LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062322\
Data File : BF128969.D
Acq On : 23 Jun 2022 23:31
Operator : CG\JU
Sample : N3462-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2-3-5-20220622

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-BF060222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128969.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.928	444	449	460	rVB	28759	42927	2.02%	0.164%
2	5.357	519	522	538	rBV	2001023	2041221	96.02%	7.784%
3	6.387	693	697	710	rBV	2068415	2125753	100.00%	8.106%
4	6.475	710	712	721	rVB	20500	21517	1.01%	0.082%
5	6.557	721	726	729	rBV2	40846	40414	1.90%	0.154%
6	6.722	751	754	761	rVB	701571	622184	29.27%	2.373%
7	6.793	761	766	772	rBV3	16621	25639	1.21%	0.098%
8	7.293	846	851	854	rBV	1140260	1033422	48.61%	3.941%
9	7.322	854	856	859	rVB	34217	26730	1.26%	0.102%
10	8.010	966	973	975	rBV	620913	582345	27.39%	2.221%
11	8.028	975	976	980	rVB	123085	78219	3.68%	0.298%
12	8.598	1070	1073	1076	rVB	31369	25519	1.20%	0.097%
13	8.722	1091	1094	1097	rVB	35542	25798	1.21%	0.098%
14	9.087	1151	1156	1159	rBV	2241499	1819342	85.59%	6.938%
15	9.163	1165	1169	1171	rBV	28409	23413	1.10%	0.089%
16	9.357	1196	1202	1206	rBV4	16550	21306	1.00%	0.081%
17	9.763	1264	1271	1274	rBV	700136	573423	26.98%	2.187%
18	9.792	1274	1276	1280	rVB	154897	120929	5.69%	0.461%
19	9.969	1302	1306	1309	rBV	58902	51786	2.44%	0.197%
20	10.310	1361	1364	1369	rVB	96317	77301	3.64%	0.295%
21	10.375	1369	1375	1377	rBV	20417	23970	1.13%	0.091%
22	10.551	1401	1405	1412	rBV	775330	750872	35.32%	2.863%
23	10.663	1421	1424	1432	rVB4	27897	47555	2.24%	0.181%
24	10.857	1451	1457	1460	rBV4	17086	22434	1.06%	0.086%
25	11.057	1488	1491	1495	rVB	47930	39626	1.86%	0.151%
26	11.110	1495	1500	1503	rVV4	29289	38780	1.82%	0.148%
27	11.145	1503	1506	1510	rVB	51904	45745	2.15%	0.174%
28	11.251	1520	1524	1526	rBV	543620	536334	25.23%	2.045%
29	11.275	1526	1528	1531	rVV	906139	653166	30.73%	2.491%
30	11.322	1531	1536	1540	rVB	194013	188313	8.86%	0.718%
31	11.486	1557	1564	1570	rBV2	122555	133868	6.30%	0.510%
32	11.539	1570	1573	1578	rVV4	20436	26024	1.22%	0.099%
33	11.639	1587	1590	1598	rVB3	38129	43215	2.03%	0.165%
34	11.751	1605	1609	1611	rBV	77264	65369	3.08%	0.249%
35	11.780	1611	1614	1617	rVV	123507	104010	4.89%	0.397%
36	11.828	1619	1622	1624	rVV	47267	40892	1.92%	0.156%

LSC Area Percent Report

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Sample : N3462-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2-3-5-20220622

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 >
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Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.863	1624	1628	1630	rVV	160887	157464	7.41%	0.600%
38	11.886	1630	1632	1637	rVB	51927	42491	2.00%	0.162%
39	12.045	1656	1659	1662	rVV	63623	51698	2.43%	0.197%
40	12.080	1662	1665	1667	rVB	55715	48673	2.29%	0.186%
41	12.298	1698	1702	1705	rBV	43309	51587	2.43%	0.197%
42	12.339	1705	1709	1711	rVV3	36901	47865	2.25%	0.183%
43	12.392	1715	1718	1722	rVV2	47253	54818	2.58%	0.209%
44	12.469	1726	1731	1734	rVB	1541225	1368442	64.37%	5.218%
45	12.527	1739	1741	1744	rVB2	37288	31223	1.47%	0.119%
46	12.610	1752	1755	1759	rVB2	43968	42300	1.99%	0.161%
47	12.692	1763	1769	1775	rBV2	1214926	1467198	69.02%	5.595%
48	12.739	1775	1777	1780	rBV	54531	51031	2.40%	0.195%
49	12.775	1780	1783	1786	rVB	58120	52685	2.48%	0.201%
50	12.810	1786	1789	1790	rBV	89676	74395	3.50%	0.284%
51	12.833	1790	1793	1800	rVB	1470408	1407643	66.22%	5.368%
52	12.916	1801	1807	1810	rBV2	71511	136247	6.41%	0.520%
53	12.945	1810	1812	1815	rBV	45114	39694	1.87%	0.151%
54	12.998	1817	1821	1823	rBV4	88136	123227	5.80%	0.470%
55	13.022	1823	1825	1828	rVB	219359	184550	8.68%	0.704%
56	13.057	1828	1831	1833	rBV2	27846	29153	1.37%	0.111%
57	13.086	1833	1836	1839	rBV	183656	153167	7.21%	0.584%
58	13.122	1839	1842	1844	rVV2	110614	121528	5.72%	0.463%
59	13.145	1844	1846	1850	rVB	72720	66497	3.13%	0.254%
60	13.180	1850	1852	1855	rVB2	35022	26364	1.24%	0.101%
61	13.216	1855	1858	1861	rBV	58022	54770	2.58%	0.209%
62	13.245	1861	1863	1867	rBV2	55014	65578	3.08%	0.250%
63	13.333	1876	1878	1883	rVB2	25779	23499	1.11%	0.090%
64	13.410	1887	1891	1894	rBV5	33106	56655	2.67%	0.216%
65	13.445	1894	1897	1900	rVV	66000	61454	2.89%	0.234%
66	13.504	1904	1907	1909	rBV3	36579	38377	1.81%	0.146%
67	13.533	1909	1912	1915	rVB	111259	97216	4.57%	0.371%
68	13.639	1927	1930	1933	rBV	183683	173302	8.15%	0.661%
69	13.669	1933	1935	1937	rVV	123436	101403	4.77%	0.387%
70	13.692	1937	1939	1941	rVV	108979	114575	5.39%	0.437%
71	13.745	1945	1948	1951	rVB	109858	101868	4.79%	0.388%
72	13.886	1965	1972	1976	rBV2	980811	1626957	76.54%	6.204%
73	13.922	1976	1978	1981	rVV	870374	673288	31.67%	2.568%
74	13.998	1985	1991	1994	rBV2	201962	295114	13.88%	1.125%
75	14.045	1997	1999	2004	rVV5	49299	91944	4.33%	0.351%
76	14.086	2004	2006	2008	rVV	83024	84838	3.99%	0.324%

LSC Area Percent Report

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Sample : N3462-08
Misc :
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Instrument :
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ClientSampleId :
SB-2-3-5-20220622

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
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Start Thrs: 0.2 Max Peaks: 100
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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	14.127	2011	2013	2015	rVB	100721	79920	3.76%	0.305%
78	14.210	2025	2027	2029	rBV2	29641	27602	1.30%	0.105%
79	14.239	2030	2032	2035	rVV2	70196	71339	3.36%	0.272%
80	14.280	2035	2039	2042	rVV	156255	155969	7.34%	0.595%
81	14.316	2042	2045	2047	rVB2	54441	50807	2.39%	0.194%
82	14.404	2058	2060	2062	rBV	71397	60271	2.84%	0.230%
83	14.421	2062	2063	2066	rVB	76133	61151	2.88%	0.233%
84	14.592	2089	2092	2100	rBV4	85622	123460	5.81%	0.471%
85	14.763	2118	2121	2125	rBV2	62671	82054	3.86%	0.313%
86	14.921	2143	2148	2151	rBV	728169	1084798	51.03%	4.137%
87	15.021	2162	2165	2169	rBV	114963	122110	5.74%	0.466%
88	15.210	2193	2197	2203	rVB	400892	518288	24.38%	1.976%
89	15.274	2203	2208	2212	rVB	545652	630184	29.65%	2.403%
90	15.333	2213	2218	2220	rVV	348725	433821	20.41%	1.654%
91	15.357	2220	2222	2229	rVB2	164908	232815	10.95%	0.888%
92	16.374	2393	2395	2401	rVB5	43214	51455	2.42%	0.196%
93	16.739	2451	2457	2464	rVB	242399	454233	21.37%	1.732%
94	17.162	2523	2529	2539	rVB	162442	352662	16.59%	1.345%

Sum of corrected areas: 26223078

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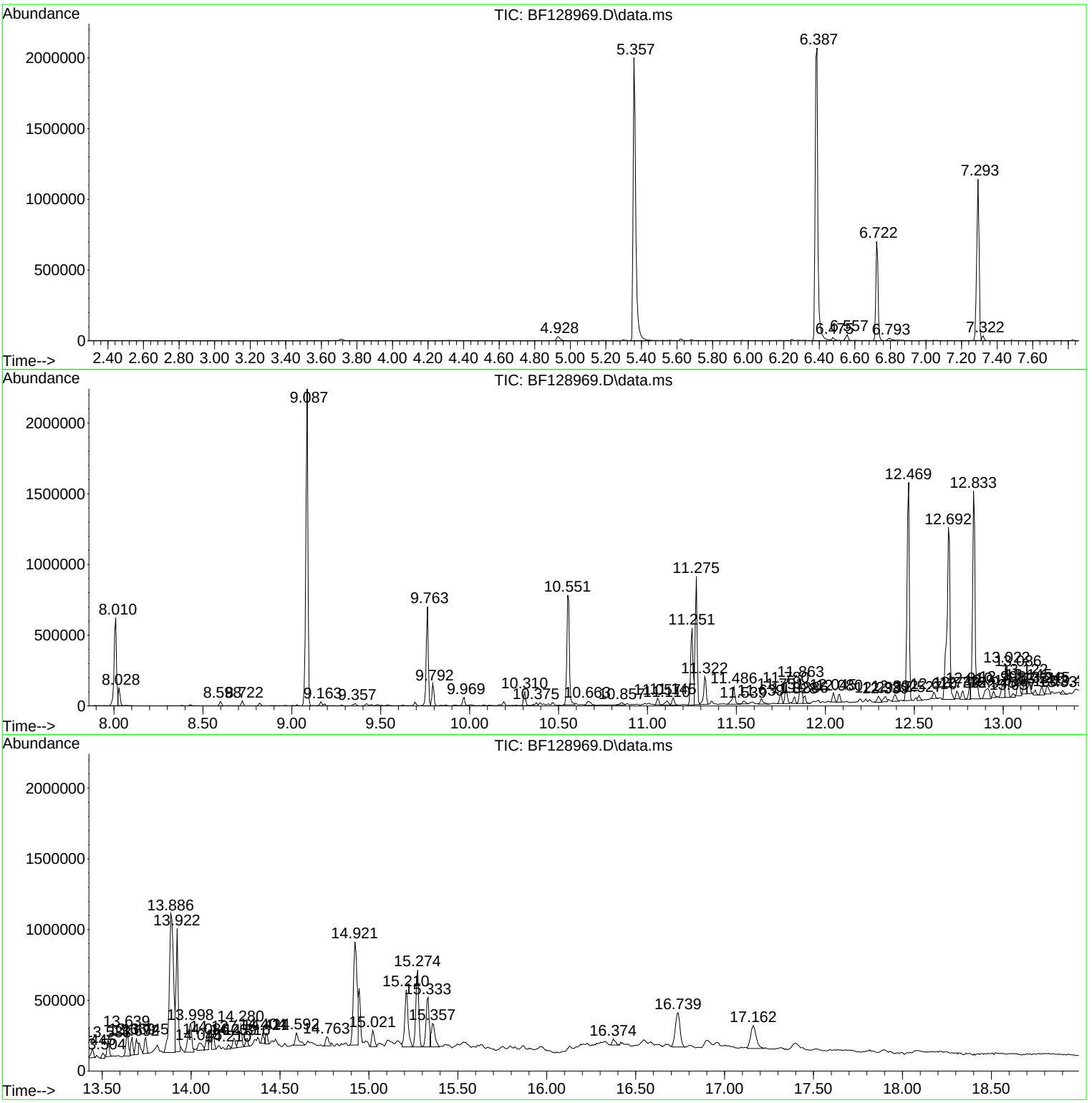
Instrument :
BNA_F
ClientSampleId :
SB-2-3-5-20220622

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.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\BF062322\
Data File : BF128969.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

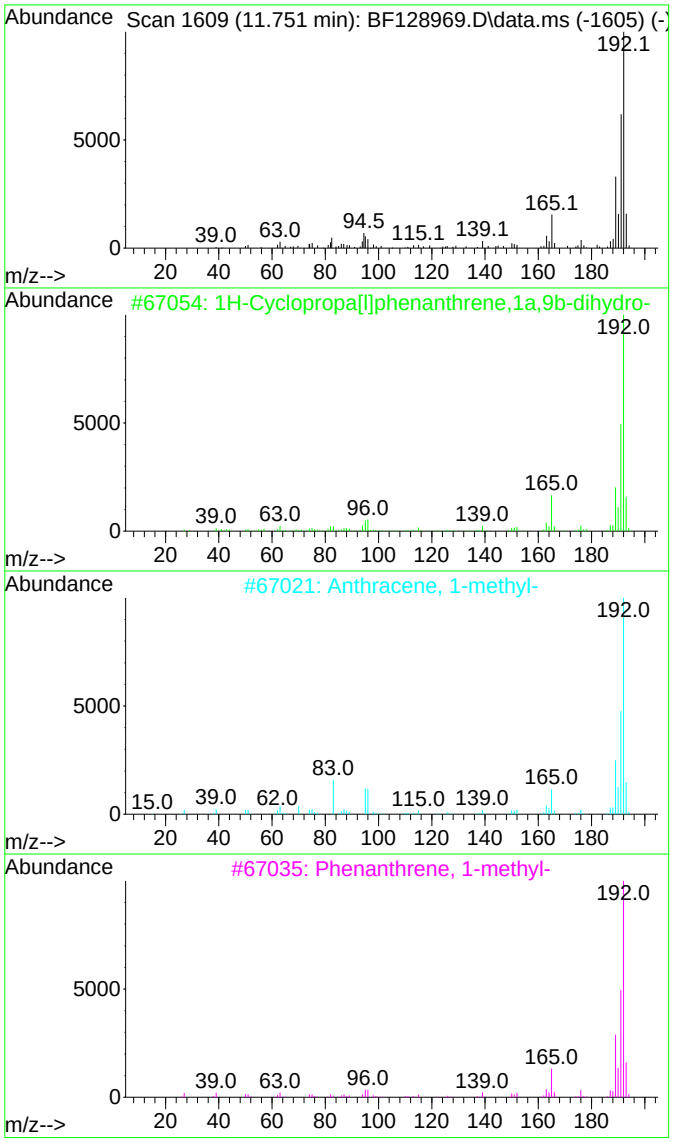
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

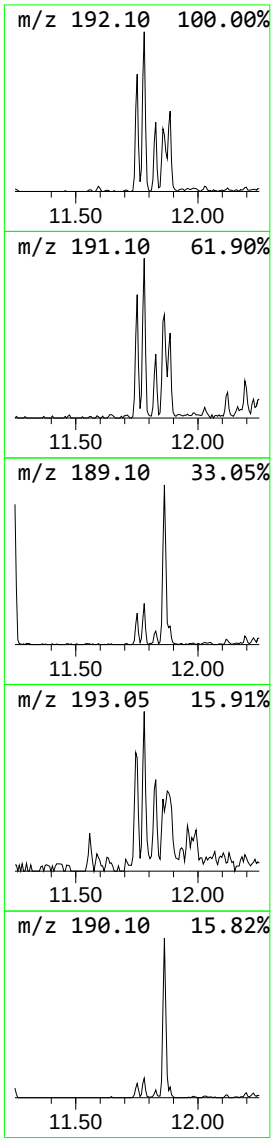
****

Peak Number 1 1H-Cyclopropa[l]phenanthren... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.751	2.44 ng	65369	Phenanthrene-d10	11.251

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	96
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	94
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
4	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	93
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062322\
Data File : BF128969.D
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Sample : N3462-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

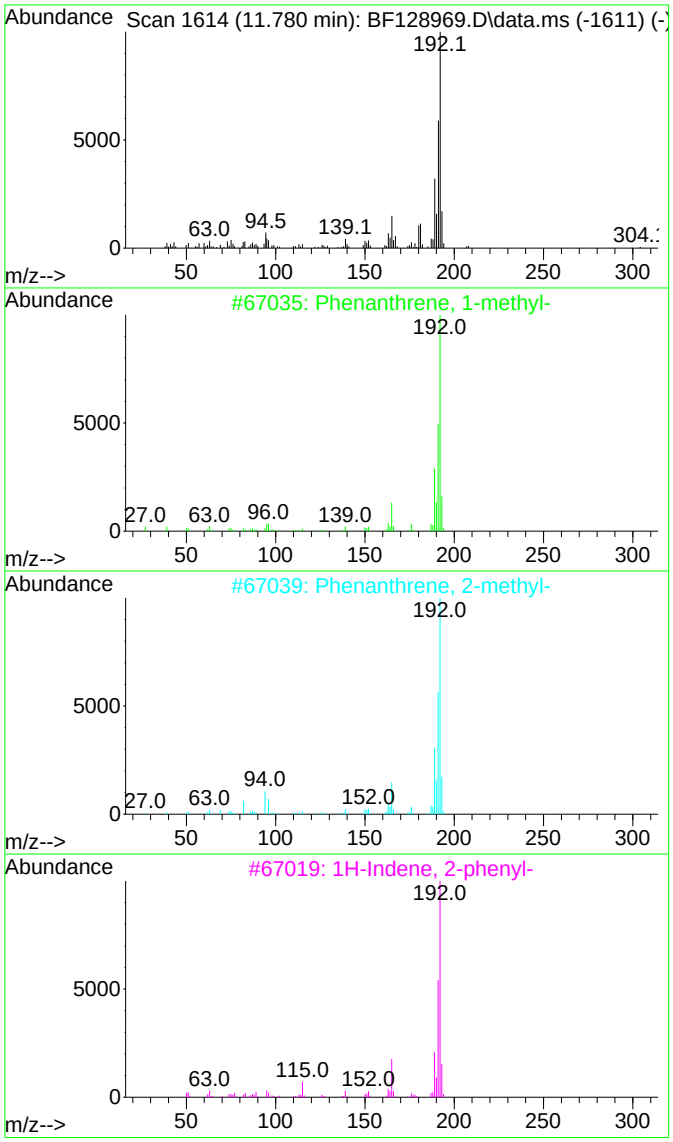
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

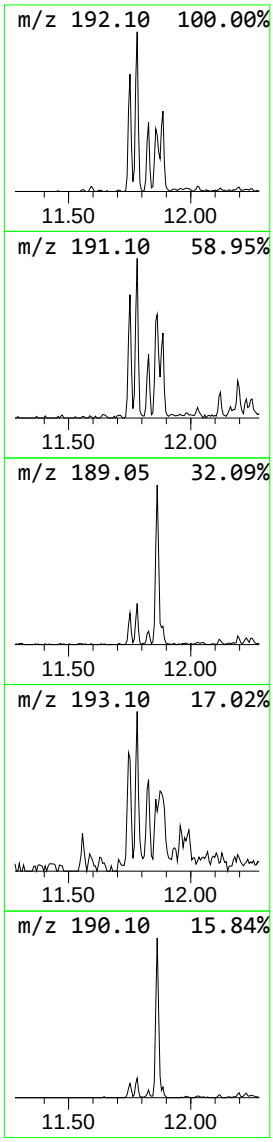
****

Peak Number 2 Phenanthrene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.781	3.88 ng	104010	Phenanthrene-d10	11.251

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	94
3	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	89
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	89
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	89





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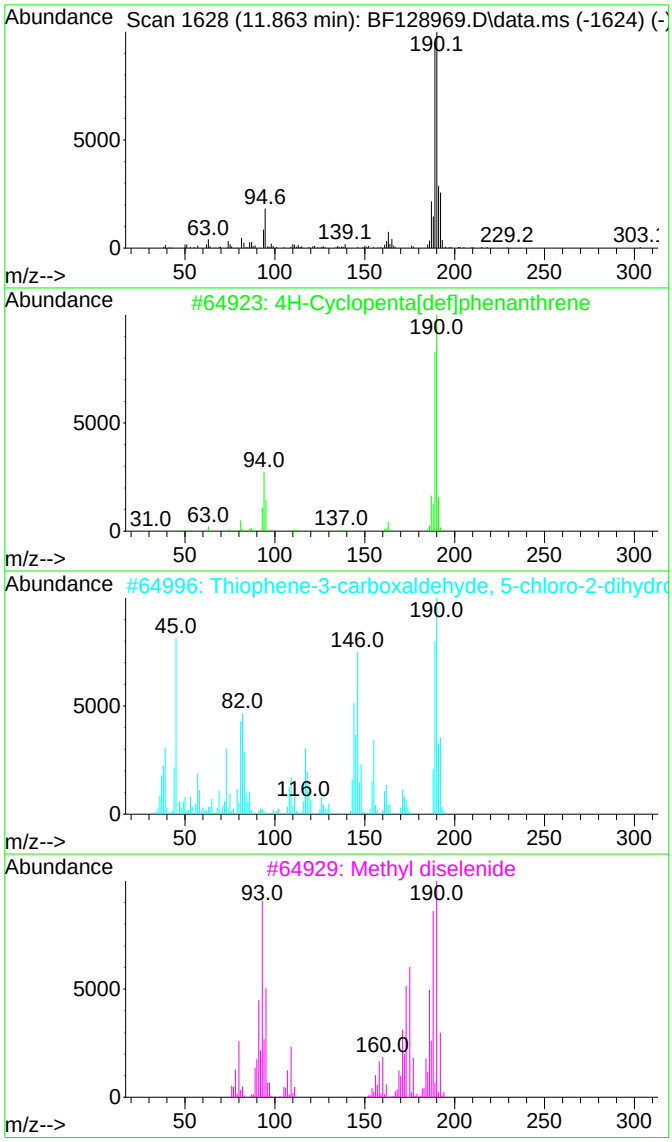
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

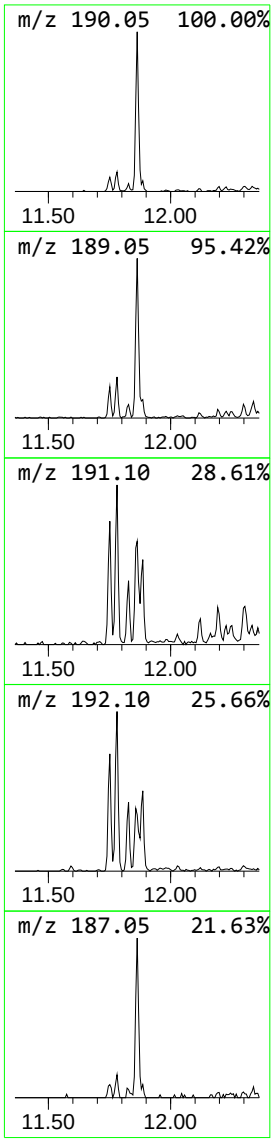
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	5.87 ng	157464	Phenanthrene-d10	11.251

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	52
3	Methyl diselenide	190	C2H6Se2	007101-31-7	49
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
5	1-Aminocyclopentanecarboxylic ac...	389	C20H36ClNO4	1000329-17-2	27





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

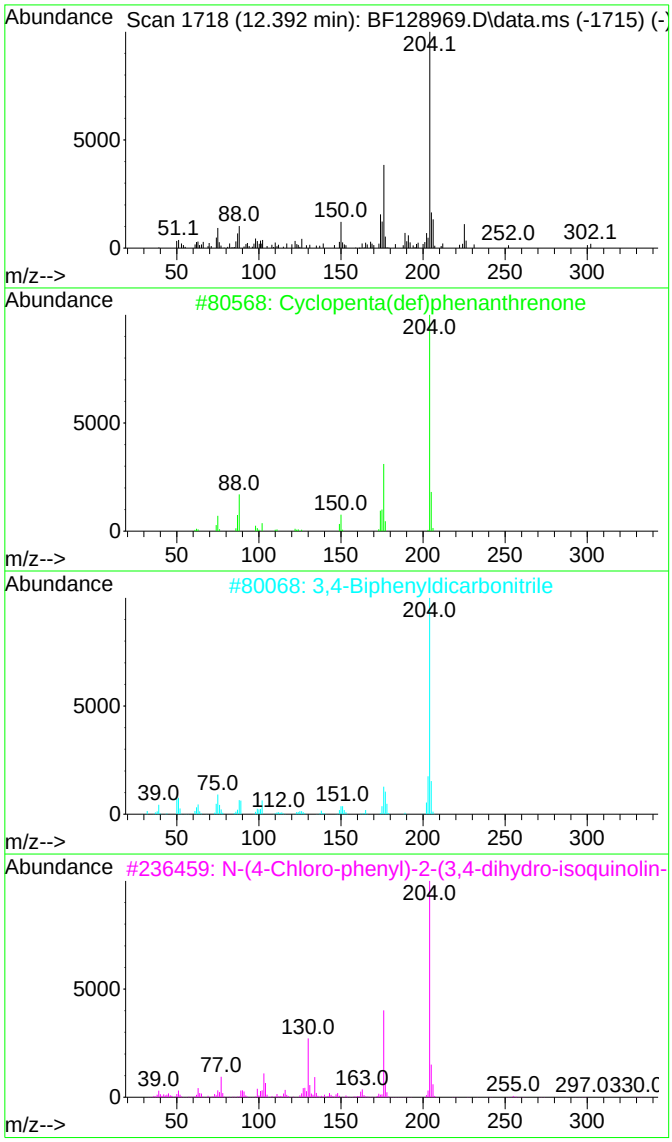
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

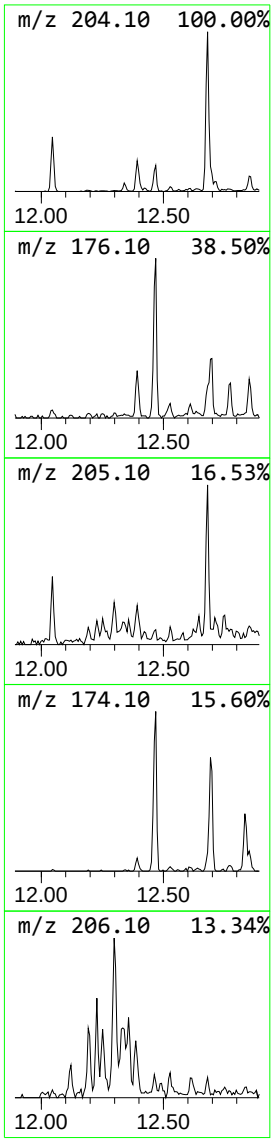
****

Peak Number 4 Cyclopenta(def)phenanthrenone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.392	2.04 ng	54818	Phenanthrene-d10	11.251

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	87
2	3,4-Biphenyldicarbonitrile	204	C14H8N2	004128-63-6	59
3	N-(4-Chloro-phenyl)-2-(3,4-dihyd...	330	C17H15ClN2OS	1010296-34-3	53
4	[1,1'-Biphenyl]-4,4'-dicarbonitrile	204	C14H8N2	001591-30-6	50
5	5,6,7,8-Tetrahydrothieno[2,3-b]q...	204	C11H12N2S	122914-50-5	50





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Data File : BF128969.D
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Sample : N3462-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2-3-5-20220622

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

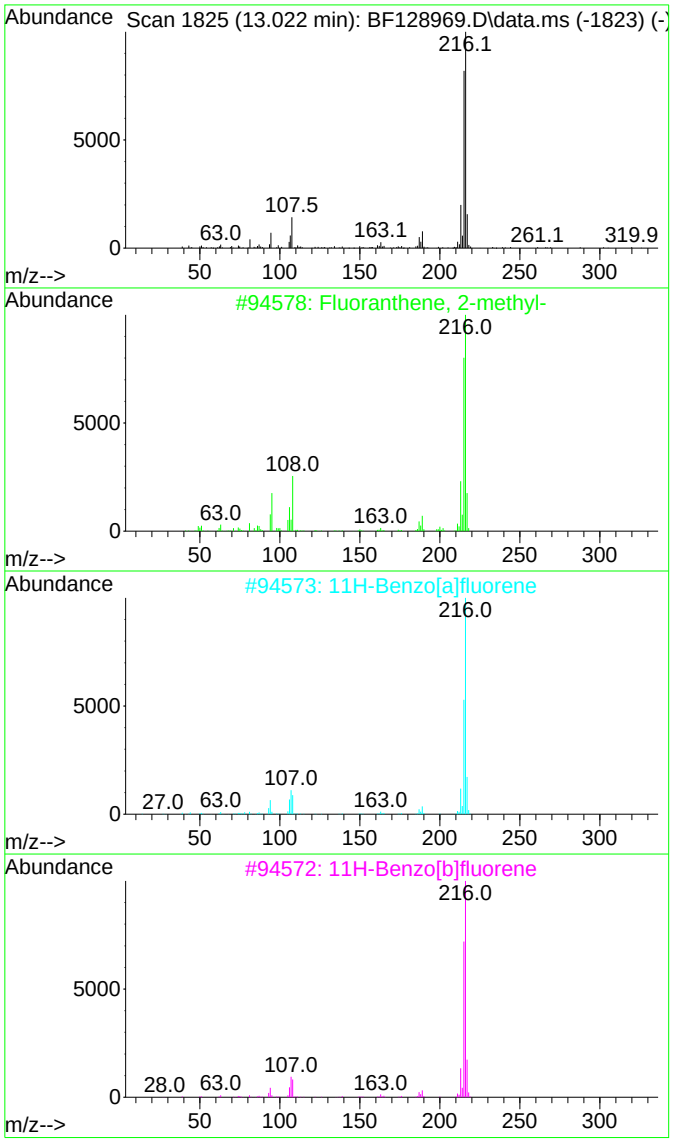
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

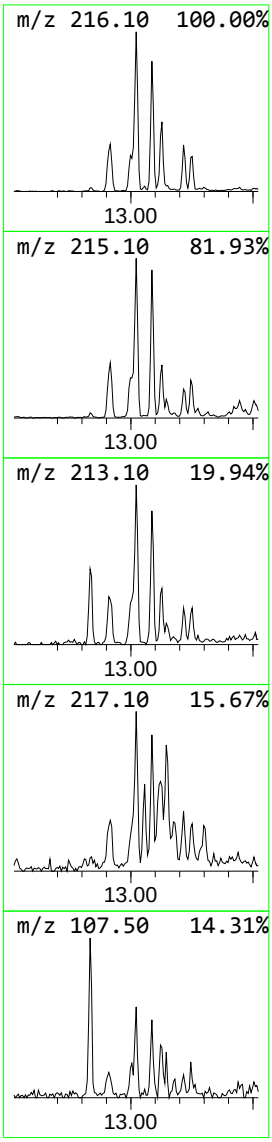
****

Peak Number 5 Fluoranthene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.022	2.27 ng	184550	Chrysene-d12	13.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	94
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	94
3	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	94
4	Pyrene, 1-methyl-	216	C17H12	002381-21-7	91
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	87





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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2-3-5-20220622

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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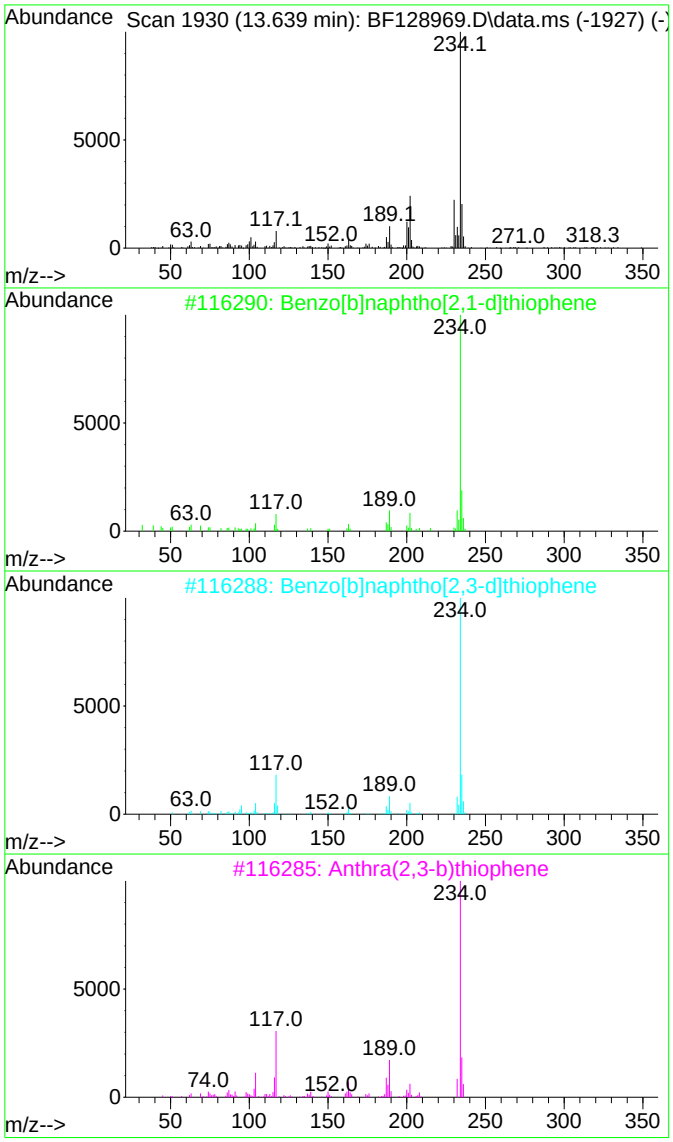
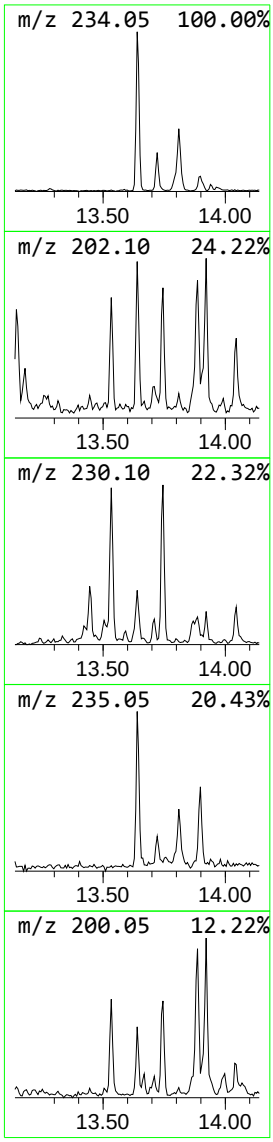
Peak Number 6 Benzo[b]naphtho[2,1-d]thiop... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.639	2.13 ng	173302	Chrysene-d12	13.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]naphtho[2,1-d]thiophene	234	C16H10S	000239-35-0	76
2	Benzo[b]naphtho[2,3-d]thiophene	234	C16H10S	000243-46-9	70
3	Anthra(2,3-b)thiophene	234	C16H10S	022108-55-0	70
4	Benzo[b]naphtho[1,2-d]thiophene	234	C16H10S	000205-43-6	52
5	5,6,8,9,10,11-Hexahydrobenz[a]an...	234	C18H18	067064-61-3	47





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Data File : BF128969.D
Acq On : 23 Jun 2022 23:31
Operator : CG\JU
Sample : N3462-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2-3-5-20220622

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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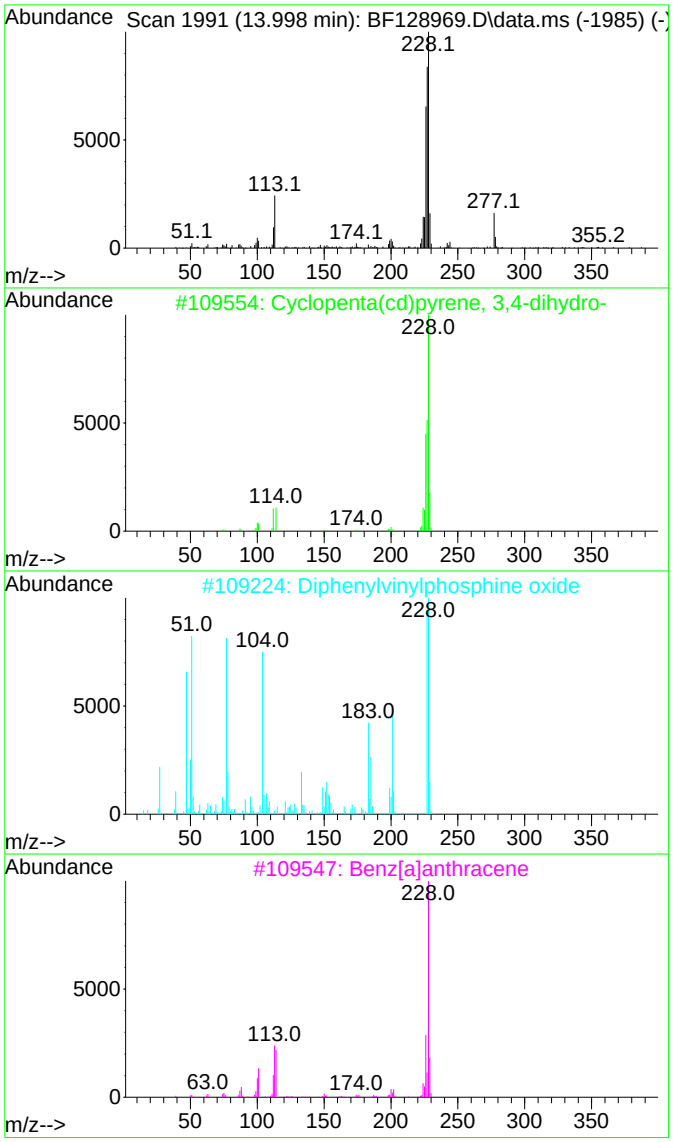
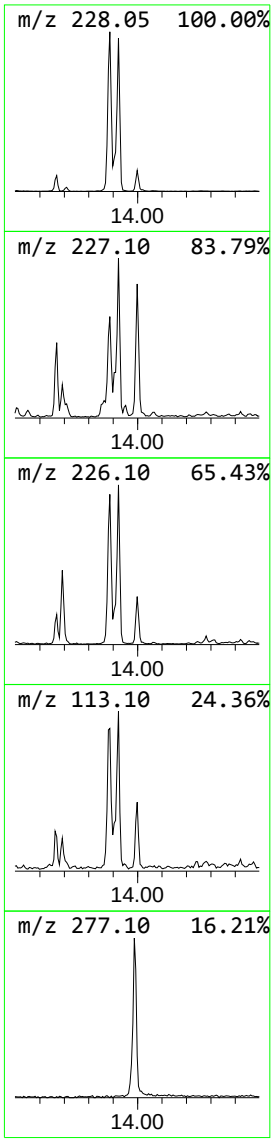
Peak Number 7 Cyclopenta(cd)pyrene, 3,4-d... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.998	3.63 ng	295114	Chrysene-d12	13.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(cd)pyrene, 3,4-dihydro-	228	C18H12	025732-74-5	87
2	Diphenylvinylphosphine oxide	228	C14H13OP	002096-78-8	47
3	Benz[a]anthracene	228	C18H12	000056-55-3	45
4	Chrysene	228	C18H12	000218-01-9	43
5	1(2H)-Phenanthrenone, 3,4,9,10-t...	228	C15H16O2	014427-61-3	38





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Operator : CG\JU
Sample : N3462-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2-3-5-20220622

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
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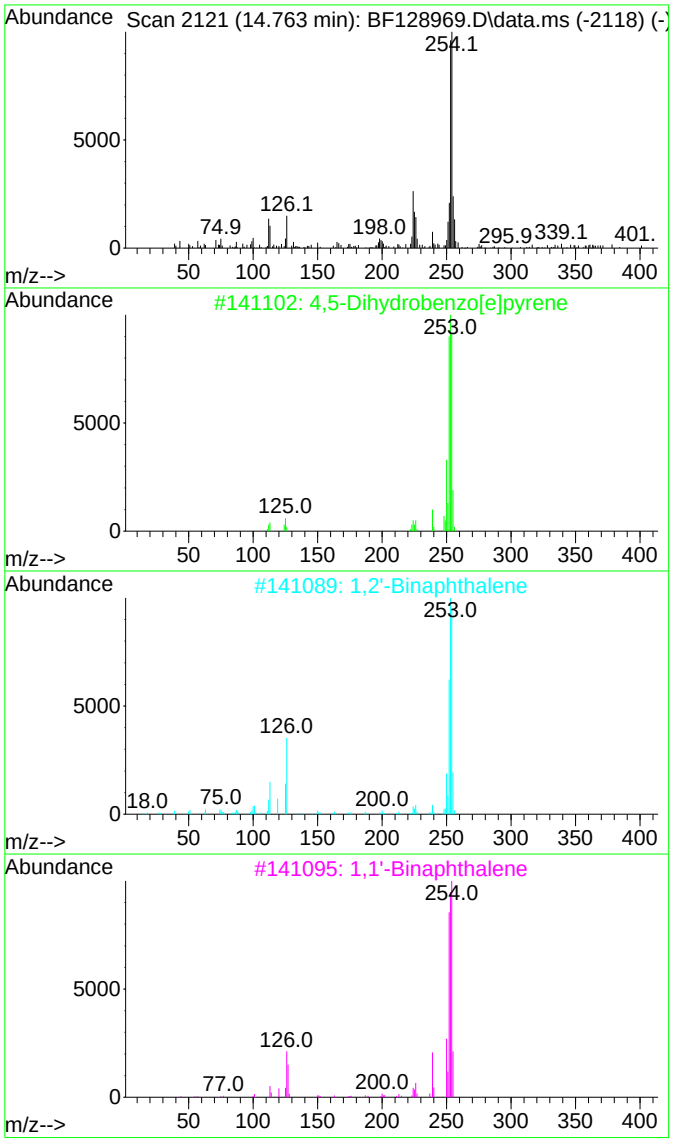
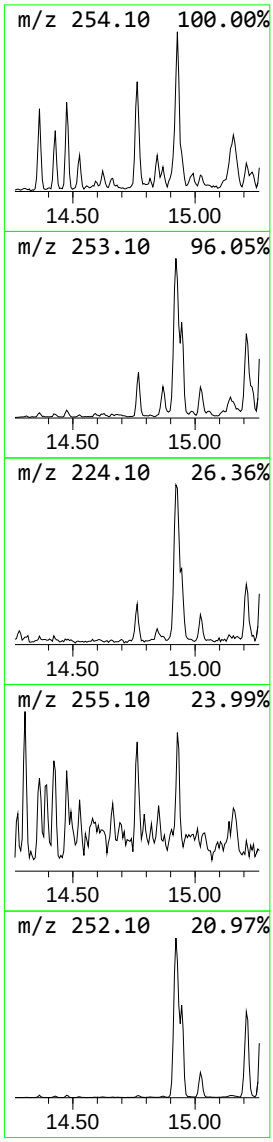
Peak Number 8 4,5-Dihydrobenzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.763	3.78 ng	82054	Perylene-d12	15.333

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,5-Dihydrobenzo[e]pyrene	254	C20H14	095676-42-9	72
2	1,2'-Binaphthalene	254	C20H14	004325-74-0	72
3	1,1'-Binaphthalene	254	C20H14	000604-53-5	68
4	9,10[1',2']-Benzenoanthracene, 9...	254	C20H14	000477-75-8	64
5	Benzo[a]pyrene, 4,5-dihydro-	254	C20H14	057652-66-1	64





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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2-3-5-20220622

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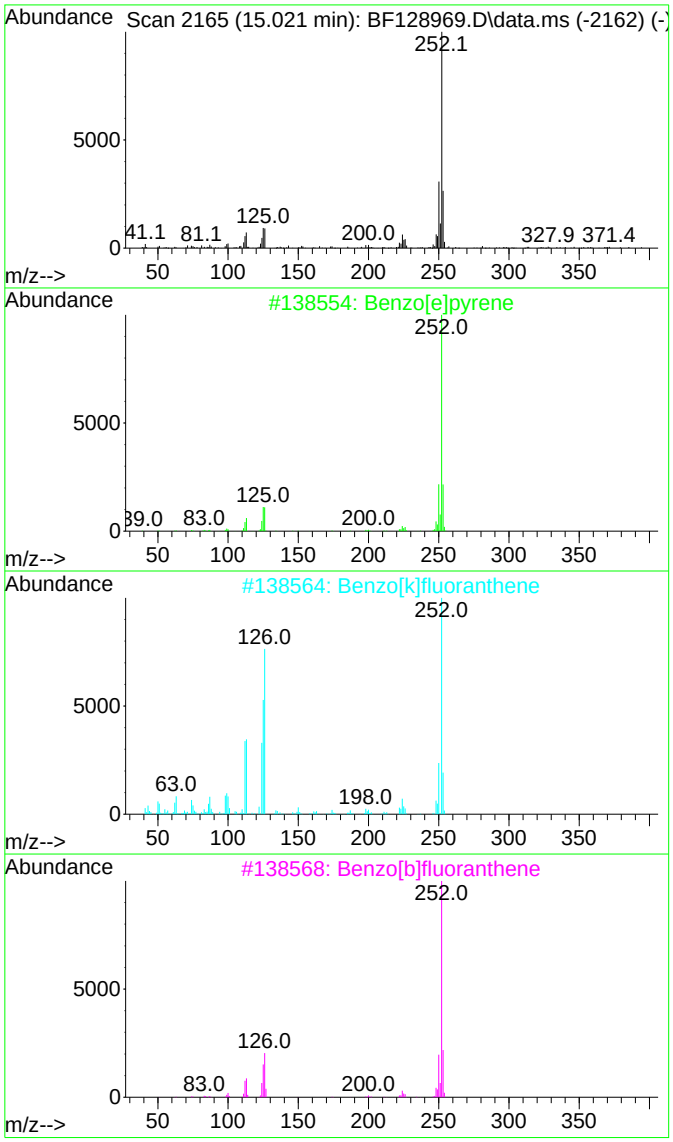
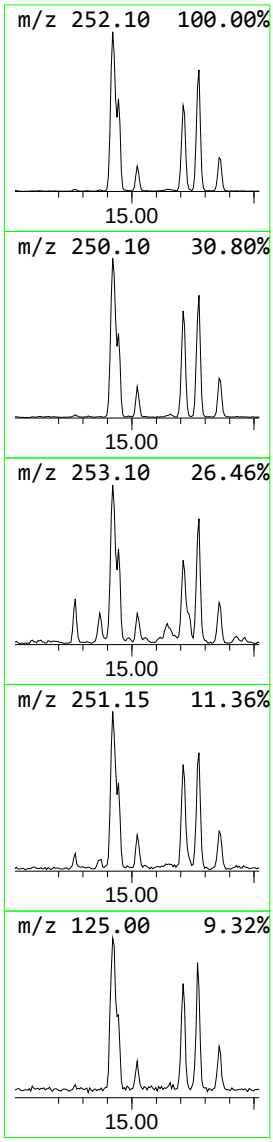
Peak Number 9 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.021	5.63 ng	122110	Perylene-d12	15.333

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	95
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	91
4	Benzo[a]pyrene	252	C20H12	000050-32-8	90
5	Perylene	252	C20H12	000198-55-0	90





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Data File : BF128969.D
Acq On : 23 Jun 2022 23:31
Operator : CG\JU
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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2-3-5-20220622

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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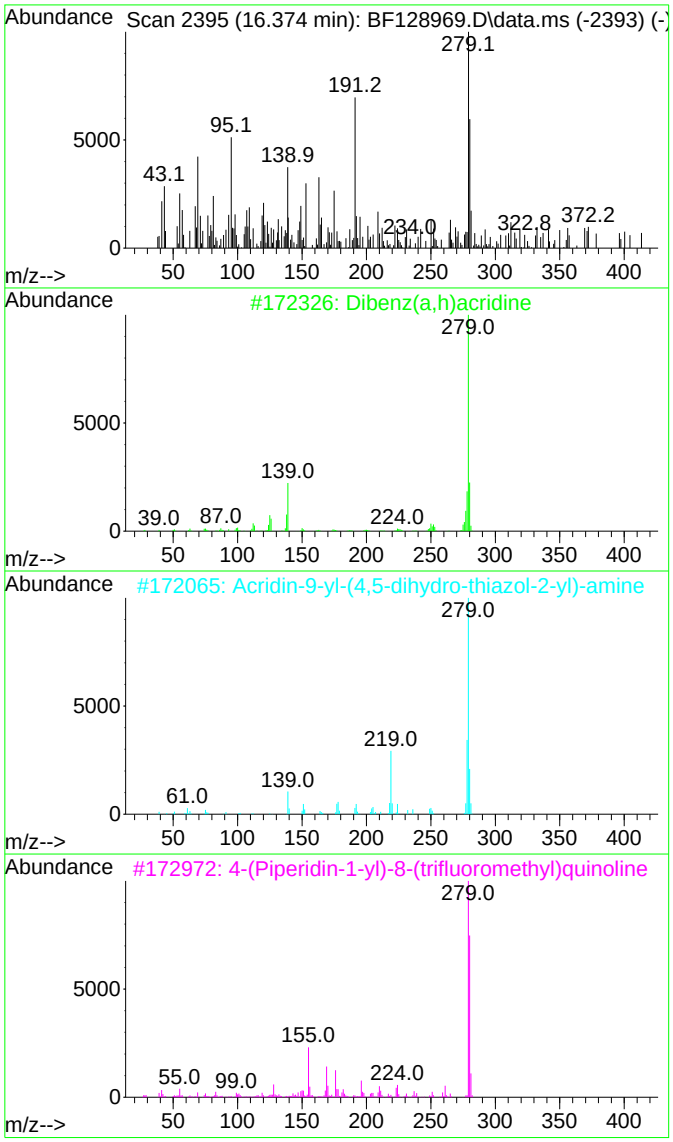
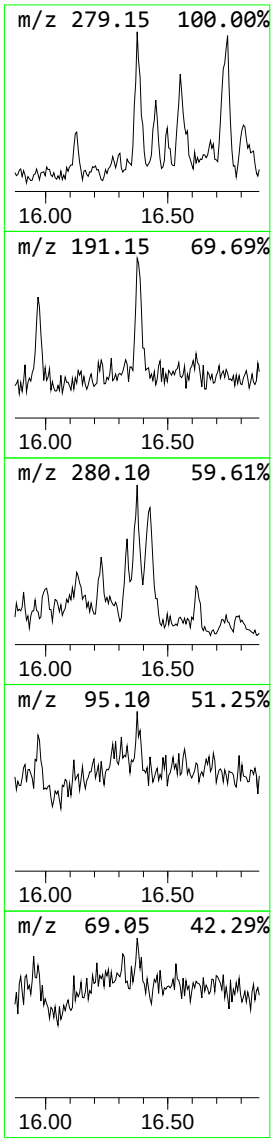
Peak Number 11 unknown16.374 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.374	2.37 ng	51455	Perylene-d12	15.333

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenz(a,h)acridine	279	C21H13N	000226-36-8	43
2	Acridin-9-yl-(4,5-dihydro-thiazo...	279	C16H13N3S	1000317-53-9	38
3	4-(Piperidin-1-yl)-8-(trifluorom...	280	C15H15F3N2	1020252-84-9	30
4	Benzene, 1,2-bis(2-pyridin-2-yle...	280	C20H12N2	350587-04-1	25
5	2-(3-Phenyl-1H-1,2,4-triazol-5-y...	294	C16H18N4Si	1000472-13-0	22





Tentatively Identified Compound (LSC) summary

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1H-Cyclopropa[l...	11.751	2.4	ng	65369	4	11.251	536334	20.0
Phenanthrene, 1...	11.781	3.9	ng	104010	4	11.251	536334	20.0
4H-Cyclopenta[d...	11.863	5.9	ng	157464	4	11.251	536334	20.0
Cyclopenta(def)...	12.392	2.0	ng	54818	4	11.251	536334	20.0
Fluoranthene, 2...	13.022	2.3	ng	184550	5	13.898	1626960	20.0
Benzo[b]naphtho...	13.639	2.1	ng	173302	5	13.898	1626960	20.0
Cyclopenta(cd)p...	13.998	3.6	ng	295114	5	13.898	1626960	20.0
4,5-Dihydrobenz...	14.763	3.8	ng	82054	6	15.333	433821	20.0
Benzo[e]pyrene	15.021	5.6	ng	122110	6	15.333	433821	20.0
unknown16.374	16.374	2.4	ng	51455	6	15.333	433821	20.0