

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
 Data File : BF128532.D
 Acq On : 28 May 2022 02:31
 Operator : CG\JU
 Sample : N2930-10
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P005-SS003-1824-01

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-BF052622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128532.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.075	471	474	483	rVB	89019	115007	1.44%	0.184%
2	5.457	533	539	542	rBV	4589605	4955308	62.02%	7.939%
3	6.463	704	710	713	rBV	4312121	5089528	63.70%	8.154%
4	6.840	770	774	777	rBV	1650781	1445032	18.09%	2.315%
5	7.398	863	869	872	rBV	3210213	3425129	42.87%	5.487%
6	8.122	987	992	995	rBV	1982100	1846795	23.12%	2.959%
7	9.004	1137	1142	1145	rBV2	305092	330796	4.14%	0.530%
8	9.045	1145	1149	1152	rVB	360847	290040	3.63%	0.465%
9	9.198	1169	1175	1178	rBV	5854677	5584671	69.90%	8.947%
10	9.275	1184	1188	1190	rBV2	324764	266566	3.34%	0.427%
11	9.322	1190	1196	1199	rVB	7868728	7989569	100.00%	12.800%
12	9.363	1199	1203	1206	rBV	240766	197445	2.47%	0.316%
13	9.533	1227	1232	1236	rBV	1599405	1559628	19.52%	2.499%
14	9.592	1237	1242	1245	rVV	70149	91940	1.15%	0.147%
15	9.728	1261	1265	1272	rVV	666099	581198	7.27%	0.931%
16	9.792	1273	1276	1283	rVV	349266	312665	3.91%	0.501%
17	9.875	1283	1290	1293	rVV	2291575	2172459	27.19%	3.480%
18	9.904	1293	1295	1298	rVV	794995	666695	8.34%	1.068%
19	9.933	1298	1300	1303	rVV	807063	585882	7.33%	0.939%
20	10.004	1306	1312	1315	rVB	93114	95692	1.20%	0.153%
21	10.663	1416	1424	1432	rBV	3350310	3277120	41.02%	5.250%
22	10.751	1435	1439	1444	rVB2	349546	342355	4.29%	0.548%
23	10.992	1474	1480	1487	rBV	239812	274175	3.43%	0.439%
24	11.057	1487	1491	1500	rVB6	56521	116398	1.46%	0.186%
25	11.363	1539	1543	1546	rBV	2128774	1768152	22.13%	2.833%
26	11.892	1629	1633	1637	rBV	404940	371960	4.66%	0.596%
27	12.598	1751	1753	1762	rVB2	66050	92755	1.16%	0.149%
28	12.680	1763	1767	1773	rBV	117420	129021	1.61%	0.207%
29	12.951	1809	1813	1817	rBV	4330595	4040405	50.57%	6.473%
30	13.892	1965	1973	1986	rBV5	86671	306879	3.84%	0.492%
31	14.004	1986	1992	1995	rBV2	1300125	1400603	17.53%	2.244%
32	14.104	2002	2009	2018	rBV	1013141	1258759	15.76%	2.017%
33	14.821	2128	2131	2134	rVB	92121	91143	1.14%	0.146%
34	14.868	2136	2139	2145	rVB	132471	133291	1.67%	0.214%
35	15.133	2181	2184	2188	rBV	68723	90440	1.13%	0.145%
36	15.198	2189	2195	2199	rVV	3283559	4267422	53.41%	6.837%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128532.D
Acq On : 28 May 2022 02:31
Operator : CG\JU
Sample : N2930-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P005-SS003-1824-01

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-BF052622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.468	2235	2241	2246	rBV	1007110	1200796	15.03%	1.924%
38	15.721	2276	2284	2294	rVB2	1026535	2163373	27.08%	3.466%
39	15.957	2320	2324	2330	rVB2	78332	118176	1.48%	0.189%
40	16.309	2379	2384	2385	rBV2	131380	164783	2.06%	0.264%
41	16.345	2385	2390	2398	rVB	844749	1488040	18.62%	2.384%
42	16.462	2406	2410	2417	rVB5	62301	107301	1.34%	0.172%
43	16.592	2428	2432	2445	rVB8	61993	130675	1.64%	0.209%
44	17.580	2593	2600	2619	rBV5	205407	1003648	12.56%	1.608%
45	17.751	2625	2629	2640	rVB6	118197	279152	3.49%	0.447%
46	18.556	2760	2766	2774	rVB7	84509	199784	2.50%	0.320%

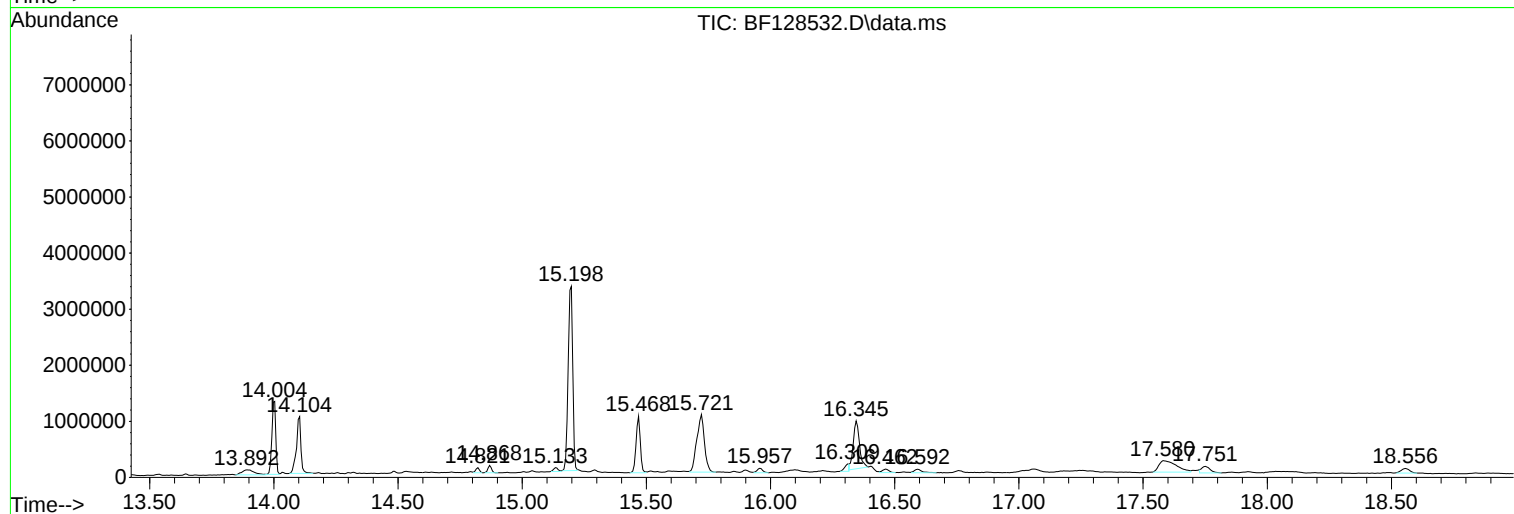
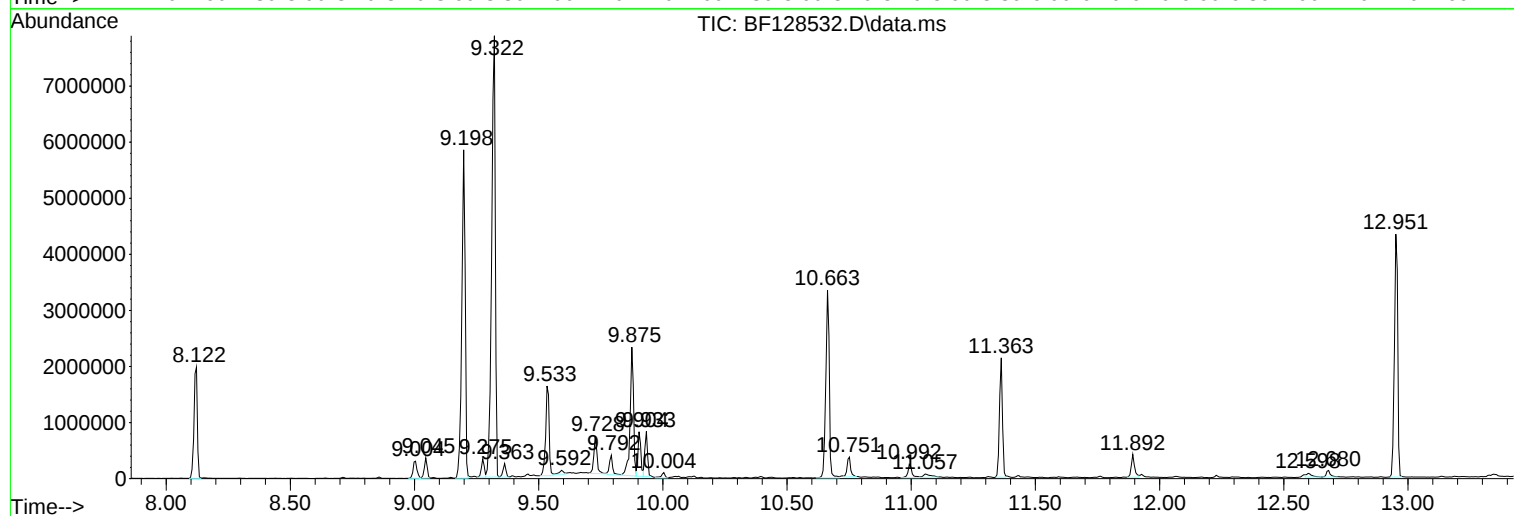
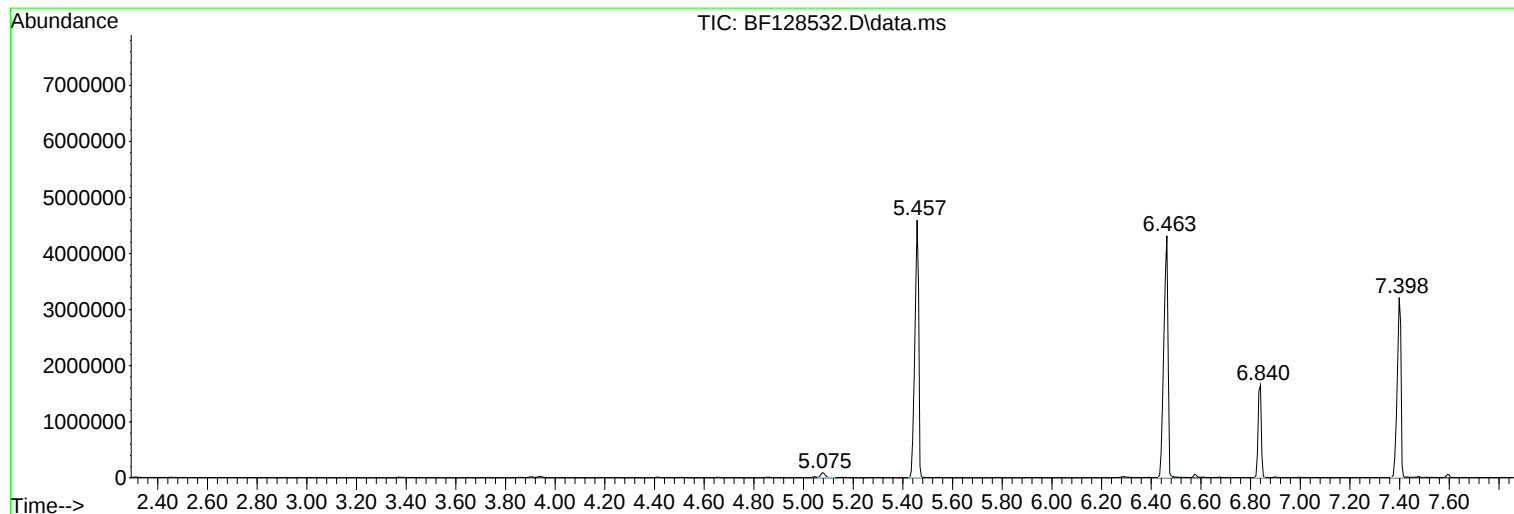
Sum of corrected areas: 62418651

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128532.D
Acq On : 28 May 2022 02:31
Operator : CG\JU
Sample : N2930-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P005-SS003-1824-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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\BF052722\
Data File : BF128532.D
Acq On : 28 May 2022 02:31
Operator : CG\JU
Sample : N2930-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P005-SS003-1824-01

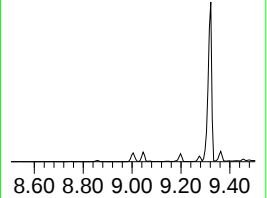
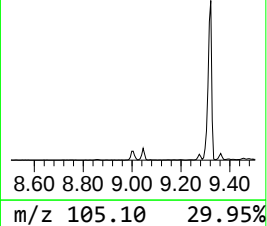
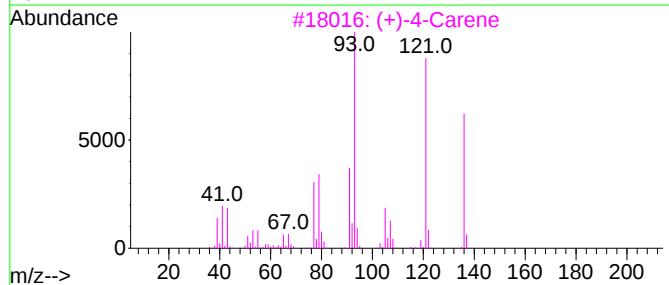
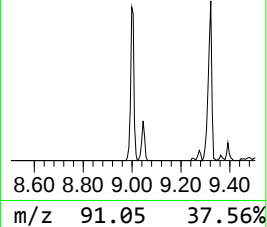
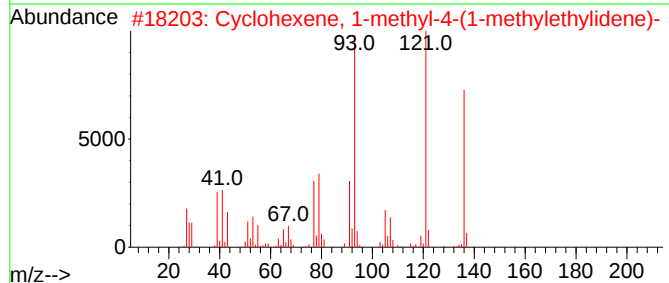
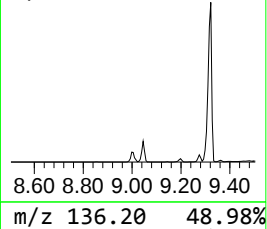
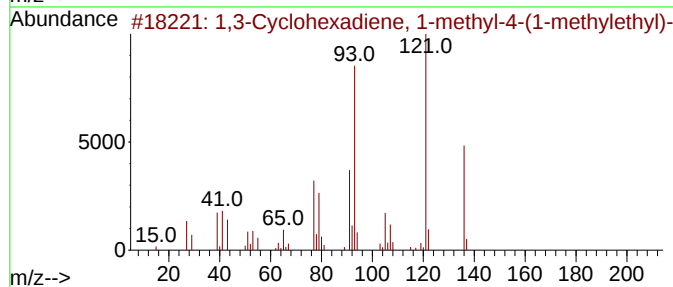
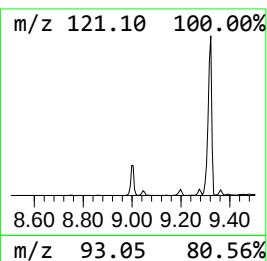
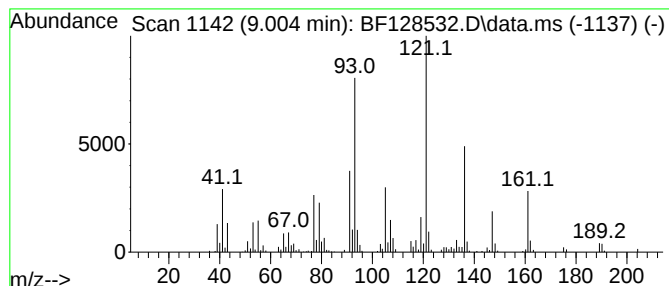
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1,3-Cyclohexadiene, 1-methy... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.004	3.05 ng	330796	Acenaphthene-d10	9.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	95
2			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	000586-62-9	94
3			(+)-4-Carene	136	C10H16	029050-33-7	94
4			2-Carene	136	C10H16	000554-61-0	94
5			Cyclohexene, 4-ethenyl-4-methyl-...	204	C15H24	020307-84-0	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128532.D
Acq On : 28 May 2022 02:31
Operator : CG\JU
Sample : N2930-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P005-SS003-1824-01

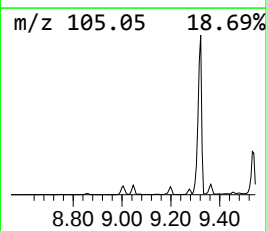
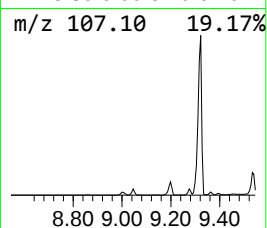
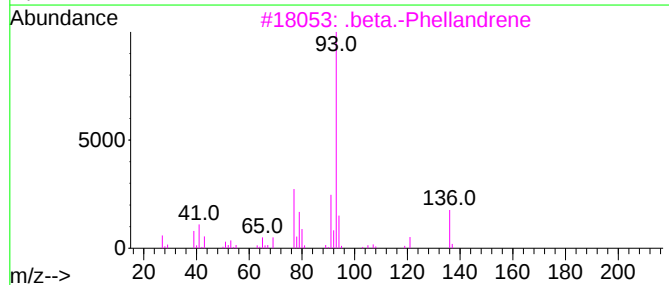
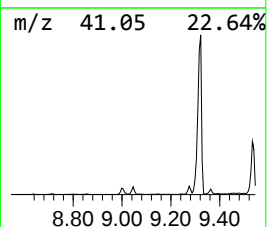
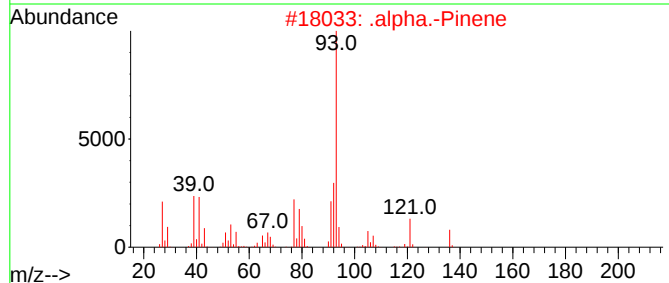
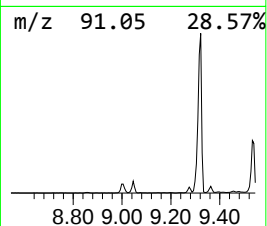
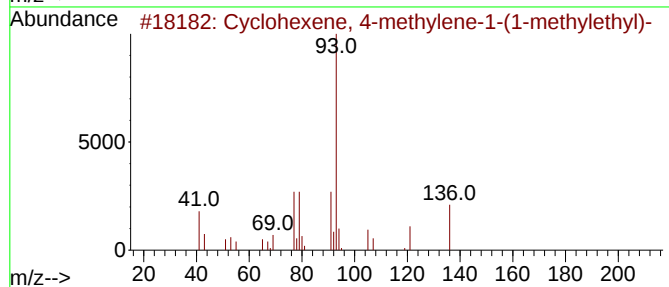
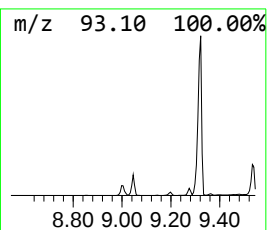
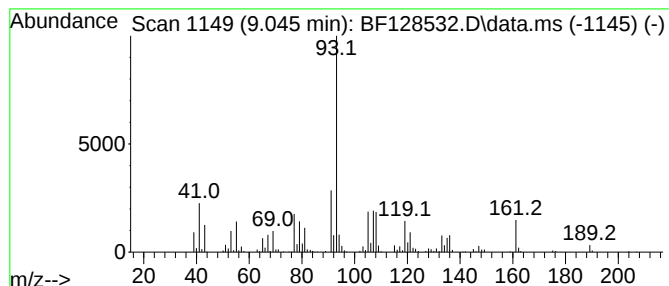
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Cyclohexene, 4-methylene-1-... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.045	2.67 ng	290040	Acenaphthene-d10	9.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 4-methylene-1-(1-me...	136	C10H16	000099-84-3	53
2			.alpha.-Pinene	136	C10H16	000080-56-8	52
3			.beta.-Phellandrene	136	C10H16	000555-10-2	47
4			isobutyranilide	163	C10H13NO	004406-41-1	46
5			Pyridine, 4-pentyl-	149	C10H15N	002961-50-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128532.D
Acq On : 28 May 2022 02:31
Operator : CG\JU
Sample : N2930-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

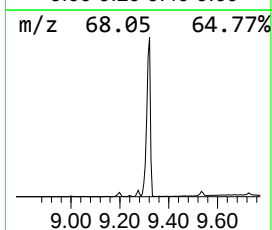
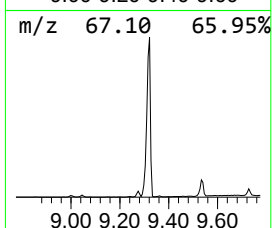
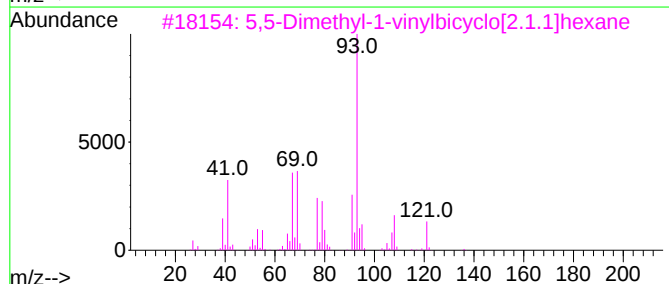
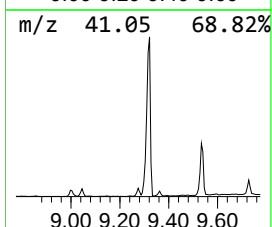
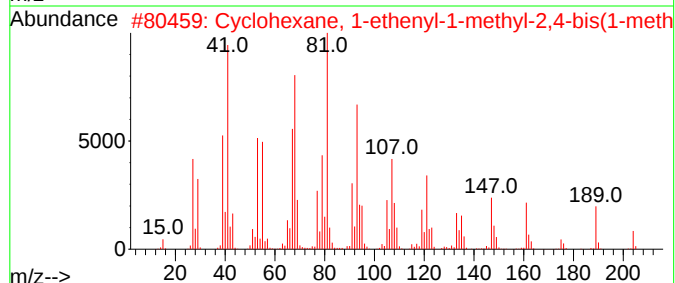
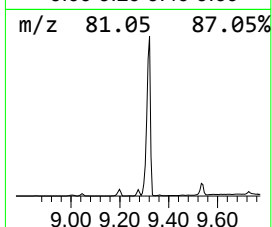
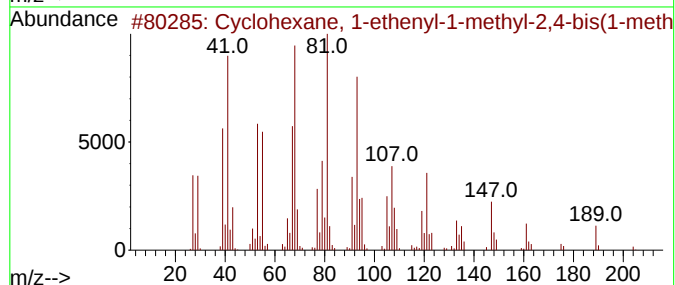
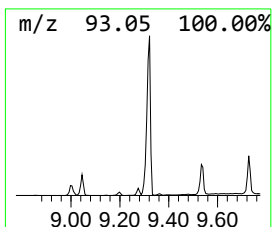
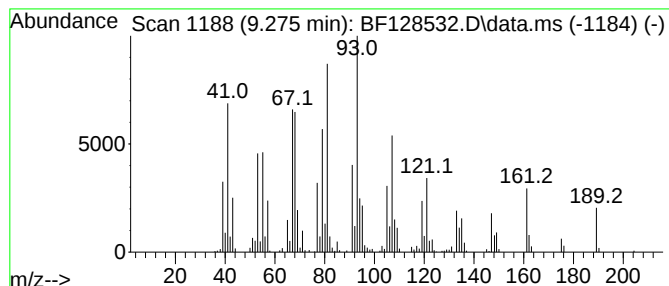
Instrument :
BNA_F
ClientSampleId :
P005-SS003-1824-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Cyclohexane, 1-ethenyl-1-me... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD		R.T.	
9.275	2.45 ng	266566	Acenaphthene-d10		9.875	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethenyl-1-methyl-...		204	C15H24	110823-68-2	59
2	Cyclohexane, 1-ethenyl-1-methyl-...		204	C15H24	000515-13-9	59
3	5,5-Dimethyl-1-vinylbicyclo[2.1....		136	C10H16	016626-39-4	49
4	Bicyclo[5.2.0]nonane, 4-methylen...		204	C15H24	1000159-38-2	38
5	1H-Pyrrole, 1-(2-furanylmethyl)-		147	C9H9NO	001438-94-4	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128532.D
Acq On : 28 May 2022 02:31
Operator : CG\JU
Sample : N2930-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P005-SS003-1824-01

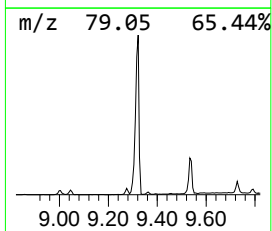
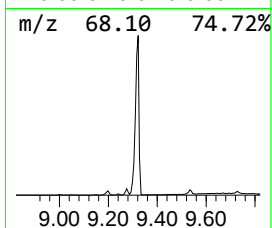
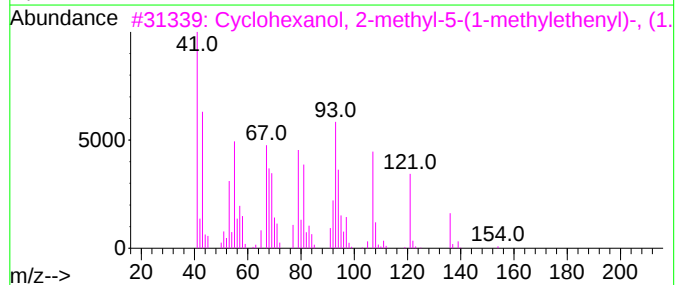
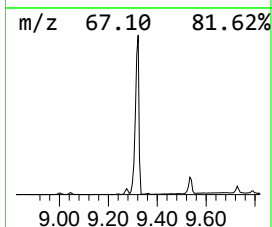
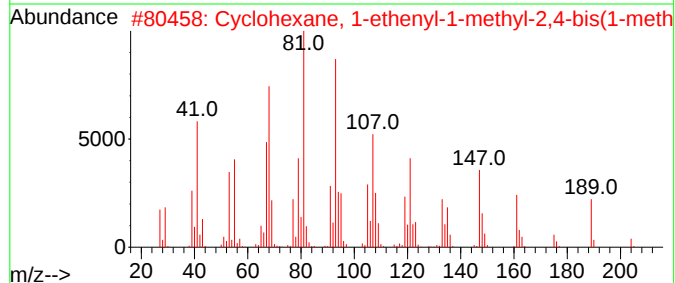
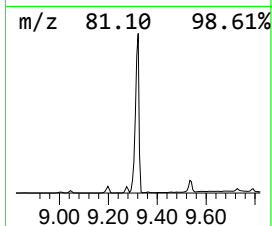
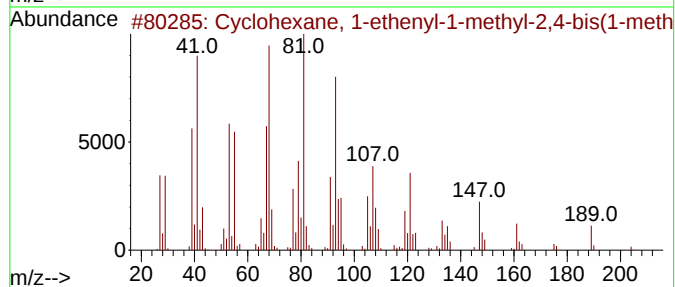
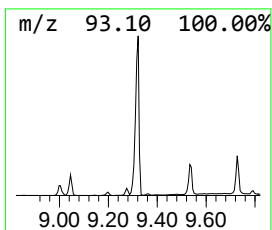
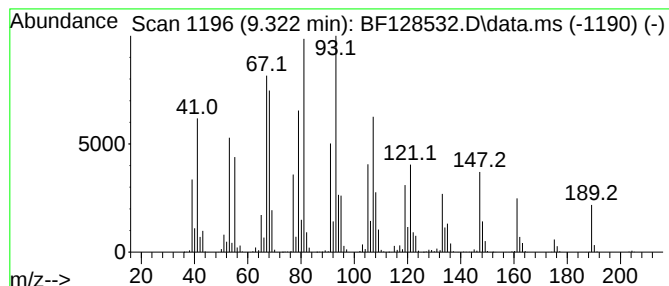
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Cyclohexanol, 2-methyl-5-(1... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.322	73.55 ng	7989570	Acenaphthene-d10	9.875

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexane, 1-ethenyl-1-methyl-...	204	C15H24	110823-68-2	86
2		Cyclohexane, 1-ethenyl-1-methyl-...	204	C15H24	000515-13-9	64
3		Cyclohexanol, 2-methyl-5-(1-meth...	154	C10H18O	018675-33-7	53
4		Cyclohexane, 1-ethenyl-1-methyl-...	204	C15H24	033880-83-0	41
5		Cyclobutane, 1,2-bis(1-methyleth...	136	C10H16	019465-02-2	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128532.D
Acq On : 28 May 2022 02:31
Operator : CG\JU
Sample : N2930-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P005-SS003-1824-01

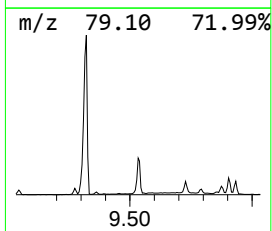
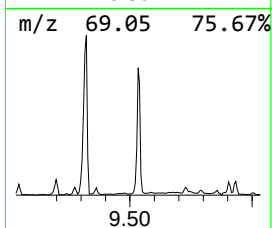
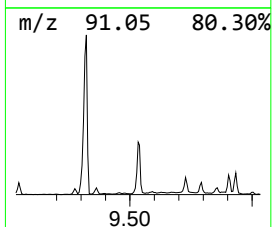
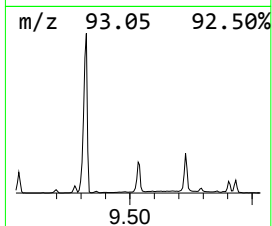
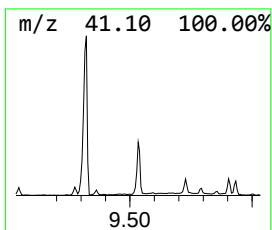
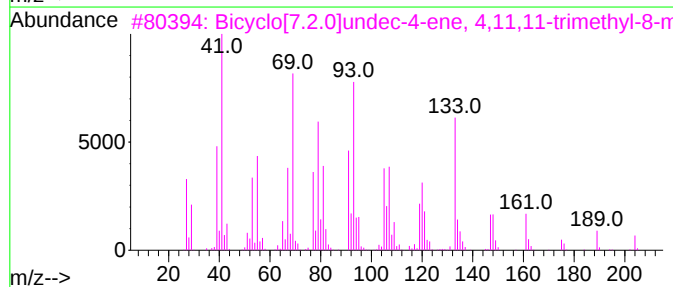
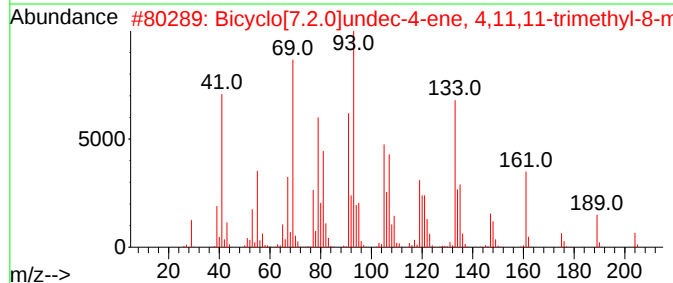
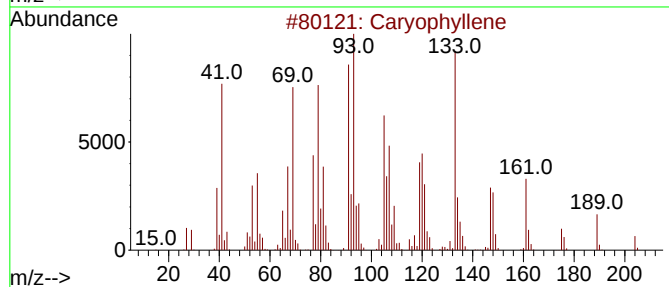
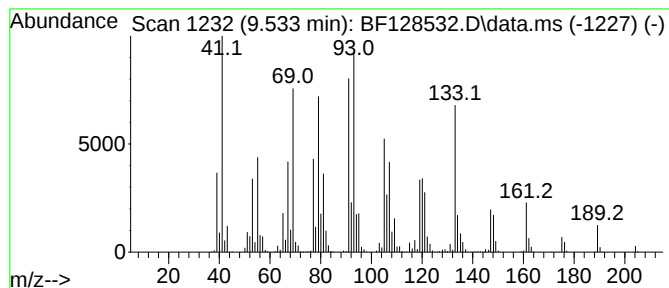
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Caryophyllene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.533	14.36 ng	1559630	Acenaphthene-d10	9.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Caryophyllene	204	C15H24	000087-44-5	99
2			Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	95
3			Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	91
4			4,11,11-trimethyl-8-methylenebic...	204	C15H24	889360-49-0	53
5			1H-Benzocycloheptene, 2,4a,5,6,7...	204	C15H24	003853-83-6	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128532.D
Acq On : 28 May 2022 02:31
Operator : CG\JU
Sample : N2930-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P005-SS003-1824-01

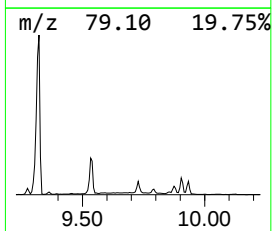
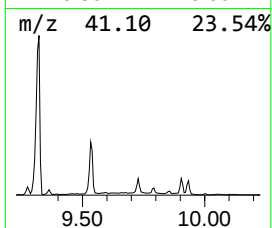
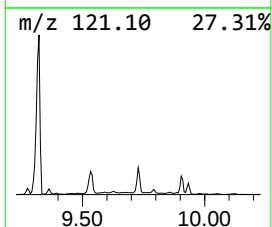
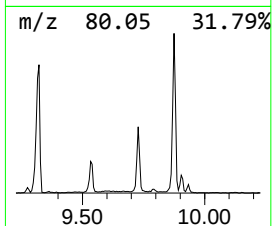
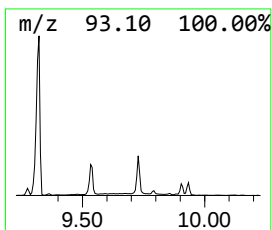
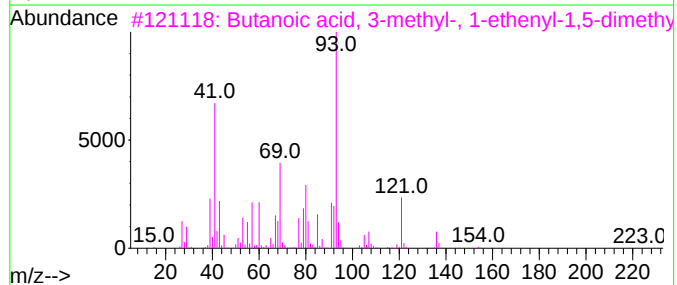
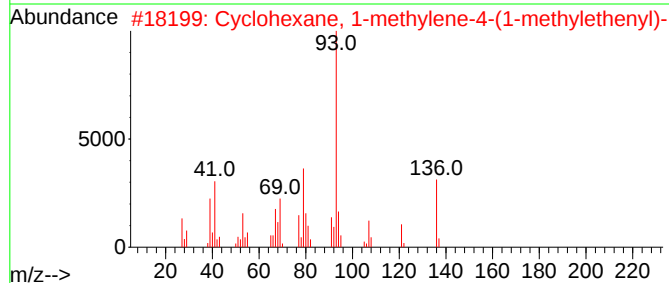
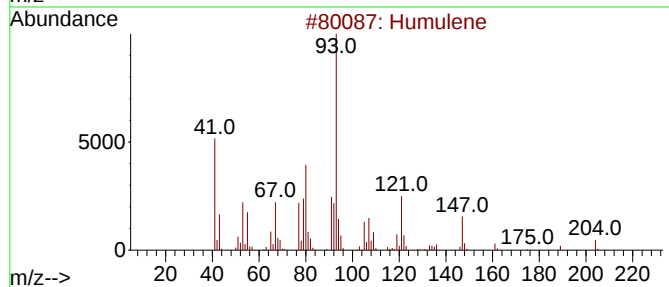
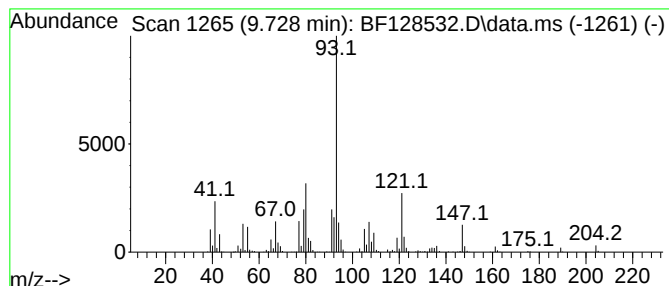
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Humulene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.728	5.35 ng	581198	Acenaphthene-d10	9.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Humulene	204	C15H24	006753-98-6	98
2			Cyclohexane, 1-methylene-4-(1-me...	136	C10H16	000499-97-8	74
3			Butanoic acid, 3-methyl-, 1-ethe...	238	C15H26O2	001118-27-0	72
4			trans-Ocimenol	154	C10H18O	007643-60-9	72
5			Linalyl acetate	196	C12H20O2	000115-95-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128532.D
Acq On : 28 May 2022 02:31
Operator : CG\JU
Sample : N2930-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P005-SS003-1824-01

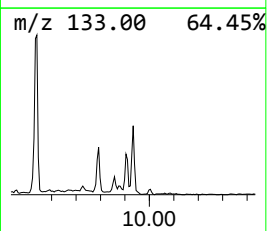
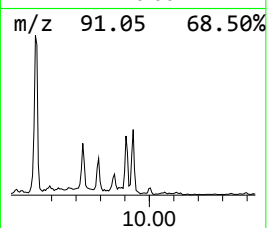
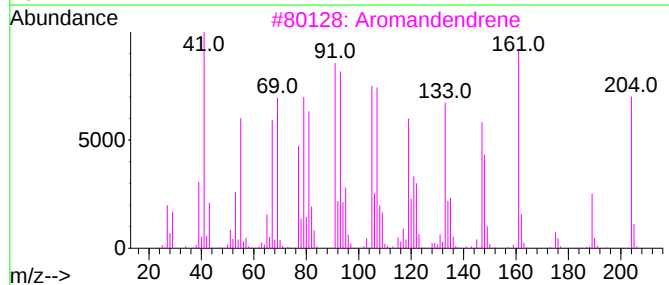
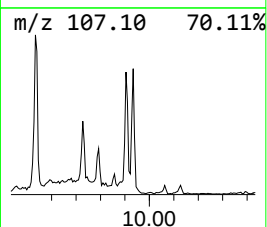
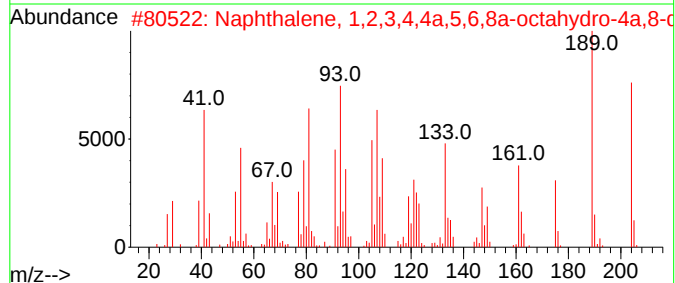
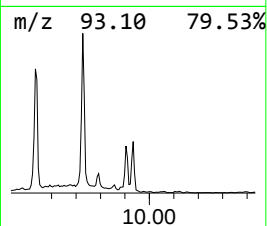
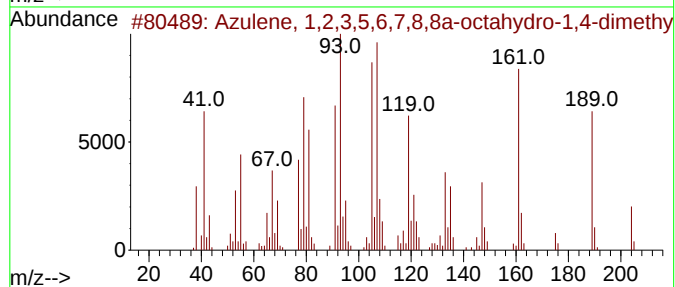
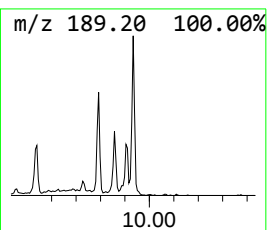
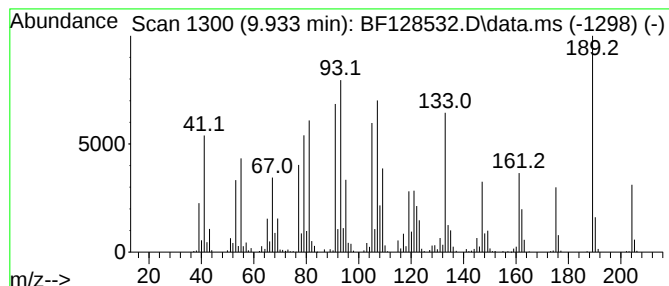
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Azulene, 1,2,3,5,6,7,8,8a-o... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.933	5.39 ng	585882	Acenaphthene-d10	9.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azulene, 1,2,3,5,6,7,8,8a-octahy...	204	C15H24	003691-11-0	70
2			Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	64
3			Aromandendrene	204	C15H24	000489-39-4	51
4			2,10,10-Trimethyltricyclo[7.1.1...	204	C14H20O	1000210-81-9	51
5			4a,8-Dimethyl-2-(prop-1-en-2-yl)...	204	C15H24	103827-22-1	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128532.D
Acq On : 28 May 2022 02:31
Operator : CG\JU
Sample : N2930-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

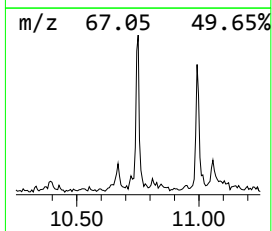
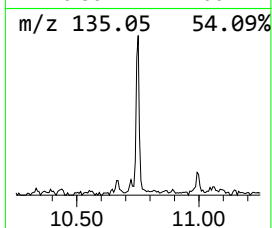
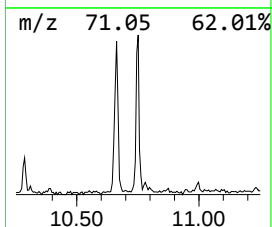
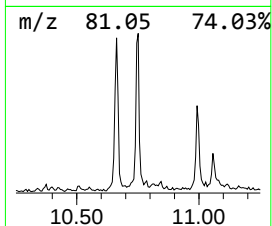
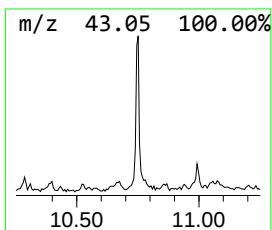
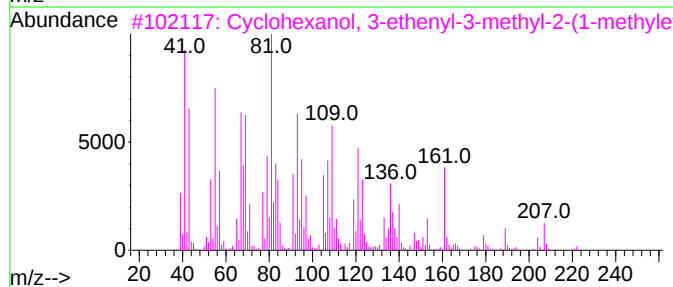
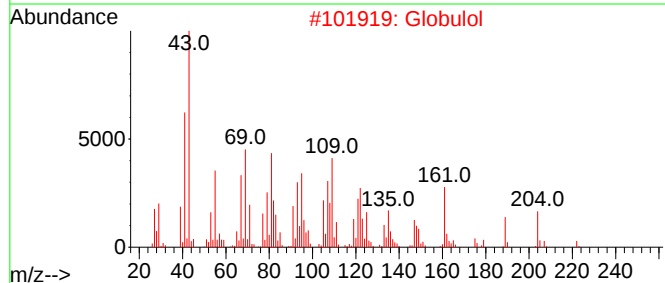
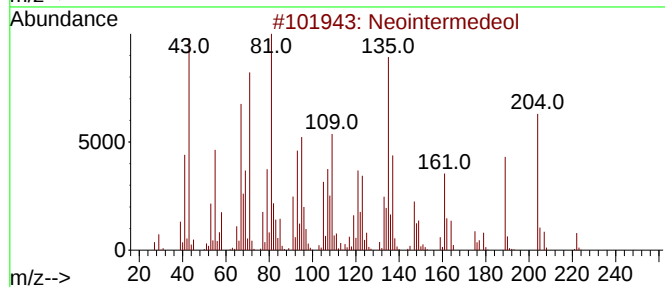
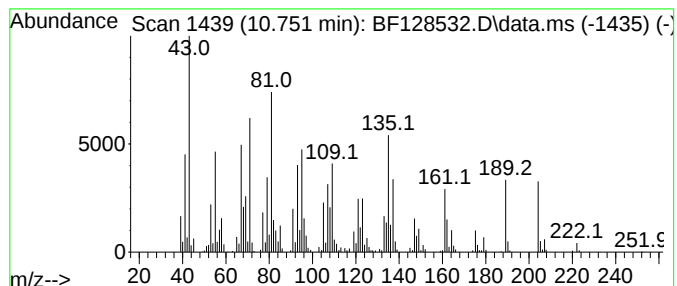
Instrument :
BNA_F
ClientSampleId :
P005-SS003-1824-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Neointermedeol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.751	3.87 ng	342355	Phenanthrene-d10	11.363	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Neointermedeol	222	C15H26O	005945-72-2	99
2	Globulol	222	C15H26O	051371-47-2	50
3	Cyclohexanol, 3-ethenyl-3-methyl...	222	C15H26O	035727-45-8	46
4	Azulene, 1,2,3,3a,4,5,6,7-octahy...	204	C15H24	022567-17-5	45
5	3-Octyne, 2,2,7-trimethyl-	152	C11H20	055402-13-6	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128532.D
Acq On : 28 May 2022 02:31
Operator : CG\JU
Sample : N2930-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P005-SS003-1824-01

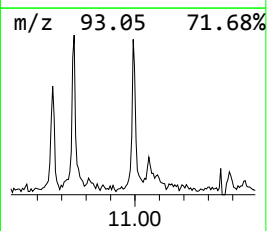
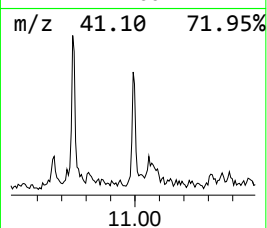
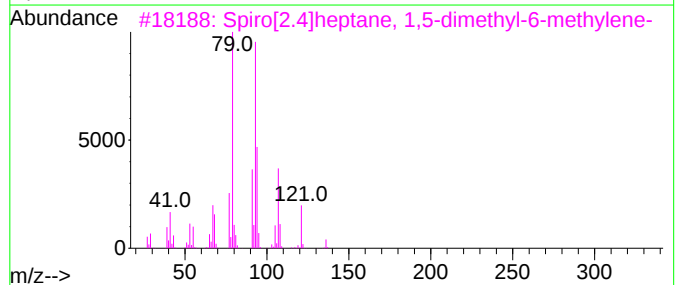
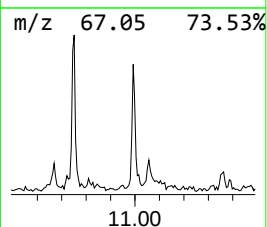
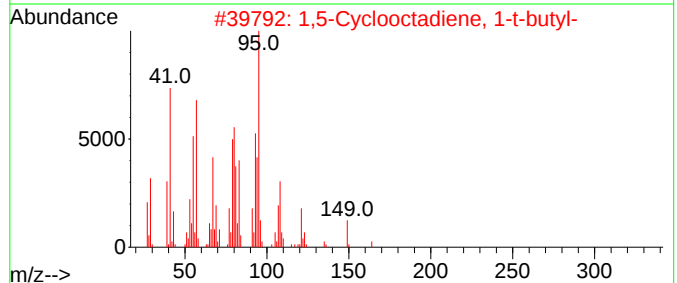
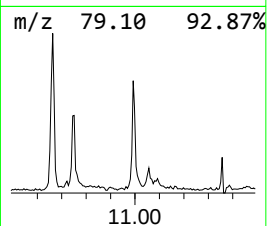
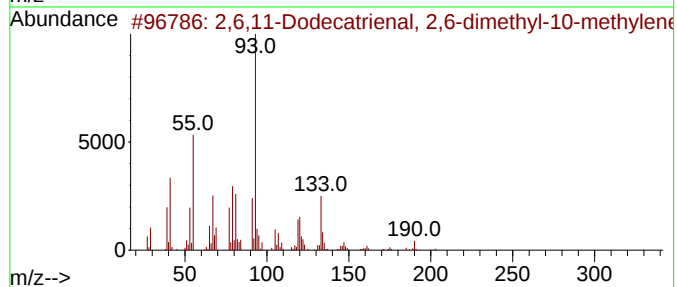
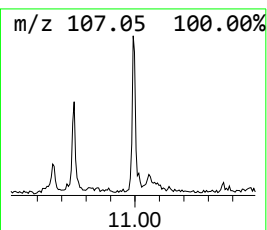
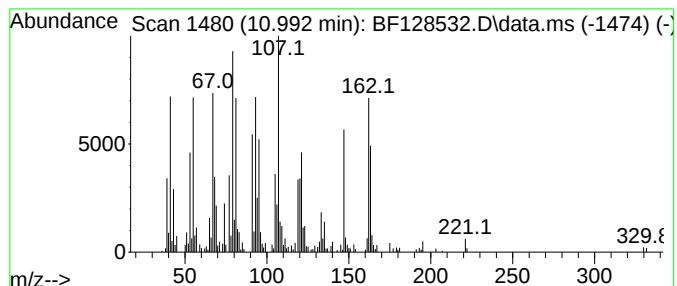
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown10.992 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.992	3.10 ng	274175	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,11-Dodecatrienal, 2,6-dimeth...	218	C15H22O	060066-88-8	47		
2	1,5-Cyclooctadiene, 1-t-butyl-	164	C12H20	1000152-18-6	43		
3	Spiro[2.4]heptane, 1,5-dimethyl-...	136	C10H16	062238-24-8	43		
4	2-Octyne	110	C8H14	002809-67-8	41		
5	Albene	162	C12H18	038451-64-8	27		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128532.D
Acq On : 28 May 2022 02:31
Operator : CG\JU
Sample : N2930-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P005-SS003-1824-01

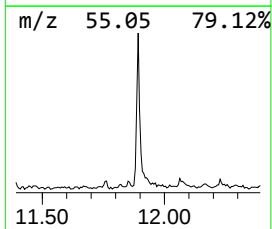
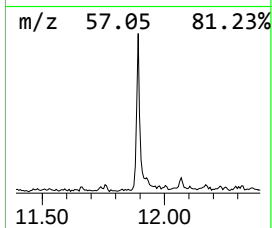
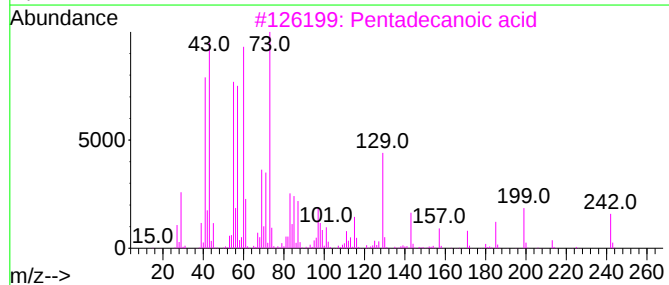
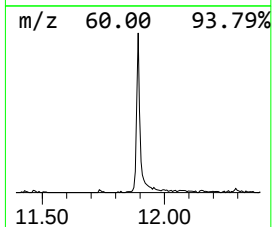
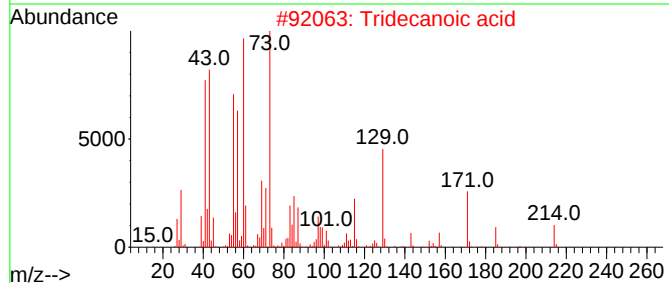
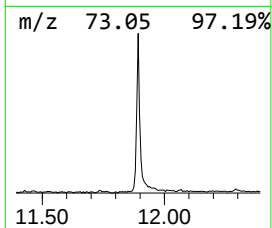
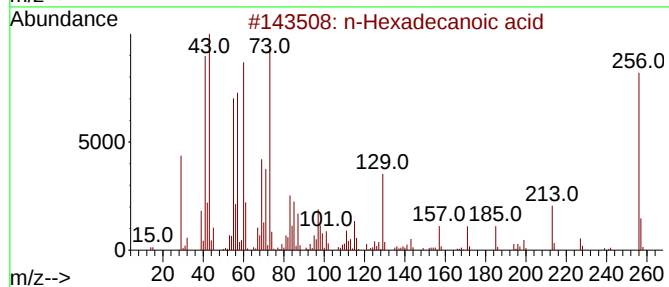
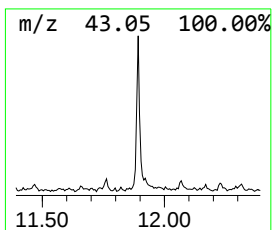
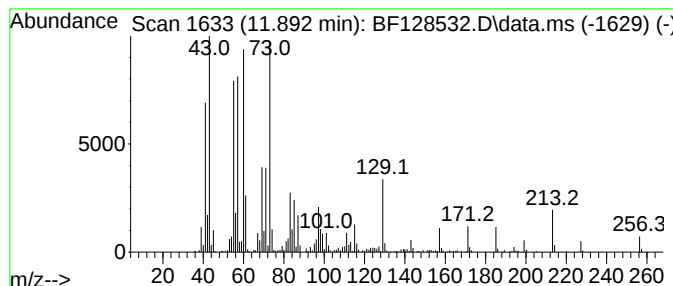
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	4.21 ng	371960	Phenanthrene-d10	11.363

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	89
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Undecanoic acid	186	C11H22O2	000112-37-8	68
5		n-Decanoic acid	172	C10H20O2	000334-48-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128532.D
Acq On : 28 May 2022 02:31
Operator : CG\JU
Sample : N2930-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

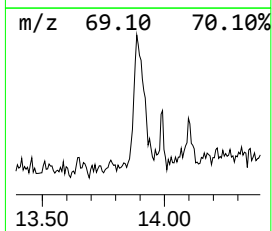
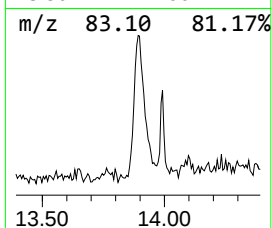
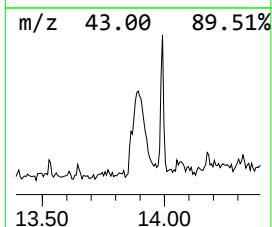
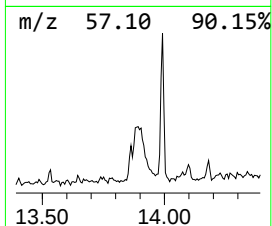
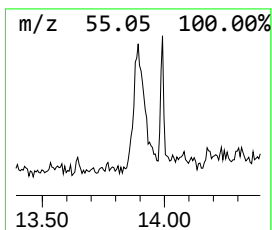
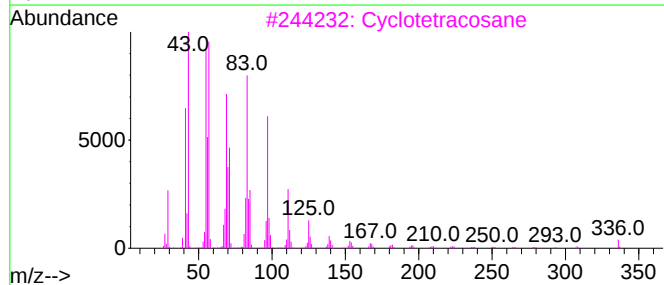
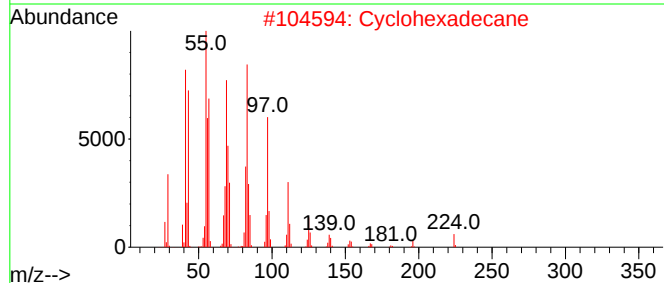
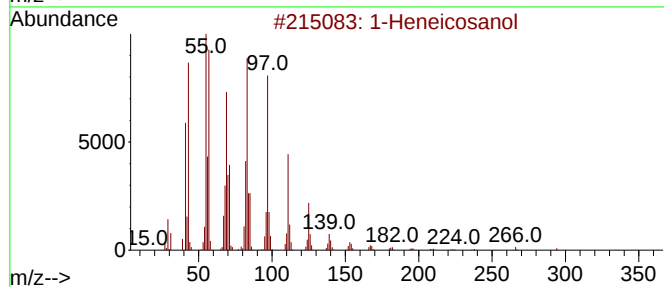
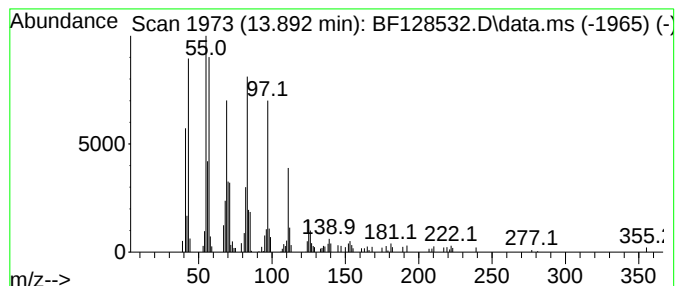
Instrument :
BNA_F
ClientSampleId :
P005-SS003-1824-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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-Heneicosanol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.892	4.38 ng	306879	Chrysene-d12	14.004	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	87
2	Cyclohexadecane	224	C16H32	000295-65-8	83
3	Cyclotetracosane	336	C24H48	000297-03-0	83
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	83
5	Cyclopentadecane	210	C15H30	000295-48-7	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128532.D
Acq On : 28 May 2022 02:31
Operator : CG\JU
Sample : N2930-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P005-SS003-1824-01

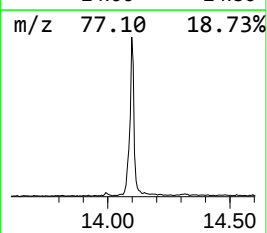
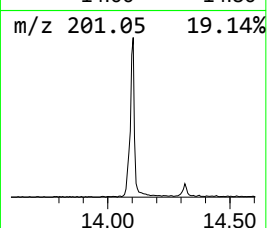
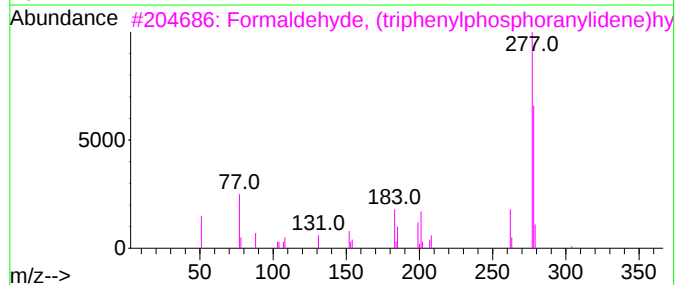
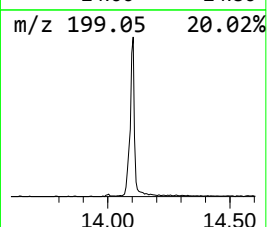
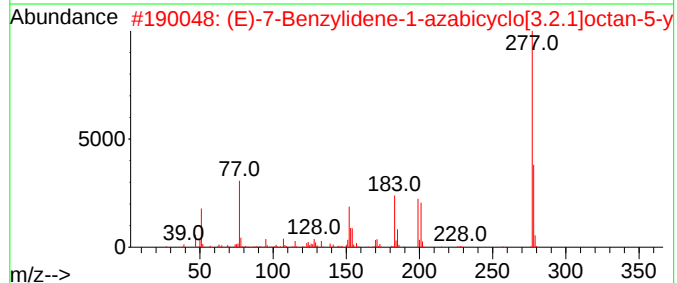
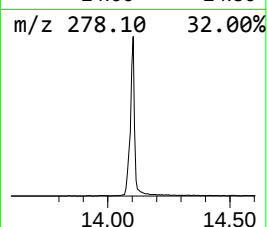
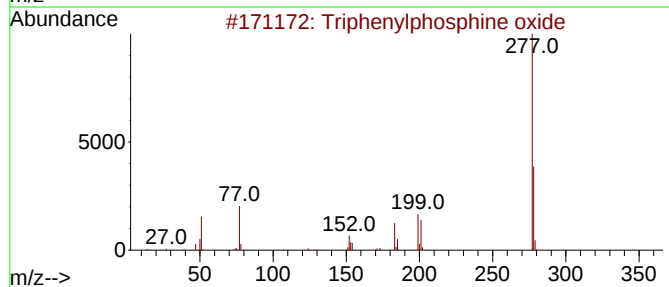
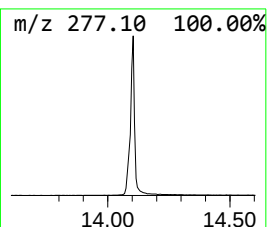
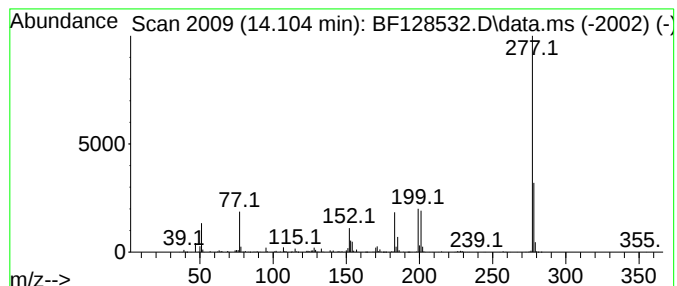
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.104	17.97 ng	1258760	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	40
4			Vanadium, cycloheptatrienyl-(pen...]	277	C17H22V	1000155-20-5	28
5			5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128532.D
Acq On : 28 May 2022 02:31
Operator : CG\JU
Sample : N2930-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

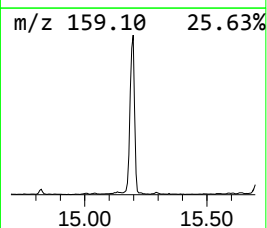
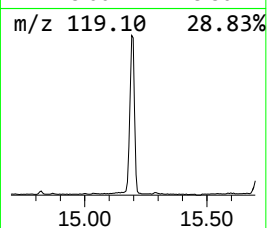
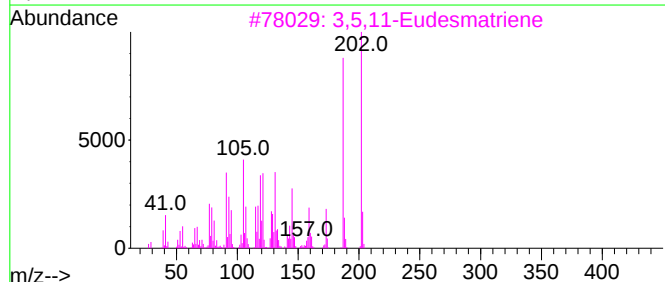
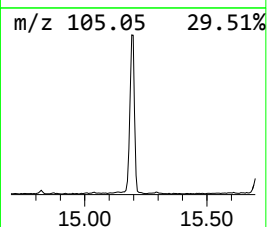
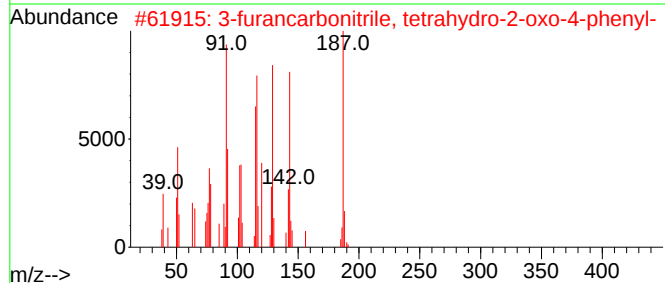
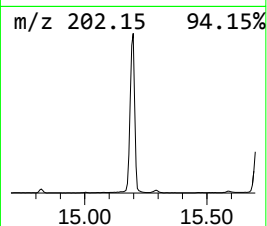
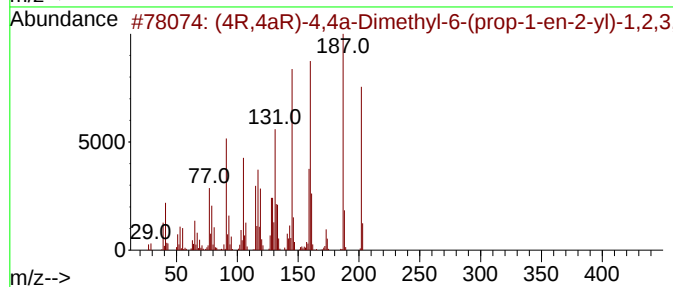
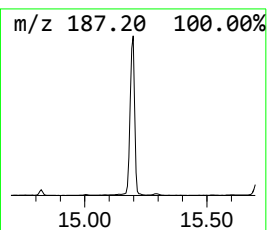
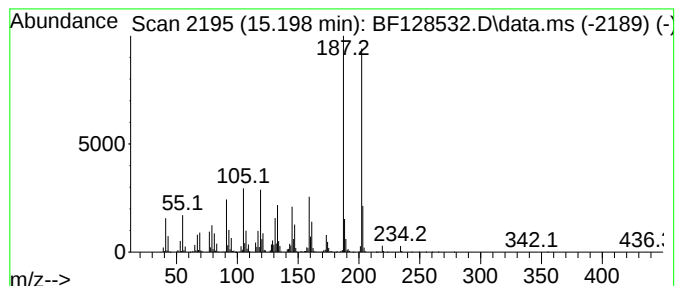
Instrument :
BNA_F
ClientSampleId :
P005-SS003-1824-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 (4R,4aR)-4,4a-Dimethyl-6-(p... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.198	71.08 ng	4267420	Perylene-d12	15.468	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(4R,4aR)-4,4a-Dimethyl-6-(prop-1...	202	C15H22	028908-26-1	87
2	3-furancarbonitrile, tetrahydro-...	187	C11H9NO2	1010395-93-6	60
3	3,5,11-Eudesmatriene	202	C15H22	193615-07-5	59
4	Pyrazol-(4H)-one, 1-(4-ethylphen...	202	C12H14N2O	107430-31-9	59
5	Cadina-1(10),6,8-triene	202	C15H22	001460-96-4	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128532.D
Acq On : 28 May 2022 02:31
Operator : CG\JU
Sample : N2930-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P005-SS003-1824-01

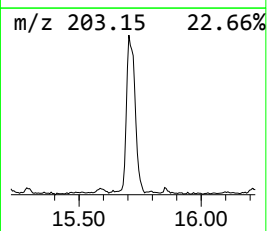
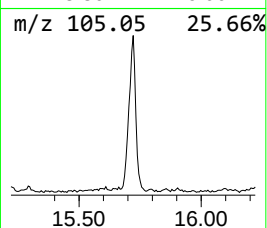
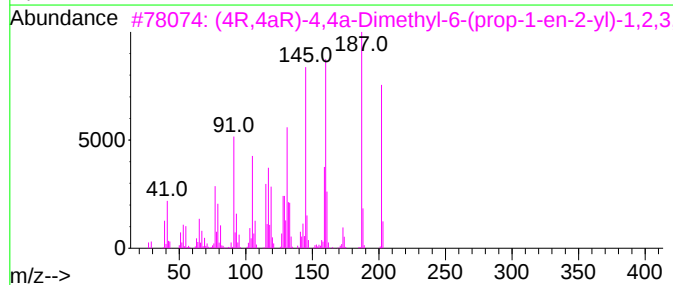
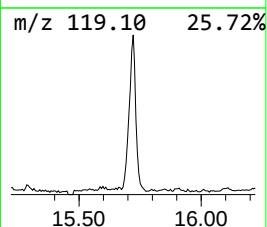
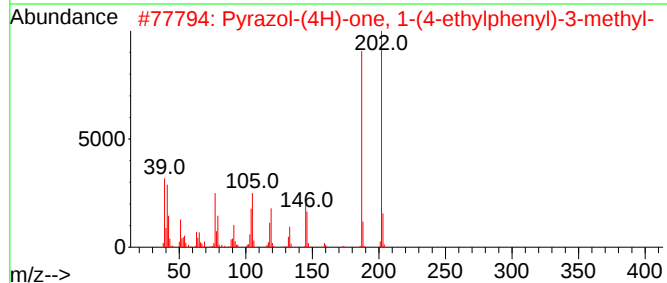
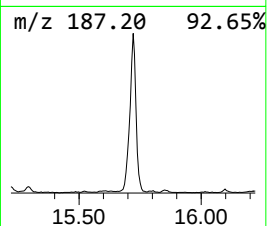
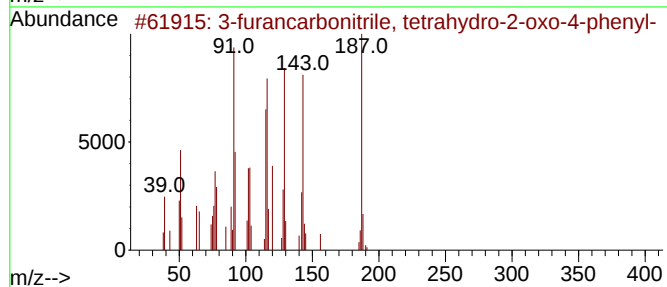
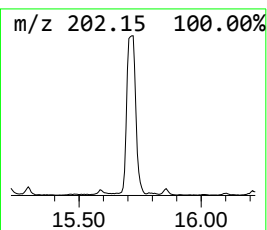
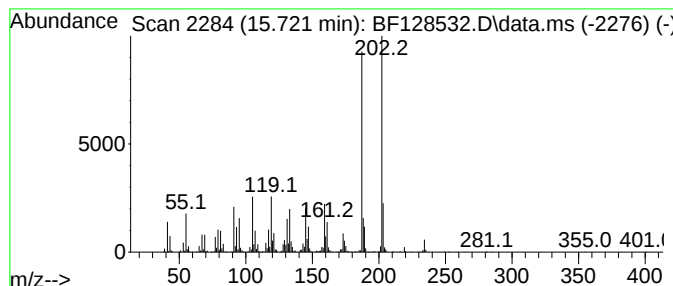
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 3-furancarbonitrile, tetrah... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.721	36.03 ng	2163370	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-furancarbonitrile, tetrahydro-...	187	C11H9N02	1010395-93-6	91
2			Pyrazol-(4H)-one, 1-(4-ethylphen...	202	C12H14N2O	107430-31-9	83
3			(4R,4aR)-4,4a-Dimethyl-6-(prop-1...	202	C15H22	028908-26-1	81
4			3,5,11-Eudesmatiene	202	C15H22	193615-07-5	72
5			Silane, trimethyl(3-phenyl-1-but...	202	C13H18Si	028129-04-6	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128532.D
Acq On : 28 May 2022 02:31
Operator : CG\JU
Sample : N2930-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P005-SS003-1824-01

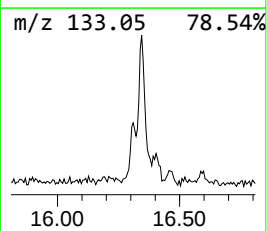
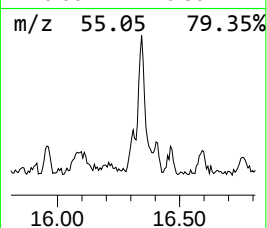
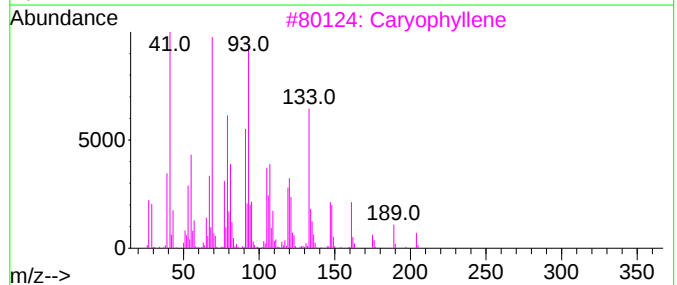
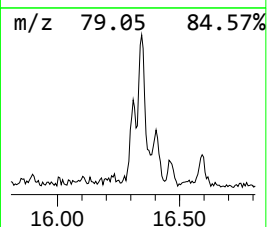
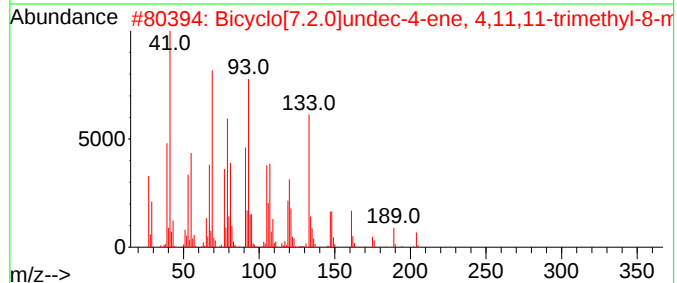
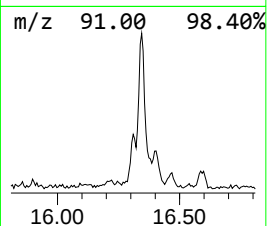
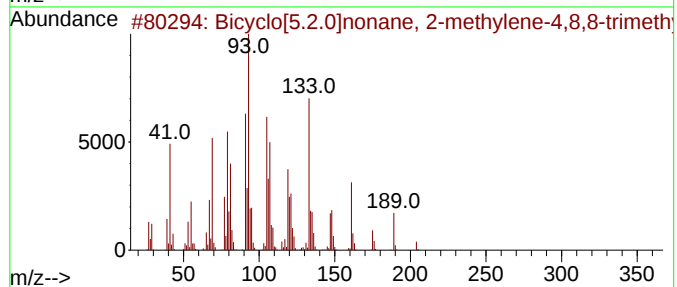
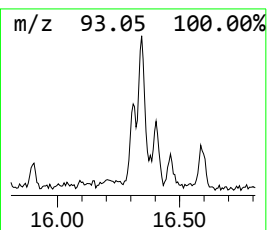
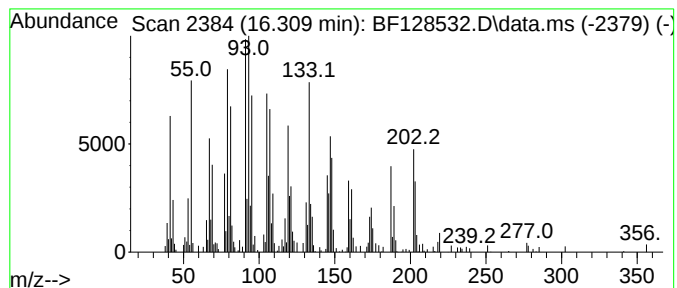
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Bicyclo[5.2.0]nonane, 2-met... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.310	2.74 ng	164783	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[5.2.0]nonane, 2-methylen...	204	C15H24	242794-76-9	90
2			Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	83
3			Caryophyllene	204	C15H24	000087-44-5	70
4			1R,3Z,9S-4,11,11-Trimethyl-8-met...	204	C15H24	1000159-39-4	64
5			Cycloheptane, 4-methylene-1-meth...	204	C15H24	1010159-38-5	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128532.D
Acq On : 28 May 2022 02:31
Operator : CG\JU
Sample : N2930-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P005-SS003-1824-01

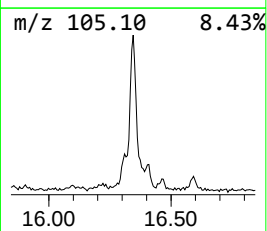
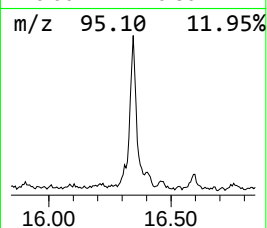
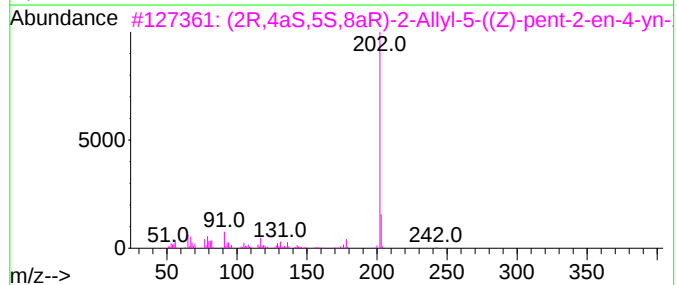
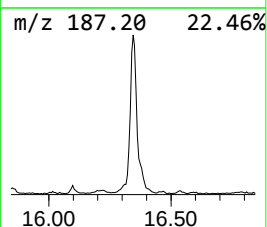
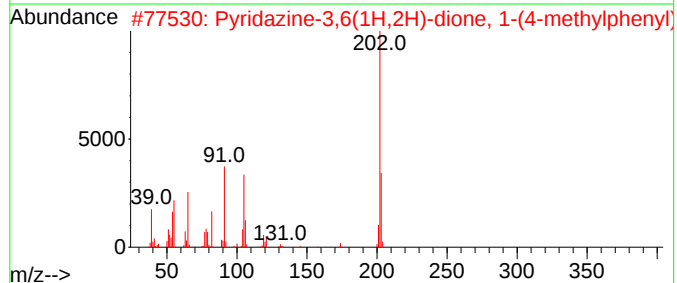
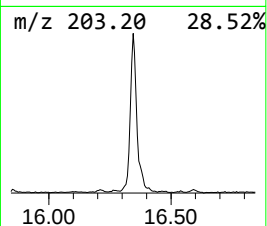
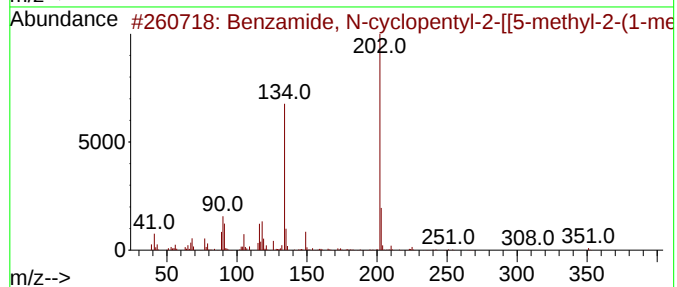
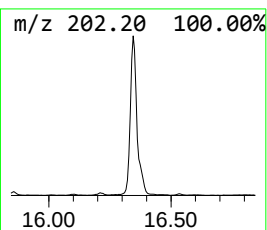
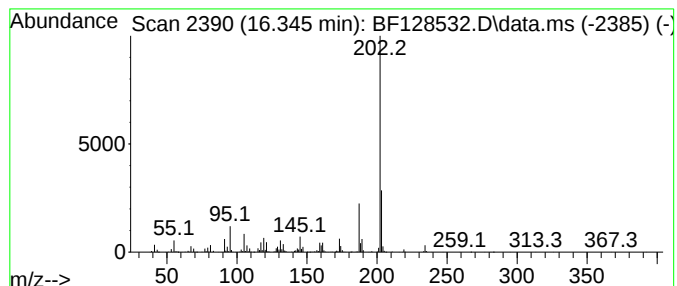
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 unknown16.345 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.345	24.78 ng	1488040	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzamide, N-cyclopentyl-2-[[5-m...	351	C23H29NO2	1000349-93-5	47
2			Pyridazine-3,6(1H,2H)-dione, 1-(...	202	C11H10N2O2	034019-60-8	47
3			(2R,4aS,5S,8aR)-2-Allyl-5-((Z)-p...	243	C17H25N	1159498-69-7	43
4			4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	43
5			Trichoclin	286	C16H14O5	065853-14-7	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128532.D
Acq On : 28 May 2022 02:31
Operator : CG\JU
Sample : N2930-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

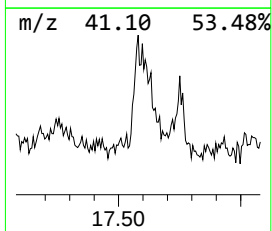
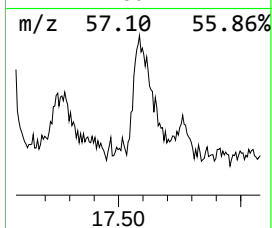
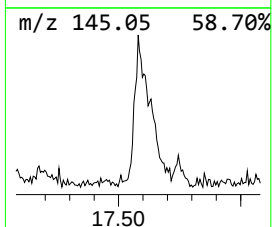
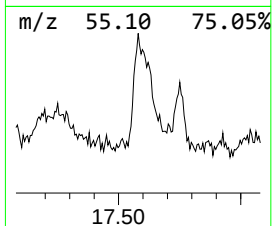
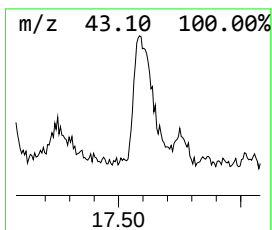
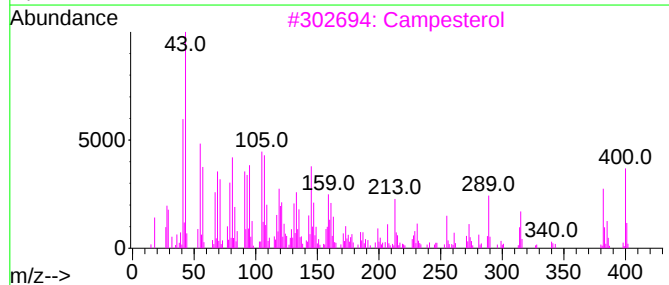
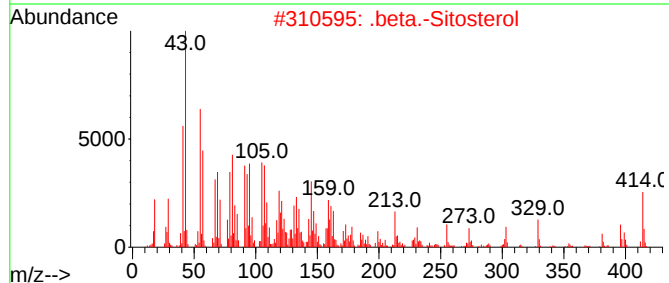
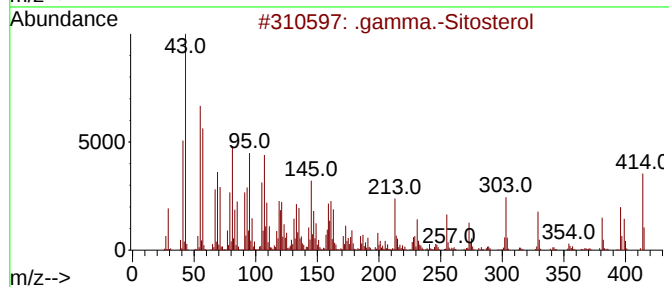
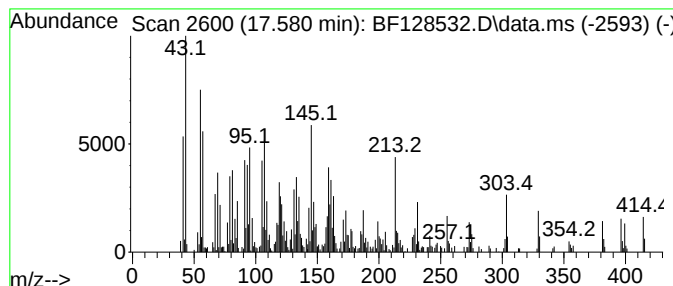
Instrument :
BNA_F
ClientSampleId :
P005-SS003-1824-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 .gamma.-Sitosterol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.580	16.72 ng	1003650	Perylene-d12	15.468	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	99
3	Campesterol	400	C28H48O	000474-62-4	58
4	(3S,8S,9S,10R,13R,14S,17R)-17-((...)	414	C29H50O	029365-29-5	49
5	Ergost-7-en-3-ol	400	C28H48O	116179-22-7	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128532.D
Acq On : 28 May 2022 02:31
Operator : CG\JU
Sample : N2930-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P005-SS003-1824-01

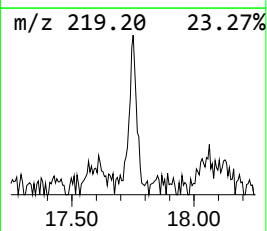
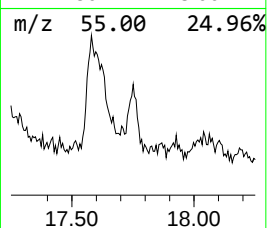
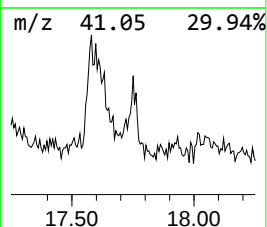
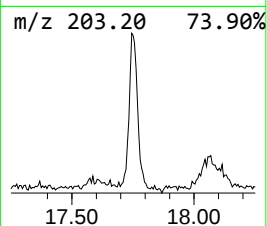
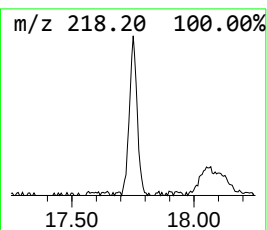
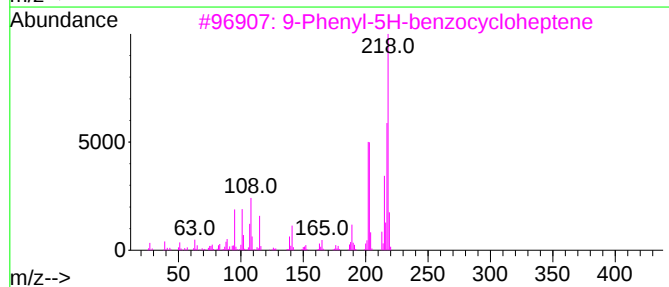
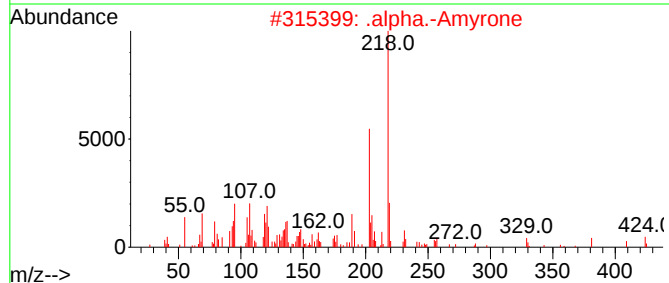
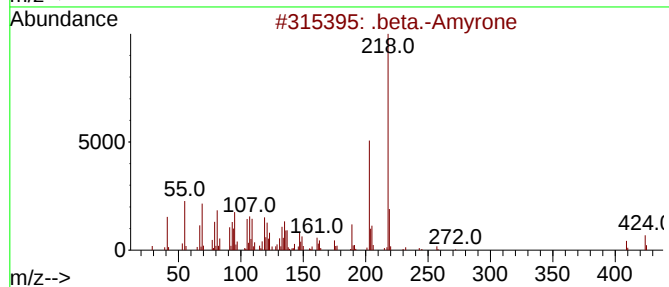
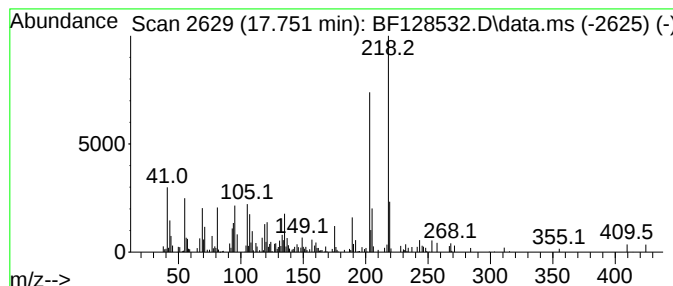
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 .beta.-Amyrone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.751	4.65 ng	279152	Perylene-d12	15.468

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.beta.-Amyrone	424	C30H48O	000638-97-1	93
2		.alpha.-Amyrone	424	C30H48O	000638-96-0	86
3		9-Phenyl-5H-benzocycloheptene	218	C17H14	138089-71-1	72
4		1,2,3,4-Tetrahydro-1-phenyl-1,2,...	218	C17H14	138089-69-7	64
5		3-Acetyl-8-methoxycoumarin	218	C12H10O4	005452-39-1	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128532.D
Acq On : 28 May 2022 02:31
Operator : CG\JU
Sample : N2930-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P005-SS003-1824-01

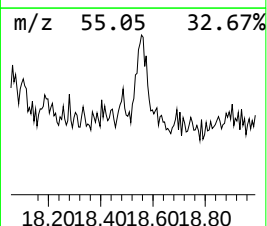
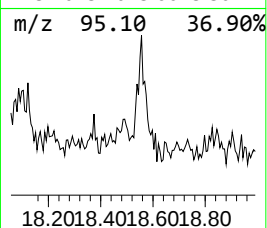
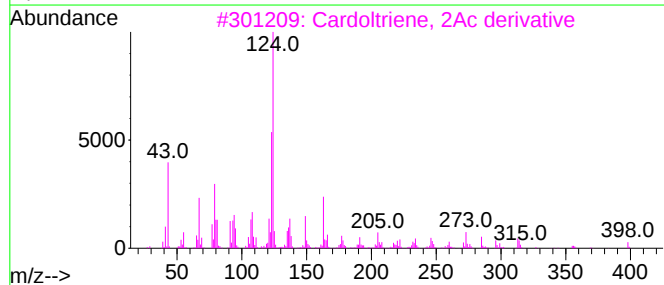
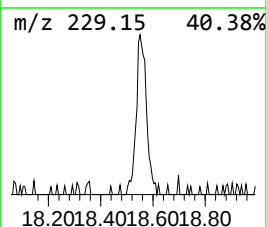
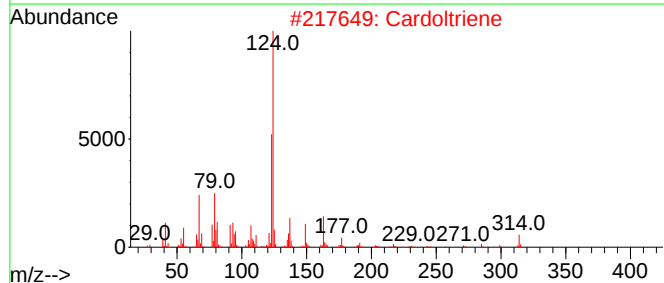
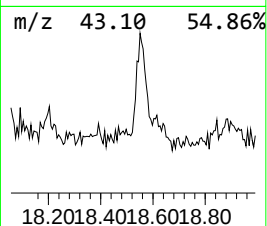
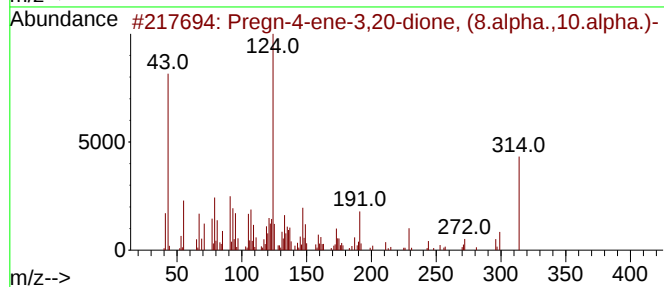
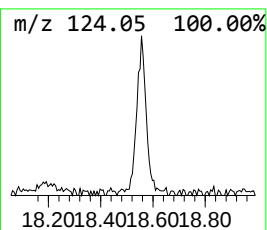
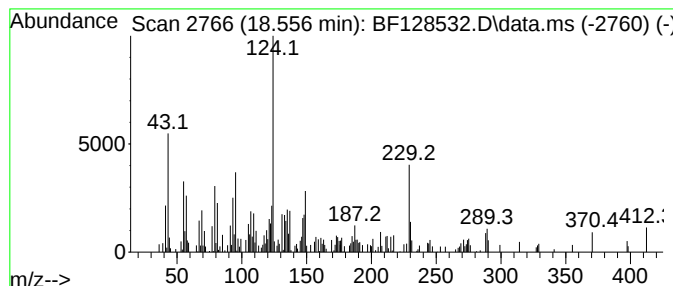
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 unknown18.556 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.556	3.33 ng	199784	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pregn-4-ene-3,20-dione, (8.alpha...	314	C21H30O2	003795-19-5	46
2			Cardoltriene	314	C21H30O2	079473-24-8	41
3			Cardoltriene, 2Ac derivative	398	C25H34O4	212835-71-7	38
4			Testosterone	288	C19H28O2	000058-22-0	35
5			Pregn-4-en-3-one, 20,21-[(1,1-d...	398	C25H39BO3	030882-66-7	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
 Data File : BF128532.D
 Acq On : 28 May 2022 02:31
 Operator : CG\JU
 Sample : N2930-10
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P005-SS003-1824-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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
1,3-Cyclohexadi...	9.004	3.0	ng	330796	3	9.875	2172460	20.0
Cyclohexene, 4-...	9.045	2.7	ng	290040	3	9.875	2172460	20.0
Cyclohexane, 1-...	9.275	2.5	ng	266566	3	9.875	2172460	20.0
Cyclohexanol, 2...	9.322	73.5	ng	7989570	3	9.875	2172460	20.0
Caryophyllene	9.533	14.4	ng	1559630	3	9.875	2172460	20.0
Humulene	9.728	5.3	ng	581198	3	9.875	2172460	20.0
4a,8-Dimethyl-2...	9.792	2.9	ng	312665	3	9.875	2172460	20.0
Azulene, 1,2,3,...	9.933	5.4	ng	585882	3	9.875	2172460	20.0
Neointermedeol	10.751	3.9	ng	342355	4	11.363	1768150	20.0
unknown10.992	10.992	3.1	ng	274175	4	11.363	1768150	20.0
n-Hexadecanoic ...	11.892	4.2	ng	371960	4	11.363	1768150	20.0
1-Heneicosanol	13.892	4.4	ng	306879	5	14.004	1400600	20.0
Triphenylphosph...	14.104	18.0	ng	1258760	5	14.004	1400600	20.0
(4R,4aR)-4,4a-D...	15.198	71.1	ng	4267420	6	15.468	1200800	20.0
3-furancarboxit...	15.721	36.0	ng	2163370	6	15.468	1200800	20.0
Bicyclo[5.2.0]n...	16.310	2.7	ng	164783	6	15.468	1200800	20.0
unknown16.345	16.345	24.8	ng	1488040	6	15.468	1200800	20.0
.gamma.-Sitosterol	17.580	16.7	ng	1003650	6	15.468	1200800	20.0
.beta.-Amyrone	17.751	4.7	ng	279152	6	15.468	1200800	20.0
unknown18.556	18.556	3.3	ng	199784	6	15.468	1200800	20.0