

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011223\
 Data File : BF132053.D
 Acq On : 12 Jan 2023 21:27
 Operator : CG\JU
 Sample : 01064-07
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-14-02

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-BF010923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132053.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	8	29	rVB2	548319	1518886	8.60%	2.008%
2	3.569	243	252	268	rBV	118401	424994	2.41%	0.562%
3	3.722	268	278	306	rBV4	209116	832531	4.71%	1.101%
4	4.293	367	375	377	rBV2	331851	583913	3.30%	0.772%
5	4.416	377	396	399	rVB	4515300	17668165	100.00%	23.355%
6	5.322	544	550	559	rBV	955107	1342166	7.60%	1.774%
7	5.387	559	561	573	rVB	267351	345517	1.96%	0.457%
8	5.546	584	588	594	rBV	299590	346963	1.96%	0.459%
9	5.687	608	612	614	rBV	475931	534206	3.02%	0.706%
10	6.251	701	708	711	rVB	996877	945770	5.35%	1.250%
11	6.434	734	739	743	rBV2	377608	522770	2.96%	0.691%
12	6.528	751	755	759	rBV2	888827	975385	5.52%	1.289%
13	6.598	764	767	771	rVV4	144580	179023	1.01%	0.237%
14	6.645	772	775	778	rBV	673109	620766	3.51%	0.821%
15	6.728	786	789	793	rBV3	353880	711366	4.03%	0.940%
16	6.775	794	797	798	rVV	687177	875761	4.96%	1.158%
17	6.798	799	801	802	rVB	889872	617774	3.50%	0.817%
18	6.916	818	821	825	rVB4	134115	189610	1.07%	0.251%
19	6.992	831	834	837	rBV	523815	415295	2.35%	0.549%
20	7.069	844	847	849	rBV	221297	234456	1.33%	0.310%
21	7.098	849	852	858	rVV2	1458328	1786156	10.11%	2.361%
22	7.175	861	865	871	rVV2	193525	427758	2.42%	0.565%
23	7.245	871	877	887	rVV2	462768	880969	4.99%	1.165%
24	7.363	892	897	901	rVV	2371989	3097295	17.53%	4.094%
25	7.428	904	908	912	rVV2	1558634	1507122	8.53%	1.992%
26	7.516	912	923	927	rVB6	101476	234849	1.33%	0.310%
27	7.716	954	957	959	rVV2	277003	307340	1.74%	0.406%
28	7.739	959	961	966	rVV	150155	201238	1.14%	0.266%
29	7.810	971	973	979	rVV4	282286	338790	1.92%	0.448%
30	7.898	979	988	990	rVV	315530	680254	3.85%	0.899%
31	8.039	1008	1012	1014	rVV4	195173	214934	1.22%	0.284%
32	8.151	1024	1031	1034	rVB2	215214	388368	2.20%	0.513%
33	8.192	1034	1038	1040	rBV	265516	235732	1.33%	0.312%
34	8.257	1045	1049	1053	rBV3	120459	178111	1.01%	0.235%
35	8.369	1063	1068	1071	rVV	2121273	2206544	12.49%	2.917%
36	8.410	1071	1075	1079	rVV2	284891	350302	1.98%	0.463%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011223\
 Data File : BF132053.D
 Acq On : 12 Jan 2023 21:27
 Operator : CG\JU
 Sample : 01064-07
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-14-02

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-BF010923.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	8.469	1080	1085	1096	rVV2	2670179	3032681	17.16%	4.009%
38	8.675	1110	1120	1124	rVV	1955296	2317099	13.11%	3.063%
39	8.716	1124	1127	1131	rVB	288188	244923	1.39%	0.324%
40	8.828	1140	1146	1148	rBV	3743473	4029705	22.81%	5.327%
41	8.845	1148	1149	1154	rVV3	367631	409173	2.32%	0.541%
42	8.975	1164	1171	1172	rBV	2391097	2615625	14.80%	3.458%
43	9.016	1172	1178	1181	rVV	2703717	4073793	23.06%	5.385%
44	9.045	1181	1183	1184	rVV	196736	179810	1.02%	0.238%
45	9.069	1184	1187	1189	rVV	2040643	2092147	11.84%	2.766%
46	9.092	1189	1191	1193	rVV	792623	575365	3.26%	0.761%
47	9.122	1193	1196	1198	rVV	654324	514117	2.91%	0.680%
48	9.163	1198	1203	1205	rVV2	1496701	1634410	9.25%	2.160%
49	9.198	1205	1209	1212	rVV	242745	255696	1.45%	0.338%
50	9.386	1232	1241	1243	rBV	483807	846742	4.79%	1.119%
51	9.610	1275	1279	1283	rVV5	246918	355602	2.01%	0.470%
52	9.663	1283	1288	1293	rVV2	507352	698951	3.96%	0.924%
53	9.728	1295	1299	1301	rVV	330469	412936	2.34%	0.546%
54	9.786	1301	1309	1313	rVV2	574922	1339649	7.58%	1.771%
55	9.828	1313	1316	1318	rVV2	176238	183763	1.04%	0.243%
56	9.863	1318	1322	1326	rVB2	273500	343337	1.94%	0.454%
57	10.369	1405	1408	1410	rVV	312590	255497	1.45%	0.338%
58	10.422	1414	1417	1420	rVB	228059	189778	1.07%	0.251%
59	10.616	1447	1450	1455	rVB2	404106	392968	2.22%	0.519%
60	11.869	1656	1663	1669	rBV	1379190	1891243	10.70%	2.500%
61	12.474	1761	1766	1769	rBV	339035	292510	1.66%	0.387%
62	12.580	1774	1784	1787	rBV	1582232	2687541	15.21%	3.553%
63	12.645	1792	1795	1803	rVB	324822	361991	2.05%	0.479%
64	12.898	1835	1838	1843	rVB	373109	320933	1.82%	0.424%
65	13.404	1921	1924	1928	rVB	212195	181083	1.02%	0.239%

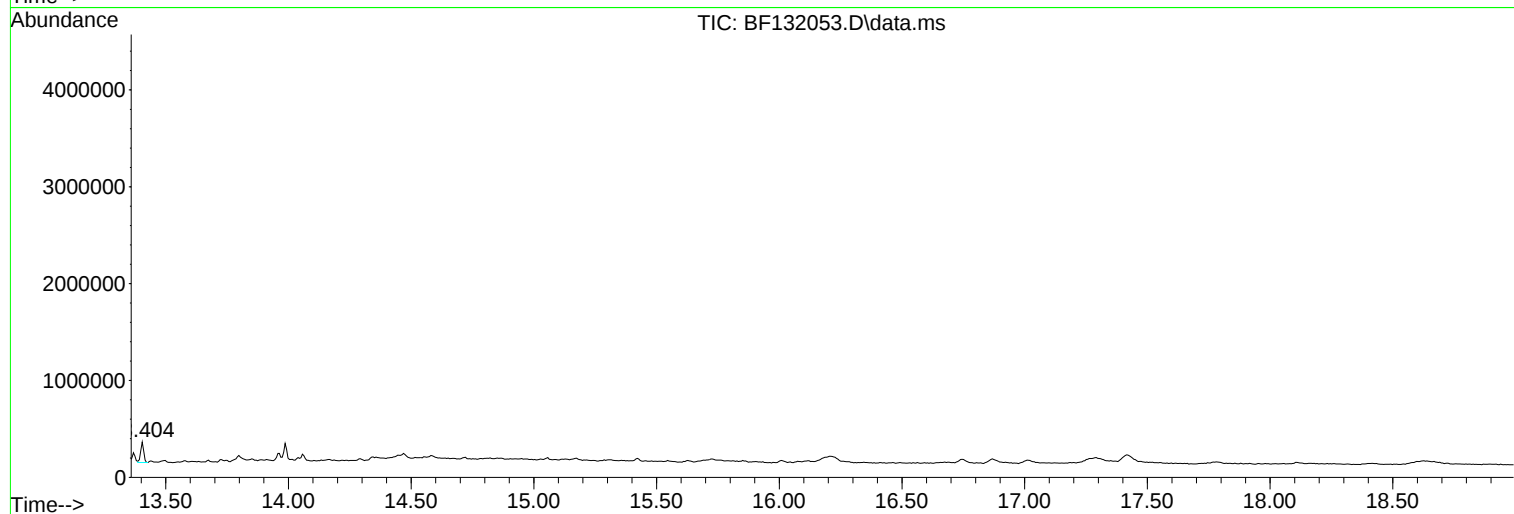
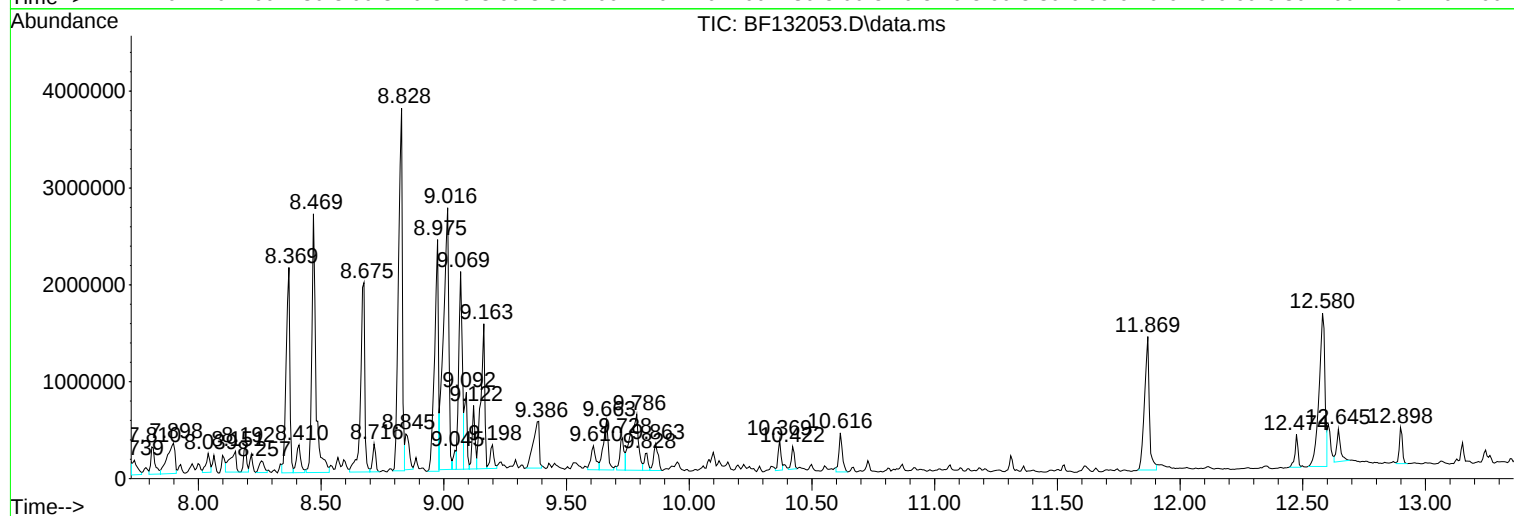
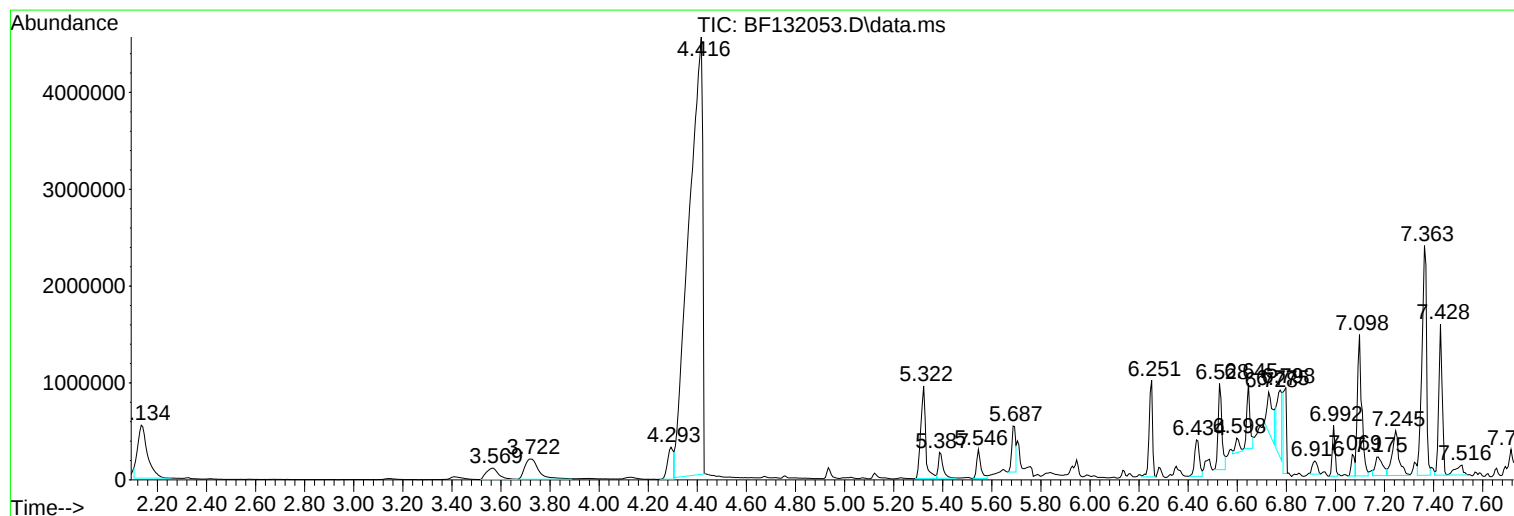
Sum of corrected areas: 75650147

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011223\
Data File : BF132053.D
Acq On : 12 Jan 2023 21:27
Operator : CG\JU
Sample : 01064-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-14-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011223\
Data File : BF132053.D
Acq On : 12 Jan 2023 21:27
Operator : CG\JU
Sample : 01064-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-14-02

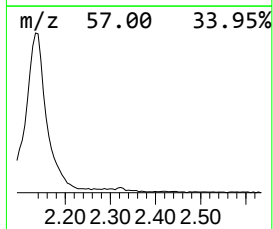
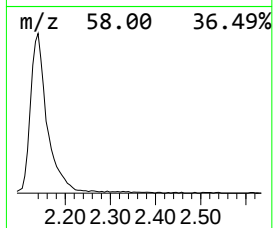
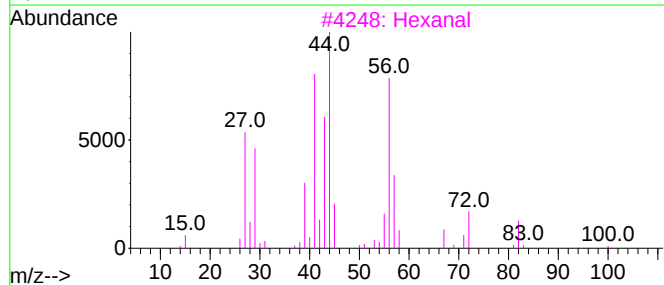
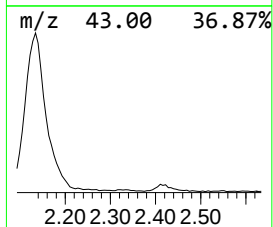
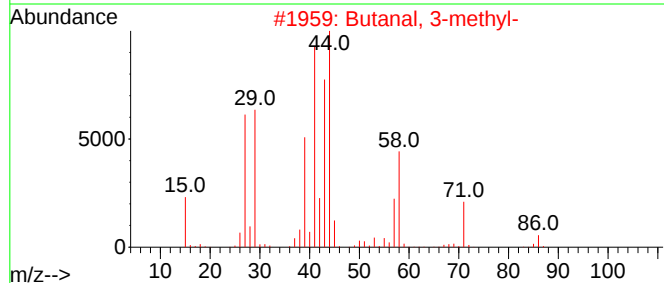
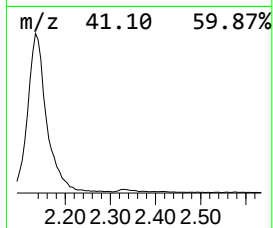
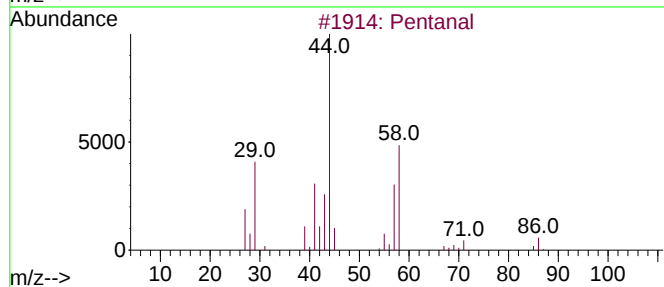
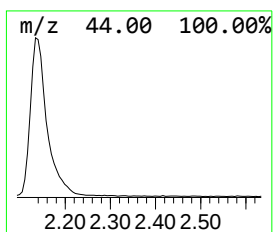
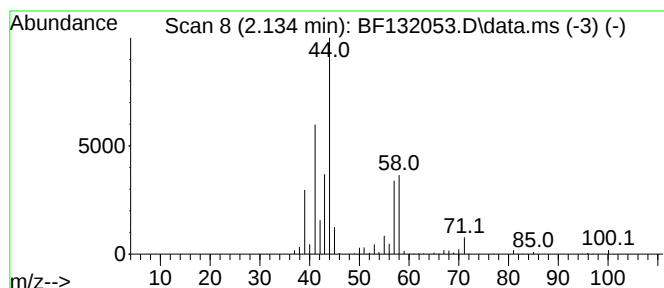
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Pentanal Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	34.69 ng	1518890	1,4-Dichlorobenzene-d4	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanal	86	C5H10O	000110-62-3	78
2			Butanal, 3-methyl-	86	C5H10O	000590-86-3	64
3			Hexanal	100	C6H12O	000066-25-1	45
4			Ethanol, 2-(2-propenyloxy)-	102	C5H10O2	000111-45-5	10
5			2-Propanamine	59	C3H9N	000075-31-0	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011223\
Data File : BF132053.D
Acq On : 12 Jan 2023 21:27
Operator : CG\JU
Sample : 01064-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-14-02

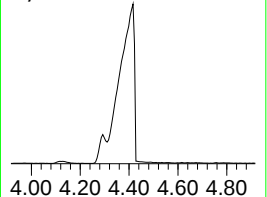
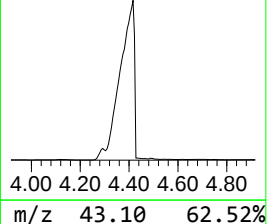
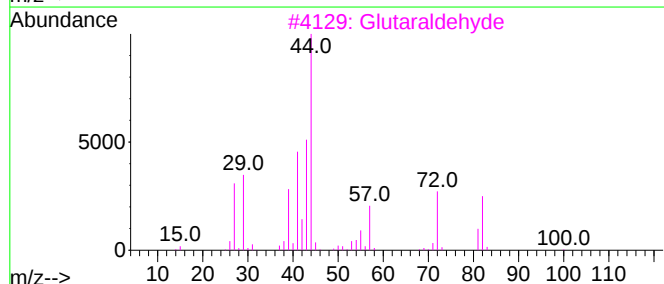
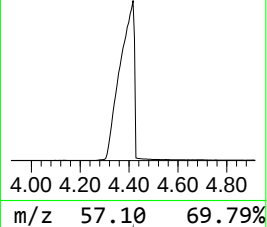
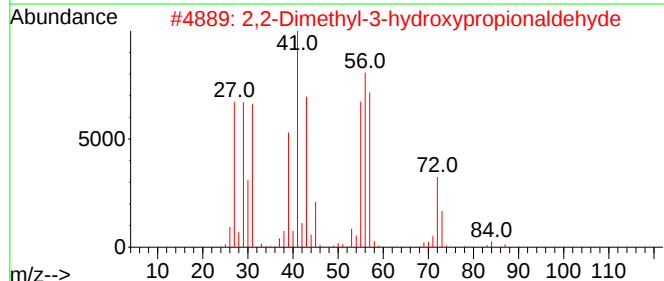
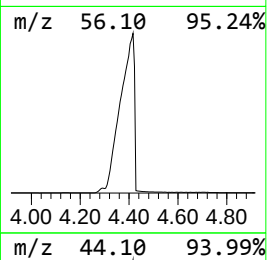
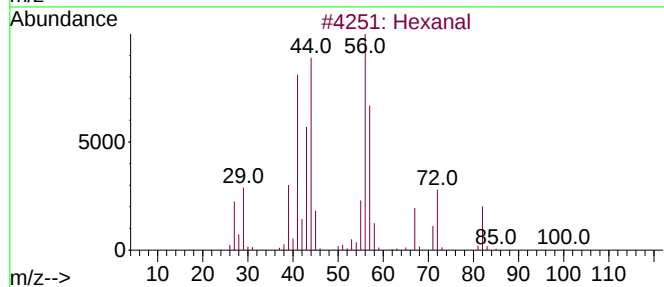
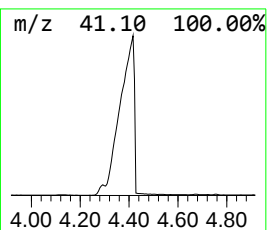
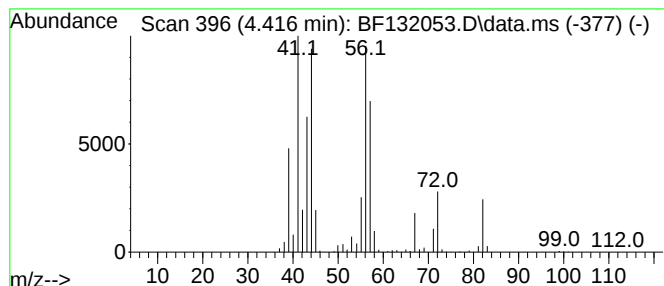
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Hexanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.416	403.49 ng	17668200	1,4-Dichlorobenzene-d4	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	81
2	2,2-Dimethyl-3-hydroxypropionald...			102	C5H10O2	000597-31-9	37
3	Glutaraldehyde			100	C5H8O2	000111-30-8	30
4	1-Butanol, 2-methyl-, (S)-			88	C5H12O	001565-80-6	22
5	Butanal			72	C4H8O	000123-72-8	16



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011223\
Data File : BF132053.D
Acq On : 12 Jan 2023 21:27
Operator : CG\JU
Sample : 01064-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

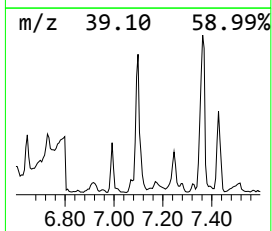
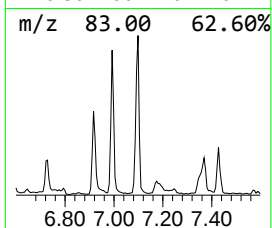
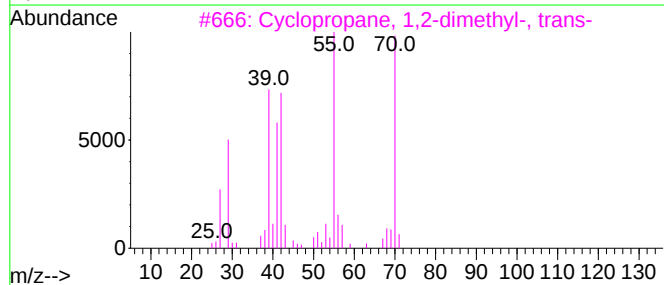
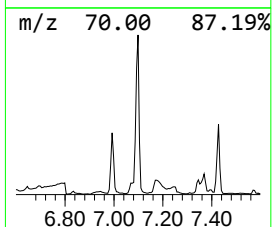
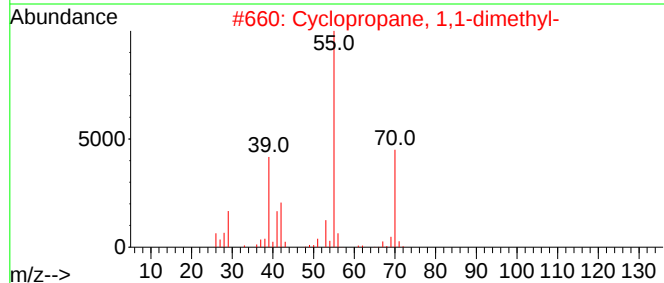
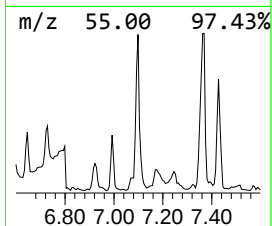
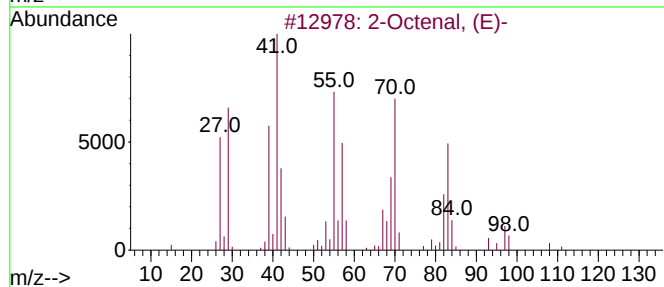
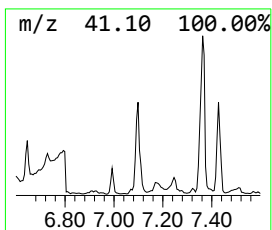
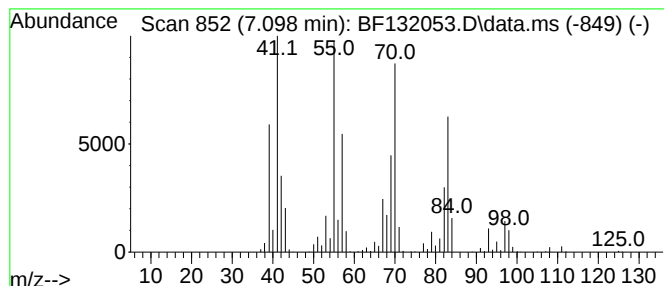
Instrument :
BNA_F
ClientSampleId :
S-14-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Octenal, (E)- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
7.098	40.79 ng	1786160	1,4-Dichlorobenzene-d4	6.769	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octenal, (E)-	126	C8H14O	002548-87-0	91
2	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	49
3	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	38
4	(E)-1,3-Butadien-1-ol	70	C4H6O	070411-98-2	38
5	(Z)-1,3-Butadien-1-ol	70	C4H6O	070415-58-6	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011223\
Data File : BF132053.D
Acq On : 12 Jan 2023 21:27
Operator : CG\JU
Sample : 01064-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-14-02

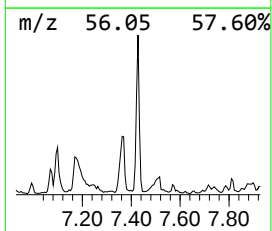
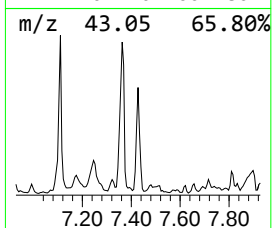
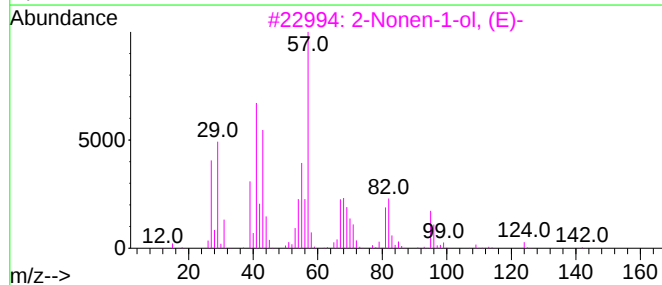
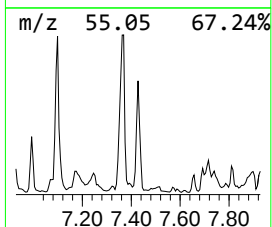
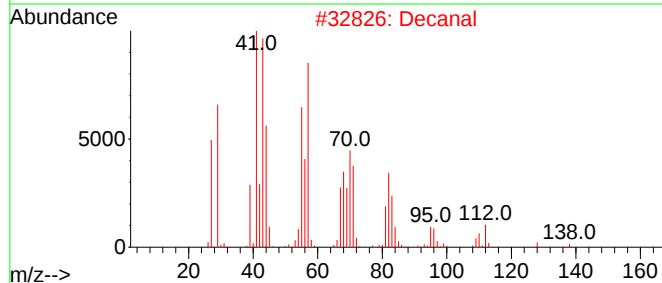
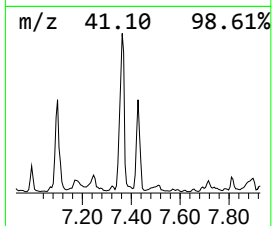
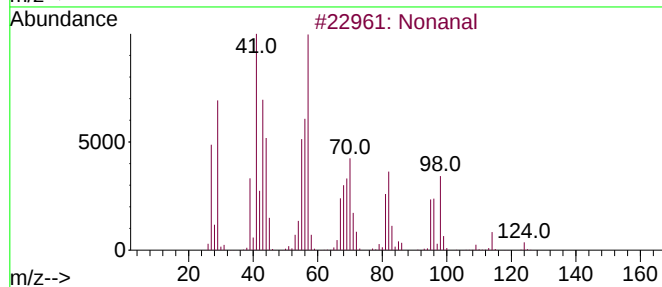
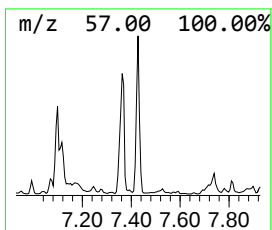
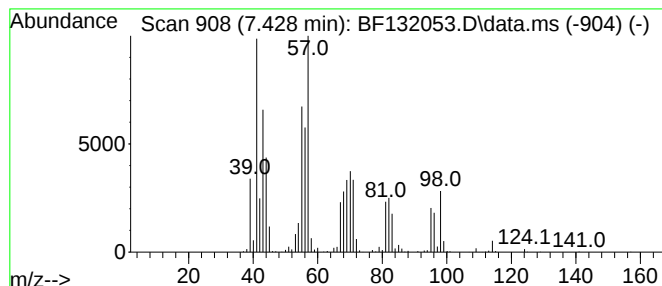
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Nonanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.428	140.24 ng	1507120	Naphthalene-d8	8.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanal			142	C9H18O	000124-19-6	78
2	Decanal			156	C10H20O	000112-31-2	50
3	2-Nonen-1-ol, (E)-			142	C9H18O	031502-14-4	38
4	2-Hepten-1-ol, (E)-			114	C7H14O	033467-76-4	30
5	1-Nonanol			144	C9H20O	000143-08-8	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011223\
Data File : BF132053.D
Acq On : 12 Jan 2023 21:27
Operator : CG\JU
Sample : 01064-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-14-02

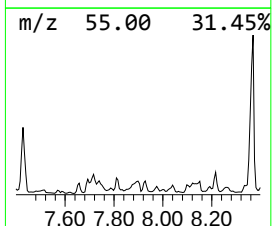
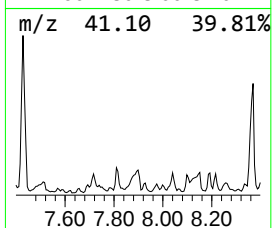
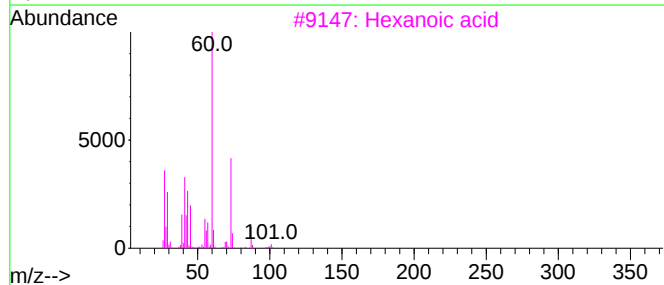
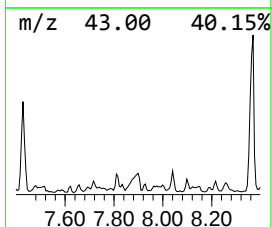
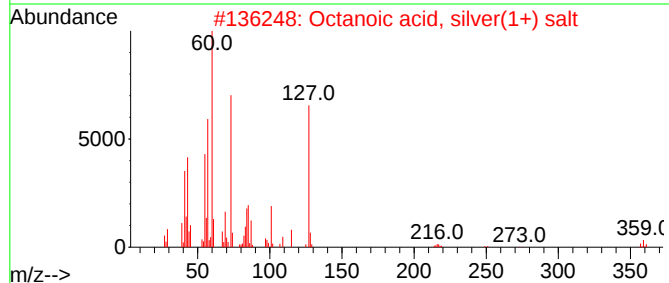
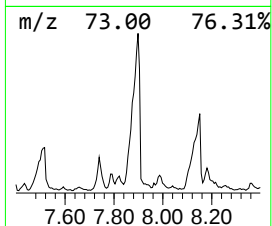
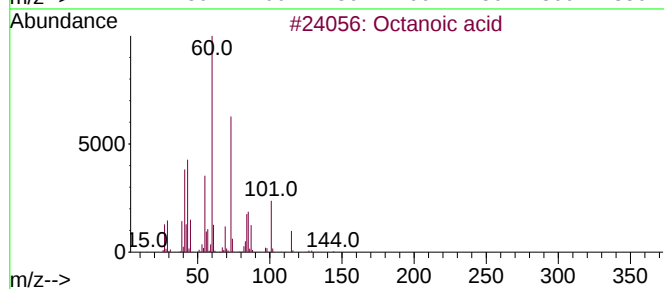
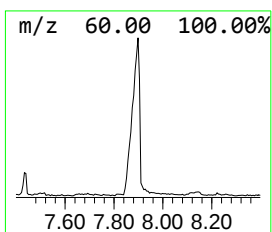
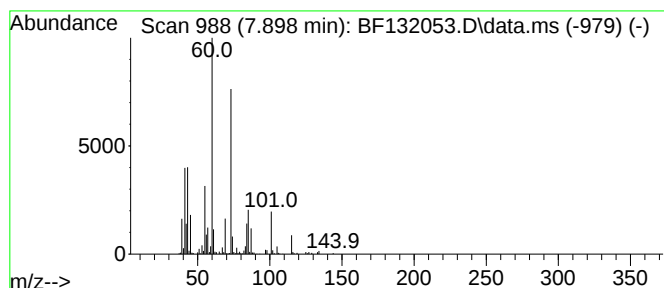
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.898	63.30 ng	680254	Naphthalene-d8	8.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octanoic acid	144	C8H16O2	000124-07-2	95
2			Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	64
3			Hexanoic acid	116	C6H12O2	000142-62-1	53
4			Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	50
5			Pentanoic acid	102	C5H10O2	000109-52-4	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011223\
Data File : BF132053.D
Acq On : 12 Jan 2023 21:27
Operator : CG\JU
Sample : 01064-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-14-02

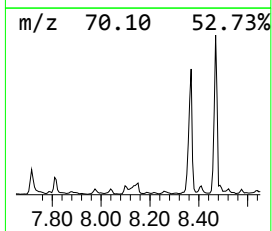
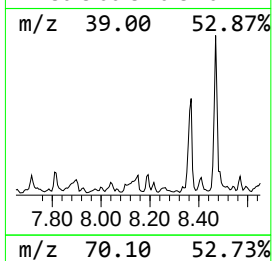
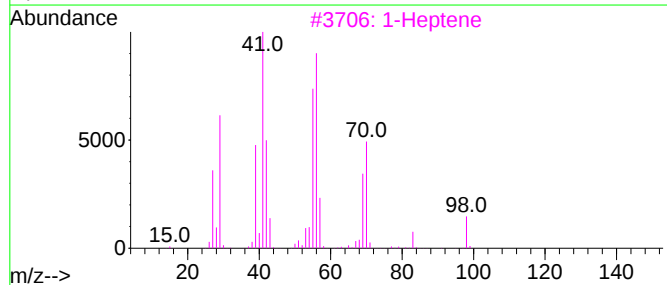
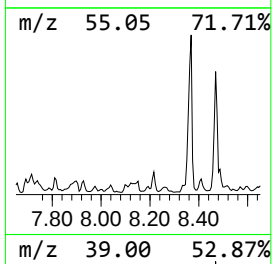
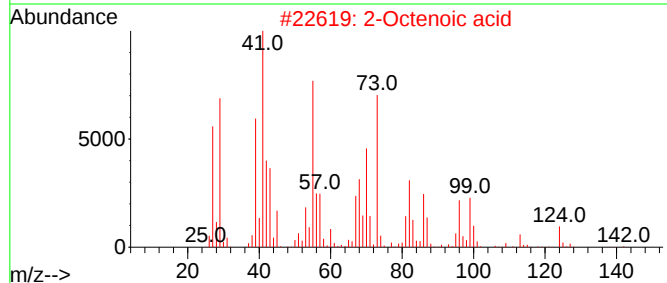
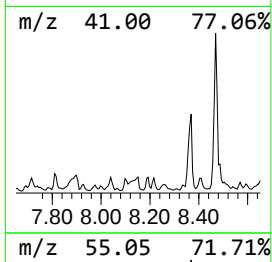
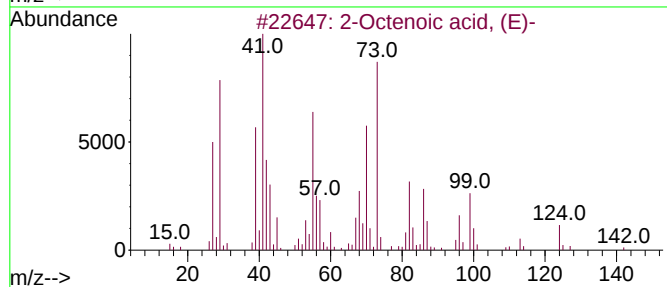
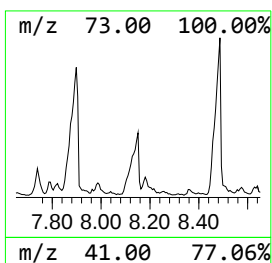
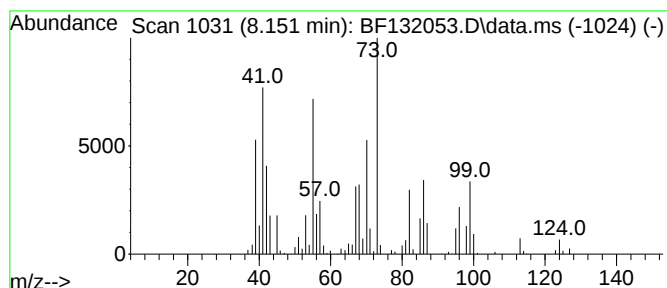
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-Octenoic acid, (E)- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.151	36.14 ng	388368	Naphthalene-d8	8.063

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Octenoic acid, (E)-	142	C8H14O2	001871-67-6	78
2		2-Octenoic acid	142	C8H14O2	001470-50-4	50
3		1-Heptene	98	C7H14	000592-76-7	38
4		2-Octenal, (E)-	126	C8H14O	002548-87-0	35
5		Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011223\
Data File : BF132053.D
Acq On : 12 Jan 2023 21:27
Operator : CG\JU
Sample : 01064-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-14-02

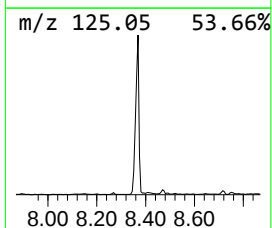
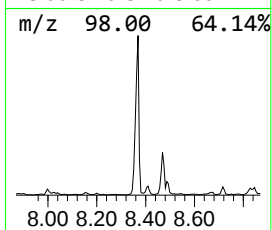
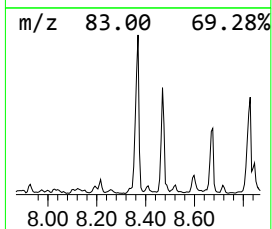
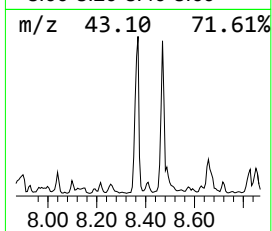
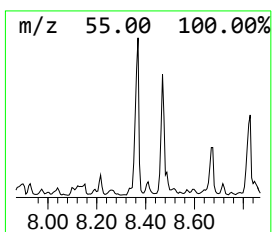
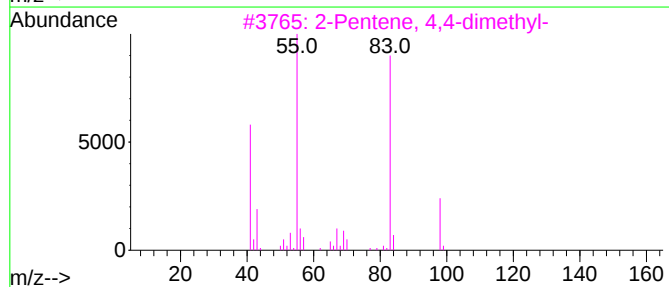
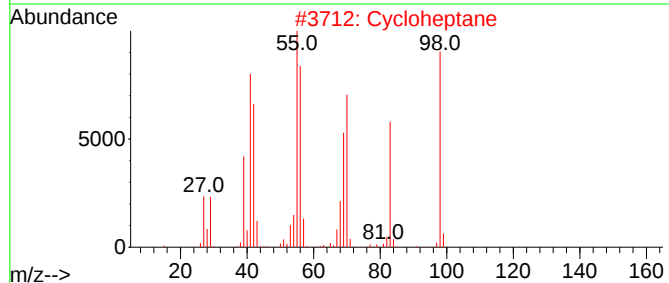
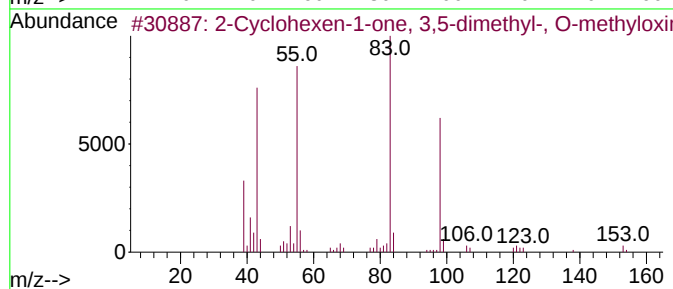
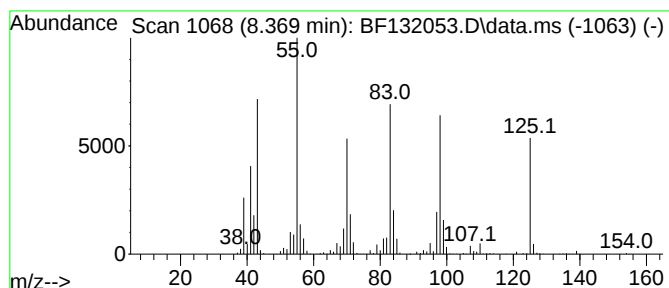
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown8.369 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.369	205.32 ng	2206540	Naphthalene-d8	8.063

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one, 3,5-dimethyl...	153	C9H15NO	056336-06-2	35	
2	Cycloheptane	98	C7H14	000291-64-5	35	
3	2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	35	
4	2-Octanol, trifluoroacetate	226	C10H17F3O2	000332-83-2	27	
5	Cyclohexanol, 1-ethenyl-	126	C8H14O	001940-19-8	27	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011223\
Data File : BF132053.D
Acq On : 12 Jan 2023 21:27
Operator : CG\JU
Sample : 01064-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

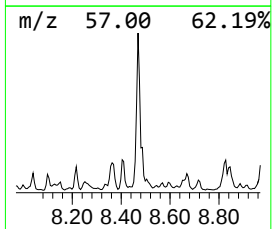
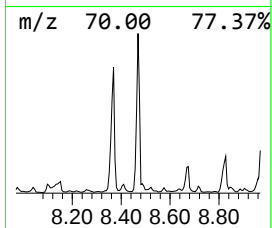
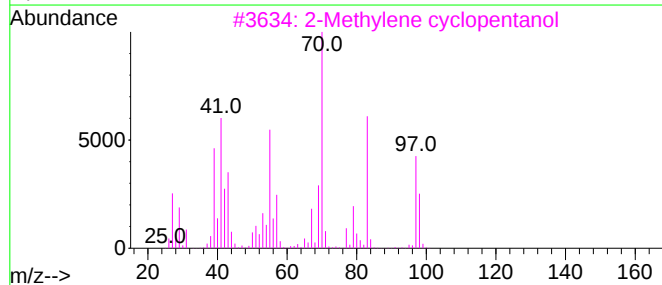
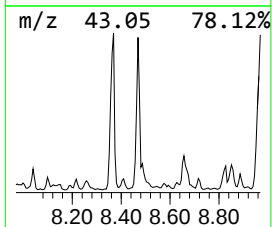
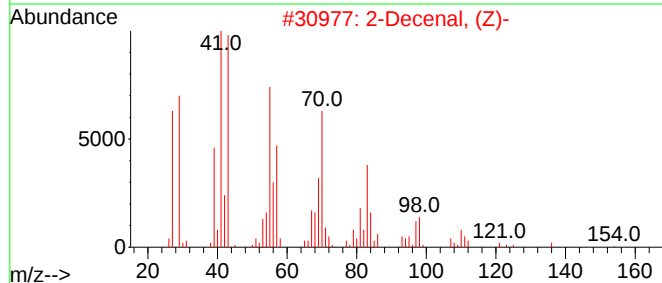
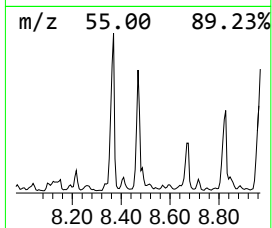
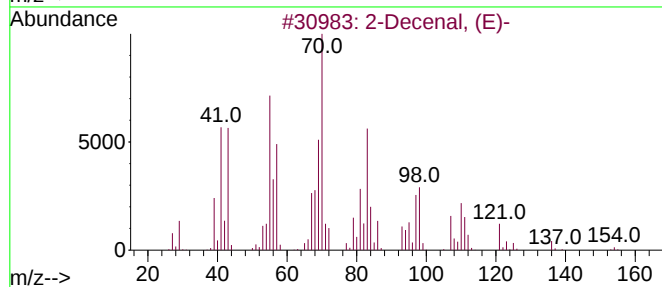
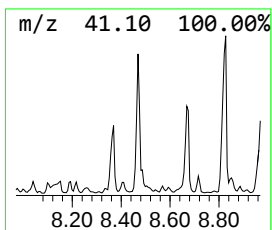
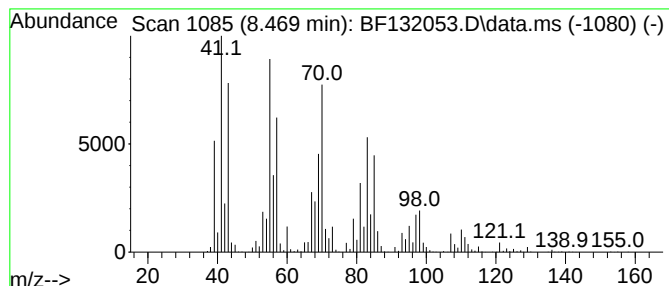
Instrument :
BNA_F
ClientSampleId :
S-14-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-Decenal, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.469	282.20 ng	3032680	Naphthalene-d8	8.063	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Decenal, (E)-	154	C10H18O	003913-81-3	72
2	2-Decenal, (Z)-	154	C10H18O	002497-25-8	58
3	2-Methylene cyclopentanol	98	C6H10O	020461-31-8	53
4	Methylamine, N-(1-ethylpentylidene...	127	C8H17N	018641-73-1	47
5	trans-1-Butyl-2-methylcyclopropane	112	C8H16	038851-70-6	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011223\
Data File : BF132053.D
Acq On : 12 Jan 2023 21:27
Operator : CG\JU
Sample : 01064-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-14-02

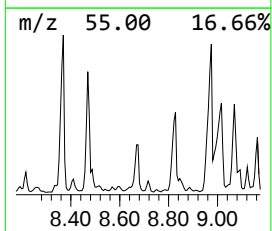
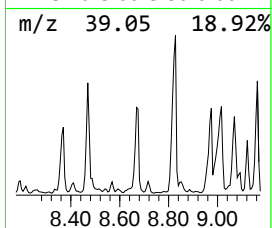
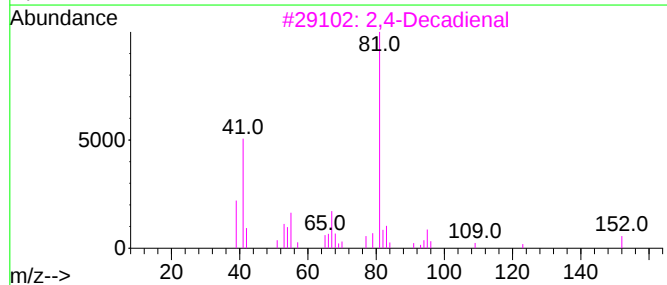
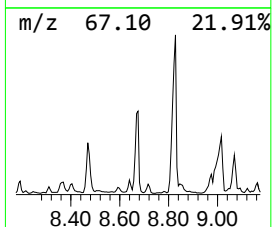
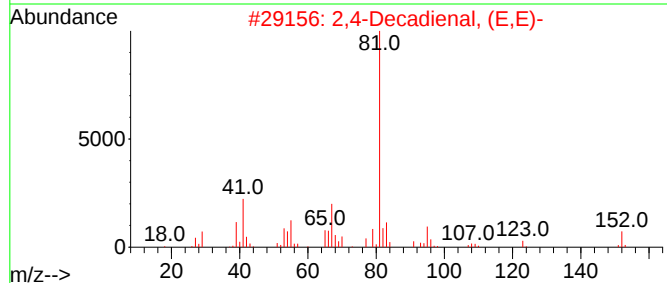
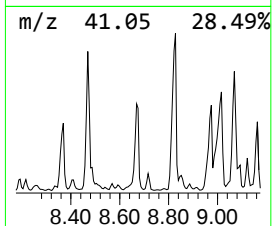
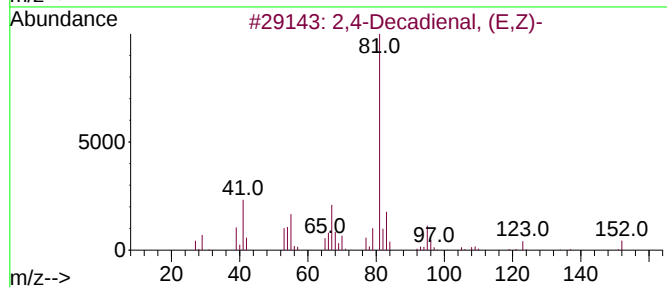
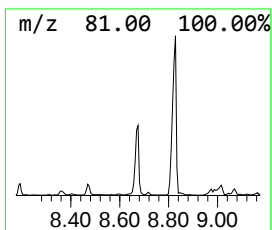
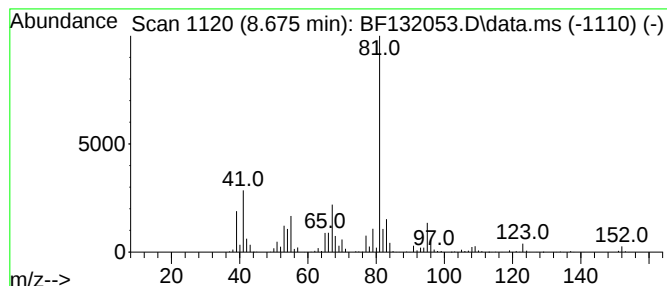
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2,4-Decadienal, (E,Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.675	215.61 ng	2317100	Naphthalene-d8	8.063

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Decadienal, (E,Z)-	152	C10H16O	025152-83-4	94	
2	2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	91	
3	2,4-Decadienal	152	C10H16O	002363-88-4	90	
4	2,4-Nonadienal, (E,E)-	138	C9H14O	005910-87-2	78	
5	2,4-Nonadienal	138	C9H14O	006750-03-4	78	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011223\
Data File : BF132053.D
Acq On : 12 Jan 2023 21:27
Operator : CG\JU
Sample : 01064-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-14-02

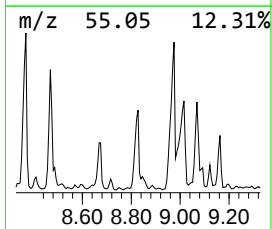
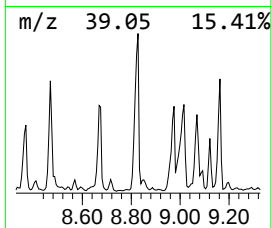
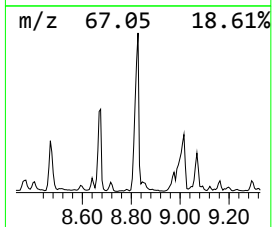
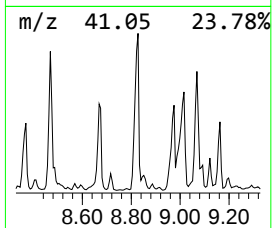
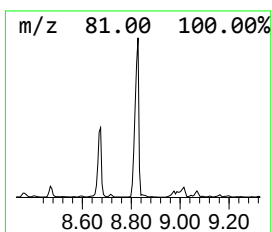
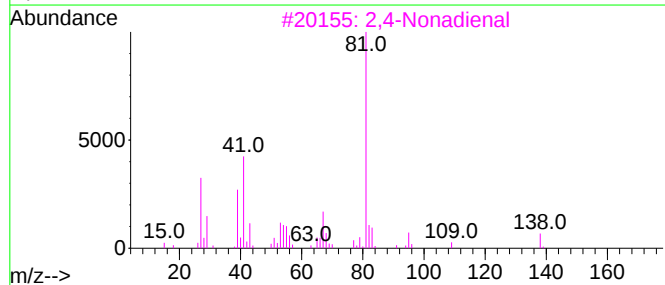
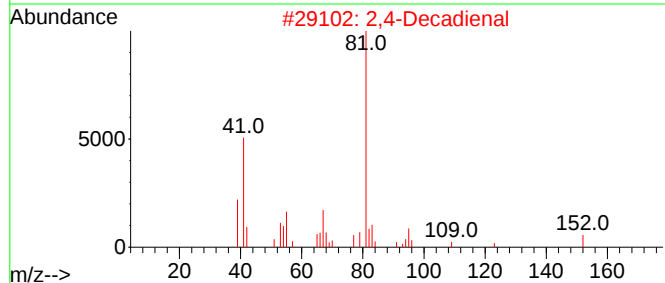
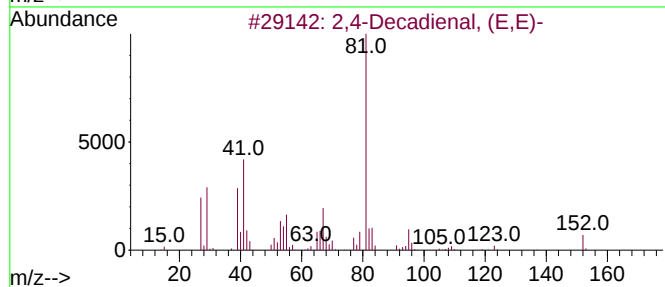
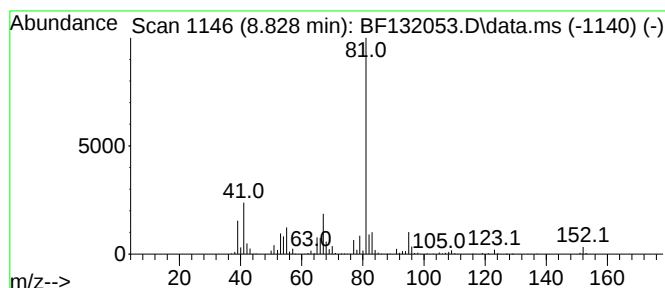
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2,4-Decadienal, (E,E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.828	374.97 ng	4029710	Naphthalene-d8	8.063

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	91	
2	2,4-Decadienal	152	C10H16O	002363-88-4	91	
3	2,4-Nonadienal	138	C9H14O	006750-03-4	83	
4	2,4-Nonadienal, (E,E)-	138	C9H14O	005910-87-2	78	
5	2,4-Octadienal, (E,E)-	124	C8H12O	030361-28-5	64	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011223\
Data File : BF132053.D
Acq On : 12 Jan 2023 21:27
Operator : CG\JU
Sample : 01064-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-14-02

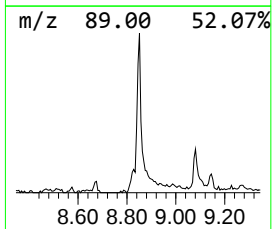
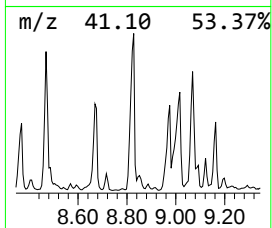
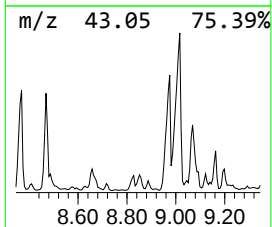
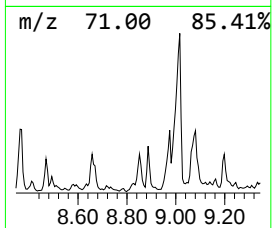
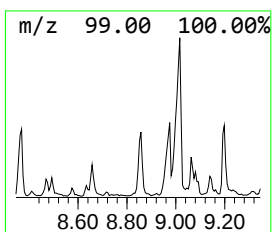
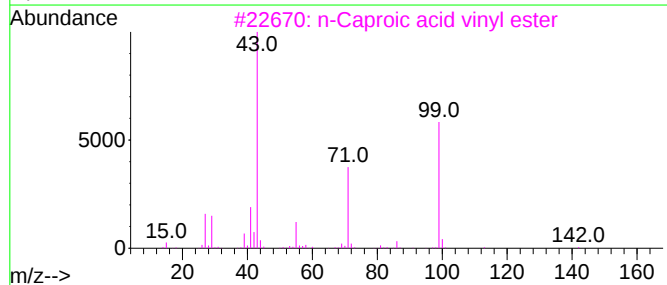
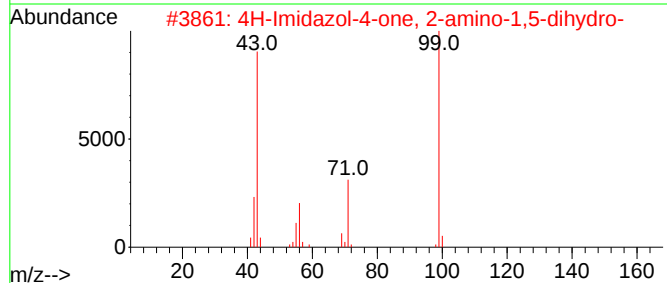
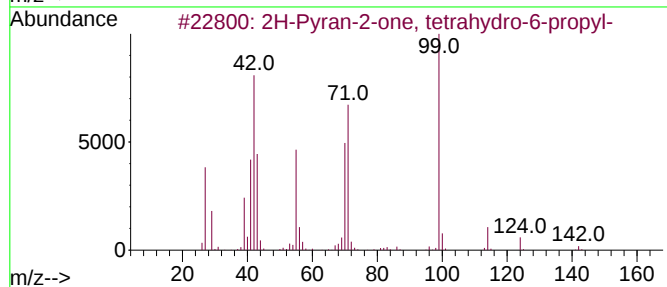
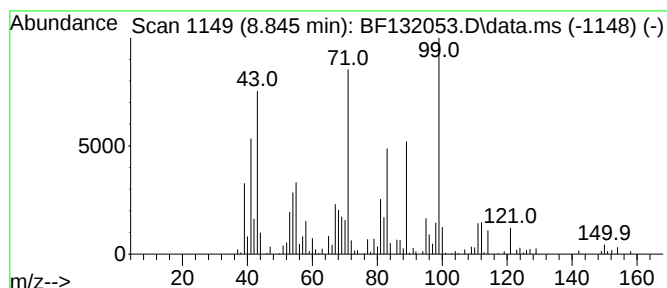
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown8.845 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.845	38.07 ng	409173	Naphthalene-d8	8.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Pyran-2-one, tetrahydro-6-pro...	142	C8H14O2	000698-76-0	49		
2	4H-Imidazol-4-one, 2-amino-1,5-d...	99	C3H5N3O	000503-86-6	46		
3	n-Caproic acid vinyl ester	142	C8H14O2	003050-69-9	43		
4	Hexanethioic acid, S-heptyl ester	230	C13H26OS	002432-80-6	43		
5	Pentanoic acid, 2-methyl-, anhyd...	214	C12H22O3	063169-61-9	43		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011223\
Data File : BF132053.D
Acq On : 12 Jan 2023 21:27
Operator : CG\JU
Sample : 01064-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-14-02

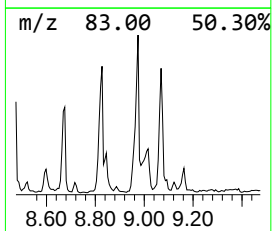
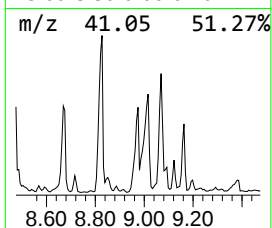
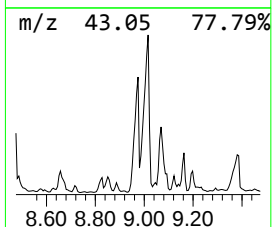
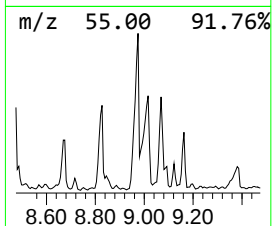
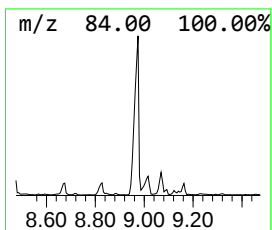
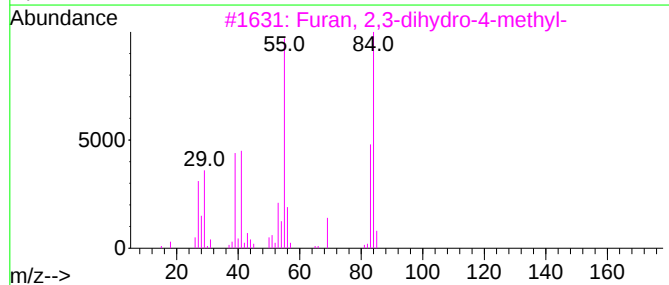
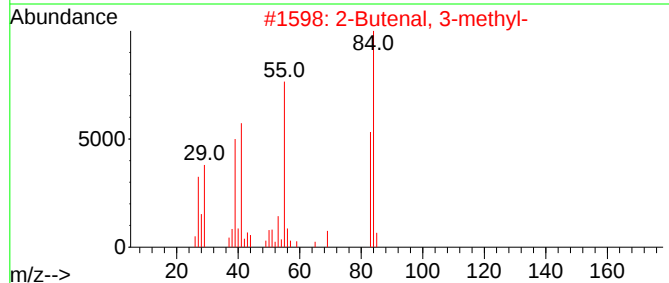
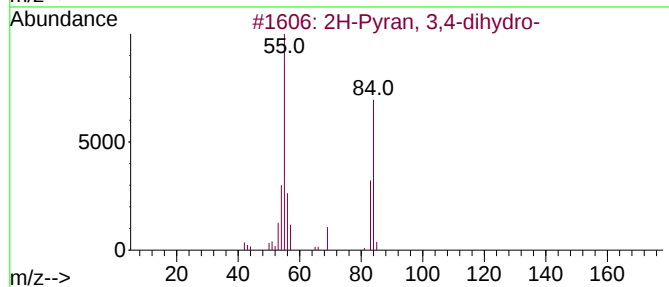
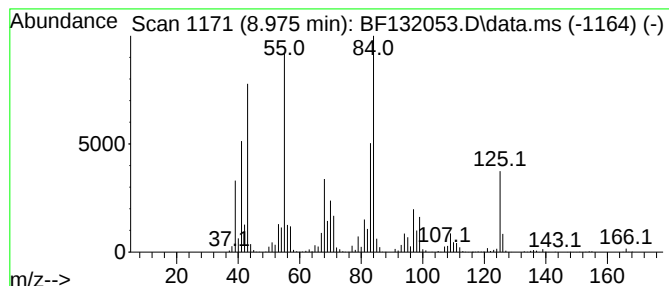
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2H-Pyran, 3,4-dihydro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.975	284.67 ng	2615630	Acenaphthene-d10	9.822

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Pyran, 3,4-dihydro-		84	C5H8O	000110-87-2	55
2	2-Butenal, 3-methyl-		84	C5H8O	000107-86-8	46
3	Furan, 2,3-dihydro-4-methyl-		84	C5H8O	034314-83-5	46
4	Octahydropyrrolo[1,2-a]pyrazine		126	C7H14N2	005654-83-1	38
5	2-Methylpiperidine		99	C6H13N	000109-05-7	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011223\
Data File : BF132053.D
Acq On : 12 Jan 2023 21:27
Operator : CG\JU
Sample : 01064-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-14-02

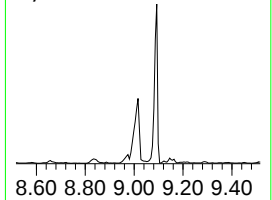
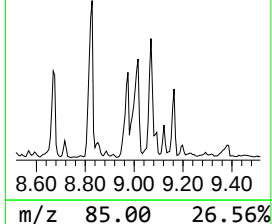
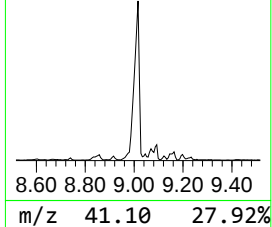
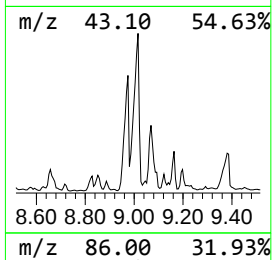
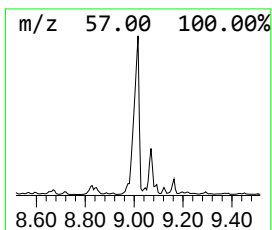
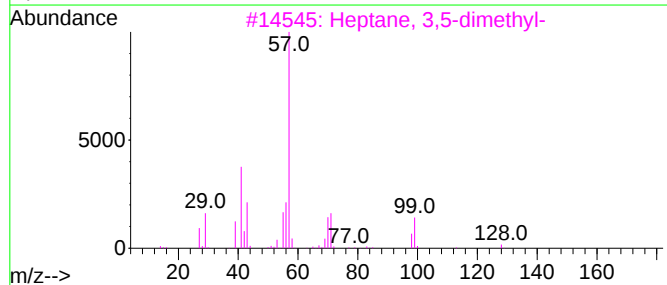
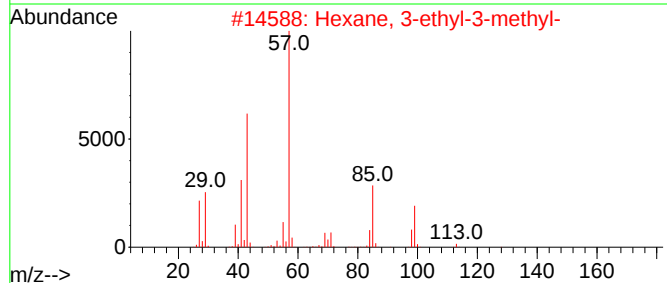
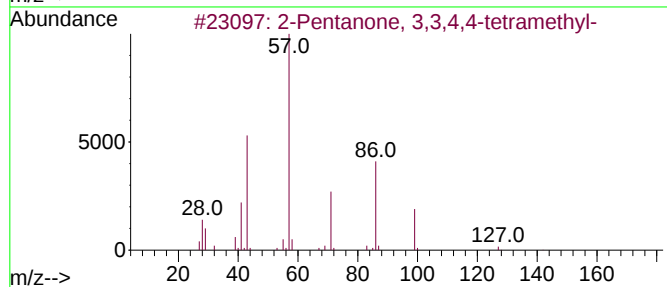
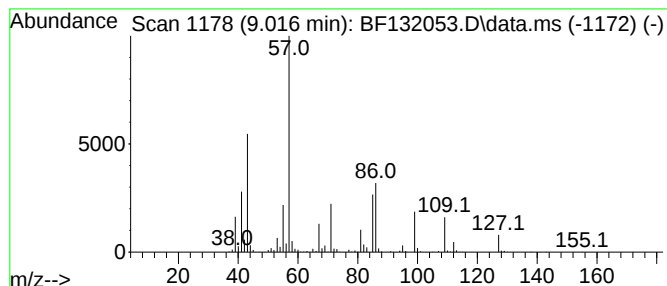
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown9.016 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.016	443.38 ng	4073790	Acenaphthene-d10	9.822

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 3,3,4,4-tetramethyl-	142	C9H18O	000865-66-7	43	
2	Hexane, 3-ethyl-3-methyl-	128	C9H20	003074-76-8	35	
3	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	27	
4	Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	27	
5	2-Nonanol, trimethylacetate	228	C14H28O2	1000463-21-6	25	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011223\
Data File : BF132053.D
Acq On : 12 Jan 2023 21:27
Operator : CG\JU
Sample : 01064-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-14-02

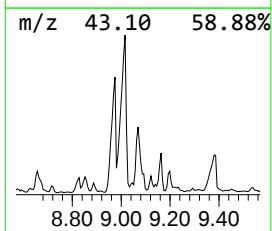
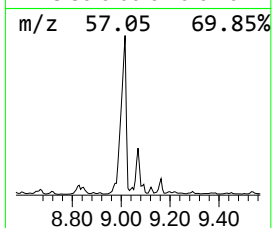
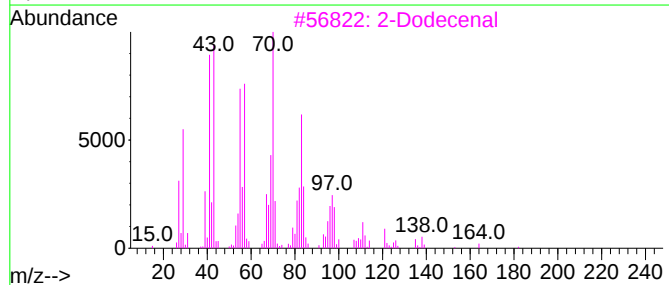
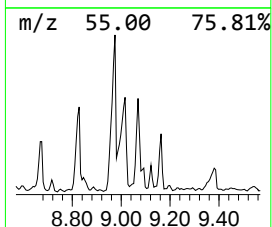
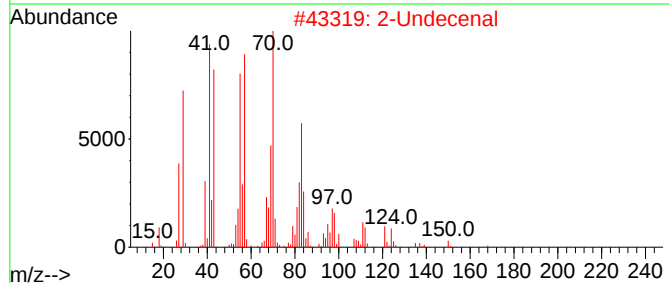
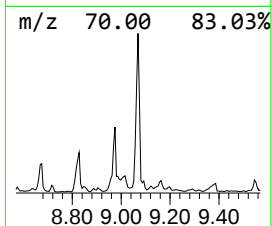
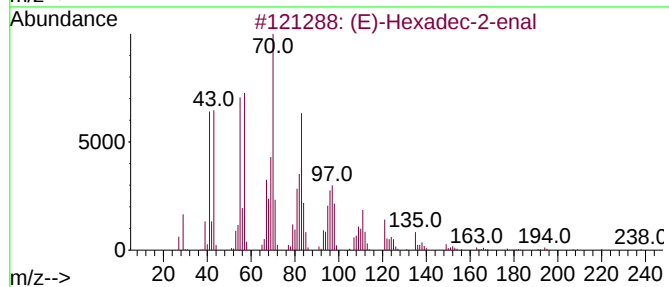
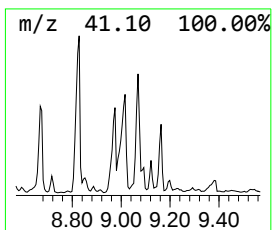
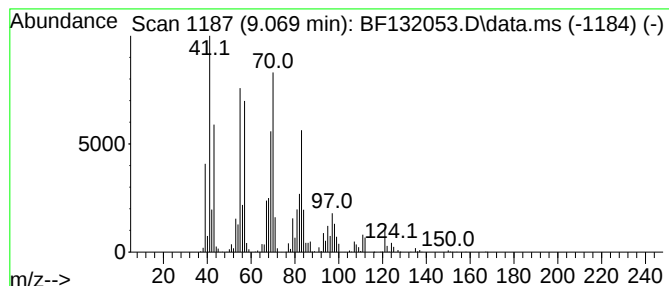
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 (E)-Hexadec-2-enal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.069	227.70 ng	2092150	Acenaphthene-d10	9.822

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		(E)-Hexadec-2-enal	238	C16H30O	022644-96-8	90
2		2-Undecenal	168	C11H20O	002463-77-6	87
3		2-Dodecenal	182	C12H22O	004826-62-4	87
4		2-Tridecenal, (E)-	196	C13H24O	007069-41-2	80
5		2-Dodecenal, (E)-	182	C12H22O	020407-84-5	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011223\
Data File : BF132053.D
Acq On : 12 Jan 2023 21:27
Operator : CG\JU
Sample : 01064-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

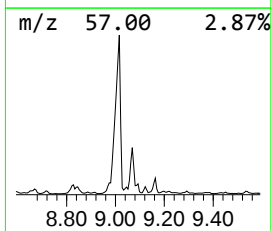
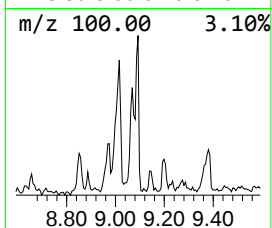
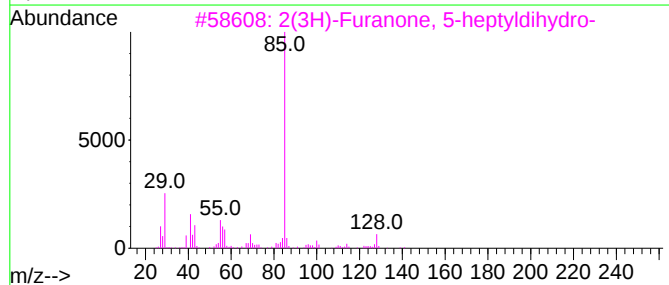
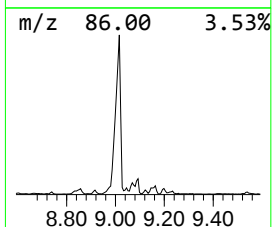
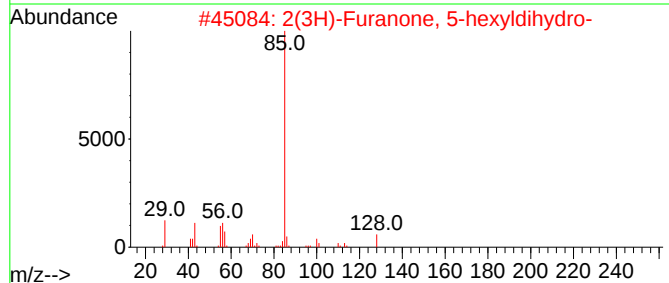
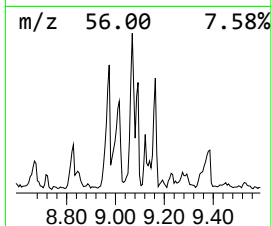
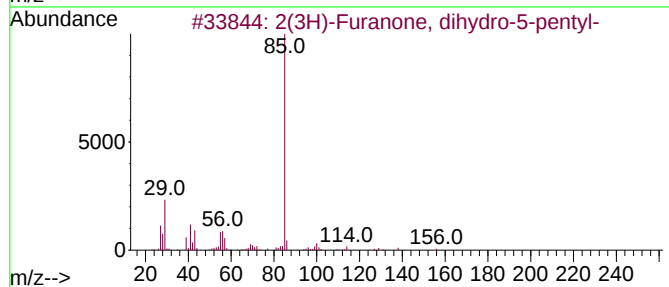
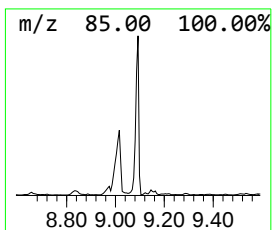
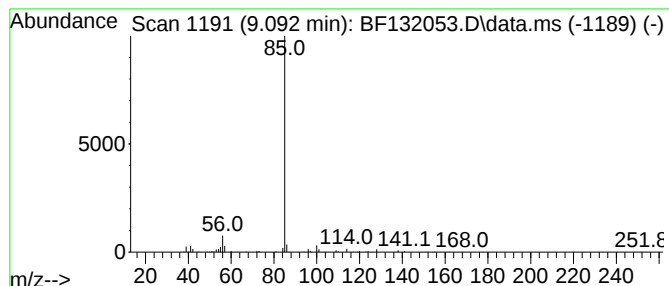
Instrument :
BNA_F
ClientSampleId :
S-14-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 2(3H)-Furanone, dihydro-5-p... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD			R.T.
9.092	62.62 ng	575365	Acenaphthene-d10			9.822
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Furanone, dihydro-5-pentyl-	156	C9H16O2		000104-61-0	83
2	2(3H)-Furanone, 5-hexyldihydro-	170	C10H18O2		000706-14-9	78
3	2(3H)-Furanone, 5-heptyldihydro-	184	C11H20O2		000104-67-6	56
4	2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2		000105-21-5	9
5	(S)-3,3,6-Trimethylhepta-1,5-die...	196	C12H20O2		003465-88-1	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011223\
Data File : BF132053.D
Acq On : 12 Jan 2023 21:27
Operator : CG\JU
Sample : 01064-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-14-02

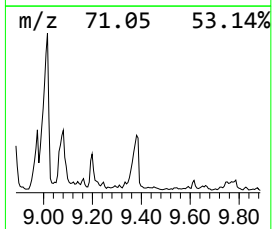
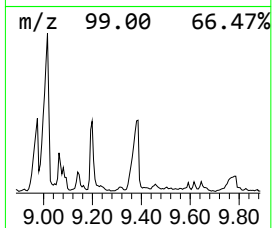
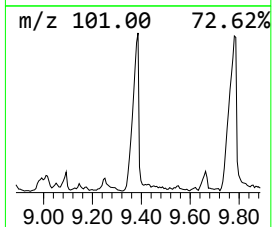
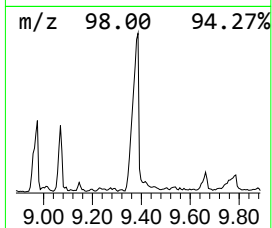
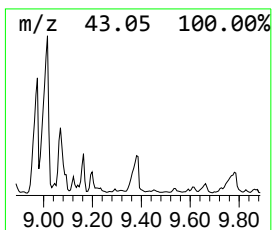
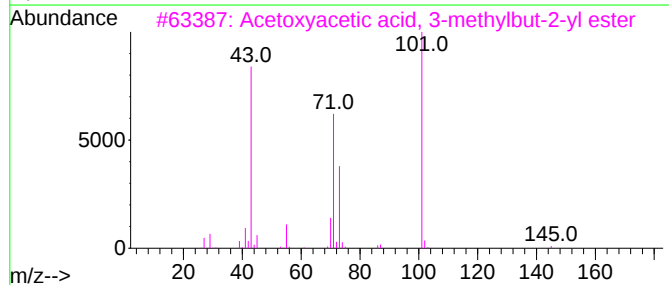
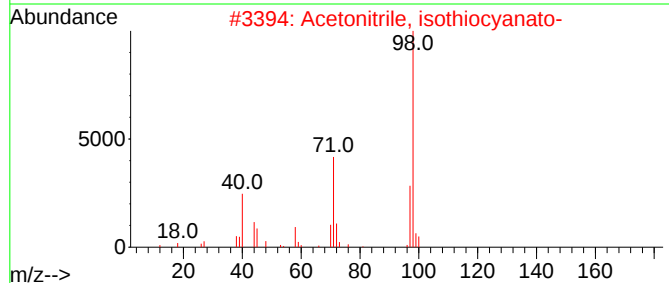
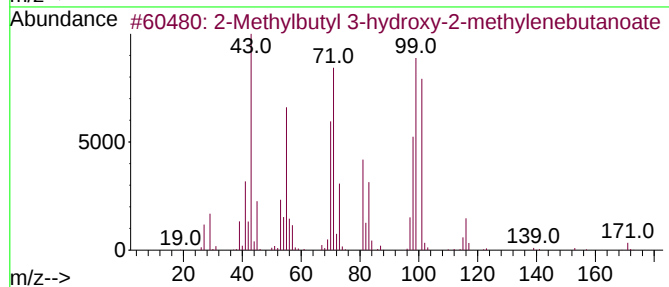
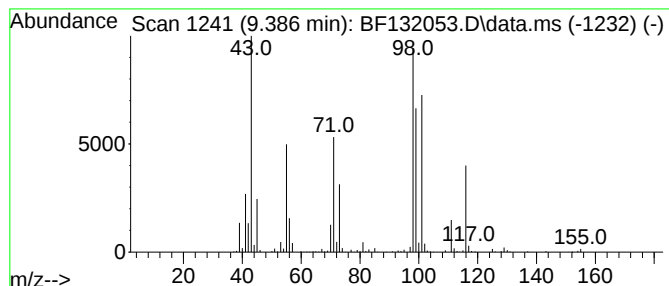
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown9.386 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.386	92.16 ng	846742	Acenaphthene-d10	9.822

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Methylbutyl 3-hydroxy-2-methyl...	186	C10H18O3	080758-69-6	47
2		Acetonitrile, isothiocyanato-	98	C3H2N2S	032772-75-1	25
3		Acetoxyacetic acid, 3-methylbut-...	188	C9H16O4	1000355-69-8	22
4		4-Methylthiazole	99	C4H5NS	000693-95-8	22
5		2H-Thiopyran, tetrahydro-2-methyl-	116	C6H12S	005161-16-0	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011223\
Data File : BF132053.D
Acq On : 12 Jan 2023 21:27
Operator : CG\JU
Sample : 01064-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-14-02

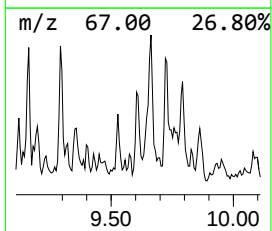
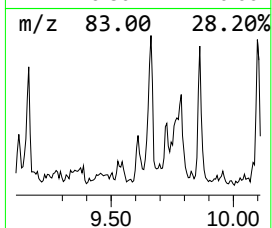
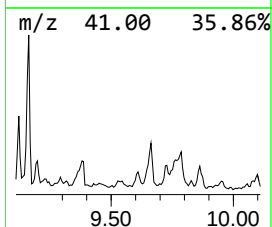
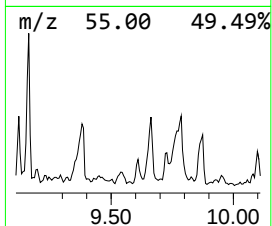
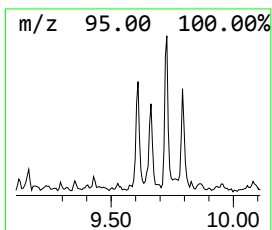
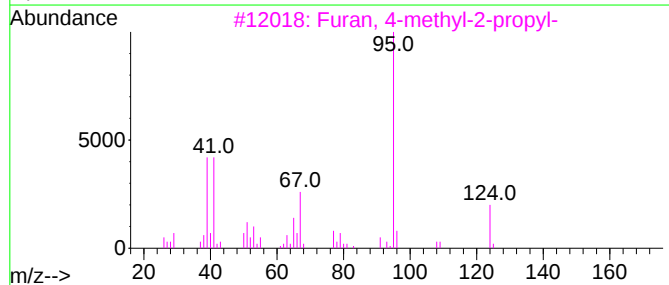
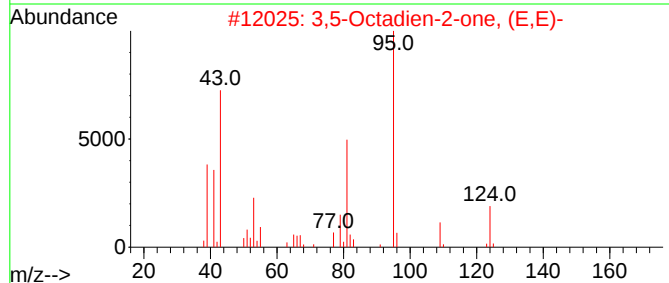
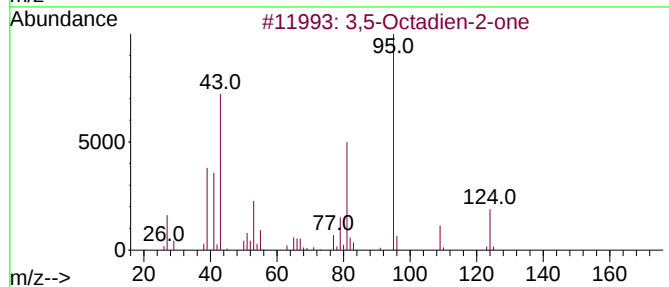
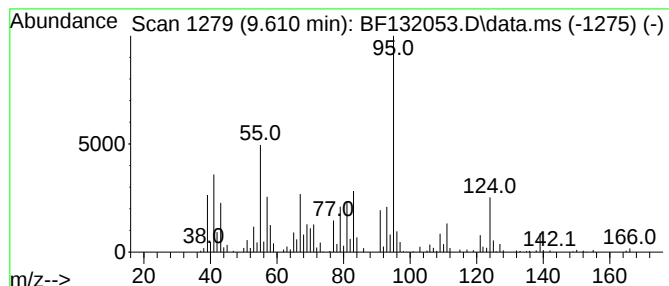
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 3,5-Octadien-2-one Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.610	38.70 ng	355602	Acenaphthene-d10	9.822

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3,5-Octadien-2-one	124	C8H12O	038284-27-4	52
2		3,5-Octadien-2-one, (E,E)-	124	C8H12O	030086-02-3	52
3		Furan, 4-methyl-2-propyl-	124	C8H12O	006148-37-4	50
4		Silane, diethyldifluoro-	124	C4H10F2Si	000358-06-5	50
5		Cycloheptane, 1-chloro-3-iodo-	258	C7H12ClI	1000337-09-8	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011223\
Data File : BF132053.D
Acq On : 12 Jan 2023 21:27
Operator : CG\JU
Sample : 01064-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-14-02

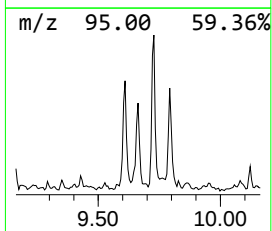
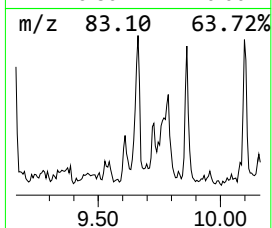
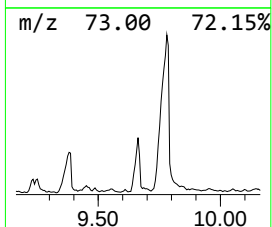
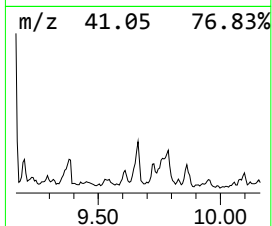
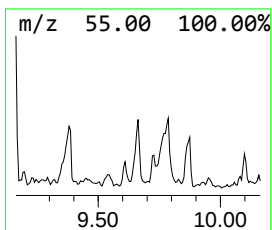
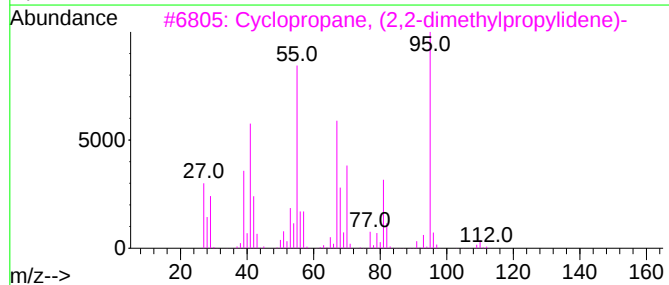
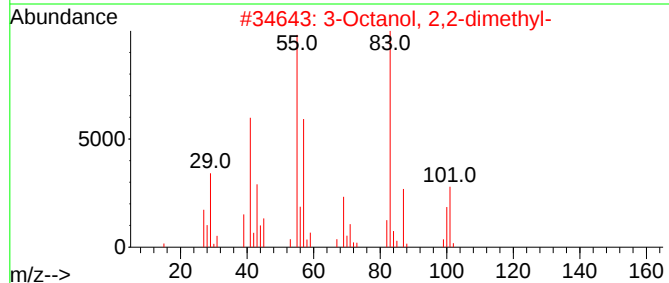
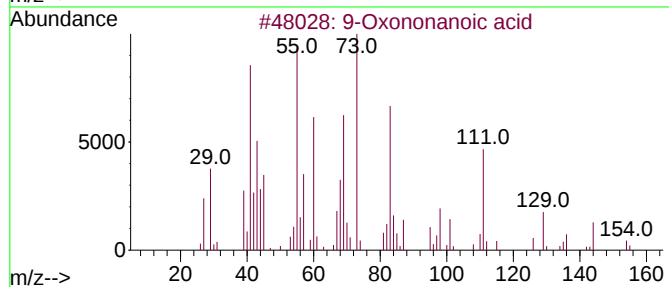
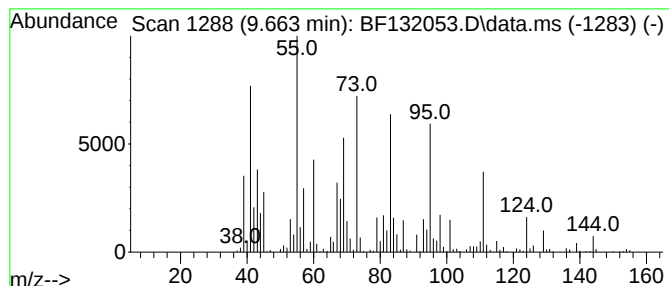
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown9.663 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.663	76.07 ng	698951	Acenaphthene-d10	9.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Oxononanoic acid	172	C9H16O3	002553-17-5	49
2			3-Octanol, 2,2-dimethyl-	158	C10H22O	019841-72-6	14
3			Cyclopropane, (2,2-dimethylpropylidene)-	110	C8H14	039647-71-7	11
4			Azeleoneitrile	150	C9H14N2	001675-69-0	11
5			1,5-Hexadiene, 2,5-dimethyl-	110	C8H14	000627-58-7	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011223\
Data File : BF132053.D
Acq On : 12 Jan 2023 21:27
Operator : CG\JU
Sample : 01064-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-14-02

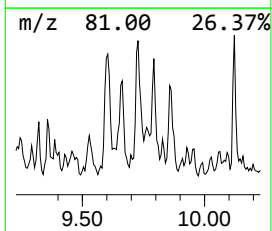
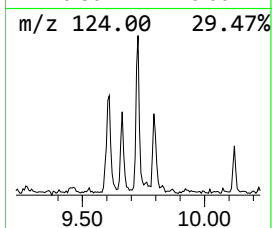
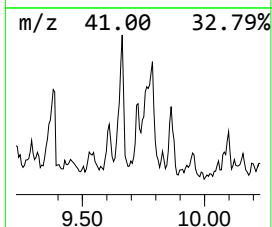
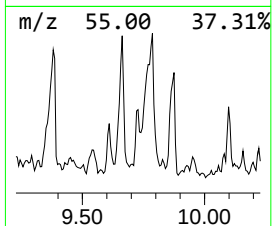
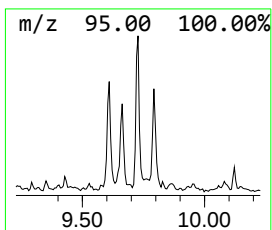
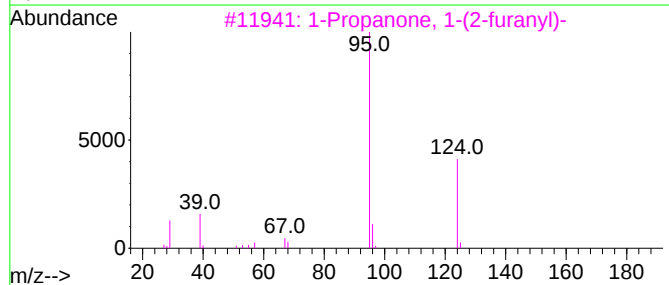
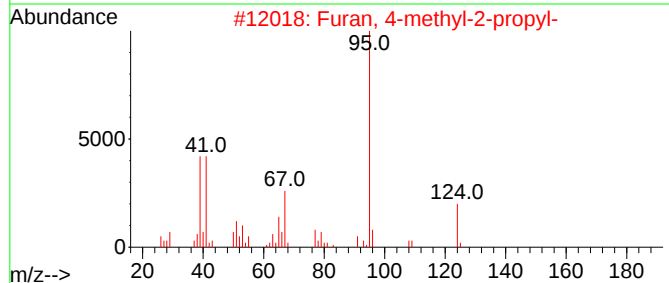
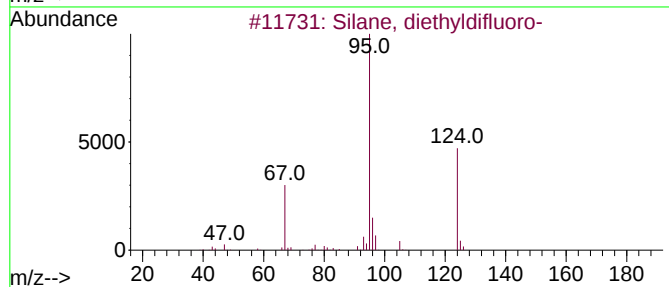
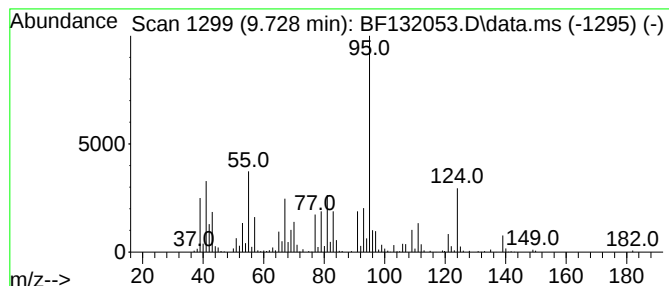
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Silane, diethyldifluoro- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.728	44.94 ng	412936	Acenaphthene-d10	9.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Silane, diethyldifluoro-	124	C4H10F2Si	000358-06-5	53
2			Furan, 4-methyl-2-propyl-	124	C8H12O	006148-37-4	50
3			1-Propanone, 1-(2-furanyl)-	124	C7H8O2	003194-15-8	49
4			1,4-Pentadiene, 2,3,4-trimethyl-	110	C8H14	072014-90-5	49
5			3,5-Octadien-2-one, (E,E)-	124	C8H12O	030086-02-3	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011223\
Data File : BF132053.D
Acq On : 12 Jan 2023 21:27
Operator : CG\JU
Sample : 01064-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

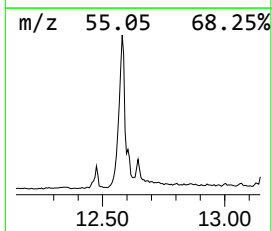
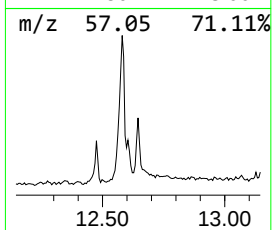
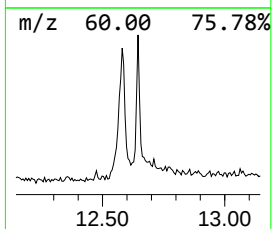
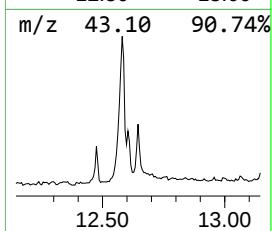
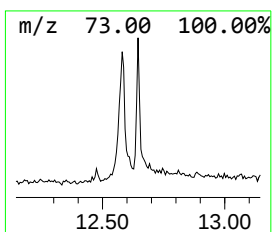
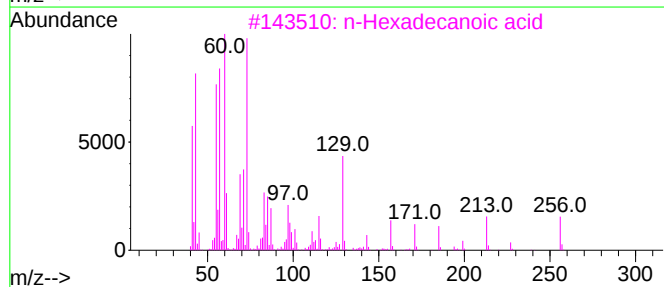
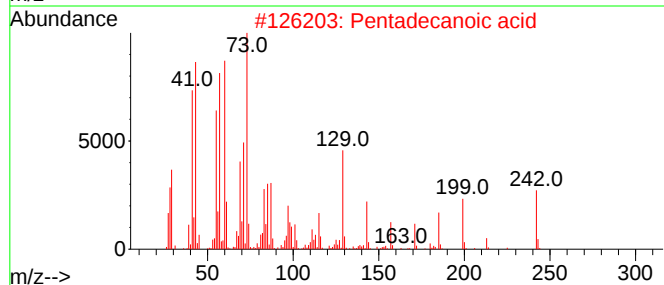
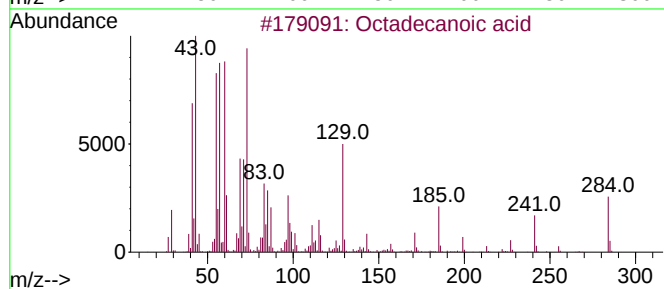
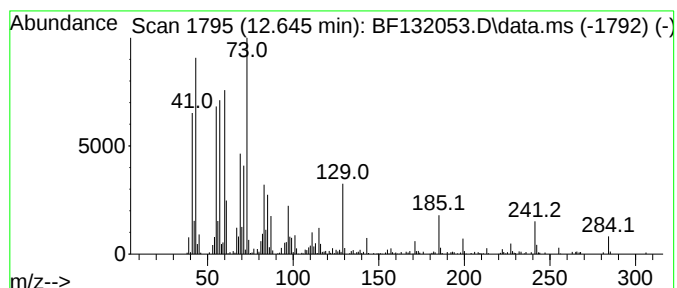
Instrument :
BNA_F
ClientSampleId :
S-14-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Octadecanoic acid Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.645	39.98 ng	361991	Chrysene-d12		13.963	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	97
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	89
3	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	87
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	70
5	8-Methylnonanoic acid		172	C10H20O2	005963-14-4	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011223\
 Data File : BF132053.D
 Acq On : 12 Jan 2023 21:27
 Operator : CG\JU
 Sample : 01064-07
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-14-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.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
Pentanal	2.134	34.7	ng	1518890	1	6.769	875761	20.0
Hexanal	4.416	403.5	ng	17668200	1	6.769	875761	20.0
2-Octenal, (E)-	7.098	40.8	ng	1786160	1	6.769	875761	20.0
Nonanal	7.428	140.2	ng	1507120	2	8.063	214934	20.0
Octanoic acid	7.898	63.3	ng	680254	2	8.063	214934	20.0
2-Octenoic acid...	8.151	36.1	ng	388368	2	8.063	214934	20.0
unknown8.369	8.369	205.3	ng	2206540	2	8.063	214934	20.0
2-Decenal, (E)-	8.469	282.2	ng	3032680	2	8.063	214934	20.0
2,4-Decadienal,...	8.675	215.6	ng	2317100	2	8.063	214934	20.0
2,4-Decadienal,...	8.828	375.0	ng	4029710	2	8.063	214934	20.0
unknown8.845	8.845	38.1	ng	409173	2	8.063	214934	20.0
2H-Pyran, 3,4-d...	8.975	284.7	ng	2615630	3	9.822	183763	20.0
unknown9.016	9.016	443.4	ng	4073790	3	9.822	183763	20.0
(E)-Hexadec-2-enal	9.069	227.7	ng	2092150	3	9.822	183763	20.0
2(3H)-Furanone,...	9.092	62.6	ng	575365	3	9.822	183763	20.0
unknown9.386	9.386	92.2	ng	846742	3	9.822	183763	20.0
3,5-Octadien-2-one	9.610	38.7	ng	355602	3	9.822	183763	20.0
unknown9.663	9.663	76.1	ng	698951	3	9.822	183763	20.0
Silane, diethyl...	9.728	44.9	ng	412936	3	9.822	183763	20.0
Octadecanoic acid	12.645	40.0	ng	361991	5	13.963	181083	20.0