

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
 Data File : BF130203.D
 Acq On : 09 Sep 2022 19:42
 Operator : CG\JU
 Sample : N4549-02
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-47

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-BF083122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130203.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.857	92	97	102	rBV	78227	127317	2.90%	0.356%
2	4.157	312	318	323	rBV2	140969	194766	4.44%	0.544%
3	4.246	328	333	337	rBV	157441	190149	4.33%	0.531%
4	4.881	438	441	448	rVB	101702	116915	2.66%	0.327%
5	5.298	507	512	515	rBV	1777959	1783828	40.64%	4.982%
6	6.292	678	681	682	rBV	87578	75044	1.71%	0.210%
7	6.322	682	686	691	rVB	1400081	1214029	27.66%	3.390%
8	6.692	745	749	752	rBV	970621	750918	17.11%	2.097%
9	6.887	779	782	785	rVB	101886	76964	1.75%	0.215%
10	7.040	802	808	814	rBV4	49303	97079	2.21%	0.271%
11	7.134	820	824	827	rBV	105327	105022	2.39%	0.293%
12	7.204	834	836	840	rVV2	63011	57878	1.32%	0.162%
13	7.263	840	846	848	rVB	2219675	2448870	55.79%	6.839%
14	7.292	848	851	857	rVB3	62237	78936	1.80%	0.220%
15	7.351	857	861	864	rBV3	60490	68901	1.57%	0.192%
16	7.557	891	896	899	rVB4	61237	99816	2.27%	0.279%
17	7.645	903	911	915	rBV5	74640	152597	3.48%	0.426%
18	7.704	918	921	922	rBV2	46951	49809	1.13%	0.139%
19	7.787	931	935	937	rBV2	46363	49057	1.12%	0.137%
20	7.892	950	953	961	rVB2	302523	530747	12.09%	1.482%
21	7.975	961	967	970	rBV	1338198	1164639	26.53%	3.252%
22	8.069	980	983	984	rBV2	55777	57235	1.30%	0.160%
23	8.169	996	1000	1001	rBV3	78215	84103	1.92%	0.235%
24	8.222	1006	1009	1013	rBV4	205578	260457	5.93%	0.727%
25	8.322	1020	1026	1027	rBV3	117975	170081	3.87%	0.475%
26	8.357	1027	1032	1035	rVB3	164444	232276	5.29%	0.649%
27	8.392	1035	1038	1040	rBV2	55193	66288	1.51%	0.185%
28	8.451	1045	1048	1052	rVB5	162805	195522	4.45%	0.546%
29	8.510	1054	1058	1061	rBV	136936	138725	3.16%	0.387%
30	8.563	1061	1067	1071	rVB6	176251	311483	7.10%	0.870%
31	8.598	1071	1073	1077	rBV2	80331	109608	2.50%	0.306%
32	8.639	1077	1080	1084	rBV3	84104	100084	2.28%	0.280%
33	8.704	1087	1091	1095	rBV5	274989	483891	11.02%	1.351%
34	8.786	1102	1105	1106	rBV2	81121	52343	1.19%	0.146%
35	8.804	1106	1108	1110	rVB3	96460	67428	1.54%	0.188%
36	8.834	1110	1113	1115	rBV3	77896	96195	2.19%	0.269%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130203.D
Acq On : 09 Sep 2022 19:42
Operator : CG\JU
Sample : N4549-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-47

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	8.857	1115	1117	1122	rVB	205166	205377	4.68%	0.574%
38	8.922	1124	1128	1129	rBV2	158546	191677	4.37%	0.535%
39	8.957	1132	1134	1139	rVB4	67987	96836	2.21%	0.270%
40	9.010	1140	1143	1146	rBV3	183190	169683	3.87%	0.474%
41	9.051	1146	1150	1153	rVB	4835718	4389715	100.00%	12.259%
42	9.081	1153	1155	1156	rBV	75365	63492	1.45%	0.177%
43	9.098	1156	1158	1161	rVV2	207802	198056	4.51%	0.553%
44	9.133	1161	1164	1166	rVV	174063	174686	3.98%	0.488%
45	9.151	1166	1167	1171	rVV3	135320	194575	4.43%	0.543%
46	9.251	1175	1184	1187	rBV6	238020	459561	10.47%	1.283%
47	9.363	1198	1203	1204	rBV3	99242	162813	3.71%	0.455%
48	9.392	1205	1208	1211	rVV2	599351	510827	11.64%	1.427%
49	9.475	1219	1222	1225	rVB2	166266	220157	5.02%	0.615%
50	9.539	1229	1233	1234	rBV3	99413	136374	3.11%	0.381%
51	9.581	1238	1240	1241	rBV	93461	81626	1.86%	0.228%
52	9.698	1247	1260	1261	rBV	1214323	2350159	53.54%	6.563%
53	9.722	1261	1264	1273	rVB	1304018	1289392	29.37%	3.601%
54	9.792	1273	1276	1278	rBV3	85304	106528	2.43%	0.297%
55	9.875	1288	1290	1291	rBV	72474	51061	1.16%	0.143%
56	9.898	1292	1294	1298	rVB2	164796	166870	3.80%	0.466%
57	9.998	1308	1311	1313	rBV2	157047	186756	4.25%	0.522%
58	10.033	1315	1317	1319	rVV2	236868	231843	5.28%	0.647%
59	10.086	1323	1326	1328	rVV2	369919	320123	7.29%	0.894%
60	10.110	1328	1330	1332	rVB2	159994	122745	2.80%	0.343%
61	10.139	1333	1335	1336	rBV	110315	81350	1.85%	0.227%
62	10.192	1342	1344	1348	rBV2	146497	117377	2.67%	0.328%
63	10.304	1361	1363	1365	rBV2	113731	100815	2.30%	0.282%
64	10.486	1390	1394	1396	rBV	1374113	1601134	36.47%	4.471%
65	10.516	1396	1399	1402	rVB	2646547	2353101	53.60%	6.571%
66	10.639	1417	1420	1422	rBV3	167034	209226	4.77%	0.584%
67	11.045	1487	1489	1492	rBV	219345	171704	3.91%	0.480%
68	11.204	1514	1516	1520	rVB	928961	720441	16.41%	2.012%
69	11.322	1534	1536	1538	rVB	338926	255068	5.81%	0.712%
70	11.533	1570	1572	1576	rVB2	205408	193946	4.42%	0.542%
71	11.610	1582	1585	1590	rBV2	322267	429973	9.80%	1.201%
72	11.763	1608	1611	1616	rVB2	313186	327419	7.46%	0.914%
73	11.827	1619	1622	1625	rVB	497500	427254	9.73%	1.193%
74	12.045	1657	1659	1663	rVB2	270104	221362	5.04%	0.618%
75	12.539	1741	1743	1747	rVB	247763	214714	4.89%	0.600%
76	12.792	1782	1786	1793	rVB	3117764	3072536	69.99%	8.581%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130203.D
Acq On : 09 Sep 2022 19:42
Operator : CG\JU
Sample : N4549-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-47

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-BF083122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	13.833	1960	1963	1967	rVB	681074	632453	14.41%	1.766%
78	15.239	2197	2202	2206	rBV	650750	738238	16.82%	2.062%

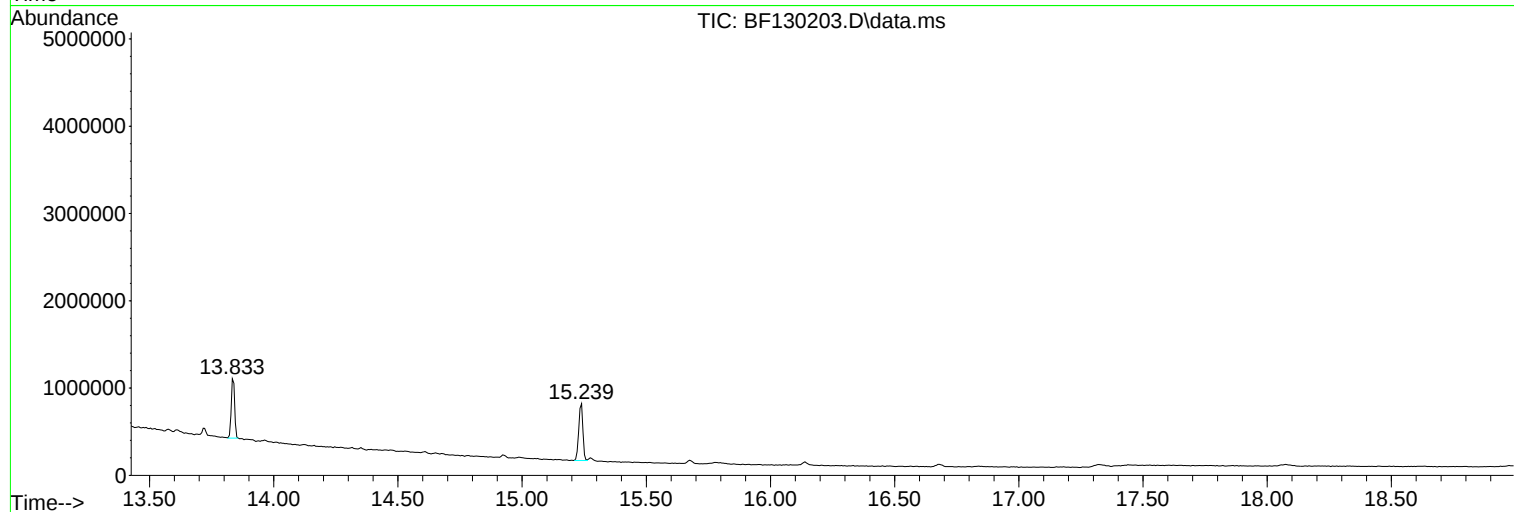
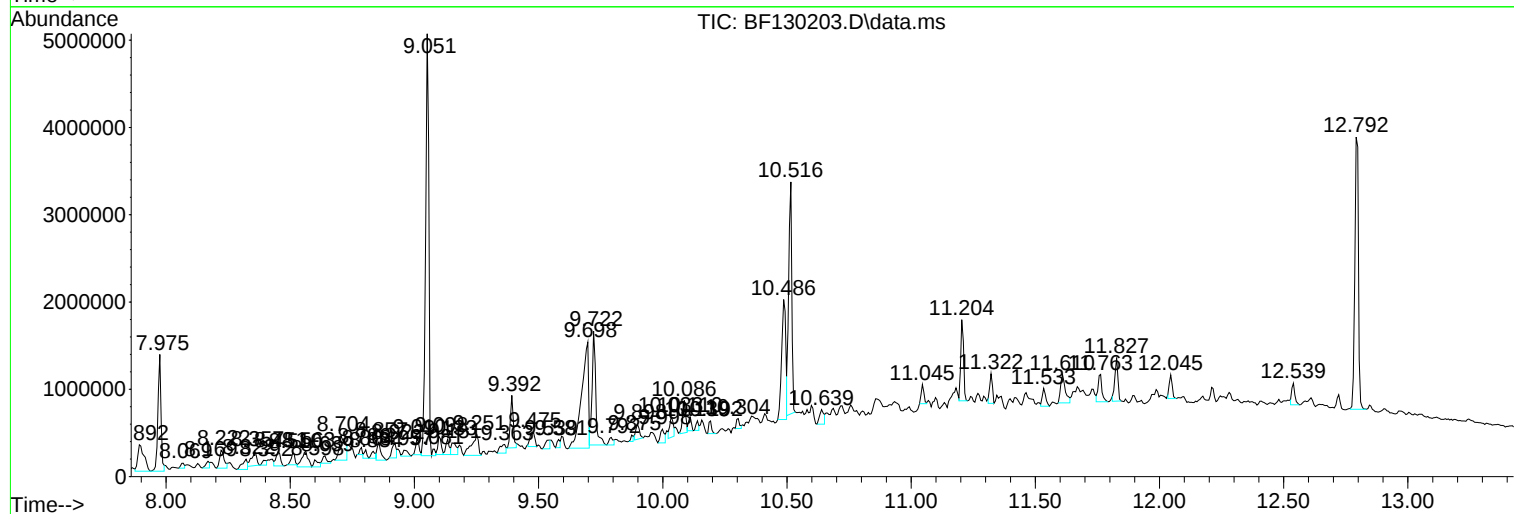
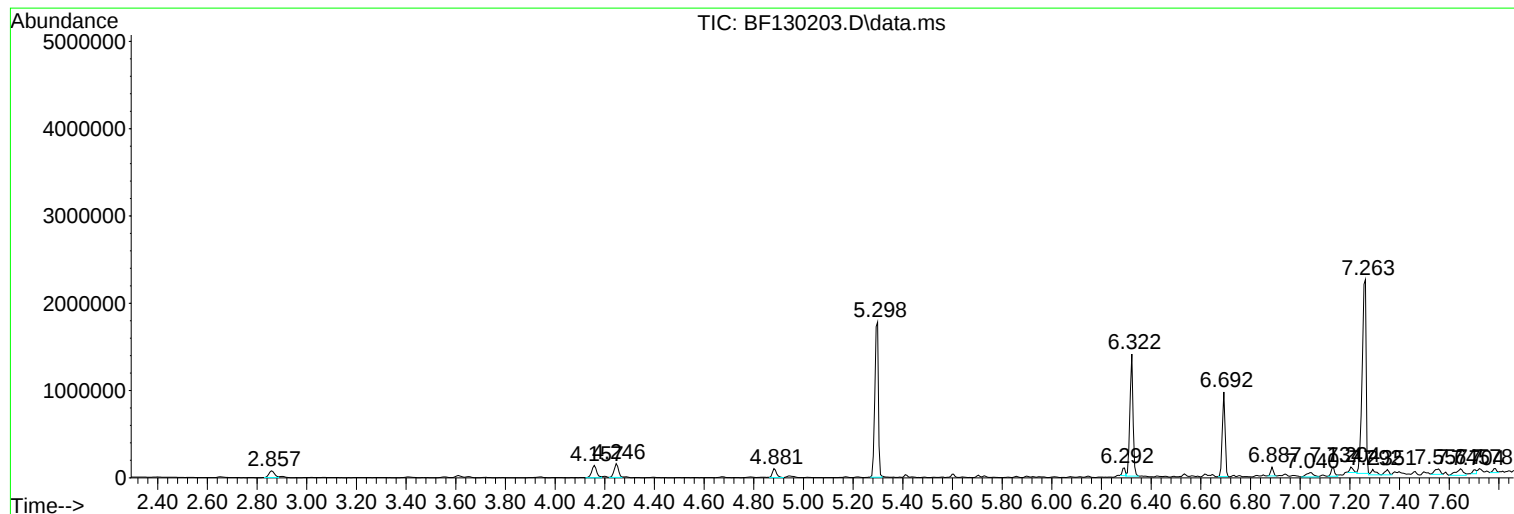
Sum of corrected areas: 35808043

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130203.D
Acq On : 09 Sep 2022 19:42
Operator : CG\JU
Sample : N4549-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-47

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.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\BF090922\
Data File : BF130203.D
Acq On : 09 Sep 2022 19:42
Operator : CG\JU
Sample : N4549-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-47

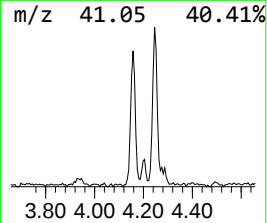
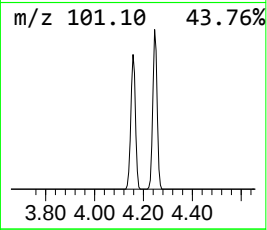
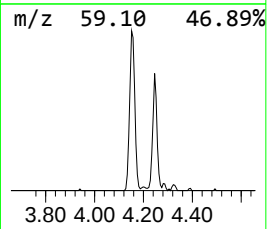
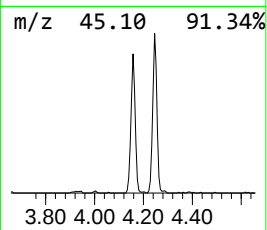
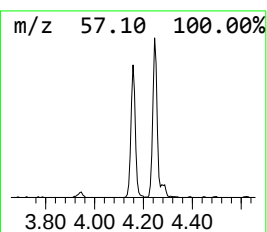
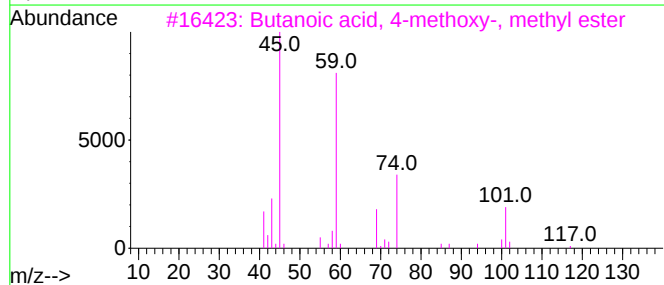
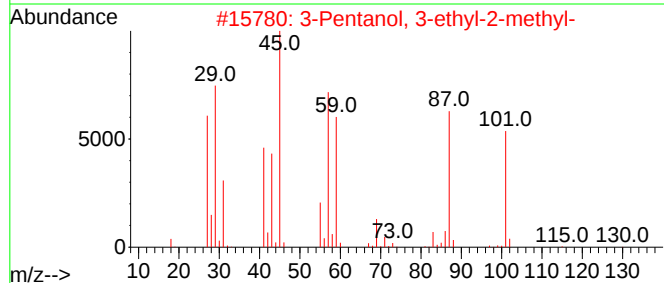
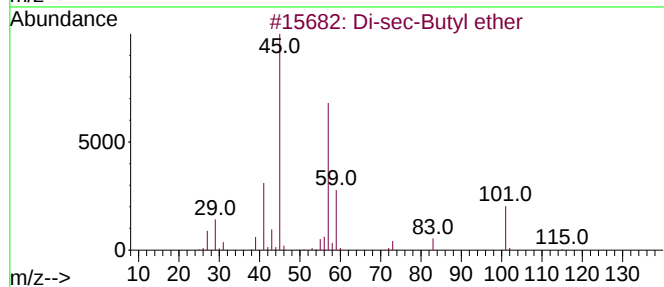
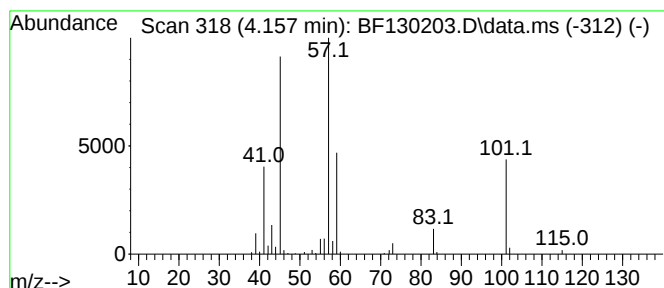
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Di-sec-Butyl ether Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.157	5.19 ng	194766	1,4-Dichlorobenzene-d4	6.692

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-sec-Butyl ether	130	C8H18O	006863-58-7	74
2			3-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	000597-05-7	72
3			Butanoic acid, 4-methoxy-, methy...	132	C6H12O3	029006-01-7	64
4			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	50
5			Ethene, (2-methoxyethoxy)-	102	C5H10O2	001663-35-0	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130203.D
Acq On : 09 Sep 2022 19:42
Operator : CG\JU
Sample : N4549-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-47

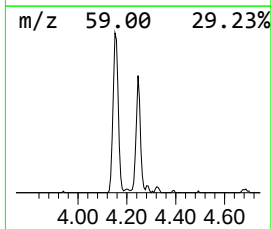
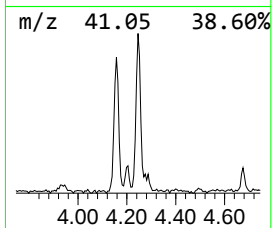
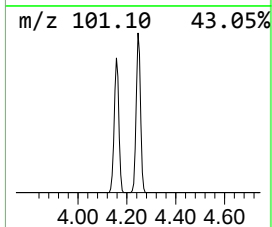
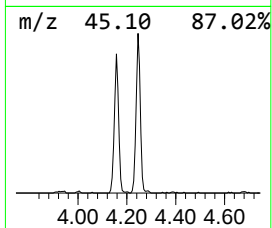
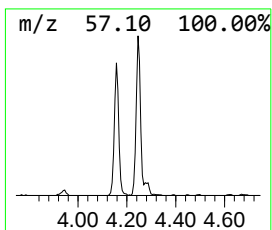
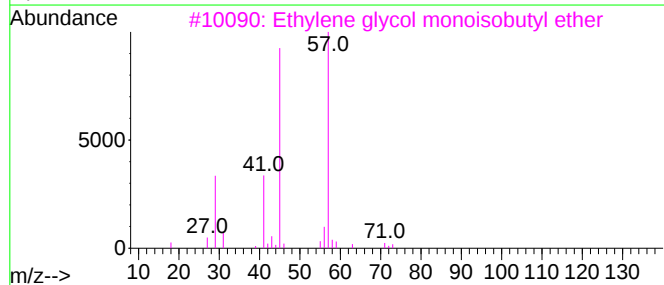
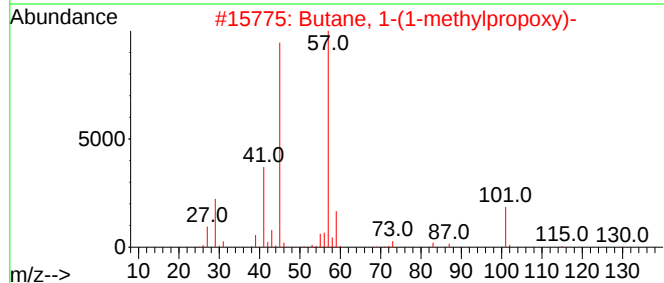
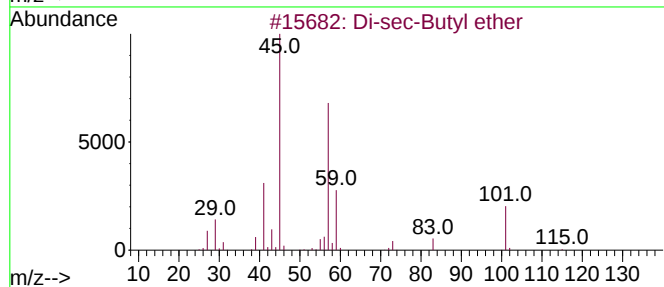
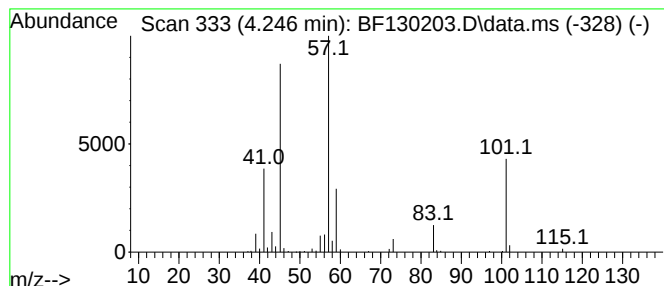
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 1-(1-methylpropoxy)- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.246	5.06 ng	190149	1,4-Dichlorobenzene-d4	6.692

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-sec-Butyl ether	130	C8H18O	006863-58-7	83
2			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	50
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	47
4			Diethyl carbitol	162	C8H18O3	000112-36-7	47
5			Boronic acid, ethyl-, diethyl ester	130	C6H15BO2	053907-92-9	36



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130203.D
Acq On : 09 Sep 2022 19:42
Operator : CG\JU
Sample : N4549-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-47

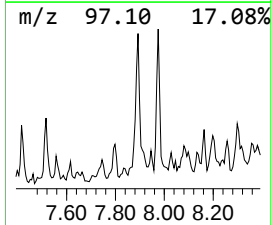
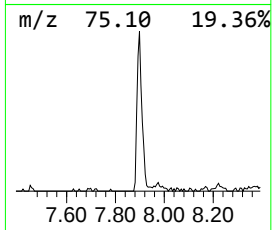
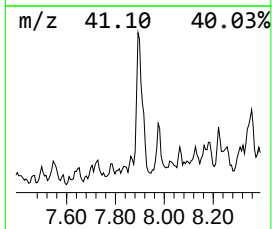
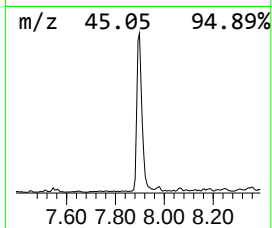
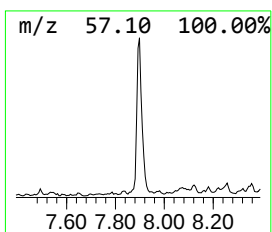
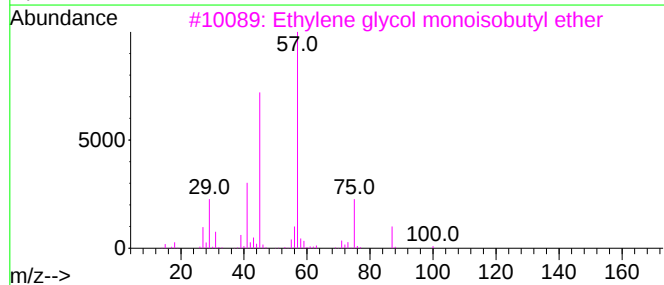
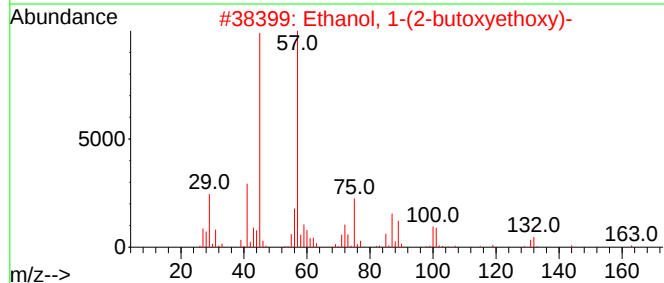
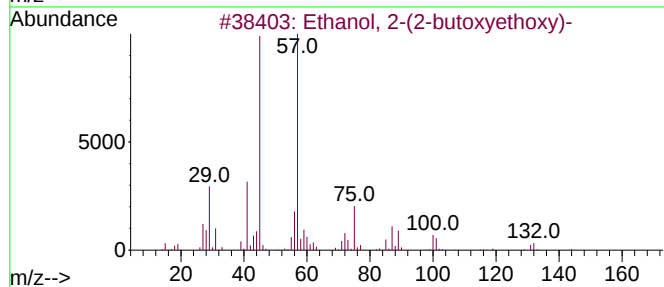
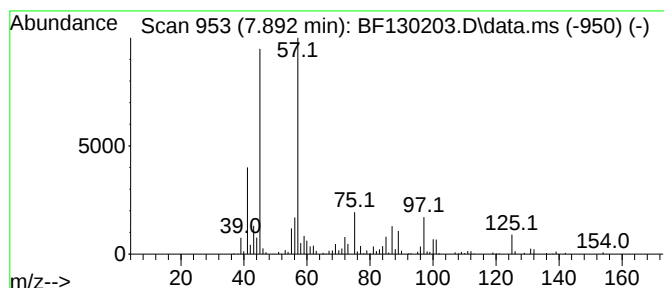
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.892	9.11 ng	530747	Naphthalene-d8	7.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	80
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	80
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	53
4			Di-sec-Butyl ether	130	C8H18O	006863-58-7	47
5			Ethane, 1-isothiocyanato-2-methoxy-	117	C4H7NOS	038663-85-3	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130203.D
Acq On : 09 Sep 2022 19:42
Operator : CG\JU
Sample : N4549-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-47

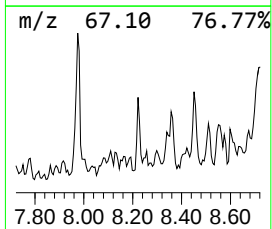
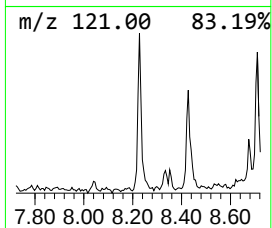
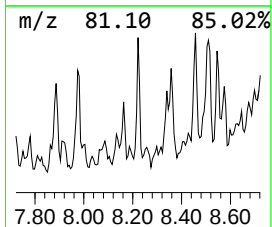
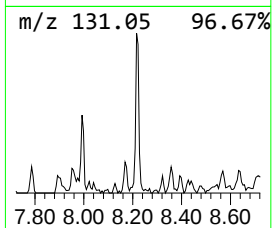
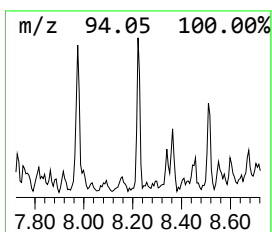
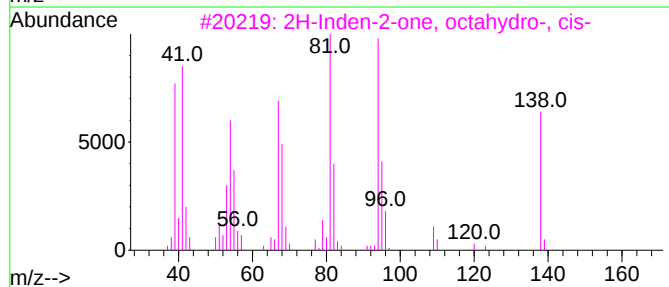
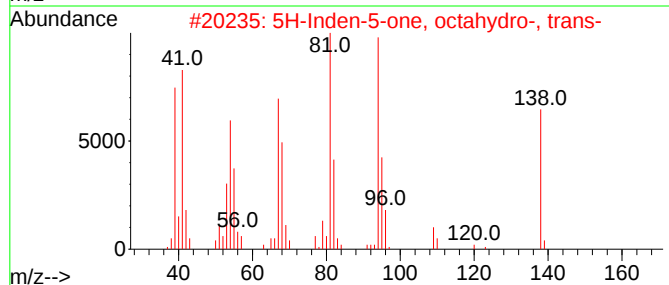
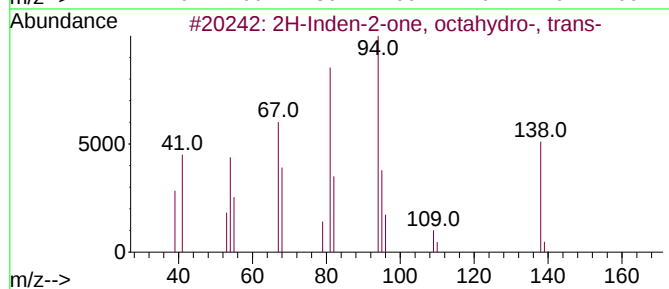
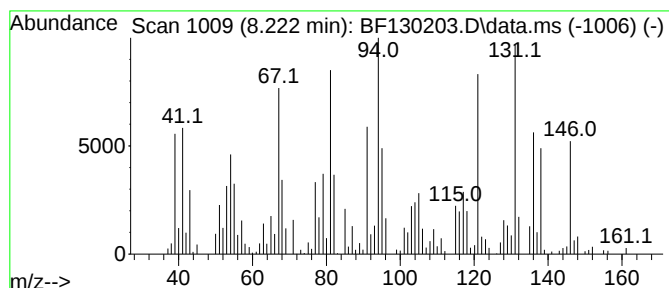
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 2H-Inden-2-one, octahydro-,... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.222	4.47 ng	260457	Naphthalene-d8	7.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2H-Inden-2-one, octahydro-, trans-	138	C9H14O	016484-17-6	70
2			5H-Inden-5-one, octahydro-, trans-	138	C9H14O	004668-81-9	64
3			2H-Inden-2-one, octahydro-, cis-	138	C9H14O	005689-04-3	62
4			2H-Inden-2-one, octahydro-	138	C9H14O	041894-93-3	45
5			Bicyclo[3.3.1]nonan-2-one	138	C9H14O	002568-17-4	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130203.D
Acq On : 09 Sep 2022 19:42
Operator : CG\JU
Sample : N4549-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-47

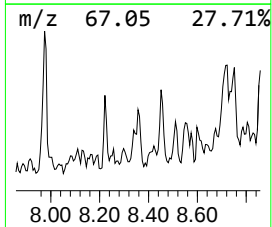
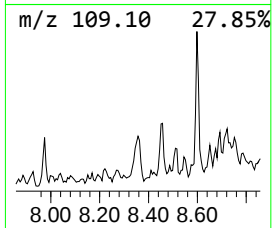
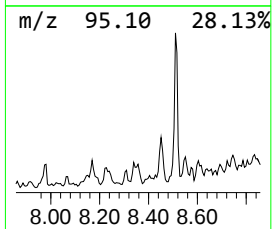
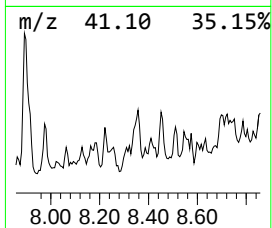
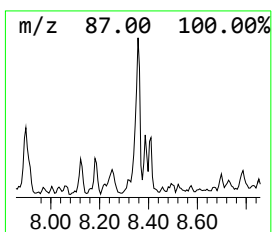
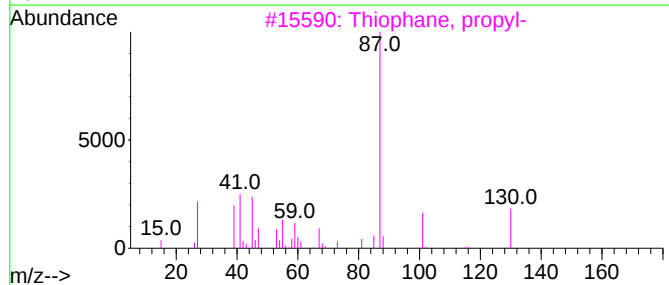
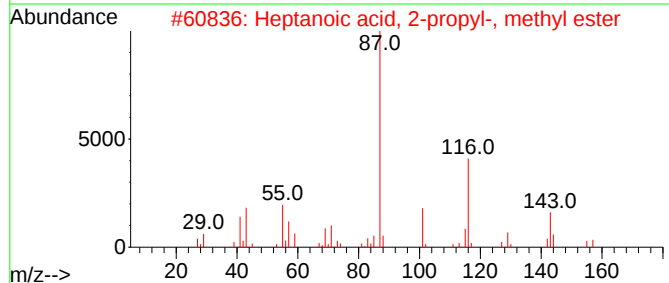
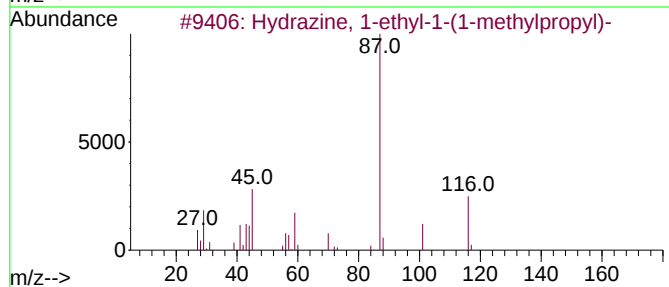
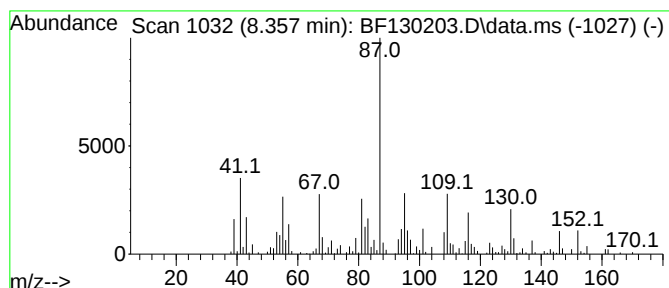
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown8.357 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.357	3.99 ng	232276	Naphthalene-d8	7.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydrazine, 1-ethyl-1-(1-methylpr...	116	C6H16N2	020325-97-7	38
2			Heptanoic acid, 2-propyl-, methy...	186	C11H22O2	056247-53-1	38
3			Thiophane, propyl-	130	C7H14S	001551-34-4	35
4			Hydrazine, 1,1-dipropyl-	116	C6H16N2	004986-50-9	35
5			Bicyclo[2.2.1]heptane-2-carboxyl...	154	C9H14O2	035520-81-1	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130203.D
Acq On : 09 Sep 2022 19:42
Operator : CG\JU
Sample : N4549-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-47

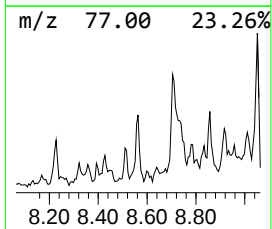
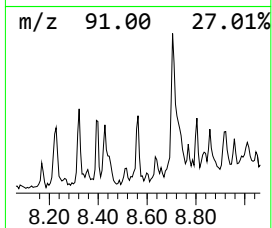
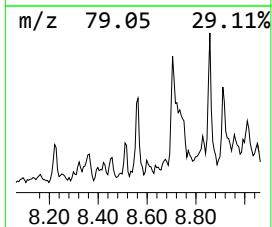
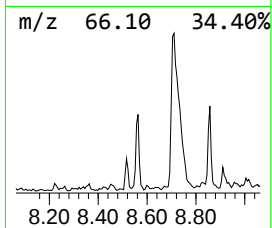
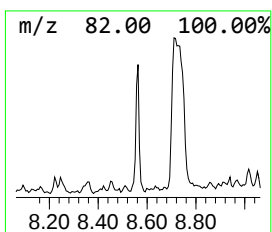
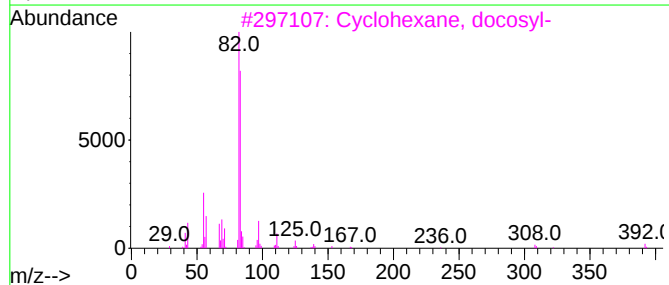
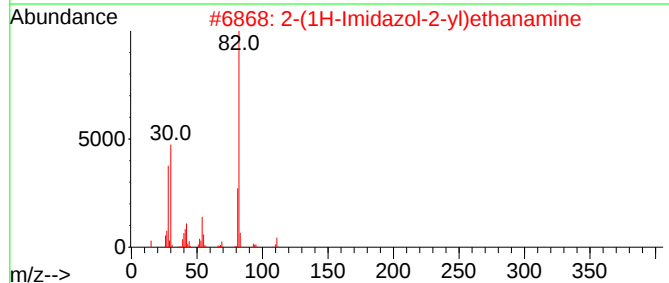
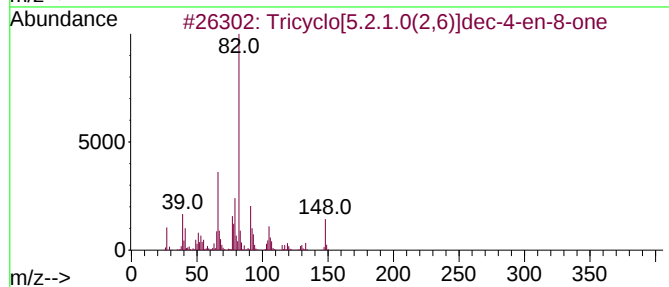
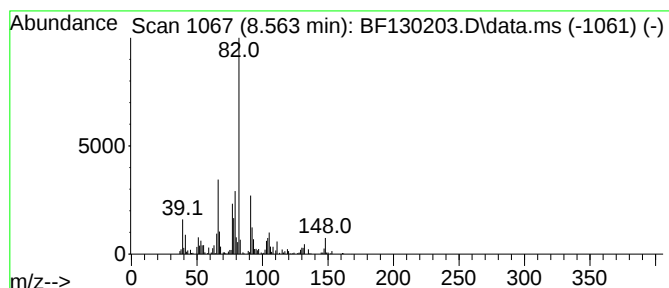
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tricyclo[5.2.1.0(2,6)]dec-4... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.563	5.35 ng	311483	Naphthalene-d8	7.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricyclo[5.2.1.0(2,6)]dec-4-en-8...	148	C10H12O	1000191-39-7	78
2			2-(1H-Imidazol-2-yl)ethanamine	111	C5H9N3	1000487-02-8	22
3			Cyclohexane, docosyl-	392	C28H56	061828-07-7	10
4			Fumaric acid, cis-hex-3-enyl hep...	436	C27H48O4	1000348-87-2	10
5			3-Hexen-1-ol, benzoate, (Z)-	204	C13H16O2	025152-85-6	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130203.D
Acq On : 09 Sep 2022 19:42
Operator : CG\JU
Sample : N4549-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-47

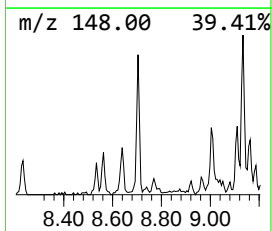
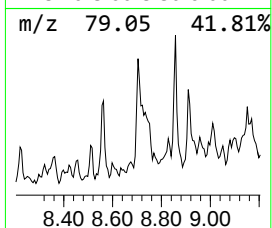
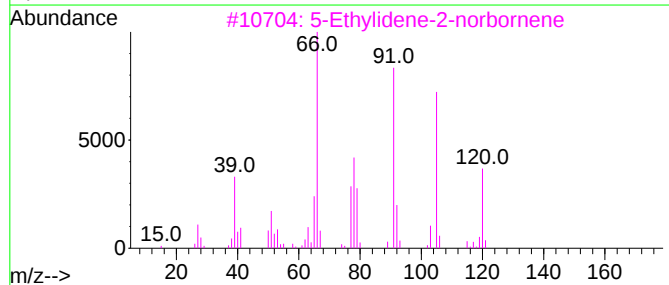
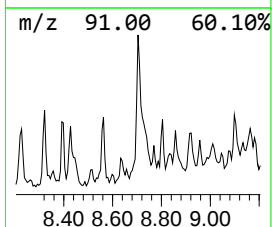
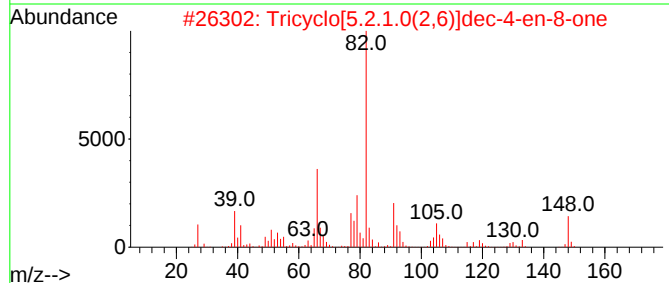
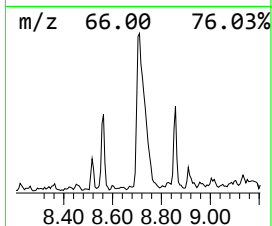
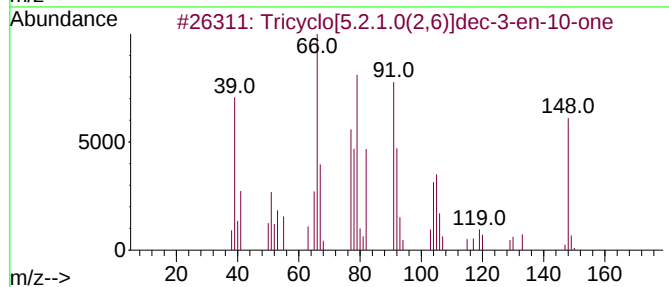
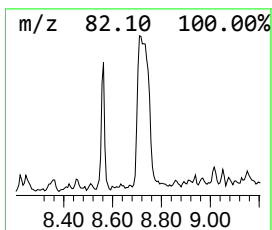
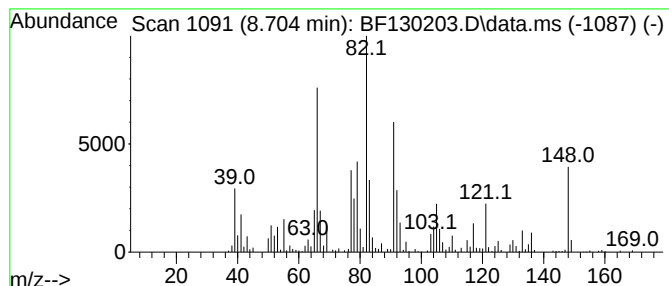
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tricyclo[5.2.1.0(2,6)]dec-3... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.704	8.31 ng	483891	Naphthalene-d8	7.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricyclo[5.2.1.0(2,6)]dec-3-en-1...	148	C10H12O	1000289-10-5	59
2			Tricyclo[5.2.1.0(2,6)]dec-4-en-8...	148	C10H12O	1000191-39-7	58
3			5-Ethylidene-2-norbornene	120	C9H12	016219-75-3	50
4			3-Hexenedinitrile	106	C6H6N2	001119-85-3	47
5			Bicyclo[3.2.0]hept-2-ene, 6-meth...	106	C8H10	038695-51-1	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130203.D
Acq On : 09 Sep 2022 19:42
Operator : CG\JU
Sample : N4549-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-47

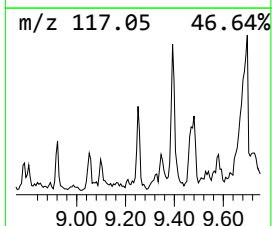
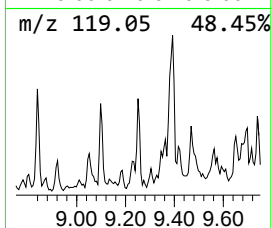
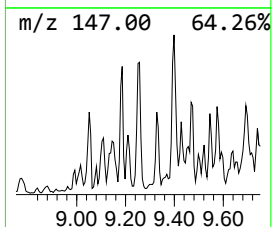
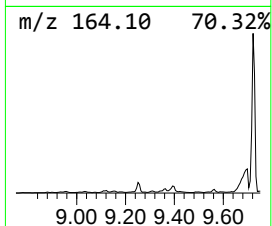
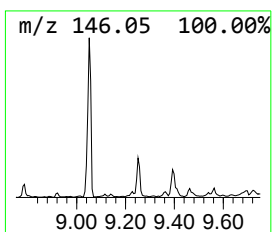
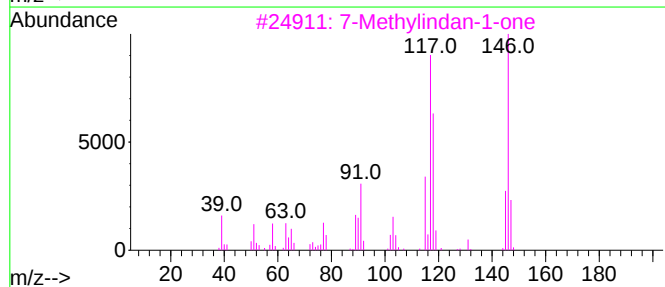
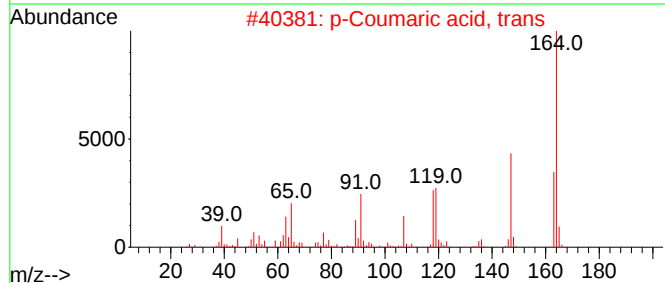
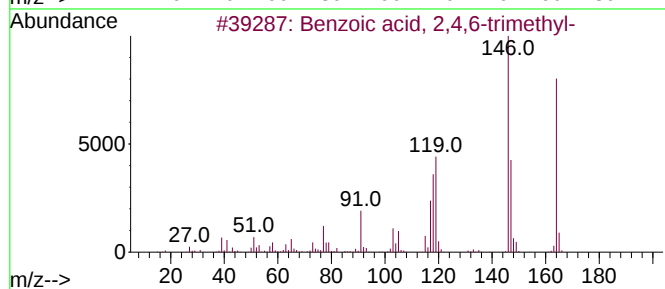
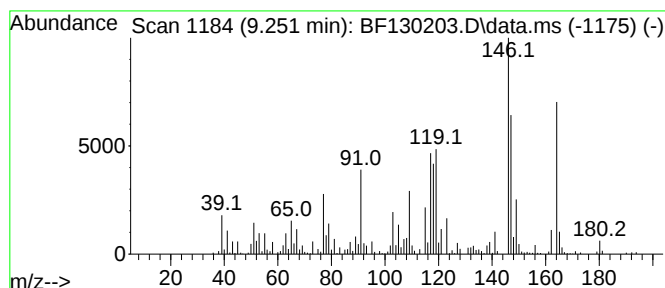
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzoic acid, 2,4,6-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.251	7.13 ng	459561	Acenaphthene-d10	9.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2,4,6-trimethyl-	164	C10H12O2	000480-63-7	76
2			p-Coumaric acid, trans	164	C9H8O3	000501-98-4	50
3			7-Methylindan-1-one	146	C10H10O	039627-61-7	49
4			Benzoic acid, 2,4,5-trimethyl-	164	C10H12O2	000528-90-5	46
5			p-Coumaric acid	164	C9H8O3	007400-08-0	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130203.D
Acq On : 09 Sep 2022 19:42
Operator : CG\JU
Sample : N4549-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

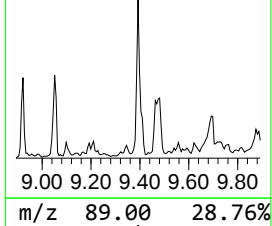
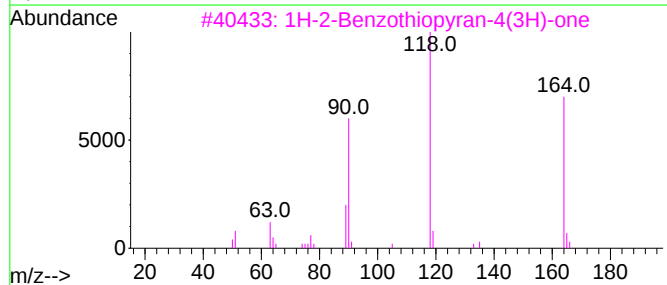
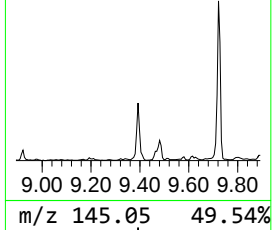
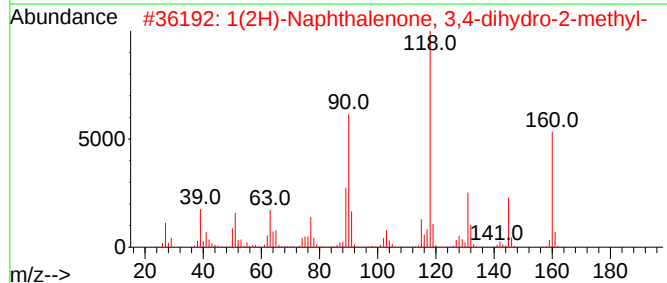
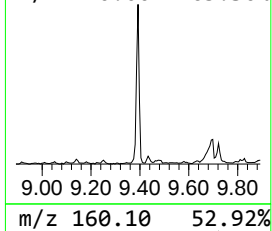
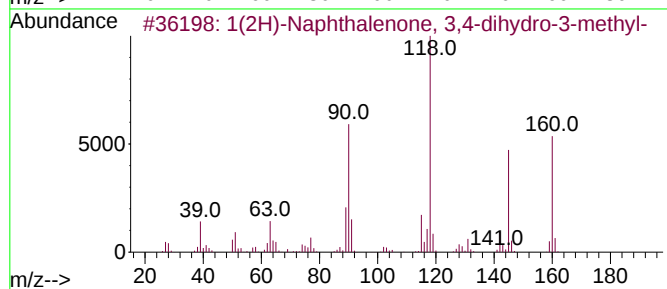
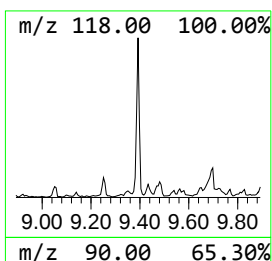
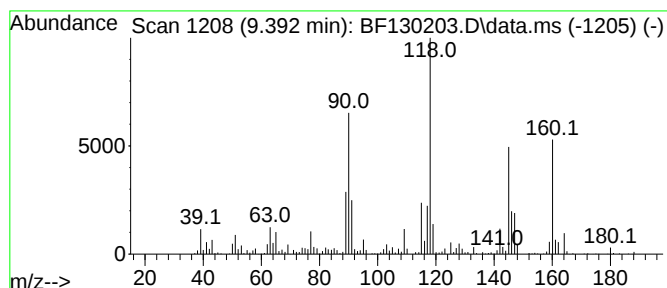
Instrument :
BNA_F
ClientSampleId :
MW-47

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1(2H)-Naphthalenone, 3,4-di... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD			R.T.
9.392	7.92 ng	510827	Acenaphthene-d10			9.722
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1(2H)-Naphthalenone, 3,4-dihydro...		160	C11H12O	014944-23-1	91
2	1(2H)-Naphthalenone, 3,4-dihydro...		160	C11H12O	001590-08-5	70
3	1H-2-Benzothiopyran-4(3H)-one		164	C9H8OS	004426-76-0	50
4	Naphthalene, 1,2,3,4-tetrahydro-...		160	C12H16	007524-63-2	49
5	Coumarin		146	C9H6O2	000091-64-5	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130203.D
Acq On : 09 Sep 2022 19:42
Operator : CG\JU
Sample : N4549-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-47

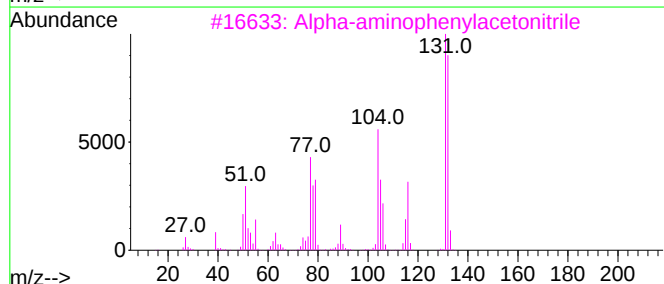
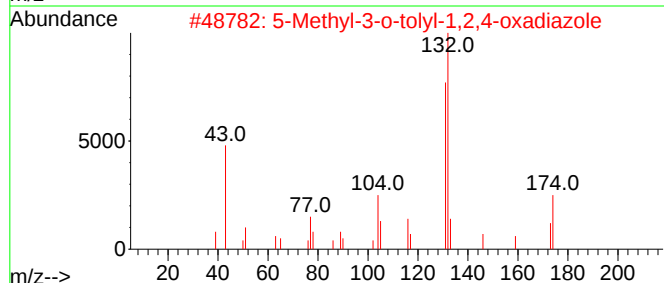
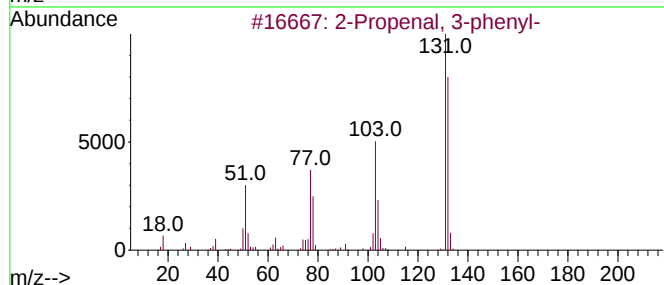
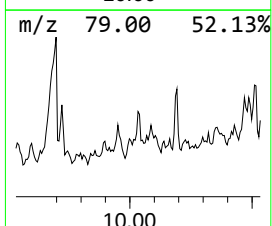
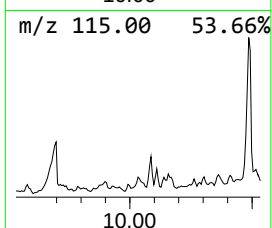
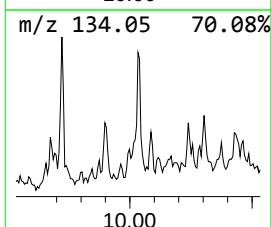
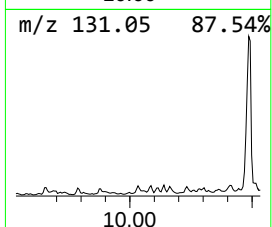
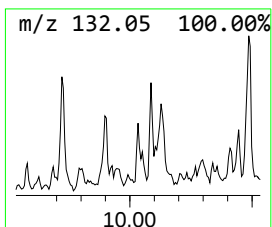
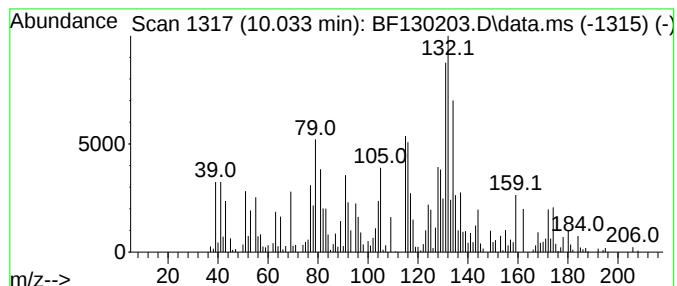
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown10.033 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.033	3.60 ng	231843	Acenaphthene-d10	9.722

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propenal, 3-phenyl-	132	C9H8O	000104-55-2	42
2		5-Methyl-3-o-tolyl-1,2,4-oxadiazole	174	C10H10N2O	087944-75-0	38
3		Alpha-aminophenylacetonitrile	132	C8H8N2	016750-42-8	35
4		1H-Indazole, 3-methyl-	132	C8H8N2	1000316-00-2	30
5		5-Methylbenzimidazole	132	C8H8N2	000614-97-1	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130203.D
Acq On : 09 Sep 2022 19:42
Operator : CG\JU
Sample : N4549-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

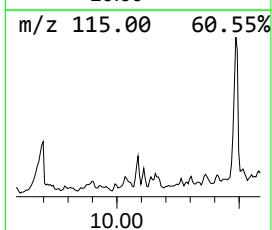
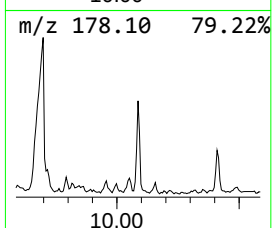
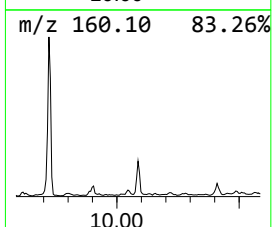
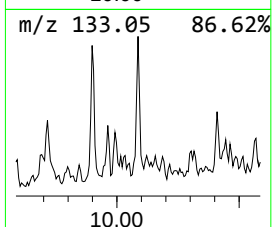
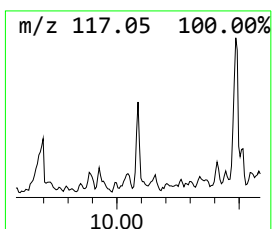
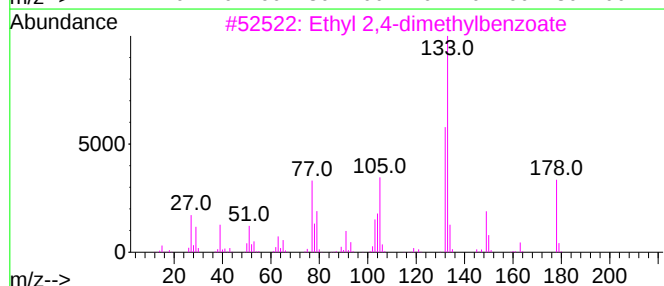
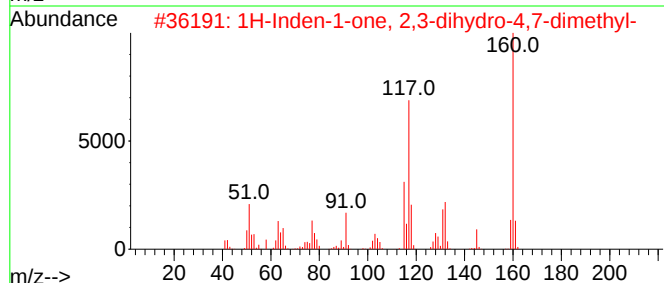
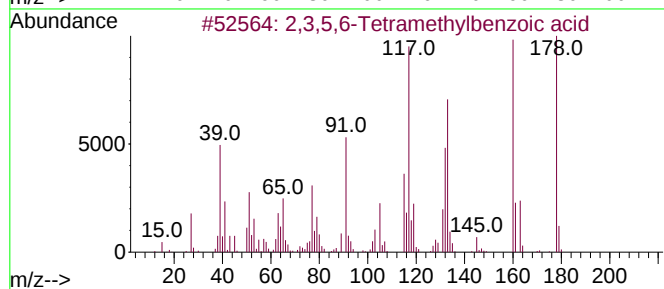
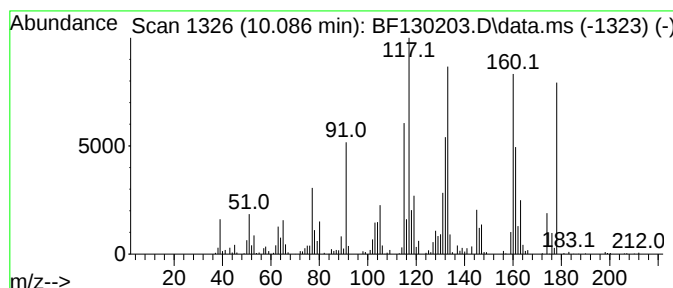
Instrument :
BNA_F
ClientSampleId :
MW-47

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2,3,5,6-Tetramethylbenzoic ... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD			R.T.
10.086	4.97 ng	320123	Acenaphthene-d10			9.722
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,3,5,6-Tetramethylbenzoic acid		178	C11H14O2	002604-45-7	93
2	1H-Inden-1-one, 2,3-dihydro-4,7-...		160	C11H12O	005037-60-5	46
3	Ethyl 2,4-dimethylbenzoate		178	C11H14O2	033499-42-2	42
4	1H-Inden-1-one, 2,3-dihydro-5,7-...		160	C11H12O	006682-69-5	38
5	2,4-Dimethylstyrene		132	C10H12	002234-20-0	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130203.D
Acq On : 09 Sep 2022 19:42
Operator : CG\JU
Sample : N4549-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

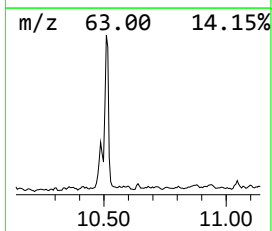
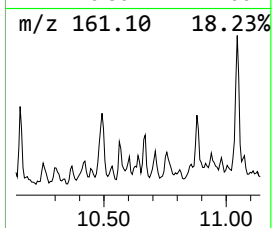
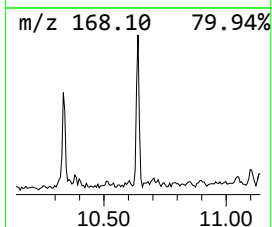
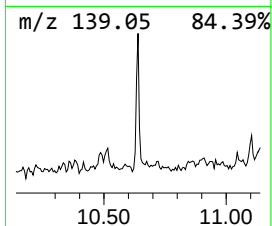
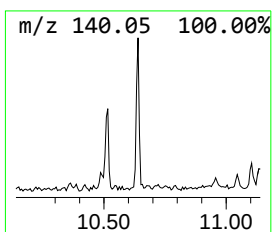
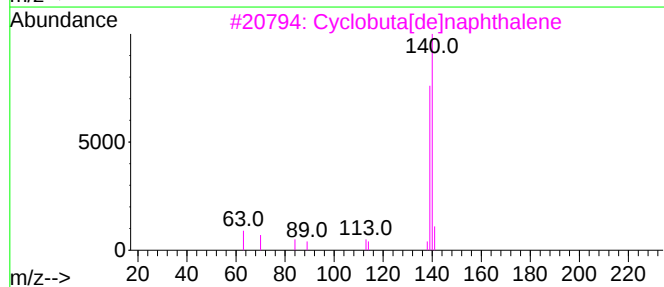
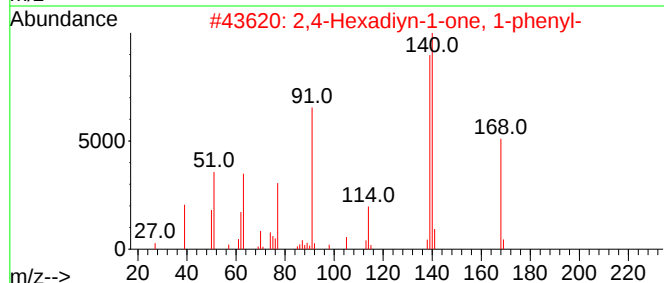
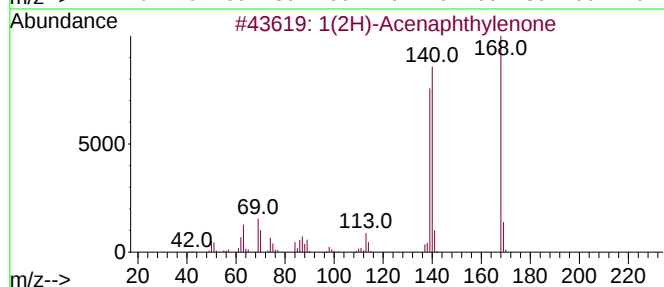
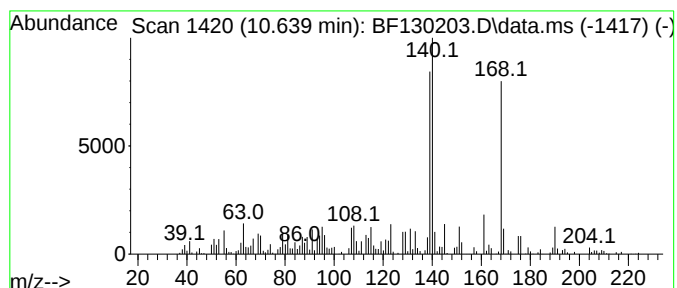
Instrument :
BNA_F
ClientSampleId :
MW-47

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1(2H)-Acenaphthylenone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.639	5.81 ng	209226	Phenanthrene-d10		11.204	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1(2H)-Acenaphthylenone		168	C12H8O	002235-15-6	90
2	2,4-Hexadiyn-1-one, 1-phenyl-		168	C12H8O	000495-74-9	74
3	Cyclobuta[de]naphthalene		140	C11H8	024973-91-9	55
4	1H-Inden-1-one, 4,7-difluoro-2,3...		168	C9H6F2O	130408-16-1	50
5	Benzene, 1,3,5-trimethoxy-		168	C9H12O3	000621-23-8	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130203.D
Acq On : 09 Sep 2022 19:42
Operator : CG\JU
Sample : N4549-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-47

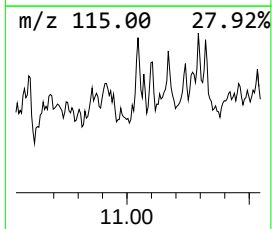
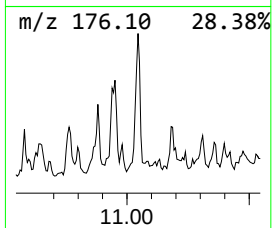
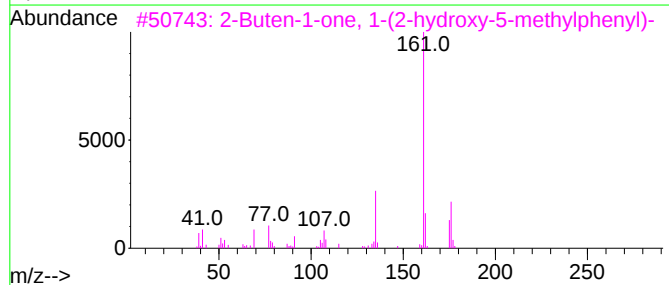
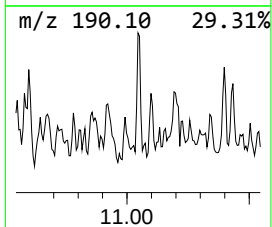
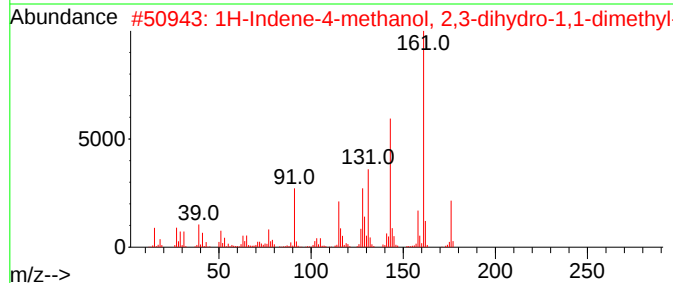
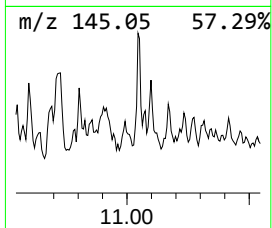
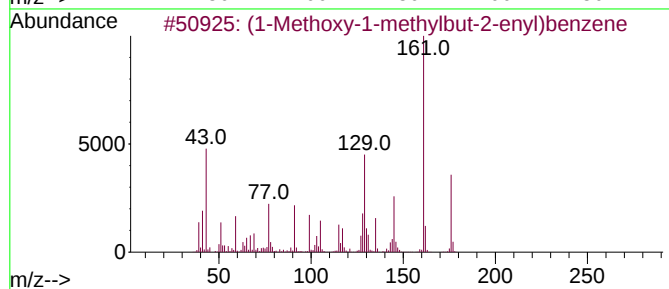
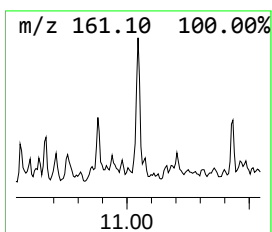
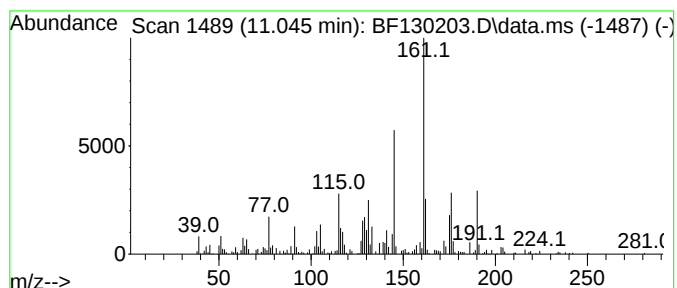
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 (1-Methoxy-1-methylbut-2-en... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.045	4.77 ng	171704	Phenanthrene-d10	11.204

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		(1-Methoxy-1-methylbut-2-enyl)be...	176	C12H16O	1000211-11-5	53
2		1H-Indene-4-methanol, 2,3-dihydr...	176	C12H16O	055591-09-8	46
3		2-Buten-1-one, 1-(2-hydroxy-5-me...	176	C11H12O2	005631-63-0	38
4		Benzene, 2-methyl-1,4-bis(1-meth...	176	C13H20	058502-85-5	38
5		Benzofuran, 2,3-dihydro-2,2,5,6-...	176	C12H16O	063577-97-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130203.D
Acq On : 09 Sep 2022 19:42
Operator : CG\JU
Sample : N4549-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-47

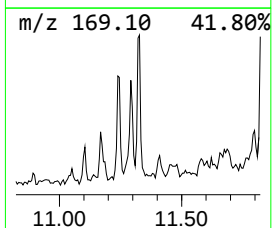
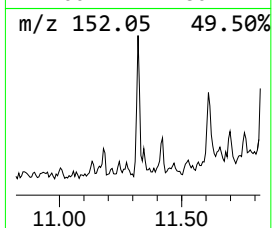
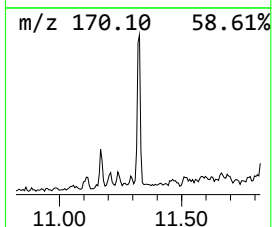
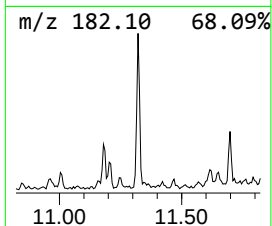
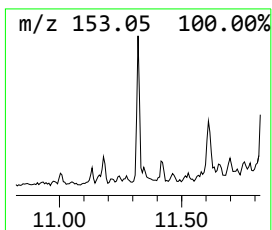
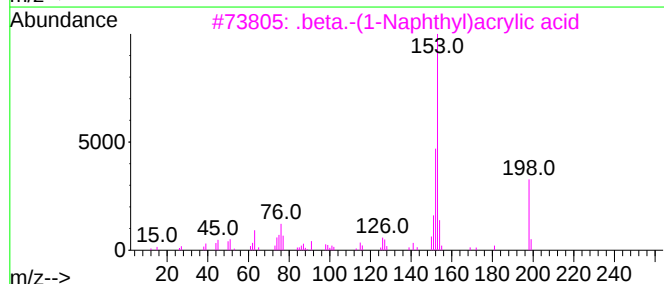
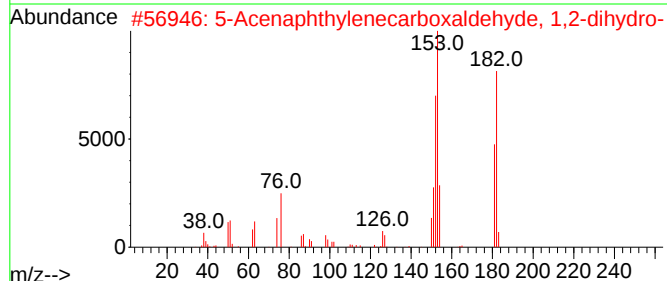
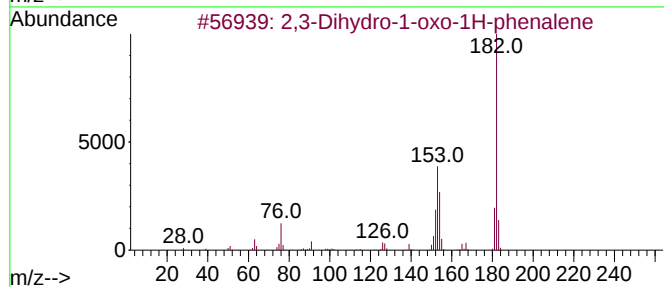
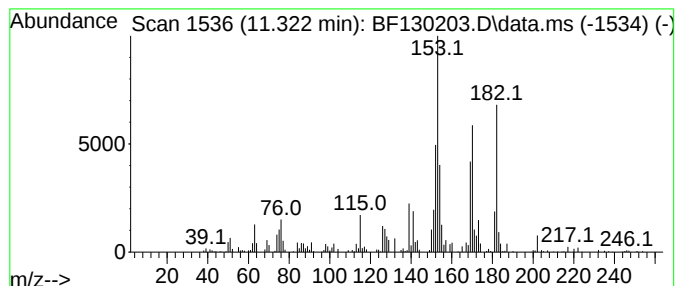
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 2,3-Dihydro-1-oxo-1H-phenalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.322	7.08 ng	255068	Phenanthrene-d10	11.204

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Dihydro-1-oxo-1H-phenalene	182	C13H10O	000518-85-4	70	
2	5-Acenaphthylenecarboxaldehyde, ...	182	C13H10O	1000362-64-3	60	
3	.beta.-(1-Naphthyl)acrylic acid	198	C13H10O2	013026-12-5	35	
4	2-(methylamino)-5,6-dihydro-1,3-...	182	C8H10N2OS	1000285-58-7	30	
5	[1,1'-Biphenyl]-4-carboxaldehyde	182	C13H10O	003218-36-8	25	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130203.D
Acq On : 09 Sep 2022 19:42
Operator : CG\JU
Sample : N4549-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

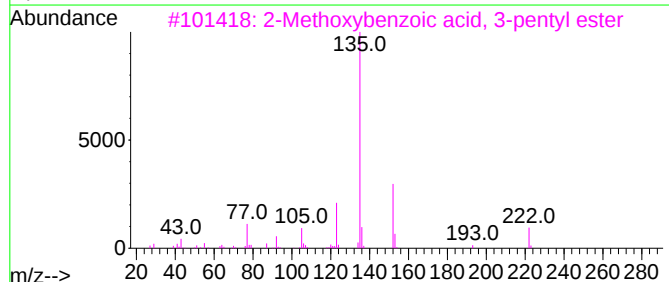
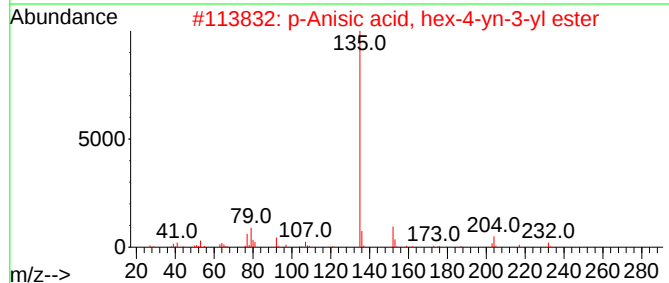
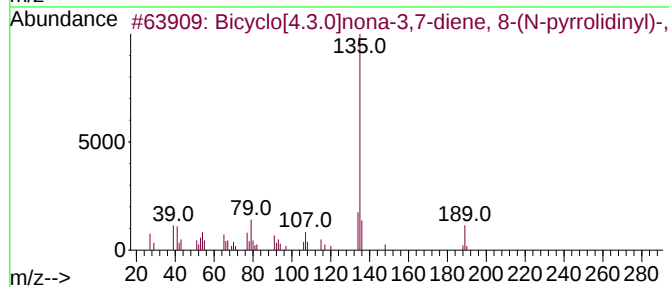
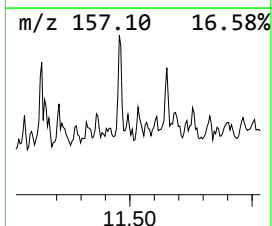
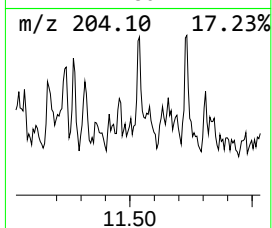
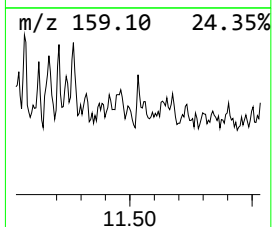
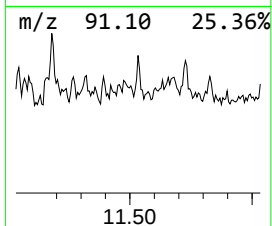
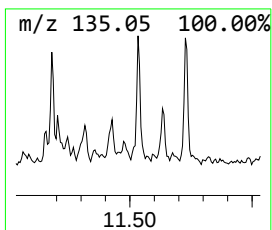
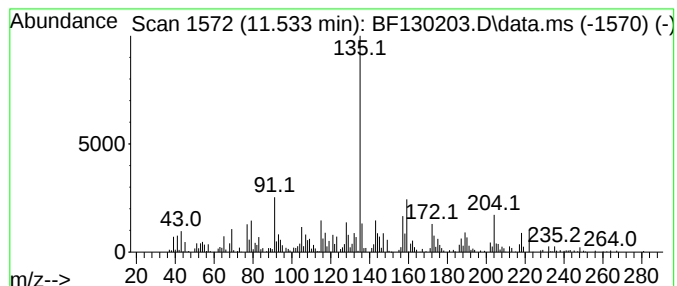
Instrument :
BNA_F
ClientSampleId :
MW-47

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown11.533 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.533	5.38 ng	193946	Phenanthrene-d10	11.204	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[4.3.0]nona-3,7-diene, 8-...	189	C13H19N	1000137-75-8	49
2	p-Anisic acid, hex-4-yn-3-yl ester	232	C14H16O3	1000299-19-4	49
3	2-Methoxybenzoic acid, 3-pentyl ...	222	C13H18O3	1000325-58-0	49
4	2-tert-Butylphenol, 0-ethoxycarb...	222	C13H18O3	1000487-37-8	46
5	1-n-Pentyladamantane	206	C15H26	050782-11-1	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130203.D
Acq On : 09 Sep 2022 19:42
Operator : CG\JU
Sample : N4549-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

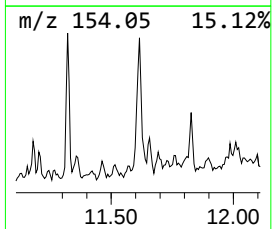
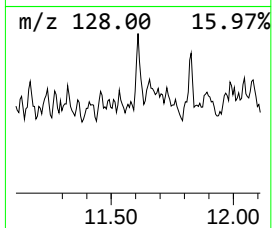
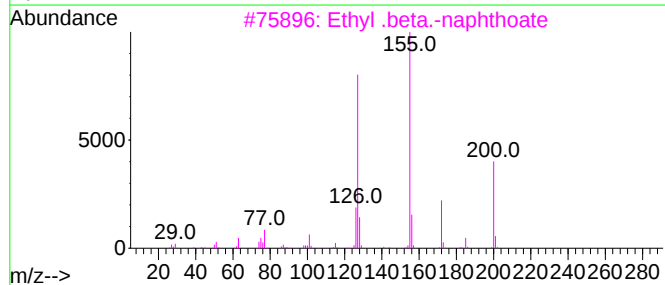
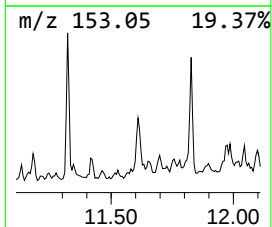
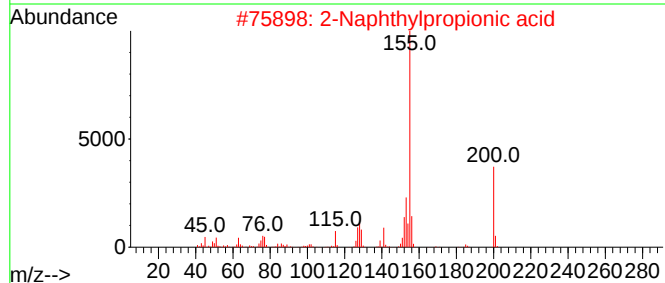
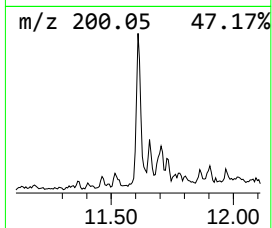
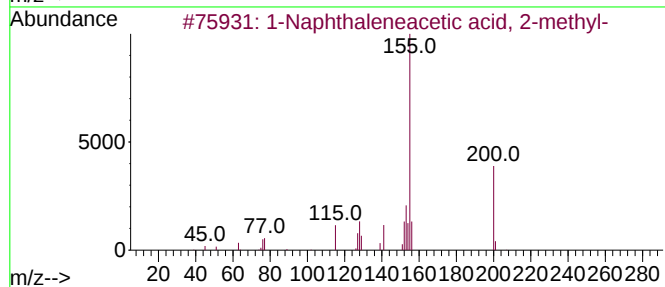
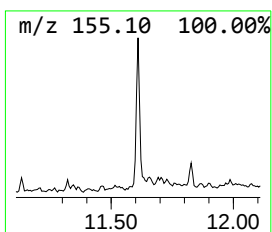
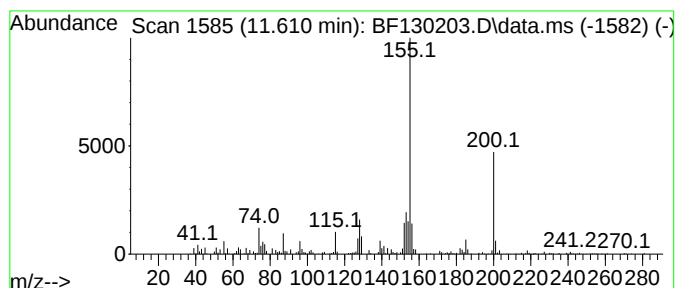
Instrument :
BNA_F
ClientSampleId :
MW-47

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 1-Naphthaleneacetic acid, 2... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.610	11.94 ng	429973	Phenanthrene-d10	11.204
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		1-Naphthaleneacetic acid, 2-methyl-	200 C13H12O2	000085-08-5 93
2		2-Naphthylpropionic acid	200 C13H12O2	1000129-24-1 72
3		Ethyl .beta.-naphthoate	200 C13H12O2	003007-91-8 64
4		1-Naphthalenecarboxylic acid, et...	200 C13H12O2	003007-97-4 59
5		Formic acid, (4-chloro-2-methoxy...	200 C9H9ClO3	1000368-24-1 59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130203.D
Acq On : 09 Sep 2022 19:42
Operator : CG\JU
Sample : N4549-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

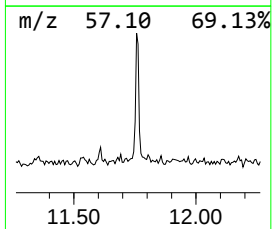
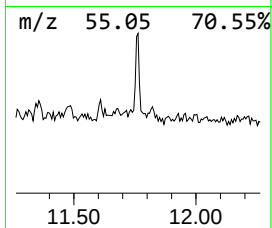
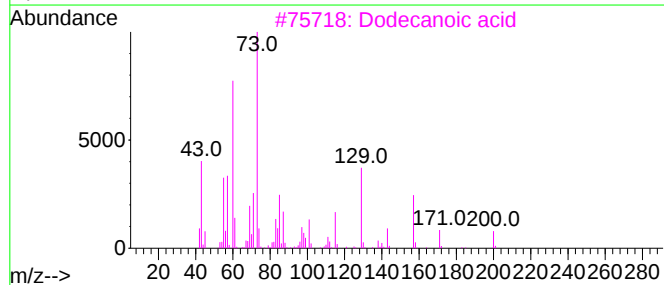
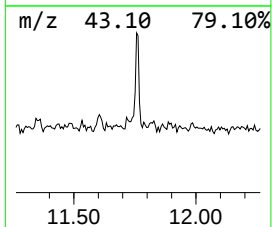
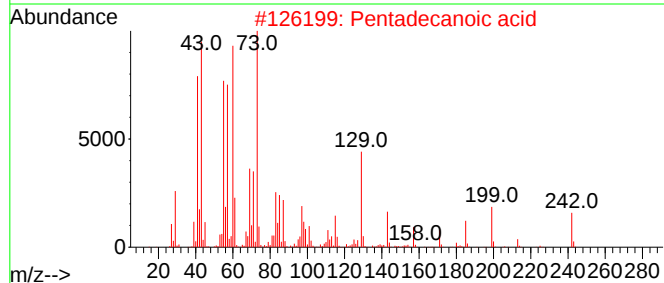
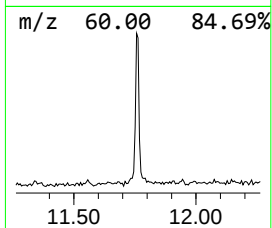
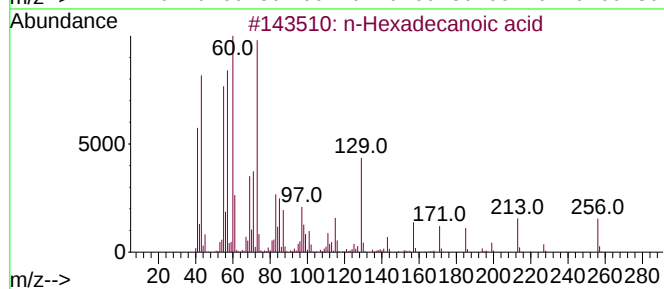
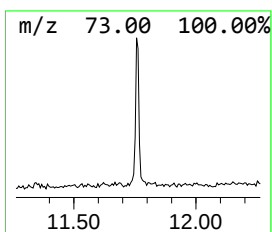
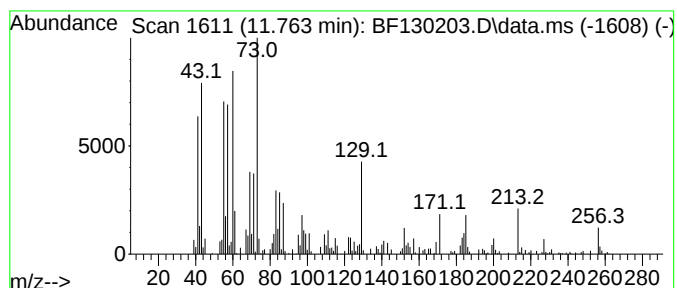
Instrument :
BNA_F
ClientSampleId :
MW-47

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.763	9.09 ng	327419	Phenanthrene-d10	11.204	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3	Dodecanoic acid	200	C12H24O2	000143-07-7	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Tridecanoic acid	214	C13H26O2	000638-53-9	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130203.D
Acq On : 09 Sep 2022 19:42
Operator : CG\JU
Sample : N4549-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

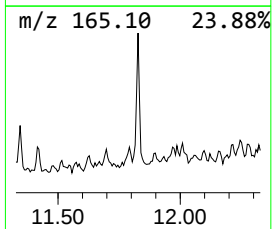
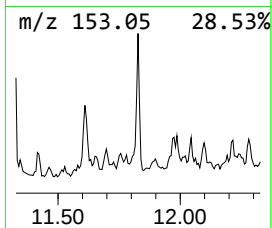
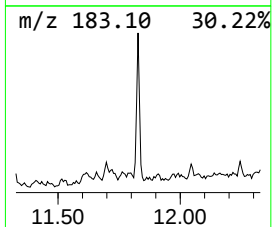
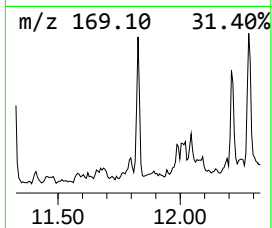
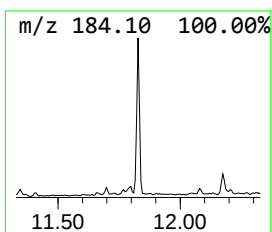
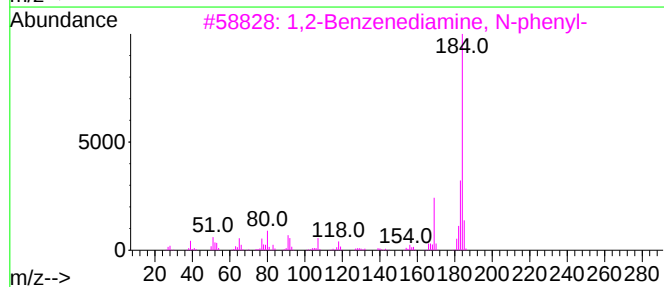
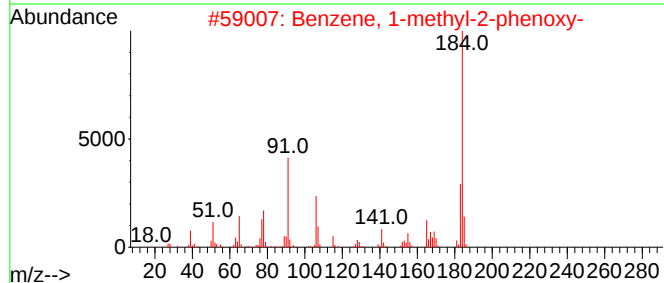
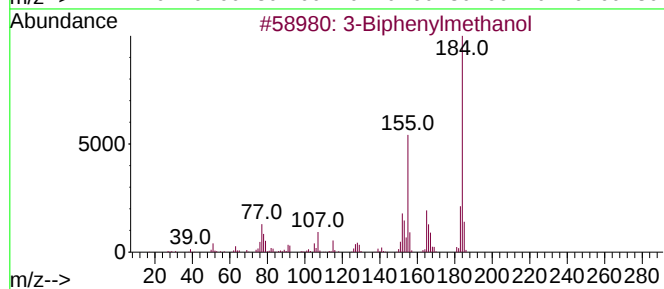
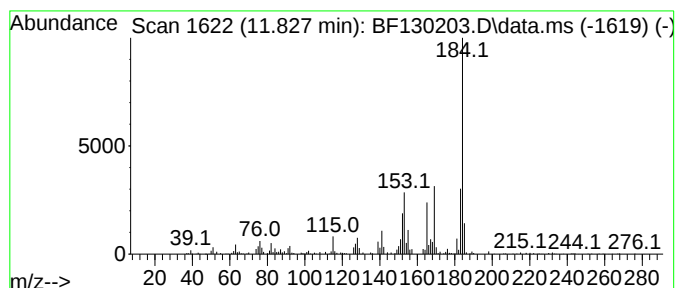
Instrument :
BNA_F
ClientSampleId :
MW-47

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 3-Biphenylmethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.827	11.86 ng	427254	Phenanthrene-d10	11.204
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		3-Biphenylmethanol	184 C13H12O	069605-90-9 68
2		Benzene, 1-methyl-2-phenoxy-	184 C13H12O	003991-61-5 62
3		1,2-Benzenediamine, N-phenyl-	184 C12H12N2	000534-85-0 52
4		6-Cyano-5-methoxyquinoline	184 C11H8N2O	1000241-27-7 49
5		[1,1'-Biphenyl]-2,2'-diamine	184 C12H12N2	001454-80-4 49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130203.D
Acq On : 09 Sep 2022 19:42
Operator : CG\JU
Sample : N4549-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

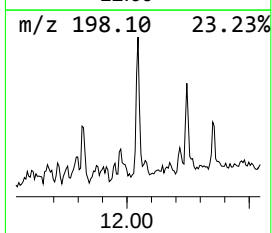
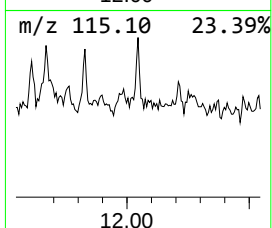
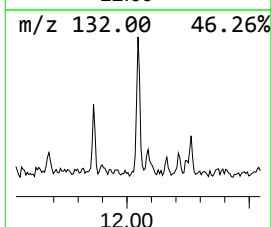
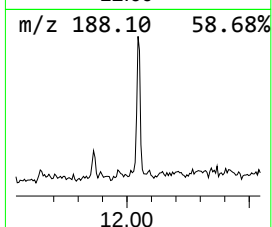
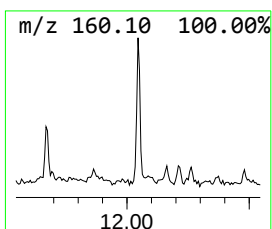
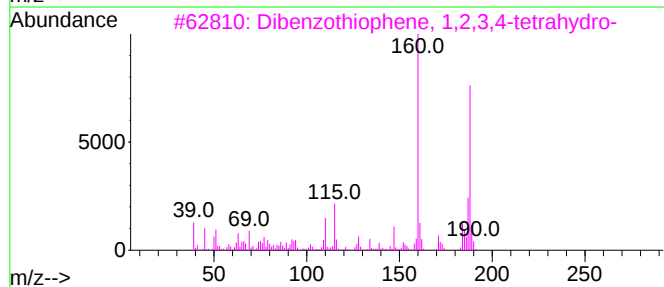
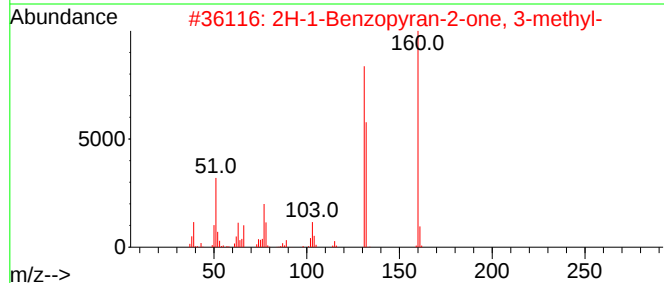
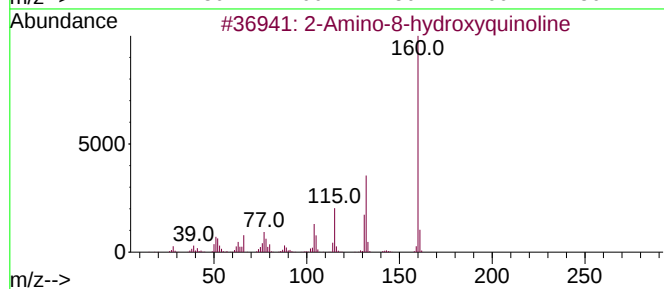
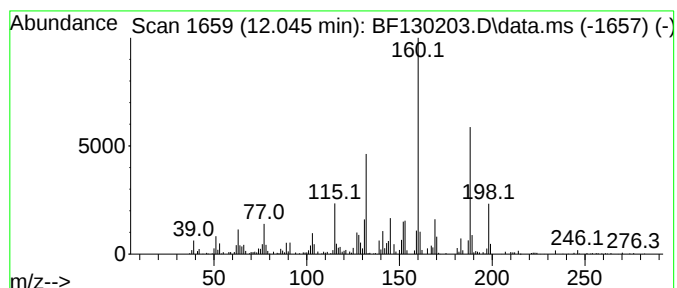
Instrument :
BNA_F
ClientSampleId :
MW-47

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 2-Amino-8-hydroxyquinoline Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.045	6.15 ng	221362	Phenanthrene-d10	11.204
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		2-Amino-8-hydroxyquinoline	160 C9H8N2O	070125-16-5 55
2		2H-1-Benzopyran-2-one, 3-methyl-	160 C10H8O2	002445-82-1 55
3		Dibenzothiophene, 1,2,3,4-tetrahydro-	188 C12H12S	016587-33-0 46
4		1,4-Methanonaphthalen-6-ol, 1,2,3,4-tetrahydro-	160 C11H12O	050838-54-5 46
5		2-Dibenzofuranol, 6,7,8,9-tetrahydro-	188 C12H12O2	001133-79-5 43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130203.D
Acq On : 09 Sep 2022 19:42
Operator : CG\JU
Sample : N4549-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-47

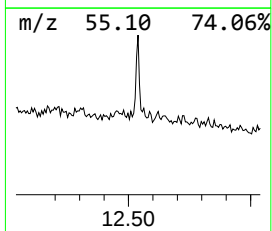
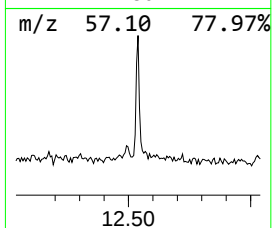
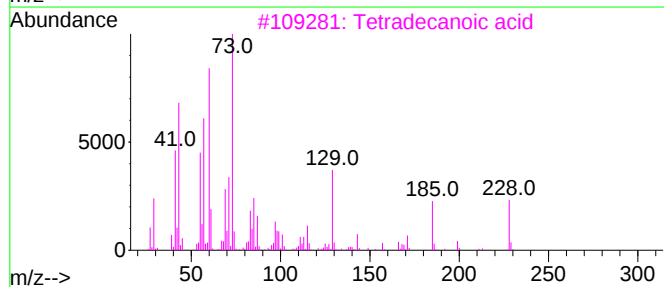
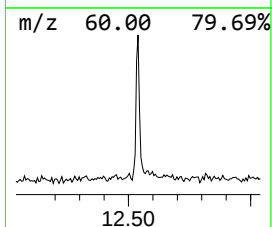
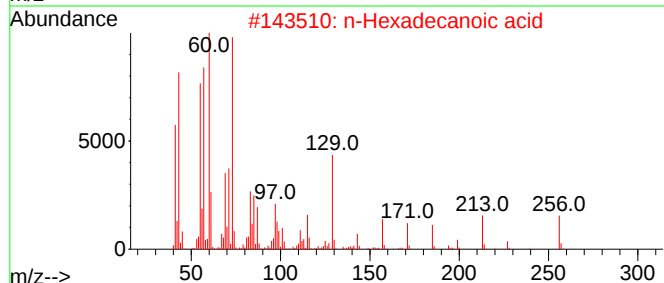
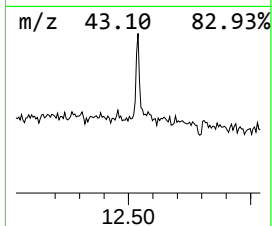
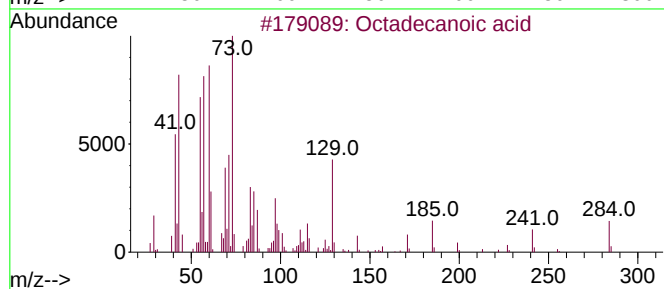
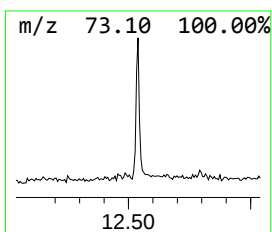
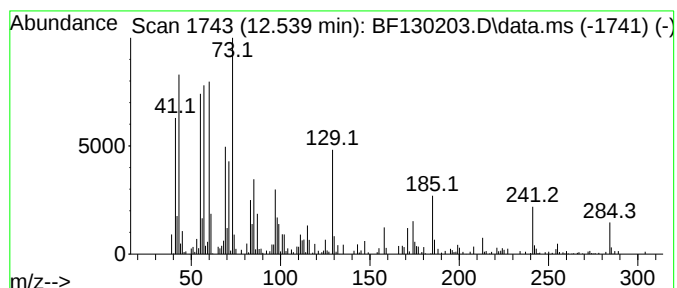
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.539	6.79 ng	214714	Chrysene-d12	13.833

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	95
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	70
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130203.D
Acq On : 09 Sep 2022 19:42
Operator : CG\JU
Sample : N4549-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-47

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.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
Di-sec-Butyl ether	4.157	5.2	ng	194766	1	6.692	750918	20.0
Butane, 1-(1-me...	4.246	5.1	ng	190149	1	6.692	750918	20.0
Ethanol, 2-(2-b...	7.892	9.1	ng	530747	2	7.975	1164640	20.0
2H-Inden-2-one,...	8.222	4.5	ng	260457	2	7.975	1164640	20.0
unknown8.357	8.357	4.0	ng	232276	2	7.975	1164640	20.0
Tricyclo[5.2.1....	8.563	5.3	ng	311483	2	7.975	1164640	20.0
Tricyclo[5.2.1....	8.704	8.3	ng	483891	2	7.975	1164640	20.0
Benzoic acid, 2...	9.251	7.1	ng	459561	3	9.722	1289390	20.0
1(2H)-Naphthale...	9.392	7.9	ng	510827	3	9.722	1289390	20.0
unknown10.033	10.033	3.6	ng	231843	3	9.722	1289390	20.0
2,3,5,6-Tetrame...	10.086	5.0	ng	320123	3	9.722	1289390	20.0
1(2H)-Acenaphth...	10.639	5.8	ng	209226	4	11.204	720441	20.0
(1-Methoxy-1-me...	11.045	4.8	ng	171704	4	11.204	720441	20.0
2,3-Dihydro-1-o...	11.322	7.1	ng	255068	4	11.204	720441	20.0
unknown11.533	11.533	5.4	ng	193946	4	11.204	720441	20.0
1-Naphthaleneac...	11.610	11.9	ng	429973	4	11.204	720441	20.0
n-Hexadecanoic ...	11.763	9.1	ng	327419	4	11.204	720441	20.0
3-Biphenylmethanol	11.827	11.9	ng	427254	4	11.204	720441	20.0
2-Amino-8-hydro...	12.045	6.2	ng	221362	4	11.204	720441	20.0
Octadecanoic acid	12.539	6.8	ng	214714	5	13.833	632453	20.0