

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120820\
 Data File : BF122591.D
 Acq On : 8 Dec 2020 16:41
 Operator : JU/CG
 Sample : L4971-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 5S1-A-D-COMP

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-BF120520.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122591.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	17	21	30	rVB	71199	116261	3.65%	0.325%
2	2.681	96	101	110	rVB	34587	59907	1.88%	0.168%
3	4.416	392	396	402	rBV	642979	725152	22.75%	2.028%
4	4.710	437	446	453	rBV5	39916	94478	2.96%	0.264%
5	4.822	461	465	474	rVB4	59592	88287	2.77%	0.247%
6	5.045	497	503	509	rVB	856504	1036061	32.50%	2.897%
7	5.457	568	573	576	rBV	3108344	2951585	92.58%	8.253%
8	5.851	636	640	645	rVB	148137	124258	3.90%	0.347%
9	5.910	645	650	653	rBV4	31692	57658	1.81%	0.161%
10	6.010	662	667	670	rVB2	113268	112911	3.54%	0.316%
11	6.275	706	712	715	rBV2	47015	53909	1.69%	0.151%
12	6.345	722	724	731	rVB3	40886	53607	1.68%	0.150%
13	6.469	740	745	750	rBV	2949171	3071620	96.35%	8.589%
14	6.651	773	776	778	rBV	131002	124668	3.91%	0.349%
15	6.839	804	808	811	rBV	1118503	912467	28.62%	2.552%
16	6.898	813	818	821	rBV3	47094	67943	2.13%	0.190%
17	7.157	858	862	865	rBV2	58313	74843	2.35%	0.209%
18	7.239	872	876	882	rVB2	74409	88072	2.76%	0.246%
19	7.398	900	903	906	rVB	2047078	1824248	57.22%	5.101%
20	7.545	925	928	934	rVB2	50866	71624	2.25%	0.200%
21	7.604	934	938	944	rVV	53548	62750	1.97%	0.175%
22	7.681	948	951	955	rVB4	40365	55564	1.74%	0.155%
23	7.863	981	982	987	rVB2	87181	90639	2.84%	0.253%
24	8.122	1022	1026	1030	rBV	1522629	1269072	39.81%	3.549%
25	8.292	1050	1055	1058	rVB2	74403	81428	2.55%	0.228%
26	8.504	1088	1091	1094	rBV2	81584	90006	2.82%	0.252%
27	8.539	1094	1097	1102	rBV2	63995	92209	2.89%	0.258%
28	8.604	1106	1108	1112	rBV3	101874	102073	3.20%	0.285%
29	8.645	1112	1115	1116	rBV	168044	133699	4.19%	0.374%
30	8.663	1116	1118	1120	rVV	70608	55207	1.73%	0.154%
31	8.704	1122	1125	1126	rVV	170969	153976	4.83%	0.431%
32	8.739	1129	1131	1134	rVV2	103145	104365	3.27%	0.292%
33	8.769	1134	1136	1138	rVB	116992	88947	2.79%	0.249%
34	8.804	1139	1142	1145	rVB2	130112	131942	4.14%	0.369%
35	8.857	1145	1151	1152	rBV3	97204	154365	4.84%	0.432%
36	8.886	1153	1156	1159	rBV2	124215	147101	4.61%	0.411%

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

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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	8.945	1163	1166	1168	rVB2	161246	133764	4.20%	0.374%
38	8.975	1169	1171	1173	rBV3	67160	73401	2.30%	0.205%
39	9.039	1180	1182	1185	rBV3	136343	168931	5.30%	0.472%
40	9.104	1190	1193	1196	rBV2	266253	355105	11.14%	0.993%
41	9.175	1203	1205	1206	rBV	196182	148870	4.67%	0.416%
42	9.198	1206	1209	1212	rVV	3709375	3188061	100.00%	8.915%
43	9.227	1212	1214	1220	rVV4	218678	369424	11.59%	1.033%
44	9.275	1220	1222	1226	rVB	151217	114893	3.60%	0.321%
45	9.316	1226	1229	1233	rBV3	142566	200916	6.30%	0.562%
46	9.392	1239	1242	1246	rVB3	351990	442561	13.88%	1.238%
47	9.445	1249	1251	1253	rVB2	144971	111020	3.48%	0.310%
48	9.557	1267	1270	1272	rBV	96459	89589	2.81%	0.251%
49	9.592	1273	1276	1280	rBV	393540	450991	14.15%	1.261%
50	9.680	1288	1291	1294	rVB2	177366	170624	5.35%	0.477%
51	9.751	1301	1303	1306	rBV	270230	226955	7.12%	0.635%
52	9.880	1321	1325	1328	rBV	1676192	1500324	47.06%	4.195%
53	10.345	1402	1404	1406	rBV2	243707	214545	6.73%	0.600%
54	10.416	1414	1416	1418	rVB2	295674	208799	6.55%	0.584%
55	10.533	1434	1436	1438	rVB2	396899	290665	9.12%	0.813%
56	10.580	1442	1444	1446	rBV	260730	205541	6.45%	0.575%
57	10.669	1455	1459	1464	rBV	2098791	1989042	62.39%	5.562%
58	10.739	1469	1471	1473	rBV	490017	405728	12.73%	1.135%
59	10.827	1483	1486	1489	rBV2	462017	480583	15.07%	1.344%
60	10.892	1495	1497	1502	rVB	497453	559483	17.55%	1.564%
61	11.210	1549	1551	1552	rBV2	304988	229493	7.20%	0.642%
62	11.310	1566	1568	1573	rBV3	490778	799453	25.08%	2.235%
63	11.368	1575	1578	1582	rVV2	1262302	1337603	41.96%	3.740%
64	11.598	1614	1617	1619	rBV	658152	626268	19.64%	1.751%
65	11.821	1652	1655	1657	rBV2	709915	719161	22.56%	2.011%
66	12.692	1801	1803	1808	rVB3	1174055	1088948	34.16%	3.045%
67	12.957	1844	1848	1851	rBV	2805102	2552068	80.05%	7.136%
68	14.010	2024	2027	2030	rBV	1088388	937018	29.39%	2.620%
69	15.468	2272	2275	2279	rVB	695153	849171	26.64%	2.375%

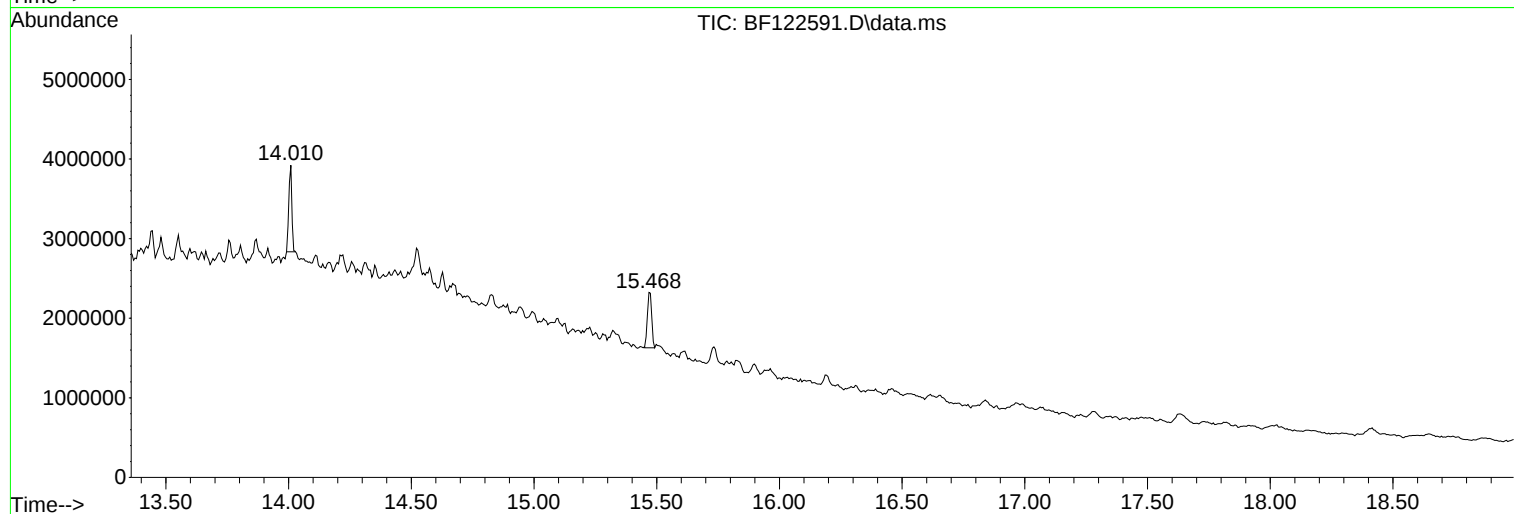
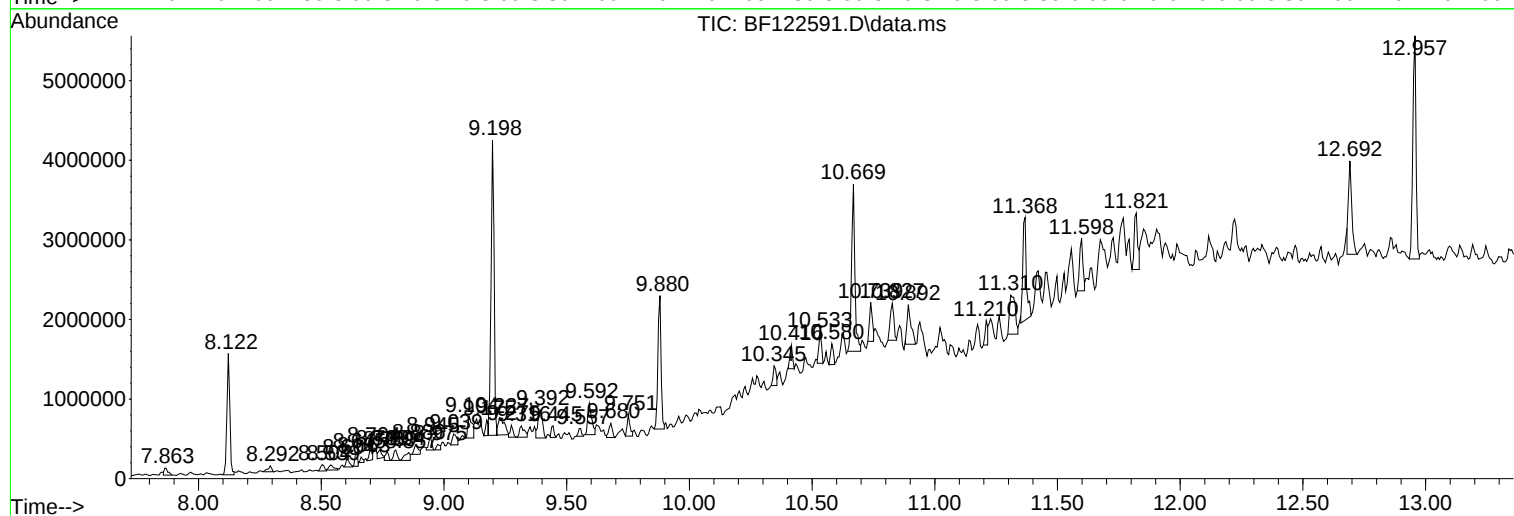
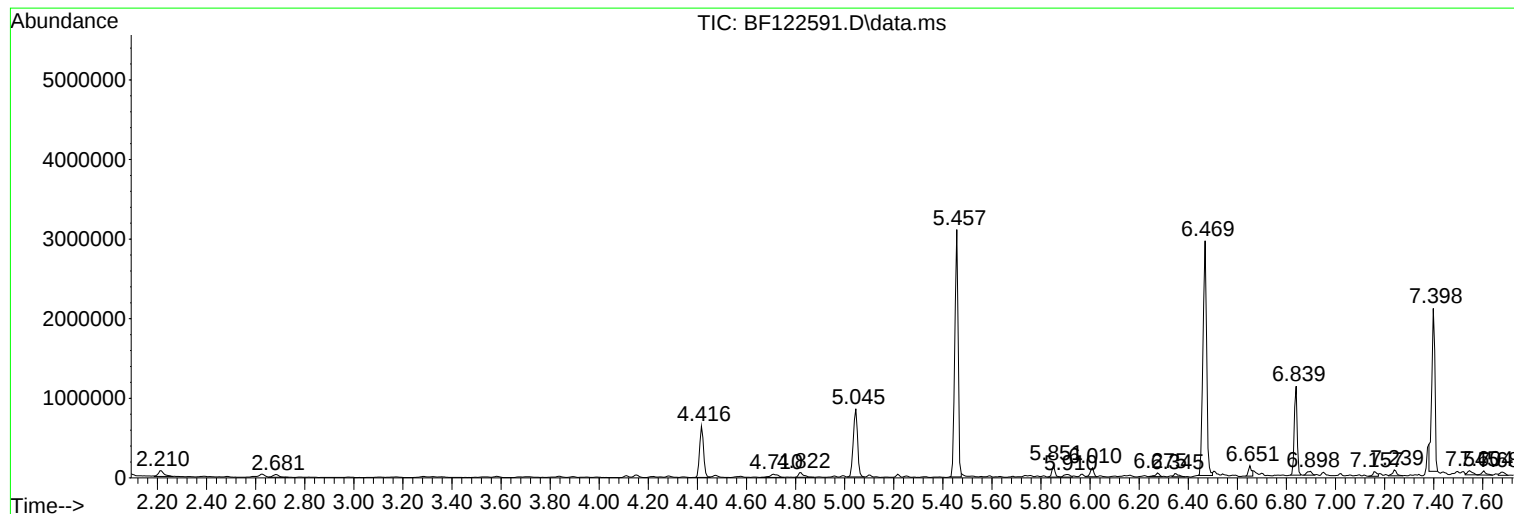
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Sample : L4971-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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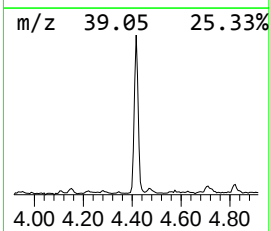
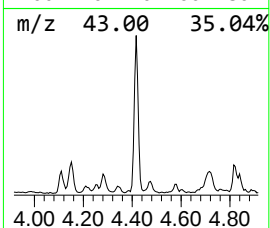
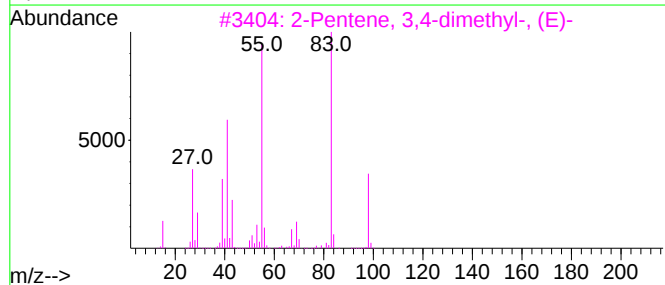
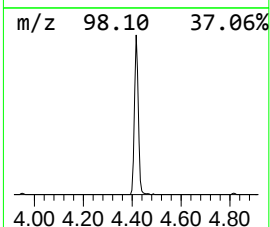
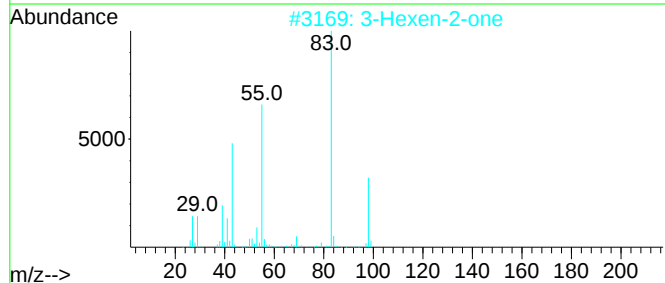
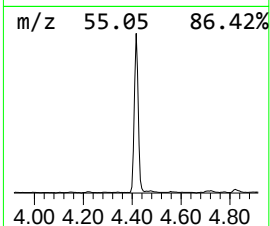
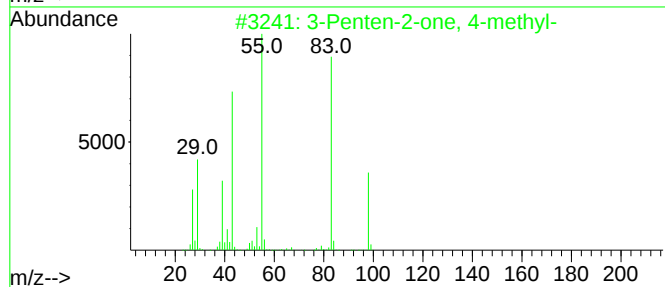
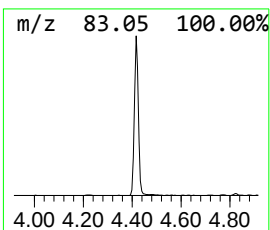
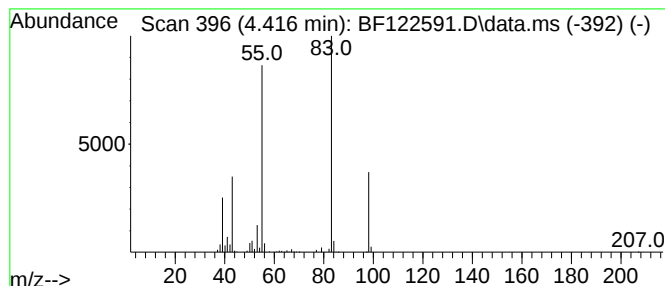
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.416	15.89 ng	725152	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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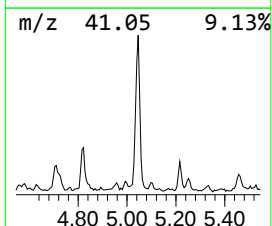
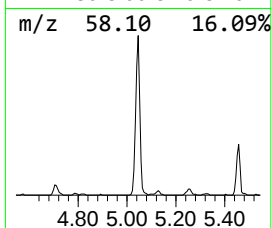
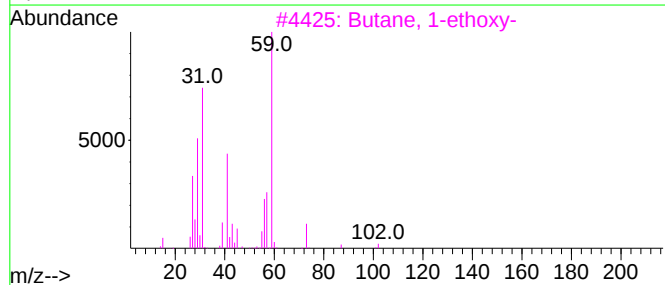
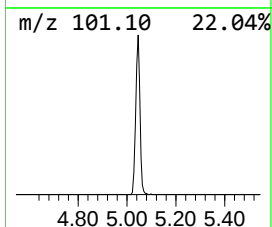
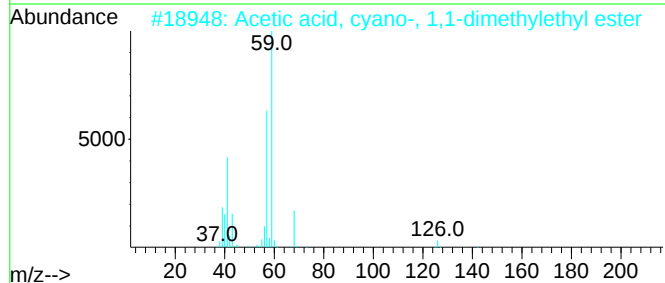
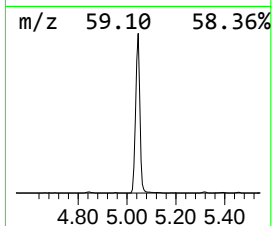
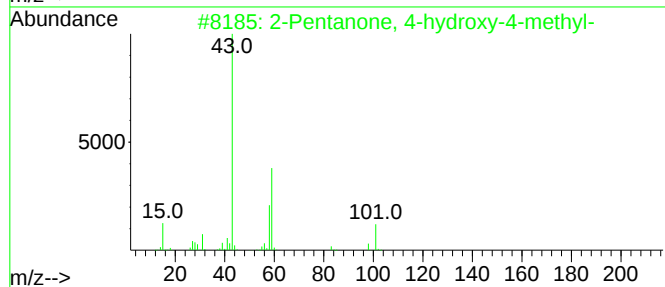
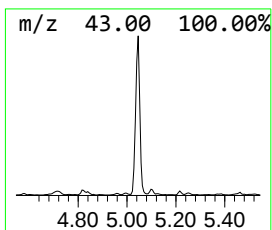
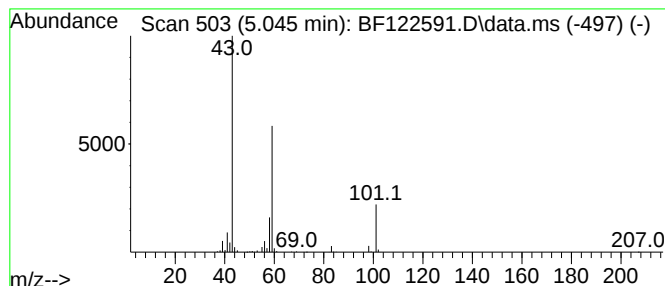
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.045	22.71 ng	1036060	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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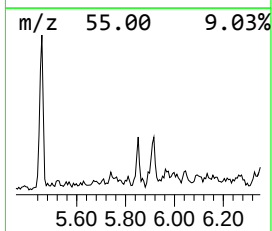
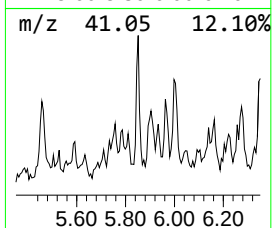
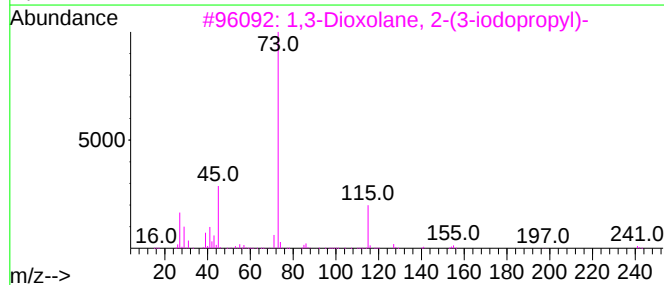
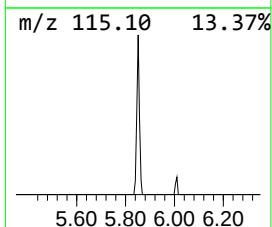
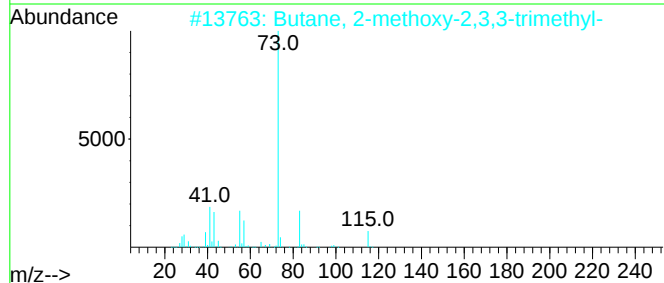
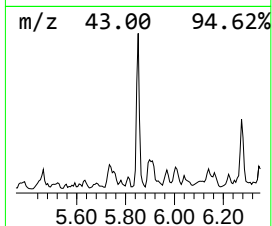
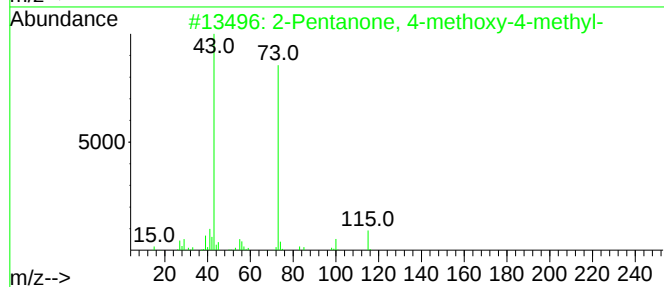
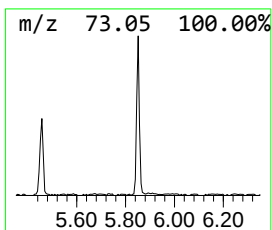
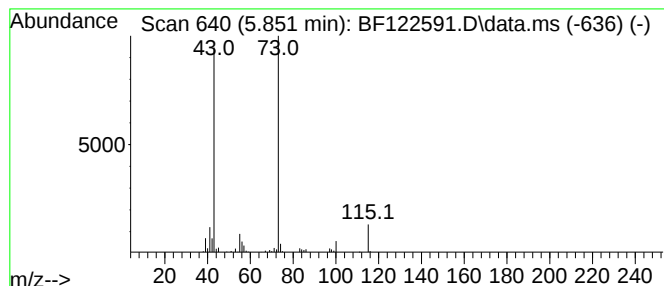
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.851	2.72 ng	124258	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	72
2			Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	35
3			1,3-Dioxolane, 2-(3-iodopropyl)-	242	C6H11IO2	058135-25-4	28
4			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	27
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	22



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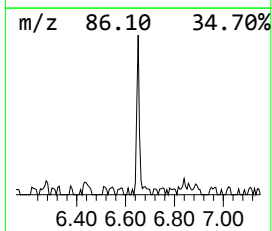
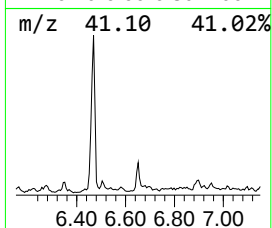
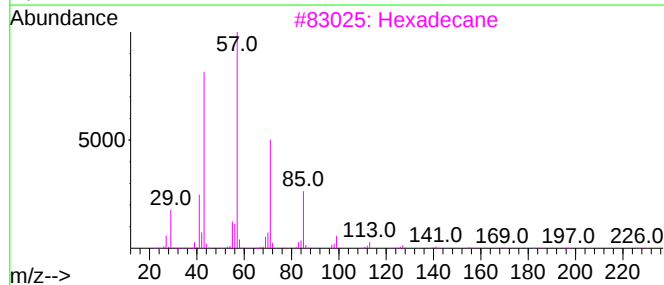
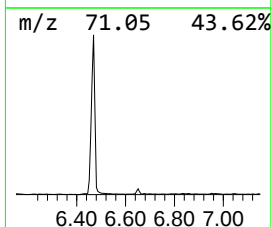
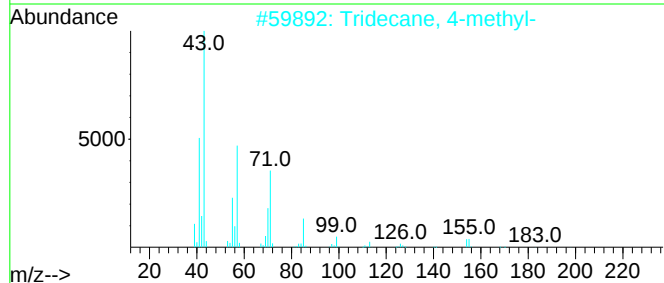
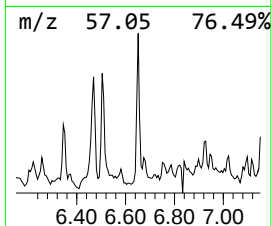
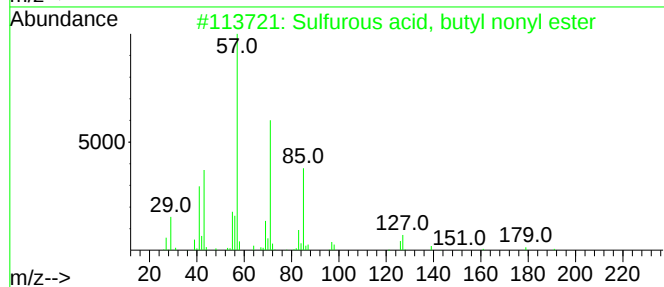
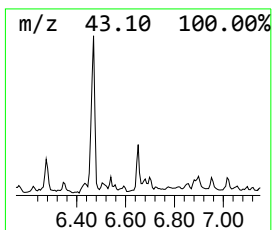
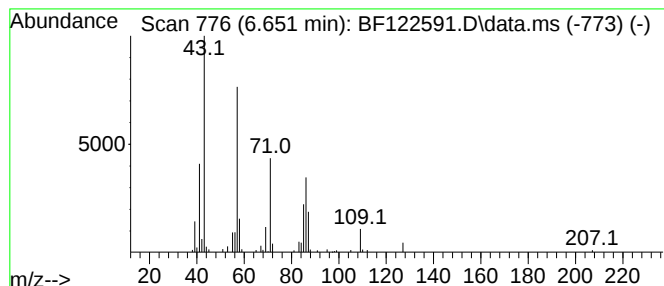
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Sulfurous acid, butyl nonyl... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.651	2.73 ng	124668	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	53
2			Tridecane, 4-methyl-	198	C14H30	026730-12-1	50
3			Hexadecane	226	C16H34	000544-76-3	50
4			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	50
5			Heptane, 2,6-dimethyl-	128	C9H20	001072-05-5	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120820\
Data File : BF122591.D
Acq On : 8 Dec 2020 16:41
Operator : JU/CG
Sample : L4971-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

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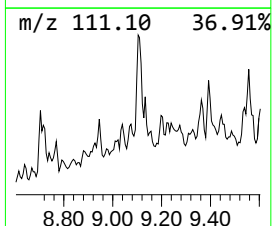
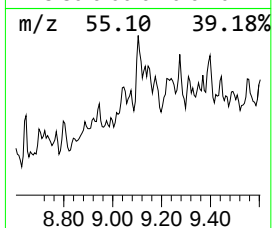
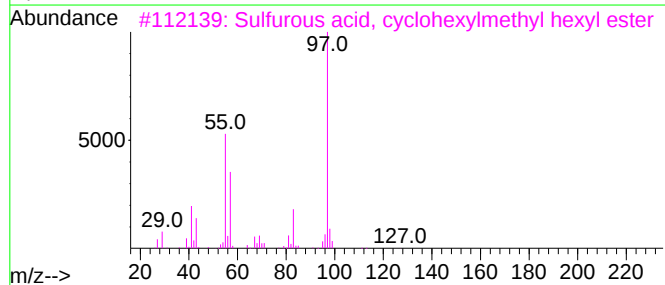
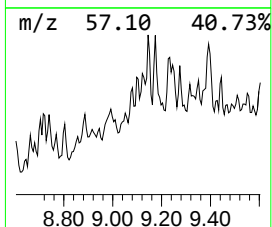
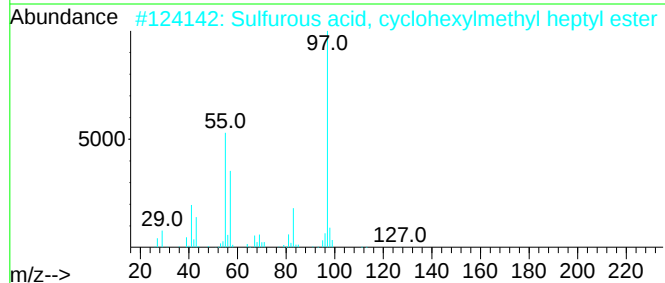
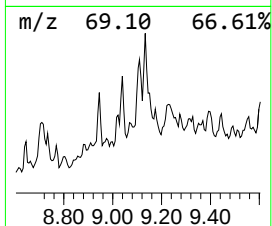
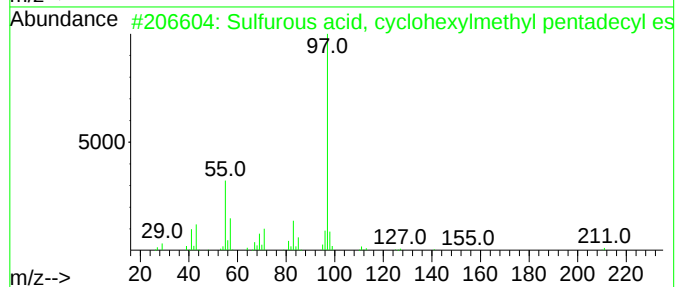
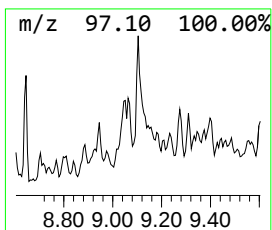
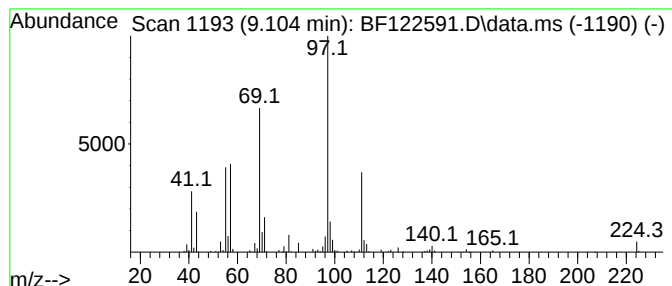
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Sulfurous acid, cyclohexylm... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.104	4.73 ng	355105	Acenaphthene-d10	9.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, cyclohexylmethyl...	388	C22H44O3S	1000309-22-3	53
2			Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	50
3			Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-6	50
4			Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	50
5			1-(Trimethylsilyl)-1-propyne	112	C6H12Si	006224-91-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120820\
Data File : BF122591.D
Acq On : 8 Dec 2020 16:41
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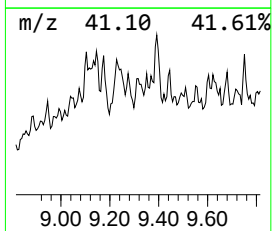
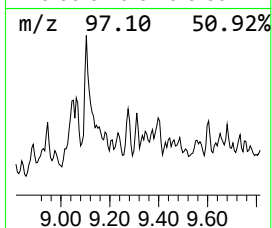
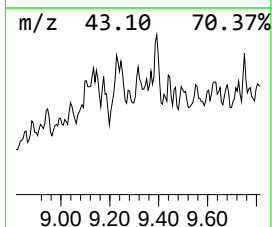
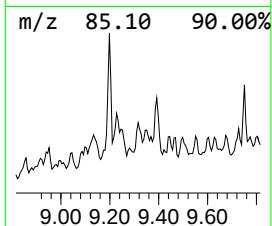
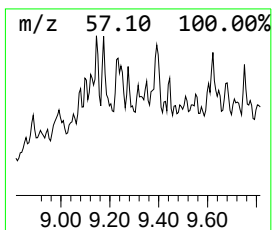
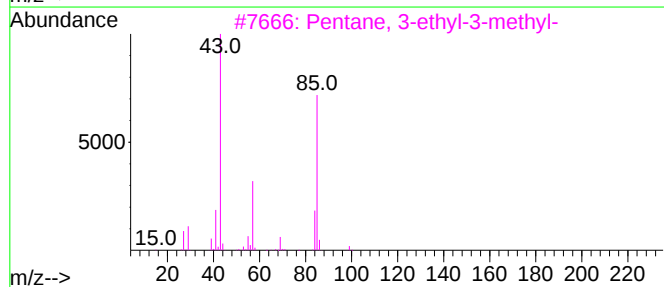
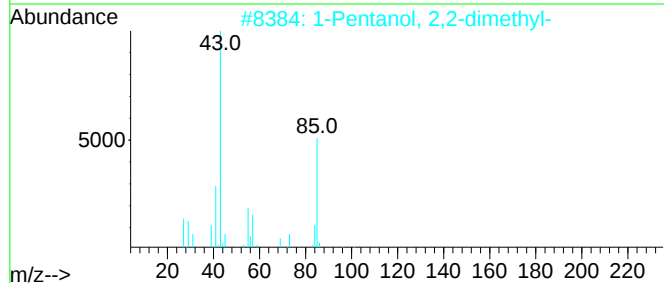
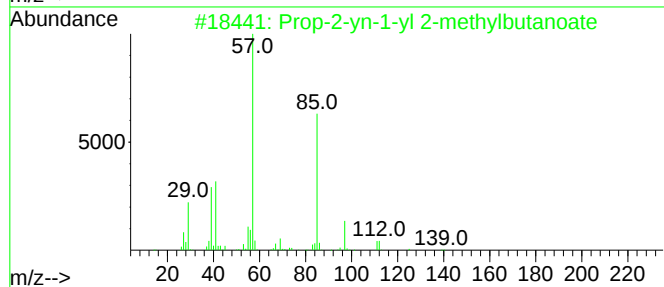
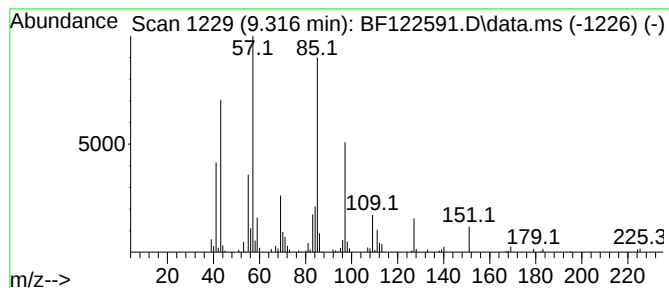
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown9.31 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.316	2.68 ng	200916	Acenaphthene-d10	9.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Prop-2-yn-1-yl 2-methylbutanoate	140	C8H12O2	1000372-70-8	43
2			1-Pentanol, 2,2-dimethyl-	116	C7H16O	002370-12-9	38
3			Pentane, 3-ethyl-3-methyl-	114	C8H18	001067-08-9	38
4			Hexane, 1,1'-oxybis-	186	C12H26O	000112-58-3	38
5			Butanoic acid, 3-methyl-, propyl...	144	C8H16O2	000557-00-6	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120820\
Data File : BF122591.D
Acq On : 8 Dec 2020 16:41
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Sample : L4971-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

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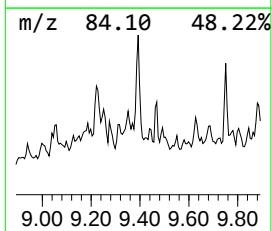
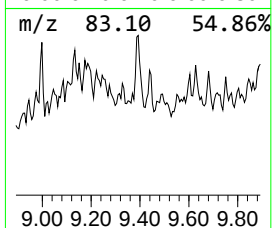
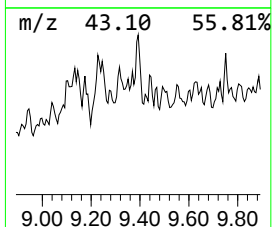
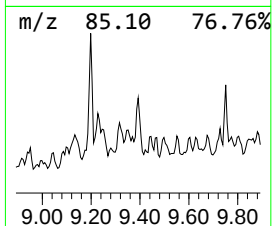
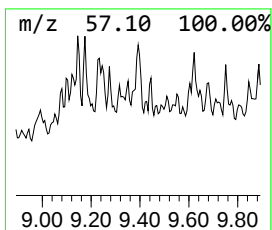
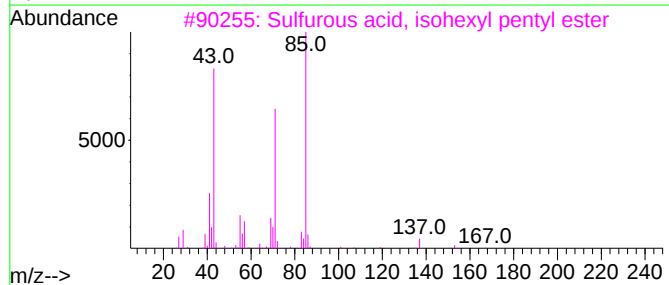
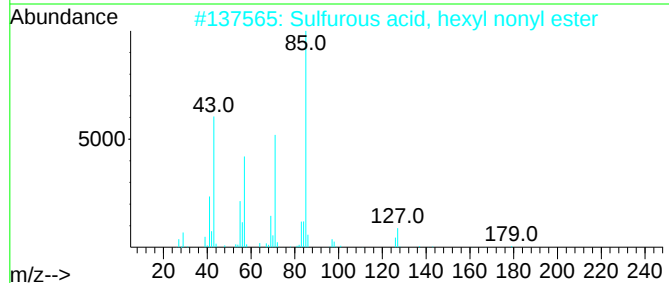
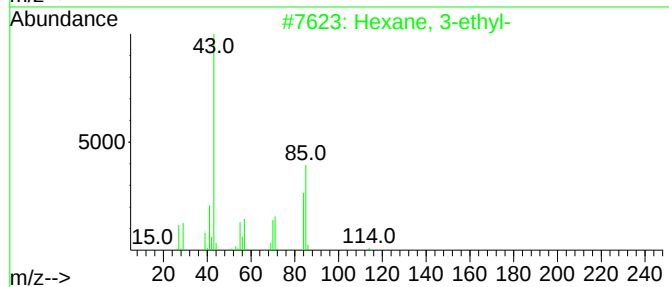
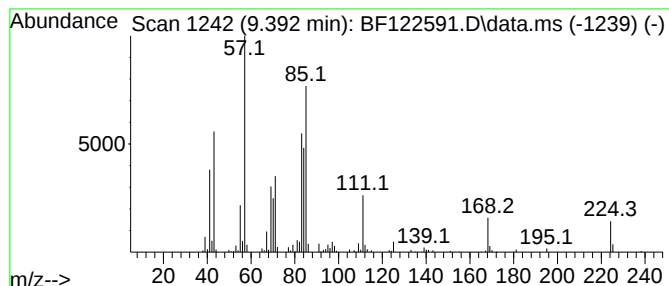
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown9.39 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.392	5.90 ng	442561	Acenaphthene-d10	9.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-ethyl-	114	C8H18	000619-99-8	38
2			Sulfurous acid, hexyl nonyl ester	292	C15H32O3S	1000309-13-1	35
3			Sulfurous acid, isohexyl pentyl ...	236	C11H24O3S	1000309-14-0	35
4			Decane, 5,6-dimethyl-	170	C12H26	001636-43-7	35
5			Tridecane, 5-methyl-	198	C14H30	025117-31-1	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120820\
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Acq On : 8 Dec 2020 16:41
Operator : JU/CG
Sample : L4971-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

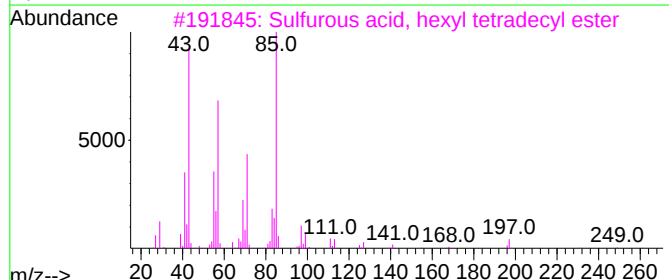
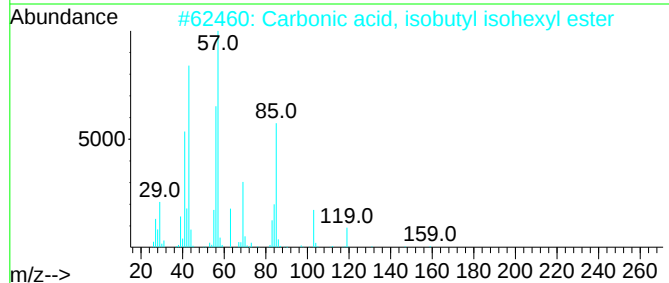
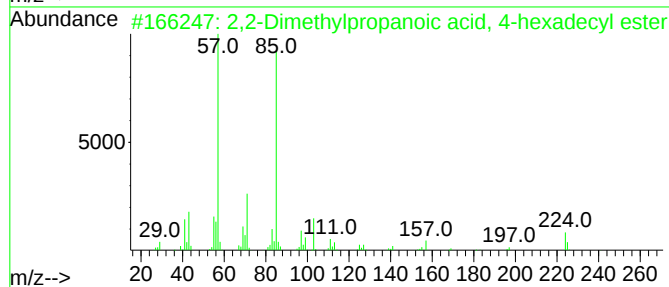
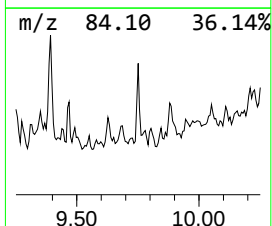
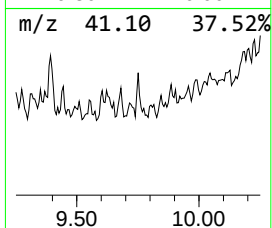
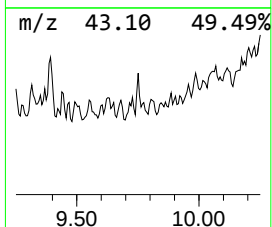
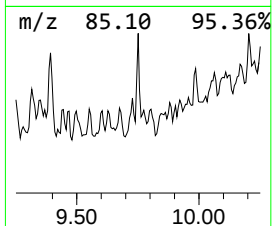
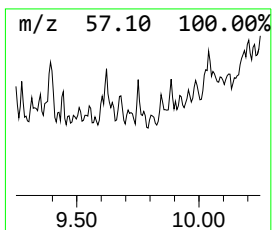
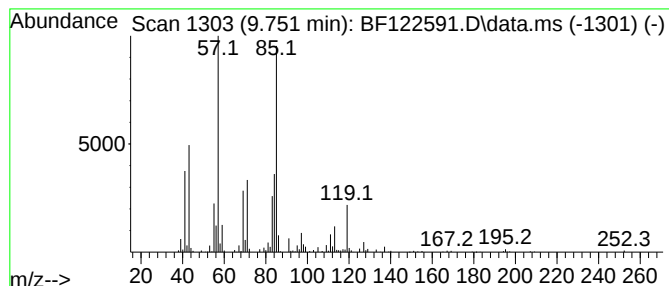
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 2,2-Dimethylpropanoic acid,... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.751	3.03 ng	226955	Acenaphthene-d10	9.880	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2-Dimethylpropanoic acid, 4-he...	326	C21H42O2	1000282-85-5	53
2	Carbonic acid, isobutyl isohexyl...	202	C11H22O3	1000314-60-3	53
3	Sulfurous acid, hexyl tetradecyl...	362	C20H42O3S	1000309-13-6	50
4	3-Hexanone, 2,5-dimethyl-	128	C8H16O	001888-57-9	47
5	Malonic acid, 3-methylpentyl pen...	398	C24H46O4	1000348-28-8	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120820\
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Misc :
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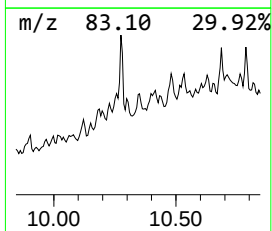
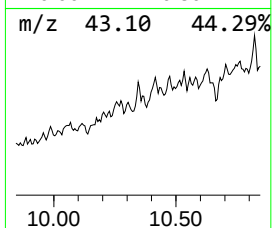
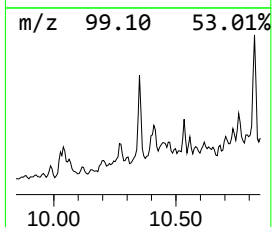
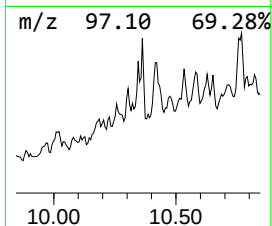
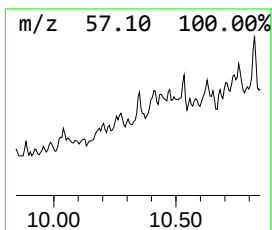
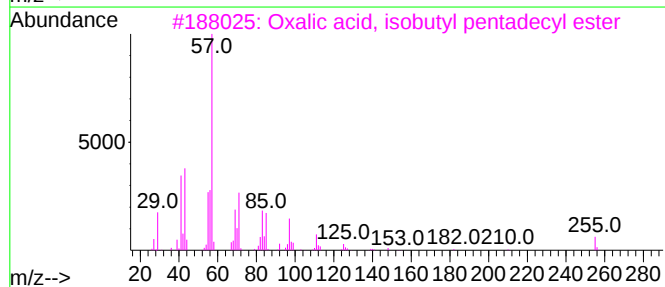
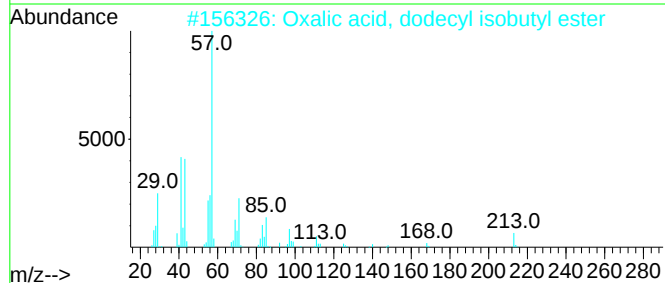
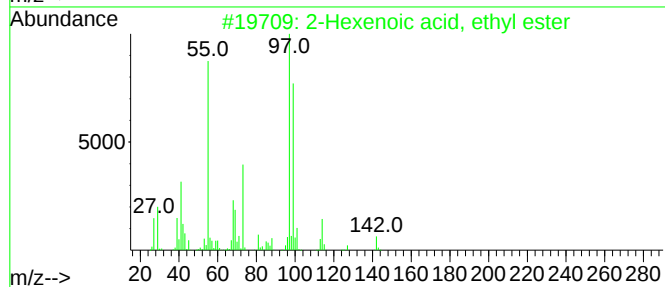
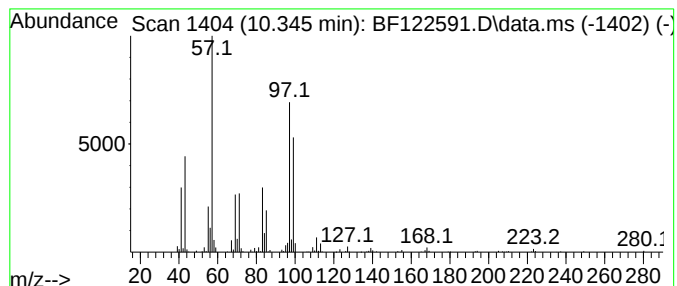
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown10.34 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.345	2.86 ng	214545	Acenaphthene-d10	9.880	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexenoic acid, ethyl ester	142	C8H14O2	001552-67-6	43
2	Oxalic acid, dodecyl isobutyl ester	314	C18H34O4	1000309-37-7	38
3	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	38
4	Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	35
5	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120820\
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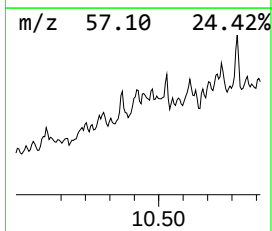
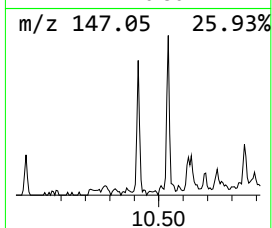
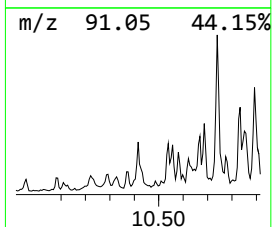
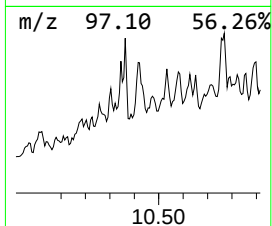
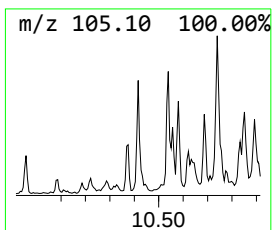
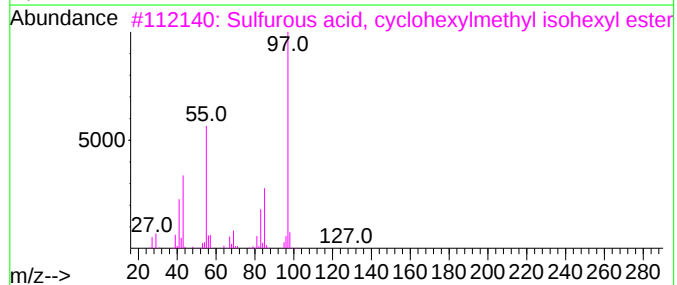
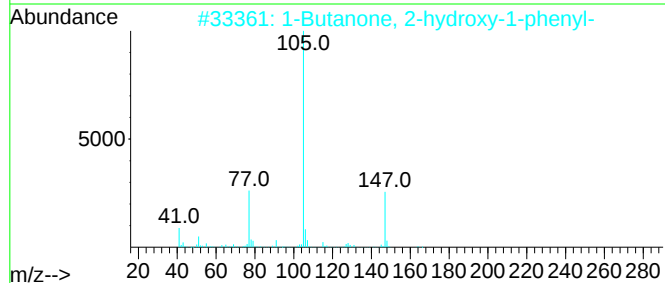
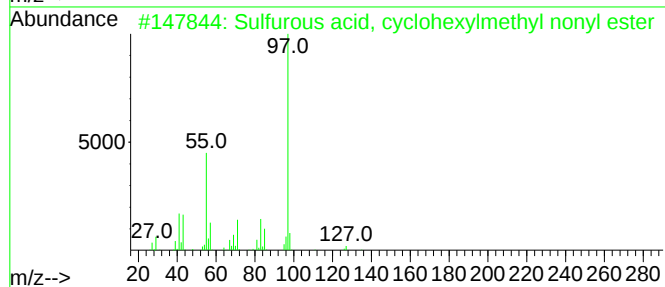
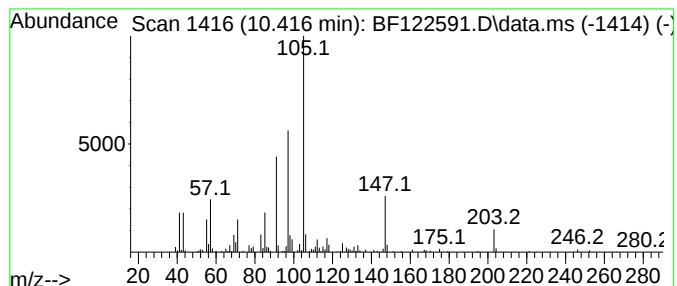
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown10.41 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.416	2.78 ng	208799	Acenaphthene-d10	9.880	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, cyclohexylmethyl...	304	C16H32O3S	1000309-21-8	22
2	1-Butanone, 2-hydroxy-1-phenyl-	164	C10H12O2	016183-46-3	22
3	Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-5	16
4	Tetrahydropyran-4-ol, 2,2-dimeth...	255	C13H21NO2S	1000316-43-9	12
5	Sulfurous acid, cyclohexylmethyl...	416	C24H48O3S	1000309-22-5	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120820\
Data File : BF122591.D
Acq On : 8 Dec 2020 16:41
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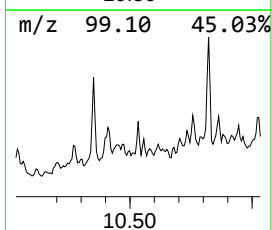
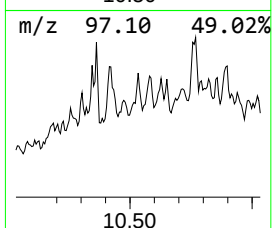
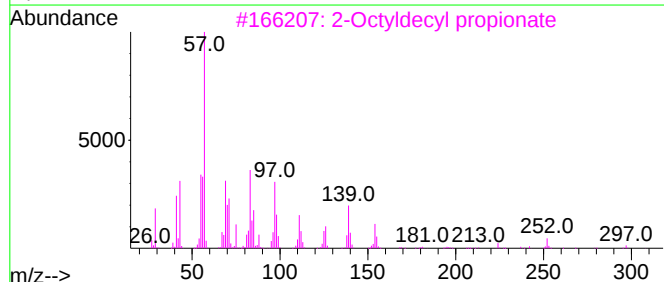
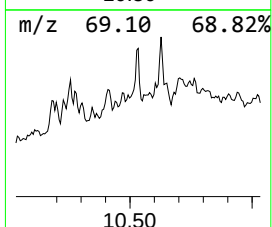
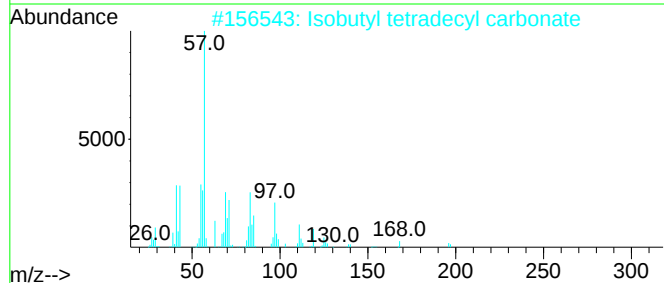
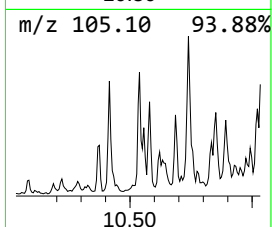
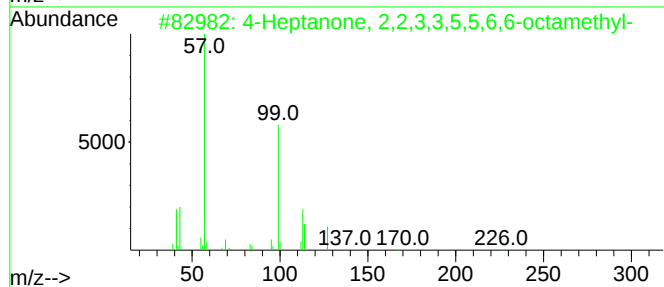
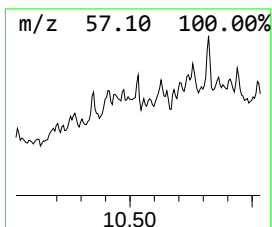
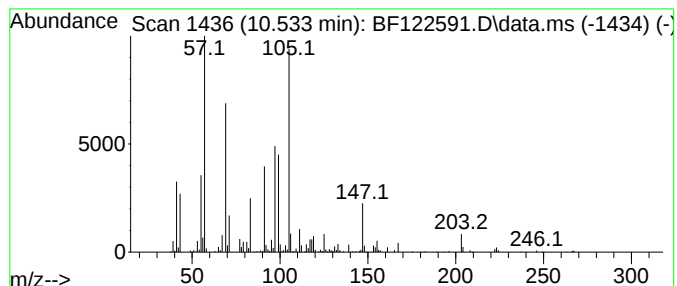
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown10.53 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.533	3.87 ng	290665	Acenaphthene-d10	9.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanone, 2,2,3,3,5,5,6,6-oct...	226	C15H30O	016424-66-1	12
2			Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	10
3			2-Octyldecyl propionate	326	C21H42O2	1000368-56-3	10
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	9
5			2-Thiopheneacetic acid, 3,5-dime...	252	C14H20O2S	1000278-92-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120820\
Data File : BF122591.D
Acq On : 8 Dec 2020 16:41
Operator : JU/CG
Sample : L4971-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
5S1-A-D-COMP

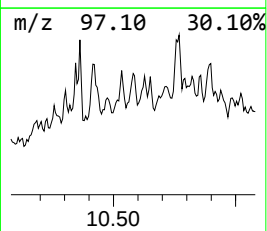
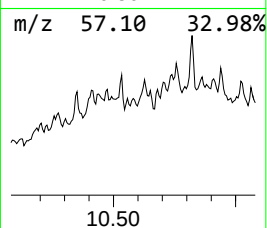
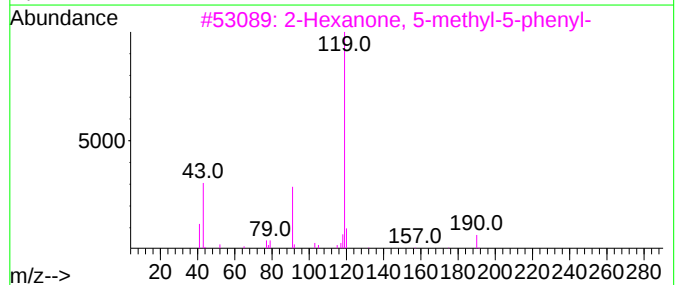
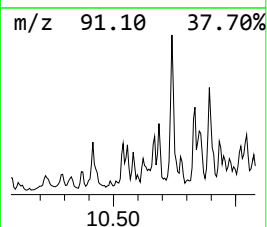
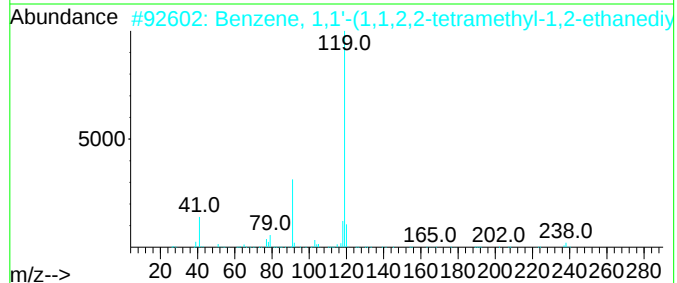
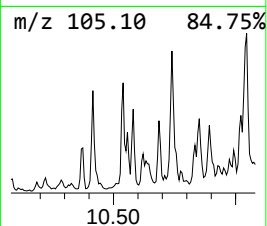
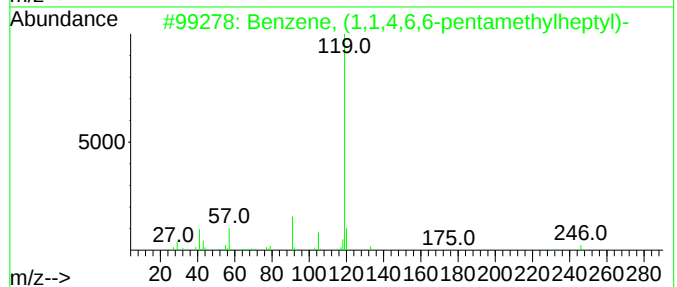
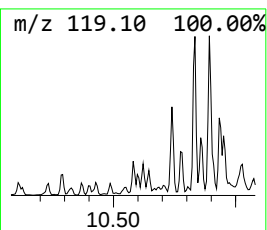
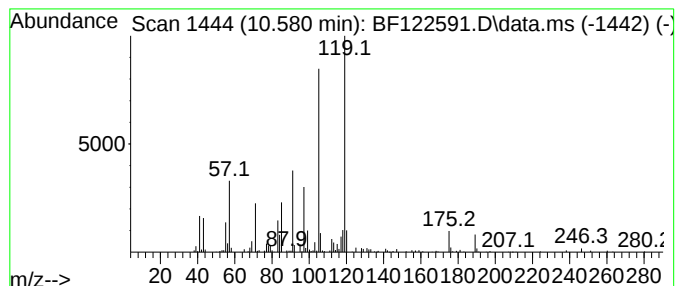
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown10.58 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.580	2.74 ng	205541	Acenaphthene-d10	9.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1,1,4,6,6-pentamethylh...	246	C18H30	055134-07-1	43
2			Benzene, 1,1'-(1,1,2,2-tetrameth...	238	C18H22	001889-67-4	38
3			2-Hexanone, 5-methyl-5-phenyl-	190	C13H18O	014128-61-1	38
4			Ethanone, 2-bromo-1-(4-methylphe...	212	C9H9BrO	000619-41-0	38
5			Tridecane, 2-methyl-2-phenyl-	274	C20H34	027854-41-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120820\
Data File : BF122591.D
Acq On : 8 Dec 2020 16:41
Operator : JU/CG
Sample : L4971-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

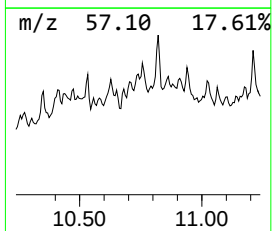
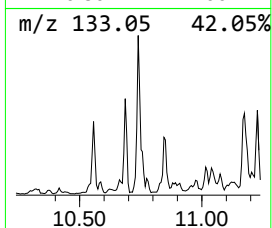
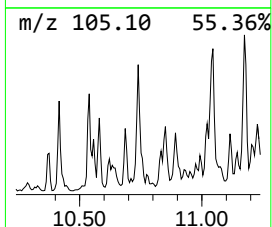
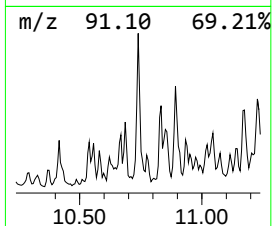
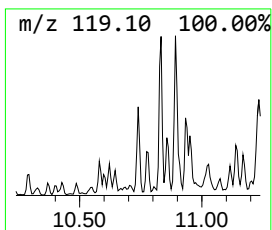
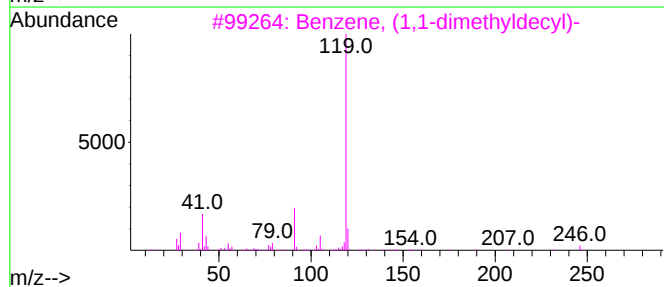
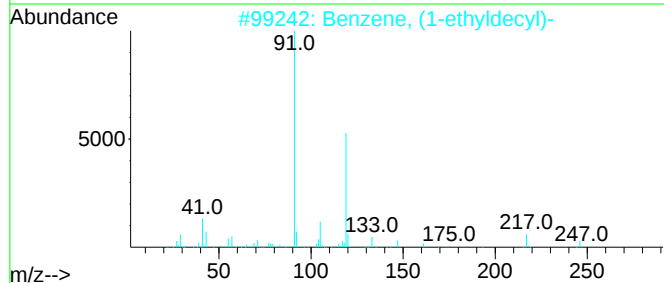
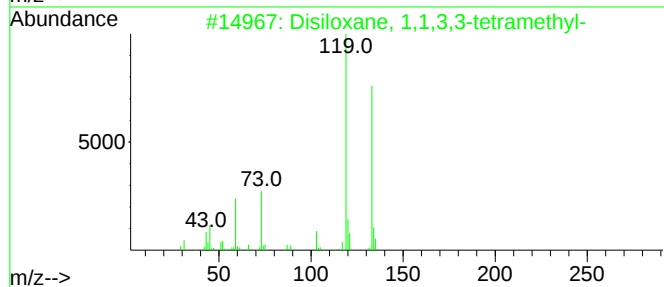
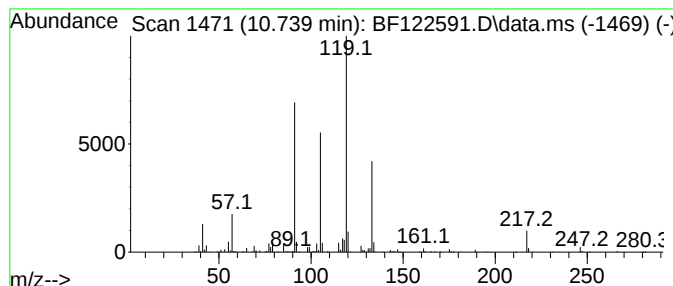
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ClientSampleId :
5S1-A-D-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Disiloxane, 1,1,3,3-tetrame... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.739	6.07 ng	405728	Phenanthrene-d10		11.368	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Disiloxane, 1,1,3,3-tetramethyl-		134	C4H14OSi2	003277-26-7	64
2	Benzene, (1-ethyldecyl)-		246	C18H30	002400-00-2	62
3	Benzene, (1,1-dimethyldecyl)-		246	C18H30	027854-40-6	53
4	Benzene, 1-ethyl-2,4-dimethyl-		134	C10H14	000874-41-9	50
5	2,4,4,6-Tetramethyl-6-phenyl-1-h...		230	C17H26	1000293-27-9	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120820\
Data File : BF122591.D
Acq On : 8 Dec 2020 16:41
Operator : JU/CG
Sample : L4971-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
5S1-A-D-COMP

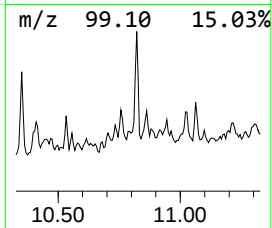
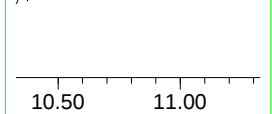
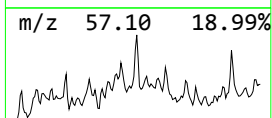
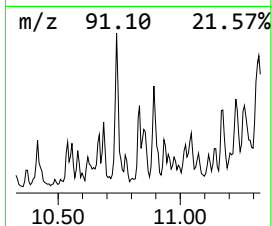
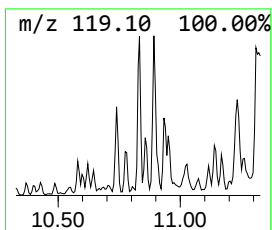
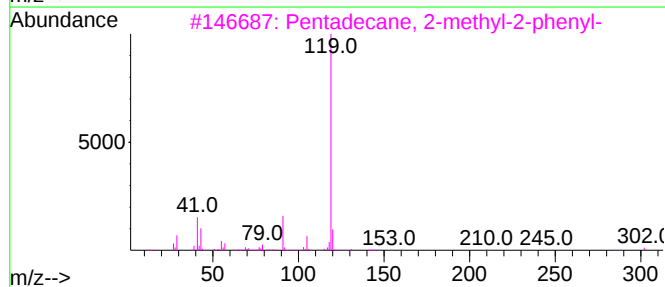
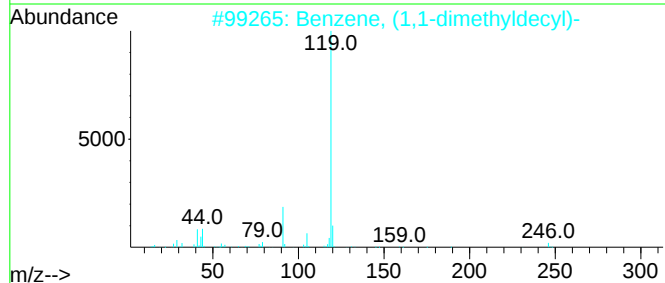
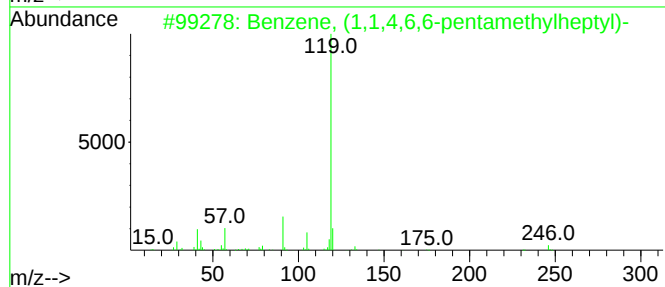
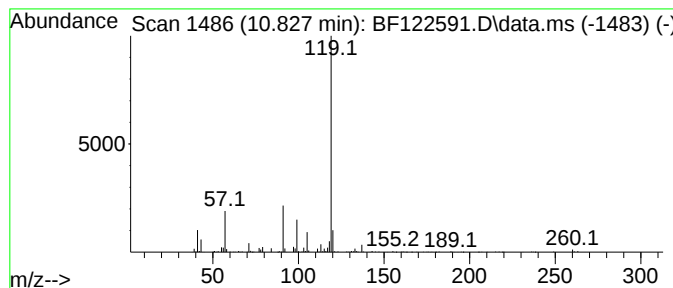
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Pentadecane, 2-methyl-2-phe... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.827	7.19 ng	480583	Phenanthrene-d10	11.368

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1,1,4,6,6-pentamethylh...	246	C18H30	055134-07-1	64
2			Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	59
3			Pentadecane, 2-methyl-2-phenyl-	302	C22H38	029138-94-1	59
4			3-Methylbenzoic acid, 4-chloro-2...	260	C15H13ClO2	1000331-26-6	50
5			1,3-Benzenediol, o-(2-methylbenz...	228	C14H12O3	1000330-73-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120820\
Data File : BF122591.D
Acq On : 8 Dec 2020 16:41
Operator : JU/CG
Sample : L4971-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
5S1-A-D-COMP

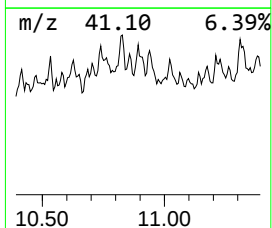
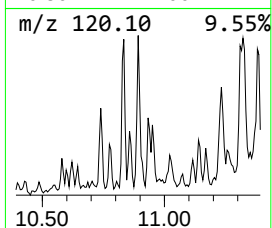
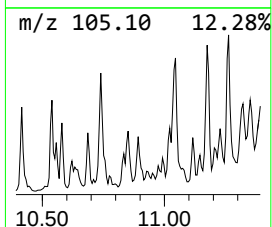
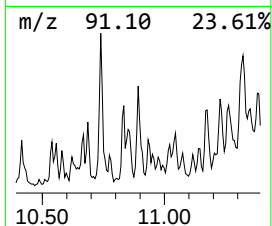
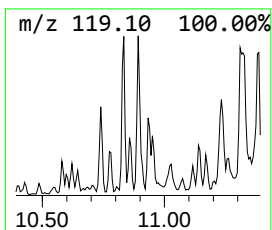
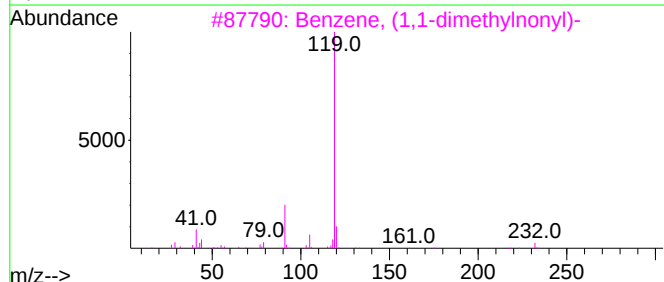
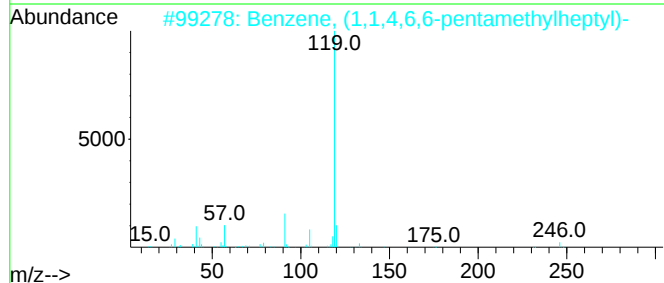
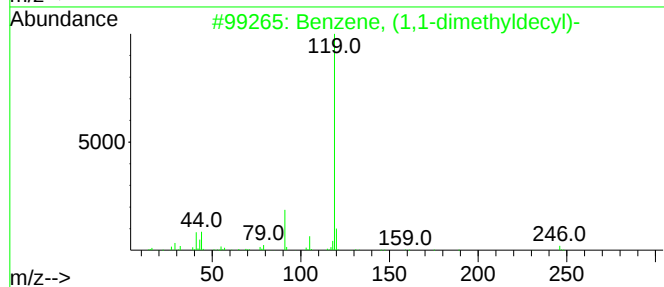
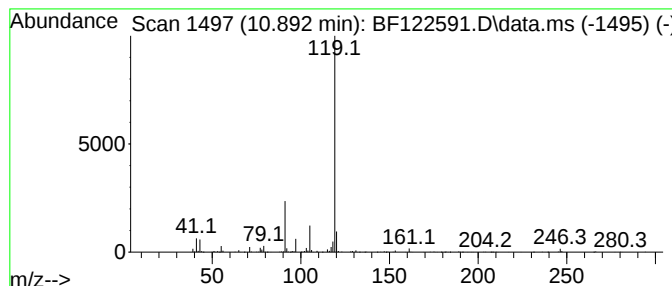
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 Benzene, (1,1-dimethyldecyl)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.892	8.37 ng	559483	Phenanthrene-d10	11.368

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	83
2			Benzene, (1,1,4,6,6-pentamethylh...	246	C18H30	055134-07-1	72
3			Benzene, (1,1-dimethylnonyl)-	232	C17H28	055191-25-8	72
4			o-Toluic acid, oct-3-en-2-yl ester	246	C16H22O2	1000292-51-3	64
5			m-Toluic acid, oct-3-en-2-yl ester	246	C16H22O2	1000292-61-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120820\
Data File : BF122591.D
Acq On : 8 Dec 2020 16:41
Operator : JU/CG
Sample : L4971-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

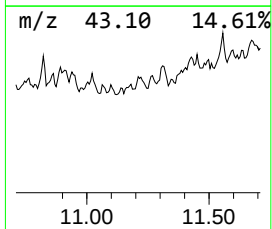
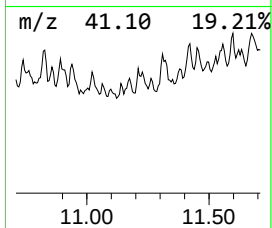
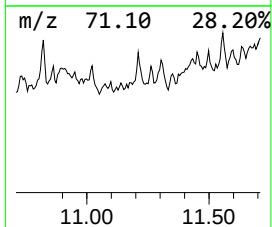
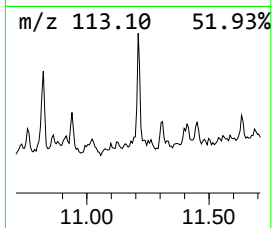
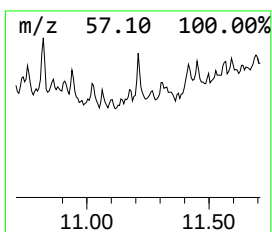
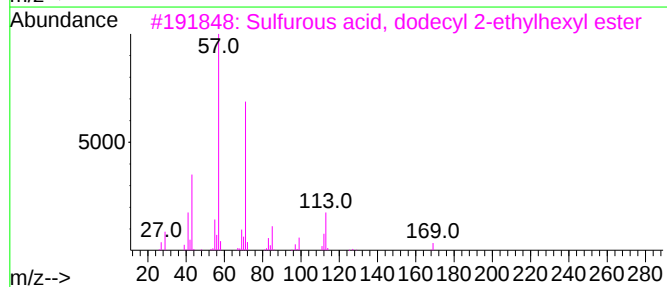
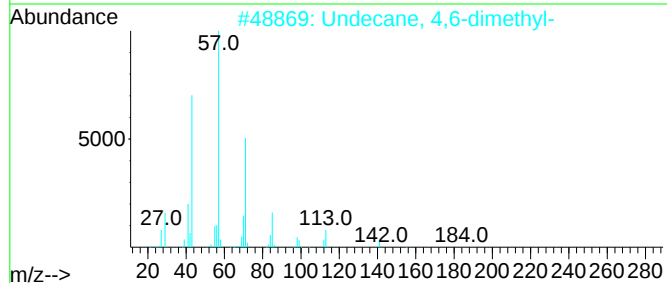
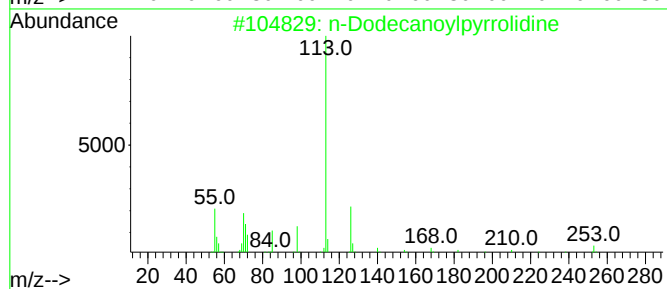
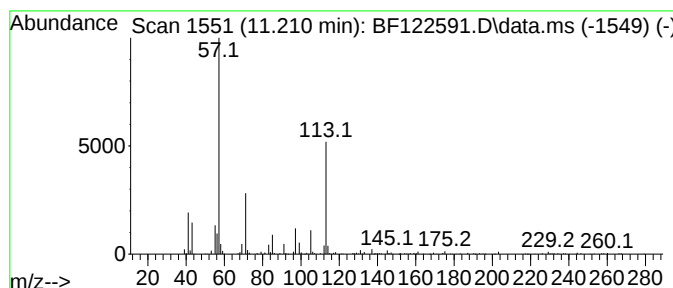
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 unknown11.21 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.210	3.43 ng	229493	Phenanthrene-d10	11.368	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Dodecanoylpyrrolidine	253	C16H31NO	070974-45-7	38
2	Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	38
3	Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	38
4	Sulfurous acid, 2-ethylhexyl tri...	376	C21H44O3S	1000309-19-6	32
5	Nonane, 2,2,4,4,6,8,8-heptamethyl-	226	C16H34	004390-04-9	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120820\
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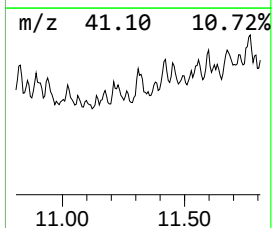
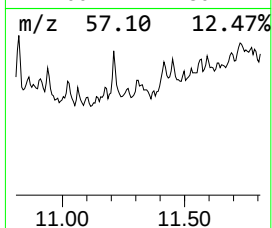
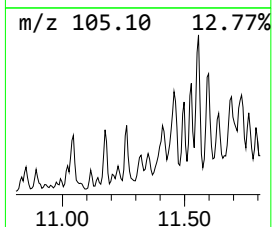
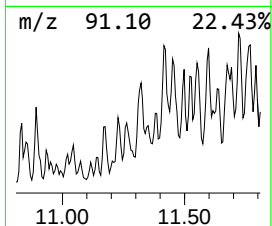
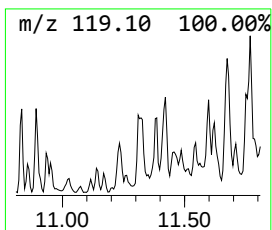
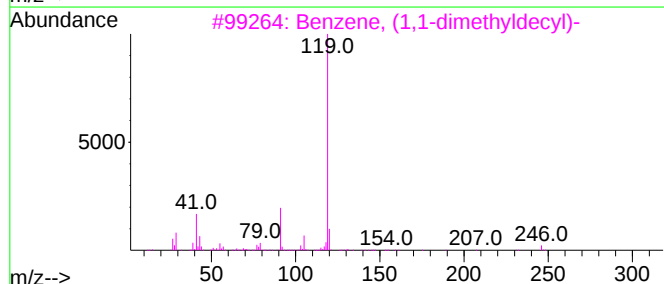
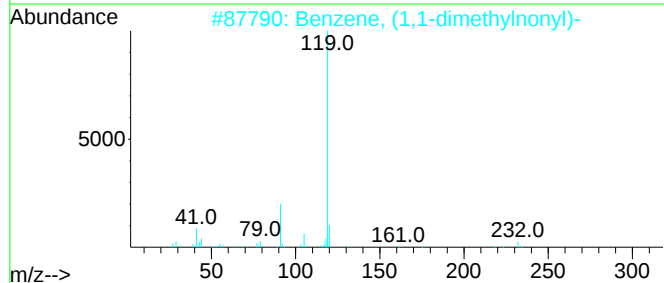
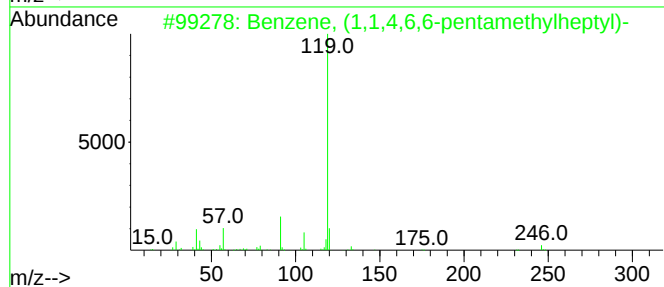
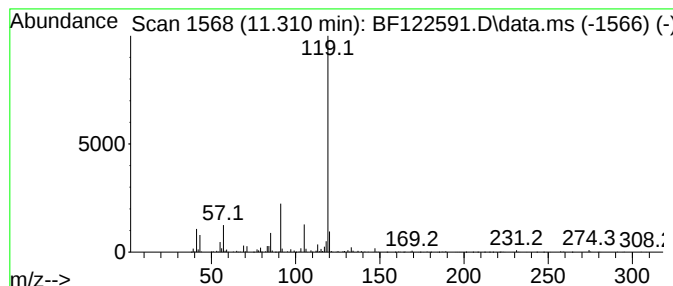
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 Benzene, (1,1,4,6,6-pentame... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.310	11.95 ng	799453	Phenanthrene-d10	11.368	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1,1,4,6,6-pentamethylh...	246	C18H30	055134-07-1	72
2	Benzene, (1,1-dimethylnonyl)-	232	C17H28	055191-25-8	64
3	Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	64
4	Pentadecane, 2-methyl-2-phenyl-	302	C22H38	029138-94-1	59
5	p-Menthane, 2,3-dibromo-8-phenyl-	372	C16H22Br2	1000152-61-6	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120820\
Data File : BF122591.D
Acq On : 8 Dec 2020 16:41
Operator : JU/CG
Sample : L4971-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

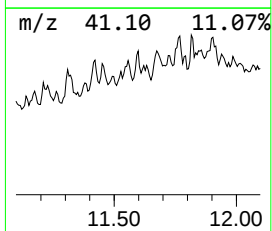
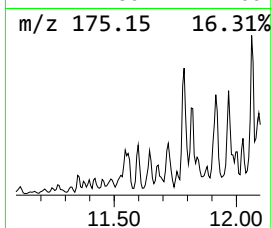
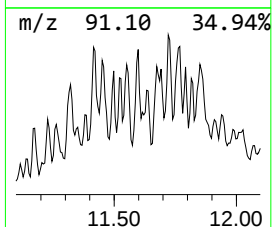
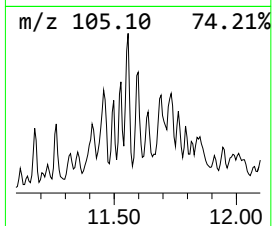
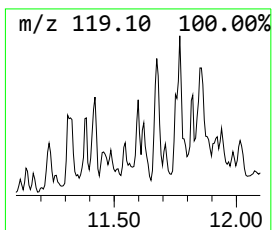
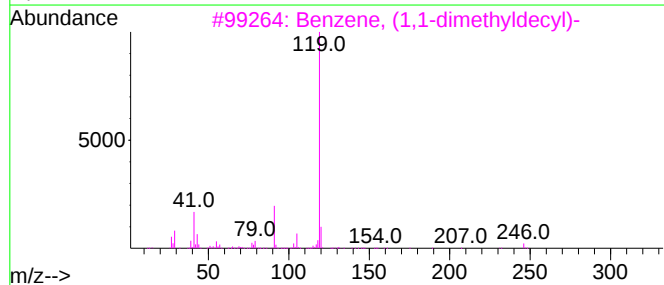
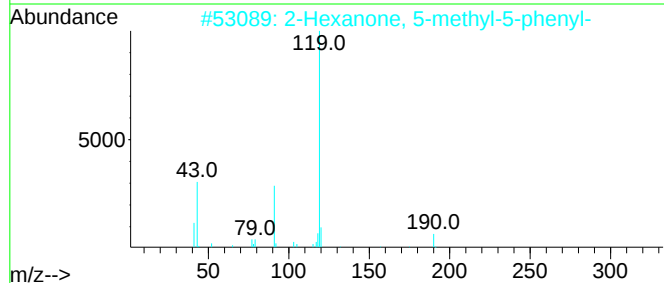
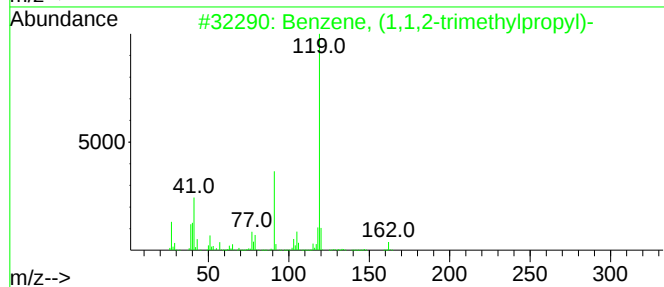
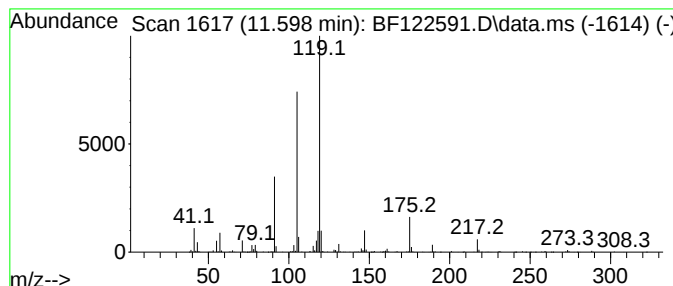
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 Benzene, (1,1,2-trimethylpr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.598	9.36 ng	626268	Phenanthrene-d10		11.368	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, (1,1,2-trimethylpropyl)-		162	C12H18	026356-11-6	53
2	2-Hexanone, 5-methyl-5-phenyl-		190	C13H18O	014128-61-1	50
3	Benzene, (1,1-dimethyldecyl)-		246	C18H30	027854-40-6	50
4	Benzamide, 3-methyl-N-allyl-		175	C11H13NO	1000339-09-8	47
5	Tridecane, 2-methyl-2-phenyl-		274	C20H34	027854-41-7	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120820\
Data File : BF122591.D
Acq On : 8 Dec 2020 16:41
Operator : JU/CG
Sample : L4971-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
5S1-A-D-COMP

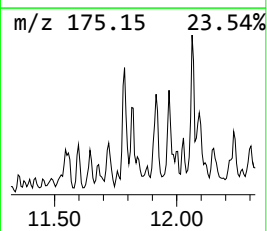
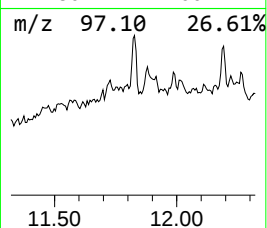
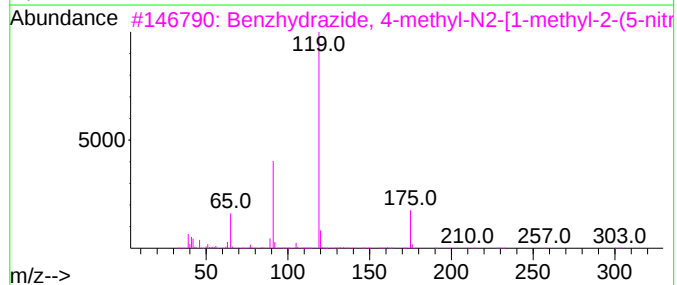
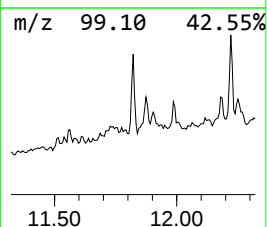
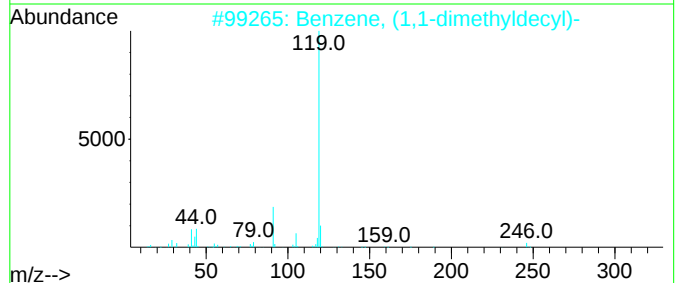
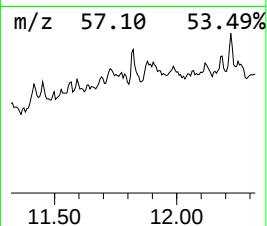
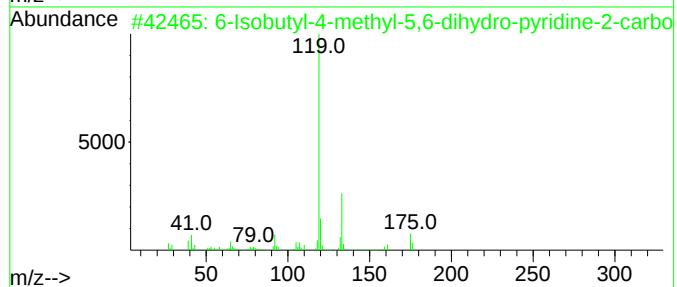
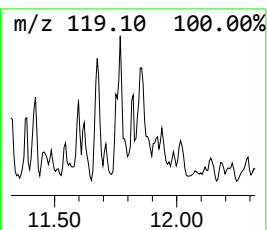
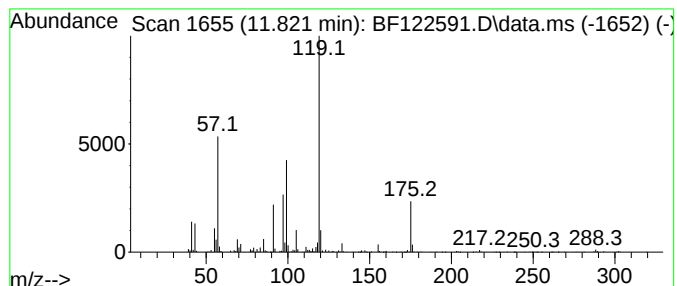
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 unknown11.82 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.821	10.75 ng	719161	Phenanthrene-d10	11.368

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		6-Isobutyl-4-methyl-5,6-dihydro-...	176	C11H16N2	1000185-72-5	43
2		Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	38
3		Benzhydrazide, 4-methyl-N2-[1-me...	303	C12H13N7O3	324021-25-2	38
4		Benzamide, 3-methyl-N-allyl-	175	C11H13NO	1000339-09-8	38
5		3-Methylbenzoic acid, 2-biphenyl...	288	C20H16O2	1000331-27-0	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120820\
Data File : BF122591.D
Acq On : 8 Dec 2020 16:41
Operator : JU/CG
Sample : L4971-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
5S1-A-D-COMP

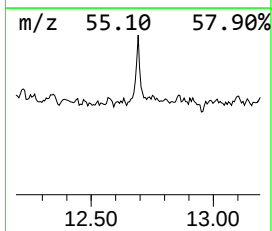
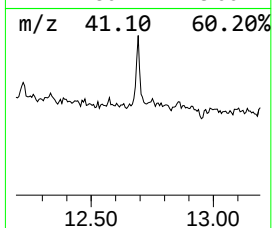
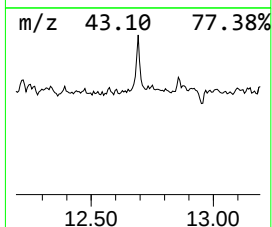
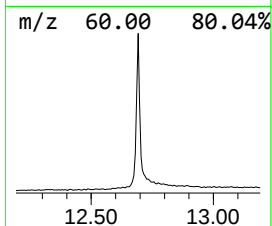
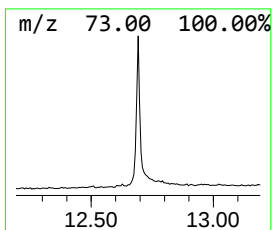
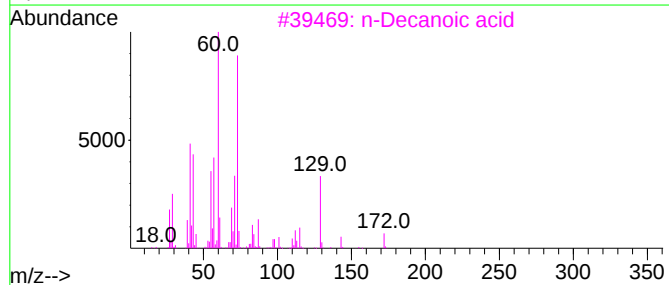
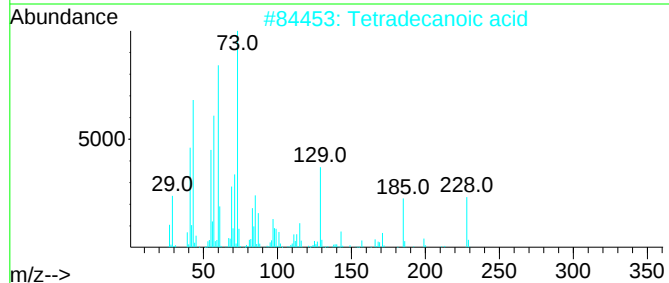
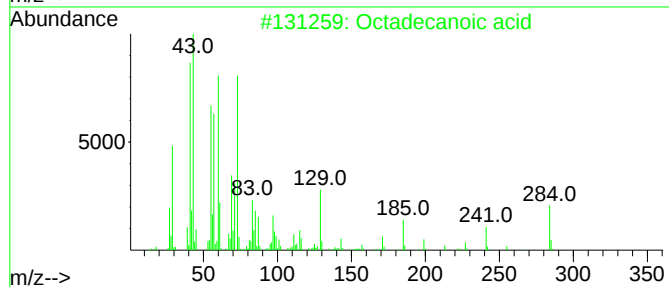
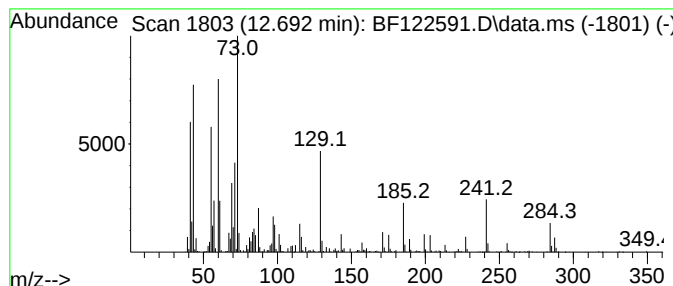
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.692	23.24 ng	1088950	Chrysene-d12	14.009

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	94
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3		n-Decanoic acid	172	C10H20O2	000334-48-5	76
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
5		Dodecanoic acid	200	C12H24O2	000143-07-7	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120820\
Data File : BF122591.D
Acq On : 8 Dec 2020 16:41
Operator : JU/CG
Sample : L4971-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
5S1-A-D-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.416	15.9	ng	725152	1	6.839	912467	20.0
2-Pentanone, 4-...	5.045	22.7	ng	1036060	1	6.839	912467	20.0
2-Pentanone, 4-...	5.851	2.7	ng	124258	1	6.839	912467	20.0
Sulfurous acid,...	6.651	2.7	ng	124668	1	6.839	912467	20.0
Sulfurous acid,...	9.104	4.7	ng	355105	3	9.880	1500320	20.0
unknown9.31	9.316	2.7	ng	200916	3	9.880	1500320	20.0
unknown9.39	9.392	5.9	ng	442561	3	9.880	1500320	20.0
2,2-Dimethylpro...	9.751	3.0	ng	226955	3	9.880	1500320	20.0
unknown10.34	10.345	2.9	ng	214545	3	9.880	1500320	20.0
unknown10.41	10.416	2.8	ng	208799	3	9.880	1500320	20.0
unknown10.53	10.533	3.9	ng	290665	3	9.880	1500320	20.0
unknown10.58	10.580	2.7	ng	205541	3	9.880	1500320	20.0
Disiloxane, 1,1...	10.739	6.1	ng	405728	4	11.368	1337600	20.0
Pentadecane, 2-...	10.827	7.2	ng	480583	4	11.368	1337600	20.0
Benzene, (1,1-d...	10.892	8.4	ng	559483	4	11.368	1337600	20.0
unknown11.21	11.210	3.4	ng	229493	4	11.368	1337600	20.0
Benzene, (1,1,4...	11.310	11.9	ng	799453	4	11.368	1337600	20.0
Benzene, (1,1,2...	11.598	9.4	ng	626268	4	11.368	1337600	20.0
unknown11.82	11.821	10.8	ng	719161	4	11.368	1337600	20.0
Octadecanoic acid	12.692	23.2	ng	1088950	5	14.009	937018	20.0