

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121322\
 Data File : BF131625.D
 Acq On : 13 Dec 2022 22:00
 Operator : CG\JU
 Sample : N5993-04
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 AOC1-S5

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: BF131625.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	10	17	rVB	406334	497711	27.49%	4.335%
2	2.251	24	28	34	rBV	29354	34563	1.91%	0.301%
3	5.092	506	511	519	rVB	187256	216402	11.95%	1.885%
4	5.498	576	580	583	rBV	1530022	1363718	75.33%	11.878%
5	6.516	748	753	756	rBV	1526057	1389472	76.76%	12.102%
6	6.881	811	815	818	rBV	422720	325055	17.96%	2.831%
7	7.445	906	911	914	rBV	919262	890531	49.19%	7.756%
8	8.169	1030	1034	1037	rVB	492305	398897	22.04%	3.474%
9	9.251	1213	1218	1221	rBV	1993875	1636383	90.40%	14.253%
10	9.933	1330	1334	1338	rBV	566004	465706	25.73%	4.056%
11	10.651	1451	1456	1459	rBV	243575	184279	10.18%	1.605%
12	10.727	1465	1469	1472	rBV	1130774	913430	50.46%	7.956%
13	11.427	1584	1588	1591	rBV	622828	492089	27.18%	4.286%
14	13.021	1855	1859	1863	rBV	2051095	1810233	100.00%	15.767%
15	13.939	2009	2015	2029	rBV5	38921	146608	8.10%	1.277%
16	14.080	2036	2039	2043	rVB	457459	381840	21.09%	3.326%
17	14.174	2051	2055	2062	rBV	31349	40718	2.25%	0.355%
18	15.586	2290	2295	2302	rBV	239280	293465	16.21%	2.556%

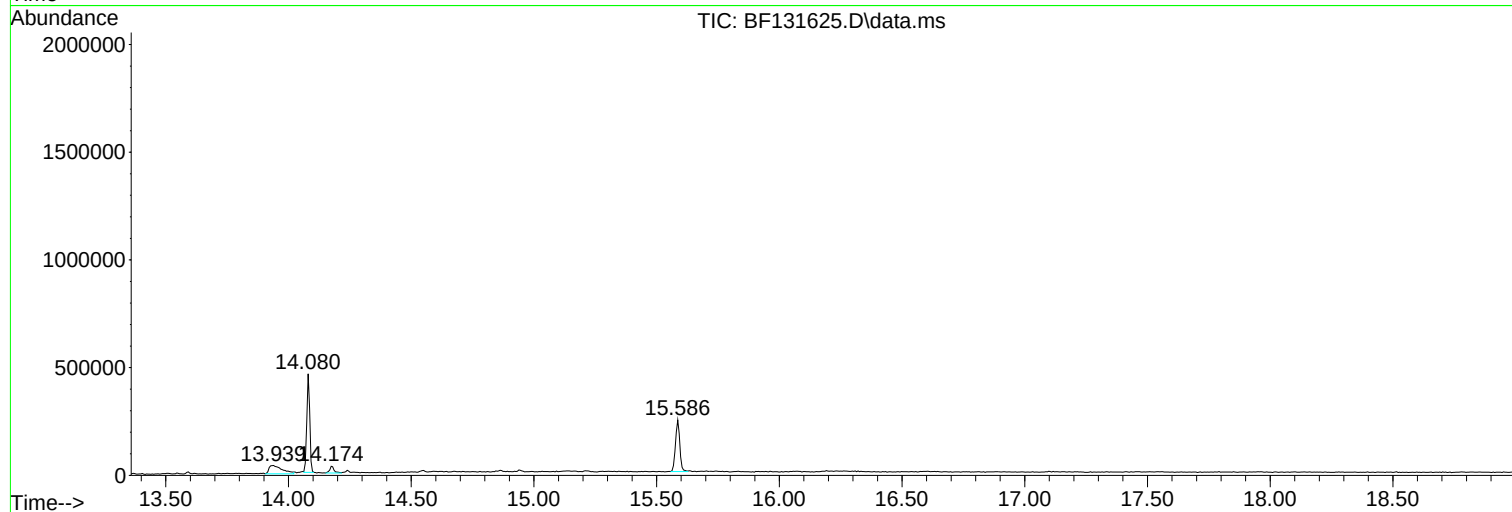
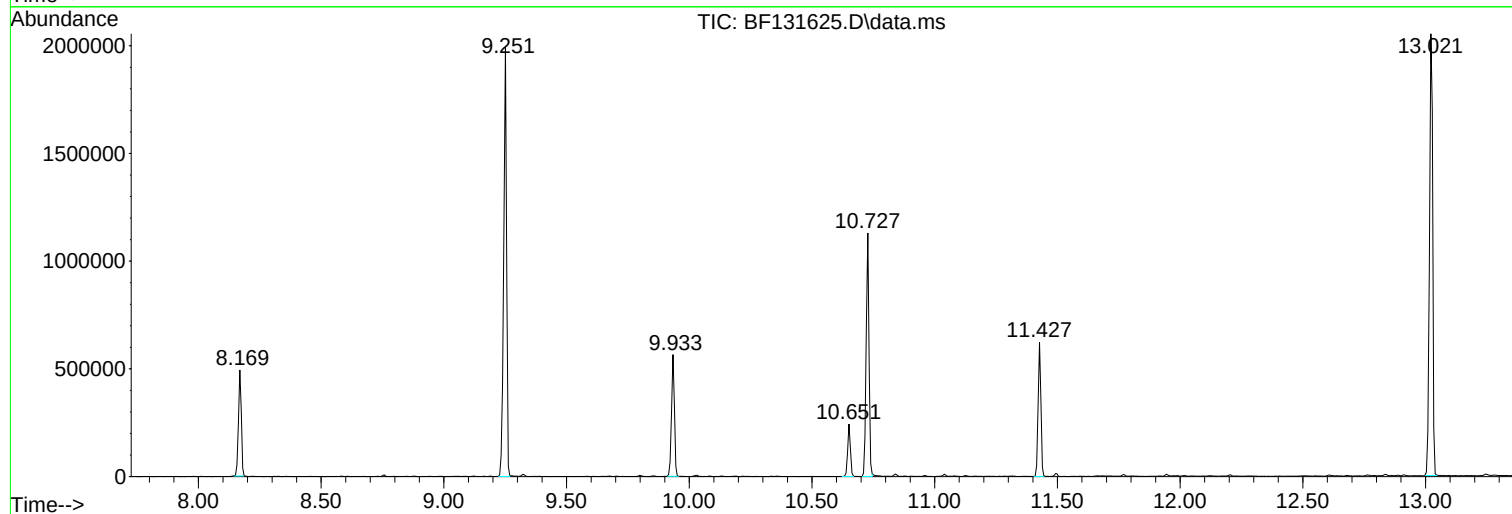
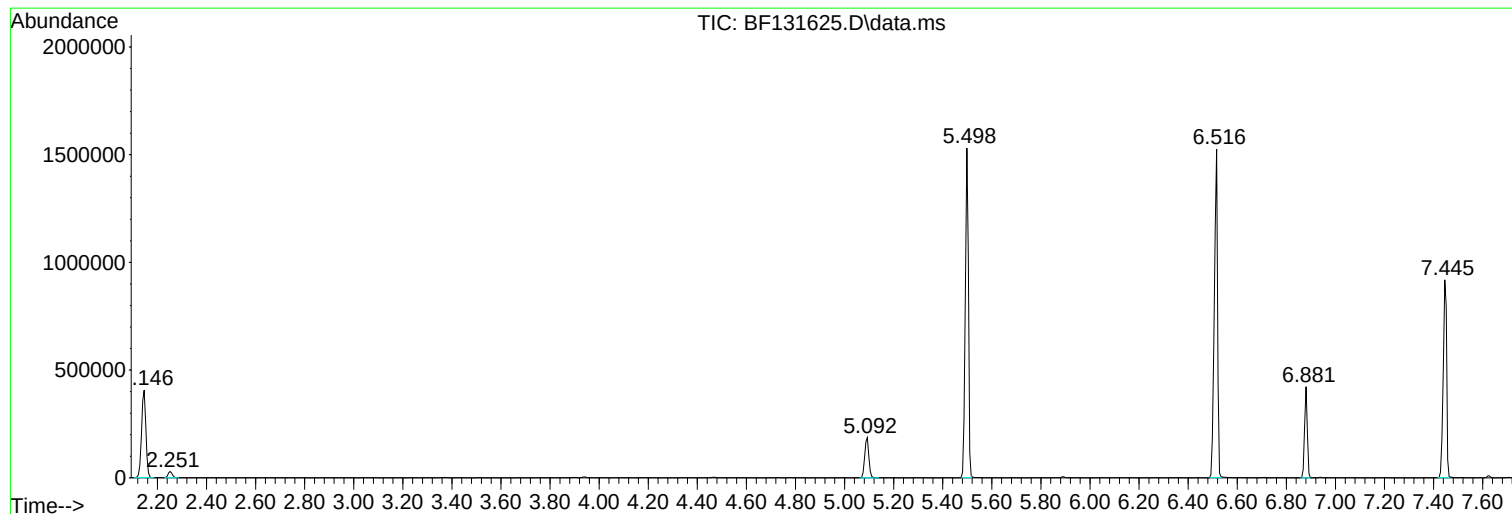
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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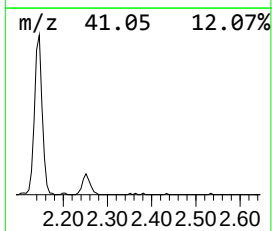
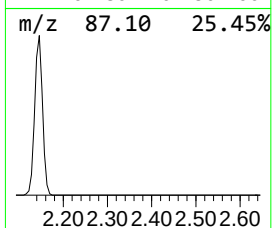
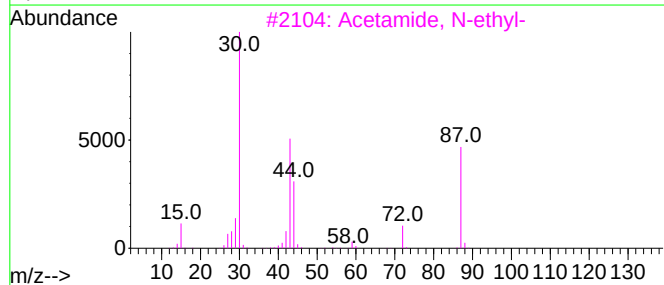
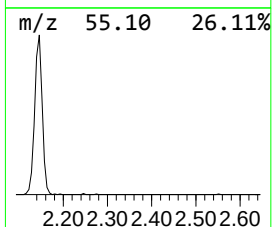
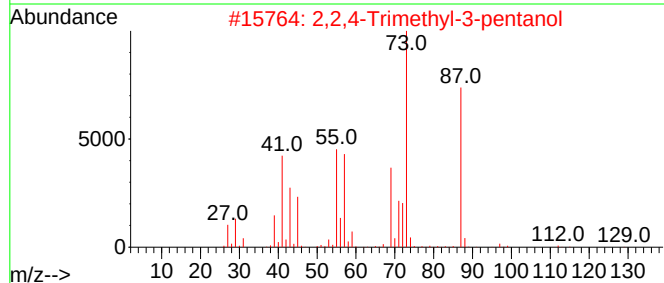
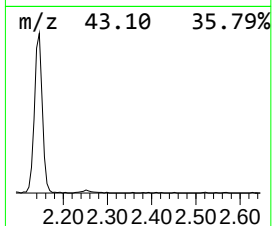
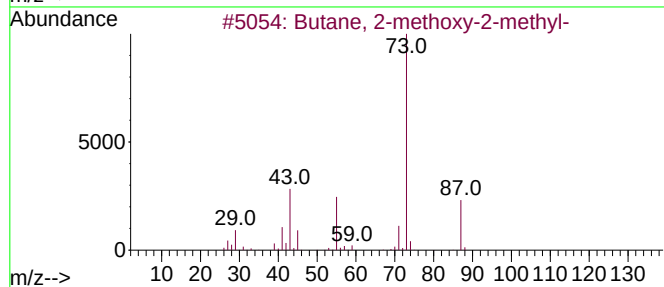
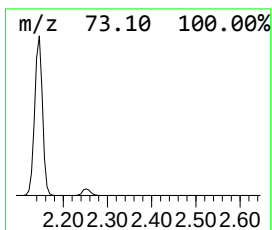
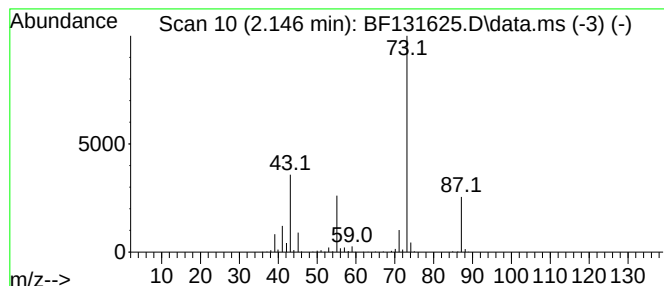
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.146	30.62 ng	497711	1,4-Dichlorobenzene-d4	6.881

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	40
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
4			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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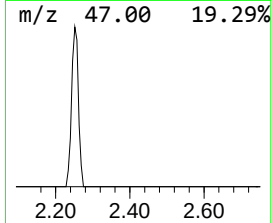
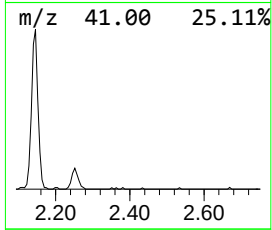
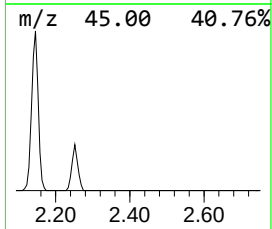
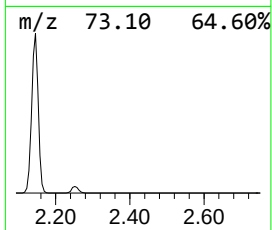
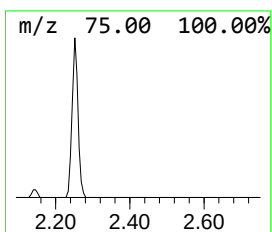
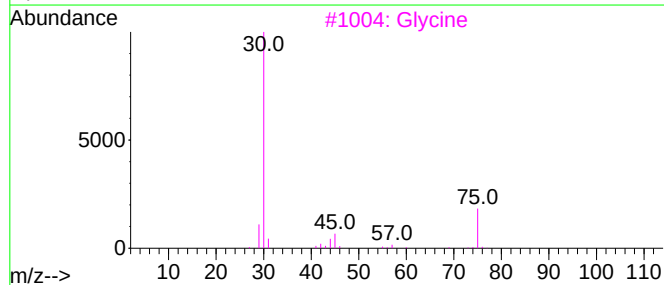
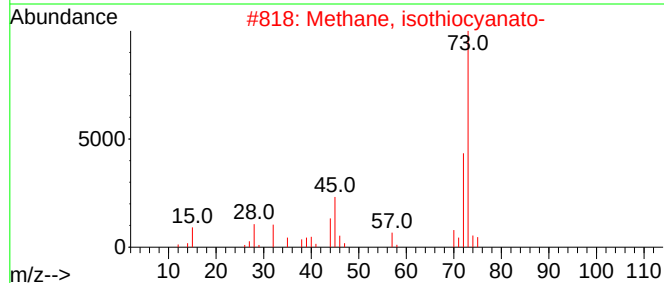
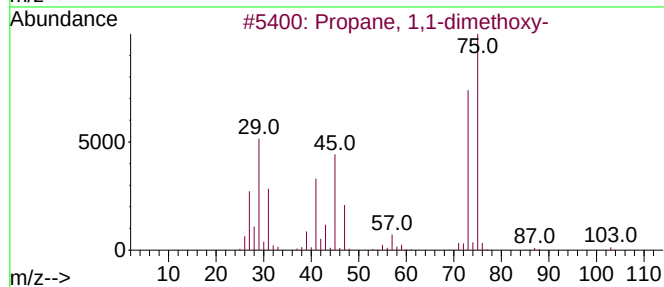
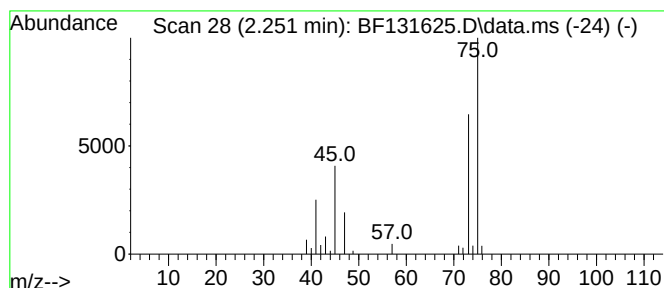
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.251	2.13 ng	34563	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	53
2			Methane, isothiocyanato-	73	C2H3NS	000556-61-6	7
3			Glycine	75	C2H5NO2	000056-40-6	7
4			Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	4
5			Methane, nitroso-	45	CH3NO	000865-40-7	4



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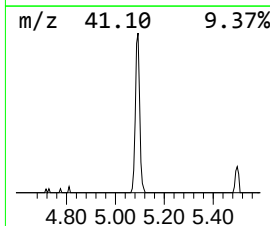
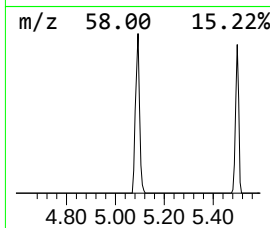
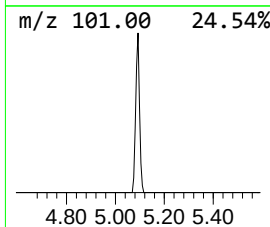
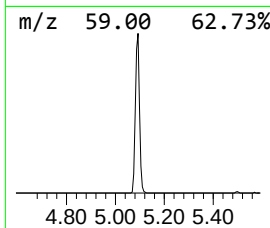
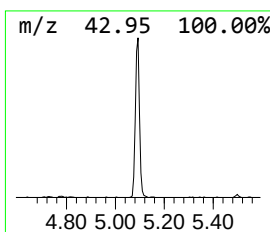
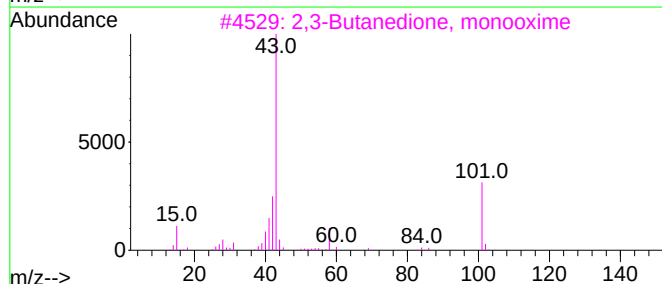
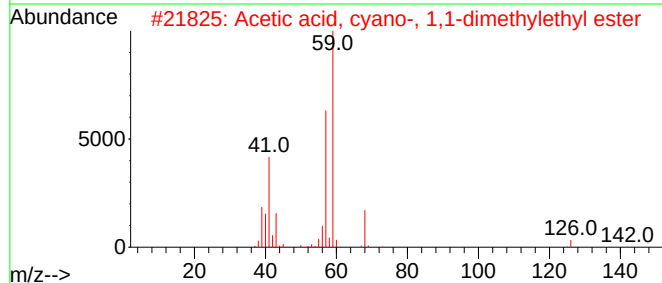
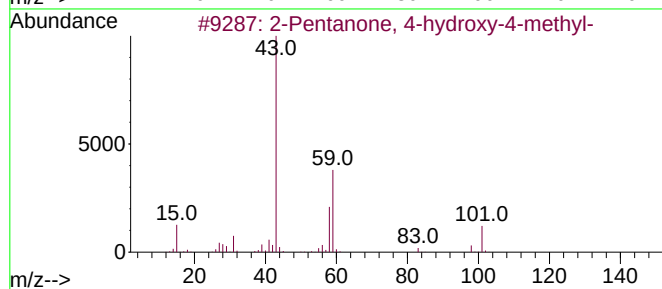
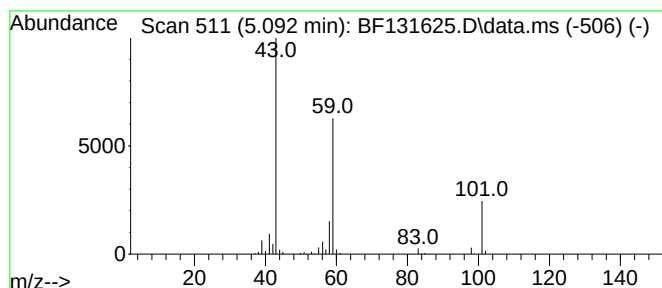
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.092	13.31 ng	216402	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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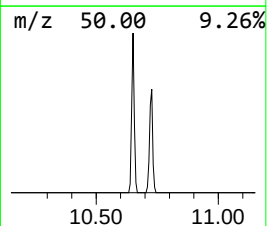
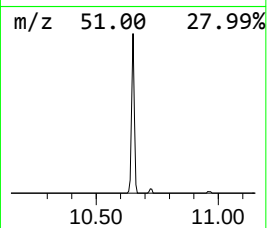
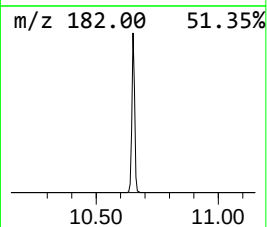
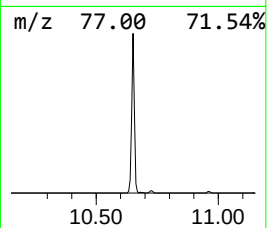
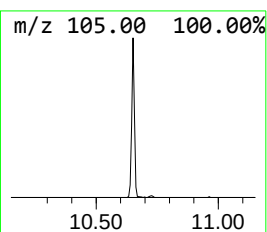
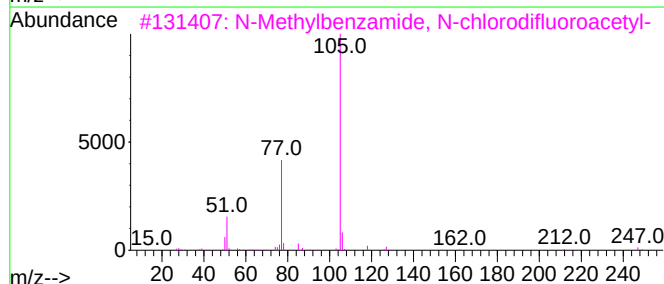
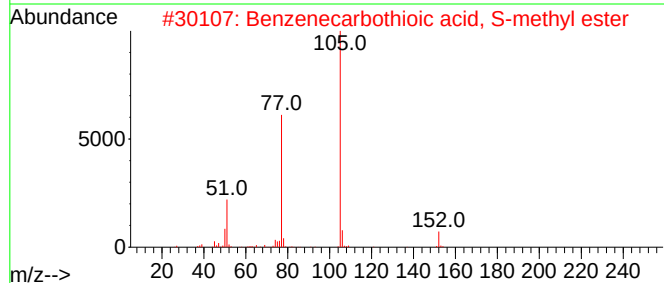
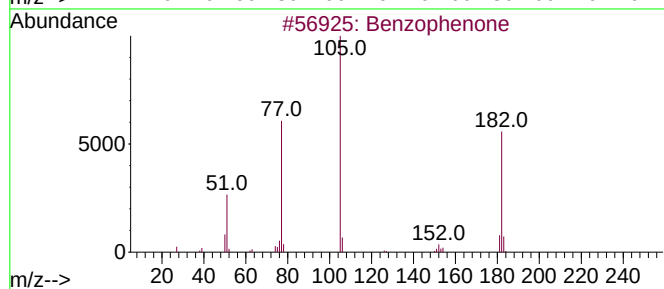
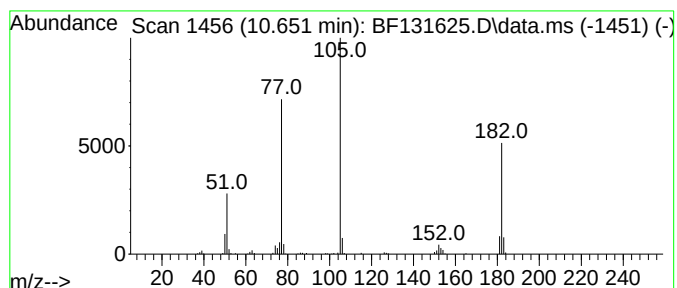
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Peak Number 4 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.651	7.91 ng	184279	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
3			N-Methylbenzamide, N-chlorodiflu...	247	C10H8ClF2NO2	1000446-98-2	50
4			Vinyl benzoate	148	C9H8O2	000769-78-8	50
5			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	50



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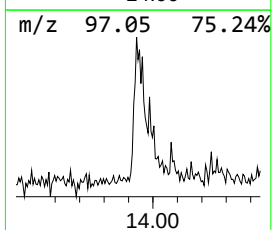
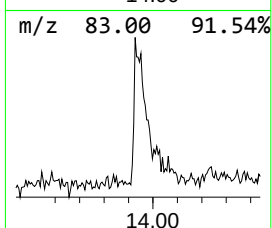
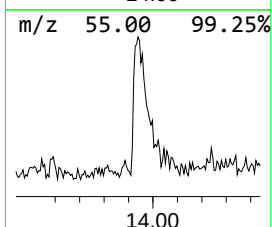
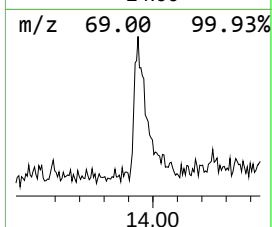
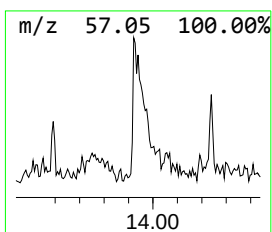
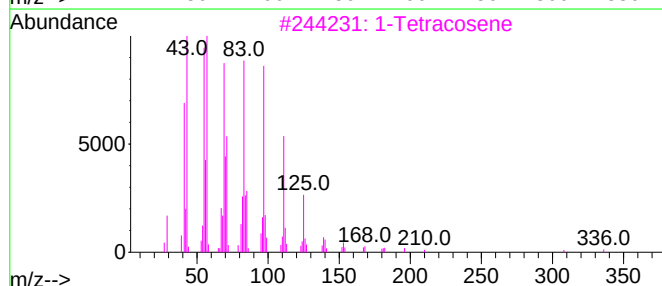
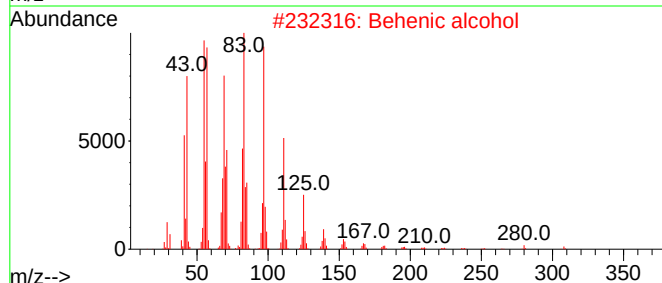
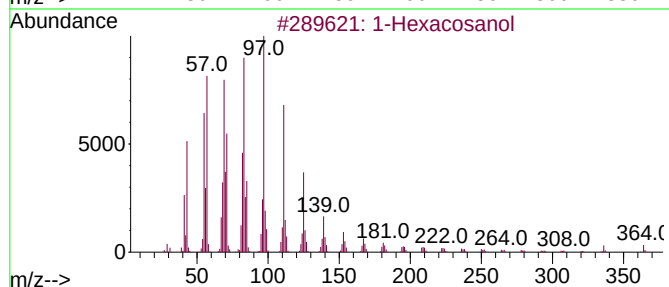
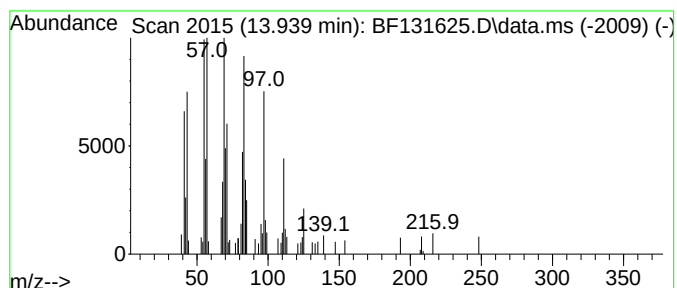
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Hexacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.939	7.68 ng	146608	Chrysene-d12	14.080	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosanol	382	C26H54O	000506-52-5	91
2	Behenic alcohol	326	C22H46O	000661-19-8	91
3	1-Tetracosene	336	C24H48	010192-32-2	90
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	87



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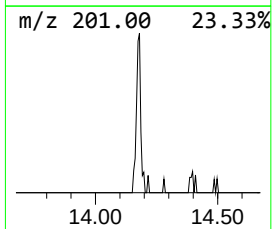
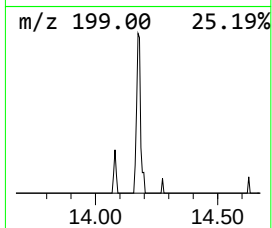
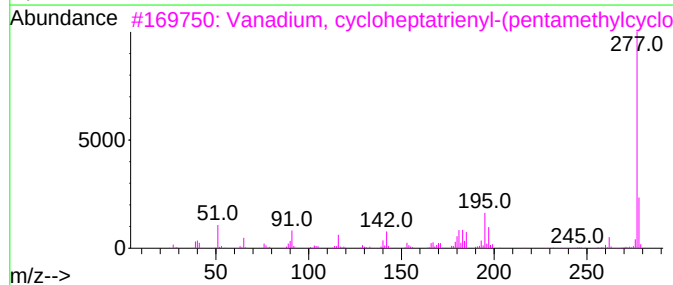
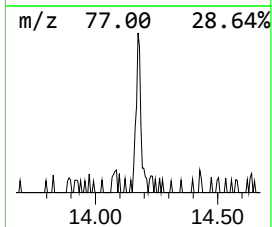
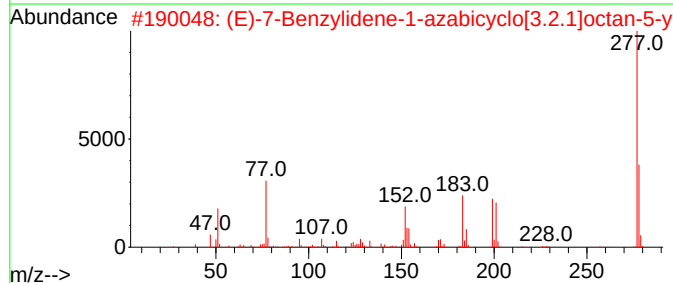
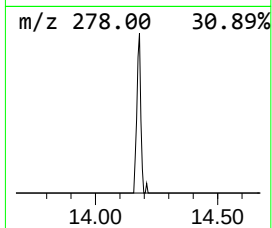
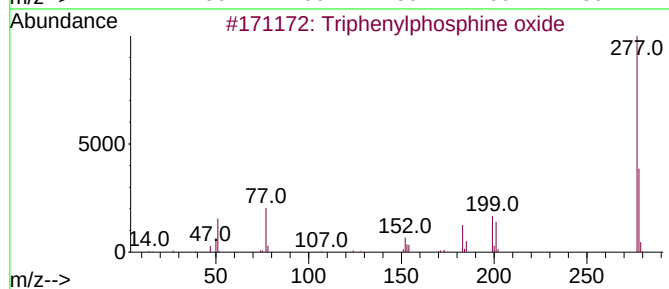
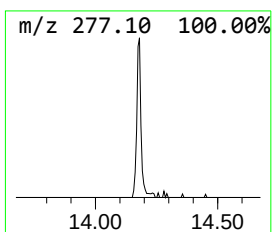
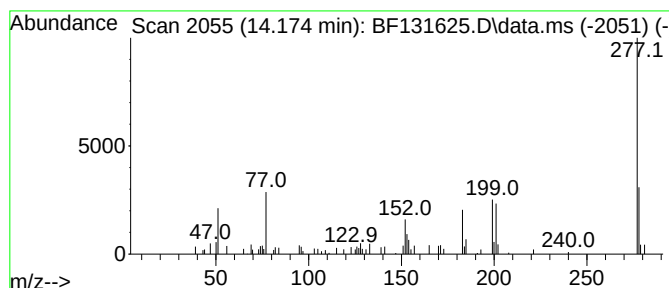
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.174	2.13 ng	40718	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	90
3			Vanadium, cycloheptatrienyl-(pen...]	277	C17H22V	1000155-20-5	47
4			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	42
5			Furo[3,2-c]quinoline, 8-bromo-2,...]	277	C13H12BrNO	1000310-92-7	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121322\
Data File : BF131625.D
Acq On : 13 Dec 2022 22:00
Operator : CG\JU
Sample : N5993-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AOC1-S5

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...	2.146	30.6	ng	497711	1	6.881	325055	20.0
Propane, 1,1-di...	2.251	2.1	ng	34563	1	6.881	325055	20.0
2-Pentanone, 4-...	5.092	13.3	ng	216402	1	6.881	325055	20.0
Benzophenone	10.651	7.9	ng	184279	3	9.933	465706	20.0
1-Hexacosanol	13.939	7.7	ng	146608	5	14.080	381840	20.0
Triphenylphosph...	14.174	2.1	ng	40718	5	14.080	381840	20.0