

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF071719\
 Data File : BF115629.D
 Acq On : 17 Jul 2019 18:30
 Operator : HP/JU
 Sample : K3835-05
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DFTPP

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 1 % of largest Peak

Max Peaks: 100

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-BF071219.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	16	25	39	rVB	717674	1023777	21.36%	2.249%
2	3.446	228	231	245	rBV	27149	62578	1.31%	0.137%
3	4.005	322	326	332	rVB	52310	66084	1.38%	0.145%
4	5.516	577	583	586	rBV	3871663	4515494	94.20%	9.920%
5	6.516	746	753	756	rBV	4145975	4793763	100.00%	10.531%
6	6.657	771	777	780	rBV	4312922	4747126	99.03%	10.428%
7	6.881	811	815	819	rBV	1243136	1010045	21.07%	2.219%
8	7.040	837	842	845	rBV	3643421	3373661	70.38%	7.411%
9	7.440	904	910	913	rBV	2471100	2778136	57.95%	6.103%
10	8.163	1028	1033	1036	rBV	1399772	1252233	26.12%	2.751%
11	9.234	1210	1215	1219	rBV	4440309	4668507	97.39%	10.256%
12	9.351	1230	1235	1244	rVB	242850	241757	5.04%	0.531%
13	9.622	1277	1281	1285	rBV	1211220	1043321	21.76%	2.292%
14	9.916	1326	1331	1334	rBV	1490334	1432588	29.88%	3.147%
15	10.504	1428	1431	1440	rBV	36208	65435	1.37%	0.144%
16	10.704	1459	1465	1468	rBV	2854988	2981036	62.19%	6.549%
17	11.398	1578	1583	1585	rBV	1468206	1412736	29.47%	3.103%
18	11.416	1585	1586	1589	rVB	96018	61213	1.28%	0.134%
19	11.657	1623	1627	1631	rBV4	32951	57606	1.20%	0.127%
20	11.922	1668	1672	1683	rVB	866899	847113	17.67%	1.861%
21	12.463	1756	1764	1774	rBV4	211098	596405	12.44%	1.310%
22	12.604	1785	1788	1791	rBV	189606	157721	3.29%	0.346%
23	12.639	1791	1794	1796	rVV	95817	77515	1.62%	0.170%
24	12.704	1801	1805	1812	rBV2	371370	373309	7.79%	0.820%
25	12.833	1822	1827	1829	rBV	149160	138117	2.88%	0.303%
26	12.980	1847	1852	1855	rBV	4061950	3843913	80.19%	8.444%
27	13.210	1888	1891	1893	rBV	59998	64739	1.35%	0.142%
28	13.551	1946	1949	1958	rVB5	43175	76627	1.60%	0.168%
29	13.898	1999	2008	2023	rVV5	168117	450137	9.39%	0.989%
30	14.027	2024	2030	2033	rVV	1078307	1043773	21.77%	2.293%
31	14.051	2033	2034	2042	rVB	82585	69218	1.44%	0.152%
32	14.498	2106	2110	2114	rBV	89116	82034	1.71%	0.180%
33	14.545	2114	2118	2125	rBV8	42419	100104	2.09%	0.220%
34	14.804	2159	2162	2166	rVB	108378	100604	2.10%	0.221%

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Stop Thrs : 0 Peak Location: TOP

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35	15.063	2202	2206	2215	rBV	69716	146158	3.05%	0.321%
36	15.145	2215	2220	2223	rBV	122284	145119	3.03%	0.319%
37	15.368	2254	2258	2264	rVB	41043	55271	1.15%	0.121%
38	15.427	2264	2268	2274	rBV	50658	63677	1.33%	0.140%
39	15.492	2274	2279	2283	rBV	724803	940175	19.61%	2.065%
40	15.521	2283	2284	2291	rVB	135321	135031	2.82%	0.297%
41	15.957	2354	2358	2363	rVB	101161	147037	3.07%	0.323%
42	16.080	2372	2379	2381	rBV7	30251	65057	1.36%	0.143%
43	16.463	2439	2444	2449	rBV	59728	104177	2.17%	0.229%
44	16.951	2523	2527	2535	rVB3	25044	49437	1.03%	0.109%
45	17.063	2542	2546	2553	rVB2	33213	61308	1.28%	0.135%

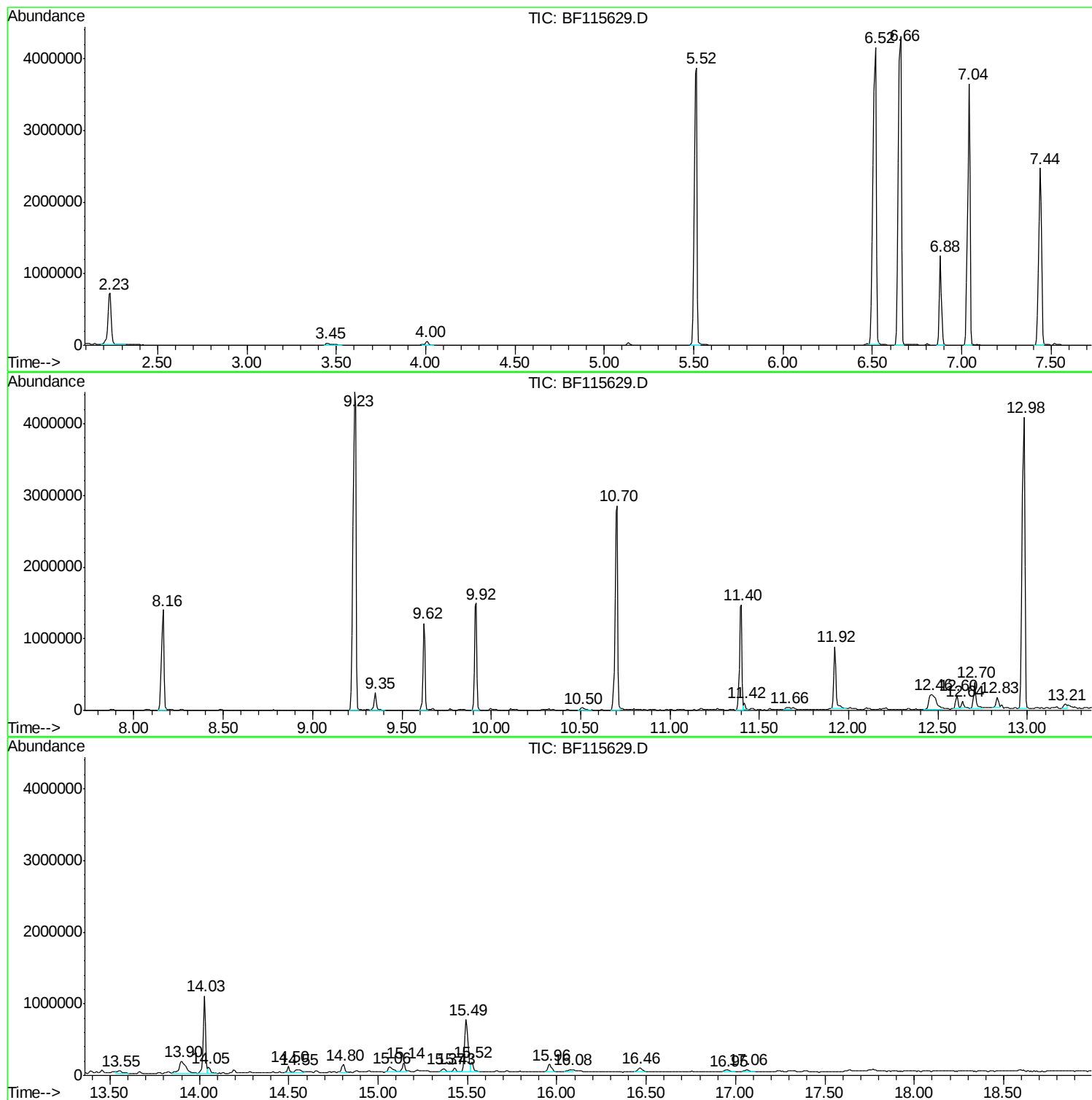
Sum of corrected areas: 45520872

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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 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.23	20.27 ng	1023780	1,4-Dichlorobenzene-d4	6.88	
Hit# of	5	Tentative ID	MW MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17

 Peak Number 2 1,3-Cyclopentanedione, 2-ch... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.66	94.00 ng	4747130	1,4-Dichlorobenzene-d4	6.88	
Hit# of	5	Tentative ID	MW MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	37
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Bicyclo[4.2.0]octa-1,3,5-triene, ...	132	C10H12	028749-81-7	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9

 Peak Number 3 1,4-Dichlorobenzene-D4 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
7.04	66.80 ng	3373660	1,4-Dichlorobenzene-d4	6.88		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dichlorobenzene-D4	150	C6D4Cl2	003855-82-1	95	
2	1,2-Dichlorobenzene-D4	150	C6D4Cl2	002199-69-1	94	
3	2-Chloro-4,6-difluoro-pyrimidine	150	C4HClF2N2	038953-30-9	50	
4	9-Borabicyclo[3.3.1]nonane, 9-et...	150	C10H19B	052102-17-7	22	
5	3-Amino-1,2,4-dithiazole-5-thione	150	C2H2N2S3	006846-35-1	17	

 Peak Number 4 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
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9.35	3.38 ng	241757	Acenaphthene-d10	9.91			
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	Acetamide, N-(2-hydroxyphenyl)-	151	C8H9NO2	000614-80-2	59		
3	Acetaminophen	151	C8H9NO2	000103-90-2	59		
4	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59		
5	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	59		

 Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.			
11.92	11.99 ng	847113	Phenanthrene-d10	11.40			
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99		
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91		
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87		
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80		
5	Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	18		

 Peak Number 6 n-Nonadecanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.		
12.46	8.44 ng	596405	Phenanthrene-d10		11.40		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1			284	C19H40O	001454-84-8	95
2	n-Heptadecanol-1			256	C17H36O	001454-85-9	95
3	1-Hexadecanol			242	C16H34O	036653-82-4	93
4	Cyclotridecane			182	C13H26	000295-02-3	92
5	9-Octadecene, (E)-			252	C18H36	007206-25-9	91

 Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD			R.T.	
12.70	5.28 ng	373309	Phenanthrene-d10			11.40	
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual

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1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	52

 Peak Number 8 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	8.63 ng	450137	Chrysene-d12	14.03

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			Behenic alcohol	326	C22H46O	000661-19-8	95
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	95
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94

 Peak Number 9 Heneicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	2.14 ng	100604	Perylene-d12	15.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Triacontane	422	C30H62	000638-68-6	91
3			2-methyloctacosane	408	C29H60	1000376-72-8	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	91

 Peak Number 10 Benz[e]acephenanthrylene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	3.11 ng	146158	Perylene-d12	15.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
2			Benzo[j]fluoranthene	252	C20H12	000205-82-3	94
3			Benzo[e]pyrene	252	C20H12	000192-97-2	93

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4 Benzo[k]fluoranthene	252 C20H12	000207-08-9 93
5 Benzo[a]pyrene	252 C20H12	000050-32-8 90

 Peak Number 11 Nonadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.15	3.09 ng	145119	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	93
2	Hexacosane	366	C26H54	000630-01-3	91
3	Octacosane	394	C28H58	000630-02-4	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	90
5	Heneicosane	296	C21H44	000629-94-7	90

 Peak Number 12 Hentriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	3.13 ng	147037	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	94
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Triacontane	422	C30H62	000638-68-6	91
5	Octadecane	254	C18H38	000593-45-3	91

 Peak Number 13 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.46	2.22 ng	104177	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Triacontane	422	C30H62	000638-68-6	91
5	Hexacosane	366	C26H54	000630-01-3	91

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.23	20.3	ng	1023780	1	6.88	1010050	20.0
1,3-Cyclopentaned...	6.66	94.0	ng	4747130	1	6.88	1010050	20.0
1,4-Dichlorobenze...	7.04	66.8	ng	3373660	1	6.88	1010050	20.0
2,4,7,9-Tetrameth...	9.35	3.4	ng	241757	3	9.91	1432590	20.0
n-Hexadecanoic acid	11.92	12.0	ng	847113	4	11.40	1412740	20.0
n-Nonadecanol-1	12.46	8.4	ng	596405	4	11.40	1412740	20.0
Octadecanoic acid	12.70	5.3	ng	373309	4	11.40	1412740	20.0
1-Heneicosanol	13.90	8.6	ng	450137	5	14.03	1043770	20.0
Heneicosane	14.80	2.1	ng	100604	6	15.49	940175	20.0
Benz[e]acephenant...	15.06	3.1	ng	146158	6	15.49	940175	20.0
Nonadecane	15.15	3.1	ng	145119	6	15.49	940175	20.0
Hentriacontane	15.96	3.1	ng	147037	6	15.49	940175	20.0
Heneicosane	16.46	2.2	ng	104177	6	15.49	940175	20.0