

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP013023\
 Data File : BP013664.D
 Acq On : 31 Jan 2023 02:01
 Operator : CG/JU
 Sample : 01328-06
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 COMP-2-BORING-1-7-14

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_P\Methods\8270E-BP012623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP013664.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.211	3	4	10	rVB	1578151	1430040	11.20%	1.940%
2	5.205	337	343	356	rBV	1494343	2101802	16.46%	2.852%
3	5.675	416	423	436	rBV	3659128	5422209	42.47%	7.357%
4	7.287	689	697	712	rBV	3437509	5609175	43.94%	7.610%
5	8.146	836	843	849	rBV	767652	1246182	9.76%	1.691%
6	9.316	1034	1042	1052	rBV	1858941	2921531	22.89%	3.964%
7	10.969	1316	1323	1341	rBV	940272	1659762	13.00%	2.252%
8	13.404	1730	1737	1749	rBV	5335227	7822534	61.28%	10.613%
9	14.775	1963	1970	1979	rBV	1402944	2164848	16.96%	2.937%
10	16.128	2194	2200	2213	rBV	221119	333337	2.61%	0.452%
11	16.263	2216	2223	2237	rBV	4192469	5997655	46.98%	8.137%
12	17.528	2432	2438	2444	rBV	1856702	2718534	21.30%	3.688%
13	18.381	2579	2583	2594	rBV	351319	554864	4.35%	0.753%
14	19.604	2788	2791	2799	rBV4	126759	202008	1.58%	0.274%
15	20.063	2863	2869	2877	rVB	10026503	12765843	100.00%	17.320%
16	21.281	3072	3076	3087	rBV	837929	1268618	9.94%	1.721%
17	21.604	3126	3131	3137	rBV	2536989	3573524	27.99%	4.848%
18	21.728	3147	3152	3176	rBV	3256472	7103874	55.65%	9.638%
19	22.533	3284	3289	3312	rVB	2887432	4848806	37.98%	6.579%
20	24.180	3563	3569	3581	rVB2	1813376	3958922	31.01%	5.371%

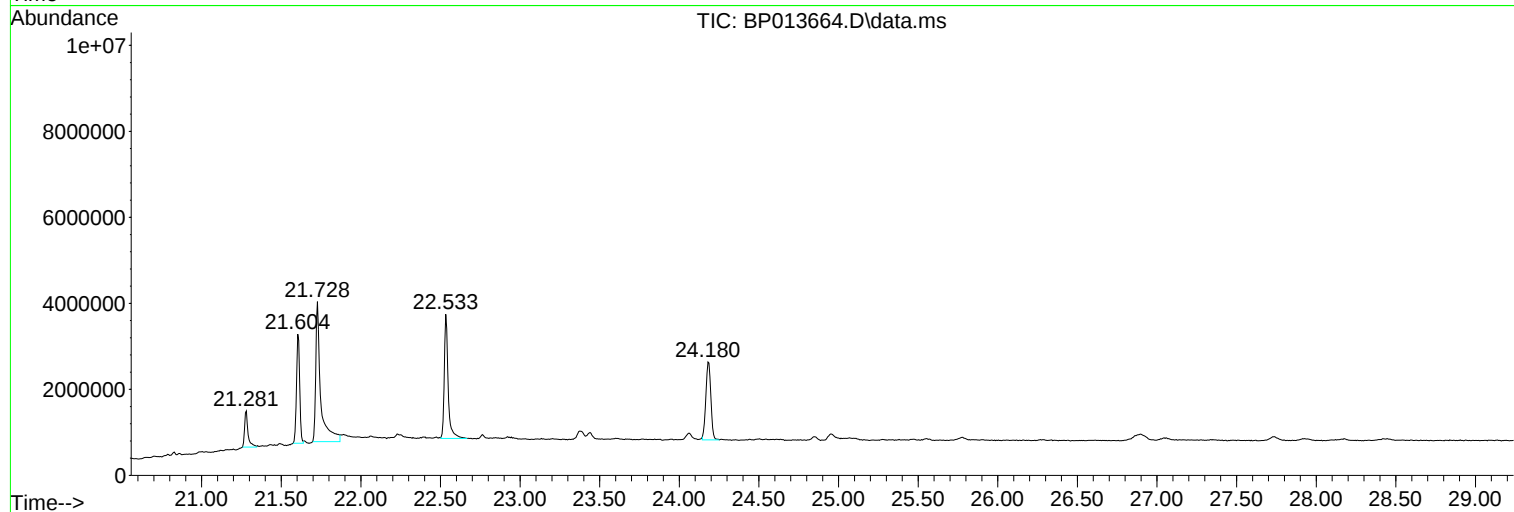
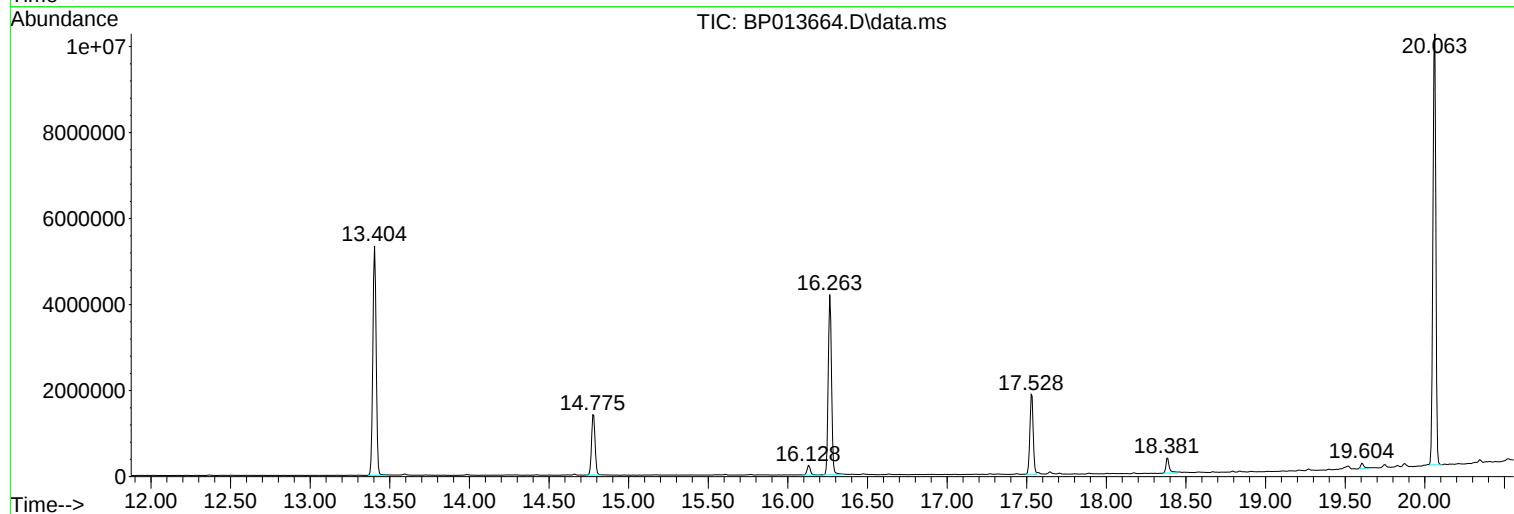
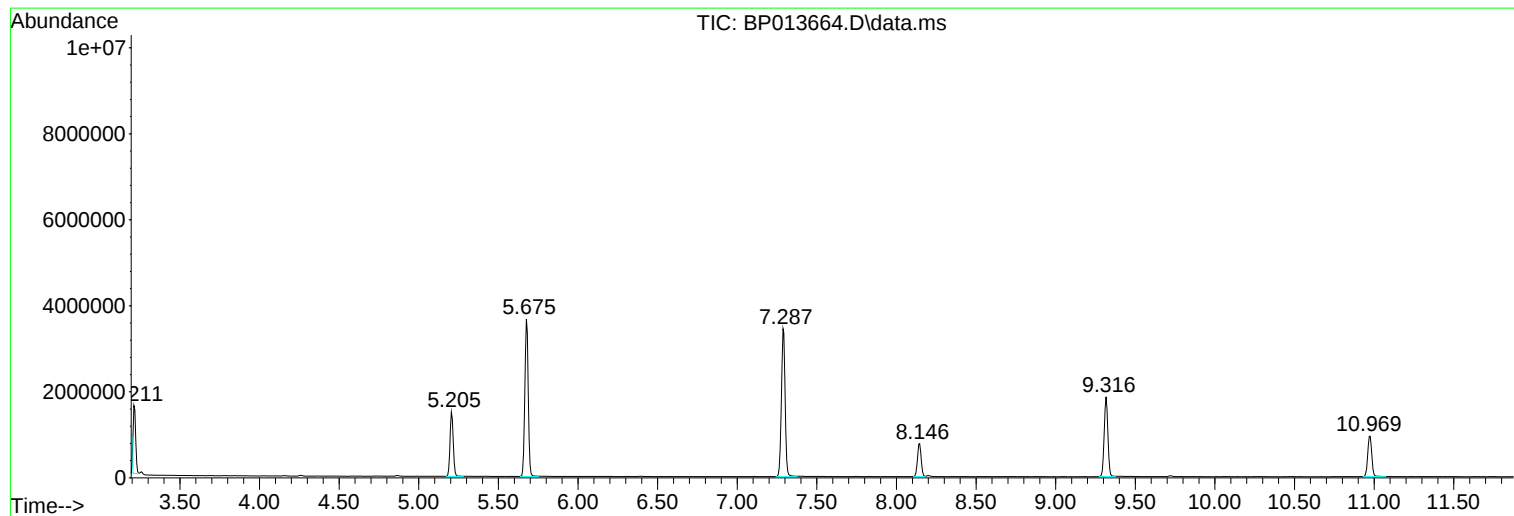
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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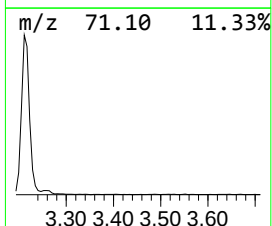
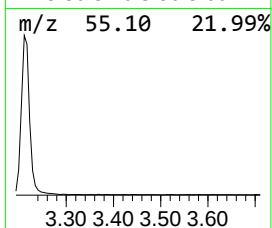
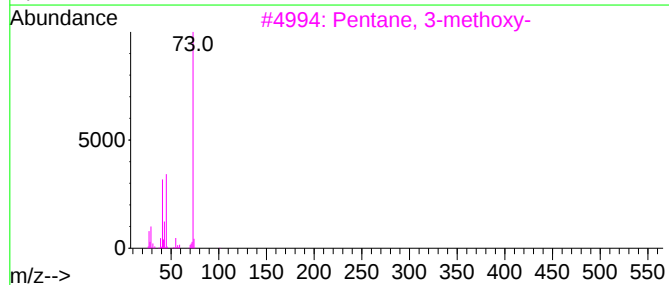
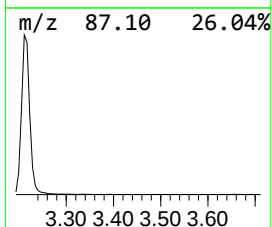
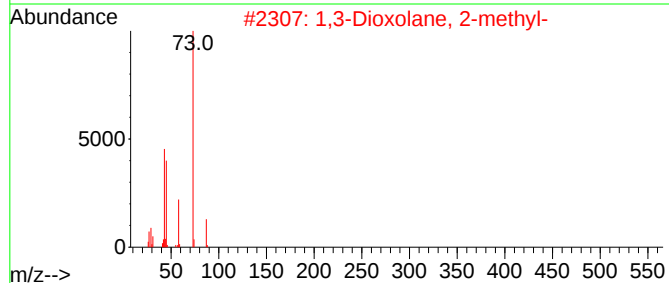
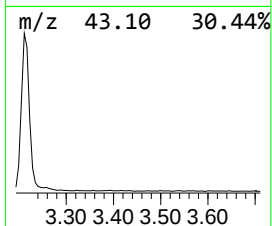
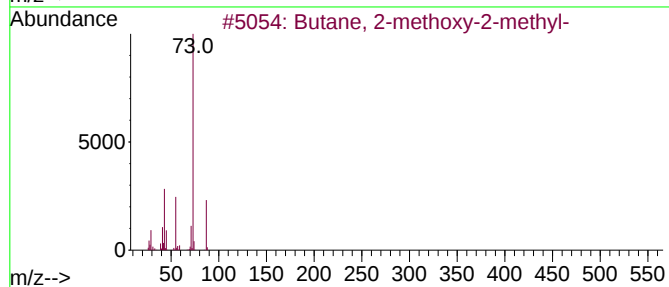
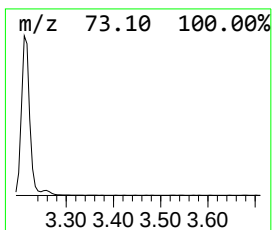
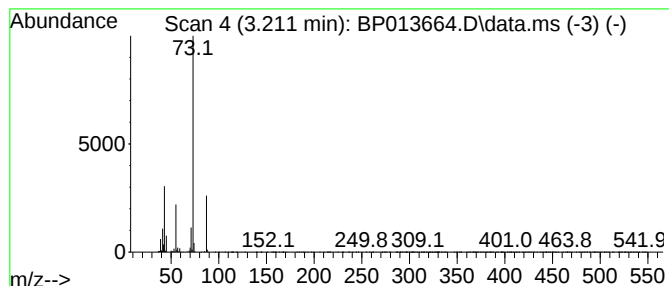
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.211	22.95 ng	1430040	1,4-Dichlorobenzene-d4	8.146

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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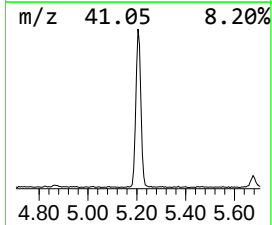
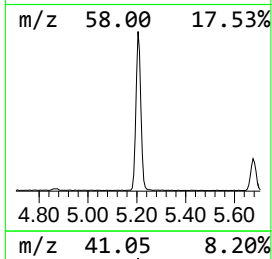
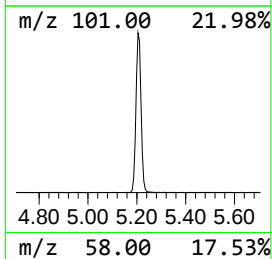
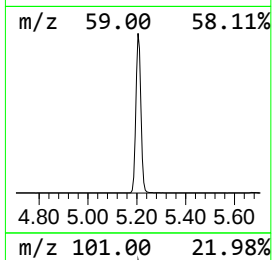
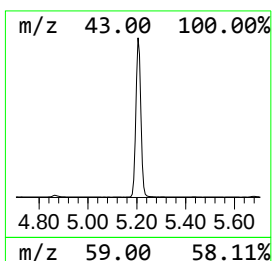
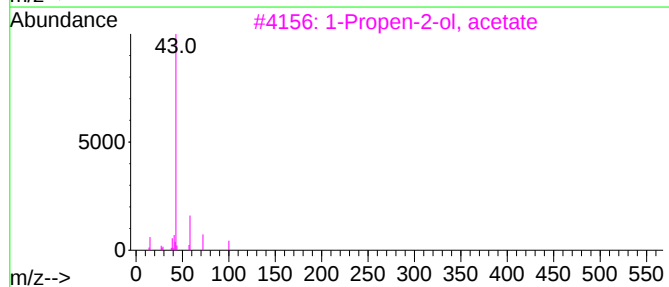
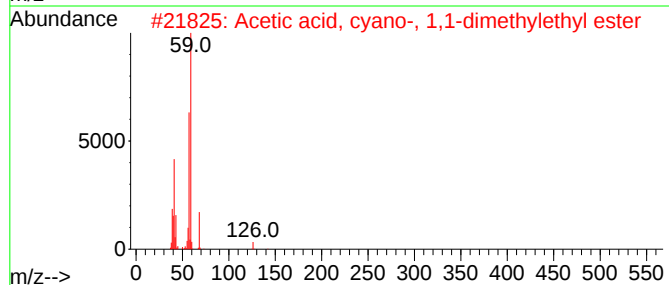
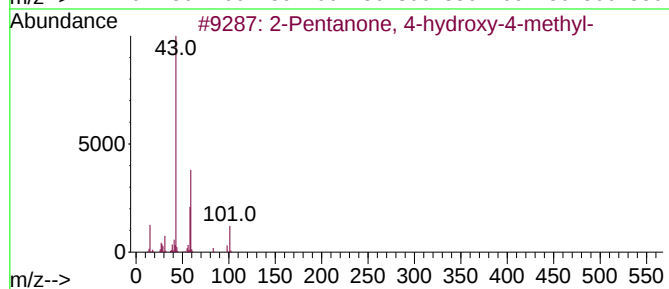
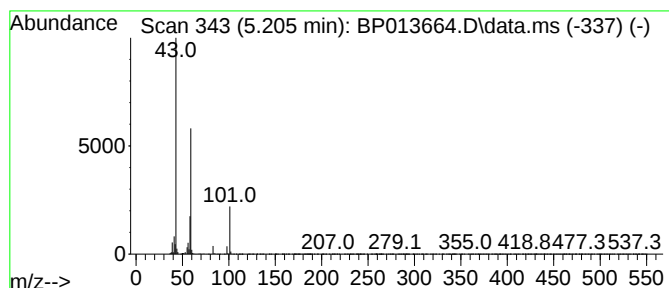
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.205	33.73 ng	2101800	1,4-Dichlorobenzene-d4	8.146

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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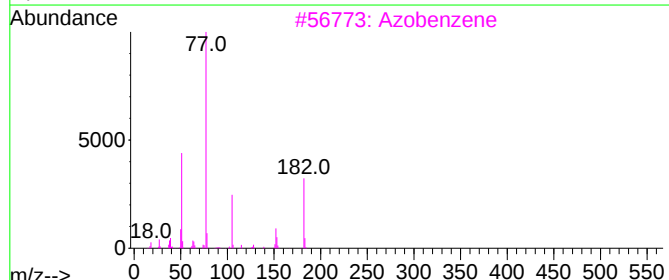
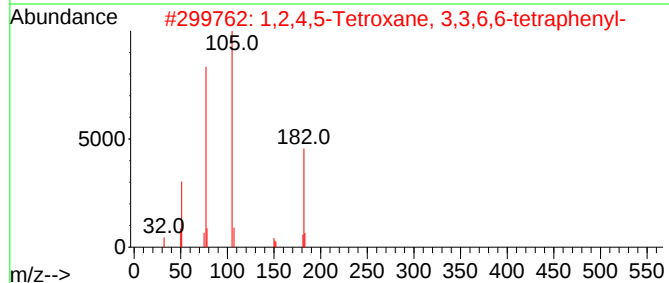
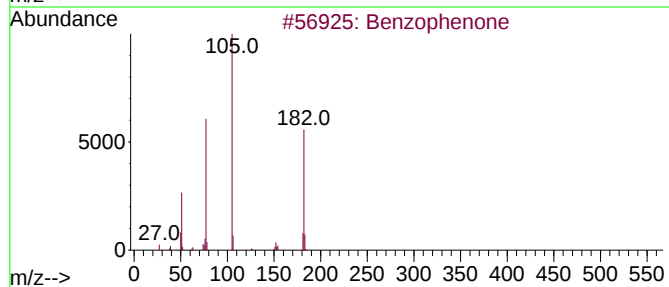
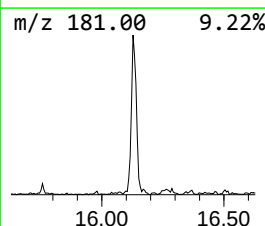
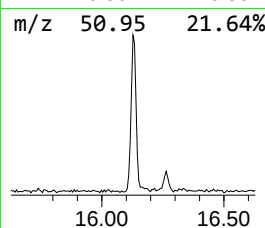
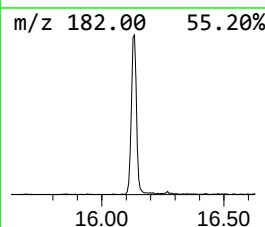
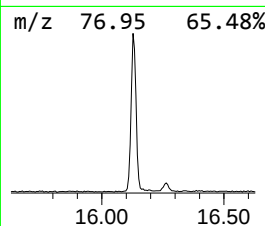
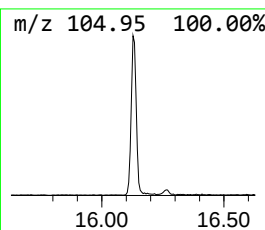
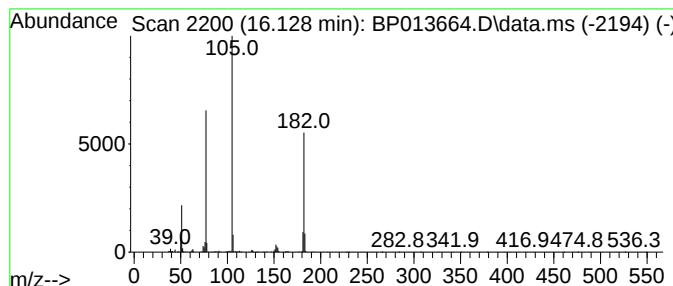
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Peak Number 3 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.128	3.08 ng	333337	Acenaphthene-d10	14.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3			Azobenzene	182	C12H10N2	000103-33-3	64
4			1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	39
5			Azobenzene, (E)-	182	C12H10N2	017082-12-1	38



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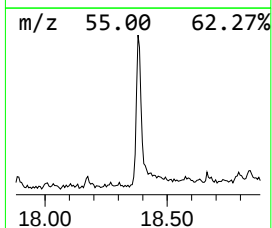
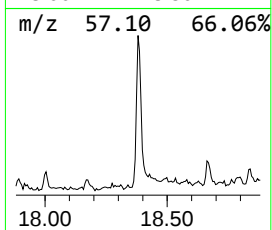
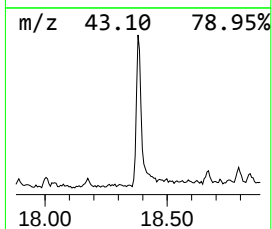
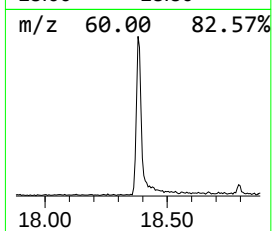
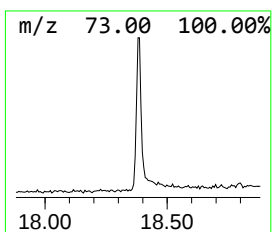
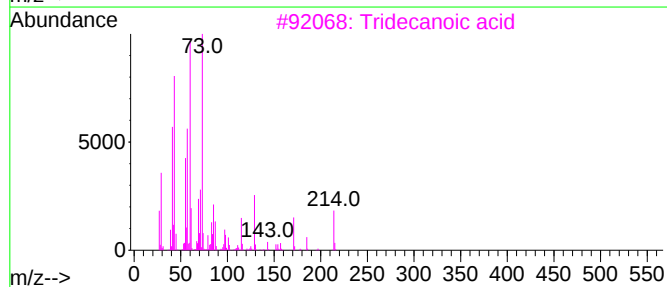
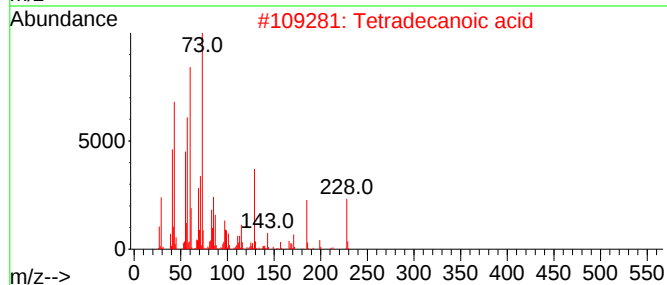
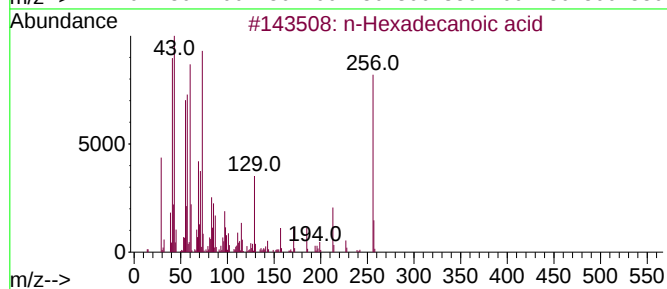
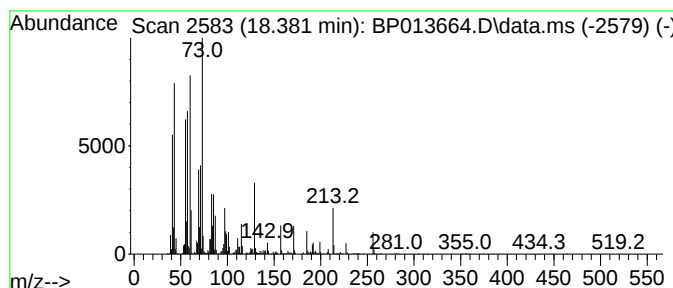
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.381	4.08 ng	554864	Phenanthrene-d10	17.528

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	89
4			Octadecanoic acid	284	C18H36O2	000057-11-4	87
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	76



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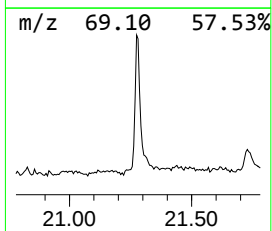
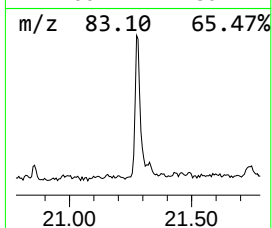
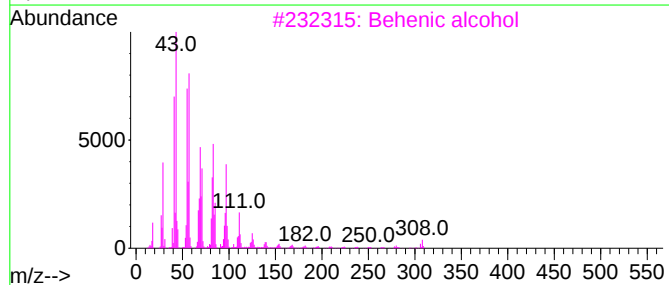
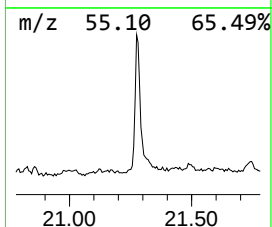
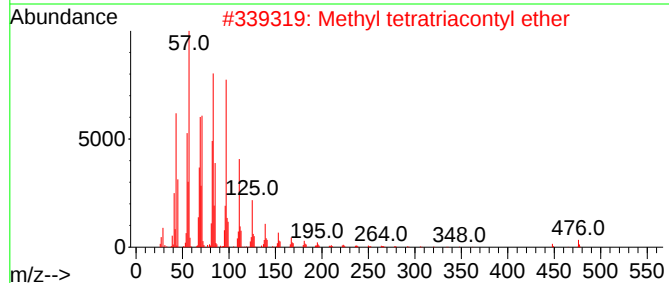
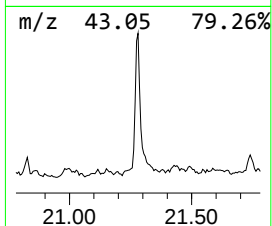
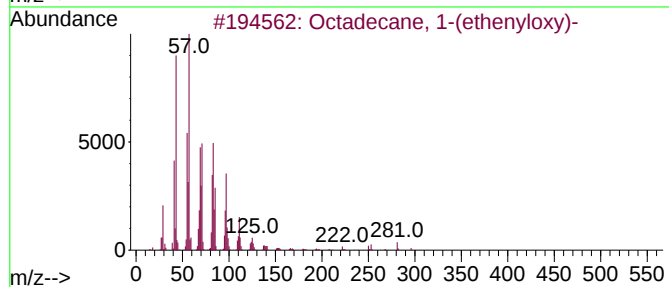
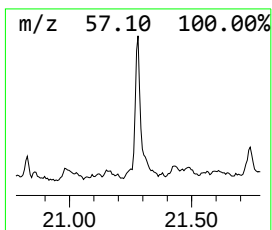
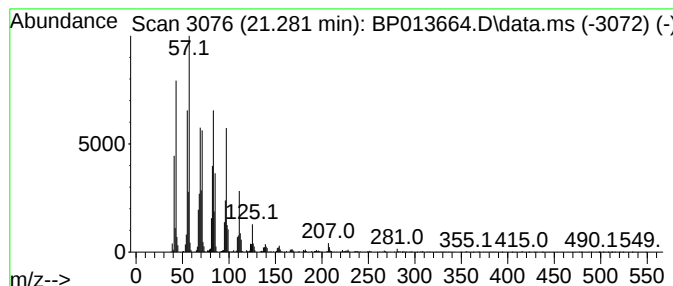
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecane, 1-(ethenyloxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.281	7.10 ng	1268620	Chrysene-d12	21.604	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	94
2	Methyl tetratriacontyl ether	509	C35H72O	1000406-30-1	91
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	17-Pentatriacontene	491	C35H70	006971-40-0	90
5	Octadecyl propyl ether	312	C21H44O	1000406-28-0	90



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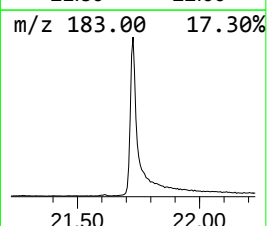
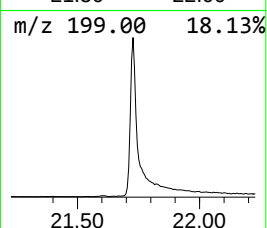
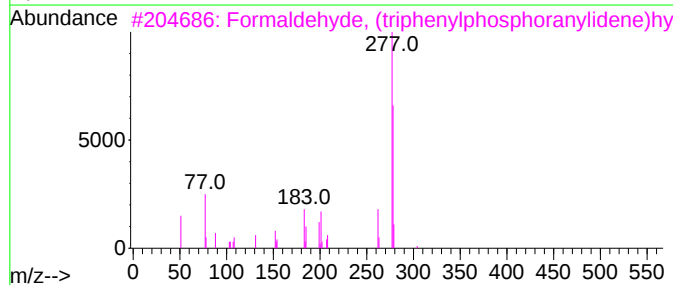
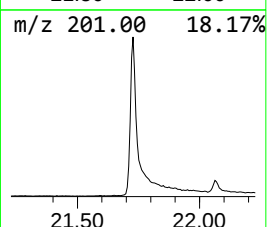
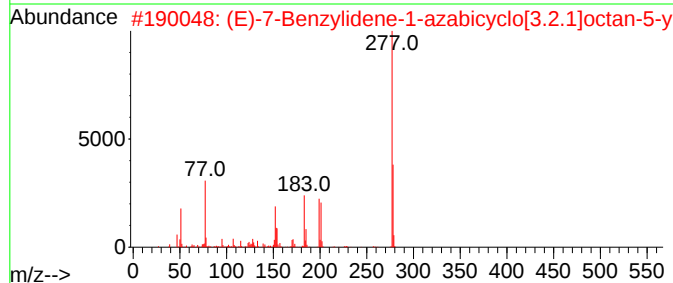
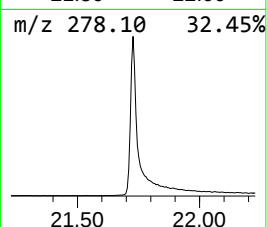
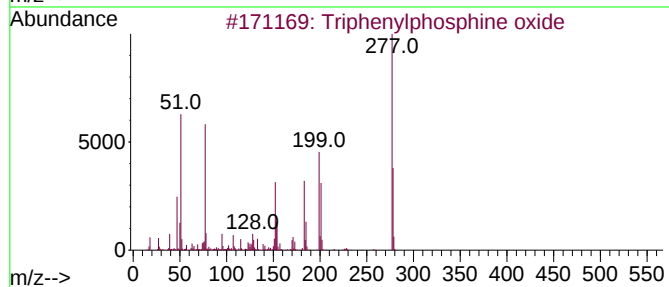
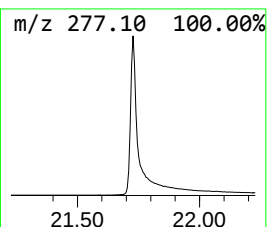
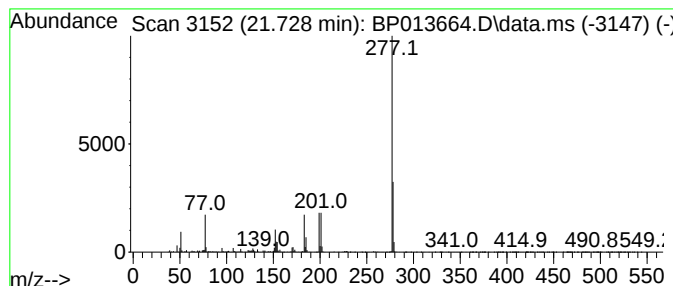
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.727	39.76 ng	7103870	Chrysene-d12	21.604

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	47
4			5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	38
5			2-Phenyl-6-(trifluoromethyl)-1H...	277	C15H10F3NO	1000387-59-3	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP013023\
Data File : BP013664.D
Acq On : 31 Jan 2023 02:01
Operator : CG/JU
Sample : 01328-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
COMP-2-BORING-1-7-14

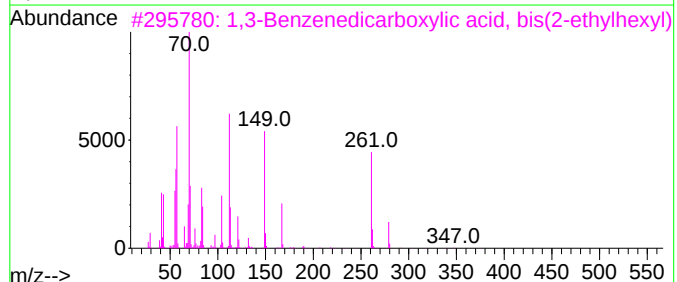
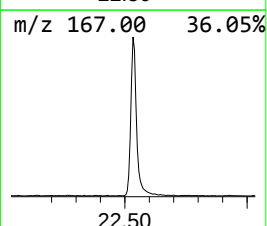
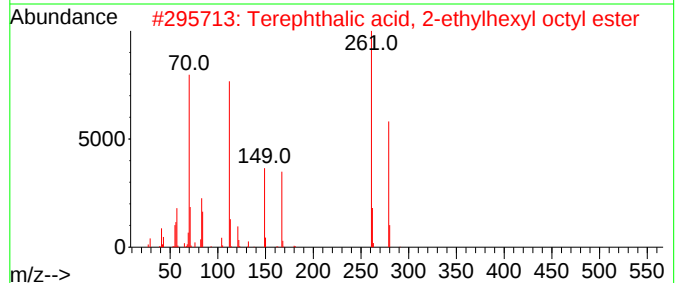
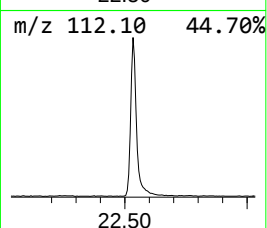
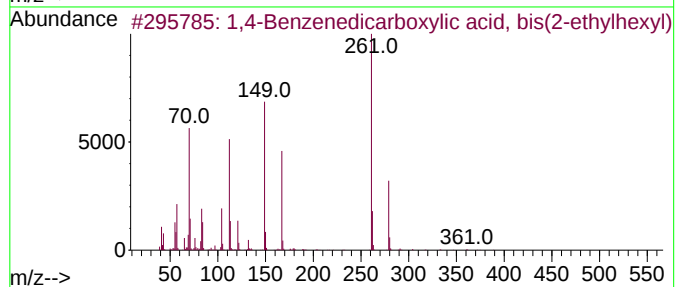
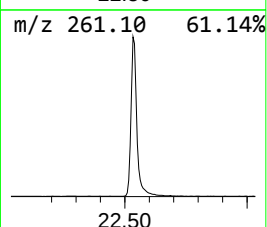
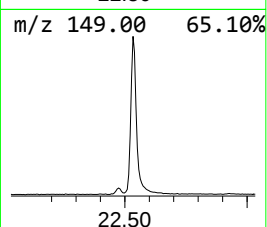
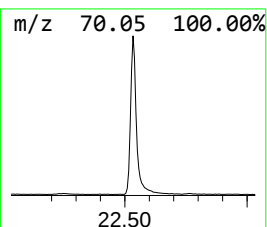
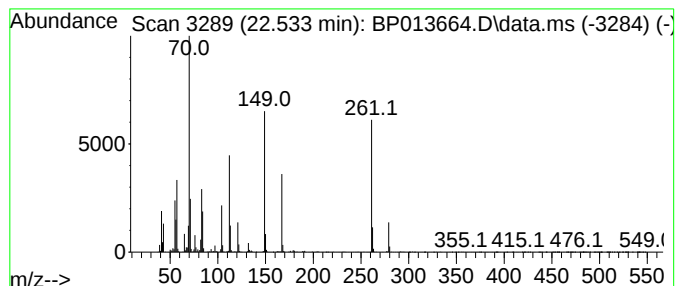
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,4-Benzenedicarboxylic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.533	27.14 ng	4848810	Chrysene-d12	21.604

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	87
2			Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	58
3			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	58
4			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	52
5			Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP013023\
Data File : BP013664.D
Acq On : 31 Jan 2023 02:01
Operator : CG/JU
Sample : 01328-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
COMP-2-BORING-1-7-14

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012623.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
Butane, 2-metho...	3.211	22.9	ng	1430040	1	8.146	1246180	20.0
2-Pentanone, 4-...	5.205	33.7	ng	2101800	1	8.146	1246180	20.0
Benzophenone	16.128	3.1	ng	333337	3	14.775	2164850	20.0
n-Hexadecanoic ...	18.381	4.1	ng	554864	4	17.528	2718530	20.0
Octadecane, 1-(...	21.281	7.1	ng	1268620	5	21.604	3573520	20.0
Triphenylphosph...	21.727	39.8	ng	7103870	5	21.604	3573520	20.0
1,4-Benzenedica...	22.533	27.1	ng	4848810	5	21.604	3573520	20.0