

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103122\
 Data File : BF130884.D
 Acq On : 31 Oct 2022 17:42
 Operator : CG\JU
 Sample : N5329-03
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CBH-594

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-BF102722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130884.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.269	23	31	36	rVB	1506623	1923153	71.10%	11.308%
2	5.163	519	523	529	rVB	129298	141709	5.24%	0.833%
3	5.557	585	590	593	rBV	1387382	1207927	44.66%	7.103%
4	6.551	755	759	763	rBV	828973	759327	28.07%	4.465%
5	6.581	763	764	769	rVB2	48760	33319	1.23%	0.196%
6	6.940	822	825	828	rBV	622679	493141	18.23%	2.900%
7	7.122	848	856	859	rBV	34863	35293	1.30%	0.208%
8	7.504	911	921	924	rBV	1668438	1755162	64.89%	10.321%
9	7.892	981	987	991	rVB3	50019	69360	2.56%	0.408%
10	7.957	995	998	1001	rBV2	33250	29362	1.09%	0.173%
11	7.992	1001	1004	1008	rVV	76439	62498	2.31%	0.367%
12	8.134	1023	1028	1035	rBV	52275	103840	3.84%	0.611%
13	8.228	1039	1044	1047	rBV	735290	599216	22.15%	3.523%
14	8.939	1162	1165	1168	rVB	40419	31163	1.15%	0.183%
15	9.039	1177	1182	1185	rVB	132818	110212	4.07%	0.648%
16	9.304	1222	1227	1230	rBV	3051582	2704798	100.00%	15.905%
17	9.639	1281	1284	1287	rBV3	27722	30731	1.14%	0.181%
18	9.986	1339	1343	1346	rBV	720430	588273	21.75%	3.459%
19	10.022	1346	1349	1352	rVB	633615	496626	18.36%	2.920%
20	10.192	1374	1378	1383	rVB	34206	29606	1.09%	0.174%
21	10.533	1433	1436	1440	rVB	195956	172367	6.37%	1.014%
22	10.780	1473	1478	1481	rBV	1675774	1456954	53.87%	8.567%
23	10.963	1506	1509	1512	rBV2	34293	48659	1.80%	0.286%
24	11.139	1536	1539	1543	rVB3	46939	53003	1.96%	0.312%
25	11.175	1543	1545	1550	rVV	42564	53248	1.97%	0.313%
26	11.222	1550	1553	1557	rVB	28921	33192	1.23%	0.195%
27	11.375	1574	1579	1582	rVB2	23025	34427	1.27%	0.202%
28	11.480	1593	1597	1599	rBV	650819	507319	18.76%	2.983%
29	11.504	1599	1601	1604	rVB	72940	52491	1.94%	0.309%
30	12.098	1699	1702	1707	rBV	38585	35445	1.31%	0.208%
31	12.698	1800	1804	1807	rBV	64738	58460	2.16%	0.344%
32	12.927	1838	1843	1845	rBV	38557	43420	1.61%	0.255%
33	12.963	1845	1849	1857	rVV	158176	213829	7.91%	1.257%
34	13.074	1863	1868	1871	rBV	2331611	2114293	78.17%	12.432%
35	14.127	2043	2047	2050	rBV	522528	437822	16.19%	2.574%
36	14.221	2059	2063	2068	rVB	96709	108017	3.99%	0.635%

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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-BF102722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.645	2300	2305	2315	rVB2	281963	378764	14.00%	2.227%
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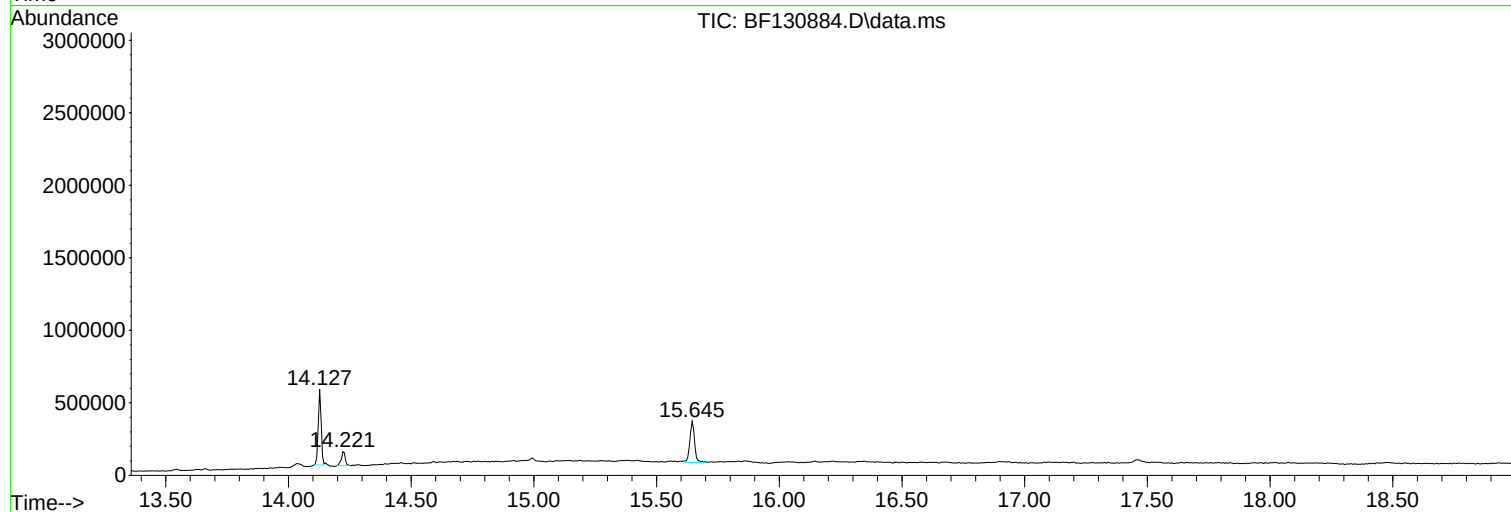
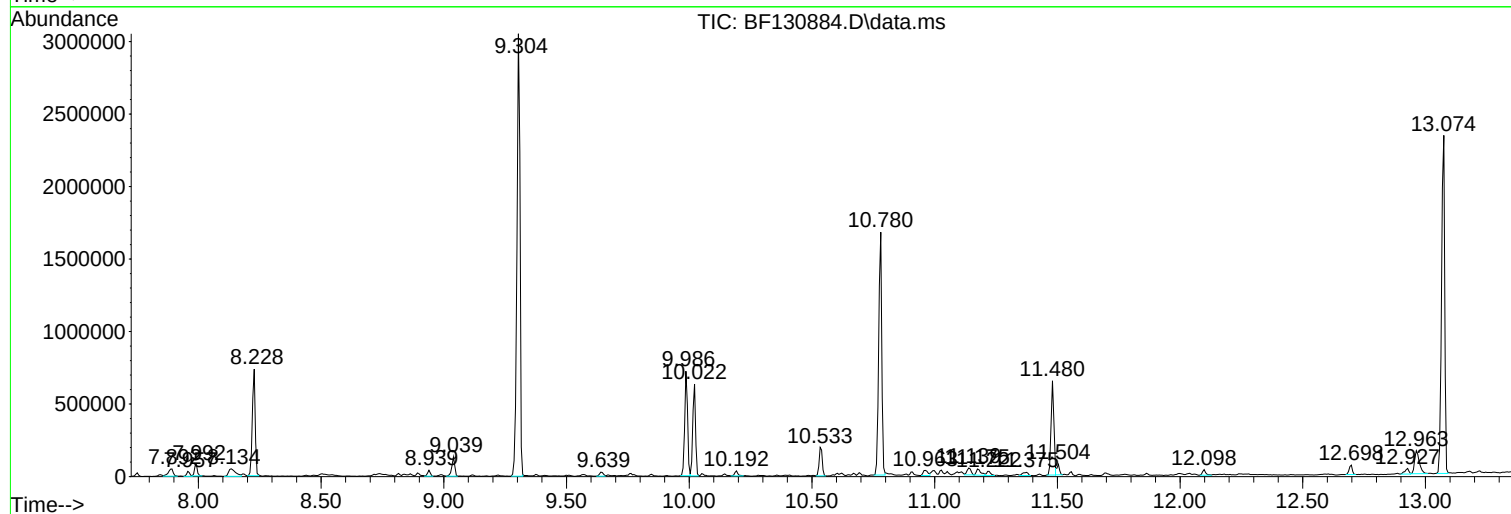
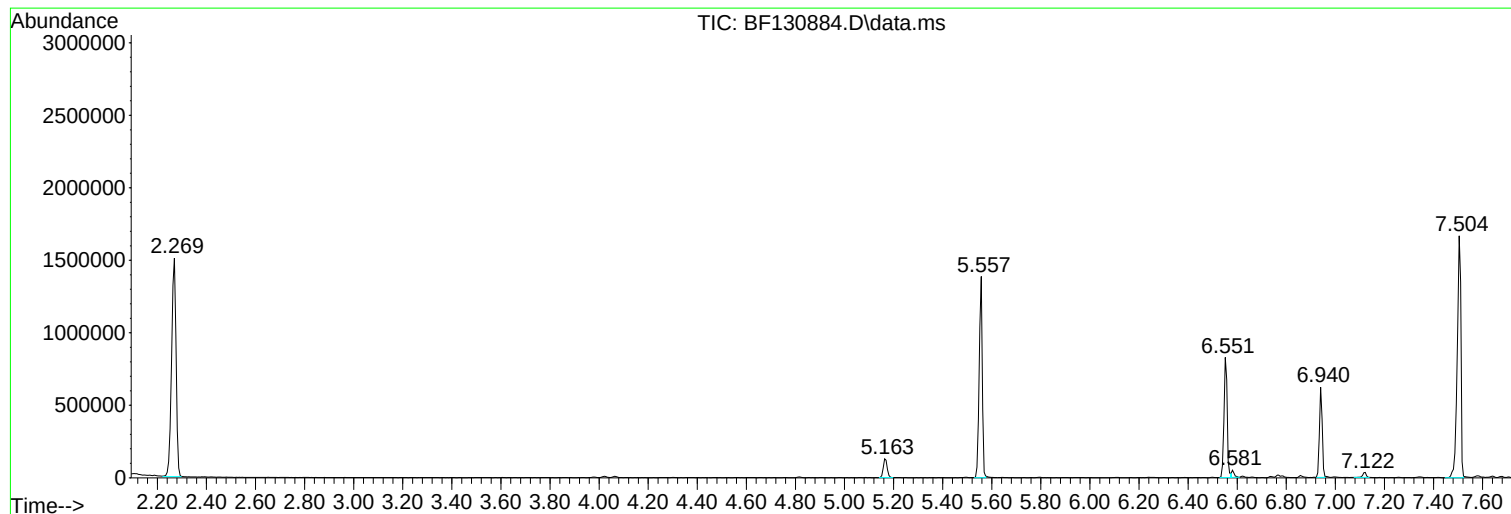
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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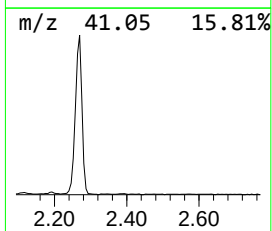
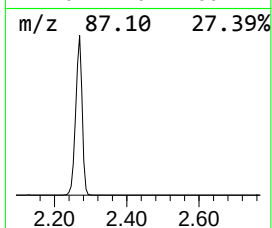
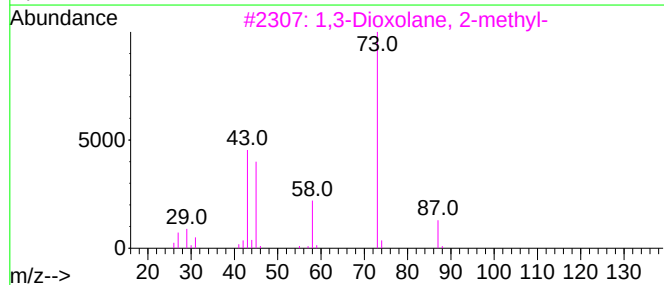
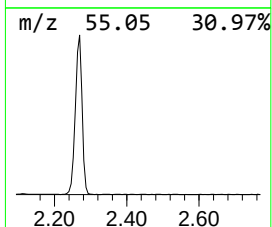
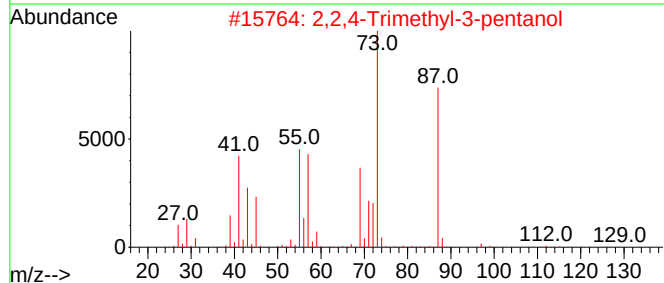
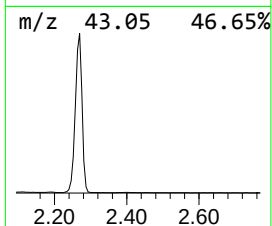
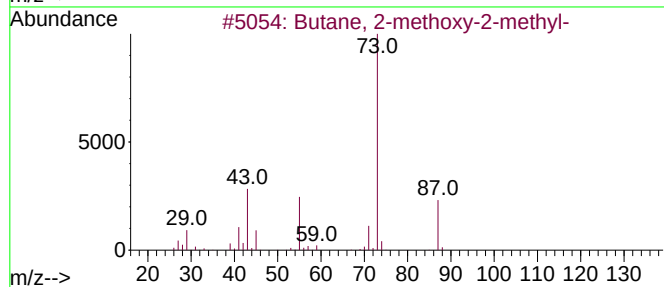
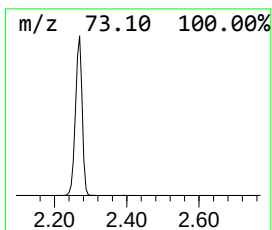
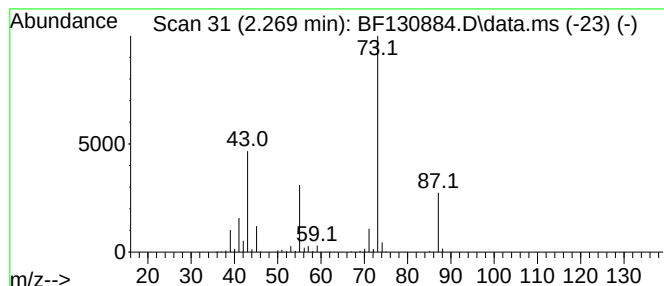
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.269	78.00 ng	1923150	1,4-Dichlorobenzene-d4	6.940

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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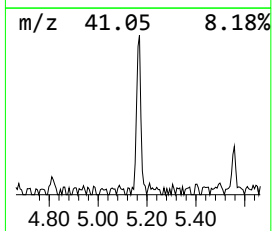
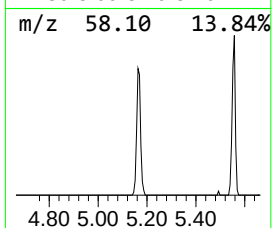
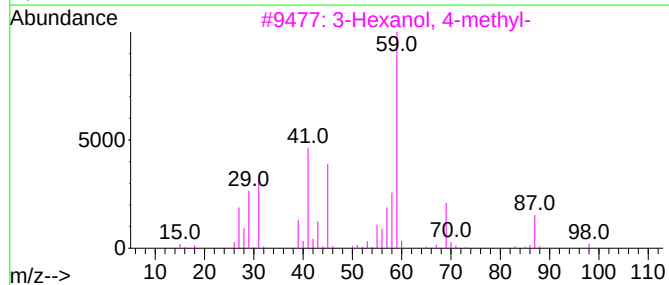
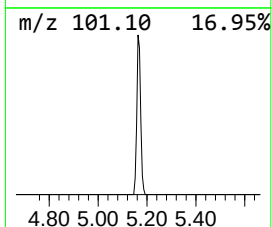
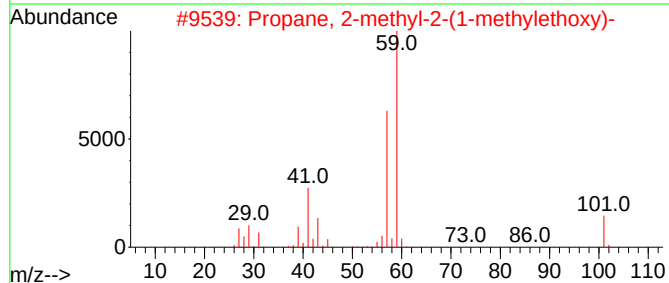
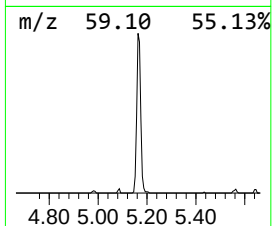
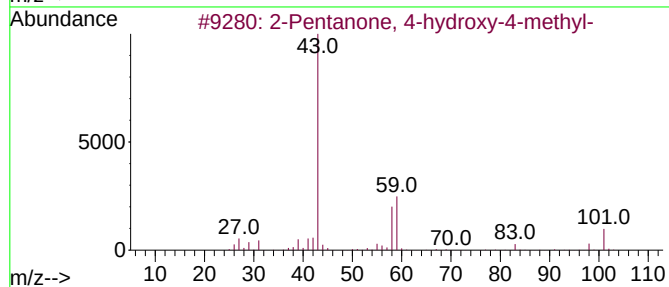
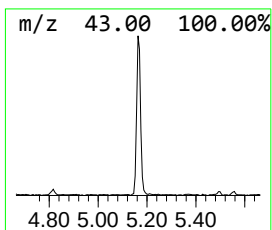
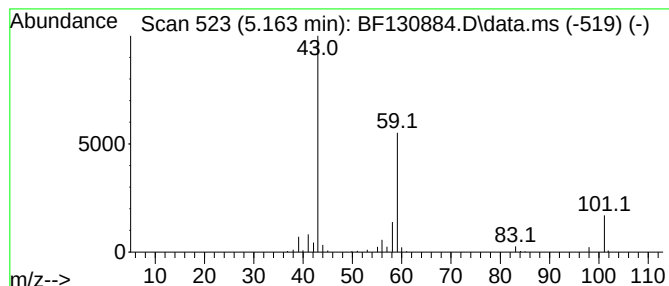
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.163	5.75 ng	141709	1,4-Dichlorobenzene-d4	6.940

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25



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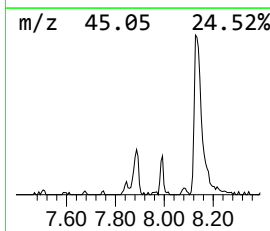
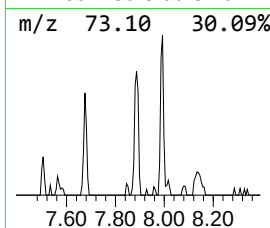
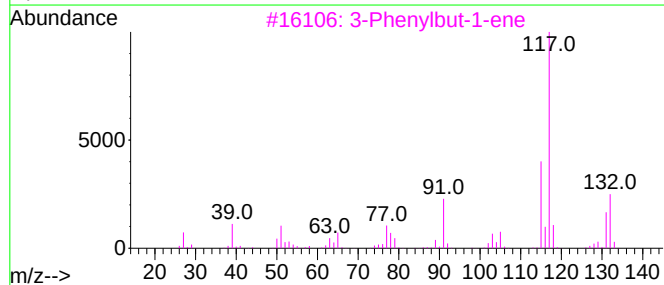
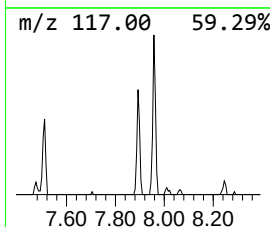
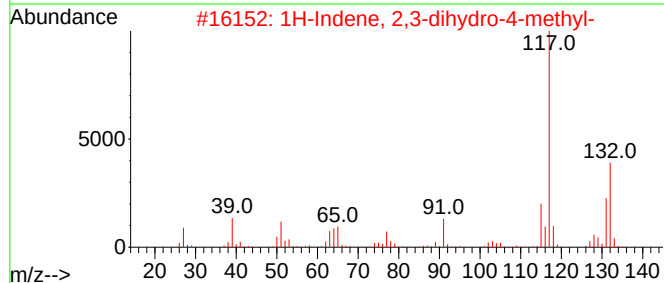
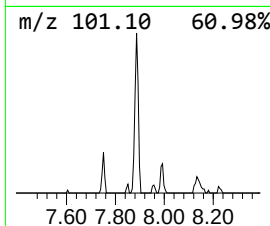
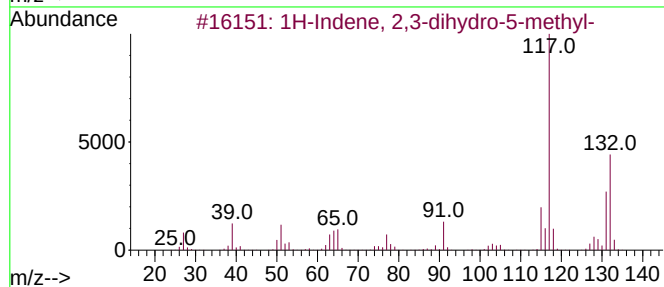
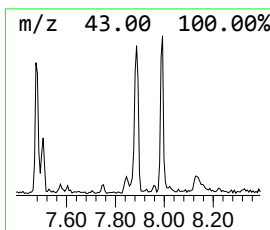
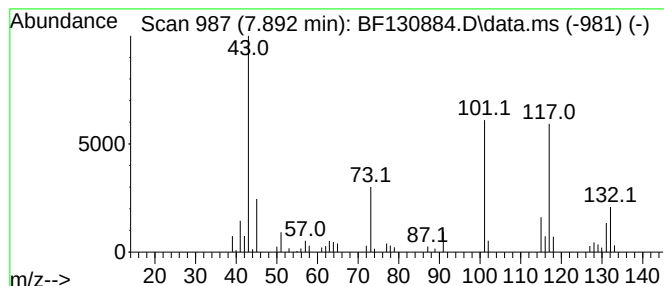
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.892	2.32 ng	69360	Naphthalene-d8	8.228

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	50
2		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	50
3		3-Phenylbut-1-ene	132	C10H12	000934-10-1	43
4		1-Phenyl-1-butene	132	C10H12	000824-90-8	41
5		Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	38



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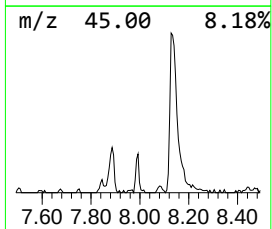
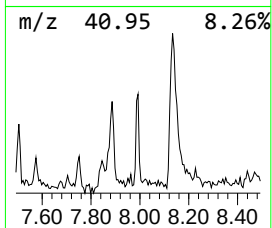
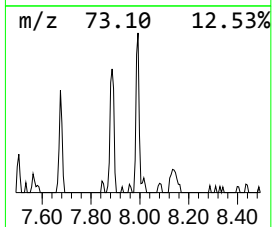
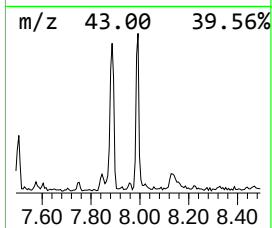
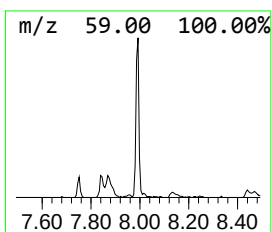
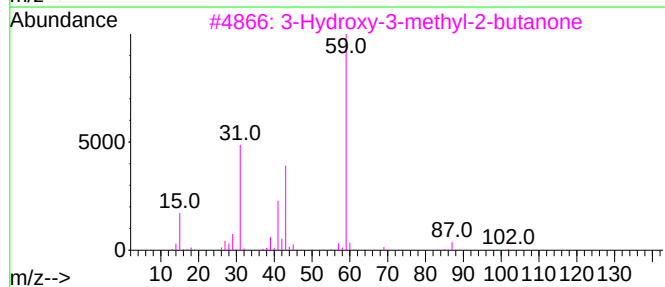
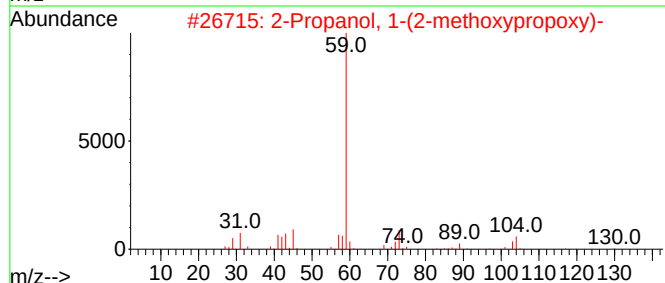
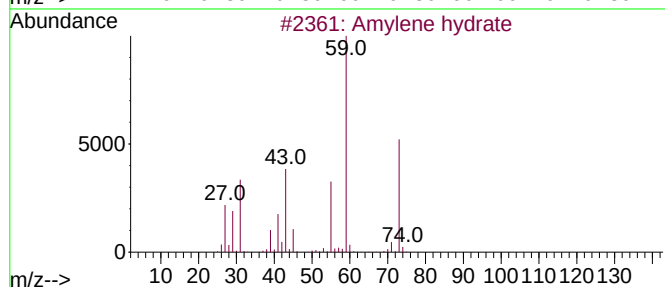
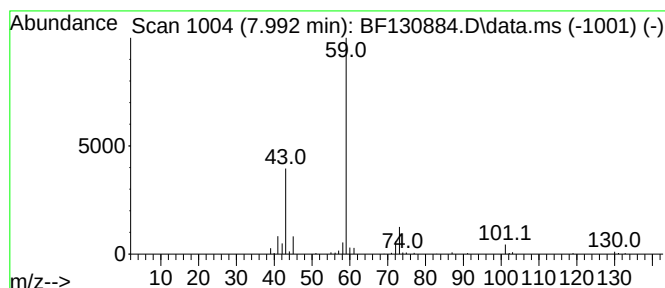
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Amylene hydrate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.992	2.09 ng	62498	Naphthalene-d8	8.228

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Amylene hydrate	88	C5H12O	000075-85-4	72
2			2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	72
3			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	59
4			Pentane, 2-methoxy-	102	C6H14O	006795-88-6	50
5			1-(1-Methoxypropan-2-yloxy)propa...	190	C9H18O4	1000367-08-6	50



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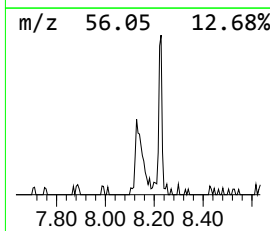
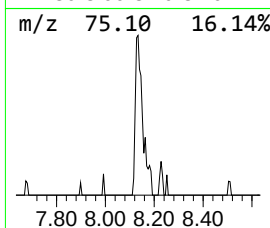
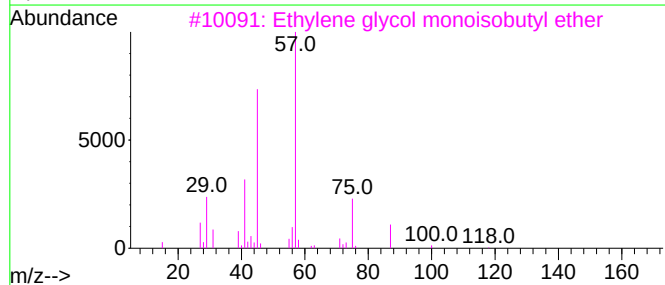
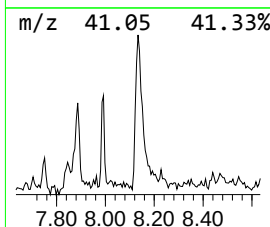
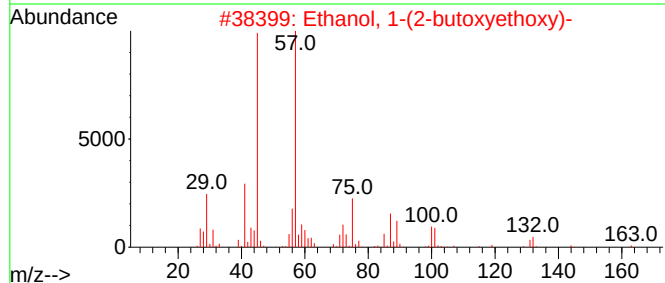
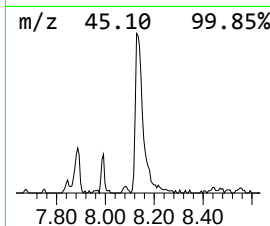
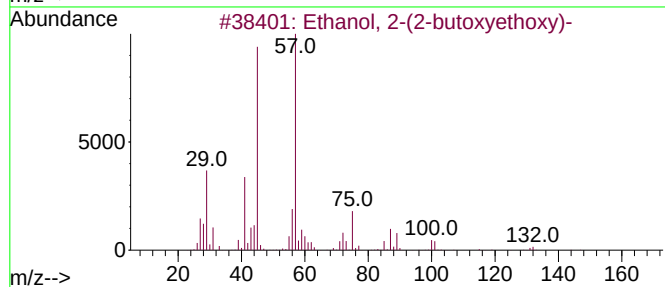
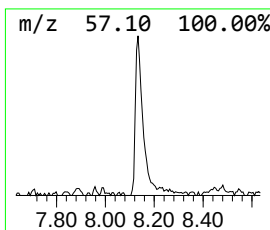
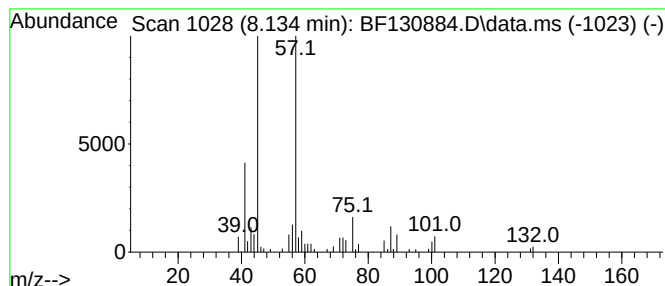
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.134	3.47 ng	103840	Naphthalene-d8	8.228

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			Tetraethylene glycol	194	C8H18O5	000112-60-7	53



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Acq On : 31 Oct 2022 17:42
Operator : CG\JU
Sample : N5329-03
Misc :
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Instrument :
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ClientSampleId :
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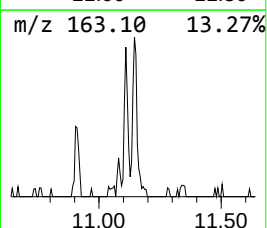
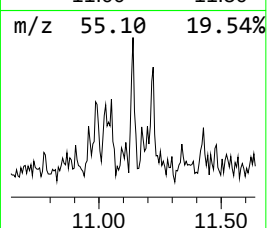
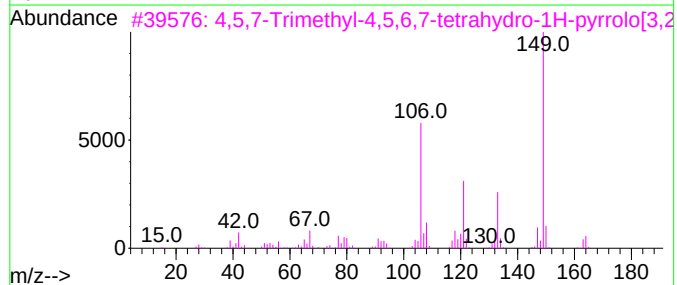
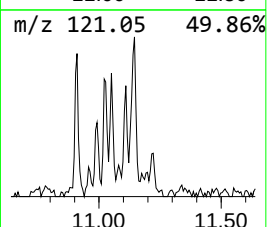
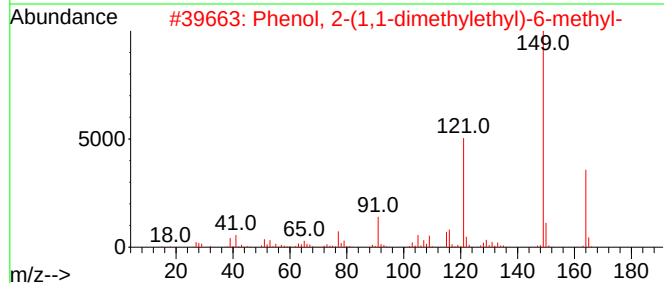
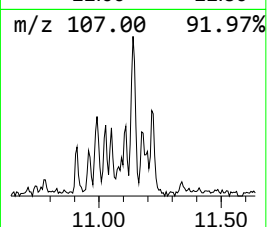
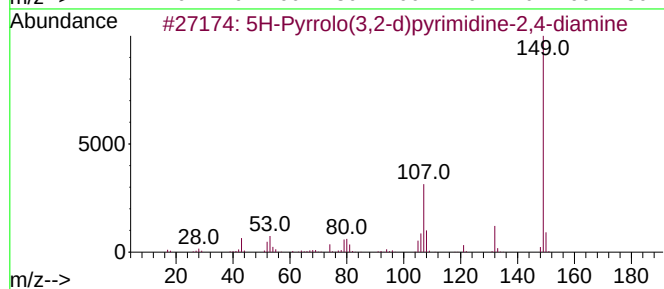
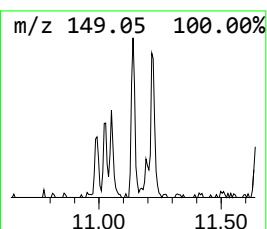
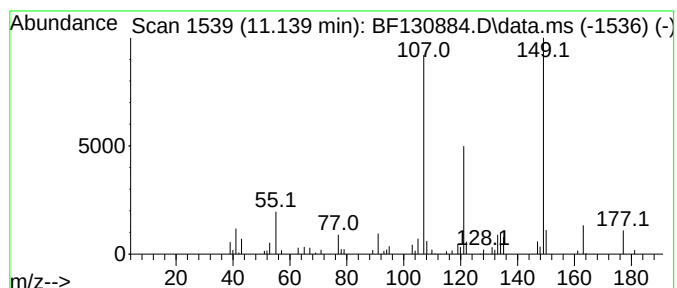
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 5H-Pyrrolo(3,2-d)pyrimidine... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.139	2.09 ng	53003	Phenanthrene-d10	11.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5H-Pyrrolo(3,2-d)pyrimidine-2,4-...	149	C6H7N5	1000244-21-4	64
2			Phenol, 2-(1,1-dimethylethyl)-6-...	164	C11H16O	002219-82-1	35
3			4,5,7-Trimethyl-4,5,6,7-tetrahyd...	164	C10H16N2	113849-86-8	35
4			2H-Indol-2-one, 1,3-dihydro-5-hy...	149	C8H7NO2	003416-18-0	35
5			3',4'-Formoxylidide	149	C9H11NO	006639-60-7	35



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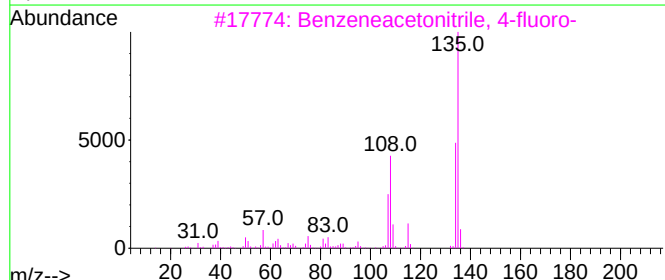
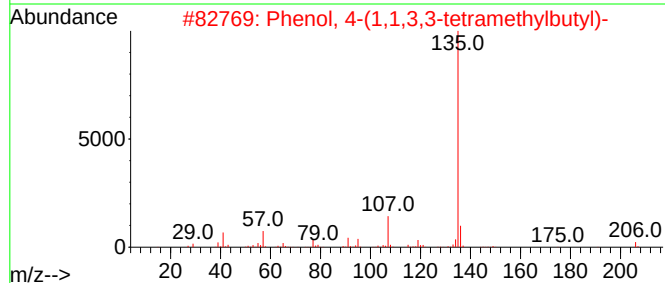
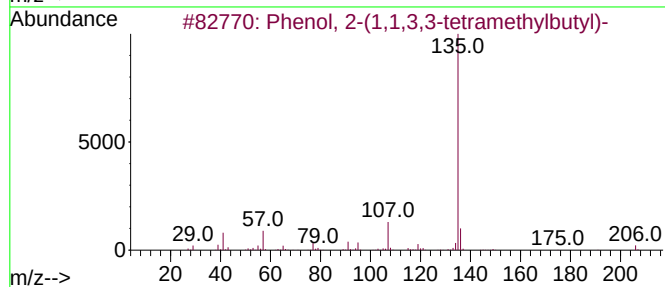
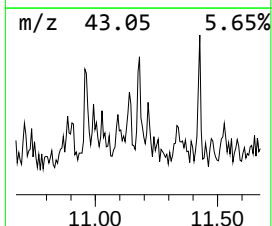
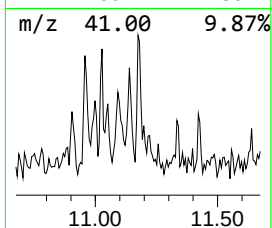
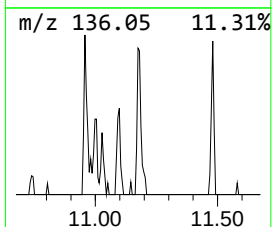
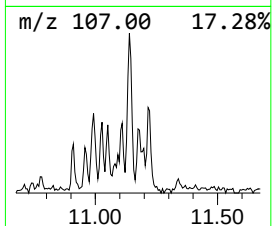
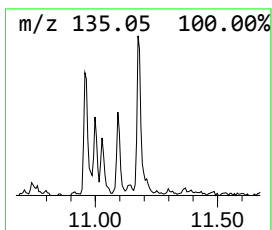
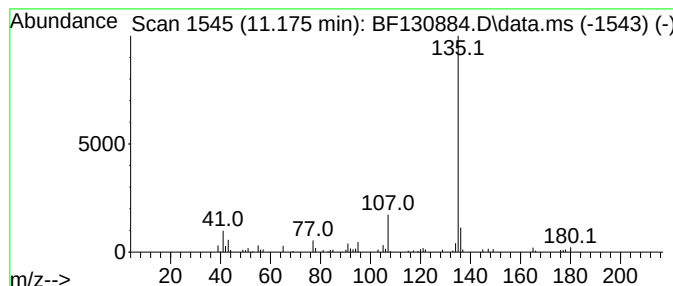
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Phenol, 2-(1,1,3,3-tetramet... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.175	2.10 ng	53248	Phenanthrene-d10		11.480	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Phenol, 2-(1,1,3,3-tetramethylbu...		206	C14H22O	003884-95-5	78
2	Phenol, 4-(1,1,3,3-tetramethylbu...		206	C14H22O	000140-66-9	78
3	Benzeneacetonitrile, 4-fluoro-		135	C8H6FN	000459-22-3	72
4	6-Methyl-1-propyl-1,2,3,4-tetra...		178	C11H18N2	1000305-41-3	72
5	4-tert-Butylphenol, 0-(n-propylo...		236	C14H20O3	1000487-25-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103122\
Data File : BF130884.D
Acq On : 31 Oct 2022 17:42
Operator : CG\JU
Sample : N5329-03
Misc :
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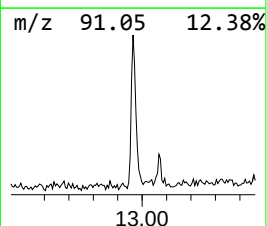
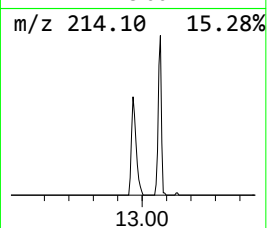
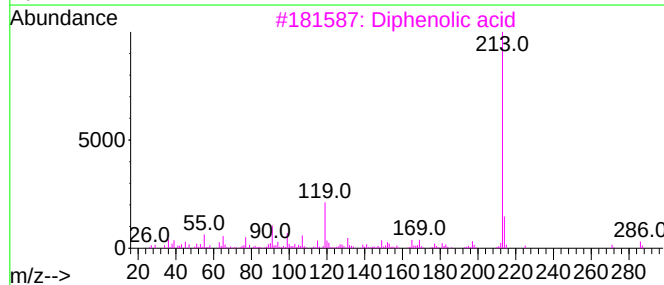
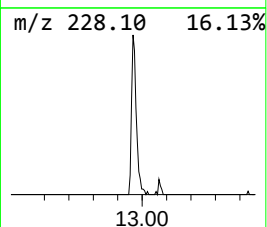
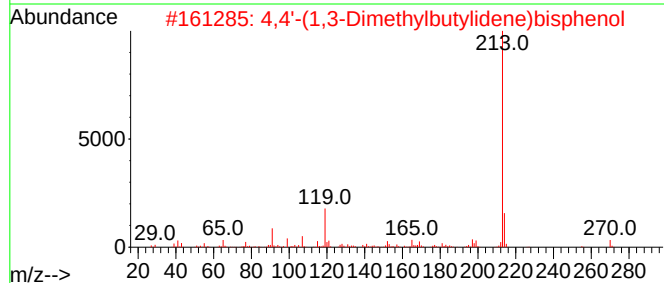
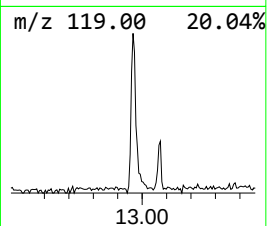
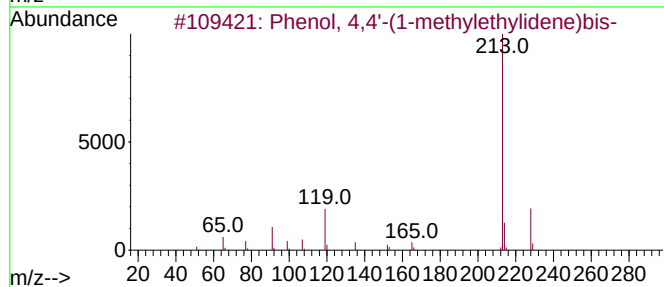
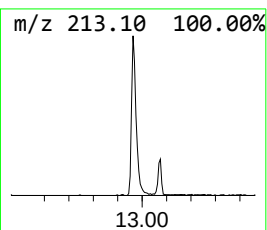
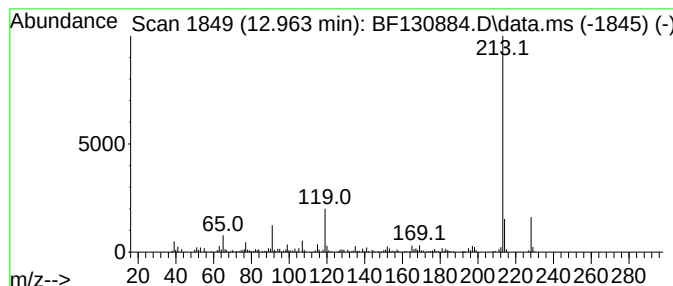
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Phenol, 4,4'-(1-methylethyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.963	9.77 ng	213829	Chrysene-d12	14.127	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	96
2	4,4'-(1,3-Dimethylbutylidene)bis...	270	C18H22O2	006807-17-6	83
3	Diphenolic acid	286	C17H18O4	000126-00-1	80
4	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	62
5	3,4'-Isopropylidenediphenol	228	C15H16O2	046765-25-7	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103122\
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Acq On : 31 Oct 2022 17:42
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Misc :
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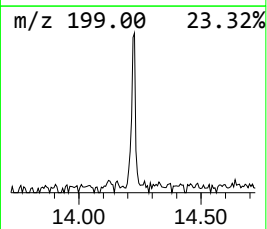
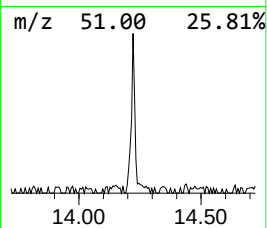
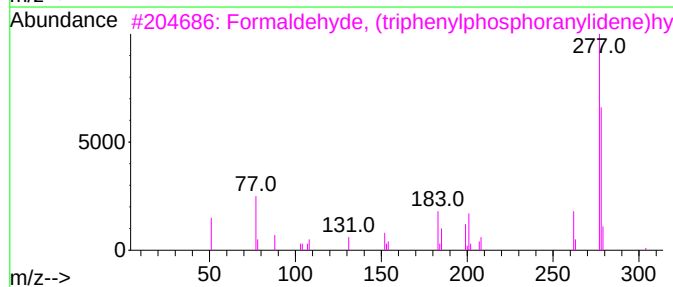
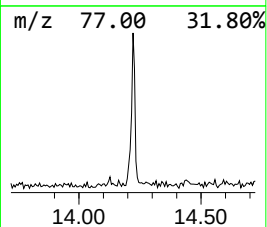
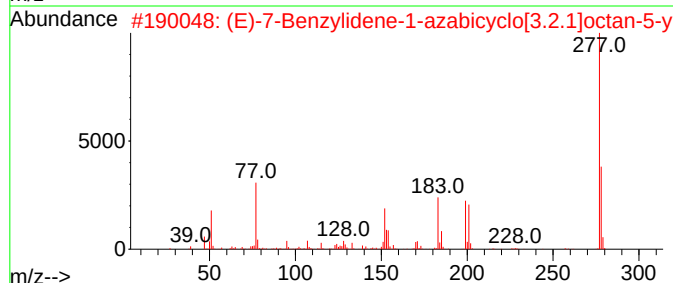
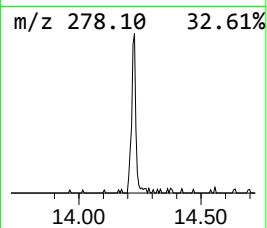
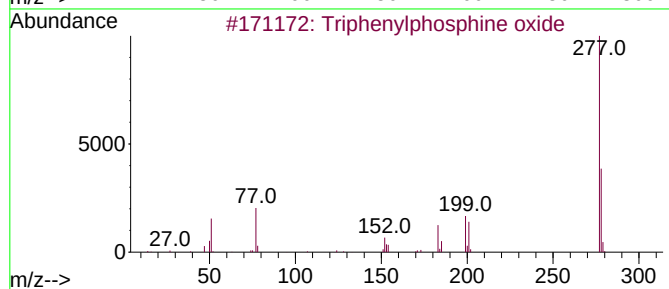
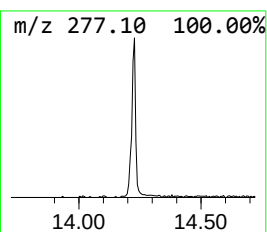
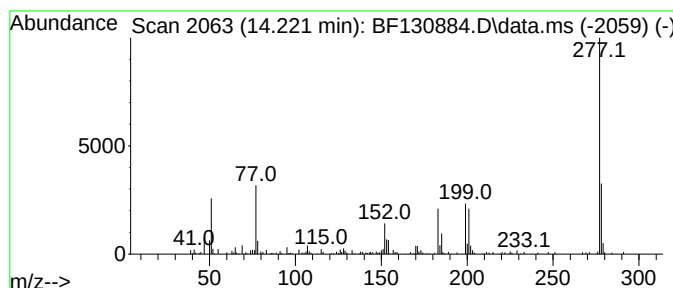
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.221	4.93 ng	108017	Chrysene-d12	14.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	50
5			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103122\
Data File : BF130884.D
Acq On : 31 Oct 2022 17:42
Operator : CG\JU
Sample : N5329-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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
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2-Pentanone, 4-...	5.163	5.8	ng	141709	1	6.940	493141	20.0
1H-Indene, 2,3-...	7.892	2.3	ng	69360	2	8.228	599216	20.0
Amylene hydrate	7.992	2.1	ng	62498	2	8.228	599216	20.0
Ethanol, 2-(2-b...	8.134	3.5	ng	103840	2	8.228	599216	20.0
5H-Pyrrolo(3,2-...	11.139	2.1	ng	53003	4	11.480	507319	20.0
Phenol, 2-(1,1,...	11.175	2.1	ng	53248	4	11.480	507319	20.0
Phenol, 4,4'-(1...	12.963	9.8	ng	213829	5	14.127	437822	20.0
Triphenylphosph...	14.221	4.9	ng	108017	5	14.127	437822	20.0