LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111320\
Data File : BF122331.D
Acq On : 13 Nov 2020 16:10
Operator : JU/CG
Sample : L4723-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-59

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: BF122331.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	17	rVB	703049	838089	20.17%	1.832%
2	5.469	570	575	578	rBV	4443217	4060353	97.71%	8.877%
3	6.481	742	747	750	rBV	4502053	4155710	100.00%	9.085%
4	6.686	778	782	788	rBV	136443	122575	2.95%	0.268%
5	6.863	809	812	816	rVB	1718597	1354207	32.59%	2.961%
6	7.422	903	907	910	rBV	3197607	2647896	63.72%	5.789%
7	8.145	1027	1030	1034	rBV	2042557	1773744	42.68%	3.878%
8	9.222	1209	1213	1217	rBV	4434503	4045780	97.35%	8.845%
9	9.616	1276	1280	1284	rBV	1087054	851554	20.49%	1.862%
10	9.904	1325	1329	1332	rBV	2478305	2021433	48.64%	4.419%
11	10.410	1411	1415	1418	rBV	126222	106970	2.57%	0.234%
12	10.686	1458	1462	1474	rBV	3163285	2712596	65.27%	5.930%
13	11.286	1562	1564	1569	rVB2	50754	57395	1.38%	0.125%
14	11.386	1577	1581	1583	rBV	2531774	2118075	50.97%	4.631%
15	11.410	1583	1585	1588	rVV	676612	524673	12.63%	1.147%
16	11.463	1591	1594	1597	rVB	81046	73883	1.78%	0.162%
17	11.610	1615	1619	1622	rBV2	49843	53069	1.28%	0.116%
18	11.886	1663	1666	1668	rBV	115792	110572	2.66%	0.242%
19	11.916	1668	1671	1675	rVV	687790	808577	19.46%	1.768%
20	11.951	1675	1677	1682	rVV2	169892	214626	5.16%	0.469%
21	11.998	1682	1685	1688	rVV	198237	238553	5.74%	0.522%
22	12.021	1688	1689	1694	rVB	110462	71686	1.73%	0.157%
23	12.186	1714	1717	1718	rBV	70134	66655	1.60%	0.146%
24	12.204	1718	1720	1725	rVB2	99338	94327	2.27%	0.206%
25	12.374	1745	1749	1754	rVB2	138353	170996	4.11%	0.374%
26	12.439	1756	1760	1763	rBV2	91298	109087	2.62%	0.238%
27	12.474	1763	1766	1768	rBV3	54835	65101	1.57%	0.142%
28	12.521	1771	1774	1778	rBV2	71397	77288	1.86%	0.169%
29	12.557	1778	1780	1783	rBV	60453	49834	1.20%	0.109%
30	12.598	1783	1787	1791	rBV	1153180	942621	22.68%	2.061%
31	12.704	1801	1805	1811	rBV3	410607	663084	15.96%	1.450%
32	12.827	1820	1826	1829	rBV	1063410	979726	23.58%	2.142%
33	12.874	1832	1834	1839	rVB2	51660	74004	1.78%	0.162%
34	12.974	1847	1851	1854	rBV	4784501	3986254	95.92%	8.715%
35	13.045	1859	1863	1866	rBV3	76498	108867	2.62%	0.238%
36	13.133	1875	1878	1880	rBV3	65355	86079	2.07%	0.188%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111320\
Data File : BF122331.D
Acq On : 13 Nov 2020 16:10
Operator : JU/CG
Sample : L4723-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-59

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	13.157	1880	1882	1884	rVB	133229	104277	2.51%	0.228%
38	13.221	1884	1893	1896	rBV2	103885	139314	3.35%	0.305%
39	13.257	1896	1899	1902	rBV2	121077	120028	2.89%	0.262%
40	13.351	1912	1915	1918	rVB	87723	64674	1.56%	0.141%
41	13.380	1918	1920	1925	rBV	75363	65359	1.57%	0.143%
42	13.457	1930	1933	1942	rVB8	29517	57800	1.39%	0.126%
43	13.657	1964	1967	1973	rVB	93179	108279	2.61%	0.237%
44	13.774	1982	1987	1990	rBV2	99992	142649	3.43%	0.312%
45	13.804	1990	1992	1994	rVV	88136	67624	1.63%	0.148%
46	13.827	1994	1996	2000	rVV2	63161	74618	1.80%	0.163%
47	13.880	2000	2005	2014	rVV3	391856	679621	16.35%	1.486%
48	14.027	2024	2030	2032	rBV2	2453833	2590348	62.33%	5.663%
49	14.051	2032	2034	2039	rVB	533890	456023	10.97%	0.997%
50	14.133	2045	2048	2051	rBV2	55935	50275	1.21%	0.110%
51	14.204	2057	2060	2063	rVB3	54535	62847	1.51%	0.137%
52	14.409	2091	2095	2098	rBV	90635	100266	2.41%	0.219%
53	14.445	2098	2101	2104	rVB	85498	77717	1.87%	0.170%
54	14.504	2105	2111	2114	rBV5	94357	128073	3.08%	0.280%
55	14.557	2118	2120	2123	rVB3	60146	58773	1.41%	0.128%
56	14.815	2158	2164	2166	rBV6	49401	80977	1.95%	0.177%
57	15.062	2201	2206	2209	rBV	424867	611733	14.72%	1.337%
58	15.168	2219	2224	2228	rVB3	66839	120364	2.90%	0.263%
59	15.368	2254	2258	2263	rVB	259270	299953	7.22%	0.656%
60	15.427	2264	2268	2274	rBV	318904	372006	8.95%	0.813%
61	15.492	2274	2279	2283	rBV	1570506	1945718	46.82%	4.254%
62	15.980	2359	2362	2366	rBV2	45259	63633	1.53%	0.139%
63	16.498	2445	2450	2452	rBV4	43859	76263	1.84%	0.167%
64	16.945	2521	2526	2535	rVB2	140957	291352	7.01%	0.637%
65	17.186	2562	2567	2571	rBV4	29739	60732	1.46%	0.133%
66	17.386	2596	2601	2610	rVB	122698	233190	5.61%	0.510%

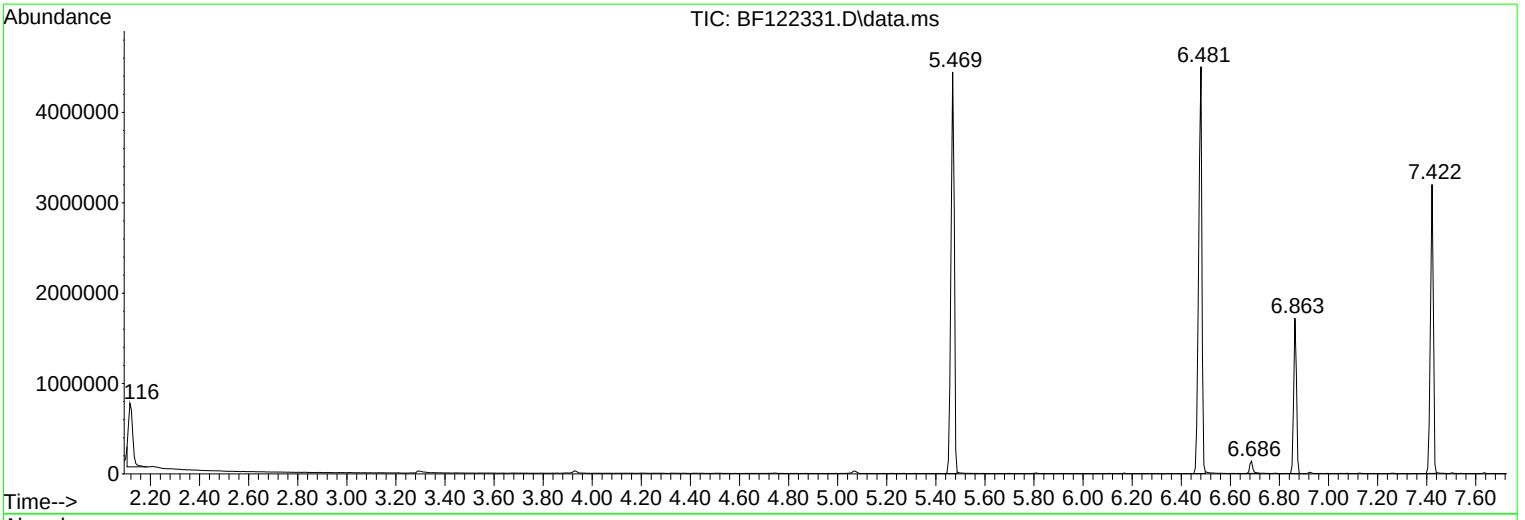
Sum of corrected areas: 45740425

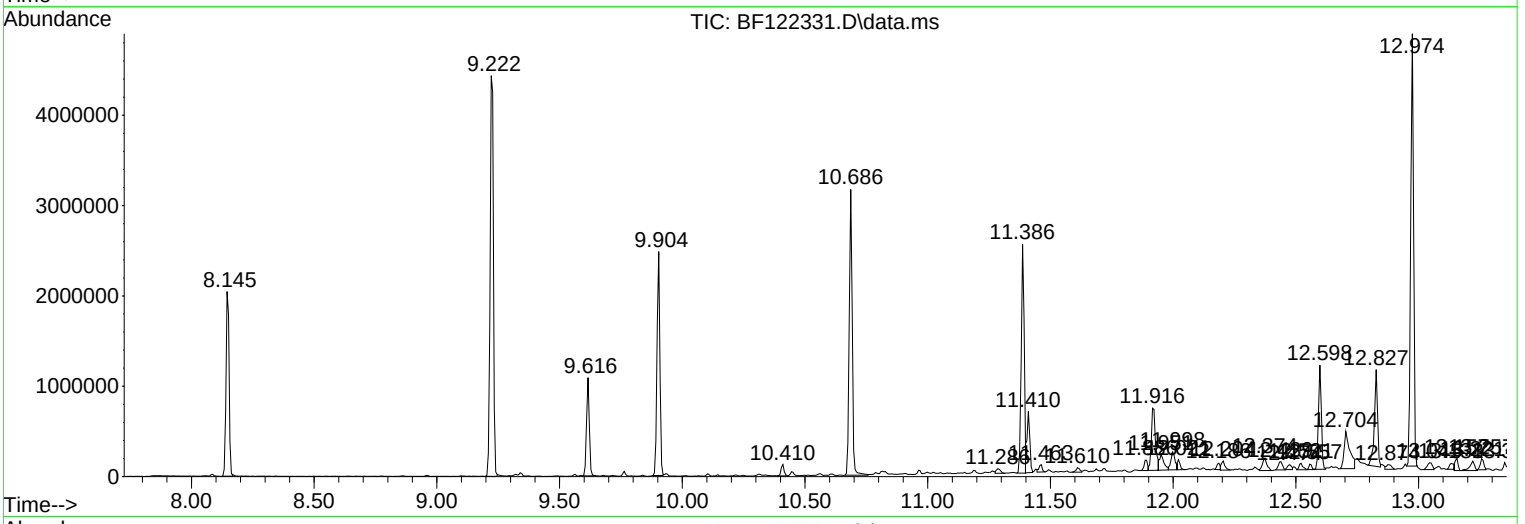
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111320\
Data File : BF122331.D
Acq On : 13 Nov 2020 16:10
Operator : JU/CG
Sample : L4723-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

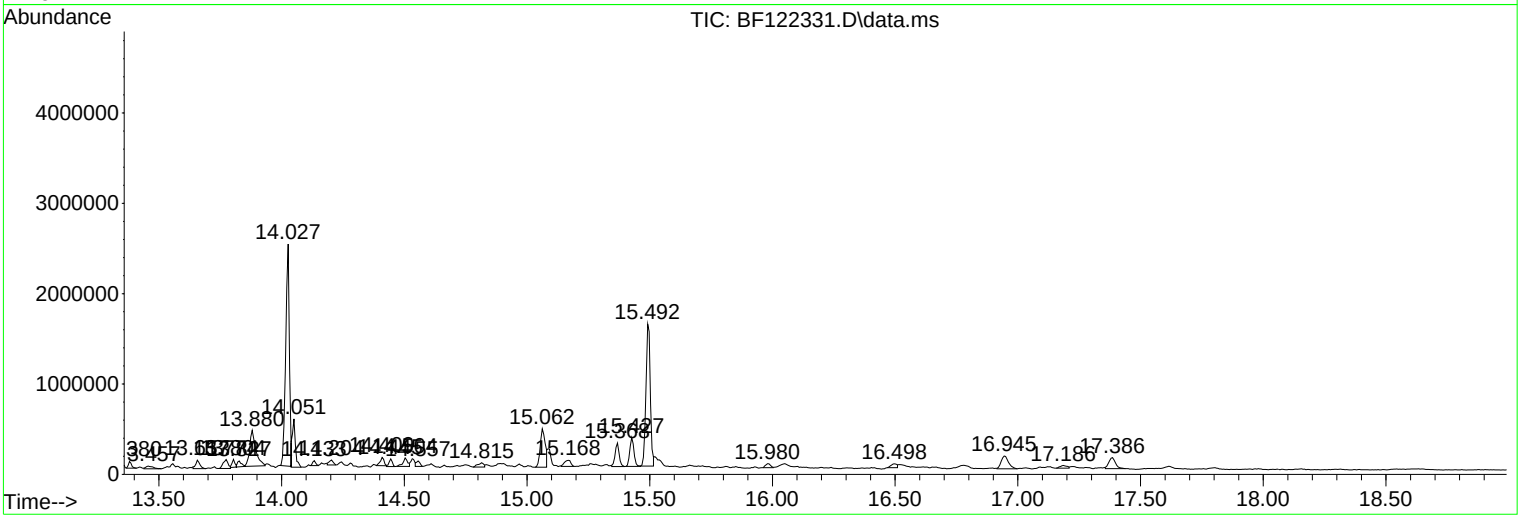
Instrument :
BNA_F
ClientSampleId :
RBR-59

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\BF111320\
Data File : BF122331.D
Acq On : 13 Nov 2020 16:10
Operator : JU/CG
Sample : L4723-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-59

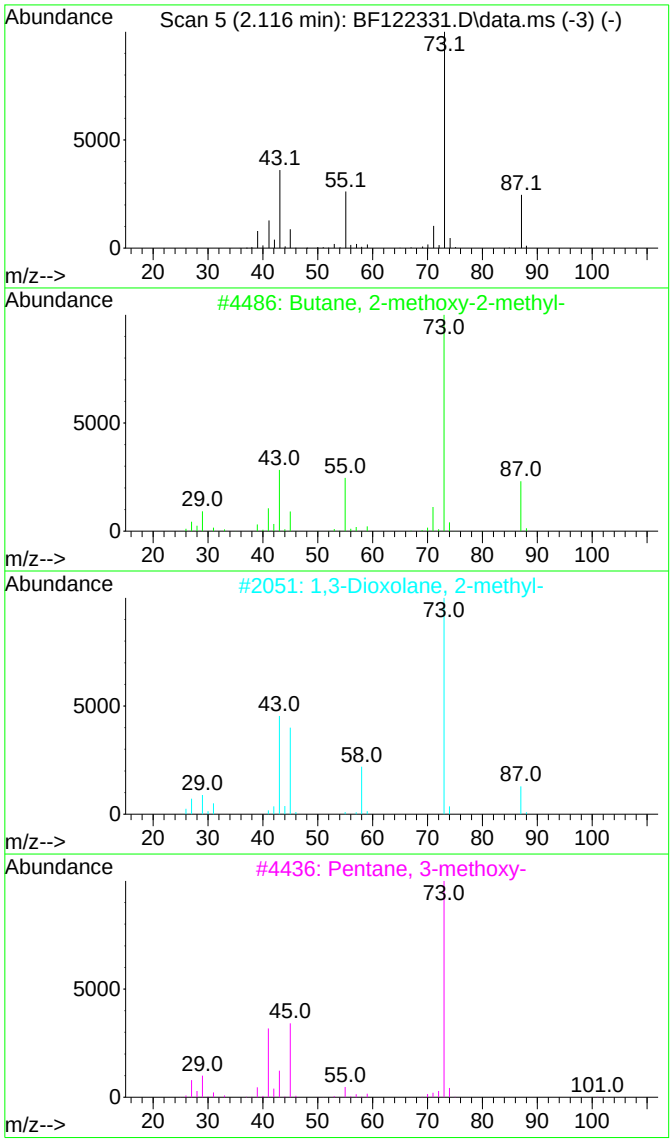
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

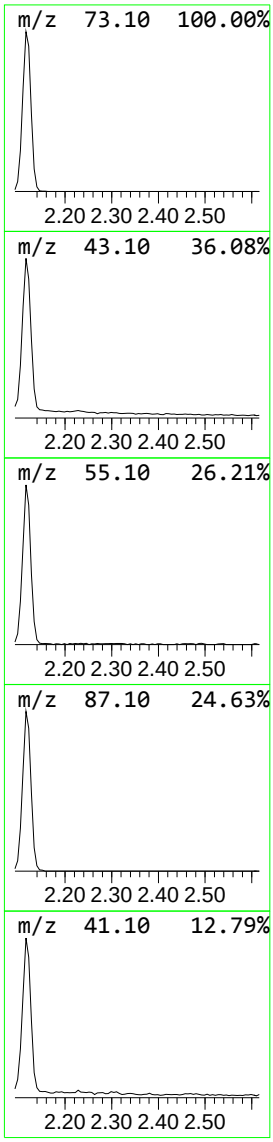
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	12.38 ng	838089	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111320\
Data File : BF122331.D
Acq On : 13 Nov 2020 16:10
Operator : JU/CG
Sample : L4723-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-59

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

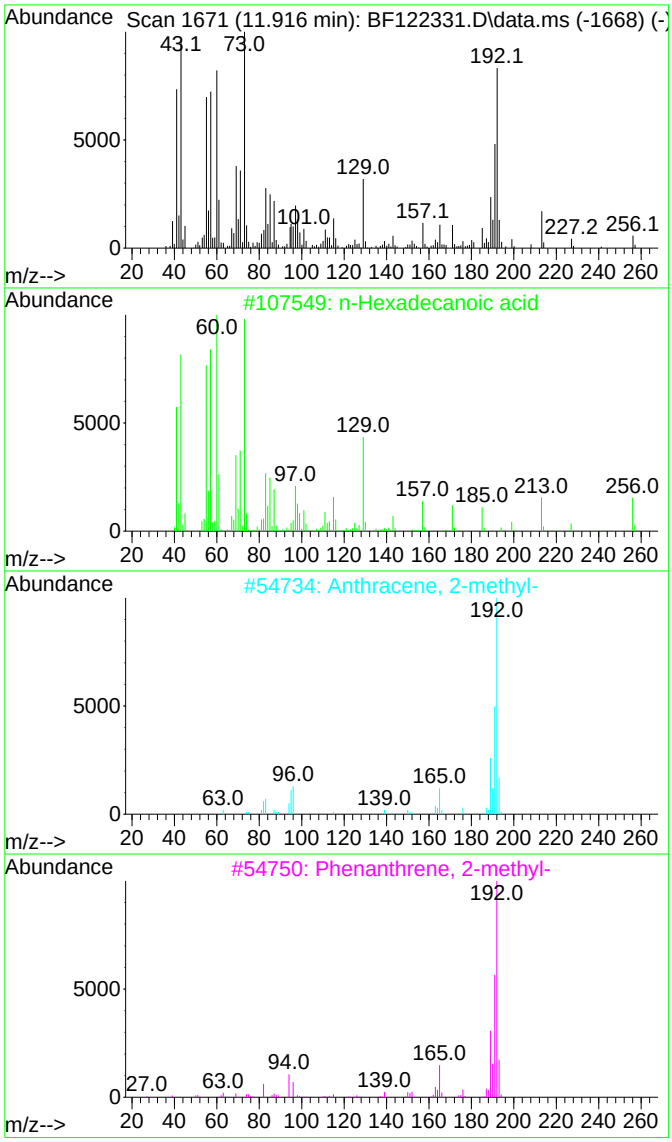
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

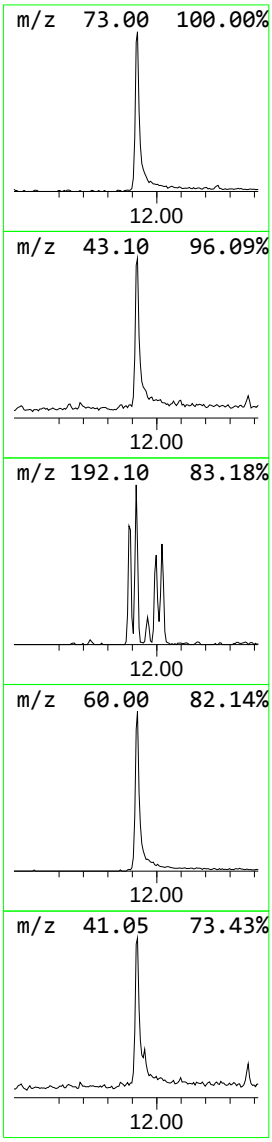
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	7.64 ng	808577	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	92





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111320\
Data File : BF122331.D
Acq On : 13 Nov 2020 16:10
Operator : JU/CG
Sample : L4723-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-59

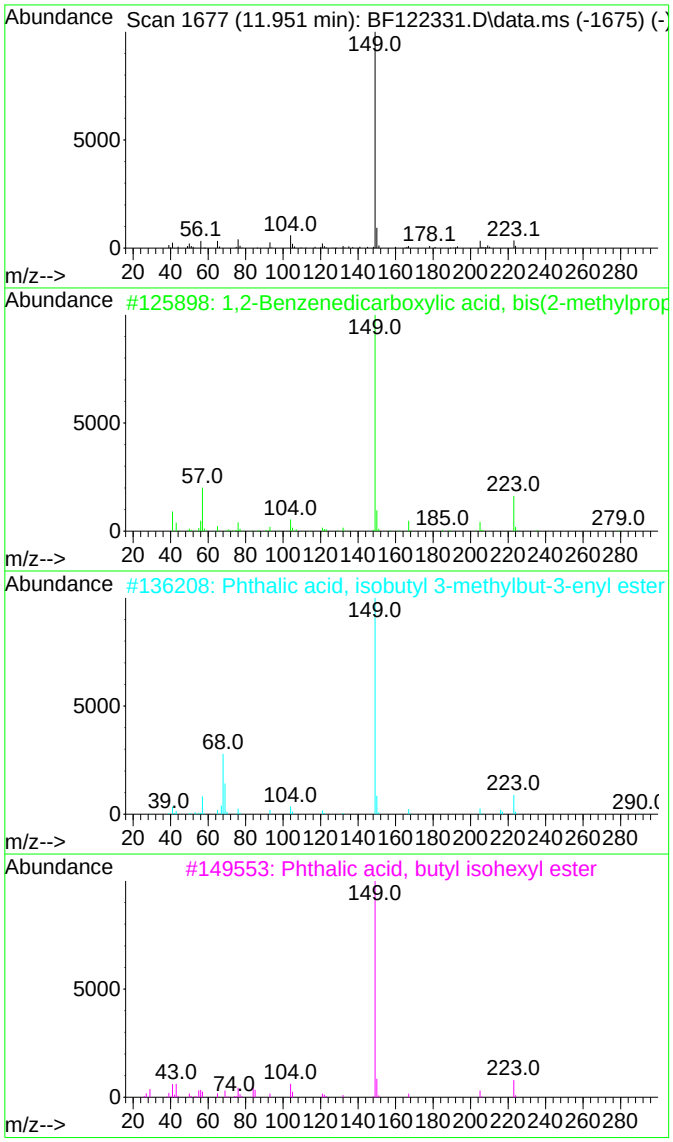
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

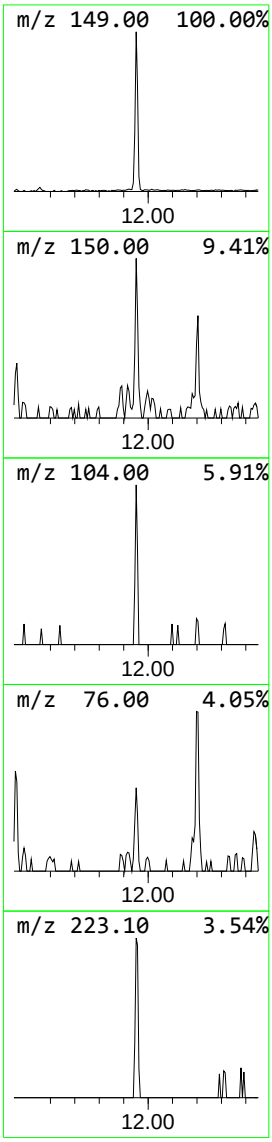
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1,2-Benzenedicarboxylic aci... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	2.03 ng	214626	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	78
2	Phthalic acid, isobutyl 3-methyl...	290	C17H22O4	1000357-10-1	78
3	Phthalic acid, butyl isohexyl ester	306	C18H26O4	1000309-03-6	78
4	Phthalic acid, butyl 3-methylbut...	290	C17H22O4	1000315-44-7	78
5	Phthalic acid, butyl hexyl ester	306	C18H26O4	1000308-99-5	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111320\
Data File : BF122331.D
Acq On : 13 Nov 2020 16:10
Operator : JU/CG
Sample : L4723-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-59

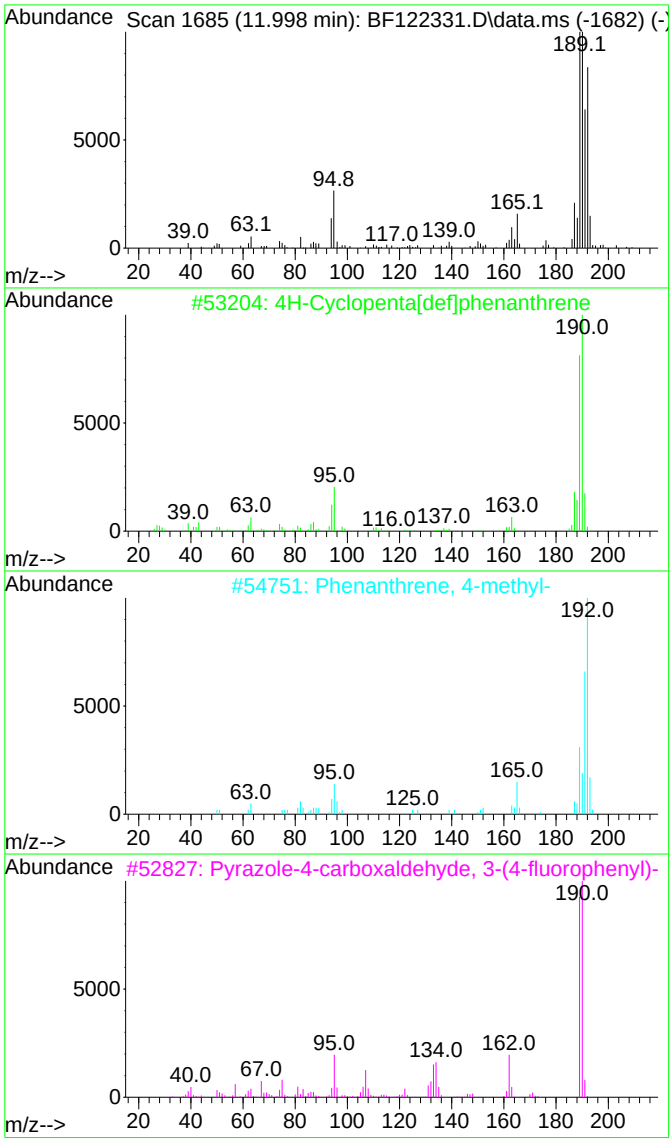
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

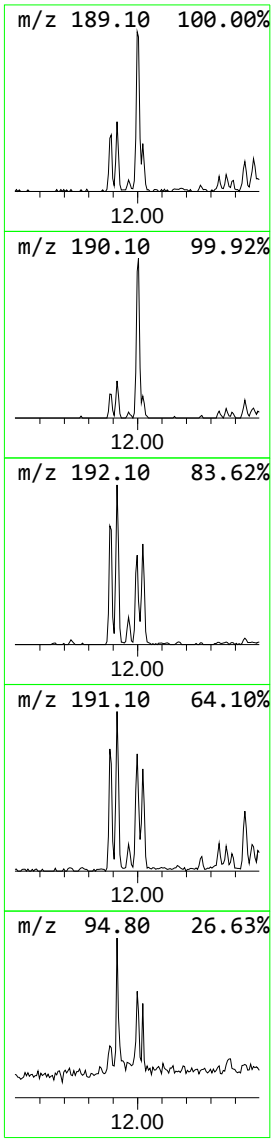
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.998	2.25 ng	238553	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	55
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	46
3	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	43
4	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	43
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111320\
Data File : BF122331.D
Acq On : 13 Nov 2020 16:10
Operator : JU/CG
Sample : L4723-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-59

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

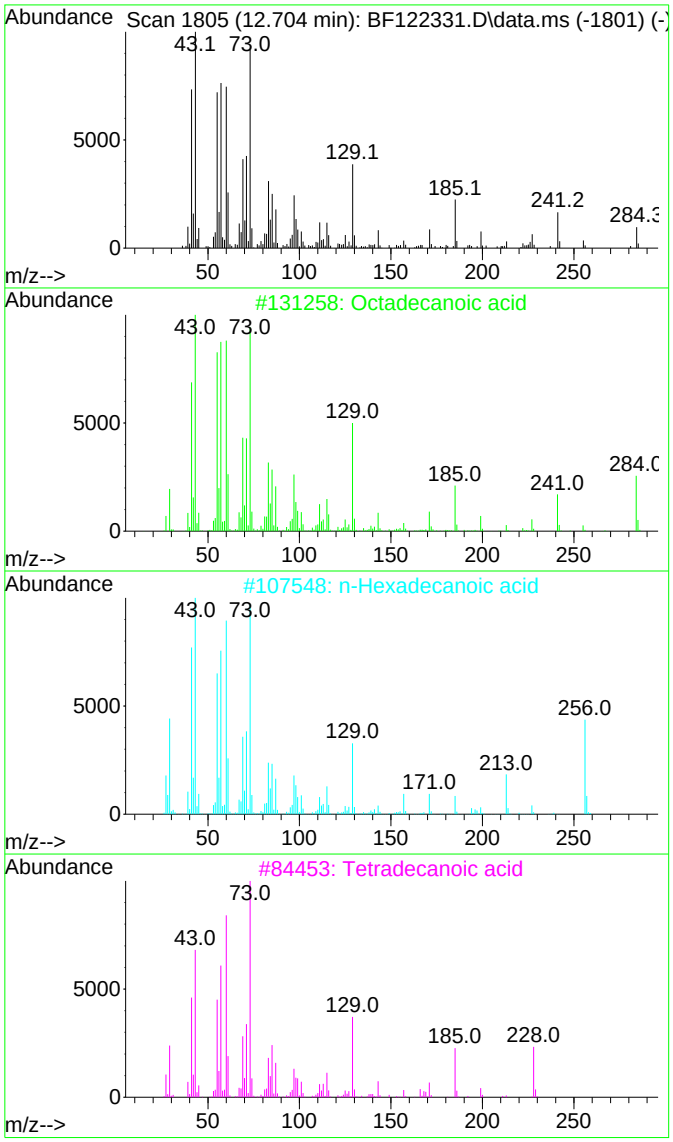
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

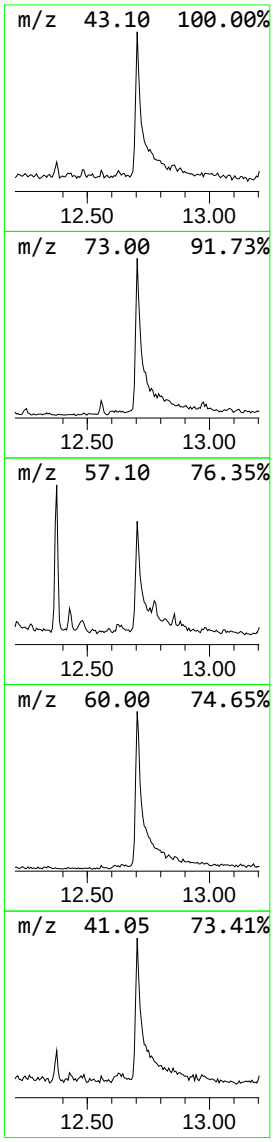
****

Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	6.26 ng	663084	Phenanthrene-d10	11.386

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	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111320\
Data File : BF122331.D
Acq On : 13 Nov 2020 16:10
Operator : JU/CG
Sample : L4723-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-59

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

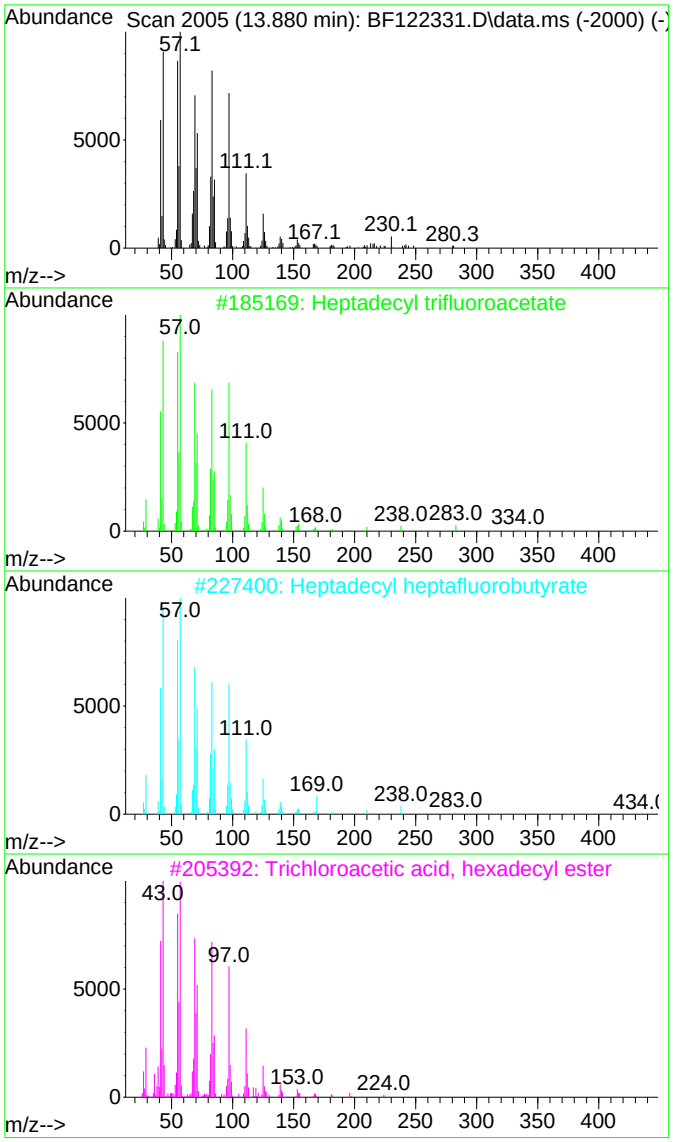
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

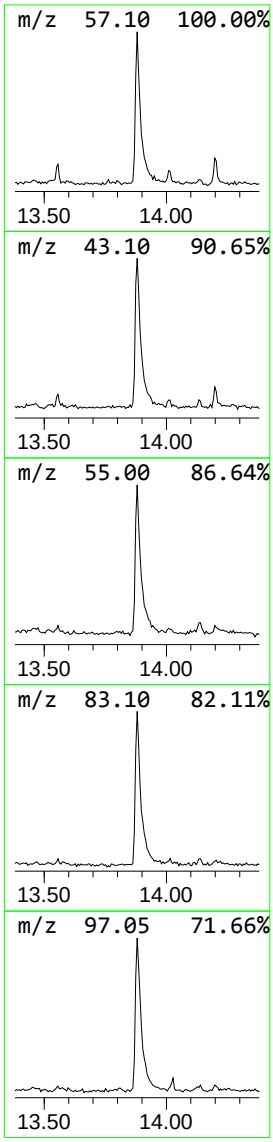
****

Peak Number 6 Heptadecyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	5.25 ng	679621	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111320\
Data File : BF122331.D
Acq On : 13 Nov 2020 16:10
Operator : JU/CG
Sample : L4723-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-59

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

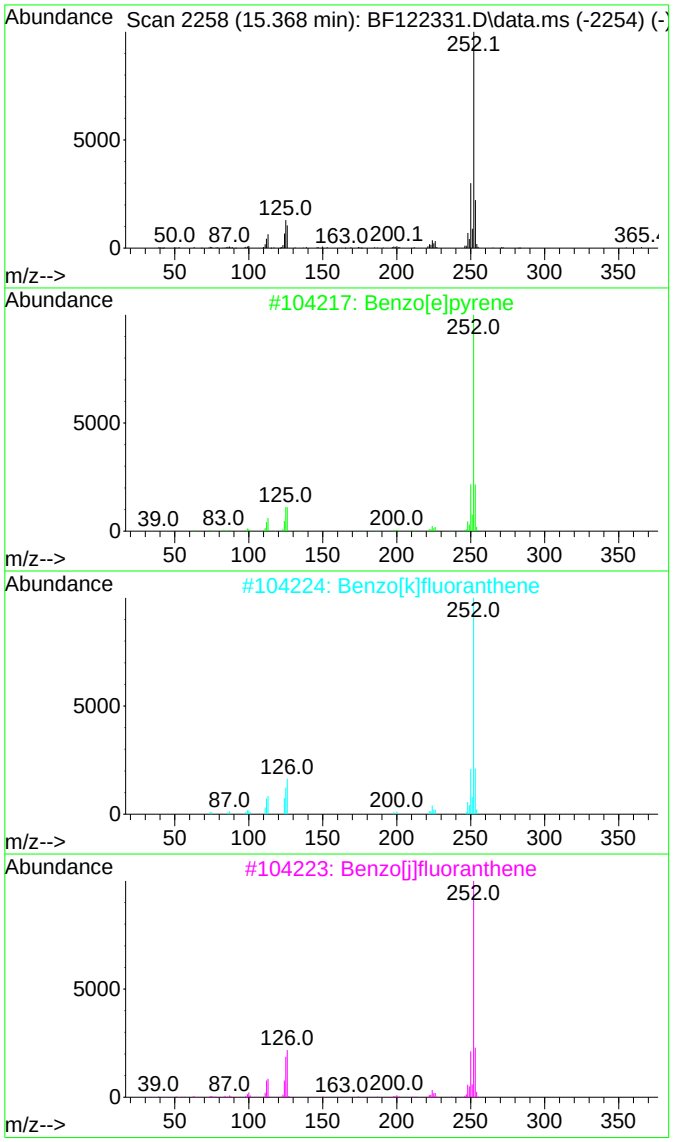
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

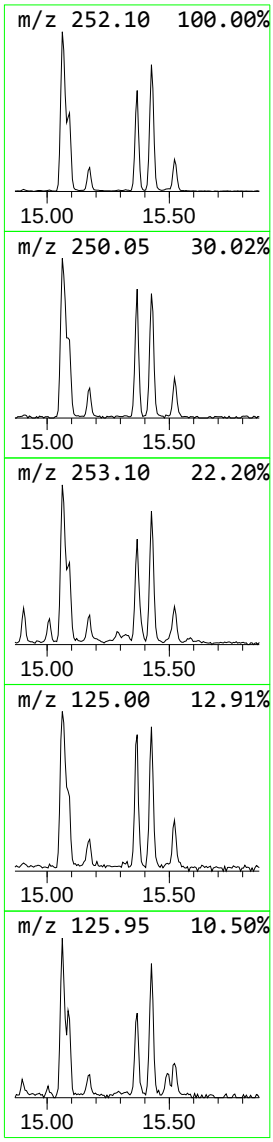
****

Peak Number 7 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.368	3.08 ng	299953	Perylene-d12	15.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	95
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
5	Perylene	252	C20H12	000198-55-0	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111320\
Data File : BF122331.D
Acq On : 13 Nov 2020 16:10
Operator : JU/CG
Sample : L4723-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-59

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...	2.116	12.4	ng	838089	1	6.863	1354210	20.0
n-Hexadecanoic ...	11.916	7.6	ng	808577	4	11.386	2118080	20.0
1,2-Benzenedica...	11.951	2.0	ng	214626	4	11.386	2118080	20.0
4H-Cyclopenta[d...	11.998	2.3	ng	238553	4	11.386	2118080	20.0
Octadecanoic acid	12.704	6.3	ng	663084	4	11.386	2118080	20.0
Heptadecyl trif...	13.880	5.3	ng	679621	5	14.027	2590350	20.0
Benzo[e]pyrene	15.368	3.1	ng	299953	6	15.492	1945720	20.0