LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052422\
Data File : BF128438.D
Acq On : 24 May 2022 16:46
Operator : CG\JU
Sample : N2981-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-15(0.5-1)

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-BF052022.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128438.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.416	190	192	206	rBV2	11850	41959	1.70%	0.194%
2	5.087	473	476	485	rVB	18031	25194	1.02%	0.117%
3	5.475	538	542	561	rBV	2037723	2152711	87.36%	9.977%
4	6.487	709	714	728	rBV	2027794	2206985	89.56%	10.229%
5	6.587	728	731	740	rVB	44219	50795	2.06%	0.235%
6	6.845	771	775	781	rBV	681937	591994	24.02%	2.744%
7	7.410	867	871	881	rBV	1526593	1520543	61.71%	7.047%
8	8.128	989	993	996	rBV	909931	788188	31.99%	3.653%
9	9.198	1171	1175	1179	rBV	2529333	2464138	100.00%	11.420%
10	9.880	1288	1291	1295	rBV	992069	861785	34.97%	3.994%
11	9.916	1295	1297	1303	rVB	47246	38199	1.55%	0.177%
12	10.433	1381	1385	1392	rVB	37992	33814	1.37%	0.157%
13	10.674	1422	1426	1433	rBV	1411360	1414521	57.40%	6.556%
14	11.222	1516	1519	1523	rBV3	20962	27008	1.10%	0.125%
15	11.374	1541	1545	1547	rBV	981006	821074	33.32%	3.805%
16	11.398	1547	1549	1554	rVB	466153	370998	15.06%	1.719%
17	11.451	1554	1558	1563	rBV	90158	80939	3.28%	0.375%
18	11.616	1580	1586	1590	rBV2	52404	65993	2.68%	0.306%
19	11.751	1606	1609	1612	rBV	58743	44312	1.80%	0.205%
20	11.863	1625	1628	1632	rBV2	89604	144217	5.85%	0.668%
21	11.898	1632	1634	1641	rVB3	142971	193766	7.86%	0.898%
22	11.992	1646	1650	1652	rVV3	79266	88907	3.61%	0.412%
23	12.010	1652	1653	1658	rVB	32643	26967	1.09%	0.125%
24	12.169	1678	1680	1684	rVB	35375	32804	1.33%	0.152%
25	12.210	1684	1687	1691	rVB	28488	27639	1.12%	0.128%
26	12.427	1720	1724	1726	rBV	30703	32718	1.33%	0.152%
27	12.521	1736	1740	1744	rBV2	23509	30467	1.24%	0.141%
28	12.592	1748	1752	1756	rBV	669571	554870	22.52%	2.572%
29	12.804	1785	1788	1789	rBV2	105799	95470	3.87%	0.442%
30	12.821	1789	1791	1796	rVB	535132	447264	18.15%	2.073%
31	12.957	1810	1814	1818	rBV	1819336	1704685	69.18%	7.901%
32	13.039	1824	1828	1833	rBV2	37709	59528	2.42%	0.276%
33	13.151	1844	1847	1849	rVB	59202	50554	2.05%	0.234%
34	13.216	1855	1858	1861	rBV	44401	41751	1.69%	0.194%
35	13.257	1861	1865	1872	rVB3	46697	71663	2.91%	0.332%
36	13.345	1878	1880	1883	rBV	25679	27741	1.13%	0.129%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052422\
Data File : BF128438.D
Acq On : 24 May 2022 16:46
Operator : CG\JU
Sample : N2981-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-15(0.5-1)

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-BF052022.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.380	1883	1886	1890	rVV4	26271	32342	1.31%	0.150%
38	13.515	1906	1909	1913	rBV4	25607	34706	1.41%	0.161%
39	13.668	1932	1935	1938	rBV	42003	37760	1.53%	0.175%
40	13.774	1947	1953	1955	rBV	65593	71072	2.88%	0.329%
41	13.798	1955	1957	1959	rVV2	43979	36158	1.47%	0.168%
42	13.827	1959	1962	1963	rVV	39757	36484	1.48%	0.169%
43	13.845	1963	1965	1967	rVV	46474	39202	1.59%	0.182%
44	13.880	1967	1971	1980	rVV3	114991	205782	8.35%	0.954%
45	13.986	1986	1989	1990	rBV	25599	26937	1.09%	0.125%
46	14.021	1990	1995	1998	rVV2	693230	845034	34.29%	3.916%
47	14.051	1998	2000	2007	rVB	270524	232147	9.42%	1.076%
48	14.115	2007	2011	2012	rBV	63934	66998	2.72%	0.311%
49	14.410	2059	2061	2064	rVB	49215	42355	1.72%	0.196%
50	14.468	2068	2071	2073	rVB	30838	28671	1.16%	0.133%
51	14.739	2114	2117	2119	rBV2	22717	25225	1.02%	0.117%
52	14.768	2120	2122	2125	rVB2	39568	35779	1.45%	0.166%
53	14.915	2144	2147	2151	rBV3	54078	62514	2.54%	0.290%
54	15.074	2169	2174	2177	rBV	269047	409532	16.62%	1.898%
55	15.186	2189	2193	2197	rBV	71502	108732	4.41%	0.504%
56	15.380	2222	2226	2233	rVB	161928	194509	7.89%	0.901%
57	15.445	2233	2237	2241	rVV	217588	260673	10.58%	1.208%
58	15.504	2243	2247	2251	rVV	447393	595127	24.15%	2.758%
59	15.539	2251	2253	2259	rVB2	65302	84958	3.45%	0.394%
60	15.921	2315	2318	2323	rVB	47894	64063	2.60%	0.297%
61	16.080	2342	2345	2353	rVB7	57692	105460	4.28%	0.489%
62	17.015	2498	2504	2513	rBV2	120831	275239	11.17%	1.276%
63	17.468	2576	2581	2593	rVB2	71292	179855	7.30%	0.834%
64	17.615	2602	2606	2618	rVB2	66706	170354	6.91%	0.790%
65	17.939	2657	2661	2665	rBV7	17684	36755	1.49%	0.170%

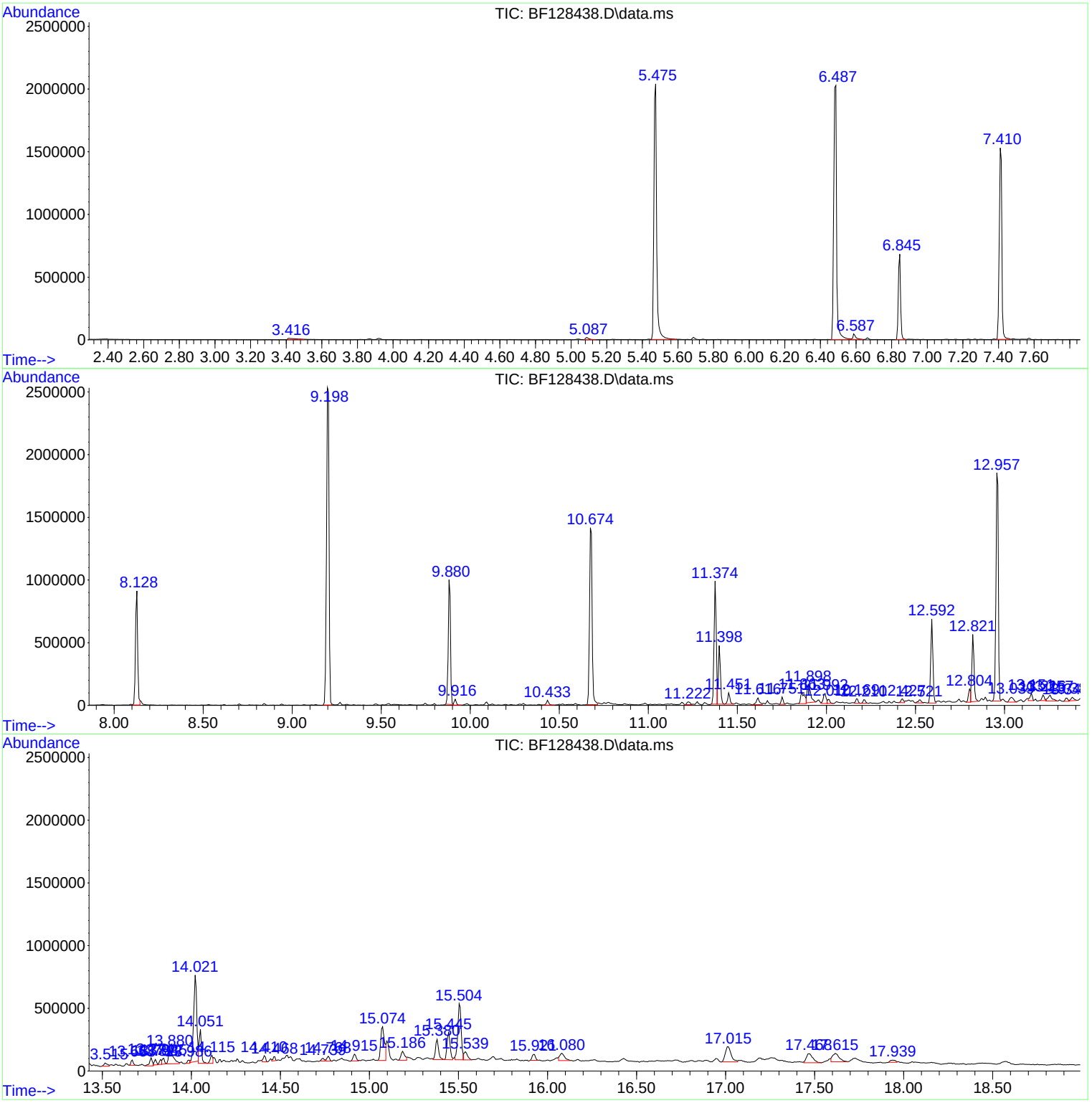
Sum of corrected areas: 21576584

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052422\
Data File : BF128438.D
Acq On : 24 May 2022 16:46
Operator : CG\JU
Sample : N2981-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-15(0.5-1)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.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\BF052422\
Data File : BF128438.D
Acq On : 24 May 2022 16:46
Operator : CG\JU
Sample : N2981-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-15(0.5-1)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

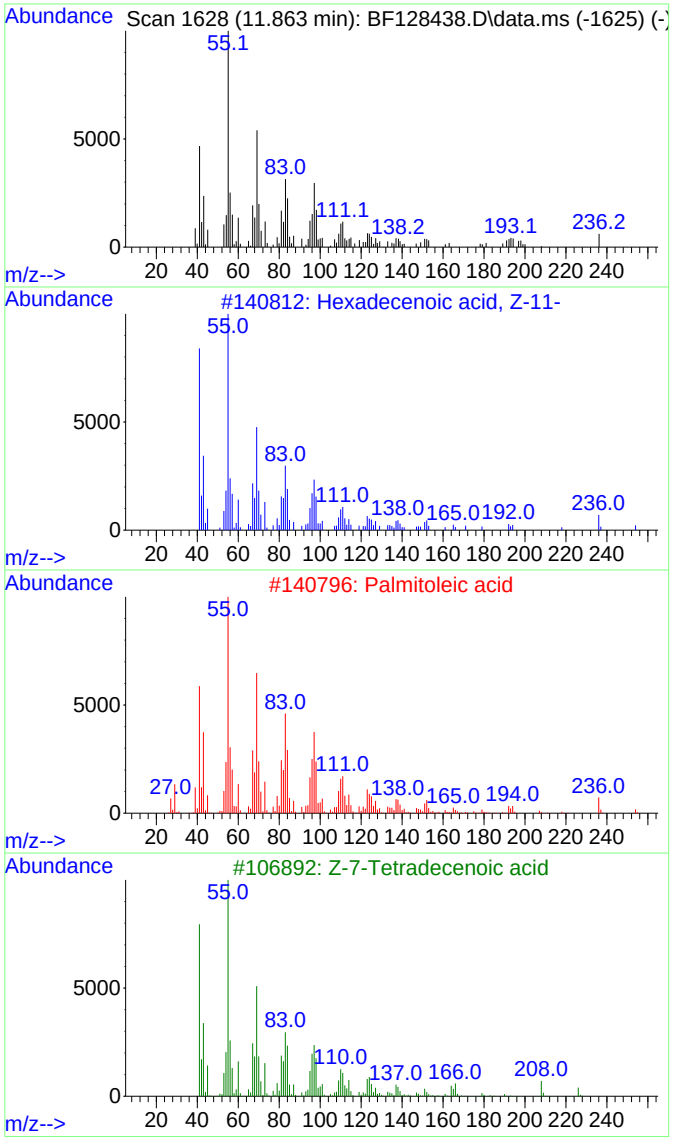
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

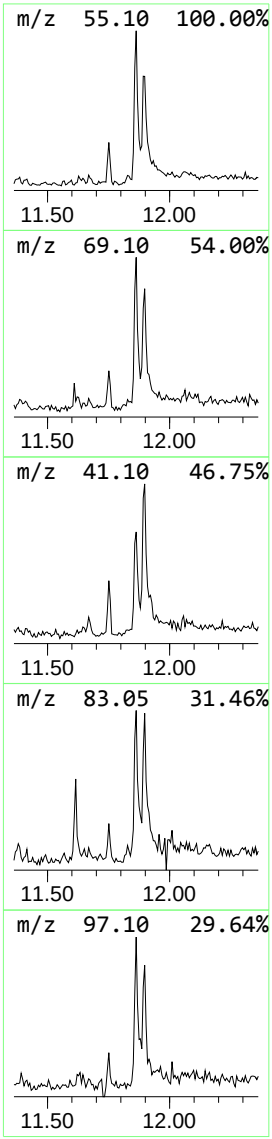
****

Peak Number 1 Hexadecenoic acid, Z-11- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	3.51 ng	144217	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	76
2	Palmitoleic acid	254	C16H30O2	000373-49-9	74
3	Z-7-Tetradecenoic acid	226	C14H26O2	1000130-98-4	58
4	cis-9-Tetradecenoic acid, heptyl...	324	C21H40O2	1010405-20-8	52
5	Oxacyclotridecan-2-one	198	C12H22O2	000947-05-7	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052422\
Data File : BF128438.D
Acq On : 24 May 2022 16:46
Operator : CG\JU
Sample : N2981-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-15(0.5-1)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

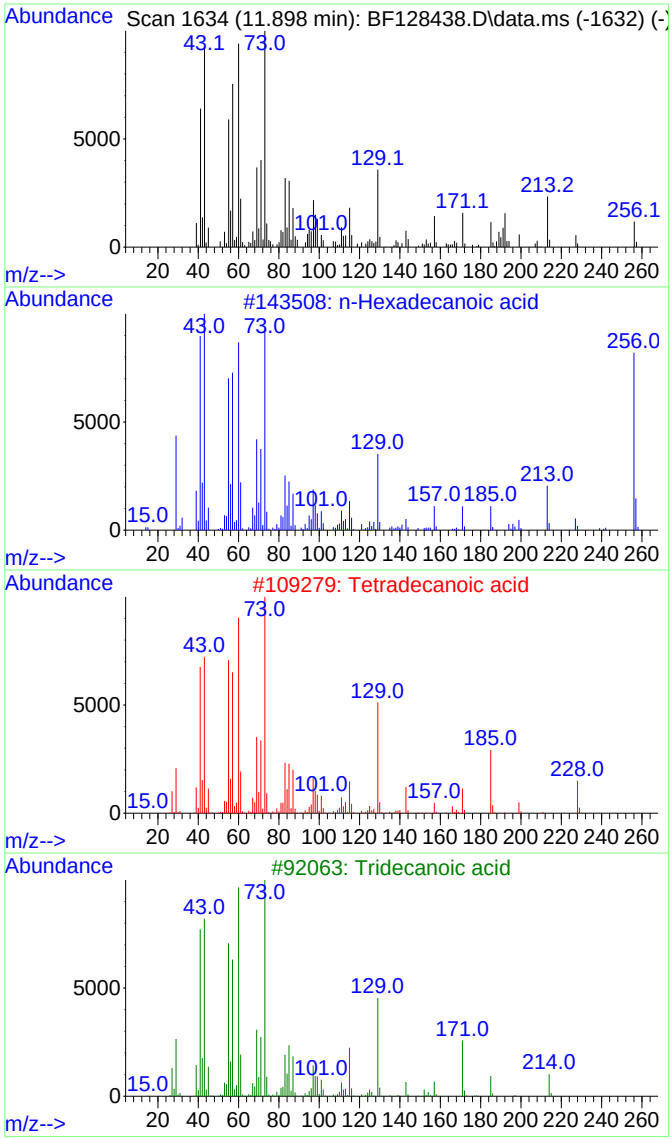
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

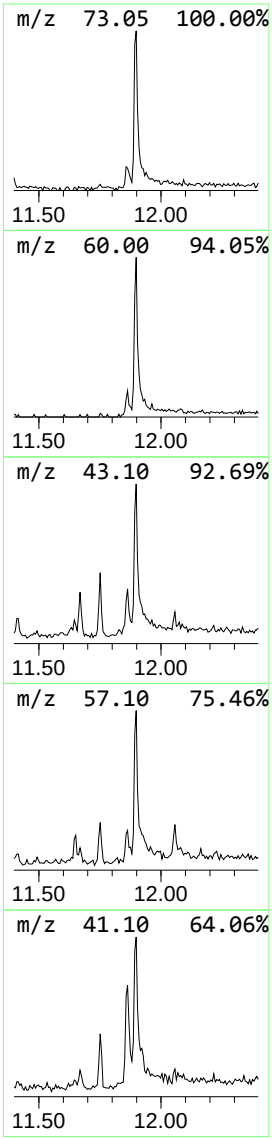
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	4.72 ng	193766	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3	Tridecanoic acid	214	C13H26O2	000638-53-9	94
4	Dodecanoic acid	200	C12H24O2	000143-07-7	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052422\
Data File : BF128438.D
Acq On : 24 May 2022 16:46
Operator : CG\JU
Sample : N2981-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-15(0.5-1)

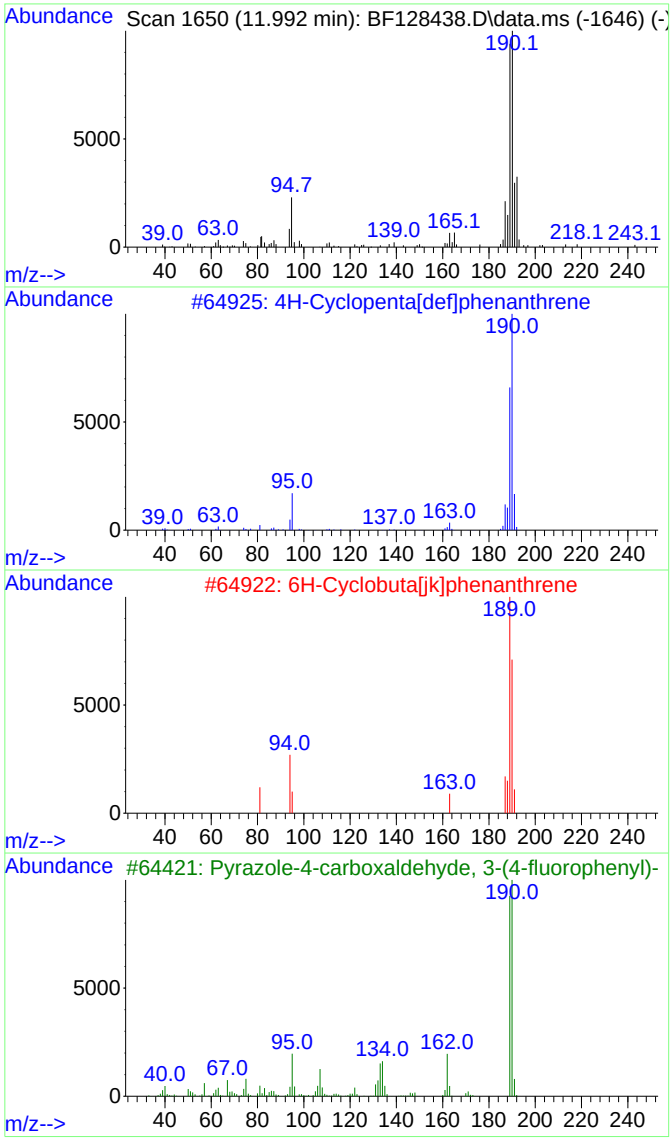
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

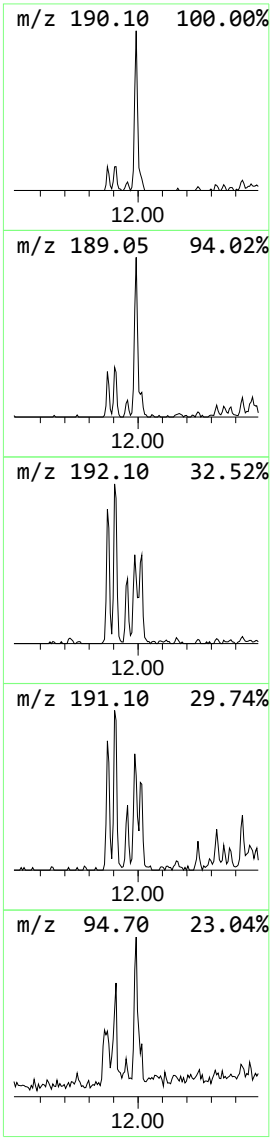
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.992	2.17 ng	88907	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	64
3	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	53
4	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052422\
Data File : BF128438.D
Acq On : 24 May 2022 16:46
Operator : CG\JU
Sample : N2981-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-15(0.5-1)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

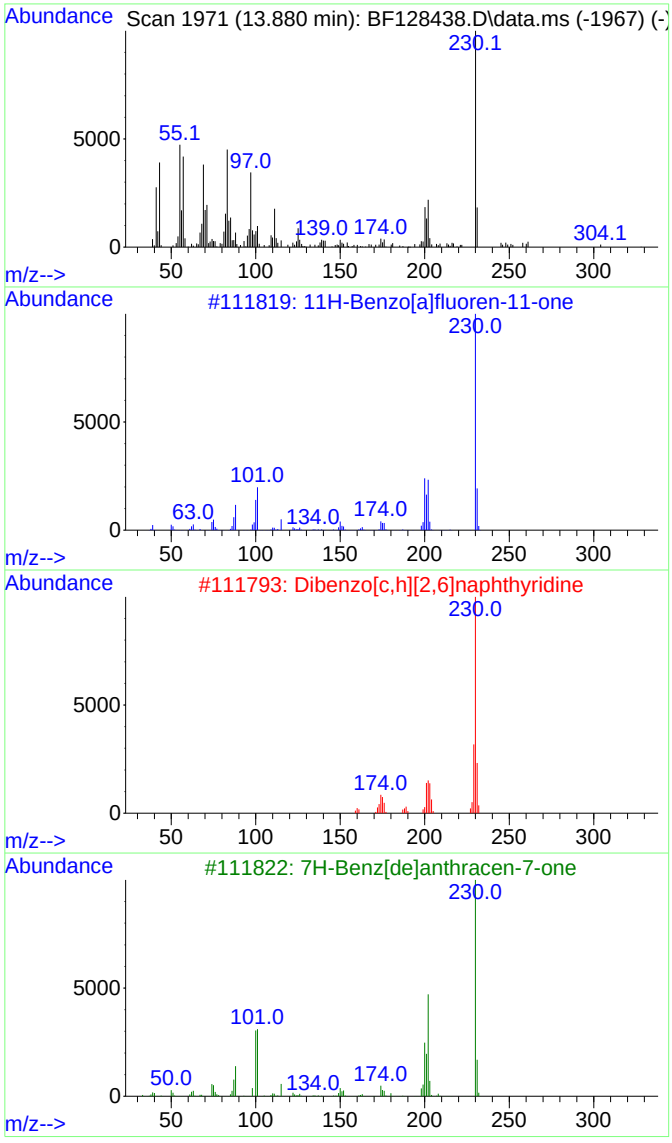
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

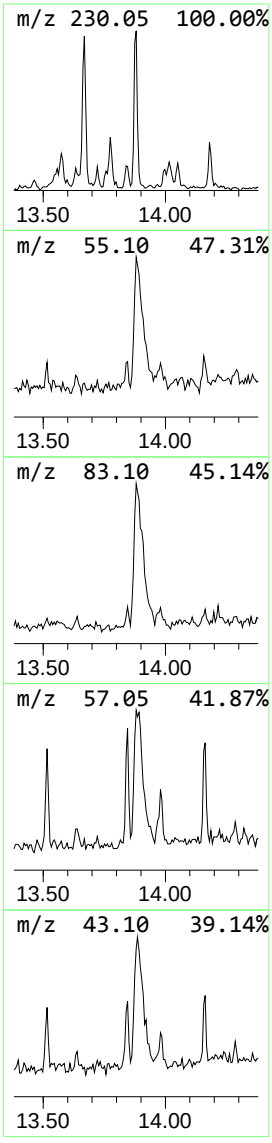
****

Peak Number 4 11H-Benzo[a]fluoren-11-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	4.87 ng	205782	Chrysene-d12	14.021

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	92
2	Dibenzo[c,h][2,6]naphthyridine	230	C16H10N2	000218-30-4	72
3	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	53
4	4-Pyrenecarbaldehyde	230	C17H10O	022245-51-8	47
5	.delta.(sup1),.alpha.-Acenaphthe...	230	C15H6N2O	014619-86-4	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052422\
Data File : BF128438.D
Acq On : 24 May 2022 16:46
Operator : CG\JU
Sample : N2981-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-15(0.5-1)

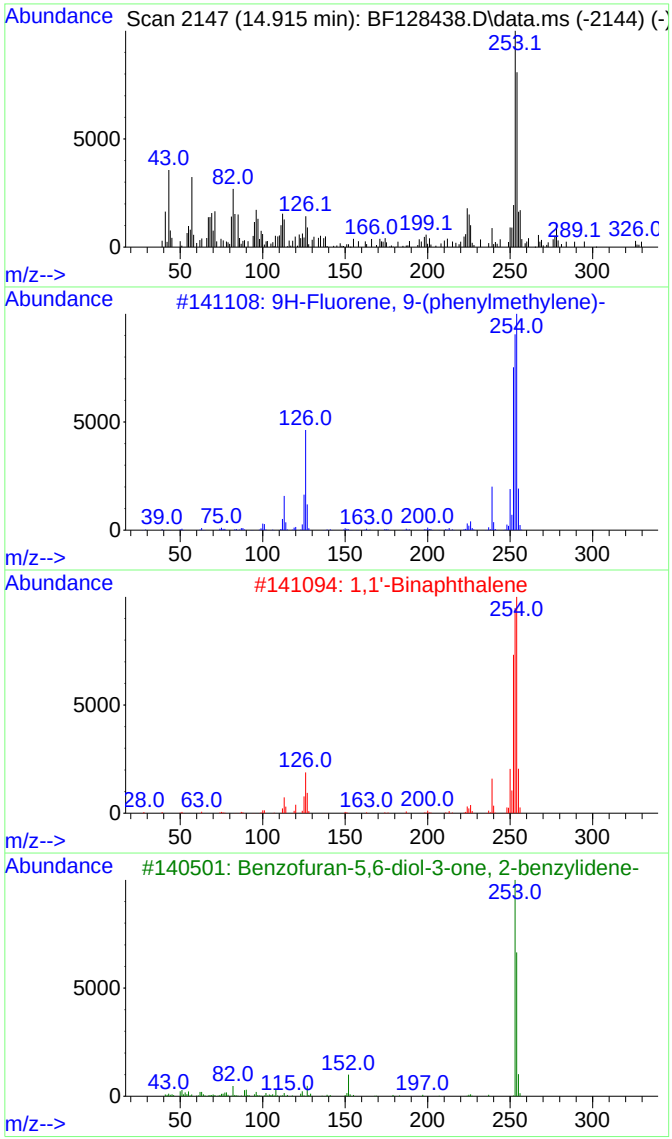
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

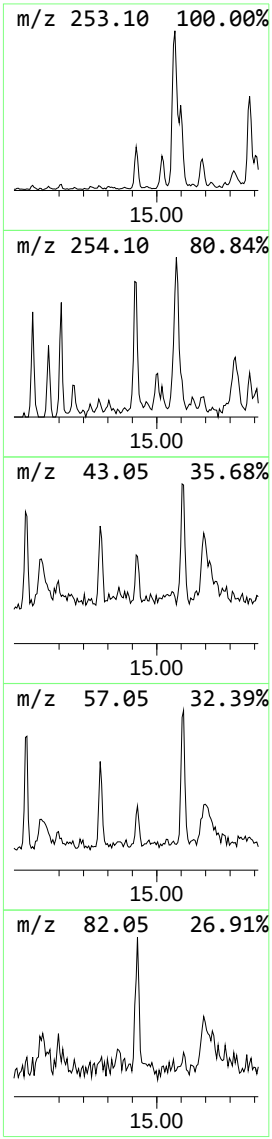
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 9H-Fluorene, 9-(phenylmethy... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.915	2.10 ng	62514	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9H-Fluorene, 9-(phenylmethylene)-	254	C20H14	001836-87-9	70
2	1,1'-Binaphthalene	254	C20H14	000604-53-5	62
3	Benzofuran-5,6-diol-3-one, 2-ben...	254	C15H10O4	1000128-65-2	58
4	1H-Pyrrolo[2,3-f]quinolin-9-ol, ...	254	C16H18N2O	1000303-71-9	58
5	3H-Pyrrolo[3,2-f]quinoline, 5-me...	254	C16H18N2O	1000350-44-1	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052422\
Data File : BF128438.D
Acq On : 24 May 2022 16:46
Operator : CG\JU
Sample : N2981-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-15(0.5-1)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

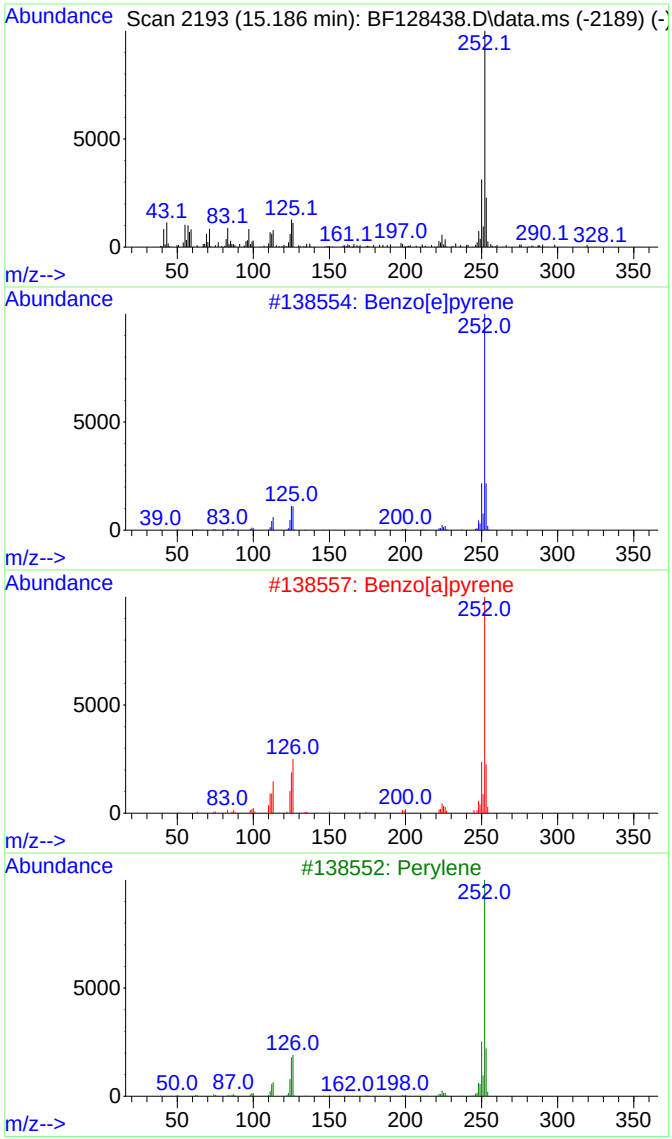
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

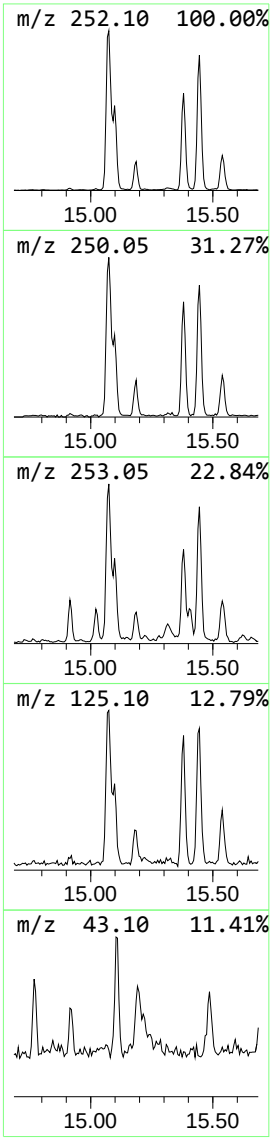
****

Peak Number 6 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.186	3.65 ng	108732	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Benzo[a]pyrene	252	C20H12	000050-32-8	95
3	Perylene	252	C20H12	000198-55-0	93
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	91
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052422\
Data File : BF128438.D
Acq On : 24 May 2022 16:46
Operator : CG\JU
Sample : N2981-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-15(0.5-1)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

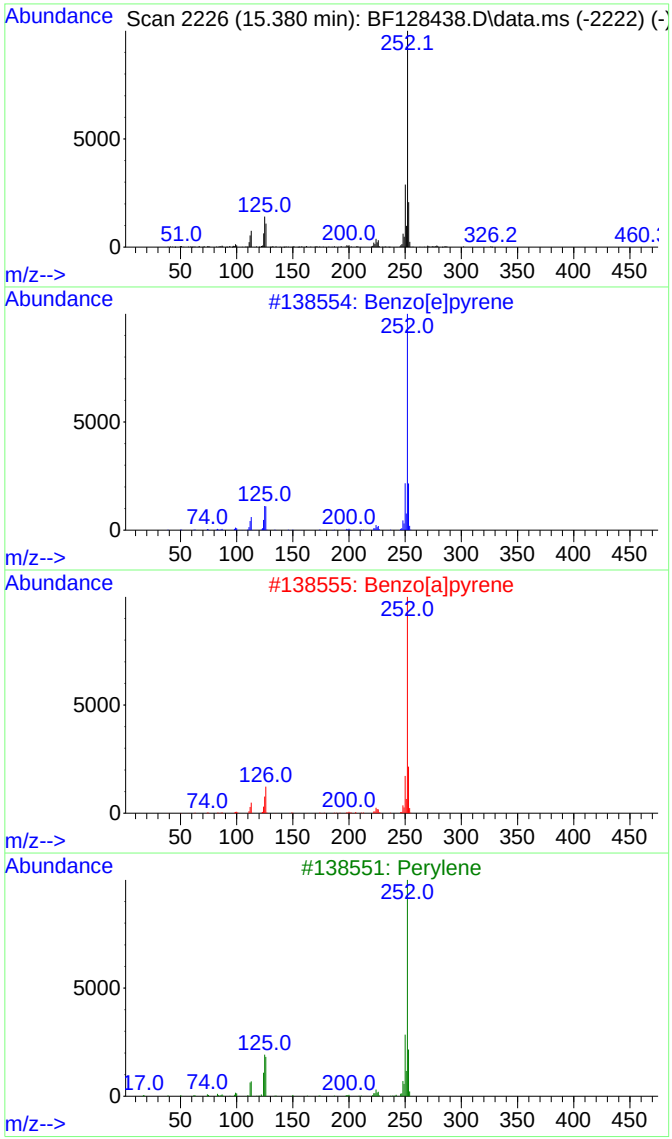
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

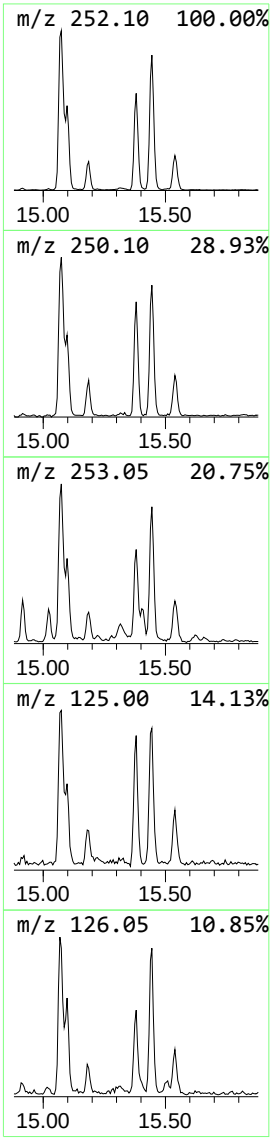
****

Peak Number 7 Perylene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.380	6.54 ng	194509	Perylene-d12	15.504

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	Perylene	252	C20H12	000198-55-0	94
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	94
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93





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Data File : BF128438.D
Acq On : 24 May 2022 16:46
Operator : CG\JU
Sample : N2981-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-15(0.5-1)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.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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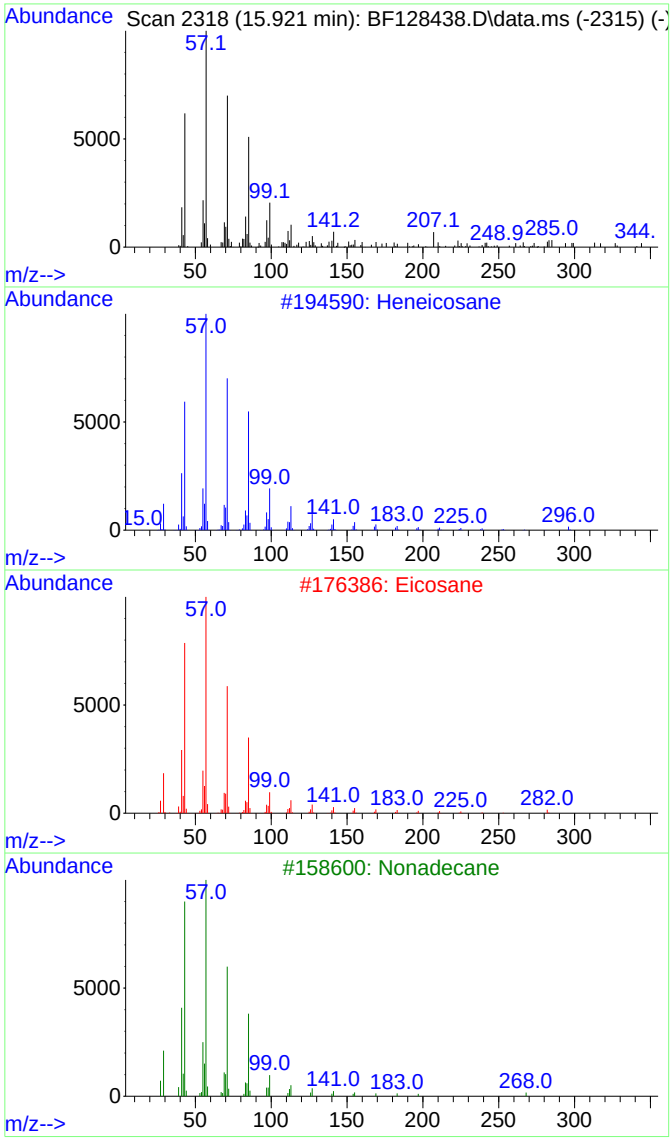
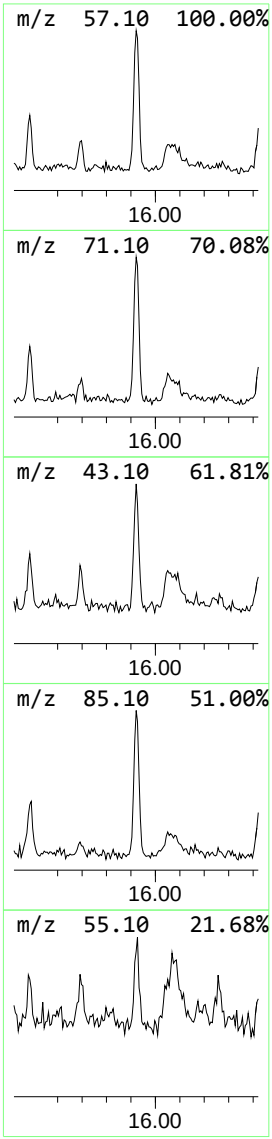
Peak Number 8 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.921	2.15 ng	64063	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Eicosane	282	C20H42	000112-95-8	90
3	Nonadecane	268	C19H40	000629-92-5	72
4	Octadecane	254	C18H38	000593-45-3	72
5	Tridecane, 6-propyl-	226	C16H34	055045-10-8	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052422\
Data File : BF128438.D
Acq On : 24 May 2022 16:46
Operator : CG\JU
Sample : N2981-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-15(0.5-1)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.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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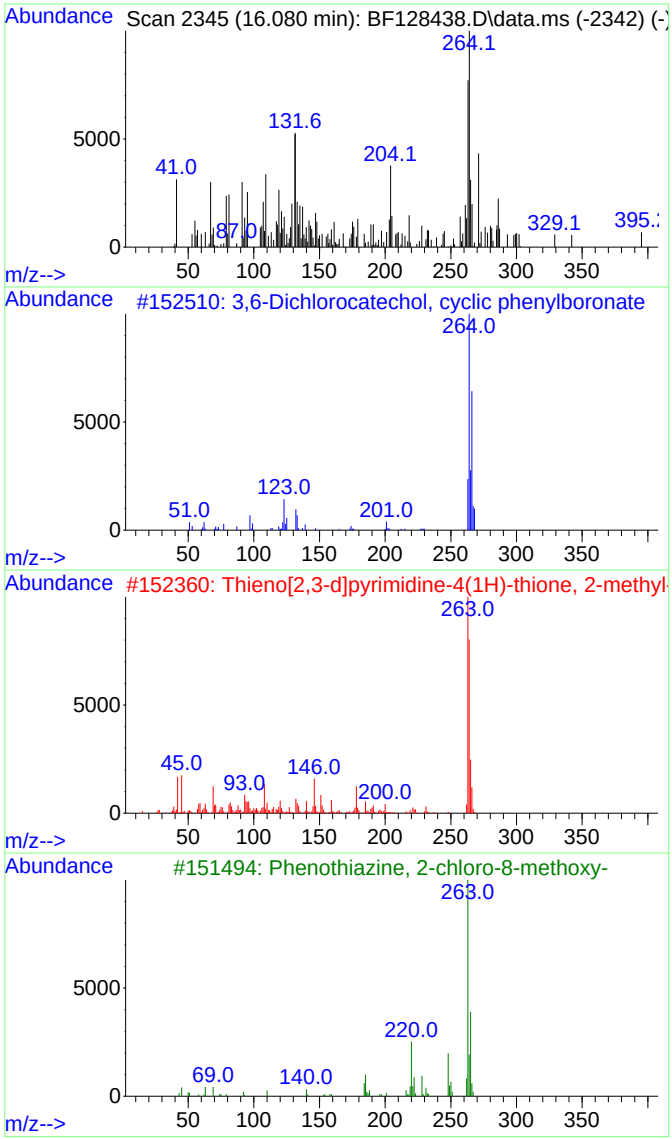
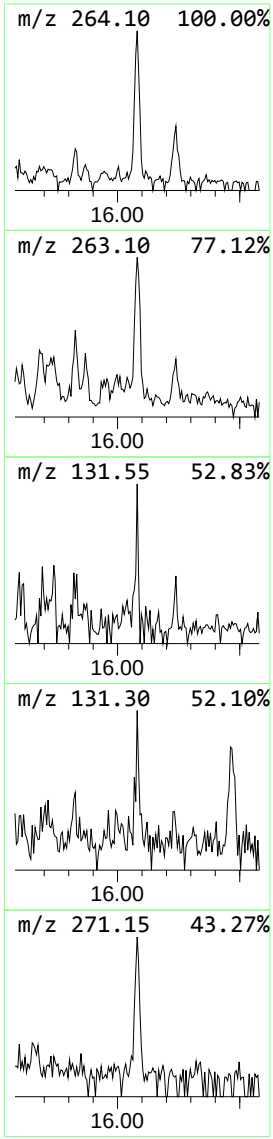
Peak Number 9 unknown16.080 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.080	3.54 ng	105460	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6-Dichlorocatechol, cyclic phe...	264	C12H7BCl2O2	1000293-25-1	18
2	Thieno[2,3-d]pyrimidine-4(1H)-th...	264	C11H8N2S3	732292-19-2	14
3	Phenothiazine, 2-chloro-8-methoxy-	263	C13H10ClNOS	017800-09-8	14
4	N-(4-Bromo-2-methylphenyl)-2-chl...	261	C9H9BrClNO	096686-51-0	11
5	1,2,4-Cyclopentanetrione, 3-isov...	264	C15H20O4	003613-60-3	11





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052422\
Data File : BF128438.D
Acq On : 24 May 2022 16:46
Operator : CG\JU
Sample : N2981-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-15(0.5-1)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.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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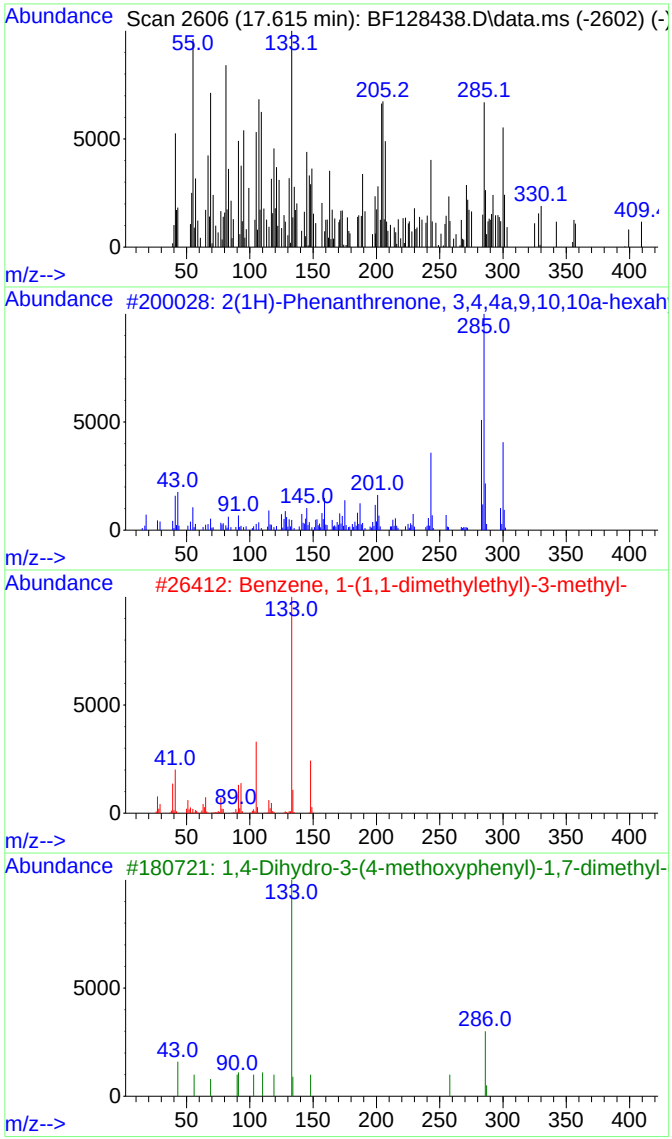
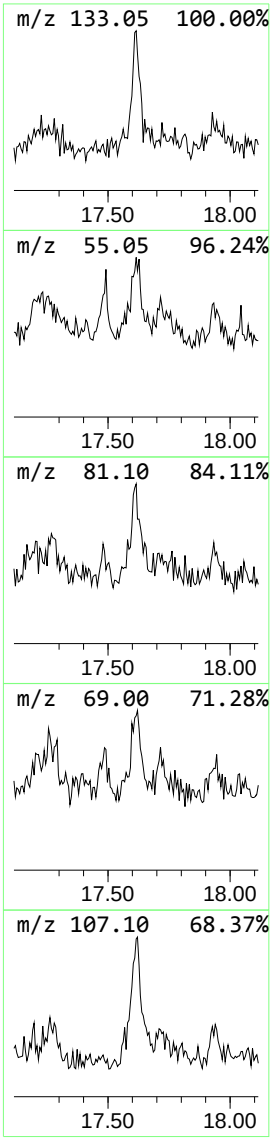
Peak Number 10 unknown17.615 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.615	5.72 ng	170354	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Phenanthrenone, 3,4,4a,9,1...	300	C20H28O2	006755-93-7	25
2	Benzene, 1-(1,1-dimethylethyl)-3...	148	C11H16	001075-38-3	25
3	1,4-Dihydro-3-(4-methoxyphenyl)-...	286	C13H14N6O2	116471-39-7	18
4	6-Cyclobutyl-3-(4-methoxyphenyl)...	286	C14H14N4OS	1000411-10-6	18
5	6H-Benzofuro[3,2-c][1]benzopyran...	300	C17H16O5	003187-52-8	18





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052422\
Data File : BF128438.D
Acq On : 24 May 2022 16:46
Operator : CG\JU
Sample : N2981-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-15(0.5-1)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.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
Hexadecenoic ac...	11.863	3.5	ng	144217	4	11.374	821074	20.0
n-Hexadecanoic ...	11.898	4.7	ng	193766	4	11.374	821074	20.0
4H-Cyclopenta[d...	11.992	2.2	ng	88907	4	11.374	821074	20.0
11H-Benzo[a]flu...	13.880	4.9	ng	205782	5	14.021	845034	20.0
9H-Fluorene, 9-...	14.915	2.1	ng	62514	6	15.504	595127	20.0
Benzo[e]pyrene	15.186	3.6	ng	108732	6	15.504	595127	20.0
Perylene	15.380	6.5	ng	194509	6	15.504	595127	20.0
Heneicosane	15.921	2.1	ng	64063	6	15.504	595127	20.0
unknown16.080	16.080	3.5	ng	105460	6	15.504	595127	20.0
unknown17.615	17.615	5.7	ng	170354	6	15.504	595127	20.0