LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030722\
Data File : BF127238.D
Acq On : 07 Mar 2022 23:52
Operator : CG\JU
Sample : N1790-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUM-18

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-BF021622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127238.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.104	475	479	486	rVB	35373	44835	2.03%	0.239%
2	5.498	542	546	559	rBV	1998055	1801017	81.64%	9.614%
3	6.510	713	718	730	rBV	2003036	1883187	85.37%	10.052%
4	6.875	777	780	784	rBV	761343	607742	27.55%	3.244%
5	7.440	872	876	879	rBV	1331862	1279578	58.01%	6.830%
6	8.157	995	998	1002	rBV	908964	828478	37.56%	4.422%
7	9.234	1177	1181	1184	rBV	2516851	2205925	100.00%	11.775%
8	9.345	1197	1200	1204	rBV	32341	31593	1.43%	0.169%
9	9.922	1294	1298	1301	rBV	988349	907893	41.16%	4.846%
10	9.951	1301	1303	1306	rVB	33947	25889	1.17%	0.138%
11	10.710	1428	1432	1436	rBV	1690773	1425491	64.62%	7.609%
12	11.351	1538	1541	1545	rVB4	25874	24942	1.13%	0.133%
13	11.410	1547	1551	1553	rBV	1081041	891382	40.41%	4.758%
14	11.433	1553	1555	1558	rVV	376401	282213	12.79%	1.506%
15	11.486	1560	1564	1566	rVB	55845	47658	2.16%	0.254%
16	11.645	1586	1591	1594	rBV	36068	37916	1.72%	0.202%
17	11.792	1612	1616	1619	rVB	55031	46415	2.10%	0.248%
18	11.910	1634	1636	1638	rBV	47421	37603	1.70%	0.201%
19	11.939	1638	1641	1644	rVB	66333	56291	2.55%	0.300%
20	12.022	1652	1655	1658	rBV2	64158	76875	3.48%	0.410%
21	12.045	1658	1659	1665	rVB2	31577	25138	1.14%	0.134%
22	12.210	1684	1687	1689	rBV	30468	27094	1.23%	0.145%
23	12.233	1689	1691	1695	rVB	50409	46322	2.10%	0.247%
24	12.463	1726	1730	1732	rBV	32452	35480	1.61%	0.189%
25	12.498	1732	1736	1739	rVV4	108342	107272	4.86%	0.573%
26	12.551	1742	1745	1748	rVB	29318	30004	1.36%	0.160%
27	12.627	1754	1758	1761	rBV	590317	474325	21.50%	2.532%
28	12.804	1786	1788	1791	rBV3	39072	42353	1.92%	0.226%
29	12.839	1791	1794	1795	rVV2	94884	97737	4.43%	0.522%
30	12.857	1795	1797	1800	rVV	468336	373141	16.92%	1.992%
31	12.904	1803	1805	1809	rVB2	25752	26547	1.20%	0.142%
32	12.998	1817	1821	1824	rVB	2105683	1756741	79.64%	9.377%
33	13.069	1829	1833	1838	rBV3	31328	53204	2.41%	0.284%
34	13.157	1845	1848	1850	rBV4	26650	32579	1.48%	0.174%
35	13.186	1850	1853	1855	rVB2	49206	47901	2.17%	0.256%
36	13.251	1855	1864	1867	rBV3	51642	102786	4.66%	0.549%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030722\
Data File : BF127238.D
Acq On : 07 Mar 2022 23:52
Operator : CG\JU
Sample : N1790-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUM-18

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-BF021622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.286	1867	1870	1873	rVB3	35661	39047	1.77%	0.208%
38	13.516	1906	1909	1912	rVB2	24597	24940	1.13%	0.133%
39	13.692	1936	1939	1944	rVB	39316	42161	1.91%	0.225%
40	13.804	1953	1958	1961	rBV2	45301	56856	2.58%	0.303%
41	13.833	1961	1963	1965	rVV	36981	42502	1.93%	0.227%
42	13.886	1969	1972	1973	rVV	48933	54271	2.46%	0.290%
43	13.921	1973	1978	1983	rVB3	110110	161980	7.34%	0.865%
44	14.057	1996	2001	2004	rBV2	612070	663844	30.09%	3.544%
45	14.080	2004	2005	2013	rVB	180070	139450	6.32%	0.744%
46	14.157	2014	2018	2021	rVB3	28968	44715	2.03%	0.239%
47	14.445	2064	2067	2070	rVB	29446	25453	1.15%	0.136%
48	14.480	2070	2073	2076	rBV4	22931	25666	1.16%	0.137%
49	14.592	2085	2092	2096	rBV3	38277	73777	3.34%	0.394%
50	14.968	2154	2156	2159	rVB4	34039	31017	1.41%	0.166%
51	15.110	2175	2180	2183	rBV	166397	254626	11.54%	1.359%
52	15.163	2187	2189	2195	rVB2	45521	47570	2.16%	0.254%
53	15.221	2195	2199	2202	rBV	26186	30492	1.38%	0.163%
54	15.415	2228	2232	2239	rVB	102084	129044	5.85%	0.689%
55	15.480	2239	2243	2250	rBV	119965	169603	7.69%	0.905%
56	15.551	2250	2255	2258	rBV	410475	521990	23.66%	2.786%
57	15.763	2288	2291	2295	rVB6	20050	26920	1.22%	0.144%
58	15.992	2327	2330	2335	rVB2	43277	64171	2.91%	0.343%
59	17.051	2505	2510	2516	rVB2	66177	123749	5.61%	0.661%
60	17.515	2582	2589	2599	rBV2	53804	118459	5.37%	0.632%

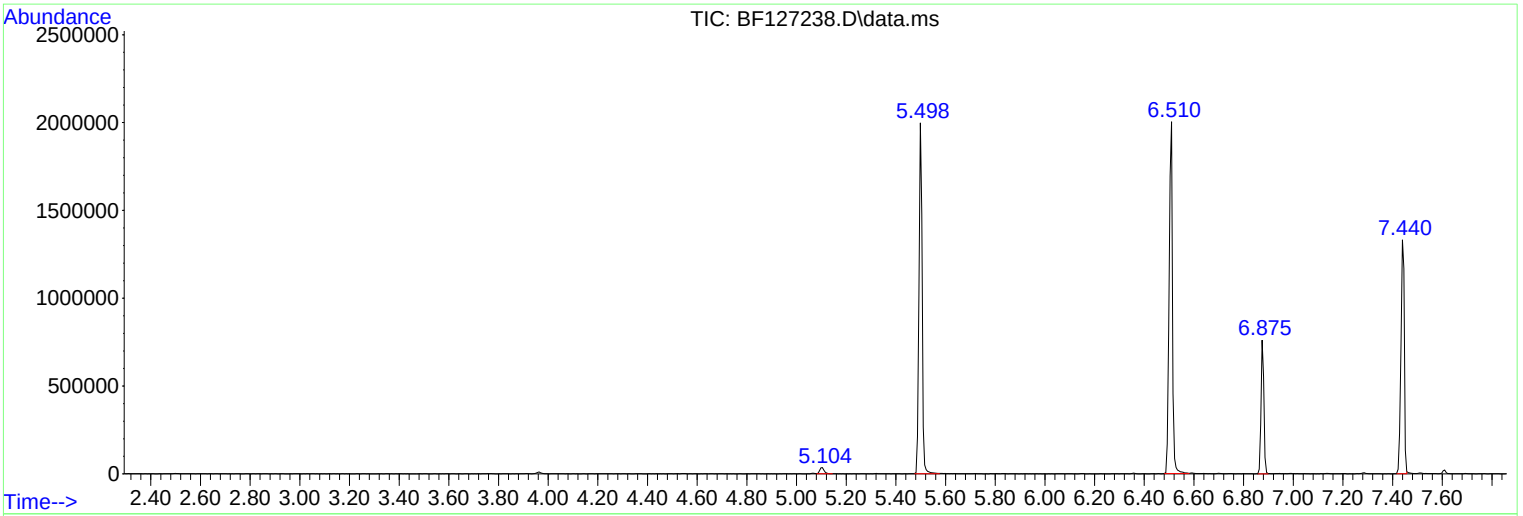
Sum of corrected areas: 18733850

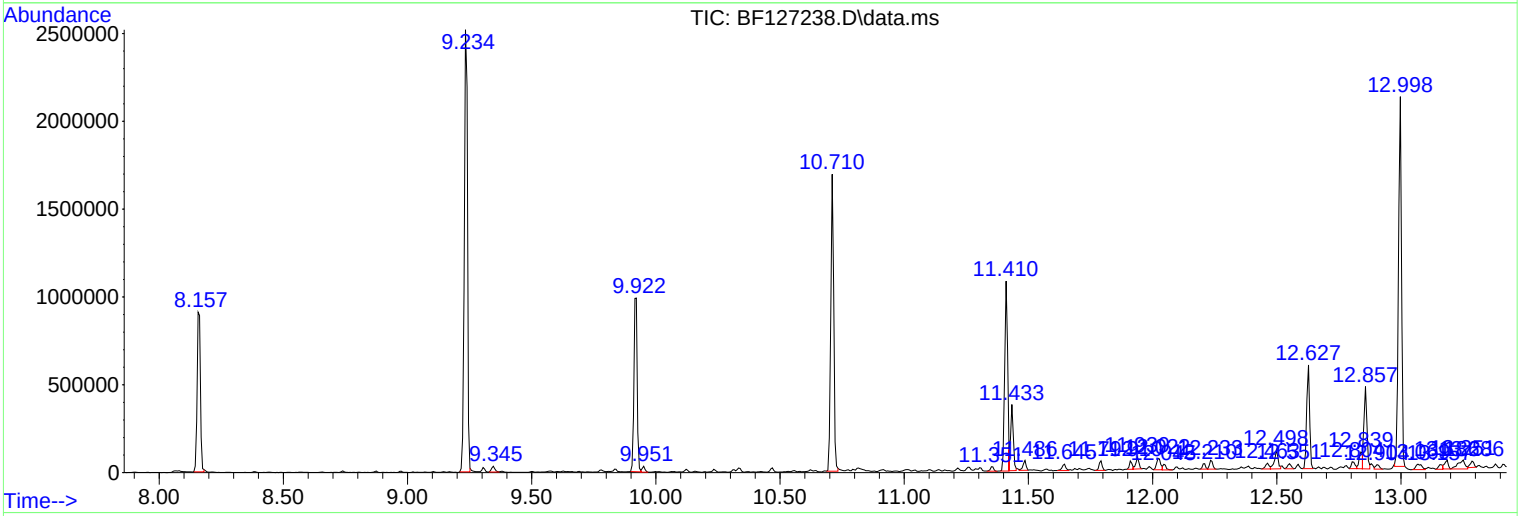
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030722\
Data File : BF127238.D
Acq On : 07 Mar 2022 23:52
Operator : CG\JU
Sample : N1790-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

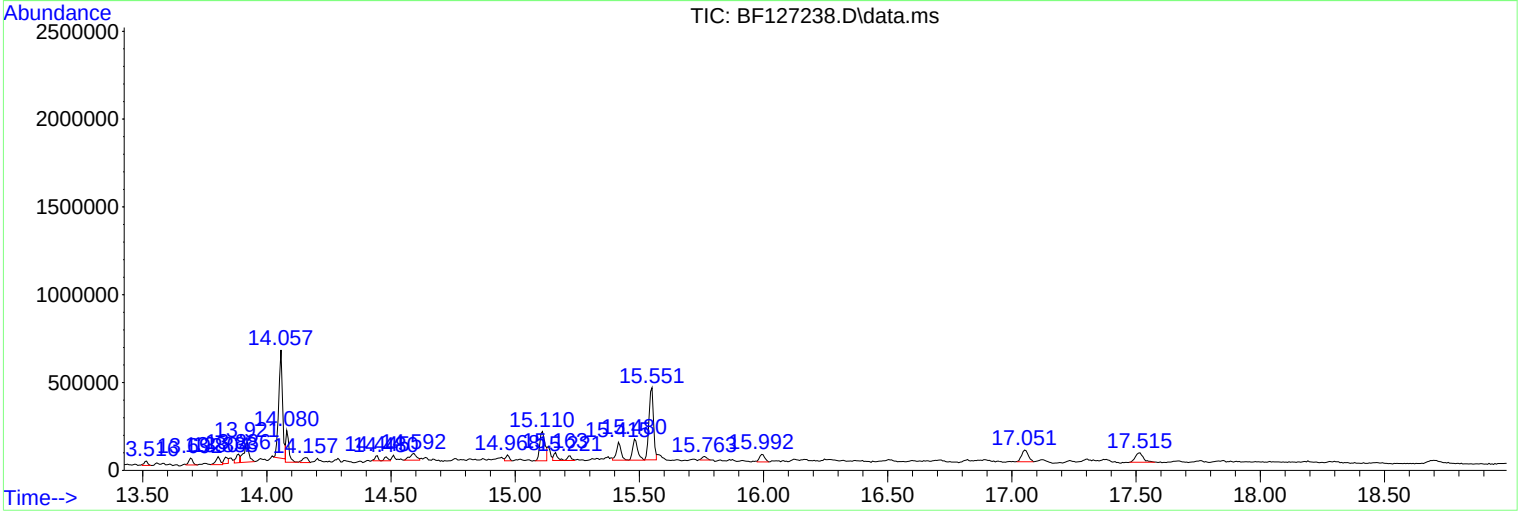
Instrument :
BNA_F
ClientSampleId :
DUM-18

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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\BF030722\
Data File : BF127238.D
Acq On : 07 Mar 2022 23:52
Operator : CG\JU
Sample : N1790-03
Misc :
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Instrument :
BNA_F
ClientSampleId :
DUM-18

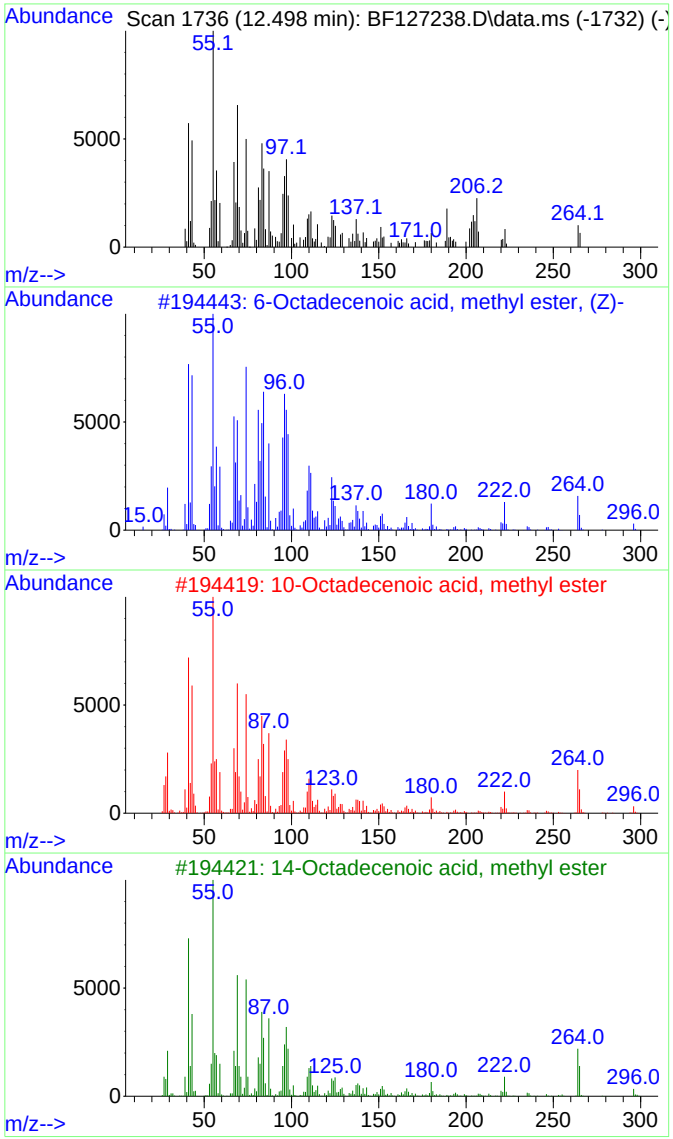
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

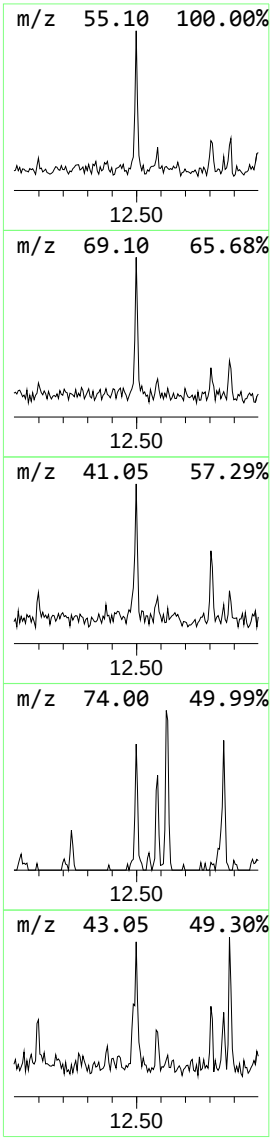
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 6-Octadecenoic acid, methyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.498	2.41 ng	107272	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	93
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	90
3	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	83
4	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	83
5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030722\
Data File : BF127238.D
Acq On : 07 Mar 2022 23:52
Operator : CG\JU
Sample : N1790-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUM-18

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

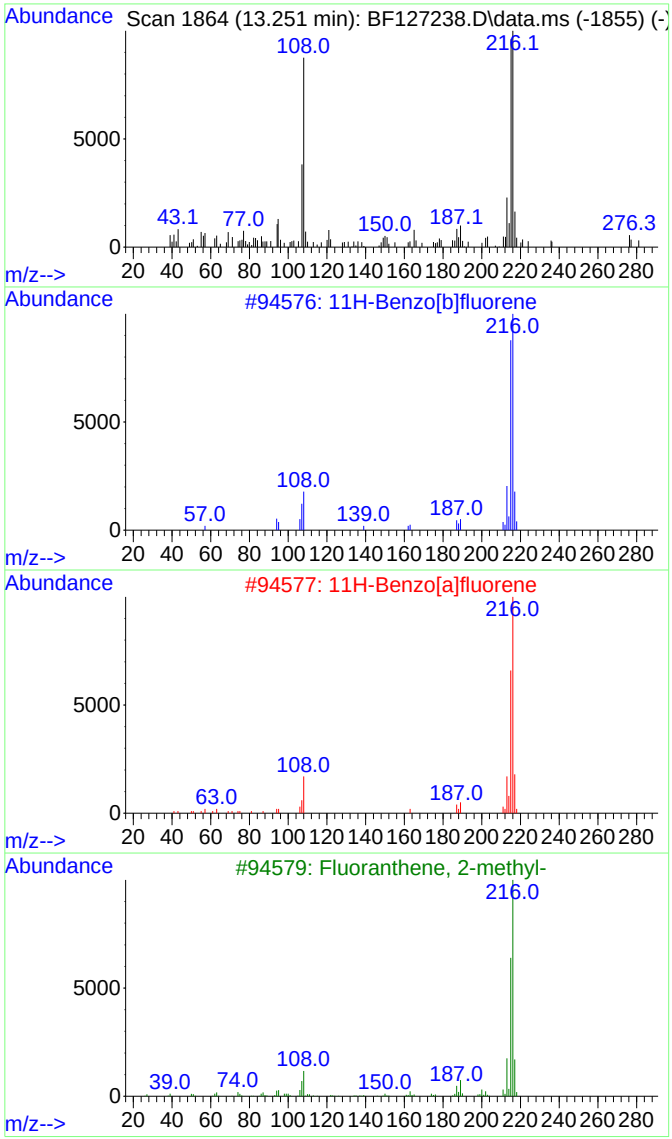
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

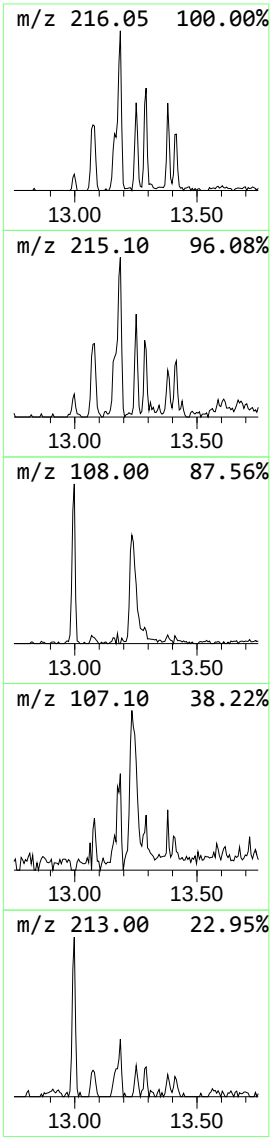
****

Peak Number 2 11H-Benzo[b]fluorene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.251	3.10 ng	102786	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	86
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	76
4	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	60
5	Pyrene, 1-methyl-	216	C17H12	002381-21-7	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030722\
Data File : BF127238.D
Acq On : 07 Mar 2022 23:52
Operator : CG\JU
Sample : N1790-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUM-18

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

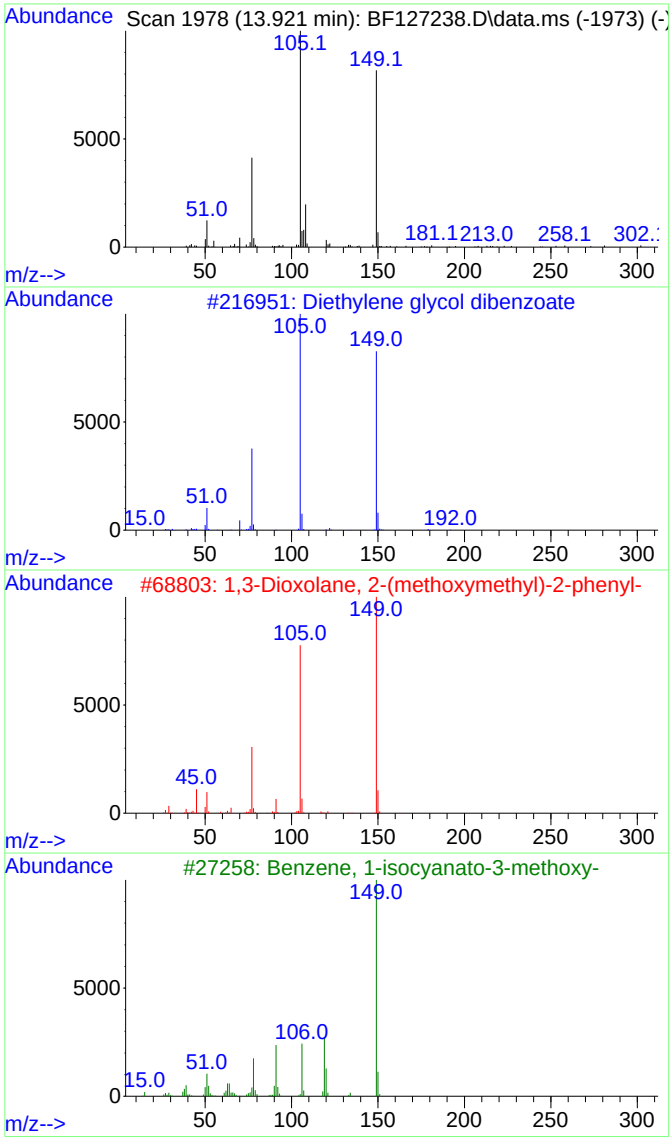
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

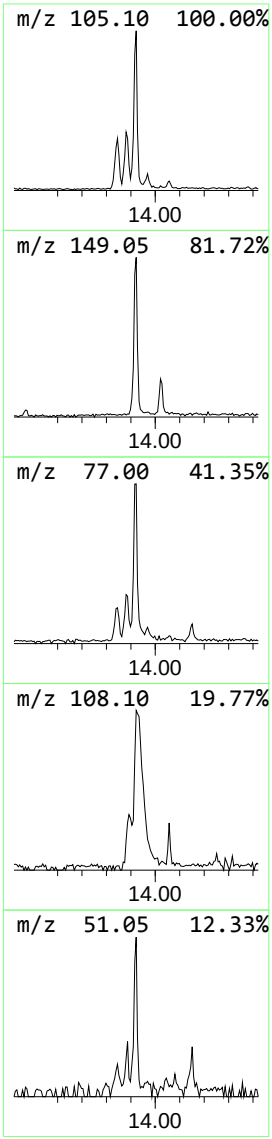
****

Peak Number 3 Diethylene glycol dibenzoate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.922	4.88 ng	161980	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	72
2	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	53
3	Benzene, 1-isocyanato-3-methoxy-	149	C8H7NO2	018908-07-1	43
4	Crotonic acid, 2-benzamido-, met...	219	C12H13NO3	105909-91-9	27
5	Benzamide, N-(5-methyl-3-isoxazo...	202	C11H10N2O2	013053-85-5	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030722\
Data File : BF127238.D
Acq On : 07 Mar 2022 23:52
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Sample : N1790-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUM-18

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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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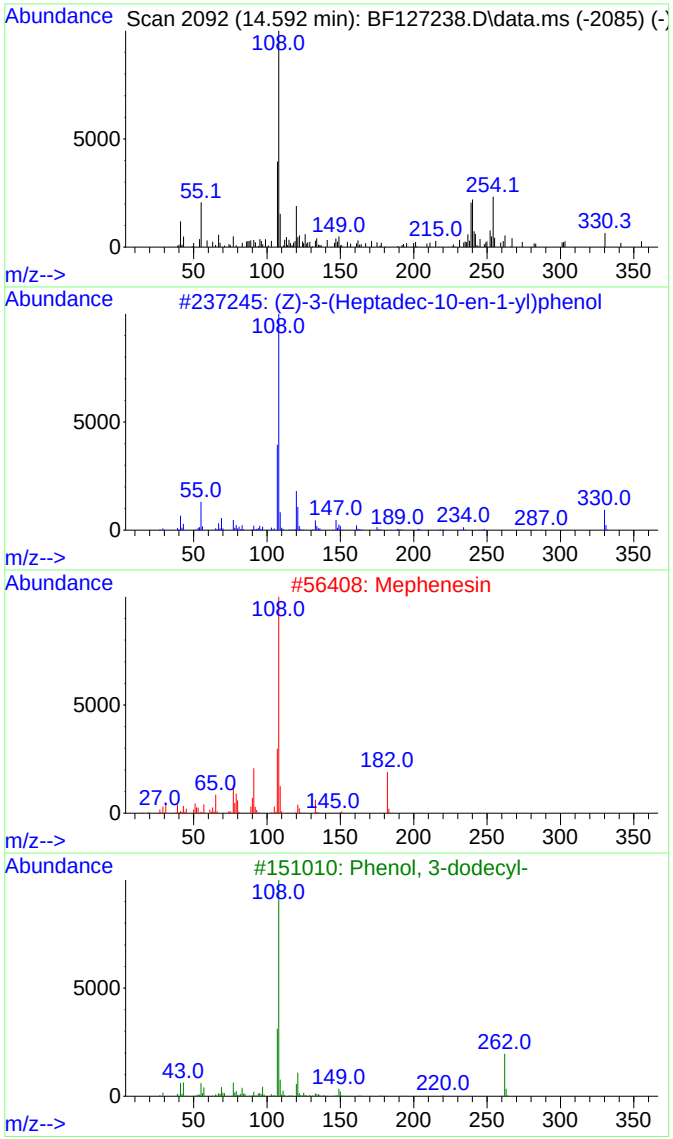
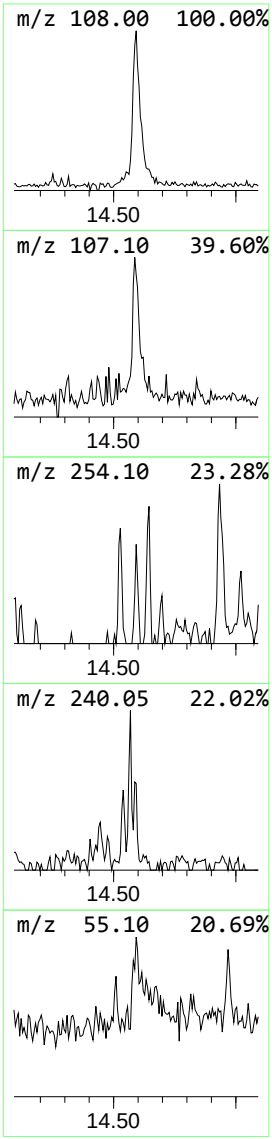
Peak Number 4 unknown14.592 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.592	2.22 ng	73777	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-3-(Heptadec-10-en-1-yl)phenol	330	C23H38O	111047-33-7	47
2	Mephenesin	182	C10H14O3	000059-47-2	43
3	Phenol, 3-dodecyl-	262	C18H30O	029665-57-4	38
4	(Z)-3-(Pentadec-10-en-1-yl)pheny...	344	C23H36O2	1000478-00-3	38
5	Oxalic acid, ethyl 2-methylpheny...	208	C11H12O4	1000309-59-1	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030722\
Data File : BF127238.D
Acq On : 07 Mar 2022 23:52
Operator : CG\JU
Sample : N1790-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUM-18

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

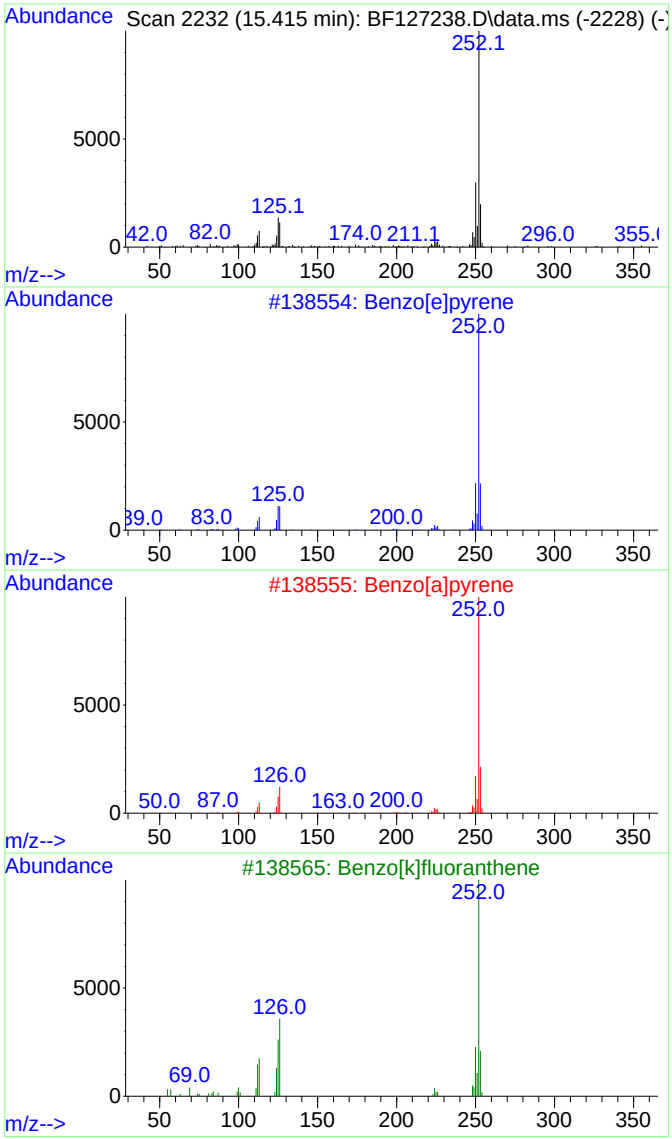
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

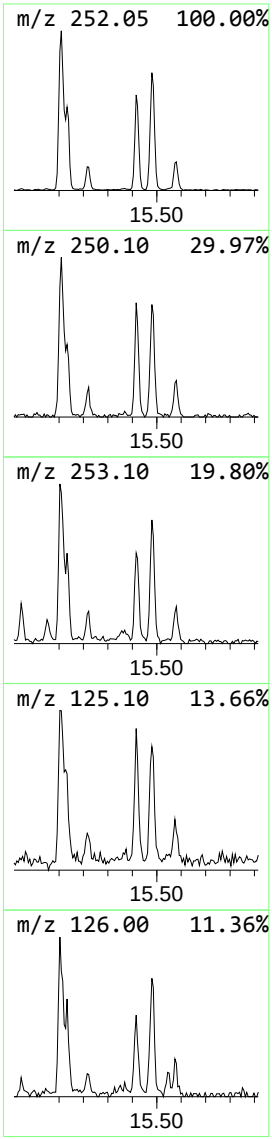
****

Peak Number 5 Benzo[e]pyrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.416	4.94 ng	129044	Perylene-d12	15.551

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	96
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
5	Perylene	252	C20H12	000198-55-0	94





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Data File : BF127238.D
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Operator : CG\JU
Sample : N1790-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUM-18

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

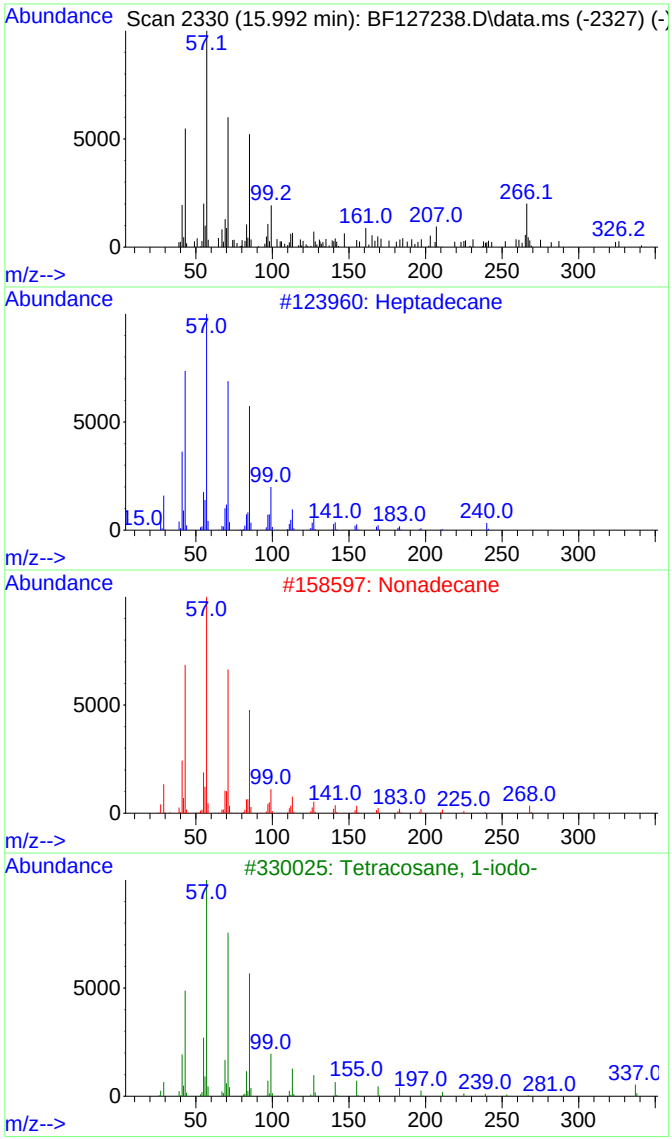
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

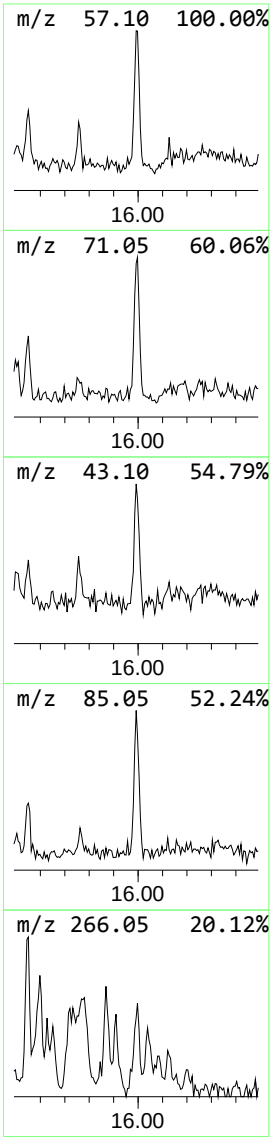
****

Peak Number 6 Heptadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.992	2.46 ng	64171	Perylene-d12	15.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	86
2	Nonadecane	268	C19H40	000629-92-5	64
3	Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	64
4	Hexadecane	226	C16H34	000544-76-3	64
5	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030722\
Data File : BF127238.D
Acq On : 07 Mar 2022 23:52
Operator : CG\JU
Sample : N1790-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUM-18

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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
6-Octadecenoic ...	12.498	2.4	ng	107272	4	11.410	891382	20.0
11H-Benzo[b]flu...	13.251	3.1	ng	102786	5	14.057	663844	20.0
Diethylene glyc...	13.922	4.9	ng	161980	5	14.057	663844	20.0
unknown14.592	14.592	2.2	ng	73777	5	14.057	663844	20.0
Benzo[e]pyrene	15.416	4.9	ng	129044	6	15.551	521990	20.0
Heptadecane	15.992	2.5	ng	64171	6	15.551	521990	20.0