LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101821\
Data File : BF125884.D
Acq On : 18 Oct 2021 18:52
Operator : JU/CG
Sample : M4249-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP1-(S)

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-BF100721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125884.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.039	498	502	507	rVB	29231	38447	1.05%	0.100%
2	5.439	565	570	573	rBV	3292581	3037510	82.64%	7.921%
3	6.451	736	742	745	rBV	2952224	2982830	81.15%	7.779%
4	6.822	802	805	808	rBV	1194501	907077	24.68%	2.365%
5	7.380	895	900	903	rBV	2213014	1936759	52.69%	5.051%
6	8.004	1002	1006	1013	rBV	248348	205363	5.59%	0.536%
7	8.104	1019	1023	1026	rBV	1548622	1245213	33.88%	3.247%
8	8.816	1140	1144	1147	rVB	44387	37866	1.03%	0.099%
9	8.910	1156	1160	1165	rVB	49460	41889	1.14%	0.109%
10	9.174	1201	1205	1209	rBV	3873496	3675536	100.00%	9.585%
11	9.439	1246	1250	1254	rBV2	41649	50488	1.37%	0.132%
12	9.510	1259	1262	1265	rBV	67544	67298	1.83%	0.175%
13	9.716	1293	1297	1301	rBV	114437	93648	2.55%	0.244%
14	9.857	1317	1321	1324	rBV	1435646	1325418	36.06%	3.456%
15	9.886	1324	1326	1329	rVB	85537	63330	1.72%	0.165%
16	10.057	1351	1355	1359	rBV	77232	62989	1.71%	0.164%
17	10.398	1410	1413	1419	rVB	150003	132979	3.62%	0.347%
18	10.639	1450	1454	1457	rBV	2257216	1896367	51.59%	4.945%
19	10.945	1496	1506	1509	rBV2	45608	64337	1.75%	0.168%
20	11.233	1553	1555	1561	rVB	66092	54500	1.48%	0.142%
21	11.333	1569	1572	1574	rBV	1257242	1112673	30.27%	2.902%
22	11.357	1574	1576	1580	rVV	980801	805350	21.91%	2.100%
23	11.410	1580	1585	1588	rVB	246225	209474	5.70%	0.546%
24	11.668	1626	1629	1633	rVB2	52629	47411	1.29%	0.124%
25	11.839	1654	1658	1660	rBV	171271	157545	4.29%	0.411%
26	11.863	1660	1662	1666	rVV	282558	234171	6.37%	0.611%
27	11.910	1666	1670	1673	rVV2	76201	70675	1.92%	0.184%
28	11.951	1673	1677	1679	rVV2	273685	295677	8.04%	0.771%
29	11.968	1679	1680	1684	rVB	127977	92697	2.52%	0.242%
30	12.133	1705	1708	1710	rBV	100980	90118	2.45%	0.235%
31	12.151	1710	1711	1715	rVB2	62599	51245	1.39%	0.134%
32	12.386	1747	1751	1754	rBV	103902	101358	2.76%	0.264%
33	12.421	1754	1757	1759	rVV2	64271	76954	2.09%	0.201%
34	12.468	1762	1765	1770	rVB	105688	109232	2.97%	0.285%
35	12.545	1775	1778	1782	rVB	1647137	1392172	37.88%	3.630%
36	12.639	1792	1794	1797	rVB	78425	66662	1.81%	0.174%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101821\
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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP1-(S)

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-BF100721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.698	1802	1804	1811	rVB2	49127	60290	1.64%	0.157%
38	12.774	1811	1817	1823	rBV	1631212	1583377	43.08%	4.129%
39	12.821	1823	1825	1830	rVB2	56031	66679	1.81%	0.174%
40	12.892	1833	1837	1838	rBV	87361	67067	1.82%	0.175%
41	12.921	1838	1842	1845	rVV	3175919	2719606	73.99%	7.092%
42	12.992	1849	1854	1858	rBV2	109109	177851	4.84%	0.464%
43	13.080	1865	1869	1870	rBV2	96571	99562	2.71%	0.260%
44	13.104	1870	1873	1876	rVB	194842	200347	5.45%	0.522%
45	13.168	1876	1884	1886	rBV	135159	149307	4.06%	0.389%
46	13.204	1886	1890	1893	rVV	175519	170878	4.65%	0.446%
47	13.233	1893	1895	1898	rVB2	40992	38502	1.05%	0.100%
48	13.262	1898	1900	1903	rBV2	37306	37438	1.02%	0.098%
49	13.298	1903	1906	1909	rVB	102777	75174	2.05%	0.196%
50	13.327	1909	1911	1915	rBV	109872	93655	2.55%	0.244%
51	13.604	1955	1958	1963	rVB	164858	162195	4.41%	0.423%
52	13.715	1972	1977	1980	rBV2	136684	197076	5.36%	0.514%
53	13.751	1980	1983	1984	rVV	140977	137101	3.73%	0.358%
54	13.768	1984	1986	1990	rVV2	130906	169354	4.61%	0.442%
55	13.815	1990	1994	2001	rVV2	206862	280668	7.64%	0.732%
56	13.886	2004	2006	2013	rVB2	33364	50998	1.39%	0.133%
57	13.968	2013	2020	2023	rBV2	1511495	2177794	59.25%	5.679%
58	13.998	2023	2025	2030	rVB	792950	690019	18.77%	1.799%
59	14.074	2036	2038	2041	rVB	116440	85763	2.33%	0.224%
60	14.109	2041	2044	2046	rVV	101021	92588	2.52%	0.241%
61	14.157	2050	2052	2054	rVB	56605	48023	1.31%	0.125%
62	14.192	2054	2058	2061	rBV2	65507	90175	2.45%	0.235%
63	14.227	2061	2064	2066	rVB3	43062	41774	1.14%	0.109%
64	14.321	2077	2080	2082	rBV	50846	58467	1.59%	0.152%
65	14.357	2082	2086	2089	rVV	178966	198371	5.40%	0.517%
66	14.392	2089	2092	2095	rVV	98434	107540	2.93%	0.280%
67	14.451	2095	2102	2104	rVV3	98093	162979	4.43%	0.425%
68	14.480	2104	2107	2109	rVV2	107753	126796	3.45%	0.331%
69	14.504	2109	2111	2114	rVV3	92264	95608	2.60%	0.249%
70	14.551	2114	2119	2124	rVB4	60204	101404	2.76%	0.264%
71	14.656	2134	2137	2140	rBV2	39545	57024	1.55%	0.149%
72	14.727	2145	2149	2155	rBV2	269448	343485	9.35%	0.896%
73	14.821	2162	2165	2167	rBV2	62688	70052	1.91%	0.183%
74	14.909	2177	2180	2183	rBV2	41820	47476	1.29%	0.124%
75	14.998	2190	2195	2198	rBV	692678	1026638	27.93%	2.677%
76	15.104	2210	2213	2218	rVB	147050	147245	4.01%	0.384%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101821\
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Acq On : 18 Oct 2021 18:52
Operator : JU/CG
Sample : M4249-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP1-(S)

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-BF100721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	15.192	2225	2228	2230	rBV2	36741	48846	1.33%	0.127%
78	15.298	2242	2246	2251	rVB	376645	441945	12.02%	1.152%
79	15.356	2251	2256	2262	rBV	552869	654445	17.81%	1.707%
80	15.421	2262	2267	2270	rVV	784257	997728	27.15%	2.602%
81	15.445	2270	2271	2279	rVB2	175172	199329	5.42%	0.520%
82	15.845	2334	2339	2342	rBV2	20981	42278	1.15%	0.110%
83	15.886	2342	2346	2351	rVV7	24352	49223	1.34%	0.128%
84	16.845	2504	2509	2518	rVB2	183835	363132	9.88%	0.947%
85	17.027	2535	2540	2544	rBV	36028	57160	1.56%	0.149%
86	17.080	2545	2549	2553	rBV3	22191	38082	1.04%	0.099%
87	17.280	2576	2583	2595	rBV	135233	270772	7.37%	0.706%
88	17.509	2619	2622	2630	rVB3	25651	44295	1.21%	0.116%

Sum of corrected areas: 38346839

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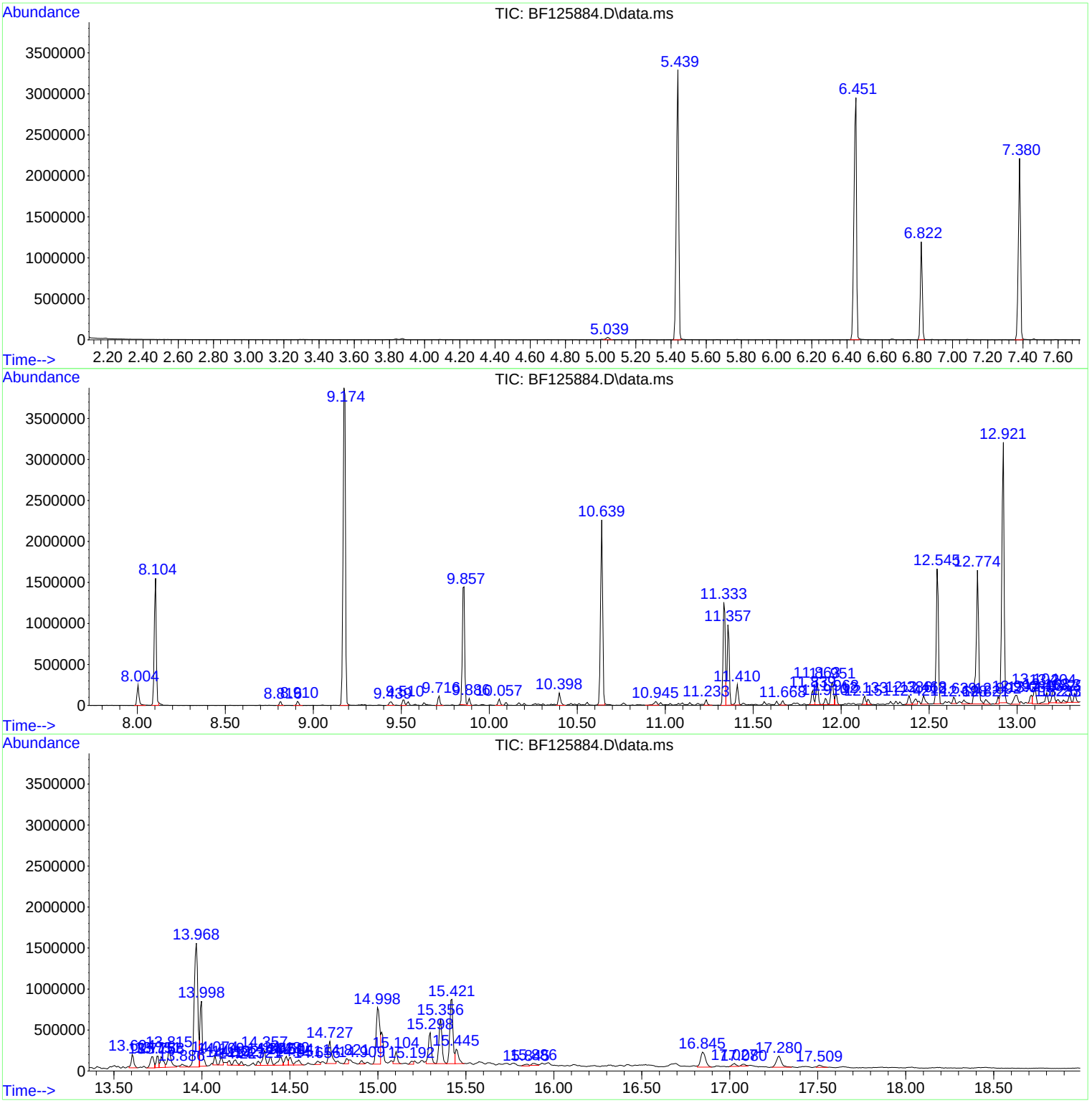
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-(S)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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\BF101821\
Data File : BF125884.D
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Operator : JU/CG
Sample : M4249-01
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Instrument :
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ClientSampleId :
TP1-(S)

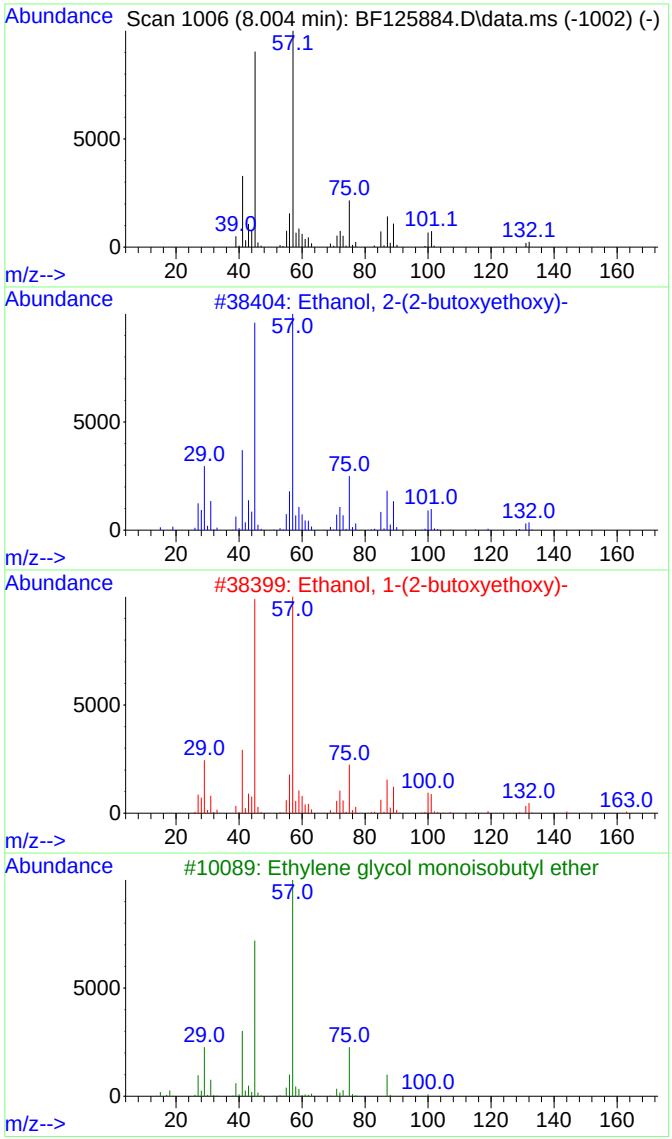
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

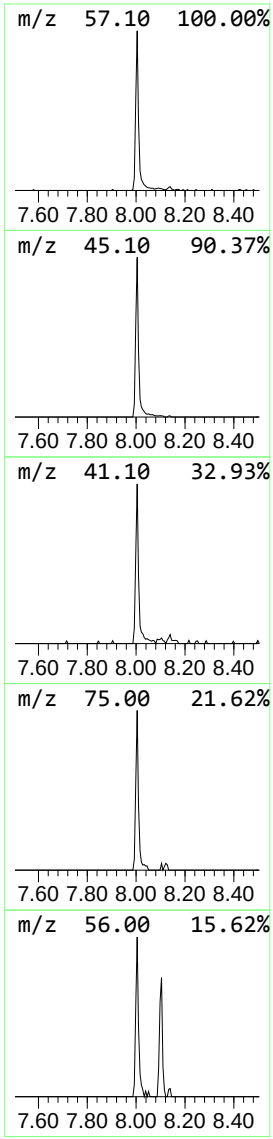
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.004	3.30 ng	205363	Naphthalene-d8	8.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	91
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101821\
Data File : BF125884.D
Acq On : 18 Oct 2021 18:52
Operator : JU/CG
Sample : M4249-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-(S)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

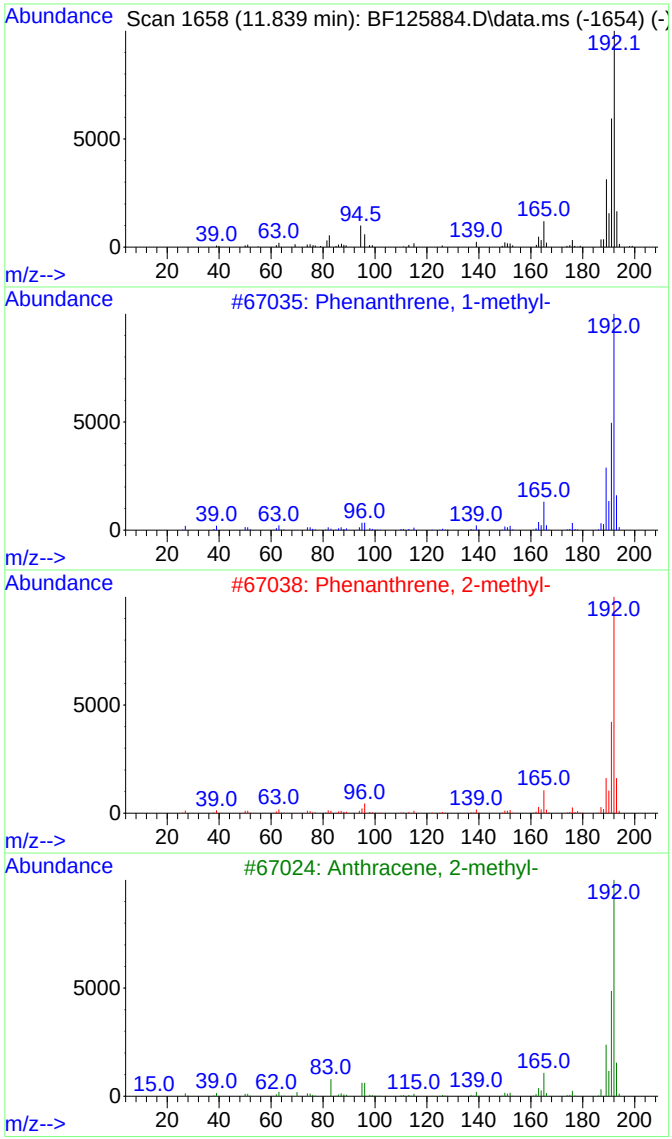
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

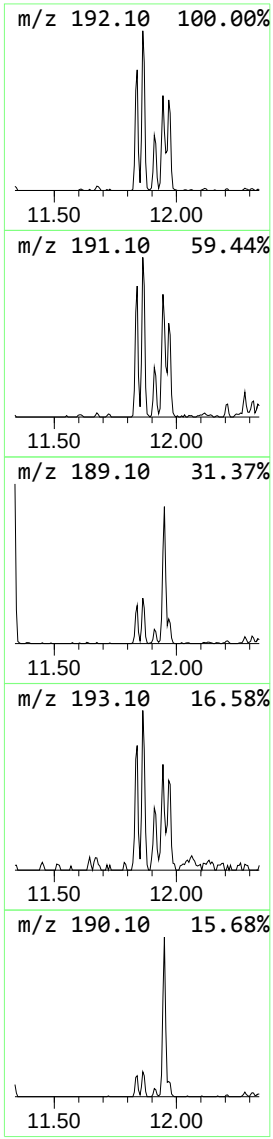
****

Peak Number 3 Phenanthrene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	2.83 ng	157545	Phenanthrene-d10	11.333

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	97
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	95
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	94





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Operator : JU/CG
Sample : M4249-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-(S)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

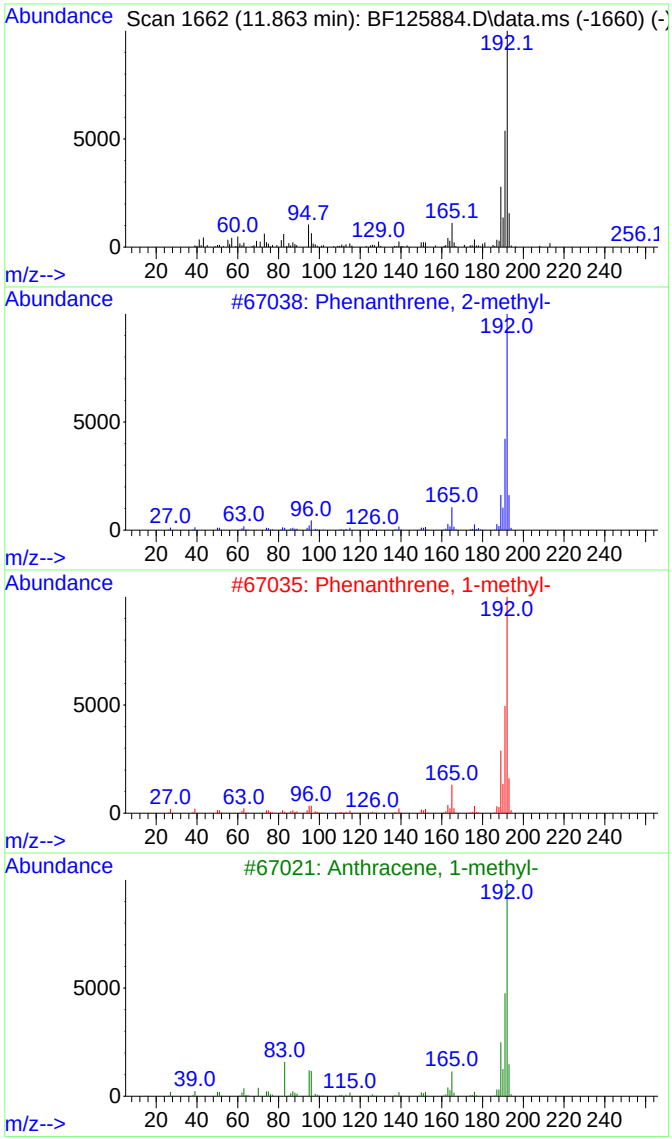
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

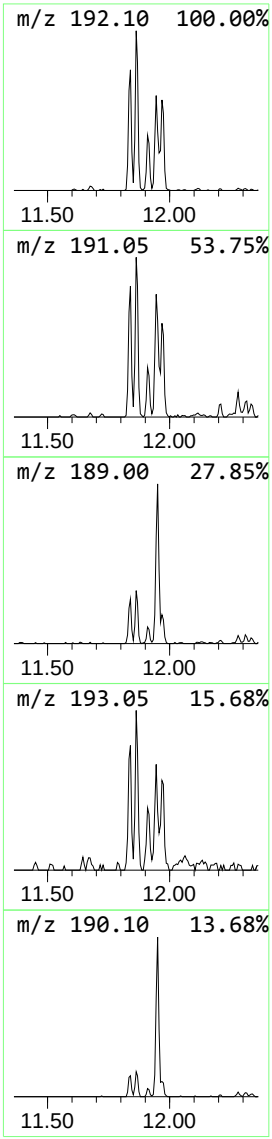
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	4.21 ng	234171	Phenanthrene-d10	11.333

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101821\
Data File : BF125884.D
Acq On : 18 Oct 2021 18:52
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Sample : M4249-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-(S)

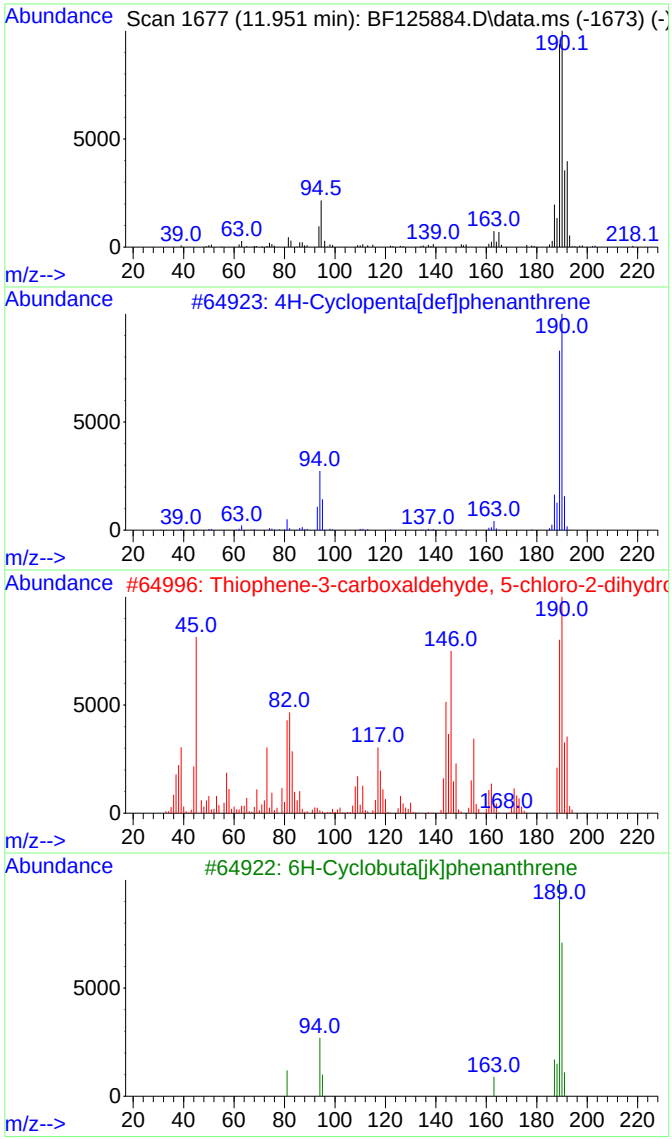
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

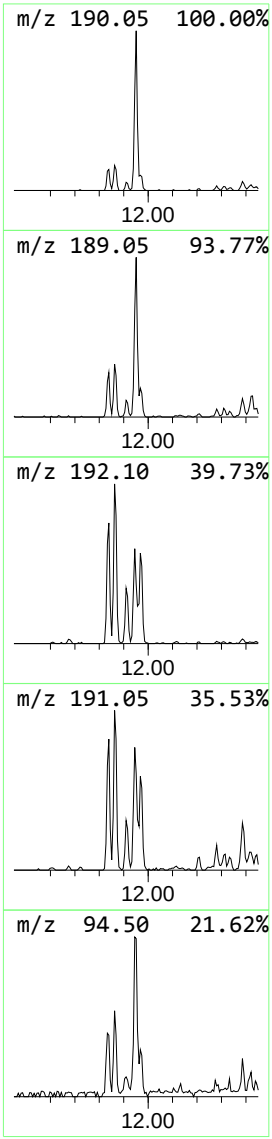
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	5.31 ng	295677	Phenanthrene-d10	11.333

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	76
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	50
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	45
4	Methyl diselenide	190	C2H6Se2	007101-31-7	43
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42





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Data File : BF125884.D
Acq On : 18 Oct 2021 18:52
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Sample : M4249-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-(S)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

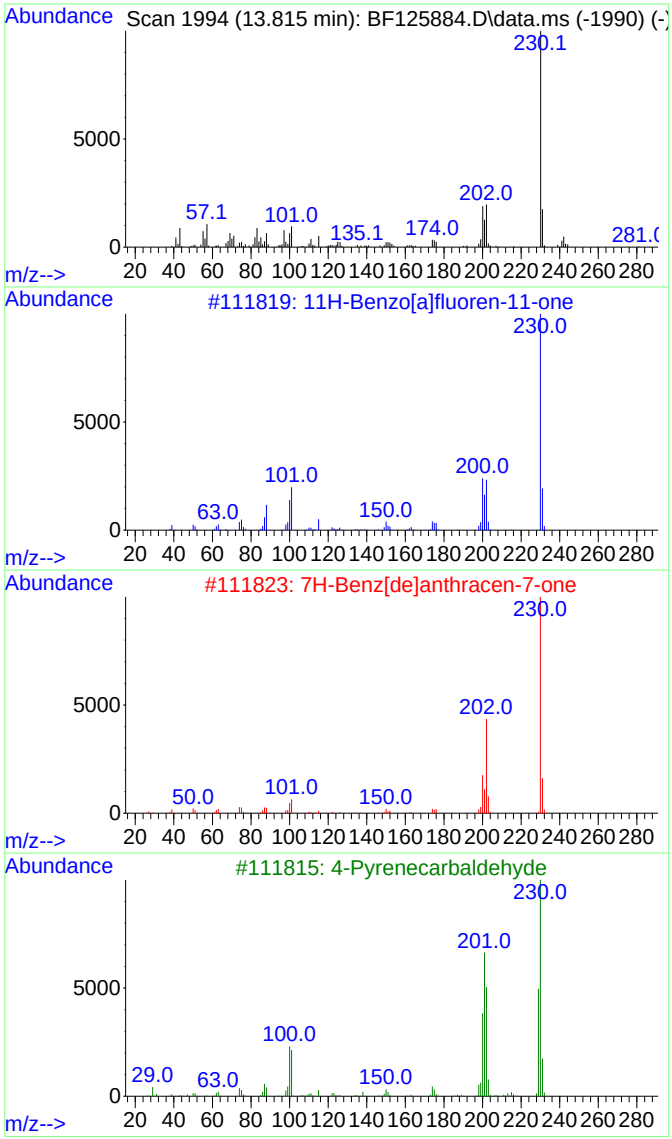
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

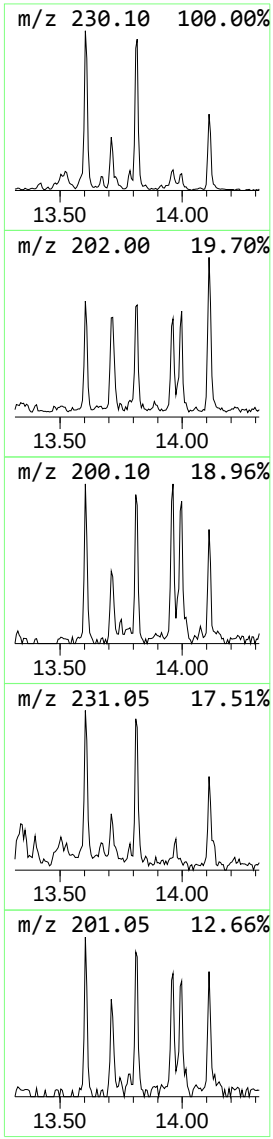
****

Peak Number 6 11H-Benzo[a]fluoren-11-one Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.815	2.58 ng	280668	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	94
2	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	90
3	4-Pyrenecarbaldehyde	230	C17H10O	022245-51-8	72
4	1-Pyrenecarboxaldehyde	230	C17H10O	003029-19-4	72
5	o-Terphenyl	230	C18H14	000084-15-1	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101821\
Data File : BF125884.D
Acq On : 18 Oct 2021 18:52
Operator : JU/CG
Sample : M4249-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-(S)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

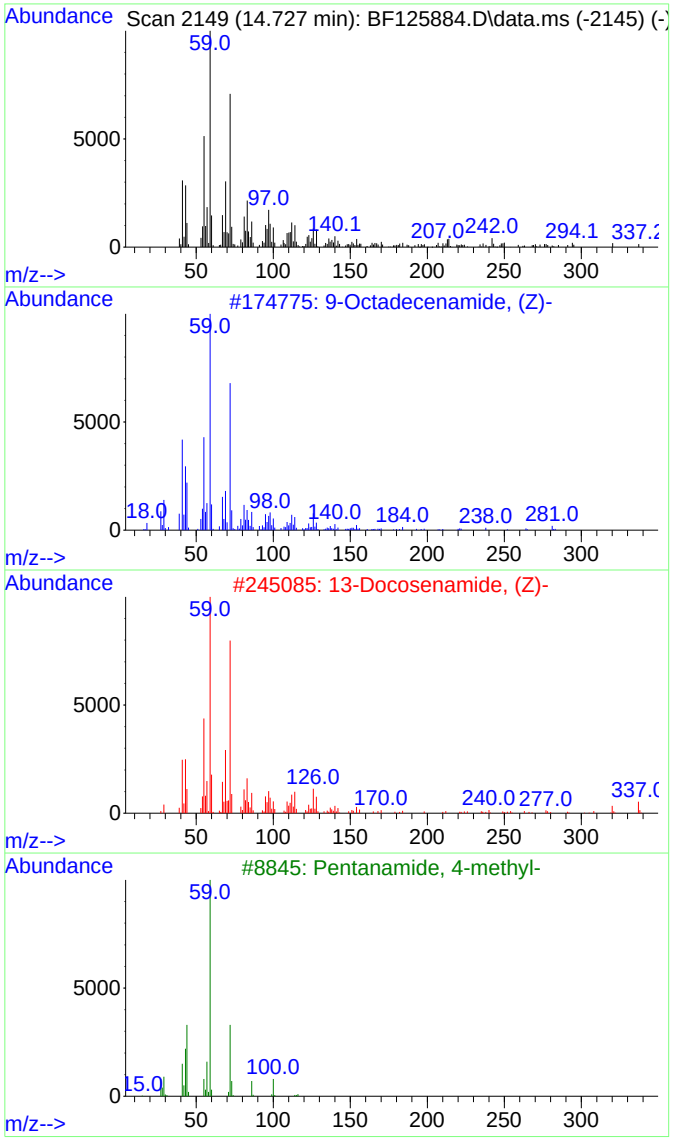
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

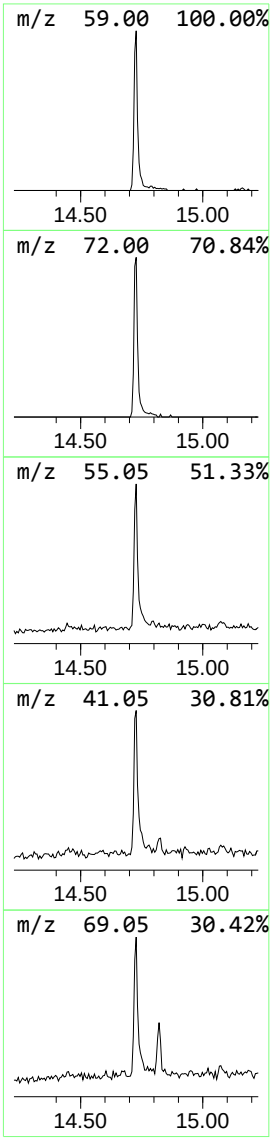
****

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.727	6.89 ng	343485	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	95
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	90
3	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	50
4	Palmitoleamide	253	C16H31NO	106010-22-4	43
5	2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	38





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Data File : BF125884.D
Acq On : 18 Oct 2021 18:52
Operator : JU/CG
Sample : M4249-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP1-(S)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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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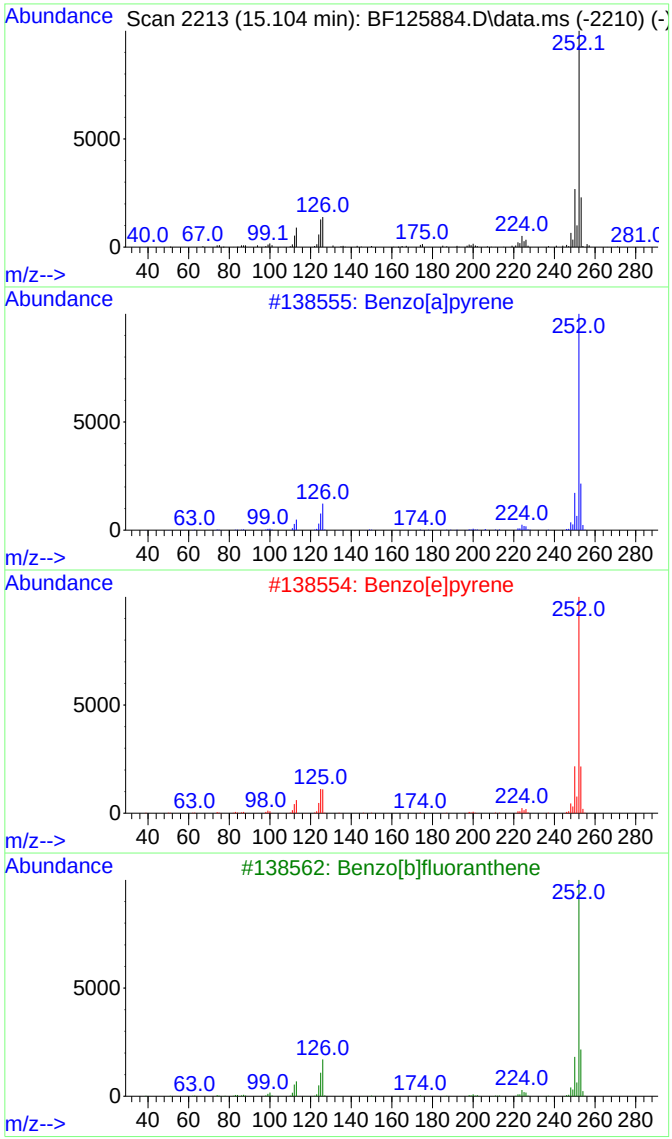
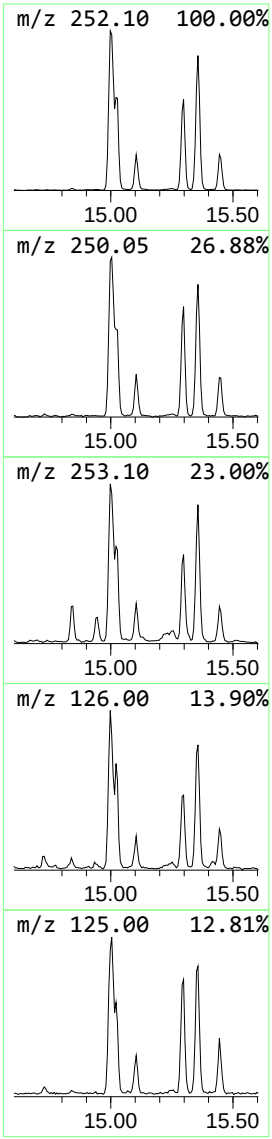
Peak Number 8 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.104	2.95 ng	147245	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene	252	C20H12	000050-32-8	96
2	Benzo[e]pyrene	252	C20H12	000192-97-2	96
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	91
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101821\
Data File : BF125884.D
Acq On : 18 Oct 2021 18:52
Operator : JU/CG
Sample : M4249-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-(S)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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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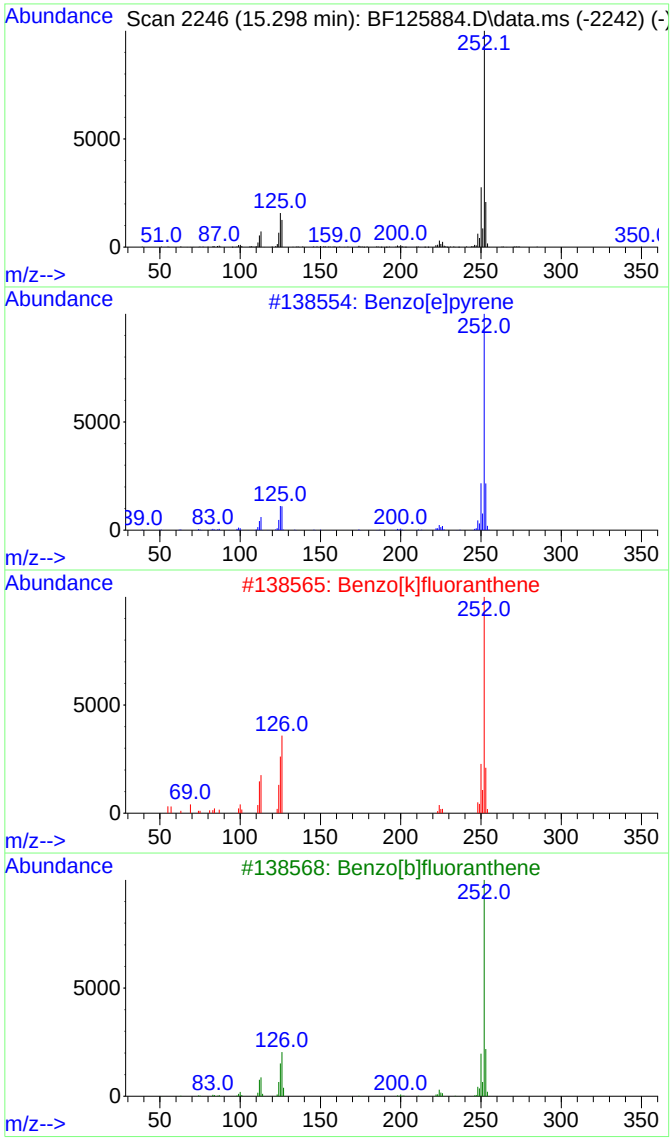
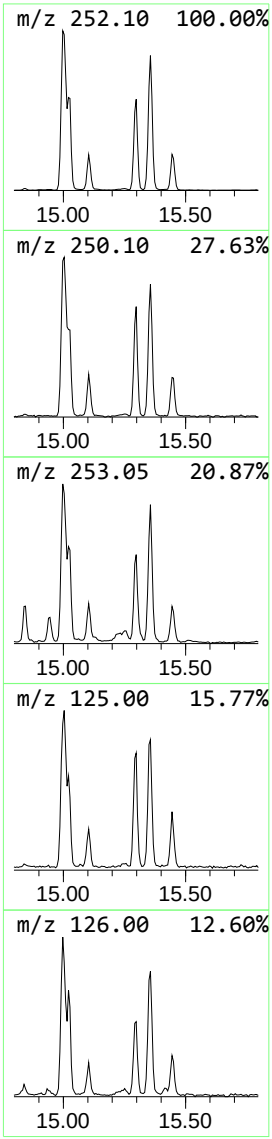
Peak Number 9 Perylene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.298	8.86 ng	441945	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
4	Benzo[a]pyrene	252	C20H12	000050-32-8	93
5	Perylene	252	C20H12	000198-55-0	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101821\
Data File : BF125884.D
Acq On : 18 Oct 2021 18:52
Operator : JU/CG
Sample : M4249-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP1-(S)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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
Ethanol, 2-(2-b...	8.004	3.3	ng	205363	2	8.104	1245210	20.0
Phenanthrene, 1...	11.839	2.8	ng	157545	4	11.333	1112670	20.0
Phenanthrene, 2...	11.863	4.2	ng	234171	4	11.333	1112670	20.0
4H-Cyclopenta[d...	11.951	5.3	ng	295677	4	11.333	1112670	20.0
11H-Benzo[a]flu...	13.815	2.6	ng	280668	5	13.974	2177790	20.0
9-Octadecenamid...	14.727	6.9	ng	343485	6	15.421	997728	20.0
Benzo[e]pyrene	15.104	3.0	ng	147245	6	15.421	997728	20.0
Perylene	15.298	8.9	ng	441945	6	15.421	997728	20.0