LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100522\
Data File : BF130535.D
Acq On : 05 Oct 2022 18:07
Operator : CG\JU
Sample : N4960-03 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAT-02-100322

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-BF091422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130535.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.487	233	238	244	rBV3	6083	10371	1.61%	0.166%
2	4.793	457	460	470	rBV	27749	34386	5.35%	0.549%
3	5.234	532	535	547	rBV	131630	164318	25.54%	2.624%
4	6.275	709	712	728	rBV	122085	157756	24.52%	2.519%
5	6.634	769	773	780	rBV	455346	400960	62.33%	6.402%
6	7.199	865	869	879	rBV	95999	98548	15.32%	1.573%
7	7.916	987	991	994	rBV	532464	473576	73.62%	7.561%
8	8.728	1124	1129	1135	rVB2	11354	15155	2.36%	0.242%
9	8.987	1170	1173	1182	rVB	204724	179363	27.88%	2.864%
10	9.075	1182	1188	1192	rBV3	10657	13101	2.04%	0.209%
11	9.257	1215	1219	1222	rBV3	11044	14420	2.24%	0.230%
12	9.328	1227	1231	1233	rBV	18551	18706	2.91%	0.299%
13	9.440	1248	1250	1255	rVB2	10171	12976	2.02%	0.207%
14	9.522	1262	1264	1270	rBV	23449	22884	3.56%	0.365%
15	9.604	1275	1278	1280	rBV	12739	12190	1.89%	0.195%
16	9.663	1284	1288	1291	rVV	576176	455651	70.83%	7.275%
17	9.692	1291	1293	1297	rVB	23760	23184	3.60%	0.370%
18	9.769	1303	1306	1310	rVB5	7675	9387	1.46%	0.150%
19	9.869	1319	1323	1325	rBV	18294	17958	2.79%	0.287%
20	9.904	1328	1329	1337	rVB5	12070	12794	1.99%	0.204%
21	9.981	1337	1342	1345	rBV4	11835	16844	2.62%	0.269%
22	10.016	1345	1348	1353	rVB2	11069	15151	2.36%	0.242%
23	10.063	1353	1356	1359	rBV5	9303	11326	1.76%	0.181%
24	10.098	1359	1362	1364	rBV2	12937	9471	1.47%	0.151%
25	10.210	1378	1381	1387	rVB	33461	39325	6.11%	0.628%
26	10.275	1387	1392	1394	rBV5	7649	12151	1.89%	0.194%
27	10.322	1397	1400	1403	rVV3	16335	19428	3.02%	0.310%
28	10.369	1405	1408	1412	rVB2	9558	12187	1.89%	0.195%
29	10.451	1417	1422	1427	rBV	107117	104181	16.19%	1.663%
30	10.569	1439	1442	1451	rVB2	62035	79375	12.34%	1.267%
31	10.757	1469	1474	1476	rBV4	15530	19901	3.09%	0.318%
32	10.781	1476	1478	1484	rVV3	13566	19435	3.02%	0.310%
33	10.839	1485	1488	1490	rVB3	9028	9097	1.41%	0.145%
34	10.904	1497	1499	1504	rVB6	12717	13580	2.11%	0.217%
35	10.951	1504	1507	1511	rBV5	9694	12457	1.94%	0.199%
36	11.022	1516	1519	1520	rVV	16490	16257	2.53%	0.260%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100522\
Data File : BF130535.D
Acq On : 05 Oct 2022 18:07
Operator : CG\JU
Sample : N4960-03 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAT-02-100322

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-BF091422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.039	1520	1522	1527	rVB2	30869	36204	5.63%	0.578%
38	11.145	1536	1540	1542	rBV	520250	461556	71.75%	7.369%
39	11.169	1542	1544	1547	rVV	173671	139235	21.64%	2.223%
40	11.216	1549	1552	1556	rVV	38424	37010	5.75%	0.591%
41	11.257	1556	1559	1562	rVV2	11300	13203	2.05%	0.211%
42	11.445	1588	1591	1593	rBV2	19144	16820	2.61%	0.269%
43	11.475	1593	1596	1598	rVV	21993	21989	3.42%	0.351%
44	11.510	1598	1602	1605	rVV	41353	49850	7.75%	0.796%
45	11.557	1607	1610	1613	rVB2	15865	17774	2.76%	0.284%
46	11.645	1622	1625	1627	rBV	62420	53226	8.27%	0.850%
47	11.675	1627	1630	1633	rVB	63948	57508	8.94%	0.918%
48	11.716	1633	1637	1640	rBV2	45395	53658	8.34%	0.857%
49	11.751	1640	1643	1646	rVV	79550	84322	13.11%	1.346%
50	11.775	1646	1647	1653	rVB	44507	40638	6.32%	0.649%
51	11.851	1657	1660	1663	rBV2	14845	15920	2.47%	0.254%
52	11.881	1663	1665	1668	rVB3	12822	10767	1.67%	0.172%
53	11.939	1672	1675	1677	rBV2	26557	24487	3.81%	0.391%
54	12.069	1695	1697	1698	rBV2	15115	12877	2.00%	0.206%
55	12.086	1698	1700	1703	rVB	23302	18270	2.84%	0.292%
56	12.122	1703	1706	1708	rBV2	29984	32226	5.01%	0.515%
57	12.192	1715	1718	1721	rBV	73682	76387	11.87%	1.220%
58	12.228	1721	1724	1727	rVV4	40757	56781	8.83%	0.907%
59	12.281	1730	1733	1737	rBV2	24572	39809	6.19%	0.636%
60	12.351	1742	1745	1749	rBV	212628	175994	27.36%	2.810%
61	12.581	1779	1784	1786	rBV	269089	256250	39.83%	4.091%
62	12.604	1786	1788	1791	rVV3	36676	43124	6.70%	0.689%
63	12.639	1792	1794	1798	rVB2	24704	27187	4.23%	0.434%
64	12.728	1805	1809	1815	rVB	230618	243701	37.88%	3.891%
65	12.798	1818	1821	1828	rVV4	31073	48058	7.47%	0.767%
66	12.904	1833	1839	1842	rVB	59542	95399	14.83%	1.523%
67	12.975	1848	1851	1854	rVB	39371	36984	5.75%	0.591%
68	13.010	1854	1857	1861	rBV	59944	62293	9.68%	0.995%
69	13.104	1870	1873	1875	rVB	43582	39803	6.19%	0.636%
70	13.133	1875	1878	1881	rBV	55986	46855	7.28%	0.748%
71	13.528	1940	1945	1948	rBV3	36211	68629	10.67%	1.096%
72	13.775	1982	1987	1990	rBV2	608938	643293	100.00%	10.271%
73	14.780	2155	2158	2164	rVB	66870	106472	16.55%	1.700%
74	15.110	2211	2214	2219	rVV	57349	67045	10.42%	1.070%
75	15.163	2220	2223	2231	rVB	277782	373666	58.09%	5.966%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100522\
Data File : BF130535.D
Acq On : 05 Oct 2022 18:07
Operator : CG\JU
Sample : N4960-03 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAT-02-100322

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-BF091422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

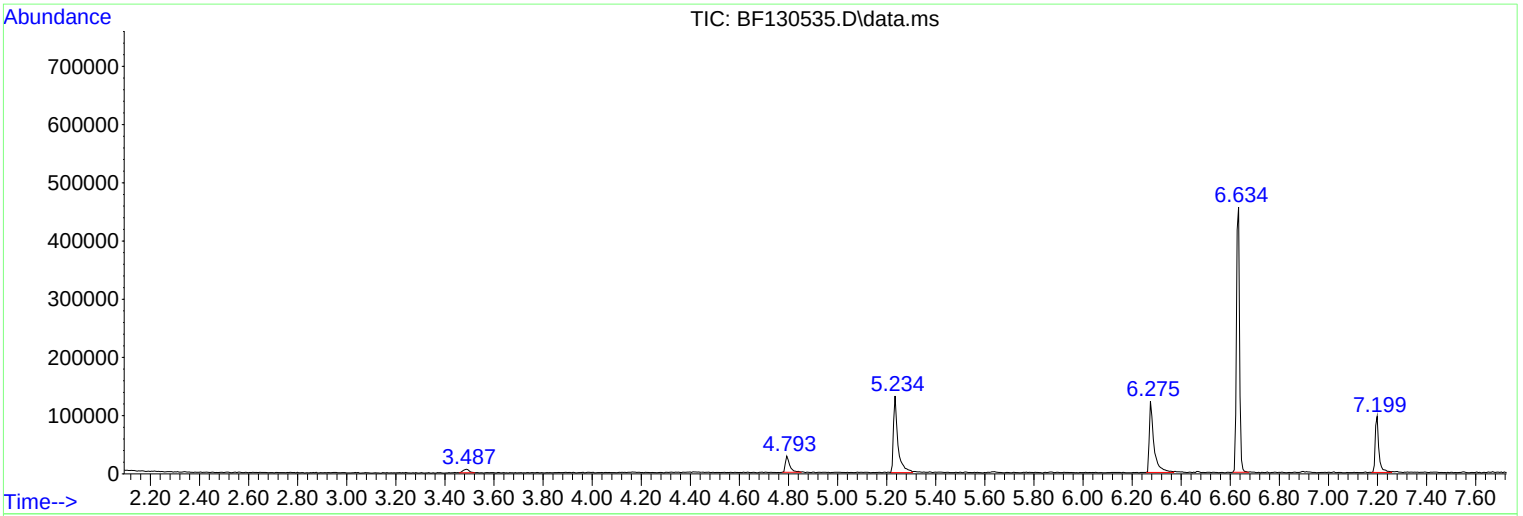
Sum of corrected areas: 6263120

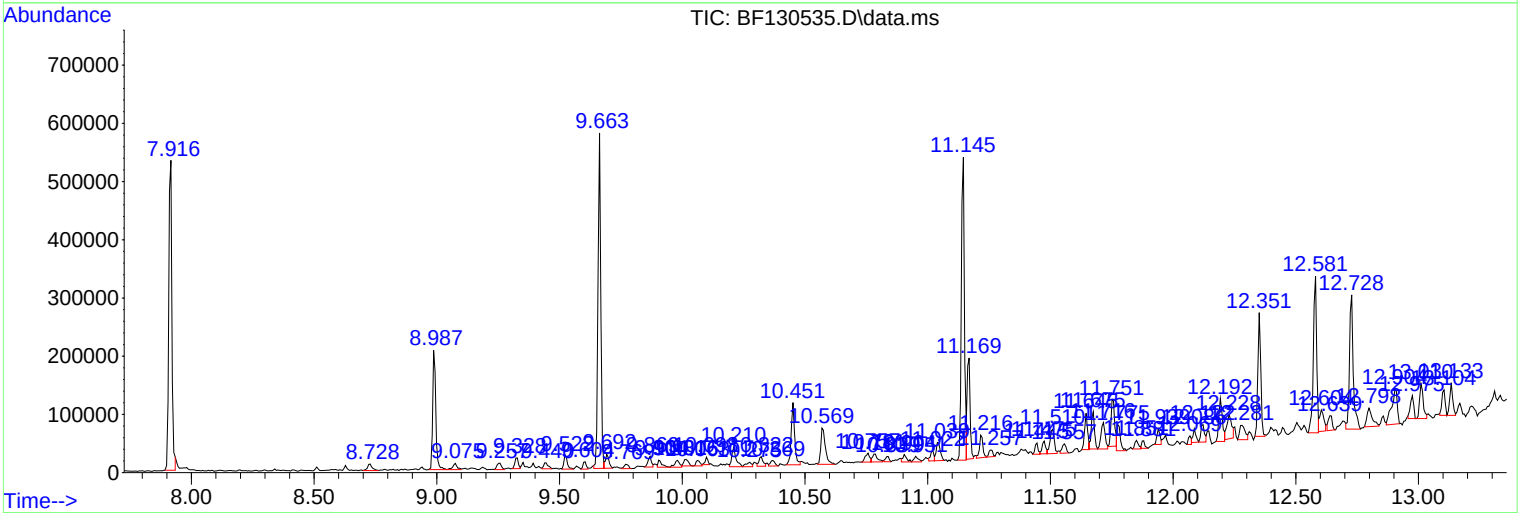
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100522\
Data File : BF130535.D
Acq On : 05 Oct 2022 18:07
Operator : CG\JU
Sample : N4960-03 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

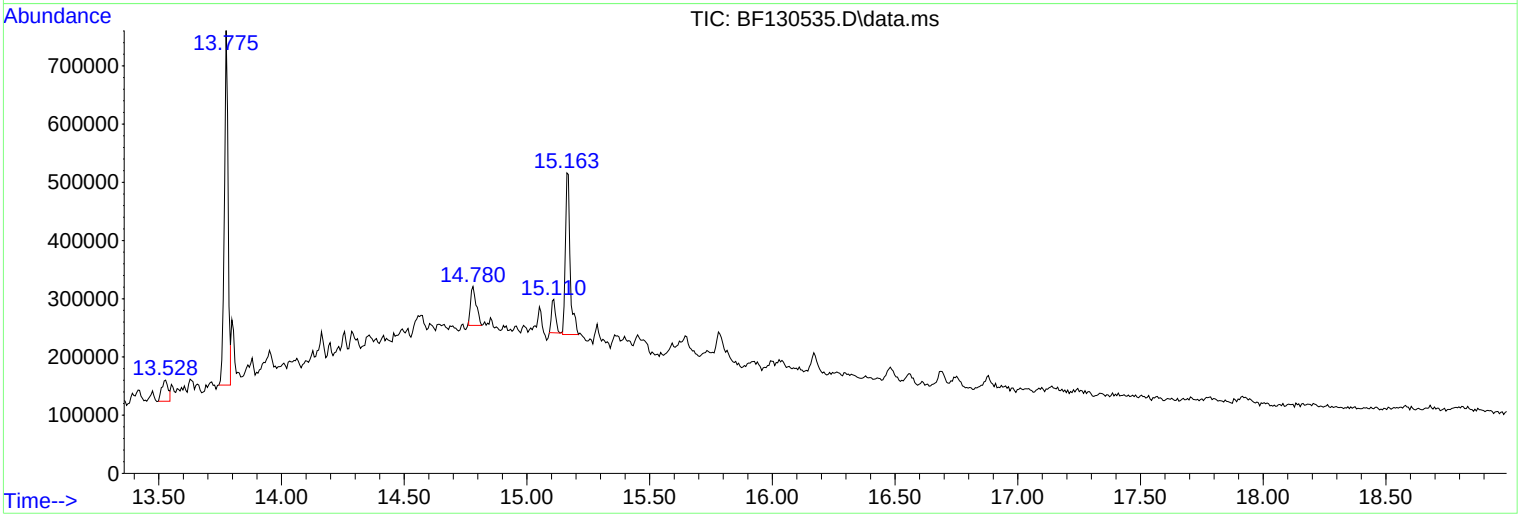
Instrument :
BNA_F
ClientSampleId :
PAT-02-100322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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\BF100522\
Data File : BF130535.D
Acq On : 05 Oct 2022 18:07
Operator : CG\JU
Sample : N4960-03 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAT-02-100322

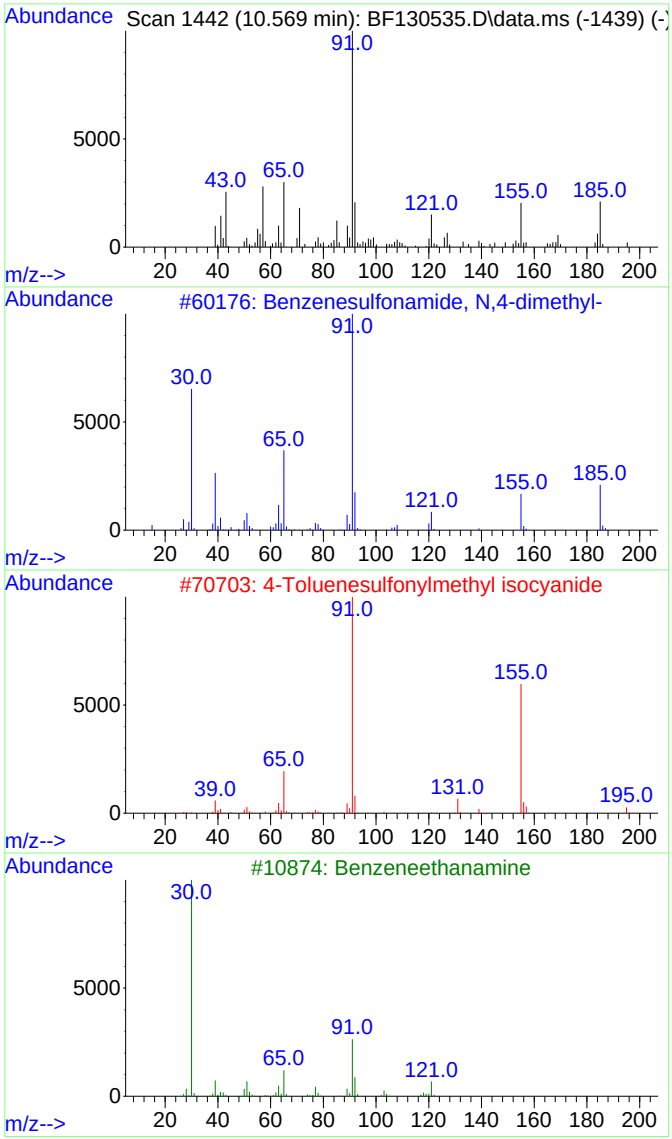
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

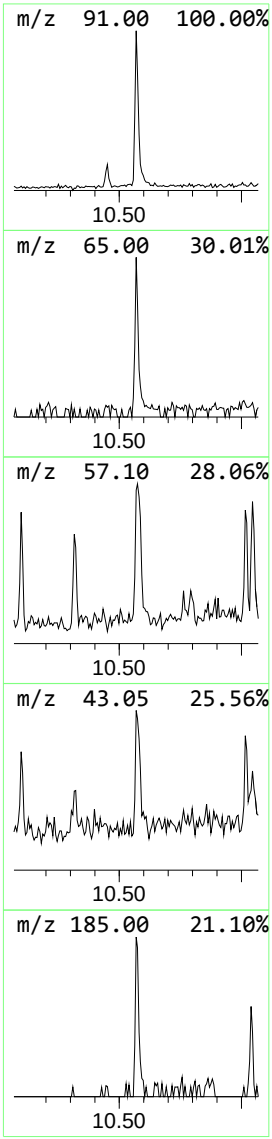
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Benzenesulfonamide, N,4-dim... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.569	3.44 ng	79375	Phenanthrene-d10	11.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	91
2	4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	46
3	Benzeneethanamine	121	C8H11N	000064-04-0	43
4	Benzenesulfonamide, N,4-dimethyl...	214	C8H10N2O3S	000080-11-5	38
5	Benzenesulfonamide, N-cyano-4-me...	272	C14H12N2O2S	1000327-63-5	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100522\
Data File : BF130535.D
Acq On : 05 Oct 2022 18:07
Operator : CG\JU
Sample : N4960-03 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAT-02-100322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

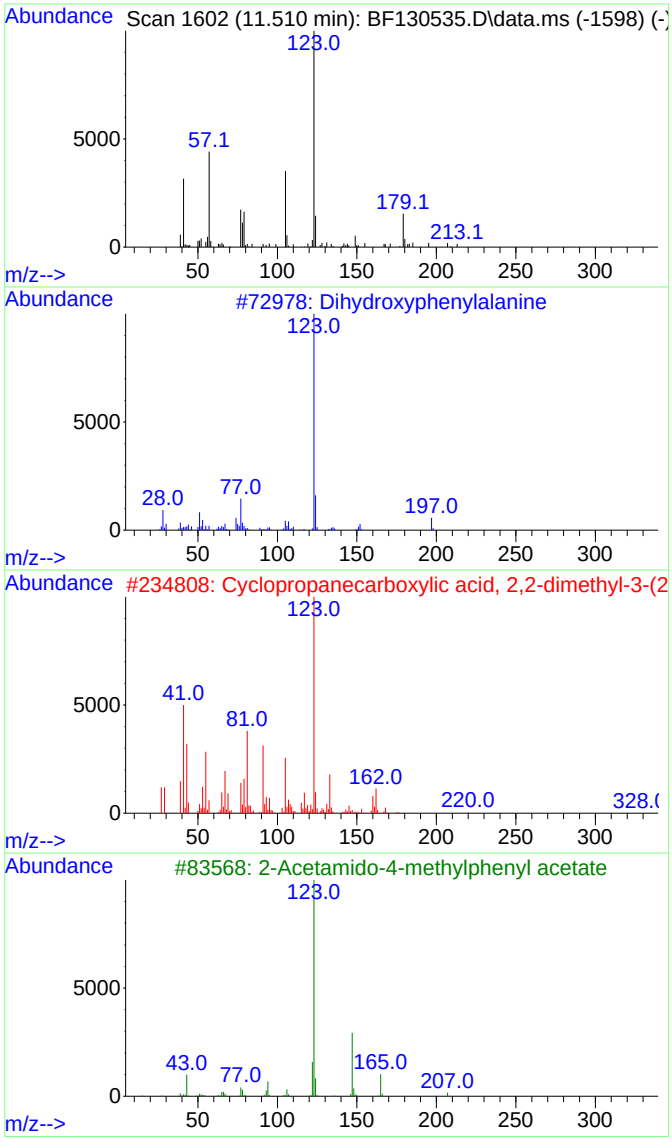
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

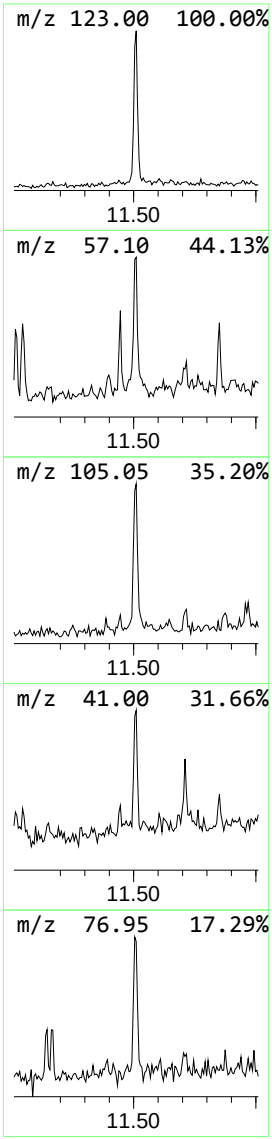
****

Peak Number 2 unknown11.510 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.510	2.16 ng	49850	Phenanthrene-d10	11.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dihydroxyphenylalanine	197	C9H11NO4	000063-84-3	40
2	Cyclopropanecarboxylic acid, 2,2...	328	C21H28O3	000121-21-1	38
3	2-Acetamido-4-methylphenyl acetate	207	C11H13NO3	1000373-46-9	38
4	Niacin	123	C6H5NO2	000059-67-6	38
5	Benzoic acid, octadecyl ester	374	C25H42O2	010578-34-4	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100522\
Data File : BF130535.D
Acq On : 05 Oct 2022 18:07
Operator : CG\JU
Sample : N4960-03 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAT-02-100322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

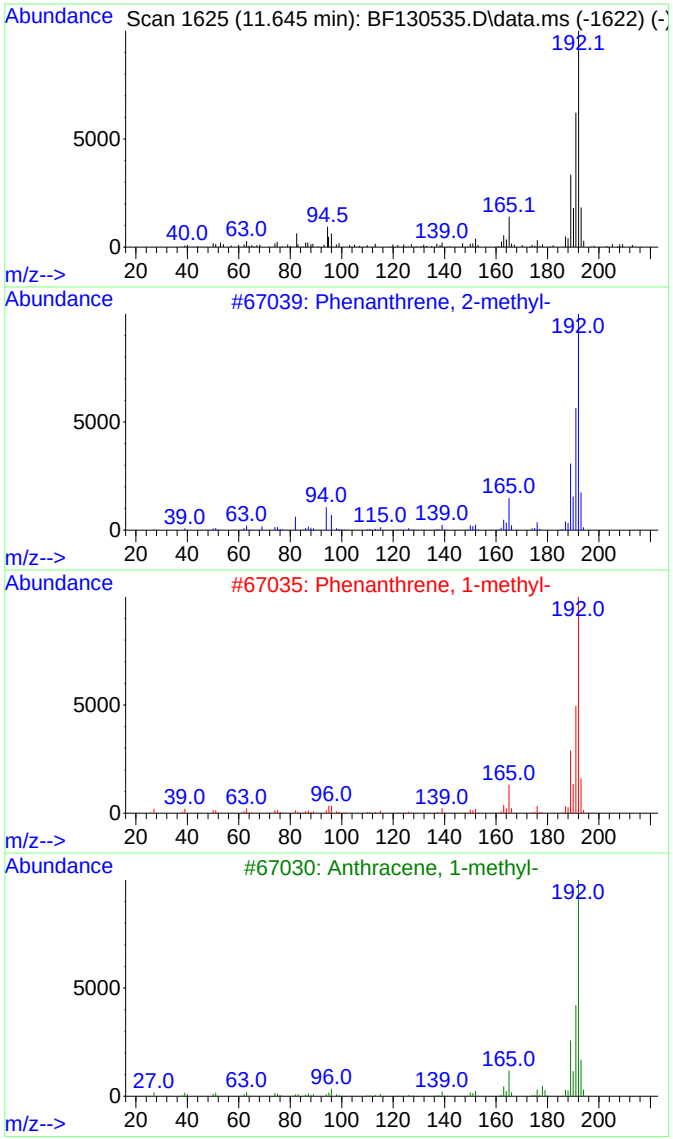
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

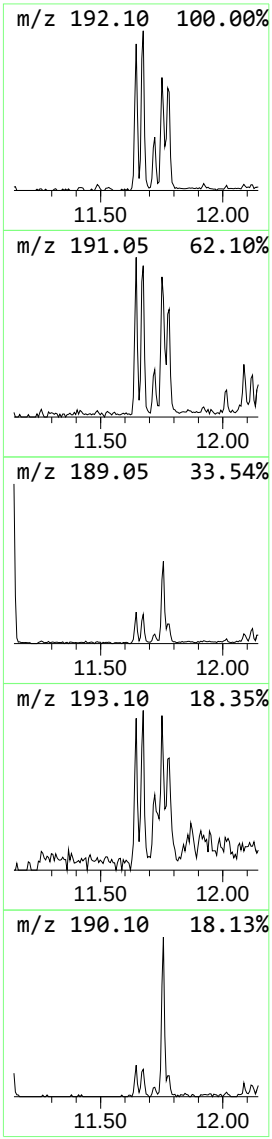
****

Peak Number 3 Phenanthrene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.645	2.31 ng	53226	Phenanthrene-d10	11.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
4	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	93
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100522\
Data File : BF130535.D
Acq On : 05 Oct 2022 18:07
Operator : CG\JU
Sample : N4960-03 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAT-02-100322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

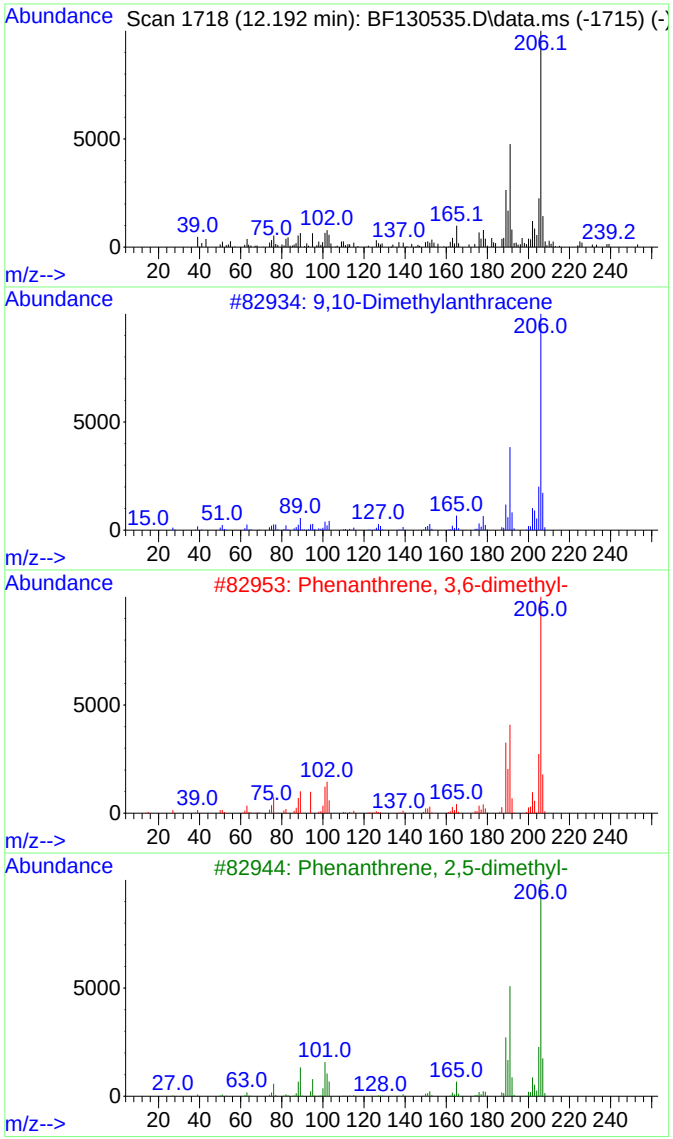
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

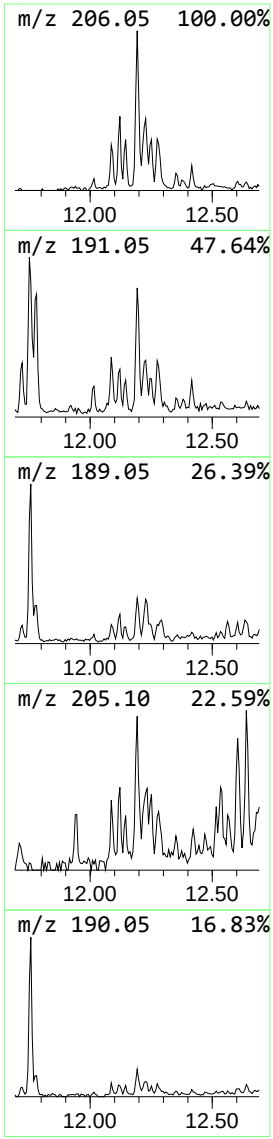
****

Peak Number 4 9,10-Dimethylanthracene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.192	3.31 ng	76387	Phenanthrene-d10	11.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Dimethylanthracene	206	C16H14	000781-43-1	94
2	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	93
3	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	93
4	Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	90
5	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100522\
Data File : BF130535.D
Acq On : 05 Oct 2022 18:07
Operator : CG\JU
Sample : N4960-03 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAT-02-100322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

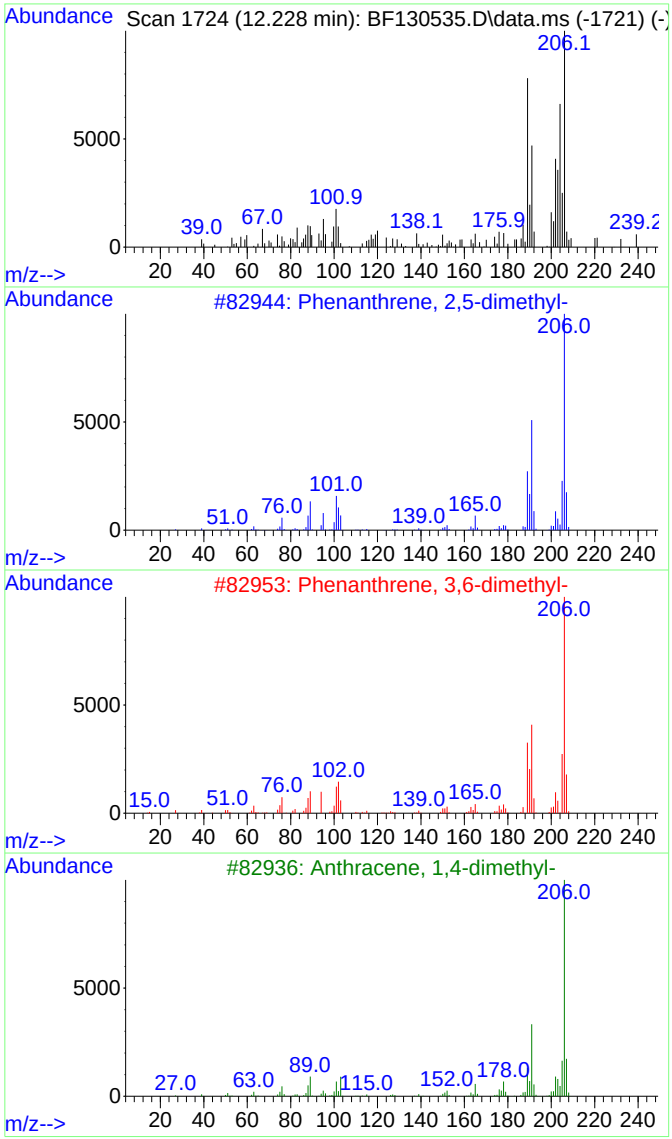
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

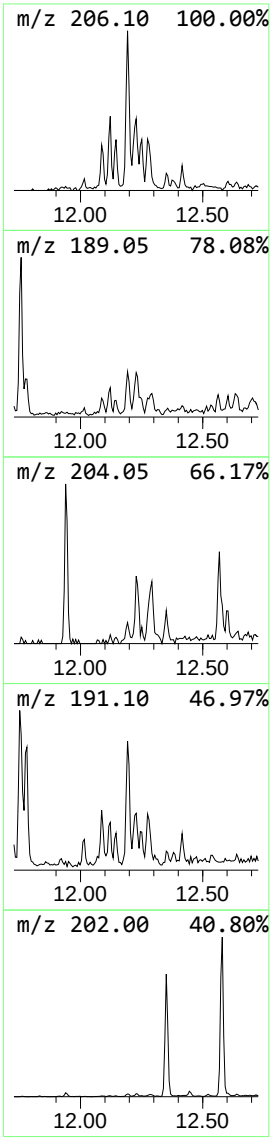
****

Peak Number 5 Phenanthrene, 2,5-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.228	2.46 ng	56781	Phenanthrene-d10	11.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	50
2	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	50
3	Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	46
4	3,5-Dichloro-4-hydroxybenzoic acid	206	C7H4Cl2O3	003336-41-2	46
5	9,10-Dimethylanthracene	206	C16H14	000781-43-1	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100522\
Data File : BF130535.D
Acq On : 05 Oct 2022 18:07
Operator : CG\JU
Sample : N4960-03 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAT-02-100322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

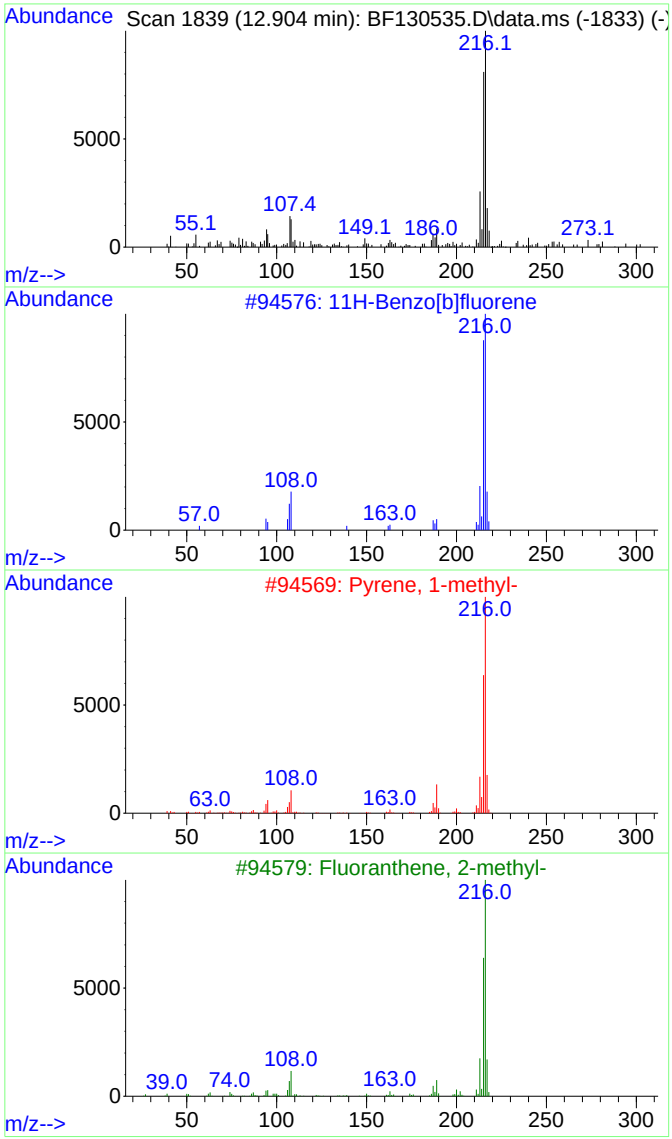
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

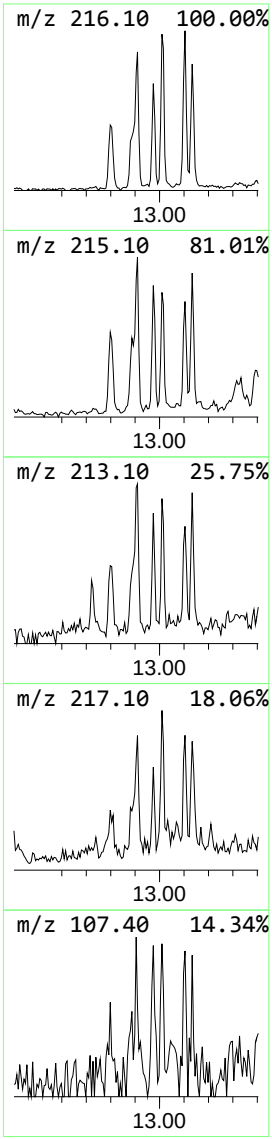
****

Peak Number 6 11H-Benzo[b]fluorene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.904	2.97 ng	95399	Chrysene-d12	13.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	91
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	86
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100522\
Data File : BF130535.D
Acq On : 05 Oct 2022 18:07
Operator : CG\JU
Sample : N4960-03 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAT-02-100322

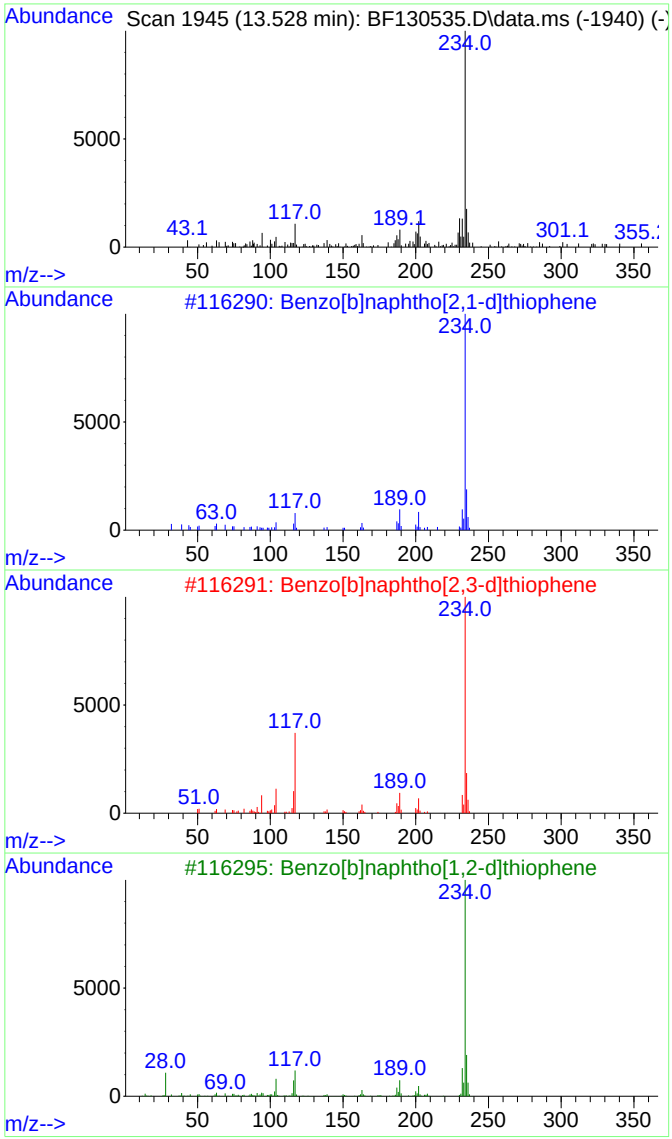
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

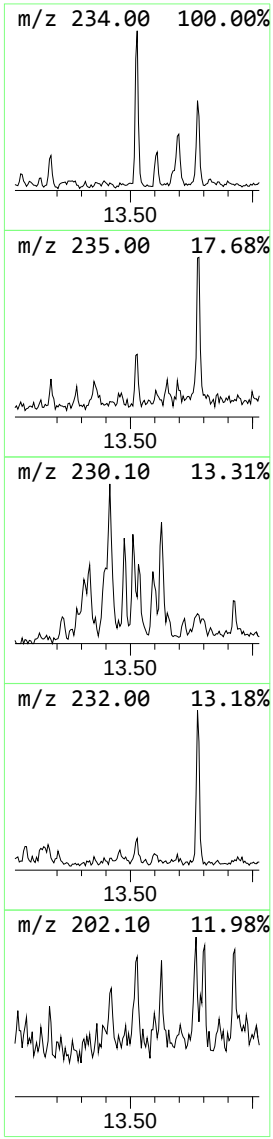
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzo[b]naphtho[2,1-d]thiop... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.528	2.13 ng	68629	Chrysene-d12	13.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]naphtho[2,1-d]thiophene	234	C16H10S	000239-35-0	95
2	Benzo[b]naphtho[2,3-d]thiophene	234	C16H10S	000243-46-9	87
3	Benzo[b]naphtho[1,2-d]thiophene	234	C16H10S	000205-43-6	81
4	Anthra(2,3-b)thiophene	234	C16H10S	022108-55-0	74
5	Phenanthro[4,3-b]thiophene	234	C16H10S	000195-68-6	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100522\
Data File : BF130535.D
Acq On : 05 Oct 2022 18:07
Operator : CG\JU
Sample : N4960-03 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAT-02-100322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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
Benzenesulfonam...	10.569	3.4	ng	79375	4	11.145	461556	20.0
unknown11.510	11.510	2.2	ng	49850	4	11.145	461556	20.0
Phenanthrene, 2...	11.645	2.3	ng	53226	4	11.145	461556	20.0
9,10-Dimethylan...	12.192	3.3	ng	76387	4	11.145	461556	20.0
Phenanthrene, 2...	12.228	2.5	ng	56781	4	11.145	461556	20.0
11H-Benzo[b]flu...	12.904	3.0	ng	95399	5	13.775	643293	20.0
Benzo[b]naphtho...	13.528	2.1	ng	68629	5	13.775	643293	20.0