

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102519\
 Data File : BF117544.D
 Acq On : 25 Oct 2019 18:53
 Operator : JU
 Sample : K5500-09
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 800-50-(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	5.357	553	556	576	rBV	677504	779465	91.40%	10.384%
2	6.387	727	731	748	rBV	746001	837596	98.22%	11.158%
3	6.504	748	751	758	rVV	857586	852801	100.00%	11.360%
4	6.728	786	789	800	rBV	223569	206276	24.19%	2.748%
5	6.887	812	816	829	rBV	691247	611494	71.70%	8.146%
6	7.292	882	885	900	rBV	442678	480739	56.37%	6.404%
7	8.010	1004	1007	1028	rBV	258140	247831	29.06%	3.301%
8	9.081	1186	1189	1199	rBV	774299	702651	82.39%	9.360%
9	9.416	1243	1246	1249	rBV	13056	11358	1.33%	0.151%
10	9.481	1252	1257	1265	rVV	109554	98698	11.57%	1.315%
11	9.763	1301	1305	1313	rVB	291102	251131	29.45%	3.345%
12	10.557	1436	1440	1450	rBV	397473	398647	46.75%	5.311%
13	10.675	1454	1460	1466	rVB6	6317	11136	1.31%	0.148%
14	11.251	1554	1558	1560	rBV	221493	215626	25.28%	2.872%
15	11.269	1560	1561	1565	rVB	26755	23912	2.80%	0.319%
16	11.492	1594	1599	1601	rBV6	7542	10179	1.19%	0.136%
17	11.775	1644	1647	1655	rVB2	53702	61684	7.23%	0.822%
18	11.863	1659	1662	1664	rBV3	8975	8631	1.01%	0.115%
19	12.298	1733	1736	1740	rBV4	8149	11984	1.41%	0.160%
20	12.333	1740	1742	1744	rVB2	12969	10238	1.20%	0.136%
21	12.463	1761	1764	1767	rBV	60411	57921	6.79%	0.772%
22	12.492	1767	1769	1773	rVV4	15607	19792	2.32%	0.264%
23	12.563	1776	1781	1785	rBV5	22622	34592	4.06%	0.461%
24	12.616	1787	1790	1793	rBV5	11987	12487	1.46%	0.166%
25	12.692	1798	1803	1807	rBV	54368	69348	8.13%	0.924%
26	12.827	1822	1826	1833	rVB	666596	609109	71.42%	8.114%
27	13.057	1863	1865	1869	rBV4	15343	19588	2.30%	0.261%
28	13.257	1895	1899	1902	rBV2	73849	83483	9.79%	1.112%
29	13.292	1902	1905	1911	rVV4	44940	62645	7.35%	0.835%
30	13.404	1921	1924	1928	rBV5	17235	25940	3.04%	0.346%
31	13.627	1960	1962	1963	rBV2	15421	10206	1.20%	0.136%
32	13.733	1977	1980	1988	rVB2	83343	146595	17.19%	1.953%
33	13.863	1999	2002	2004	rBV	71365	69207	8.12%	0.922%
34	13.892	2004	2007	2010	rBV	239812	239627	28.10%	3.192%

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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	15.333	2248	2252	2256	rVB2	149498	214118	25.11%	2.852%
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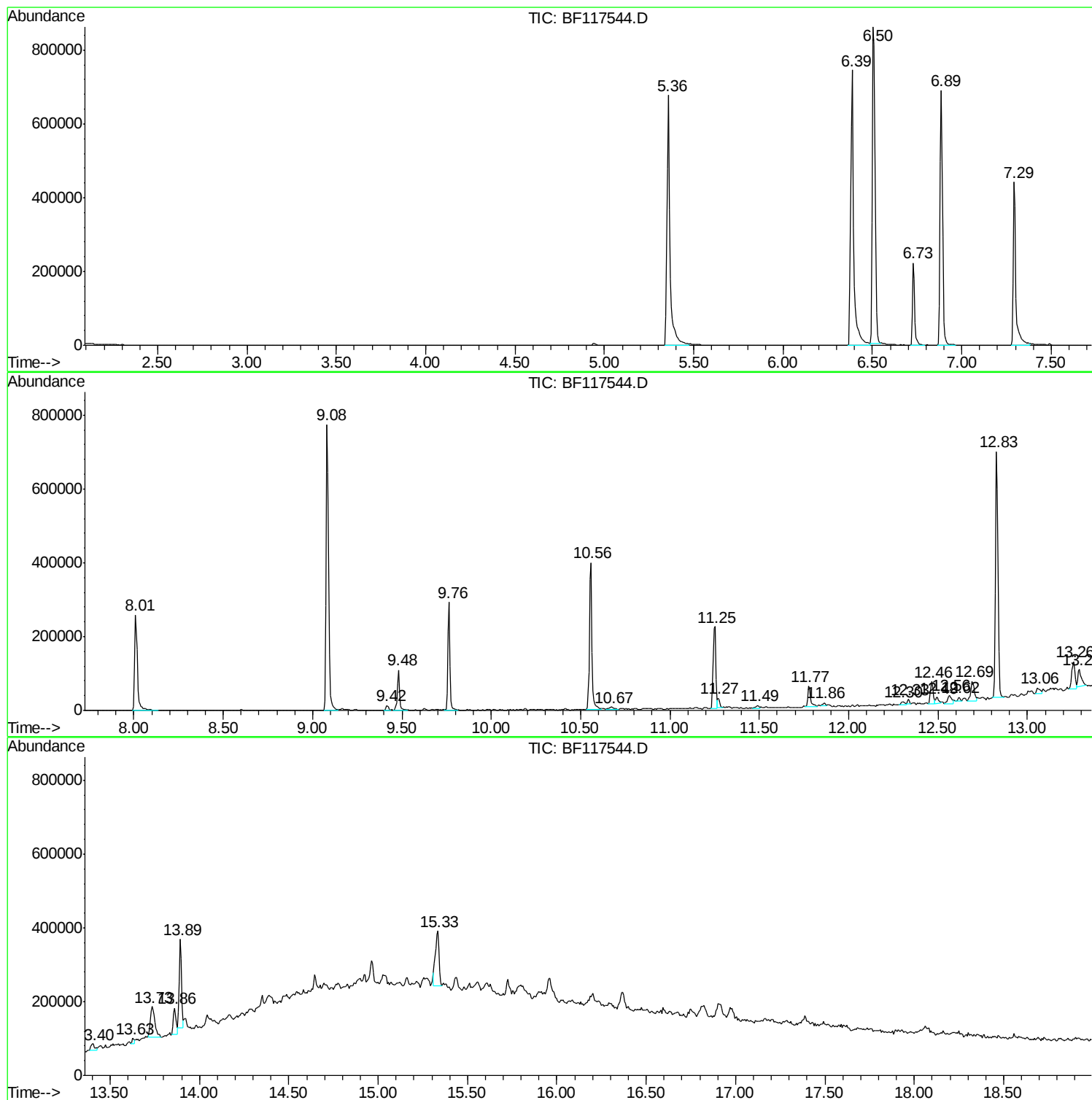
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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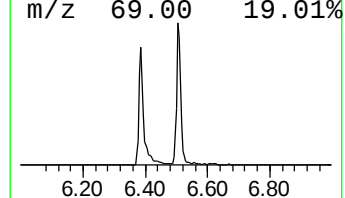
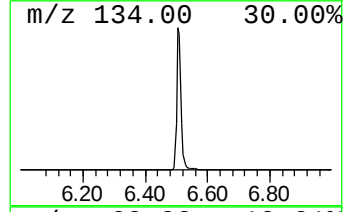
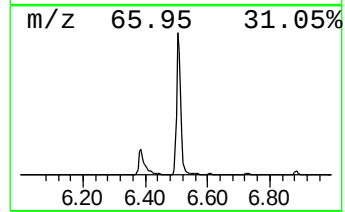
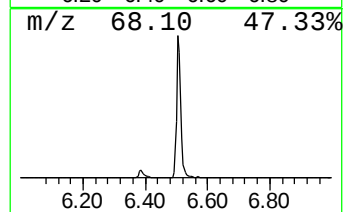
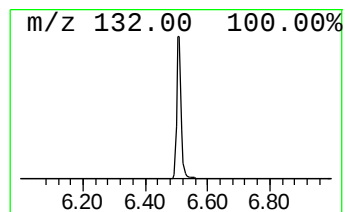
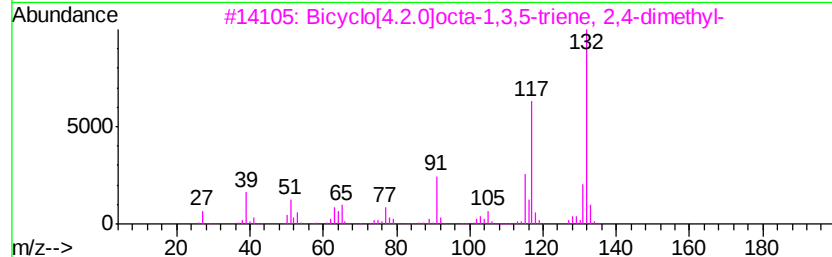
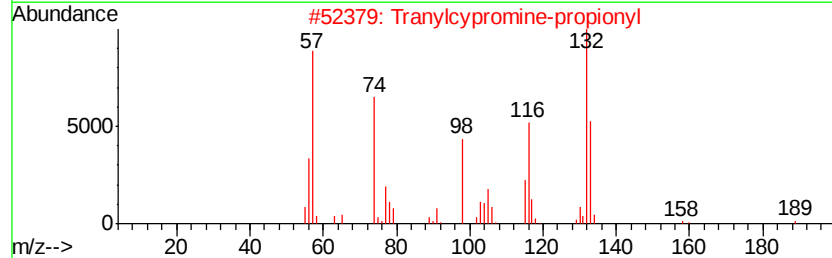
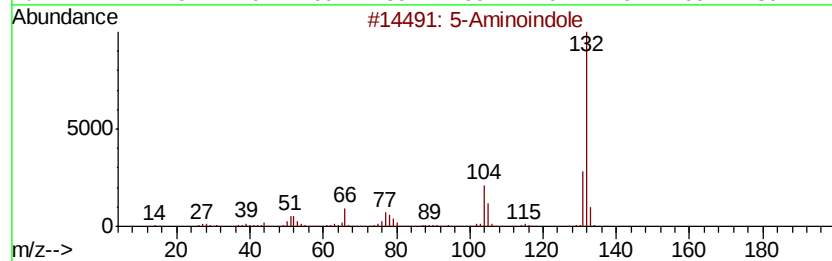
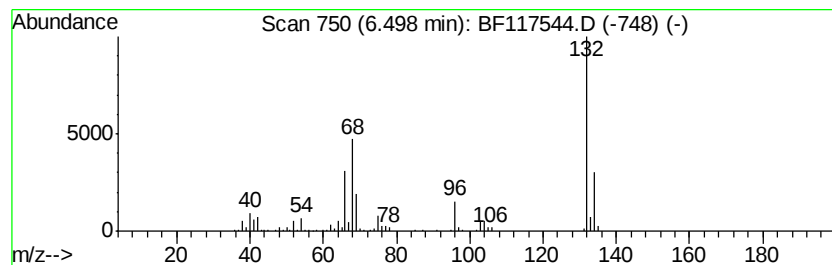
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	82.69 ng	852801	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	12
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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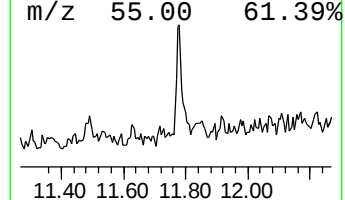
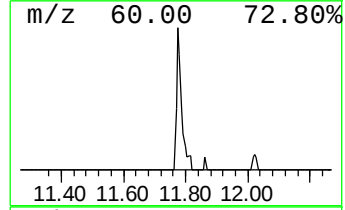
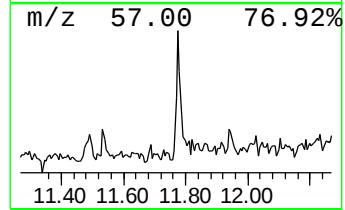
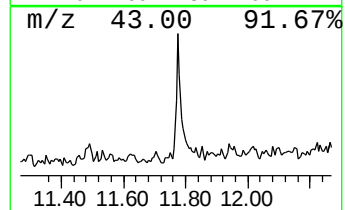
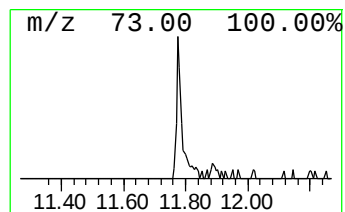
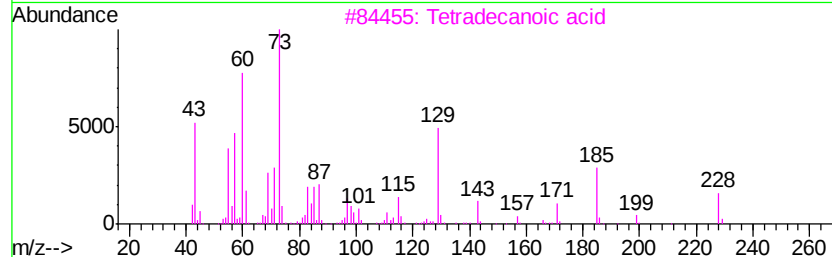
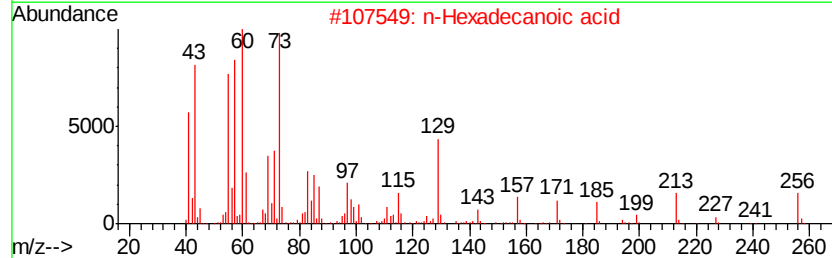
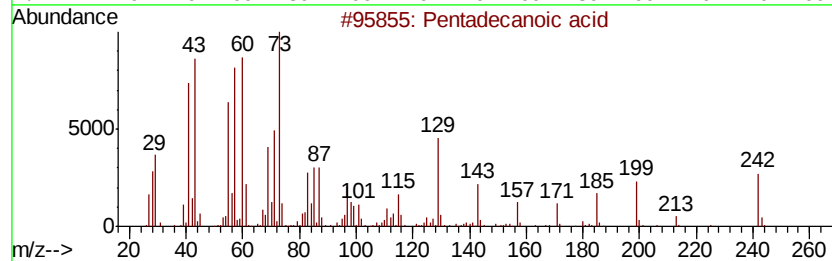
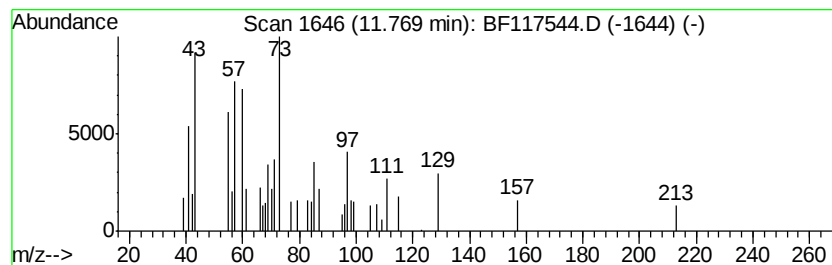
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	5.72 ng	61684	Phenanthrene-d10	11.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	43
5		n-Decanoic acid	172	C10H20O2	000334-48-5	43



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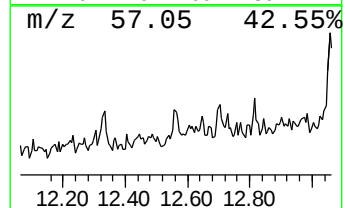
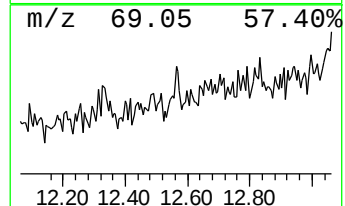
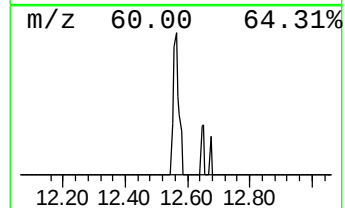
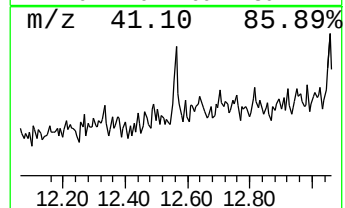
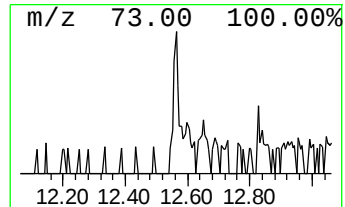
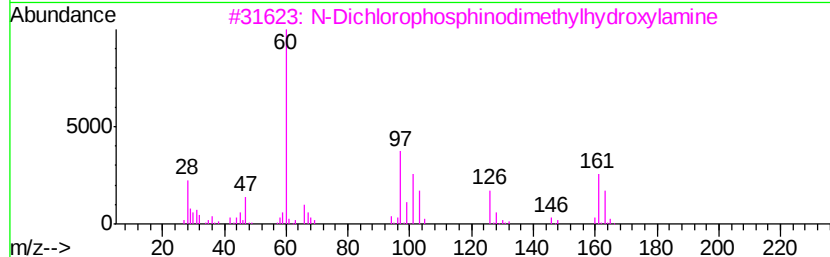
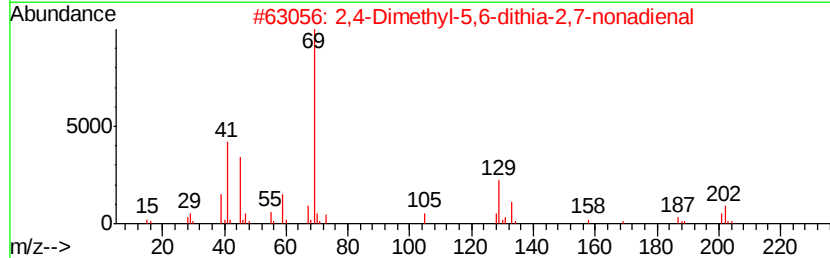
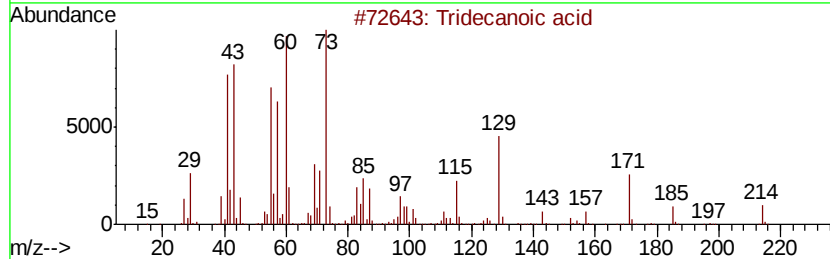
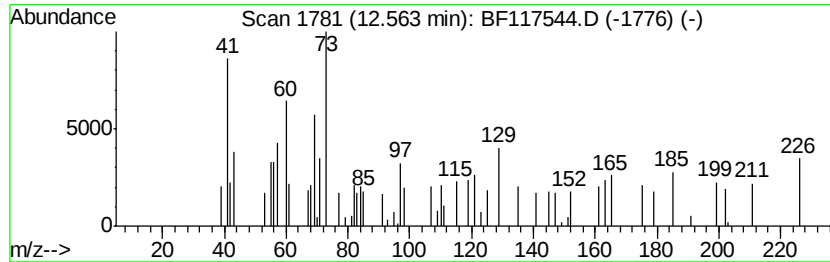
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown12.56 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.56	3.21 ng	34592	Phenanthrene-d10	11.25	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	14
2	2,4-Dimethyl-5,6-dithia-2,7-nona...	202	C9H14OS2	1000322-30-5	9
3	N-Dichlorophosphinodimethylhydro...	161	C2H6Cl2NOP	022692-23-5	9
4	l-Gala-l-ido-octitol	242	C8H18O8	1000130-11-9	9
5	n-Decanoic acid	172	C10H20O2	000334-48-5	8



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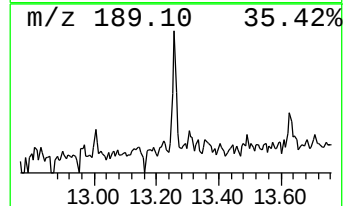
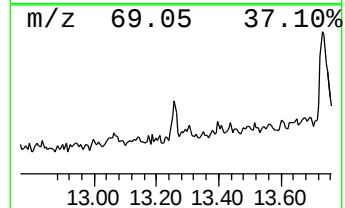
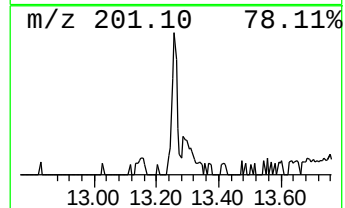
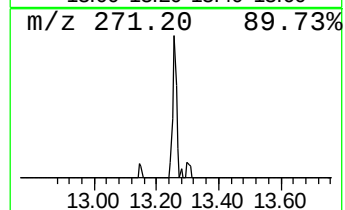
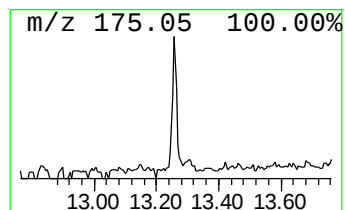
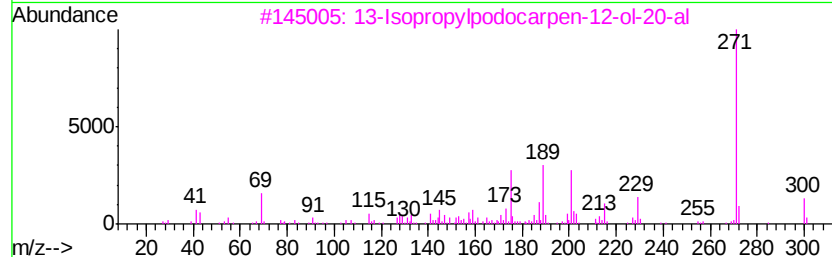
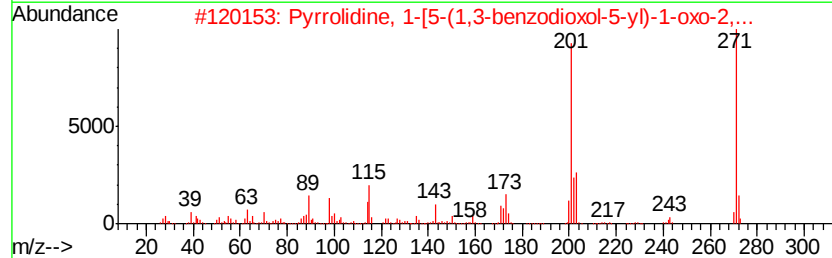
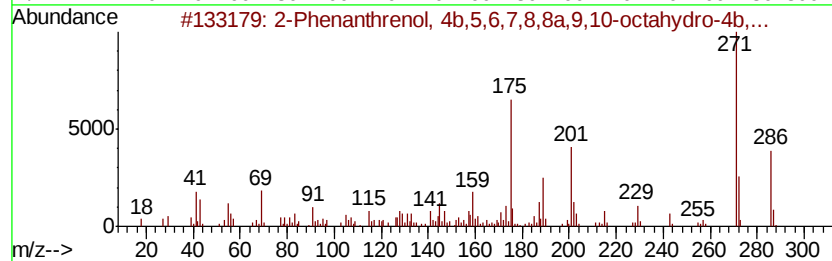
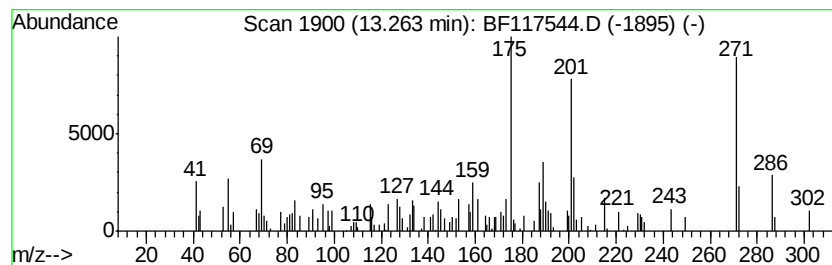
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.26	6.97 ng	83483	Chrysene-d12	13.89		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	59	
2	Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	38	
3	13-Isopropylpodocarpin-12-ol-20-al	300	C20H28O2	024035-37-8	35	
4	Dihydroapohemanthamine	271	C16H17NO3	001153-01-1	25	
5	2,2-Bis(4'-methoxyphenyl)-2-etho...	286	C18H22O3	1000283-53-7	22	



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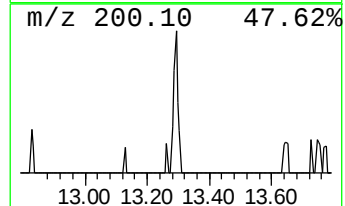
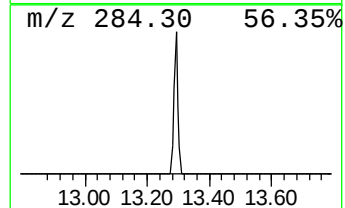
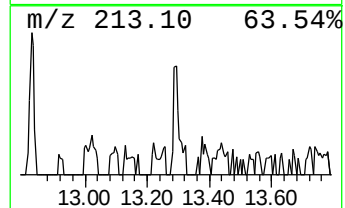
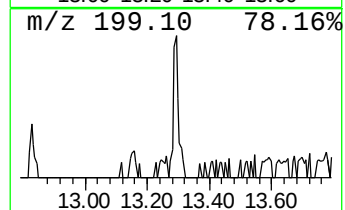
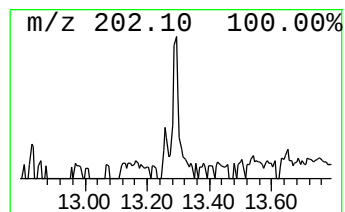
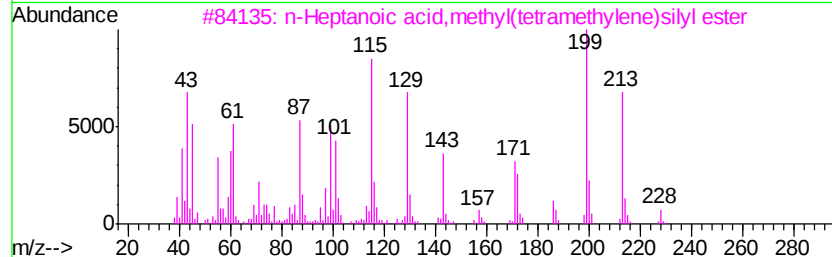
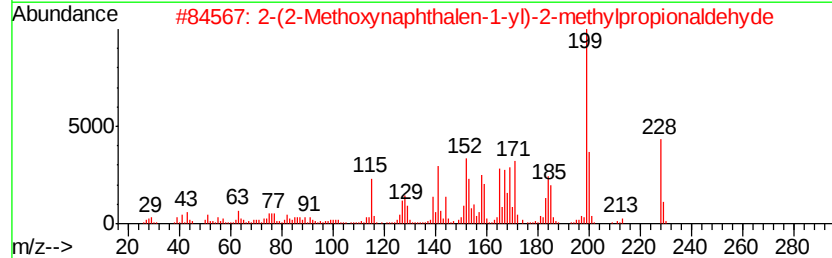
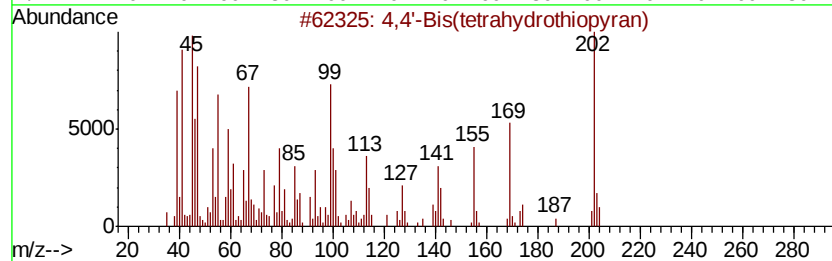
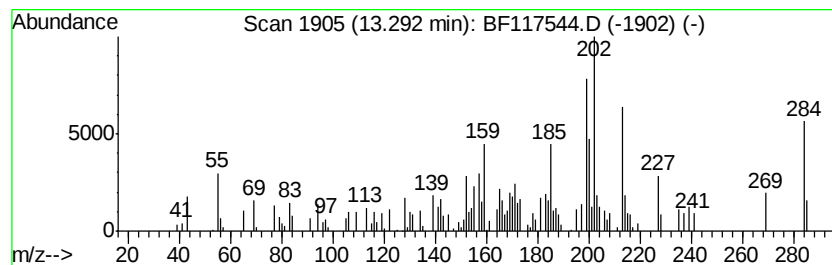
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TIC Integration Parameters: LSCINT.P

Peak Number 6 4,4'-Bis(tetrahydrothiopyran) Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.29	5.23 ng	62645	Chrysene-d12	13.89		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	56	
2	2-(2-Methoxynaphthalen-1-yl)-2-m...	228	C15H16O2	032454-20-9	35	
3	n-Heptanoic acid,methyl(tetramet...	228	C12H24O2Si	1000217-03-6	18	
4	4-Methoxy-naphthalene-1-carboxyl...	202	C12H10O3	1000317-85-4	18	
5	.beta.-D-Glucopyranoside, methyl...	320	C16H32O6	1000157-04-8	18	



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102519\
Data File : BF117544.D
Acq On : 25 Oct 2019 18:53
Operator : JU
Sample : K5500-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
800-50-(0-2)

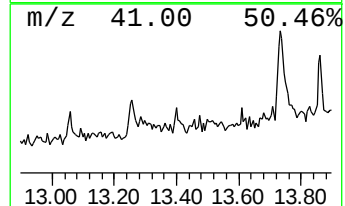
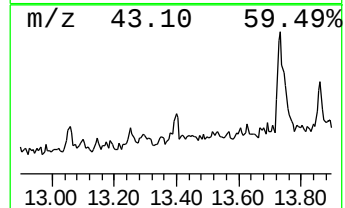
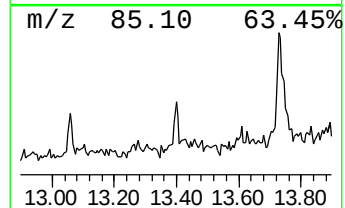
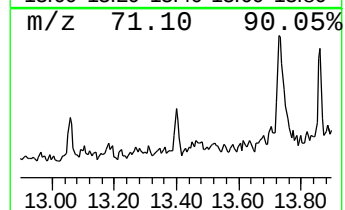
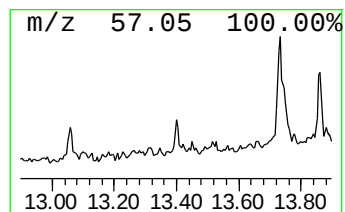
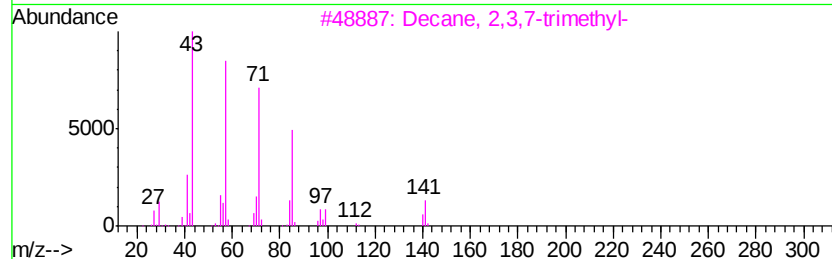
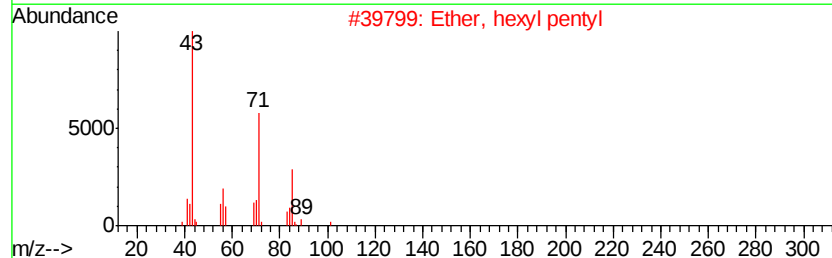
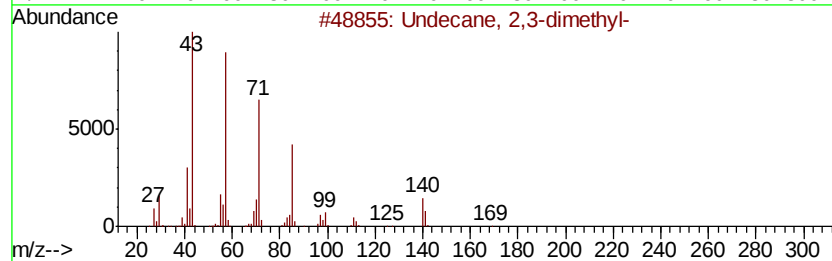
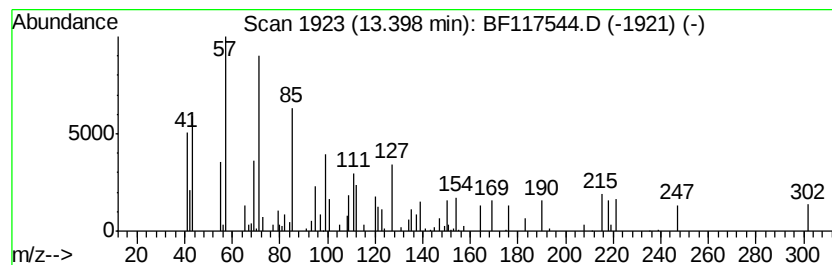
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown13.40 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.40	2.17 ng	25940	Chrysene-d12	13.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Undecane, 2,3-dimethyl-	184	C13H28	017312-77-5	35
2		Ether, hexyl pentyl	172	C11H24O	032357-83-8	27
3		Decane, 2,3,7-trimethyl-	184	C13H28	062238-13-5	27
4		Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	27
5		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102519\
Data File : BF117544.D
Acq On : 25 Oct 2019 18:53
Operator : JU
Sample : K5500-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

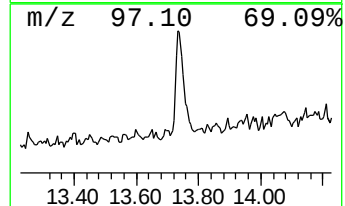
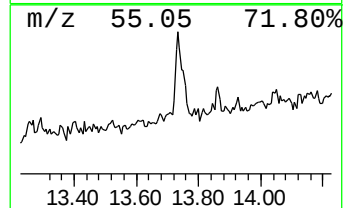
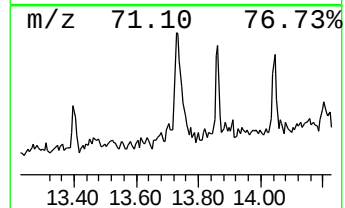
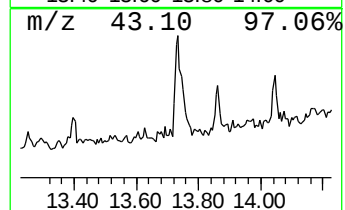
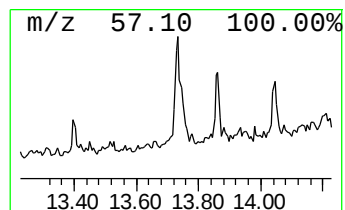
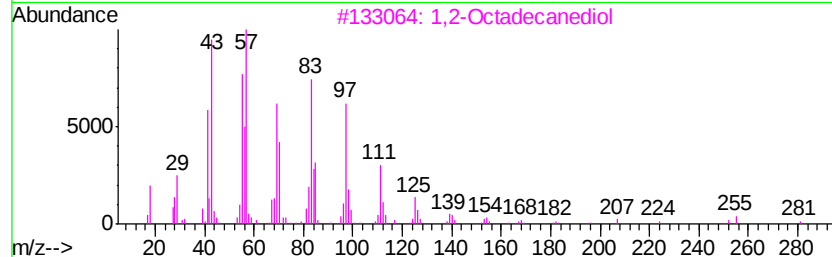
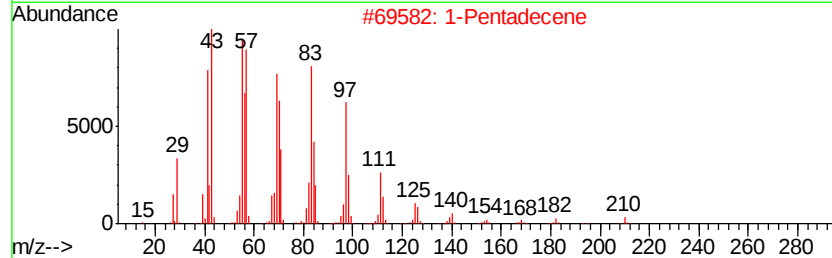
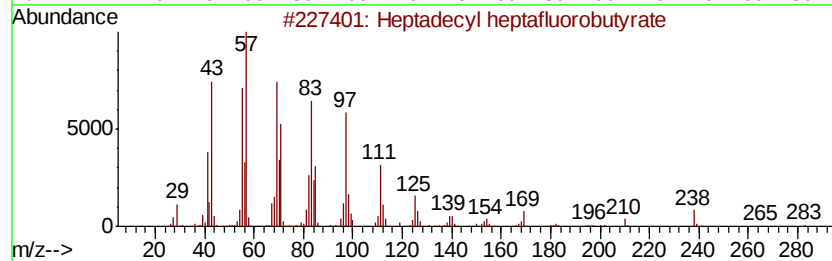
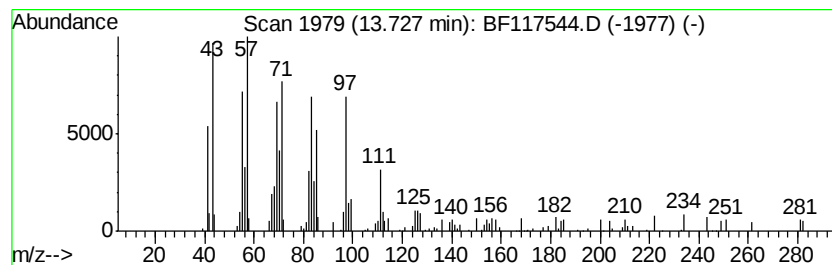
Instrument :
BNA_F
ClientSampleId :
800-50-(0-2)

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 8 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.		
13.73	12.24 ng	146595	Chrysene-d12		13.89		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2			1-Pentadecene	210	C15H30	013360-61-7	76
3			1,2-Octadecanediol	286	C18H38O2	020294-76-2	58
4			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	53
5			Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102519\
Data File : BF117544.D
Acq On : 25 Oct 2019 18:53
Operator : JU
Sample : K5500-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
800-50-(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	82.7	ng	852801	1	6.73	206276	20.0
Pentadecanoic acid	11.77	5.7	ng	61684	4	11.25	215626	20.0
unknown12.56	12.56	3.2	ng	34592	4	11.25	215626	20.0
2-Phenanthrenol, ...	13.26	7.0	ng	83483	5	13.89	239627	20.0
4,4'-Bis(tetrahyd...	13.29	5.2	ng	62645	5	13.89	239627	20.0
unknown13.40	13.40	2.2	ng	25940	5	13.89	239627	20.0
Heptadecyl heptaf...	13.73	12.2	ng	146595	5	13.89	239627	20.0