LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080123\
Data File : BF134557.D
Acq On : 01 Aug 2023 19:56
Operator : CG\JU
Sample : 03645-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-(1-5)

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-BF080123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134557.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.040	492	502	508	rVB2	35743	58451	1.11%	0.145%
2	5.422	561	567	570	rBV	4364823	4711196	89.43%	11.723%
3	6.422	730	737	740	rBV	4240654	4913175	93.27%	12.226%
4	6.792	796	800	803	rBV	1535480	1259039	23.90%	3.133%
5	7.351	889	895	898	rBV	3306868	3095447	58.76%	7.703%
6	8.069	1012	1017	1020	rBV	2024862	1723832	32.72%	4.290%
7	9.145	1195	1200	1204	rBV	5253313	5267764	100.00%	13.108%
8	9.269	1217	1221	1224	rVB	374966	331116	6.29%	0.824%
9	9.539	1263	1267	1272	rBV	343162	277128	5.26%	0.690%
10	9.822	1309	1315	1318	rBV	2177014	1849638	35.11%	4.603%
11	10.610	1444	1449	1452	rBV	3601570	3367983	63.94%	8.381%
12	10.739	1467	1471	1480	rVB3	59322	88503	1.68%	0.220%
13	10.910	1495	1500	1504	rBV4	42237	56070	1.06%	0.140%
14	11.186	1545	1547	1551	rBV2	98351	97976	1.86%	0.244%
15	11.310	1564	1568	1570	rBV	2147518	1814792	34.45%	4.516%
16	11.333	1570	1572	1575	rVV	359838	273194	5.19%	0.680%
17	11.380	1575	1580	1583	rVB2	132052	130966	2.49%	0.326%
18	11.616	1617	1620	1623	rBV2	75504	68456	1.30%	0.170%
19	11.851	1655	1660	1664	rBV2	497438	495549	9.41%	1.233%
20	11.880	1664	1665	1669	rVB	76771	63420	1.20%	0.158%
21	11.921	1669	1672	1674	rBV	61960	61921	1.18%	0.154%
22	12.027	1686	1690	1695	rVB2	54054	54191	1.03%	0.135%
23	12.521	1770	1774	1777	rBV	468100	395021	7.50%	0.983%
24	12.639	1791	1794	1799	rBV3	119574	138321	2.63%	0.344%
25	12.751	1807	1813	1816	rBV2	339957	375166	7.12%	0.934%
26	12.792	1817	1820	1823	rBV2	65746	60069	1.14%	0.149%
27	12.904	1835	1839	1843	rBV	4873066	4754154	90.25%	11.830%
28	13.151	1878	1881	1883	rBV	103865	89240	1.69%	0.222%
29	13.492	1936	1939	1942	rVB	90211	76438	1.45%	0.190%
30	13.815	1991	1994	2001	rVB2	367888	426392	8.09%	1.061%
31	13.951	2012	2017	2020	rBV	1366275	1335085	25.34%	3.322%
32	13.974	2020	2021	2024	rVB	169918	95222	1.81%	0.237%
33	14.139	2047	2049	2052	rBV	88151	72512	1.38%	0.180%
34	14.451	2099	2102	2106	rVB	107847	98405	1.87%	0.245%
35	14.733	2147	2150	2152	rBV2	60166	64723	1.23%	0.161%
36	14.757	2152	2154	2159	rVB2	72298	70725	1.34%	0.176%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080123\
Data File : BF134557.D
Acq On : 01 Aug 2023 19:56
Operator : CG\JU
Sample : 03645-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-(1-5)

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-BF080123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.986	2189	2193	2196	rBV	151280	234087	4.44%	0.582%
38	15.098	2208	2212	2214	rBV2	83436	105756	2.01%	0.263%
39	15.280	2240	2243	2250	rVB	91847	122625	2.33%	0.305%
40	15.345	2250	2254	2259	rVB	126111	154814	2.94%	0.385%
41	15.409	2260	2265	2269	rBV	971382	1185493	22.50%	2.950%
42	15.939	2351	2355	2359	rBV	52253	79166	1.50%	0.197%
43	15.980	2359	2362	2368	rVB2	57871	95759	1.82%	0.238%
44	16.868	2509	2513	2522	rVB2	46754	97875	1.86%	0.244%

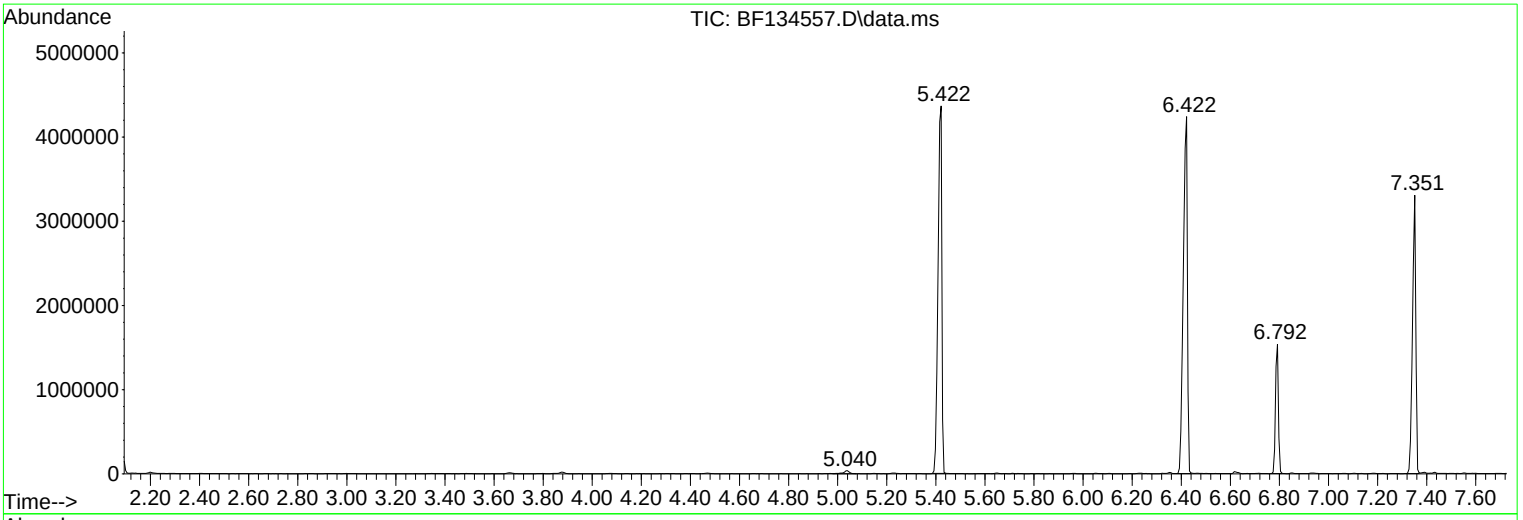
Sum of corrected areas: 40186855

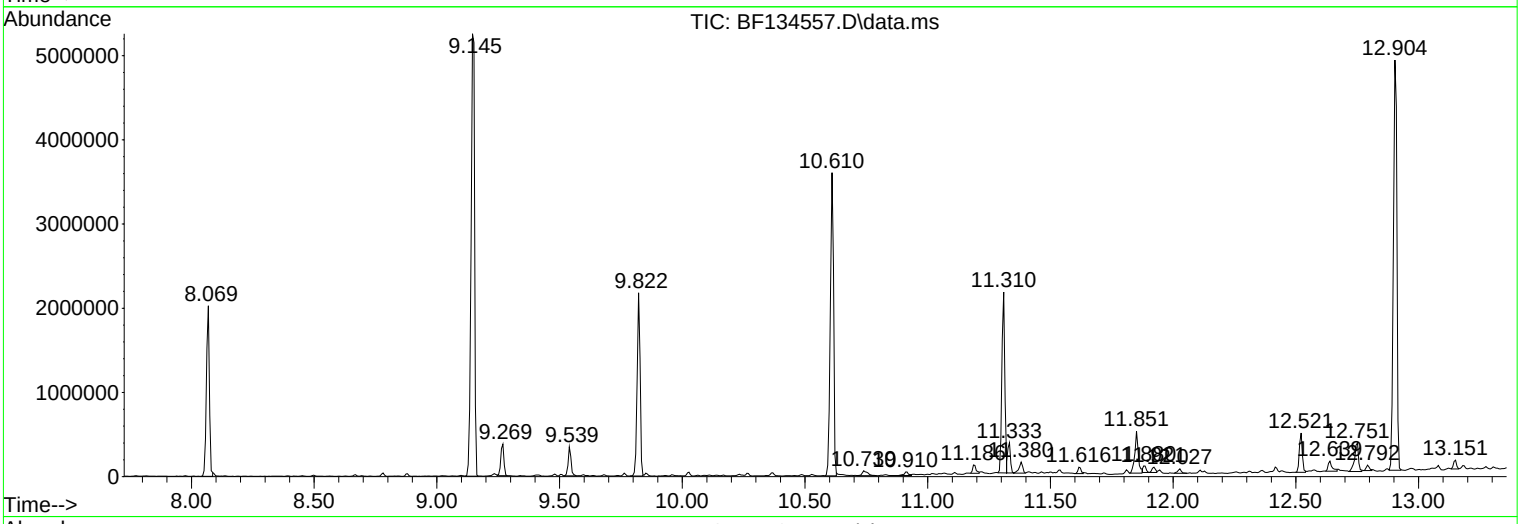
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080123\
Data File : BF134557.D
Acq On : 01 Aug 2023 19:56
Operator : CG\JU
Sample : 03645-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

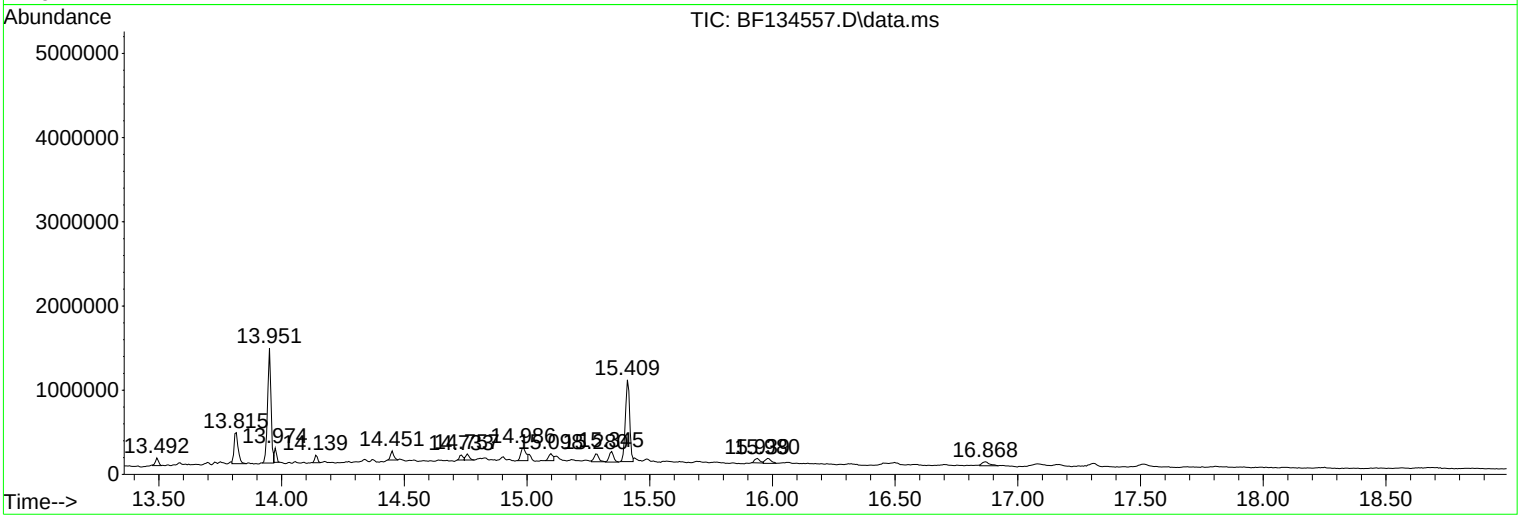
Instrument :
BNA_F
ClientSampleId :
SB-04-(1-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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\BF080123\
Data File : BF134557.D
Acq On : 01 Aug 2023 19:56
Operator : CG\JU
Sample : 03645-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-(1-5)

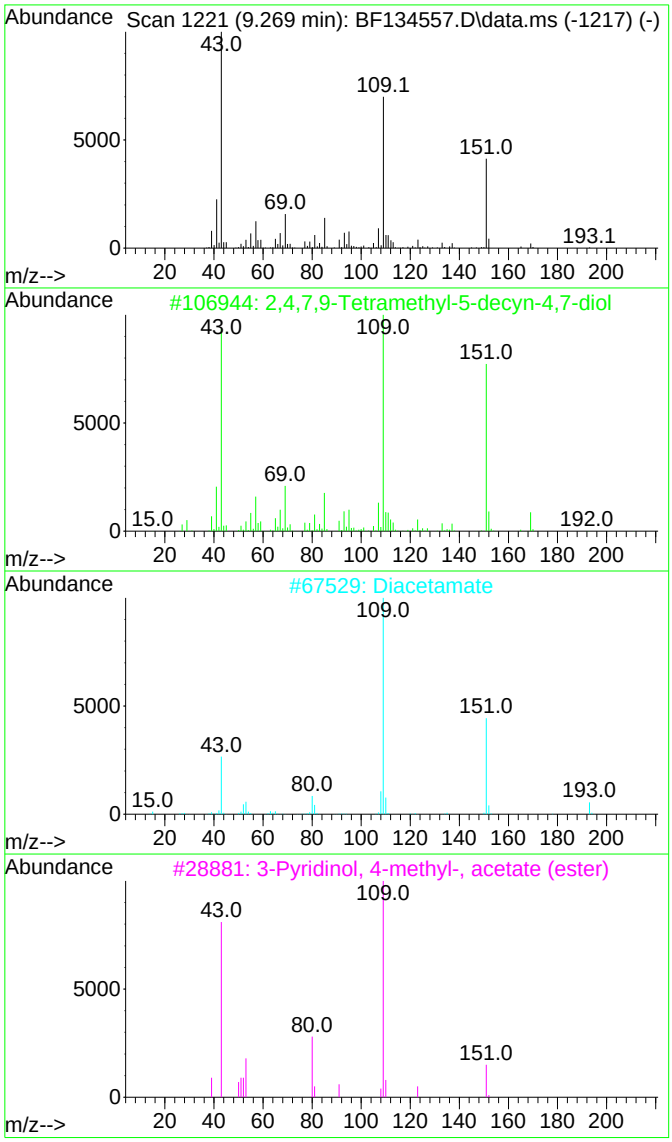
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

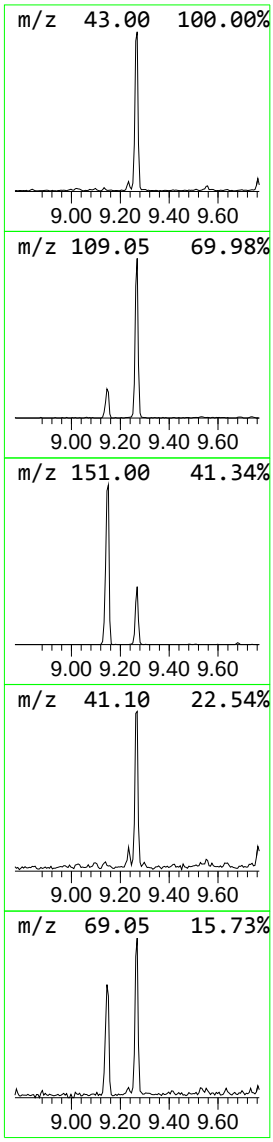
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.269	3.58 ng	331116	Acenaphthene-d10	9.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	Diacetamate	193	C10H11NO3	002623-33-8	53
3	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	53
4	Metacetamol	151	C8H9NO2	000621-42-1	53
5	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080123\
Data File : BF134557.D
Acq On : 01 Aug 2023 19:56
Operator : CG\JU
Sample : 03645-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-(1-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

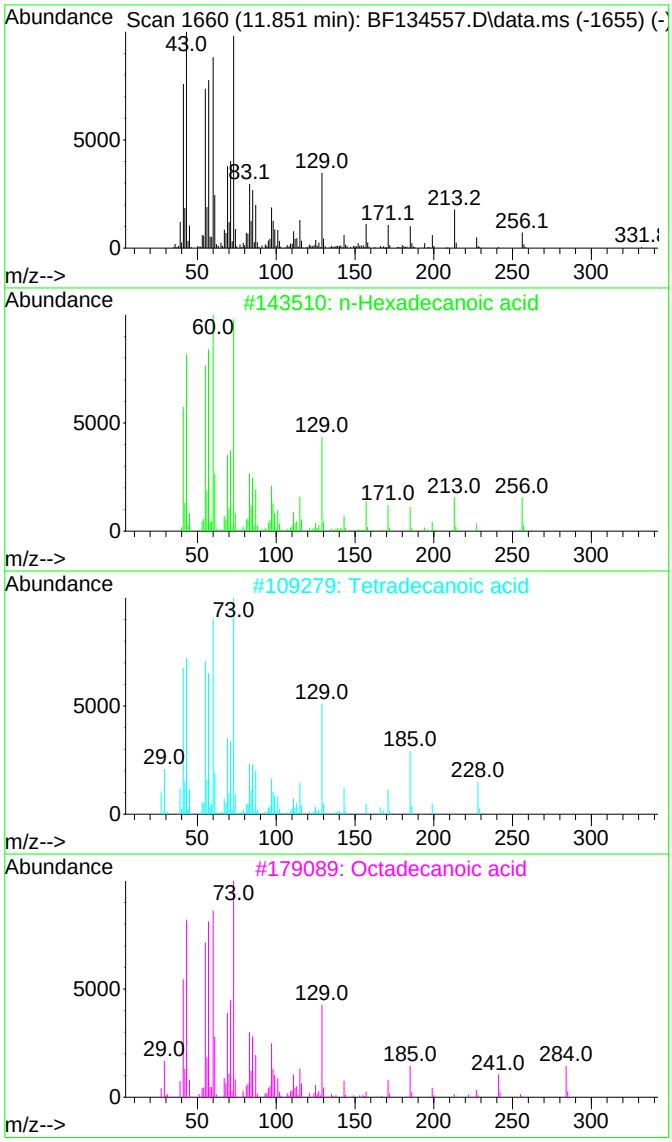
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

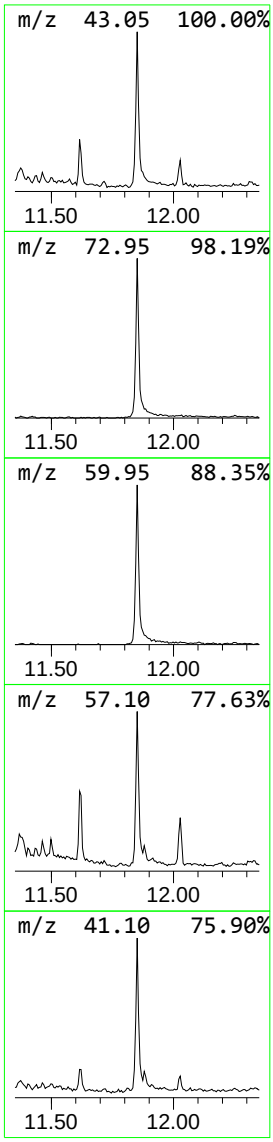
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.851	5.46 ng	495549	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	Octadecanoic acid	284	C18H36O2	000057-11-4	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	Tridecanoic acid	214	C13H26O2	000638-53-9	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080123\
Data File : BF134557.D
Acq On : 01 Aug 2023 19:56
Operator : CG\JU
Sample : 03645-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-(1-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

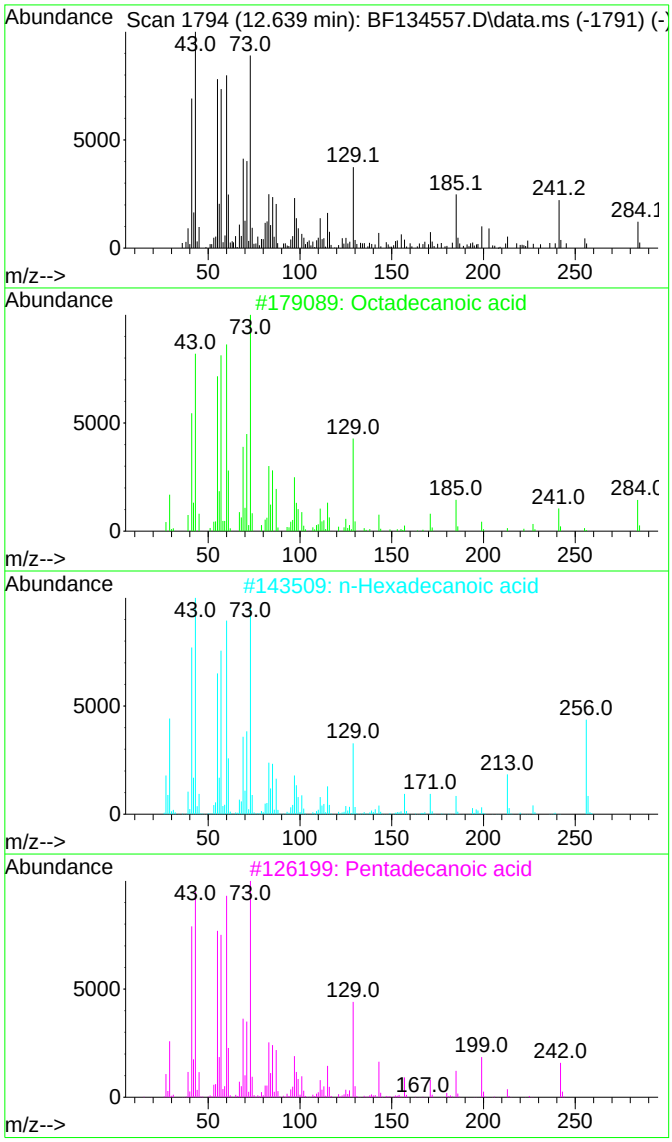
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

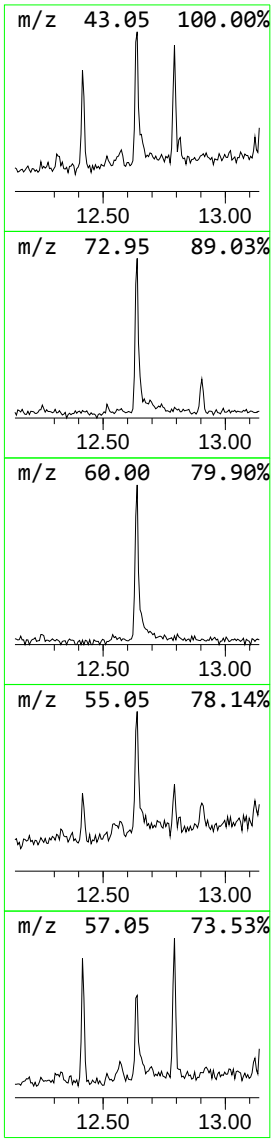
****

Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.639	2.07 ng	138321	Chrysene-d12	13.951

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080123\
Data File : BF134557.D
Acq On : 01 Aug 2023 19:56
Operator : CG\JU
Sample : 03645-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-(1-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

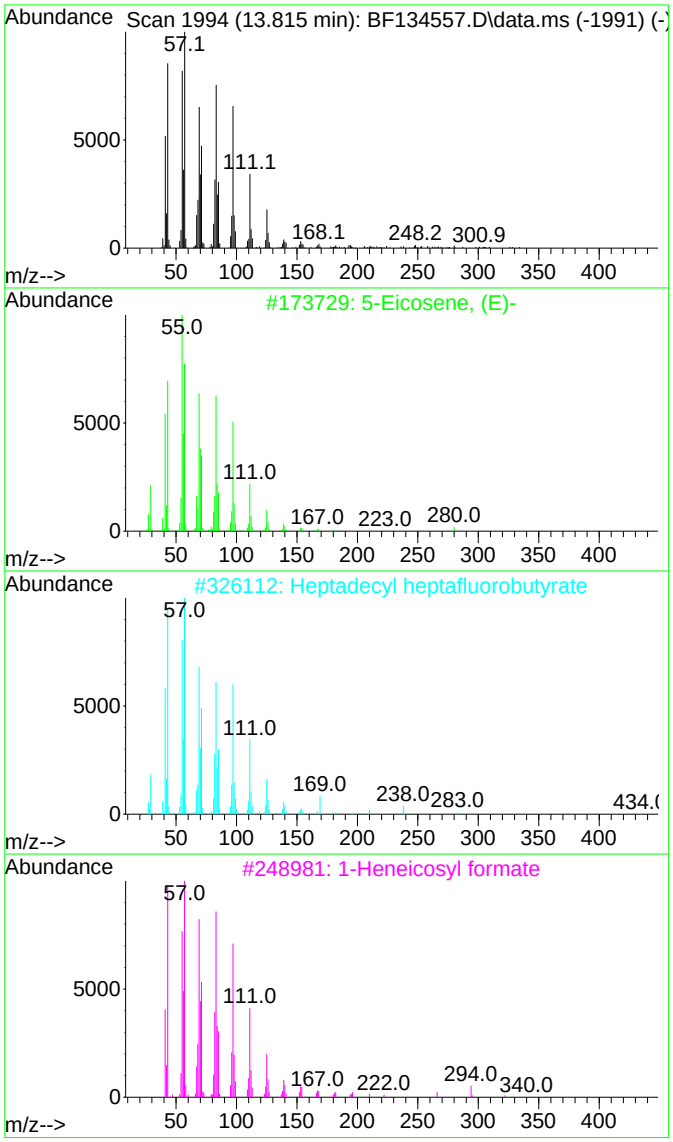
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

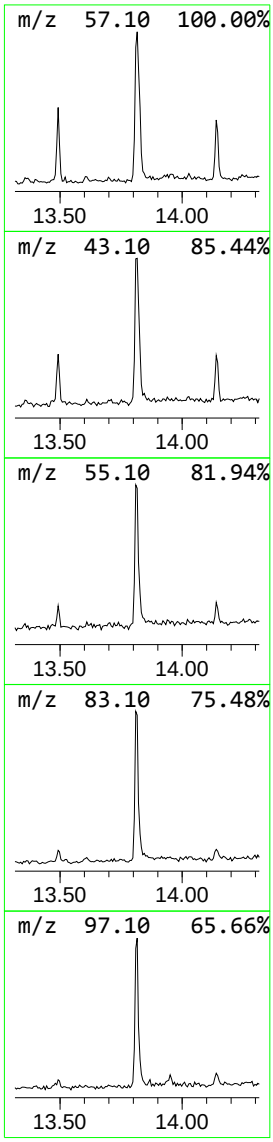
****

Peak Number 4 5-Eicosene, (E)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	6.39 ng	426392	Chrysene-d12	13.951

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	95
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
5	Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080123\
Data File : BF134557.D
Acq On : 01 Aug 2023 19:56
Operator : CG\JU
Sample : 03645-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-(1-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

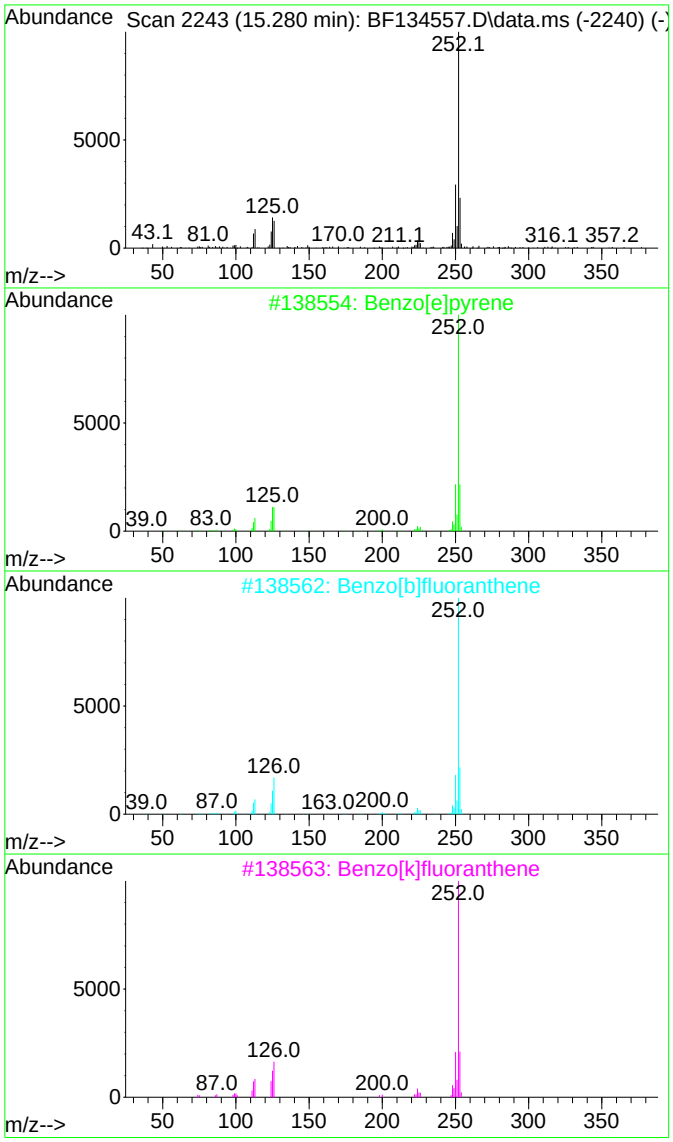
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

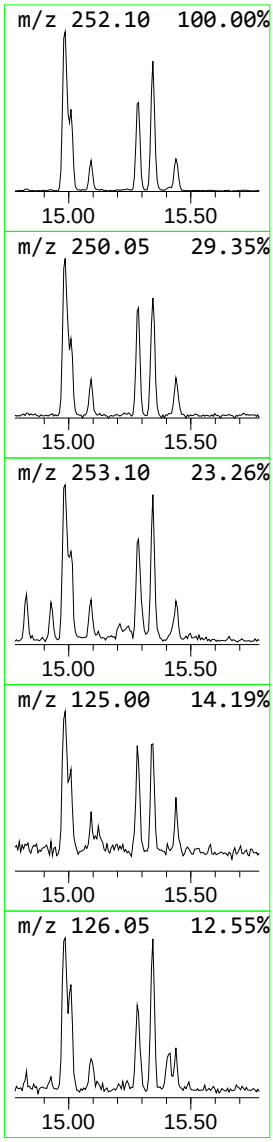
****

Peak Number 5 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.280	2.07 ng	122625	Perylene-d12	15.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	97
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
4	Benzo[a]pyrene	252	C20H12	000050-32-8	95
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	95





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080123\
Data File : BF134557.D
Acq On : 01 Aug 2023 19:56
Operator : CG\JU
Sample : 03645-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-(1-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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
2,4,7,9-Tetrame...	9.269	3.6	ng	331116	3	9.822	1849640	20.0
n-Hexadecanoic ...	11.851	5.5	ng	495549	4	11.310	1814790	20.0
Octadecanoic acid	12.639	2.1	ng	138321	5	13.951	1335090	20.0
5-Eicosene, (E)-	13.816	6.4	ng	426392	5	13.951	1335090	20.0
Benzo[e]pyrene	15.280	2.1	ng	122625	6	15.410	1185490	20.0