LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120320\
Data File : BF122538.D
Acq On : 3 Dec 2020 15:25
Operator : JU/CG
Sample : L4911-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SK-12-1-SPC

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-BF110920.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122538.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	6	11	17	rVB	231218	306524	6.32%	0.743%
2	2.257	25	29	38	rVB	58224	81082	1.67%	0.196%
3	5.081	505	509	514	rBV	55853	67402	1.39%	0.163%
4	5.481	572	577	580	rBV	4041879	3905761	80.50%	9.461%
5	6.487	743	748	766	rBV	3672170	4185911	86.27%	10.140%
6	6.851	807	810	814	rBV	1367159	1188466	24.49%	2.879%
7	7.416	901	906	909	rBV	2773000	2600322	53.59%	6.299%
8	8.139	1025	1029	1032	rBV	1823950	1509523	31.11%	3.657%
9	9.216	1207	1212	1215	rBV	5141693	4505064	92.85%	10.913%
10	9.610	1276	1279	1286	rBV	160961	171305	3.53%	0.415%
11	9.757	1301	1304	1310	rVB	63219	57453	1.18%	0.139%
12	9.892	1323	1327	1336	rBV	1818608	1832086	37.76%	4.438%
13	10.686	1457	1462	1473	rBV	2946299	3155794	65.04%	7.645%
14	10.810	1478	1483	1490	rVB2	81569	145289	2.99%	0.352%
15	11.280	1560	1563	1568	rVB	63257	62986	1.30%	0.153%
16	11.380	1576	1580	1583	rBV	2094013	1893838	39.03%	4.588%
17	11.404	1583	1584	1588	rVV	258179	168253	3.47%	0.408%
18	11.457	1590	1593	1596	rVB	105255	94123	1.94%	0.228%
19	11.616	1617	1620	1628	rBV3	35339	65763	1.36%	0.159%
20	11.910	1667	1670	1677	rBV2	440969	489921	10.10%	1.187%
21	11.992	1681	1684	1687	rBV2	61270	65200	1.34%	0.158%
22	12.433	1756	1759	1763	rBV	60562	79105	1.63%	0.192%
23	12.516	1771	1773	1779	rVB	58446	54015	1.11%	0.131%
24	12.592	1783	1786	1790	rVV	739557	624523	12.87%	1.513%
25	12.698	1800	1804	1817	rBV3	566528	848150	17.48%	2.055%
26	12.822	1820	1825	1831	rVB	746541	750323	15.46%	1.818%
27	12.969	1846	1850	1859	rVB	4889654	4851925	100.00%	11.753%
28	13.045	1859	1863	1866	rVV2	64218	101185	2.09%	0.245%
29	13.104	1870	1873	1875	rVV	85096	73823	1.52%	0.179%
30	13.127	1875	1877	1879	rVV3	72258	86853	1.79%	0.210%
31	13.151	1879	1881	1884	rVB2	84407	71337	1.47%	0.173%
32	13.257	1895	1899	1902	rBV2	105728	129784	2.67%	0.314%
33	13.469	1933	1935	1938	rVB	54612	50242	1.04%	0.122%
34	13.657	1964	1967	1972	rVB	106393	110288	2.27%	0.267%
35	13.769	1983	1986	1989	rBV2	66935	71851	1.48%	0.174%
36	13.821	1993	1995	2000	rVV2	57051	63964	1.32%	0.155%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120320\
Data File : BF122538.D
Acq On : 3 Dec 2020 15:25
Operator : JU/CG
Sample : L4911-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SK-12-1-SPC

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-BF110920.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.869	2000	2003	2007	rVB	94919	95263	1.96%	0.231%
38	13.939	2008	2015	2023	rBV4	213546	702918	14.49%	1.703%
39	14.021	2024	2029	2032	rVV2	1878315	2166933	44.66%	5.249%
40	14.045	2032	2033	2042	rVB	410380	334044	6.88%	0.809%
41	14.186	2055	2057	2063	rVB5	50252	59520	1.23%	0.144%
42	14.410	2093	2095	2098	rVB	70610	58045	1.20%	0.141%
43	14.445	2098	2101	2104	rVB2	57612	56880	1.17%	0.138%
44	14.492	2105	2109	2114	rBV4	63016	82819	1.71%	0.201%
45	14.880	2172	2175	2177	rBV2	39889	54414	1.12%	0.132%
46	15.063	2202	2206	2209	rBV	382997	547779	11.29%	1.327%
47	15.174	2222	2225	2228	rVB	64698	66047	1.36%	0.160%
48	15.368	2254	2258	2264	rVB	222545	284918	5.87%	0.690%
49	15.427	2264	2268	2274	rVV	195901	239153	4.93%	0.579%
50	15.492	2274	2279	2292	rVB	1079095	1562153	32.20%	3.784%
51	16.957	2522	2528	2534	rBV2	107077	221127	4.56%	0.536%
52	17.192	2564	2568	2575	rBV3	28047	64021	1.32%	0.155%
53	17.398	2597	2603	2610	rVB	82021	166404	3.43%	0.403%

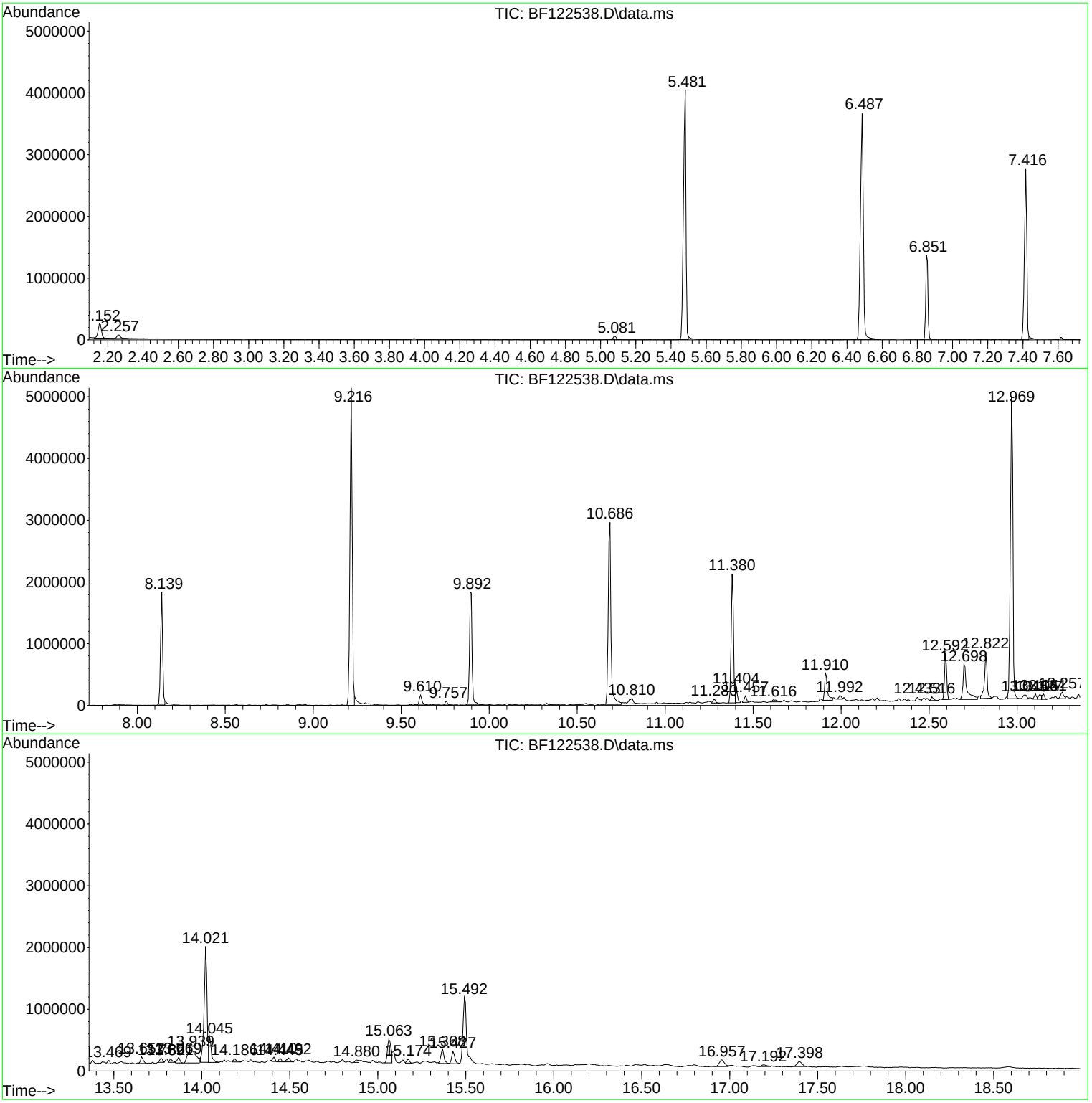
Sum of corrected areas: 41281872

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120320\
Data File : BF122538.D
Acq On : 3 Dec 2020 15:25
Operator : JU/CG
Sample : L4911-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SK-12-1-SPC

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120320\
Data File : BF122538.D
Acq On : 3 Dec 2020 15:25
Operator : JU/CG
Sample : L4911-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SK-12-1-SPC

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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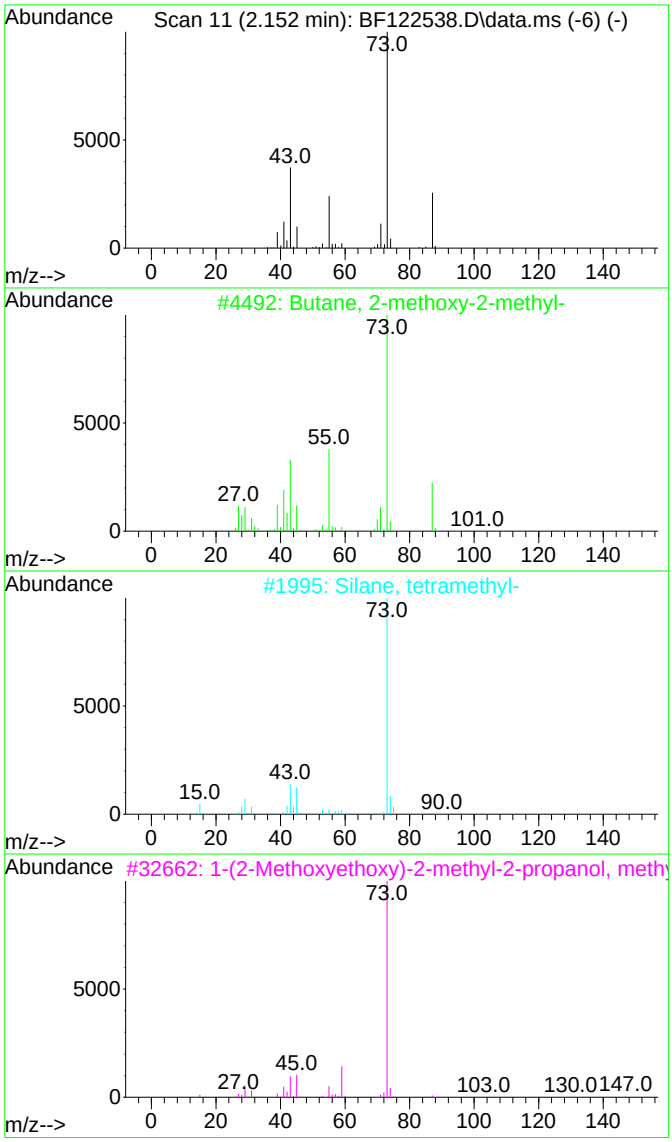
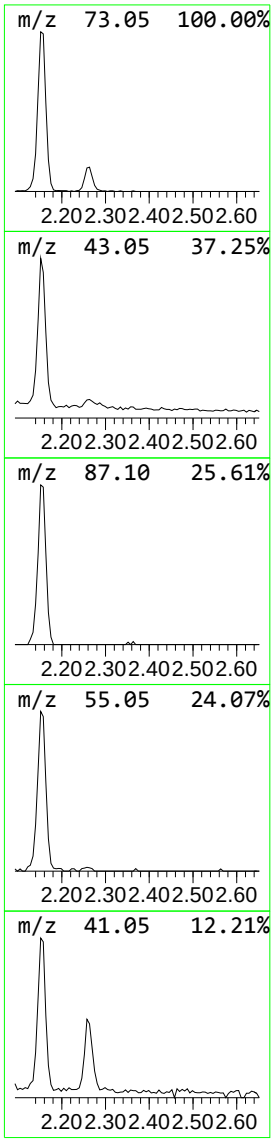
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	5.16 ng	306524	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	43
3	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	25
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120320\
Data File : BF122538.D
Acq On : 3 Dec 2020 15:25
Operator : JU/CG
Sample : L4911-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SK-12-1-SPC

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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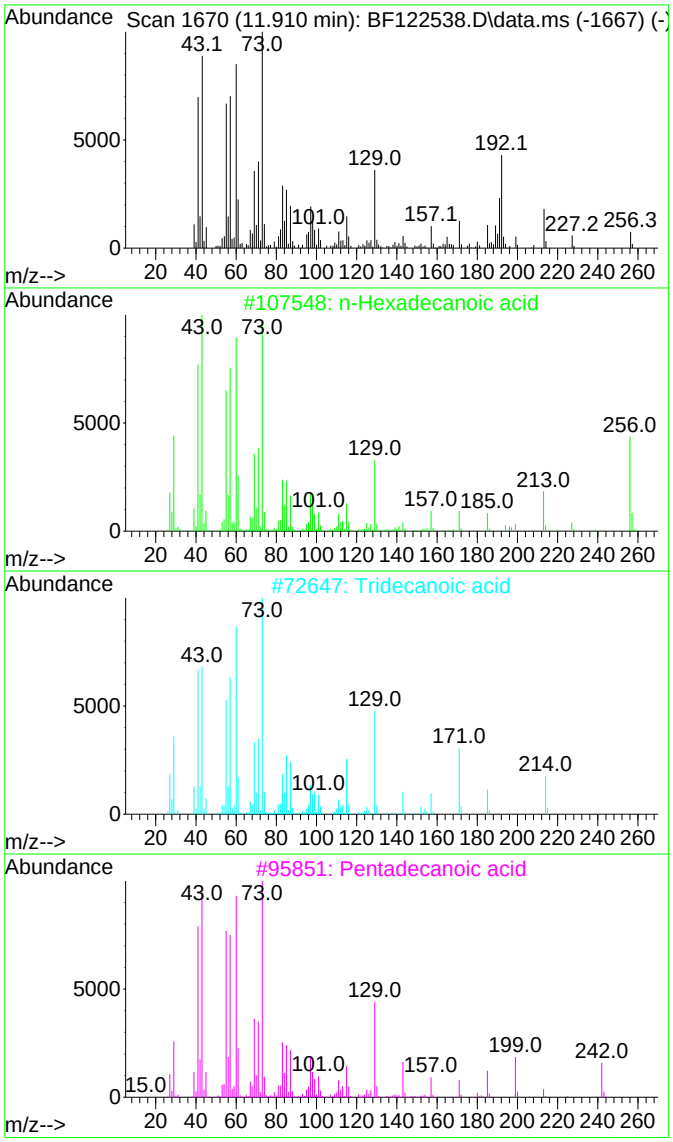
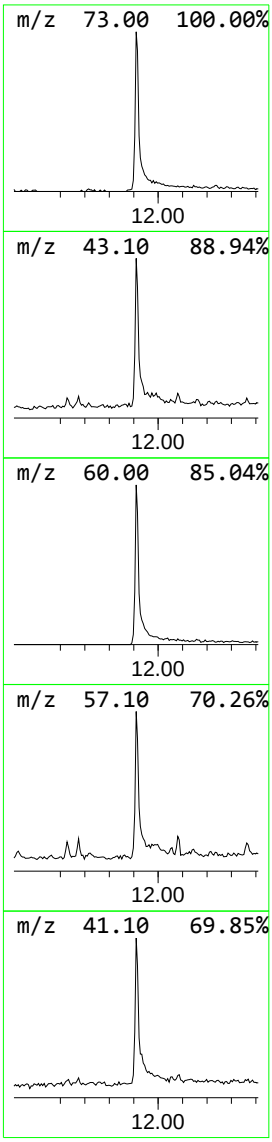
Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	5.17 ng	489921	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	20





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120320\
Data File : BF122538.D
Acq On : 3 Dec 2020 15:25
Operator : JU/CG
Sample : L4911-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SK-12-1-SPC

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

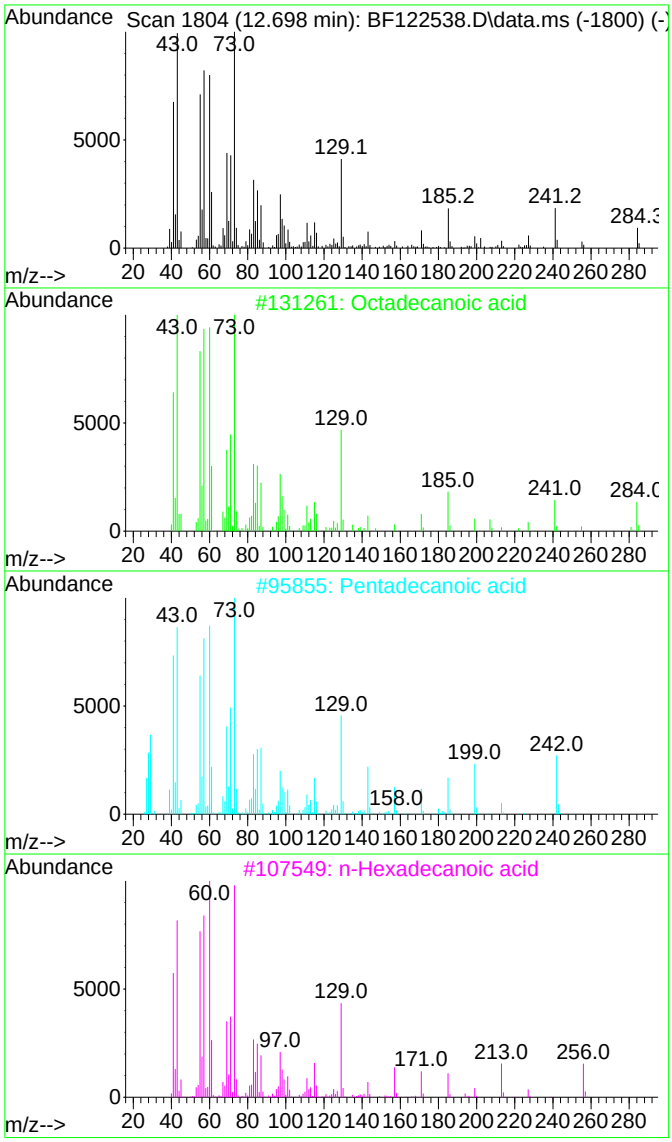
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

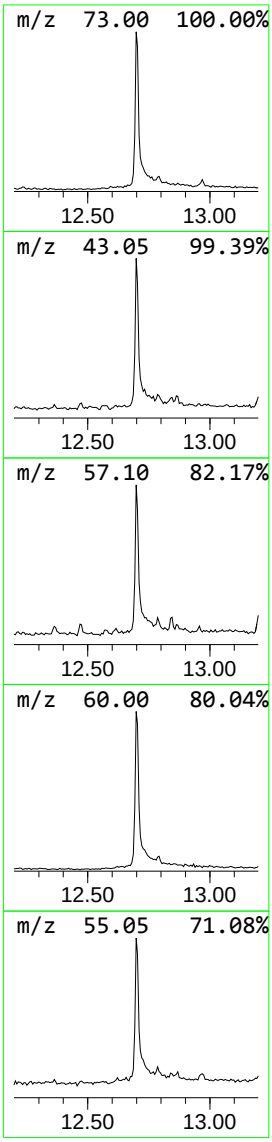
****

Peak Number 3 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.698	8.96 ng	848150	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120320\
Data File : BF122538.D
Acq On : 3 Dec 2020 15:25
Operator : JU/CG
Sample : L4911-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SK-12-1-SPC

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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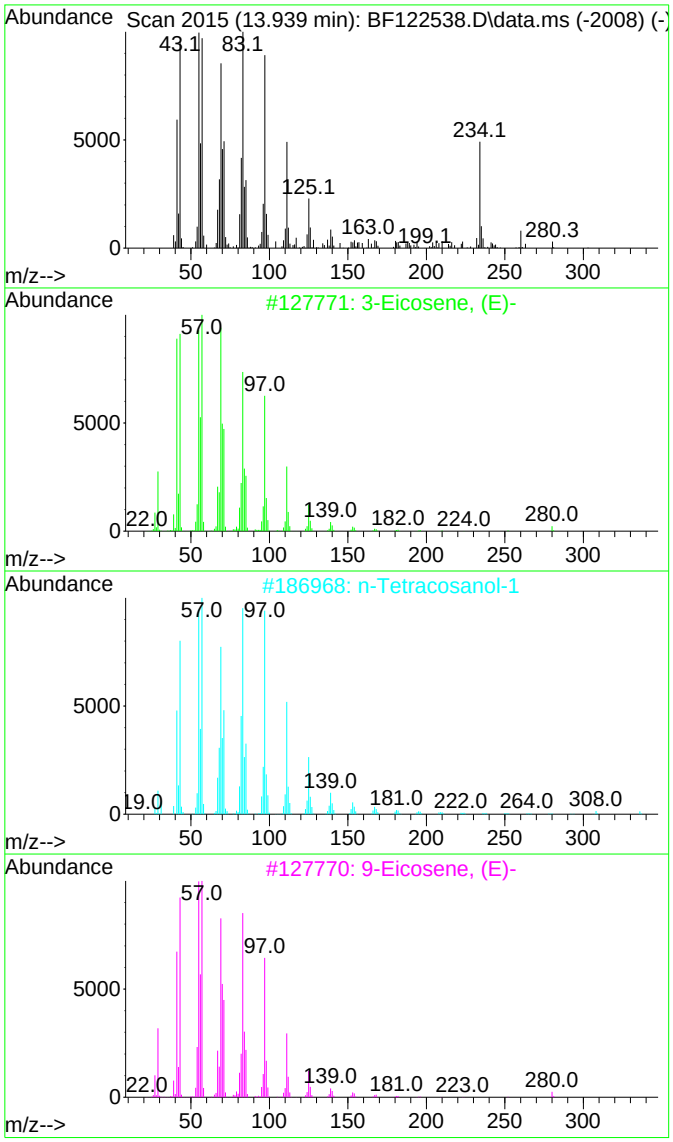
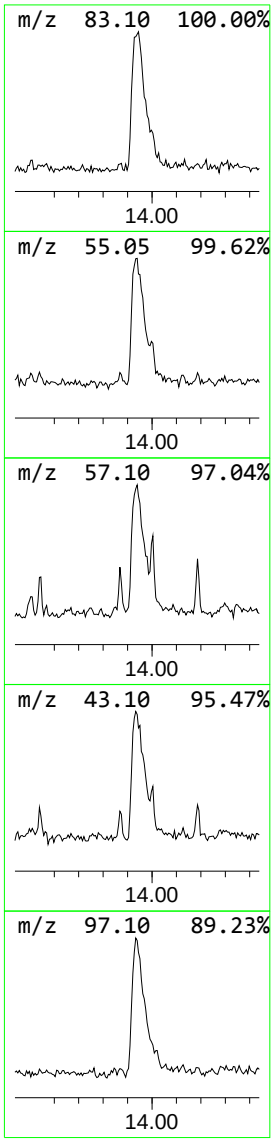
Peak Number 4 3-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.939	6.49 ng	702918	Chrysene-d12	14.021

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
4	1-Heneicosanol	312	C21H44O	015594-90-8	91
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120320\
Data File : BF122538.D
Acq On : 3 Dec 2020 15:25
Operator : JU/CG
Sample : L4911-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SK-12-1-SPC

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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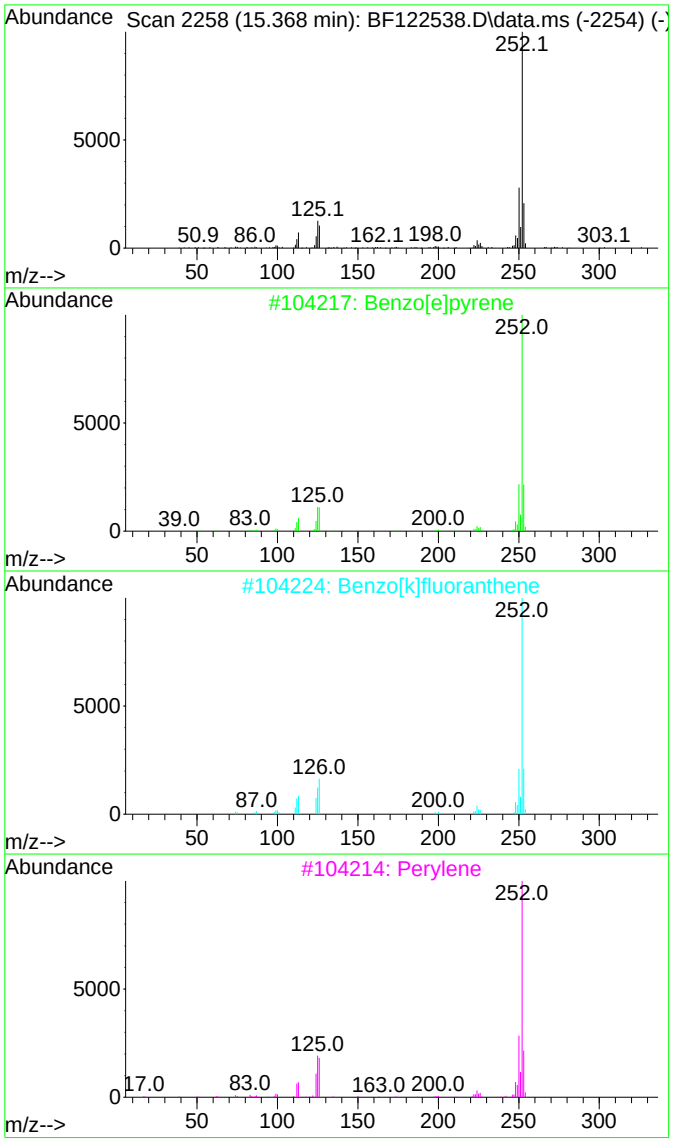
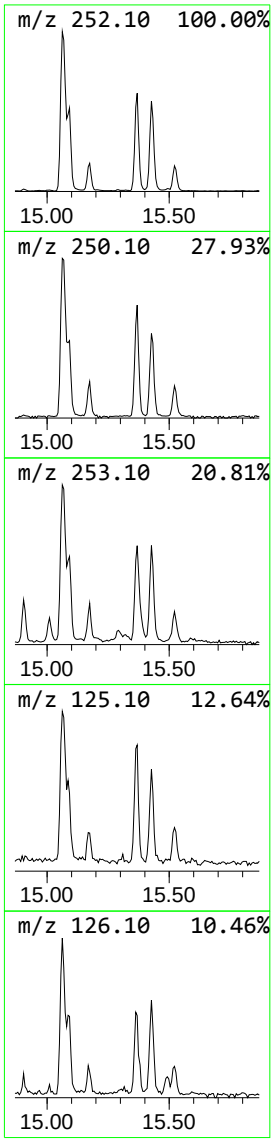
Peak Number 5 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.368	3.65 ng	284918	Perylene-d12	15.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3	Perylene	252	C20H12	000198-55-0	97
4	Benzo[a]pyrene	252	C20H12	000050-32-8	96
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	95





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120320\
Data File : BF122538.D
Acq On : 3 Dec 2020 15:25
Operator : JU/CG
Sample : L4911-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SK-12-1-SPC

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.152	5.2	ng	306524	1	6.857	1188470	20.0
n-Hexadecanoic ...	11.910	5.2	ng	489921	4	11.380	1893840	20.0
Octadecanoic acid	12.698	9.0	ng	848150	4	11.380	1893840	20.0
3-Eicosene, (E)-	13.939	6.5	ng	702918	5	14.021	2166930	20.0
Benzo[e]pyrene	15.368	3.6	ng	284918	6	15.492	1562150	20.0