

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022118\
 Data File : BF103136.D
 Acq On : 21 Feb 2018 15:11
 Operator : SJ/JU
 Sample : J1623-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-1-2

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\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	2.157	5	12	23	rVB	1267936	1686821	36.16%	3.865%
2	5.081	504	509	513	rBV	52011	63324	1.36%	0.145%
3	5.128	513	517	526	rVB	108122	170640	3.66%	0.391%
4	5.504	576	581	585	rBV	4173256	4664347	100.00%	10.686%
5	6.516	747	753	756	rBV	3837192	4594877	98.51%	10.527%
6	6.651	771	776	779	rBV	4312379	4544531	97.43%	10.412%
7	6.875	811	814	818	rBV	1284898	1113364	23.87%	2.551%
8	7.034	837	841	845	rBV	3610787	3523520	75.54%	8.072%
9	7.445	905	911	914	rBV	3025999	3103697	66.54%	7.111%
10	8.157	1029	1032	1048	rBV	1496506	1523134	32.65%	3.490%
11	9.233	1210	1215	1225	rBV	4375305	4508916	96.67%	10.330%
12	9.628	1278	1282	1290	rVB	198691	211019	4.52%	0.483%
13	9.833	1314	1317	1321	rBV	103041	82391	1.77%	0.189%
14	9.916	1327	1331	1335	rBV2	1715957	1516212	32.51%	3.474%
15	10.333	1399	1402	1405	rVB	154053	117834	2.53%	0.270%
16	10.710	1461	1466	1477	rBV	2430390	2510749	53.83%	5.752%
17	10.804	1480	1482	1490	rVB	95336	101084	2.17%	0.232%
18	11.404	1580	1584	1587	rBV	1396197	1322753	28.36%	3.030%
19	11.427	1587	1588	1593	rVV	363371	244017	5.23%	0.559%
20	11.480	1593	1597	1600	rVB	60653	61644	1.32%	0.141%
21	11.922	1666	1672	1673	rBV2	69897	107433	2.30%	0.246%
22	12.016	1685	1688	1691	rBV2	62178	75744	1.62%	0.174%
23	12.469	1758	1765	1767	rBV3	119349	152127	3.26%	0.349%
24	12.492	1767	1769	1774	rVB3	88166	91807	1.97%	0.210%
25	12.621	1787	1791	1795	rBV	401621	369731	7.93%	0.847%
26	12.851	1823	1830	1833	rBV	385168	406180	8.71%	0.931%
27	12.992	1849	1854	1857	rBV	3098538	3136027	67.23%	7.185%
28	13.033	1859	1861	1863	rVV	76475	57864	1.24%	0.133%
29	13.827	1993	1996	1999	rBV2	54116	70504	1.51%	0.162%
30	13.868	2000	2003	2006	rVV2	243561	262458	5.63%	0.601%
31	13.904	2006	2009	2015	rVB	415192	429248	9.20%	0.983%
32	14.051	2029	2034	2037	rBV2	1159384	1275340	27.34%	2.922%
33	14.074	2037	2038	2046	rVB	203908	161970	3.47%	0.371%
34	14.510	2109	2112	2119	rBV5	49160	88874	1.91%	0.204%

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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	15.104	2210	2213	2216	rBV	139860	200266	4.29%	0.459%
36	15.480	2274	2277	2282	rVB	103935	124062	2.66%	0.284%
37	15.545	2283	2288	2298	rBV	677618	974482	20.89%	2.233%

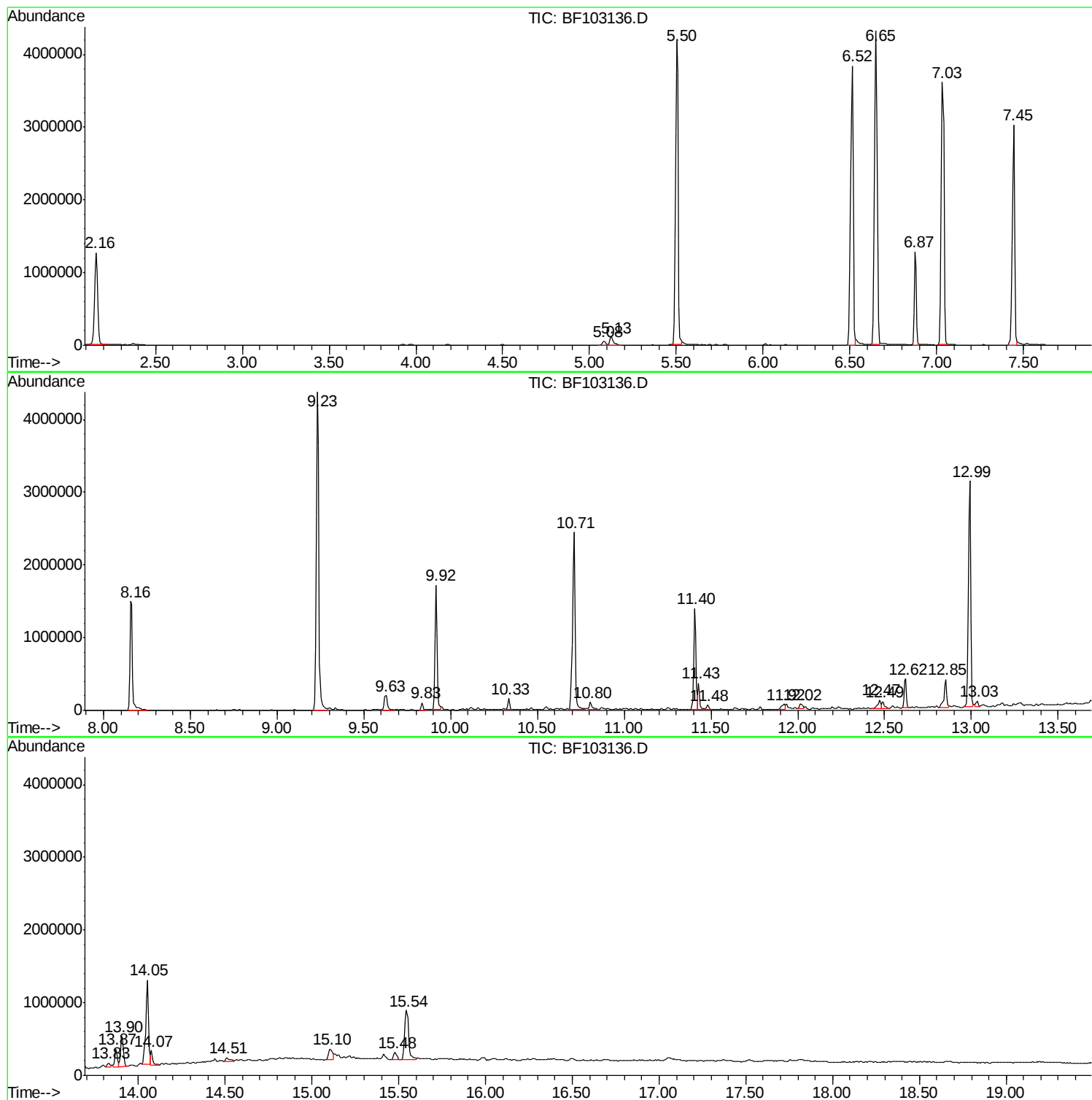
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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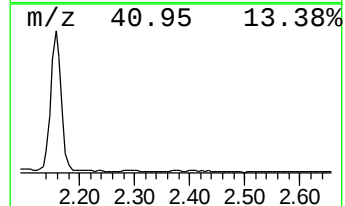
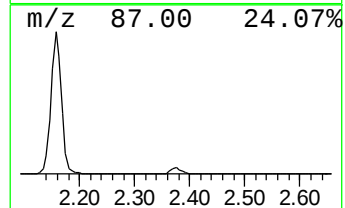
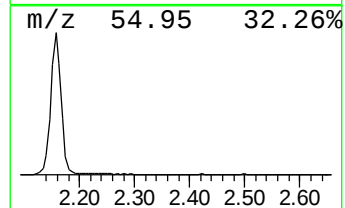
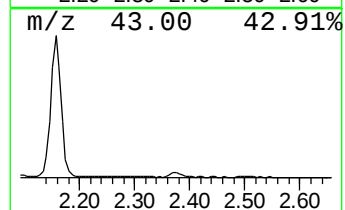
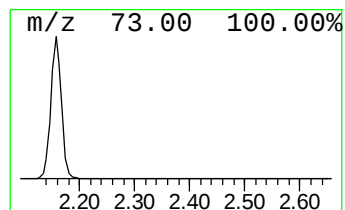
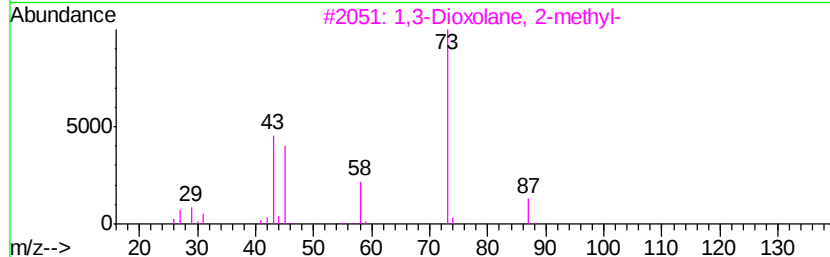
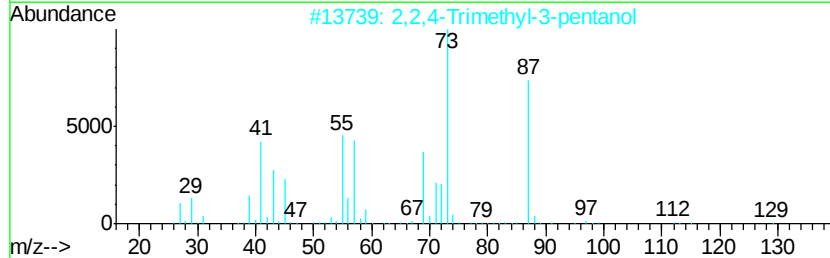
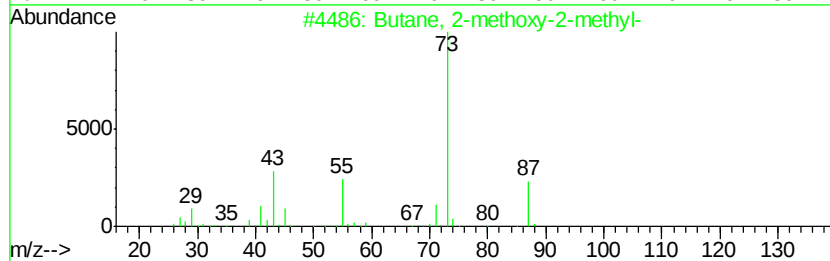
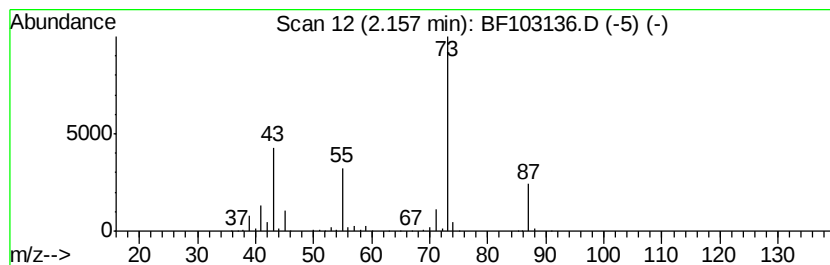
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	30.30 ng	1686820	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		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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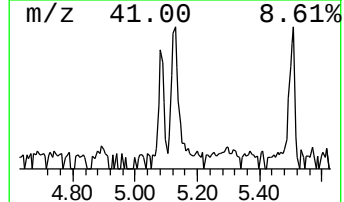
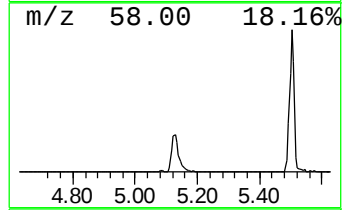
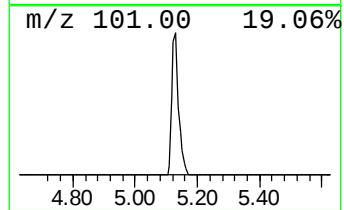
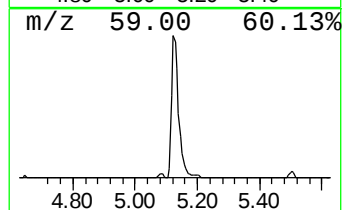
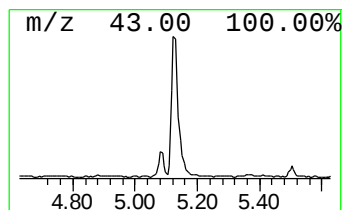
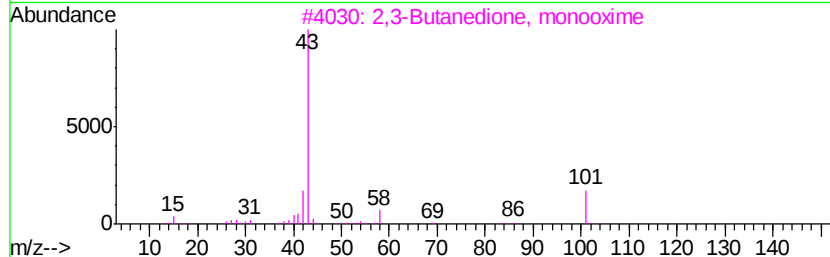
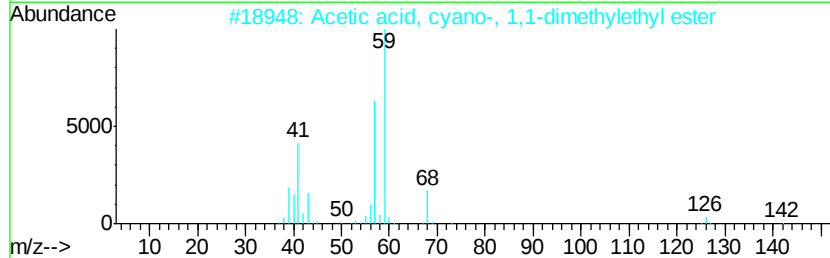
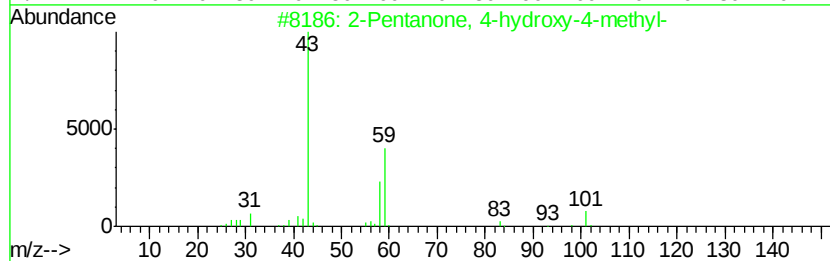
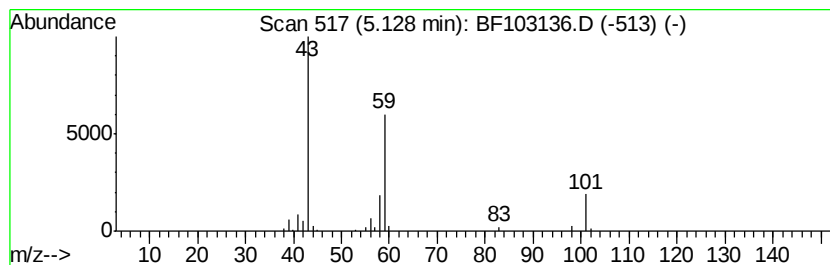
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	3.07 ng	170640	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			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4			Acetone	58	C3H6O	000067-64-1	10
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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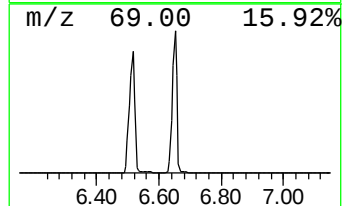
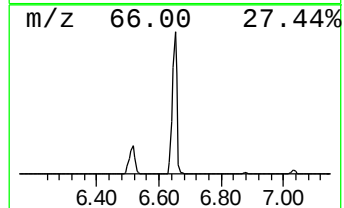
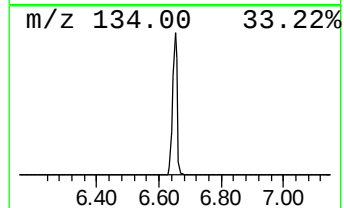
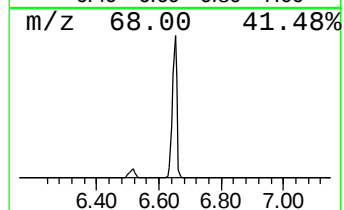
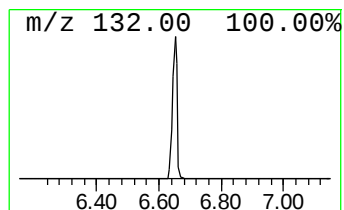
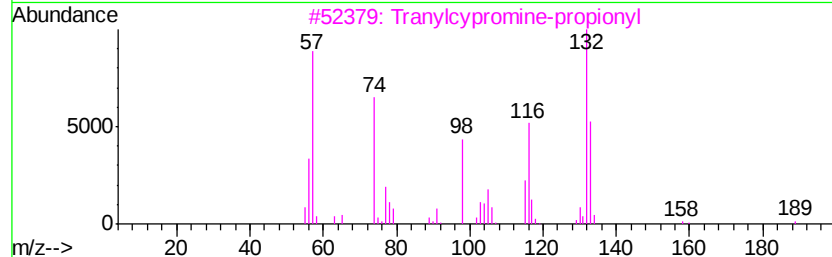
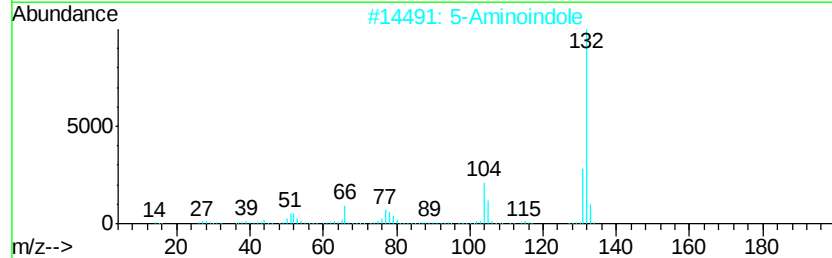
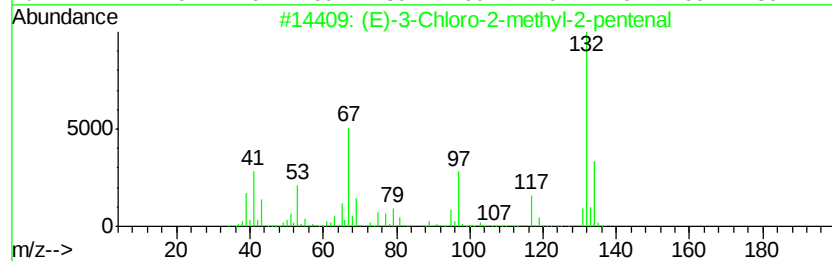
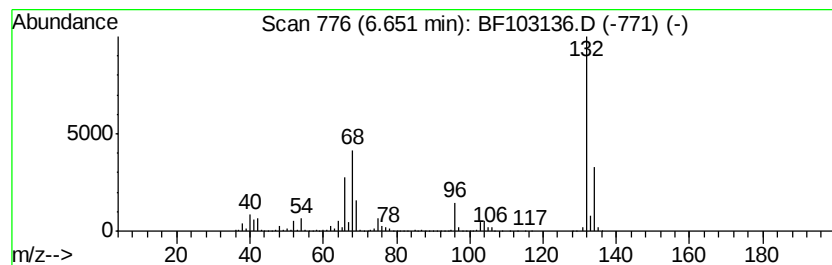
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	81.64 ng	4544530	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	Tranvlcvpromine-propionyl	189	C12H15NO	1000123-86-3	10	
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9	
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9	



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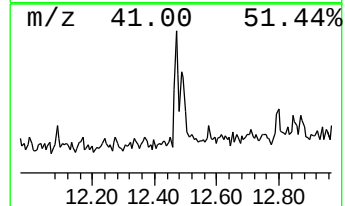
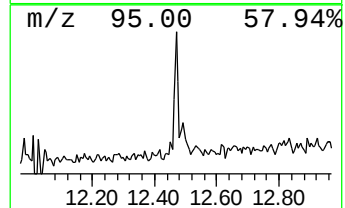
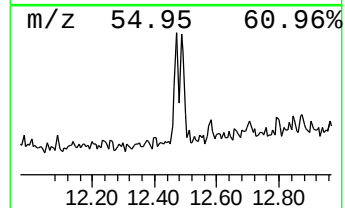
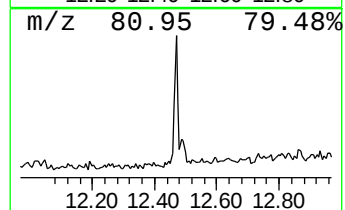
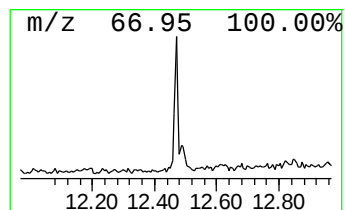
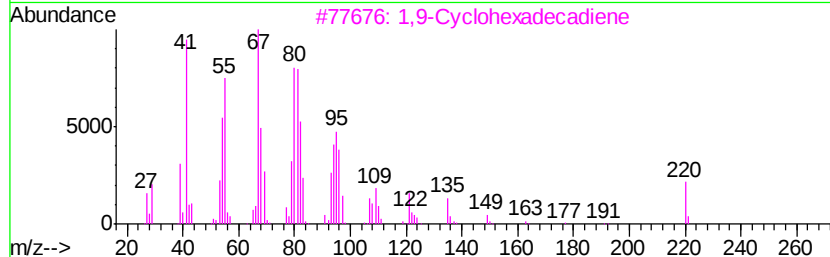
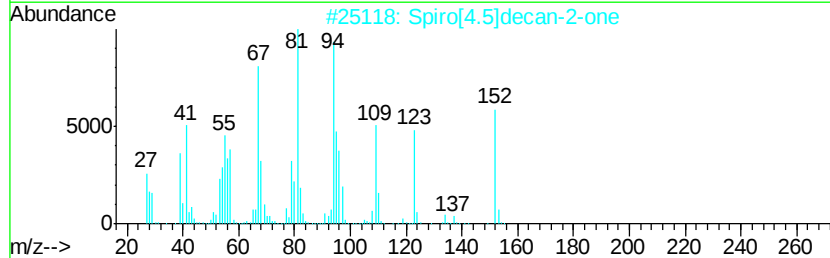
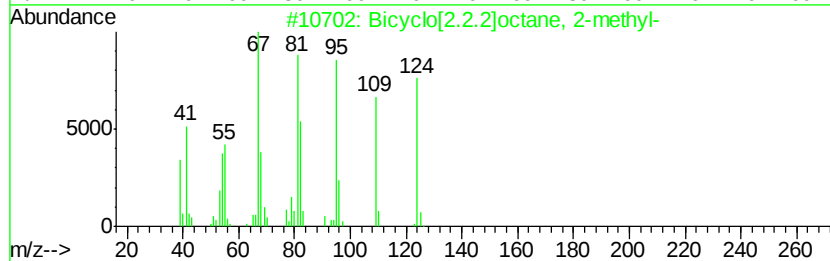
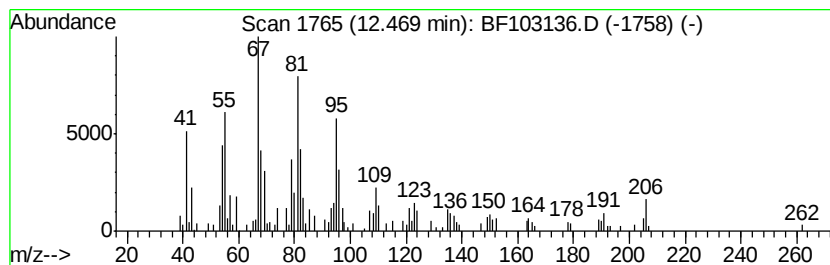
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Bicyclo[2.2.2]octane, 2-met... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.47	2.30 ng	152127	Phenanthrene-d10	11.40

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bicyclo[2.2.2]octane, 2-methyl-	124	C9H16	000766-53-0	90
2		Spiro[4.5]decan-2-one	152	C10H16O	003643-16-1	90
3		1,9-Cyclohexadecadiene	220	C16H28	004277-06-9	87
4		8-Hexadecyne	222	C16H30	019781-86-3	83
5		1-Tridecyne	180	C13H24	026186-02-7	80



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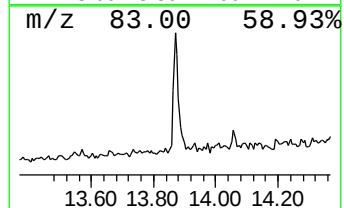
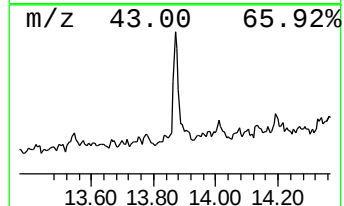
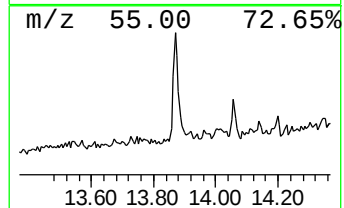
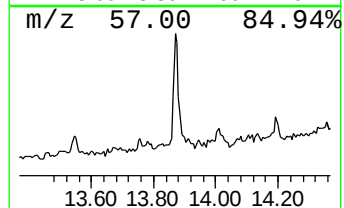
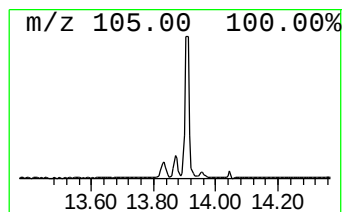
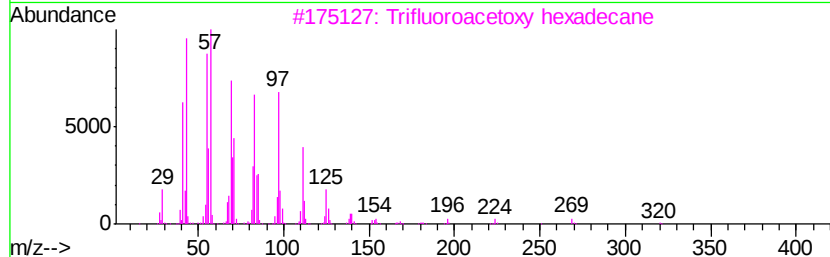
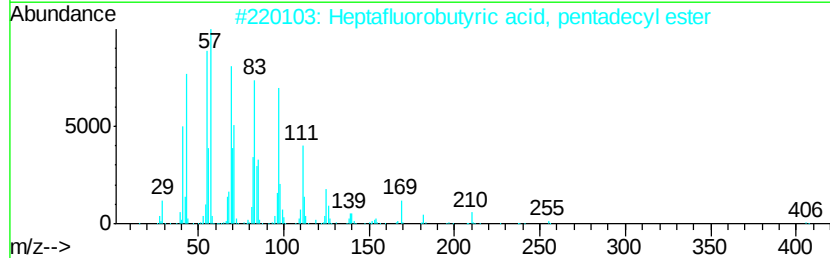
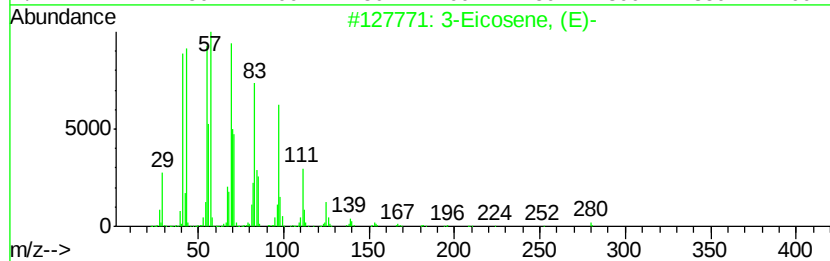
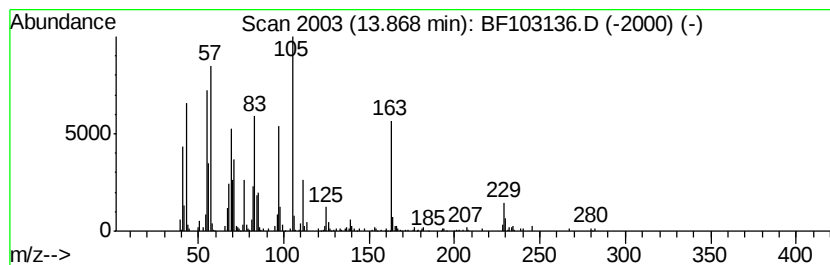
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 3-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.87	4.12 ng	262458	Chrysene-d12	14.05		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Eicosene, (E)-	280	C20H40	074685-33-9	86
2		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	60
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	60
4		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	60
5		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	60



Data Path : Z:\HPCHEM1\BNA F\DATA\BF022118\
Data File : BF103136.D
Acq On : 21 Feb 2018 15:11
Operator : SJ/JU
Sample : J1623-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-2

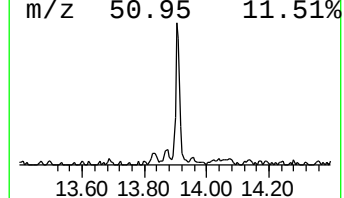
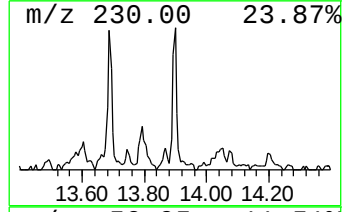
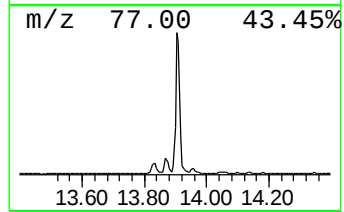
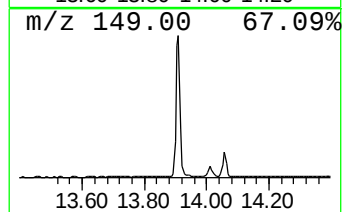
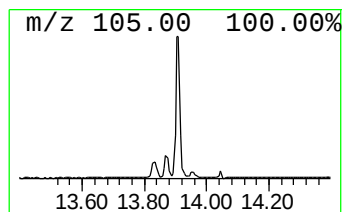
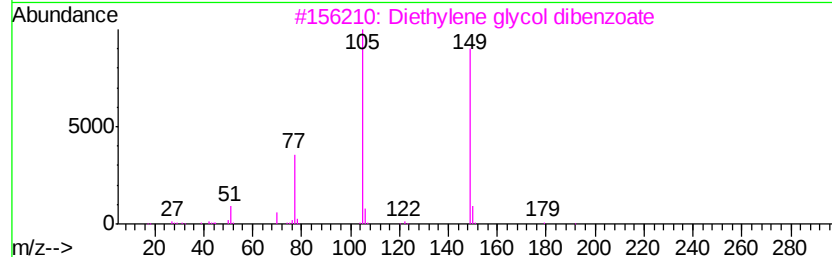
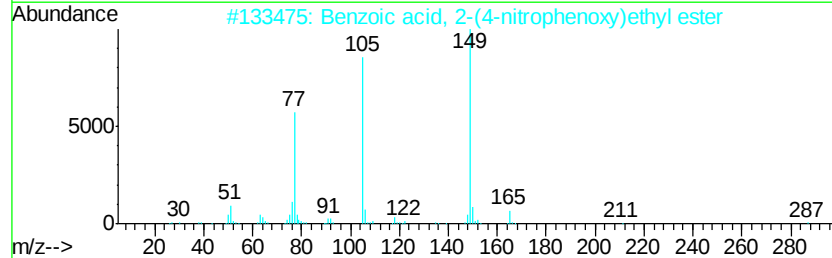
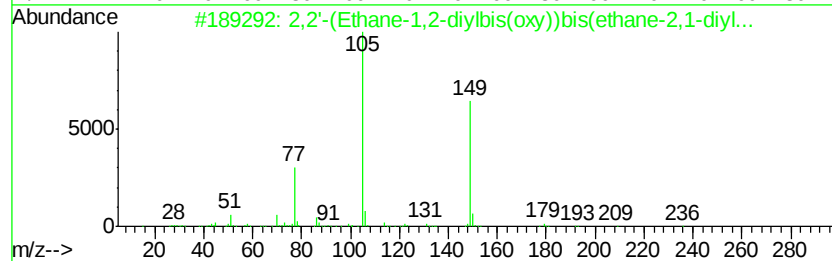
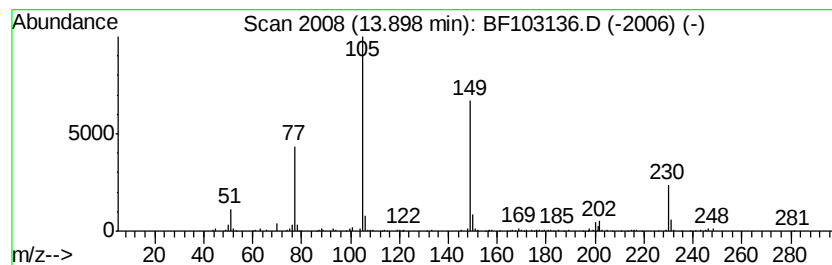
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2,2'-(Ethane-1,2-diylbis(ox... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	6.73 ng	429248	Chrysene-d12	14.05

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2'	-	(Ethane-1,2-diylbis(oxv))bi...	358	C20H22O6	1000366-99-4	83
2	Benzoic acid,	2-	(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	72
3	Diethylene glycol	dibenzoate		314	C18H18O5	000120-55-8	59
4	2-Methyl-4-hydroxy	benzoxazole		149	C8H7NO2	051110-60-2	43
5	1,3,4-Oxadiazolium,	5-hydroxy-2,	...	238	C14H10N2O2	024660-41-1	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022118\
Data File : BF103136.D
Acq On : 21 Feb 2018 15:11
Operator : SJ/JU
Sample : J1623-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-2

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...	2.16	30.3	ng	1686820	1	6.87	1113360	20.0
2-Pentanone, 4-hy...	5.13	3.1	ng	170640	1	6.87	1113360	20.0
unknown6.65	6.65	81.6	ng	4544530	1	6.87	1113360	20.0
Bicyclo[2.2.2]oct...	12.47	2.3	ng	152127	4	11.40	1322750	20.0
3-Eicosene, (E)-	13.87	4.1	ng	262458	5	14.05	1275340	20.0
2,2'-(Ethane-1,2-...	13.90	6.7	ng	429248	5	14.05	1275340	20.0