

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF103019\
 Data File : BF117622.D
 Acq On : 30 Oct 2019 14:12
 Operator : JU
 Sample : K5542-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 54-54-(0-1.2)

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	4.916	478	481	505	rBV	83752	131896	14.63%	1.629%
2	5.351	552	555	579	rBV	531483	759834	84.29%	9.385%
3	6.387	727	731	747	rBV	625901	857845	95.16%	10.595%
4	6.504	747	751	766	rVB	950318	901456	100.00%	11.134%
5	6.728	785	789	802	rVB	221388	216405	24.01%	2.673%
6	6.881	812	815	830	rBV	709805	638751	70.86%	7.889%
7	7.292	882	885	905	rBV	392276	502687	55.76%	6.209%
8	8.010	1004	1007	1027	rBV	222159	280831	31.15%	3.469%
9	9.080	1185	1189	1201	rBV	965995	878438	97.45%	10.850%
10	9.480	1254	1257	1268	rBV	75021	83177	9.23%	1.027%
11	9.757	1301	1304	1320	rVB	293462	312594	34.68%	3.861%
12	10.557	1436	1440	1455	rBV	381848	442957	49.14%	5.471%
13	11.251	1554	1558	1567	rBV	224657	275748	30.59%	3.406%
14	11.774	1645	1647	1656	rBV4	17173	23415	2.60%	0.289%
15	12.468	1761	1765	1770	rBV	42075	46032	5.11%	0.569%
16	12.698	1798	1804	1811	rBV	44421	53797	5.97%	0.664%
17	12.827	1822	1826	1833	rBV	778378	688178	76.34%	8.500%
18	13.392	1918	1922	1925	rBV2	14890	17545	1.95%	0.217%
19	13.739	1976	1981	1988	rBV5	21394	51860	5.75%	0.641%
20	13.892	2002	2007	2011	rBV	239773	273016	30.29%	3.372%
21	14.039	2029	2032	2034	rBV	23636	19828	2.20%	0.245%
22	14.345	2081	2084	2089	rBV	29949	27080	3.00%	0.334%
23	14.386	2089	2091	2096	rBV5	9277	12745	1.41%	0.157%
24	14.639	2132	2134	2138	rVB	33865	29872	3.31%	0.369%
25	14.710	2144	2146	2149	rVB2	32139	27479	3.05%	0.339%
26	14.874	2172	2174	2176	rBV2	11829	14313	1.59%	0.177%
27	14.933	2180	2184	2185	rVV2	25952	35558	3.94%	0.439%
28	14.957	2185	2188	2195	rVB2	52047	67137	7.45%	0.829%
29	15.274	2240	2242	2245	rBV	14709	17612	1.95%	0.218%
30	15.333	2245	2252	2261	rVB	165466	277007	30.73%	3.421%
31	15.721	2314	2318	2322	rVB3	27772	41248	4.58%	0.509%
32	15.945	2354	2356	2362	rVB7	24195	34219	3.80%	0.423%
33	16.186	2392	2397	2401	rBV4	20226	33139	3.68%	0.409%
34	16.351	2423	2425	2429	rVB4	19275	22622	2.51%	0.279%

LSC Area Percent Report

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54-54-(0-1.2)

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-BF101819.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

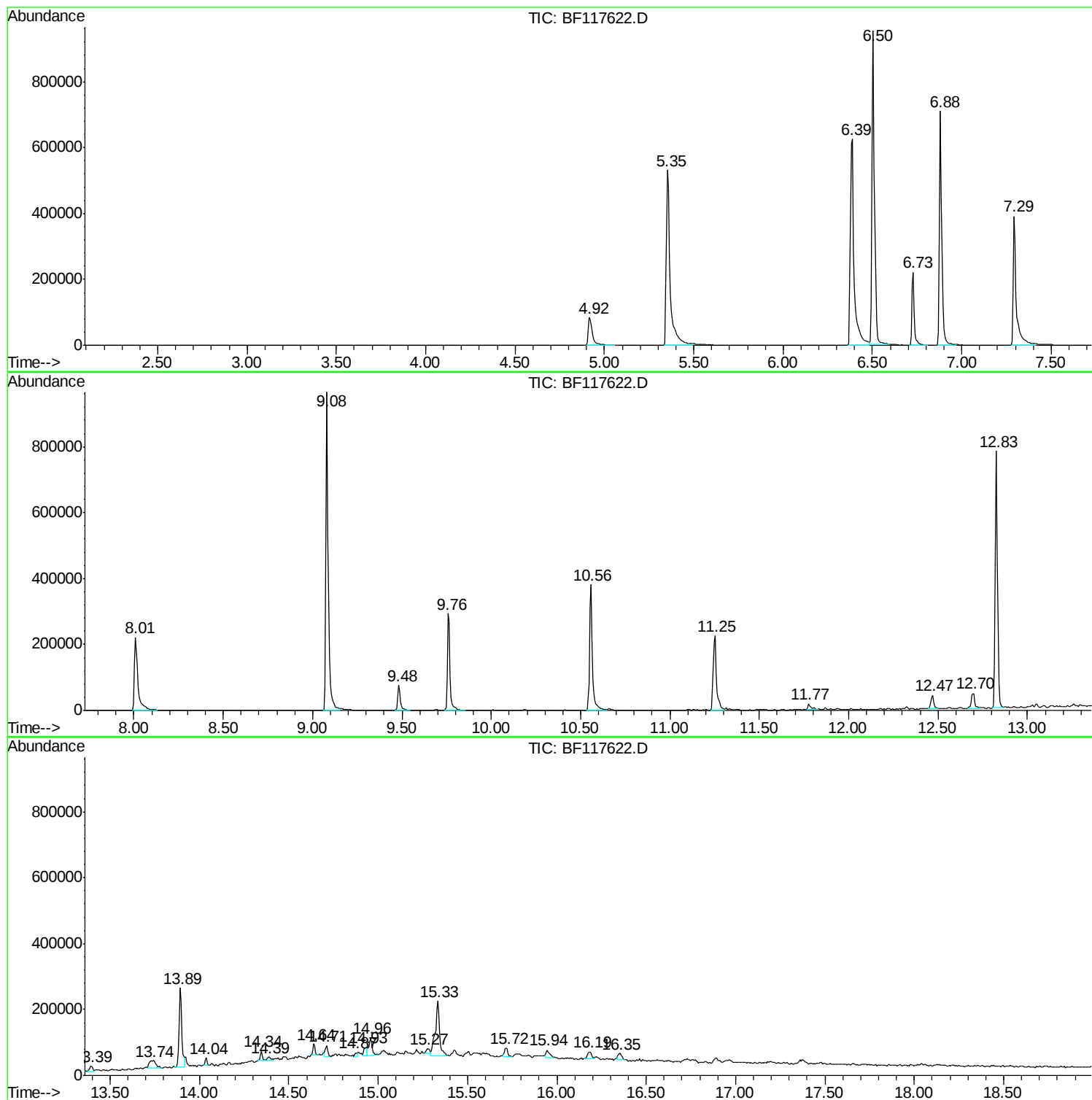
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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ClientSampled :
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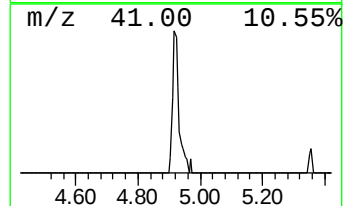
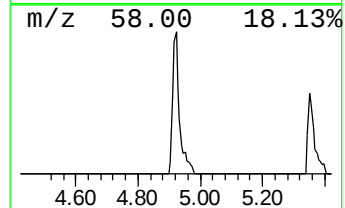
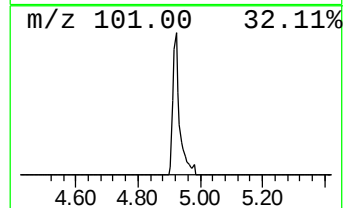
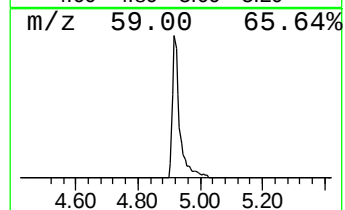
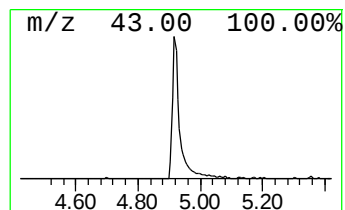
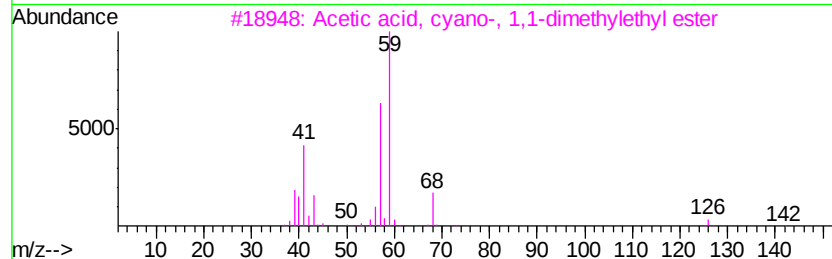
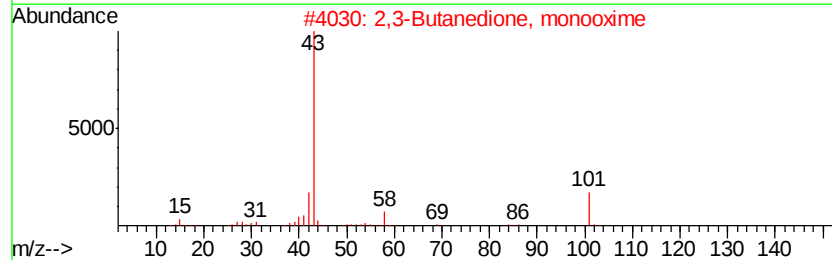
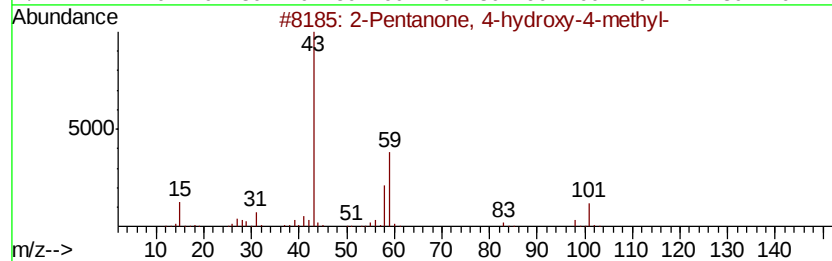
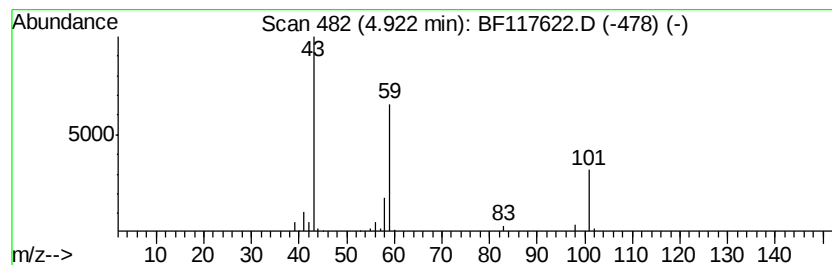
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	12.19 ng	131896	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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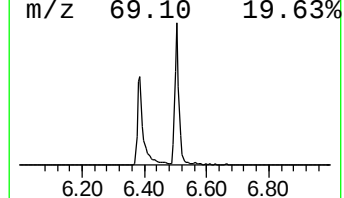
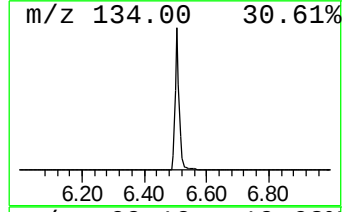
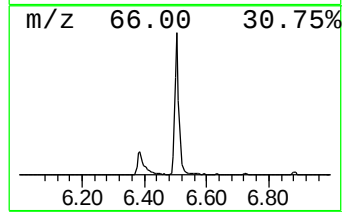
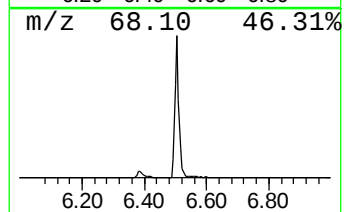
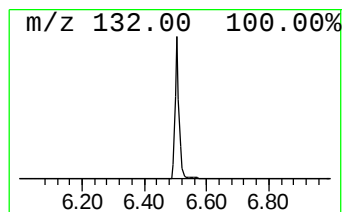
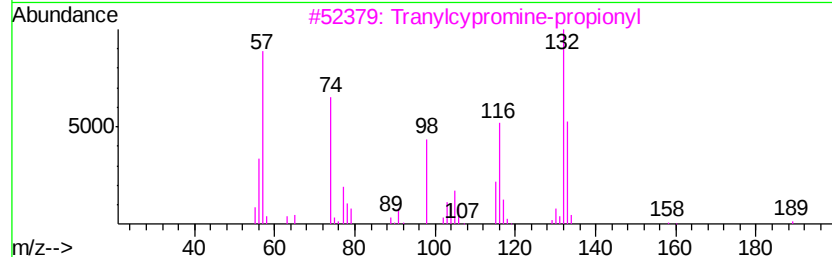
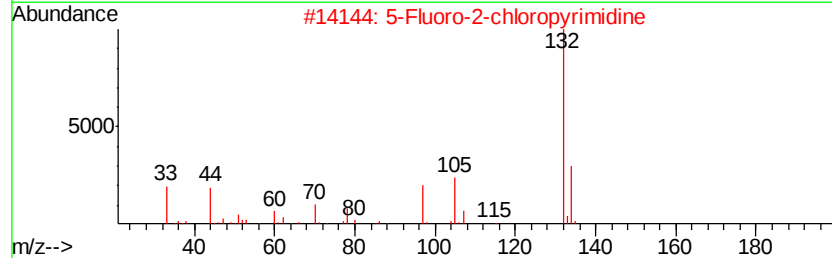
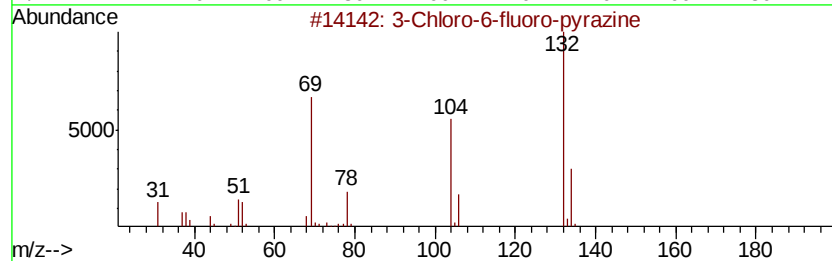
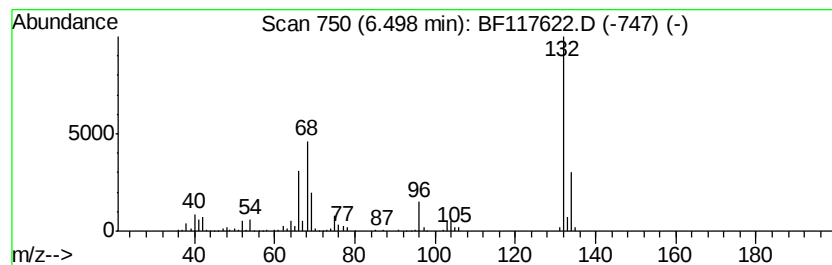
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	83.31 ng	901456	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	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		Xenon	132	Xe	007440-63-3	9



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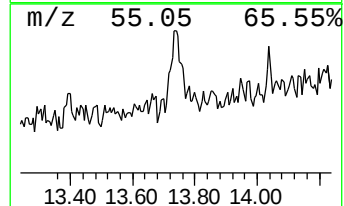
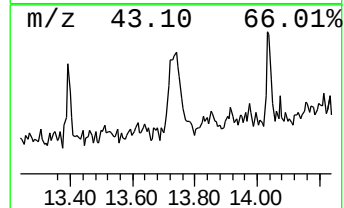
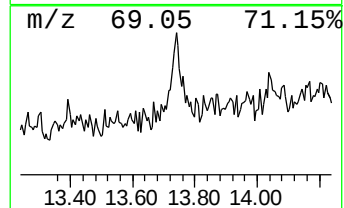
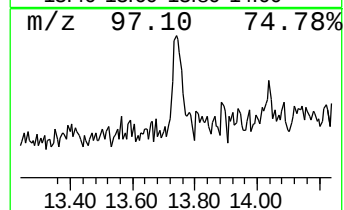
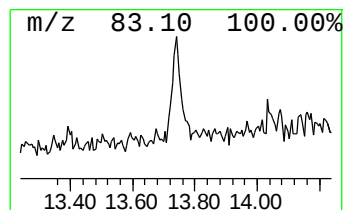
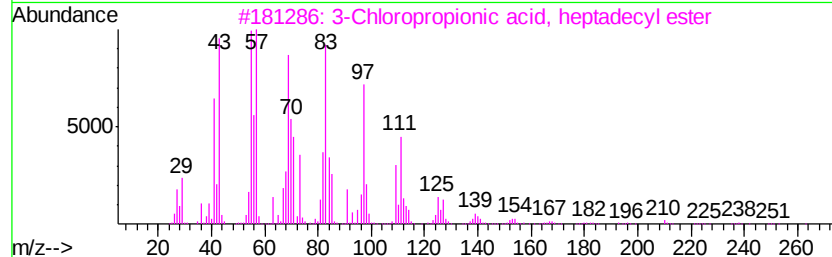
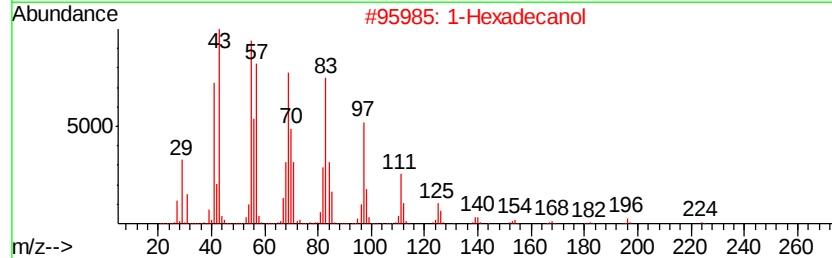
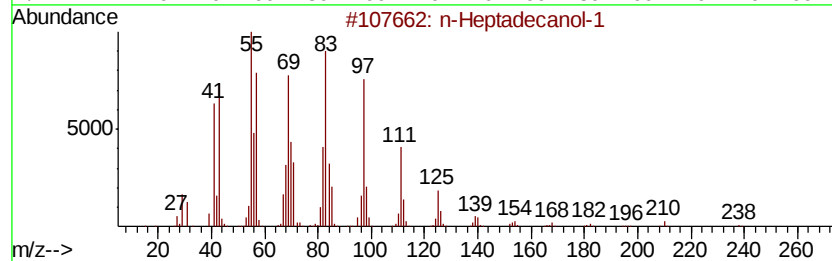
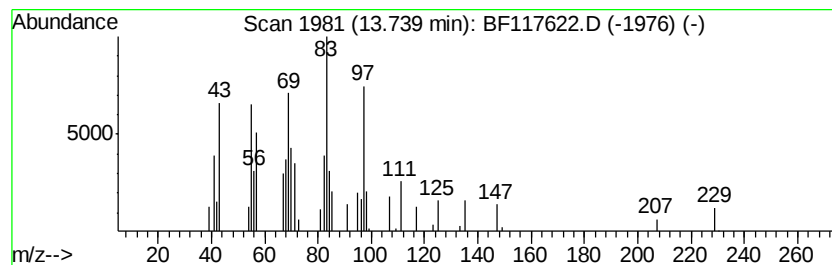
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Heptadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.74	3.80 ng	51860	Chrysene-d12	13.89	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Heptadecanol-1	256	C17H36O	001454-85-9	87
2	1-Hexadecanol	242	C16H34O	036653-82-4	87
3	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	86
4	Chloroacetic acid, tetradecyl ester	290	C16H31ClO2	018277-86-6	74
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	74



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 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 54-54-(0-1.2)

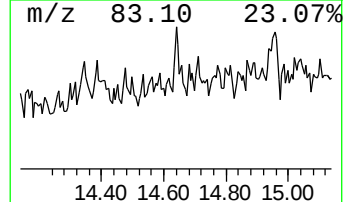
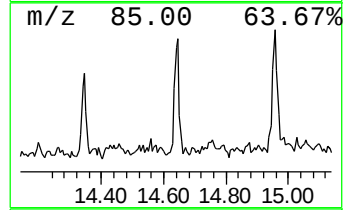
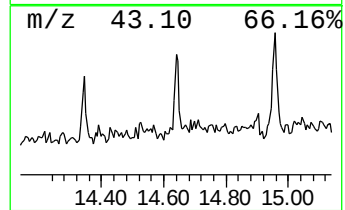
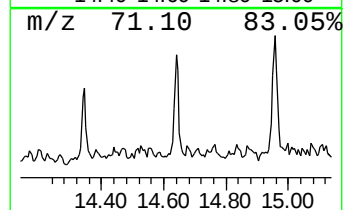
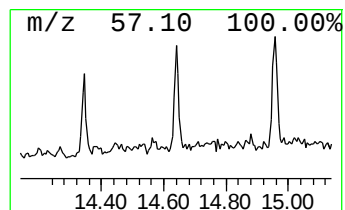
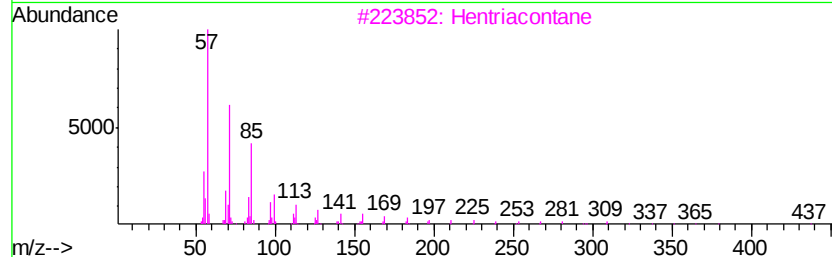
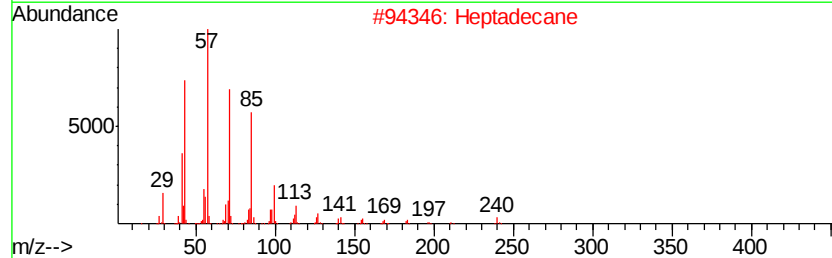
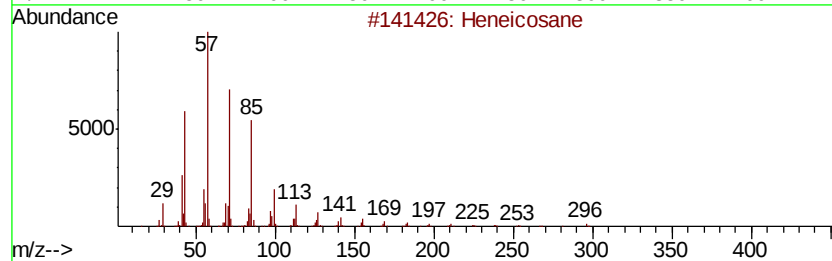
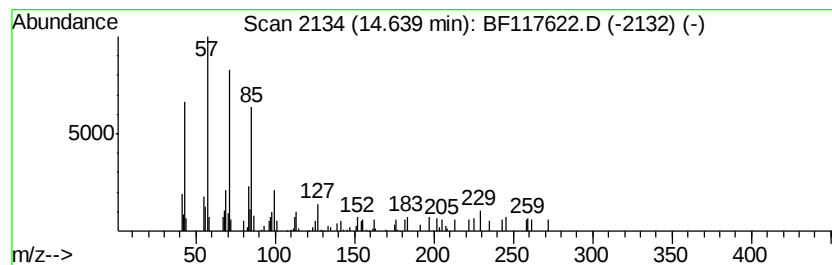
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 5 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.16 ng	29872	Perylene-d12	15.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	64
2	Heptadecane		240	C17H36	000629-78-7	64
3	Hentriacontane		437	C31H64	000630-04-6	59
4	Dodecane, 3-methyl-		184	C13H28	017312-57-1	59
5	Hexadecane, 1-iodo-		352	C16H33I	000544-77-4	59



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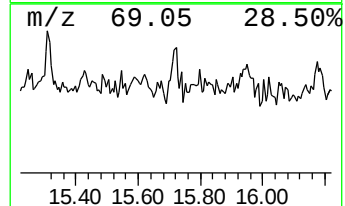
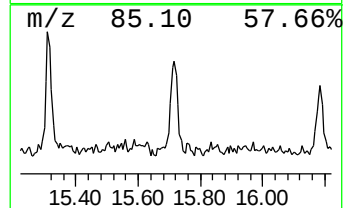
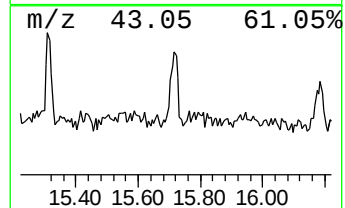
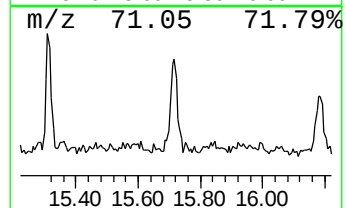
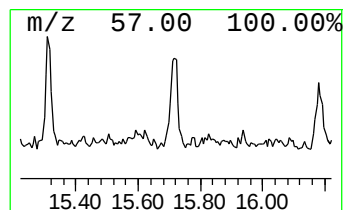
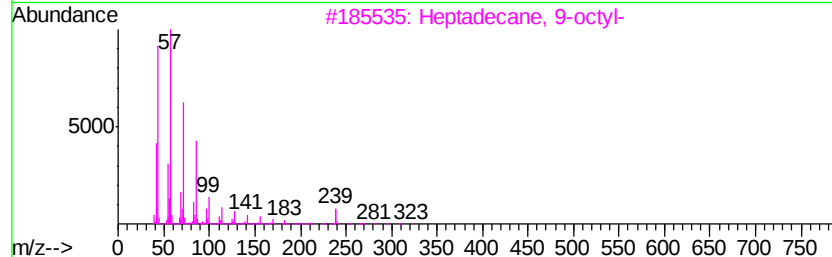
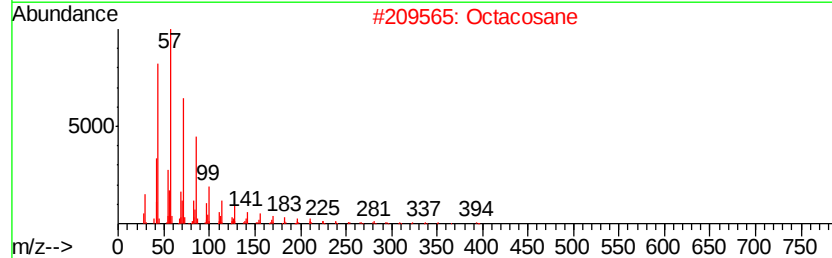
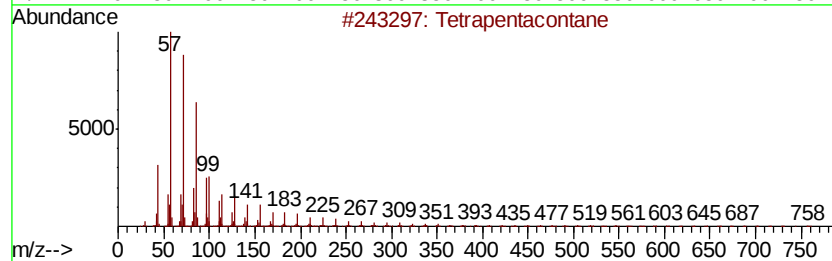
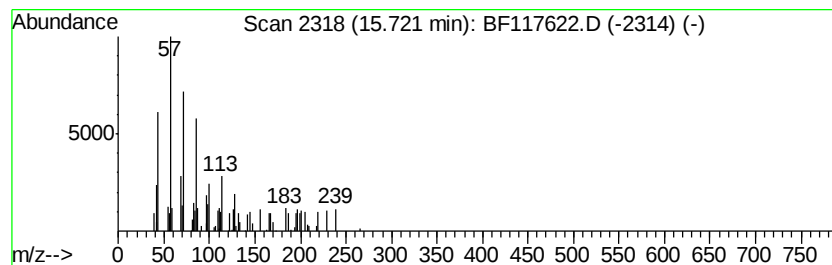
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Tetrapentacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	2.98 ng	41248	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetrapentacontane	759	C54H110	005856-66-6	52
2		Octacosane	394	C28H58	000630-02-4	52
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	50
4		Heptadecane	240	C17H36	000629-78-7	50
5		Heneicosane	296	C21H44	000629-94-7	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
Data File : BF117622.D
Acq On : 30 Oct 2019 14:12
Operator : JU
Sample : K5542-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
54-54-(0-1.2)

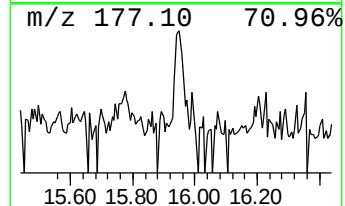
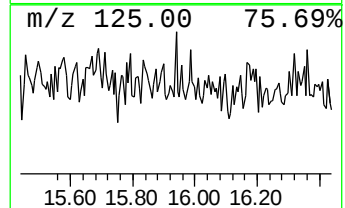
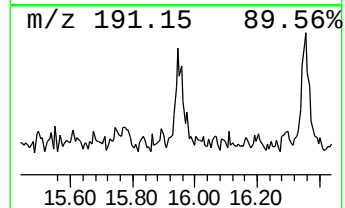
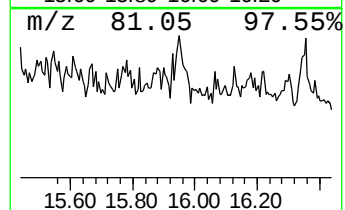
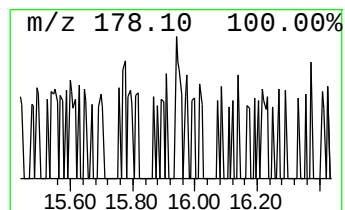
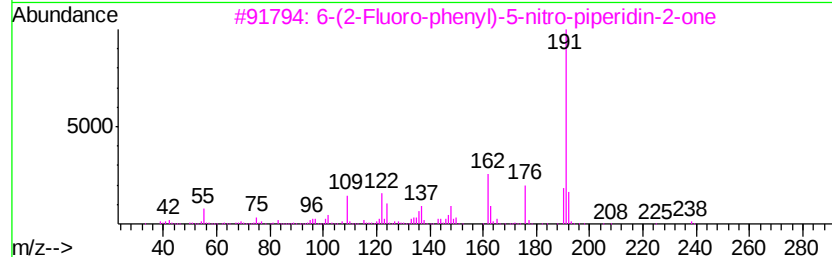
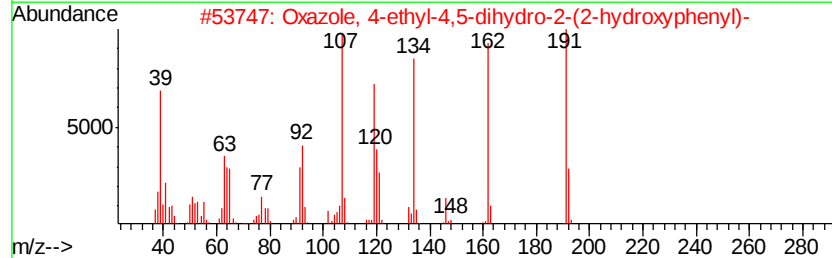
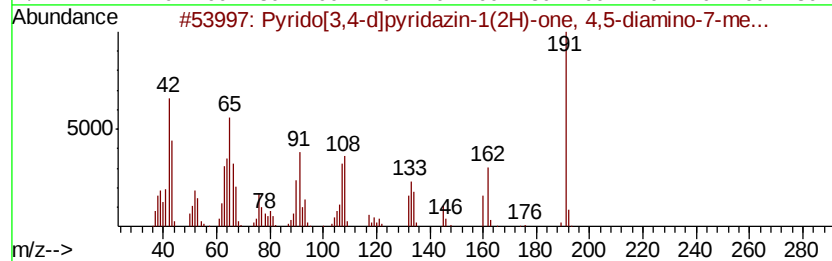
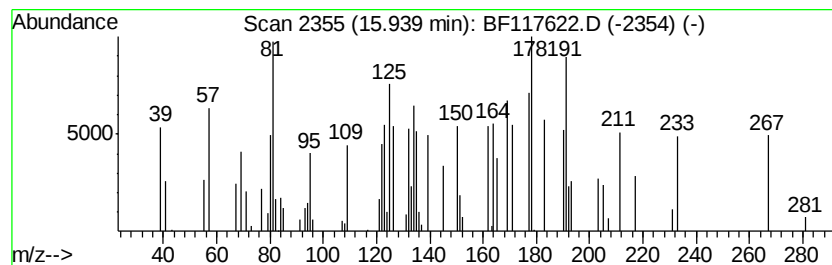
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.94 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	2.47 ng	34219	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrido[3,4-d]pyridazin-1(2H)-one...	191	C8H9N5O	1000263-69-7	25
2		Oxazole, 4-ethyl-4,5-dihydro-2-(...	191	C11H13N02	1000142-01-8	18
3		6-(2-Fluoro-phenyl)-5-nitro-pipe...	238	C11H11FN2O3	1000275-16-4	12
4		Amiphenazole	191	C9H9N3S	000490-55-1	10
5		2-Fluoro-6-trifluoromethylbenzoi...	308	C14H16F4O3	1000357-30-8	10



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
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Acq On : 30 Oct 2019 14:12
Operator : JU
Sample : K5542-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

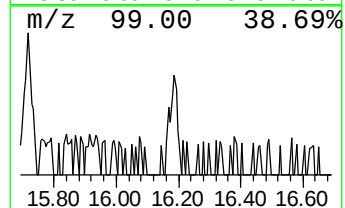
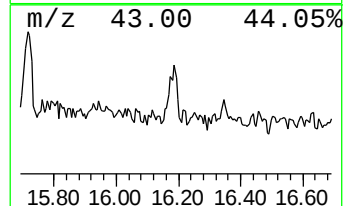
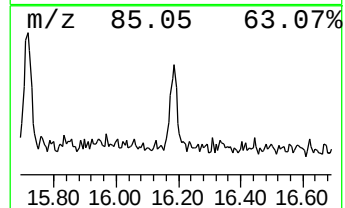
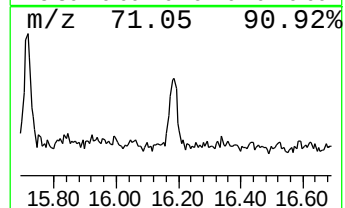
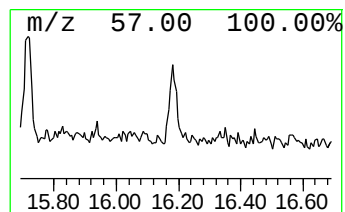
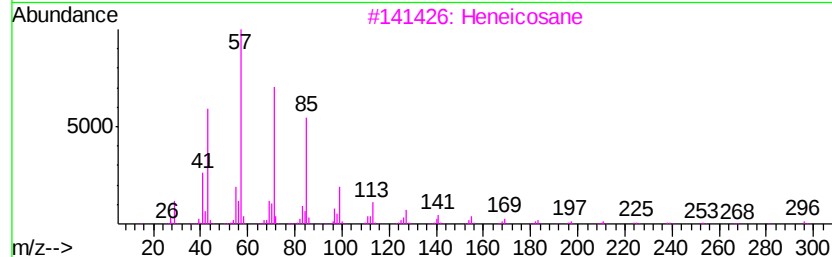
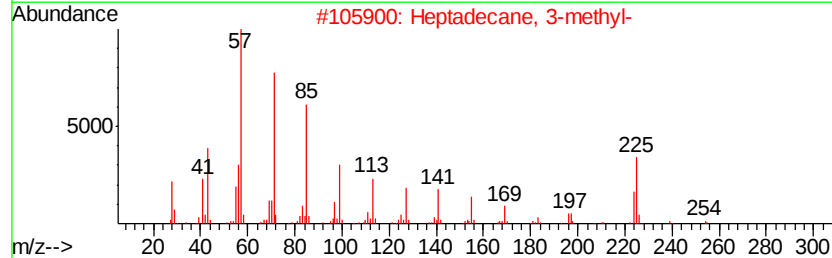
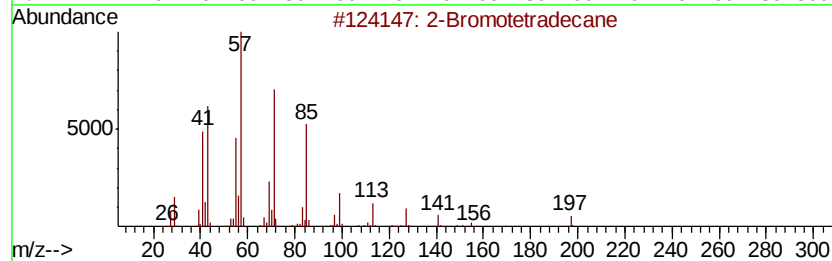
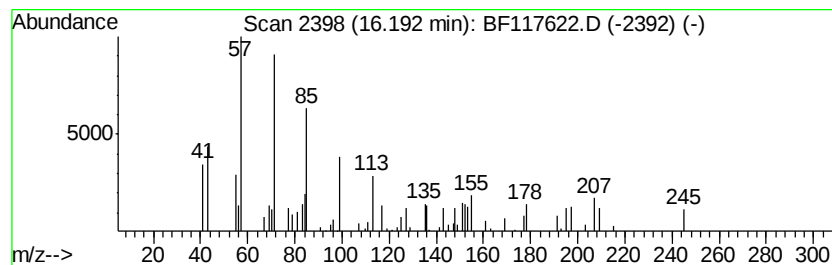
Instrument :
BNA_F
ClientSampleId :
54-54-(0-1.2)

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 2-Bromotetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	2.39 ng	33139	Perylene-d12	15.33
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Bromotetradecane	276 C14H29Br	074036-95-6	64
2	Heptadecane, 3-methyl-	254 C18H38	006418-44-6	64
3	Heneicosane	296 C21H44	000629-94-7	59
4	Hexadecane	226 C16H34	000544-76-3	53
5	Sulfurous acid, 2-ethylhexyl hex...	278 C14H30O3S	1000309-20-2	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF103019\
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Operator : JU
Sample : K5542-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
54-54-(0-1.2)

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
2-Pentanone, 4-hy...	4.92	12.2	ng	131896	1	6.73	216405	20.0
unknown6.50	6.50	83.3	ng	901456	1	6.73	216405	20.0
n-Heptadecanol-1	13.74	3.8	ng	51860	5	13.89	273016	20.0
Heneicosane	14.64	2.2	ng	29872	6	15.33	277007	20.0
Tetrapentacontane	15.72	3.0	ng	41248	6	15.33	277007	20.0
unknown15.94	15.94	2.5	ng	34219	6	15.33	277007	20.0
2-Bromotetradecane	16.19	2.4	ng	33139	6	15.33	277007	20.0