

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042622\
 Data File : BF127931.D
 Acq On : 27 Apr 2022 00:03
 Operator : CG\JU
 Sample : N2502-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 C1

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-BF042222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127931.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.498	528	546	549	rVB	8747617	31862739	40.27%	9.986%
2	5.557	551	556	561	rBV	2799509	3417465	4.32%	1.071%
3	5.610	561	565	582	rVV	2263600	3831453	4.84%	1.201%
4	5.810	594	599	604	rBV	3484696	3290827	4.16%	1.031%
5	6.116	648	651	655	rBV	995836	866218	1.09%	0.271%
6	6.404	697	700	703	rVV	1083939	899442	1.14%	0.282%
7	6.475	707	712	714	rBV	4709476	4490510	5.68%	1.407%
8	6.516	714	719	722	rVV3	2852704	4511268	5.70%	1.414%
9	6.557	722	726	729	rVB	7652919	8804978	11.13%	2.760%
10	6.634	735	739	742	rBV	4881098	4644347	5.87%	1.456%
11	6.681	742	747	758	rVV	548462	1660207	2.10%	0.520%
12	6.781	758	764	767	rVB	8818684	11906665	15.05%	3.732%
13	6.945	788	792	794	rBV	1143741	934200	1.18%	0.293%
14	7.004	798	802	805	rVB	5485988	5909039	7.47%	1.852%
15	7.234	812	841	842	rBV4	10835557	79115588	100.00%	24.796%
16	7.422	870	873	875	rBV	1145620	1063280	1.34%	0.333%
17	7.492	881	885	888	rVB	1692940	1454404	1.84%	0.456%
18	7.545	888	894	896	rBV	2555681	3003271	3.80%	0.941%
19	7.745	926	928	931	rVB	1361222	1007039	1.27%	0.316%
20	8.234	1007	1011	1013	rVV	1312108	1225389	1.55%	0.384%
21	9.304	1187	1193	1196	rBV	4423854	4216761	5.33%	1.322%
22	9.986	1303	1309	1312	rVV	1148291	987565	1.25%	0.310%
23	10.433	1382	1385	1389	rBV	859419	835939	1.06%	0.262%
24	10.657	1419	1423	1426	rVV	909180	1066479	1.35%	0.334%
25	10.692	1426	1429	1433	rVV2	1433745	1900611	2.40%	0.596%
26	10.739	1433	1437	1440	rVV	1927963	2960292	3.74%	0.928%
27	10.775	1440	1443	1448	rVV3	3499569	4915858	6.21%	1.541%
28	10.916	1459	1467	1471	rVV2	5050603	9621204	12.16%	3.015%
29	10.975	1471	1477	1480	rVV	7187079	14792203	18.70%	4.636%
30	11.016	1480	1484	1487	rVV2	8240343	16795855	21.23%	5.264%
31	11.051	1487	1490	1492	rVV2	8513996	12618804	15.95%	3.955%
32	11.075	1492	1494	1496	rVV	7779634	7378605	9.33%	2.313%
33	11.110	1496	1500	1501	rVV2	5833846	7961003	10.06%	2.495%
34	11.169	1505	1510	1512	rVV4	8605571	15346557	19.40%	4.810%
35	11.210	1512	1517	1520	rVV2	8092645	16461529	20.81%	5.159%
36	11.245	1520	1523	1527	rVV2	7371644	9385149	11.86%	2.941%

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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-BF042222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.310	1530	1534	1536	rVV3	712596	894855	1.13%	0.280%
38	11.363	1540	1543	1547	rVV2	1535103	2414191	3.05%	0.757%
39	11.416	1550	1552	1558	rVB3	1005358	1311191	1.66%	0.411%
40	11.492	1559	1565	1567	rBV2	905672	1293938	1.64%	0.406%
41	11.757	1608	1610	1613	rVB	1023485	819778	1.04%	0.257%
42	12.169	1677	1680	1683	rBV	1256184	1013080	1.28%	0.318%
43	12.563	1744	1747	1750	rBV	1682067	1468529	1.86%	0.460%
44	12.669	1762	1765	1768	rBV3	627626	798559	1.01%	0.250%
45	12.704	1768	1771	1774	rVV	897998	907176	1.15%	0.284%
46	12.939	1808	1811	1814	rVB2	1501225	1212633	1.53%	0.380%
47	13.074	1831	1834	1837	rVB	2293751	2180333	2.76%	0.683%
48	13.298	1869	1872	1875	rBV	1910366	1964876	2.48%	0.616%
49	13.651	1929	1932	1937	rVB3	1471800	1648901	2.08%	0.517%

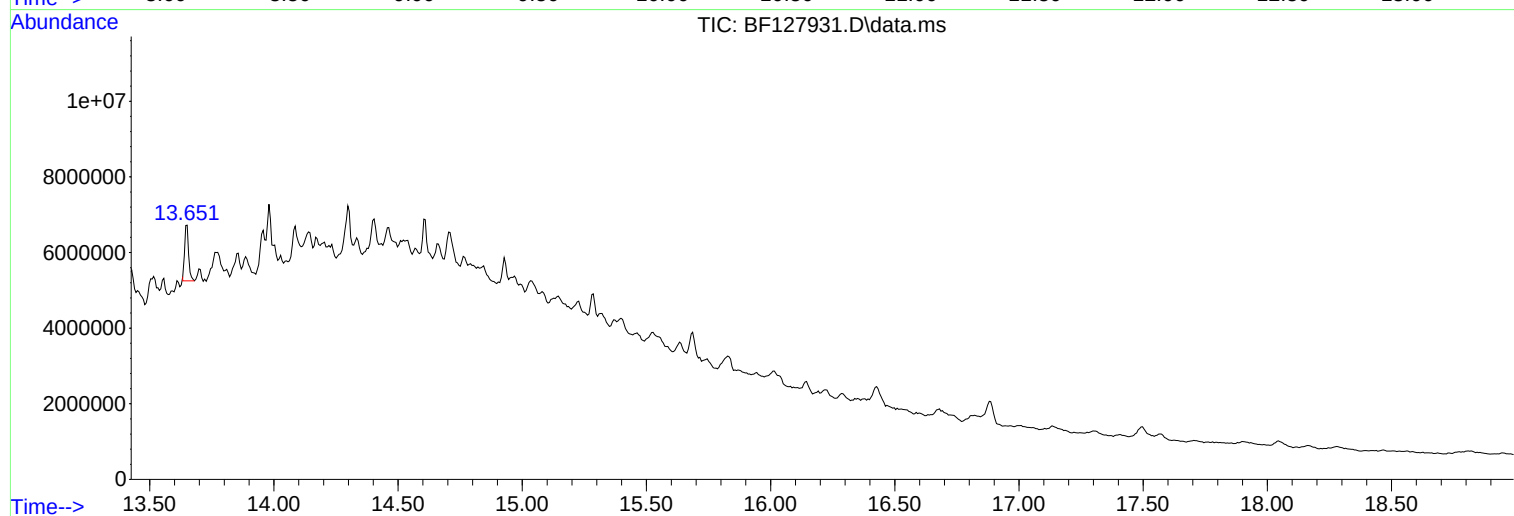
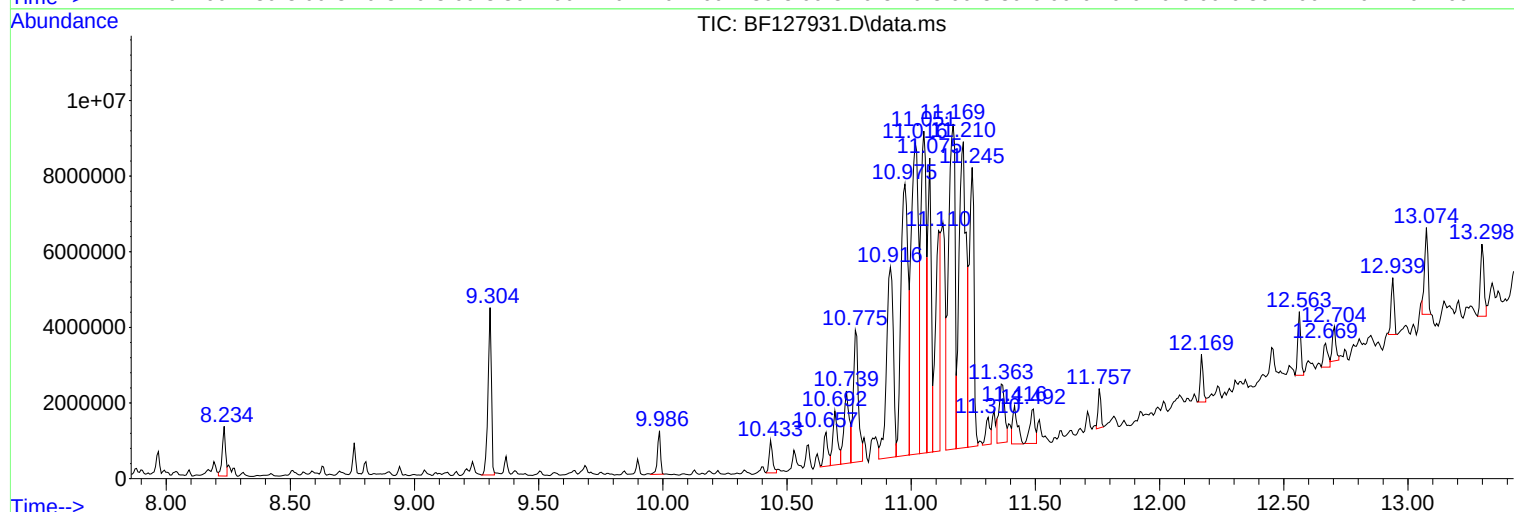
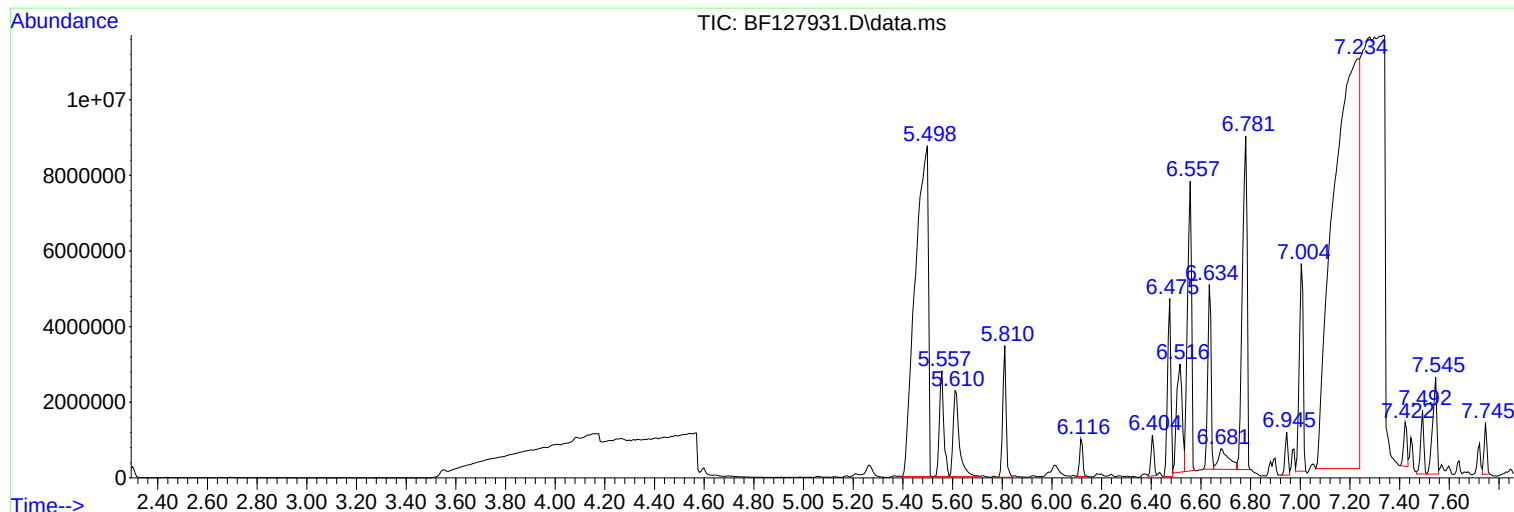
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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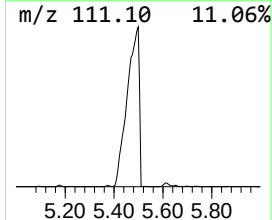
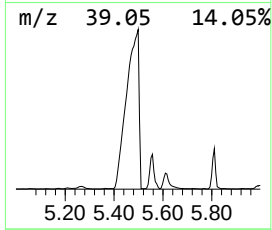
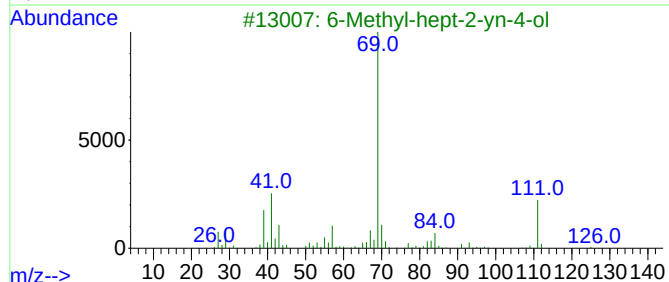
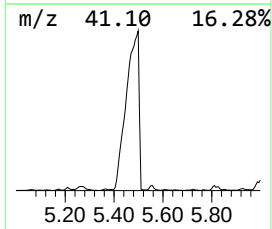
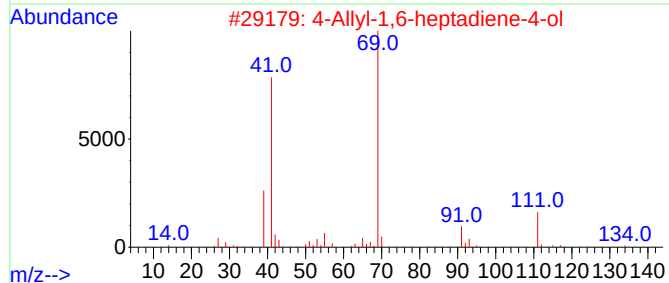
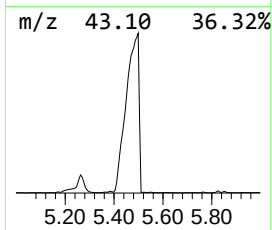
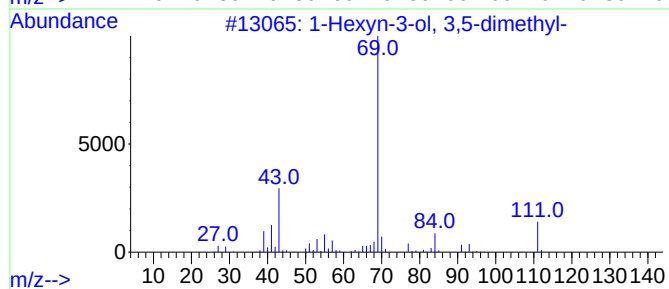
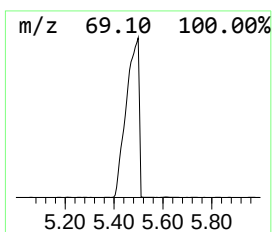
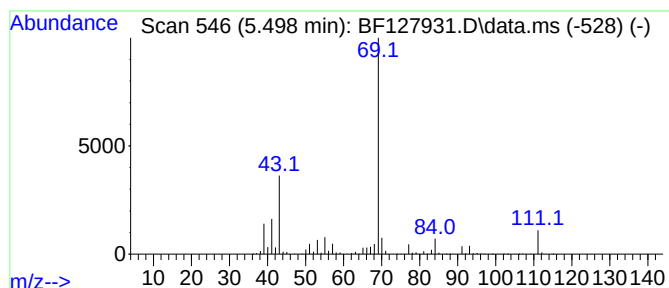
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Hexyn-3-ol, 3,5-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.498	682.14 ng	31862700	1,4-Dichlorobenzene-d4	6.945

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexyn-3-ol, 3,5-dimethyl-	126	C8H14O	000107-54-0	86	
2	4-Allyl-1,6-heptadiene-4-ol	152	C10H16O	010202-75-2	50	
3	6-Methyl-hept-2-yn-4-ol	126	C8H14O	060018-69-1	50	
4	1-Hexyn-3-ol, 3-methyl-	112	C7H12O	004339-05-3	45	
5	Trifluoroacetyl-lavandulol	250	C12H17F3O2	028673-24-7	45	



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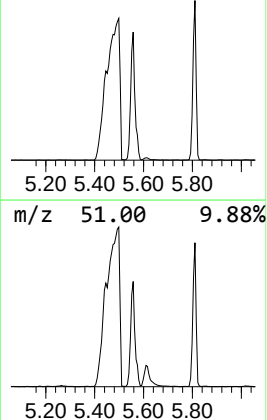
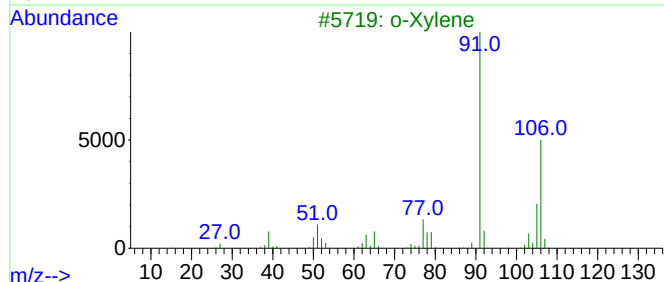
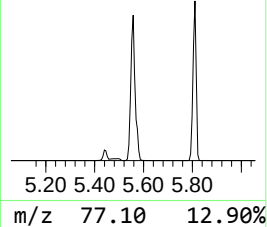
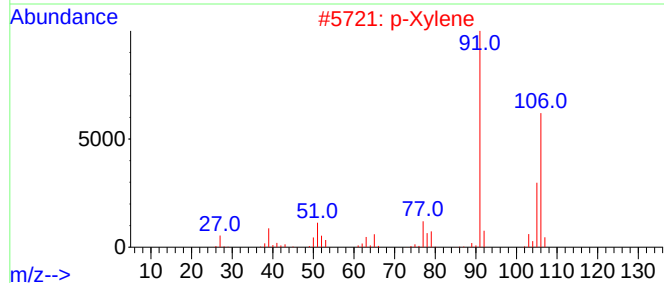
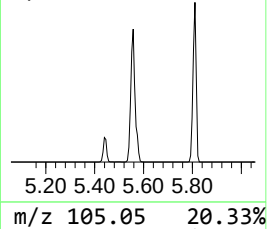
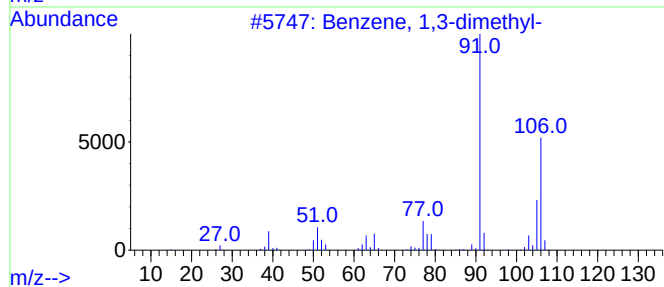
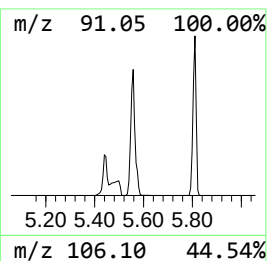
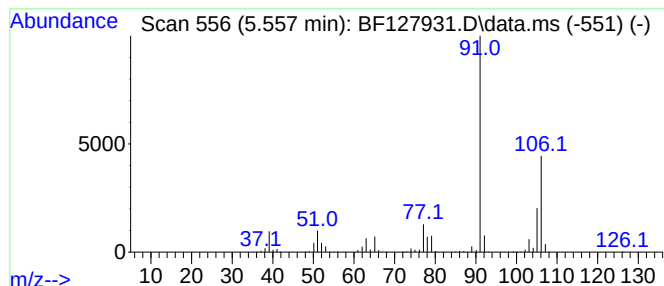
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzene, 1,3-dimethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.557	73.16 ng	3417470	1,4-Dichlorobenzene-d4	6.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	97
2			p-Xylene	106	C8H10	000106-42-3	97
3			o-Xylene	106	C8H10	000095-47-6	97
4			Ethylbenzene	106	C8H10	000100-41-4	87
5			Cyclopentene, 1-ethenyl-3-methyl...	106	C8H10	061142-07-2	86



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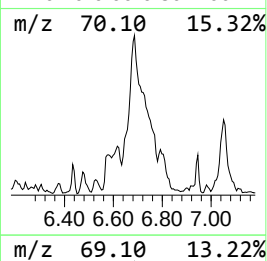
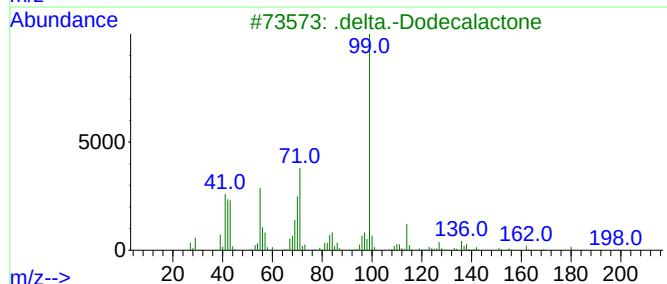
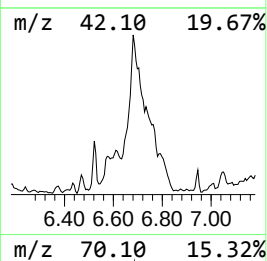
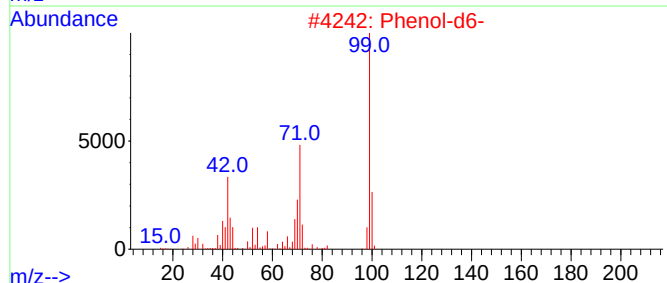
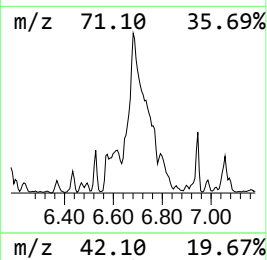
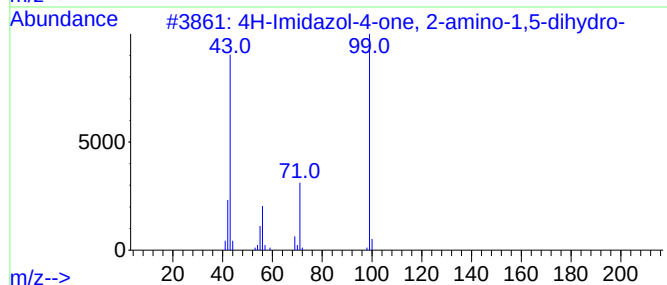
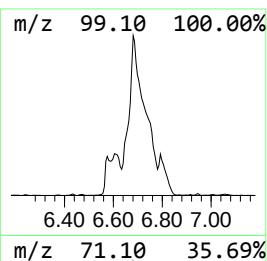
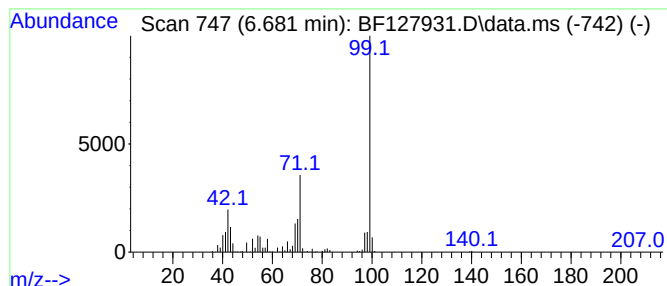
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 4H-Imidazol-4-one, 2-amino-... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.681	35.54 ng	1660210	1,4-Dichlorobenzene-d4	6.945

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4H-Imidazol-4-one, 2-amino-1,5-d...	99	C3H5N3O	000503-86-6	64
2		Phenol-d6-	100	C6D6O	013127-88-3	56
3		.delta.-Dodecalactone	198	C12H22O2	000713-95-1	56
4		Hexanoic acid, 4-octyl ester	228	C14H28O2	1010160-13-3	56
5		2-Piperidinone	99	C5H9NO	000675-20-7	52



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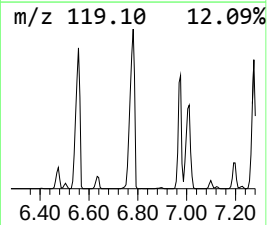
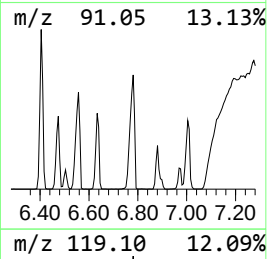
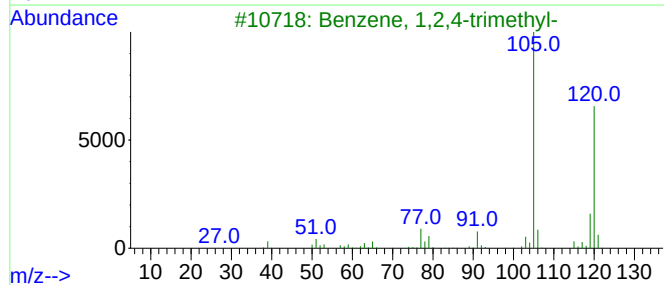
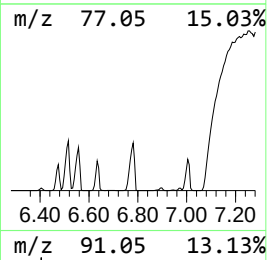
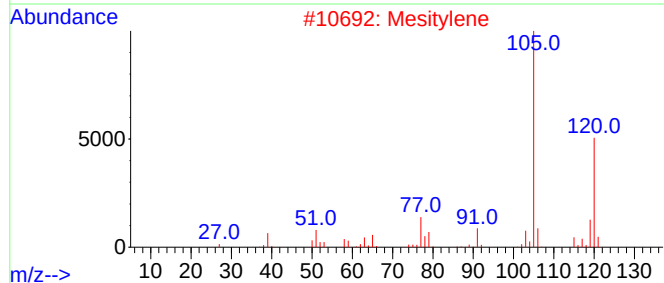
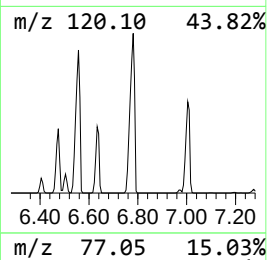
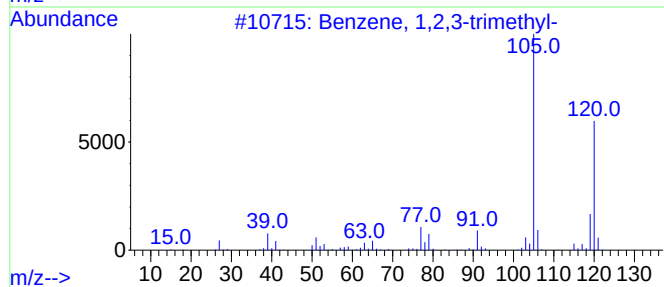
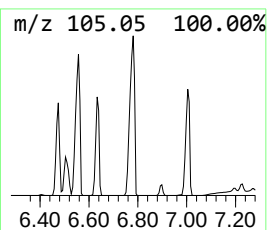
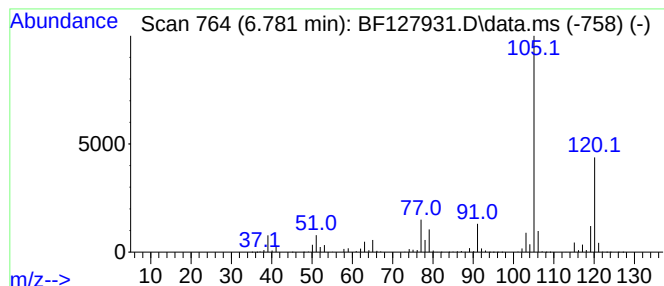
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzene, 1,2,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.781	254.91 ng	11906700	1,4-Dichlorobenzene-d4	6.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2			Mesitylene	120	C9H12	000108-67-8	97
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



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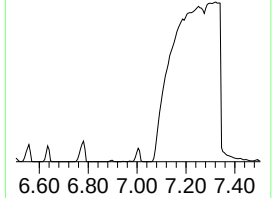
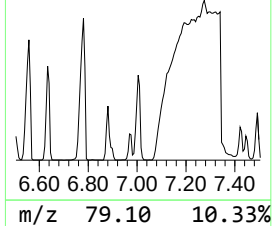
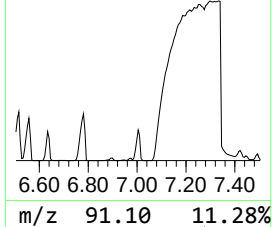
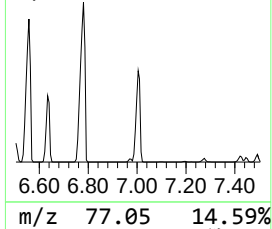
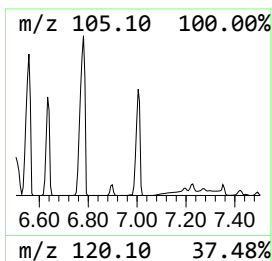
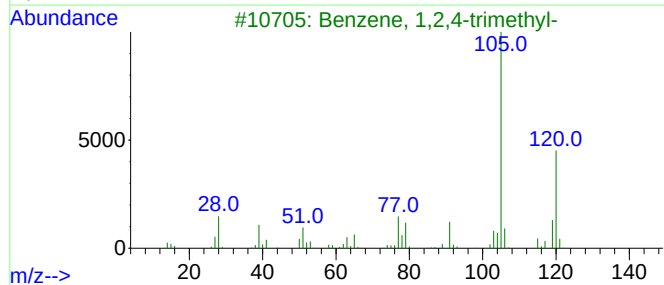
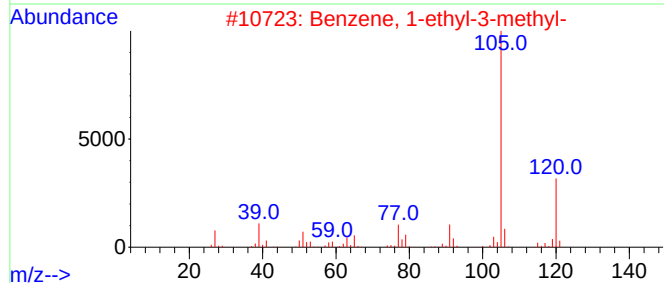
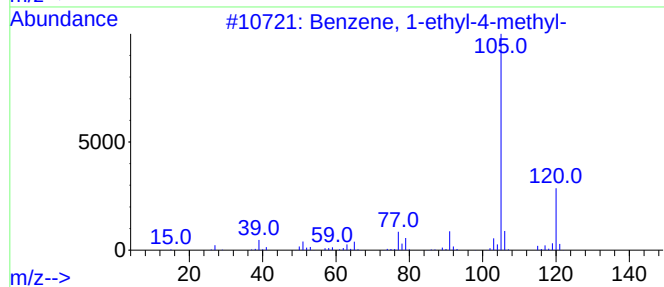
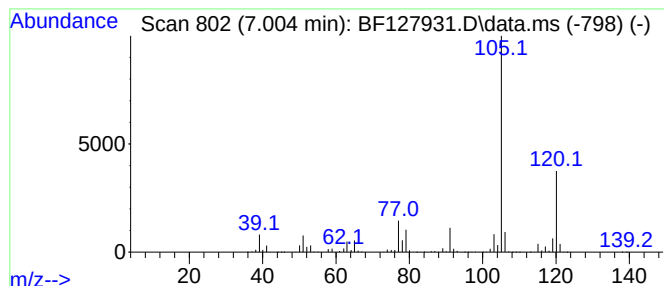
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzene, 1-ethyl-4-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.004	126.51 ng	5909040	1,4-Dichlorobenzene-d4	6.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042622\
Data File : BF127931.D
Acq On : 27 Apr 2022 00:03
Operator : CG\JU
Sample : N2502-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

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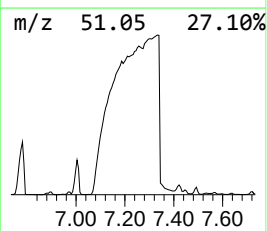
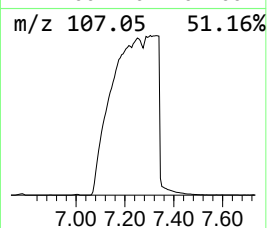
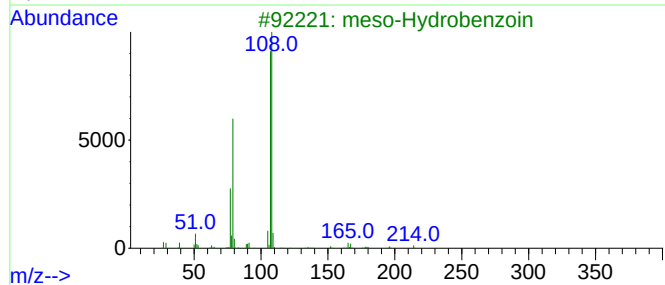
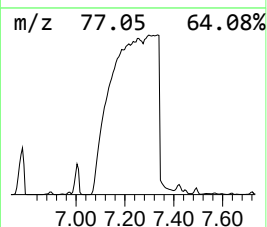
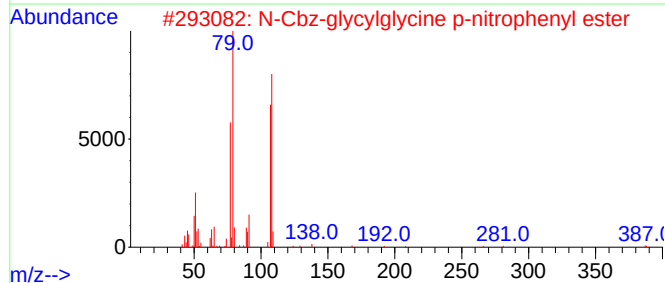
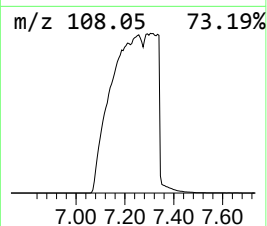
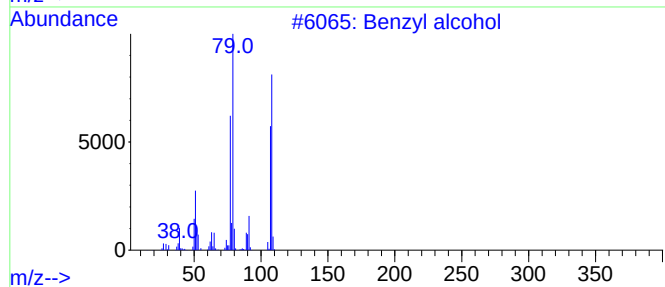
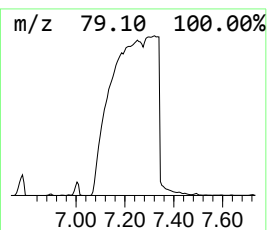
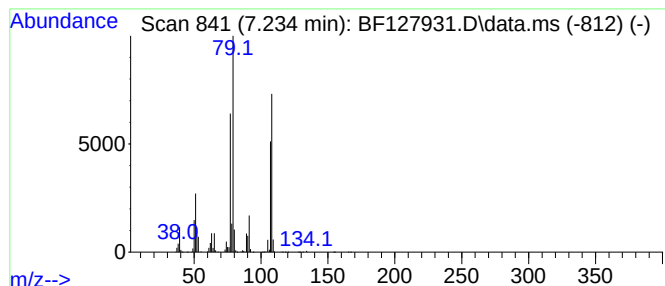
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 N-Cbz-glycylglycine p-nitro... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.234	1693.76 ng	79115600	1,4-Dichlorobenzene-d4	6.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzyl alcohol	108	C7H8O	000100-51-6	98
2			N-Cbz-glycylglycine p-nitropheny...	387	C18H17N3O7	013574-81-7	91
3			meso-Hydrobenzoin	214	C14H14O2	000579-43-1	83
4			1,2-Propanediol, 1-phenyl-	152	C9H12O2	001855-09-0	78
5			Furan, 2-(2-propenyl)-	108	C7H8O	075135-41-0	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042622\
Data File : BF127931.D
Acq On : 27 Apr 2022 00:03
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Sample : N2502-01
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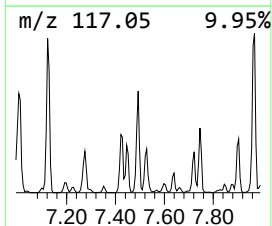
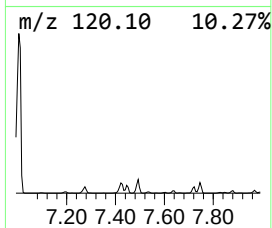
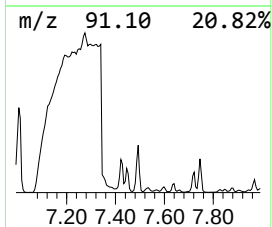
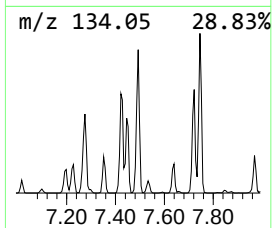
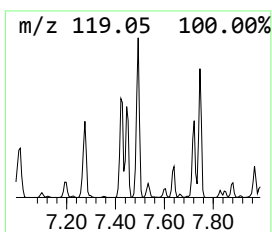
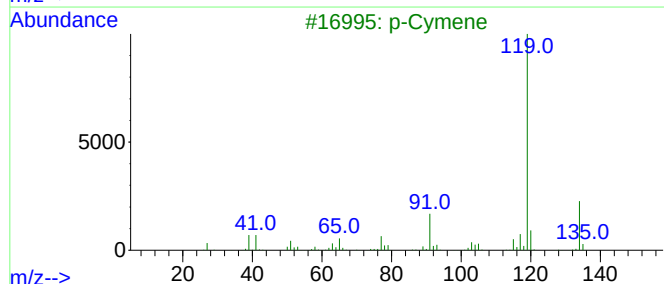
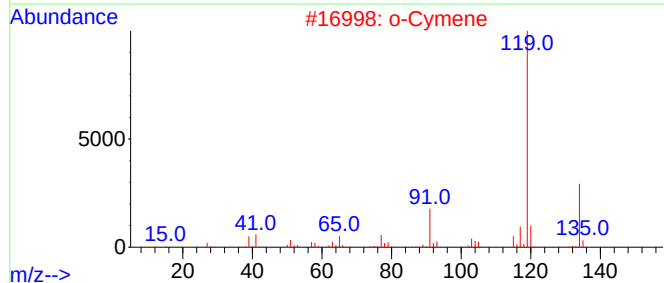
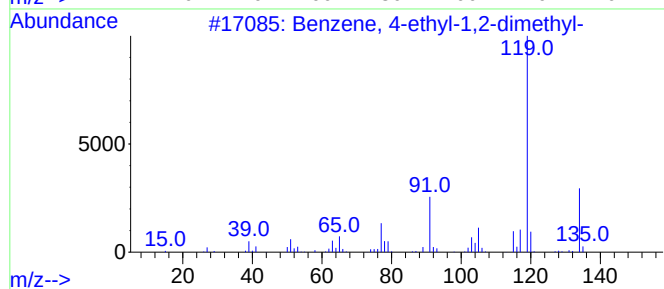
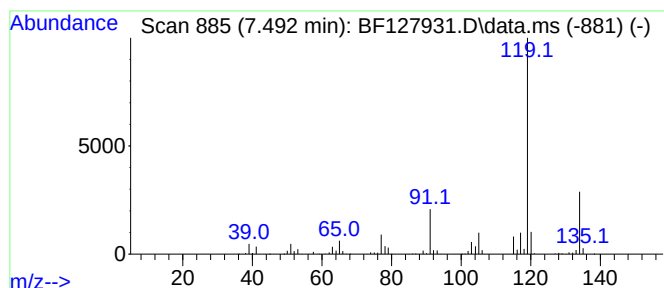
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.492	31.14 ng	1454400	1,4-Dichlorobenzene-d4	6.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2			o-Cymene	134	C10H14	000527-84-4	95
3			p-Cymene	134	C10H14	000099-87-6	95
4			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
5			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042622\
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Operator : CG\JU
Sample : N2502-01
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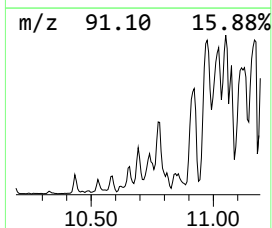
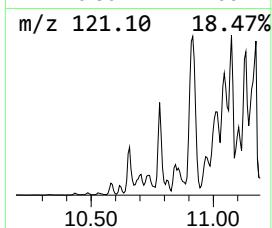
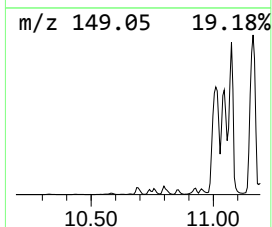
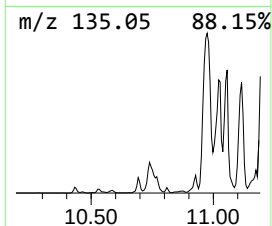
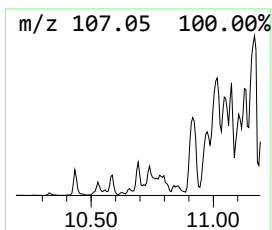
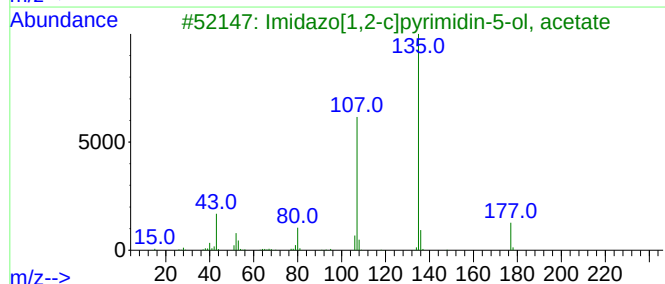
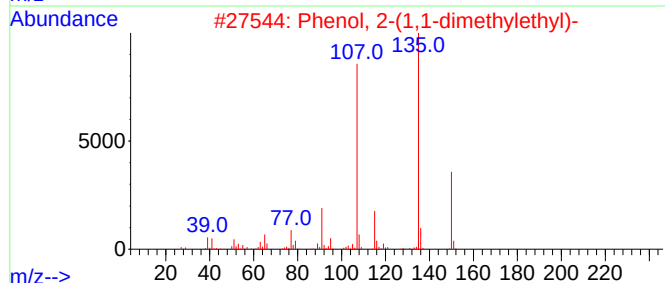
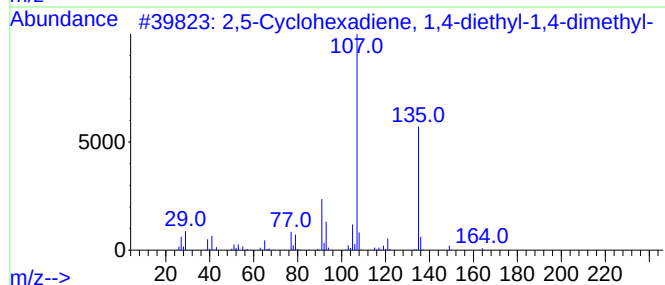
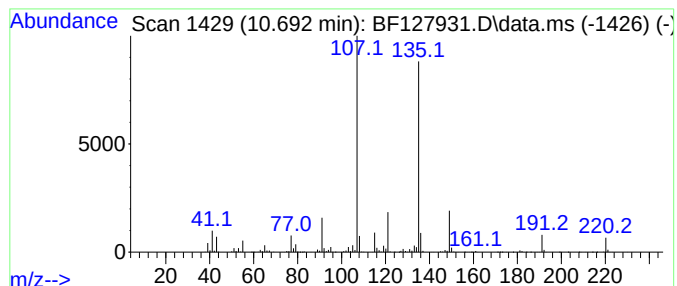
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2,5-Cyclohexadiene, 1,4-die... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.692	38.49 ng	1900610	Acenaphthene-d10	9.986	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene, 1,4-diethyl-...	164	C12H20	1000150-21-6	64
2	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	64
3	Imidazo[1,2-c]pyrimidin-5-ol, ac...	177	C8H7N3O2	1000509-01-4	59
4	1,5,6,7-Tetrahydro-4-indolone	135	C8H9NO	013754-86-4	59
5	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042622\
Data File : BF127931.D
Acq On : 27 Apr 2022 00:03
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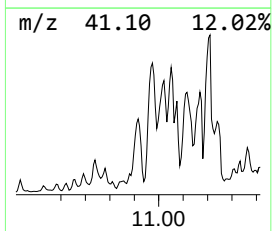
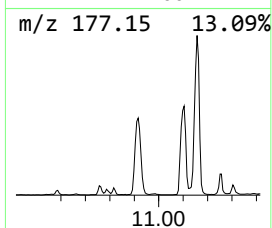
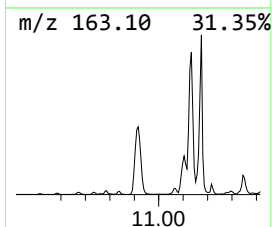
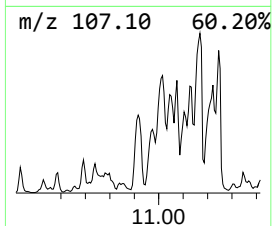
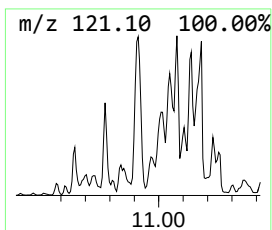
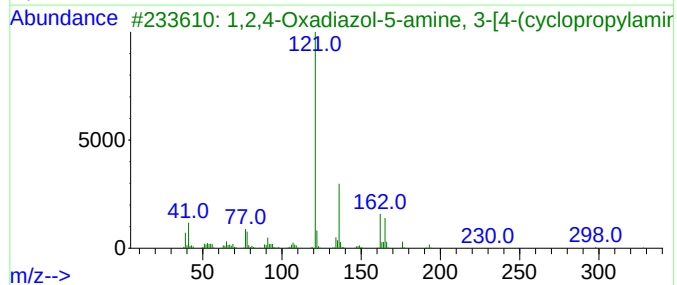
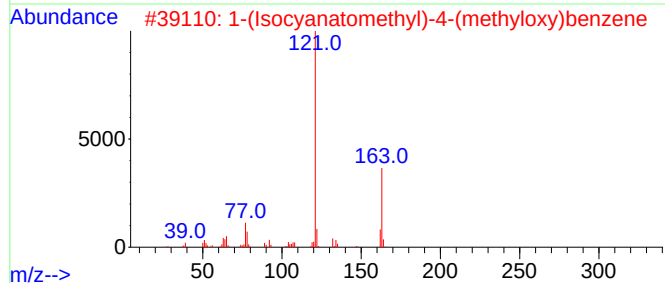
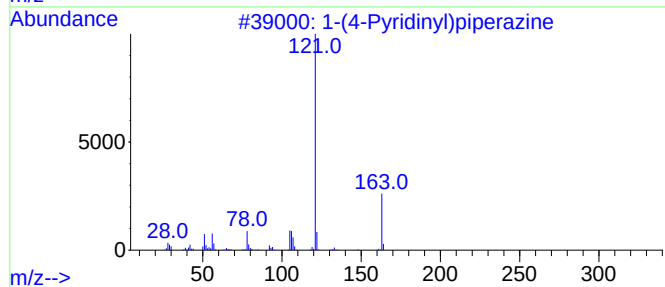
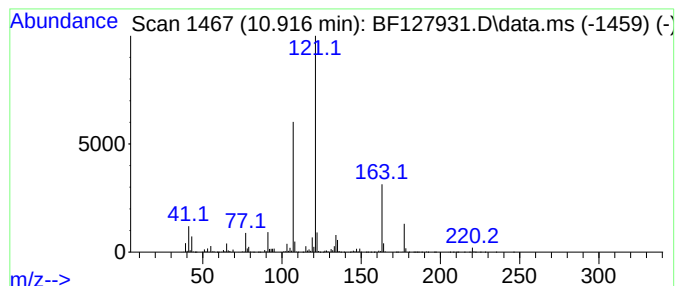
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-(4-Pyridinyl)piperazine Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.916	148.71 ng	9621200	Phenanthrene-d10	11.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-(4-Pyridinyl)piperazine	163	C9H13N3	001008-91-9	50
2			1-(Isocyanatomethyl)-4-(methylox...	163	C9H9NO2	056651-60-6	50
3			1,2,4-Oxadiazol-5-amine, 3-[4-(c...	328	C15H16N6O3	1000351-08-7	47
4			2-sec-Butylphenol, 0-ethoxycarbo...	222	C13H18O3	1000487-26-4	46
5			N-Allyl-p-hydroxybenzamide	177	C10H11NO2	090921-72-5	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042622\
Data File : BF127931.D
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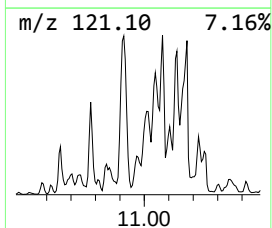
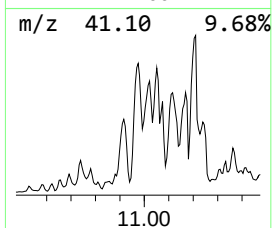
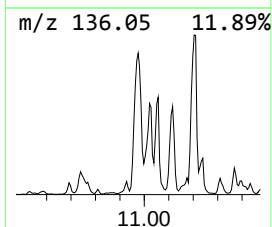
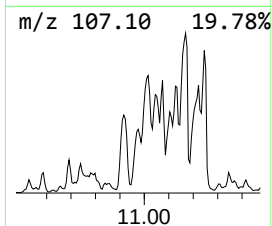
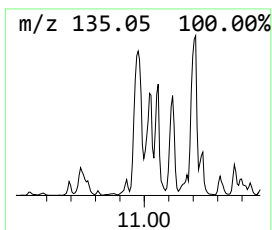
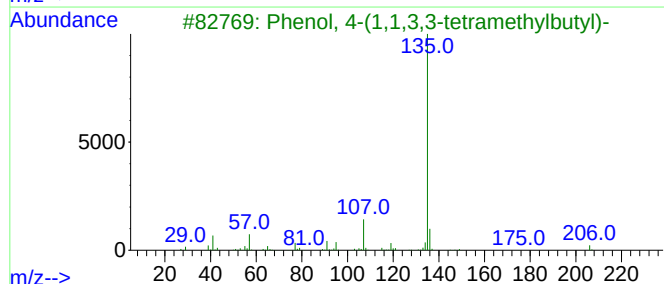
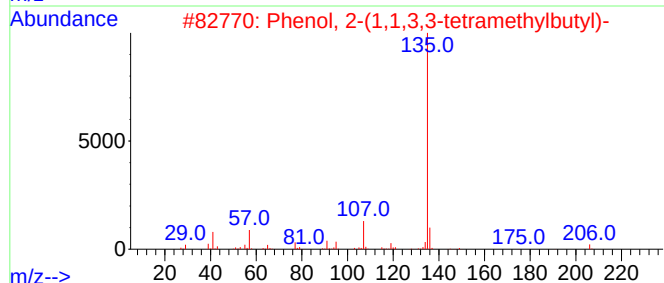
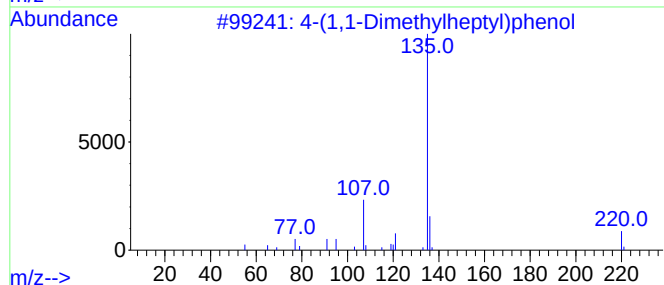
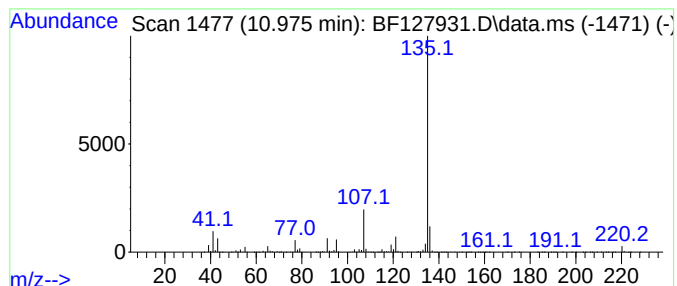
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 4-(1,1-Dimethylheptyl)phenol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.975	228.64 ng	14792200	Phenanthrene-d10	11.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-(1,1-Dimethylheptyl)phenol	220	C15H24O	1000384-80-3	91
2			Phenol, 2-(1,1,3,3-tetramethylbu...	206	C14H22O	003884-95-5	90
3			Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	90
4			4-(1,1-Dimethylpropyl)phenyl ace...	206	C13H18O2	1000373-45-3	83
5			Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042622\
Data File : BF127931.D
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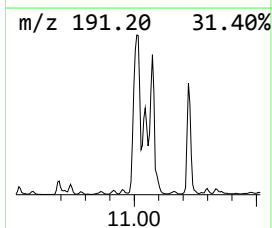
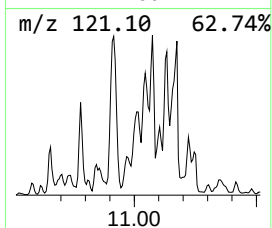
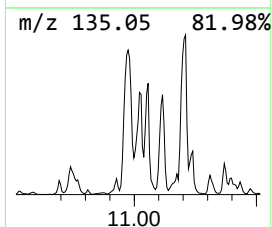
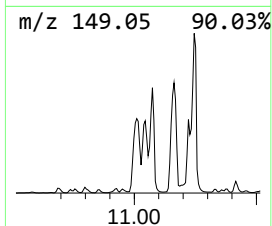
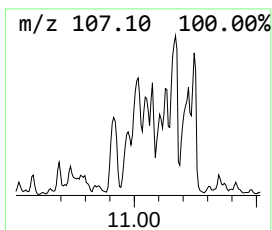
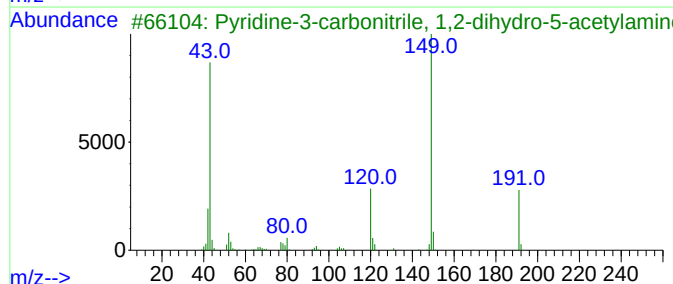
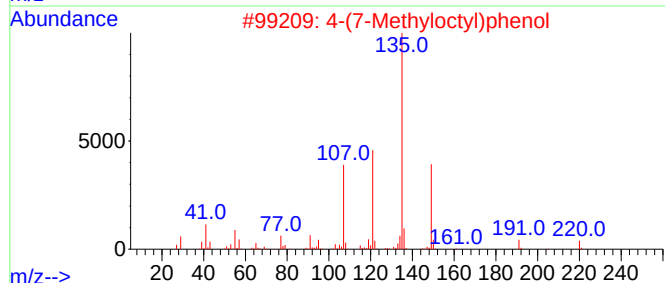
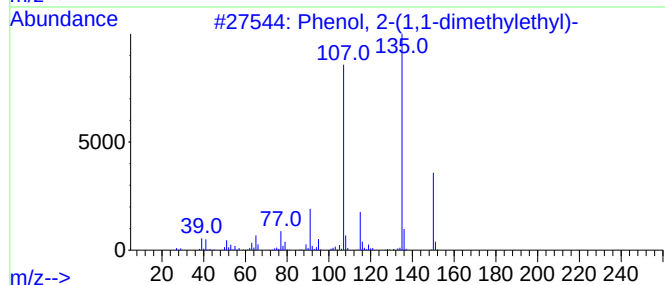
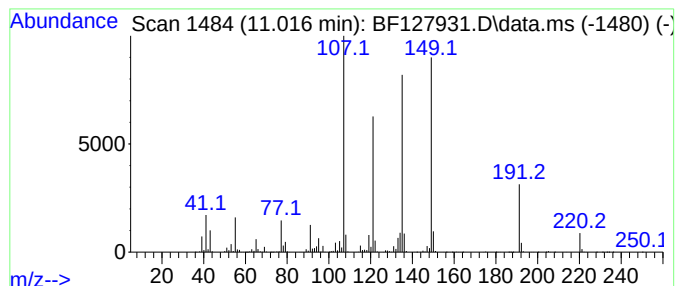
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown11.016 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.016	259.61 ng	16795900	Phenanthrene-d10	11.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	43
2			4-(7-Methyloctyl)phenol	220	C15H24O	024518-48-7	30
3			Pyridine-3-carbonitrile, 1,2-dih...	191	C9H9N3O2	220098-92-0	30
4			1-Isopropenyl-3-propenylcyclop...	150	C11H18	1000192-81-2	30
5			2-tert-Butyl-6-methylphenol, 2-m...	220	C15H24O	1000395-19-4	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042622\
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Misc :
ALS Vial : 19 Sample Multiplier: 1

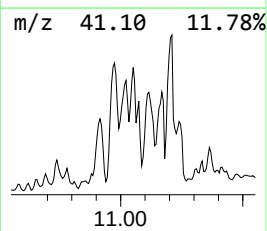
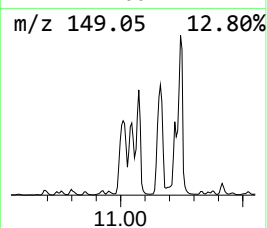
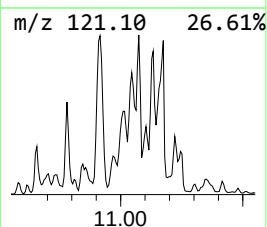
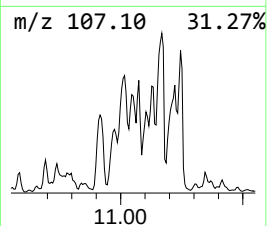
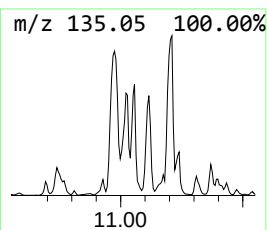
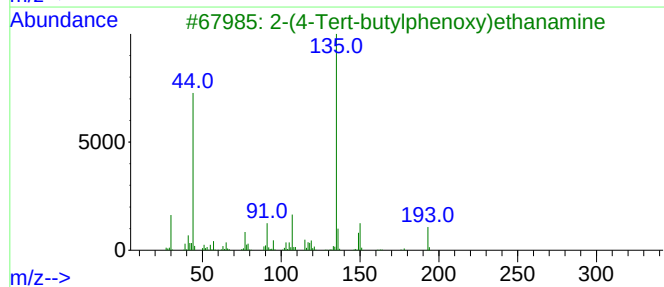
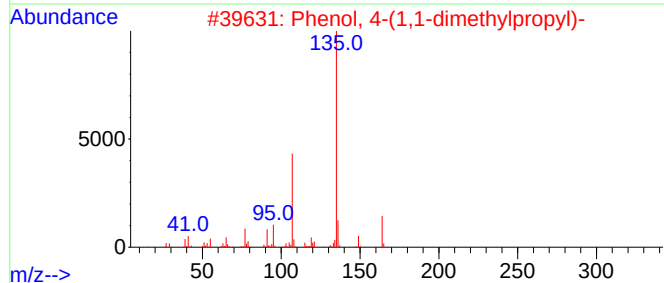
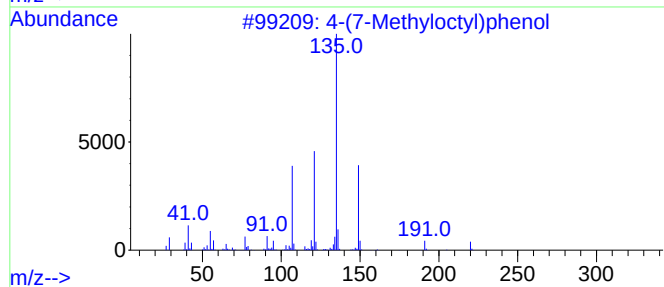
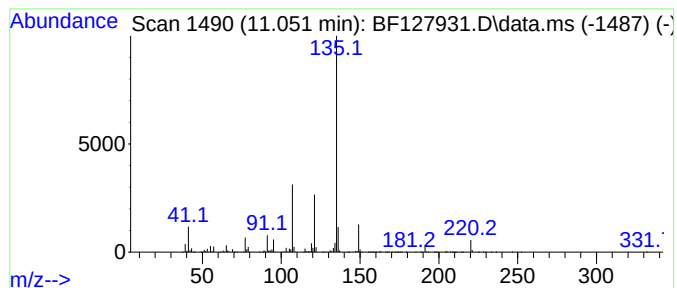
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 4-(7-Methyloctyl)phenol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.051	195.04 ng	12618800	Phenanthrene-d10	11.492
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		4-(7-Methyloctyl)phenol	220 C15H24O	024518-48-7 80
2		Phenol, 4-(1,1-dimethylpropyl)-	164 C11H16O	000080-46-6 72
3		2-(4-Tert-butylphenoxy)ethanamine	193 C12H19NO	050634-73-6 64
4		Phenol, 4-(1,1,3,3-tetramethylbu...	206 C14H22O	000140-66-9 64
5		((1,2-Diethylethylene)bis(p-phen...	354 C22H26O4	004547-76-6 64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042622\
Data File : BF127931.D
Acq On : 27 Apr 2022 00:03
Operator : CG\JU
Sample : N2502-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

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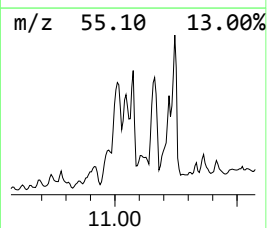
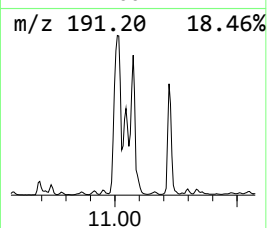
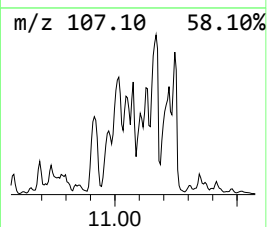
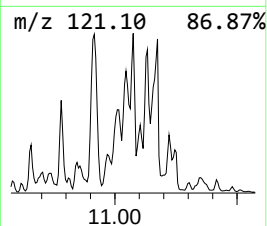
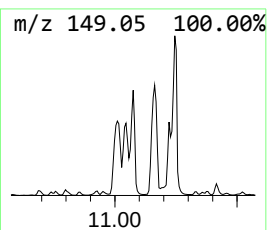
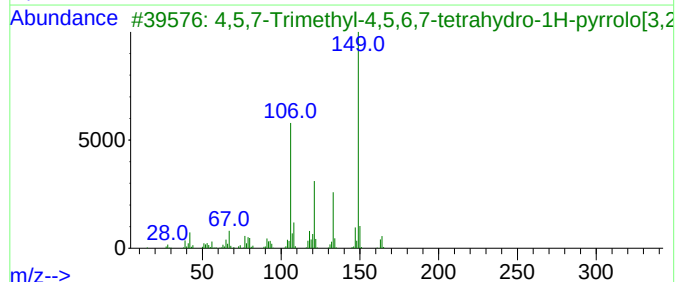
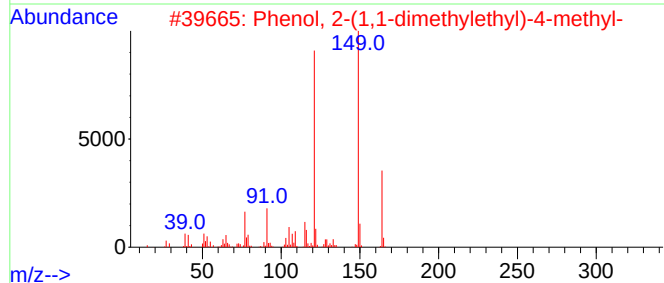
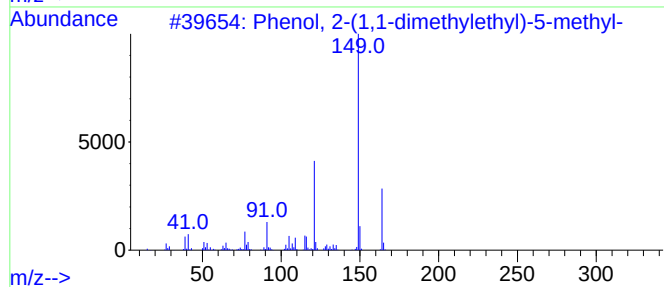
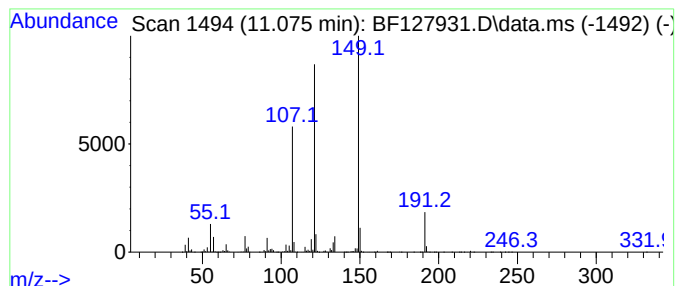
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Phenol, 2-(1,1-dimethylethy... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.075	114.05 ng	7378610	Phenanthrene-d10	11.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-(1,1-dimethylethyl)-5-...	164	C11H16O	000088-60-8	59
2			Phenol, 2-(1,1-dimethylethyl)-4-...	164	C11H16O	002409-55-4	59
3			4,5,7-Trimethyl-4,5,6,7-tetrahyd...	164	C10H16N2	113849-86-8	35
4			Phenol, 2-methyl-4-(1,1,3,3-tetr...	220	C15H24O	002219-84-3	35
5			1-(2,6-Dimethyl-4-propoxyphenyl)...	220	C14H20O2	1000190-22-3	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042622\
Data File : BF127931.D
Acq On : 27 Apr 2022 00:03
Operator : CG\JU
Sample : N2502-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

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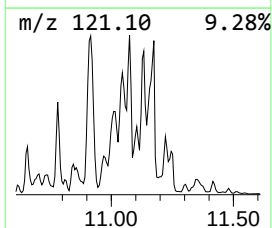
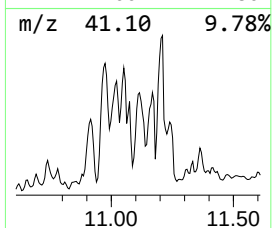
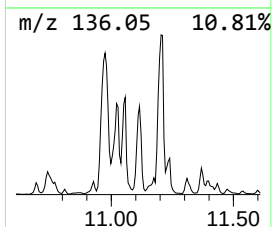
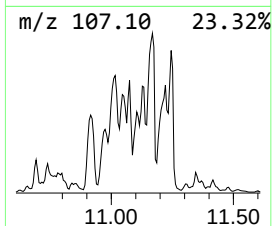
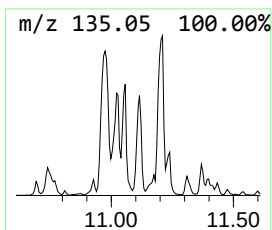
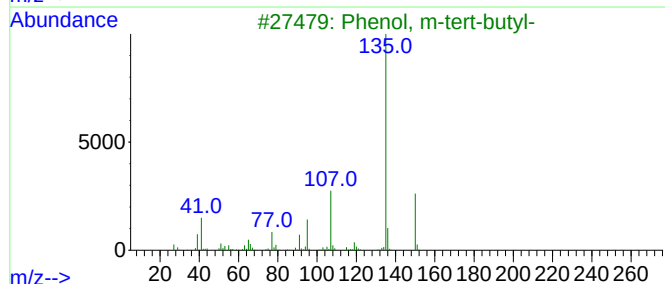
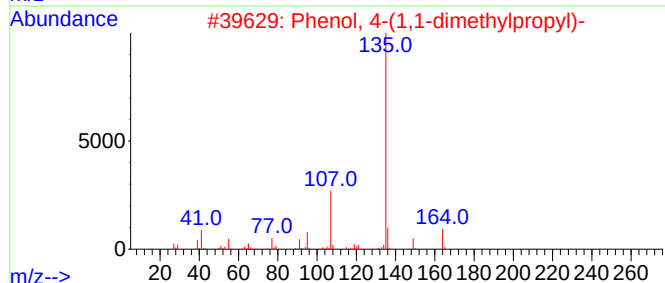
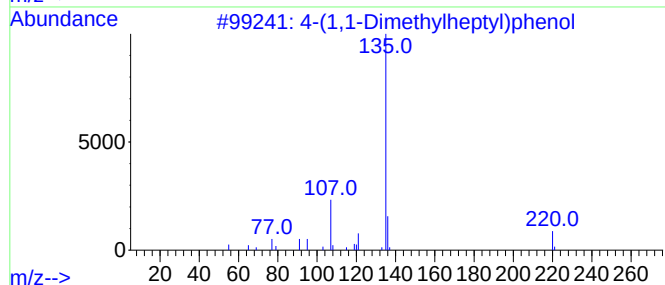
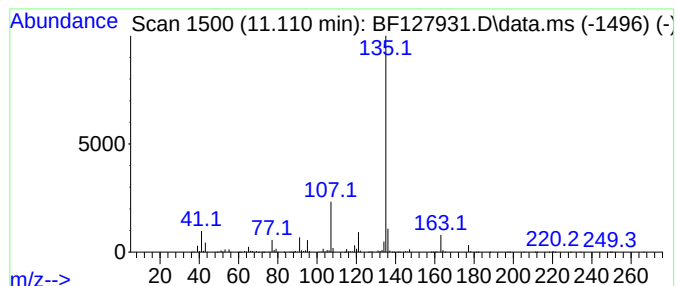
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Phenol, 4-(1,1-dimethylprop... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.110	123.05 ng	7961000	Phenanthrene-d10	11.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-(1,1-Dimethylheptyl)phenol	220	C15H24O	1000384-80-3	90
2			Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	72
3			Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	64
4			5(6H)-Quinazolinone, 2-amino-7,8...	163	C8H9N3O	1000338-03-0	64
5			Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042622\
Data File : BF127931.D
Acq On : 27 Apr 2022 00:03
Operator : CG\JU
Sample : N2502-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

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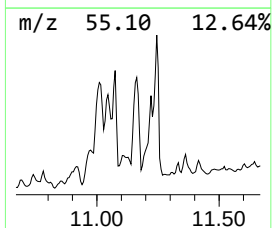
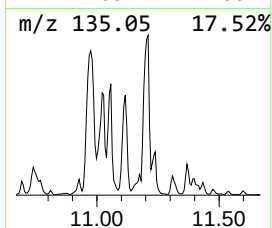
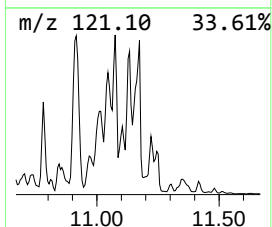
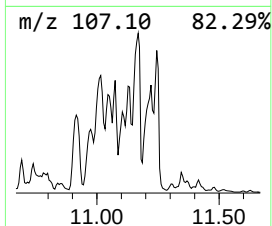
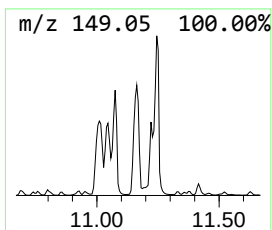
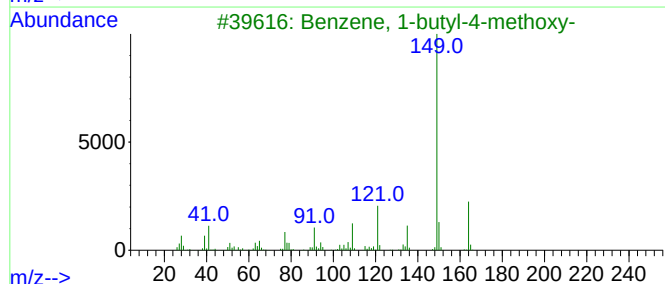
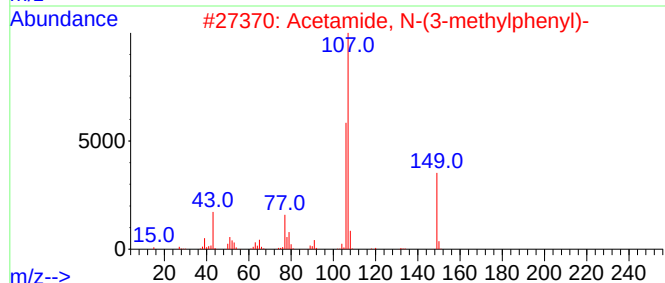
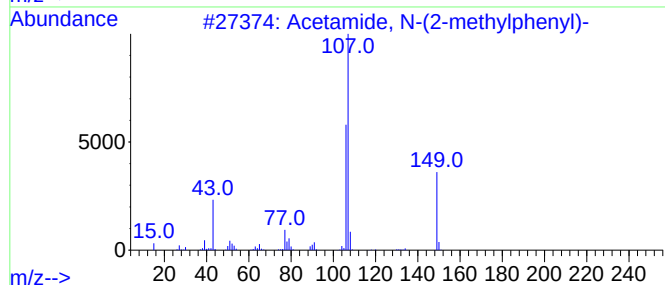
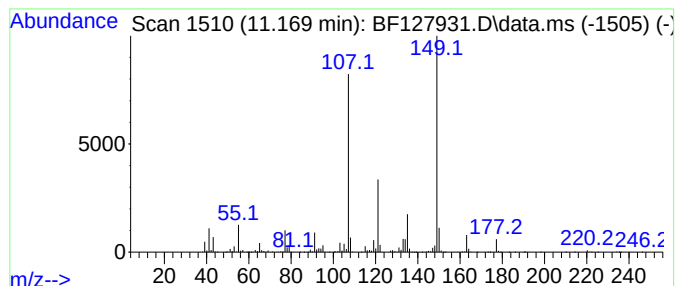
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown11.169 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.169	237.21 ng	15346600	Phenanthrene-d10	11.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetamide, N-(2-methylphenyl)-	149	C9H11NO	000120-66-1	49
2			Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	47
3			Benzene, 1-butyl-4-methoxy-	164	C11H16O	018272-84-9	46
4			Phenol, 4-(1,1-dimethylethyl)-2-...	164	C11H16O	000098-27-1	43
5			Methyl (1s,3s,5R,7S)-3-methylada...	208	C13H20O2	1010504-39-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042622\
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Acq On : 27 Apr 2022 00:03
Operator : CG\JU
Sample : N2502-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

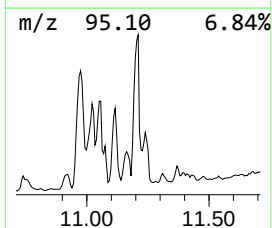
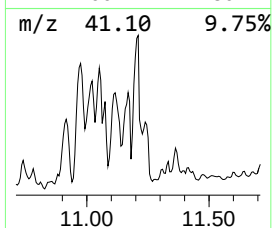
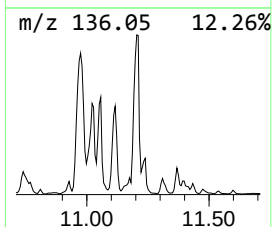
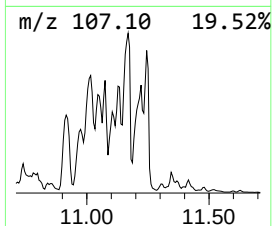
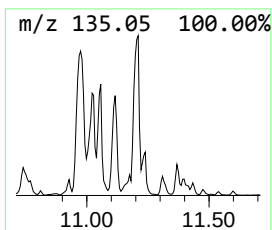
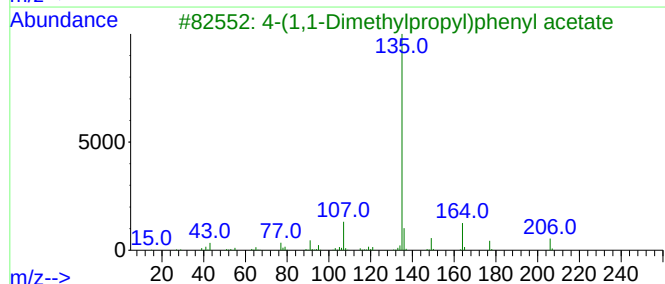
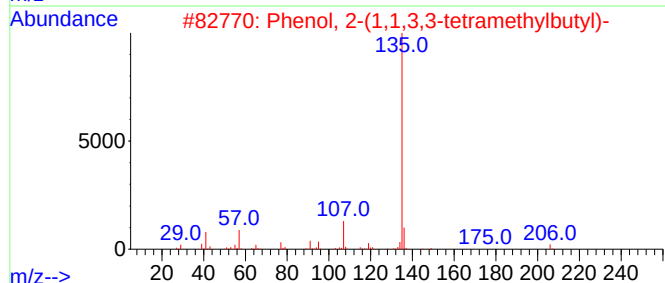
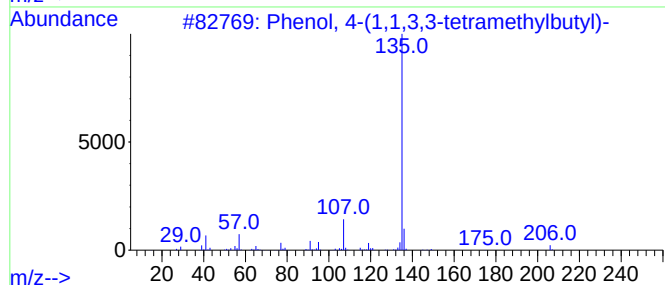
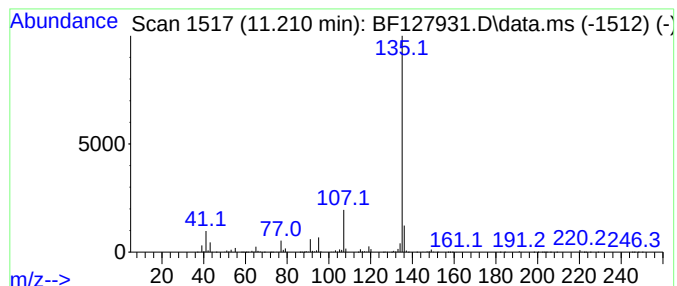
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Phenol, 4-(1,1,3,3-tetramet... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.210	254.44 ng	16461500	Phenanthrene-d10	11.492	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	90
2	Phenol, 2-(1,1,3,3-tetramethylbu...	206	C14H22O	003884-95-5	87
3	4-(1,1-Dimethylpropyl)phenyl ace...	206	C13H18O2	1000373-45-3	83
4	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	78
5	Hexestrol, O-(n-propyloxycarbonyl)-	356	C22H28O4	1000487-65-1	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042622\
Data File : BF127931.D
Acq On : 27 Apr 2022 00:03
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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
C1

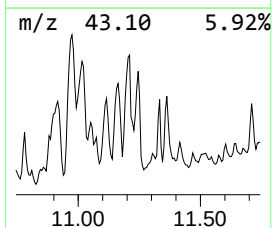
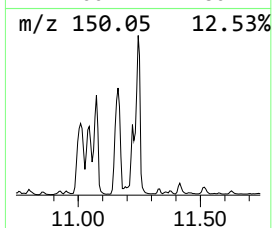
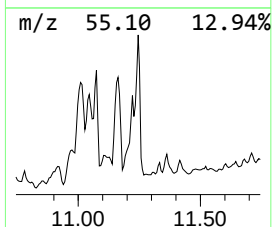
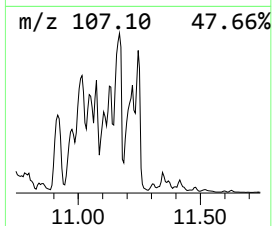
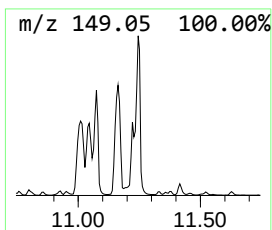
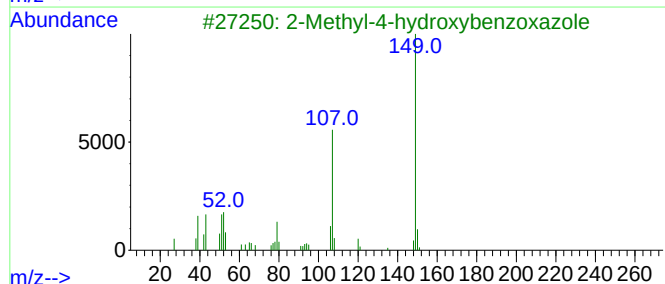
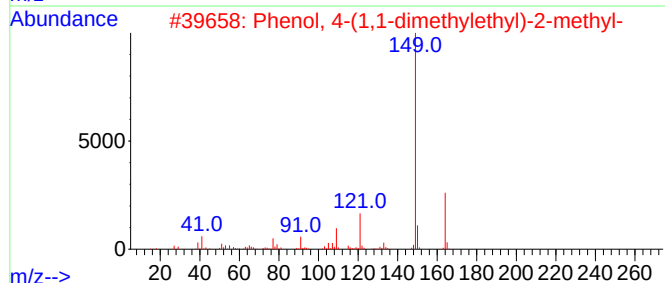
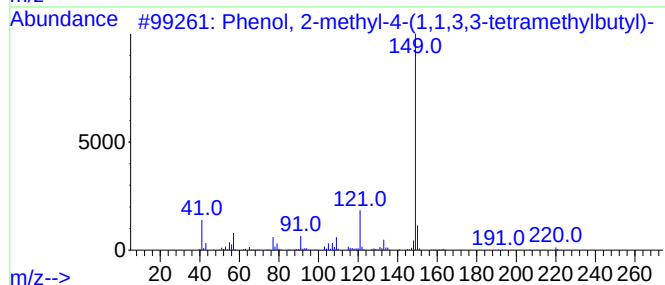
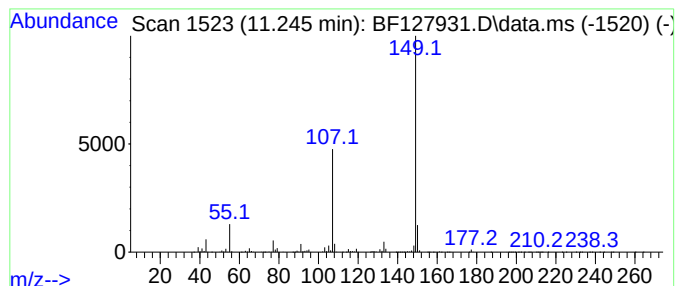
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Phenol, 2-methyl-4-(1,1,3,3... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.245	145.06 ng	9385150	Phenanthrene-d10	11.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-methyl-4-(1,1,3,3-tetr...	220	C15H24O	002219-84-3	50
2			Phenol, 4-(1,1-dimethylethyl)-2-...	164	C11H16O	000098-27-1	40
3			2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	40
4			Hexestrol dimethyl ether	298	C20H26O2	000130-78-9	38
5			2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	28



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042622\
Data File : BF127931.D
Acq On : 27 Apr 2022 00:03
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Misc :
ALS Vial : 19 Sample Multiplier: 1

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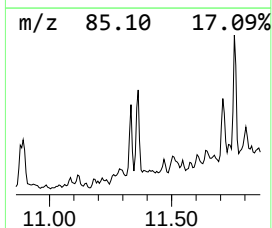
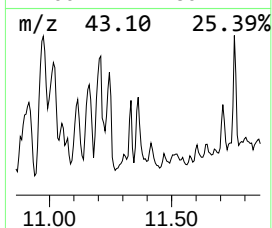
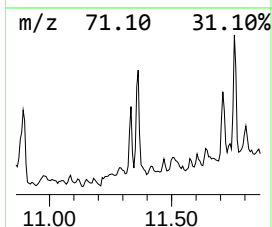
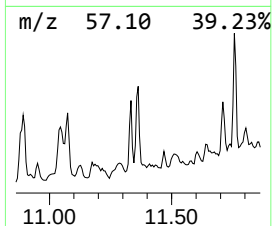
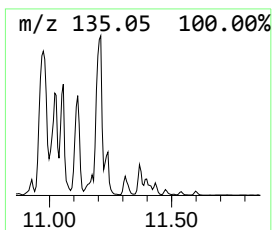
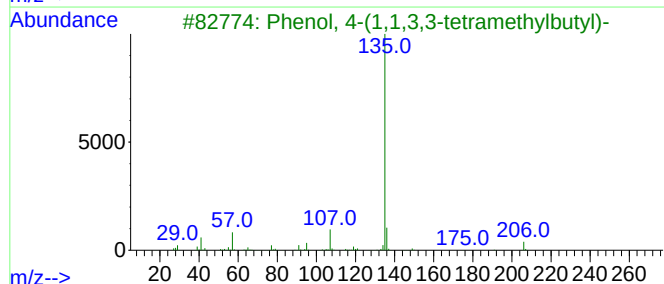
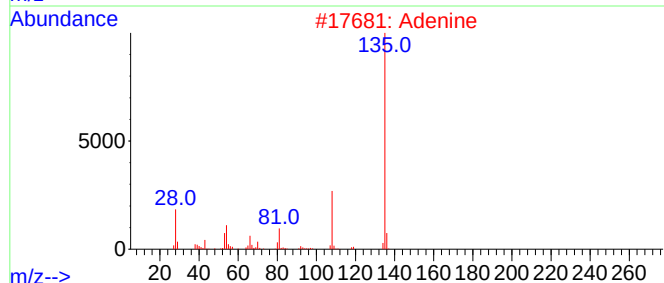
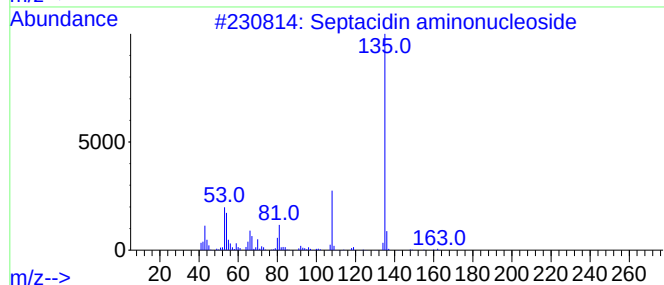
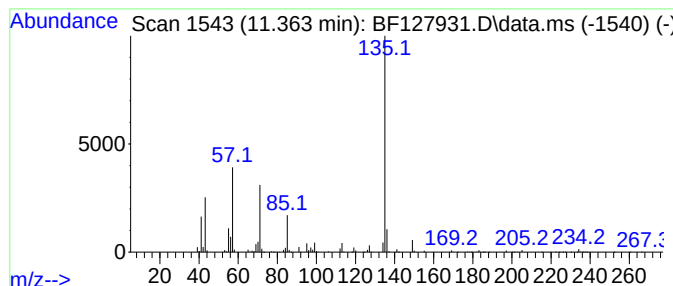
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Septacidin aminonucleoside Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.363	37.32 ng	2414190	Phenanthrene-d10	11.492

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Septacidin aminonucleoside	326	C12H18N6O5	003059-05-0	50
2		Adenine	135	C5H5N5	000073-24-5	40
3		Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	40
4		Phenol, 2-(1,1,3,3-tetramethylbu...	206	C14H22O	003884-95-5	36
5		4-(1,1-Dimethylpropyl)phenyl ace...	206	C13H18O2	1000373-45-3	36



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042622\
Data File : BF127931.D
Acq On : 27 Apr 2022 00:03
Operator : CG\JU
Sample : N2502-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

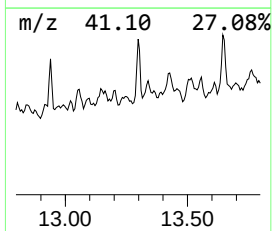
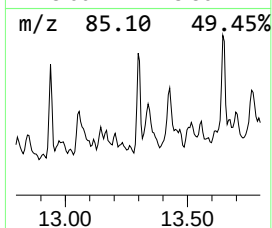
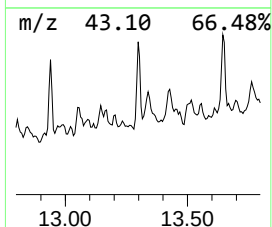
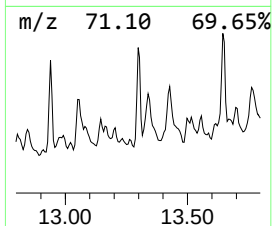
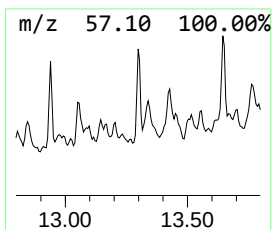
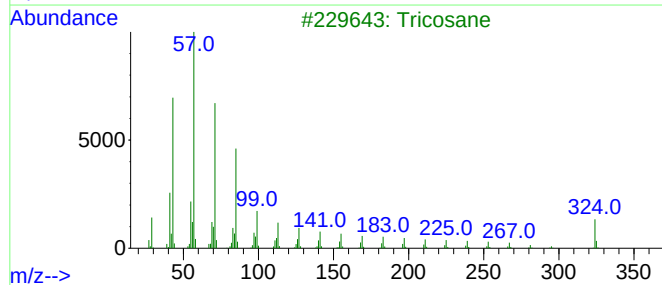
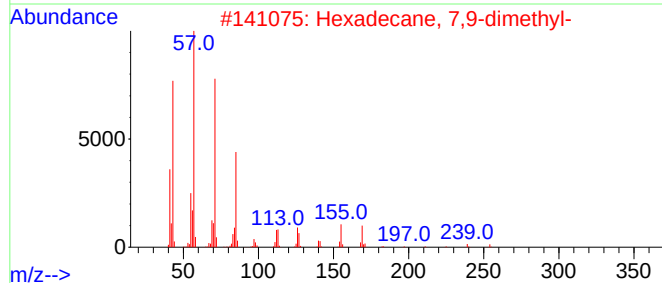
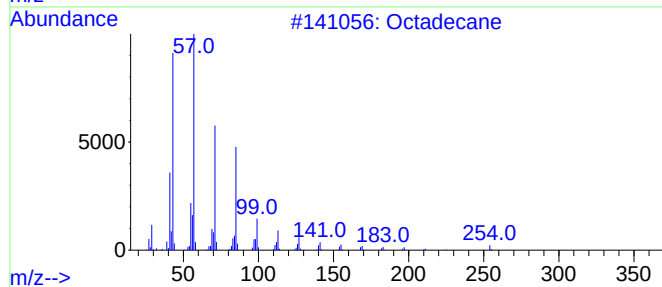
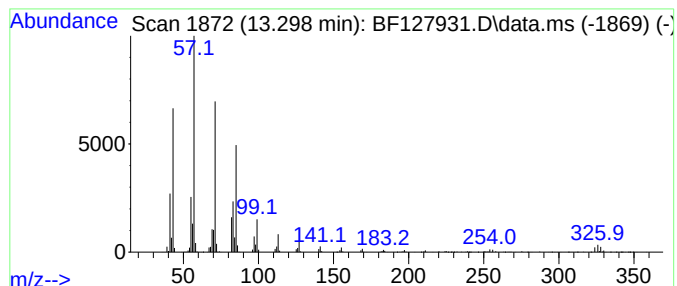
Instrument :
BNA_F
ClientSampleId :
C1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Octadecane Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.298	23.83 ng	1964880	Chrysene-d12		14.145	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecane		254	C18H38	000593-45-3	86
2	Hexadecane, 7,9-dimethyl-		254	C18H38	021164-95-4	86
3	Tricosane		324	C23H48	000638-67-5	81
4	Heneicosane		296	C21H44	000629-94-7	74
5	Tetradecane, 1-iodo-		324	C14H29I	019218-94-1	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042622\
 Data File : BF127931.D
 Acq On : 27 Apr 2022 00:03
 Operator : CG\JU
 Sample : N2502-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 C1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexyn-3-ol, 3...	5.498	682.1	ng	31862700	1	6.945	934200	20.0
Benzene, 1,3-di...	5.557	73.2	ng	3417470	1	6.945	934200	20.0
4H-Imidazol-4-o...	6.681	35.5	ng	1660210	1	6.945	934200	20.0
Benzene, 1,2,3-...	6.781	254.9	ng	11906700	1	6.945	934200	20.0
Benzene, 1-ethy...	7.004	126.5	ng	5909040	1	6.945	934200	20.0
N-Cbz-glycylgly...	7.234	1693.8	ng	79115600	1	6.945	934200	20.0
Benzene, 4-ethy...	7.492	31.1	ng	1454400	1	6.945	934200	20.0
2,5-Cyclohexadi...	10.692	38.5	ng	1900610	3	9.986	987565	20.0
1-(4-Pyridinyl)...	10.916	148.7	ng	9621200	4	11.492	1293940	20.0
4-(1,1-Dimethyl...	10.975	228.6	ng	14792200	4	11.492	1293940	20.0
unknown11.016	11.016	259.6	ng	16795900	4	11.492	1293940	20.0
4-(7-Methylocty...	11.051	195.0	ng	12618800	4	11.492	1293940	20.0
Phenol, 2-(1,1-...	11.075	114.1	ng	7378610	4	11.492	1293940	20.0
Phenol, 4-(1,1-...	11.110	123.1	ng	7961000	4	11.492	1293940	20.0
unknown11.169	11.169	237.2	ng	15346600	4	11.492	1293940	20.0
Phenol, 4-(1,1,...	11.210	254.4	ng	16461500	4	11.492	1293940	20.0
Phenol, 2-methy...	11.245	145.1	ng	9385150	4	11.492	1293940	20.0
Septacidin amin...	11.363	37.3	ng	2414190	4	11.492	1293940	20.0
Octadecane	13.298	23.8	ng	1964880	5	14.145	1648900	20.0