

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102819\
 Data File : BF117563.D
 Acq On : 28 Oct 2019 16:04
 Operator : JU
 Sample : K5501-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 187-88-(0-2)

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % 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-BF101819.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	5.351	552	555	579	rBV	651755	820863	81.06%	7.948%
2	6.381	726	730	747	rBV	831082	932648	92.10%	9.030%
3	6.504	747	751	769	rVB	938055	973801	96.17%	9.429%
4	6.728	785	789	799	rBV	224109	229789	22.69%	2.225%
5	6.881	811	815	826	rBV	786453	708210	69.94%	6.857%
6	7.292	881	885	913	rBV	523082	577886	57.07%	5.595%
7	8.010	1003	1007	1033	rBV	251707	300696	29.69%	2.911%
8	9.081	1185	1189	1202	rBV	1157865	1012631	100.00%	9.805%
9	9.481	1254	1257	1267	rBV	97696	96845	9.56%	0.938%
10	9.757	1301	1304	1308	rBV	367870	333164	32.90%	3.226%
11	9.792	1308	1310	1318	rVB2	20403	22460	2.22%	0.217%
12	10.551	1436	1439	1456	rBV	542153	561440	55.44%	5.436%
13	11.245	1554	1557	1559	rBV	367669	310048	30.62%	3.002%
14	11.269	1559	1561	1567	rVV	168647	169670	16.76%	1.643%
15	11.327	1567	1571	1578	rVB	30293	38181	3.77%	0.370%
16	11.492	1594	1599	1604	rBV3	14796	23272	2.30%	0.225%
17	11.775	1645	1647	1655	rVB2	61225	67189	6.64%	0.651%
18	11.863	1659	1662	1665	rBV	26080	25924	2.56%	0.251%
19	12.463	1760	1764	1773	rBV	265403	251815	24.87%	2.438%
20	12.692	1796	1803	1810	rBV	226583	264232	26.09%	2.558%
21	12.827	1822	1826	1829	rBV	992974	828683	81.83%	8.024%
22	12.910	1836	1840	1845	rVB3	8877	13935	1.38%	0.135%
23	13.021	1851	1859	1862	rBV	24722	37909	3.74%	0.367%
24	13.086	1868	1870	1873	rBV	19856	18334	1.81%	0.178%
25	13.127	1873	1877	1884	rVB4	14114	23656	2.34%	0.229%
26	13.645	1963	1965	1967	rBV2	9278	11059	1.09%	0.107%
27	13.727	1975	1979	1989	rVB4	84742	147497	14.57%	1.428%
28	13.892	1998	2007	2010	rBV2	257598	362917	35.84%	3.514%
29	13.916	2010	2011	2018	rVV	89064	80295	7.93%	0.777%
30	13.998	2020	2025	2030	rVB	26423	26932	2.66%	0.261%
31	14.286	2069	2074	2077	rBV2	18086	20305	2.01%	0.197%
32	14.645	2133	2135	2139	rVB4	17199	14832	1.46%	0.144%
33	14.716	2143	2147	2151	rVB	238423	211793	20.92%	2.051%
34	14.921	2179	2182	2185	rBV	91353	119955	11.85%	1.161%

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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

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35	14.951	2185	2187	2193	rVB3	46036	71565	7.07%	0.693%
36	15.033	2198	2201	2204	rVB	18301	21570	2.13%	0.209%
37	15.215	2227	2232	2235	rBV	49357	57230	5.65%	0.554%
38	15.274	2239	2242	2246	rBV	81285	89848	8.87%	0.870%
39	15.327	2246	2251	2256	rBV	168183	223662	22.09%	2.166%
40	15.551	2287	2289	2295	rVB6	7153	13602	1.34%	0.132%
41	15.721	2314	2318	2322	rVB3	16610	23689	2.34%	0.229%
42	15.804	2328	2332	2342	rVB3	12238	31267	3.09%	0.303%
43	16.745	2485	2492	2500	rBV2	40757	89754	8.86%	0.869%
44	17.180	2560	2566	2576	rVB2	30097	66873	6.60%	0.647%

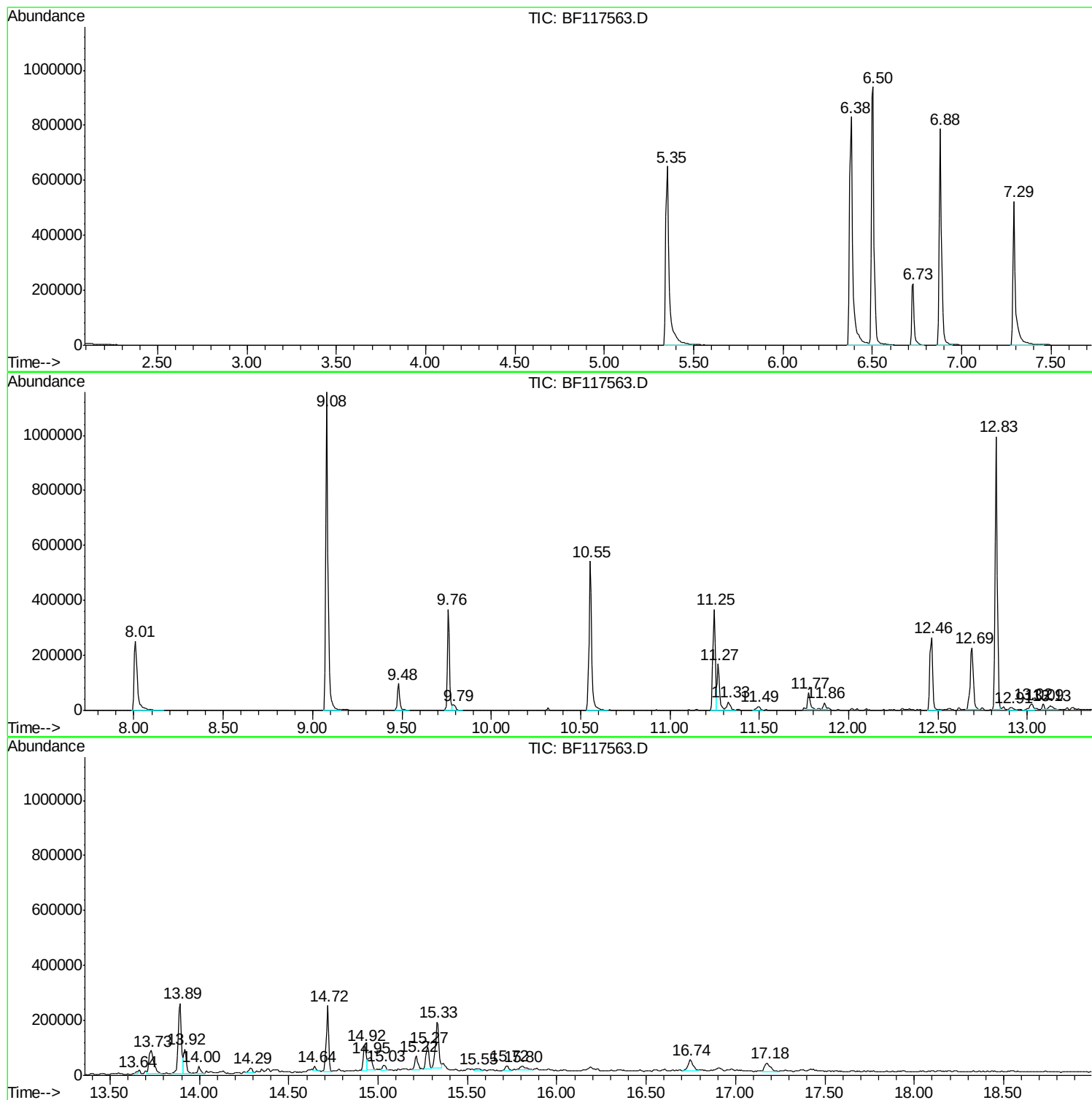
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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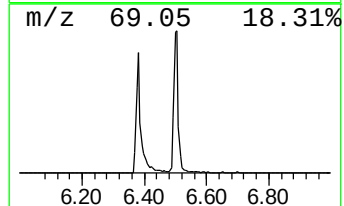
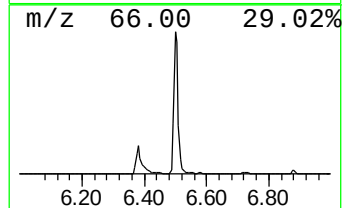
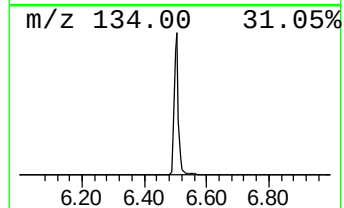
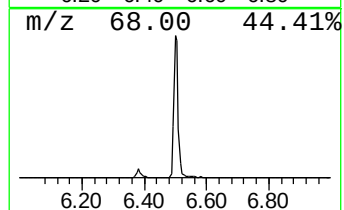
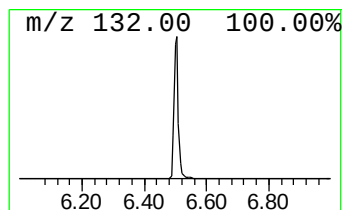
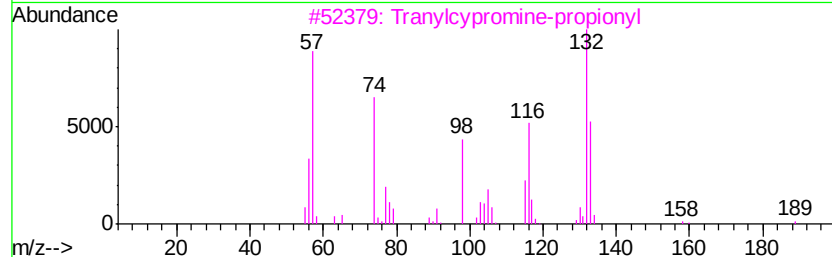
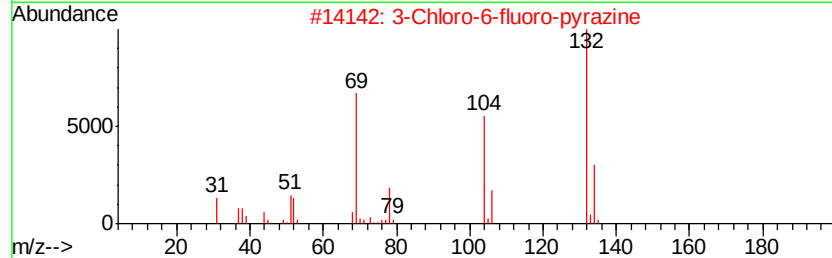
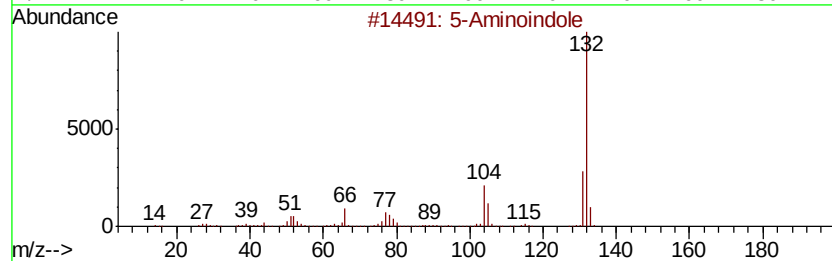
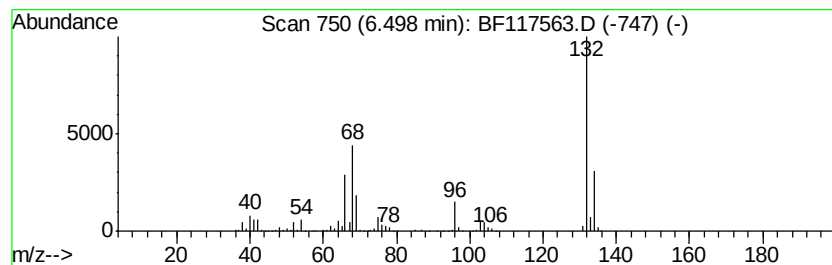
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	84.76 ng	973801	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	22
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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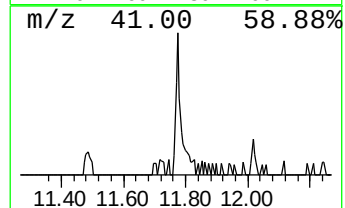
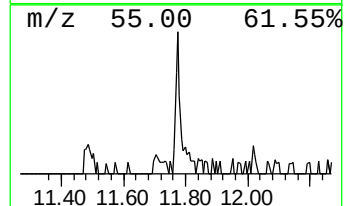
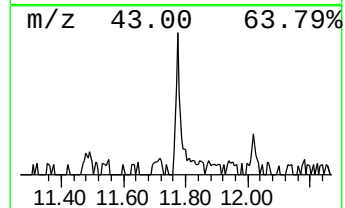
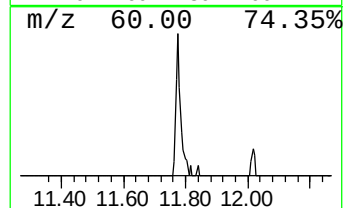
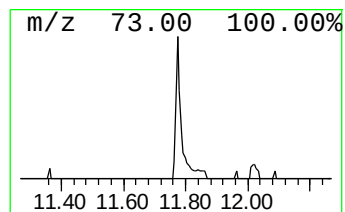
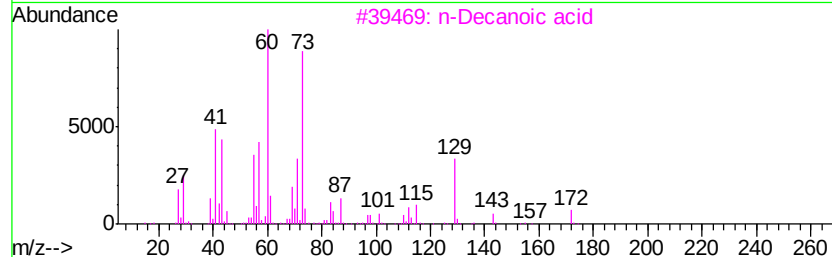
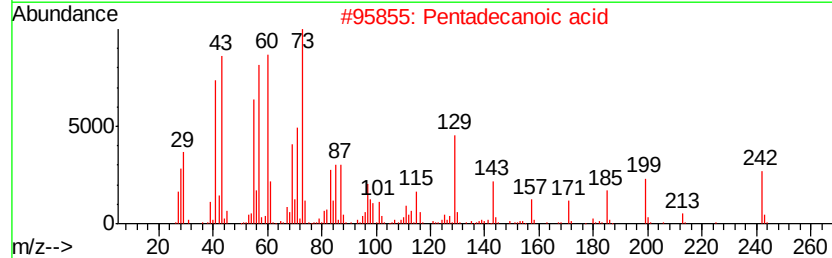
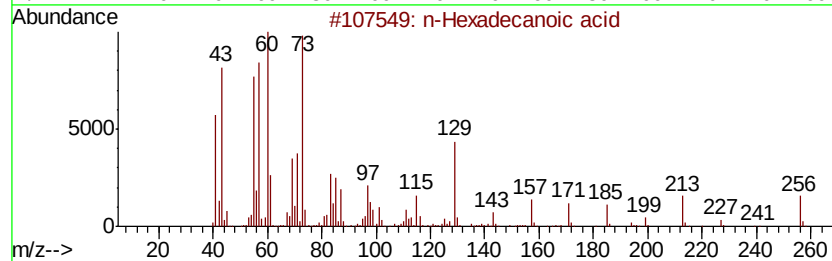
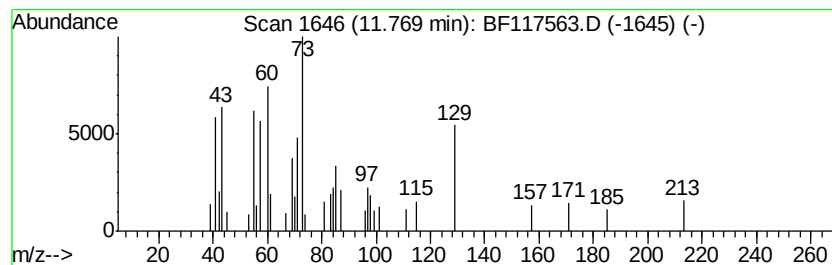
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	4.33 ng	67189	Phenanthrene-d10	11.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3		n-Decanoic acid	172	C10H20O2	000334-48-5	59
4		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	59
5		Sedoheptulosan	192	C7H12O6	000469-90-9	22



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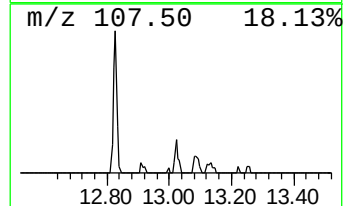
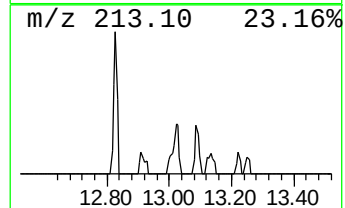
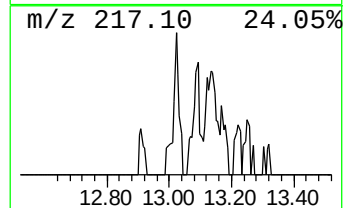
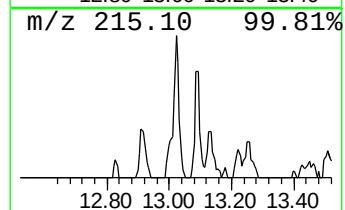
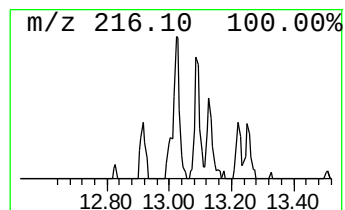
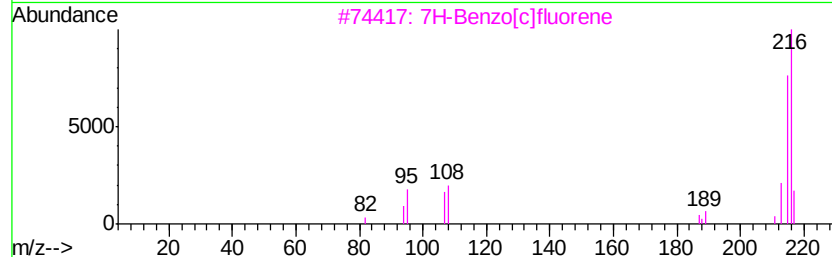
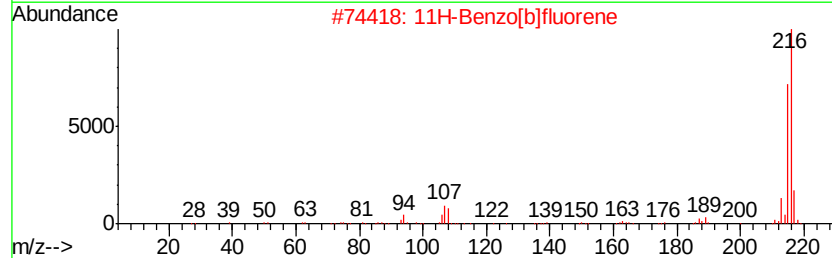
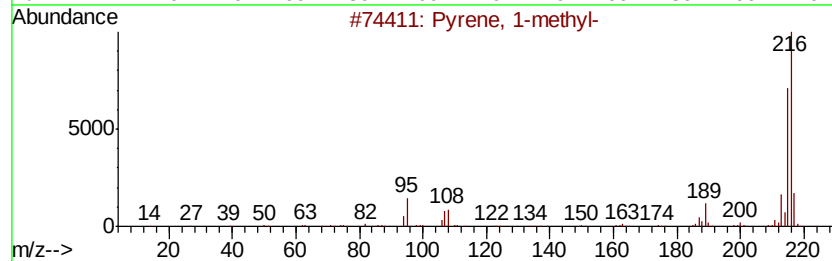
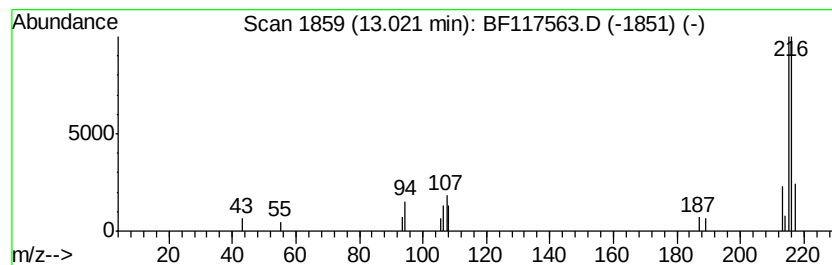
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pyrene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.02	2.09 ng	37909	Chrysene-d12	13.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrene, 1-methyl-	216	C17H12	002381-21-7	86
2		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	86
3		7H-Benzo[c]fluorene	216	C17H12	000205-12-9	72
4		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	64
5		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	64



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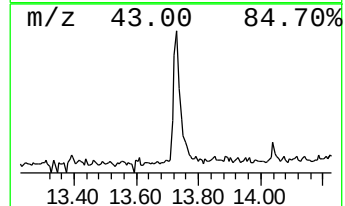
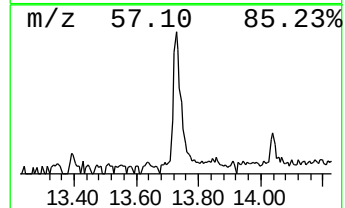
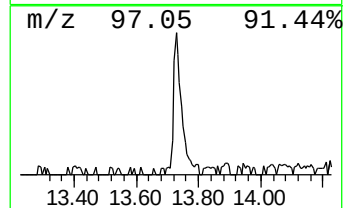
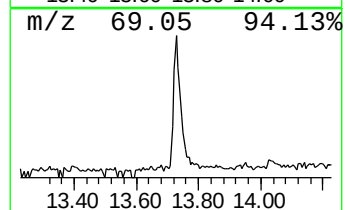
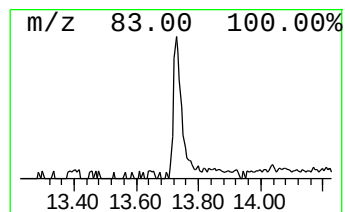
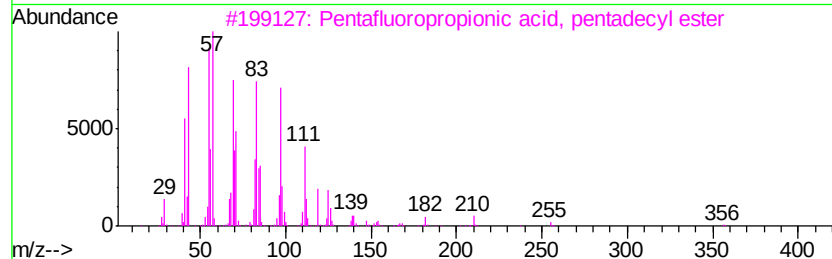
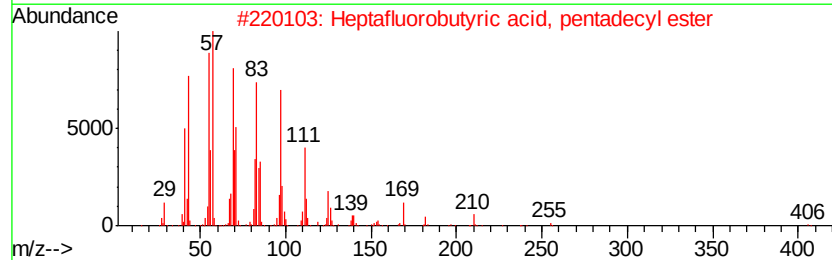
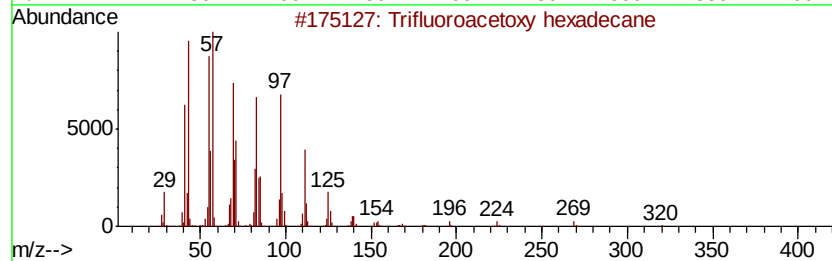
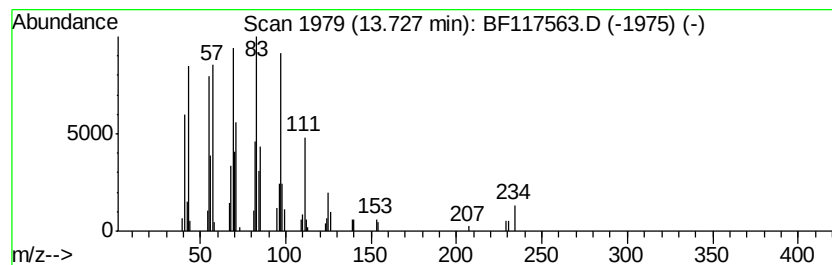
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	8.13 ng	147497	Chrysene-d12	13.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
2		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
3		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5		1-Heneicosanol	312	C21H44O	015594-90-8	90



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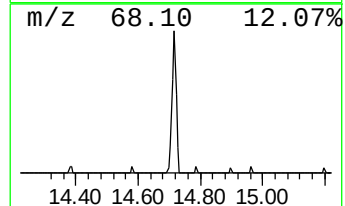
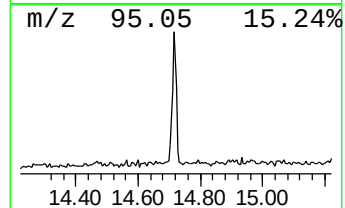
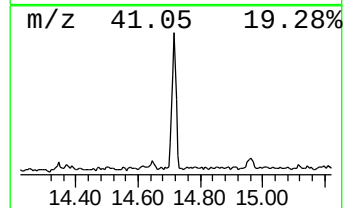
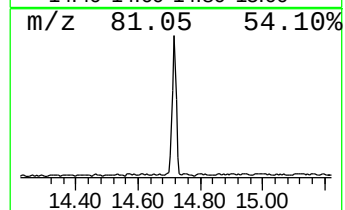
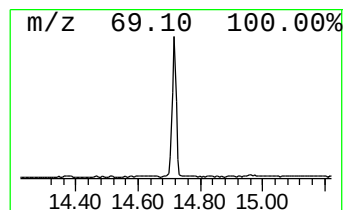
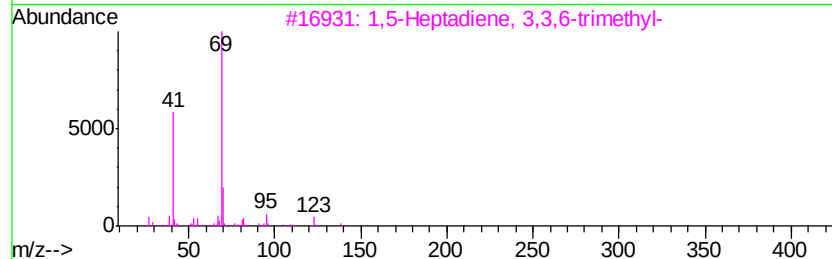
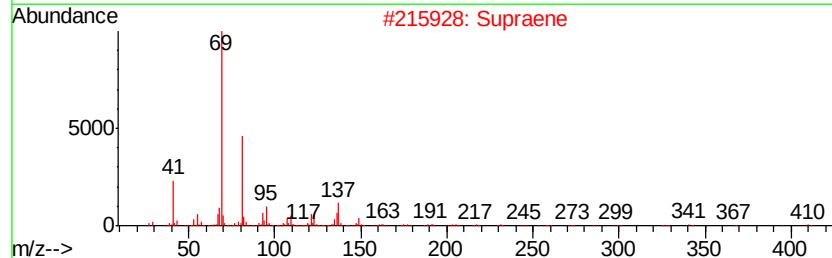
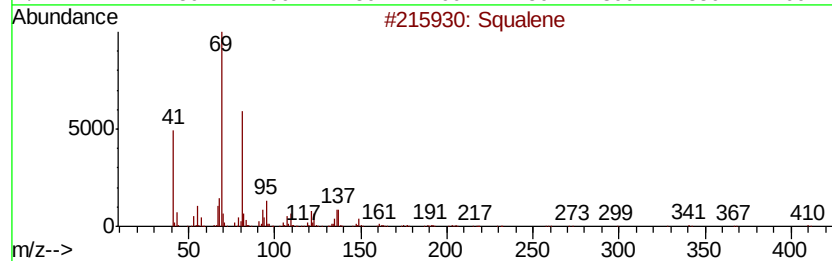
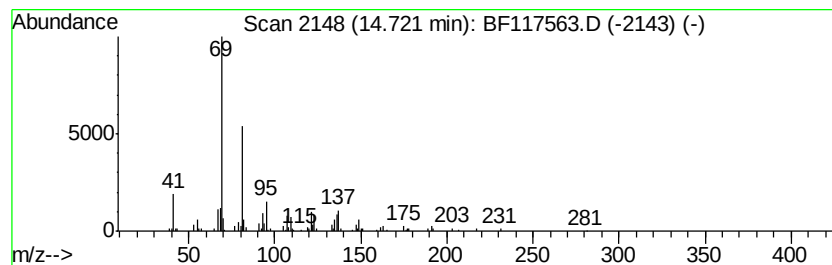
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

Peak Number 6 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	18.94 ng	211793	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	53
4		2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	53
5		1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102819\
Data File : BF117563.D
Acq On : 28 Oct 2019 16:04
Operator : JU
Sample : K5501-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
187-88-(0-2)

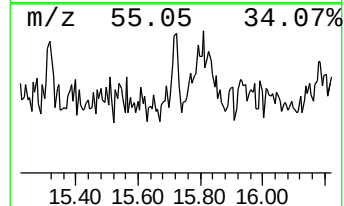
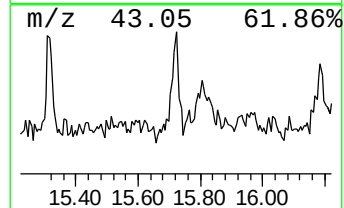
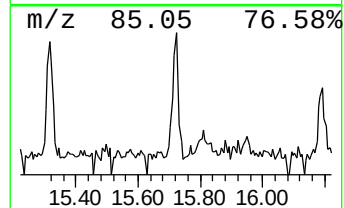
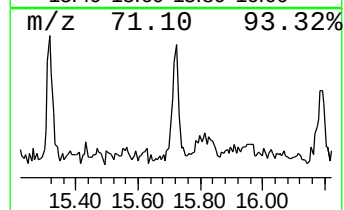
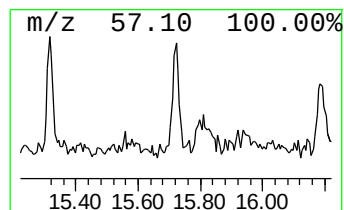
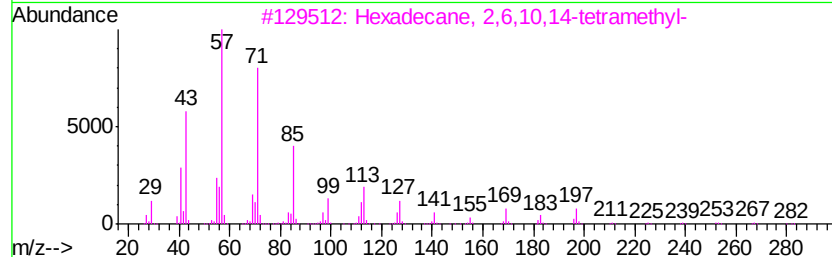
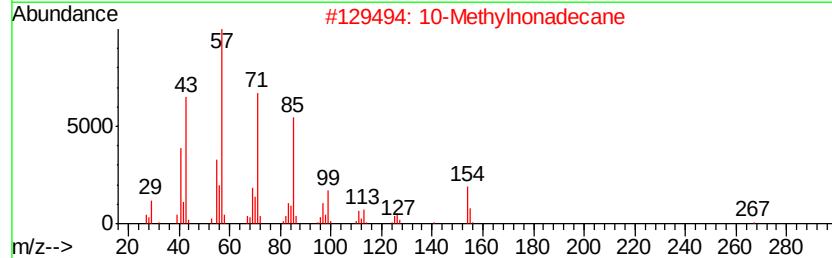
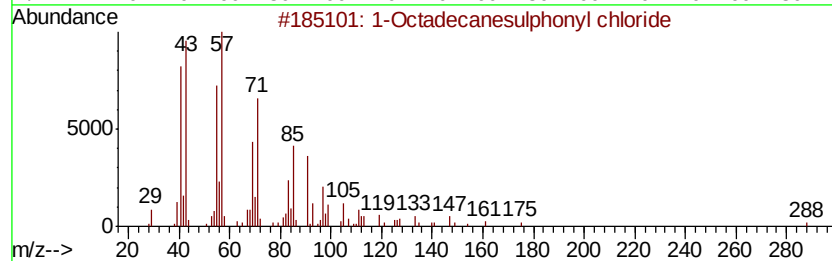
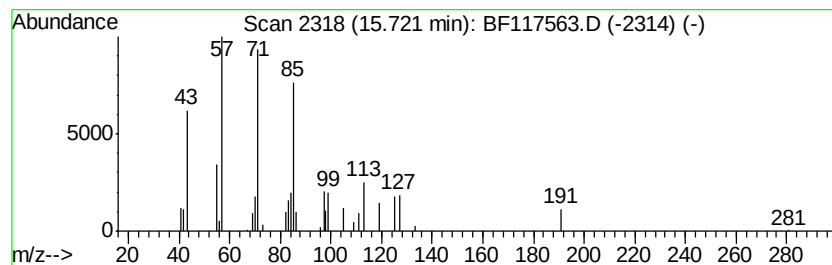
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Octadecanesulphonyl chloride Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	2.12 ng	23689	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	59
2		10-Methylnonadecane	282	C20H42	056862-62-5	59
3		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	59
4		Decane, 2,4,6-trimethyl-	184	C13H28	062108-27-4	53
5		Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102819\
Data File : BF117563.D
Acq On : 28 Oct 2019 16:04
Operator : JU
Sample : K5501-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

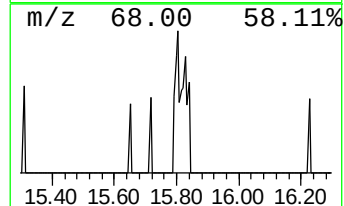
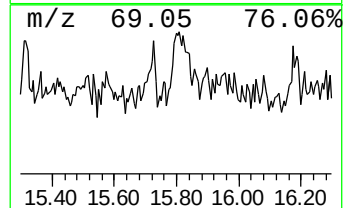
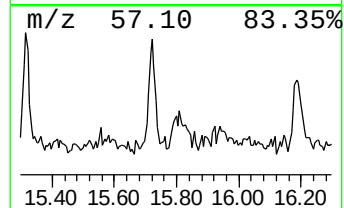
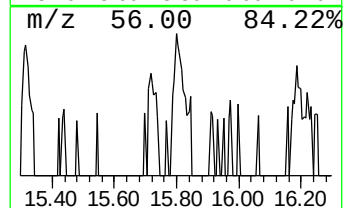
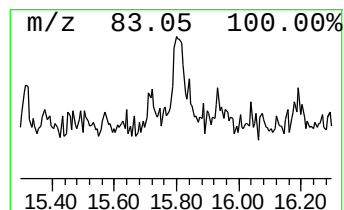
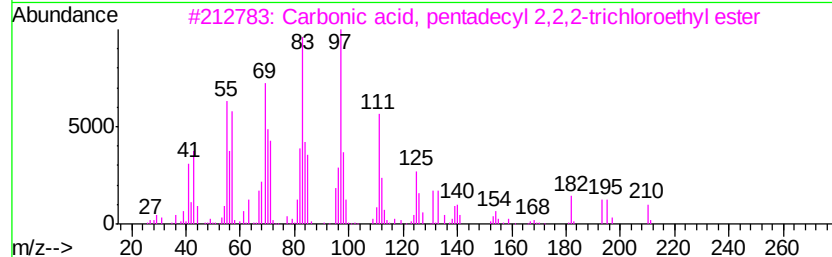
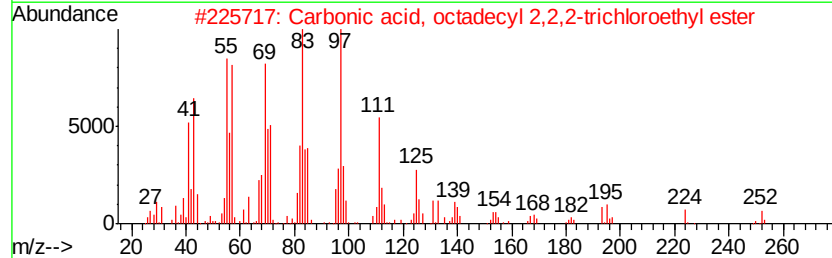
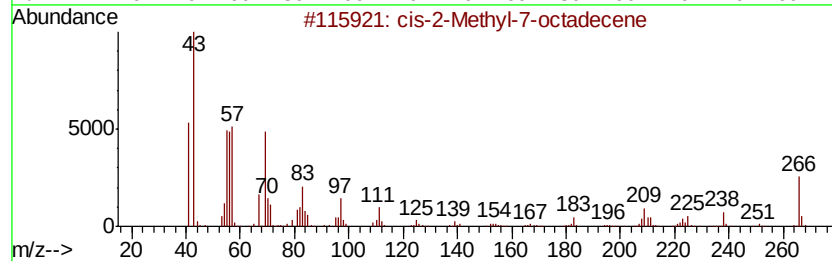
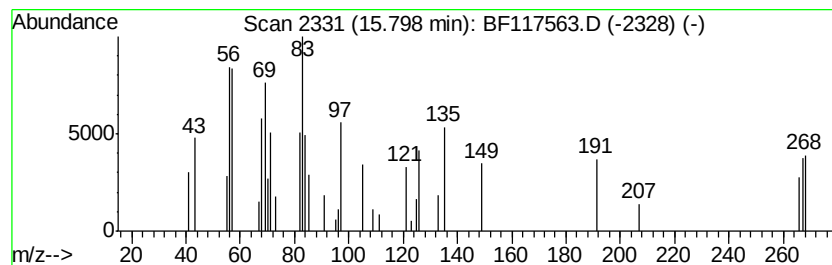
Instrument :
BNA_F
ClientSampleId :
187-88-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown15.80 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.80	2.80 ng	31267	Perylene-d12	15.33
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		cis-2-Methyl-7-octadecene	266 C19H38	035354-39-3 16
2		Carbonic acid, octadecyl 2,2,2-t...	444 C21H39Cl303	1000314-56-3 14
3		Carbonic acid, pentadecyl 2,2,2-...	402 C18H33Cl303	1000314-56-1 14
4		4-Methyl-2,3-hexadien-1-ol	112 C7H12O	1000196-09-6 14
5		Cetene	224 C16H32	000629-73-2 14



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102819\
Data File : BF117563.D
Acq On : 28 Oct 2019 16:04
Operator : JU
Sample : K5501-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
187-88-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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
unknown6.50	6.50	84.8	ng	973801	1	6.73	229789	20.0
n-Hexadecanoic acid	11.77	4.3	ng	67189	4	11.25	310048	20.0
Pyrene, 1-methyl-	13.02	2.1	ng	37909	5	13.89	362917	20.0
Trifluoroacetoxy ...	13.73	8.1	ng	147497	5	13.89	362917	20.0
Squalene	14.72	18.9	ng	211793	6	15.33	223662	20.0
1-Octadecanesulph...	15.72	2.1	ng	23689	6	15.33	223662	20.0
unknown15.80	15.80	2.8	ng	31267	6	15.33	223662	20.0