

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
 Data File : BF102848.D
 Acq On : 8 Feb 2018 11:42
 Operator : SJ/JU
 Sample : J1469-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WABUT-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-BF020318.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	2.152	7	11	20	rVB	377128	516385	10.19%	1.091%
2	5.110	511	514	523	rVB	137489	174068	3.44%	0.368%
3	5.498	575	580	584	rBV	4430319	4821787	95.17%	10.184%
4	6.510	746	752	756	rBV	4357575	5066262	100.00%	10.701%
5	6.651	771	776	780	rBV	4575069	4726341	93.29%	9.983%
6	6.881	811	815	819	rBV	1540449	1280224	25.27%	2.704%
7	7.039	838	842	845	rBV	3864766	3495083	68.99%	7.382%
8	7.445	905	911	914	rBV	3325422	3223734	63.63%	6.809%
9	8.163	1029	1033	1037	rBV	1932436	1708228	33.72%	3.608%
10	9.239	1211	1216	1219	rBV	4682929	4626790	91.33%	9.772%
11	9.316	1224	1229	1231	rVV	114255	145590	2.87%	0.308%
12	9.357	1231	1236	1238	rVB3	47747	60010	1.18%	0.127%
13	9.627	1277	1282	1285	rBV	521912	524730	10.36%	1.108%
14	9.845	1312	1319	1323	rBV	275807	310199	6.12%	0.655%
15	9.922	1328	1332	1341	rVB	1973180	1852854	36.57%	3.913%
16	10.075	1354	1358	1361	rBV2	78262	81140	1.60%	0.171%
17	10.163	1370	1373	1378	rBV4	48025	62663	1.24%	0.132%
18	10.345	1401	1404	1407	rVB	300843	234229	4.62%	0.495%
19	10.563	1437	1441	1444	rBV	86379	97365	1.92%	0.206%
20	10.710	1458	1466	1470	rBV	2804209	2988013	58.98%	6.311%
21	10.739	1470	1471	1476	rVB3	93749	98952	1.95%	0.209%
22	10.816	1481	1484	1489	rVV2	323968	322061	6.36%	0.680%
23	11.263	1557	1560	1563	rBV	117155	113183	2.23%	0.239%
24	11.292	1563	1565	1571	rVB2	51093	61994	1.22%	0.131%
25	11.410	1581	1585	1588	rBV	1893678	1718080	33.91%	3.629%
26	11.733	1635	1640	1646	rVB8	31072	54505	1.08%	0.115%
27	11.927	1669	1673	1677	rBV	277853	267844	5.29%	0.566%
28	12.621	1788	1791	1801	rBV	86327	136931	2.70%	0.289%
29	12.710	1803	1806	1814	rBV6	46977	71680	1.41%	0.151%
30	12.992	1850	1854	1858	rBV	3644000	3872152	76.43%	8.178%
31	13.874	2001	2004	2012	rBV	335146	390709	7.71%	0.825%
32	14.021	2025	2029	2030	rBV	54645	57294	1.13%	0.121%
33	14.045	2030	2033	2037	rVV	1249225	1189794	23.48%	2.513%
34	14.510	2108	2112	2119	rBV	302072	345854	6.83%	0.730%

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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.815	2160	2164	2168	rBV2	39076	58068	1.15%	0.123%
36	15.157	2218	2222	2225	rBV	351627	382311	7.55%	0.807%
37	15.527	2280	2285	2297	rVB	781116	1096631	21.65%	2.316%
38	15.751	2319	2323	2329	rBV3	66069	95468	1.88%	0.202%
39	15.992	2358	2364	2369	rBV	242334	367312	7.25%	0.776%
40	16.039	2369	2372	2378	rVV5	44541	69512	1.37%	0.147%
41	16.803	2498	2502	2509	rVB4	54364	108005	2.13%	0.228%
42	17.115	2551	2555	2561	rVB3	52834	100607	1.99%	0.212%
43	17.198	2565	2569	2576	rVB8	45429	90307	1.78%	0.191%
44	17.615	2634	2640	2650	rVB7	83943	201216	3.97%	0.425%
45	18.680	2814	2821	2826	rBV9	31404	79704	1.57%	0.168%

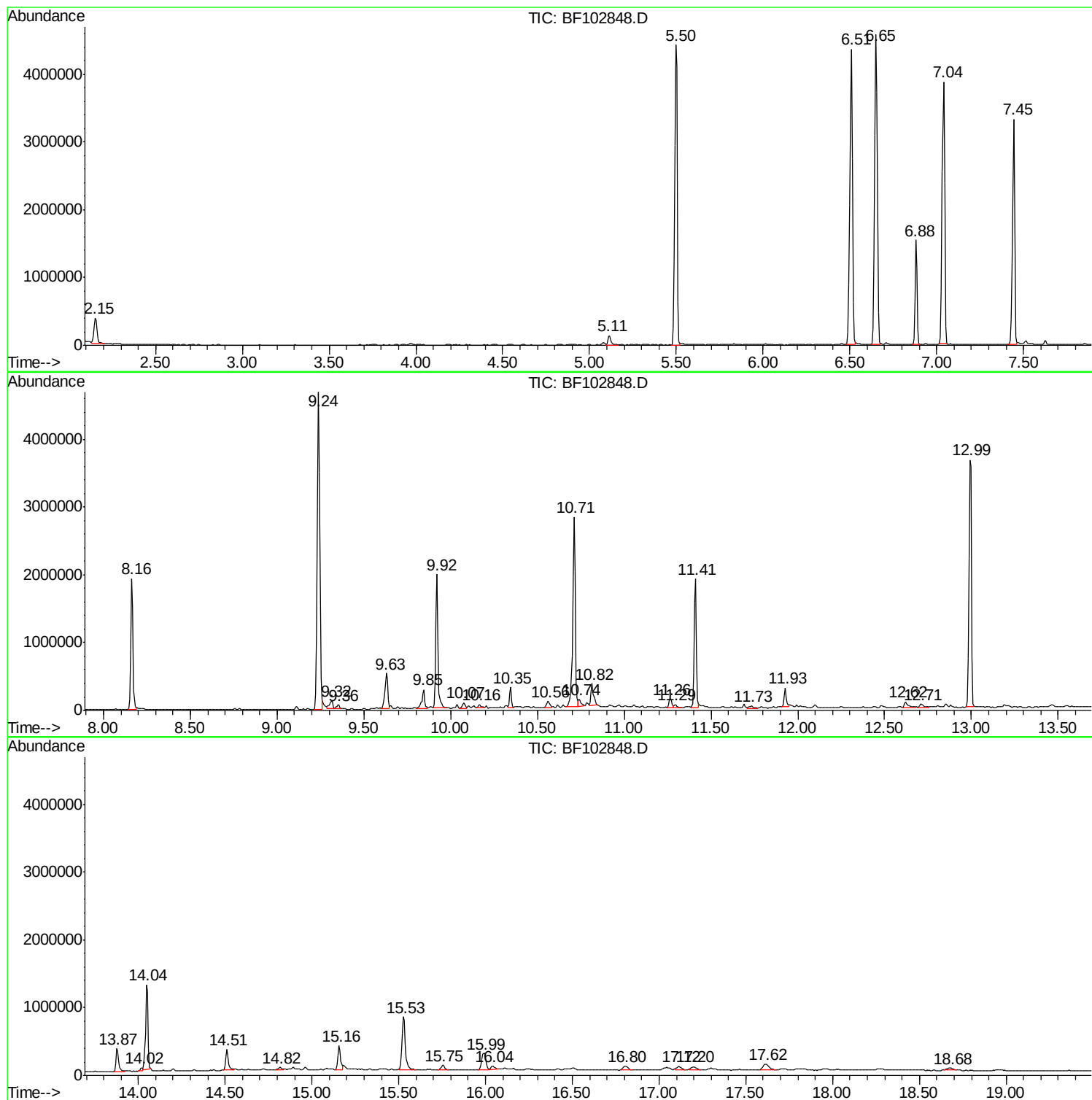
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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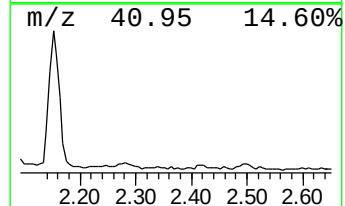
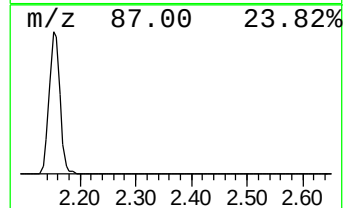
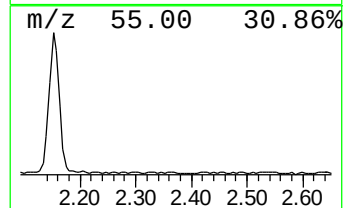
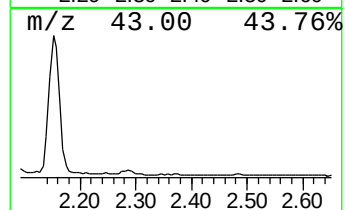
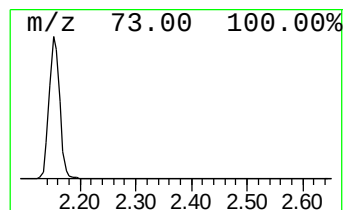
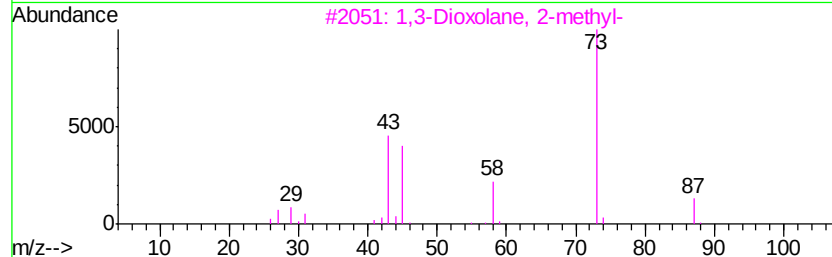
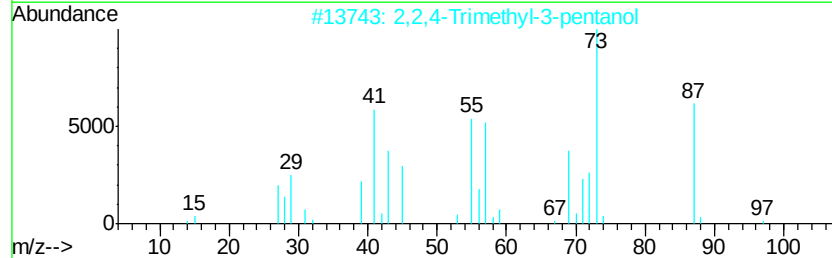
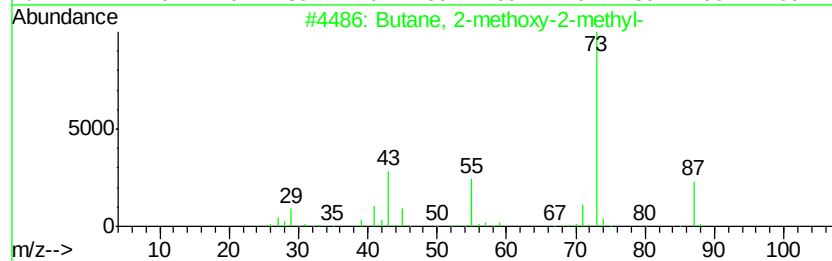
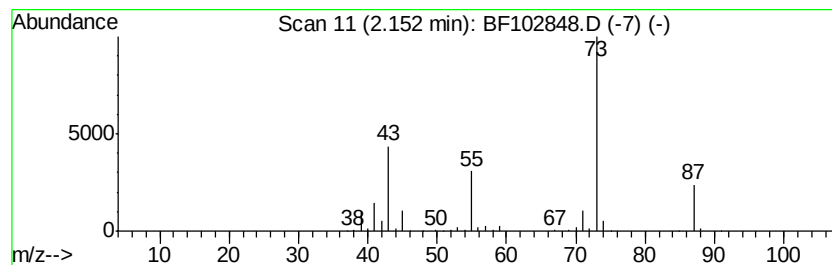
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	8.07 ng	516385	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	10



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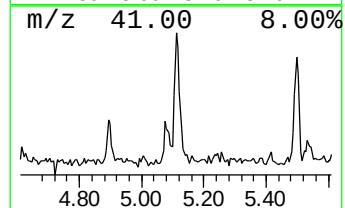
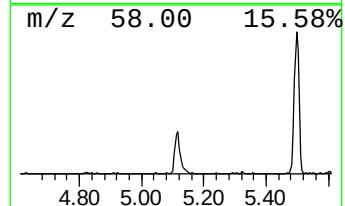
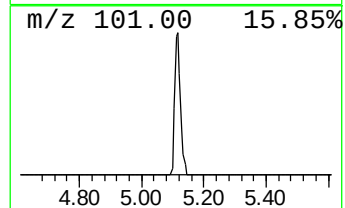
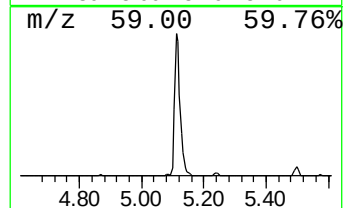
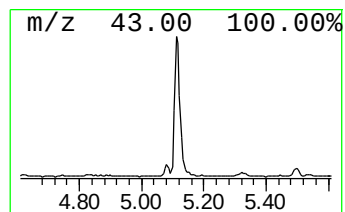
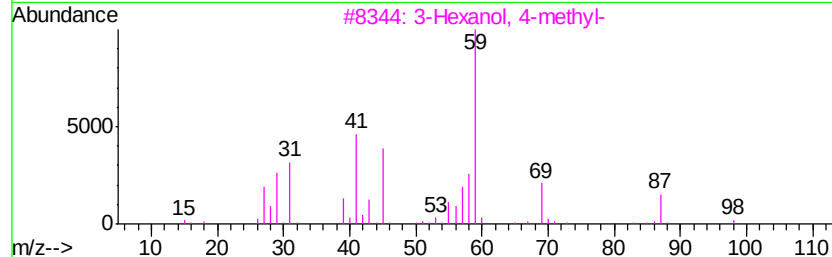
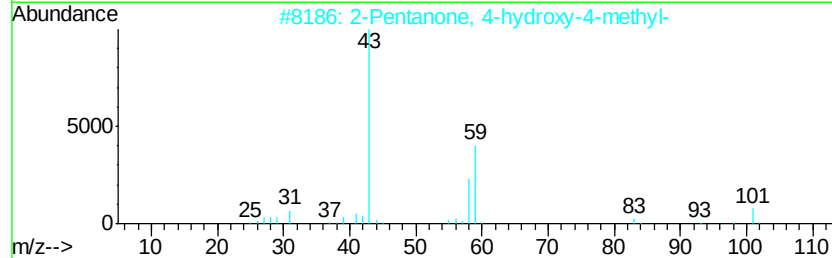
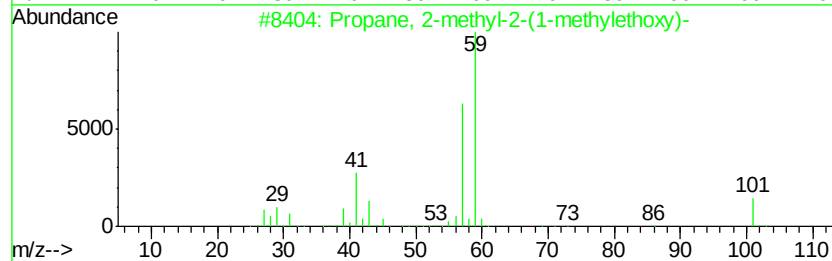
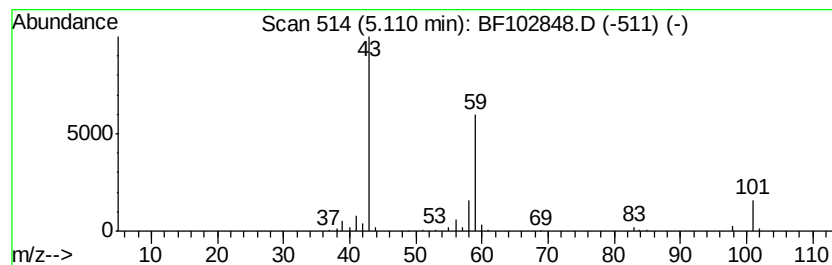
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 2-methyl-2-(1-meth... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	2.72 ng	174068	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5		1,2-Butanediol	90	C4H10O2	000584-03-2	28



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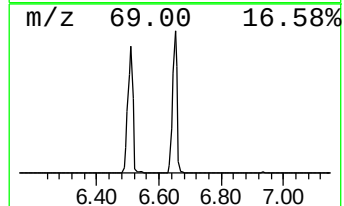
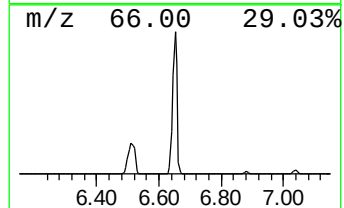
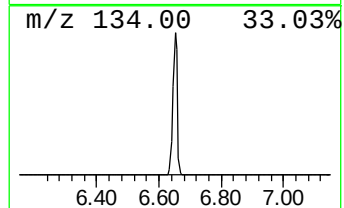
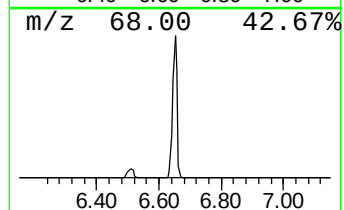
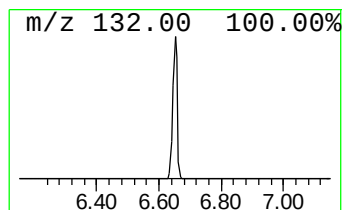
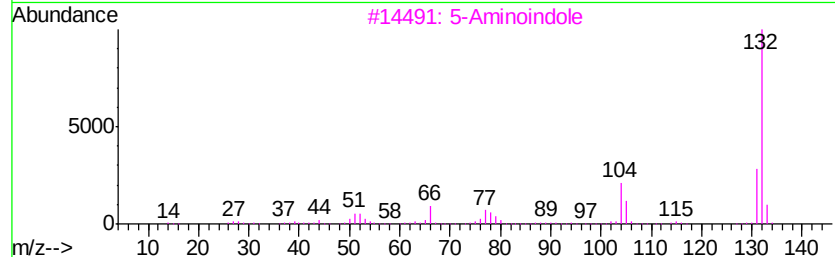
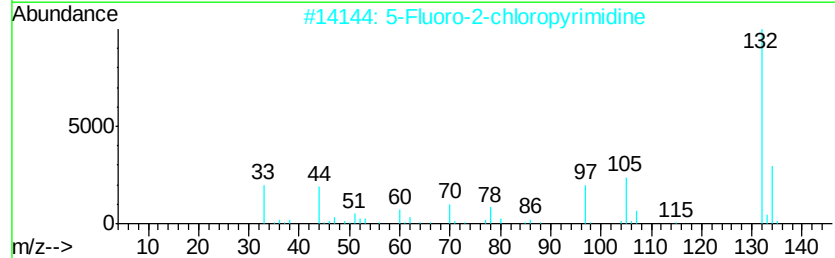
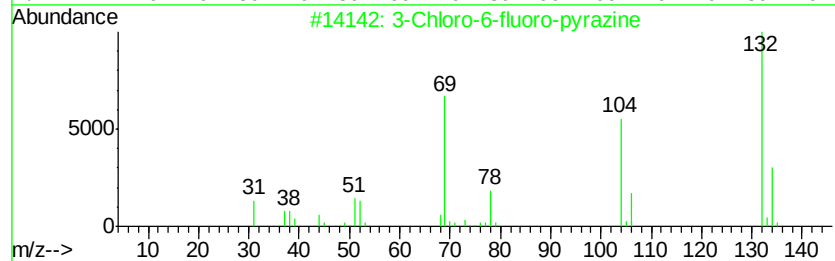
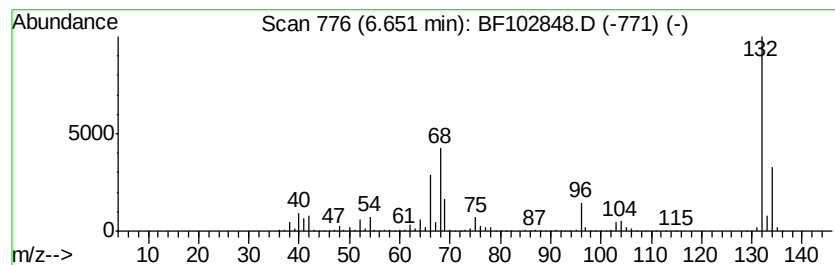
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	73.84 ng	4726340	1,4-Dichlorobenzene-d4	6.88

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		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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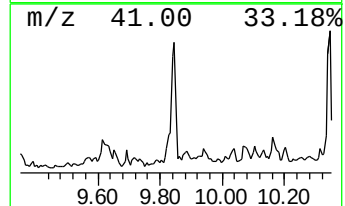
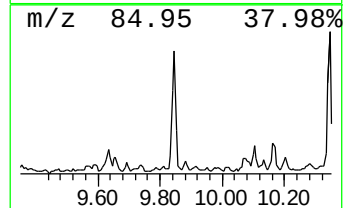
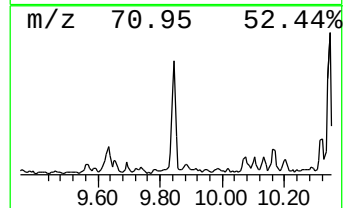
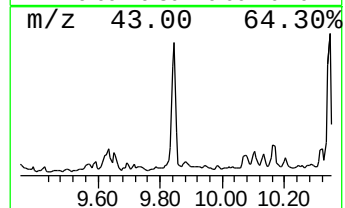
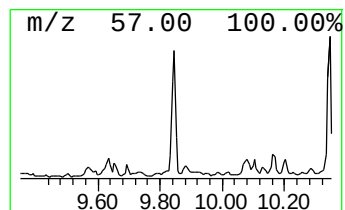
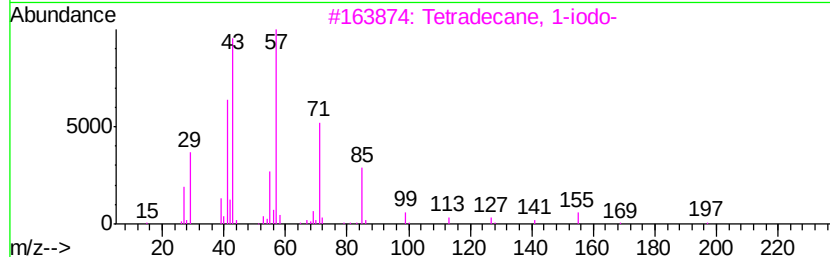
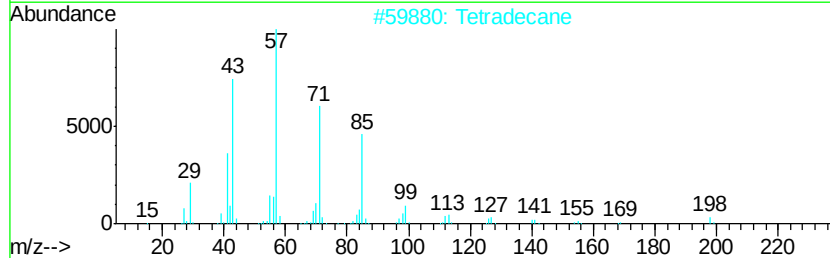
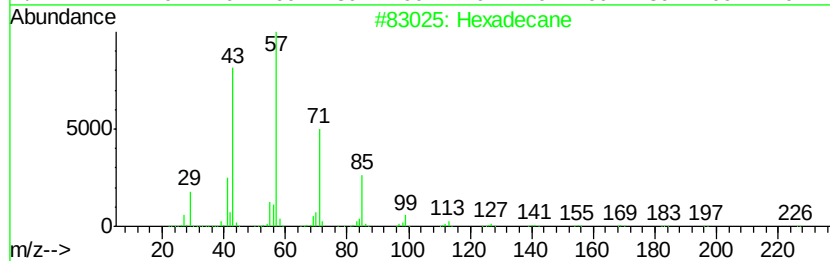
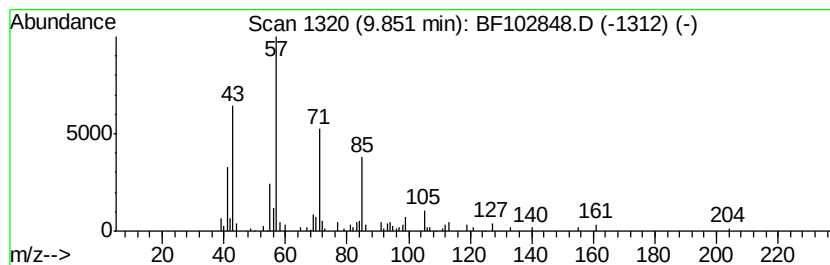
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.85	3.35 ng	310199	Acenaphthene-d10	9.92
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	91
2	Tetradecane	198 C14H30	000629-59-4	90
3	Tetradecane, 1-iodo-	324 C14H29I	019218-94-1	86
4	Sulfurous acid, 2-ethylhexyl hex...	278 C14H30O3S	1000309-20-2	78
5	Decane, 2,4-dimethyl-	170 C12H26	002801-84-5	78



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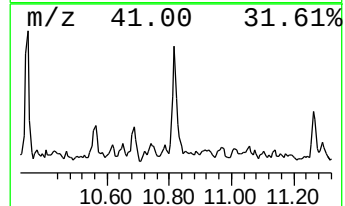
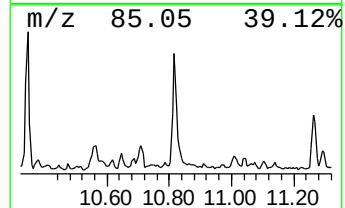
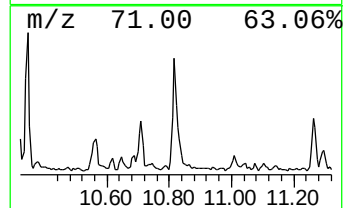
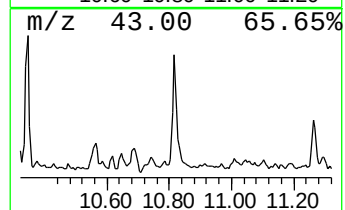
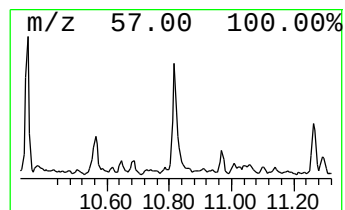
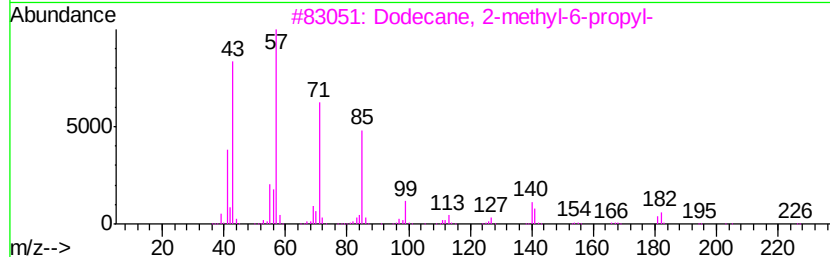
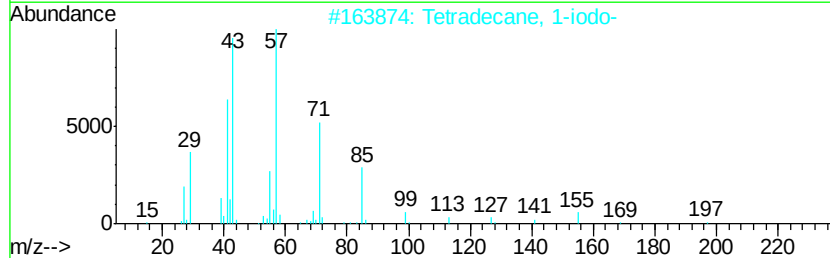
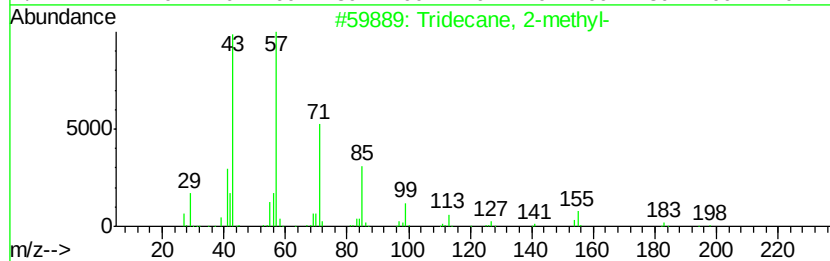
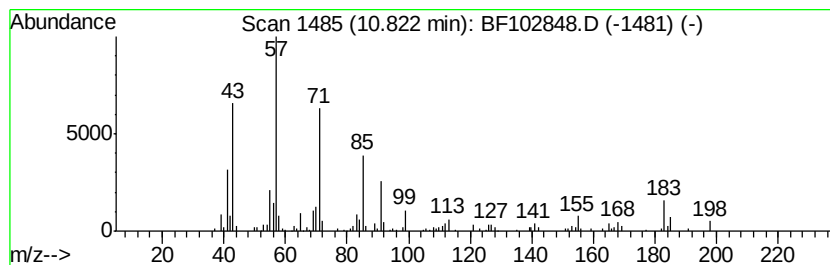
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tridecane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.82	3.75 ng	322061	Phenanthrene-d10		11.41
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 2-methyl-	198	C14H30	001560-96-9	64
2	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	64
3	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	64
4	Decane, 3-methyl-	156	C11H24	013151-34-3	58
5	Heptacosane	380	C27H56	000593-49-7	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
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Operator : SJ/JU
Sample : J1469-01
Misc :
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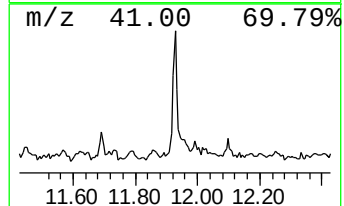
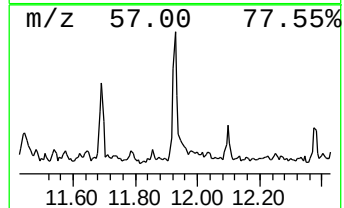
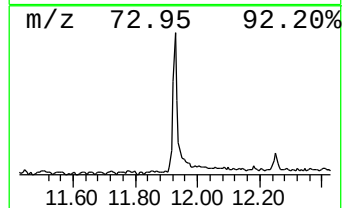
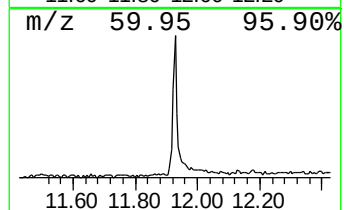
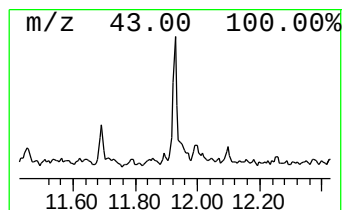
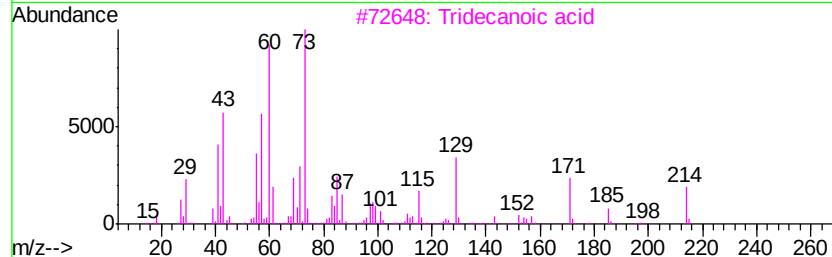
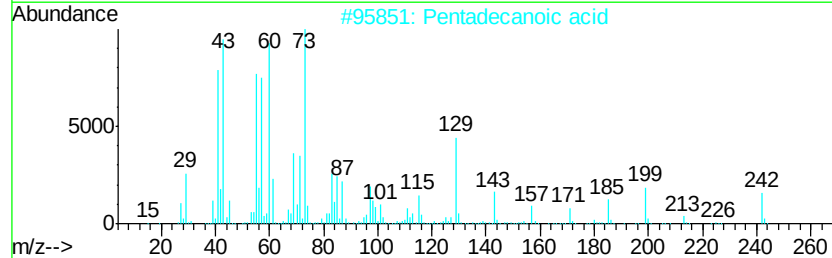
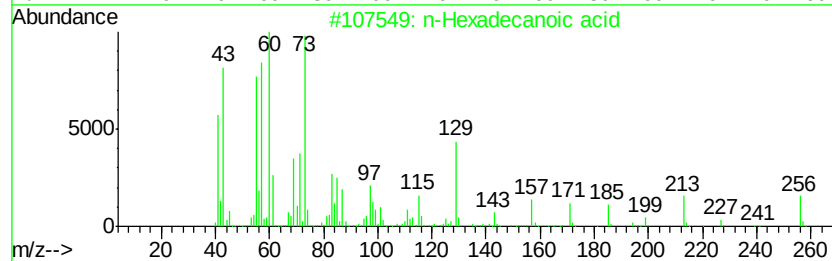
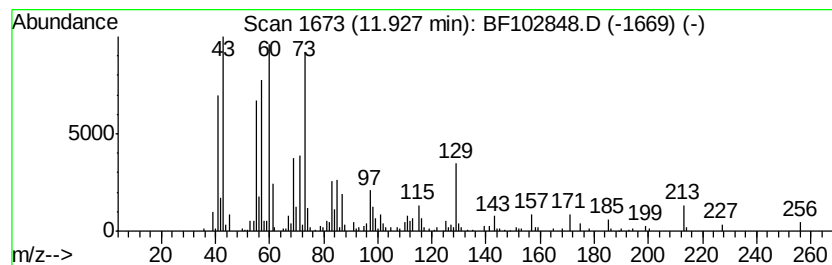
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.93	3.12 ng	267844	Phenanthrene-d10	11.41	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
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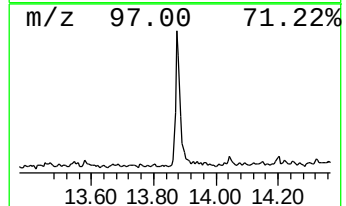
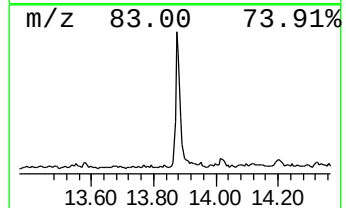
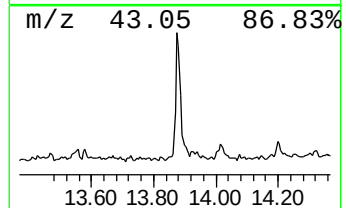
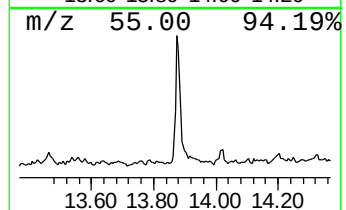
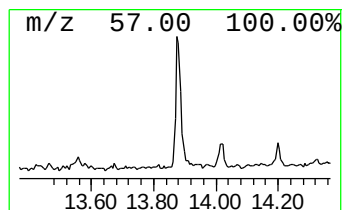
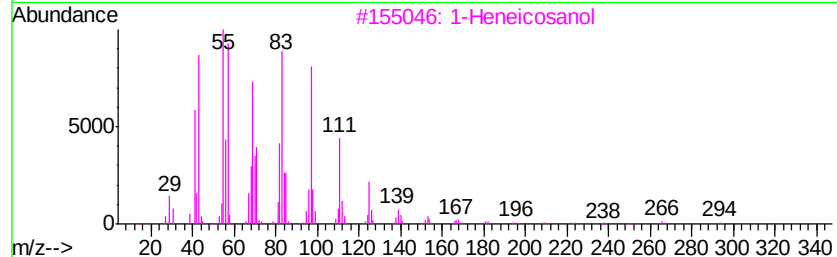
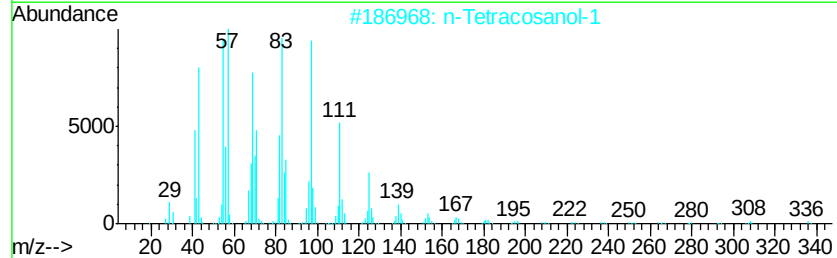
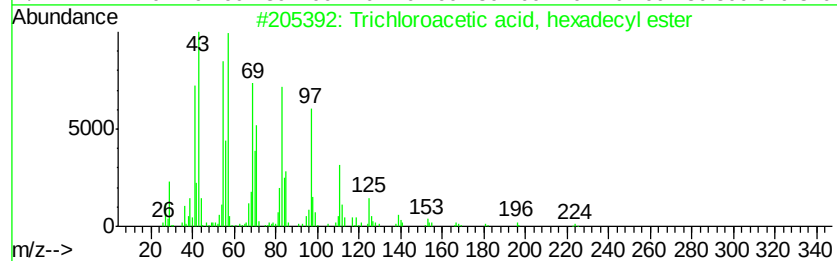
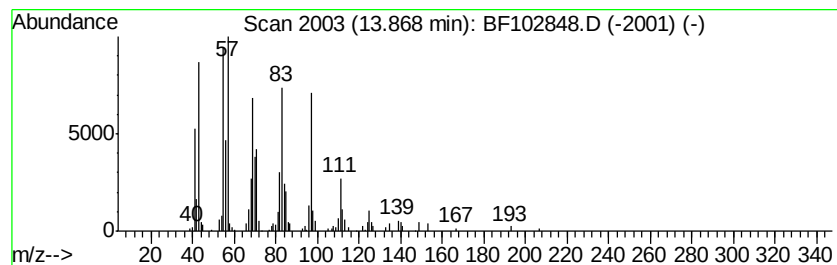
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Trichloroacetic acid, hexad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	6.57 ng	390709	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3		1-Heneicosanol	312	C21H44O	015594-90-8	94
4		Octacosanol	410	C28H58O	000557-61-9	94
5		Behenic alcohol	326	C22H46O	000661-19-8	94



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Acq On : 8 Feb 2018 11:42
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Sample : J1469-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

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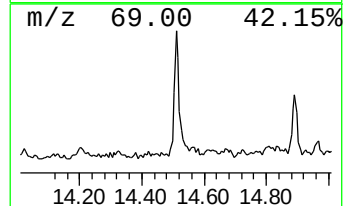
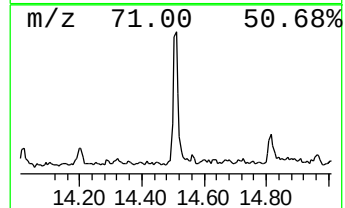
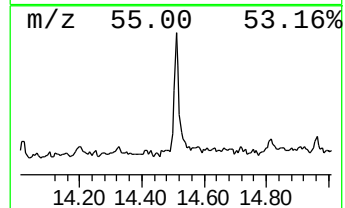
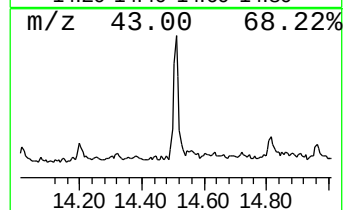
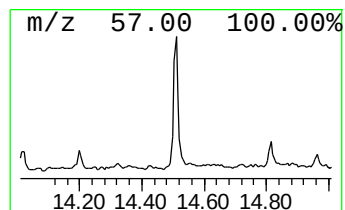
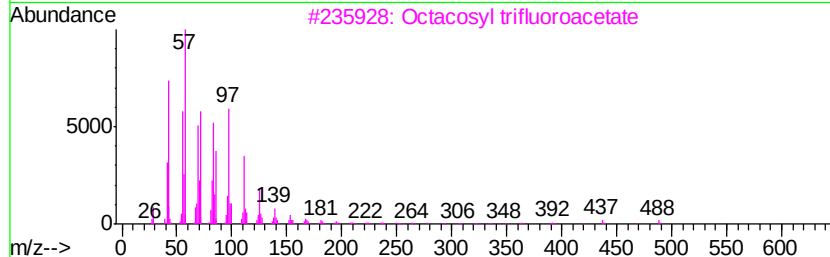
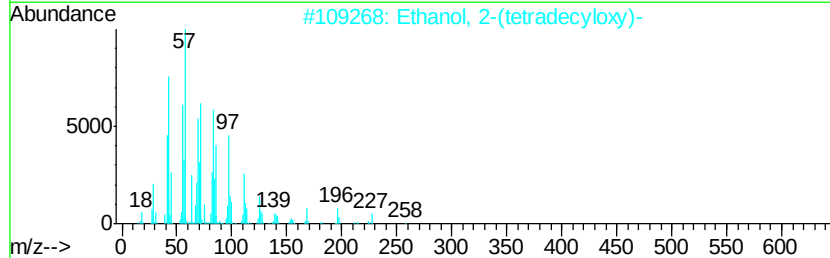
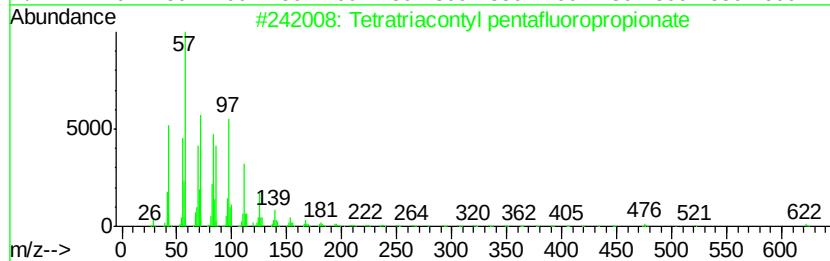
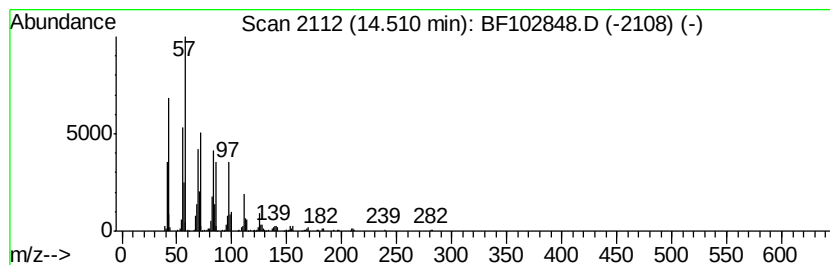
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tetratriacontyl pentafluoro... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.51	5.81 ng	345854	Chrysene-d12	14.04

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	91
2			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
4			Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1000351-81-4	91
5			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91



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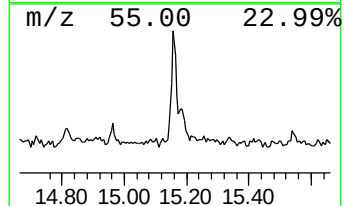
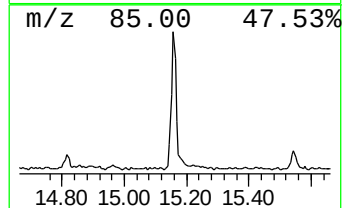
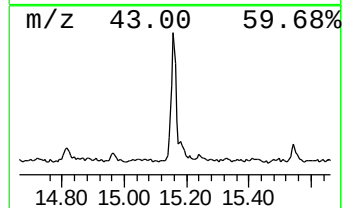
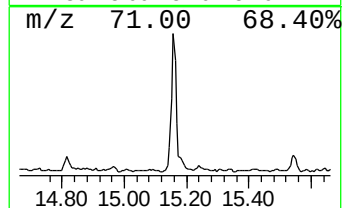
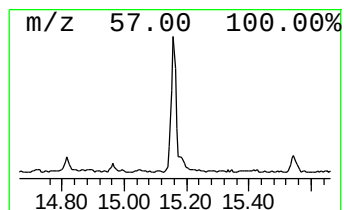
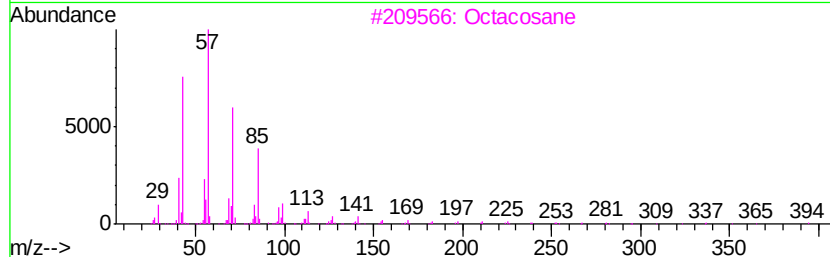
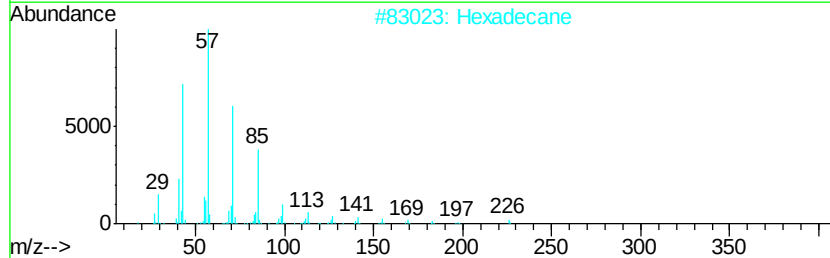
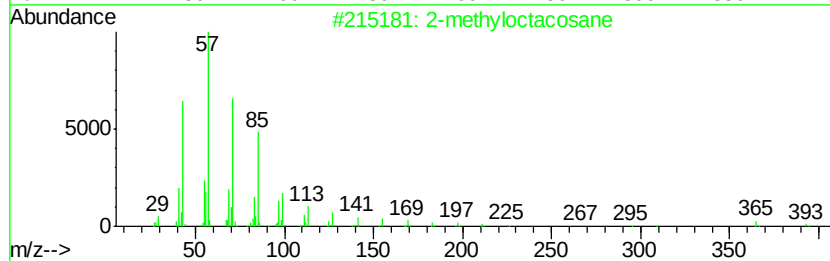
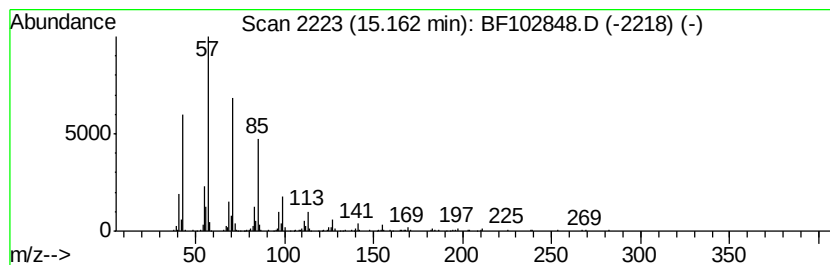
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2-methyloctacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	6.97 ng	382311	Perylene-d12	15.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	90
2		Hexadecane	226	C16H34	000544-76-3	87
3		Octacosane	394	C28H58	000630-02-4	87
4		Heptadecane	240	C17H36	000629-78-7	86
5		Undecane, 3-methyl-	170	C12H26	001002-43-3	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102848.D
Acq On : 8 Feb 2018 11:42
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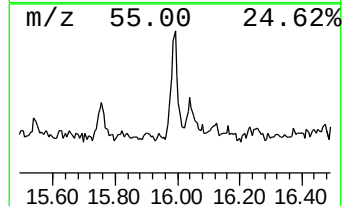
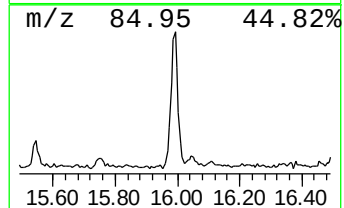
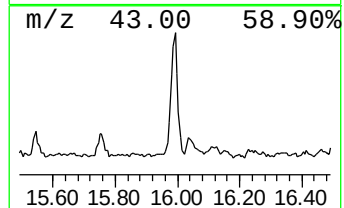
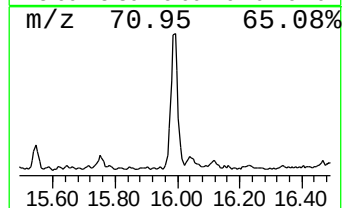
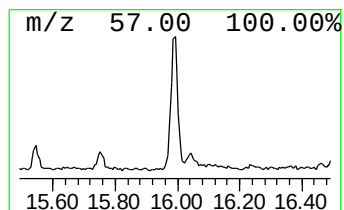
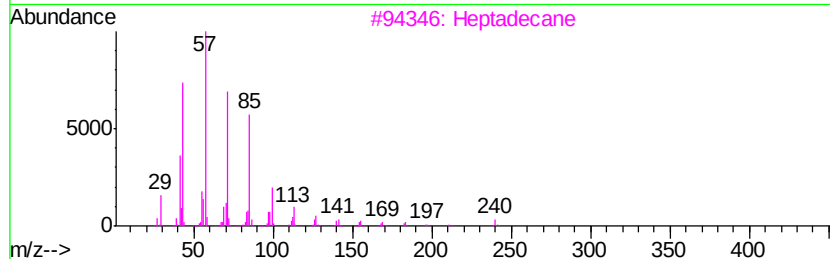
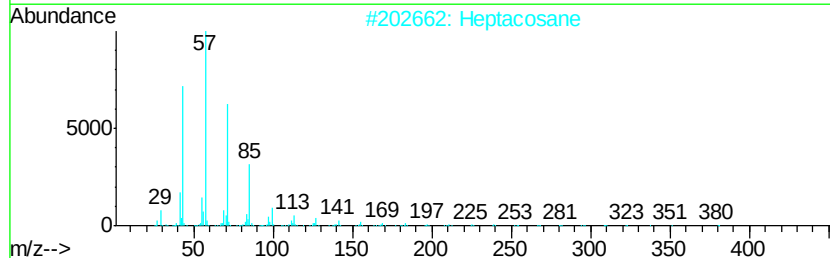
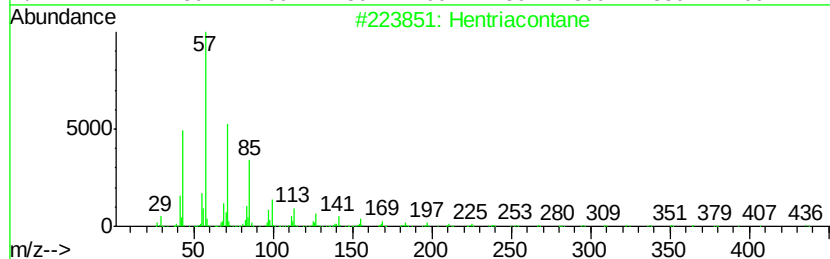
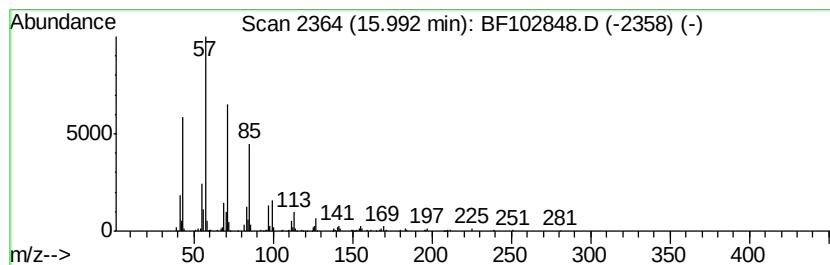
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hentriacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.99	6.70 ng	367312	Perylene-d12	15.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hentriacontane	437	C31H64	000630-04-6	91
2		Heptacosane	380	C27H56	000593-49-7	87
3		Heptadecane	240	C17H36	000629-78-7	86
4		Tridecane, 3-methyl-	198	C14H30	006418-41-3	86
5		Octacosane	394	C28H58	000630-02-4	81



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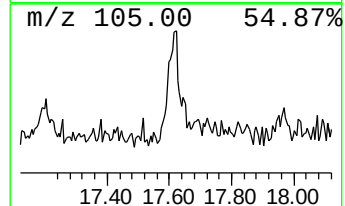
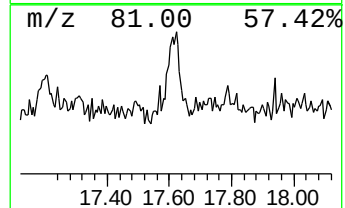
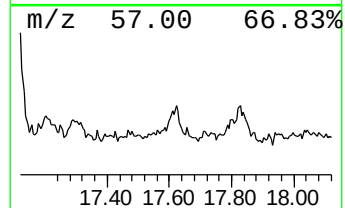
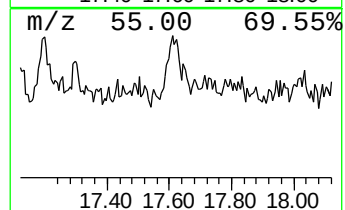
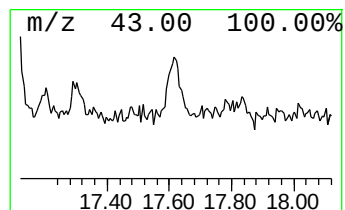
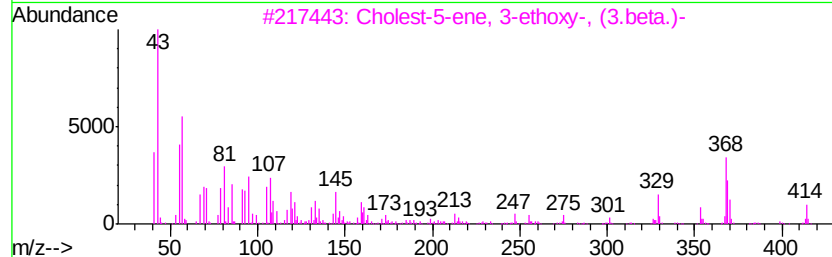
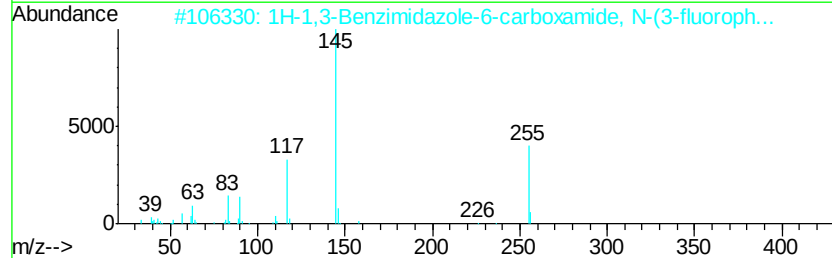
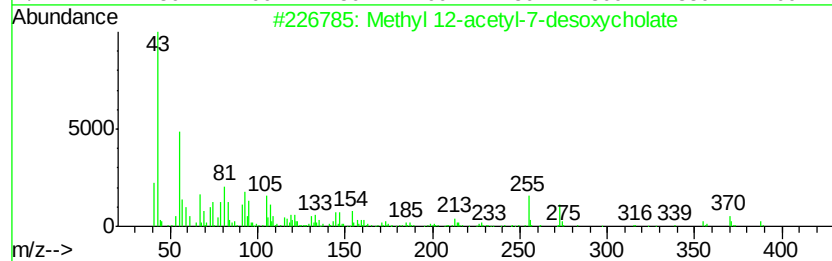
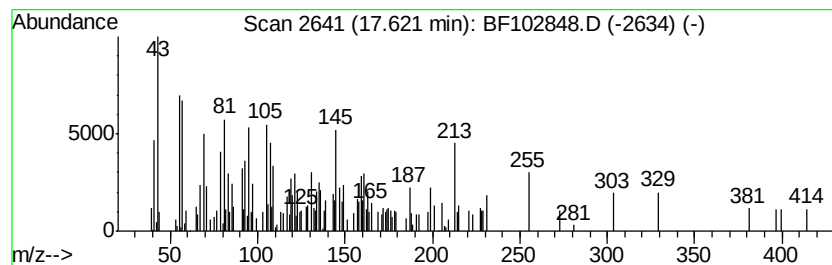
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown17.62 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.62	3.67 ng	201216	Perylene-d12	15.53
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Methyl 12-acetyl-7-desoxycholate	448 C27H44O5	055547-48-3 25
2		1H-1,3-Benzimidazole-6-carboxami...	255 C14H10FN3O	1000350-37-6 25
3		Cholest-5-ene, 3-ethoxy-, (3.beta...	414 C29H50O	000986-19-6 16
4		.beta.-Sitosterol acetate	456 C31H52O2	000915-05-9 16
5		Norflurazon	303 C12H9ClF3N3O	027314-13-2 10



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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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...	2.15	8.1 ng		516385	1	6.88	1280220	20.0
Propane, 2-methyl...	5.11	2.7 ng		174068	1	6.88	1280220	20.0
unknown6.65	6.65	73.8 ng		4726340	1	6.88	1280220	20.0
Hexadecane	9.85	3.4 ng		310199	3	9.92	1852850	20.0
Tridecane, 2-methyl-	10.82	3.8 ng		322061	4	11.41	1718080	20.0
n-Hexadecanoic acid	11.93	3.1 ng		267844	4	11.41	1718080	20.0
Trichloroacetic a...	13.87	6.6 ng		390709	5	14.04	1189790	20.0
Tetratriacontyl p...	14.51	5.8 ng		345854	5	14.04	1189790	20.0
2-methyloctacosane	15.16	7.0 ng		382311	6	15.53	1096630	20.0
Hentriacontane	15.99	6.7 ng		367312	6	15.53	1096630	20.0
unknown17.62	17.62	3.7 ng		201216	6	15.53	1096630	20.0