

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF063016\
 Data File : BF088546.D
 Acq On : 30 Jun 2016 23:23
 Operator : UM/SJ
 Sample : H3629-06
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LOCATION-5D(9-11)

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-BF063016.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	1.678	4	8	11	rVB	4955837	9214040	100.00%	14.830%
2	1.735	11	13	23	rVV	321074	734106	7.97%	1.182%
3	1.873	23	25	40	rVV	2491555	4369107	47.42%	7.032%
4	2.067	40	42	59	rVB2	121190	366013	3.97%	0.589%
5	5.004	295	299	307	rVB	737369	1450710	15.74%	2.335%
6	5.416	331	335	338	rBV	3480491	4389264	47.64%	7.065%
7	5.816	368	370	373	rBV	106524	106481	1.16%	0.171%
8	6.456	422	426	428	rVB	3737974	5442318	59.07%	8.760%
9	6.582	434	437	440	rBV	3492243	4641386	50.37%	7.470%
10	6.810	455	457	459	rBV	1131350	1096057	11.90%	1.764%
11	6.970	468	471	474	rVB	3310030	3315116	35.98%	5.336%
12	7.382	503	507	509	rBV	2852525	3409383	37.00%	5.488%
13	8.102	567	570	572	rBV	1328023	1553551	16.86%	2.500%
14	9.176	661	664	667	rBV	4043011	4471247	48.53%	7.197%
15	9.565	696	698	701	rVB	689964	634874	6.89%	1.022%
16	9.850	720	723	725	rBV	1741275	1742909	18.92%	2.805%
17	10.639	788	792	794	rBV	2343310	3313013	35.96%	5.332%
18	10.765	801	803	807	rVB	73815	100406	1.09%	0.162%
19	11.211	837	842	844	rBV2	94507	131653	1.43%	0.212%
20	11.325	849	852	853	rVV	1895003	1734068	18.82%	2.791%
21	11.393	856	858	860	rVB	93737	95469	1.04%	0.154%
22	11.862	897	899	901	rBV2	189174	218046	2.37%	0.351%
23	11.931	903	905	910	rVB2	95186	137739	1.49%	0.222%
24	12.525	955	957	960	rBV	519751	490497	5.32%	0.789%
25	12.651	966	968	974	rBV2	73680	141057	1.53%	0.227%
26	12.754	974	977	979	rVV2	610241	783778	8.51%	1.262%
27	12.914	988	991	993	rVV	3742551	3969768	43.08%	6.389%
28	13.085	1000	1006	1008	rBV	55413	103989	1.13%	0.167%
29	13.451	1035	1038	1040	rBV	125208	141005	1.53%	0.227%
30	13.851	1069	1073	1078	rBV2	79461	236812	2.57%	0.381%
31	13.954	1078	1082	1083	rVV	1265358	1840398	19.97%	2.962%
32	13.977	1083	1084	1087	rVB	178670	145454	1.58%	0.234%
33	14.948	1166	1169	1174	rBV	137254	266006	2.89%	0.428%
34	15.234	1191	1194	1196	rVB	67477	96109	1.04%	0.155%

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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 >
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35	15.291	1196	1199	1201	rBV	85218	125695	1.36%	0.202%
36	15.348	1201	1204	1207	rBV	914477	1122207	12.18%	1.806%

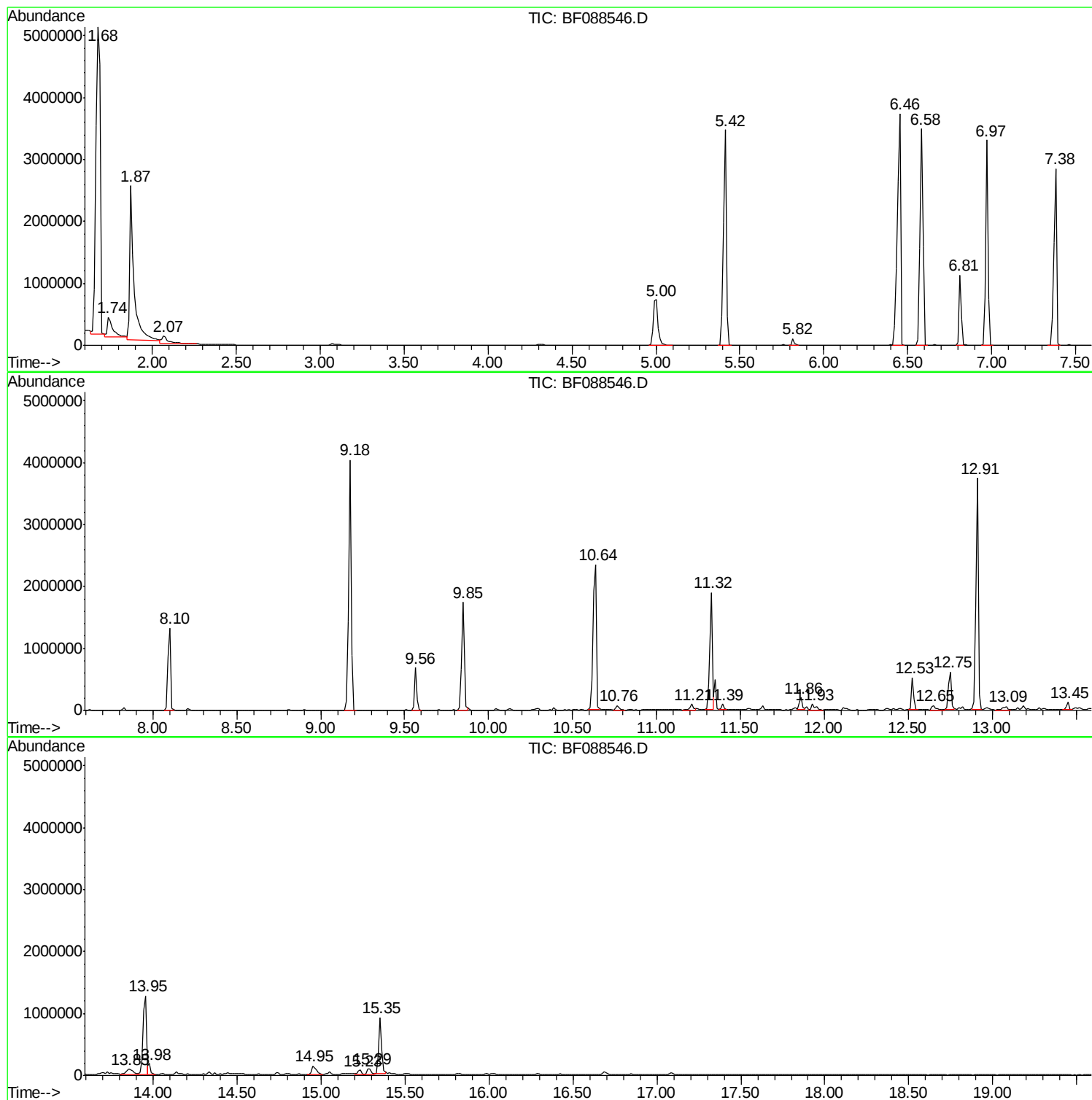
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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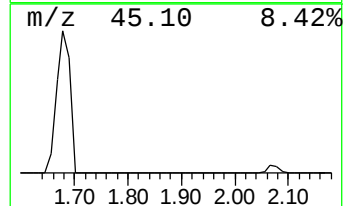
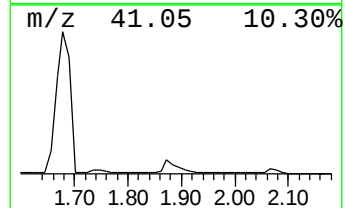
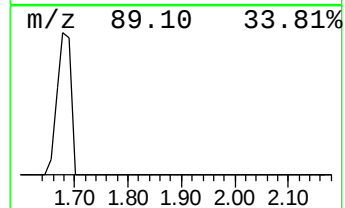
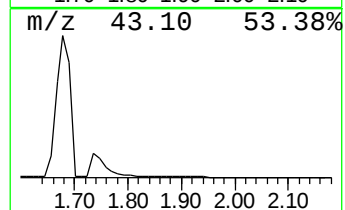
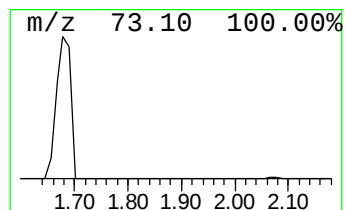
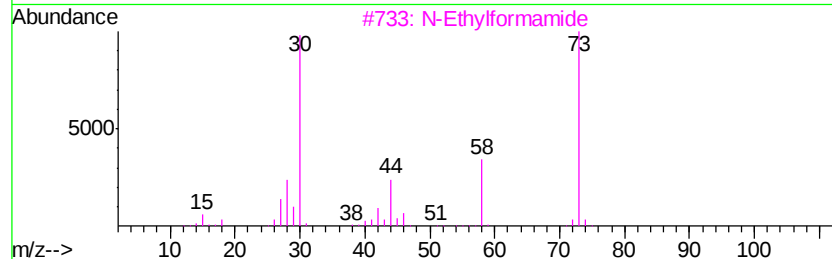
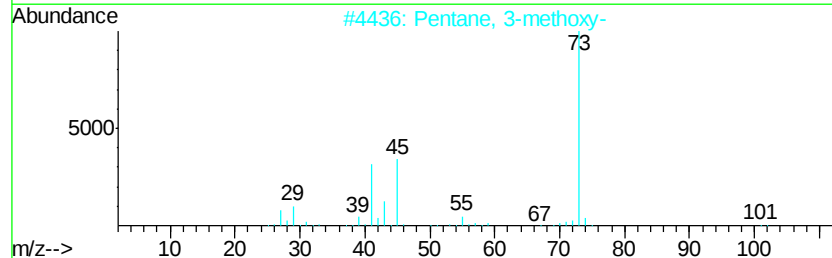
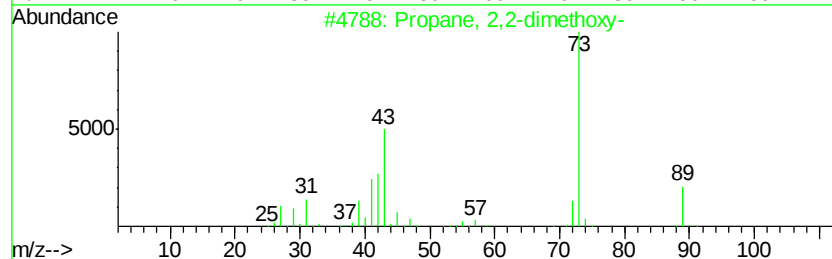
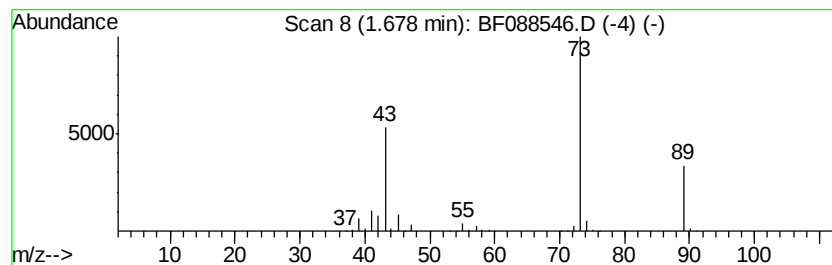
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.68	168.13 ng	9214040	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5		1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9



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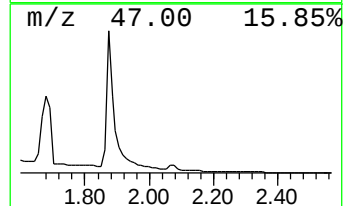
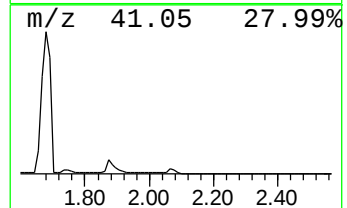
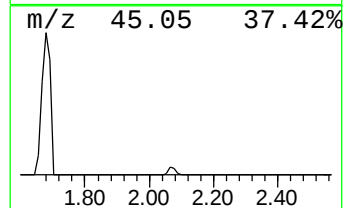
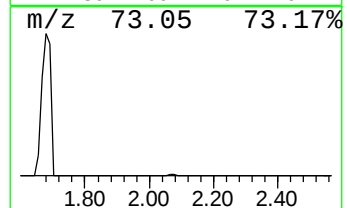
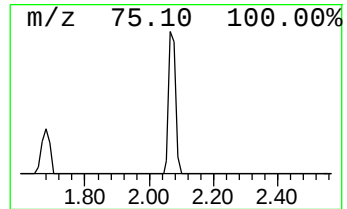
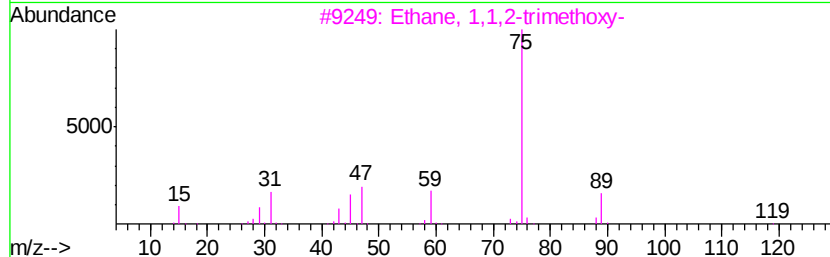
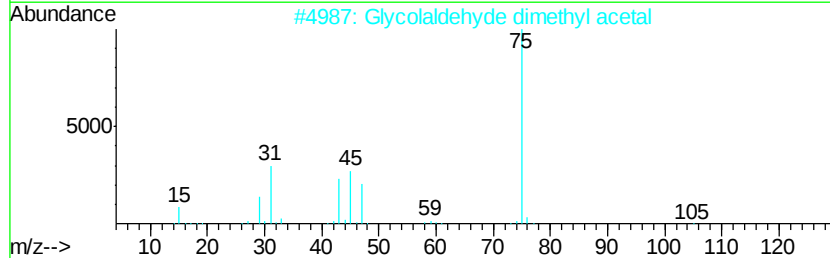
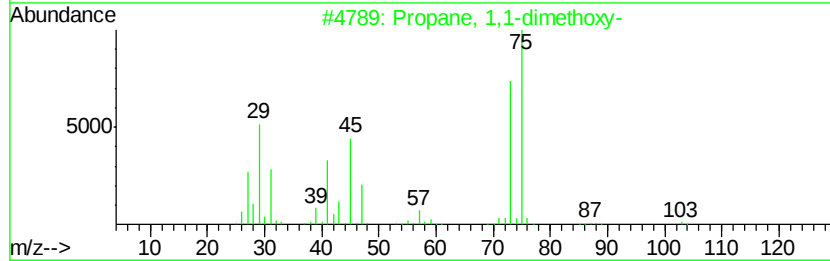
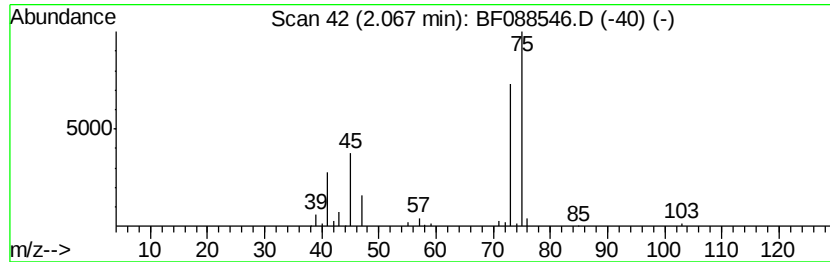
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Peak Number 4 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.07	6.68 ng	366013	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2		Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	36
3		Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	9
4		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9
5		Pentanoic acid, 2-hydroxy-, ethy...	146	C7H14O3	006938-26-7	9



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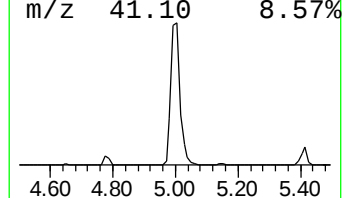
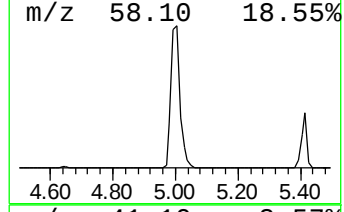
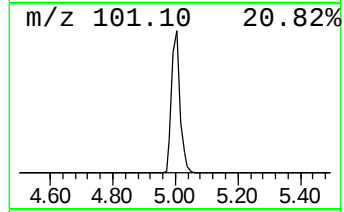
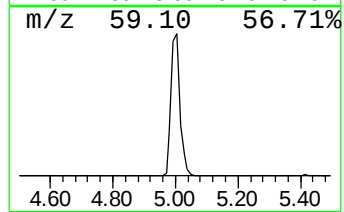
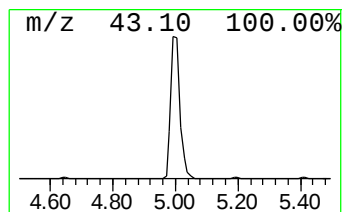
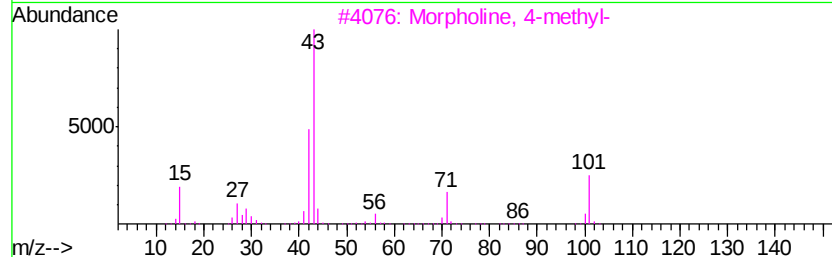
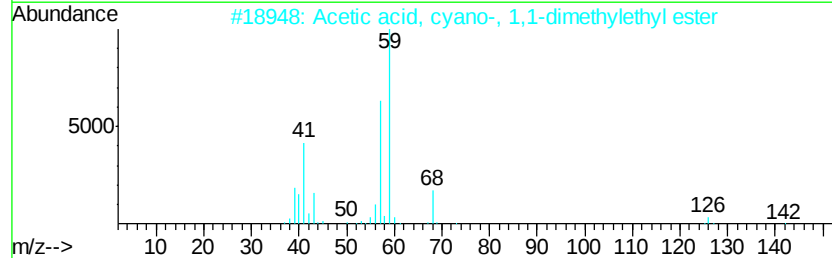
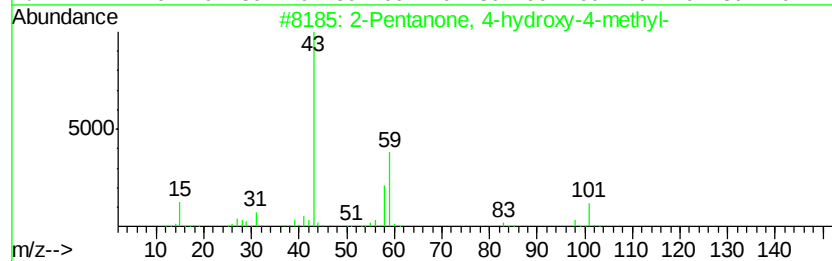
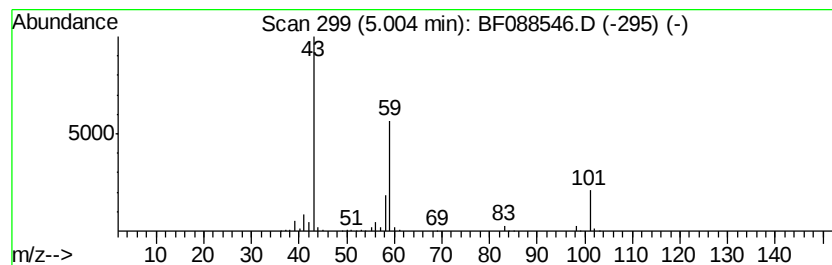
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	26.47 ng	1450710	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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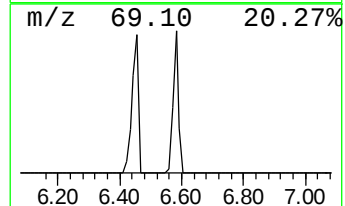
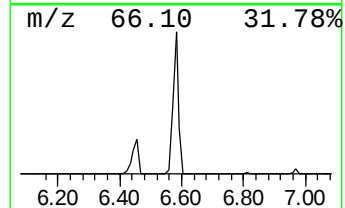
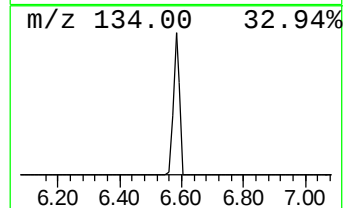
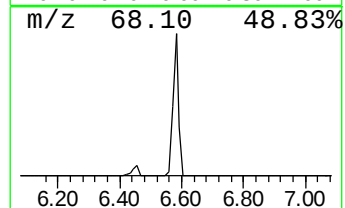
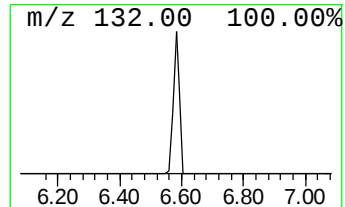
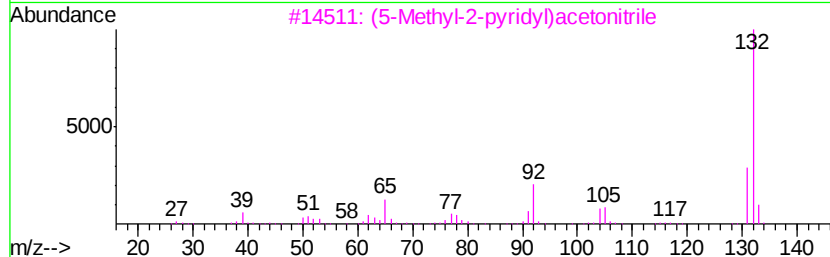
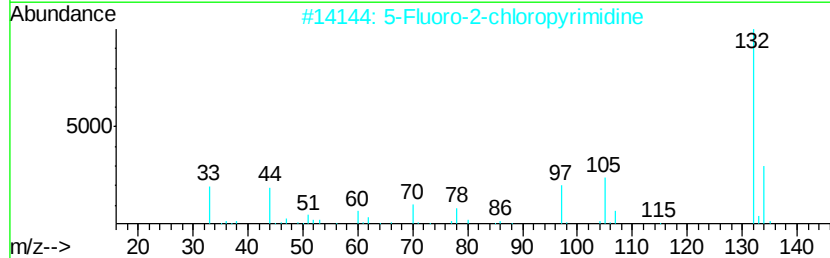
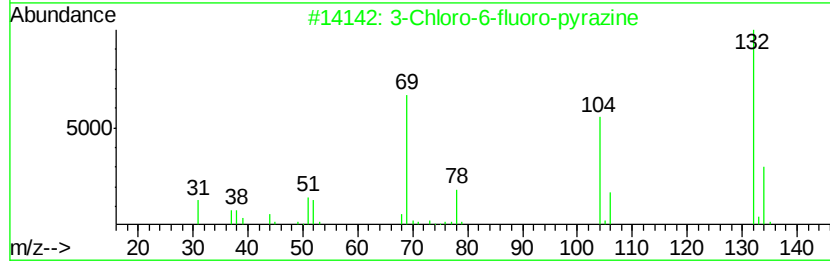
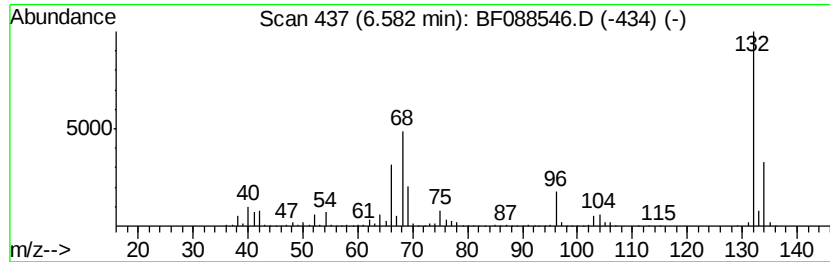
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 unknown6.58 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	84.69 ng	4641390	1,4-Dichlorobenzene-d4	6.81

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	12
3		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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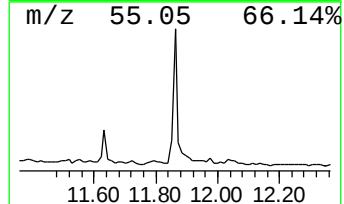
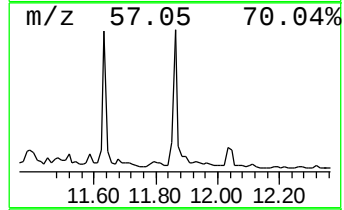
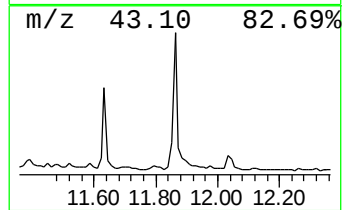
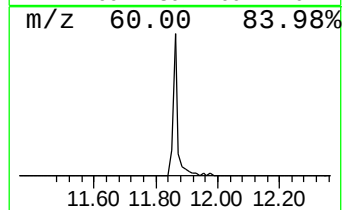
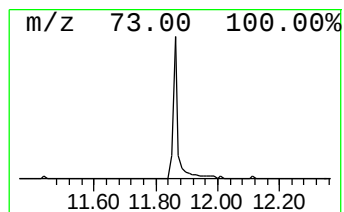
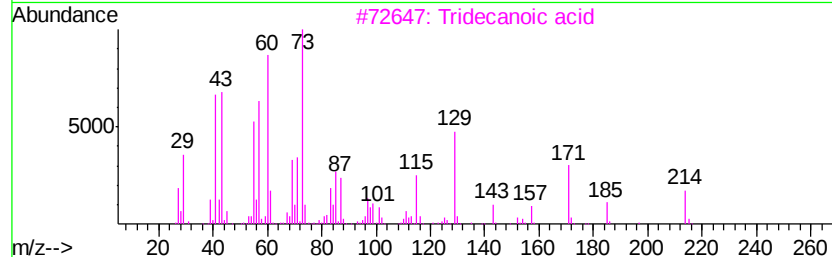
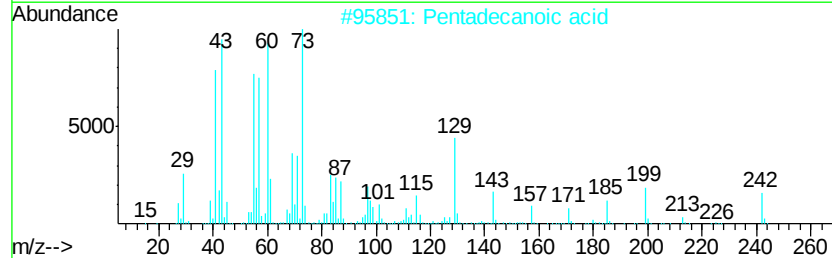
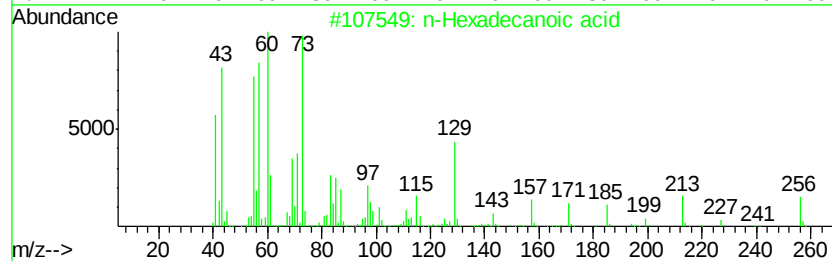
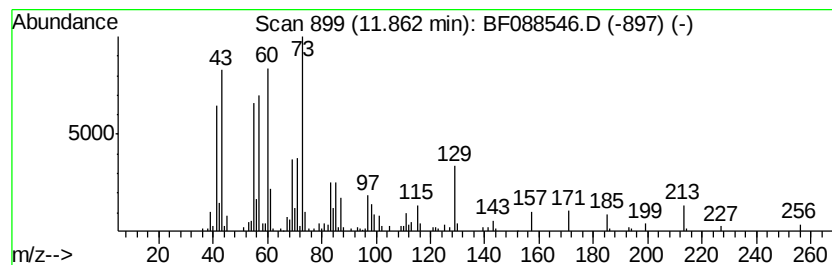
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Peak Number 8 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	2.51 ng	218046	Phenanthrene-d10	11.32

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	87
3		Tridecanoic acid	214	C13H26O2	000638-53-9	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5		Heptanoic acid	130	C7H14O2	000111-14-8	35



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Sample : H3629-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LOCATION-5D(9-11)

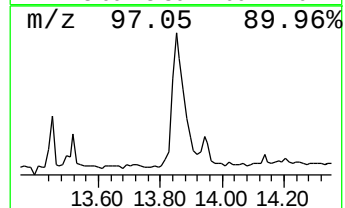
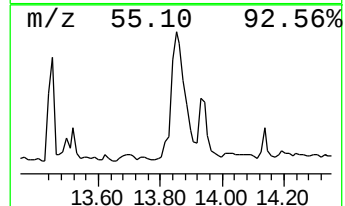
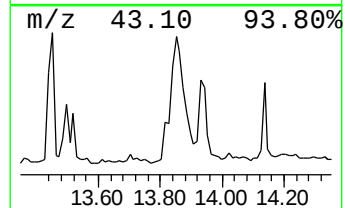
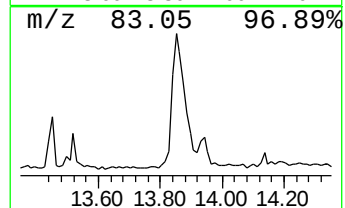
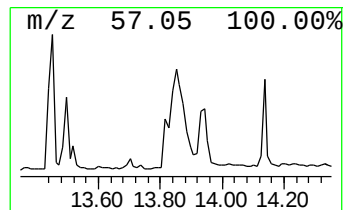
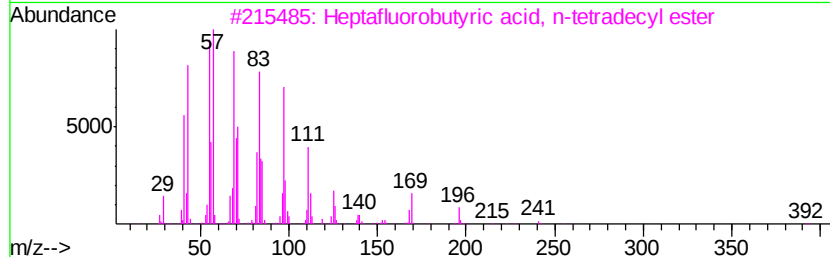
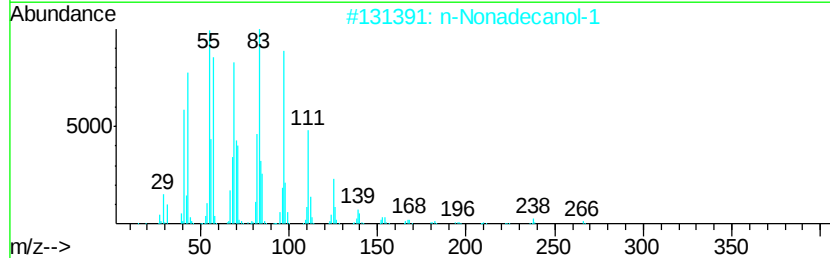
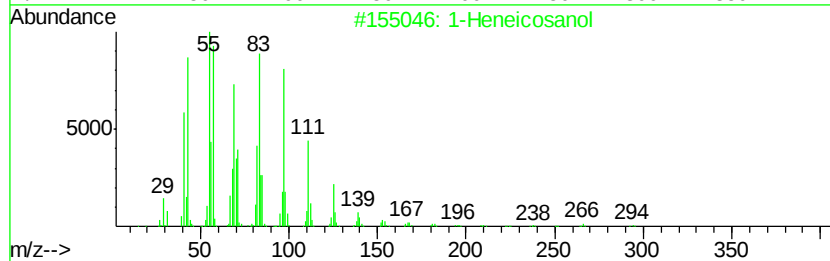
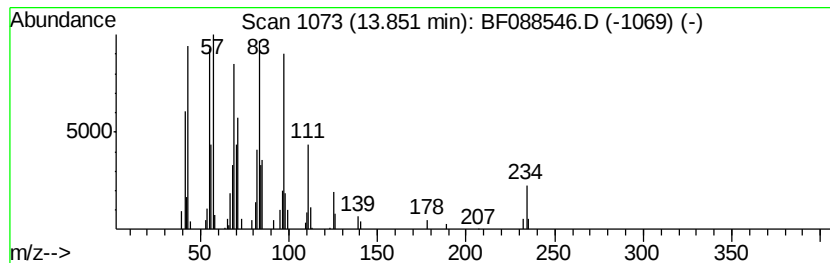
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Heneicosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	2.57 ng	236812	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	94
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
4		1-Heptacosanol	396	C27H56O	002004-39-9	94
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF063016\
Data File : BF088546.D
Acq On : 30 Jun 2016 23:23
Operator : UM/SJ
Sample : H3629-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LOCATION-5D(9-11)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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
Propane, 2,2-dime...	1.68	168.1	ng	9214040	1	6.81	1096060	20.0
Propane, 1,1-dime...	2.07	6.7	ng	366013	1	6.81	1096060	20.0
2-Pentanone, 4-hy...	5.00	26.5	ng	1450710	1	6.81	1096060	20.0
unknown6.58	6.58	84.7	ng	4641390	1	6.81	1096060	20.0
n-Hexadecanoic acid	11.86	2.5	ng	218046	4	11.32	1734070	20.0
1-Heneicosanol	13.85	2.6	ng	236812	5	13.95	1840400	20.0