

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
 Data File : BF118337.D
 Acq On : 27 Dec 2019 14:53
 Operator : JU
 Sample : K6431-12
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :

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-BF122419.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	2.122	3	6	14	rVB	452721	549275	9.52%	1.078%
2	5.069	502	507	522	rVB	557673	764519	13.25%	1.500%
3	5.475	572	576	579	rBV	3900535	3696651	64.04%	7.254%
4	6.128	683	687	691	rVB	298582	239520	4.15%	0.470%
5	6.493	743	749	756	rBV	3853767	4054474	70.24%	7.957%
6	6.551	756	759	763	rVB	539419	444872	7.71%	0.873%
7	6.628	767	772	775	rBV	4629732	4305808	74.60%	8.450%
8	6.851	806	810	818	rBV	1111624	894357	15.49%	1.755%
9	7.010	832	837	840	rBV	3984887	3355598	58.14%	6.585%
10	7.416	901	906	909	rBV	2391303	2488810	43.12%	4.884%
11	8.139	1025	1029	1045	rBV	1250773	1185393	20.54%	2.326%
12	9.216	1207	1212	1215	rBV	5549834	5101005	88.37%	10.010%
13	9.551	1266	1269	1272	rBV	98385	73347	1.27%	0.144%
14	9.610	1275	1279	1284	rBV	459449	385092	6.67%	0.756%
15	9.898	1324	1328	1335	rVB	1655043	1436482	24.89%	2.819%
16	10.698	1459	1464	1467	rBV	4055595	3673222	63.64%	7.208%
17	11.392	1578	1582	1590	rBV	1792154	1551708	26.88%	3.045%
18	11.922	1667	1672	1684	rVB	690661	761811	13.20%	1.495%
19	12.475	1764	1766	1771	rBV	222640	201953	3.50%	0.396%
20	12.610	1786	1789	1799	rBV	149072	259085	4.49%	0.508%
21	12.704	1802	1805	1811	rBV	265756	332464	5.76%	0.652%
22	12.757	1811	1814	1819	rVB	59967	87874	1.52%	0.172%
23	12.845	1824	1829	1832	rVV2	131768	129439	2.24%	0.254%
24	12.986	1848	1853	1856	rBV	6021157	5772044	100.00%	11.327%
25	13.145	1877	1880	1883	rBV2	57667	60347	1.05%	0.118%
26	13.186	1883	1887	1889	rBV2	106592	111364	1.93%	0.219%
27	13.280	1900	1903	1908	rBV4	40859	58049	1.01%	0.114%
28	13.498	1938	1940	1945	rBV	263651	307512	5.33%	0.603%
29	13.551	1945	1949	1951	rVB2	122455	131167	2.27%	0.257%
30	13.745	1979	1982	1988	rBV2	175309	236664	4.10%	0.464%
31	13.874	2001	2004	2014	rVB	868348	954222	16.53%	1.873%
32	14.016	2025	2028	2029	rBV	96520	87423	1.51%	0.172%
33	14.045	2029	2033	2037	rVV	1344920	1328155	23.01%	2.606%
34	14.198	2055	2059	2067	rBV	301634	309162	5.36%	0.607%

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35	14.504	2107	2111	2120	rBV2	466307	551380	9.55%	1.082%
36	14.810	2157	2163	2167	rBV	431734	505099	8.75%	0.991%
37	14.886	2173	2176	2180	rVB	73673	76603	1.33%	0.150%
38	15.098	2209	2212	2217	rBV	57702	102931	1.78%	0.202%
39	15.157	2217	2222	2225	rBV	441178	499743	8.66%	0.981%
40	15.474	2273	2276	2281	rBV	50407	74209	1.29%	0.146%
41	15.539	2281	2287	2297	rVB	1279455	1678355	29.08%	3.294%
42	15.986	2357	2363	2367	rBV	304027	473725	8.21%	0.930%
43	16.039	2367	2372	2380	rVB2	174506	320319	5.55%	0.629%
44	16.415	2431	2436	2443	rBV4	147682	289077	5.01%	0.567%
45	16.498	2444	2450	2461	rVB3	170563	343859	5.96%	0.675%
46	17.045	2538	2543	2548	rBV5	35210	74477	1.29%	0.146%
47	17.098	2548	2552	2562	rVB4	57551	134902	2.34%	0.265%
48	17.192	2563	2568	2580	rVB4	65221	158734	2.75%	0.312%
49	17.615	2633	2640	2652	rVB8	101828	254959	4.42%	0.500%
50	18.656	2812	2817	2826	rVB9	36005	89954	1.56%	0.177%

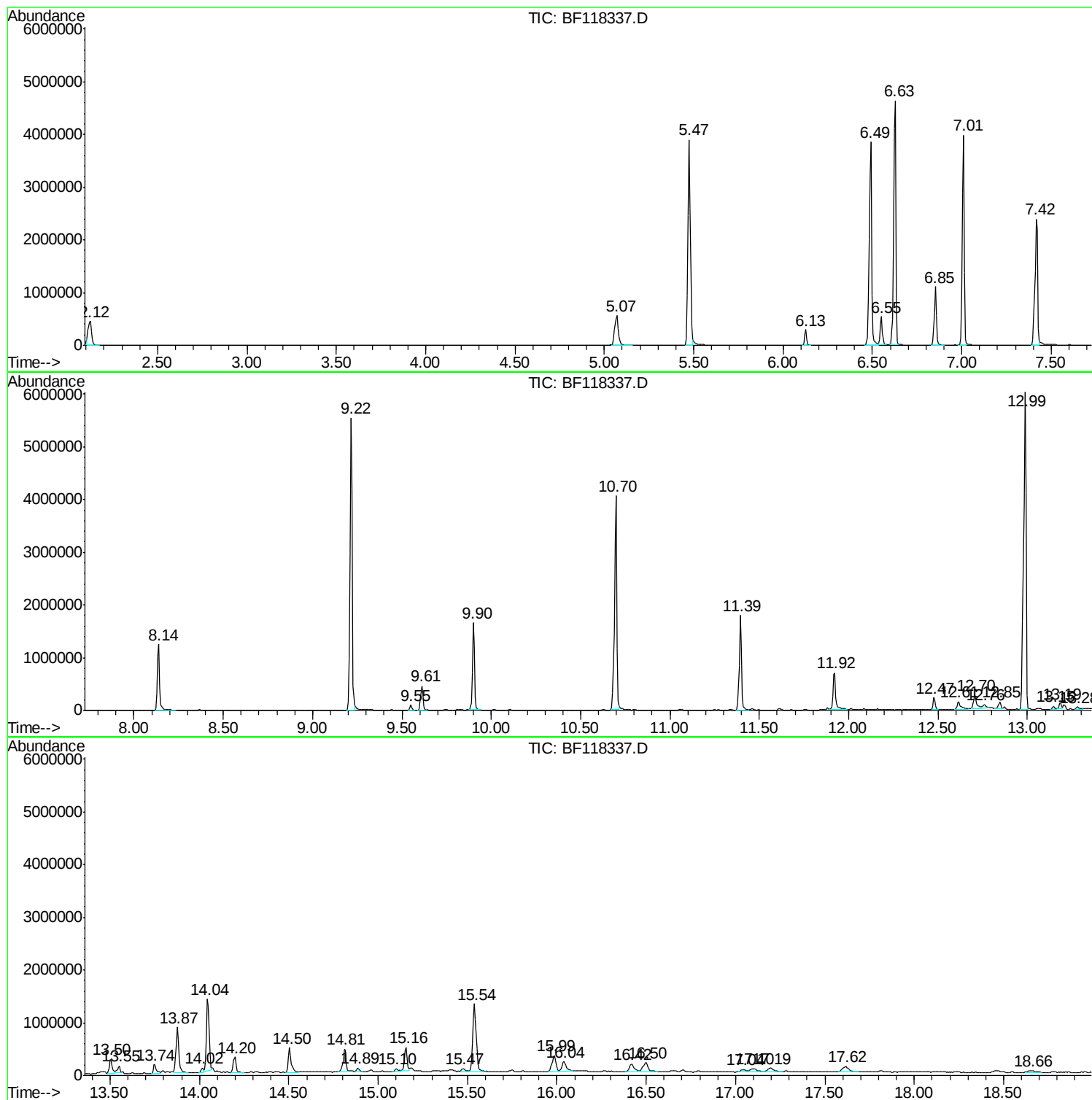
Sum of corrected areas: 50957194

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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 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.12	12.28 ng	549275	1,4-Dichlorobenzene-d4	6.85	
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	40
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.07	17.10 ng	764519	1,4-Dichlorobenzene-d4	6.85	
Hit# of	5	Tentative ID	MW MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Acetone	58	C3H6O	000067-64-1	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9

Peak Number 3 Bicyclo[3.1.1]hept-2-ene, 3... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.13	5.36 ng	239520	1,4-Dichlorobenzene-d4	6.85	
Hit# of	5	Tentative ID	MW MolForm	CAS#	Qual
1	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	94
2	.alpha.-Pinene	136	C10H16	000080-56-8	94
3	(+)-3-Carene	136	C10H16	000498-15-7	91
4	(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	91
5	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91

Peak Number 4 3-Chloro-6-fluoro-pyrazine Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
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6.63	96.29 ng	4305810	1,4-Dichlorobenzene-d4	6.85			
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4			Bicyclo[4.2.0]octa-1,3,5-triene, ...	132	C10H12	028749-81-7	9
5			2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9

 Peak Number 5 1,2-Dichlorobenzene-D4 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.			
7.01	75.04 ng	3355600	1,4-Dichlorobenzene-d4	6.85			
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Dichlorobenzene-D4	150	C6D4Cl2	002199-69-1	95
2			1,4-Dichlorobenzene-D4	150	C6D4Cl2	003855-82-1	95
3			2-Cyclohexene-1,4-dione, 5,6-dic...	370	C15H12Cl2N2O5	324051-46-9	27
4			9-Borabicyclo[3.3.1]nonane, 9-et...	150	C10H19B	052102-17-7	22
5			2,3,5-Tri-O-p-nitrobenzoyl-.alph...	606	C27H18N4O13	1000129-91-5	16

 Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.			
11.92	9.82 ng	761811	Phenanthrene-d10	11.39			
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	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5			Dodecanoic acid	200	C12H24O2	000143-07-7	53

 Peak Number 7 Fluoranthene Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD			R.T.	
12.61	3.34 ng	259085	Phenanthrene-d10			11.39	
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual

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1	Fluoranthene	202	C16H10	000206-44-0	97
2	Pyrene	202	C16H10	000129-00-0	90
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	76
4	1,4-Pentadiyn-3-one, 1,5-diphenyl-	230	C17H10O	015814-30-9	50
5	1H-Indole-3-propanoic acid, 1-(t...	275	C15H21NO2Si	056196-72-6	38

 Peak Number 8 Octadecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	4.29 ng	332464	Phenanthrene-d10	11.39

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	58
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	53
4		Undecanoic acid	186	C11H22O2	000112-37-8	25
5		Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	20

 Peak Number 9 Naphthalene, 1,1'-methylene... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	4.63 ng	307512	Chrysene-d12	14.05

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 1,1'-methylenebis[d...	288	C21H36	055125-02-5	46
2		cis, cis-2-Ethylbicyclo[4.4.0]de...	166	C12H22	066660-40-0	43
3		Naphthalene, 1-(1,1-dimethylethy...	194	C14H26	056292-64-9	43
4		Naphthalene, 2-butyldecahydro-	194	C14H26	006305-52-8	38
5		3-Iodomethyl-3,6,6-trimethyl-cyc...	264	C10H17I	1000193-08-2	35

 Peak Number 10 10,12-Tricosadiynoic acid, ... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	3.56 ng	236664	Chrysene-d12	14.05

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		10,12-Tricosadiynoic acid, methy...	360	C24H40O2	1000333-59-4	42
2		(Z,Z)-.alpha.-Farnesene	204	C15H24	1000293-03-1	25
3		Pimaric acid	302	C20H30O2	000127-27-5	25

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4 4-Methyl-benzoic acid (4-propyl-... 272 C17H24N20 1000275-81-2 22
 5 Bicyclo[3.1.1]hept-2-ene, 2,6-di... 204 C15H24 017699-05-7 18

 Peak Number 11 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.		
13.87	14.37 ng	954222	Chrysene-d12		14.05		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2			1-Heneicosanol	312	C21H44O	015594-90-8	93
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
5			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93

 Peak Number 12 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.		
14.20	4.66 ng	309162	Chrysene-d12		14.05		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	94
2			Hexacosane	366	C26H54	000630-01-3	91
3			2-methyloctacosane	408	C29H60	1000376-72-8	91
4			triacontane	422	C30H62	000638-68-6	91
5			Pentacosane	352	C25H52	000629-99-2	91

 Peak Number 13 Tricosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.50	8.30 ng	551380	Chrysene-d12		14.05
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	93
2	Hexadecane	226	C16H34	000544-76-3	91
3	Heptadecane	240	C17H36	000629-78-7	91
4	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	91
5	Tetracosane	338	C24H50	000646-31-1	91

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Peak Number 14 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	6.02 ng	505099	Perylene-d12	15.54
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	95
2	Hentriacontane	437 C31H64	000630-04-6	91
3	Tetracosane	338 C24H50	000646-31-1	91
4	2-methyloctacosane	408 C29H60	1000376-72-8	91
5	Heneicosane	296 C21H44	000629-94-7	91

Peak Number 15 Tetracosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	5.96 ng	499743	Perylene-d12	15.54
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Tetracosane	338 C24H50	000646-31-1	91
2	Heneicosane	296 C21H44	000629-94-7	91
3	triacontane	422 C30H62	000638-68-6	91
4	2-methyloctacosane	408 C29H60	1000376-72-8	91
5	Hexadecane, 1-iodo-	352 C16H33I	000544-77-4	91

Peak Number 16 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.99	5.65 ng	473725	Perylene-d12	15.54
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptadecane	240 C17H36	000629-78-7	93
2	Heneicosane	296 C21H44	000629-94-7	91
3	Hexacosane	366 C26H54	000630-01-3	91
4	triacontane	422 C30H62	000638-68-6	91
5	2-methyloctacosane	408 C29H60	1000376-72-8	91

Peak Number 17 Cyclohexane, 1,2-dimethyl-3... Concentration Rank 16

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16.04	3.82 ng	320319	Perylene-d12	15.54			
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	81
2			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	70
3			Octacosanol	410	C28H58O	000557-61-9	64
4			1-Heptacosanol	396	C27H56O	002004-39-9	60
5			Octacosyl acetate	452	C30H60O2	018206-97-8	53

 Peak Number 18 Cholesterol Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.42	3.44 ng	289077	Perylene-d12		15.54	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cholesterol	386	C27H46O	000057-88-5	99
2		26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	91
3		4-(cis-2,3,4,trans-6-Tetramethyl...	386	C20H26N4O4	1000243-17-5	35
4		1-Oxaspiro[4.4]nonane-4-carboxam...	273	C16H19N03	1000319-97-0	18
5		Methyl cholate	422	C25H42O5	001448-36-8	14

 Peak Number 19 Octadecane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD		R.T.		
16.50	4.10 ng	343859	Perylene-d12		15.54		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	93
2			Triacontane	422	C30H62	000638-68-6	91
3			Tetracosane	338	C24H50	000646-31-1	91
4			Hexacosane	366	C26H54	000630-01-3	91
5			Heneicosane	296	C21H44	000629-94-7	91

 Peak Number 20 .gamma.-Sitosterol Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD			R.T.
17.62	3.04 ng	254959	Perylene-d12			15.54
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF122719\
Data File : BF118337.D
Acq On : 27 Dec 2019 14:53
Operator : JU
Sample : K6431-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

1	.gamma.-Sitosterol	414	C29H500	000083-47-6	91
2	1-Methyl-1-n-octyloxy-1-silacycl...	228	C13H280Si	1000216-91-0	53
3	.beta.-Sitosterol	414	C29H500	000083-46-5	53
4	Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H500	000986-19-6	25
5	Cholest-7-en-3-ol, 4,4-dimethyl-...	414	C29H500	006384-28-7	11

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF122719\
 Data File : BF118337.D
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 BNA_F
 ClientSampleId :

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.12	12.3	ng	549275	1	6.85	894357	20.0
2-Pentanone, 4-hy...	5.07	17.1	ng	764519	1	6.85	894357	20.0
Bicyclo[3.1.1]hep...	6.13	5.4	ng	239520	1	6.85	894357	20.0
3-Chloro-6-fluoro...	6.63	96.3	ng	4305810	1	6.85	894357	20.0
1,2-Dichlorobenze...	7.01	75.0	ng	3355600	1	6.85	894357	20.0
n-Hexadecanoic acid	11.92	9.8	ng	761811	4	11.39	1551710	20.0
Fluoranthene	12.61	3.3	ng	259085	4	11.39	1551710	20.0
Octadecanoic acid	12.70	4.3	ng	332464	4	11.39	1551710	20.0
Naphthalene, 1,1'...	13.50	4.6	ng	307512	5	14.05	1328160	20.0
10,12-Tricosadiyn...	13.74	3.6	ng	236664	5	14.05	1328160	20.0
Heptadecyl heptaf...	13.87	14.4	ng	954222	5	14.05	1328160	20.0
Eicosane	14.20	4.7	ng	309162	5	14.05	1328160	20.0
Tricosane	14.50	8.3	ng	551380	5	14.05	1328160	20.0
Hexadecane	14.81	6.0	ng	505099	6	15.54	1678360	20.0
Tetracosane	15.16	6.0	ng	499743	6	15.54	1678360	20.0
Heptadecane	15.99	5.6	ng	473725	6	15.54	1678360	20.0
Cyclohexane, 1,2-...	16.04	3.8	ng	320319	6	15.54	1678360	20.0
Cholesterol	16.42	3.4	ng	289077	6	15.54	1678360	20.0
Octadecane	16.50	4.1	ng	343859	6	15.54	1678360	20.0
.gamma.-Sitosterol	17.62	3.0	ng	254959	6	15.54	1678360	20.0