

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042718\
 Data File : BF104901.D
 Acq On : 28 Apr 2018 00:13
 Operator : JU/SJ
 Sample : J2590-01
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

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:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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	5.016	494	498	508	rBV	96689	137470	4.35%	0.515%
2	5.422	562	567	570	rBV	2738408	2725883	86.29%	10.218%
3	6.445	736	741	758	rBV	2325225	2912136	92.18%	10.916%
4	6.575	758	763	766	rBV	3075190	2883661	91.28%	10.810%
5	6.798	797	801	805	rBV	761882	608983	19.28%	2.283%
6	6.957	823	828	831	rBV	2573627	2297212	72.72%	8.611%
7	7.369	893	898	901	rBV	1822810	1770245	56.04%	6.636%
8	8.081	1015	1019	1035	rBV	786397	808955	25.61%	3.032%
9	9.163	1198	1203	1206	rBV	3181652	3159142	100.00%	11.842%
10	9.551	1264	1269	1277	rBV	325777	310985	9.84%	1.166%
11	9.763	1301	1305	1308	rBV	61909	54274	1.72%	0.203%
12	9.839	1314	1318	1326	rBV2	956429	840562	26.61%	3.151%
13	10.263	1387	1390	1392	rVB	81008	69043	2.19%	0.259%
14	10.480	1421	1427	1429	rBV	26239	31919	1.01%	0.120%
15	10.633	1449	1453	1462	rBV	1770077	1776873	56.25%	6.661%
16	10.733	1467	1470	1474	rBV	77842	77073	2.44%	0.289%
17	11.327	1568	1571	1574	rBV	746696	712536	22.55%	2.671%
18	11.351	1574	1575	1581	rVB	117237	91721	2.90%	0.344%
19	11.851	1655	1660	1668	rBV3	71354	97791	3.10%	0.367%
20	12.545	1775	1778	1782	rBV	229283	198767	6.29%	0.745%
21	12.774	1812	1817	1824	rBV	200617	226012	7.15%	0.847%
22	12.922	1837	1842	1845	rBV	2488585	2440822	77.26%	9.150%
23	13.110	1866	1874	1877	rBV4	23713	45066	1.43%	0.169%
24	13.804	1988	1992	1996	rBV	246835	252016	7.98%	0.945%
25	13.839	1996	1998	2005	rVB	42592	43299	1.37%	0.162%
26	13.980	2014	2022	2025	rBV	681993	748939	23.71%	2.807%
27	14.004	2025	2026	2029	rVB	96269	56804	1.80%	0.213%
28	14.721	2145	2148	2154	rVB	196395	192417	6.09%	0.721%
29	15.021	2195	2199	2202	rBV	72554	108652	3.44%	0.407%
30	15.321	2247	2250	2256	rVB	37274	40377	1.28%	0.151%
31	15.380	2257	2260	2265	rVB	54001	67057	2.12%	0.251%
32	15.445	2266	2271	2275	rBV	369036	486849	15.41%	1.825%
33	17.357	2591	2596	2605	rBV6	32417	89692	2.84%	0.336%
34	17.615	2634	2640	2653	rBV8	89426	313698	9.93%	1.176%

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Operator : JU/SJ
Sample : J2590-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

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

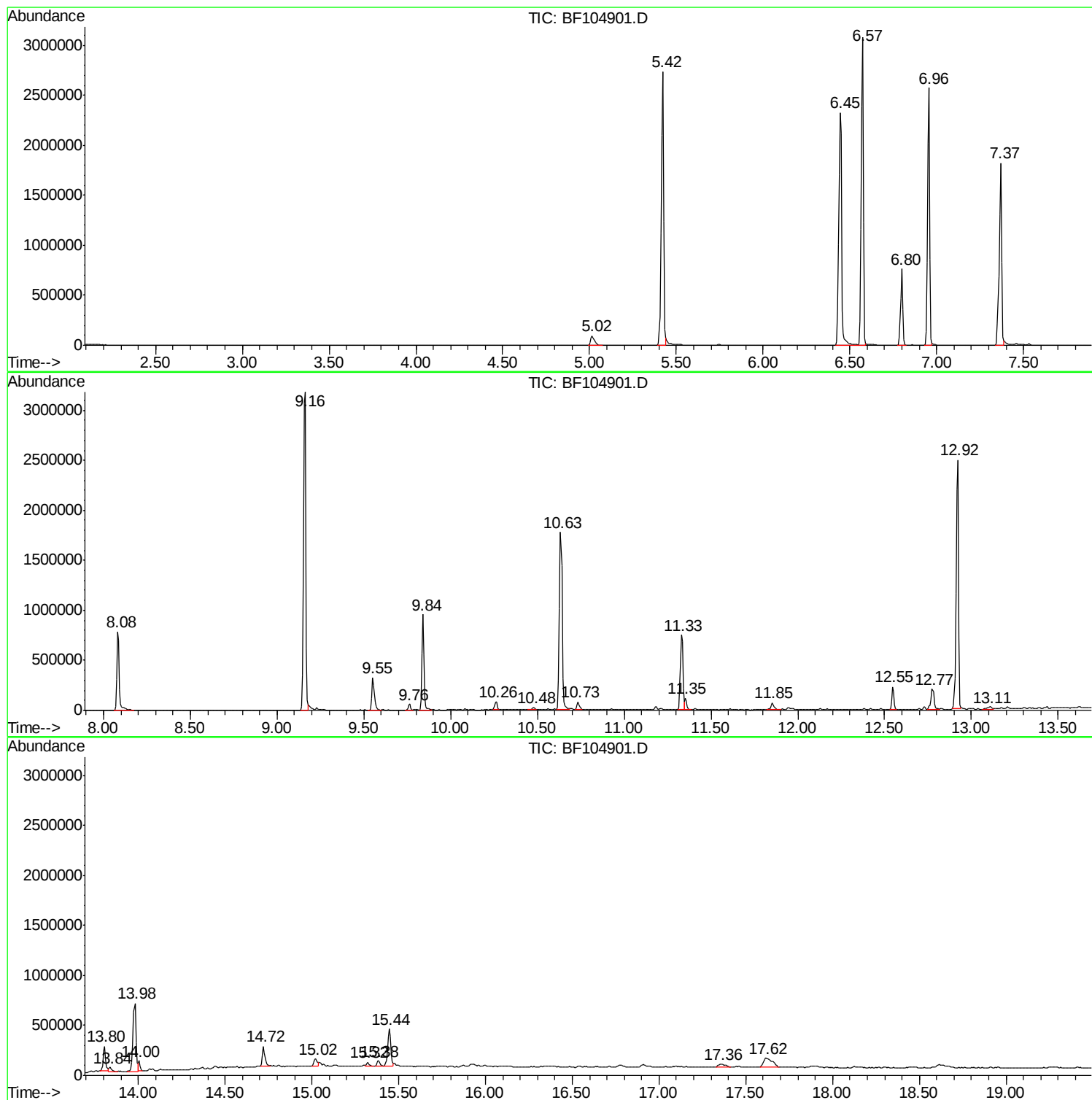
Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 26676931

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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.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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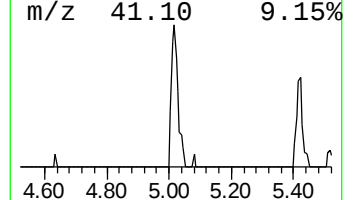
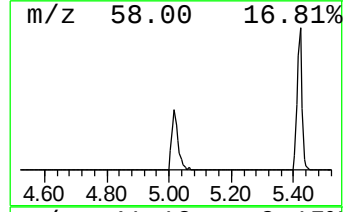
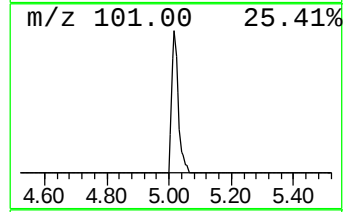
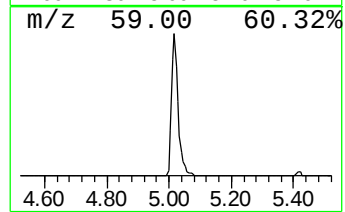
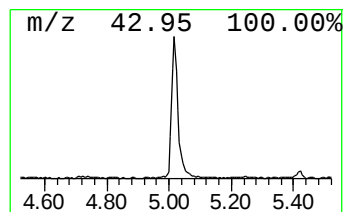
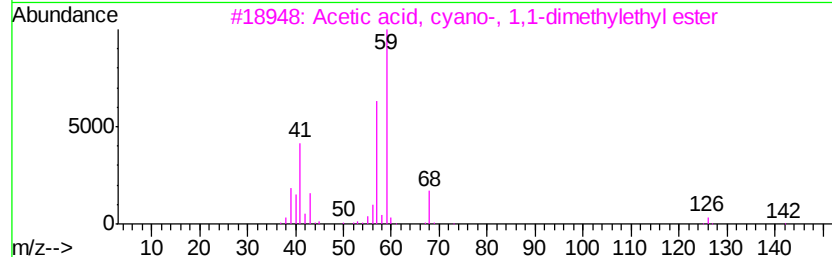
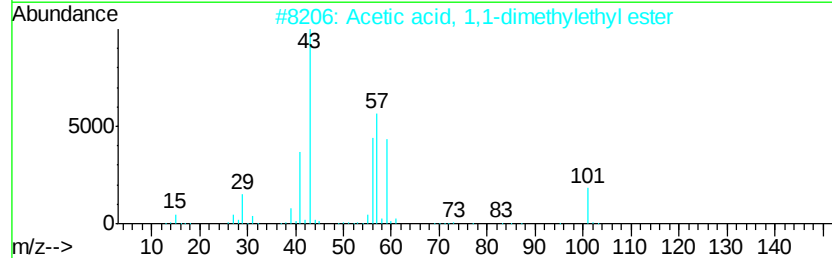
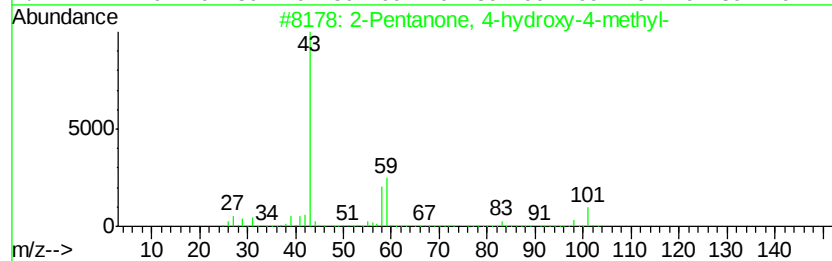
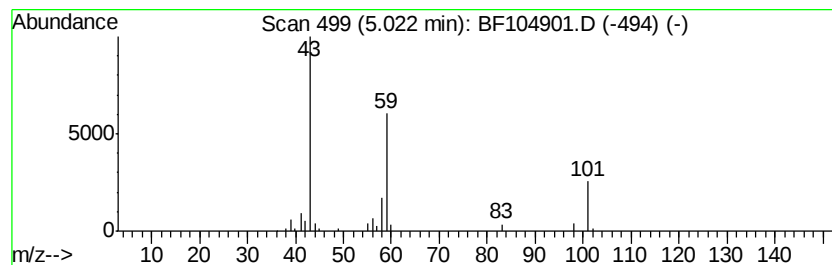
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	4.51 ng	137470	1,4-Dichlorobenzene-d4	6.80

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38	
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17	
4	Acetone	58	C3H6O	000067-64-1	9	
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9	



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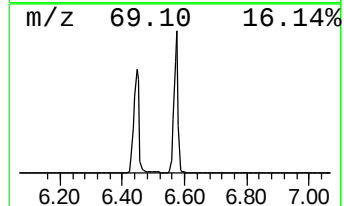
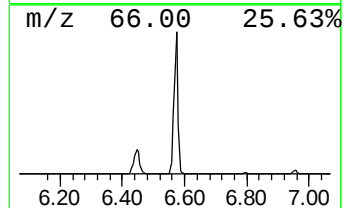
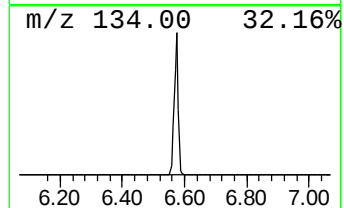
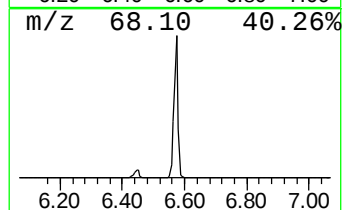
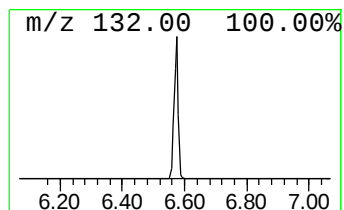
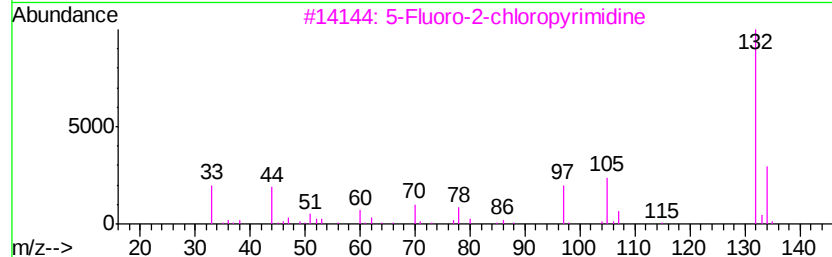
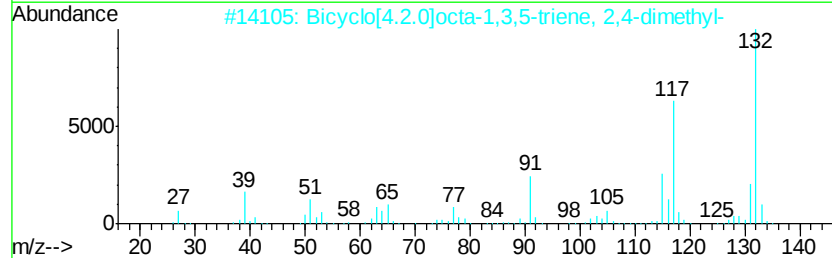
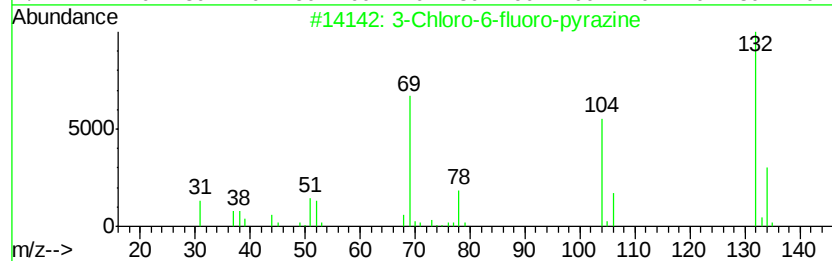
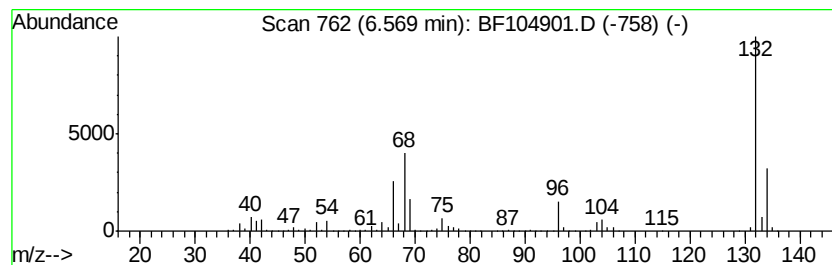
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	94.70 ng	2883660	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



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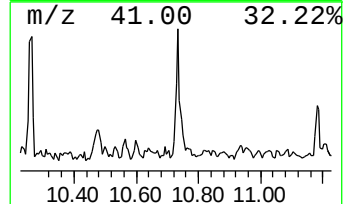
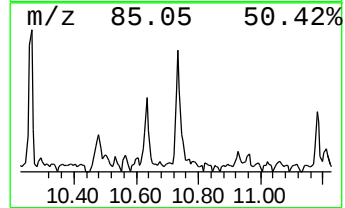
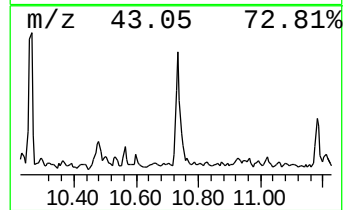
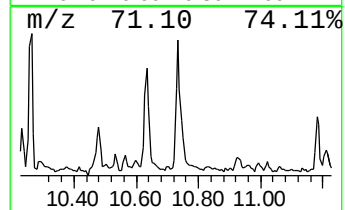
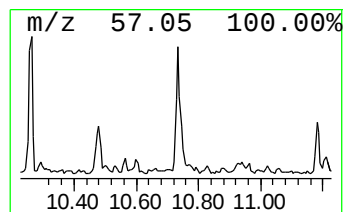
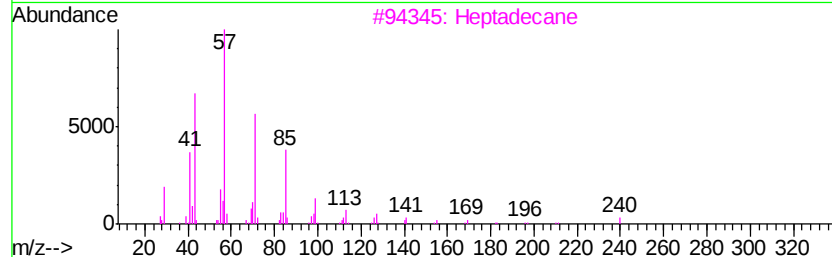
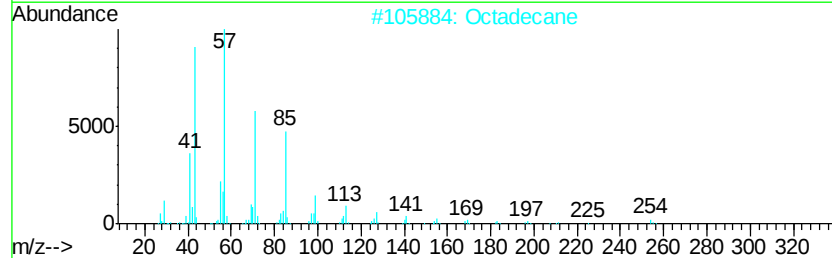
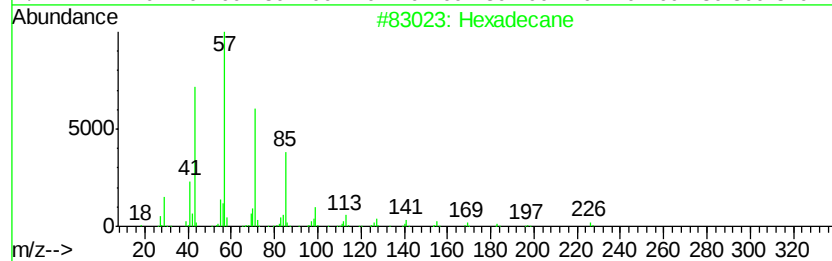
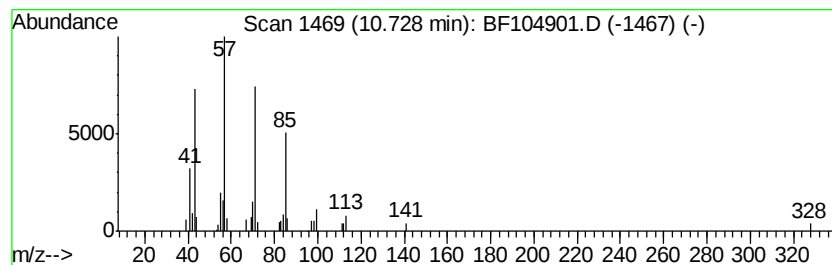
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.73	2.16 ng	77073	Phenanthrene-d10	11.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	91
2		Octadecane	254	C18H38	000593-45-3	91
3		Heptadecane	240	C17H36	000629-78-7	91
4		Tetradecane	198	C14H30	000629-59-4	91
5		Eicosane	282	C20H42	000112-95-8	90



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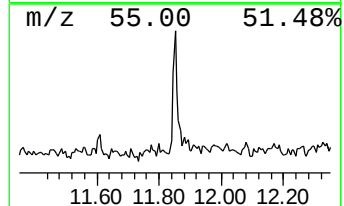
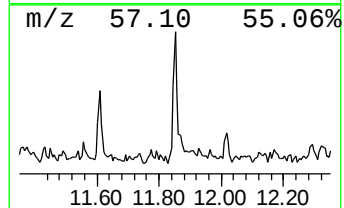
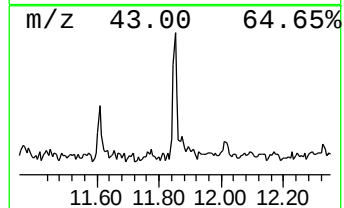
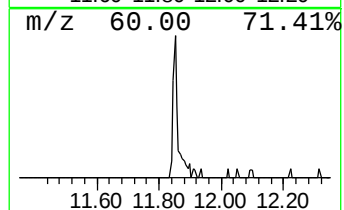
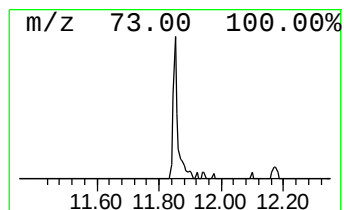
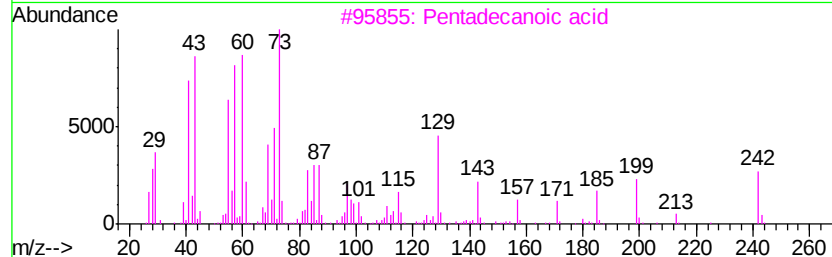
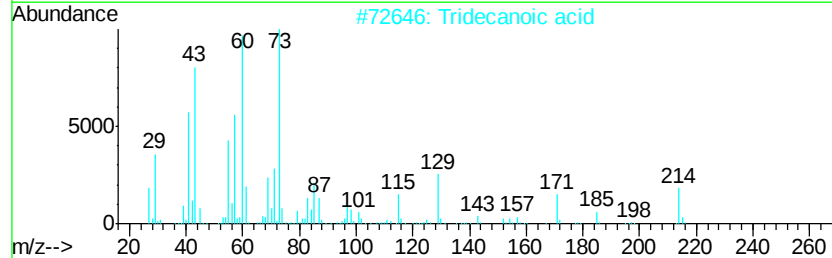
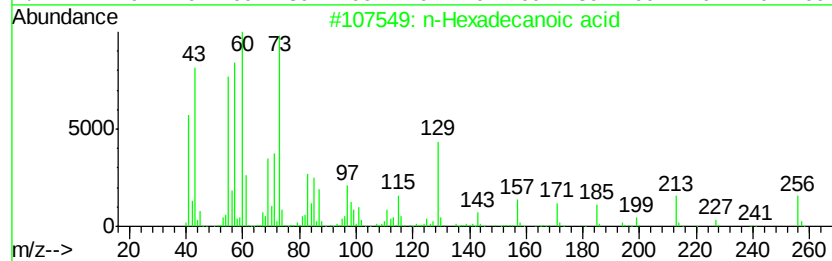
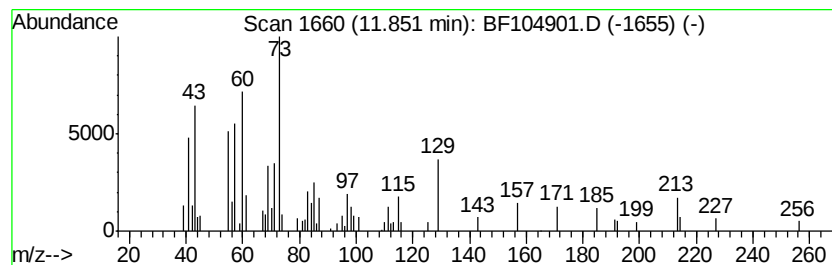
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	2.74 ng	97791	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	87
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5		n-Decanoic acid	172	C10H20O2	000334-48-5	38



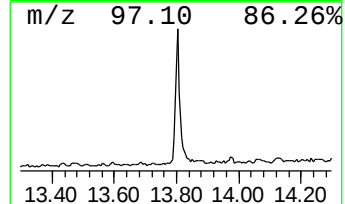
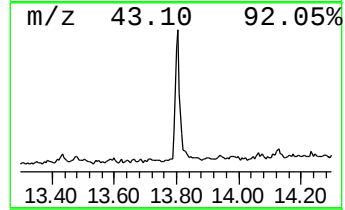
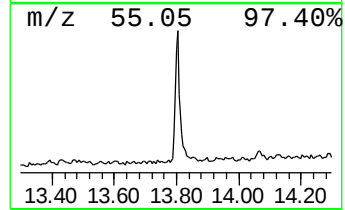
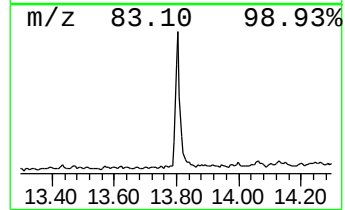
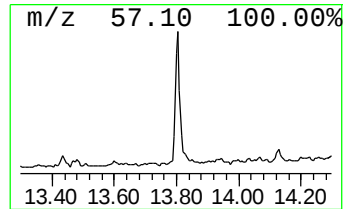
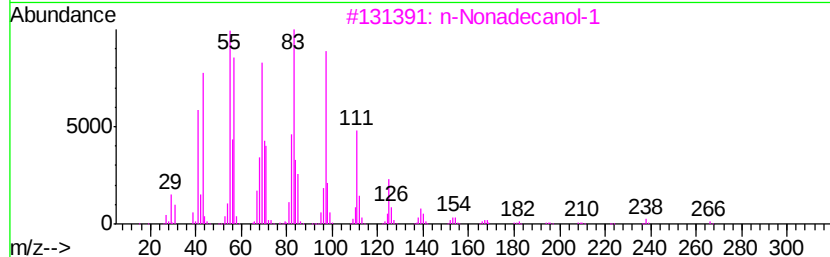
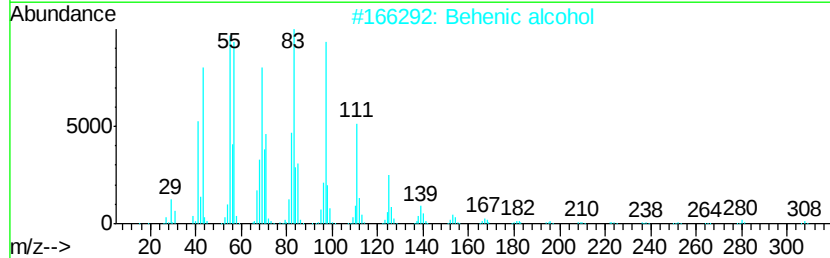
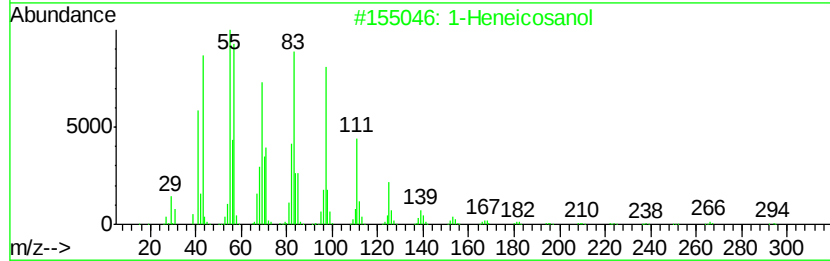
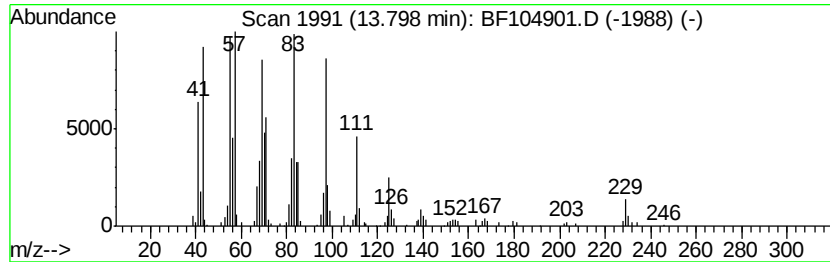
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.80	6.73 ng	252016	Chrysene-d12	13.98	
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	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	93



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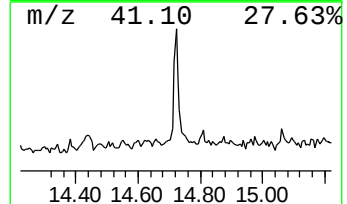
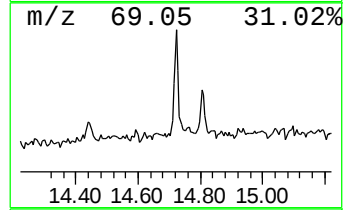
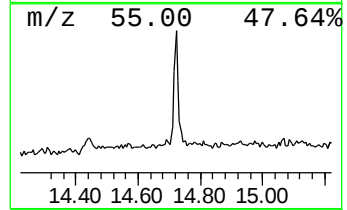
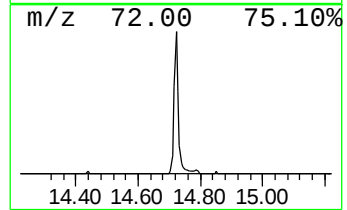
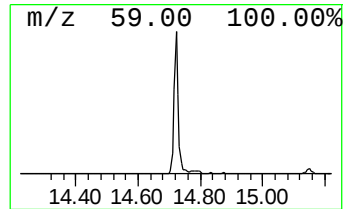
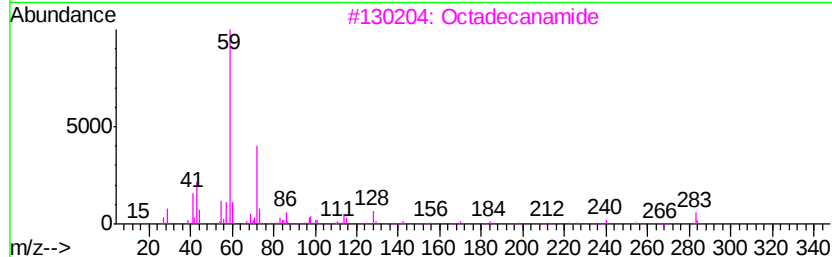
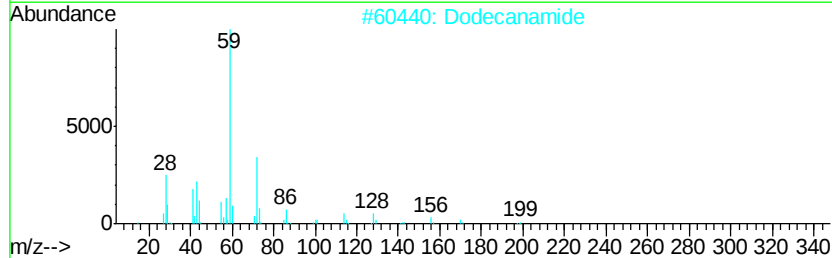
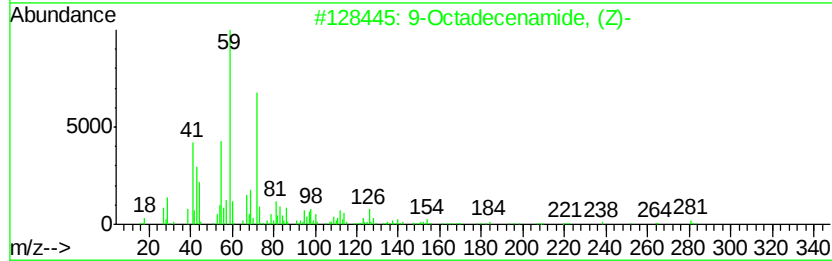
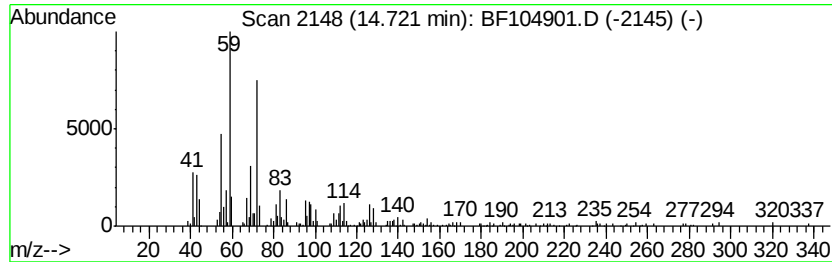
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	7.90 ng	192417	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2		Dodecanamide	199	C12H25NO	001120-16-7	50
3		Octadecanamide	283	C18H37NO	000124-26-5	47
4		Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	43
5		Decanamide-	171	C10H21NO	002319-29-1	43



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104901.D
Acq On : 28 Apr 2018 00:13
Operator : JU/SJ
Sample : J2590-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

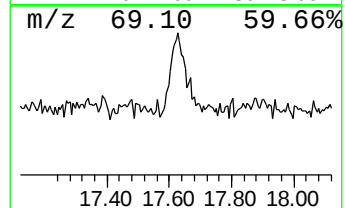
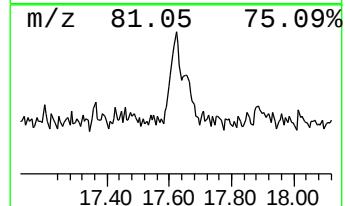
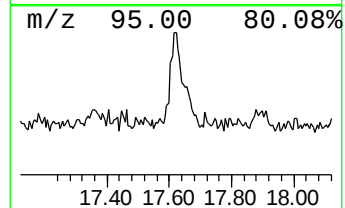
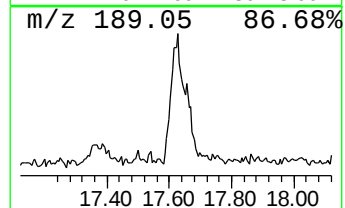
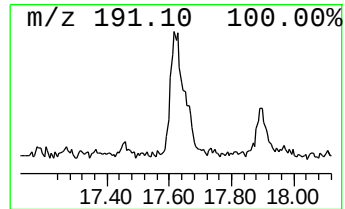
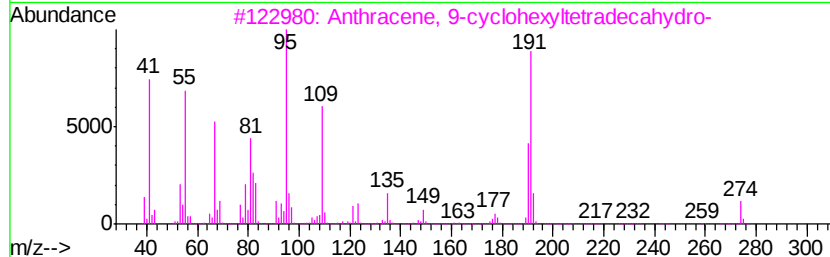
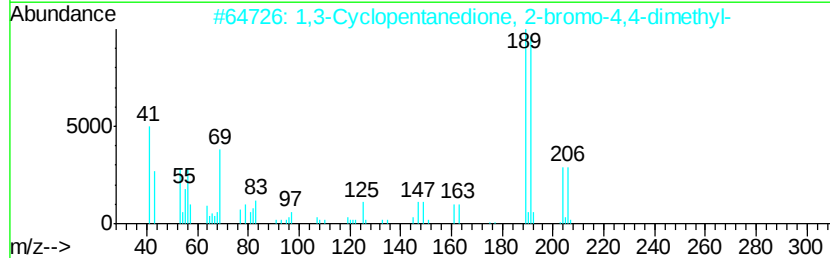
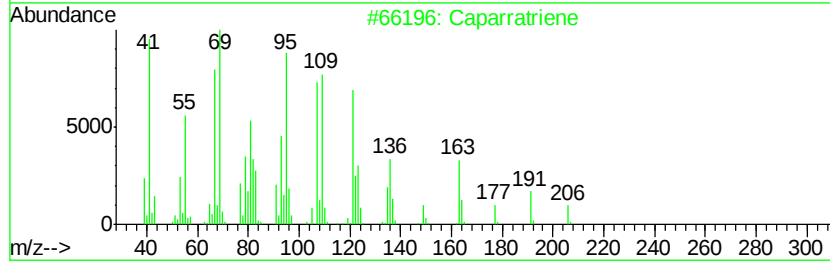
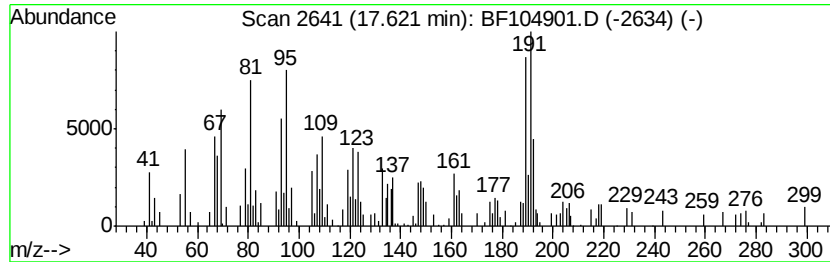
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Caparratriene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.62	12.89 ng	313698	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Caparratriene	206	C15H26	1000374-08-7	53
2		1,3-Cyclopentanedione, 2-bromo-4...	204	C7H9BrO2	057157-02-5	45
3		Anthracene, 9-cyclohexyltetradec...	274	C20H34	055255-70-4	41
4		4-(2', 4', 4'-trimethyl-viciclo[4...	204	C14H20O	1000373-94-4	20
5		Spiro[4-oxatricyclo[5.3.0.0(2,6)...]	276	C18H28O2	1000156-82-9	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042718\
Data File : BF104901.D
Acq On : 28 Apr 2018 00:13
Operator : JU/SJ
Sample : J2590-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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...	5.02	4.5	ng	137470	1	6.80	608983	20.0
unknown6.57	6.57	94.7	ng	2883660	1	6.80	608983	20.0
Hexadecane	10.73	2.2	ng	77073	4	11.33	712536	20.0
n-Hexadecanoic acid	11.85	2.7	ng	97791	4	11.33	712536	20.0
1-Heneicosanol	13.80	6.7	ng	252016	5	13.98	748939	20.0
9-Octadecenamide, ...	14.72	7.9	ng	192417	6	15.44	486849	20.0
Caparratriene	17.62	12.9	ng	313698	6	15.44	486849	20.0