

Data Path : U:\HPCHEM1\BNA F\DATA\BF012618\
 Data File : BF102482.D
 Acq On : 26 Jan 2018 21:23
 Operator : SJ/JU
 Sample : J1257-03 5X
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-12(0-5)

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-BF012218.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	4.893	474	477	486	rBV	40510	50274	4.36%	0.380%
2	5.281	539	543	548	rBV	68312	108346	9.40%	0.819%
3	5.328	548	551	570	rVB	656162	742454	64.42%	5.612%
4	6.240	703	706	709	rBV	90477	79403	6.89%	0.600%
5	6.269	709	711	714	rVV	49802	45117	3.91%	0.341%
6	6.316	714	719	724	rVB2	41662	45359	3.94%	0.343%
7	6.369	724	728	743	rBV	585986	878124	76.19%	6.637%
8	6.492	745	749	754	rVV	852401	800614	69.47%	6.051%
9	6.540	754	757	764	rVB2	157181	161385	14.00%	1.220%
10	6.722	784	788	794	rBV	993623	939269	81.50%	7.099%
11	6.775	794	797	804	rVB3	35002	45424	3.94%	0.343%
12	6.834	804	807	810	rBV	41197	37326	3.24%	0.282%
13	6.875	810	814	817	rBV	668422	603117	52.33%	4.559%
14	6.992	831	834	837	rVB2	61143	67740	5.88%	0.512%
15	7.034	838	841	843	rBV	50919	45748	3.97%	0.346%
16	7.251	875	878	880	rBV	68375	52693	4.57%	0.398%
17	7.281	880	883	887	rBV2	378624	384669	33.38%	2.907%
18	7.492	916	919	921	rBV	54400	44154	3.83%	0.334%
19	7.875	981	984	988	rBV3	35083	42227	3.66%	0.319%
20	8.004	1003	1006	1009	rBV	1420582	1152535	100.00%	8.711%
21	8.057	1012	1015	1017	rVV3	43022	50387	4.37%	0.381%
22	8.081	1017	1019	1028	rVB6	32187	57001	4.95%	0.431%
23	8.292	1053	1055	1059	rVB4	38983	40487	3.51%	0.306%
24	8.351	1061	1065	1068	rBV5	24530	37337	3.24%	0.282%
25	8.422	1073	1077	1078	rVV2	49977	54405	4.72%	0.411%
26	8.463	1082	1084	1087	rVB2	49223	44519	3.86%	0.336%
27	8.681	1119	1121	1125	rVB4	37634	47301	4.10%	0.358%
28	8.716	1125	1127	1130	rBV	55189	61226	5.31%	0.463%
29	8.804	1139	1142	1151	rVB4	41259	83908	7.28%	0.634%
30	8.875	1151	1154	1158	rBV5	27378	41367	3.59%	0.313%
31	8.992	1171	1174	1176	rBV3	44583	46869	4.07%	0.354%
32	9.016	1176	1178	1182	rVB2	59695	56005	4.86%	0.423%
33	9.075	1185	1188	1197	rVV	845116	795094	68.99%	6.010%
34	9.151	1197	1201	1204	rVV2	87318	105395	9.14%	0.797%

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35	9.345	1232	1234	1239	rBV4	37427	47130	4.09%	0.356%
36	9.457	1250	1253	1255	rBV	200008	179527	15.58%	1.357%
37	9.516	1261	1263	1267	rVB4	40053	35813	3.11%	0.271%
38	9.616	1277	1280	1283	rBV	167230	174253	15.12%	1.317%
39	9.663	1285	1288	1290	rVB	215730	178531	15.49%	1.349%
40	9.686	1290	1292	1293	rBV	49189	39392	3.42%	0.298%
41	9.733	1297	1300	1301	rVV2	75629	78833	6.84%	0.596%
42	9.757	1301	1304	1308	rVV	1271777	1080200	93.72%	8.164%
43	9.786	1308	1309	1313	rVB3	65648	68925	5.98%	0.521%
44	10.004	1344	1346	1349	rBV3	46525	52929	4.59%	0.400%
45	10.122	1363	1366	1369	rVB3	78954	78019	6.77%	0.590%
46	10.157	1369	1372	1375	rBV3	194629	190190	16.50%	1.438%
47	10.186	1375	1377	1379	rVV	44370	39047	3.39%	0.295%
48	10.210	1379	1381	1383	rVV2	52847	41159	3.57%	0.311%
49	10.551	1436	1439	1442	rBV	264731	295292	25.62%	2.232%
50	10.669	1455	1459	1466	rBV	431063	517400	44.89%	3.911%
51	11.133	1535	1538	1542	rVB	449297	432115	37.49%	3.266%
52	11.245	1554	1557	1559	rBV	1000273	854095	74.11%	6.456%
53	11.269	1559	1561	1566	rVB	237475	235257	20.41%	1.778%
54	11.486	1596	1598	1601	rVB	190971	150484	13.06%	1.137%
55	12.463	1762	1764	1767	rBV	320168	254691	22.10%	1.925%
56	12.692	1801	1803	1805	rBV	492400	359921	31.23%	2.720%

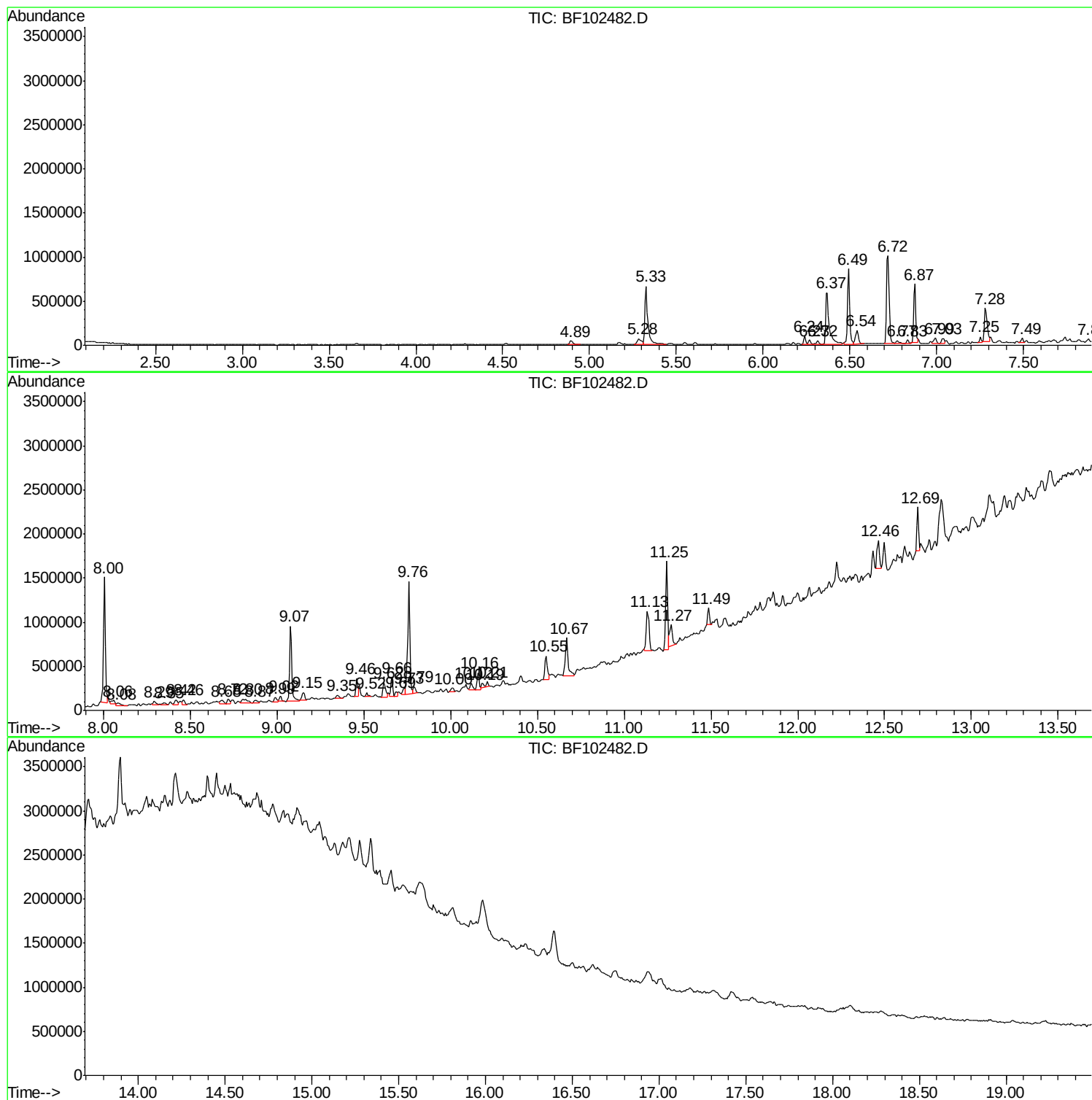
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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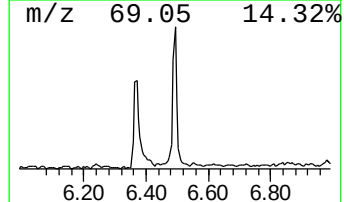
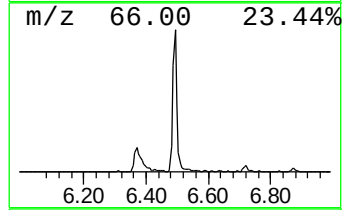
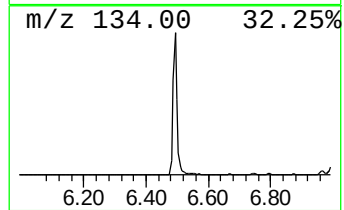
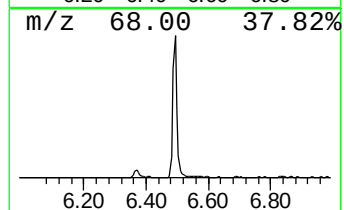
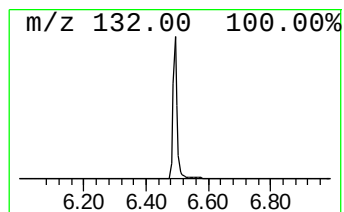
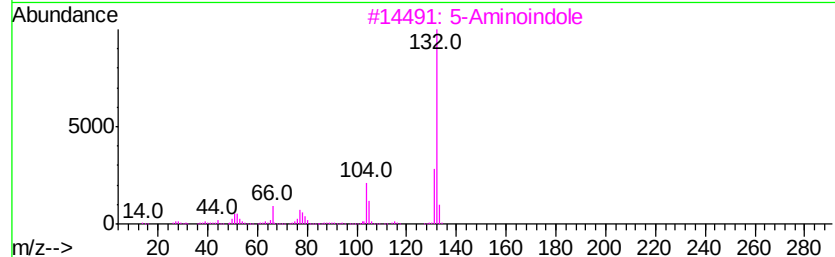
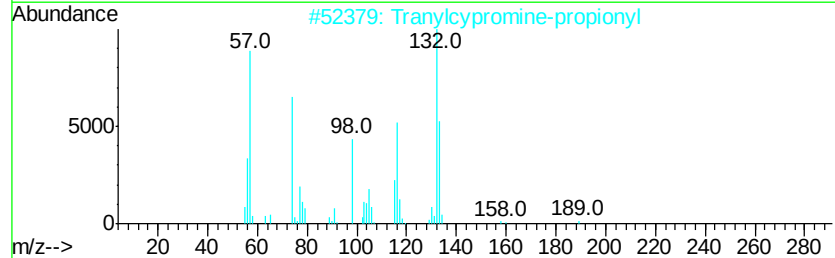
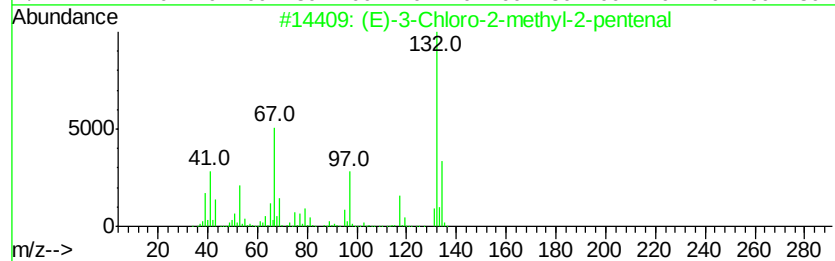
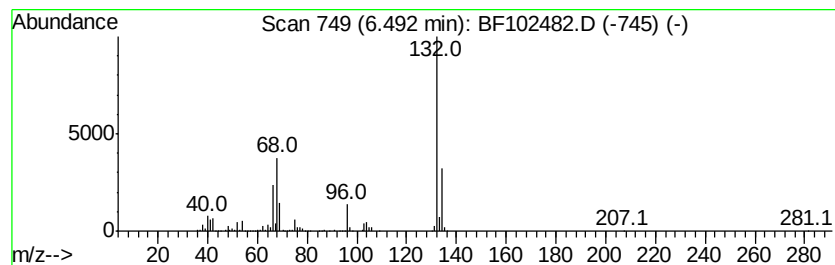
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	17.05 ng	800614	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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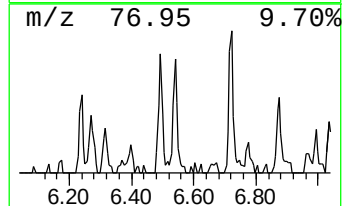
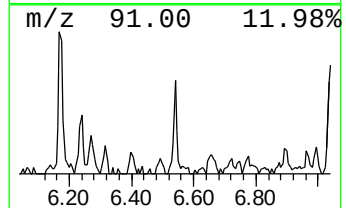
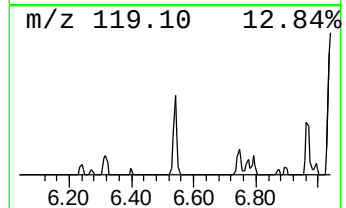
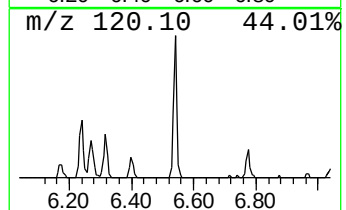
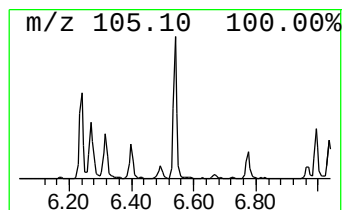
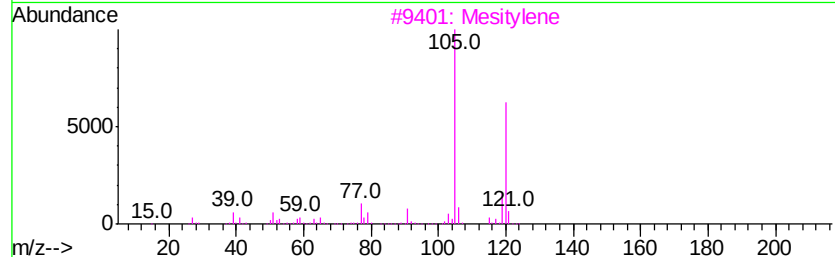
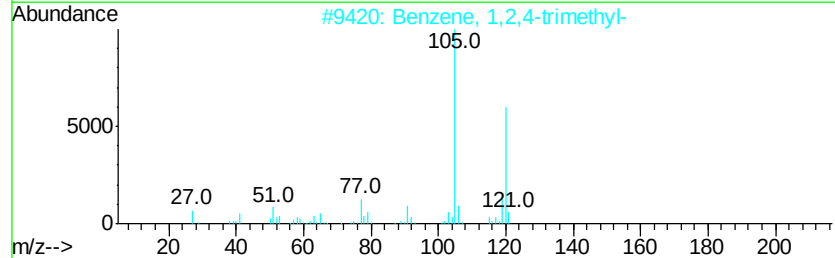
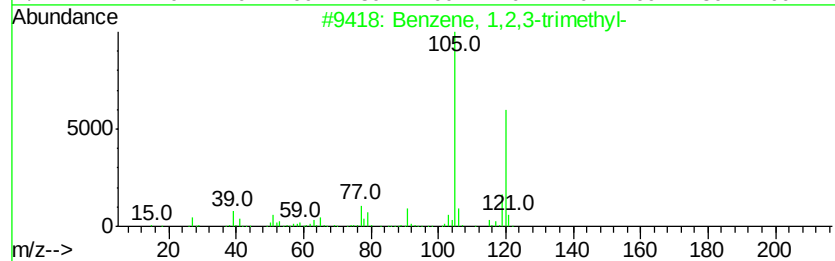
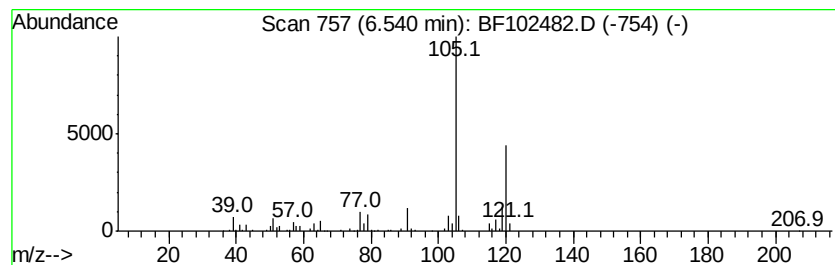
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzene, 1,2,3-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	3.44 ng	161385	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
3		Mesitylene	120	C9H12	000108-67-8	91
4		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90



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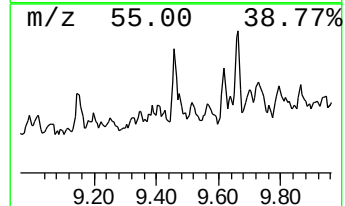
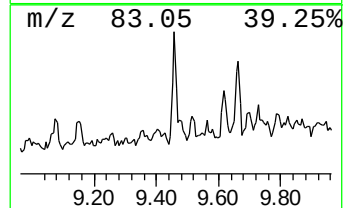
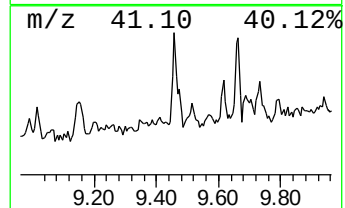
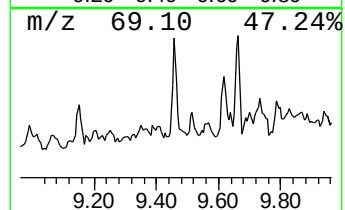
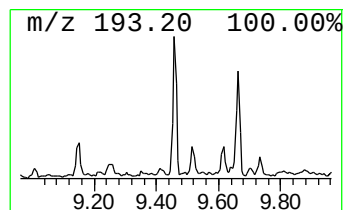
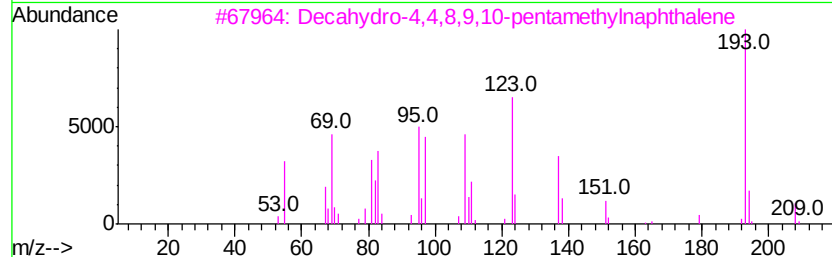
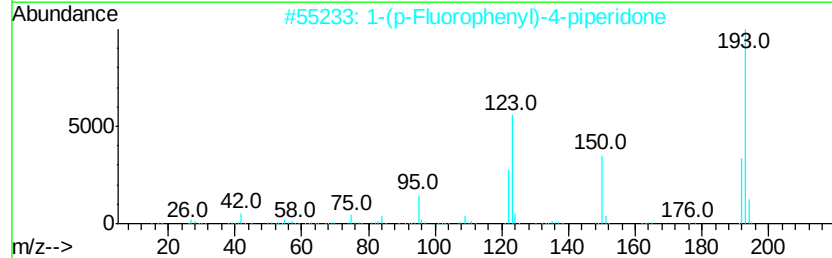
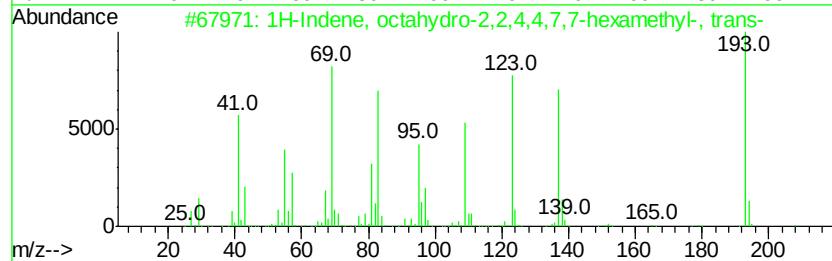
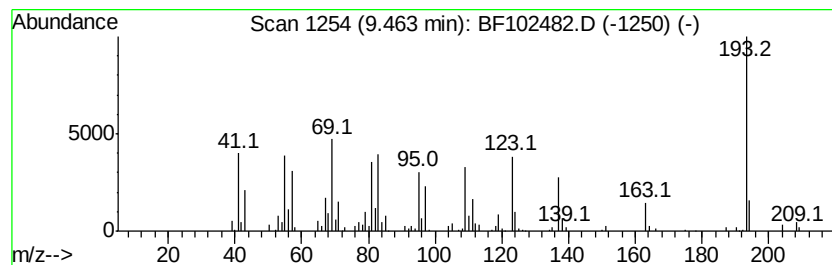
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Peak Number 4 1H-Indene, octahydro-2,2,4,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.46	3.32 ng	179527	Acenaphthene-d10	9.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	59
2		1-(p-Fluorophenyl)-4-piperidone	193	C11H12FN0	1000238-56-7	46
3		Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	43
4		2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	37
5		S-Phenyl 5-(phenylthio)pentaneth...	302	C17H18OS2	1000234-40-7	37



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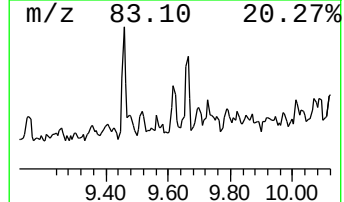
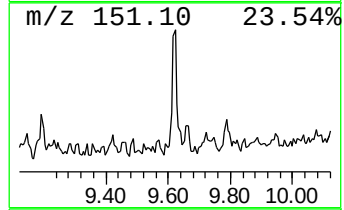
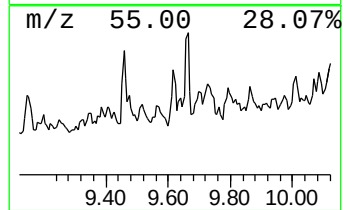
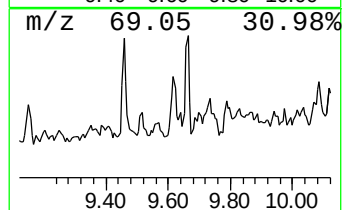
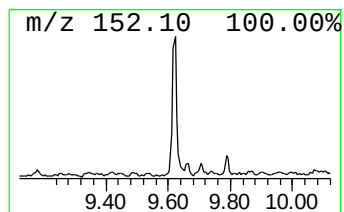
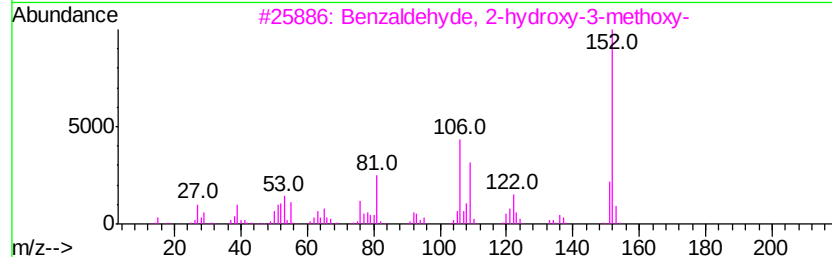
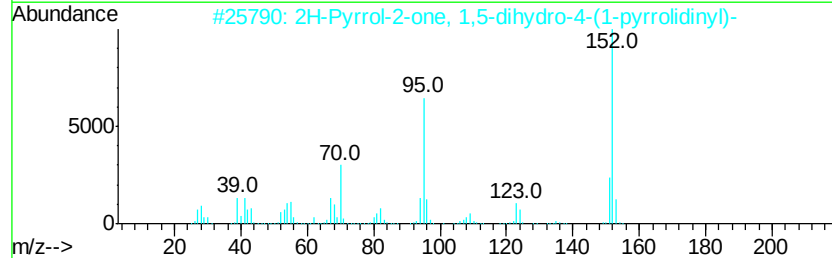
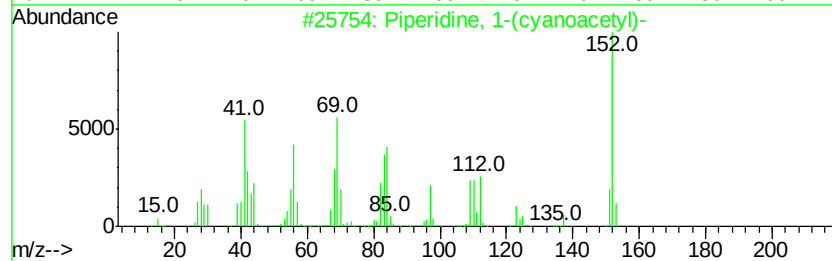
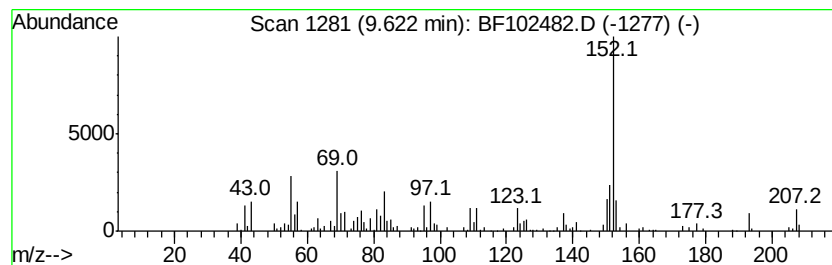
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Piperidine, 1-(cyanoacetyl)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.62	3.23 ng	174253	Acenaphthene-d10	9.76

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Piperidine, 1-(cyanoacetyl)-	152	C8H12N2O	015029-30-8	50
2		2H-Pyrrol-2-one, 1,5-dihydro-4-(...	152	C8H12N2O	105776-93-0	46
3		Benzaldehyde, 2-hydroxy-3-methoxy-	152	C8H8O3	000148-53-8	43
4		Biphenylene	152	C12H8	000259-79-0	42
5		Acenaphthylene	152	C12H8	000208-96-8	38



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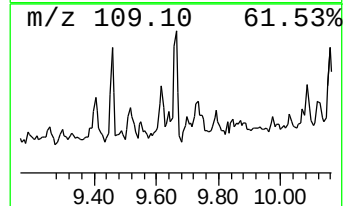
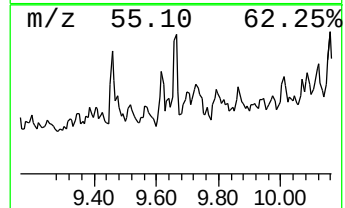
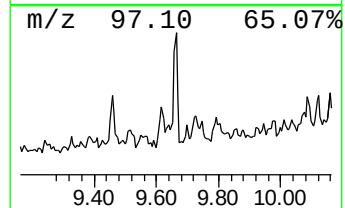
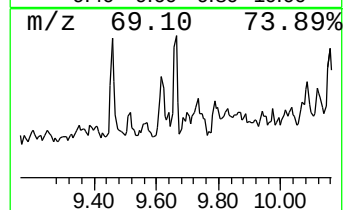
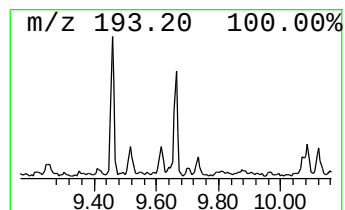
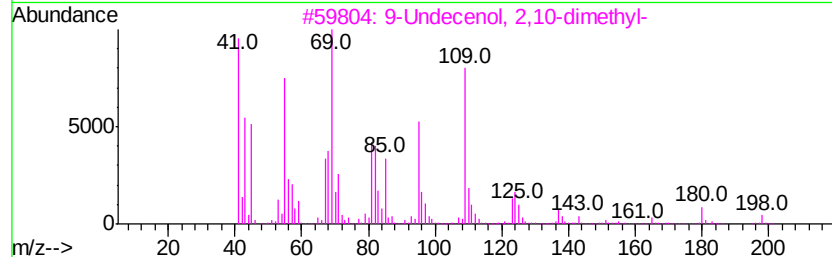
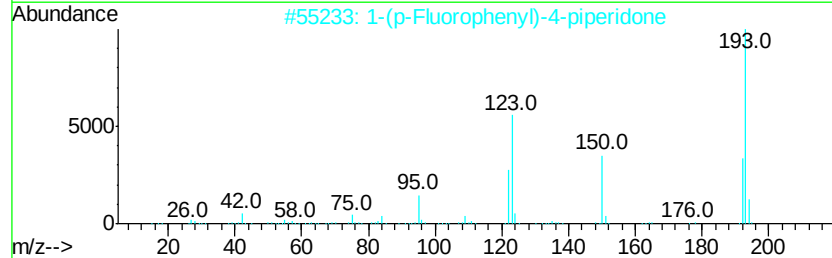
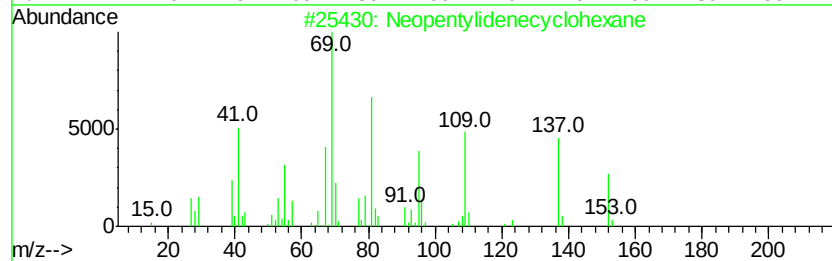
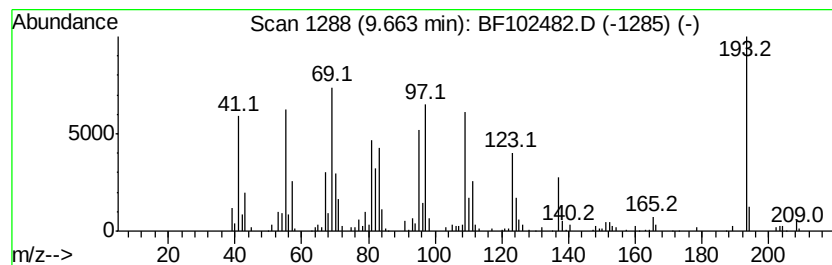
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown9.66 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.66	3.31 ng	178531	Acenaphthene-d10	9.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Neopentylidenecyclohexane	152	C11H20	039546-80-0	27
2		1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	22
3		9-Undecenol, 2,10-dimethyl-	198	C13H26O	1000131-86-0	22
4		Cyclopentane, (2-methylpropyl)-	126	C9H18	003788-32-7	20
5		2(5H)-Furanone, 5,5-dimethyl-	112	C6H8O2	020019-64-1	18



Data Path : U:\HPCHEM1\BNA F\DATA\BF012618\
Data File : BF102482.D
Acq On : 26 Jan 2018 21:23
Operator : SJ/JU
Sample : J1257-03 5X
Misc :
ALS Vial : 21 Sample Multiplier: 1

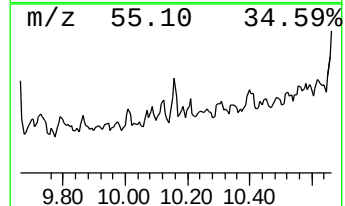
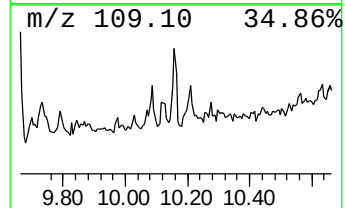
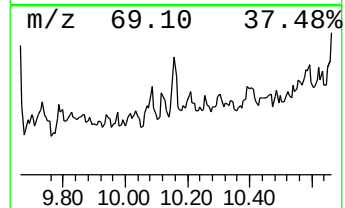
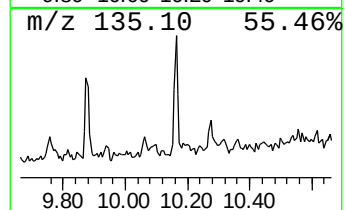
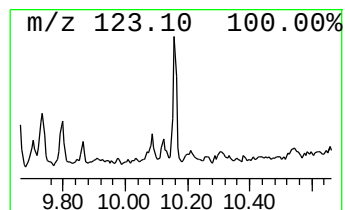
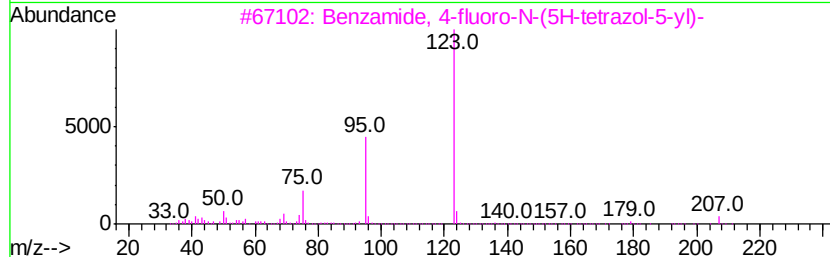
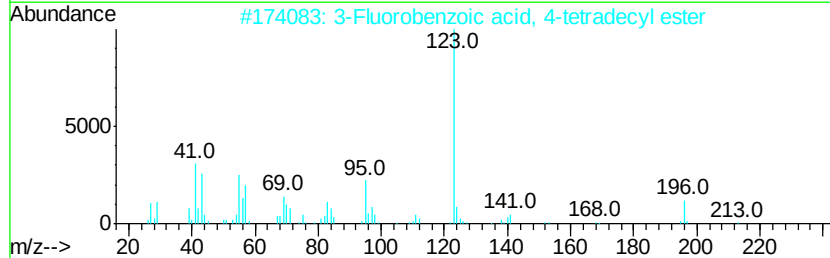
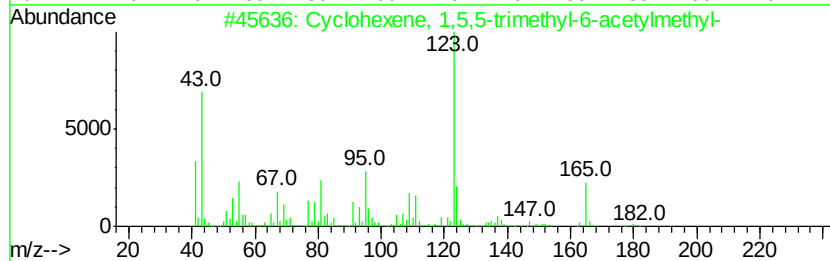
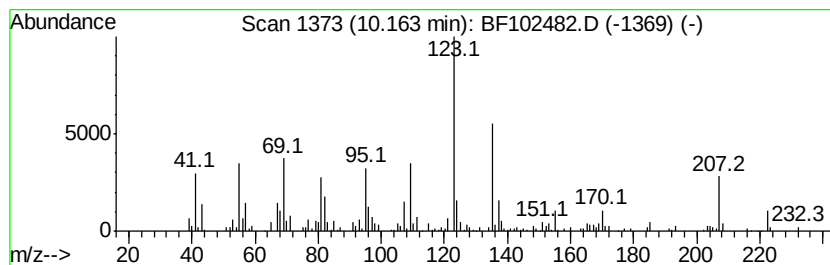
Instrument :
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ClientSampleId :
WC-12(0-5)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclohexene, 1,5,5-trimethy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.16	3.52 ng	190190	Acenaphthene-d10	9.76	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 1,5,5-trimethyl-6-a...	180	C12H20O	211563-96-1	52
2	3-Fluorobenzoic acid, 4-tetradec...	336	C21H33F02	1000280-60-6	47
3	Benzamide, 4-fluoro-N-(5H-tetraz...	207	C8H6FN5O	1000262-68-4	47
4	4-Fluorobenzoic acid, 4-pentadec...	350	C22H35F02	1000280-68-5	47
5	3-Fluorobenzoic acid, 3-tridecyl...	322	C20H31F02	1000280-60-3	47



Data Path : U:\HPCHEM1\BNA F\DATA\BF012618\
Data File : BF102482.D
Acq On : 26 Jan 2018 21:23
Operator : SJ/JU
Sample : J1257-03 5X
Misc :
ALS Vial : 21 Sample Multiplier: 1

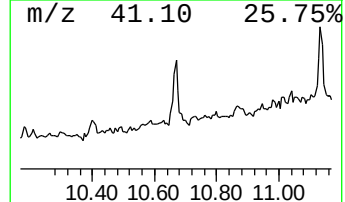
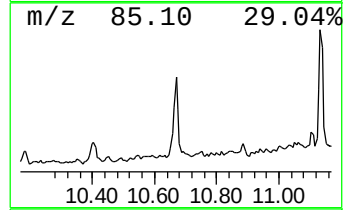
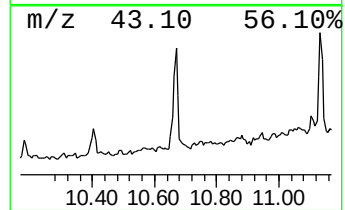
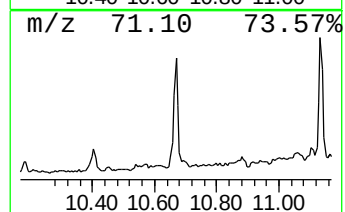
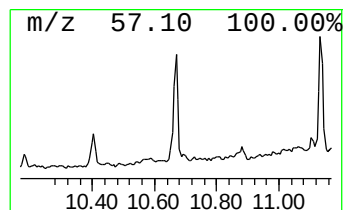
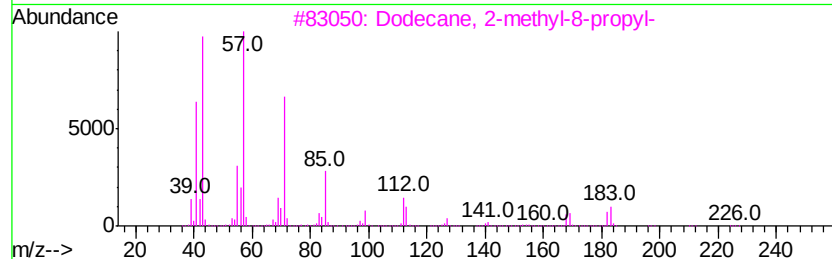
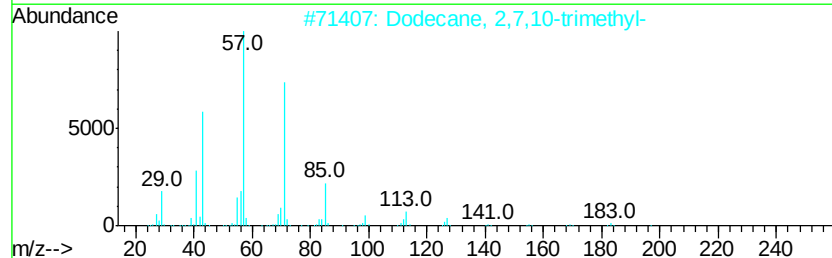
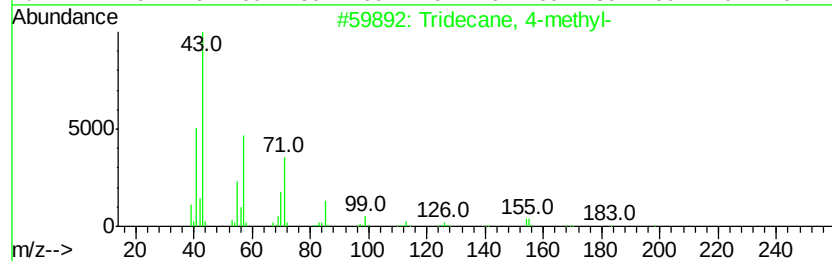
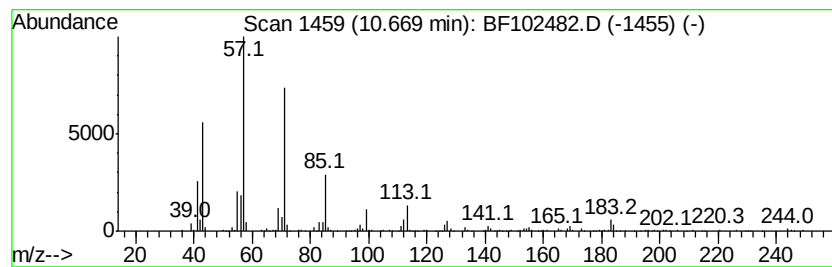
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tridecane, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	12.12 ng	517400	Phenanthrene-d10	11.25
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Tridecane, 4-methyl-	198 C14H30	026730-12-1 87
2		Dodecane, 2,7,10-trimethyl-	212 C15H32	074645-98-0 86
3		Dodecane, 2-methyl-8-propyl-	226 C16H34	055045-07-3 86
4		Pentadecane, 7-methyl-	226 C16H34	006165-40-8 81
5		Dodecane, 2,6,11-trimethyl-	212 C15H32	031295-56-4 80



Data Path : U:\HPCHEM1\BNA_F\DATA\BF012618\
Data File : BF102482.D
Acq On : 26 Jan 2018 21:23
Operator : SJ/JU
Sample : J1257-03 5X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-12(0-5)

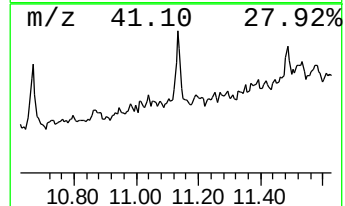
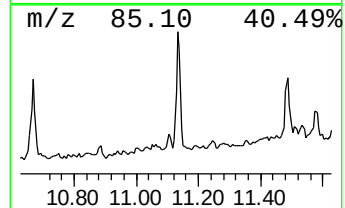
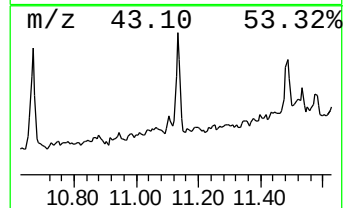
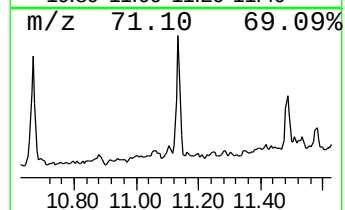
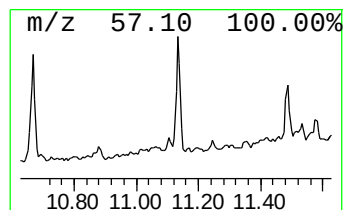
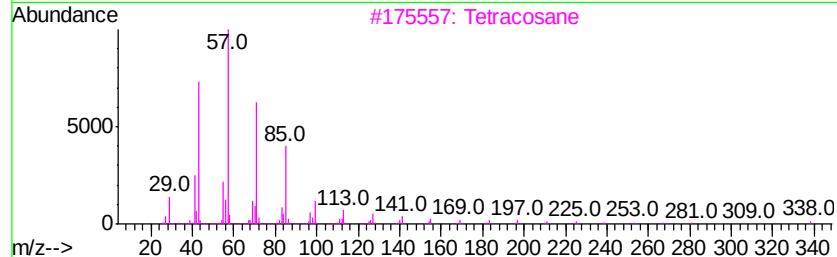
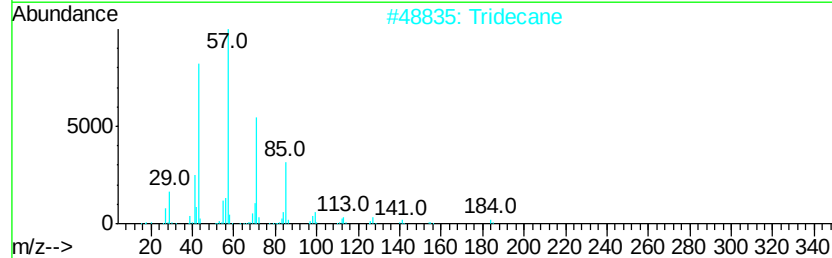
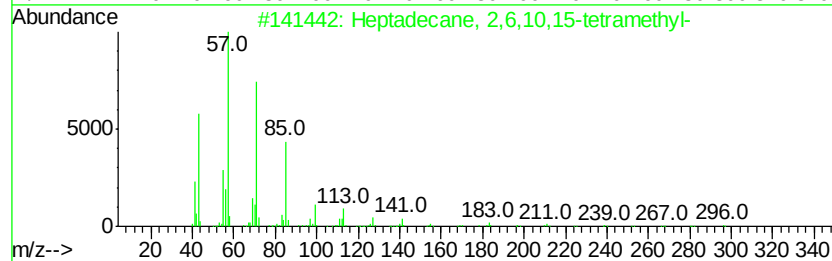
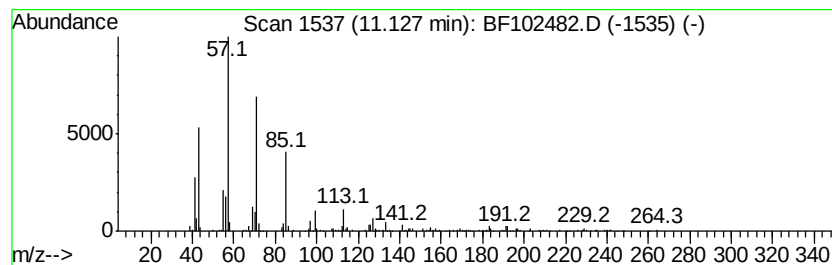
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecane, 2,6,10,15-tetr... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.13	10.12 ng	432115	Phenanthrene-d10	11.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
2		Tridecane	184	C13H28	000629-50-5	90
3		Tetracosane	338	C24H50	000646-31-1	90
4		Heneicosane	296	C21H44	000629-94-7	90
5		Heptacosane	380	C27H56	000593-49-7	90



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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-12(0-5)

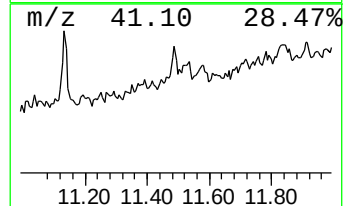
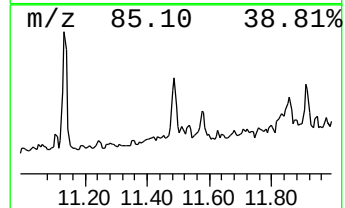
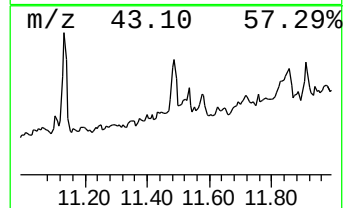
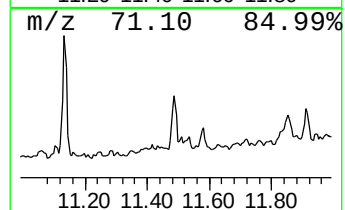
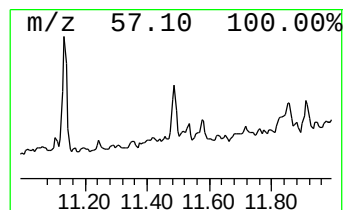
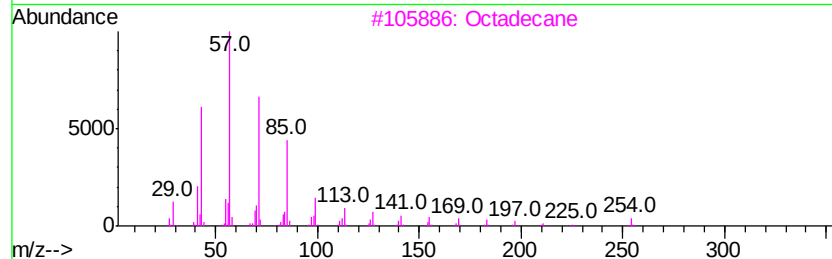
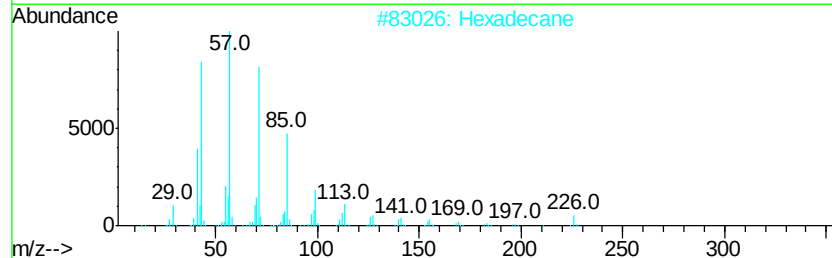
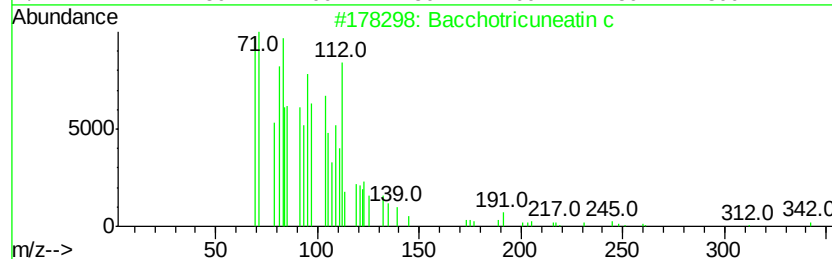
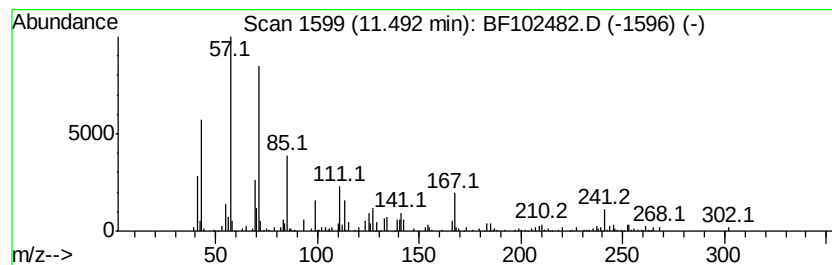
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Bacchotricuneatin c Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.49	3.52 ng	150484	Phenanthrene-d10	11.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bacchotricuneatin c	342	C20H22O5	066563-30-2	80
2		Hexadecane	226	C16H34	000544-76-3	74
3		Octadecane	254	C18H38	000593-45-3	74
4		Heptadecane	240	C17H36	000629-78-7	74
5		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	72



Data Path : U:\HPCHEM1\BNA_F\DATA\BF012618\
Data File : BF102482.D
Acq On : 26 Jan 2018 21:23
Operator : SJ/JU
Sample : J1257-03 5X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-12(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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
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Benzene, 1,2,3-tr...	6.54	3.4	ng	161385	1	6.72	939269	20.0
1H-Indene, octahy...	9.46	3.3	ng	179527	3	9.76	1080200	20.0
Piperidine, 1-(cy...	9.62	3.2	ng	174253	3	9.76	1080200	20.0
unknown9.66	9.66	3.3	ng	178531	3	9.76	1080200	20.0
Cyclohexene, 1,5,...	10.16	3.5	ng	190190	3	9.76	1080200	20.0
Tridecane, 4-methyl-	10.67	12.1	ng	517400	4	11.25	854095	20.0
Heptadecane, 2,6,...	11.13	10.1	ng	432115	4	11.25	854095	20.0
Bacchotricuneatin c	11.49	3.5	ng	150484	4	11.25	854095	20.0