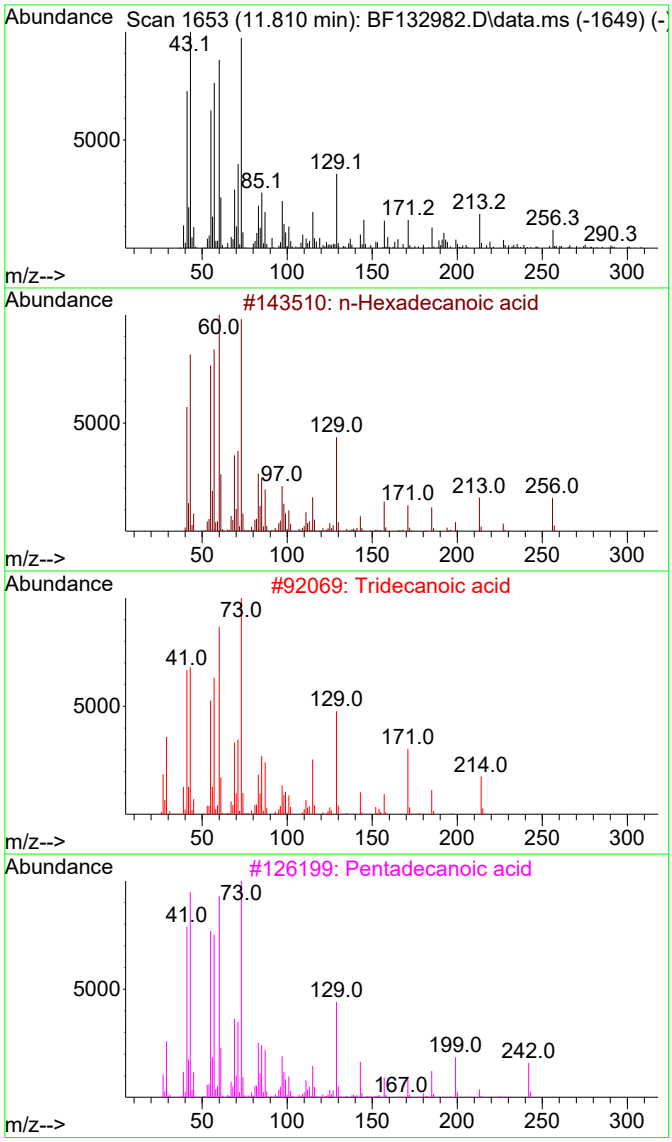
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

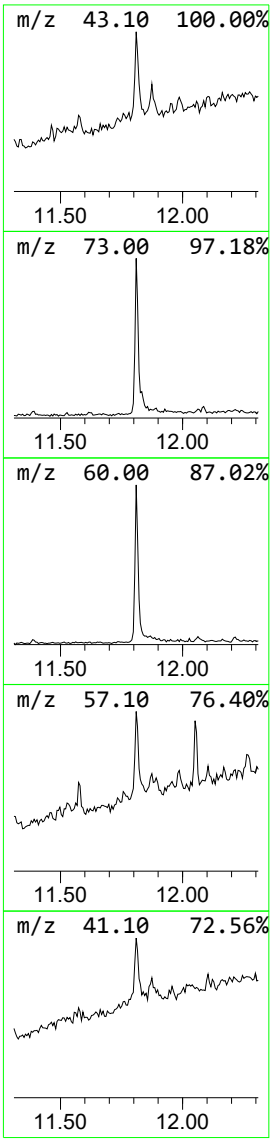
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.810	8.45 ng	540819	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Isopropyl palmitate	298	C19H38O2	000142-91-6	80
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	76





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Operator : CG\JU
Sample : 02389-27 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
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SPB-7WC-23-04-17

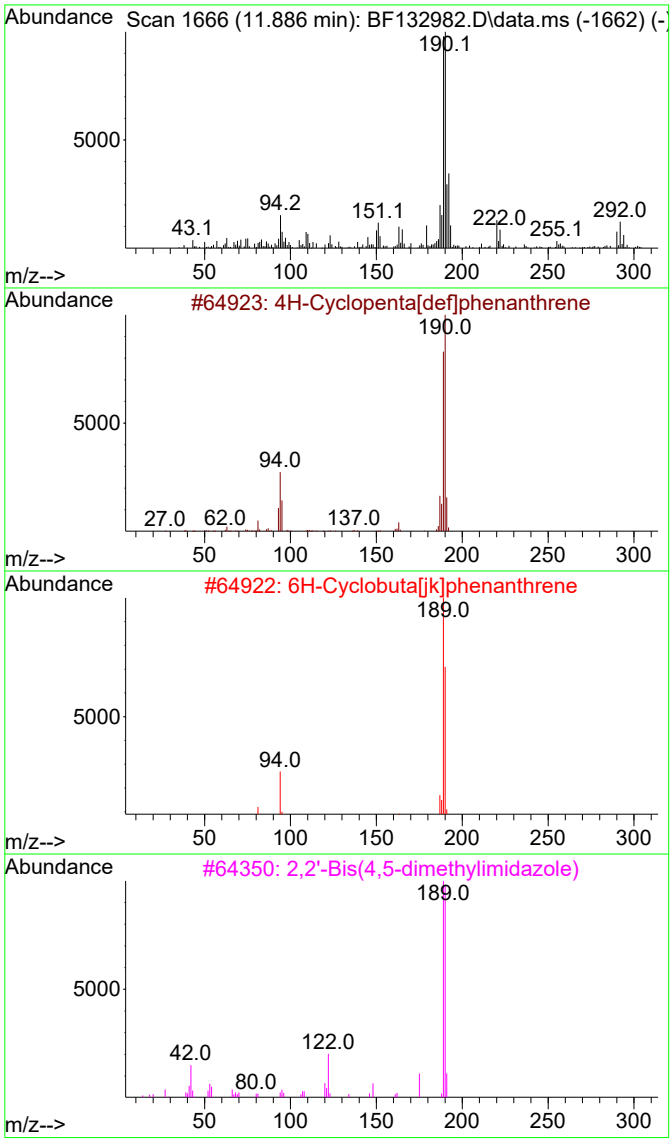
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

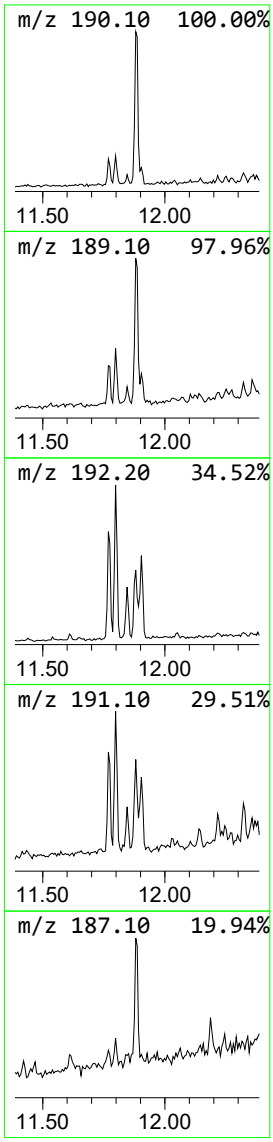
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	5.46 ng	349461	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	59
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	50
4	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	38
5	1-Aminocyclopentanecarboxylic ac...	389	C20H36ClNO4	1000329-17-2	27





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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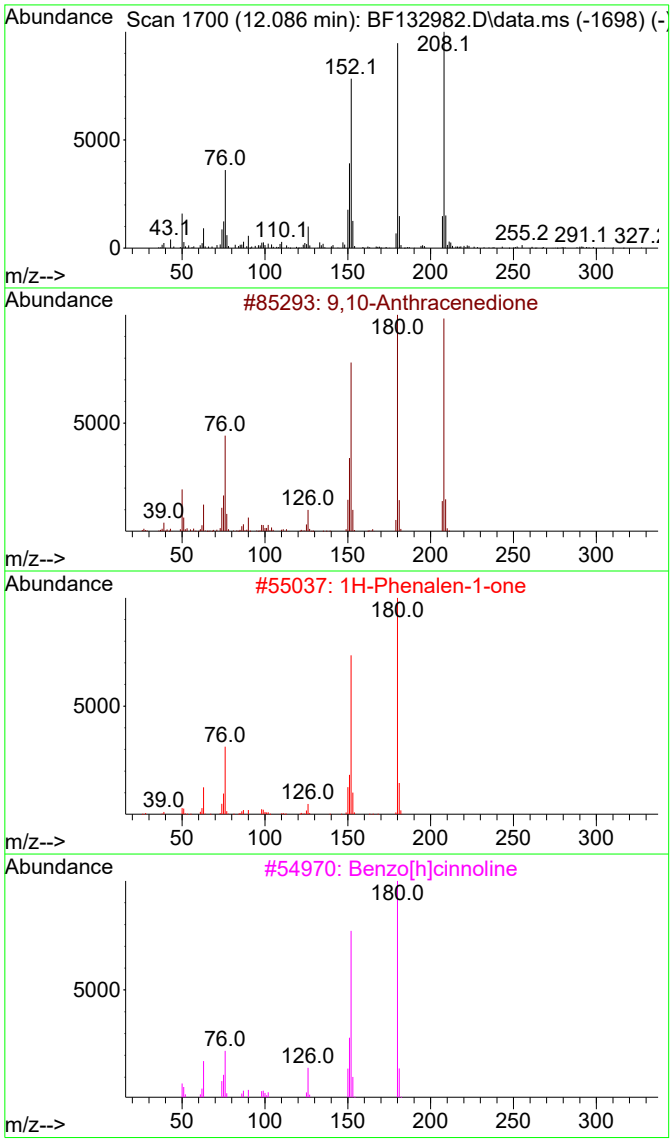
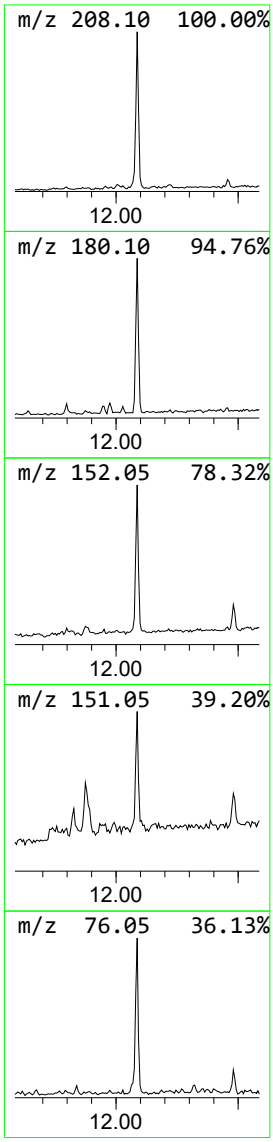
****

Peak Number 6 9,10-Anthracenedione Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.086	3.10 ng	198212	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	99
2	1H-Phenalen-1-one	180	C13H8O	000548-39-0	78
3	Benzo[h]cinnoline	180	C12H8N2	000230-31-9	70
4	9H-Fluoren-9-one	180	C13H8O	000486-25-9	70
5	Benzo[c]cinnoline	180	C12H8N2	000230-17-1	64





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BNA_F
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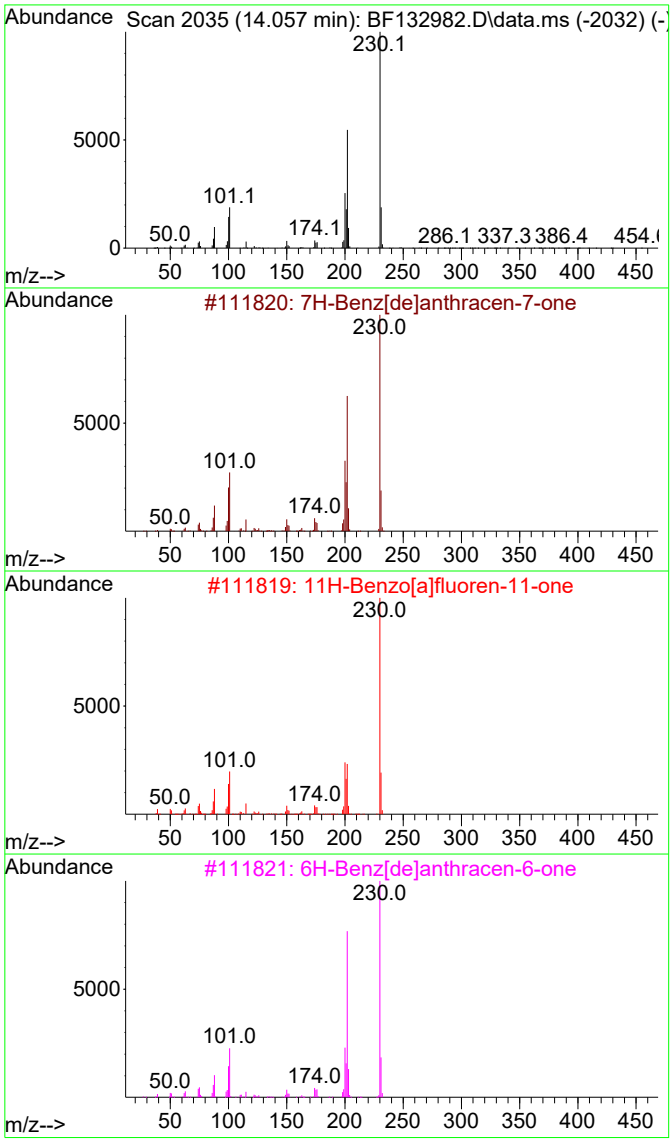
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

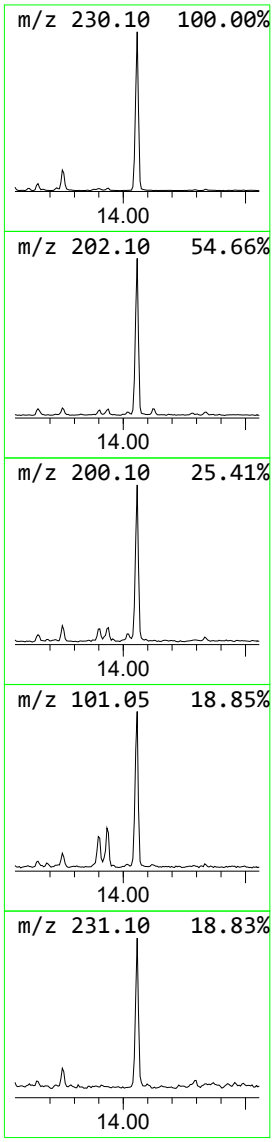
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 7H-Benz[de]anthracen-7-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.057	11.42 ng	1117160	Chrysene-d12	13.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	98
2	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	98
3	6H-Benz[de]anthracen-6-one	230	C17H10O	080252-14-8	94
4	Pyrene	202	C16H10	000129-00-0	94
5	1-Pyrenecarboxaldehyde	230	C17H10O	003029-19-4	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042123\
Data File : BF132982.D
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

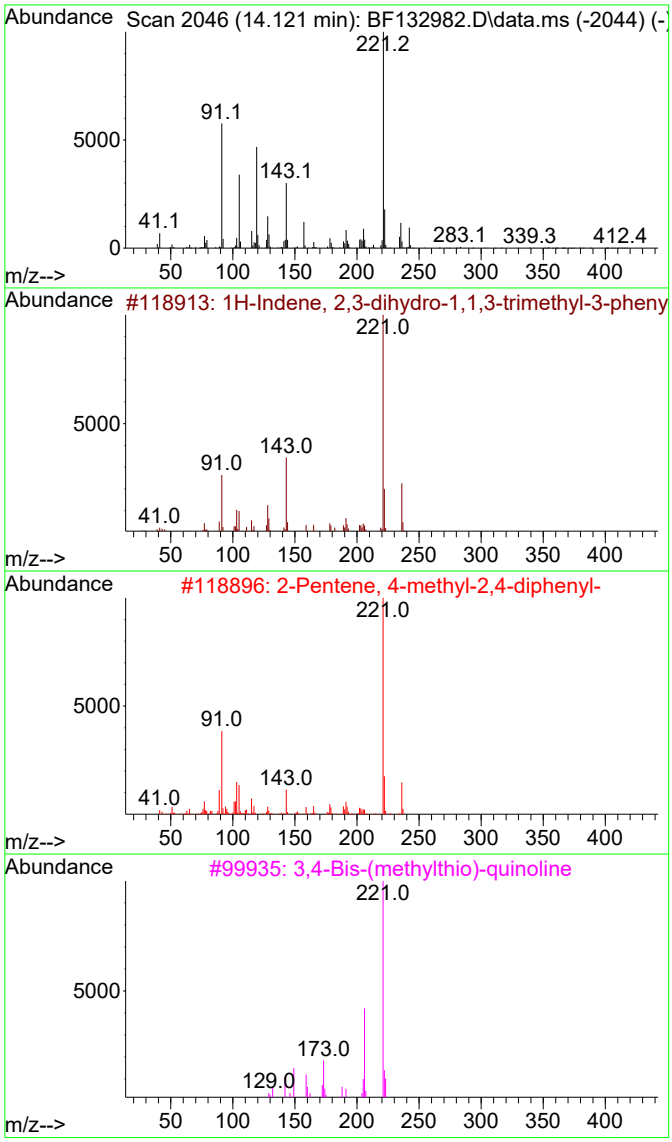
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

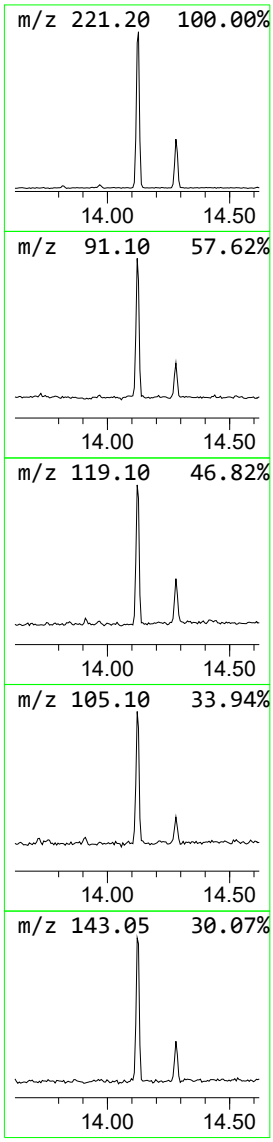
****

Peak Number 8 unknown14.121 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.121	13.68 ng	1337730	Chrysene-d12	13.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	50
2	2-Pentene, 4-methyl-2,4-diphenyl-	236	C18H20	006258-73-7	47
3	3,4-Bis-(methylthio)-quinoline	221	C11H11NS2	074579-34-3	47
4	Indole, 5-(4-methylphenyl)-N-met...	221	C16H15N	1000380-54-7	43
5	N-Methyl-m-hemipimide	221	C11H11NO4	092288-92-1	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042123\
Data File : BF132982.D
Acq On : 21 Apr 2023 22:05
Operator : CG\JU
Sample : 02389-27 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPB-7WC-23-04-17

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

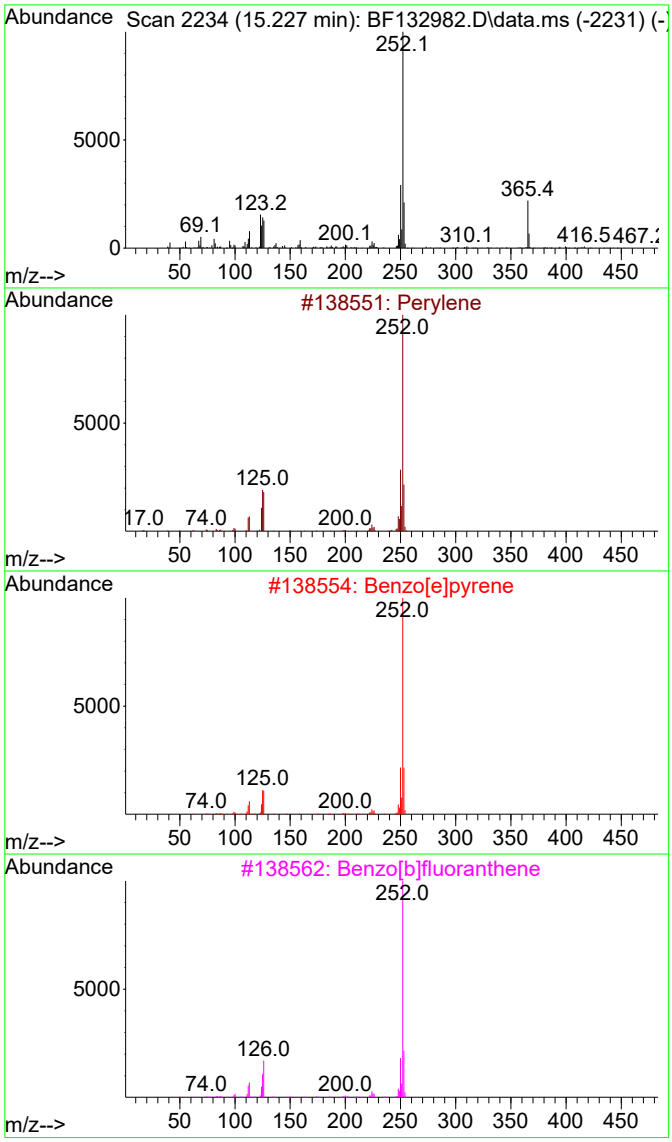
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

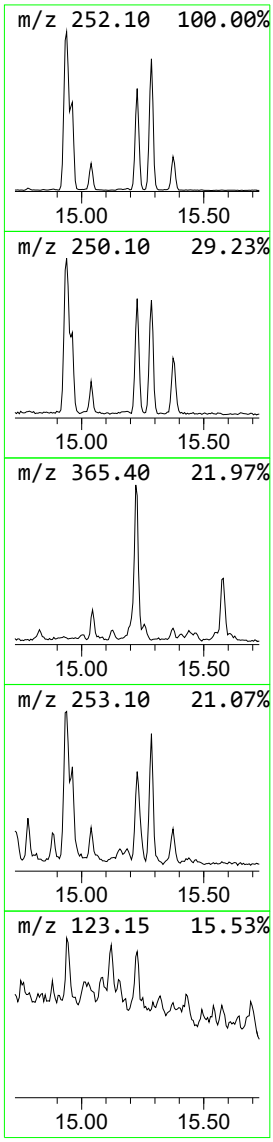
****

Peak Number 9 Perylene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.227	31.30 ng	869521	Perylene-d12	15.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	99
2	Benzo[e]pyrene	252	C20H12	000192-97-2	98
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	97
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042123\
Data File : BF132982.D
Acq On : 21 Apr 2023 22:05
Operator : CG\JU
Sample : 02389-27 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPB-7WC-23-04-17

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Stannane, tribu...	10.422	7.8	ng	635143	3	9.786	1622290	20.0
Benzenamine, 3,...	10.710	2.3	ng	150052	4	11.269	1280700	20.0
1H-Indene, 2,3-...	10.880	2.6	ng	169191	4	11.269	1280700	20.0
n-Hexadecanoic ...	11.810	8.4	ng	540819	4	11.269	1280700	20.0
4H-Cyclopenta[d...	11.886	5.5	ng	349461	4	11.269	1280700	20.0
9,10-Anthracene...	12.086	3.1	ng	198212	4	11.269	1280700	20.0
7H-Benz[de]anth...	14.057	11.4	ng	1117160	5	13.910	1955690	20.0
unknown14.121	14.121	13.7	ng	1337730	5	13.910	1955690	20.0
Perylene	15.227	31.3	ng	869521	6	15.345	555563	20.0