

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110321\
 Data File : BF126026.D
 Acq On : 3 Nov 2021 18:48
 Operator : JU/CG
 Sample : M4427-02 5X
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FDR-BH-5-20211029-6.5-7

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-BF110321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126026.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.451	568	572	576	rBV	905998	759478	8.66%	0.484%
2	6.463	740	744	752	rBV	859291	826296	9.42%	0.527%
3	6.657	773	777	779	rBV	351559	291076	3.32%	0.186%
4	6.851	806	810	814	rVB	1200756	1025132	11.68%	0.654%
5	7.034	837	841	845	rVB	172104	157999	1.80%	0.101%
6	7.081	845	849	850	rBV	98439	110457	1.26%	0.070%
7	7.234	870	875	877	rBV2	96659	123354	1.41%	0.079%
8	7.381	897	900	902	rBV	495065	485552	5.53%	0.310%
9	7.404	902	904	906	rVV	674518	558279	6.36%	0.356%
10	7.457	910	913	916	rVB	1003565	811402	9.25%	0.517%
11	7.492	916	919	921	rBV2	135411	143669	1.64%	0.092%
12	7.534	923	926	928	rVB2	128622	122668	1.40%	0.078%
13	7.663	941	948	951	rBV5	173585	349191	3.98%	0.223%
14	7.704	951	955	958	rVB3	94824	149749	1.71%	0.095%
15	7.798	965	971	974	rBV2	217718	335577	3.82%	0.214%
16	7.828	974	976	981	rVB	208304	216767	2.47%	0.138%
17	7.945	992	996	1000	rVB	217039	216472	2.47%	0.138%
18	8.004	1000	1006	1009	rBV2	625194	673341	7.67%	0.429%
19	8.133	1023	1028	1034	rVB	1610996	1398034	15.93%	0.891%
20	8.186	1034	1037	1040	rVB3	111564	130198	1.48%	0.083%
21	8.228	1040	1044	1047	rBV4	133375	226359	2.58%	0.144%
22	8.263	1047	1050	1053	rVV3	118700	154269	1.76%	0.098%
23	8.292	1053	1055	1059	rVB2	270268	329603	3.76%	0.210%
24	8.339	1060	1063	1065	rBV	386445	346912	3.95%	0.221%
25	8.369	1066	1068	1071	rVB2	223910	232227	2.65%	0.148%
26	8.404	1071	1074	1076	rBV2	148927	141208	1.61%	0.090%
27	8.486	1082	1088	1090	rBV5	159263	309023	3.52%	0.197%
28	8.522	1090	1094	1096	rBV2	389081	476793	5.43%	0.304%
29	8.551	1096	1099	1101	rBV	256169	240896	2.75%	0.154%
30	8.581	1101	1104	1108	rBV2	381044	380402	4.34%	0.243%
31	8.616	1108	1110	1114	rBV3	227054	244416	2.79%	0.156%
32	8.657	1114	1117	1119	rBV	1865035	1428468	16.28%	0.911%
33	8.675	1119	1120	1122	rVB2	248681	144572	1.65%	0.092%
34	8.716	1122	1127	1128	rBV4	640095	761180	8.68%	0.485%
35	8.733	1128	1130	1132	rVV2	635748	640923	7.30%	0.409%
36	8.781	1136	1138	1141	rVB3	345390	291315	3.32%	0.186%

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Integrator: RTE

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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

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37	8.822	1141	1145	1148	rBV3	810368	1211392	13.81%	0.772%
38	8.898	1149	1158	1161	rBV4	1081849	2172967	24.77%	1.385%
39	9.063	1183	1186	1189	rBV4	845016	905293	10.32%	0.577%
40	9.116	1193	1195	1198	rBV	1700897	1962738	22.37%	1.251%
41	9.369	1236	1238	1240	rBV	770841	654750	7.46%	0.417%
42	9.416	1242	1246	1249	rVB2	2404733	2873635	32.75%	1.832%
43	9.463	1252	1254	1257	rBV2	1056403	983216	11.21%	0.627%
44	9.569	1270	1272	1275	rVB2	529892	402233	4.58%	0.256%
45	9.616	1277	1280	1283	rBV2	1472456	1600661	18.24%	1.020%
46	9.769	1304	1306	1314	rVB2	1128518	1543104	17.59%	0.984%
47	9.857	1319	1321	1323	rBV2	600437	530503	6.05%	0.338%
48	9.886	1323	1326	1328	rBV	1318592	1272445	14.50%	0.811%
49	9.969	1338	1340	1342	rBV	894810	670662	7.64%	0.428%
50	10.098	1359	1362	1365	rBV4	889082	975140	11.11%	0.622%
51	10.127	1365	1367	1368	rBV	537598	493476	5.62%	0.315%
52	10.386	1407	1411	1414	rVB2	2811998	2951892	33.64%	1.882%
53	10.433	1414	1419	1425	rVB3	2823213	4104555	46.78%	2.617%
54	10.563	1437	1441	1445	rBV2	3687349	6006113	68.45%	3.829%
55	10.598	1445	1447	1449	rVV2	2869166	2515991	28.67%	1.604%
56	10.639	1452	1454	1456	rVV	3731887	3379228	38.51%	2.154%
57	10.663	1456	1458	1461	rVV	2821754	2729313	31.11%	1.740%
58	10.704	1463	1465	1467	rVB	2394452	1752565	19.97%	1.117%
59	10.727	1467	1469	1471	rBV2	794499	656728	7.48%	0.419%
60	10.763	1471	1475	1478	rVV	6000691	5971889	68.06%	3.807%
61	10.798	1478	1481	1484	rVB2	2290901	2388385	27.22%	1.523%
62	10.851	1484	1490	1492	rBV	5365041	6366946	72.56%	4.059%
63	10.874	1492	1494	1497	rVB2	2650469	2757266	31.42%	1.758%
64	10.916	1497	1501	1505	rBV	5941563	6130957	69.87%	3.909%
65	10.957	1505	1508	1509	rBV2	2377117	2329766	26.55%	1.485%
66	11.045	1520	1523	1528	rVB3	2134003	3281387	37.40%	2.092%
67	11.127	1535	1537	1540	rVB	1534292	1550027	17.67%	0.988%
68	11.157	1540	1542	1545	rBV	861847	688069	7.84%	0.439%
69	11.186	1545	1547	1551	rVB	2134279	2058667	23.46%	1.312%
70	11.251	1551	1558	1561	rBV	4064474	7291589	83.10%	4.649%
71	11.333	1569	1572	1577	rBV2	3877479	6388203	72.81%	4.073%
72	11.380	1577	1580	1581	rVV	1946491	2072789	23.62%	1.321%
73	11.404	1581	1584	1587	rVV2	3163208	3581939	40.82%	2.284%
74	11.433	1587	1589	1592	rVV	2819008	2899762	33.05%	1.849%
75	11.469	1593	1595	1599	rVV3	1557566	2227922	25.39%	1.420%
76	11.504	1599	1601	1605	rVB3	1845434	2445331	27.87%	1.559%

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 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 >
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77	11.539	1605	1607	1609	rBV	812394	683287	7.79%	0.436%
78	11.569	1609	1612	1616	rVB2	1882049	2135399	24.34%	1.361%
79	11.610	1616	1619	1622	rBV	4050621	4670837	53.23%	2.978%
80	11.651	1622	1626	1630	rVB2	1834029	2685596	30.61%	1.712%
81	11.704	1630	1635	1638	rBV2	5645551	8774288	100.00%	5.594%
82	11.792	1644	1650	1652	rBV	3962371	6333198	72.18%	4.038%
83	11.839	1655	1658	1660	rBV	2154135	1963874	22.38%	1.252%
84	11.939	1672	1675	1677	rBV	2236658	2161974	24.64%	1.378%
85	12.080	1697	1699	1702	rBV2	1229873	1078544	12.29%	0.688%
86	14.010	2024	2027	2031	rBV3	1728116	2352874	26.82%	1.500%
87	15.051	2201	2204	2214	rVB	875535	1822564	20.77%	1.162%
88	15.351	2252	2255	2261	rVB	899324	1185461	13.51%	0.756%
89	15.415	2263	2266	2269	rVB	840986	912467	10.40%	0.582%
90	15.474	2274	2276	2279	rVB	617159	648900	7.40%	0.414%
91	16.927	2519	2523	2529	rVB2	410954	749270	8.54%	0.478%
92	17.368	2594	2598	2612	rVB	288440	686176	7.82%	0.437%

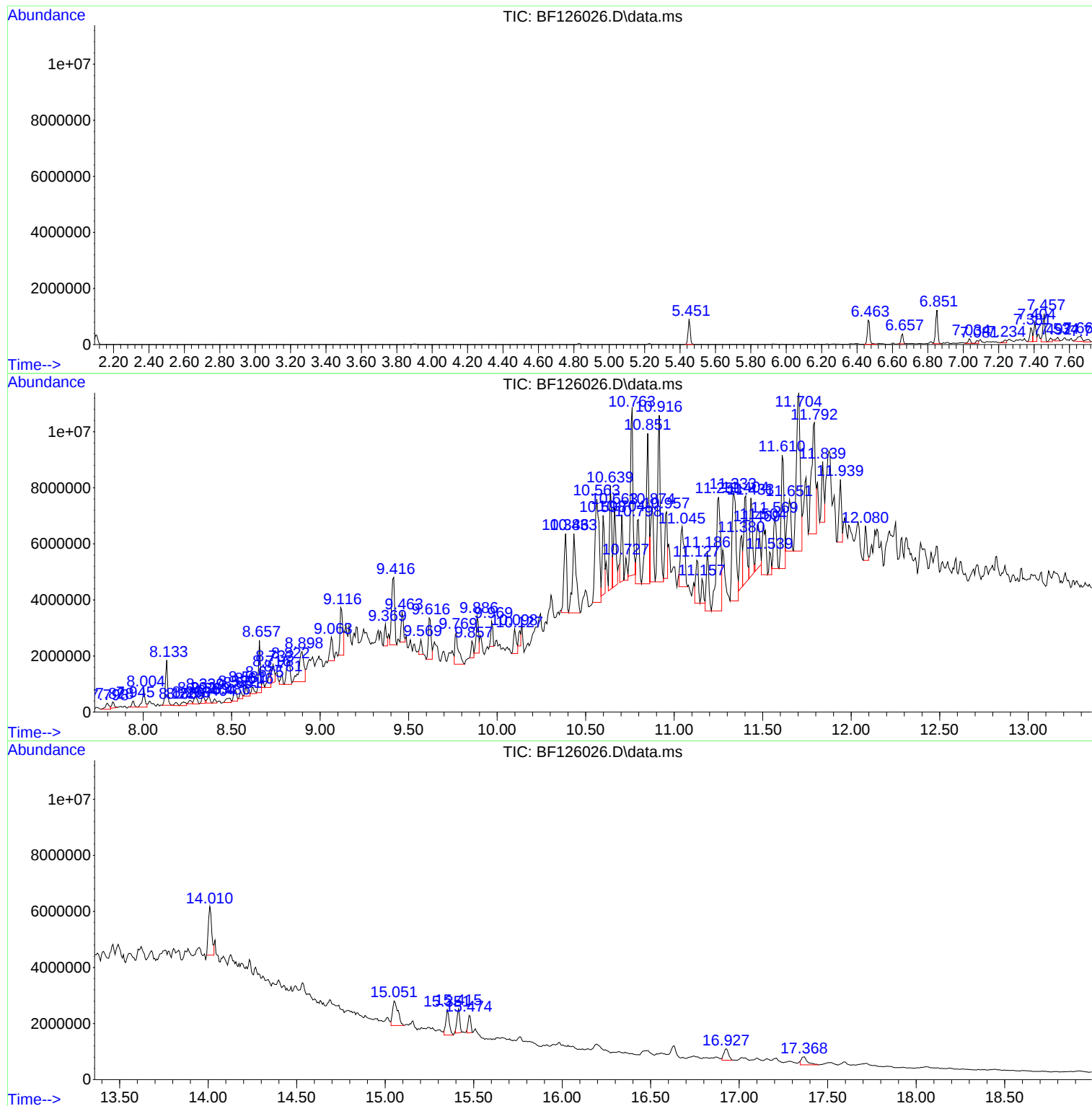
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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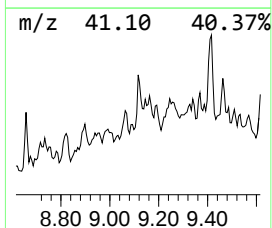
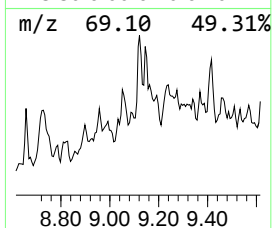
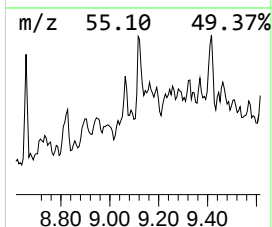
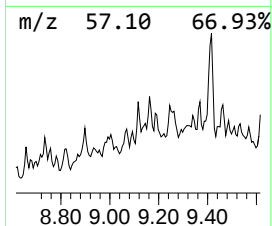
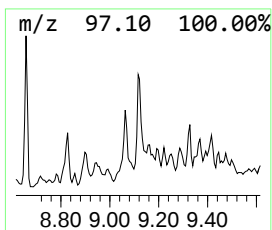
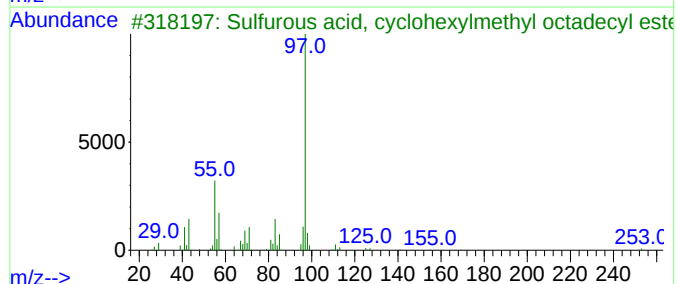
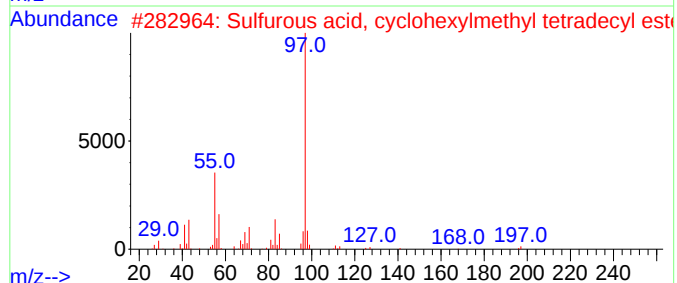
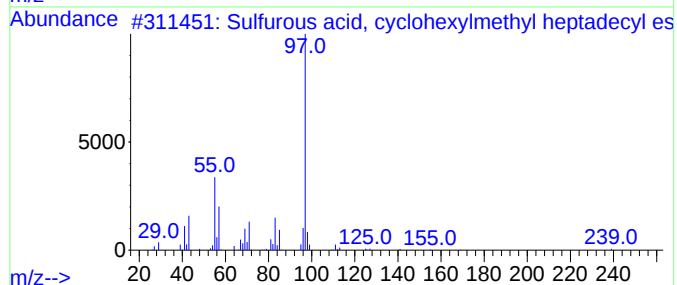
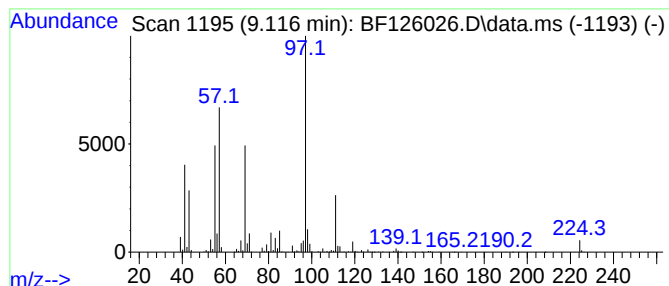
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Sulfurous acid, cyclohexylm... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.116	30.85 ng	1962740	Acenaphthene-d10	9.886

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Sulfurous acid, cyclohexylmethyl...	416	C24H48O3S	1000309-22-5	64
2		Sulfurous acid, cyclohexylmethyl...	374	C21H42O3S	1000309-22-2	64
3		Sulfurous acid, cyclohexylmethyl...	430	C25H50O3S	1000309-22-6	64
4		2,4,4,6,6,8,8-Heptamethyl-2-nonene	224	C16H32	039761-73-4	64
5		Sulfurous acid, cyclohexylmethyl...	360	C20H40O3S	1000309-22-1	64



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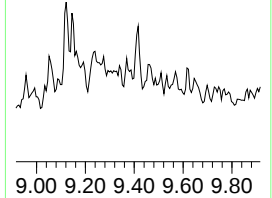
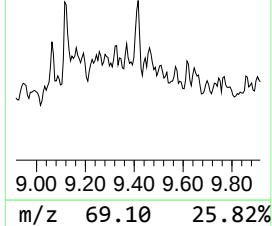
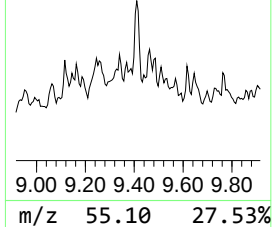
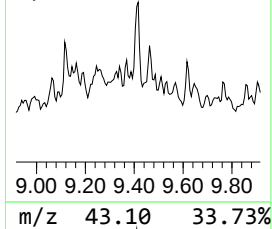
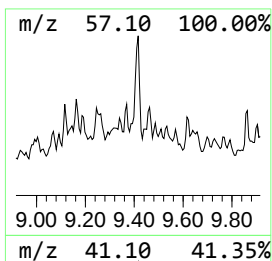
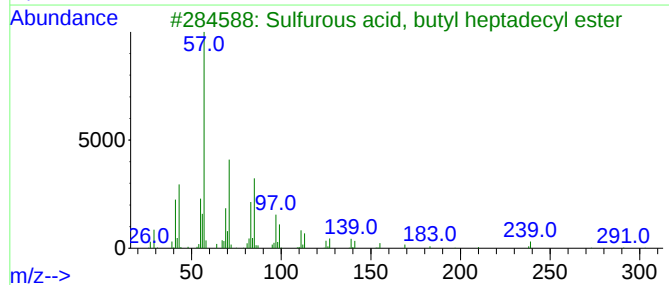
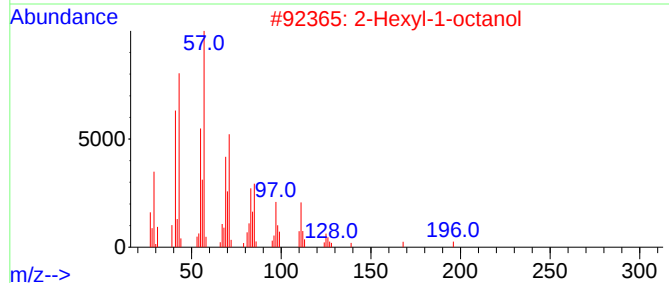
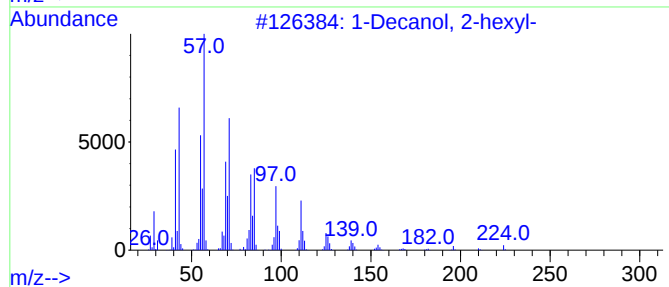
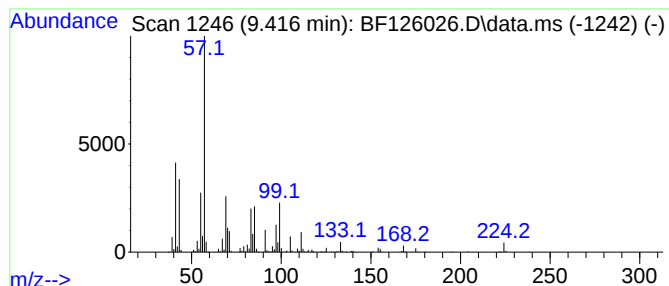
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Decanol, 2-hexyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.416	45.17 ng	2873640	Acenaphthene-d10	9.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-			242	C16H34O	002425-77-6	53
2	2-Hexyl-1-octanol			214	C14H30O	019780-79-1	53
3	Sulfurous acid, butyl heptadecyl...			376	C21H44O3S	1000309-18-4	50
4	2-Azido-2,4,4,6,6,8,8-heptamethy...			267	C16H33N3	1000293-29-1	47
5	Butyl decyl ether			214	C14H30O	1000406-40-2	40



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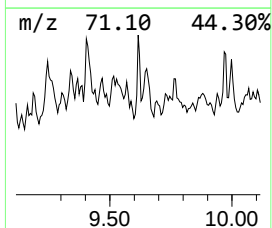
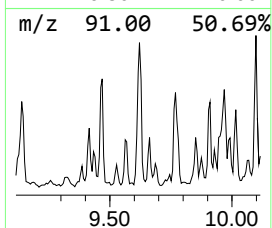
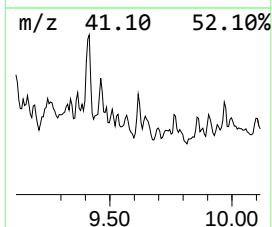
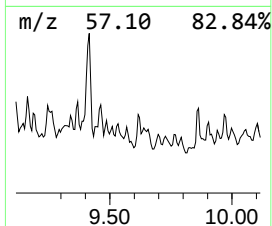
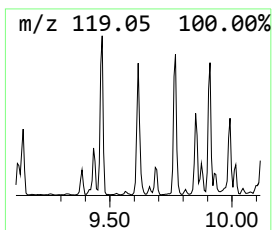
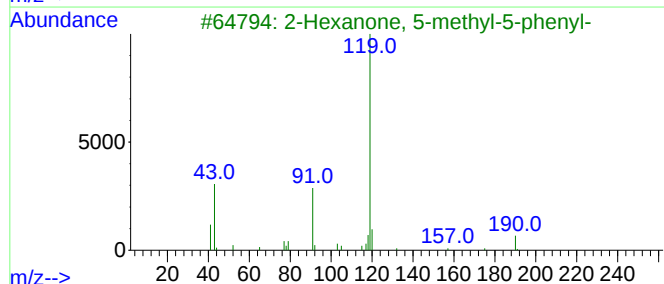
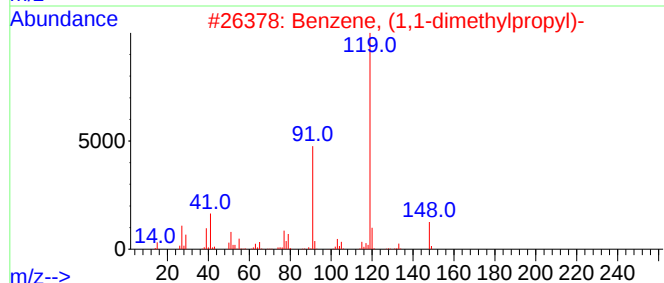
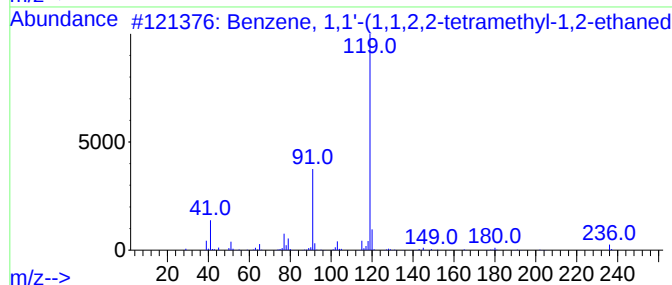
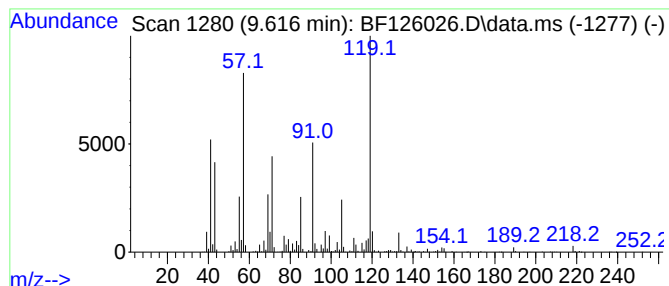
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown9.616 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.616	25.16 ng	1600660	Acenaphthene-d10	9.886	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(1,1,2,2-tetrameth...	238	C18H22	001889-67-4	41
2	Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	35
3	2-Hexanone, 5-methyl-5-phenyl-	190	C13H18O	014128-61-1	35
4	1-Chloro-2-methyl-2-phenylpropane	168	C10H13Cl	000515-40-2	35
5	Benzene, (1,1-dimethylbutyl)-	162	C12H18	001985-57-5	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110321\
Data File : BF126026.D
Acq On : 3 Nov 2021 18:48
Operator : JU/CG
Sample : M4427-02 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

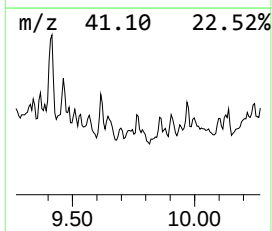
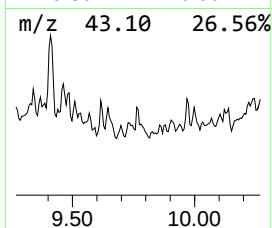
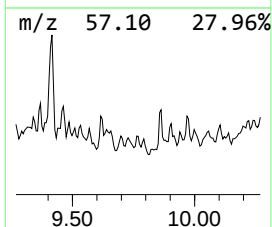
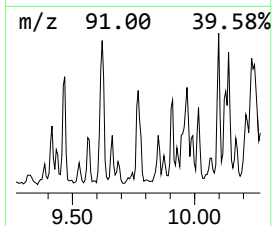
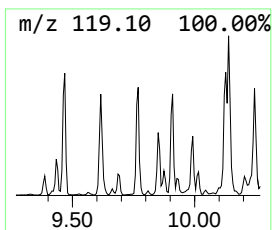
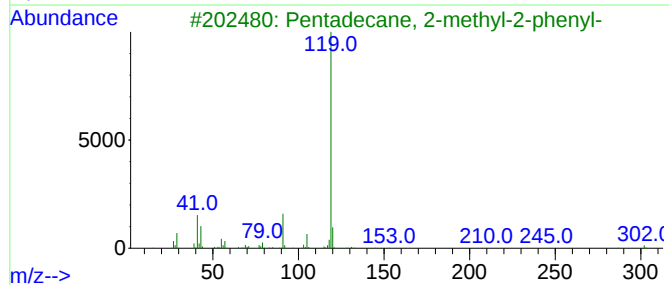
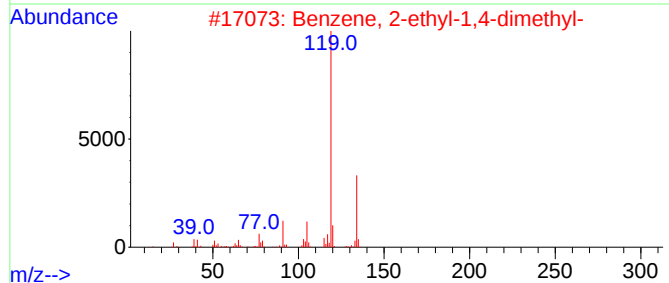
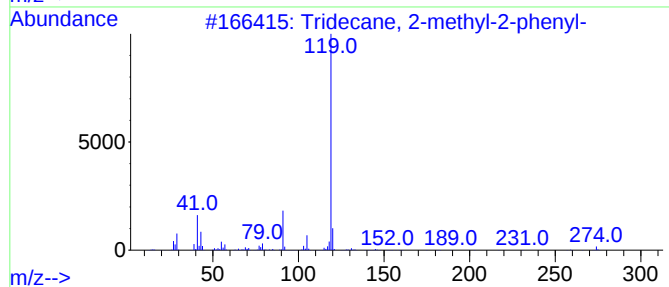
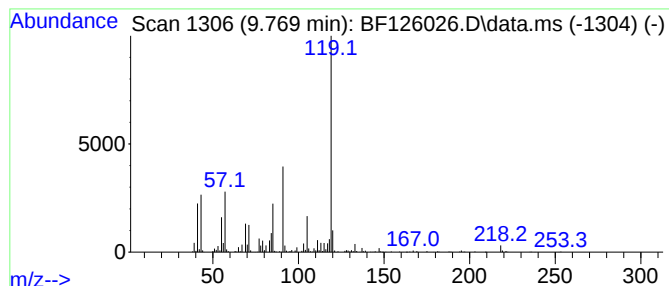
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ClientSampleId :
FDR-BH-5-20211029-6.5-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Tridecane, 2-methyl-2-phenyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.769	24.25 ng	1543100	Acenaphthene-d10	9.886	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 2-methyl-2-phenyl-	274	C20H34	027854-41-7	59
2	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	59
3	Pentadecane, 2-methyl-2-phenyl-	302	C22H38	029138-94-1	59
4	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	59
5	Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110321\
Data File : BF126026.D
Acq On : 3 Nov 2021 18:48
Operator : JU/CG
Sample : M4427-02 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FDR-BH-5-20211029-6.5-7

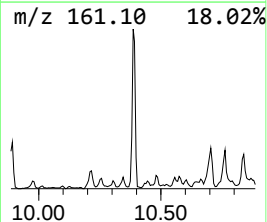
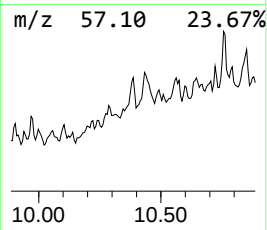
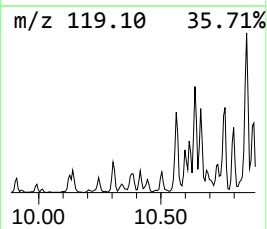
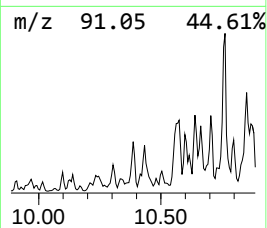
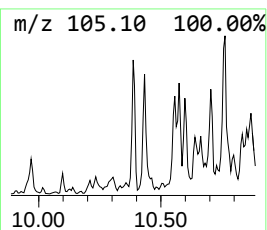
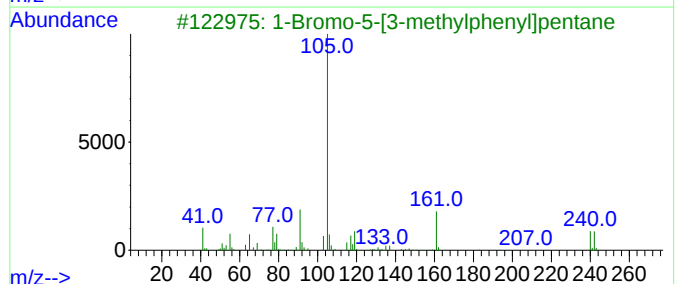
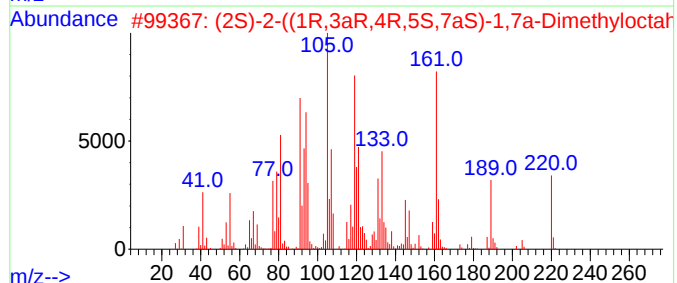
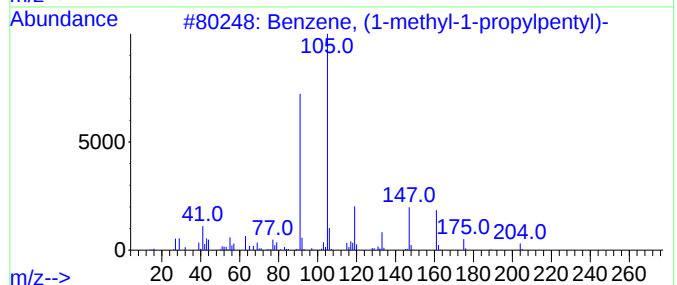
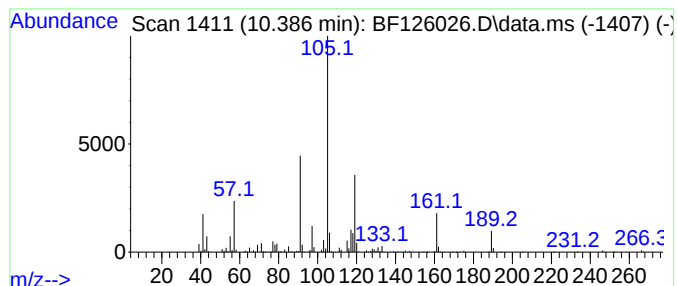
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown10.386 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.386	46.40 ng	2951890	Acenaphthene-d10	9.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methyl-1-propylpentyl)-	204	C15H24	054932-91-1	45
2			(2S)-2-((1R,3aR,4R,5S,7aS)-1,7a...	220	C15H24O	030810-34-5	38
3			1-Bromo-5-[3-methylphenyl]pentane	240	C12H17Br	1000211-83-1	37
4			Benzaldehyde, 4-[(2-methylphenyl...	226	C15H14O2	1000338-23-1	14
5			Succinic acid, 2-chloro-6-fluoro...	350	C18H16ClF04	1000389-75-0	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110321\
Data File : BF126026.D
Acq On : 3 Nov 2021 18:48
Operator : JU/CG
Sample : M4427-02 5X
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ALS Vial : 13 Sample Multiplier: 1

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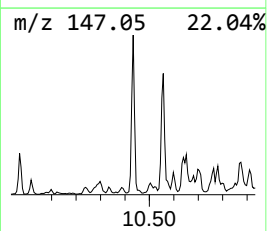
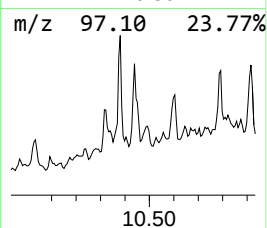
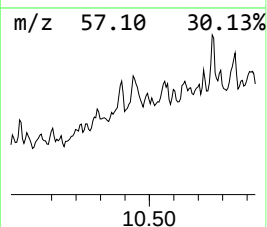
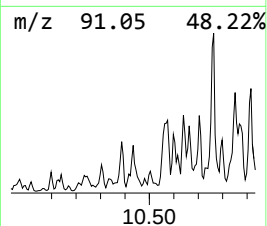
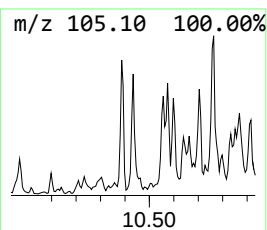
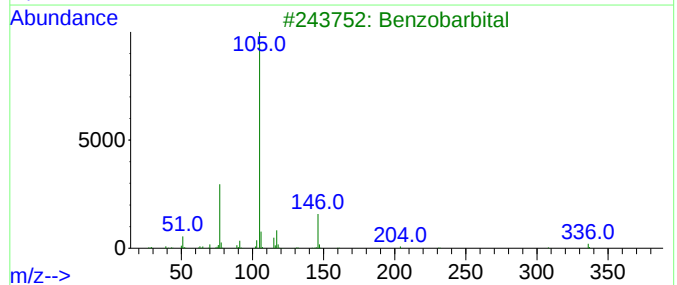
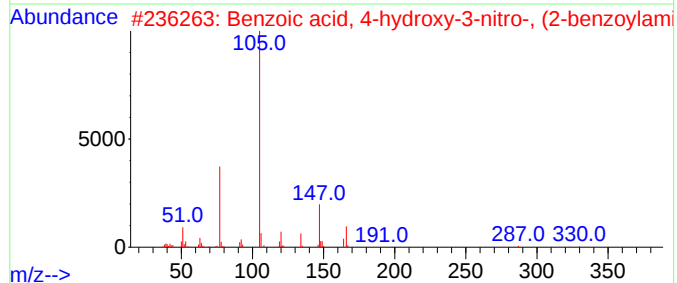
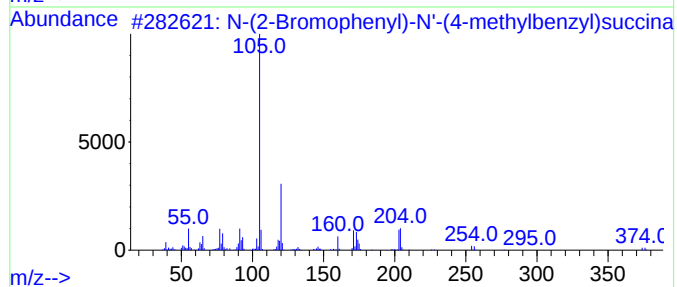
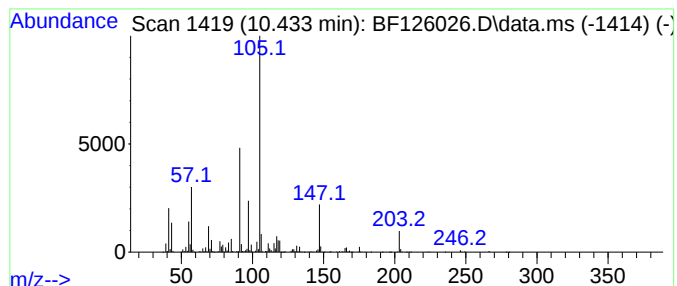
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown10.433 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.433	64.51 ng	4104560	Acenaphthene-d10	9.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-(2-Bromophenyl)-N'-(4-methylbe...	374	C18H19BrN2O2	328019-20-1	32
2			Benzoic acid, 4-hydroxy-3-nitro-...	330	C16H14N2O6	346661-98-1	32
3			Benzobarbital	336	C19H16N2O4	000744-80-9	27
4			Succinic acid, phenethyl 2,3-dic...	366	C18H16Cl2O4	1000358-00-7	14
5			3-phenylbutyric acid, 2,2,2-trif...	246	C12H13F3O2	1000376-55-4	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110321\
Data File : BF126026.D
Acq On : 3 Nov 2021 18:48
Operator : JU/CG
Sample : M4427-02 5X
Misc :
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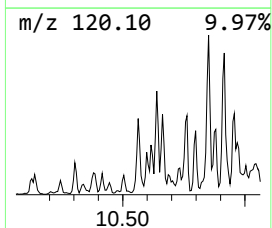
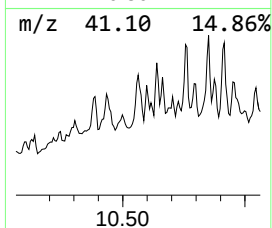
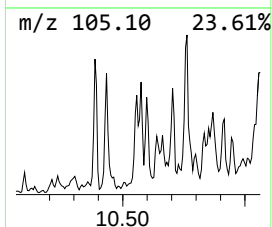
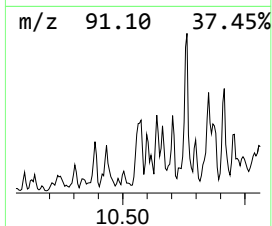
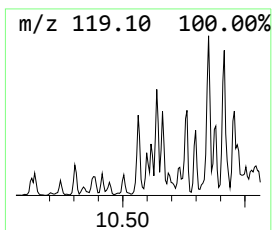
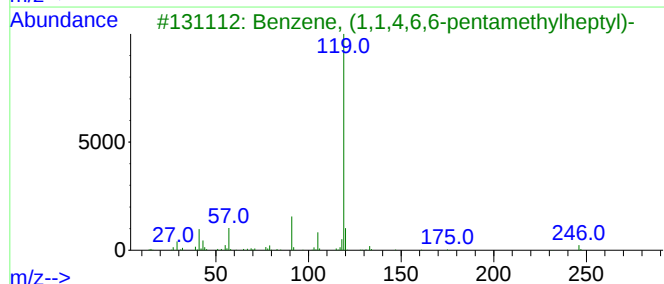
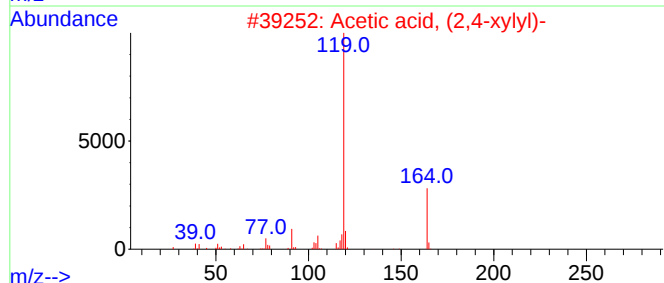
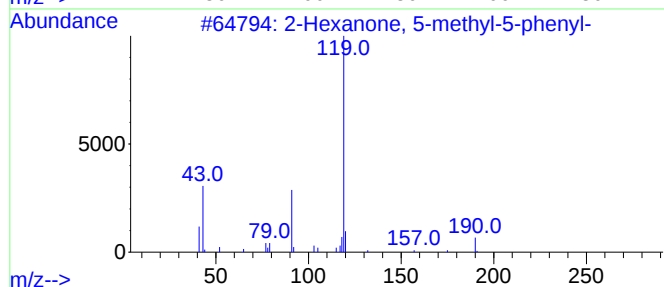
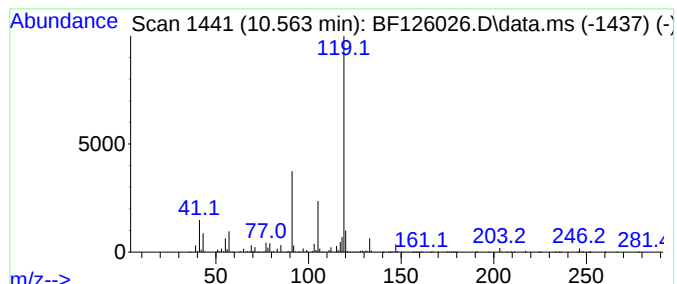
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-Hexanone, 5-methyl-5-phenyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
10.563	94.40 ng	6006110	Acenaphthene-d10			9.886
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Hexanone, 5-methyl-5-phenyl-		190	C13H18O	014128-61-1	62
2	Acetic acid, (2,4-xylyl)-		164	C10H12O2	006331-04-0	59
3	Benzene, (1,1,4,6,6-pentamethylh...		246	C18H30	055134-07-1	59
4	Benzene, (1,1-dimethyldecyl)-		246	C18H30	027854-40-6	58
5	(6-Chloro-2-methylhexan-2-yl)ben...		210	C13H19Cl	1417621-45-4	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110321\
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Sample : M4427-02 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

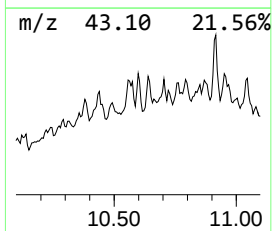
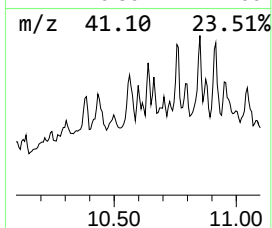
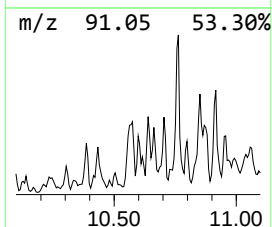
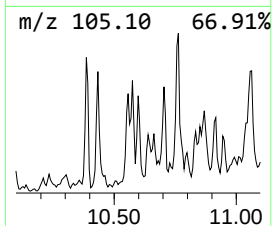
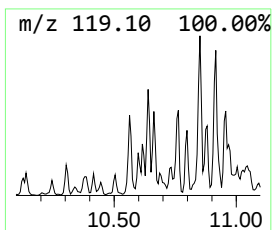
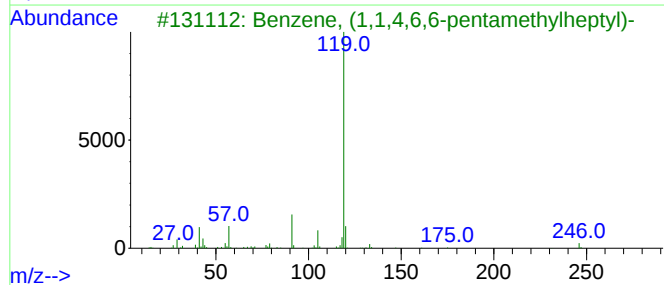
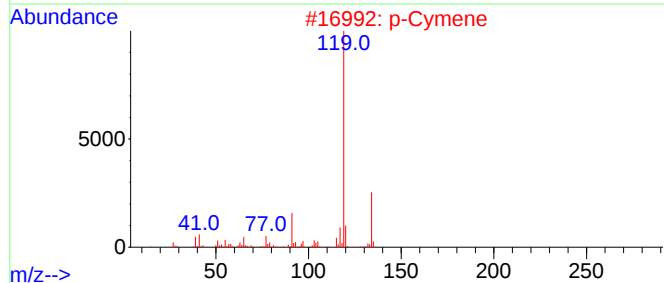
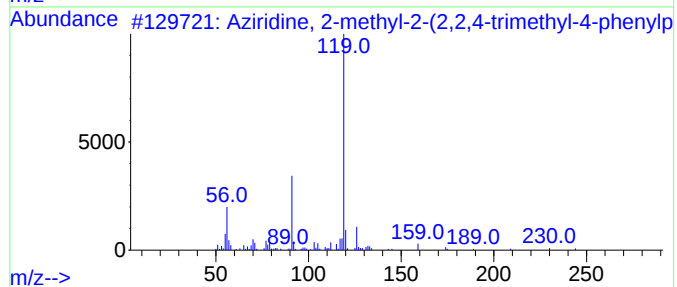
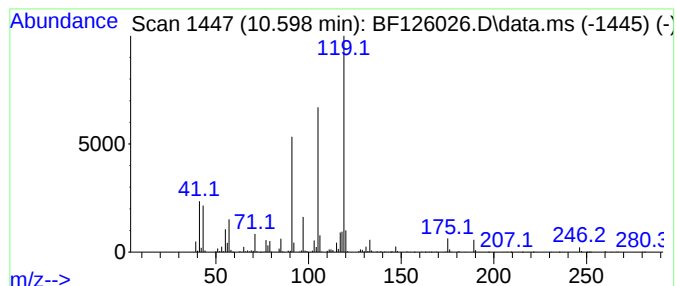
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Aziridine, 2-methyl-2-(2,2,... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.598	39.55 ng	2515990	Acenaphthene-d10	9.886	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aziridine, 2-methyl-2-(2,2,4-tri...	245	C17H27N	1000293-28-5	64
2	p-Cymene	134	C10H14	000099-87-6	59
3	Benzene, (1,1,4,6,6-pentamethylh...	246	C18H30	055134-07-1	59
4	1,3,8-p-Menthatriene	134	C10H14	018368-95-1	53
5	Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110321\
Data File : BF126026.D
Acq On : 3 Nov 2021 18:48
Operator : JU/CG
Sample : M4427-02 5X
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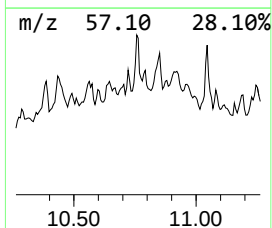
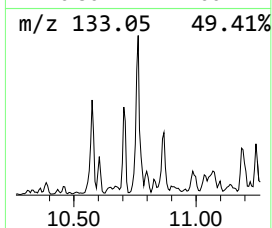
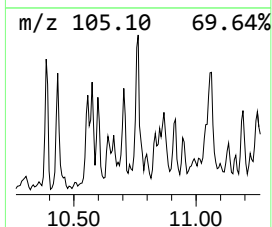
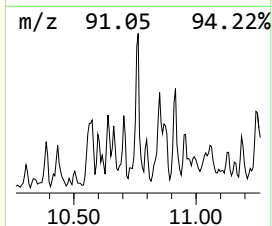
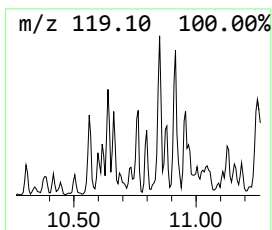
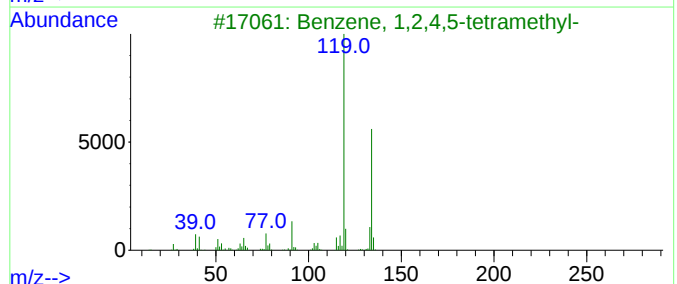
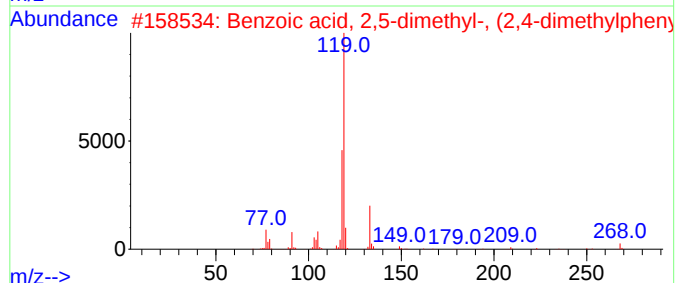
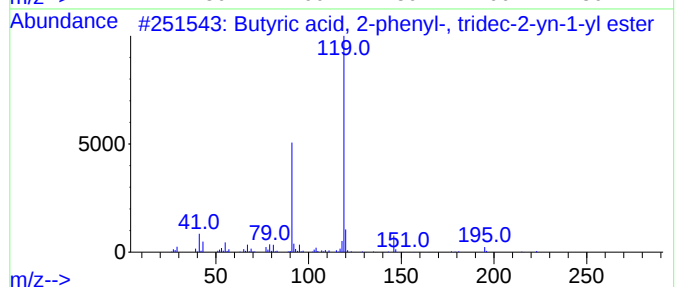
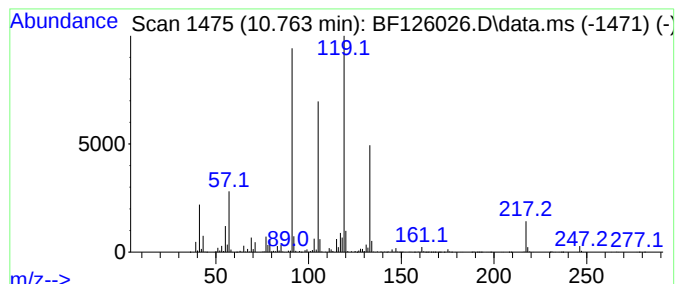
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Butyric acid, 2-phenyl-, tr... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.763	57.62 ng	5971890	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyric acid, 2-phenyl-, tridec-...	342	C23H34O2	1000406-92-1	50
2			Benzoic acid, 2,5-dimethyl-, (2,...	268	C18H20O2	055000-48-1	50
3			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	47
4			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	47
5			Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110321\
Data File : BF126026.D
Acq On : 3 Nov 2021 18:48
Operator : JU/CG
Sample : M4427-02 5X
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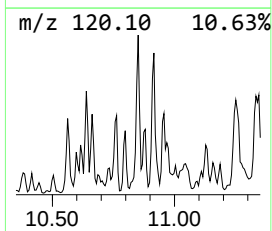
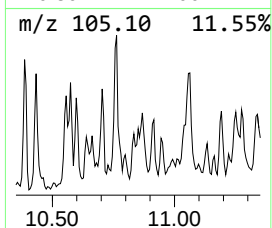
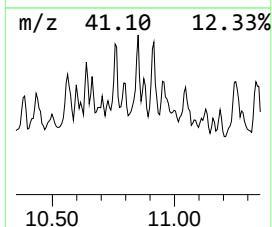
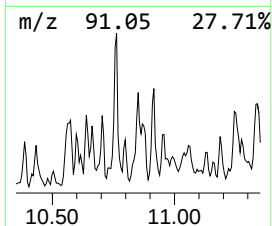
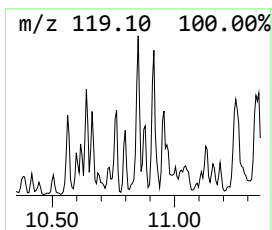
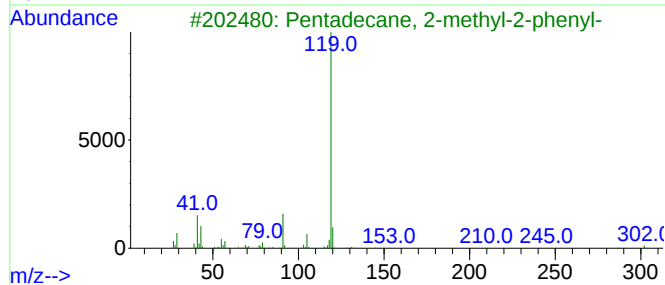
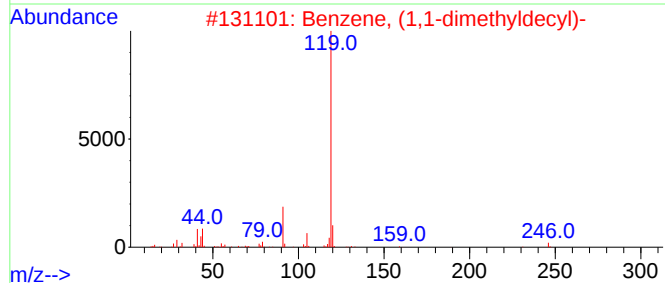
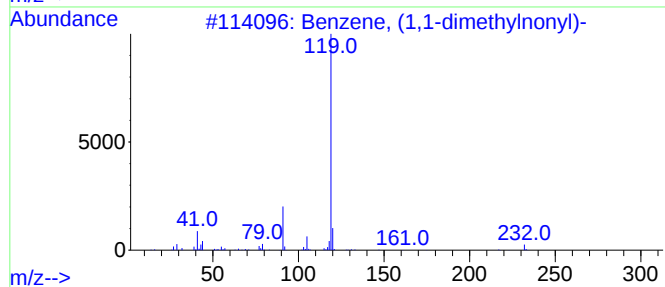
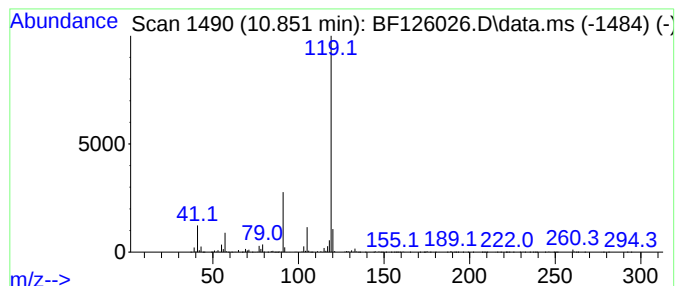
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzene, (1,1-dimethylnonyl)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.851	61.43 ng	6366950	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1,1-dimethylnonyl)-	232	C17H28	055191-25-8	87
2			Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	78
3			Pentadecane, 2-methyl-2-phenyl-	302	C22H38	029138-94-1	78
4			Cumene hydroperoxide, TMS deriva...	224	C12H20O2Si	018057-16-4	78
5			Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110321\
Data File : BF126026.D
Acq On : 3 Nov 2021 18:48
Operator : JU/CG
Sample : M4427-02 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

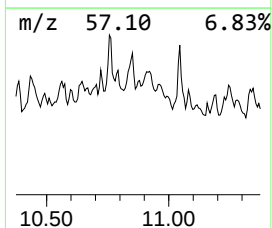
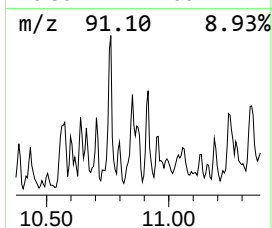
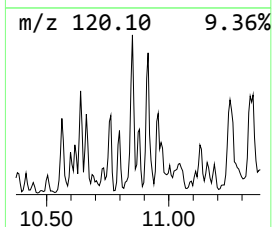
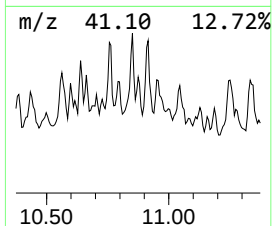
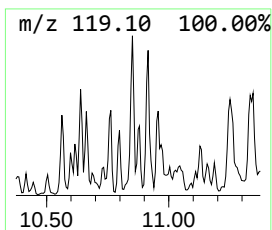
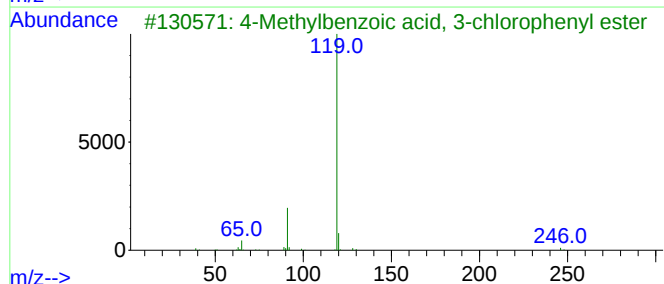
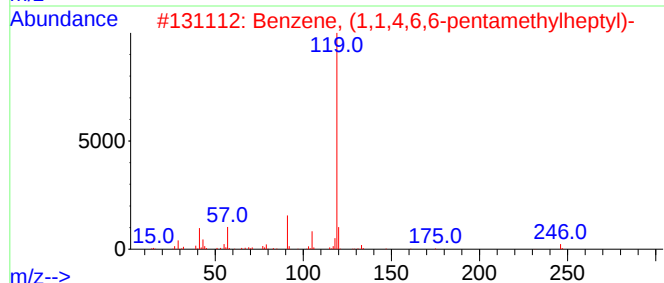
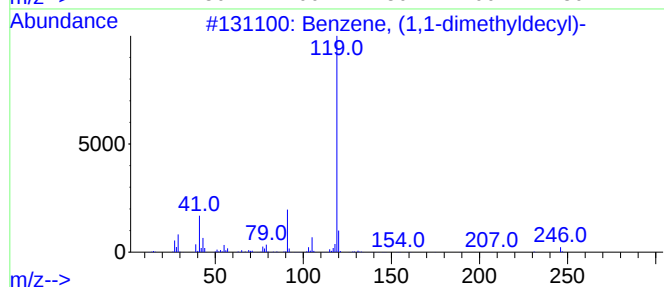
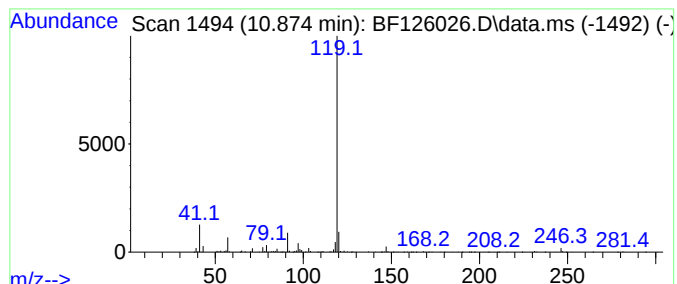
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ClientSampleId :
FDR-BH-5-20211029-6.5-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Benzene, (1,1,4,6,6-pentame... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD			R.T.
10.874	26.60 ng	2757270	Phenanthrene-d10			11.374
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, (1,1-dimethyldecyl)-		246	C18H30	027854-40-6	86
2	Benzene, (1,1,4,6,6-pentamethylh...		246	C18H30	055134-07-1	78
3	4-Methylbenzoic acid, 3-chloroph...		246	C14H11ClO2	1000325-60-1	64
4	Butyric acid, 2-phenyl-, tridec...		342	C23H34O2	1000406-92-1	64
5	3-Methylbenzoic acid, 3-chloroph...		246	C14H11ClO2	1010325-71-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110321\
Data File : BF126026.D
Acq On : 3 Nov 2021 18:48
Operator : JU/CG
Sample : M4427-02 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

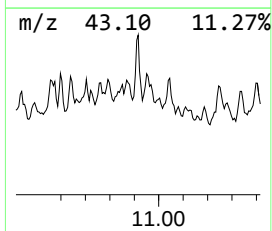
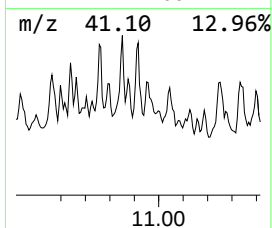
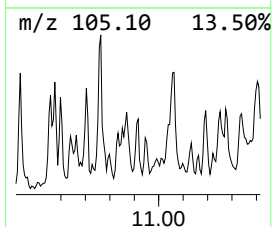
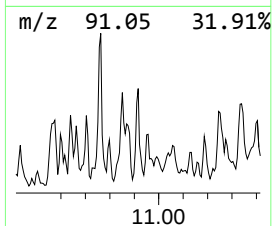
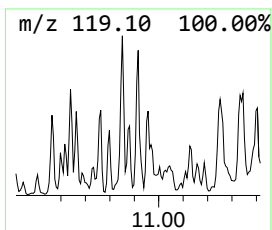
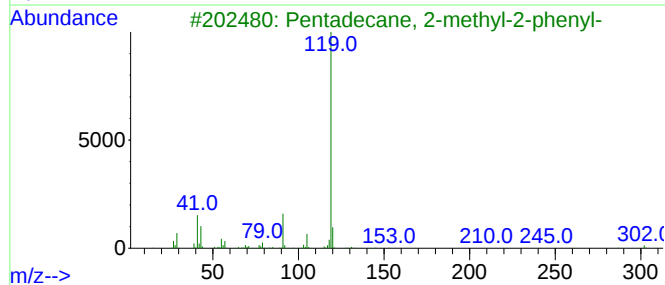
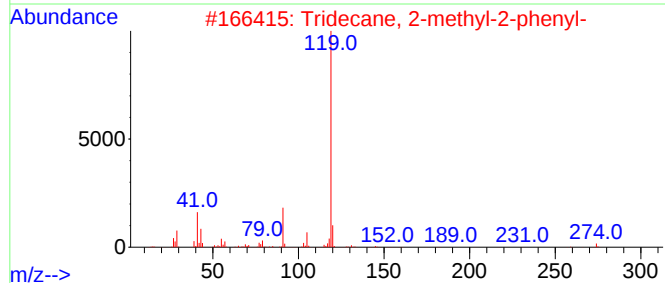
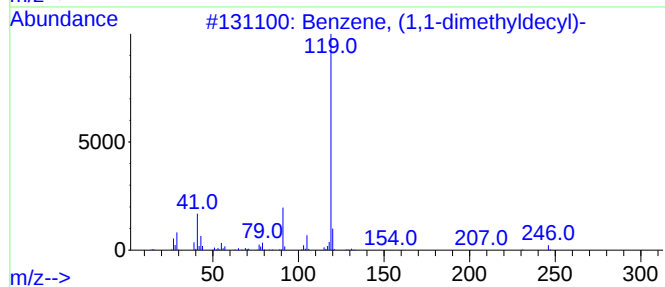
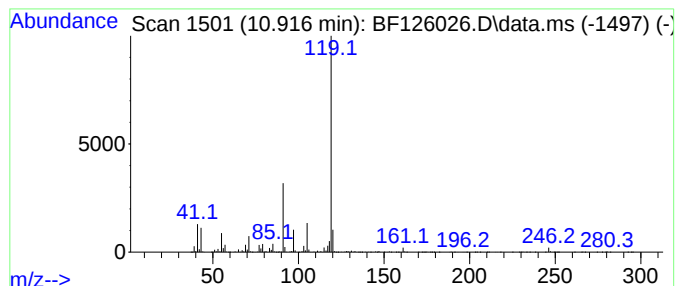
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ClientSampleId :
FDR-BH-5-20211029-6.5-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Benzene, (1,1-dimethyldecyl)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.916	59.16 ng	6130960	Phenanthrene-d10		11.374	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, (1,1-dimethyldecyl)-		246	C18H30	027854-40-6	93
2	Tridecane, 2-methyl-2-phenyl-		274	C20H34	027854-41-7	64
3	Pentadecane, 2-methyl-2-phenyl-		302	C22H38	029138-94-1	64
4	Cumene hydroperoxide, TMS deriva...		224	C12H20O2Si	018057-16-4	64
5	Benzene, (1,1-dimethylnonyl)-		232	C17H28	055191-25-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110321\
Data File : BF126026.D
Acq On : 3 Nov 2021 18:48
Operator : JU/CG
Sample : M4427-02 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FDR-BH-5-20211029-6.5-7

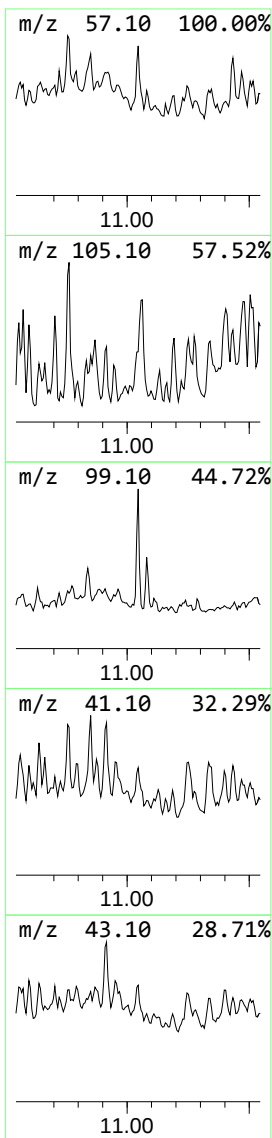
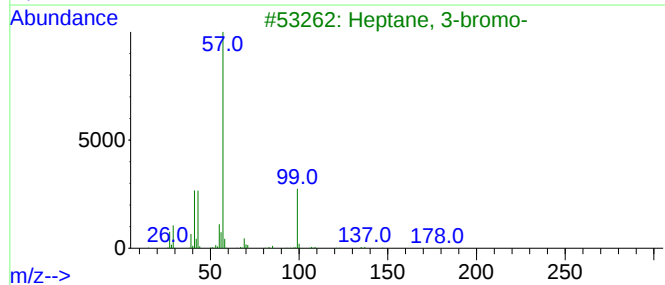
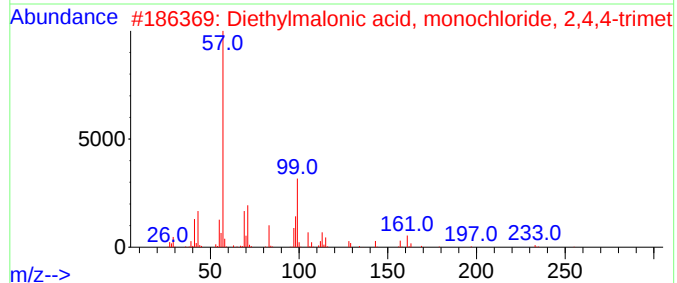
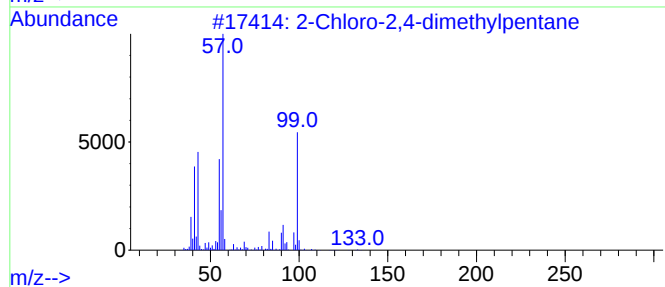
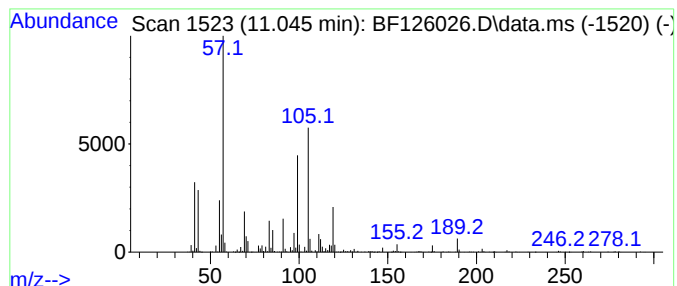
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown11.045 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.045	31.66 ng	3281390	Phenanthrene-d10	11.374

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Chloro-2,4-dimethylpentane	134	C7H15Cl	035951-33-8	37
2		Diethylmalonic acid, monochlorid...	290	C15H27ClO3	1010369-49-2	37
3		Heptane, 3-bromo-	178	C7H15Br	001974-05-6	32
4		Acetamide, N-ethenyl-N-methyl-	99	C5H9NO	003195-78-6	16
5		Tridecane, 2-methyl-	198	C14H30	001560-96-9	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110321\
Data File : BF126026.D
Acq On : 3 Nov 2021 18:48
Operator : JU/CG
Sample : M4427-02 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

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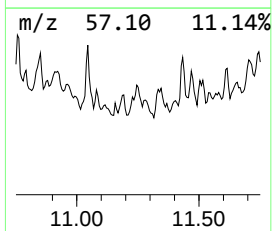
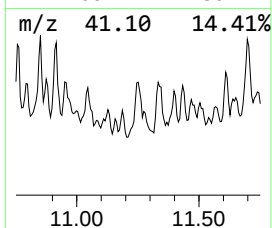
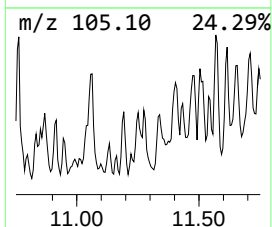
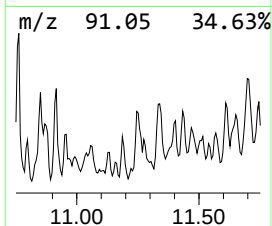
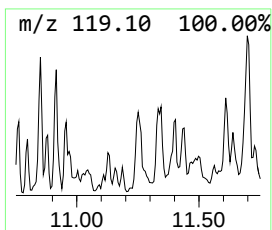
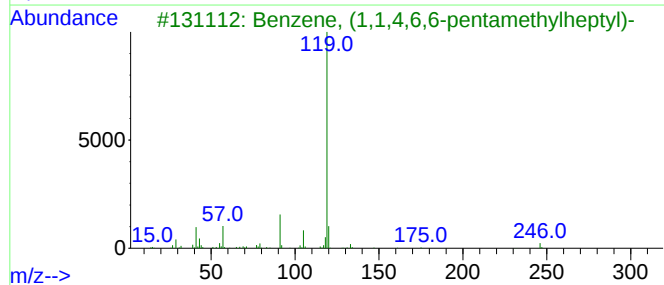
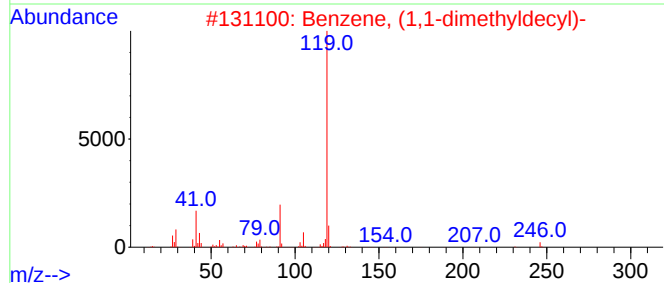
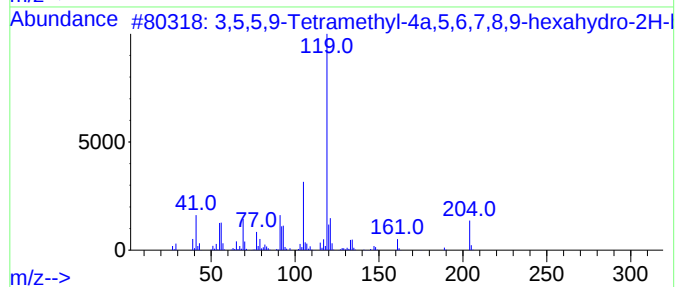
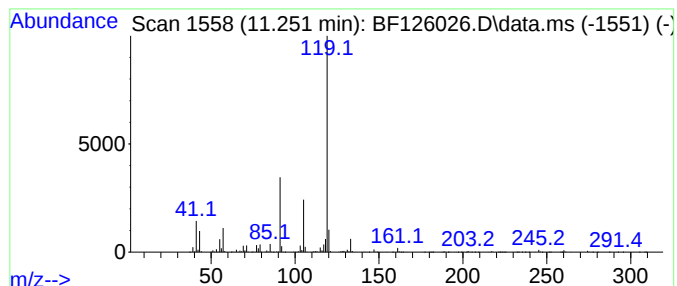
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 3,5,5,9-Tetramethyl-4a,5,6,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.251	70.36 ng	7291590	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5,5,9-Tetramethyl-4a,5,6,7,8,9...	204	C15H24	1000412-94-8	64		
2	Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	59		
3	Benzene, (1,1,4,6,6-pentamethylh...	246	C18H30	055134-07-1	59		
4	Tridecane, 2-methyl-2-phenyl-	274	C20H34	027854-41-7	59		
5	Benzene, (1,1-dimethylnonyl)-	232	C17H28	055191-25-8	58		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110321\
Data File : BF126026.D
Acq On : 3 Nov 2021 18:48
Operator : JU/CG
Sample : M4427-02 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

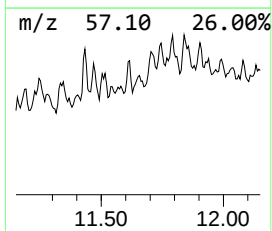
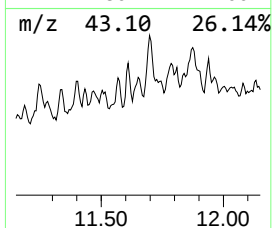
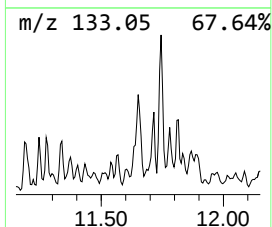
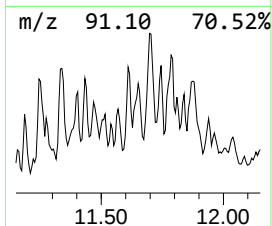
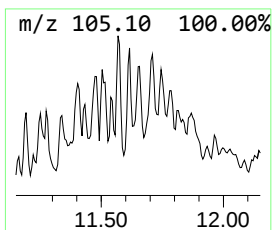
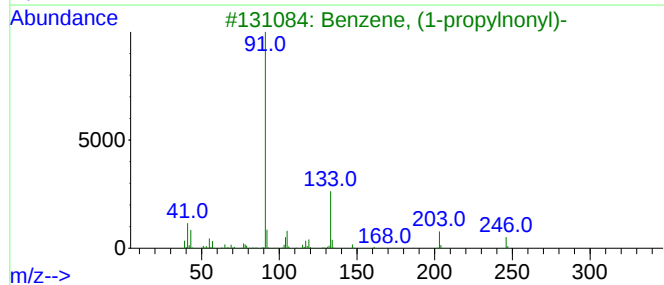
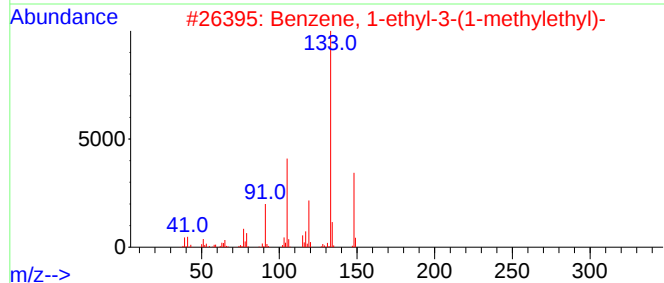
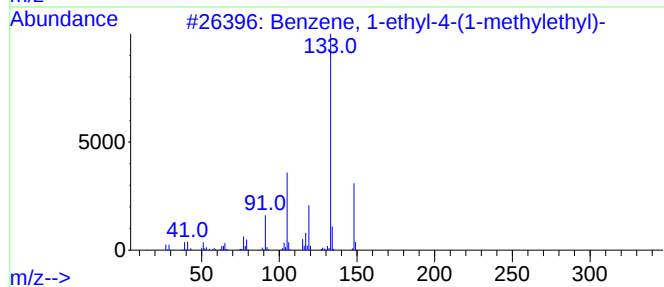
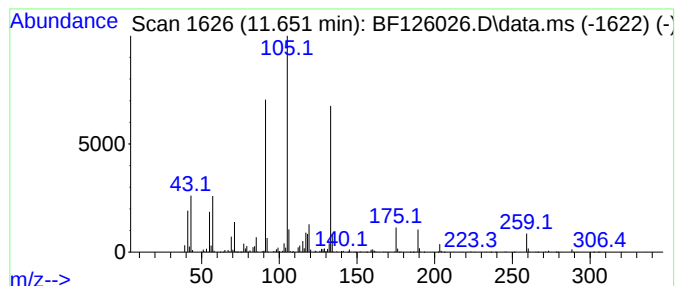
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Benzene, 1-ethyl-4-(1-methy... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD			R.T.
11.651	25.91 ng	2685600	Phenanthrene-d10			11.374
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-4-(1-methylethyl)-		148	C11H16	004218-48-8	50
2	Benzene, 1-ethyl-3-(1-methylethyl)-		148	C11H16	004920-99-4	50
3	Benzene, (1-propylnonyl)-		246	C18H30	002719-64-4	43
4	6-Aminoindazole		133	C7H7N3	006967-12-0	38
5	1H-Benzimidazol-2-amine		133	C7H7N3	000934-32-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110321\
Data File : BF126026.D
Acq On : 3 Nov 2021 18:48
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Sample : M4427-02 5X
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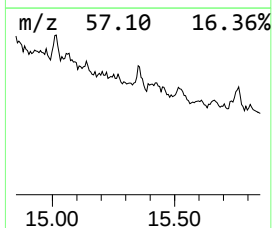
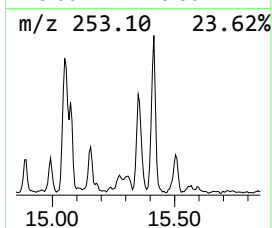
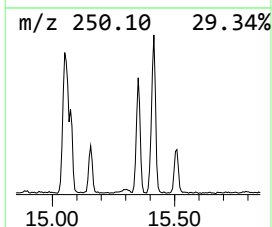
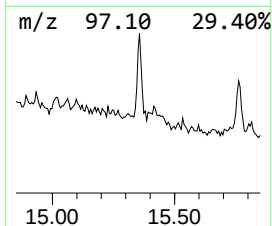
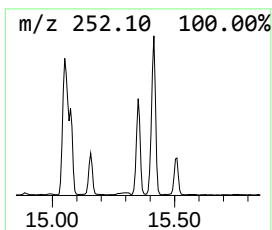
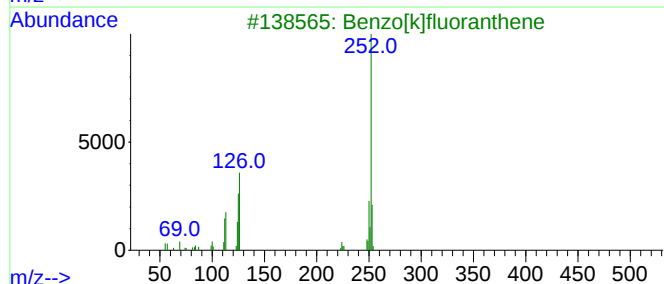
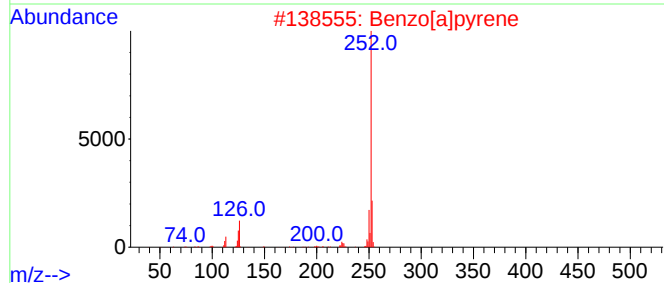
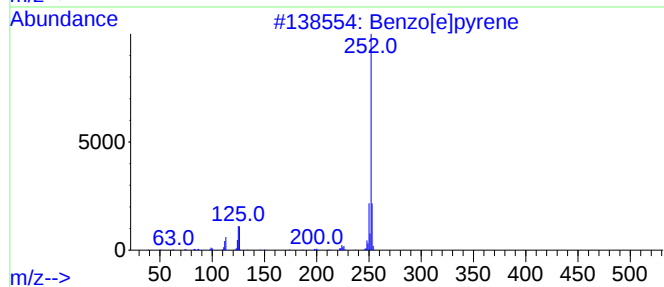
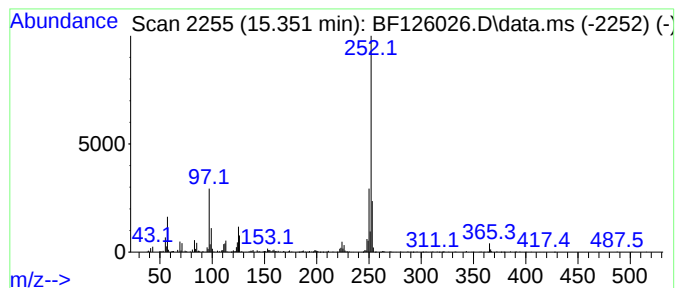
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Benzo[e]pyrene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.351	36.54 ng	1185460	Perylene-d12	15.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	93
2			Benzo[a]pyrene	252	C20H12	000050-32-8	89
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	89
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	89
5			Perylene	252	C20H12	000198-55-0	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110321\
 Data File : BF126026.D
 Acq On : 3 Nov 2021 18:48
 Operator : JU/CG
 Sample : M4427-02 5X
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FDR-BH-5-20211029-6.5-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown8.898	8.898	31.1	ng	2172970	2	8.133	1398030	20.0
Sulfurous acid,...	9.116	30.9	ng	1962740	3	9.886	1272450	20.0
1-Decanol, 2-he...	9.416	45.2	ng	2873640	3	9.886	1272450	20.0
unknown9.616	9.616	25.2	ng	1600660	3	9.886	1272450	20.0
Tridecane, 2-me...	9.769	24.3	ng	1543100	3	9.886	1272450	20.0
unknown10.386	10.386	46.4	ng	2951890	3	9.886	1272450	20.0
unknown10.433	10.433	64.5	ng	4104560	3	9.886	1272450	20.0
2-Hexanone, 5-m...	10.563	94.4	ng	6006110	3	9.886	1272450	20.0
Aziridine, 2-me...	10.598	39.5	ng	2515990	3	9.886	1272450	20.0
Butyric acid, 2...	10.763	57.6	ng	5971890	4	11.374	2072790	20.0
Benzene, (1,1-d...	10.851	61.4	ng	6366950	4	11.374	2072790	20.0
Benzene, (1,1,4...	10.874	26.6	ng	2757270	4	11.374	2072790	20.0
Benzene, (1,1-d...	10.916	59.2	ng	6130960	4	11.374	2072790	20.0
unknown11.045	11.045	31.7	ng	3281390	4	11.374	2072790	20.0
3,5,5,9-Tetrame...	11.251	70.4	ng	7291590	4	11.374	2072790	20.0
Benzene, 1-ethy...	11.651	25.9	ng	2685600	4	11.374	2072790	20.0
Benzo[e]pyrene	15.351	36.5	ng	1185460	6	15.480	648900	20.0