

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091323\
 Data File : BF135231.D
 Acq On : 13 Sep 2023 19:48
 Operator : CG\JU
 Sample : 04321-01 2X
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RT2345

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135231.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.387	557	561	569	rBV	1265663	1168089	97.68%	6.426%
2	6.404	730	734	741	rBV	1212469	1195840	100.00%	6.578%
3	6.763	791	795	802	rVB	756361	605698	50.65%	3.332%
4	7.322	887	890	894	rBV	860587	682245	57.05%	3.753%
5	7.981	1000	1002	1006	rBV3	63566	80189	6.71%	0.441%
6	8.040	1006	1012	1016	rVV	914233	930155	77.78%	5.117%
7	8.092	1018	1021	1022	rBV	70104	65139	5.45%	0.358%
8	8.269	1049	1051	1055	rBV3	84228	104121	8.71%	0.573%
9	8.334	1059	1062	1065	rVV3	183846	202761	16.96%	1.115%
10	8.387	1069	1071	1074	rVV3	101170	86872	7.26%	0.478%
11	8.422	1074	1077	1080	rVV	154360	136730	11.43%	0.752%
12	8.469	1080	1085	1086	rVV	199892	247241	20.68%	1.360%
13	8.504	1089	1091	1094	rVB	154574	140328	11.73%	0.772%
14	8.581	1102	1104	1109	rVB5	65166	71591	5.99%	0.394%
15	8.639	1110	1114	1116	rBV	423553	387586	32.41%	2.132%
16	8.675	1116	1120	1122	rVV3	65716	107145	8.96%	0.589%
17	8.728	1126	1129	1133	rVB3	134067	173115	14.48%	0.952%
18	8.781	1136	1138	1141	rBV2	93613	98133	8.21%	0.540%
19	8.816	1141	1144	1147	rBV2	101264	109224	9.13%	0.601%
20	8.845	1147	1149	1151	rBV2	68248	63961	5.35%	0.352%
21	8.869	1151	1153	1157	rBV4	108582	103973	8.69%	0.572%
22	8.922	1159	1162	1165	rVV4	139370	153487	12.84%	0.844%
23	8.998	1172	1175	1178	rBV4	155362	212829	17.80%	1.171%
24	9.034	1178	1181	1184	rVV4	171071	214626	17.95%	1.181%
25	9.069	1184	1187	1190	rVB2	278653	250755	20.97%	1.379%
26	9.122	1191	1196	1199	rBV	1121233	1062032	88.81%	5.842%
27	9.157	1199	1202	1204	rBV3	162178	158853	13.28%	0.874%
28	9.204	1205	1210	1213	rBV3	522594	829563	69.37%	4.563%
29	9.434	1246	1249	1251	rBV3	264455	289619	24.22%	1.593%
30	9.469	1252	1255	1259	rVB	607777	604263	50.53%	3.324%
31	9.504	1259	1261	1263	rBV	570119	493345	41.26%	2.714%
32	9.528	1263	1265	1268	rVV	443579	415729	34.76%	2.287%
33	9.557	1268	1270	1278	rVB6	330967	513796	42.97%	2.826%
34	9.622	1278	1281	1283	rBV3	237451	213627	17.86%	1.175%
35	9.669	1286	1289	1291	rBV2	584393	686344	57.39%	3.776%
36	9.710	1294	1296	1299	rVB	1115082	1025935	85.79%	5.644%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
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37	9.745	1299	1302	1305	rBV2	440846	604829	50.58%	3.327%
38	9.781	1305	1308	1310	rBV2	580879	678873	56.77%	3.734%
39	9.804	1310	1312	1315	rVB2	897516	839593	70.21%	4.619%
40	10.216	1379	1382	1385	rBV	1023102	994967	83.20%	5.473%
41	13.963	2016	2019	2027	rVB	562400	685955	57.36%	3.773%
42	15.421	2263	2267	2271	rBV	419306	489716	40.95%	2.694%

Sum of corrected areas: 18178872

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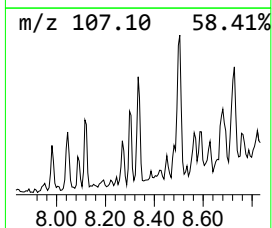
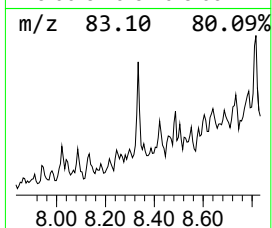
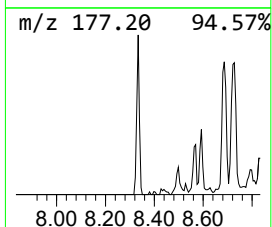
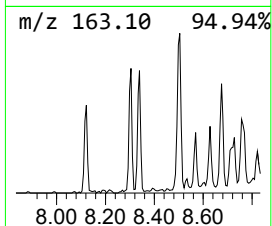
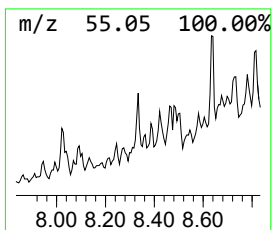
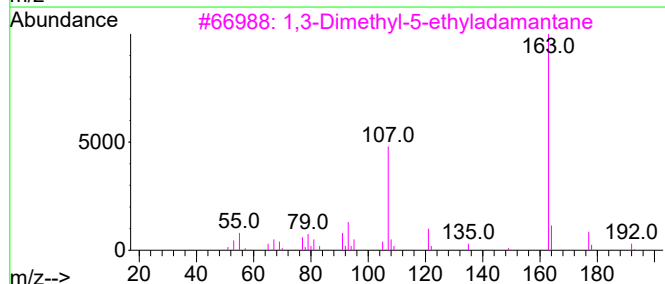
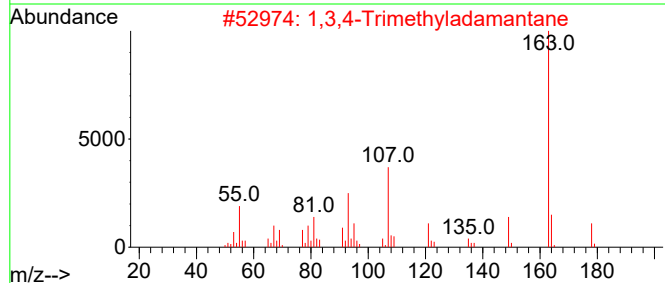
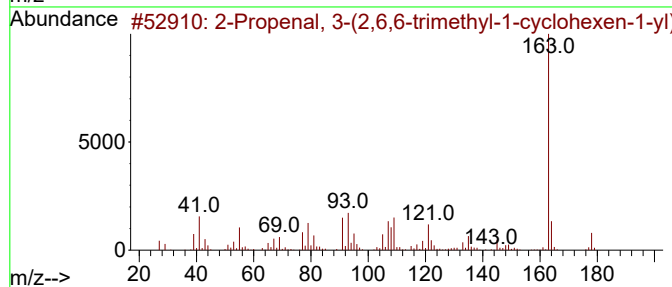
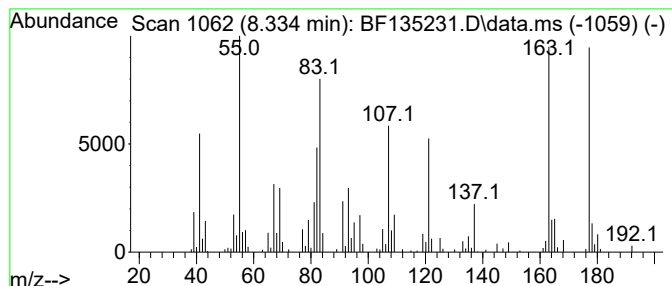
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown8.334 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.334	4.36 ng	202761	Naphthalene-d8	8.040

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenal, 3-(2,6,6-trimethyl-1...	178	C12H18O	004951-40-0	35	
2	1,3,4-Trimethyladamantane	178	C13H22	1000214-98-3	30	
3	1,3-Dimethyl-5-ethyladamantane	192	C14H24	001687-35-0	25	
4	1,2-Dimethyl-5-nitroadamantane	209	C12H19NO2	006588-68-7	22	
5	3,7-Decadiene, 2,9-dimethyl-	166	C12H22	074630-13-0	18	



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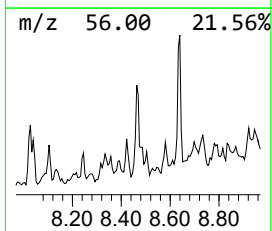
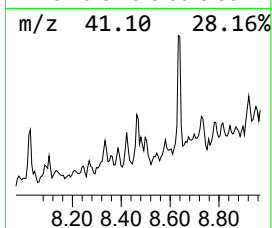
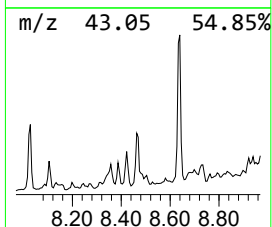
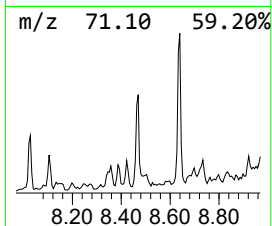
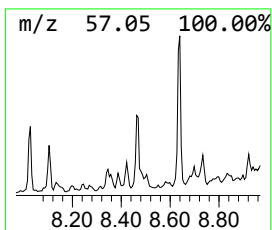
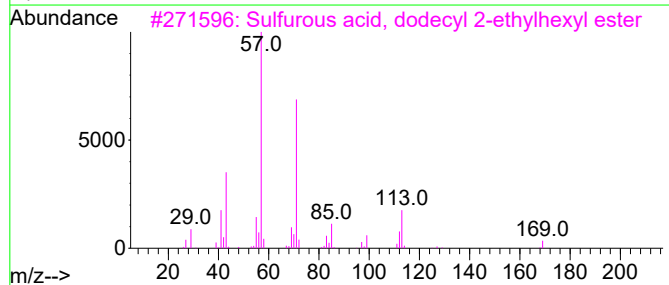
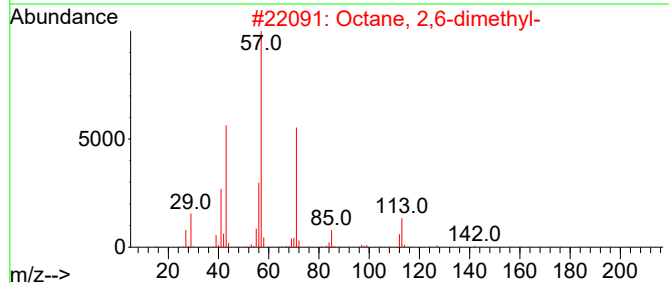
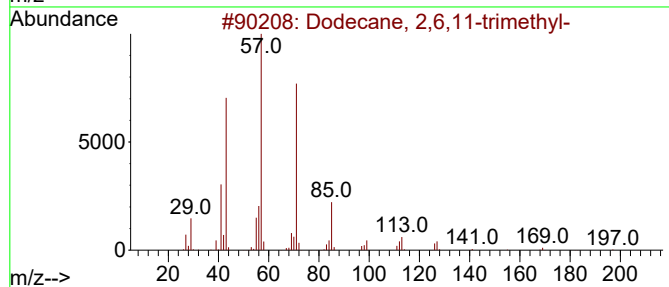
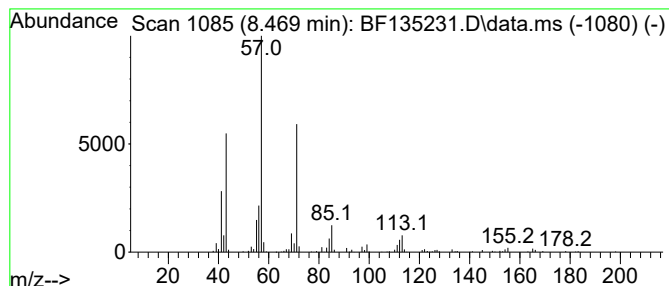
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Dodecane, 2,6,11-trimethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.469	5.32 ng	247241	Naphthalene-d8	8.040

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	78
2			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	78
3			Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	72
4			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	64
5			Nonane, 3-methyl-	142	C10H22	005911-04-6	64



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Instrument :
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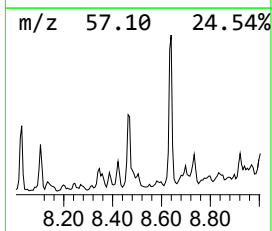
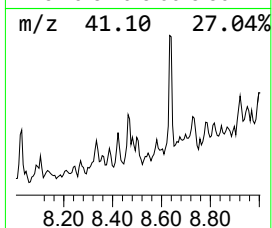
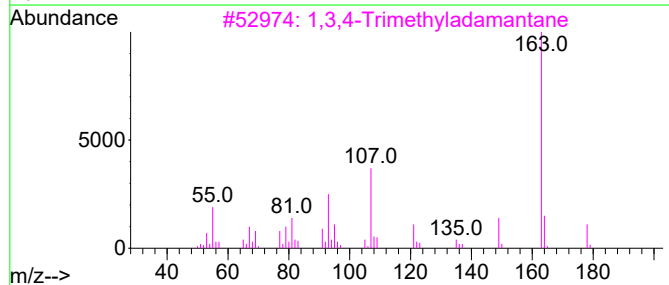
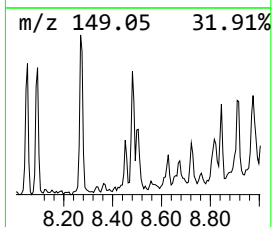
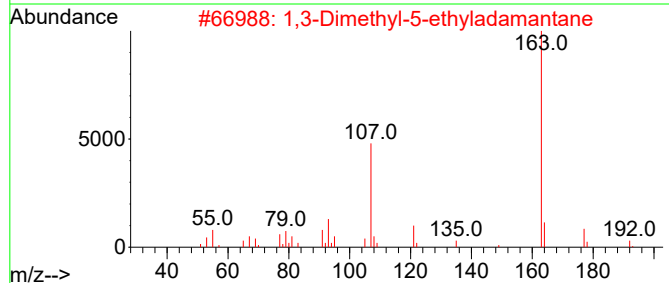
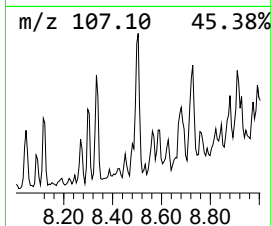
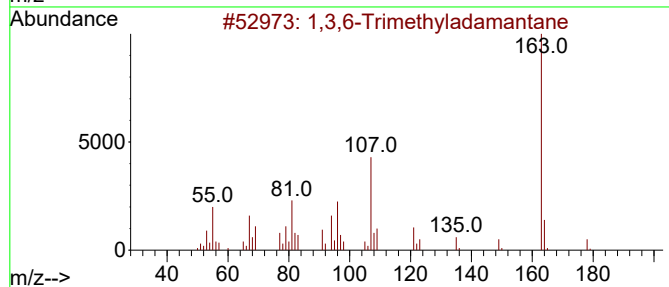
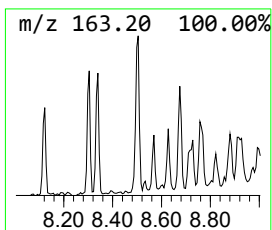
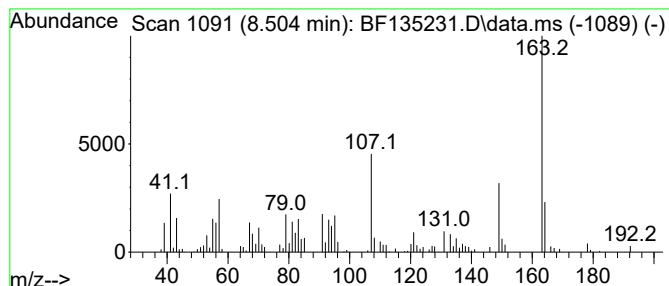
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 1,3,6-Trimethyladamantane Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.504	3.02 ng	140328	Naphthalene-d8	8.040

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3,6-Trimethyladamantane	178	C13H22	024139-37-5	72
2			1,3-Dimethyl-5-ethyladamantane	192	C14H24	001687-35-0	64
3			1,3,4-Trimethyladamantane	178	C13H22	1000214-98-3	45
4			Tricyclo[3.3.1.1(3,7)-]decane, 1...	242	C12H19Br	000941-37-7	45
5			Benzene, 1-(1,1-dimethylethyl)-4...	178	C12H18O	017269-94-2	42



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ALS Vial : 10 Sample Multiplier: 1

Instrument :
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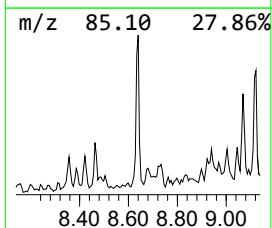
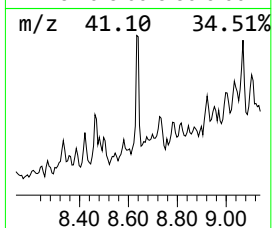
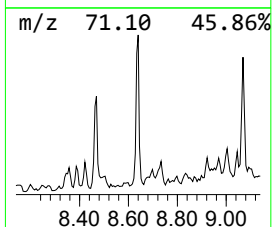
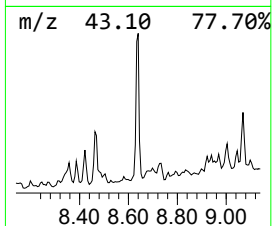
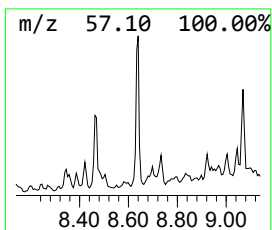
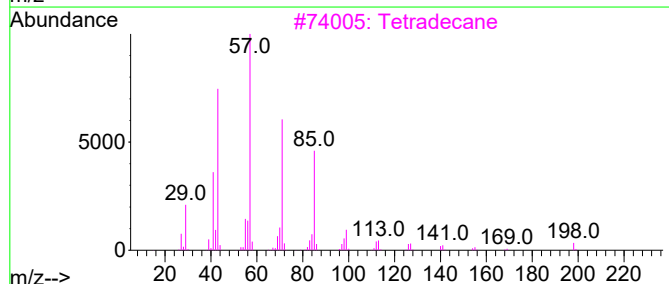
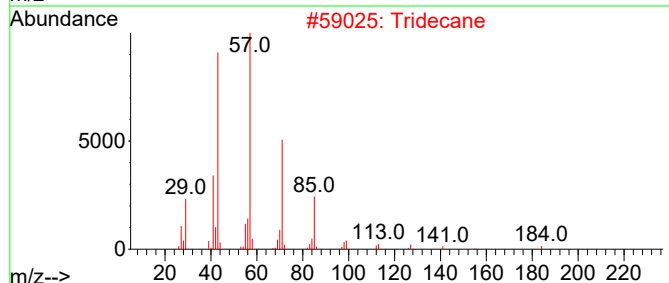
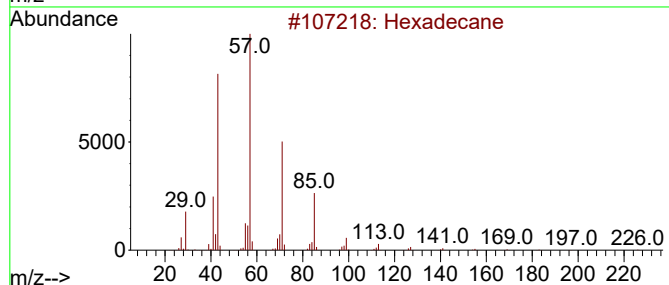
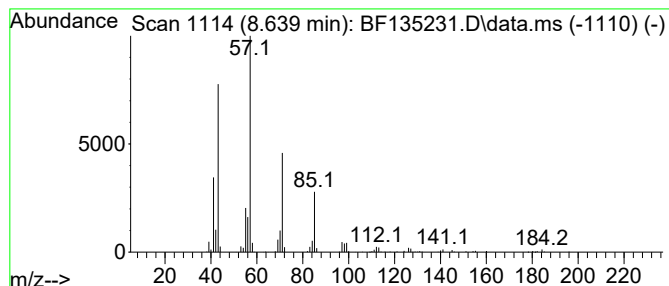
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.639	8.33 ng	387586	Naphthalene-d8	8.040

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	86
2			Tridecane	184	C13H28	000629-50-5	81
3			Tetradecane	198	C14H30	000629-59-4	78
4			Dodecane	170	C12H26	000112-40-3	78
5			Undecane, 5-ethyl-	184	C13H28	017453-94-0	72



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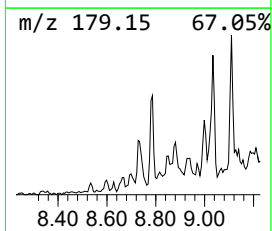
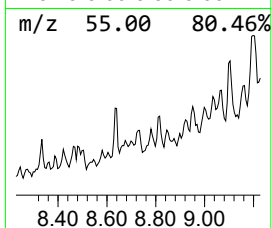
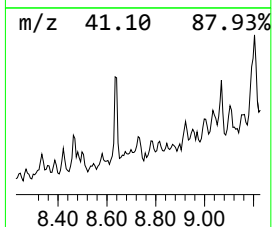
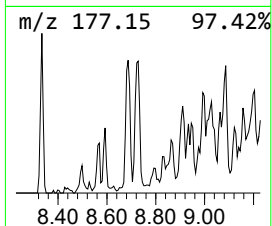
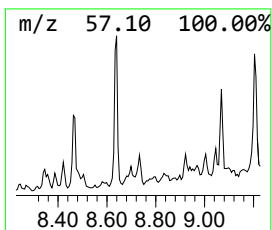
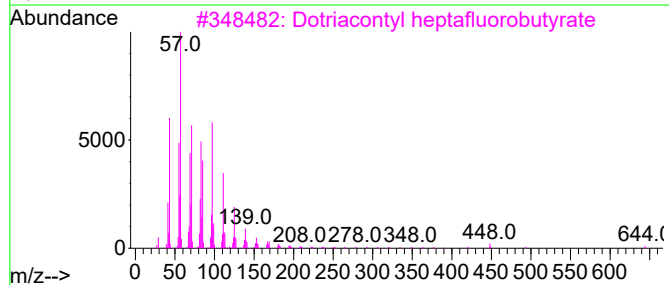
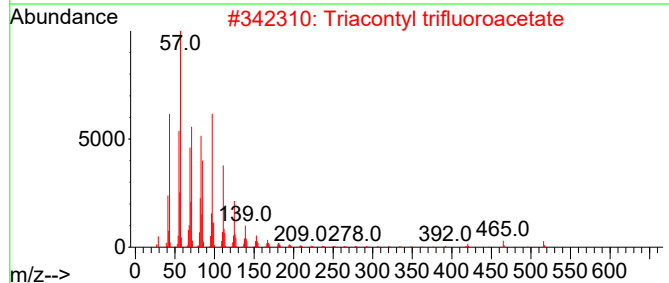
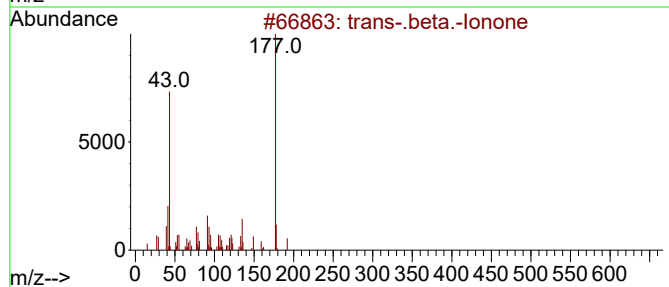
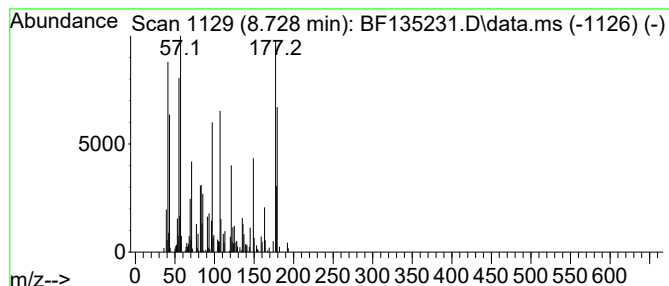
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown8.728 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.728	3.72 ng	173115	Naphthalene-d8	8.040

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-.beta.-Ionone	192	C13H20O	000079-77-6	18
2			Triacontyl trifluoroacetate	534	C32H61F3O2	1000351-75-7	15
3			Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	15
4			3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	014901-07-6	14
5			2-Cyclopropyl-4-methyl-5-pyrimid...	178	C9H10N2O2	954233-05-7	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091323\
Data File : BF135231.D
Acq On : 13 Sep 2023 19:48
Operator : CG\JU
Sample : 04321-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT2345

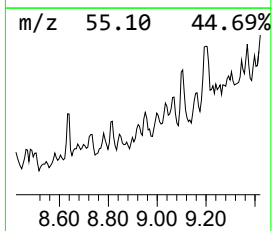
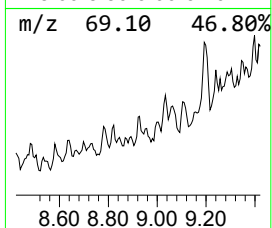
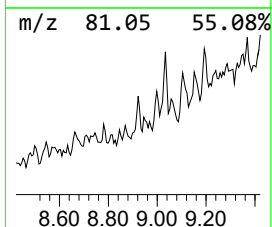
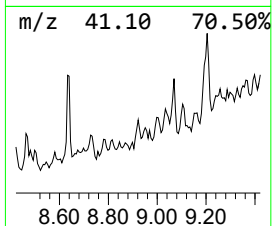
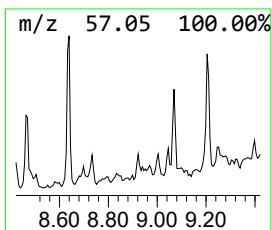
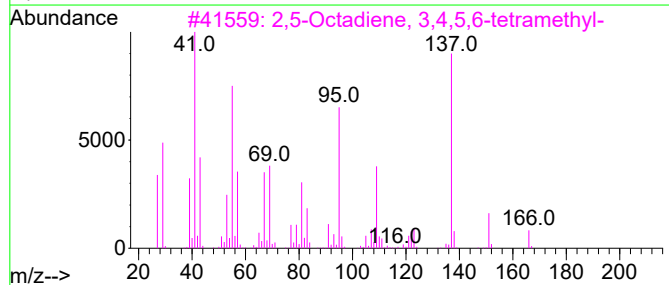
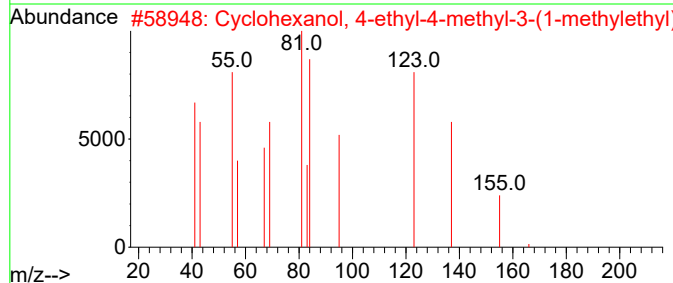
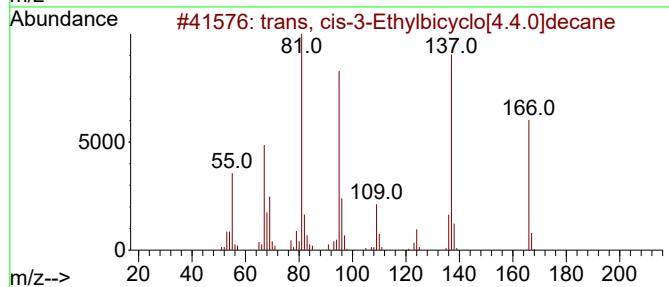
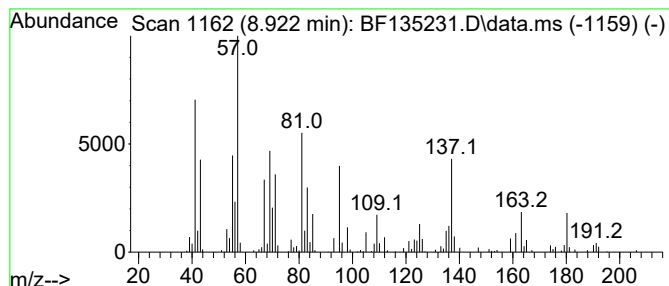
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown8.922 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.922	3.30 ng	153487	Naphthalene-d8	8.040

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans, cis-3-Ethylbicyclo[4.4.0]...	166	C12H22	066660-43-3	47
2			Cyclohexanol, 4-ethyl-4-methyl-3...	184	C12H24O	055869-52-8	38
3			2,5-Octadiene, 3,4,5,6-tetramethyl-	166	C12H22	247797-85-9	37
4			4a(2H)-Naphthalenemethanol, octa...	168	C11H20O	099992-19-5	32
5			Bicyclo[6.1.0]nonane, 9-bromo-9...	216	C10H17Br	059474-03-2	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091323\
Data File : BF135231.D
Acq On : 13 Sep 2023 19:48
Operator : CG\JU
Sample : 04321-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

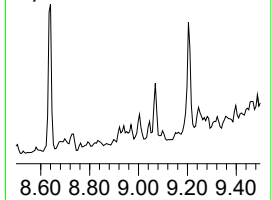
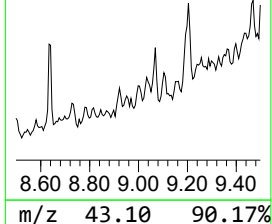
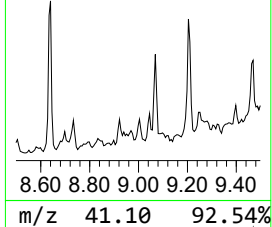
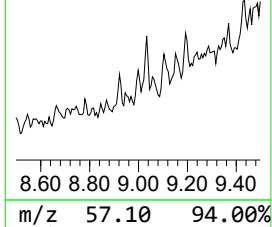
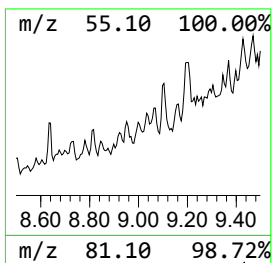
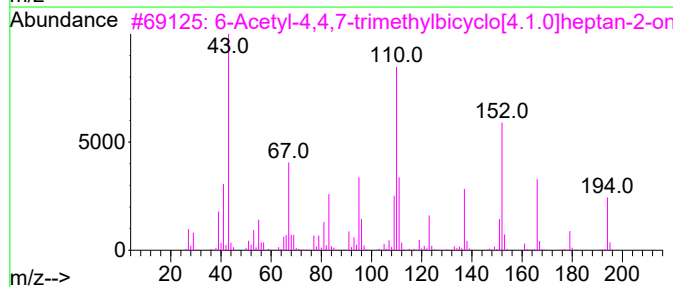
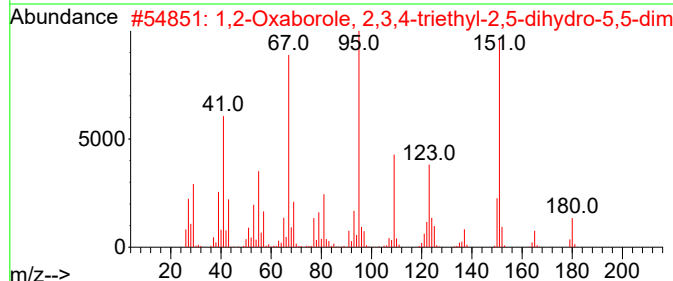
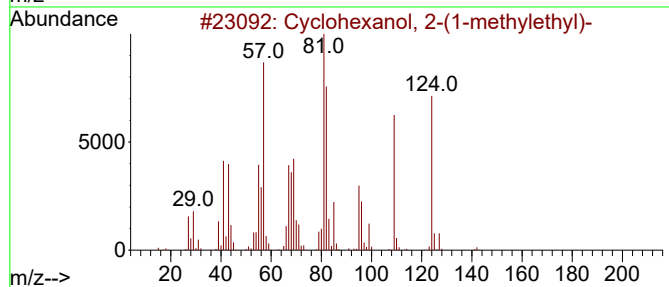
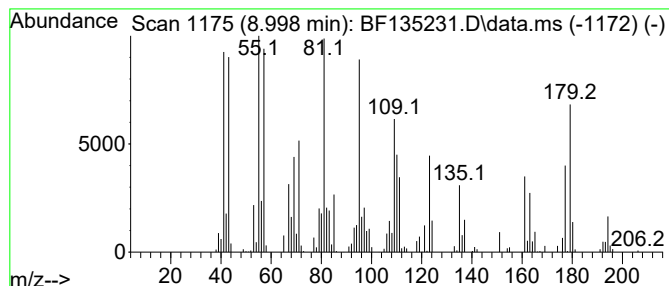
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown8.998 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD		R.T.	
8.998	5.07 ng	212829	Acenaphthene-d10		9.804	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Cyclohexanol, 2-(1-methylethyl)-		142	C9H18O	000096-07-1	38
2	1,2-Oxaborole, 2,3,4-triethyl-2,...		180	C11H21BO	061142-64-1	30
3	6-Acetyl-4,4,7-trimethylbicyclo[...]		194	C12H18O2	1000194-36-0	25
4	Divinylbis(cyclopropyl)silane		164	C10H16Si	1000109-95-2	22
5	3-Heptyne, 5-methyl-		110	C8H14	061228-09-9	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091323\
Data File : BF135231.D
Acq On : 13 Sep 2023 19:48
Operator : CG\JU
Sample : 04321-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

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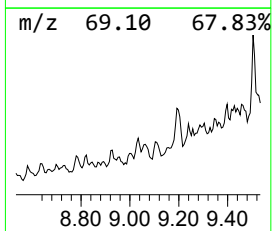
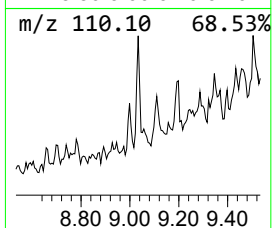
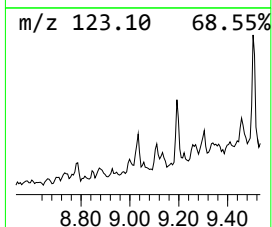
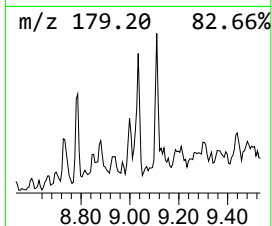
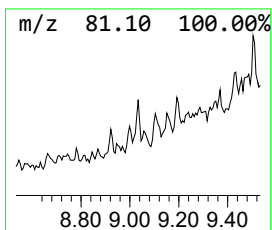
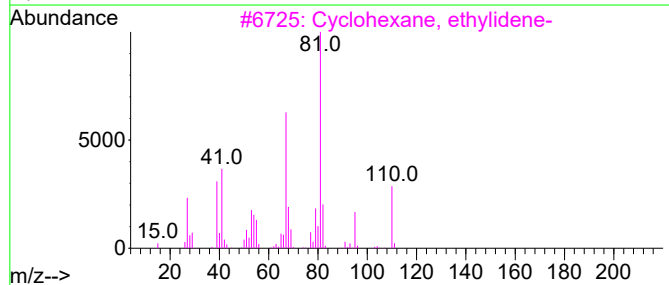
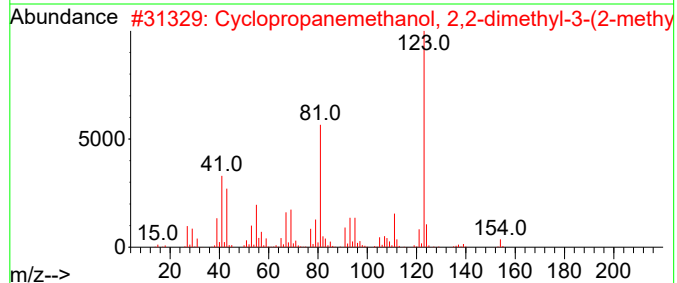
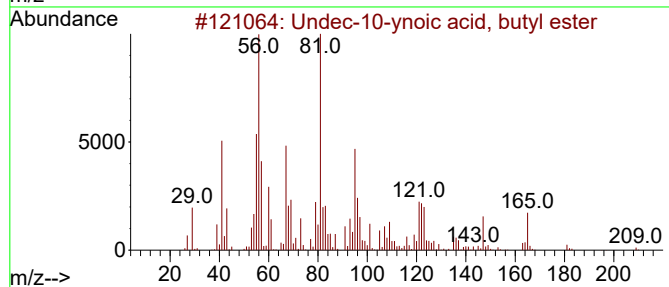
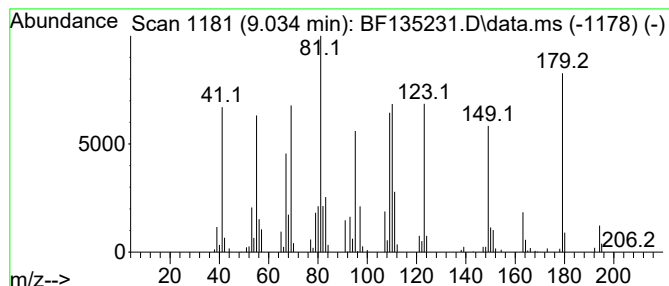
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown9.034 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.034	5.11 ng	214626	Acenaphthene-d10	9.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undec-10-ynoic acid, butyl ester	238	C15H26O2	1000406-15-7	27
2			Cyclopropanemethanol, 2,2-dimeth...	154	C10H18O	005617-92-5	25
3			Cyclohexane, ethylidene-	110	C8H14	001003-64-1	22
4			6,11-Undecadiene, 1-acetoxy-3,7-...	252	C16H28O2	1000150-66-0	22
5			Imidazolo[1,2-a]pyrimidine-2,5(1...	179	C8H9N3O2	053854-19-6	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091323\
Data File : BF135231.D
Acq On : 13 Sep 2023 19:48
Operator : CG\JU
Sample : 04321-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

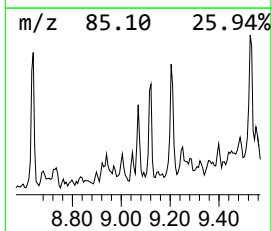
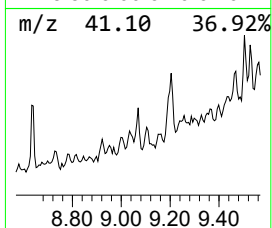
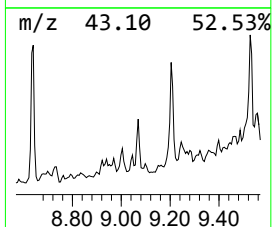
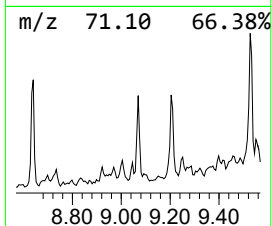
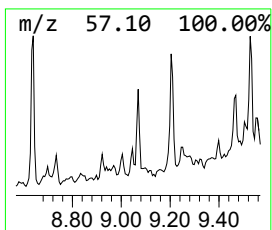
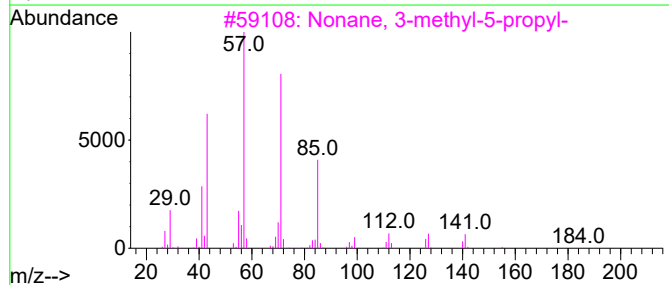
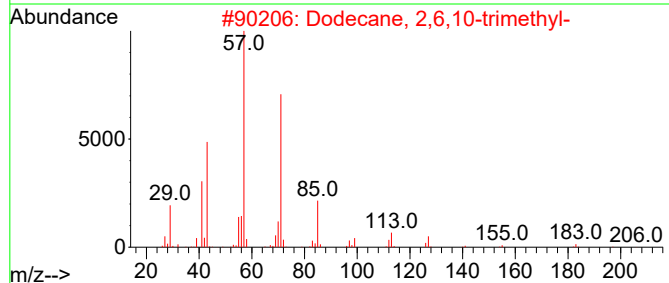
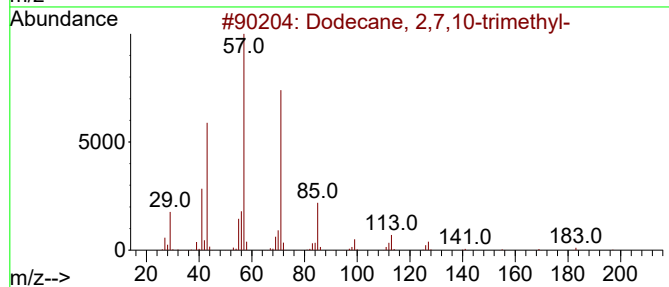
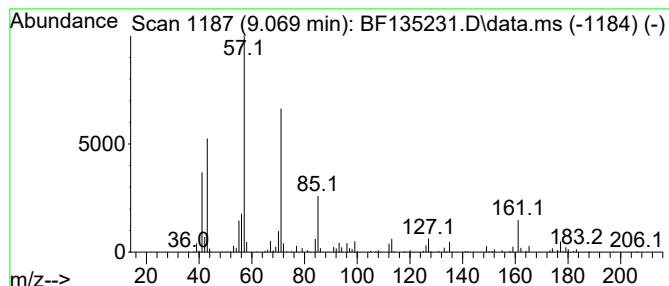
Instrument :
BNA_F
ClientSampleId :
RT2345

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Dodecane, 2,7,10-trimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.069	5.97 ng	250755	Acenaphthene-d10	9.804	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	74
2	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	72
3	Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	53
4	Octane, 2,7-dimethyl-	142	C10H22	001072-16-8	50
5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091323\
Data File : BF135231.D
Acq On : 13 Sep 2023 19:48
Operator : CG\JU
Sample : 04321-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

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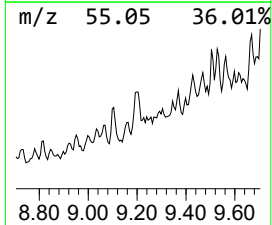
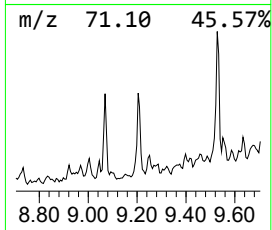
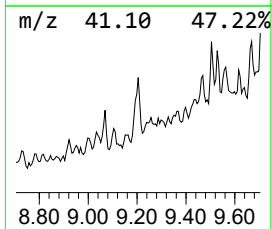
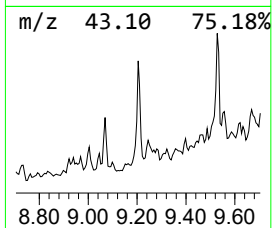
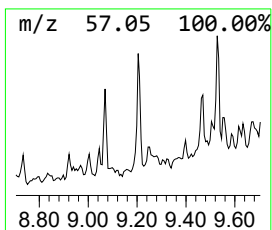
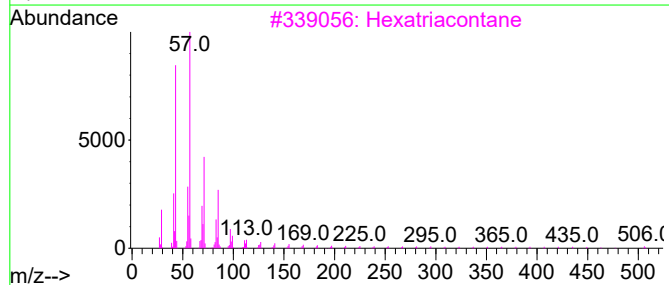
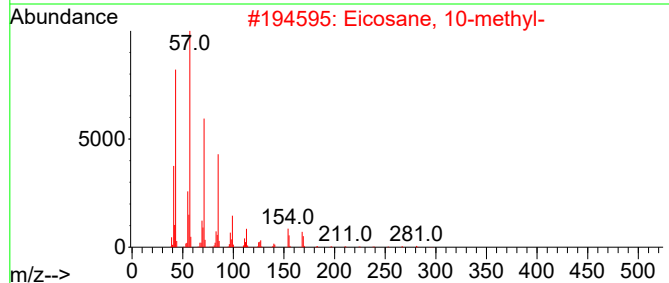
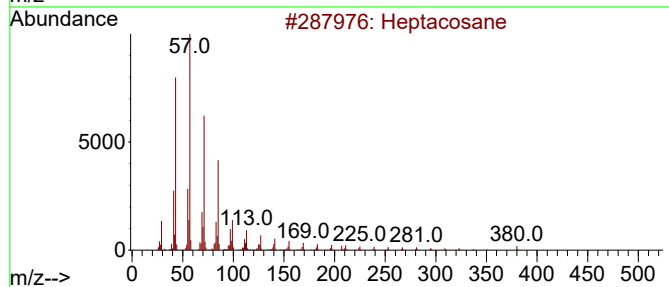
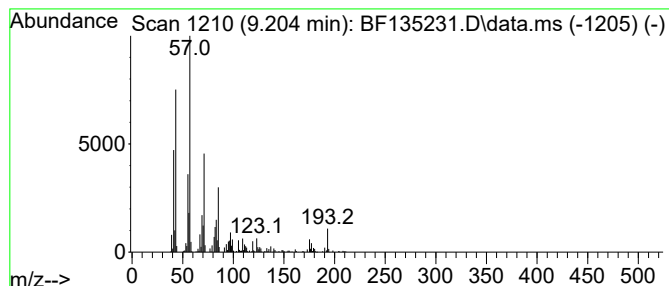
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.204	19.76 ng	829563	Acenaphthene-d10	9.804

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptacosane	380	C27H56	000593-49-7	58
2		Eicosane, 10-methyl-	296	C21H44	054833-23-7	58
3		Hexatriacontane	507	C36H74	000630-06-8	53
4		Dotriacontane	451	C32H66	000544-85-4	53
5		2-Methyltetracosane	352	C25H52	001560-78-7	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091323\
Data File : BF135231.D
Acq On : 13 Sep 2023 19:48
Operator : CG\JU
Sample : 04321-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

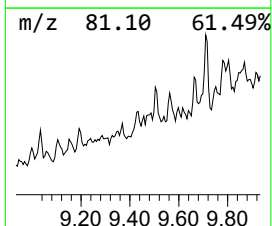
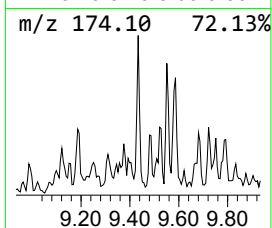
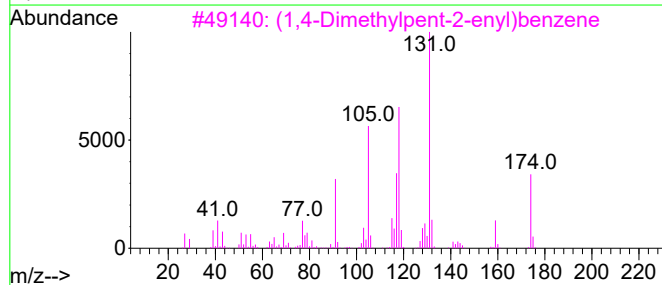
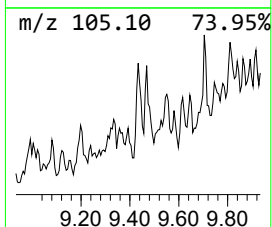
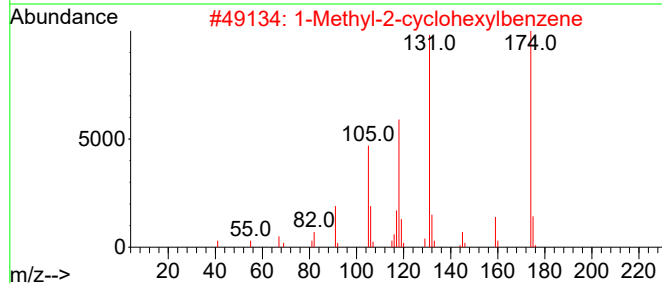
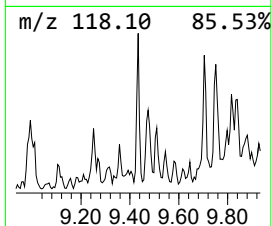
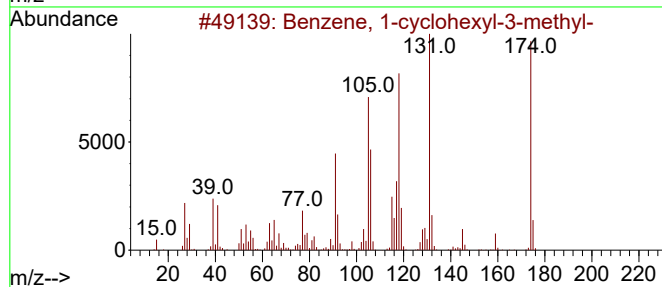
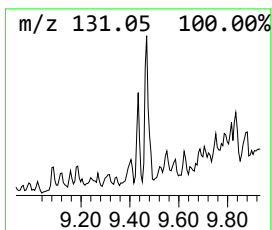
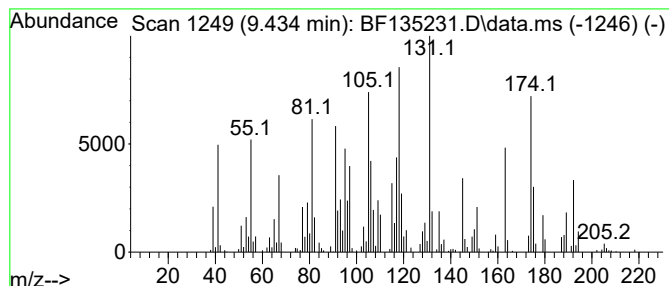
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzene, 1-cyclohexyl-3-met... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.434	6.90 ng	289619	Acenaphthene-d10	9.804	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-cyclohexyl-3-methyl-	174	C13H18	004575-46-6	78
2	1-Methyl-2-cyclohexylbenzene	174	C13H18	004501-35-3	60
3	(1,4-Dimethylpent-2-enyl)benzene	174	C13H18	1000184-97-9	55
4	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	38
5	3,6-Dimethyl-4-chromone	174	C11H10O2	057646-01-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091323\
Data File : BF135231.D
Acq On : 13 Sep 2023 19:48
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Sample : 04321-01 2X
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ALS Vial : 10 Sample Multiplier: 1

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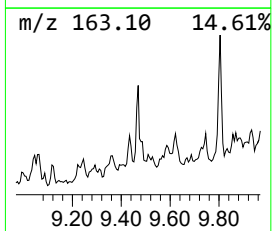
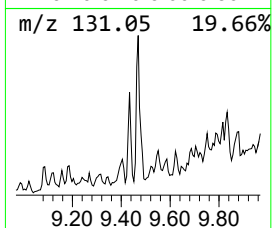
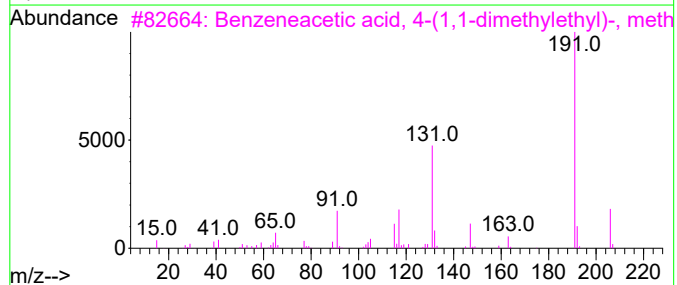
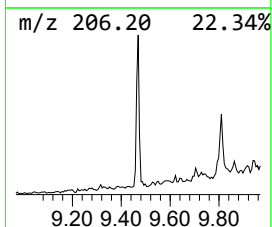
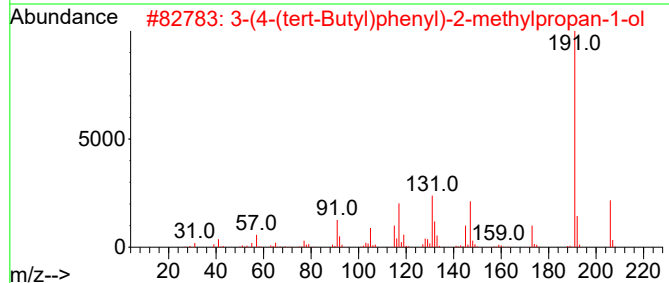
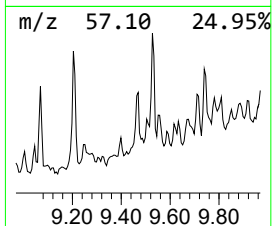
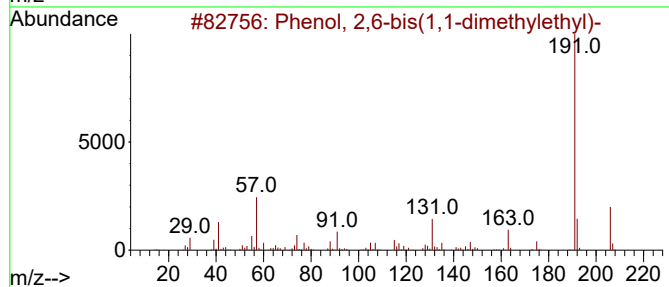
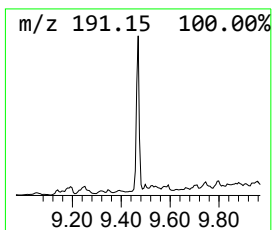
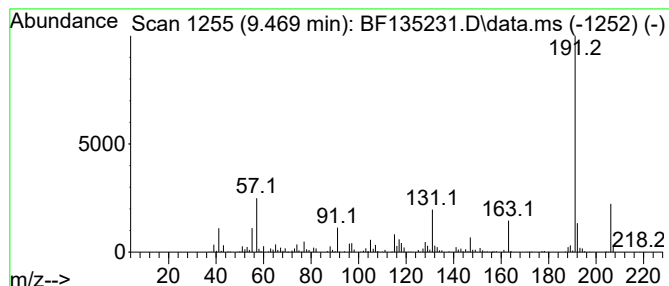
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.469	14.39 ng	604263	Acenaphthene-d10	9.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	93
2			3-(4-(tert-Butyl)phenyl)-2-methy...	206	C14H22O	056107-04-1	87
3			Benzeneacetic acid, 4-(1,1-dimet...	206	C13H18O2	003549-23-3	83
4			3-(4-tert-Butylphenyl)propanoic ...	206	C13H18O2	001208-64-6	83
5			Ethyl 4-t-butylbenzoate	206	C13H18O2	005406-57-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091323\
Data File : BF135231.D
Acq On : 13 Sep 2023 19:48
Operator : CG\JU
Sample : 04321-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

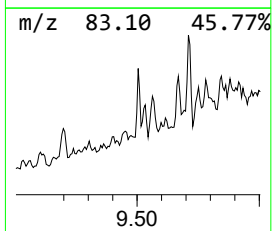
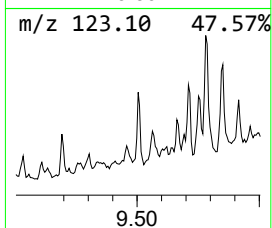
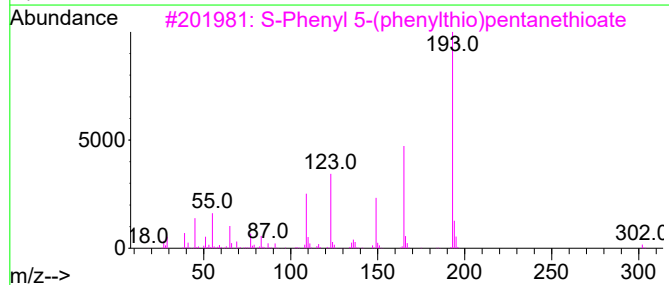
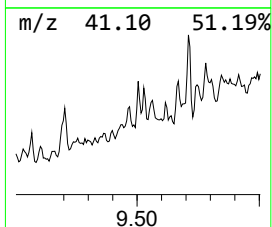
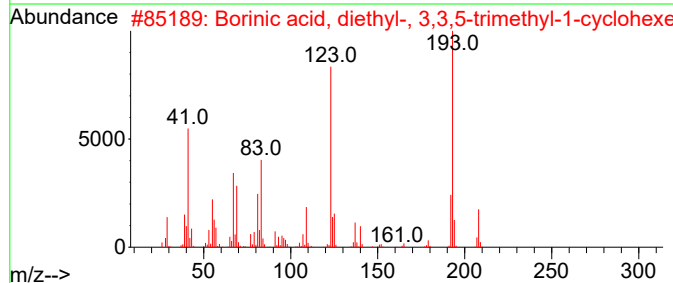
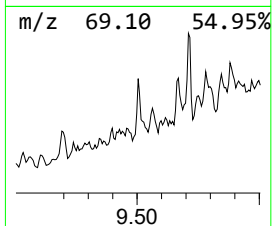
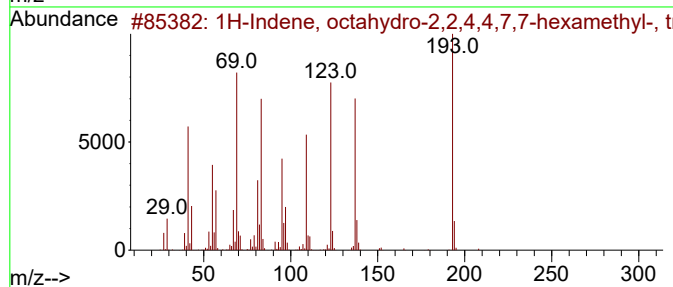
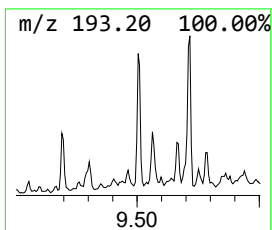
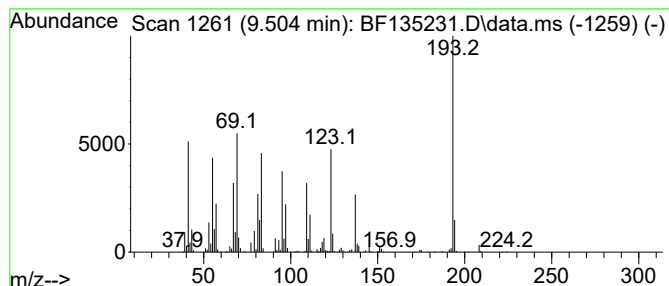
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1H-Indene, octahydro-2,2,4,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.504	11.75 ng	493345	Acenaphthene-d10	9.804	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	50
2	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	45
3	S-Phenyl 5-(phenylthio)pentaneth...	302	C17H18OS2	1000234-40-7	43
4	1-Methyl-3-(trifluoromethyl)-1H...	193	C7H10F3N3	1000511-73-1	35
5	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091323\
Data File : BF135231.D
Acq On : 13 Sep 2023 19:48
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Sample : 04321-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

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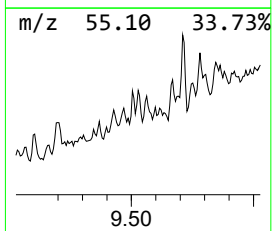
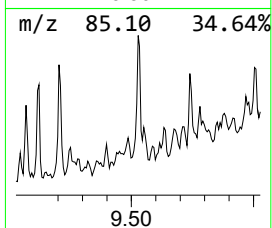
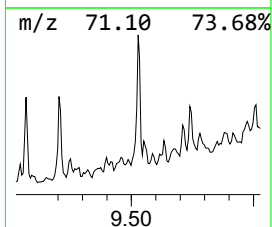
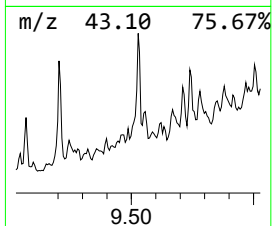
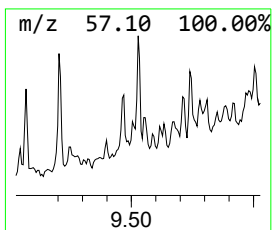
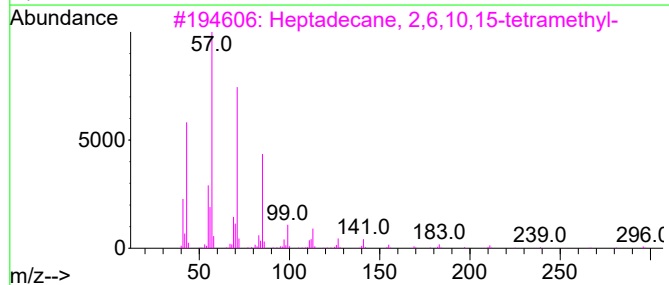
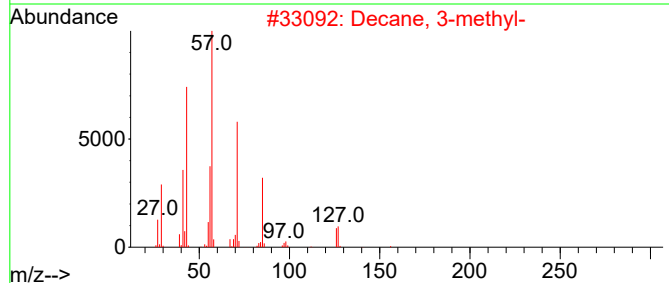
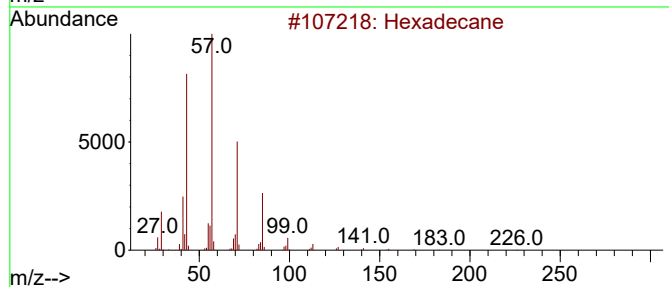
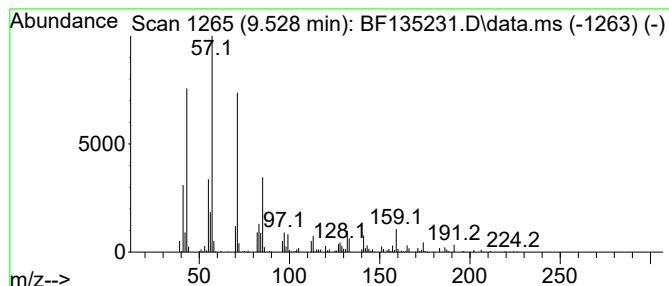
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Decane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.528	9.90 ng	415729	Acenaphthene-d10	9.804

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecane	226	C16H34	000544-76-3	78
2		Decane, 3-methyl-	156	C11H24	013151-34-3	64
3		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	64
4		Pentadecane, 7-methyl-	226	C16H34	006165-40-8	64
5		Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091323\
Data File : BF135231.D
Acq On : 13 Sep 2023 19:48
Operator : CG\JU
Sample : 04321-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

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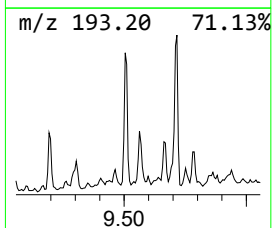
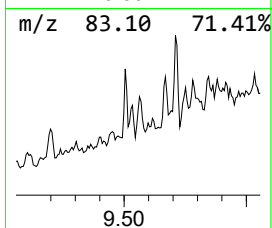
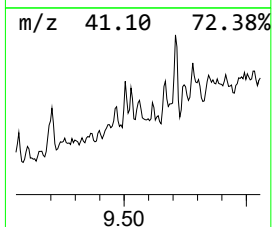
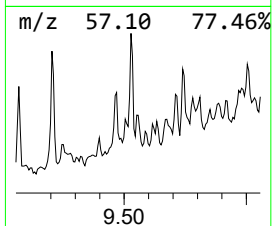
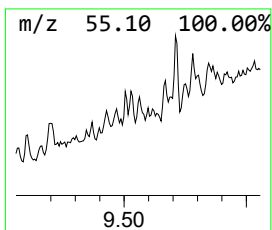
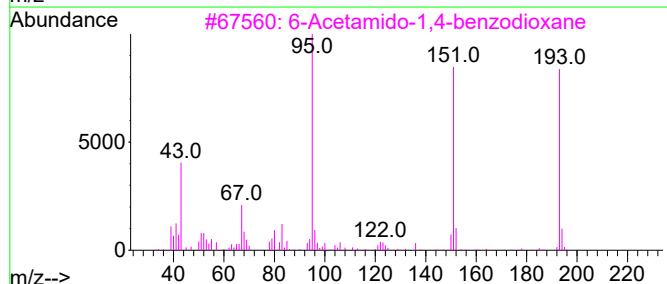
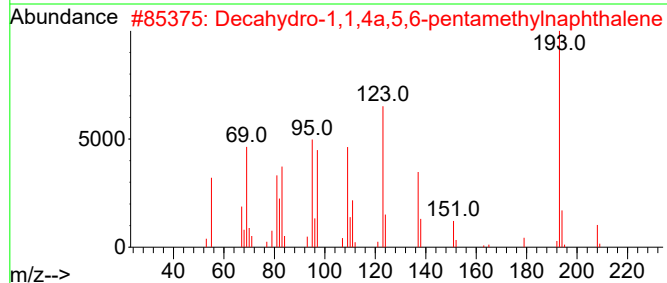
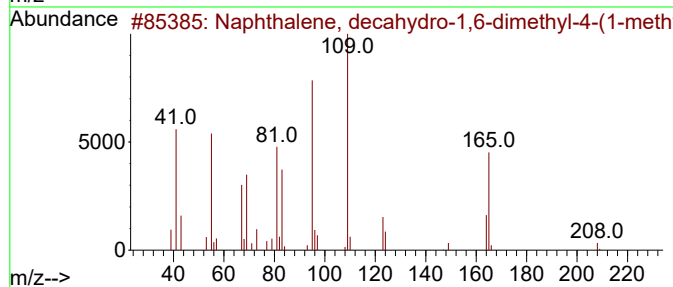
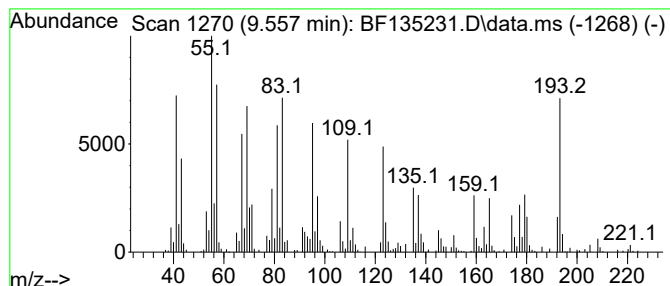
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown9.557 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.557	12.24 ng	513796	Acenaphthene-d10	9.804

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, decahydro-1,6-dimet...	208	C15H28	029788-41-8	38
2		Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	30
3		6-Acetamido-1,4-benzodioxane	193	C10H11NO3	063546-19-0	20
4		4-Amino-N-hydroxypyrazolo[3,2-c]...	193	C6H7N7O	1000443-50-2	18
5		N-(4-Methyl-2-pyrimidinyl)acetoa...	193	C9H11N3O2	000713-70-2	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091323\
Data File : BF135231.D
Acq On : 13 Sep 2023 19:48
Operator : CG\JU
Sample : 04321-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

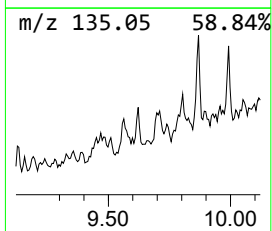
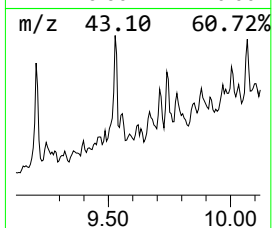
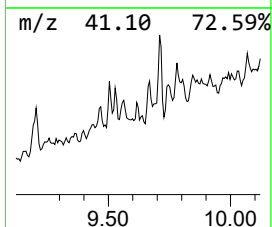
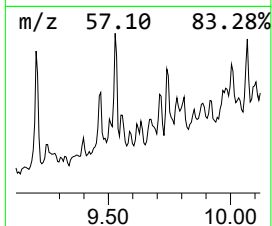
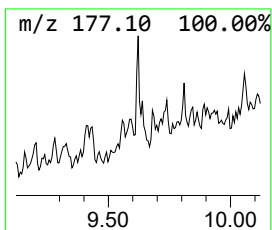
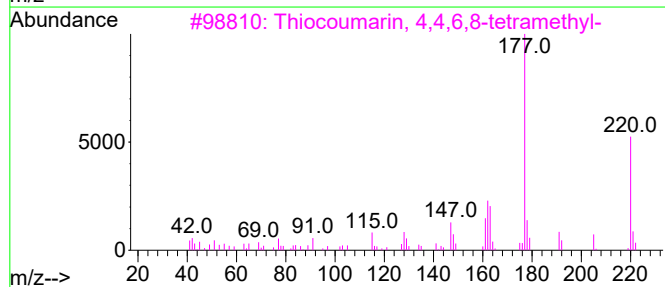
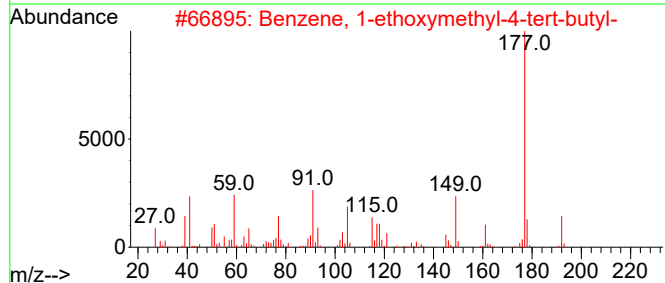
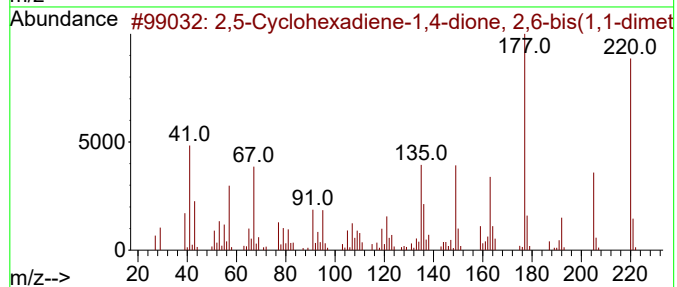
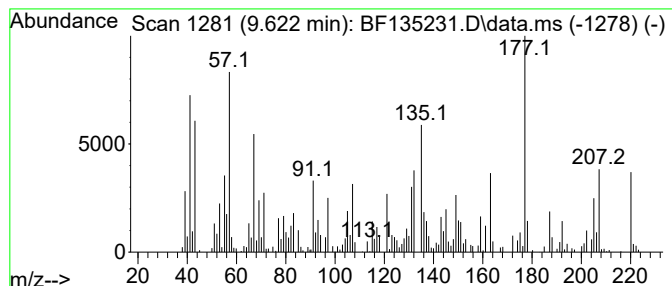
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.622	5.09 ng	213627	Acenaphthene-d10	9.804	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	86
2	Benzene, 1-ethoxymethyl-4-tert-b...	192	C13H20O	1000157-87-5	38
3	Thiocoumarin, 4,4,6,8-tetramethyl-	220	C13H16OS	1000128-90-3	38
4	3-tert-Butylbenzoic acid, methyl...	192	C12H16O2	027330-57-0	38
5	Phenylacetic acid, 2-nitro-.alph...	223	C11H13NO4	136764-87-9	20



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091323\
Data File : BF135231.D
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Sample : 04321-01 2X
Misc :
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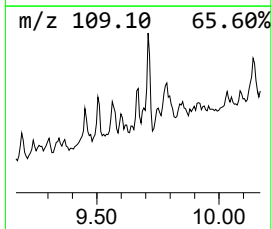
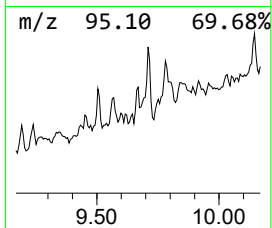
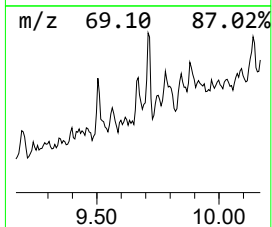
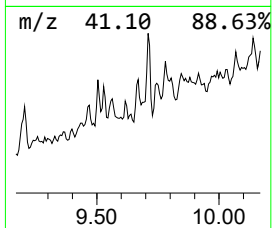
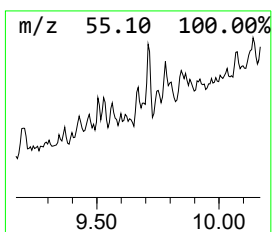
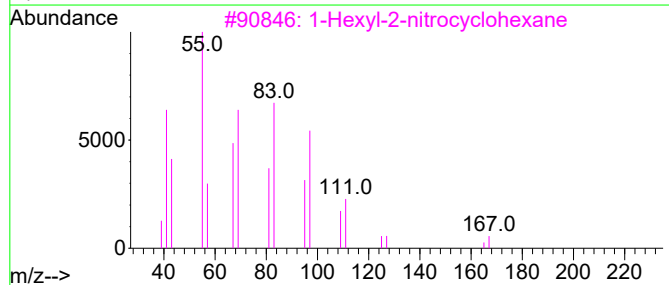
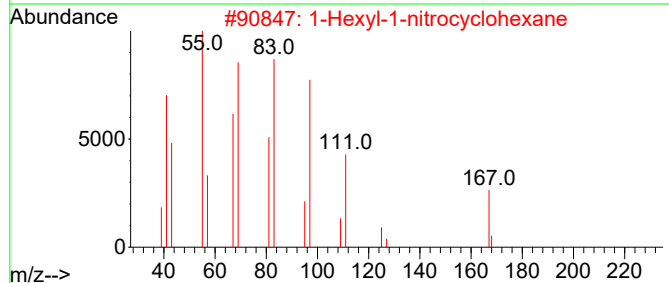
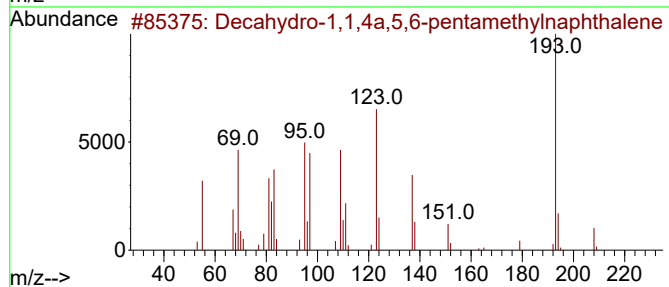
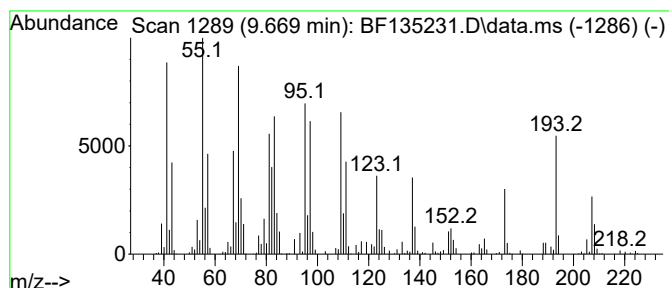
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.669	16.35 ng	686344	Acenaphthene-d10	9.804	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	53
2	1-Hexyl-1-nitrocyclohexane	213	C12H23NO2	118252-09-8	43
3	1-Hexyl-2-nitrocyclohexane	213	C12H23NO2	118252-04-3	35
4	Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	30
5	1,4-Heptadiene, 3,3,6-trimethyl-	138	C10H18	074498-89-8	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091323\
Data File : BF135231.D
Acq On : 13 Sep 2023 19:48
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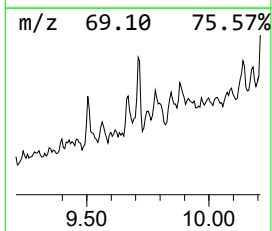
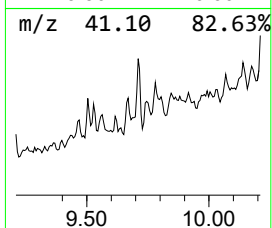
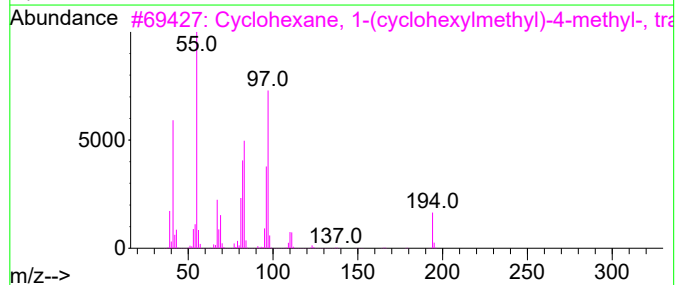
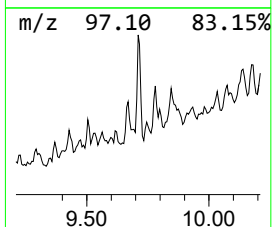
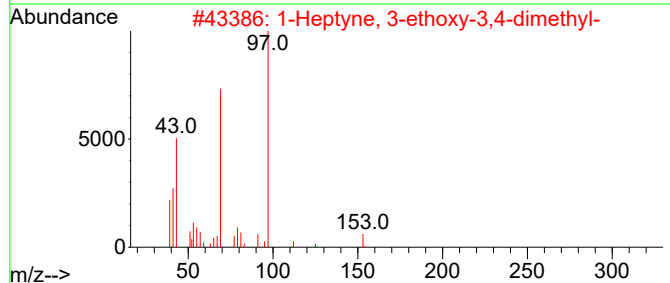
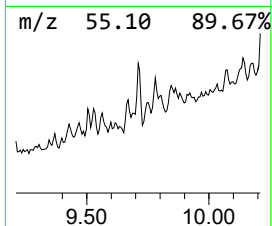
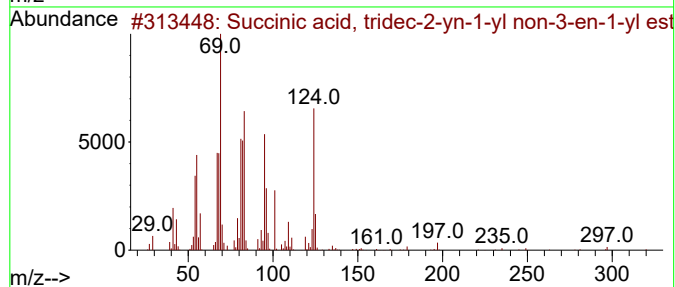
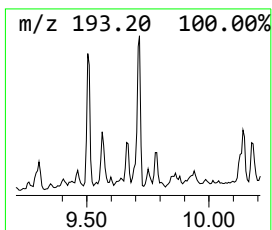
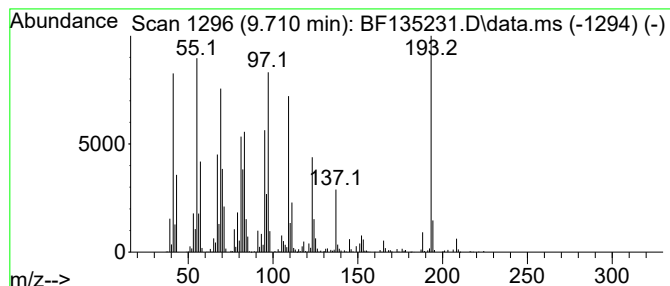
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown9.710 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.710	24.44 ng	1025940	Acenaphthene-d10	9.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Succinic acid, tridec-2-yn-1-yl ...	420	C26H44O4	1010391-10-5	25
2			1-Heptyne, 3-ethoxy-3,4-dimethyl-	168	C11H20O	054411-04-0	22
3			Cyclohexane, 1-(cyclohexylmethyl)-	194	C14H26	054823-98-2	15
4			1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	11
5			1-Hexene, 3-methyl-	98	C7H14	003404-61-3	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091323\
Data File : BF135231.D
Acq On : 13 Sep 2023 19:48
Operator : CG\JU
Sample : 04321-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT2345

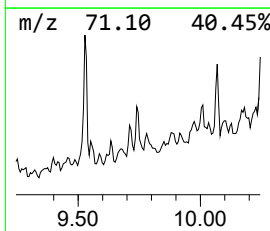
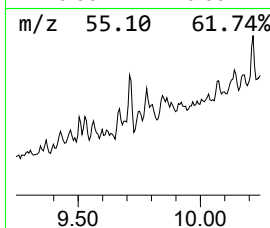
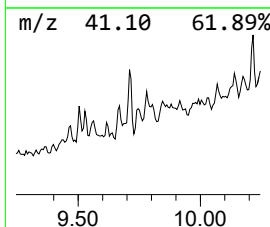
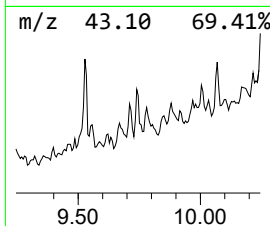
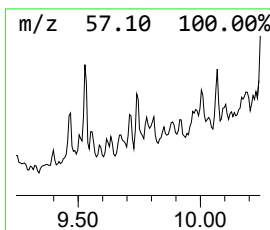
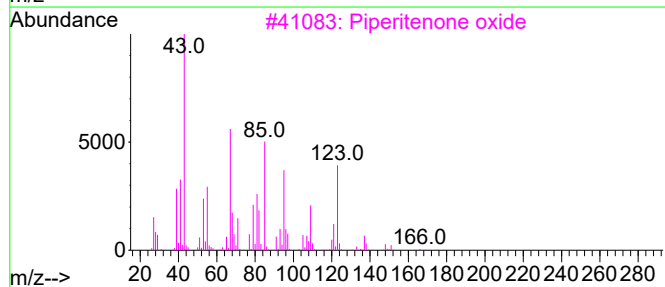
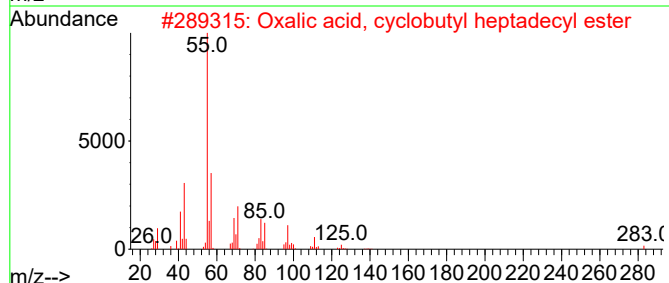
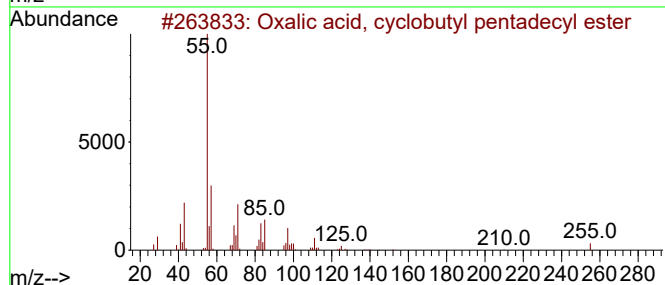
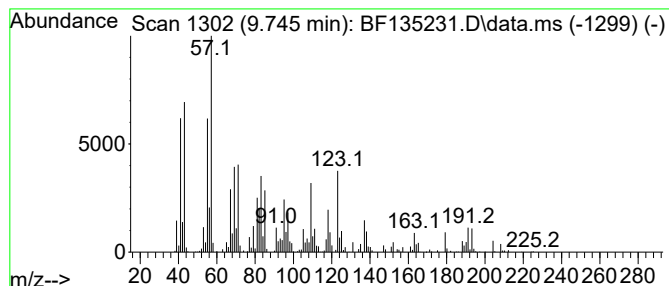
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown9.745 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.745	14.41 ng	604829	Acenaphthene-d10	9.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1010309-70-5	27
2			Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	27
3			Piperitenone oxide	166	C10H14O2	035178-55-3	27
4			Tridecane	184	C13H28	000629-50-5	25
5			Pentadecane	212	C15H32	000629-62-9	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091323\
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Operator : CG\JU
Sample : 04321-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

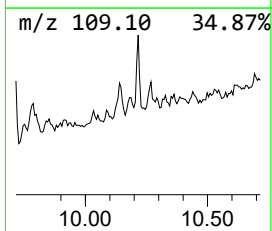
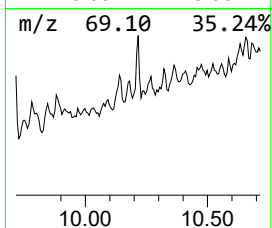
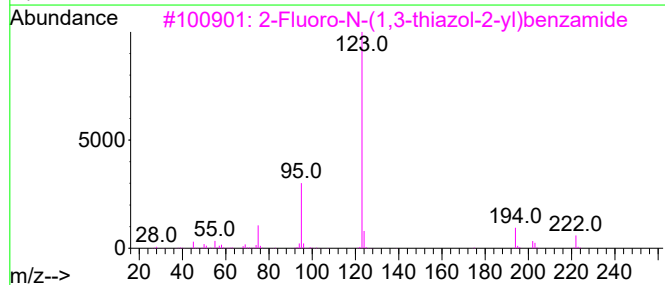
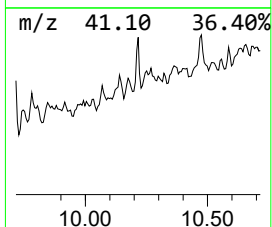
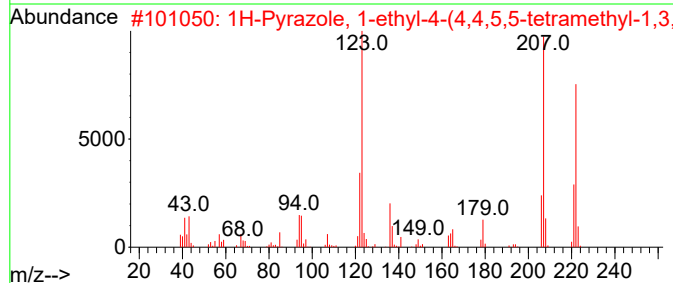
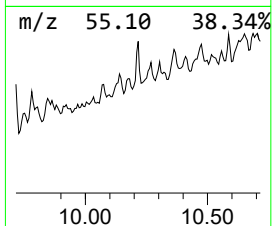
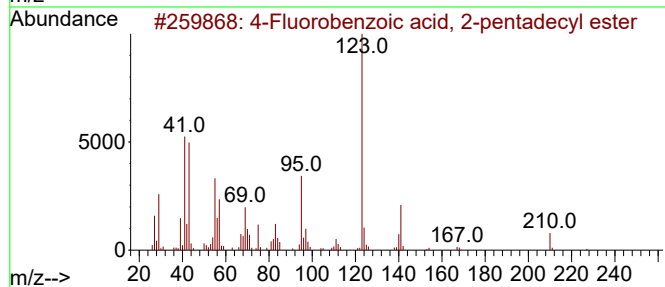
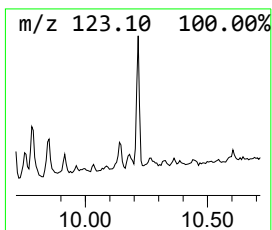
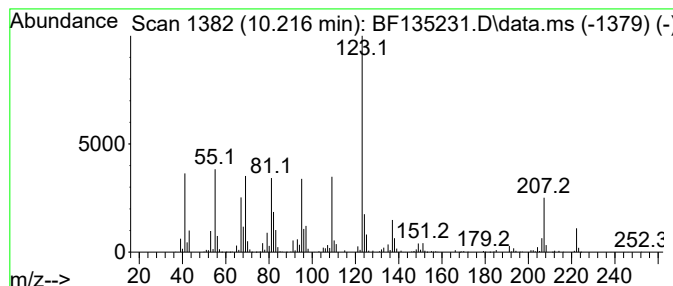
Instrument :
BNA_F
ClientSampleId :
RT2345

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 4-Fluorobenzoic acid, 2-pen... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.216	23.70 ng	994967	Acenaphthene-d10		9.804	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	4-Fluorobenzoic acid, 2-pentadec...		350	C22H35FO2	1000280-68-3	50
2	1H-Pyrazole, 1-ethyl-4-(4,4,5,5-...		222	C11H19BN2O2	1010319-69-6	50
3	2-Fluoro-N-(1,3-thiazol-2-yl)ben...		222	C10H7FN2OS	000319-38-0	47
4	4-Fluorobenzoic acid, 4-pentadec...		350	C22H35FO2	1000280-68-5	47
5	3-Buten-2-one, 4-(4-hydroxy-2,2,...		224	C13H20O3	038274-01-0	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091323\
 Data File : BF135231.D
 Acq On : 13 Sep 2023 19:48
 Operator : CG\JU
 Sample : 04321-01 2X
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RT2345

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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
unknown8.334	8.334	4.4	ng	202761	2	8.040	930155	20.0
Dodecane, 2,6,1...	8.469	5.3	ng	247241	2	8.040	930155	20.0
1,3,6-Trimethyl...	8.504	3.0	ng	140328	2	8.040	930155	20.0
Hexadecane	8.639	8.3	ng	387586	2	8.040	930155	20.0
unknown8.728	8.728	3.7	ng	173115	2	8.040	930155	20.0
unknown8.922	8.922	3.3	ng	153487	2	8.040	930155	20.0
unknown8.998	8.998	5.1	ng	212829	3	9.804	839593	20.0
unknown9.034	9.034	5.1	ng	214626	3	9.804	839593	20.0
Dodecane, 2,7,1...	9.069	6.0	ng	250755	3	9.804	839593	20.0
Heptacosane	9.204	19.8	ng	829563	3	9.804	839593	20.0
Benzene, 1-cycl...	9.434	6.9	ng	289619	3	9.804	839593	20.0
Phenol, 2,6-bis...	9.469	14.4	ng	604263	3	9.804	839593	20.0
1H-Indene, octa...	9.504	11.8	ng	493345	3	9.804	839593	20.0
Decane, 3-methyl-	9.528	9.9	ng	415729	3	9.804	839593	20.0
unknown9.557	9.557	12.2	ng	513796	3	9.804	839593	20.0
2,5-Cyclohexadi...	9.622	5.1	ng	213627	3	9.804	839593	20.0
Decahydro-1,1,4...	9.669	16.4	ng	686344	3	9.804	839593	20.0
unknown9.710	9.710	24.4	ng	1025940	3	9.804	839593	20.0
unknown9.745	9.745	14.4	ng	604829	3	9.804	839593	20.0
4-Fluorobenzoic...	10.216	23.7	ng	994967	3	9.804	839593	20.0