

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
 Data File : BF131577.D
 Acq On : 09 Dec 2022 20:49
 Operator : CG\JU
 Sample : N5947-03
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NYE-WATER-1208

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-BF120822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131577.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	15	25	30	rVB	1689500	2166790	55.94%	11.450%
2	5.128	513	517	523	rVB	168635	179403	4.63%	0.948%
3	5.528	581	585	588	rBV	1342445	1263532	32.62%	6.677%
4	6.534	752	756	764	rBV	852433	788563	20.36%	4.167%
5	6.904	816	819	823	rBV	495470	462382	11.94%	2.443%
6	7.481	910	917	920	rVB	1786178	2018314	52.10%	10.665%
7	7.834	968	977	983	rBV3	28121	54416	1.40%	0.288%
8	8.198	1034	1039	1042	rBV	672301	589808	15.23%	3.117%
9	9.281	1217	1223	1226	rVB	3954627	3873698	100.00%	20.469%
10	9.381	1236	1240	1243	rBV2	52286	77643	2.00%	0.410%
11	9.769	1302	1306	1311	rBV	53651	48426	1.25%	0.256%
12	9.886	1322	1326	1331	rVB	52927	48597	1.25%	0.257%
13	9.945	1331	1336	1337	rBV	515486	460986	11.90%	2.436%
14	9.963	1337	1339	1342	rVB	802679	605926	15.64%	3.202%
15	10.251	1384	1388	1392	rBV2	23053	39140	1.01%	0.207%
16	10.757	1467	1474	1477	rBV	2459140	2364821	61.05%	12.496%
17	11.222	1549	1553	1556	rVB	55579	48215	1.24%	0.255%
18	11.457	1589	1593	1596	rVB	749296	668379	17.25%	3.532%
19	11.839	1655	1658	1664	rVB	104807	93975	2.43%	0.497%
20	11.980	1678	1682	1685	rBV	83077	92583	2.39%	0.489%
21	12.769	1813	1816	1820	rBV	60495	68575	1.77%	0.362%
22	13.051	1859	1864	1867	rBV	1915510	1822820	47.06%	9.632%
23	13.969	2017	2020	2024	rBV3	35696	40963	1.06%	0.216%
24	14.104	2040	2043	2047	rVB	417376	375808	9.70%	1.986%
25	14.192	2055	2058	2060	rBV2	57003	67032	1.73%	0.354%
26	14.216	2060	2062	2068	rVB	295612	258985	6.69%	1.368%
27	15.621	2296	2301	2310	rVB	275593	344974	8.91%	1.823%

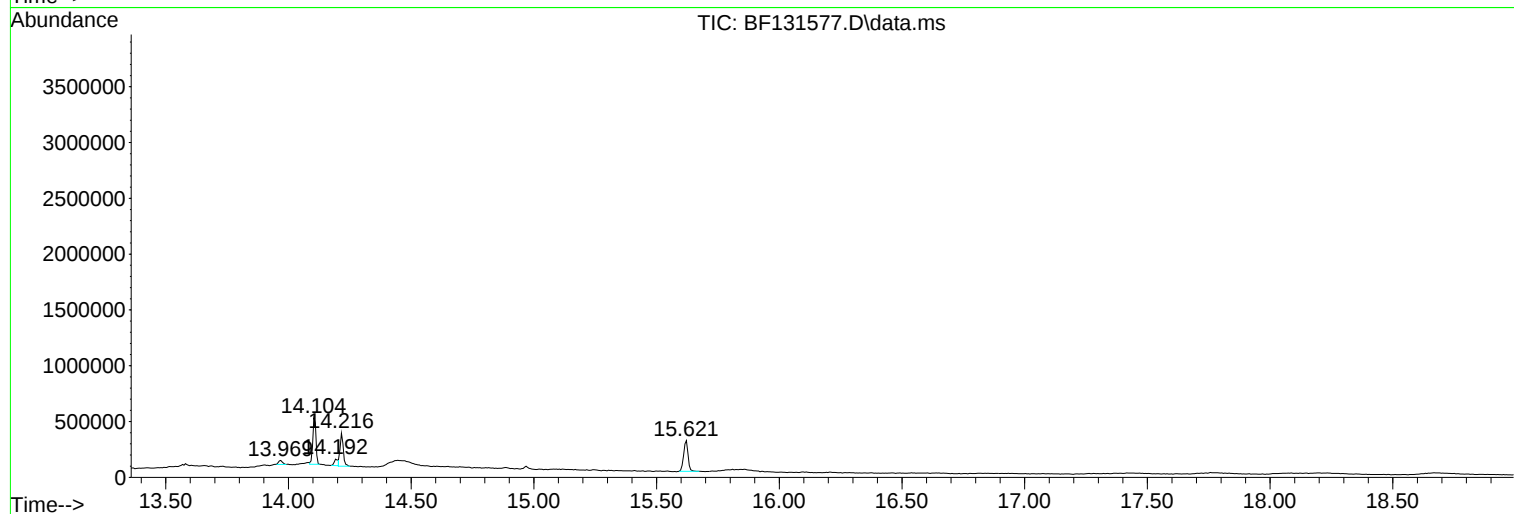
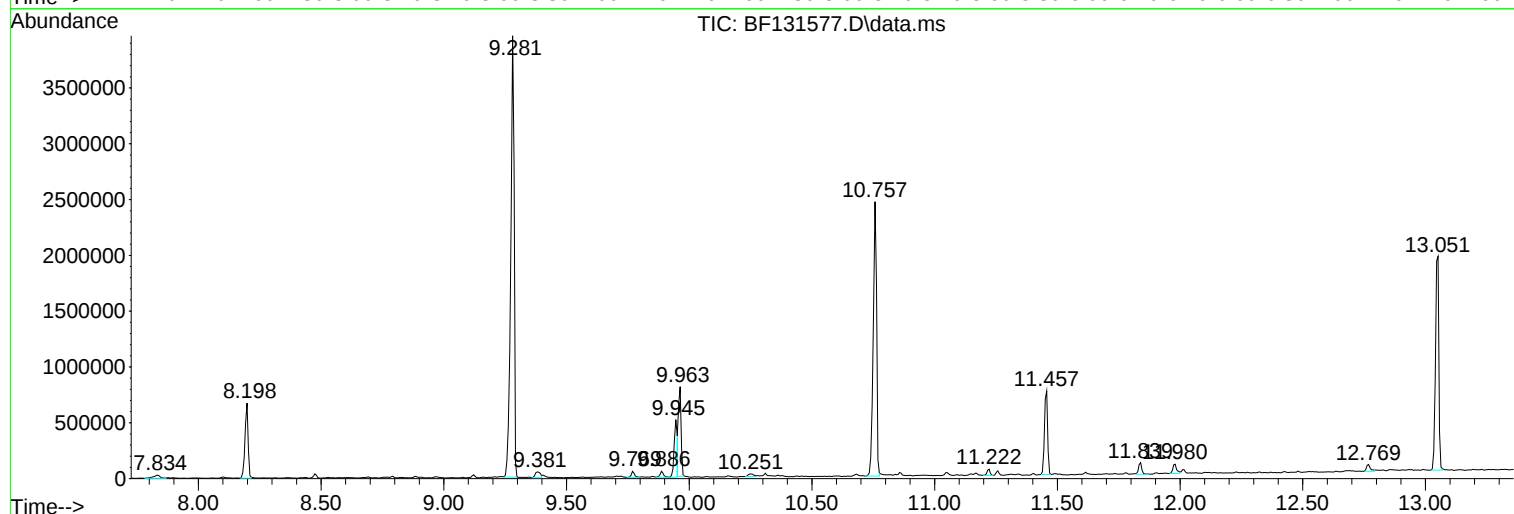
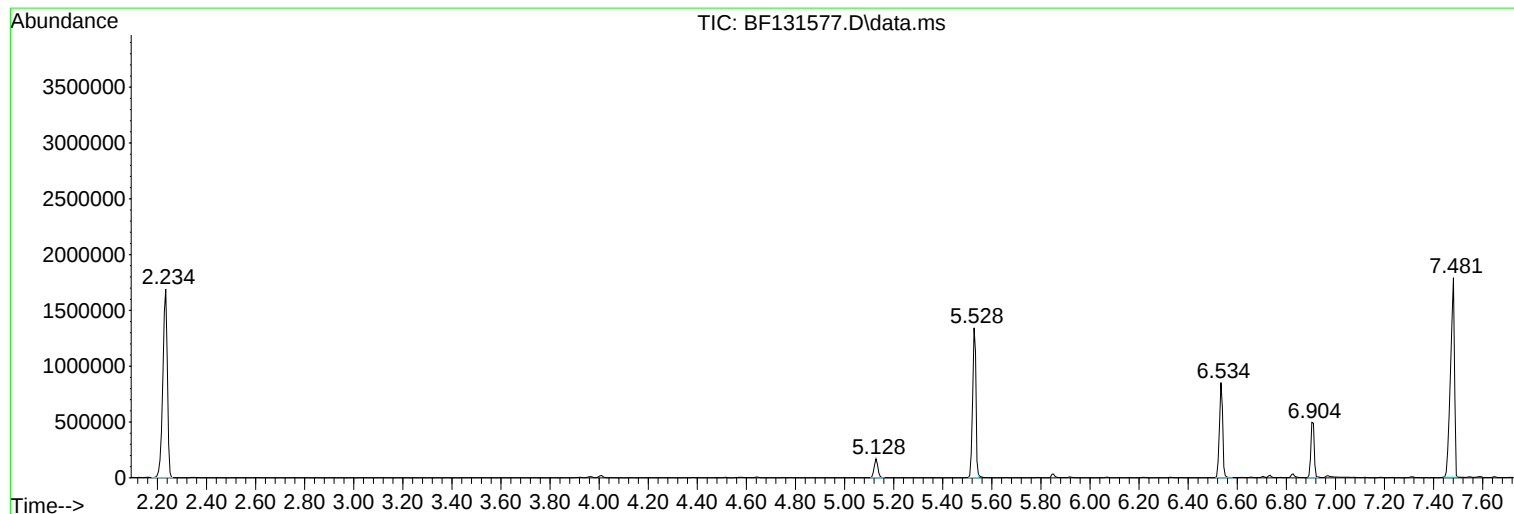
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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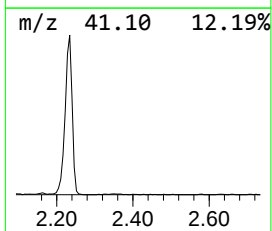
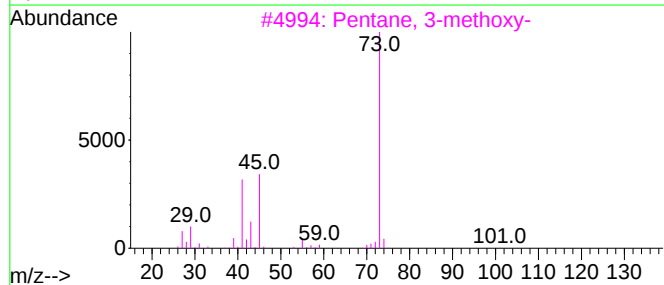
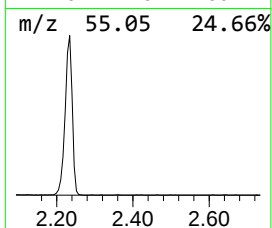
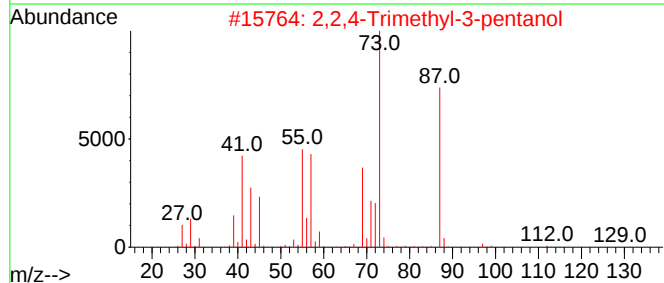
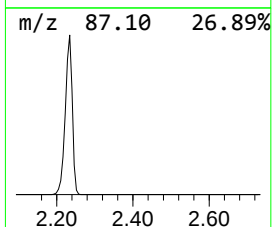
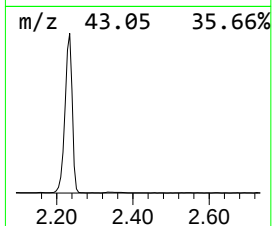
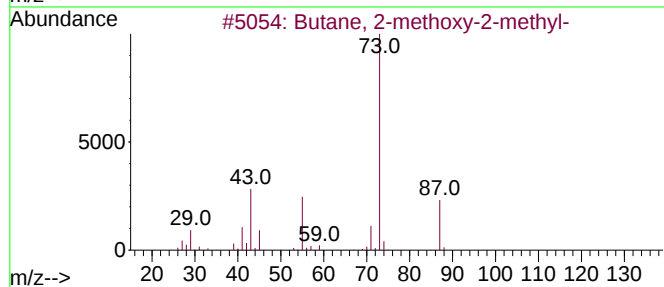
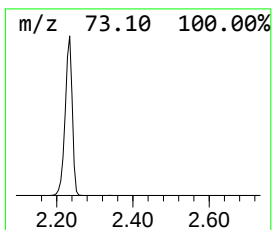
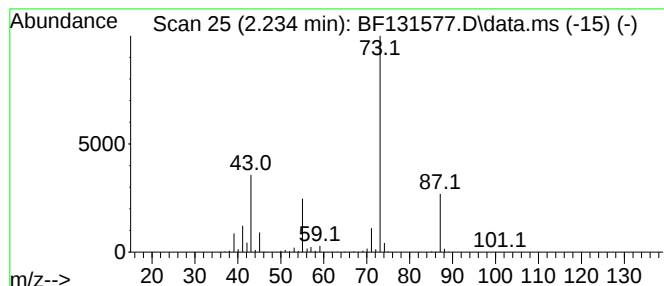
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.234	93.72 ng	2166790	1,4-Dichlorobenzene-d4	6.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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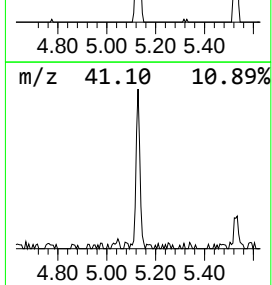
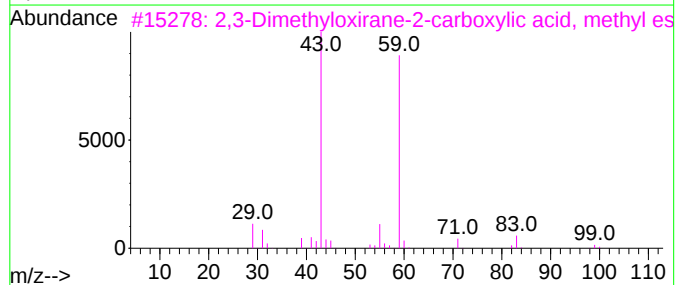
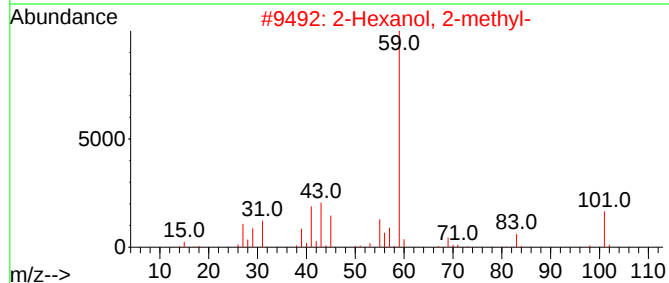
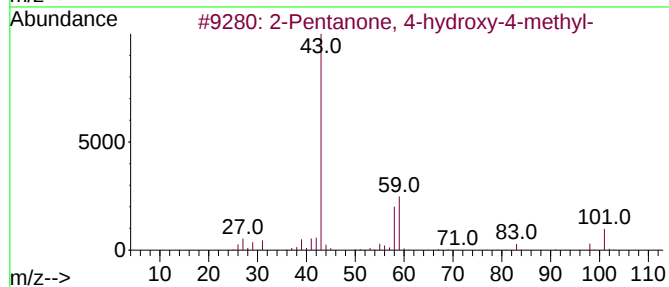
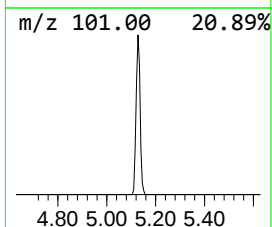
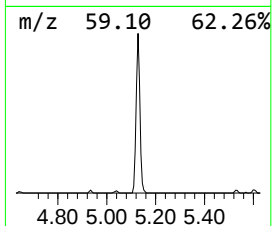
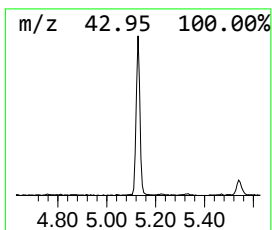
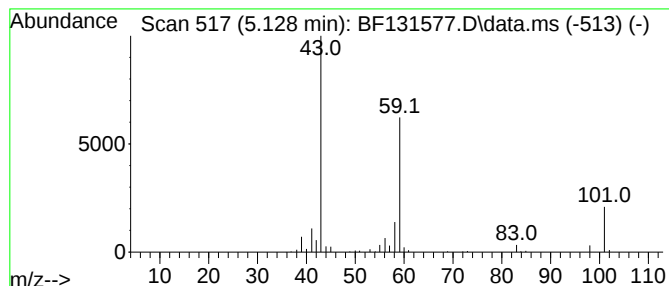
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.128	7.76 ng	179403	1,4-Dichlorobenzene-d4	6.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3			2,3-Dimethyloxirane-2-carboxylic...	130	C6H10O3	1000306-64-4	23
4			3-Pentanol	88	C5H12O	000584-02-1	17
5			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17



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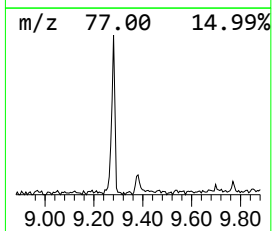
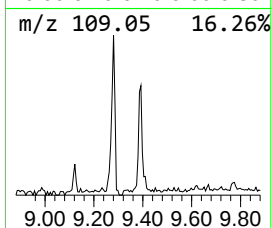
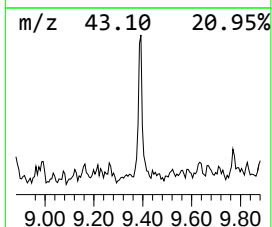
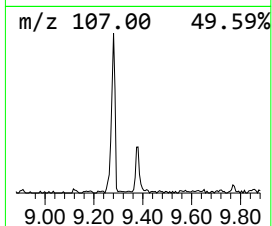
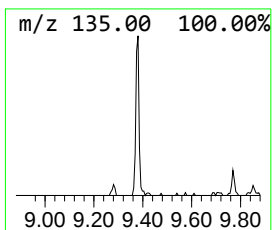
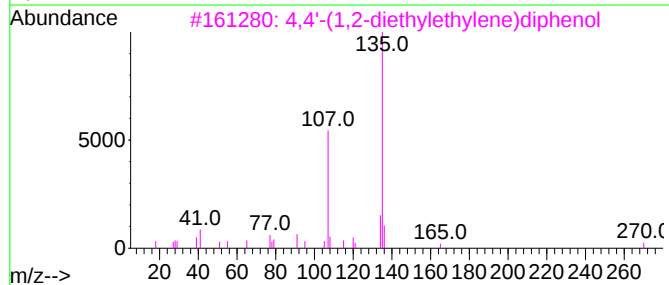
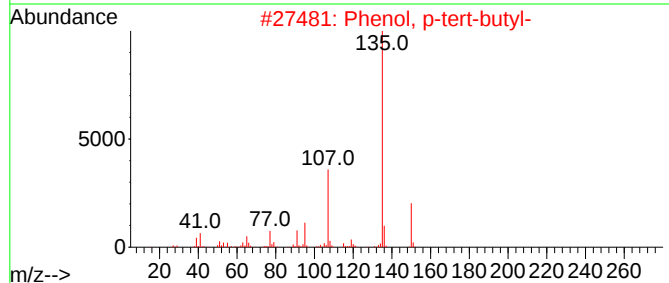
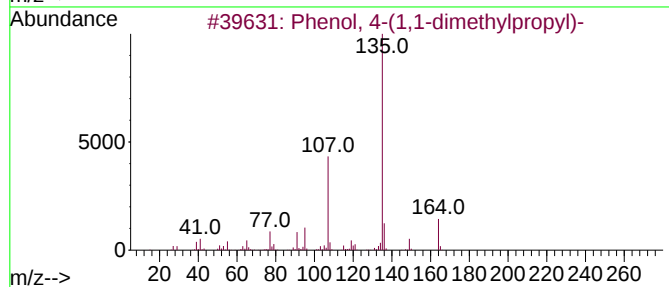
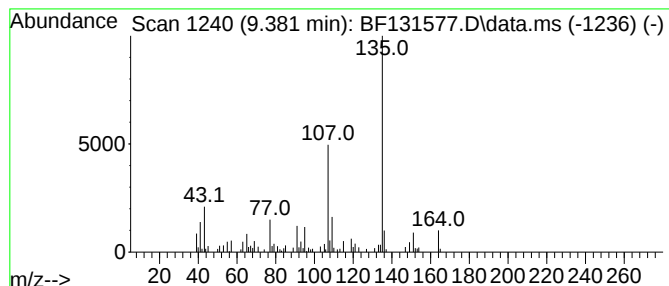
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Phenol, 4-(1,1-dimethylprop... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.381	2.56 ng	77643	Acenaphthene-d10	9.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	93
2			Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	72
3			4,4'-(1,2-diethylethylene)diphenol	270	C18H22O2	005635-50-7	59
4			Imidazo[1,2-c]pyrimidin-5-ol	135	C6H5N3O	055662-66-3	53
5			6,7-Dihydro-5H-cyclopenta[d]pyri...	135	C7H9N3	026979-06-6	53



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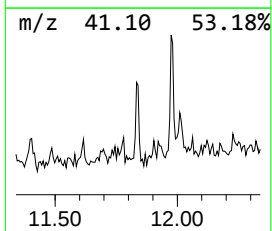
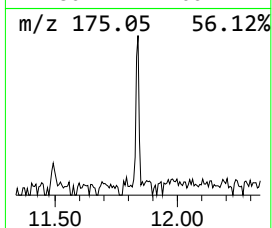
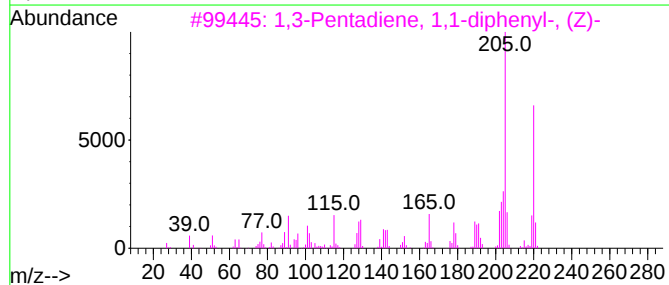
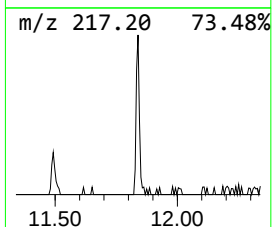
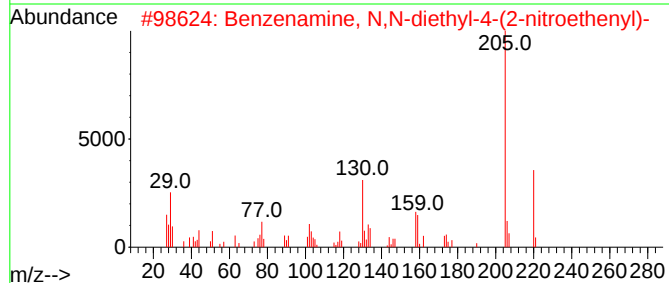
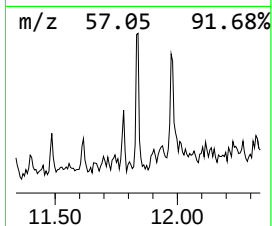
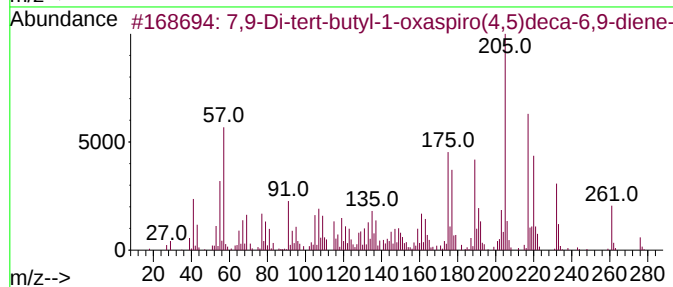
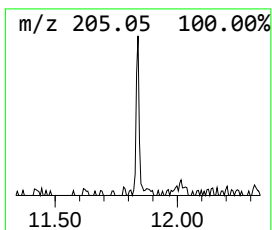
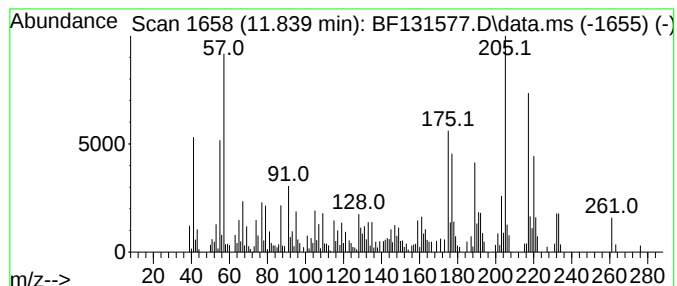
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Peak Number 4 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.839	2.81 ng	93975	Phenanthrene-d10	11.457	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	96
2	Benzenamine, N,N-diethyl-4-(2-ni...	220	C12H16N2O2	064462-51-7	51
3	1,3-Pentadiene, 1,1-diphenyl-, (Z)-	220	C17H16	015295-31-5	49
4	3-Acetylphenanthrene	220	C16H12O	002039-76-1	43
5	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	41



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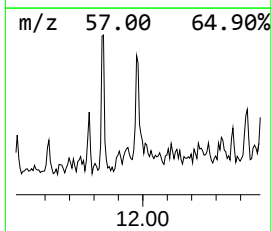
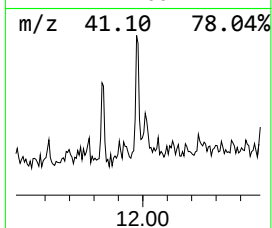
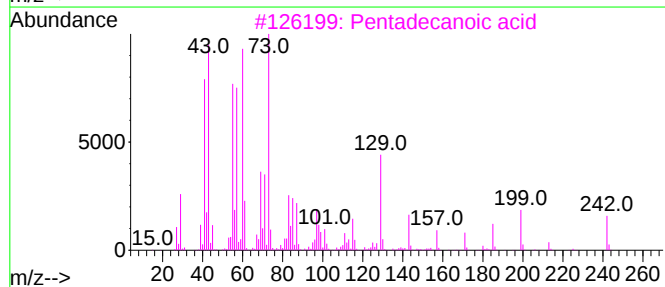
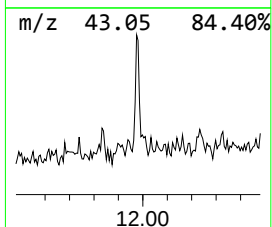
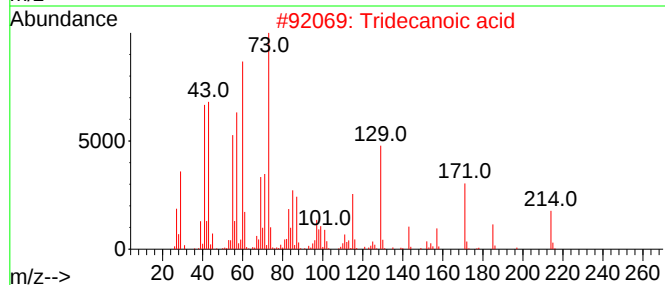
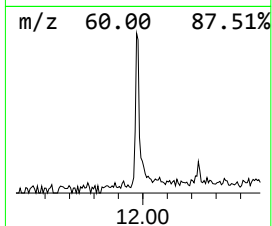
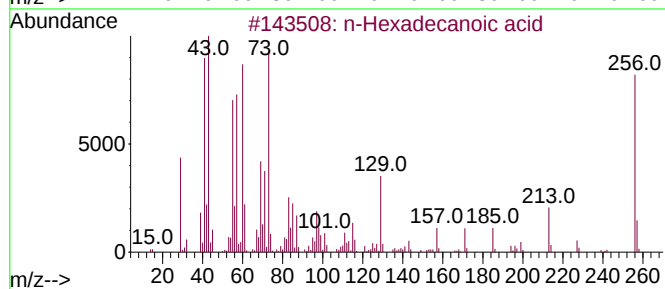
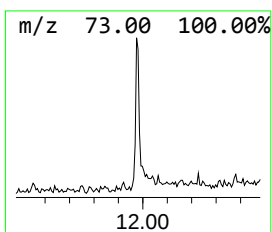
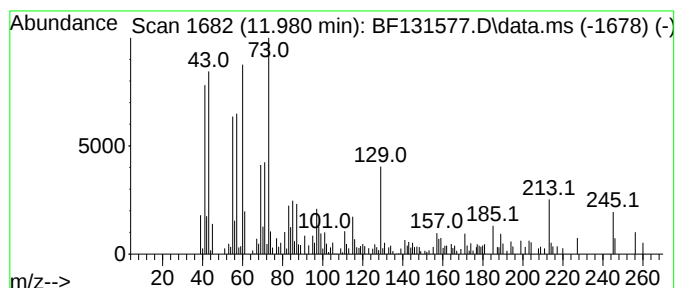
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.980	2.77 ng	92583	Phenanthrene-d10	11.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	76



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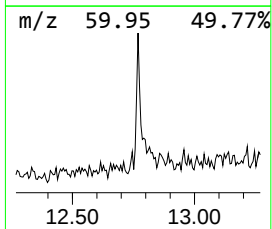
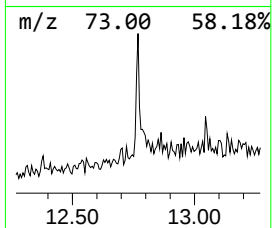
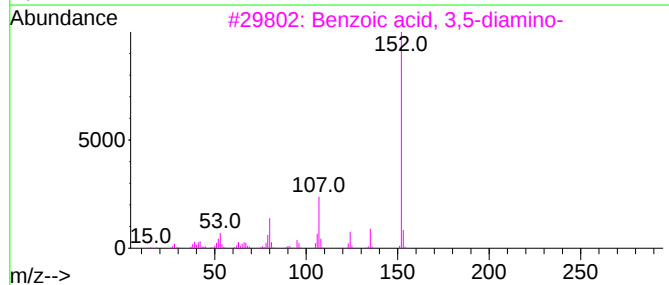
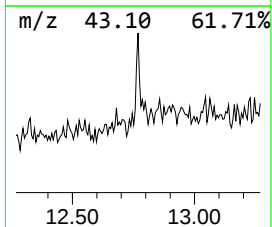
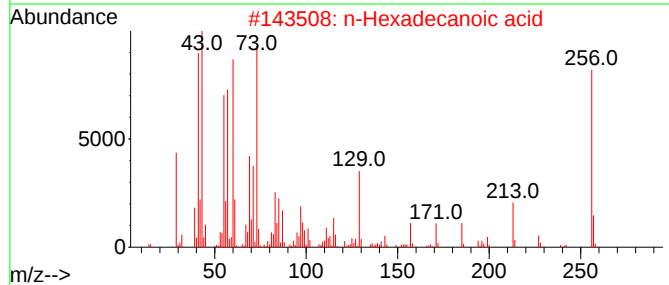
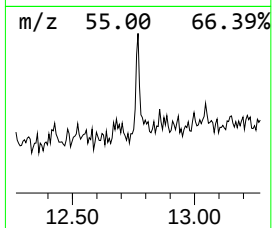
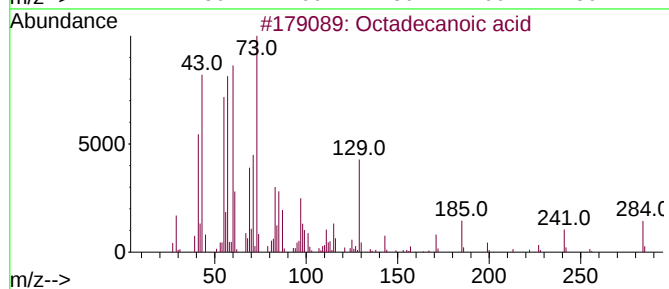
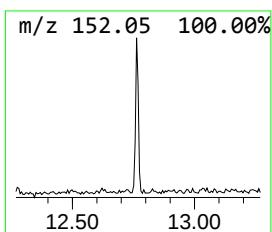
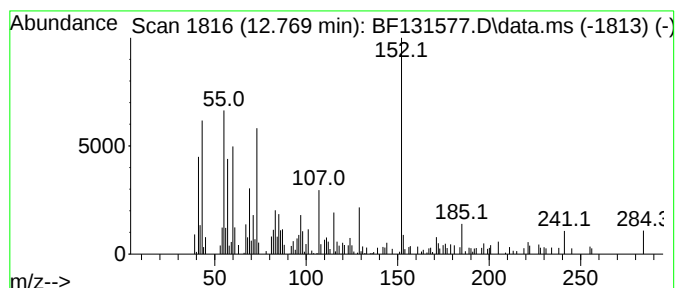
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.769	2.05 ng	68575	Phenanthrene-d10	11.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	58
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	44
3			Benzoic acid, 3,5-diamino-	152	C7H8N2O2	000535-87-5	38
4			3,4-Methylenedioxyanisole	152	C8H8O3	007228-35-5	35
5			2H-Pyrrol-2-one, 1,5-dihydro-4-(...	152	C8H12N2O	105776-93-0	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
Data File : BF131577.D
Acq On : 09 Dec 2022 20:49
Operator : CG\JU
Sample : N5947-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

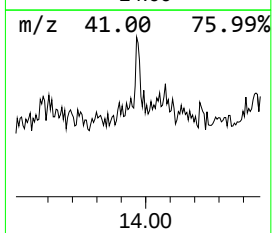
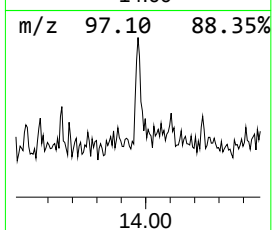
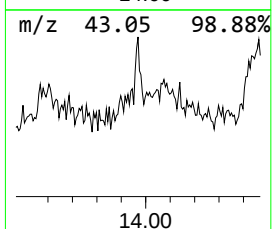
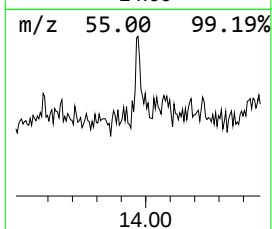
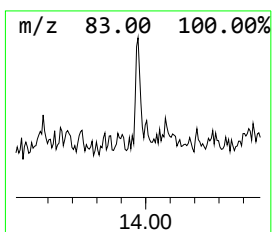
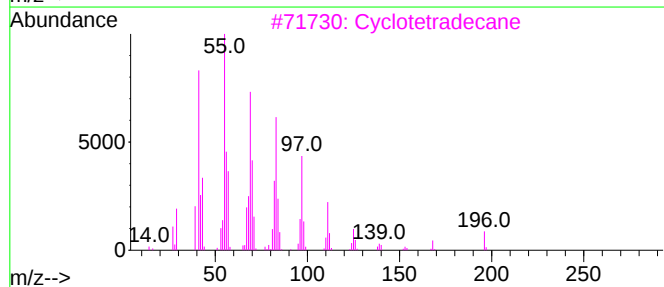
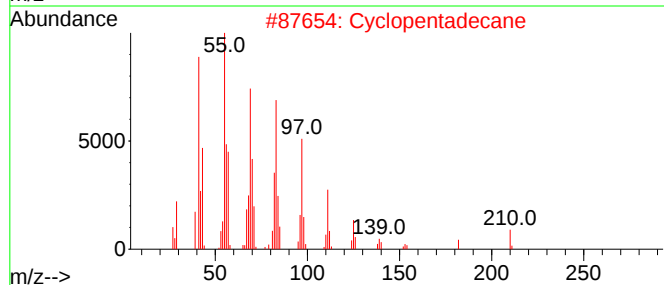
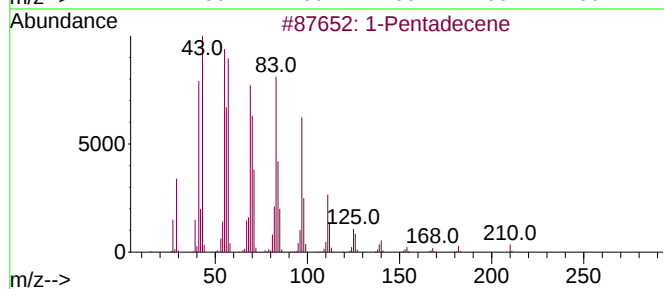
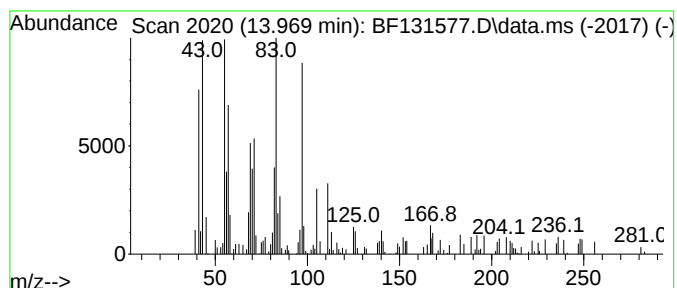
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ClientSampleId :
NYE-WATER-1208

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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 1-Pentadecene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.969	2.18 ng	40963	Chrysene-d12	14.104	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentadecene	210	C15H30	013360-61-7	76
2	Cyclopentadecane	210	C15H30	000295-48-7	55
3	Cyclotetradecane	196	C14H28	000295-17-0	51
4	Cyclododecane, ethyl-	196	C14H28	028981-49-9	51
5	Cyclopentane, 1-hexyl-3-methyl-	168	C12H24	061142-68-5	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
Data File : BF131577.D
Acq On : 09 Dec 2022 20:49
Operator : CG\JU
Sample : N5947-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NYE-WATER-1208

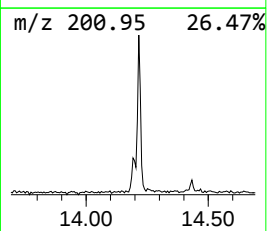
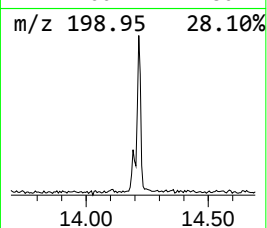
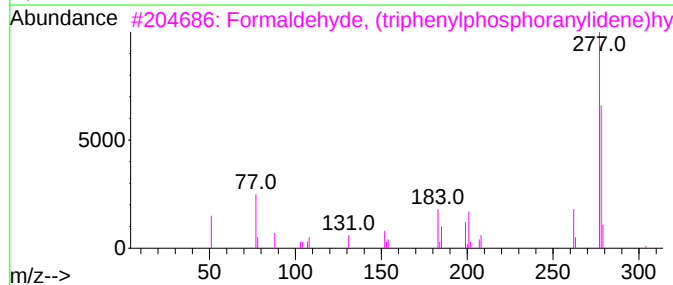
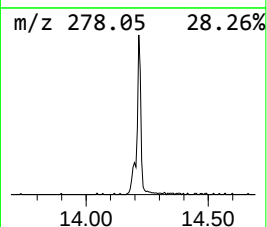
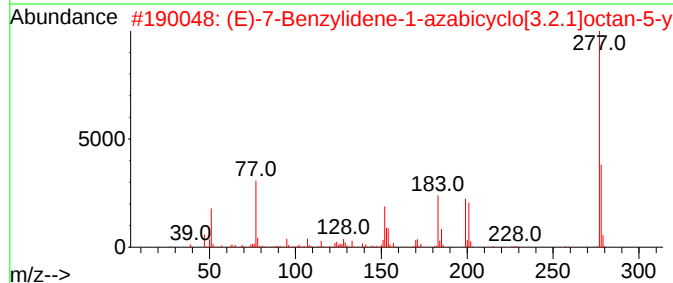
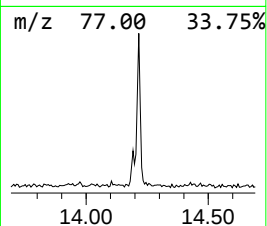
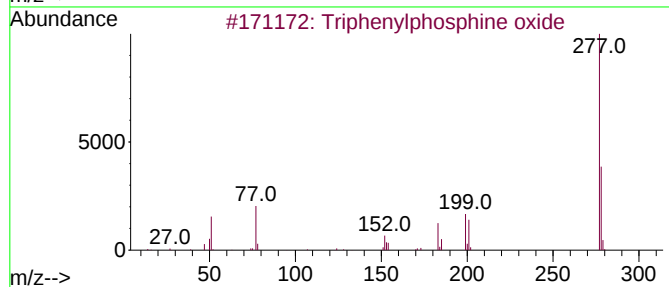
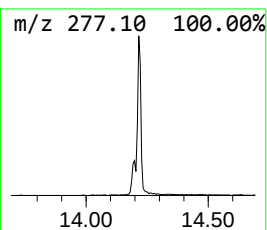
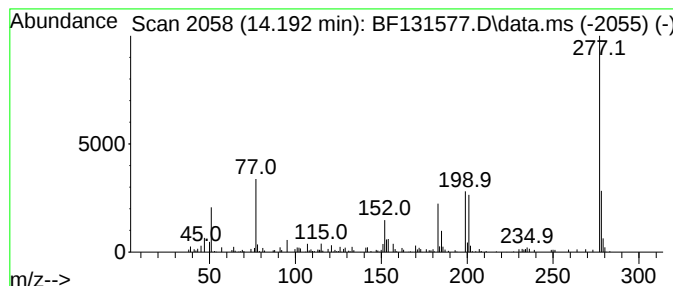
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.192	3.57 ng	67032	Chrysene-d12	14.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	50
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
4			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	38
5			Pyridine, 2-(methylthio)-3,6-dip...	277	C18H15NS	074663-72-2	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
Data File : BF131577.D
Acq On : 09 Dec 2022 20:49
Operator : CG\JU
Sample : N5947-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NYE-WATER-1208

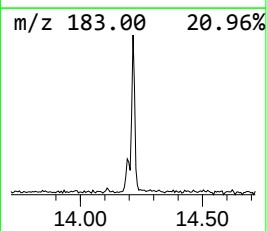
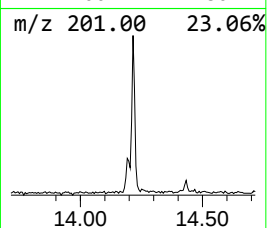
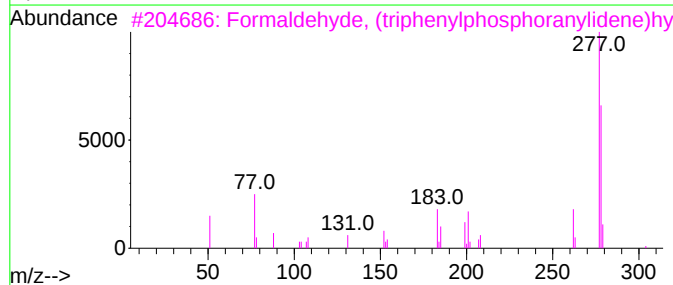
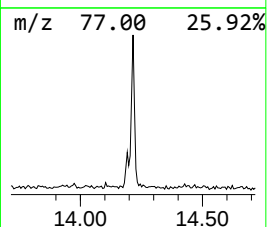
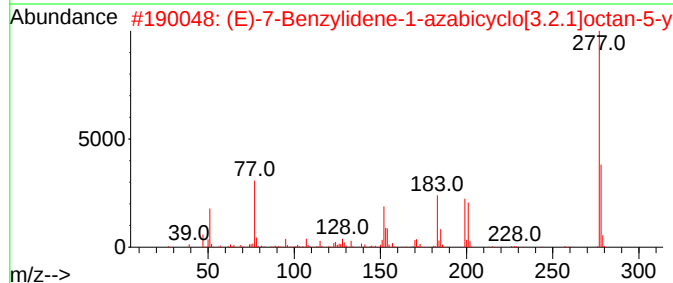
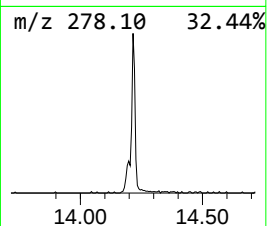
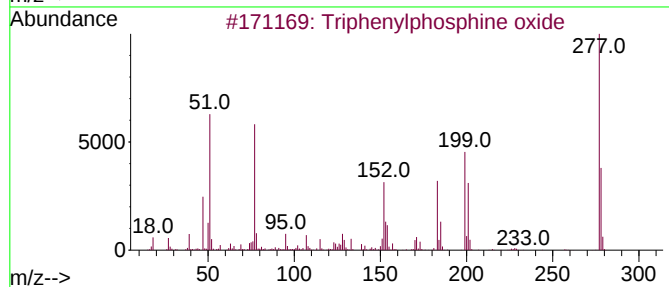
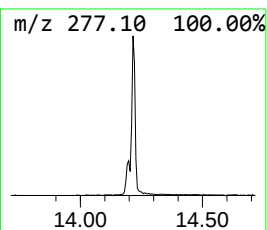
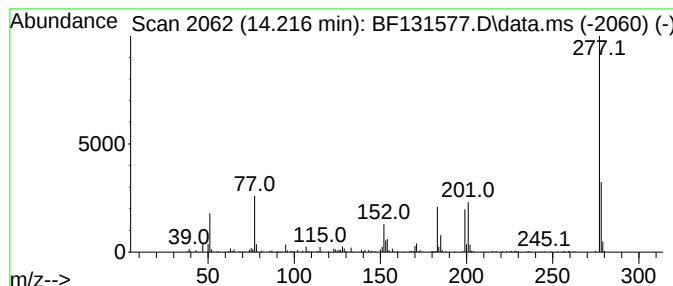
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Formaldehyde, (triphenylpho... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.216	13.78 ng	258985	Chrysene-d12	14.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	90
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	70
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4			4-Nitro-4'-methyldiphenylsulfone	277	C13H11N04S	004094-37-5	38
5			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15N02	299962-12-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
Data File : BF131577.D
Acq On : 09 Dec 2022 20:49
Operator : CG\JU
Sample : N5947-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NYE-WATER-1208

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.234	93.7	ng	2166790	1	6.910	462382	20.0
2-Pentanone, 4-...	5.128	7.8	ng	179403	1	6.910	462382	20.0
Phenol, 4-(1,1-...	9.381	2.6	ng	77643	3	9.963	605926	20.0
7,9-Di-tert-but...	11.839	2.8	ng	93975	4	11.457	668379	20.0
n-Hexadecanoic ...	11.980	2.8	ng	92583	4	11.457	668379	20.0
Octadecanoic acid	12.769	2.0	ng	68575	4	11.457	668379	20.0
1-Pentadecene	13.969	2.2	ng	40963	5	14.104	375808	20.0
Triphenylphosph...	14.192	3.6	ng	67032	5	14.104	375808	20.0
Formaldehyde, (...	14.216	13.8	ng	258985	5	14.104	375808	20.0