

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022718\
 Data File : BF103273.D
 Acq On : 27 Feb 2018 19:48
 Operator : SJ/JU
 Sample : J1672-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 72-11977-72-11982

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-BF022218.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	2.158	5	12	19	rVB	330229	449155	10.55%	1.091%
2	3.557	230	250	251	rBV	690110	3328988	78.21%	8.089%
3	5.116	512	515	529	rVB	153200	209012	4.91%	0.508%
4	5.510	577	582	592	rBV	3785408	4256599	100.00%	10.343%
5	6.522	748	754	757	rBV	3238772	4087104	96.02%	9.931%
6	6.651	771	776	780	rBV	3790472	4009982	94.21%	9.744%
7	6.875	810	814	822	rBV	1139254	997651	23.44%	2.424%
8	7.034	836	841	844	rBV	3199839	3038000	71.37%	7.382%
9	7.440	905	910	914	rBV	2515221	2733767	64.22%	6.643%
10	8.157	1028	1032	1044	rBV	1450561	1270723	29.85%	3.088%
11	8.263	1047	1050	1063	rBV	24126	59049	1.39%	0.143%
12	9.234	1210	1215	1218	rBV	4059590	3844168	90.31%	9.341%
13	9.410	1237	1245	1248	rBV	679955	1135700	26.68%	2.760%
14	9.622	1276	1281	1287	rBV	366204	320137	7.52%	0.778%
15	9.828	1313	1316	1319	rBV	125577	102051	2.40%	0.248%
16	9.863	1319	1322	1324	rVV	73828	66287	1.56%	0.161%
17	9.892	1324	1327	1328	rVV	321963	249939	5.87%	0.607%
18	9.916	1328	1331	1334	rVV	1386640	1261924	29.65%	3.066%
19	9.945	1334	1336	1339	rVB	57139	43985	1.03%	0.107%
20	10.328	1399	1401	1404	rVB	139743	111856	2.63%	0.272%
21	10.551	1433	1439	1442	rBV	34976	45091	1.06%	0.110%
22	10.710	1462	1466	1469	rBV	2037576	1979510	46.50%	4.810%
23	10.804	1479	1482	1487	rBV	78719	68708	1.61%	0.167%
24	11.210	1548	1551	1556	rBV	82230	121812	2.86%	0.296%
25	11.404	1580	1584	1587	rBV	1138236	1053734	24.76%	2.560%
26	11.428	1587	1588	1592	rVB	174210	122329	2.87%	0.297%
27	11.922	1667	1672	1677	rBV2	115933	169643	3.99%	0.412%
28	12.375	1745	1749	1756	rBV	201471	281492	6.61%	0.684%
29	12.622	1788	1791	1795	rBV	186818	170494	4.01%	0.414%
30	12.851	1825	1830	1832	rBV	131147	148515	3.49%	0.361%
31	12.869	1832	1833	1842	rVB4	86220	105408	2.48%	0.256%
32	12.992	1849	1854	1857	rBV	2728349	2721595	63.94%	6.613%
33	13.404	1921	1924	1929	rBV	202217	270986	6.37%	0.658%
34	13.869	2000	2003	2015	rVB	472057	535737	12.59%	1.302%

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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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.057	2030	2035	2044	rVB	803677	853497	20.05%	2.074%
36	14.139	2047	2049	2052	rBV2	82968	70315	1.65%	0.171%
37	14.321	2077	2080	2085	rBV	82369	113255	2.66%	0.275%
38	14.892	2175	2177	2187	rVB	93070	118420	2.78%	0.288%
39	15.563	2286	2291	2298	rVB	462902	627867	14.75%	1.526%

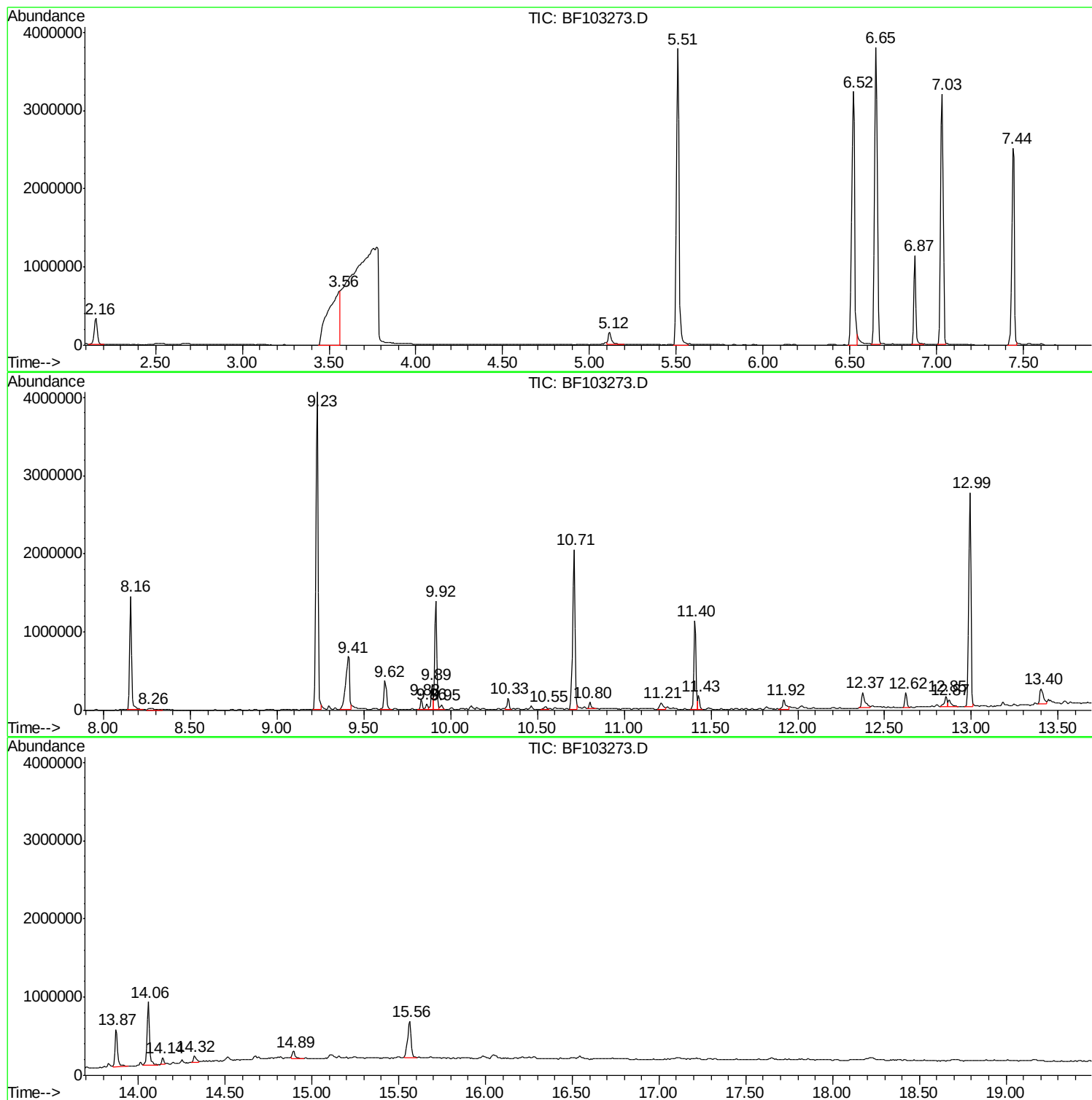
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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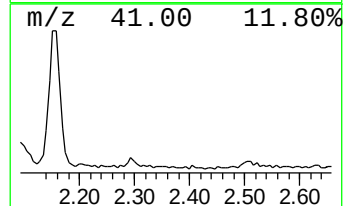
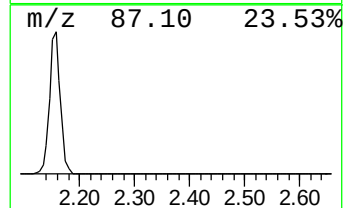
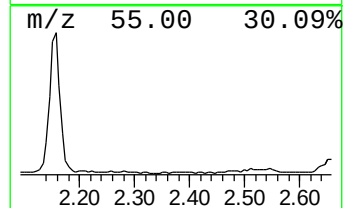
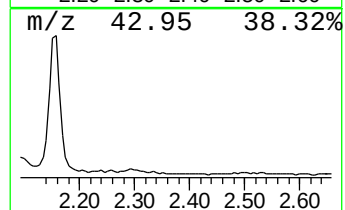
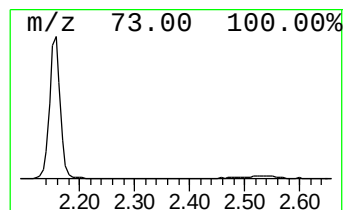
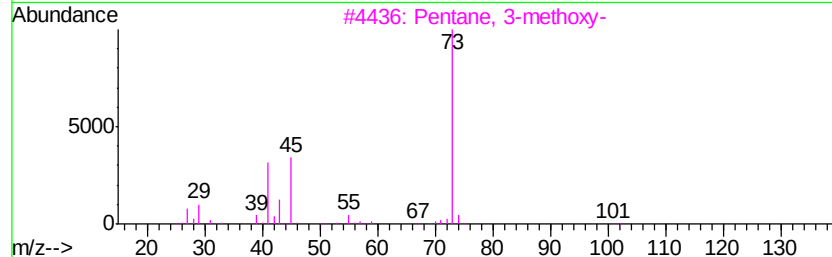
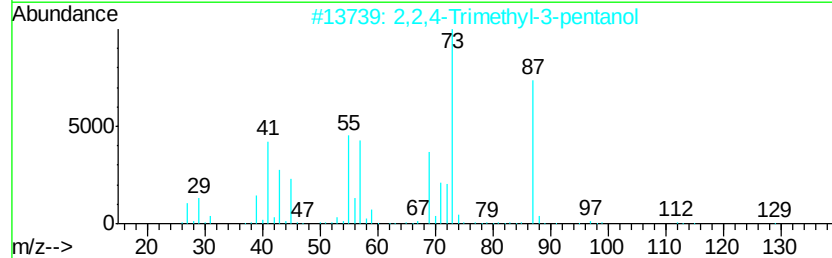
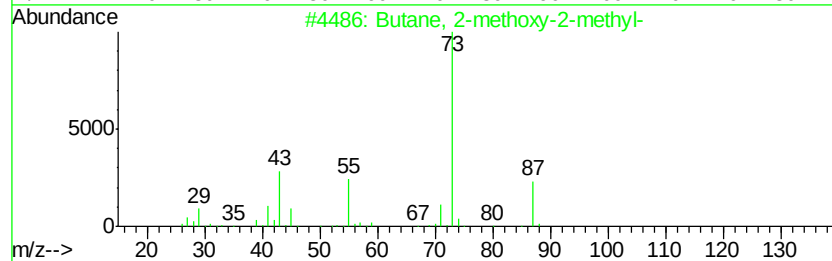
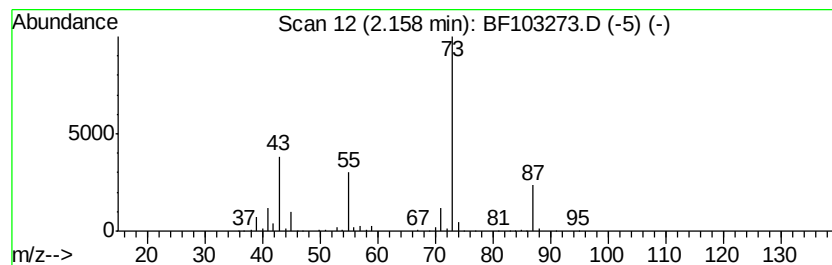
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	9.00 ng	449155	1,4-Dichlorobenzene-d4	6.87

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	40
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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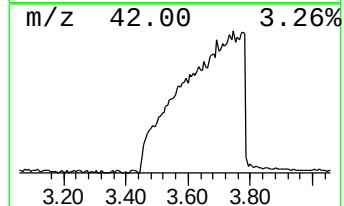
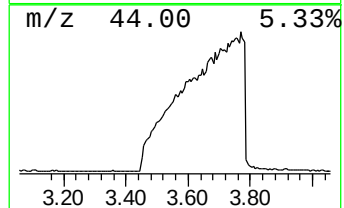
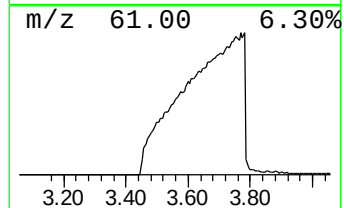
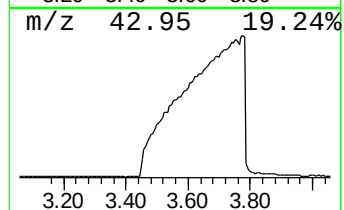
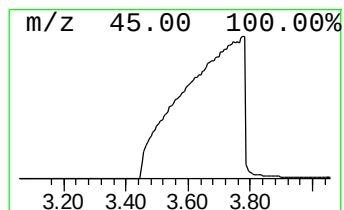
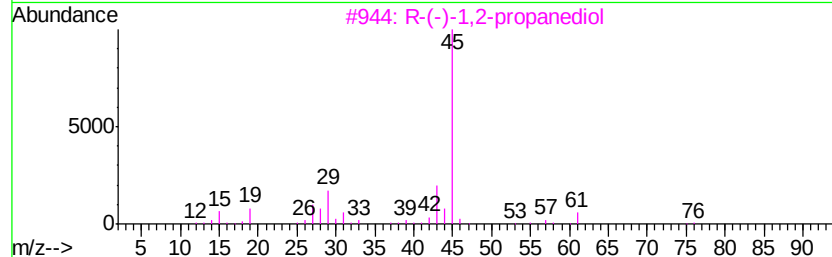
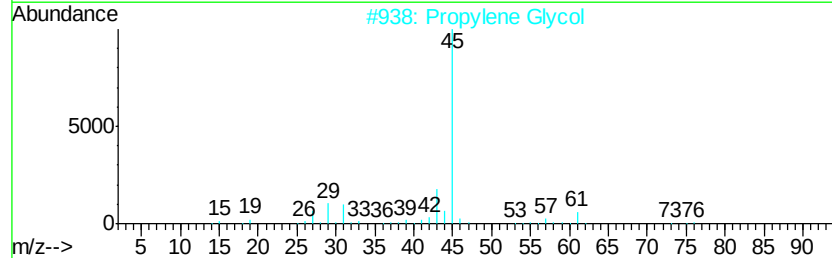
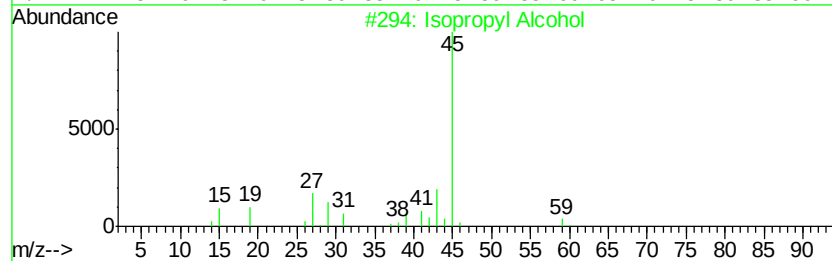
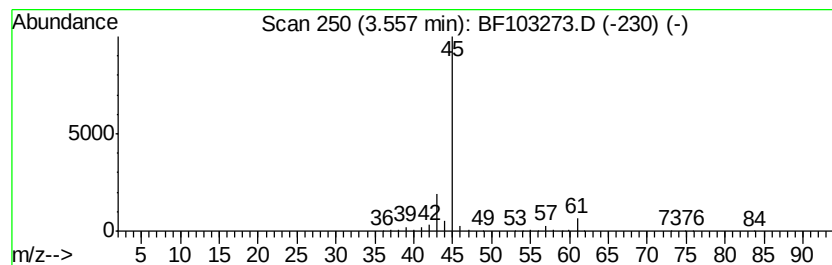
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Isopropyl Alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.56	66.74 ng	3328990	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
2		Propylene Glycol	76	C3H8O2	000057-55-6	43
3		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
4		Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9
5		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9



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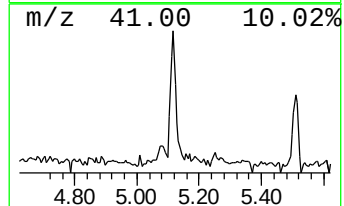
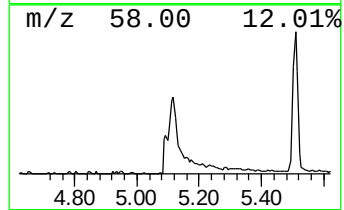
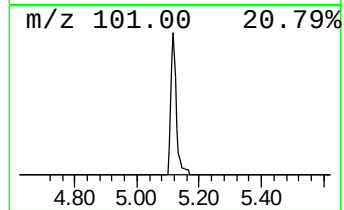
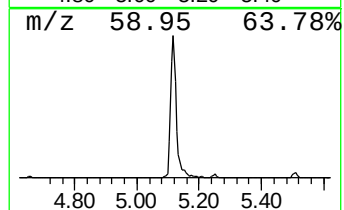
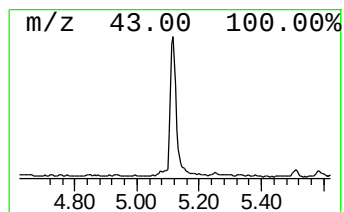
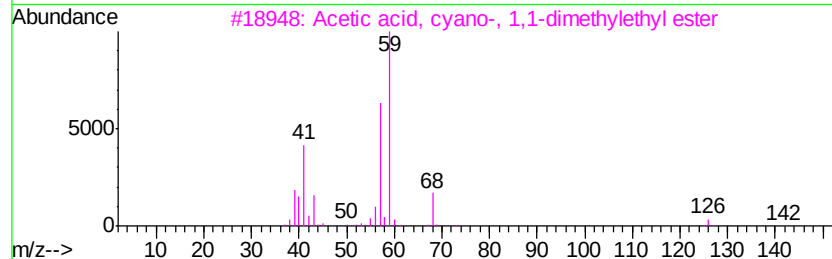
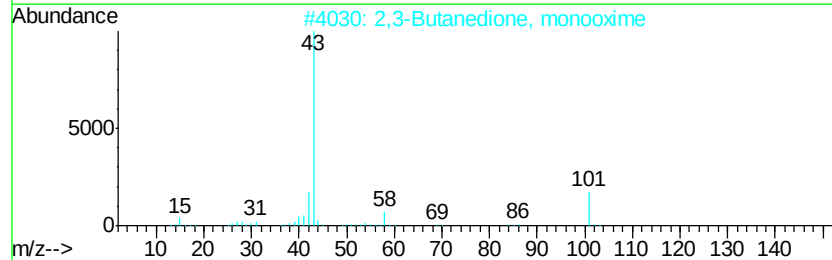
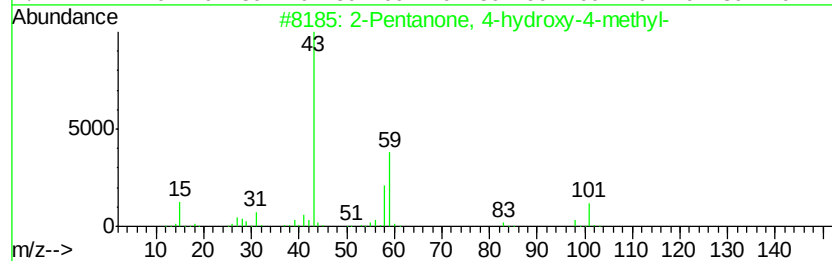
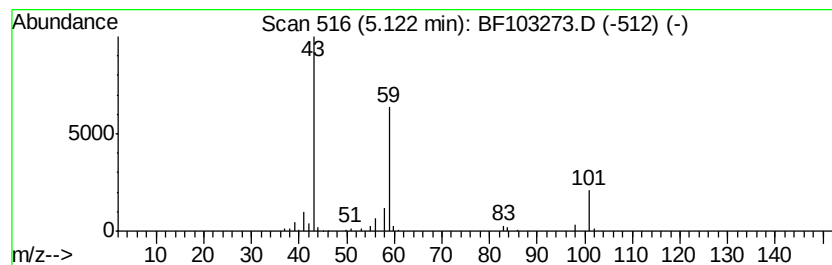
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	4.19 ng	209012	1,4-Dichlorobenzene-d4	6.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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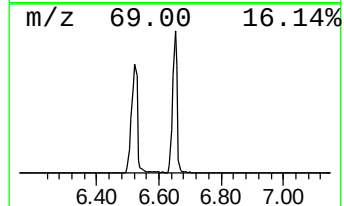
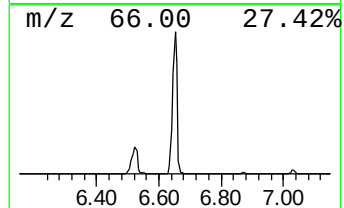
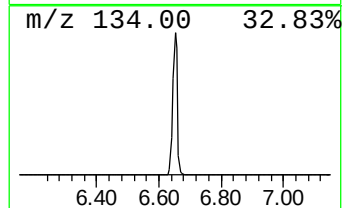
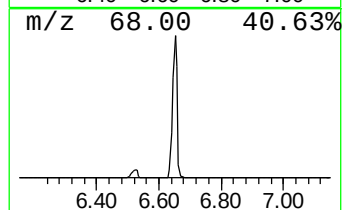
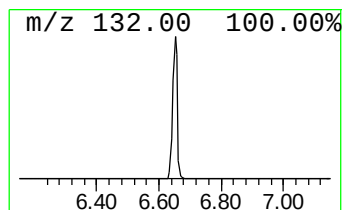
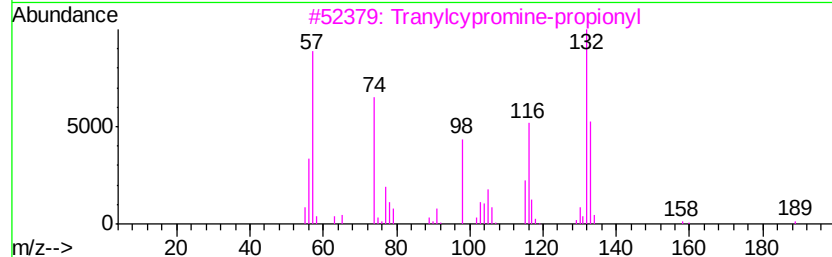
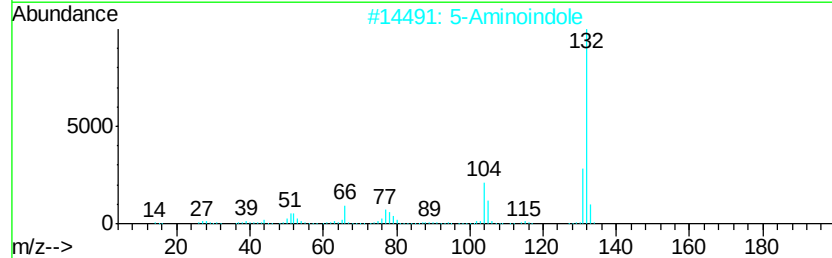
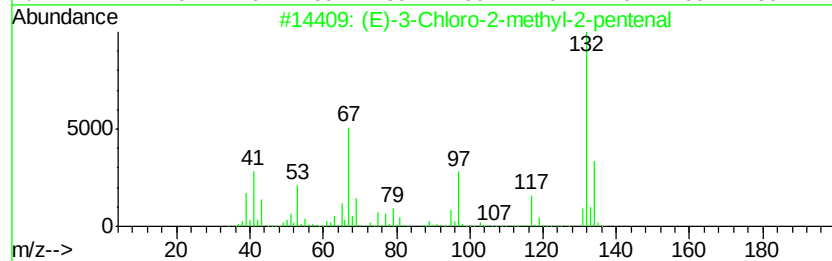
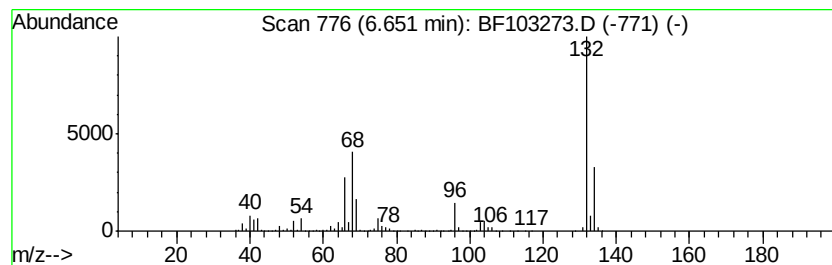
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	80.39 ng	4009980	1,4-Dichlorobenzene-d4	6.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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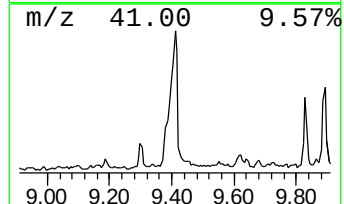
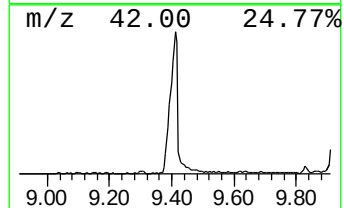
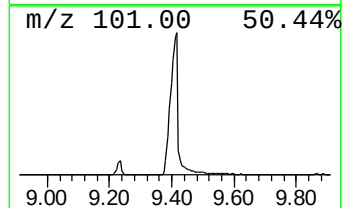
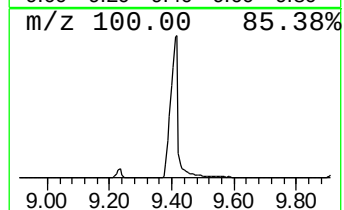
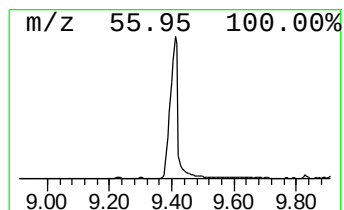
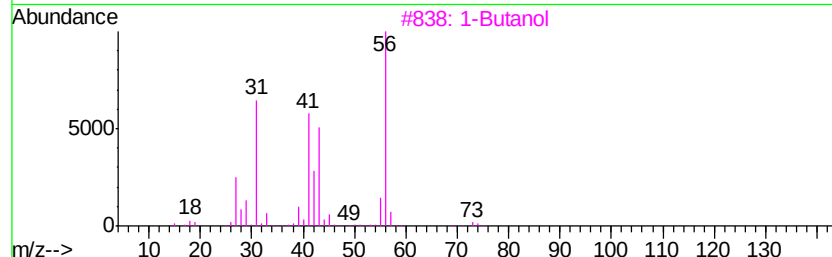
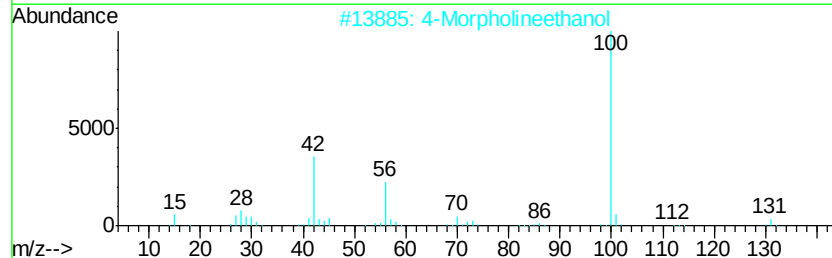
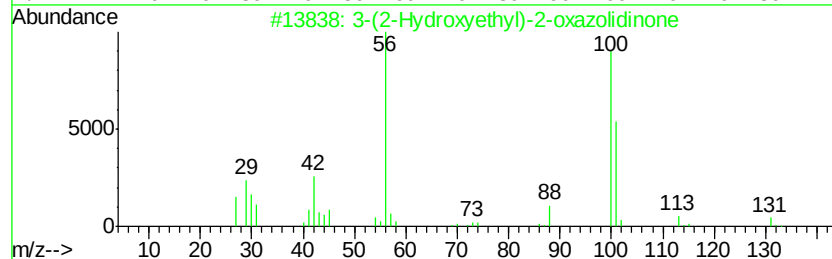
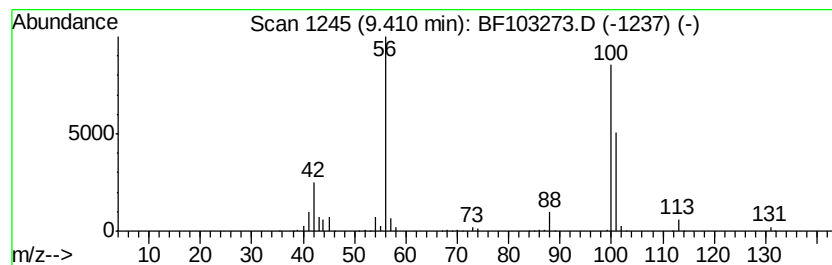
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 3-(2-Hydroxyethyl)-2-oxazol... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.41	18.00 ng	1135700	Acenaphthene-d10	9.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(2-Hydroxyethyl)-2-oxazolidinone	131	C5H9NO3	003356-88-5	83
2	4-Morpholineethanol	131	C6H13NO2	000622-40-2	35
3	1-Butanol	74	C4H10O	000071-36-3	27
4	Aminothiazole	100	C3H4N2S	000096-50-4	10
5	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022718\
Data File : BF103273.D
Acq On : 27 Feb 2018 19:48
Operator : SJ/JU
Sample : J1672-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11977-72-11982

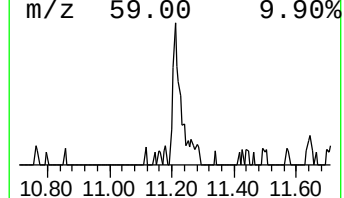
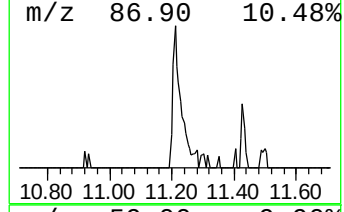
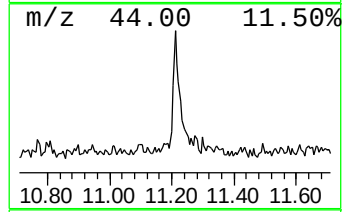
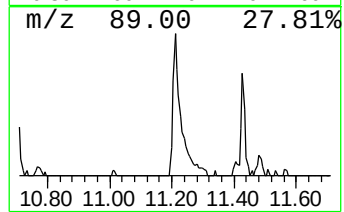
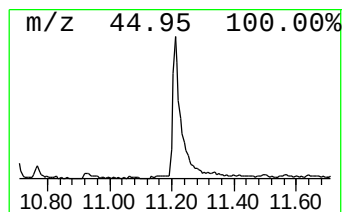
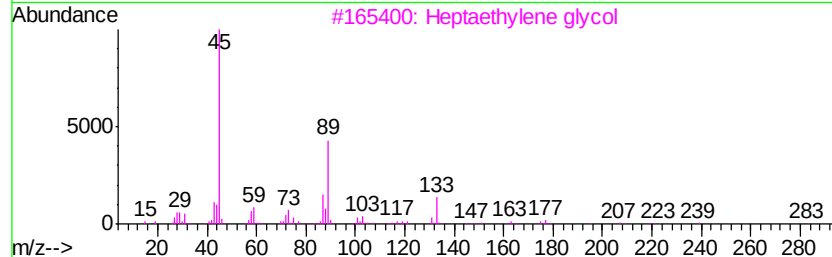
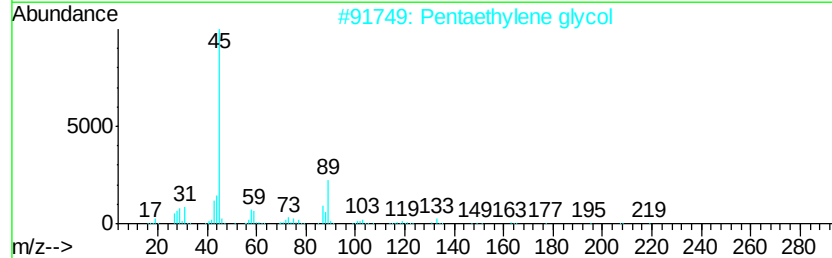
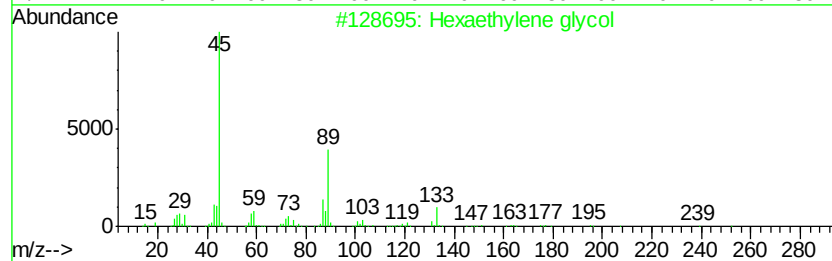
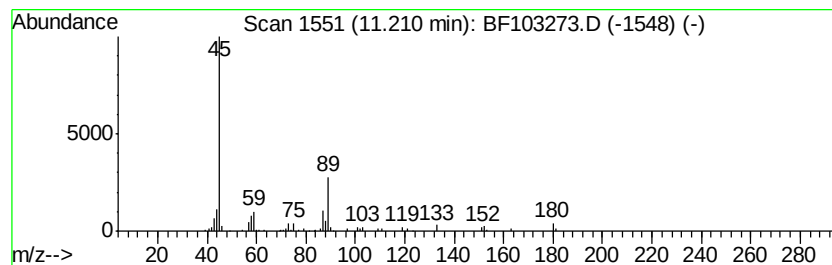
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexaethylene glycol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.21	2.31 ng	121812	Phenanthrene-d10	11.40

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexaethylene glycol	282	C12H26O7	002615-15-8	90
2			Pentaethylene glycol	238	C10H22O6	004792-15-8	80
3			Heptaethylene glycol	326	C14H30O8	005617-32-3	78
4			2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	78
5			2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	78



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022718\
Data File : BF103273.D
Acq On : 27 Feb 2018 19:48
Operator : SJ/JU
Sample : J1672-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

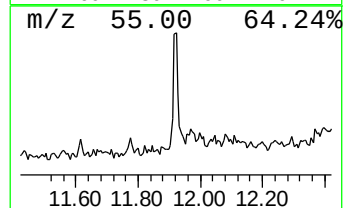
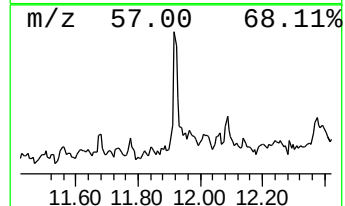
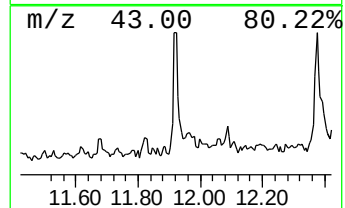
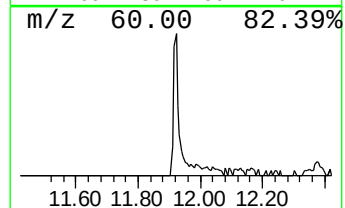
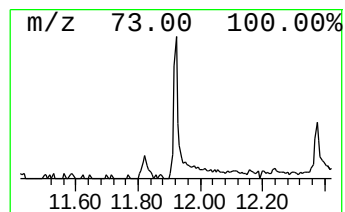
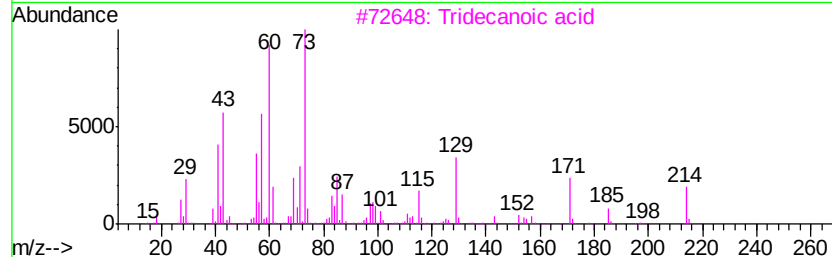
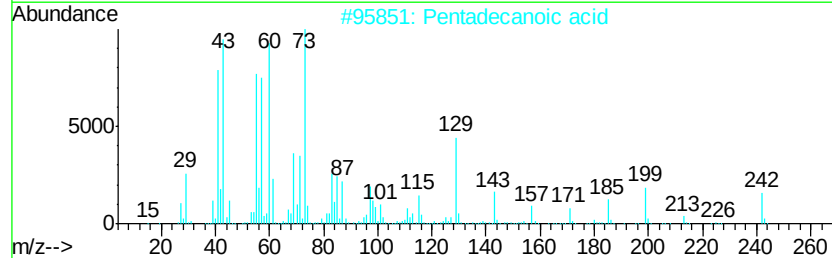
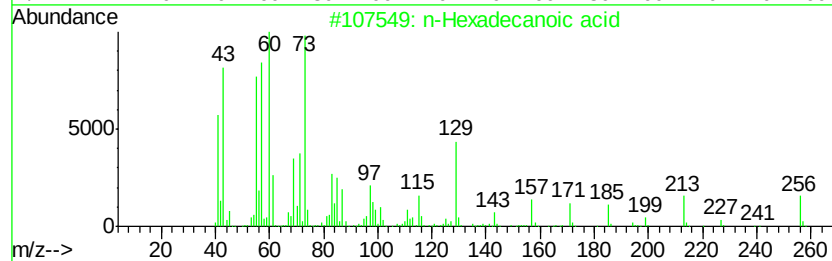
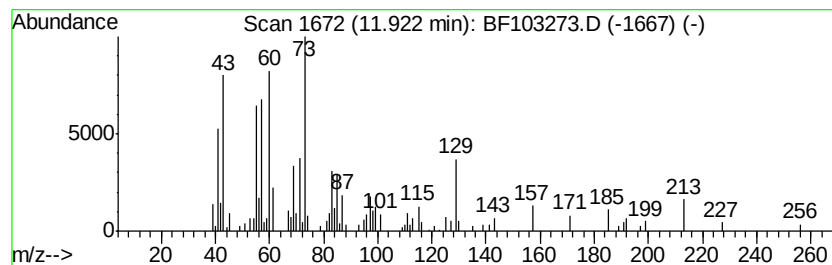
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.	
11.92	3.22 ng	169643	Phenanthrene-d10		11.40	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tridecanoic acid	214	C13H26O2	000638-53-9	80
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5		Dodecanoic acid	200	C12H24O2	000143-07-7	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF022718\
Data File : BF103273.D
Acq On : 27 Feb 2018 19:48
Operator : SJ/JU
Sample : J1672-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
72-11977-72-11982

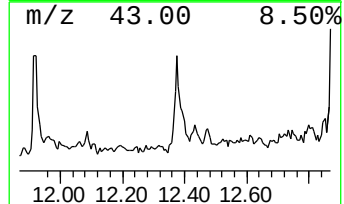
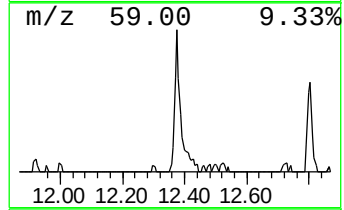
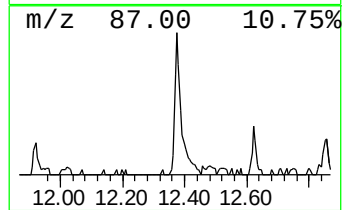
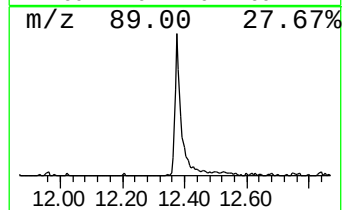
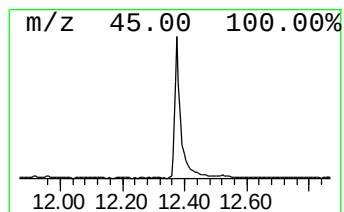
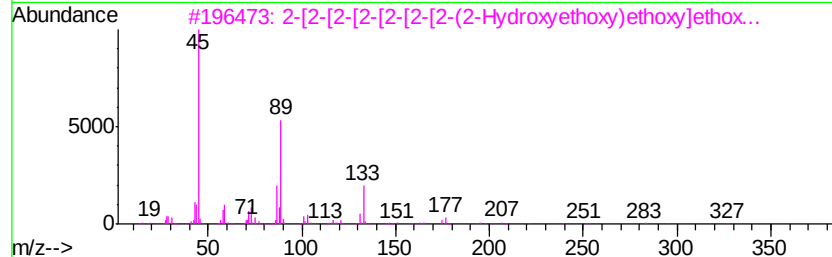
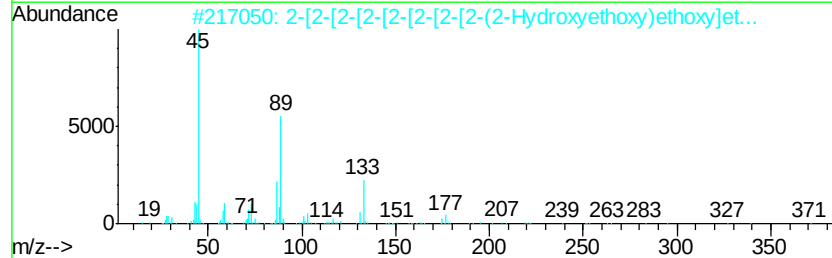
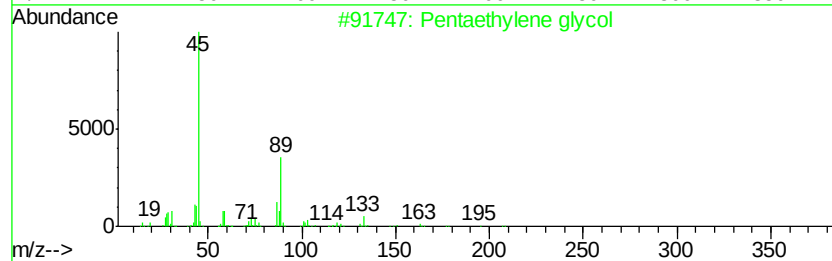
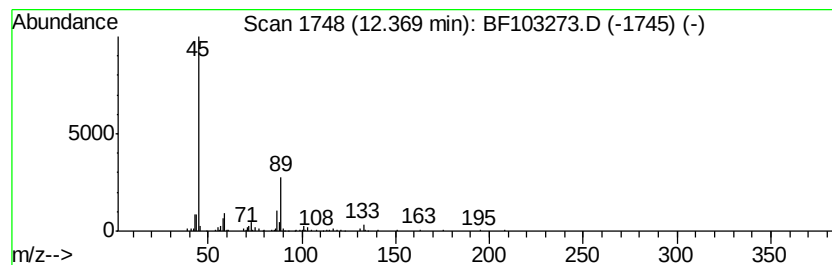
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentaethylene glycol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.37	5.34 ng	281492	Phenanthrene-d10	11.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentaethylene glycol	238	C10H22O6	004792-15-8	90
2		2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	90
3		2-[2-[2-[2-[2-[2-[2-(2-Hydroxvet...	370	C16H34O9	005117-19-1	83
4		Triethylene glycol	150	C6H14O4	000112-27-6	78
5		Tetraethyleneglycol monomethylether	208	C9H20O5	023783-42-8	78



Data Path : Z:\HPCHEM1\BNA F\DATA\BF022718\
Data File : BF103273.D
Acq On : 27 Feb 2018 19:48
Operator : SJ/JU
Sample : J1672-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

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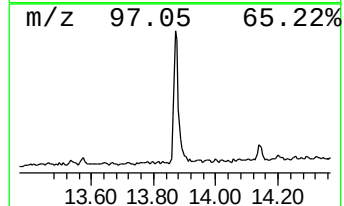
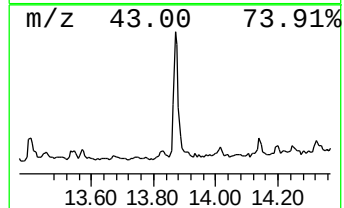
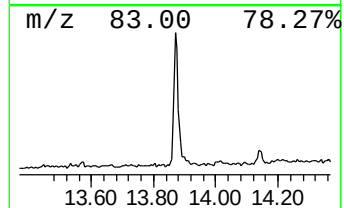
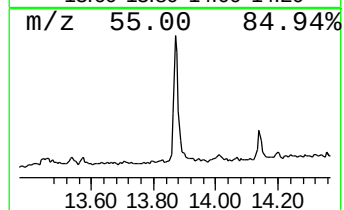
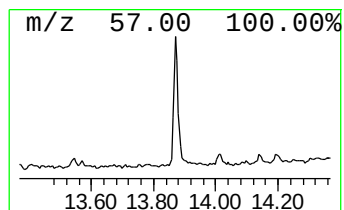
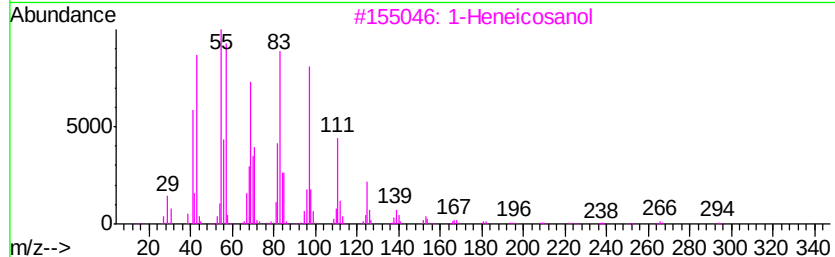
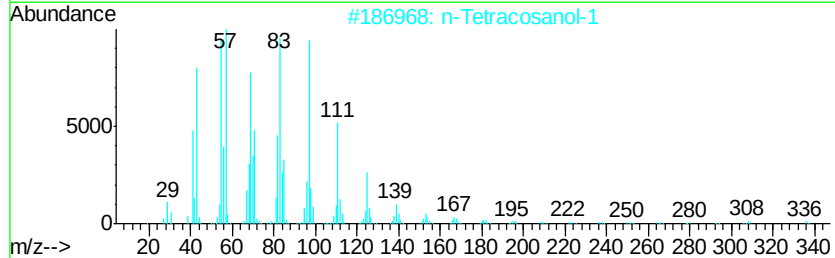
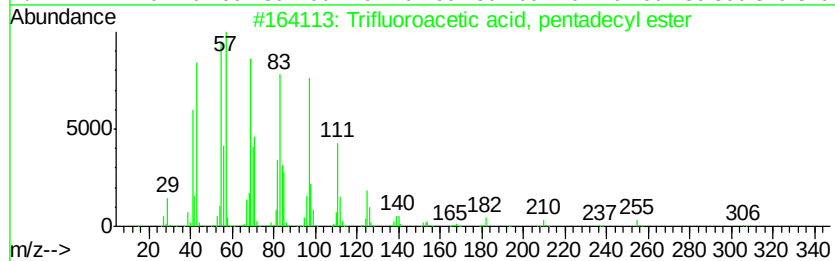
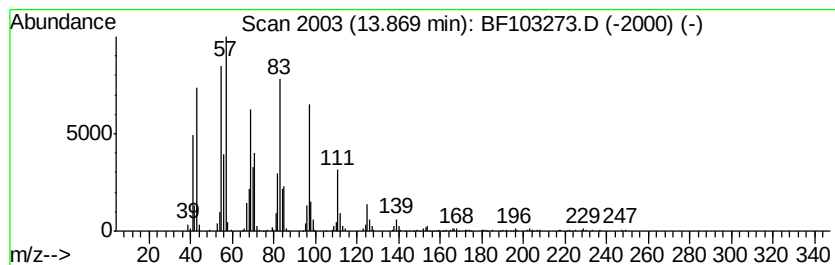
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Trifluoroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	12.55 ng	535737	Chrysene-d12	14.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3		1-Heneicosanol	312	C21H44O	015594-90-8	93
4		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
5		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF022718\
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Sample : J1672-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

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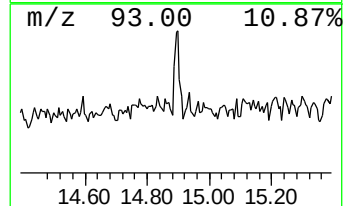
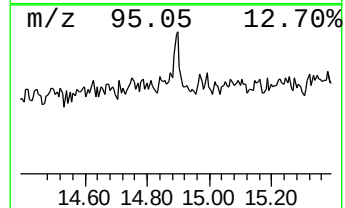
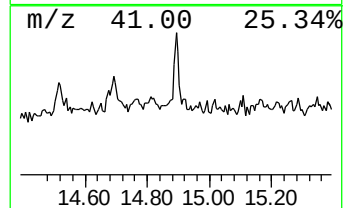
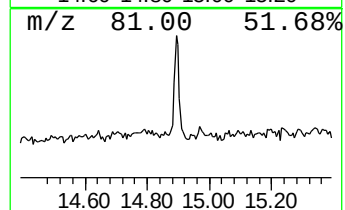
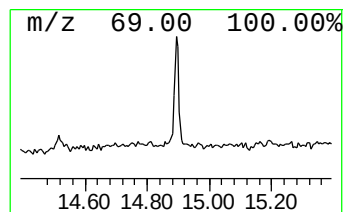
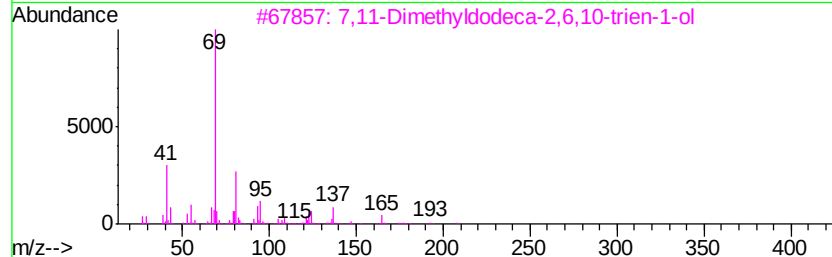
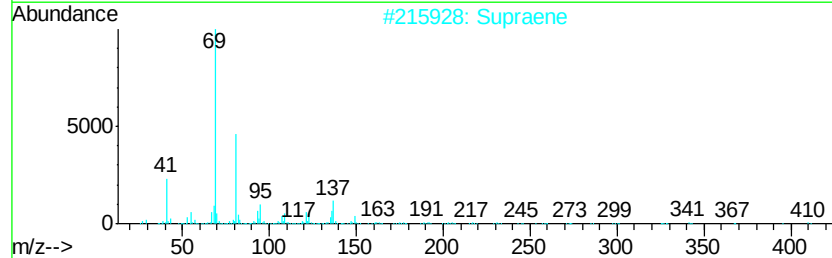
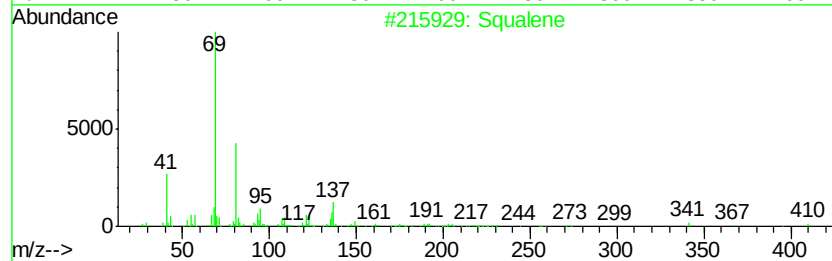
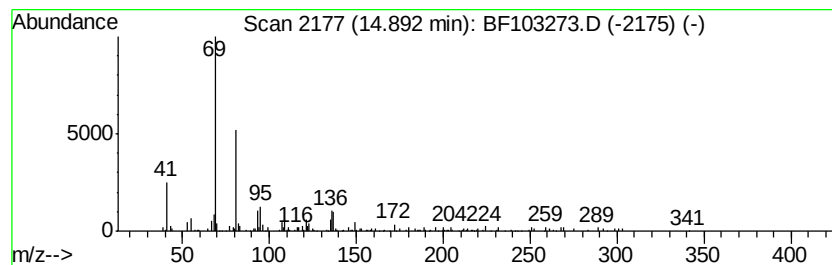
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	3.77 ng	118420	Perylene-d12	15.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	72
2		Supraene	410	C30H50	007683-64-9	64
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
4		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	59
5		3,7,11-Trimethyl-dodeca-2,6,10-t...	236	C15H24O2	007548-13-2	56



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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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...	2.16	9.0	ng	449155	1	6.87	997651	20.0
Isopropyl Alcohol	3.56	66.7	ng	3328990	1	6.87	997651	20.0
2-Pentanone, 4-hy...	5.12	4.2	ng	209012	1	6.87	997651	20.0
unknown6.65	6.65	80.4	ng	4009980	1	6.87	997651	20.0
3-(2-Hydroxyethyl...	9.41	18.0	ng	1135700	3	9.92	1261920	20.0
Hexaethylene glycol	11.21	2.3	ng	121812	4	11.40	1053730	20.0
n-Hexadecanoic acid	11.92	3.2	ng	169643	4	11.40	1053730	20.0
Pentaethylene glycol	12.37	5.3	ng	281492	4	11.40	1053730	20.0
Trifluoroacetic a...	13.87	12.6	ng	535737	5	14.06	853497	20.0
Squalene	14.89	3.8	ng	118420	6	15.56	627867	20.0