

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083021\
 Data File : BF125266.D
 Acq On : 30 Aug 2021 17:10
 Operator : JU/CG
 Sample : M3561-12
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VE1-2

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125266.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.204	11	20	26	rVB	2364253	3361310	66.44%	8.551%
2	4.010	324	327	332	rVB	56889	67899	1.34%	0.173%
3	5.122	513	516	520	rBV	135446	130738	2.58%	0.333%
4	5.528	581	585	596	rBV	1727461	1550925	30.65%	3.946%
5	6.528	752	755	765	rVB	1135143	1027636	20.31%	2.614%
6	6.910	817	820	825	rBV	1287147	1052152	20.80%	2.677%
7	7.475	912	916	919	rBV	3124655	2919556	57.71%	7.427%
8	7.851	974	980	986	rBV8	56885	118008	2.33%	0.300%
9	7.933	986	994	1002	rBV8	83519	230728	4.56%	0.587%
10	8.016	1002	1008	1014	rBV6	61686	141234	2.79%	0.359%
11	8.110	1017	1024	1032	rBV	547890	984740	19.46%	2.505%
12	8.175	1032	1035	1036	rBV2	82117	74078	1.46%	0.188%
13	8.198	1036	1039	1042	rVB	1486265	1266518	25.03%	3.222%
14	8.392	1070	1072	1076	rVB2	172585	186056	3.68%	0.473%
15	8.445	1078	1081	1084	rVV3	112069	128227	2.53%	0.326%
16	8.522	1091	1094	1097	rBV3	94839	142582	2.82%	0.363%
17	8.633	1110	1113	1117	rBV4	167230	239837	4.74%	0.610%
18	8.669	1117	1119	1122	rVB3	218675	207381	4.10%	0.528%
19	8.722	1125	1128	1129	rBV3	95697	78976	1.56%	0.201%
20	8.751	1131	1133	1135	rVB2	123311	93231	1.84%	0.237%
21	8.775	1135	1137	1141	rVB3	123207	126882	2.51%	0.323%
22	8.822	1142	1145	1147	rBV4	111863	147781	2.92%	0.376%
23	8.880	1151	1155	1158	rBV5	156678	256652	5.07%	0.653%
24	8.916	1158	1161	1164	rBV3	132217	164583	3.25%	0.419%
25	8.945	1164	1166	1168	rBV3	117438	146769	2.90%	0.373%
26	9.022	1176	1179	1181	rBV3	142500	172669	3.41%	0.439%
27	9.245	1214	1217	1218	rBV3	297476	305916	6.05%	0.778%
28	9.269	1218	1221	1225	rVB	5262862	5059425	100.00%	12.871%
29	9.351	1230	1235	1238	rBV4	239784	399276	7.89%	1.016%
30	9.386	1238	1241	1244	rBV3	259658	397357	7.85%	1.011%
31	9.457	1251	1253	1256	rBV2	207558	175486	3.47%	0.446%
32	9.533	1263	1266	1269	rBV3	383189	466887	9.23%	1.188%
33	9.598	1275	1277	1281	rVB4	263593	330989	6.54%	0.842%
34	9.657	1284	1287	1291	rVB2	468917	586550	11.59%	1.492%
35	9.727	1296	1299	1300	rBV2	237158	220582	4.36%	0.561%
36	9.816	1312	1314	1316	rBV3	262150	231167	4.57%	0.588%

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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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37	9.951	1334	1337	1340	rVB	1893039	1509397	29.83%	3.840%
38	9.986	1340	1343	1346	rBV3	383387	373561	7.38%	0.950%
39	10.269	1388	1391	1395	rBV	480848	559320	11.06%	1.423%
40	10.569	1439	1442	1447	rBV	724681	756927	14.96%	1.926%
41	10.745	1469	1472	1478	rBV	2278685	2092799	41.36%	5.324%
42	10.863	1490	1492	1495	rBV2	519202	474635	9.38%	1.207%
43	11.445	1588	1591	1594	rVB	1670813	1431937	28.30%	3.643%
44	11.980	1679	1682	1685	rVB	964885	749936	14.82%	1.908%
45	12.757	1812	1814	1819	rVB2	645652	598665	11.83%	1.523%
46	13.033	1856	1861	1864	rBV	5060536	4862213	96.10%	12.369%
47	13.933	2012	2014	2024	rVB	385016	454363	8.98%	1.156%
48	14.086	2036	2040	2043	rVB	1114549	1016579	20.09%	2.586%
49	15.586	2290	2295	2303	rVB	971548	1237193	24.45%	3.147%

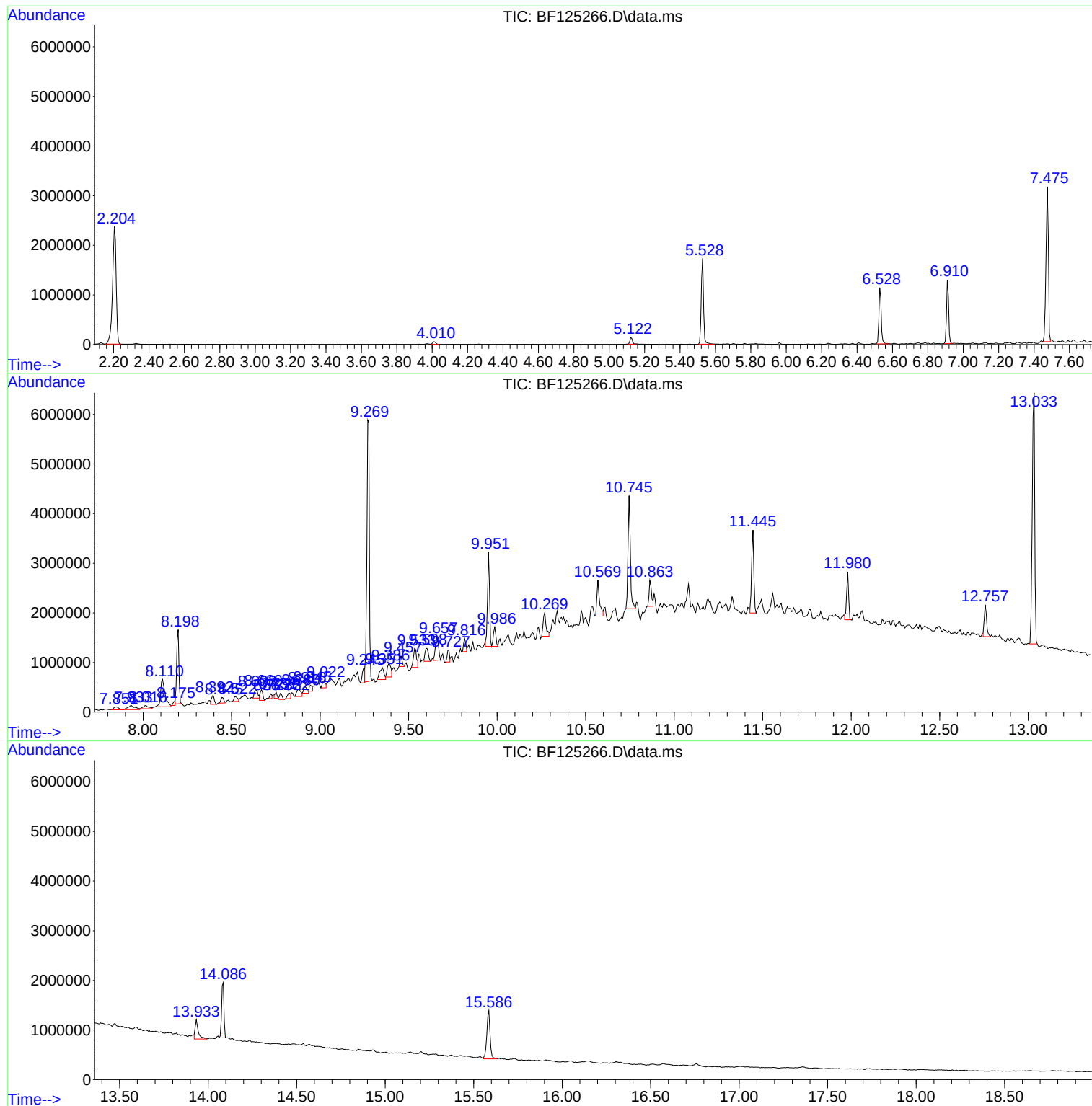
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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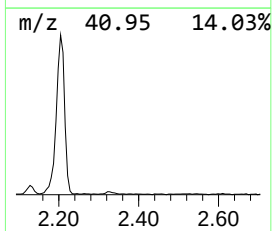
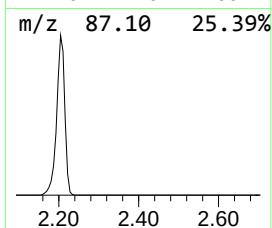
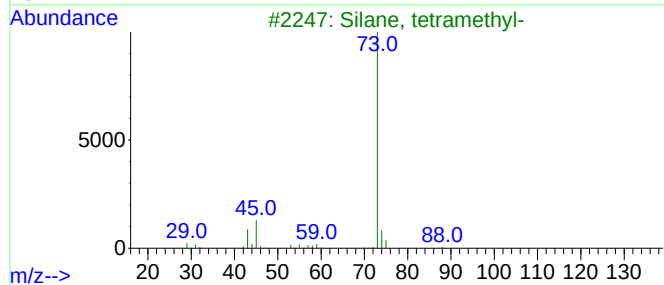
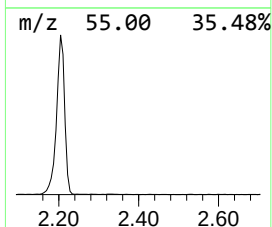
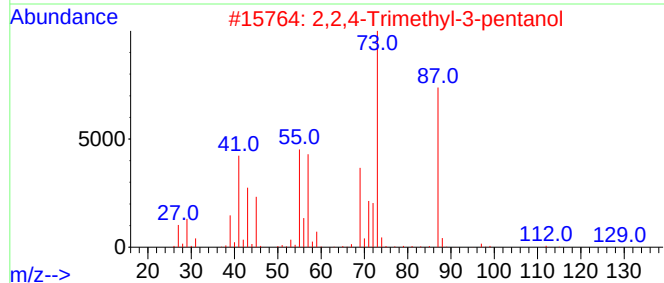
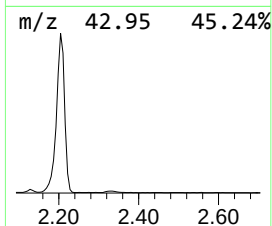
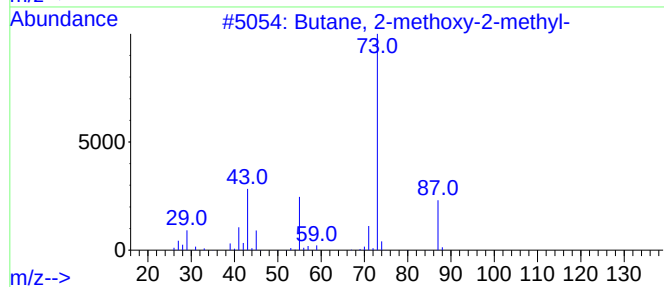
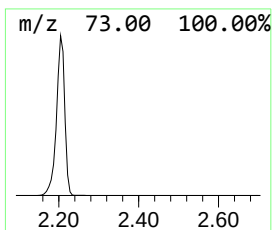
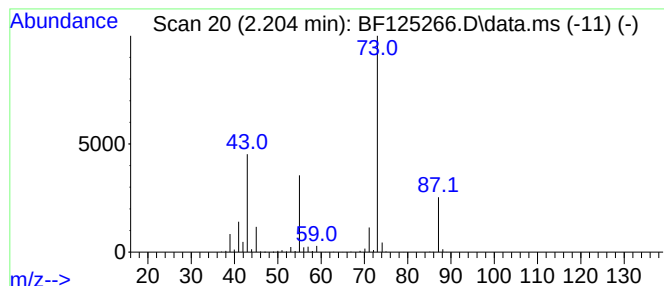
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.204	63.89 ng	3361310	1,4-Dichlorobenzene-d4	6.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
VE1-2

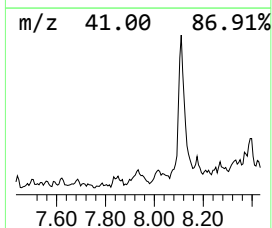
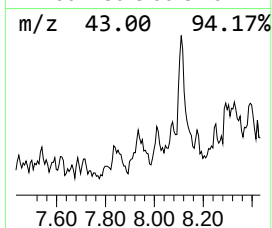
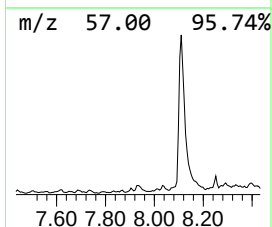
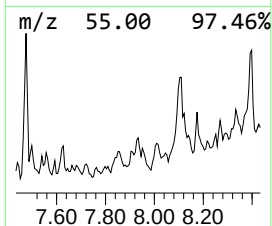
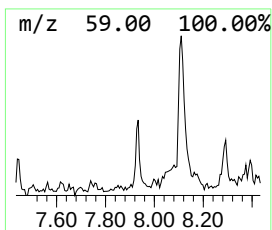
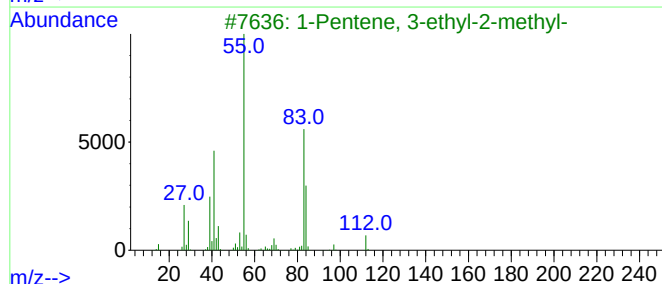
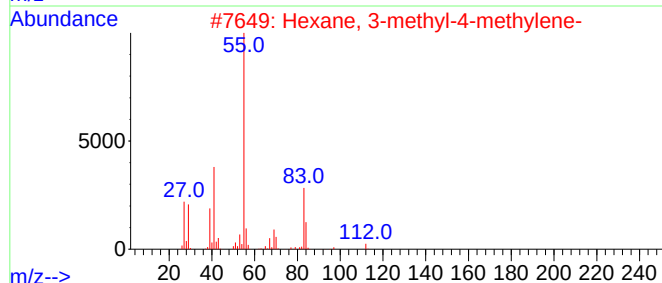
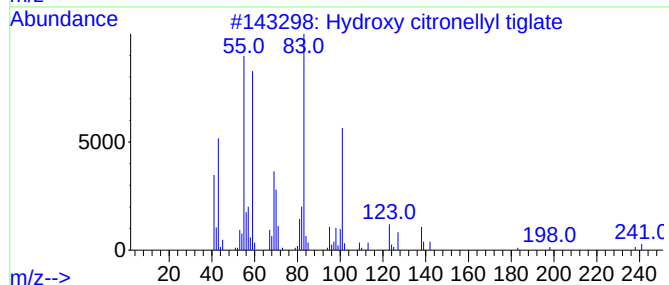
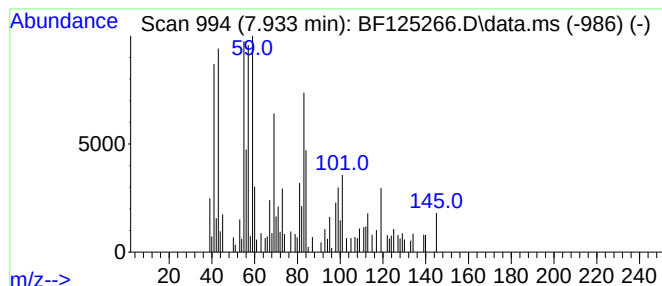
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.933 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.933	3.64 ng	230728	Naphthalene-d8	8.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydroxy citronellyl tiglate	256	C15H28O3	1000383-63-1	27
2			Hexane, 3-methyl-4-methylene-	112	C8H16	003404-67-9	22
3			1-Pentene, 3-ethyl-2-methyl-	112	C8H16	019780-66-6	22
4			Butyl aldoxime, 3-methyl-, anti	101	C5H11NO	005775-74-6	22
5			Hydrazine, 1-(5-hexenyl)-1-methyl-	128	C7H16N2	053907-78-1	14



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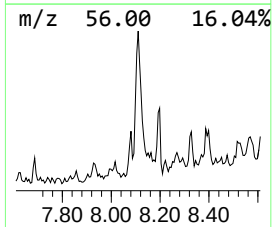
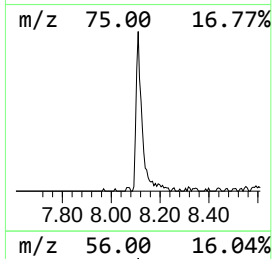
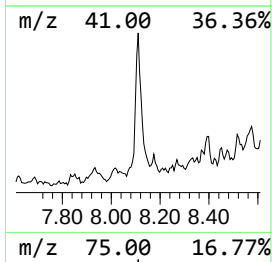
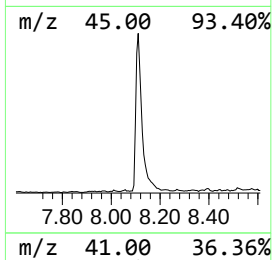
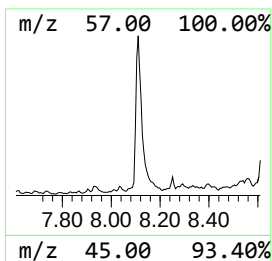
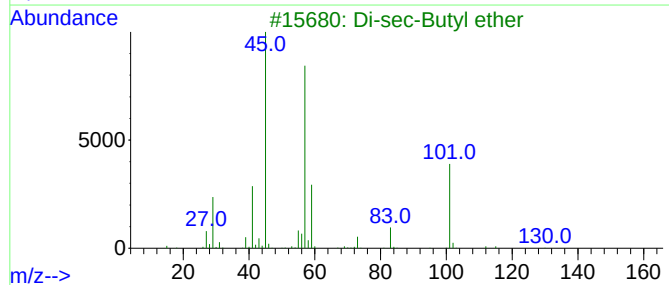
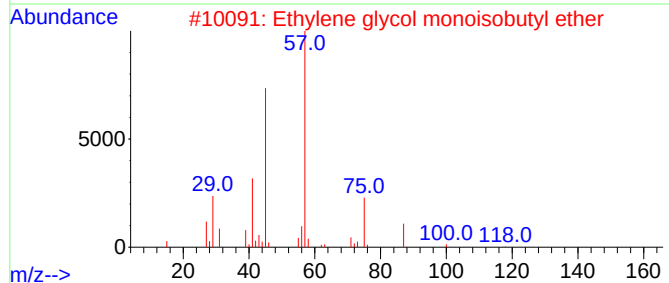
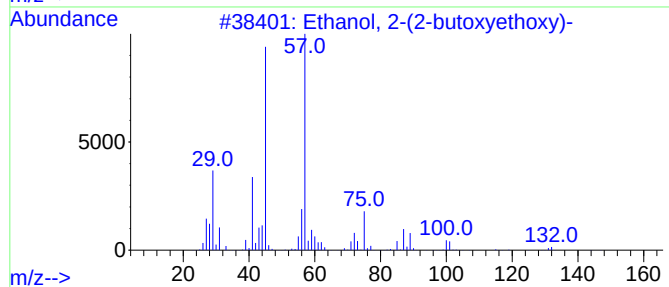
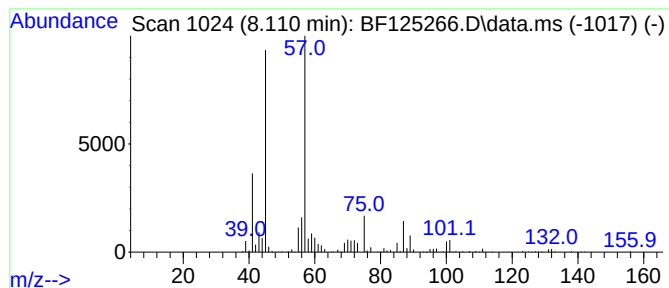
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	15.55 ng	984740	Naphthalene-d8	8.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	53
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50



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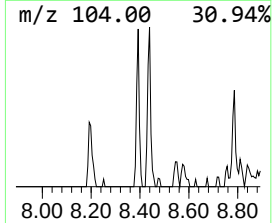
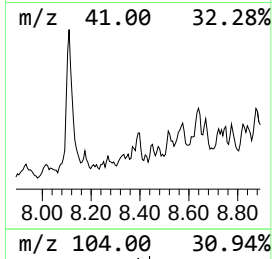
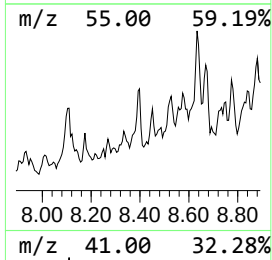
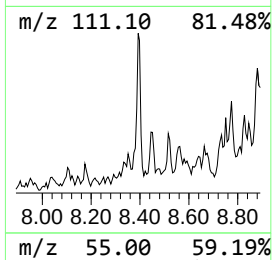
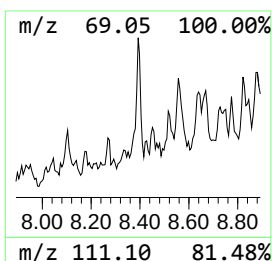
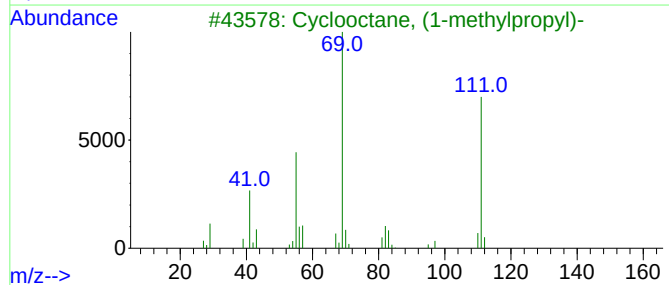
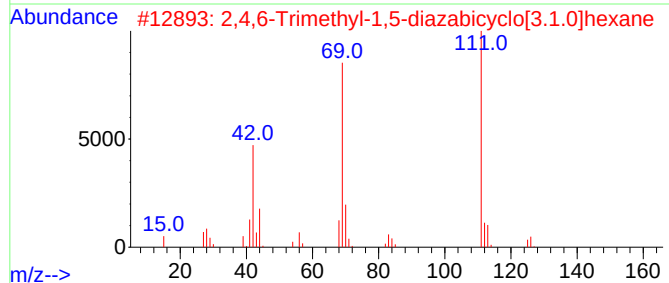
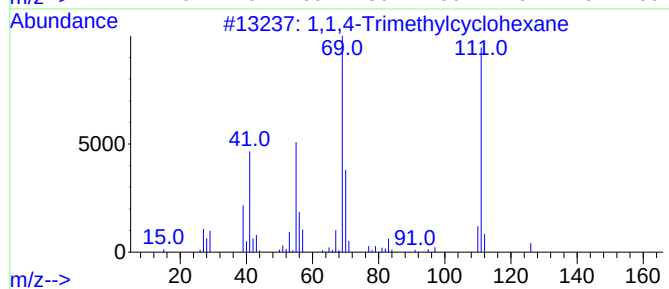
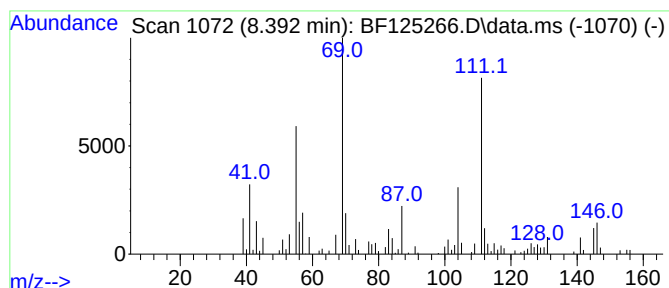
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1,1,4-Trimethylcyclohexane Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.392	2.94 ng	186056	Naphthalene-d8	8.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,1,4-Trimethylcyclohexane	126	C9H18	007094-27-1	58
2			2,4,6-Trimethyl-1,5-diazabicyclo...	126	C7H14N2	1000283-21-2	53
3			Cyclooctane, (1-methylpropyl)-	168	C12H24	016538-89-9	53
4			3-Isopropyl-5-methyl-hex-4-en-2-one	154	C10H18O	077142-85-9	53
5			Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	53



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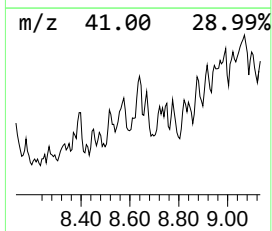
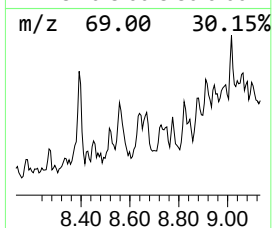
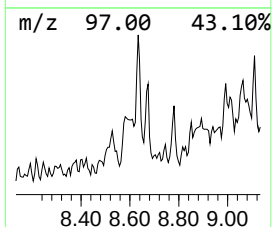
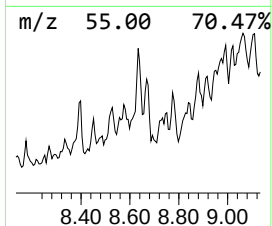
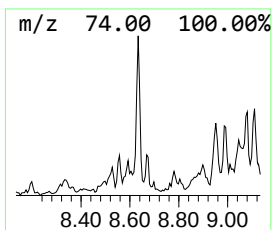
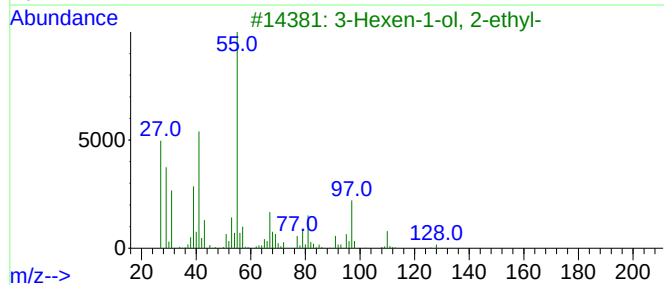
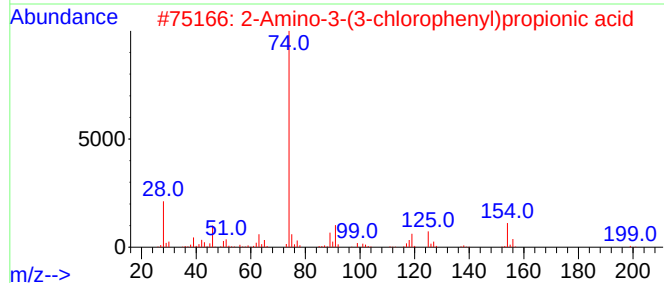
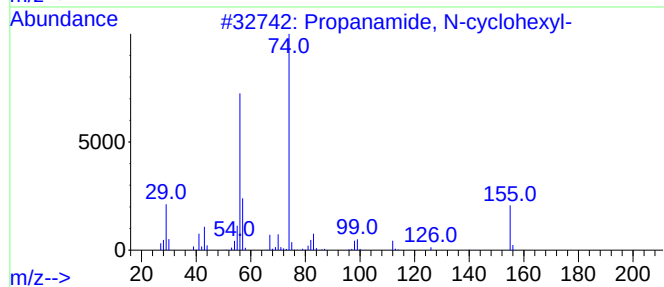
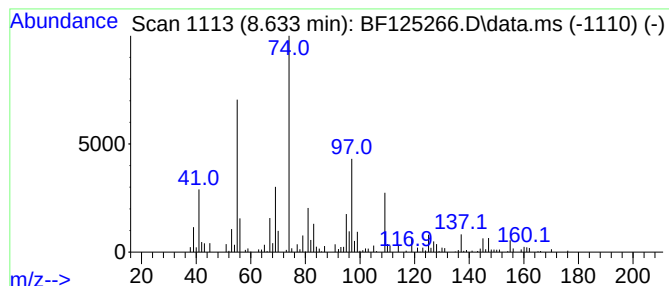
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown8.633 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.633	3.79 ng	239837	Naphthalene-d8	8.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanamide, N-cyclohexyl-	155	C9H17NO	001126-56-3	38
2			2-Amino-3-(3-chlorophenyl)propio...	199	C9H10ClNO2	1000192-11-1	25
3			3-Hexen-1-ol, 2-ethyl-	128	C8H16O	053907-73-6	14
4			Pentanoic acid, 3-methyl-, methy...	130	C7H14O2	002177-78-8	12
5			Cycloheptanemethanol	128	C8H16O	004448-75-3	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083021\
Data File : BF125266.D
Acq On : 30 Aug 2021 17:10
Operator : JU/CG
Sample : M3561-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VE1-2

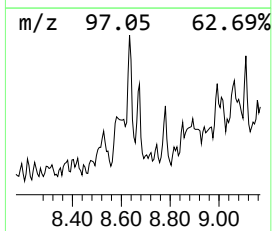
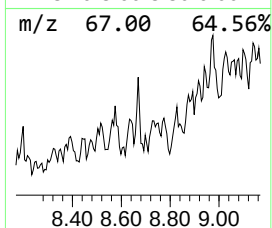
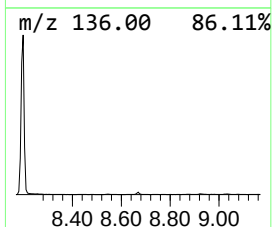
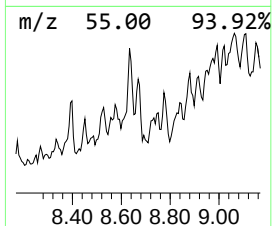
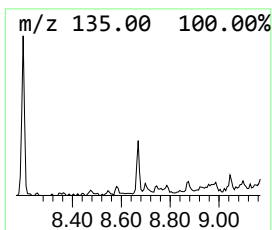
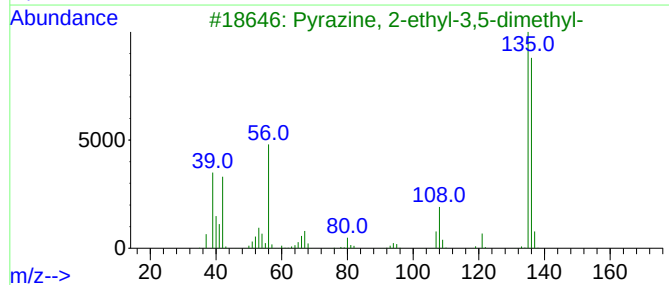
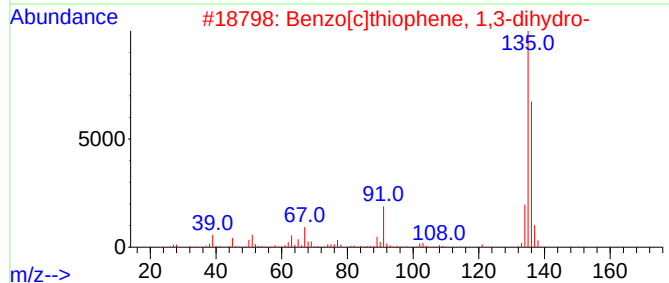
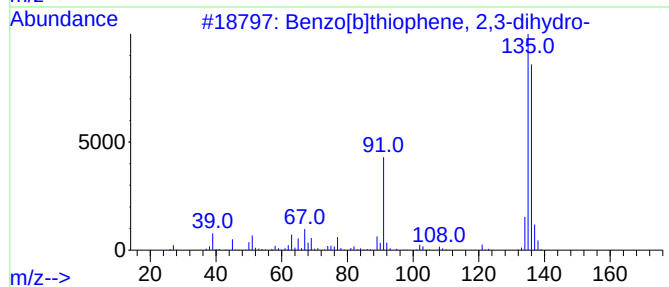
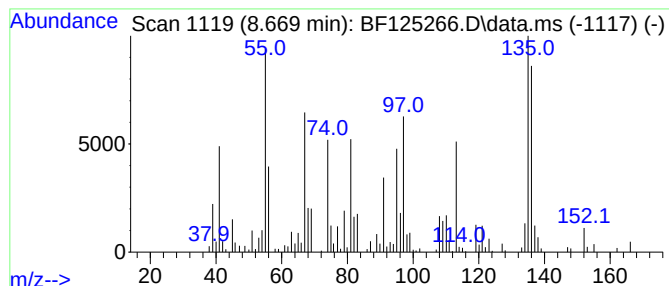
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzo[b]thiophene, 2,3-dihy... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.669	3.27 ng	207381	Naphthalene-d8	8.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]thiophene, 2,3-dihydro-	136	C8H8S	004565-32-6	50
2			Benzo[c]thiophene, 1,3-dihydro-	136	C8H8S	002471-92-3	50
3			Pyrazine, 2-ethyl-3,5-dimethyl-	136	C8H12N2	013925-07-0	43
4			Pyrazine, 3-ethyl-2,5-dimethyl-	136	C8H12N2	013360-65-1	43
5			Benzaldehyde, 4-methoxy-	136	C8H8O2	000123-11-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083021\
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Sample : M3561-12
Misc :
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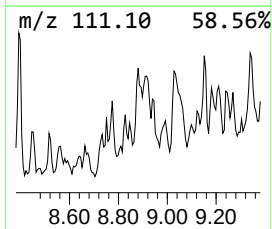
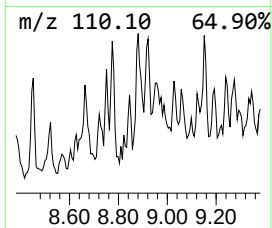
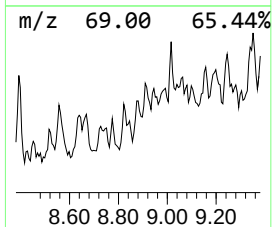
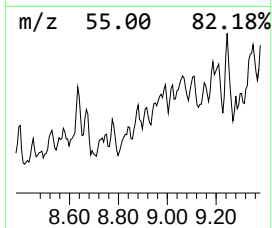
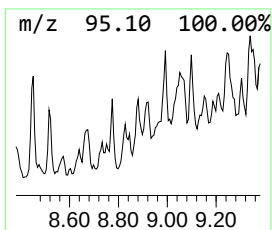
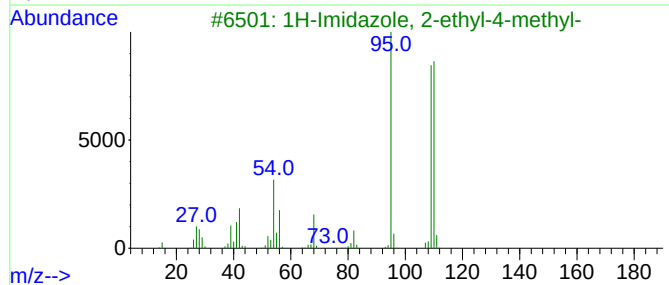
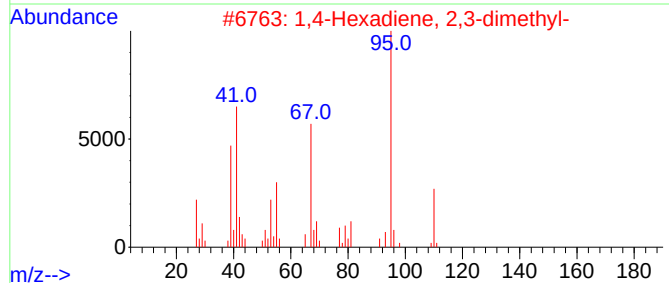
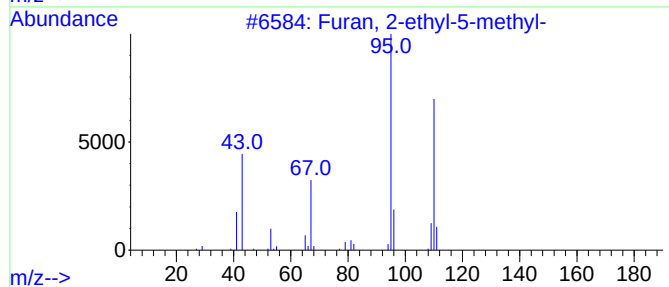
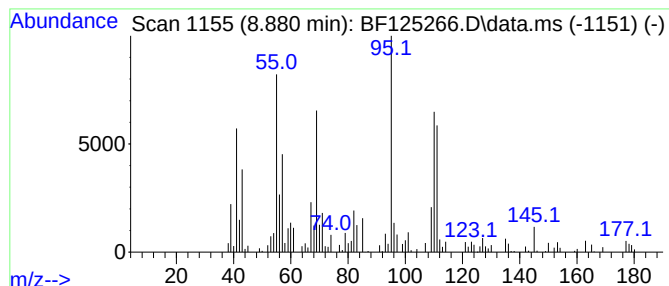
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Furan, 2-ethyl-5-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.880	4.05 ng	256652	Naphthalene-d8	8.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, 2-ethyl-5-methyl-	110	C7H10O	001703-52-2	53
2			1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	46
3			1H-Imidazole, 2-ethyl-4-methyl-	110	C6H10N2	000931-36-2	43
4			Perilla ketone	166	C10H14O2	000553-84-4	43
5			2,9-Dimethyl-5-decyne	166	C12H22	019550-56-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083021\
Data File : BF125266.D
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Sample : M3561-12
Misc :
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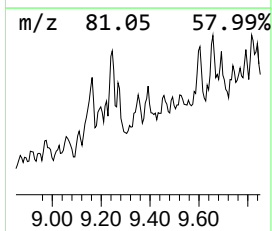
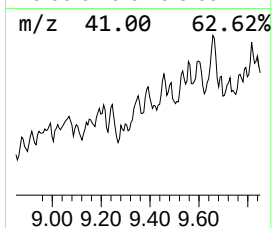
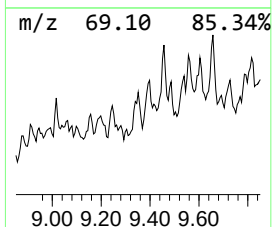
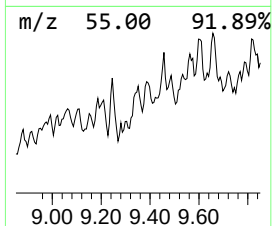
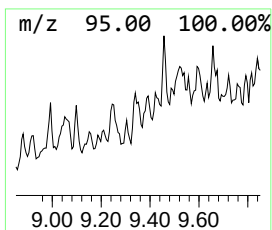
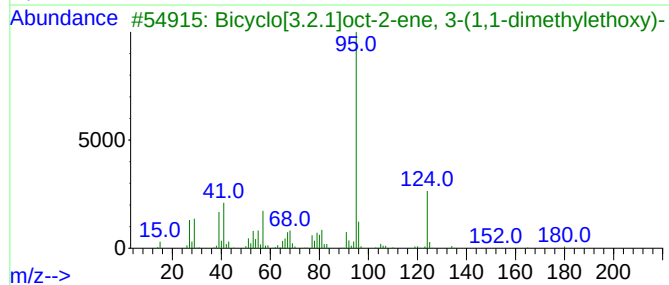
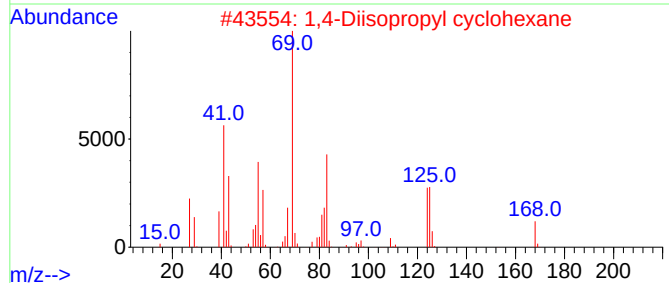
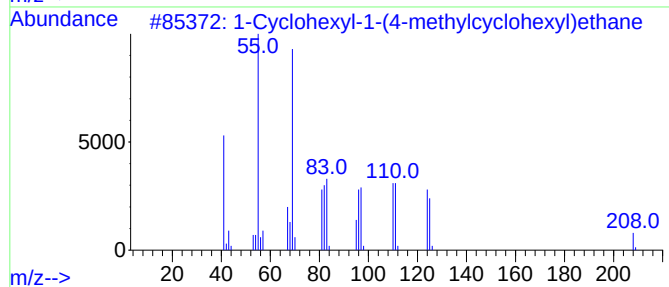
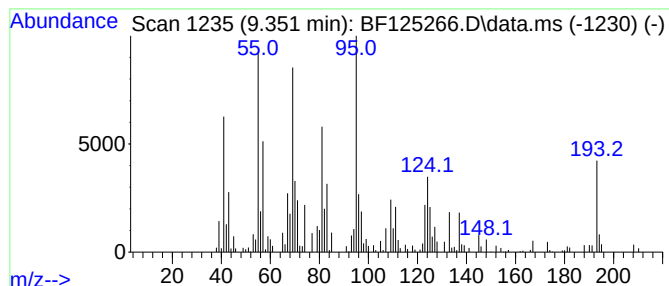
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ClientSampleId :
VE1-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 1-Cyclohexyl-1-(4-methylcyc... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.351	5.29 ng	399276	Acenaphthene-d10	9.951	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Cyclohexyl-1-(4-methylcyclohex...	208	C15H28	002027-12-5	50
2	1,4-Diisopropyl cyclohexane	168	C12H24	022907-72-8	22
3	Bicyclo[3.2.1]oct-2-ene, 3-(1,1-...	180	C12H20O	037609-41-9	22
4	Cyclopentene, 1-isopropyl-4,5-di...	138	C10H18	007712-74-5	22
5	3,5,9-Undecatrien-2-one, 6,10-di...	192	C13H20O	003548-78-5	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083021\
Data File : BF125266.D
Acq On : 30 Aug 2021 17:10
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Misc :
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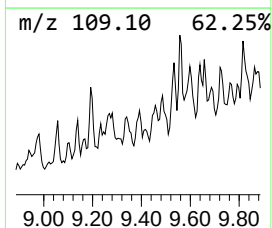
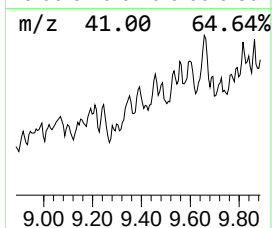
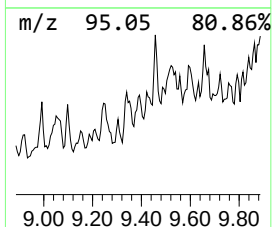
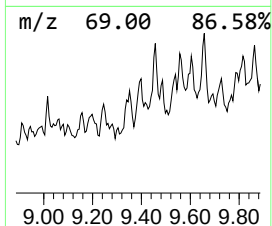
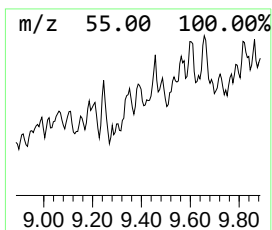
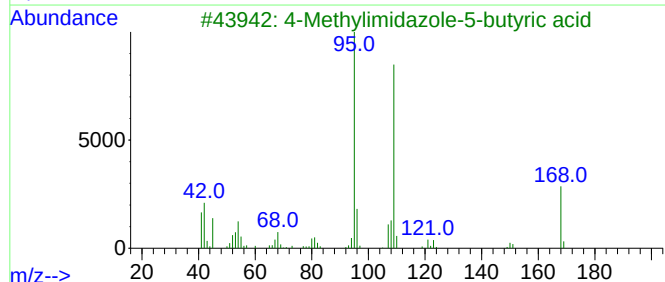
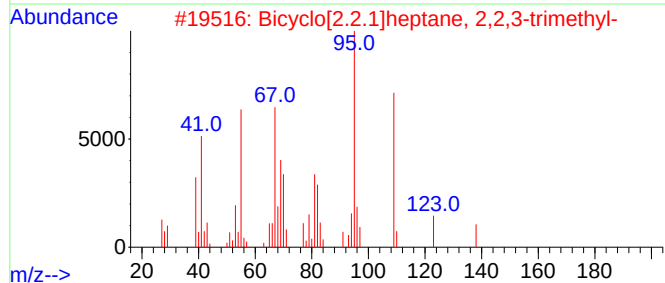
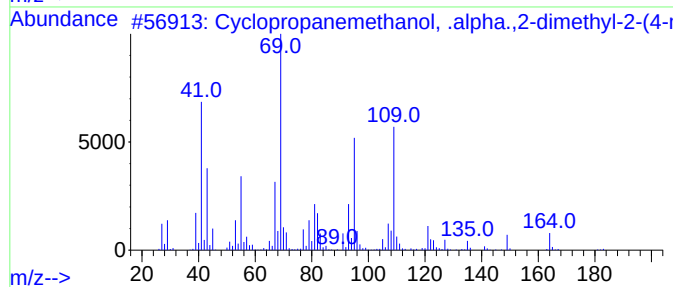
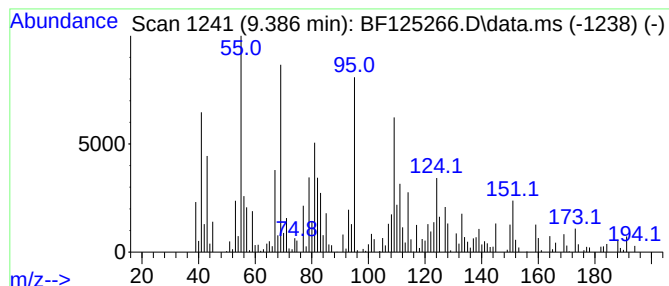
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown9.386 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.386	5.27 ng	397357	Acenaphthene-d10	9.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropanemethanol, .alpha.,2-...	182	C12H22O	121959-70-4	38
2			Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	000473-19-8	25
3			4-Methylimidazole-5-butyric acid	168	C8H12N2O2	1000129-14-7	22
4			Heptanoic acid, 2-vinyl-, ethyl ...	184	C11H20O2	091213-09-1	22
5			Perfluoro-2-azabutene	183	C3F7N	1000322-34-7	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083021\
Data File : BF125266.D
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Sample : M3561-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VE1-2

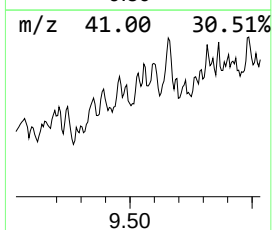
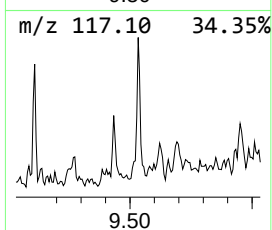
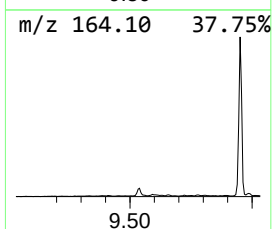
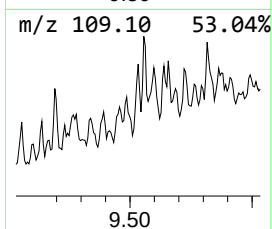
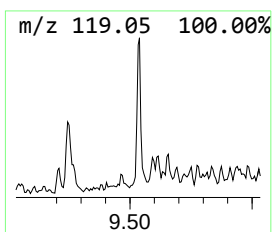
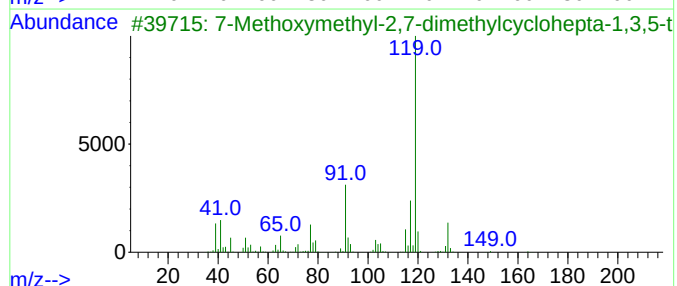
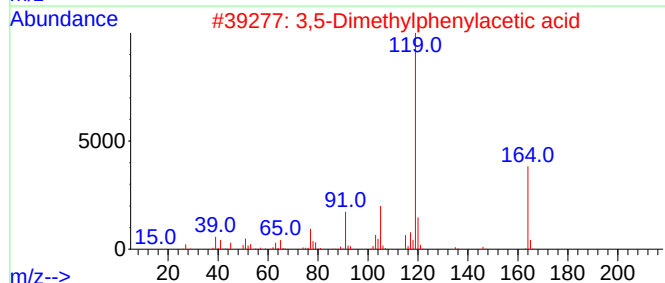
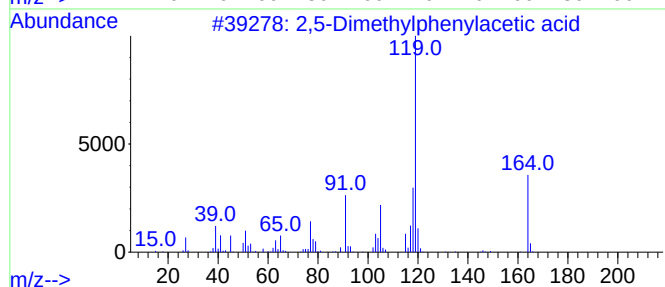
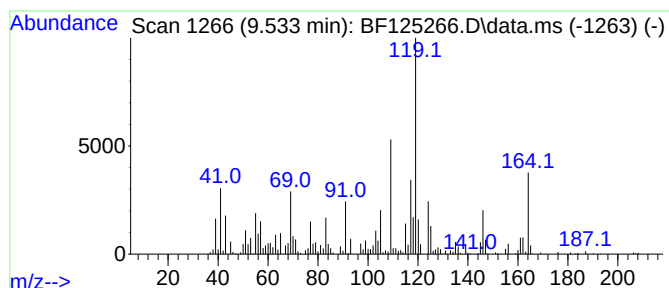
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 2,5-Dimethylphenylacetic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.533	6.19 ng	466887	Acenaphthene-d10	9.951

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,5-Dimethylphenylacetic acid	164	C10H12O2	1000342-65-5	50
2		3,5-Dimethylphenylacetic acid	164	C10H12O2	042288-46-0	45
3		7-Methoxymethyl-2,7-dimethylcycl...	164	C11H16O	073992-48-0	35
4		Benzene, 1,1'-(1,1,2,2-tetrameth...	238	C18H22	001889-67-4	35
5		o-Toluic acid, 3,5-difluoropheny...	248	C14H10F2O2	1000293-77-2	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083021\
Data File : BF125266.D
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ClientSampleId :
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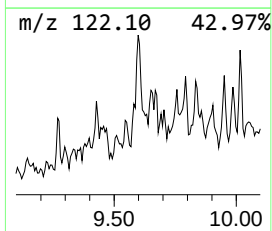
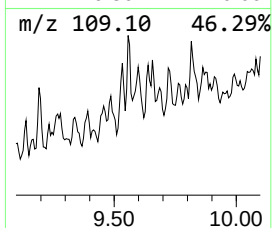
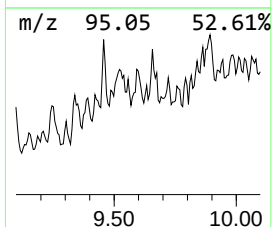
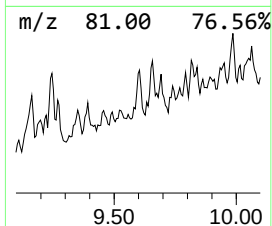
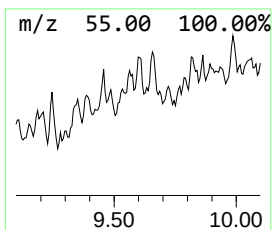
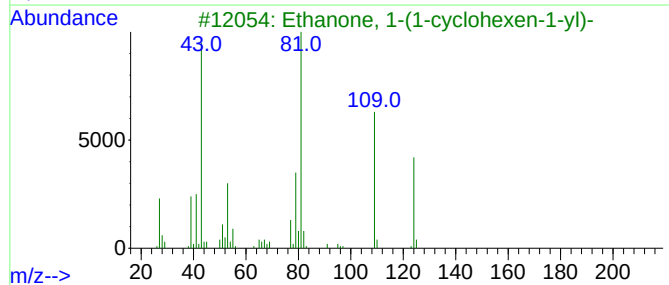
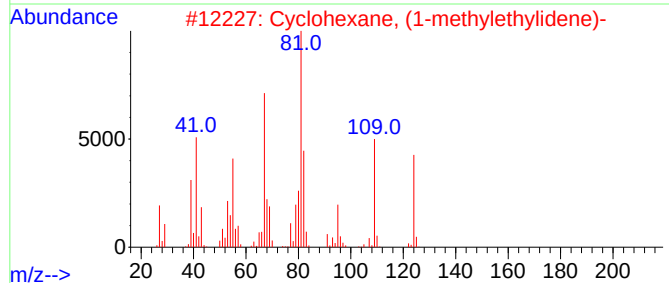
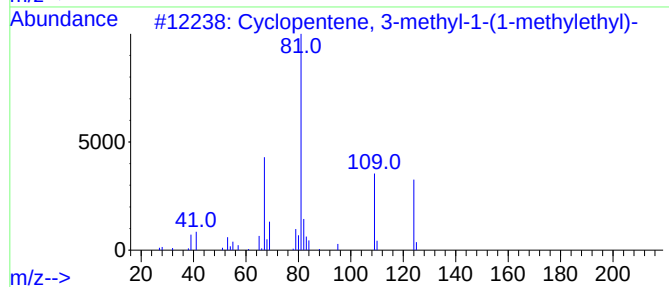
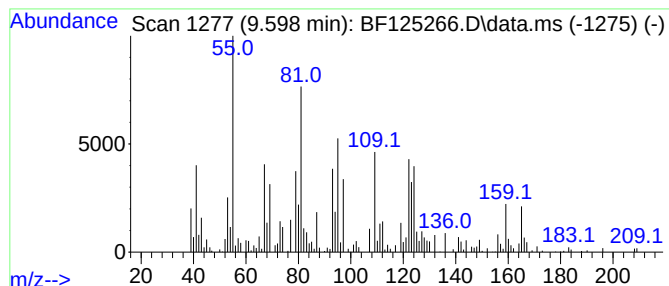
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown9.598 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.598	4.39 ng	330989	Acenaphthene-d10	9.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentene, 3-methyl-1-(1-meth...	124	C9H16	051115-02-7	41
2			Cyclohexane, (1-methylethylidene)-	124	C9H16	005749-72-4	41
3			Ethanone, 1-(1-cyclohexen-1-yl)-	124	C8H12O	000932-66-1	38
4			Bicyclo[3.3.1]nonan-3-ol, exo-	140	C9H16O	010036-08-5	27
5			Undec-10-ynoic acid, tridec-2-yn...	360	C24H40O2	1000406-96-9	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083021\
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Sample : M3561-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VE1-2

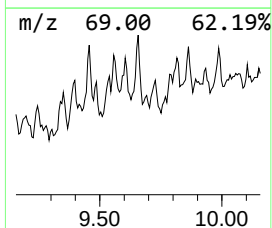
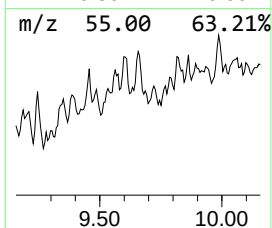
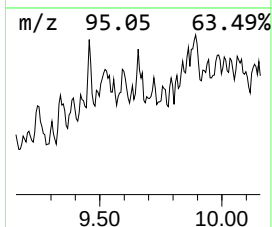
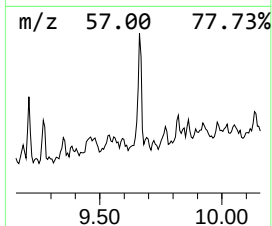
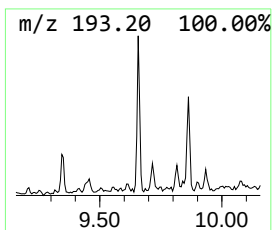
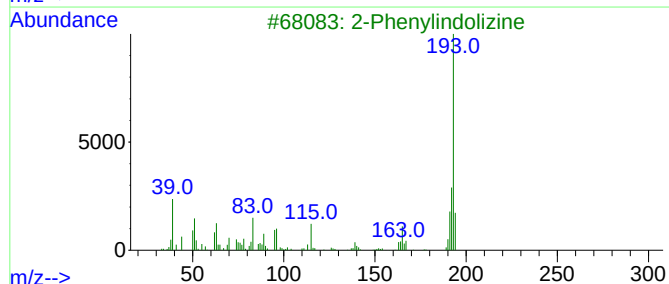
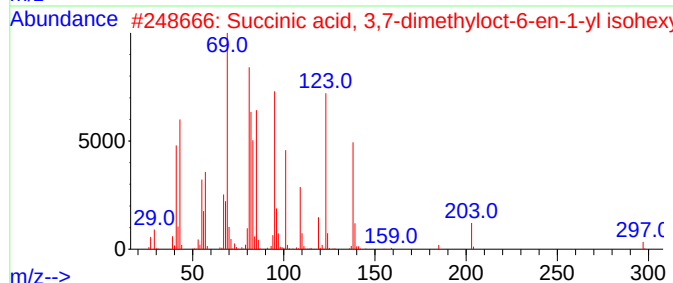
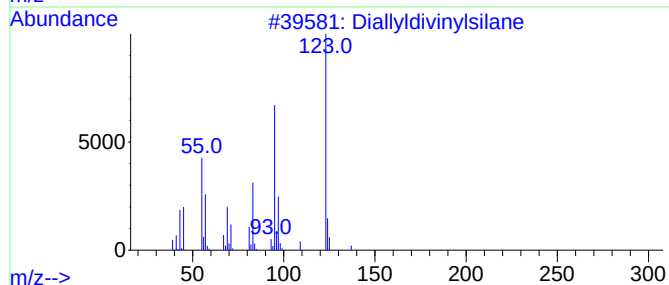
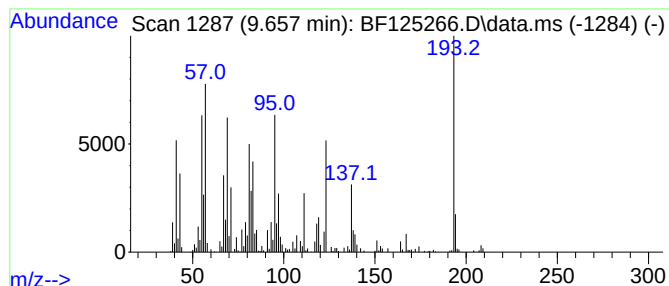
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown9.657 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.657	7.77 ng	586550	Acenaphthene-d10	9.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diallyldivinylsilane	164	C10H16Si	119901-88-1	35
2			Succinic acid, 3,7-dimethyloct-6...	340	C20H36O4	1000353-33-9	30
3			2-Phenylindolizine	193	C14H11N	025379-20-8	27
4			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	000554-59-6	25
5			9-Phenanthrenamine	193	C14H11N	000947-73-9	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083021\
Data File : BF125266.D
Acq On : 30 Aug 2021 17:10
Operator : JU/CG
Sample : M3561-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VE1-2

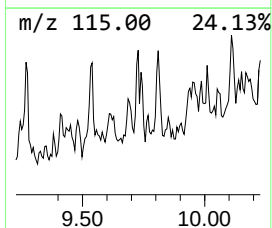
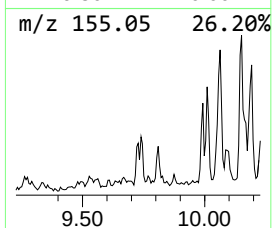
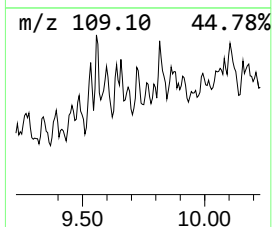
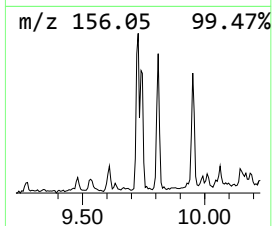
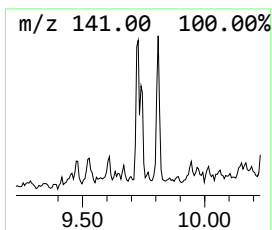
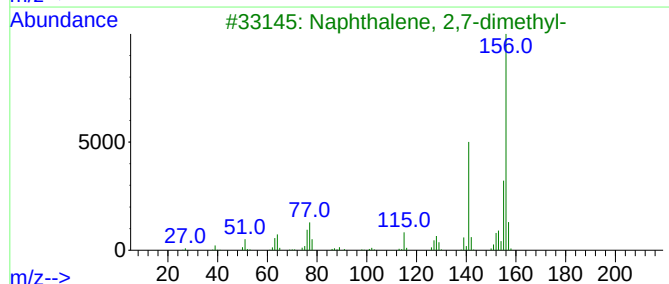
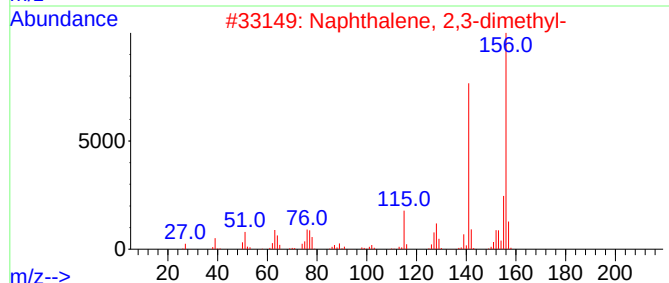
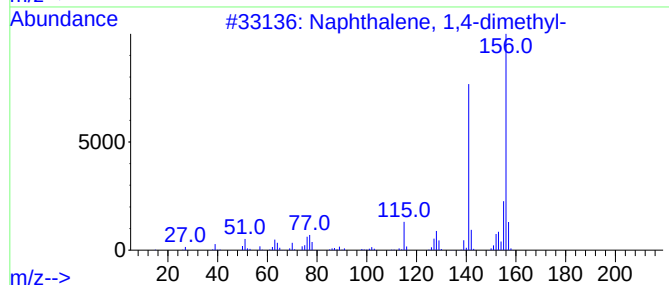
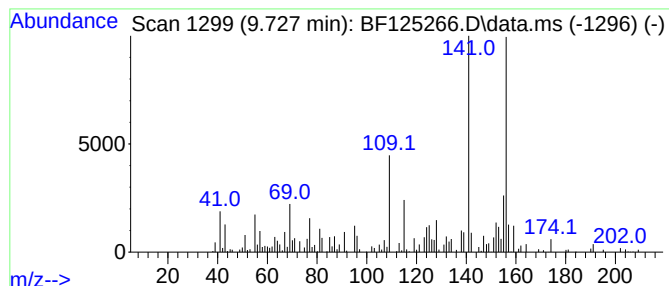
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Naphthalene, 1,4-dimethyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.727	2.92 ng	220582	Acenaphthene-d10	9.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	89
2			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	89
3			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	89
4			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	89
5			Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083021\
Data File : BF125266.D
Acq On : 30 Aug 2021 17:10
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Sample : M3561-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VE1-2

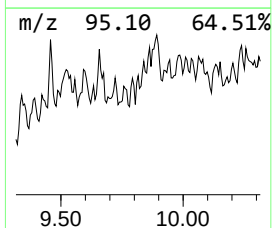
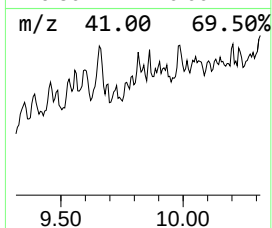
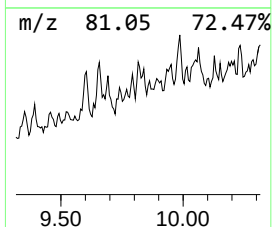
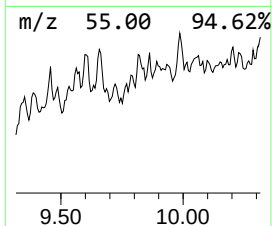
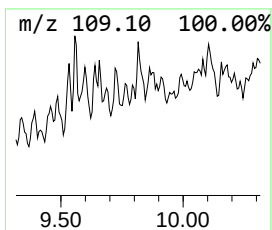
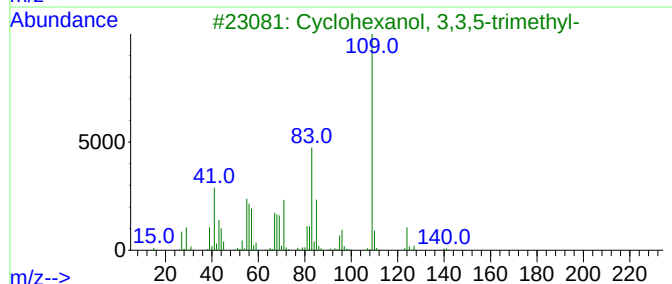
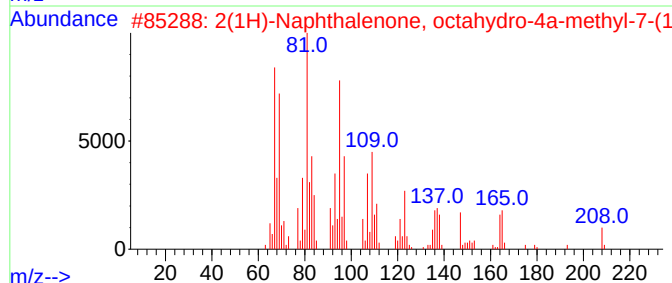
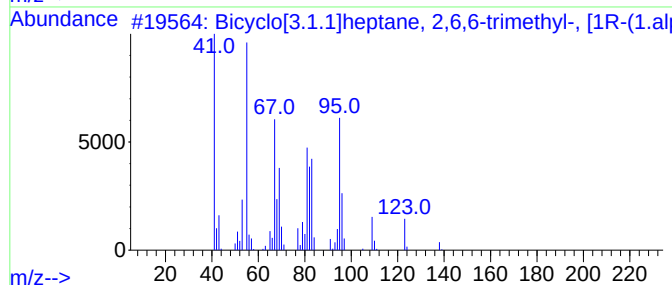
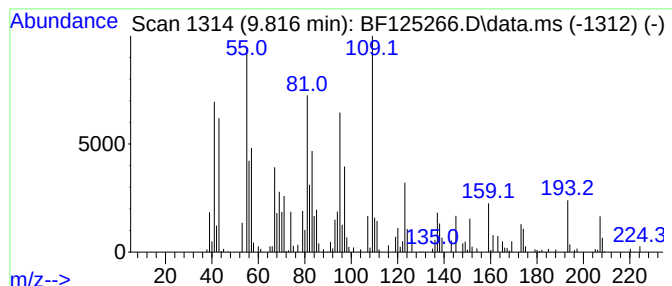
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 unknown9.816 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.816	3.06 ng	231167	Acenaphthene-d10	9.951

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	004863-59-6	41
2		2(1H)-Naphthalenone, octahydro-4...	208	C14H24O	054594-42-2	30
3		Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O	000116-02-9	27
4		Ethanone, 1-(1,3-dimethyl-3-cycl...	152	C10H16O	051733-68-7	25
5		Cyclohexaneethanol, 4-methyl-.be...	154	C10H18O	015714-12-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083021\
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Operator : JU/CG
Sample : M3561-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

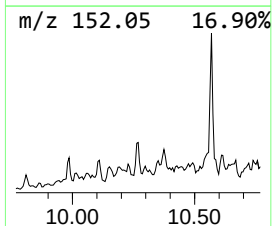
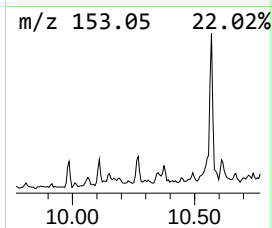
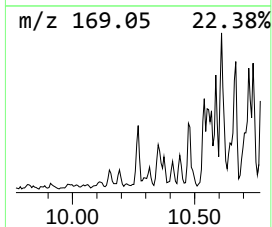
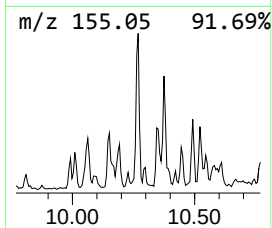
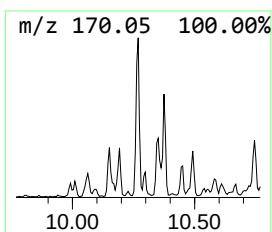
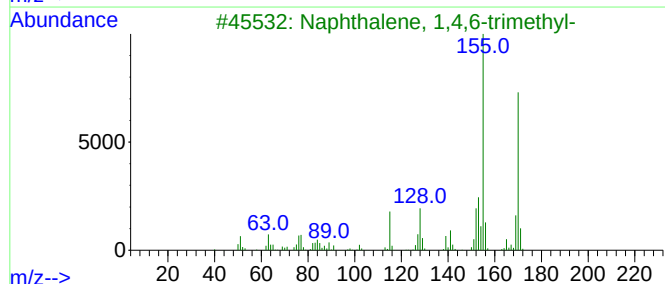
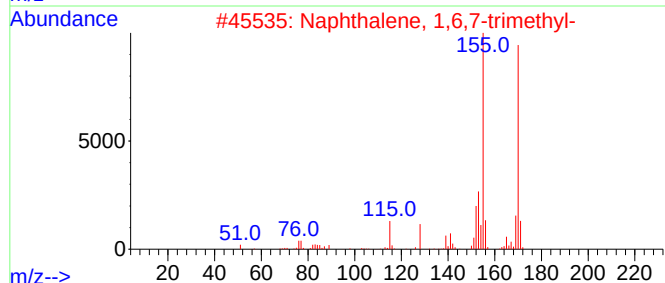
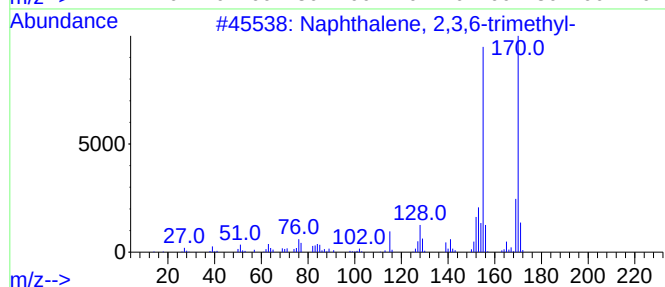
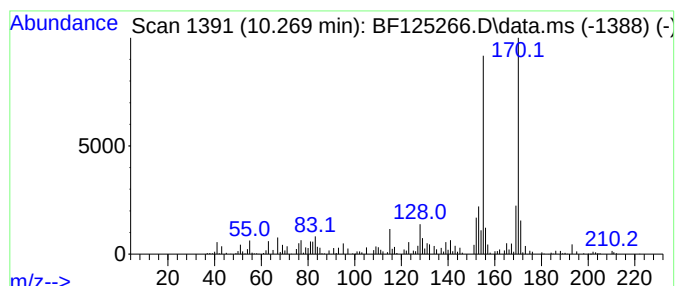
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 Naphthalene, 2,3,6-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.269	7.41 ng	559320	Acenaphthene-d10	9.951	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	98
2	Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	98
3	Naphthalene, 1,4,6-trimethyl-	170	C13H14	002131-42-2	97
4	Naphthalene, 1,4,5-trimethyl-	170	C13H14	002131-41-1	95
5	4,6,8-Trimethylazulene	170	C13H14	000941-81-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083021\
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Misc :
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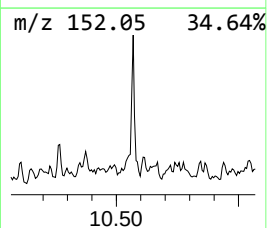
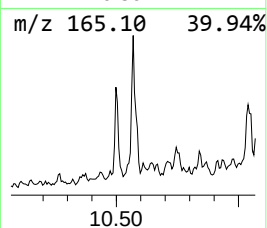
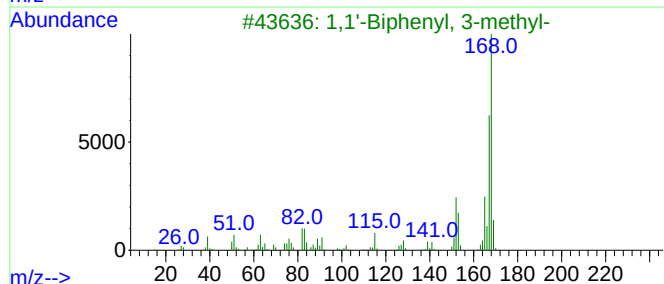
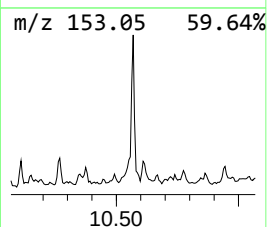
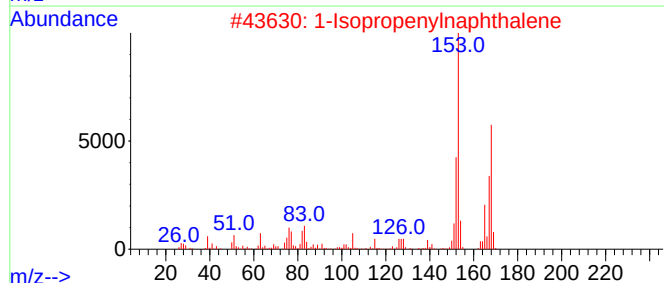
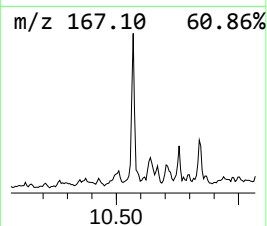
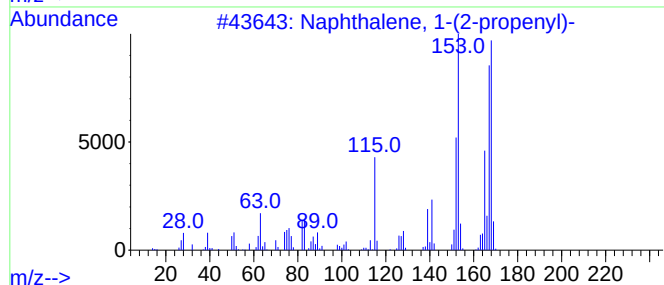
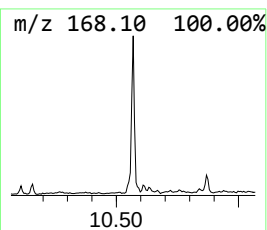
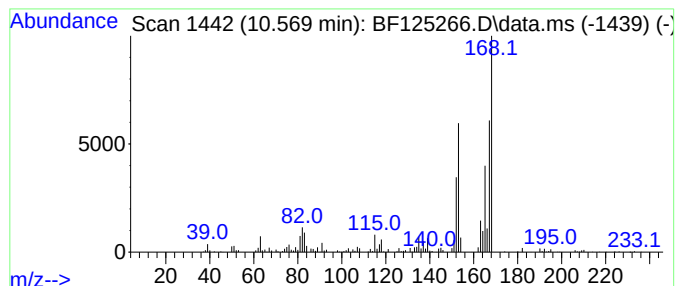
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 Naphthalene, 1-(2-propenyl)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.569	10.03 ng	756927	Acenaphthene-d10	9.951	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-(2-propenyl)-	168	C13H12	002489-86-3	76
2	1-Isopropenylnaphthalene	168	C13H12	001855-47-6	58
3	1,1'-Biphenyl, 3-methyl-	168	C13H12	000643-93-6	52
4	1,1'-Biphenyl, 4-methyl-	168	C13H12	000644-08-6	52
5	1,1'-Biphenyl, 2-methyl-	168	C13H12	000643-58-3	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083021\
Data File : BF125266.D
Acq On : 30 Aug 2021 17:10
Operator : JU/CG
Sample : M3561-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VE1-2

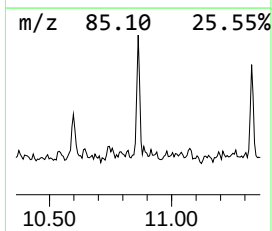
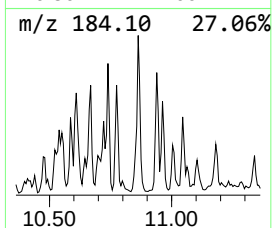
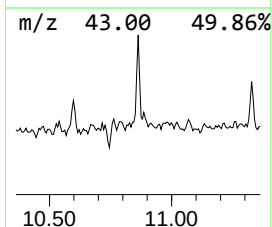
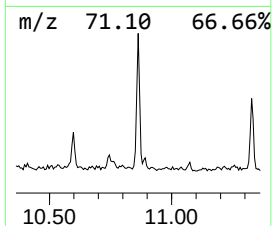
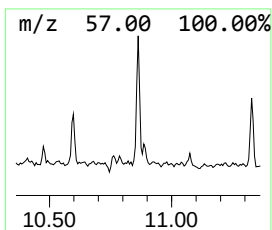
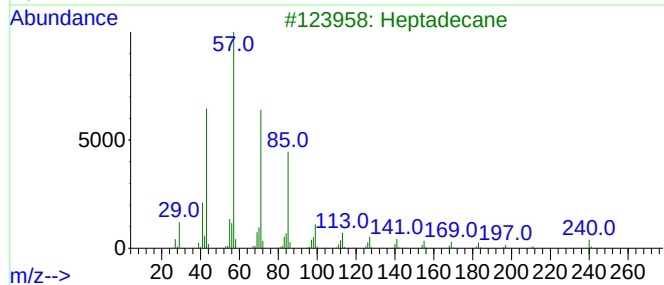
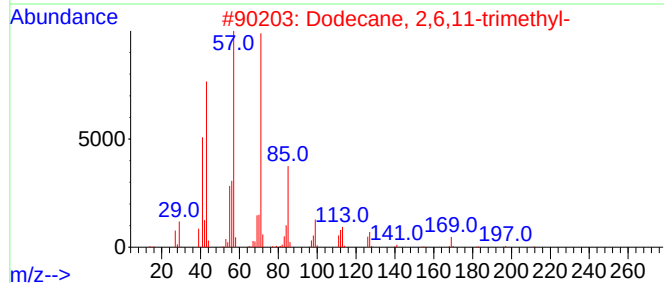
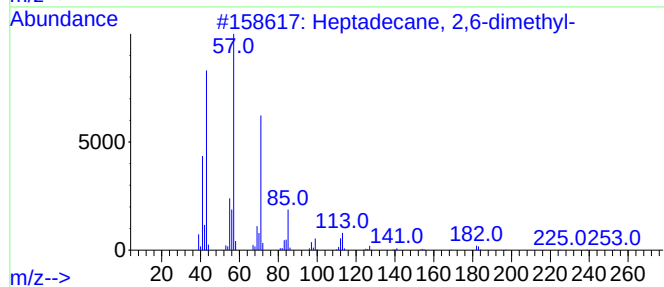
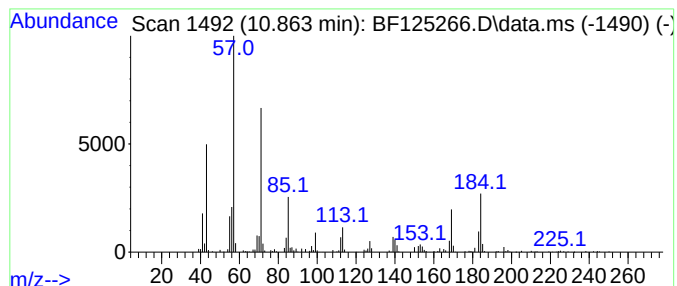
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 Heptadecane, 2,6-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.863	6.63 ng	474635	Phenanthrene-d10	11.445

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	50
2		Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	49
3		Heptadecane	240	C17H36	000629-78-7	43
4		Hexadecane	226	C16H34	000544-76-3	43
5		Sulfurous acid, 2-ethylhexyl und...	348	C19H40O3S	1000309-19-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083021\
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ALS Vial : 9 Sample Multiplier: 1

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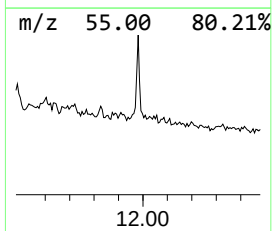
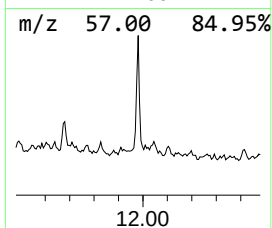
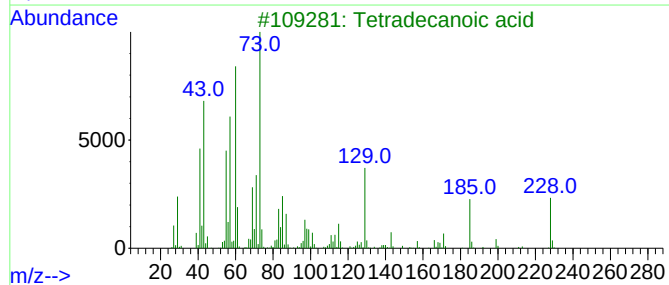
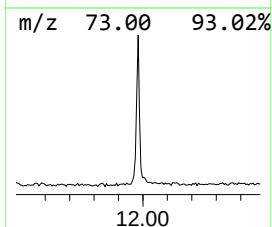
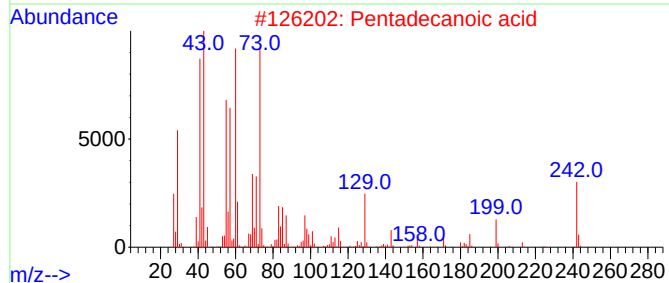
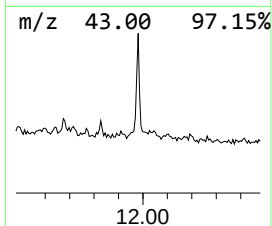
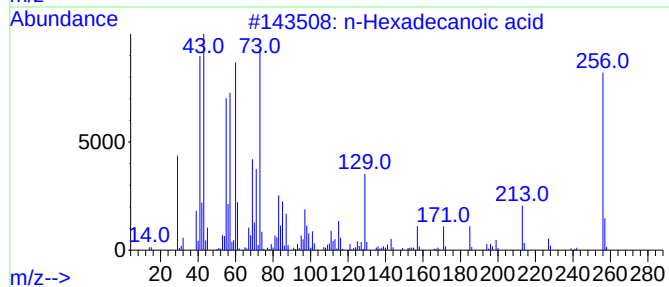
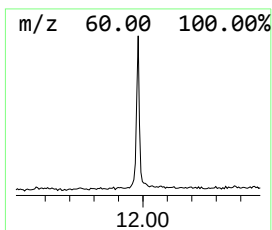
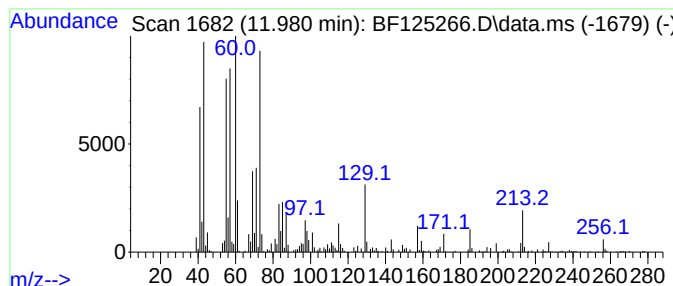
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.980	10.47 ng	749936	Phenanthrene-d10	11.445

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4		Undecanoic acid	186	C11H22O2	000112-37-8	72
5		Tridecanoic acid	214	C13H26O2	000638-53-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083021\
Data File : BF125266.D
Acq On : 30 Aug 2021 17:10
Operator : JU/CG
Sample : M3561-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VE1-2

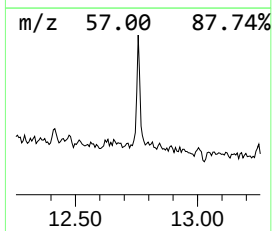
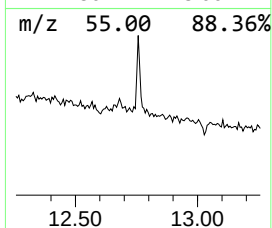
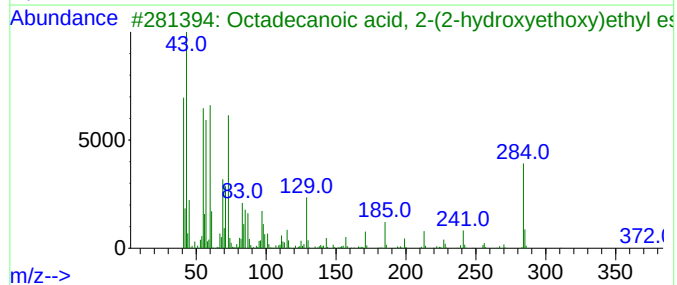
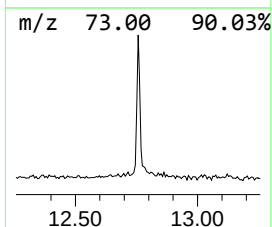
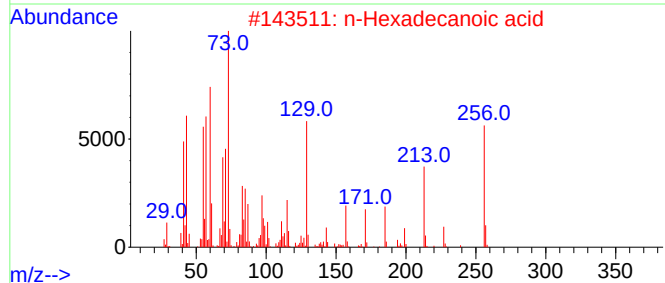
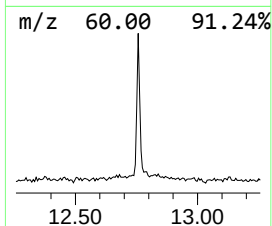
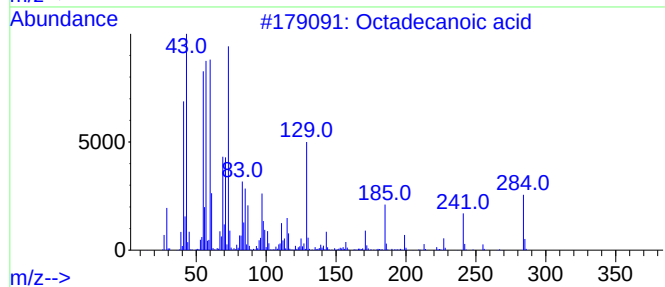
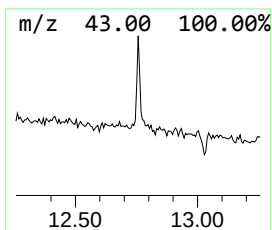
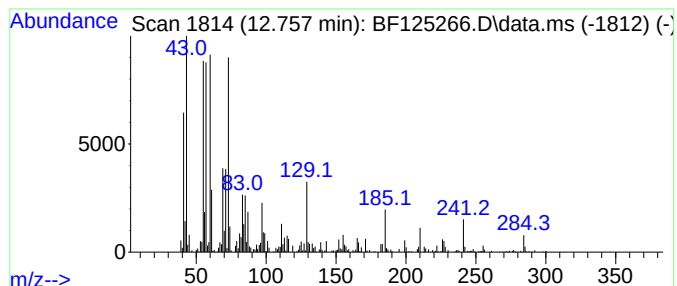
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.757	8.36 ng	598665	Phenanthrene-d10	11.445

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	98
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5		Tridecanoic acid	214	C13H26O2	000638-53-9	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083021\
Data File : BF125266.D
Acq On : 30 Aug 2021 17:10
Operator : JU/CG
Sample : M3561-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VE1-2

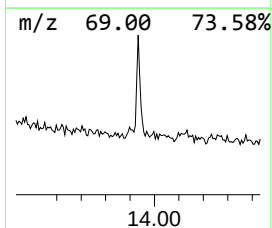
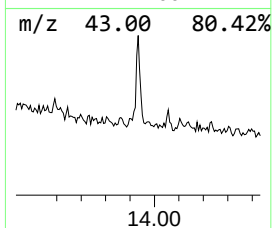
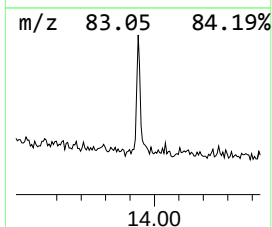
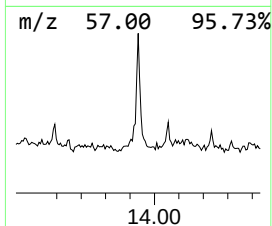
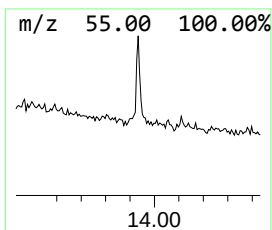
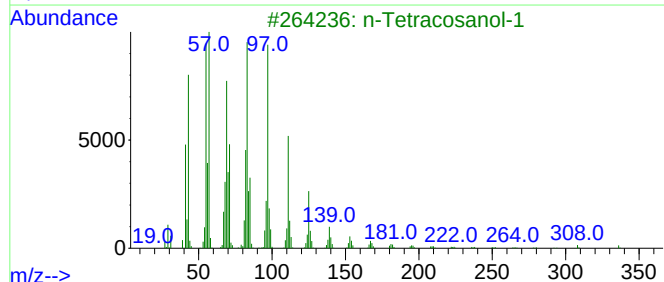
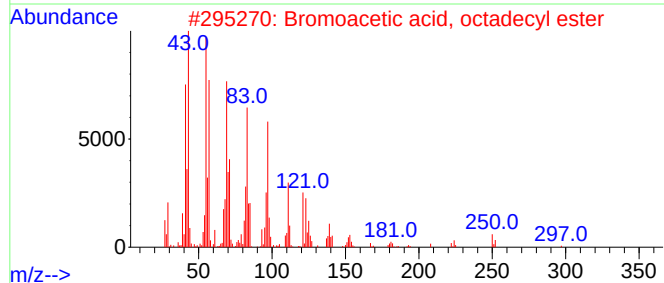
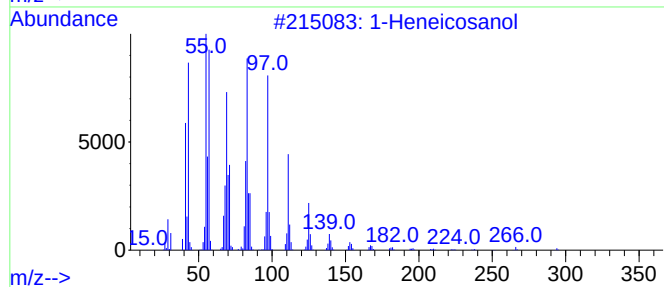
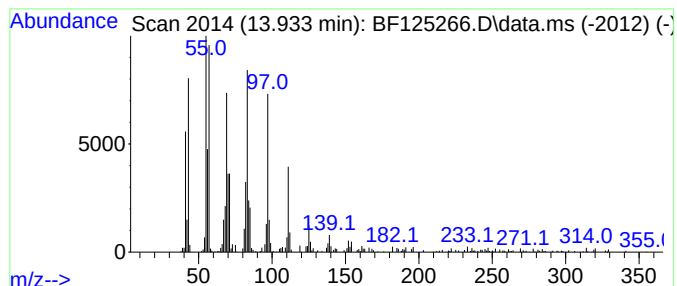
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.933	8.94 ng	454363	Chrysene-d12	14.086

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	94
2		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	91
5		9-Eicosene, (E)-	280	C20H40	074685-29-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083021\
 Data File : BF125266.D
 Acq On : 30 Aug 2021 17:10
 Operator : JU/CG
 Sample : M3561-12
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VE1-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.204	63.9	ng	3361310	1	6.910	1052150	20.0
unknown7.933	7.933	3.6	ng	230728	2	8.198	1266520	20.0
Ethanol, 2-(2-b...	8.110	15.6	ng	984740	2	8.198	1266520	20.0
1,1,4-Trimethyl...	8.392	2.9	ng	186056	2	8.198	1266520	20.0
unknown8.633	8.633	3.8	ng	239837	2	8.198	1266520	20.0
Benzo[b]thiophe...	8.669	3.3	ng	207381	2	8.198	1266520	20.0
Furan, 2-ethyl-...	8.880	4.0	ng	256652	2	8.198	1266520	20.0
1-Cyclohexyl-1-...	9.351	5.3	ng	399276	3	9.951	1509400	20.0
unknown9.386	9.386	5.3	ng	397357	3	9.951	1509400	20.0
2,5-Dimethylphe...	9.533	6.2	ng	466887	3	9.951	1509400	20.0
unknown9.598	9.598	4.4	ng	330989	3	9.951	1509400	20.0
unknown9.657	9.657	7.8	ng	586550	3	9.951	1509400	20.0
Naphthalene, 1,...	9.727	2.9	ng	220582	3	9.951	1509400	20.0
unknown9.816	9.816	3.1	ng	231167	3	9.951	1509400	20.0
Naphthalene, 2,...	10.269	7.4	ng	559320	3	9.951	1509400	20.0
Naphthalene, 1-...	10.569	10.0	ng	756927	3	9.951	1509400	20.0
Heptadecane, 2,...	10.863	6.6	ng	474635	4	11.445	1431940	20.0
n-Hexadecanoic ...	11.980	10.5	ng	749936	4	11.445	1431940	20.0
Octadecanoic acid	12.757	8.4	ng	598665	4	11.445	1431940	20.0
1-Heneicosanol	13.933	8.9	ng	454363	5	14.086	1016580	20.0