LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072523\
Data File : BF134466.D
Acq On : 25 Jul 2023 16:59
Operator : CG\JU
Sample : 03580-03 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-2

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-BF072423.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134466.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.246	24	27	39	rVB	29094	48827	3.22%	0.351%
2	5.081	505	509	514	rBV	19888	23770	1.57%	0.171%
3	5.475	572	576	591	rBV	1500234	1514767	100.00%	10.894%
4	6.475	743	746	764	rBV	1442213	1403375	92.65%	10.093%
5	6.834	804	807	816	rBV	563809	458759	30.29%	3.299%
6	7.398	899	903	912	rBV	963500	880964	58.16%	6.336%
7	8.110	1021	1024	1033	rBV	647930	520268	34.35%	3.742%
8	9.186	1203	1207	1210	rBV	1908535	1428234	94.29%	10.272%
9	9.586	1270	1275	1279	rVB	40965	40099	2.65%	0.288%
10	9.869	1319	1323	1326	rBV	696889	526700	34.77%	3.788%
11	9.898	1326	1328	1332	rVB	22081	21328	1.41%	0.153%
12	10.663	1454	1458	1469	rBV	950193	804150	53.09%	5.783%
13	11.222	1549	1553	1555	rBV2	30542	29844	1.97%	0.215%
14	11.257	1555	1559	1563	rVB	20158	27496	1.82%	0.198%
15	11.363	1573	1577	1579	rBV	692740	549797	36.30%	3.954%
16	11.386	1579	1581	1586	rVV	328220	275079	18.16%	1.978%
17	11.439	1587	1590	1593	rVV	90618	81221	5.36%	0.584%
18	11.474	1593	1596	1602	rVB8	11532	21835	1.44%	0.157%
19	11.604	1614	1618	1624	rBV2	23208	27665	1.83%	0.199%
20	11.827	1652	1656	1659	rBV5	14319	20012	1.32%	0.144%
21	11.869	1660	1663	1665	rVV	43189	42788	2.82%	0.308%
22	11.892	1665	1667	1673	rVV2	192139	213682	14.11%	1.537%
23	11.945	1673	1676	1679	rVV	30987	39837	2.63%	0.287%
24	11.980	1679	1682	1685	rVV	80953	91525	6.04%	0.658%
25	12.004	1685	1686	1691	rVB	32942	24761	1.63%	0.178%
26	12.163	1711	1713	1716	rVB	36038	30883	2.04%	0.222%
27	12.198	1716	1719	1724	rBV5	30138	38698	2.55%	0.278%
28	12.316	1734	1739	1742	rBV7	18151	31127	2.05%	0.224%
29	12.421	1754	1757	1759	rBV	34606	35274	2.33%	0.254%
30	12.516	1769	1773	1776	rVB2	25703	30472	2.01%	0.219%
31	12.586	1781	1785	1789	rBV	530896	435017	28.72%	3.129%
32	12.686	1799	1802	1805	rBV3	38489	45607	3.01%	0.328%
33	12.739	1808	1811	1813	rVV2	24832	27852	1.84%	0.200%
34	12.816	1818	1824	1829	rVV	545244	611424	40.36%	4.397%
35	12.868	1831	1833	1837	rVB2	26539	29873	1.97%	0.215%
36	12.957	1844	1848	1852	rBV	1448312	1336677	88.24%	9.613%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072523\
Data File : BF134466.D
Acq On : 25 Jul 2023 16:59
Operator : CG\JU
Sample : 03580-03 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-2

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-BF072423.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.039	1858	1862	1866	rBV4	32792	55504	3.66%	0.399%
38	13.151	1874	1881	1883	rBV2	54199	91862	6.06%	0.661%
39	13.216	1889	1892	1894	rBV	41199	38290	2.53%	0.275%
40	13.251	1896	1898	1900	rVV2	35350	32527	2.15%	0.234%
41	13.345	1912	1914	1916	rBV	26075	24313	1.61%	0.175%
42	13.374	1917	1919	1922	rVV	30683	29953	1.98%	0.215%
43	13.663	1966	1968	1975	rBV	32374	46587	3.08%	0.335%
44	13.774	1984	1987	1989	rBV	45255	42730	2.82%	0.307%
45	13.798	1989	1991	1994	rVB	33063	27527	1.82%	0.198%
46	13.827	1994	1996	1997	rBV	33195	27149	1.79%	0.195%
47	13.874	2002	2004	2008	rVV	44285	52860	3.49%	0.380%
48	14.027	2025	2030	2033	rBV2	558358	736431	48.62%	5.296%
49	14.051	2033	2034	2038	rVB	212398	151456	10.00%	1.089%
50	14.133	2046	2048	2050	rVB	45054	29460	1.94%	0.212%
51	14.292	2073	2075	2077	rBV3	37939	43098	2.85%	0.310%
52	15.086	2207	2210	2213	rBV	169428	192020	12.68%	1.381%
53	15.404	2261	2264	2271	rBV	60841	65888	4.35%	0.474%
54	15.468	2272	2275	2280	rVB	109446	129039	8.52%	0.928%
55	15.533	2282	2286	2289	rBV	252740	318247	21.01%	2.289%

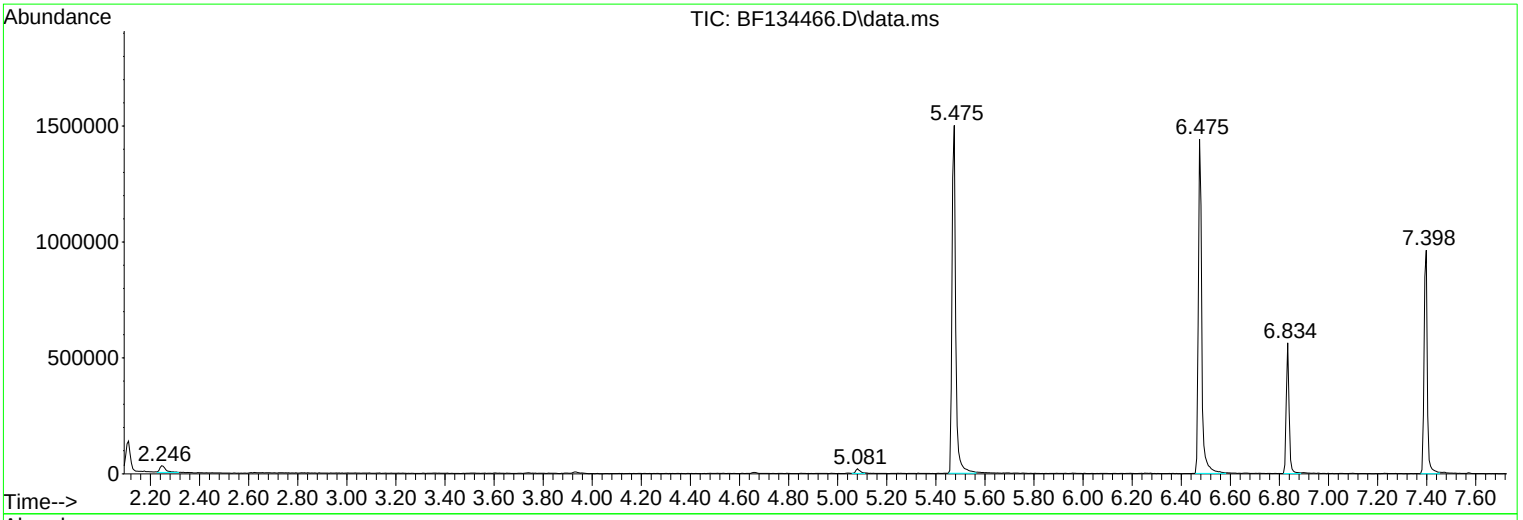
Sum of corrected areas: 13904628

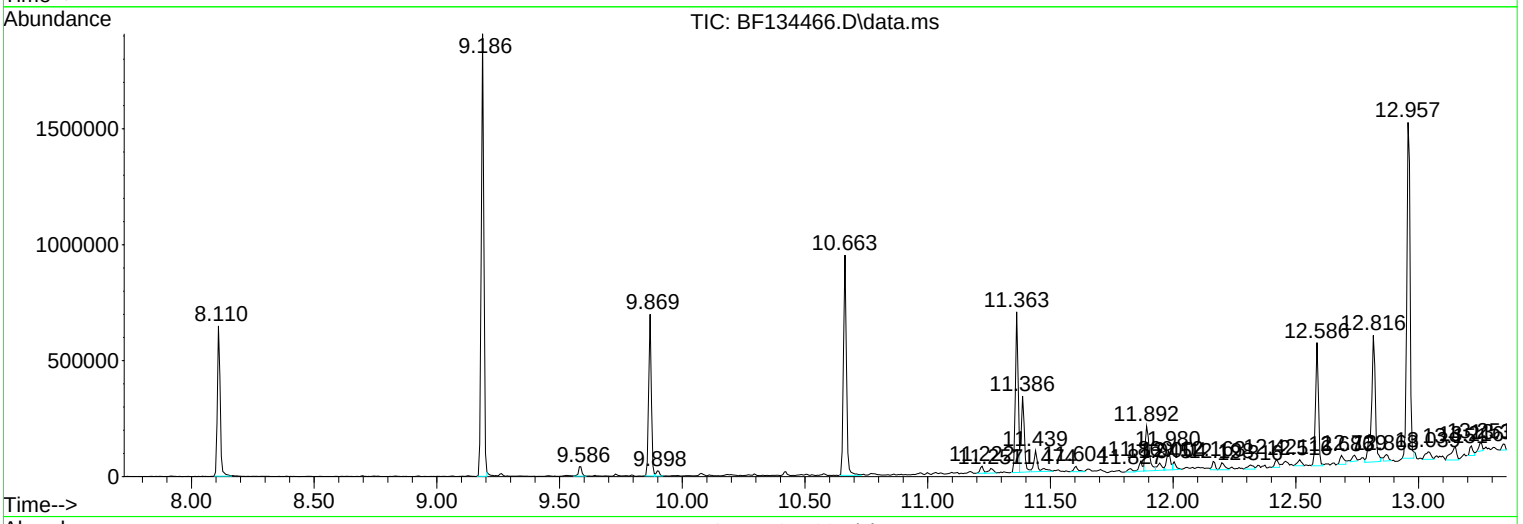
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072523\
Data File : BF134466.D
Acq On : 25 Jul 2023 16:59
Operator : CG\JU
Sample : 03580-03 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

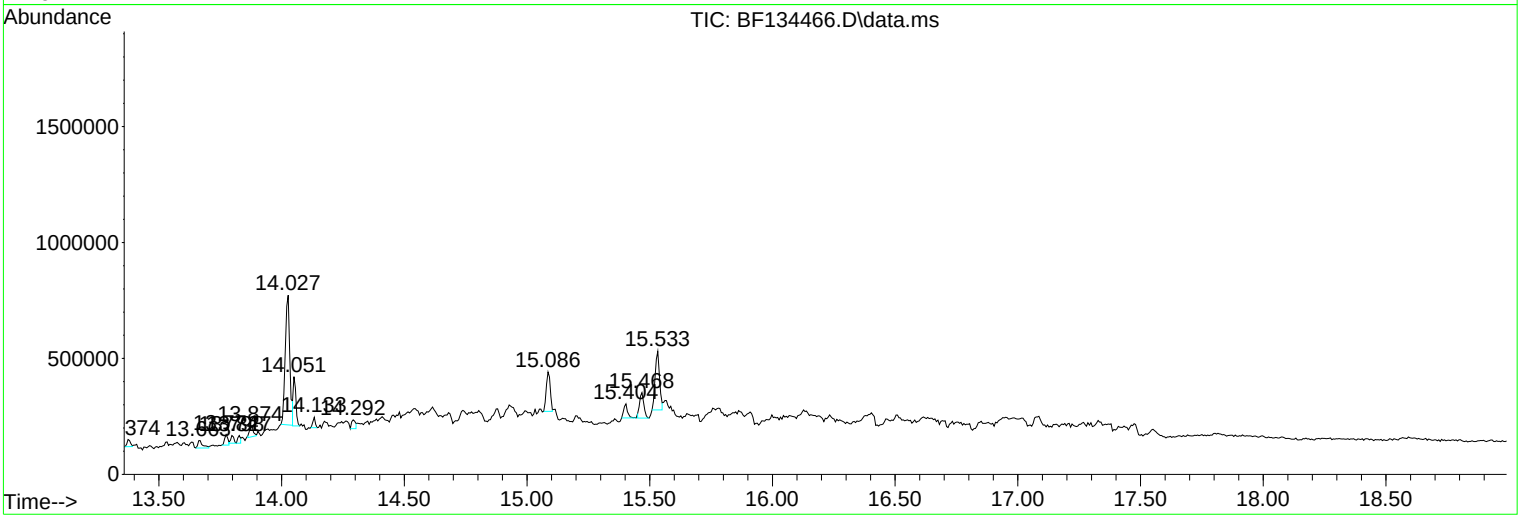
Instrument :
BNA_F
ClientSampleId :
SAMPLE-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.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\BF072523\
Data File : BF134466.D
Acq On : 25 Jul 2023 16:59
Operator : CG\JU
Sample : 03580-03 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

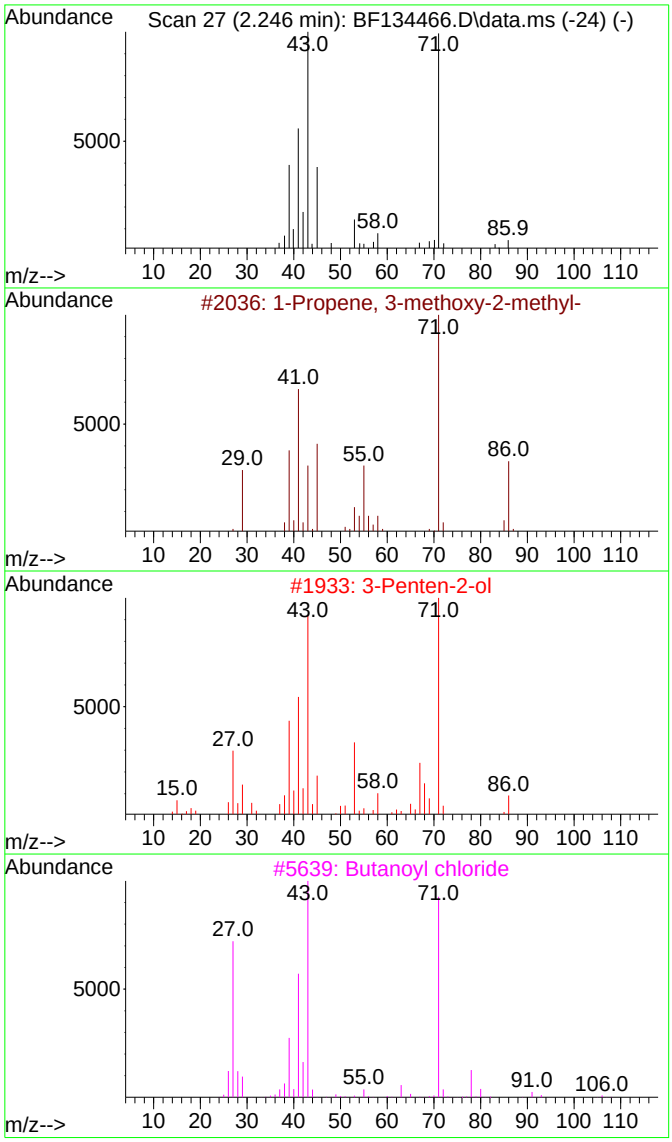
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

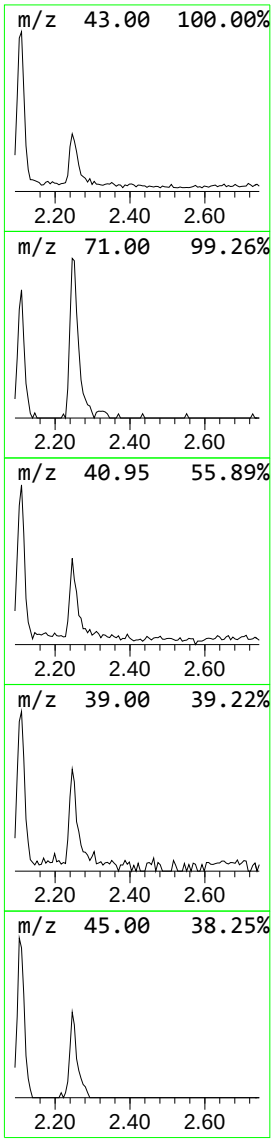
****

Peak Number 1 unknown2.246 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.246	2.13 ng	48827	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 3-methoxy-2-methyl-	86	C5H10O	022418-49-1	47
2	3-Penten-2-ol	86	C5H10O	001569-50-2	42
3	Butanoyl chloride	106	C4H7ClO	000141-75-3	38
4	1,6-Heptadien-4-ol	112	C7H12O	002883-45-6	37
5	2-Butene, 1-methoxy-, (E)-	86	C5H10O	010034-14-7	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072523\
Data File : BF134466.D
Acq On : 25 Jul 2023 16:59
Operator : CG\JU
Sample : 03580-03 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

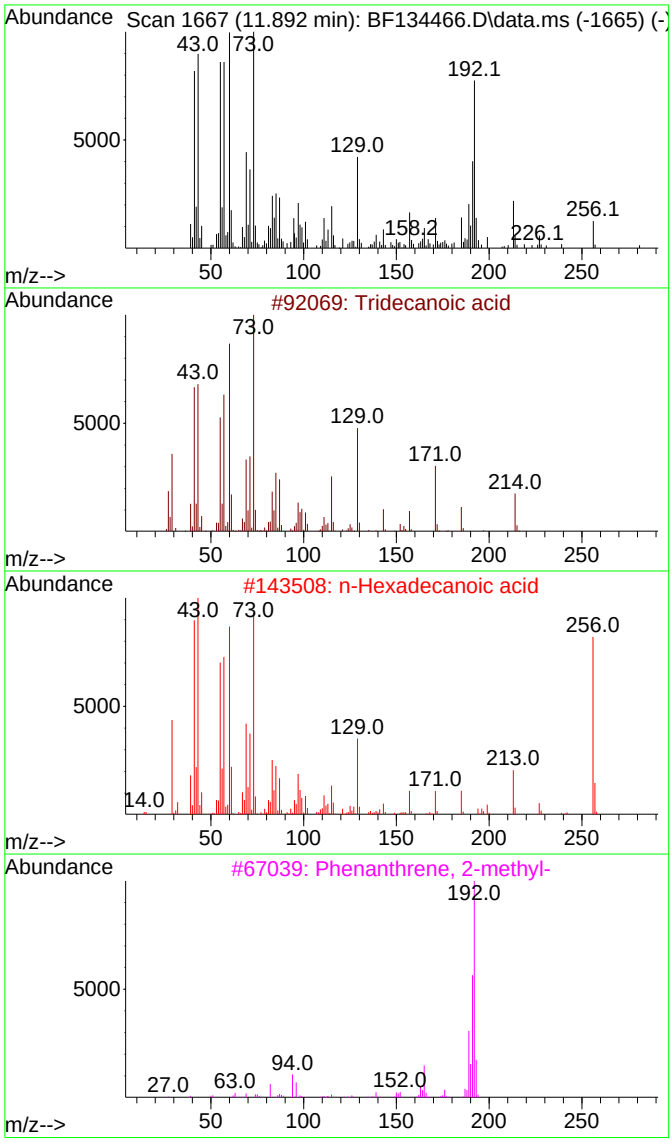
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

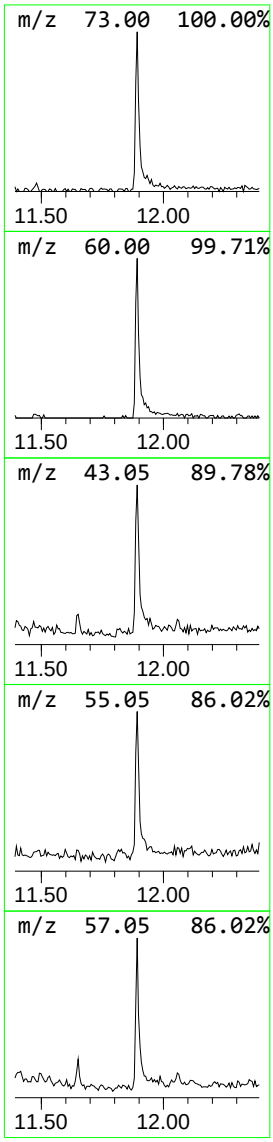
****

Peak Number 2 Tridecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	7.77 ng	213682	Phenanthrene-d10	11.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	95
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	60
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	51
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072523\
Data File : BF134466.D
Acq On : 25 Jul 2023 16:59
Operator : CG\JU
Sample : 03580-03 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-2

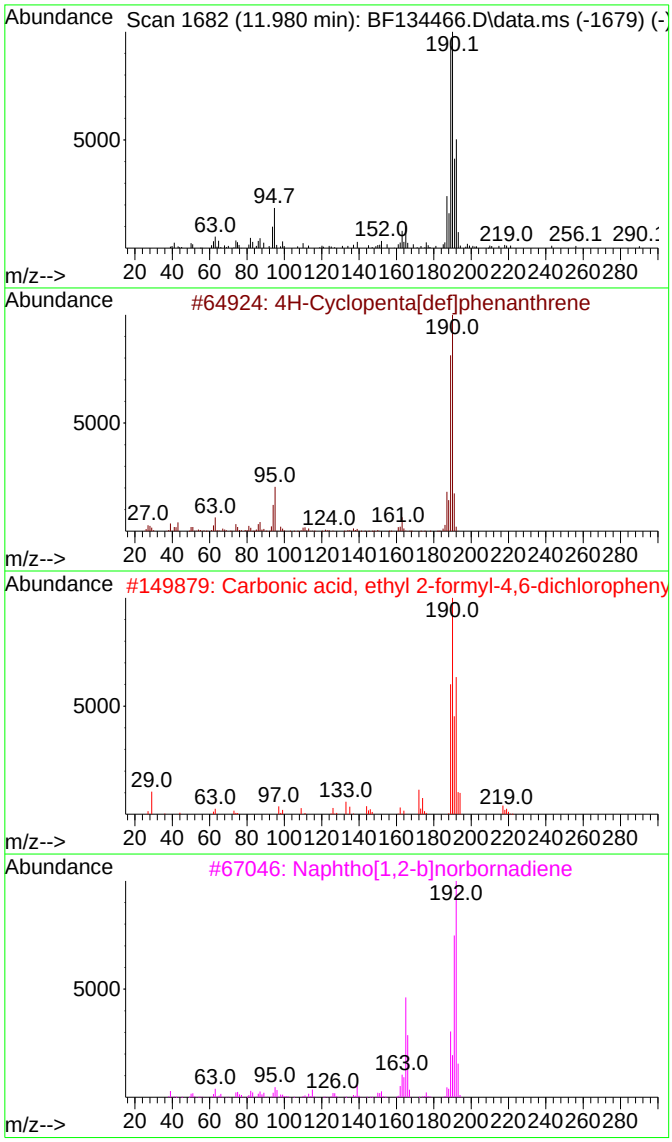
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

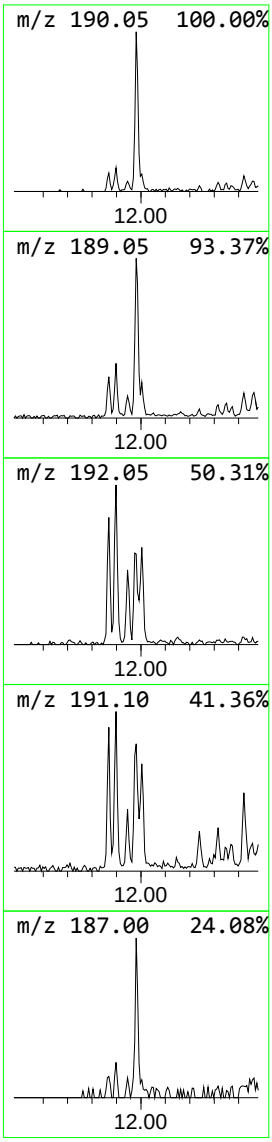
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.980	3.33 ng	91525	Phenanthrene-d10	11.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	91
2	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	50
3	Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	30
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	25
5	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	20





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072523\
Data File : BF134466.D
Acq On : 25 Jul 2023 16:59
Operator : CG\JU
Sample : 03580-03 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

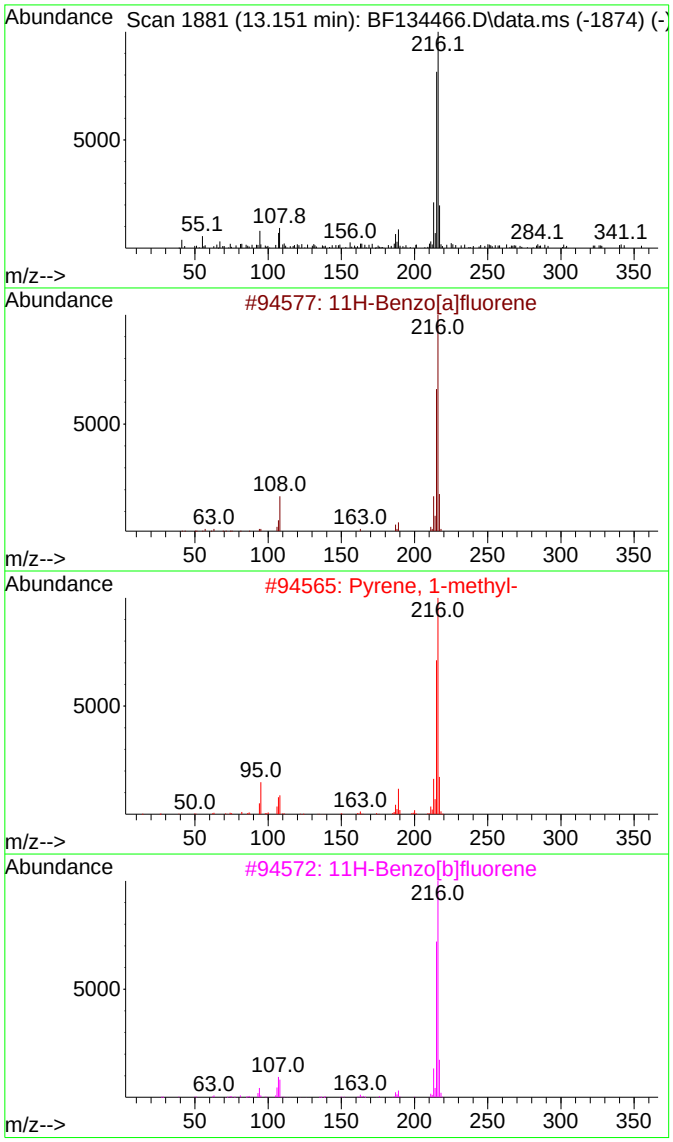
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

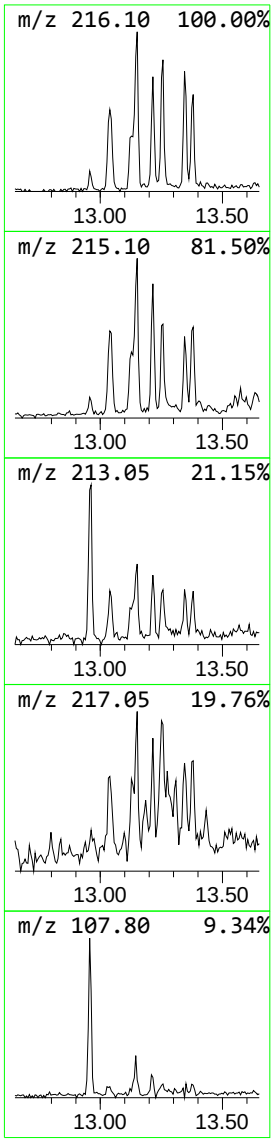
****

Peak Number 4 11H-Benzo[a]fluorene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.151	2.49 ng	91862	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	94
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	94
3	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
4	Pyrene, 2-methyl-	216	C17H12	003442-78-2	91
5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072523\
Data File : BF134466.D
Acq On : 25 Jul 2023 16:59
Operator : CG\JU
Sample : 03580-03 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

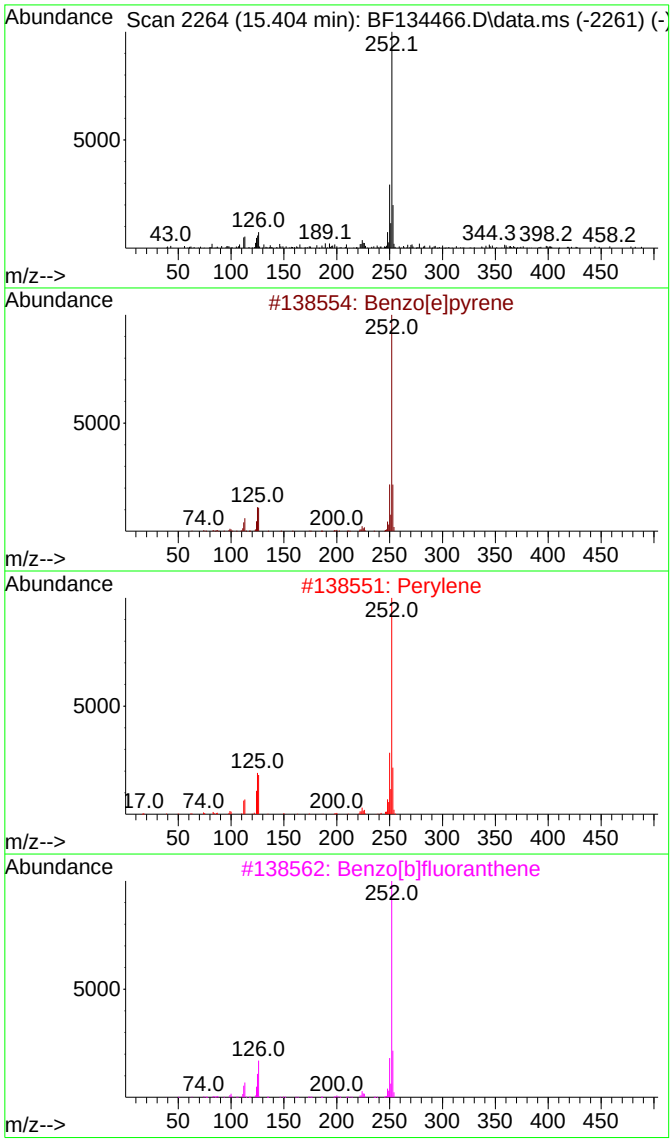
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

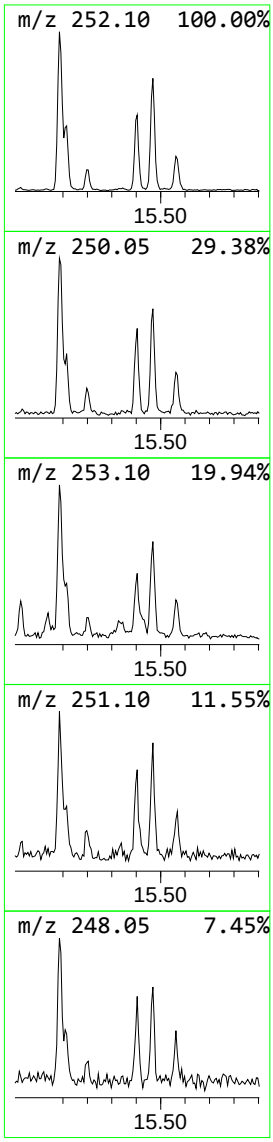
****

Peak Number 5 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.404	4.14 ng	65888	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	90
2	Perylene	252	C20H12	000198-55-0	89
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	76
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	74
5	Benzo[a]pyrene	252	C20H12	000050-32-8	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072523\
Data File : BF134466.D
Acq On : 25 Jul 2023 16:59
Operator : CG\JU
Sample : 03580-03 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.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
unknown2.246	2.246	2.1	ng	48827	1	6.834	458759	20.0
Tridecanoic acid	11.892	7.8	ng	213682	4	11.363	549797	20.0
4H-Cyclopenta[d...	11.980	3.3	ng	91525	4	11.363	549797	20.0
11H-Benzo[a]flu...	13.151	2.5	ng	91862	5	14.027	736431	20.0
Benzo[e]pyrene	15.404	4.1	ng	65888	6	15.533	318247	20.0