

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
 Data File : BP019897.D
 Acq On : 27 Feb 2024 15:27
 Operator : MA/JU
 Sample : P1523-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 20240763-COMPOSITE-39N-N-3-01

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-BP022624.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP019897.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.123	3	6	15	rVB	2966760	3555666	86.76%	10.705%
2	3.746	108	112	124	rBV3	53899	109252	2.67%	0.329%
3	3.864	128	132	136	rBV	57641	73894	1.80%	0.222%
4	3.993	150	154	160	rVB2	30450	48510	1.18%	0.146%
5	4.070	161	167	177	rVV	224420	372848	9.10%	1.123%
6	4.240	189	196	203	rBV	80997	125909	3.07%	0.379%
7	4.452	228	232	240	rVB	89983	122856	3.00%	0.370%
8	4.587	248	255	259	rBV	42646	72200	1.76%	0.217%
9	4.640	259	264	269	rVV	397567	611093	14.91%	1.840%
10	4.693	269	273	284	rVB	238999	354213	8.64%	1.066%
11	5.017	322	328	338	rBV	490453	716440	17.48%	2.157%
12	5.469	398	405	414	rBV	1454991	2169685	52.94%	6.532%
13	5.793	449	460	465	rBV	60409	103624	2.53%	0.312%
14	5.917	475	481	488	rBV4	19238	43466	1.06%	0.131%
15	6.093	502	511	516	rBV	32565	57678	1.41%	0.174%
16	6.205	526	530	544	rVB3	53748	114616	2.80%	0.345%
17	6.752	619	623	632	rVB7	41188	111112	2.71%	0.335%
18	7.069	670	677	684	rBV	1476842	2399116	58.54%	7.223%
19	7.122	684	686	692	rVB	33695	45848	1.12%	0.138%
20	7.293	706	715	722	rBV5	30631	81366	1.99%	0.245%
21	7.599	760	767	773	rBV2	81082	147805	3.61%	0.445%
22	7.893	812	817	825	rVB	393424	643761	15.71%	1.938%
23	8.058	839	845	850	rBV	33065	60202	1.47%	0.181%
24	8.140	850	859	863	rVV3	53896	108407	2.65%	0.326%
25	8.187	863	867	872	rVV5	20877	42154	1.03%	0.127%
26	8.869	978	983	988	rBV5	19442	44355	1.08%	0.134%
27	9.069	1008	1017	1027	rBV	924137	1605567	39.18%	4.834%
28	9.816	1138	1144	1154	rBV3	31898	84255	2.06%	0.254%
29	10.057	1180	1185	1191	rBV6	24164	54077	1.32%	0.163%
30	10.563	1263	1271	1276	rBV	36850	64208	1.57%	0.193%
31	10.699	1286	1294	1310	rVB	516166	919056	22.43%	2.767%
32	10.893	1318	1327	1339	rBV2	30068	81693	1.99%	0.246%
33	11.087	1351	1360	1366	rBV6	35310	104441	2.55%	0.314%
34	11.140	1366	1369	1375	rVB	28462	43226	1.05%	0.130%
35	11.346	1400	1404	1407	rBV	36771	62044	1.51%	0.187%
36	11.375	1407	1409	1415	rVB2	42339	64922	1.58%	0.195%

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.452	1415	1422	1429	rBV4	61078	118773	2.90%	0.358%
38	11.528	1429	1435	1441	rVB3	31329	64106	1.56%	0.193%
39	12.157	1531	1542	1549	rBV5	15469	46401	1.13%	0.140%
40	13.163	1701	1713	1728	rBV	2198097	3341544	81.54%	10.061%
41	13.440	1752	1760	1768	rBV	318579	511114	12.47%	1.539%
42	14.540	1940	1947	1960	rVB	855308	1293678	31.57%	3.895%
43	16.034	2191	2201	2220	rBV	1757074	2708267	66.09%	8.154%
44	17.298	2410	2416	2431	rBV	1022041	1572936	38.38%	4.736%
45	17.986	2528	2533	2538	rBV	32686	44004	1.07%	0.132%
46	18.198	2564	2569	2580	rBV	409424	603311	14.72%	1.816%
47	19.116	2722	2725	2729	rVB3	34408	41917	1.02%	0.126%
48	19.433	2775	2779	2788	rBV	171427	261894	6.39%	0.788%
49	19.869	2848	2853	2863	rVB	3407220	4098112	100.00%	12.338%
50	20.180	2903	2906	2910	rVB2	39140	44603	1.09%	0.134%
51	20.669	2985	2989	2992	rBV2	52992	63636	1.55%	0.192%
52	20.875	3021	3024	3031	rBV	69759	98568	2.41%	0.297%
53	21.122	3062	3066	3071	rBV	180394	228021	5.56%	0.687%
54	21.398	3108	3113	3121	rBV	976316	1361684	33.23%	4.100%
55	21.569	3139	3142	3146	rVB2	62308	68089	1.66%	0.205%
56	23.821	3519	3525	3534	rVB	574797	1224156	29.87%	3.686%

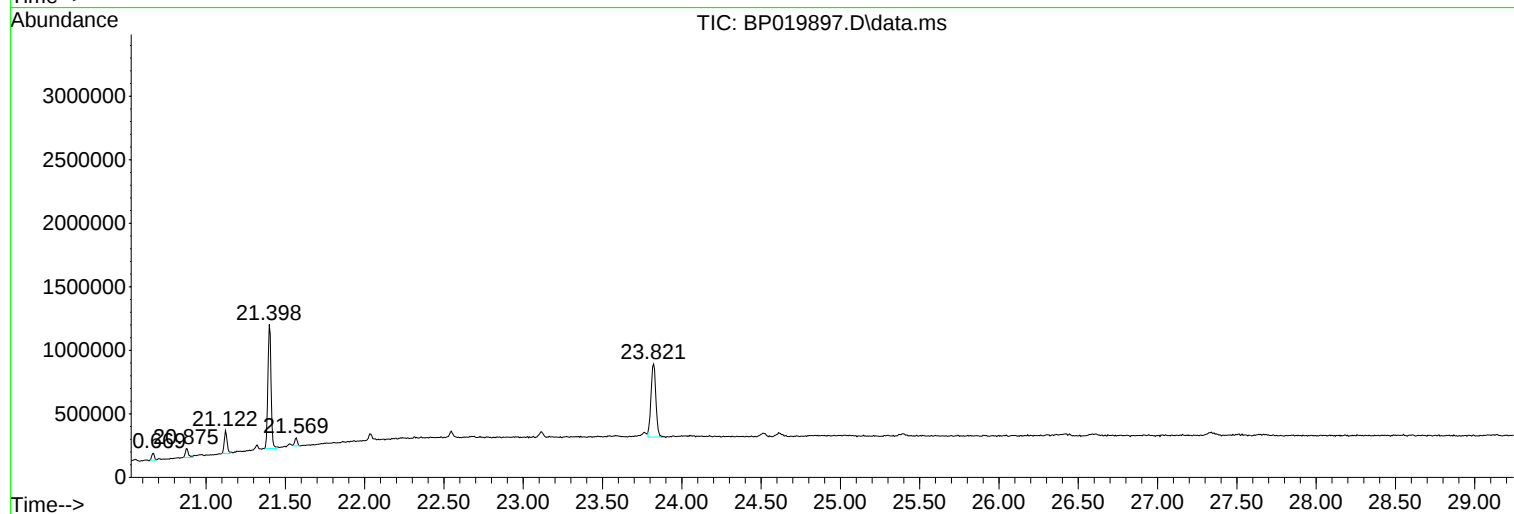
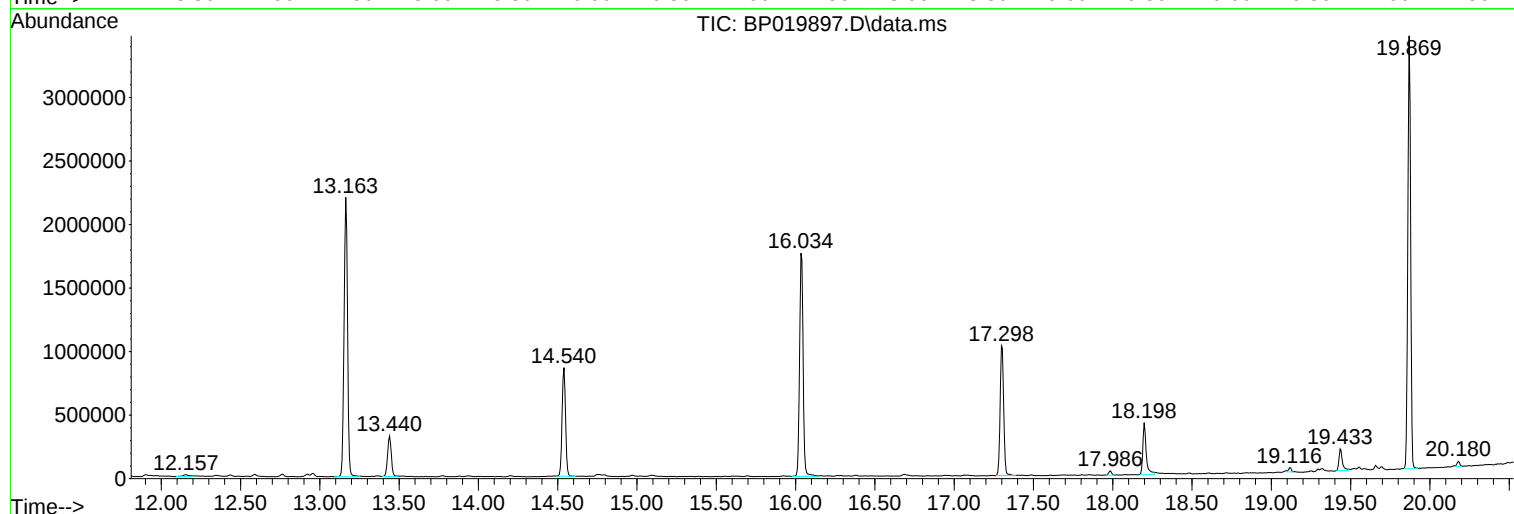
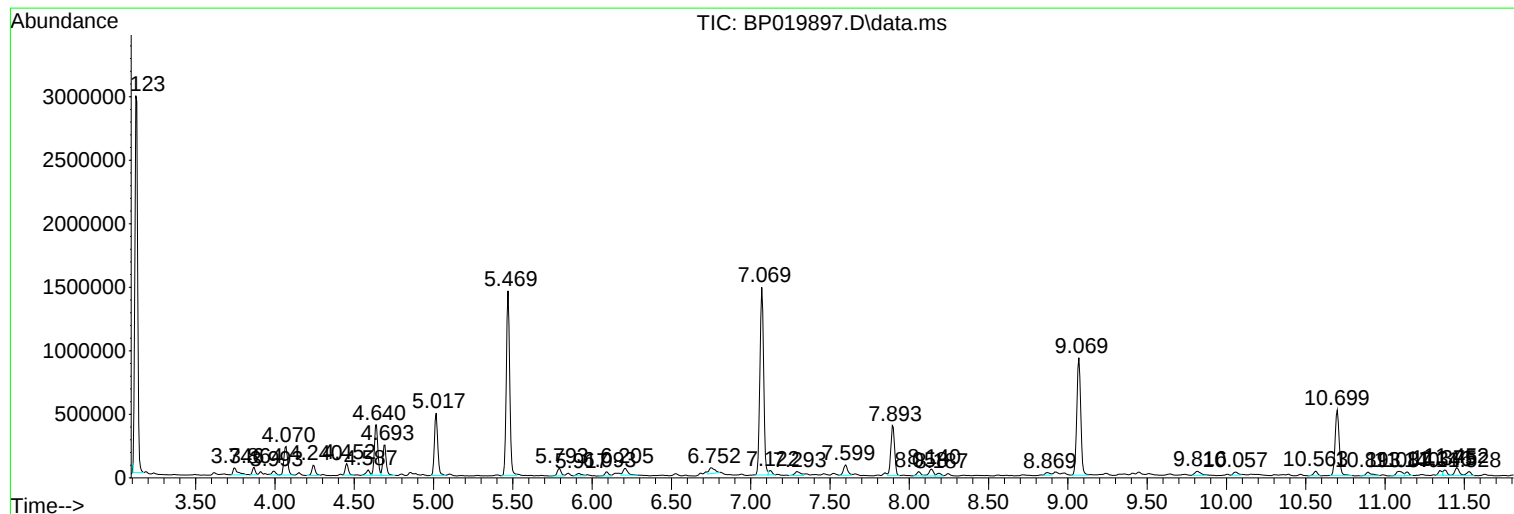
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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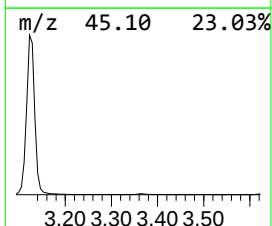
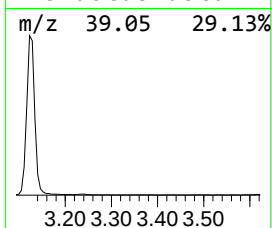
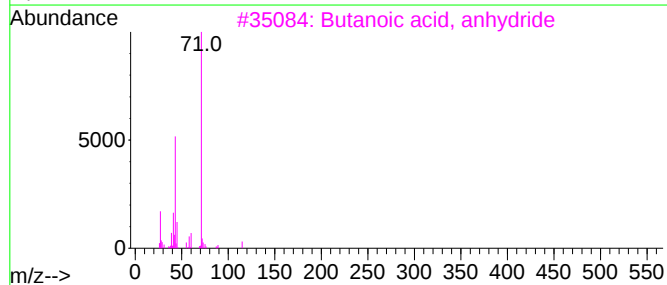
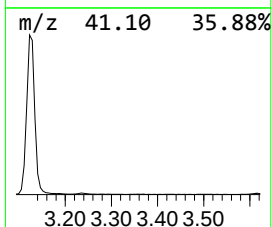
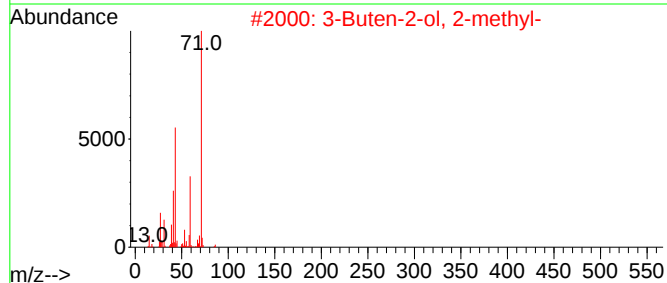
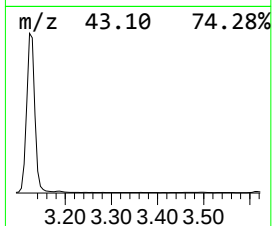
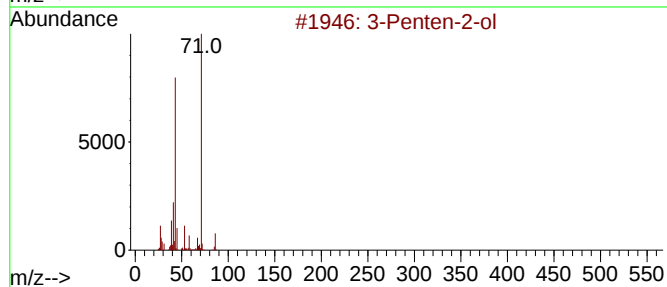
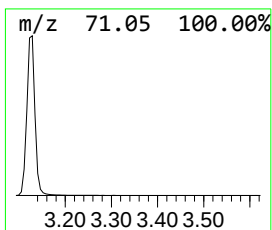
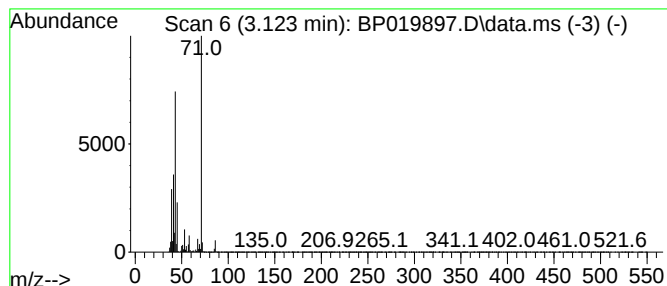
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-ol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.123	110.47 ng	3555670	1,4-Dichlorobenzene-d4	7.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-ol	86	C5H10O	001569-50-2	87
2			3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	64
3			Butanoic acid, anhydride	158	C8H14O3	000106-31-0	64
4			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	50
5			Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	45



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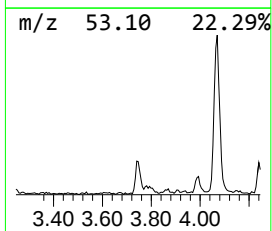
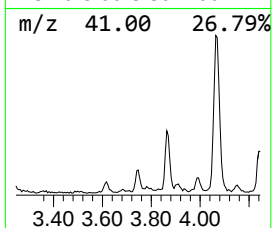
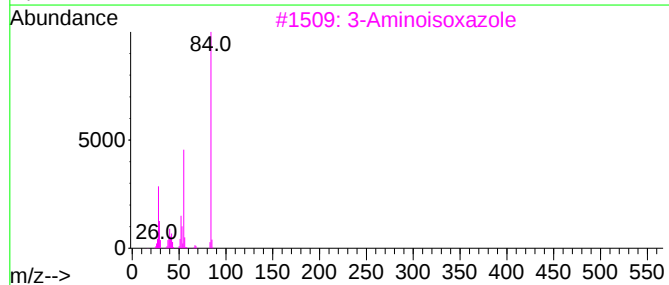
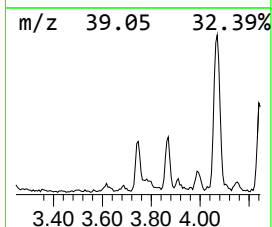
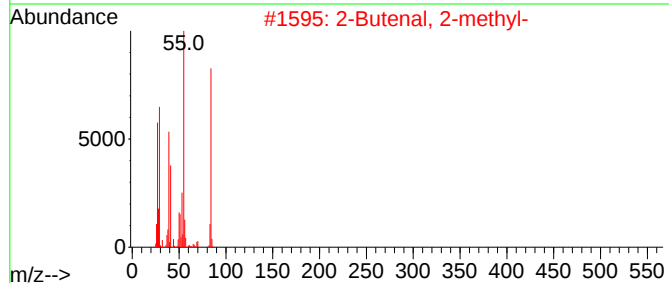
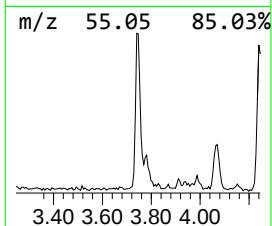
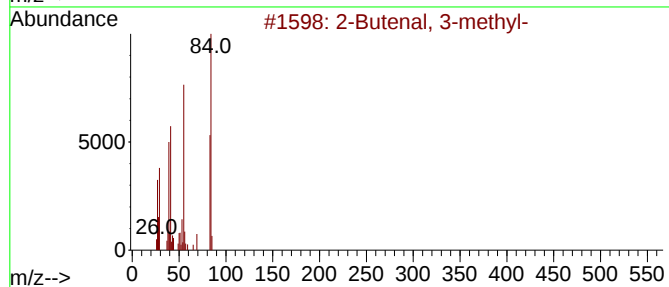
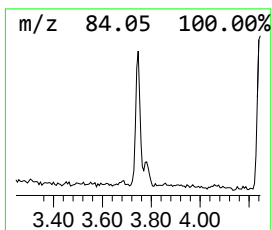
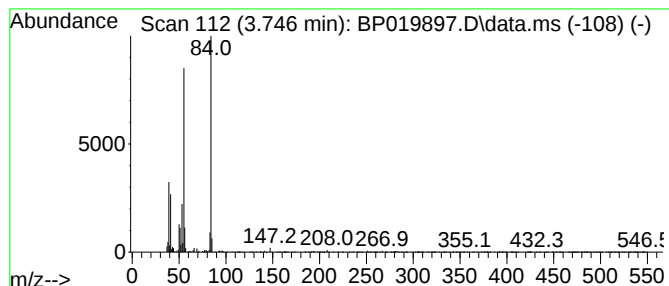
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Butenal, 3-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.746	3.39 ng	109252	1,4-Dichlorobenzene-d4	7.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butenal, 3-methyl-	84	C5H8O	000107-86-8	87
2			2-Butenal, 2-methyl-	84	C5H8O	001115-11-3	86
3			3-Aminoisoxazole	84	C3H4N2O	001750-42-1	72
4			2-Ethylacrolein	84	C5H8O	000922-63-4	72
5			Furan, 2,3-dihydro-4-methyl-	84	C5H8O	034314-83-5	45



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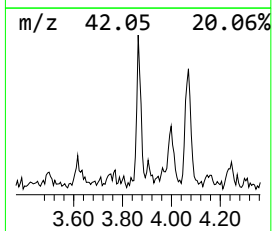
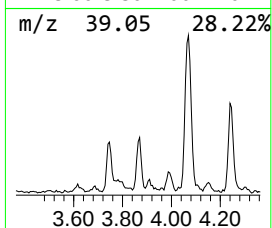
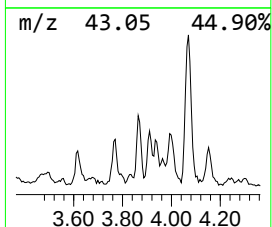
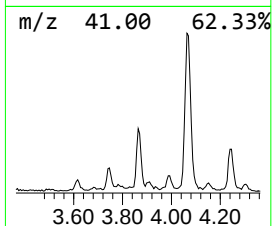
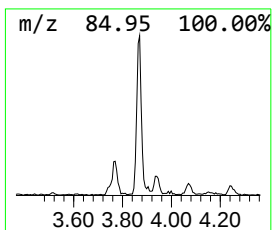
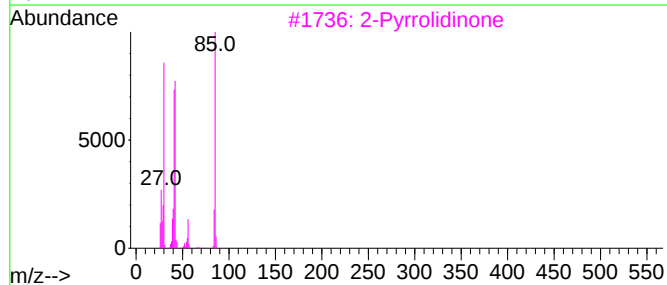
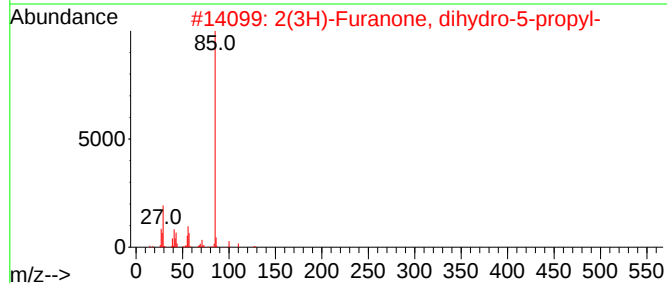
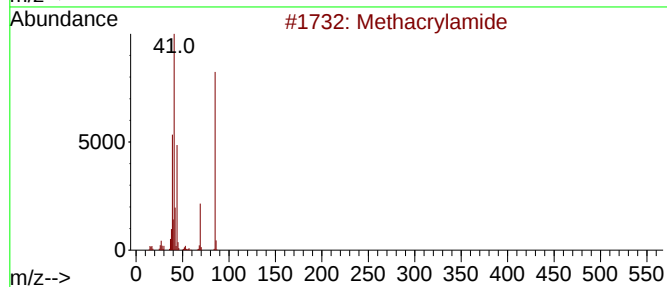
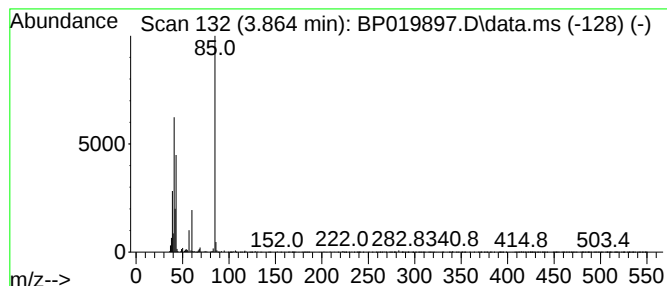
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown3.864 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.864	2.30 ng	73894	1,4-Dichlorobenzene-d4	7.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methacrylamide	85	C4H7NO	000079-39-0	49
2			2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	40
3			2-Pyrrolidinone	85	C4H7NO	000616-45-5	38
4			2H-Pyran, tetrahydro-2-methyl-	100	C6H12O	010141-72-7	38
5			5-Hydroxypentanal	102	C5H10O2	004221-03-8	33



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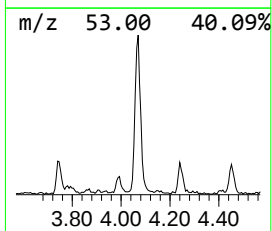
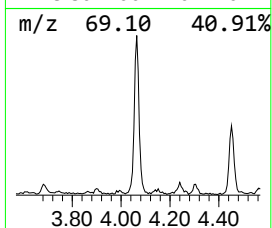
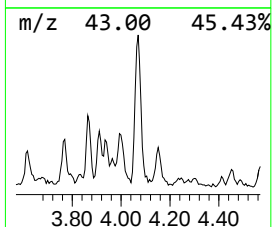
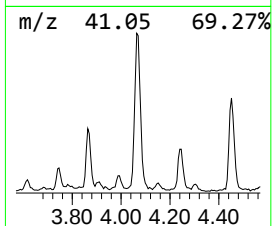
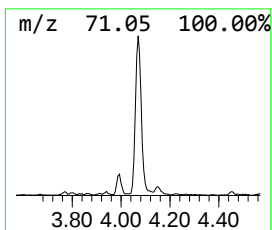
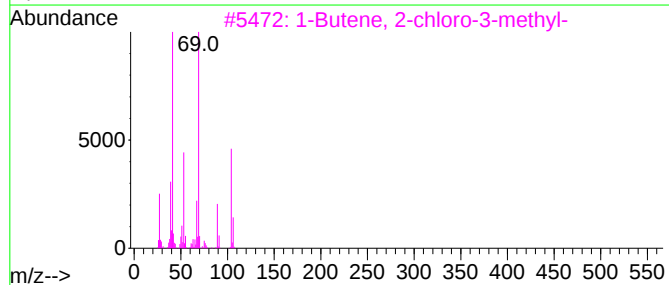
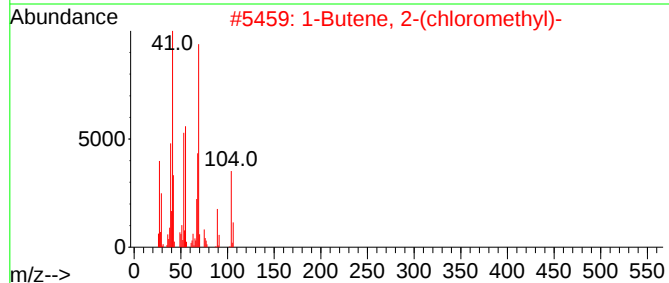
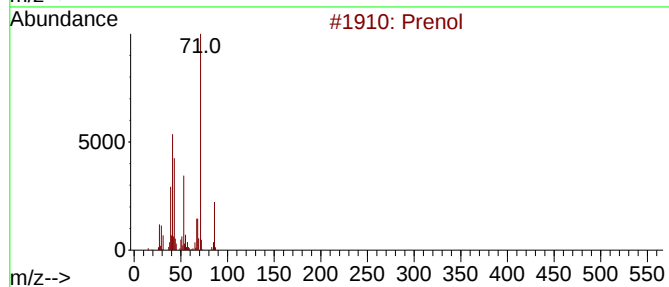
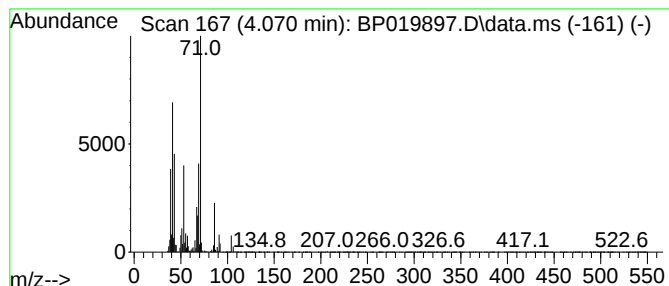
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Prenol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.070	11.58 ng	372848	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Prenol	86	C5H10O	000556-82-1	81
2	1-Butene, 2-(chloromethyl)-	104	C5H9Cl	023010-02-8	38
3	1-Butene, 2-chloro-3-methyl-	104	C5H9Cl	017773-64-7	32
4	2-Buten-1-ol, 2-methyl-	86	C5H10O	004675-87-0	27
5	trans-1-Methoxy-1-butene	86	C5H10O	010034-13-6	18



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20240763-COMPOSITE-39N-N-3-01

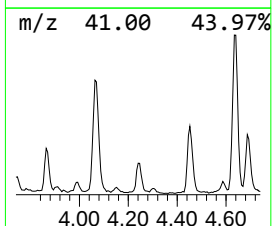
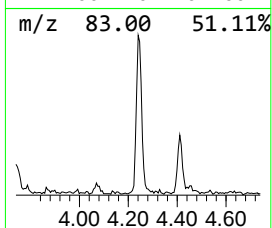
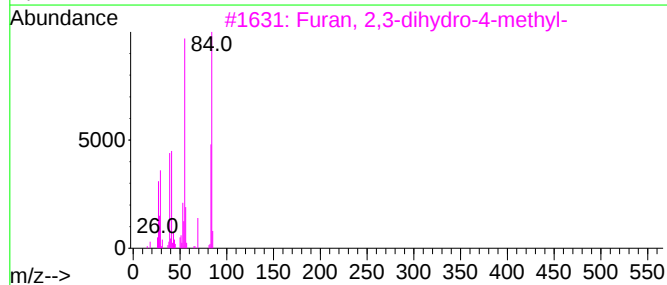
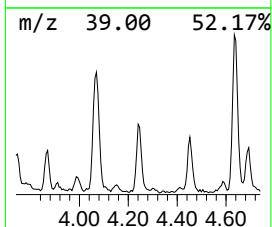
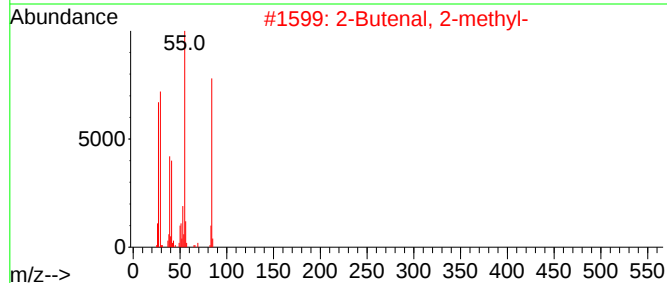
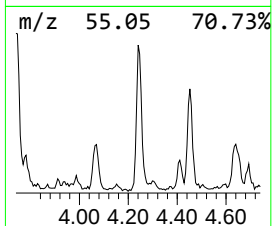
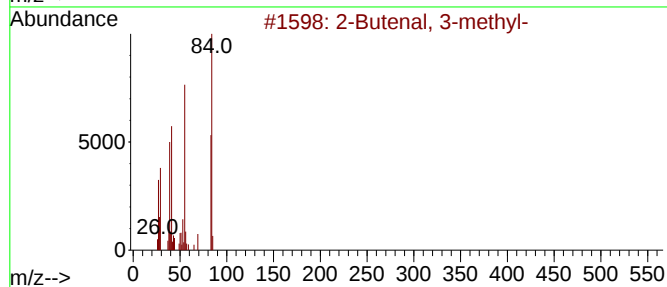
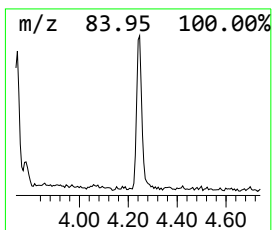
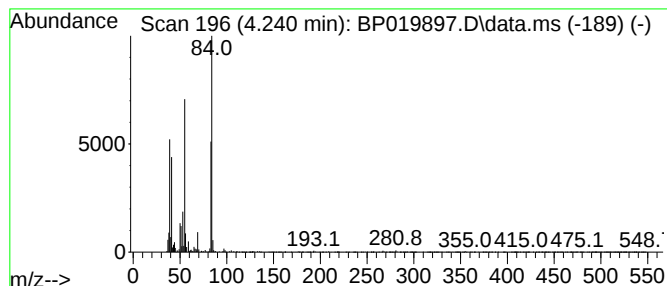
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 2-Butenal, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.240	3.91 ng	125909	1,4-Dichlorobenzene-d4	7.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butenal, 3-methyl-	84	C5H8O	000107-86-8	91
2			2-Butenal, 2-methyl-	84	C5H8O	001115-11-3	64
3			Furan, 2,3-dihydro-4-methyl-	84	C5H8O	034314-83-5	64
4			2-Butenal, 2-methyl-, (E)-	84	C5H8O	000497-03-0	47
5			2-Ethylacrolein	84	C5H8O	000922-63-4	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019897.D
Acq On : 27 Feb 2024 15:27
Operator : MA/JU
Sample : P1523-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240763-COMPOSITE-39N-N-3-01

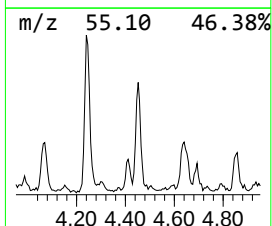
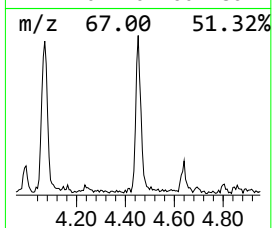
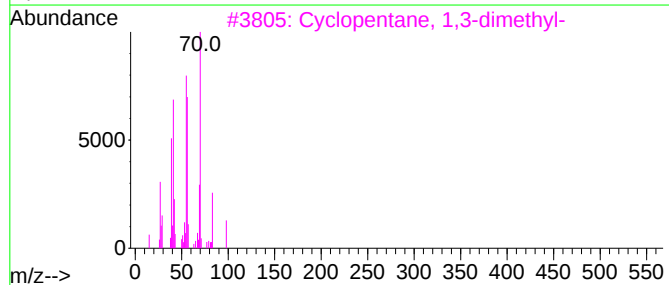
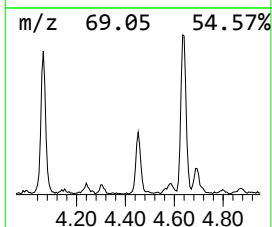
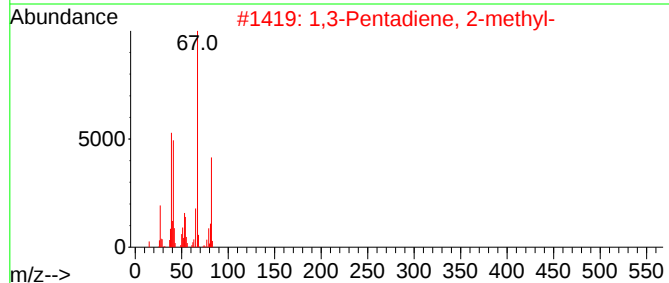
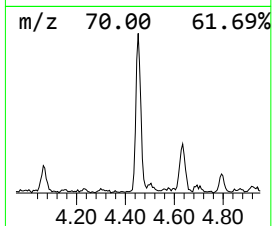
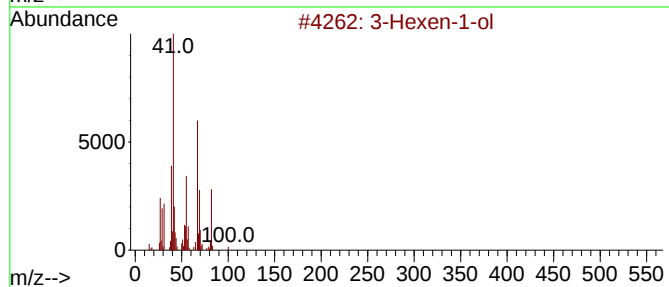
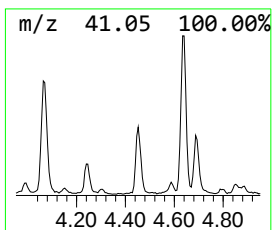
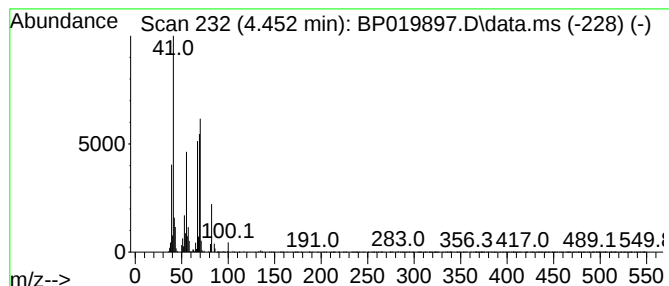
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 3-Hexen-1-ol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.452	3.82 ng	122856	1,4-Dichlorobenzene-d4	7.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-1-ol	100	C6H12O	000544-12-7	53
2			1,3-Pentadiene, 2-methyl-	82	C6H10	001118-58-7	49
3			Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	38
4			(Z)-1,3-Butadien-1-ol	70	C4H6O	070415-58-6	38
5			3-Hexen-1-ol, (Z)-	100	C6H12O	000928-96-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019897.D
Acq On : 27 Feb 2024 15:27
Operator : MA/JU
Sample : P1523-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
20240763-COMPOSITE-39N-N-3-01

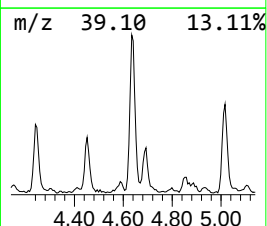
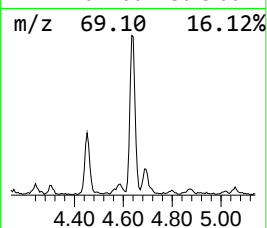
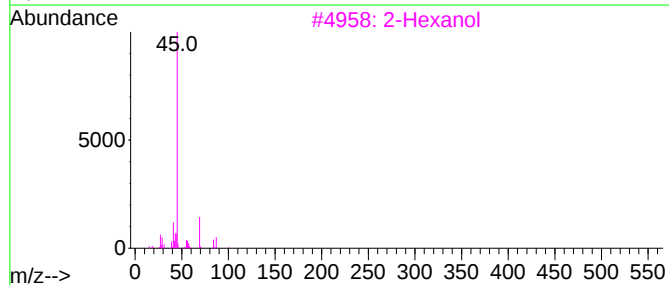
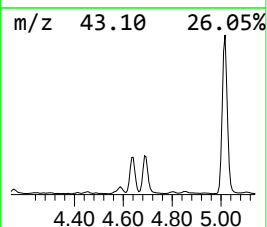
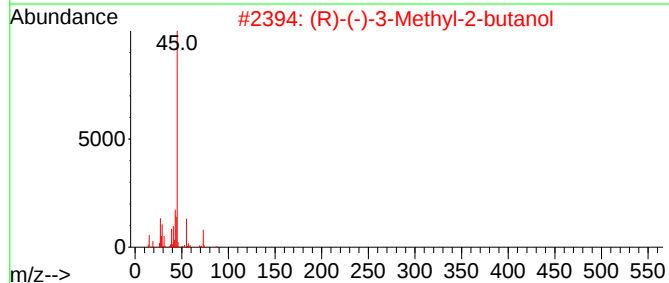
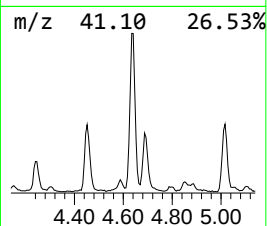
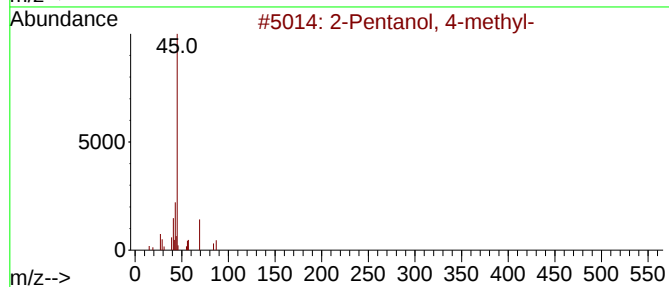
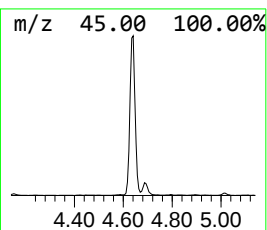
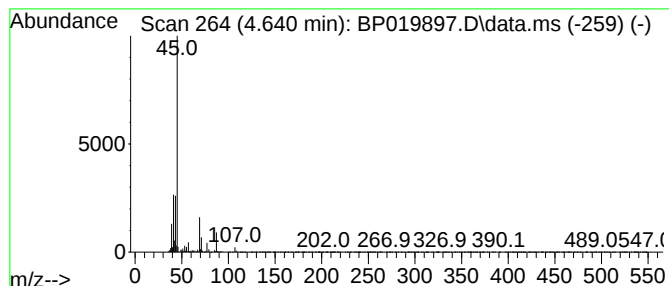
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-Pentanol, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.640	18.99 ng	611093	1,4-Dichlorobenzene-d4	7.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	72
2			(R)-(-)-3-Methyl-2-butanol	88	C5H12O	001572-93-6	42
3			2-Hexanol	102	C6H14O	000626-93-7	40
4			Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	40
5			Propanenitrile, 3-methoxy-	85	C4H7NO	000110-67-8	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019897.D
Acq On : 27 Feb 2024 15:27
Operator : MA/JU
Sample : P1523-01
Misc :
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Instrument :
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20240763-COMPOSITE-39N-N-3-01

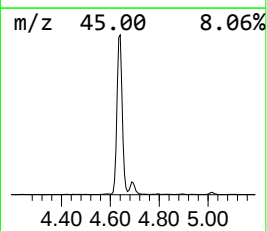
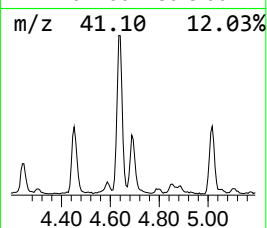
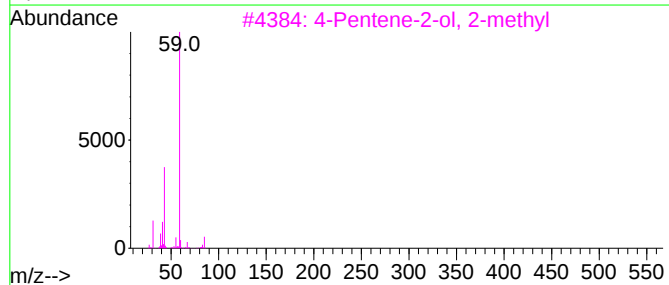
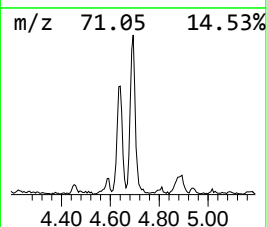
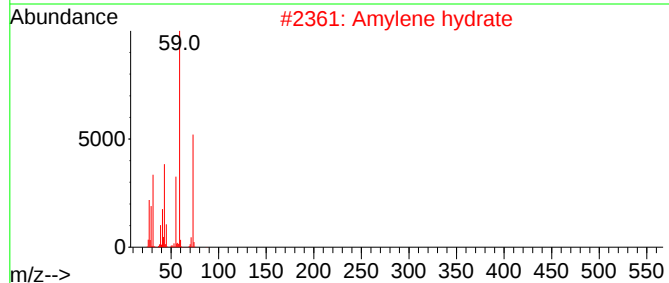
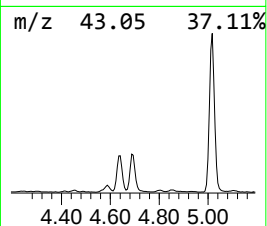
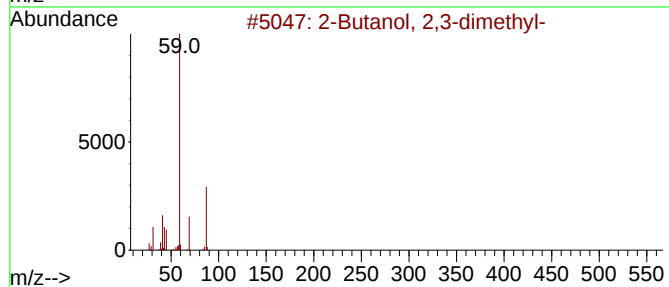
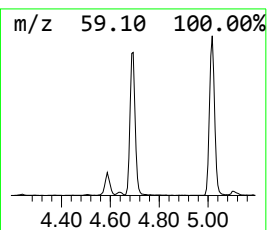
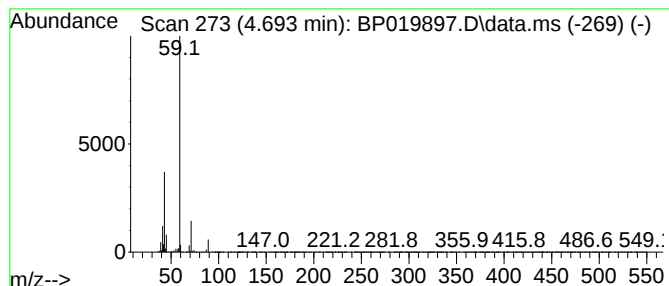
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown4.693 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.693	11.00 ng	354213	1,4-Dichlorobenzene-d4	7.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-			102	C6H14O	000594-60-5	45
2	Amylene hydrate			88	C5H12O	000075-85-4	45
3	4-Pentene-2-ol, 2-methyl			100	C6H12O	000624-97-5	36
4	2-Propanol, 1-methoxy-2-methyl-			104	C5H12O2	003587-64-2	9
5	2,3-Butanediol, 2,3-dimethyl-			118	C6H14O2	000076-09-5	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019897.D
Acq On : 27 Feb 2024 15:27
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Sample : P1523-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

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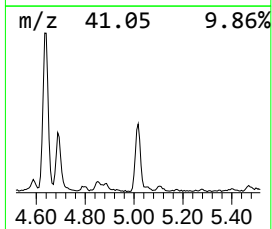
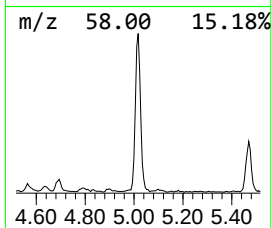
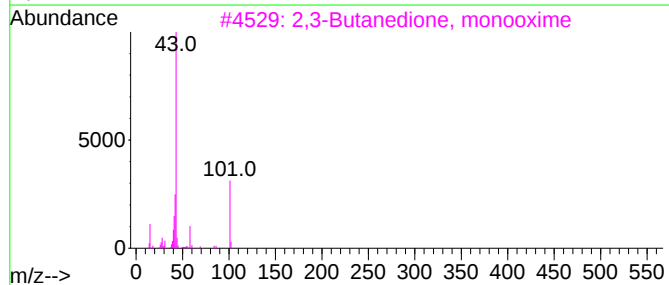
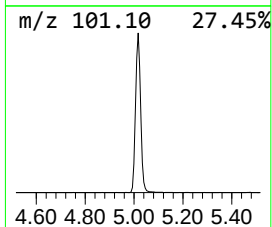
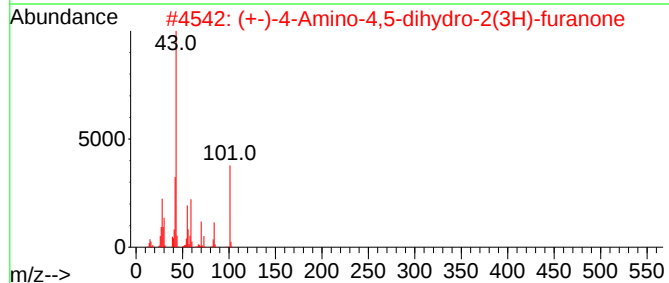
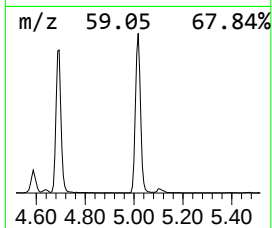
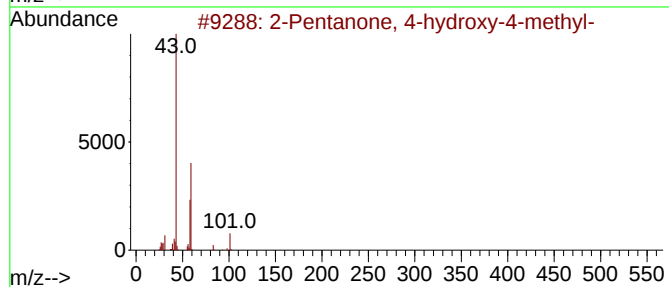
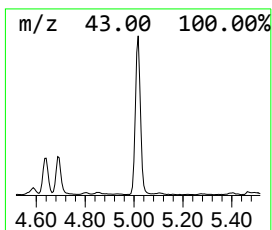
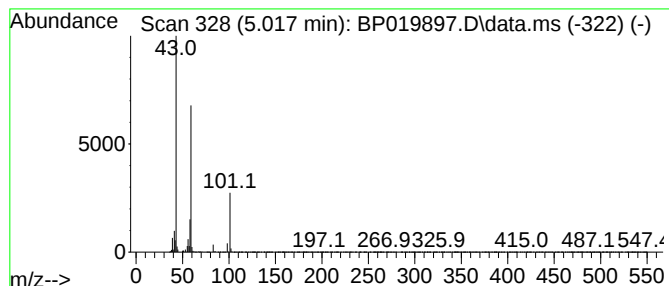
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.017	22.26 ng	716440	1,4-Dichlorobenzene-d4	7.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019897.D
Acq On : 27 Feb 2024 15:27
Operator : MA/JU
Sample : P1523-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

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20240763-COMPOSITE-39N-N-3-01

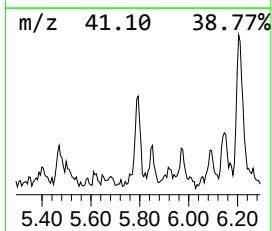
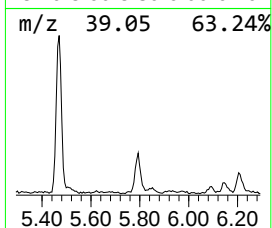
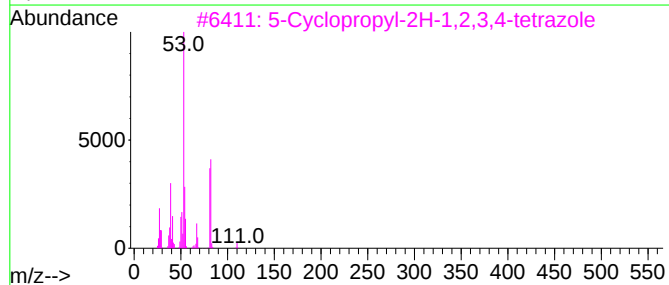
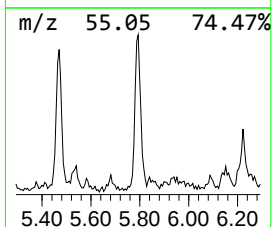
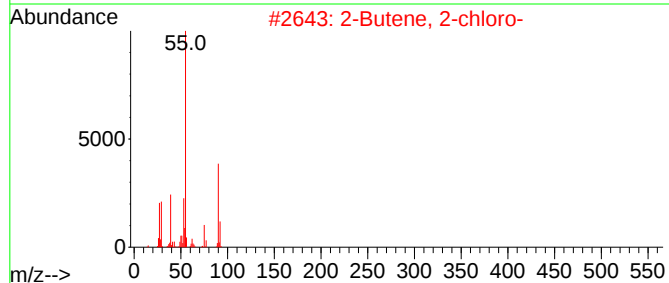
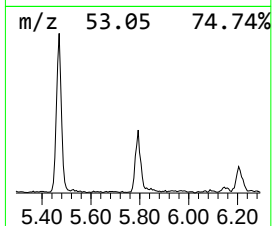
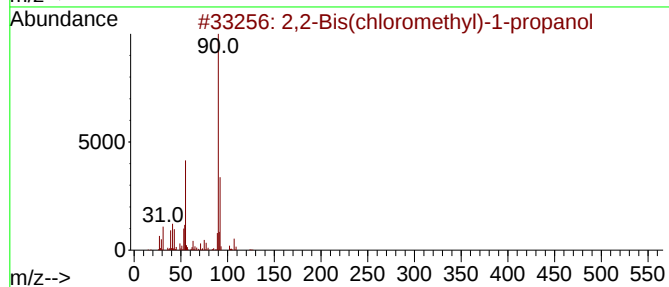
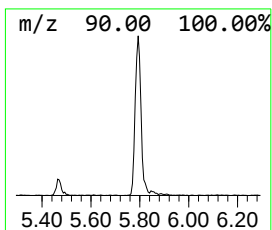
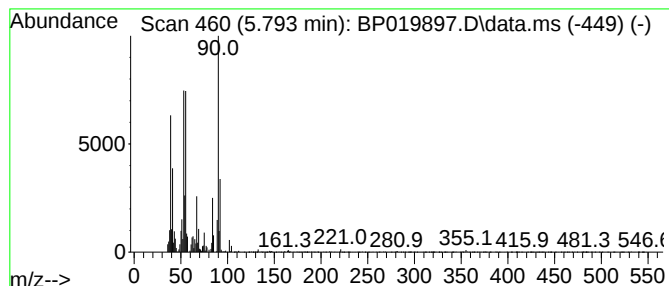
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown5.793 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.793	3.22 ng	103624	1,4-Dichlorobenzene-d4	7.893

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,2-Bis(chloromethyl)-1-propanol	156	C5H10Cl2O	005355-54-4	38
2		2-Butene, 2-chloro-	90	C4H7Cl	004461-41-0	35
3		5-Cyclopropyl-2H-1,2,3,4-tetrazole	110	C4H6N4	027943-07-3	35
4		1-Propene, 1-chloro-2-methyl-	90	C4H7Cl	000513-37-1	32
5		1-Butene, 3-chloro-	90	C4H7Cl	000563-52-0	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019897.D
Acq On : 27 Feb 2024 15:27
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Sample : P1523-01
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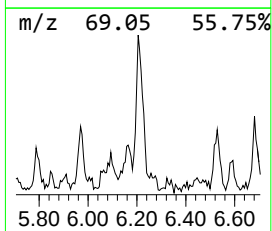
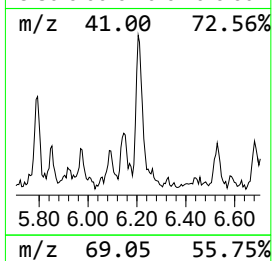
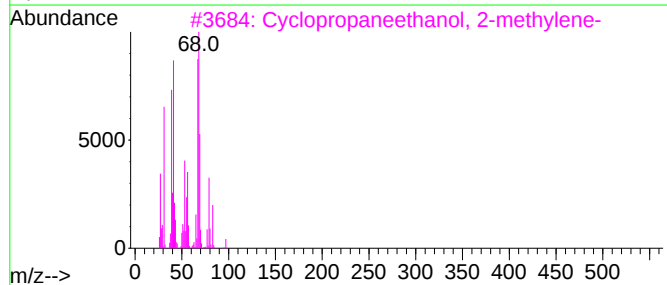
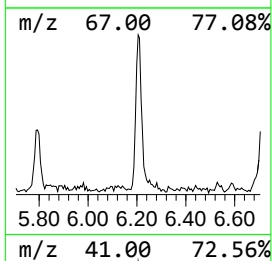
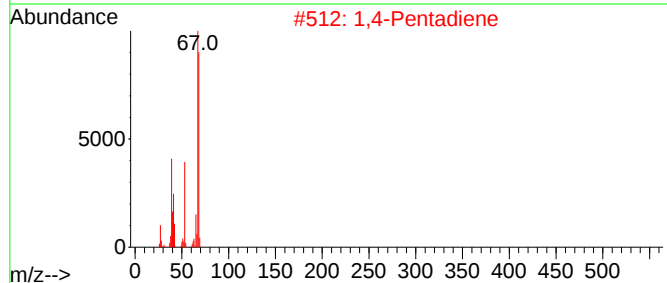
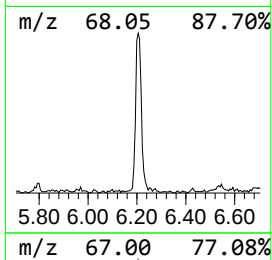
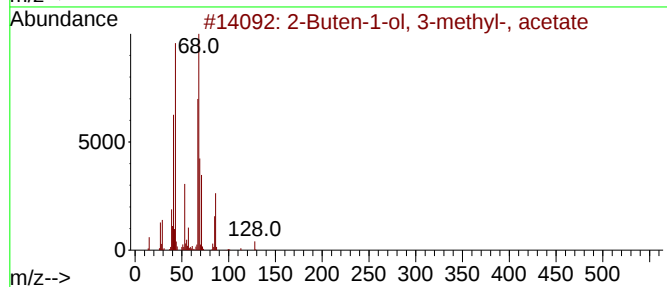
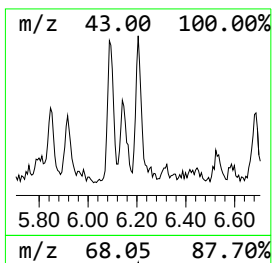
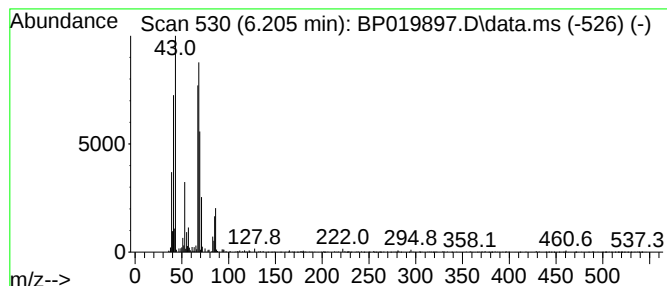
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2-Buten-1-ol, 3-methyl-, ac... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.205	3.56 ng	114616	1,4-Dichlorobenzene-d4	7.893

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Buten-1-ol, 3-methyl-, acetate	128	C7H12O2	001191-16-8	83
2		1,4-Pentadiene	68	C5H8	000591-93-5	64
3		Cyclopropaneethanol, 2-methylene-	98	C6H10O	120477-28-3	59
4		2,5-Dihydro-3-methyl-thiophene 1...	132	C5H8O2S	001193-10-8	59
5		2-Methylbut-2-en-1-yl acetate	128	C7H12O2	033425-30-8	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019897.D
Acq On : 27 Feb 2024 15:27
Operator : MA/JU
Sample : P1523-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240763-COMPOSITE-39N-N-3-01

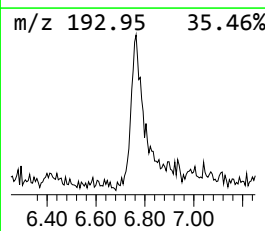
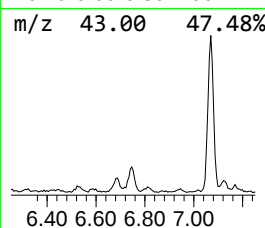
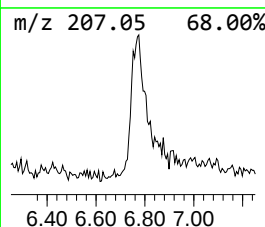
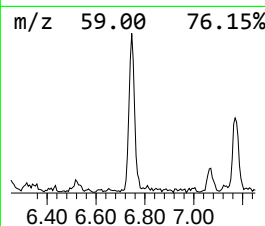
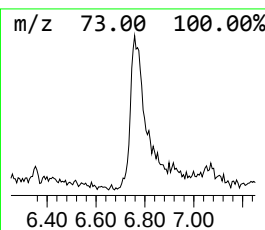
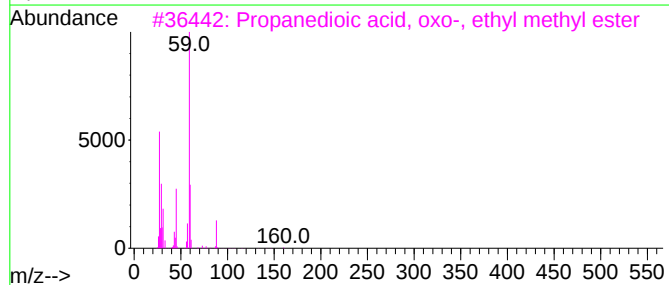
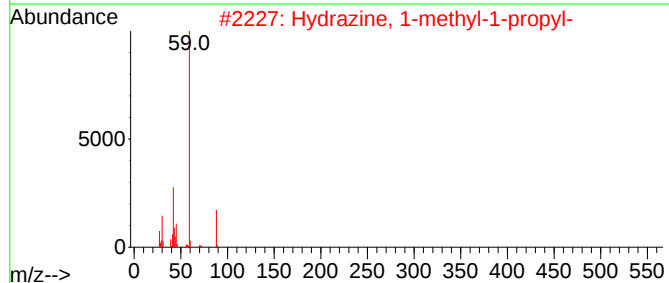
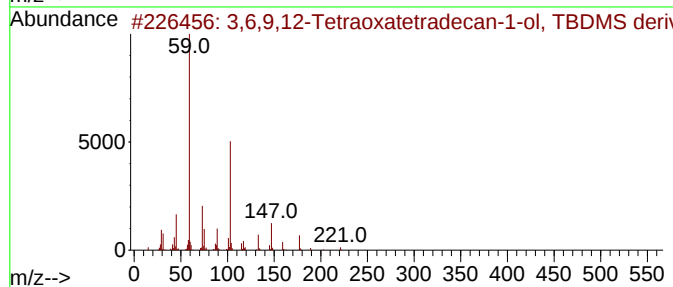
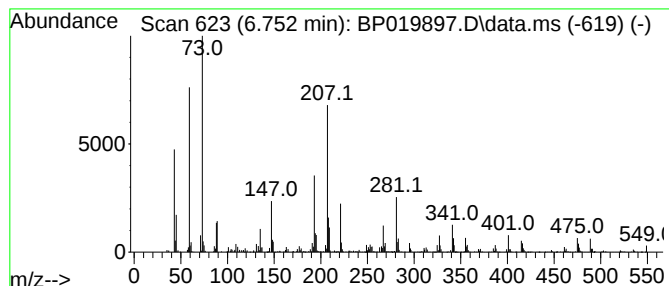
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown6.752 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.752	3.45 ng	111112	1,4-Dichlorobenzene-d4	7.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6,9,12-Tetraoxatetradecan-1-ol...	322	C15H34O5Si	1000352-09-6	35		
2	Hydrazine, 1-methyl-1-propyl-	88	C4H12N2	004986-49-6	35		
3	Propanedioic acid, oxo-, ethyl m...	160	C6H8O5	126542-89-0	35		
4	1,4-Bis(trimethylsilyl)benzene	222	C12H22Si2	013183-70-5	35		
5	Methyl 16-methoxyheptadecanoate	314	C19H38O3	1000110-18-2	35		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019897.D
Acq On : 27 Feb 2024 15:27
Operator : MA/JU
Sample : P1523-01
Misc :
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ClientSampleId :
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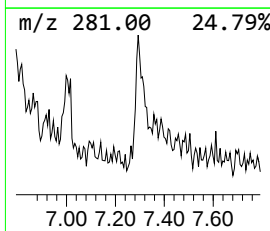
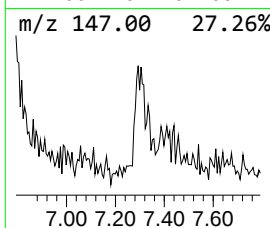
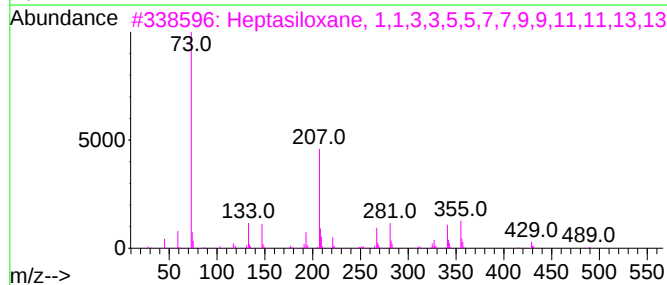
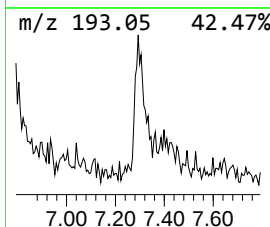
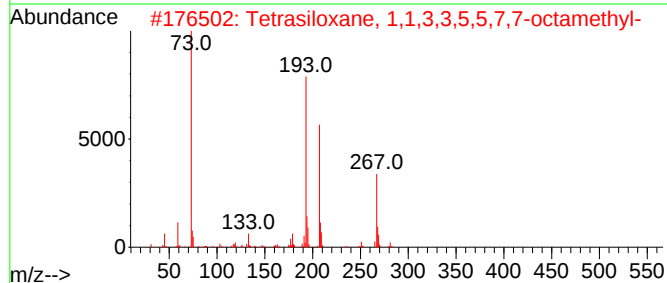
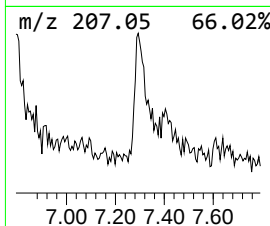
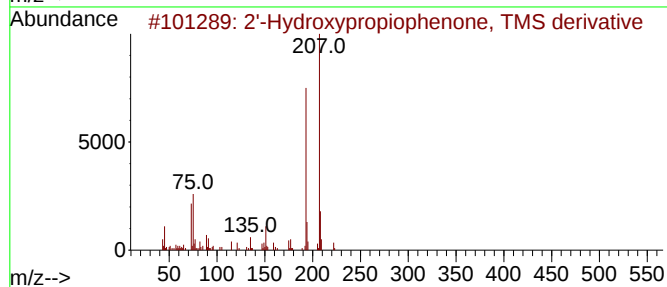
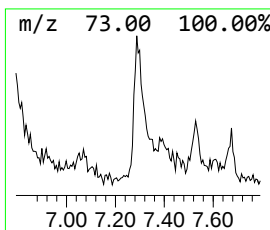
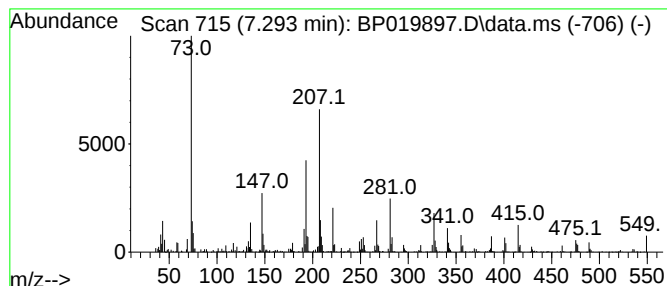
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2'-Hydroxypropiophenone, TM... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.293	2.53 ng	81366	1,4-Dichlorobenzene-d4	7.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2'-Hydroxypropiophenone, TMS der...	222	C12H18O2Si	033342-87-9	53
2			Tetrasiloxane, 1,1,3,3,5,5,7,7-o...	282	C8H26O3Si4	001000-05-1	35
3			Heptasiloxane, 1,1,3,3,5,5,7,7,9...	504	C14H44O6Si7	019095-23-9	22
4			Stannane, tributylethyl-	320	C14H32Sn	019411-60-0	20
5			Cyclohexane-1,3-dione, 2-allylam...	207	C12H17NO2	104926-37-6	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019897.D
Acq On : 27 Feb 2024 15:27
Operator : MA/JU
Sample : P1523-01
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Instrument :
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20240763-COMPOSITE-39N-N-3-01

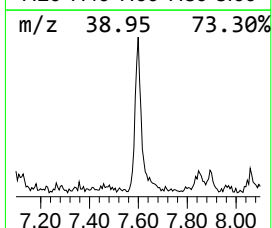
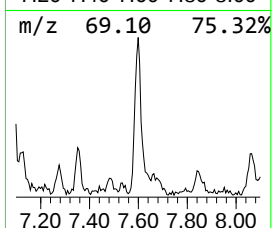
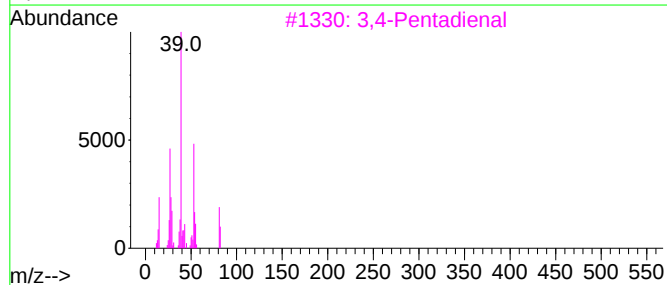
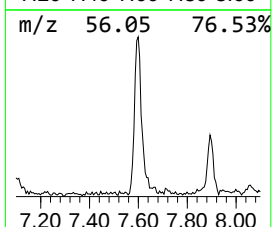
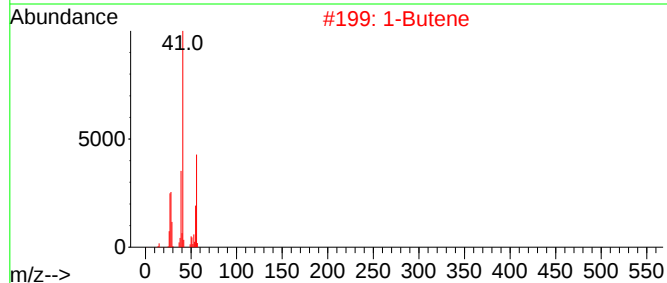
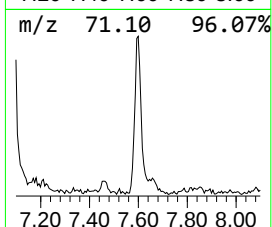
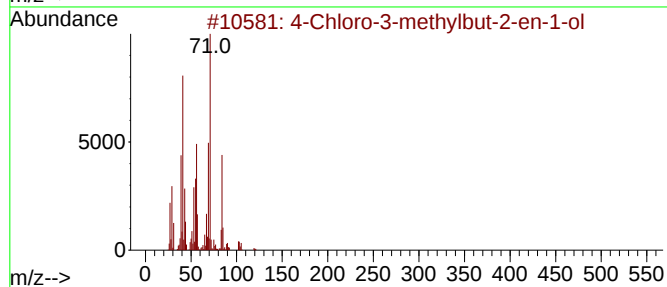
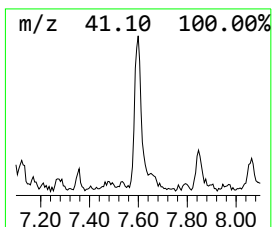
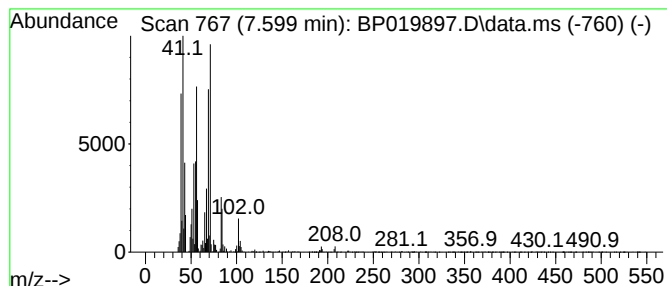
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 4-Chloro-3-methylbut-2-en-1-ol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.599	4.59 ng	147805	1,4-Dichlorobenzene-d4	7.893

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Chloro-3-methylbut-2-en-1-ol	120	C5H9ClO	053170-97-1	78
2		1-Butene	56	C4H8	000106-98-9	38
3		3,4-Pentadienal	82	C5H6O	004009-55-6	38
4		2-Butene, (Z)-	56	C4H8	000590-18-1	38
5		1-Propene, 2-methyl-	56	C4H8	000115-11-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019897.D
Acq On : 27 Feb 2024 15:27
Operator : MA/JU
Sample : P1523-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

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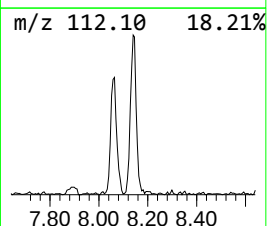
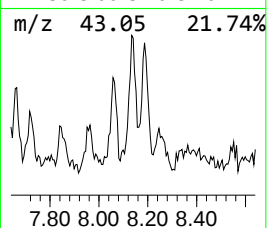
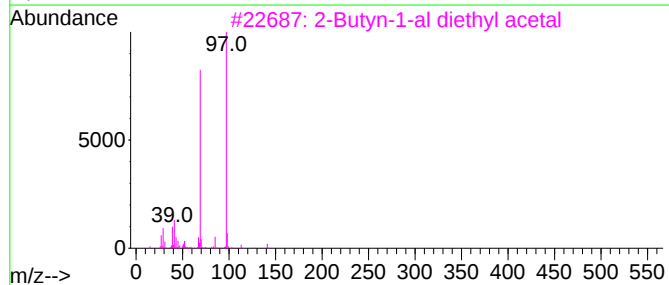
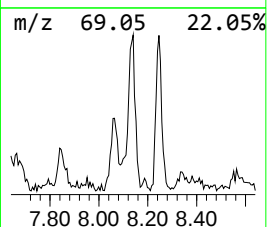
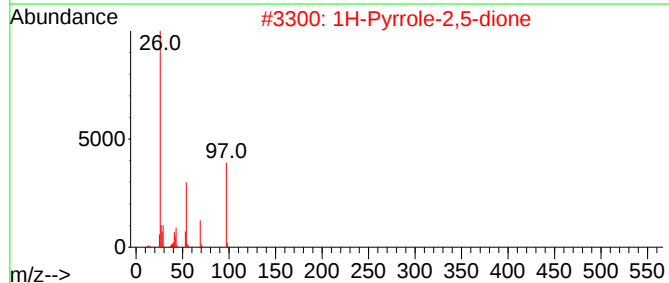
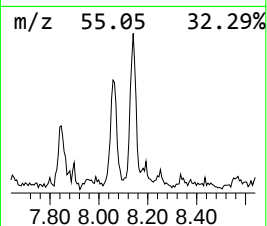
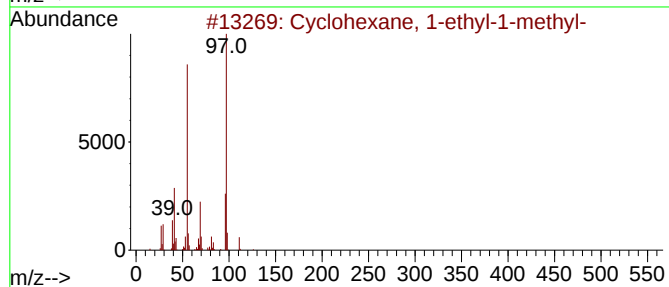
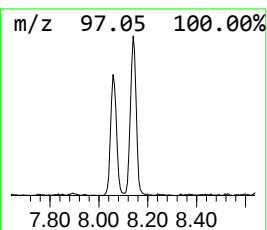
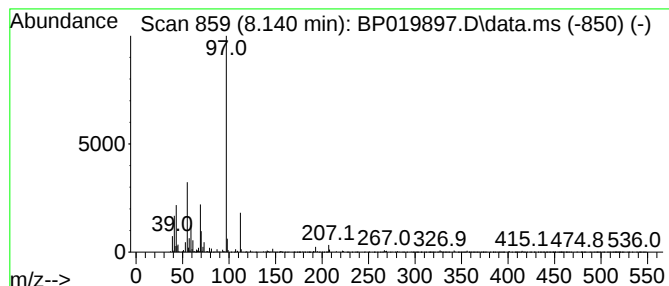
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown8.140 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.140	3.37 ng	108407	1,4-Dichlorobenzene-d4	7.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	36
2			1H-Pyrrole-2,5-dione	97	C4H3NO2	000541-59-3	33
3			2-Butyn-1-al diethyl acetal	142	C8H14O2	002806-97-5	33
4			2-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-40-4	30
5			Didecyl methylphosphonate	376	C21H45O3P	059651-63-7	28



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019897.D
Acq On : 27 Feb 2024 15:27
Operator : MA/JU
Sample : P1523-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
20240763-COMPOSITE-39N-N-3-01

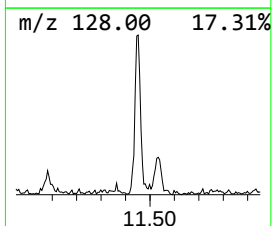
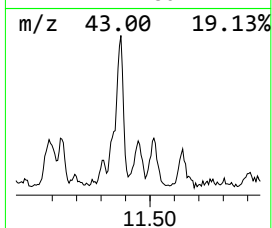
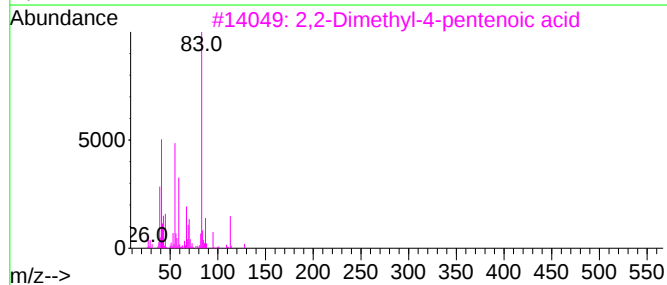
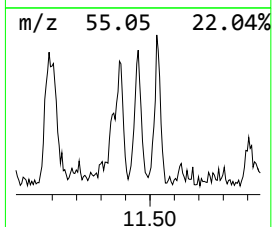
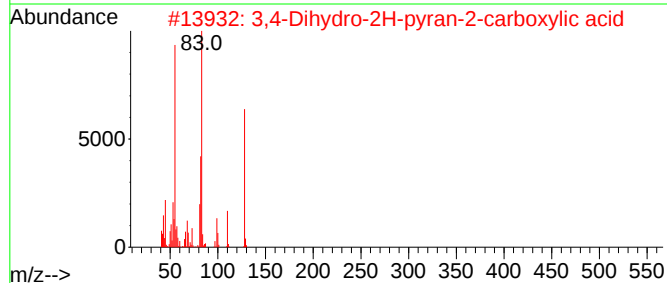
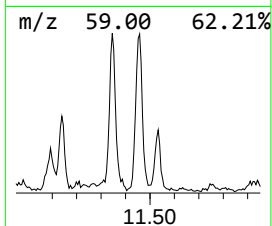
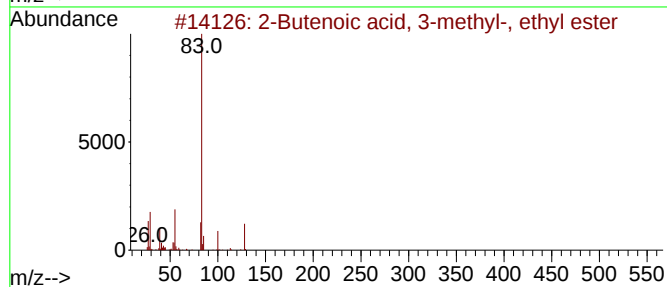
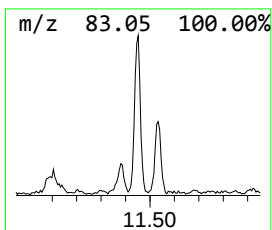
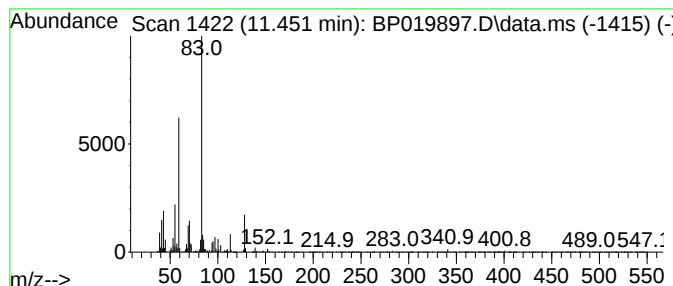
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown11.451 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.451	2.58 ng	118773	Naphthalene-d8	10.699

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butenoic acid, 3-methyl-, ethy...	128	C7H12O2	000638-10-8	47
2			3,4-Dihydro-2H-pyran-2-carboxyli...	128	C6H8O3	1010132-10-4	47
3			2,2-Dimethyl-4-pentenoic acid	128	C7H12O2	016386-93-9	47
4			3-Methyl-2-butenic acid, undec-...	252	C16H28O2	1000299-31-6	43
5			(1,2-Dichlorotrifluoroethyl)cycl...	234	C8H11Cl2F3	219904-98-0	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
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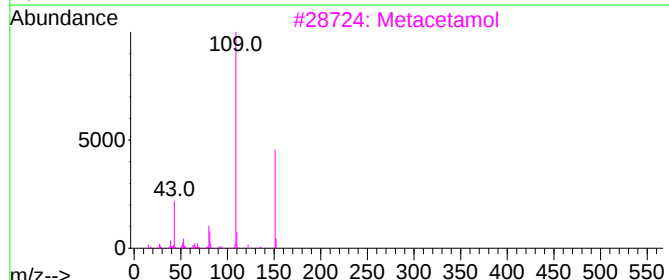
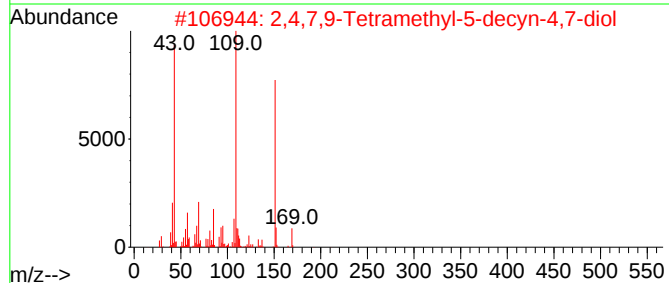
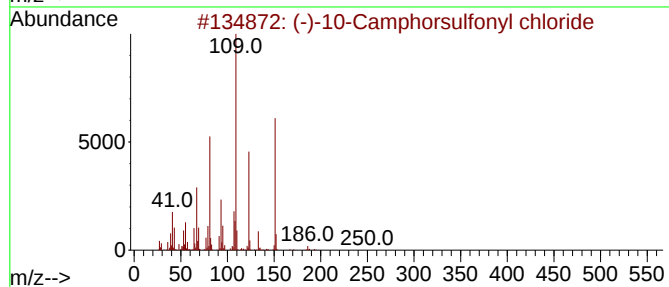
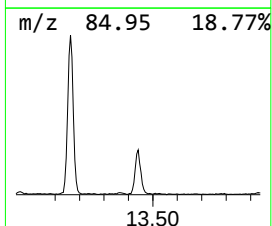
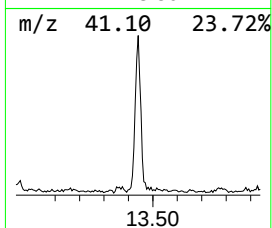
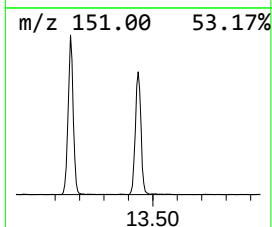
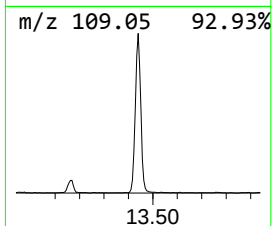
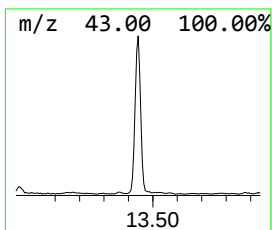
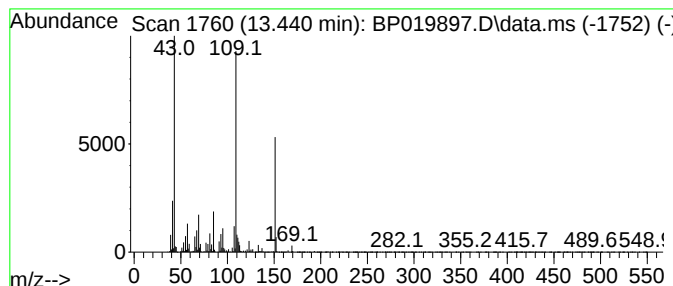
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 (-)-10-Camphorsulfonyl chlo... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD			R.T.
13.440	7.90 ng	511114	Acenaphthene-d10			14.540
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	(-)-10-Camphorsulfonyl chloride		250	C10H15ClO3S	039262-22-1	72
2	2,4,7,9-Tetramethyl-5-decyn-4,7-...		226	C14H26O2	000126-86-3	68
3	Metacetamol		151	C8H9NO2	000621-42-1	64
4	Pyridine, 2-butyl-, 1-oxide		151	C9H13NO	031396-32-4	59
5	Acetaminophen		151	C8H9NO2	000103-90-2	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019897.D
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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240763-COMPOSITE-39N-N-3-01

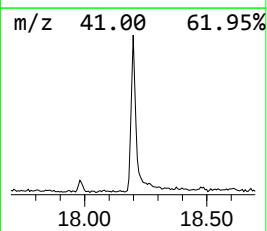
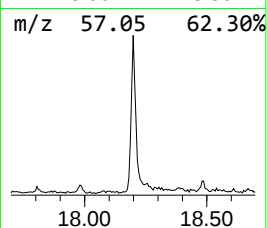
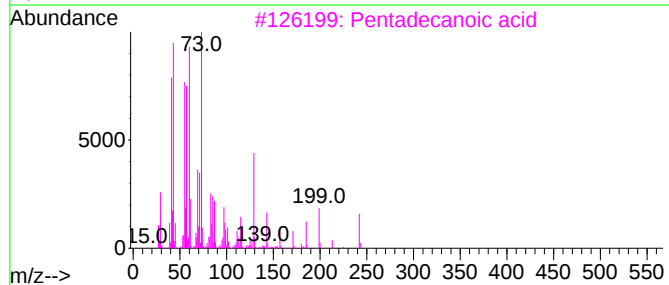
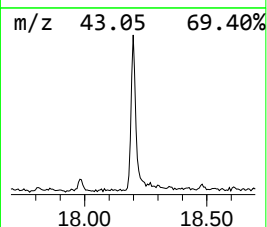
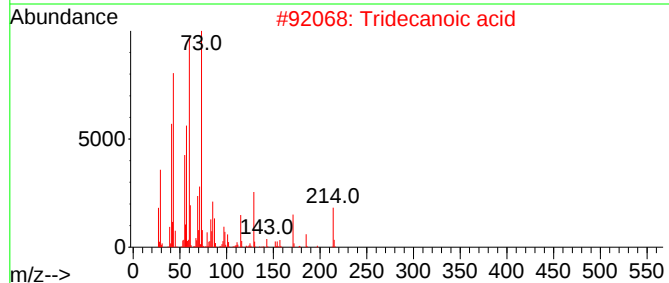
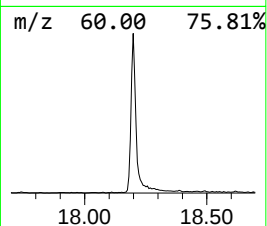
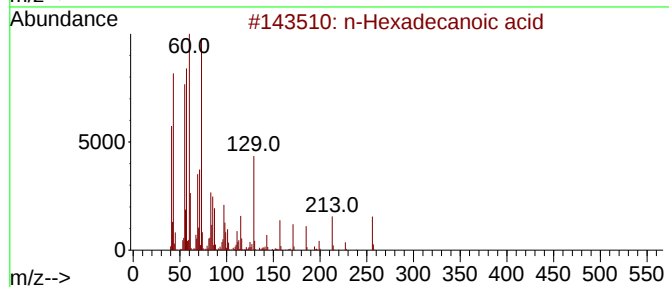
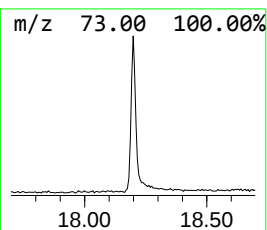
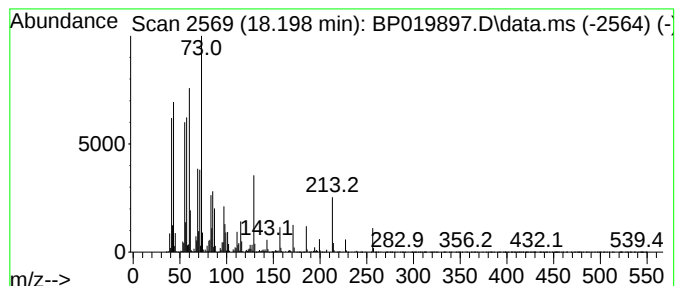
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.198	7.67 ng	603311	Phenanthrene-d10	17.298

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Octadecanoic acid	284	C18H36O2	000057-11-4	68
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019897.D
Acq On : 27 Feb 2024 15:27
Operator : MA/JU
Sample : P1523-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240763-COMPOSITE-39N-N-3-01

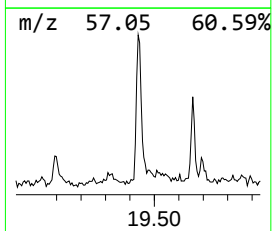
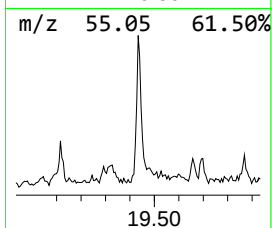
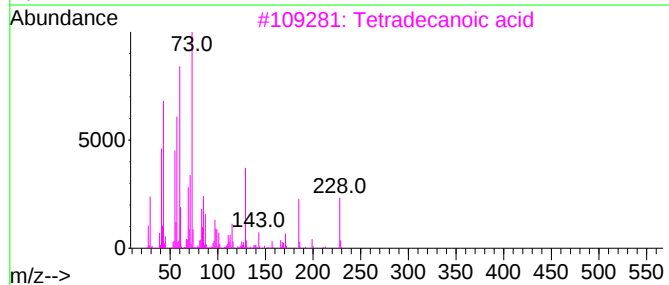
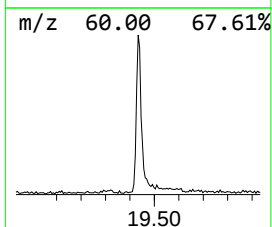
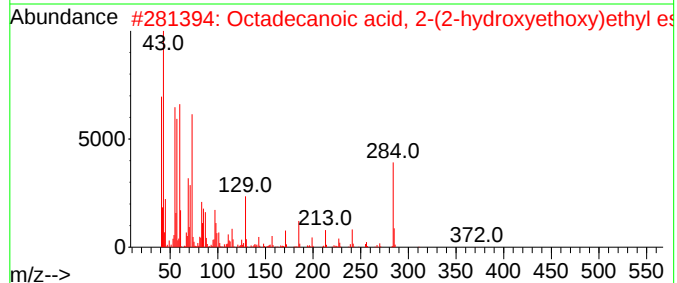
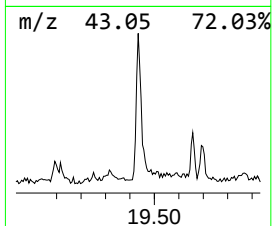
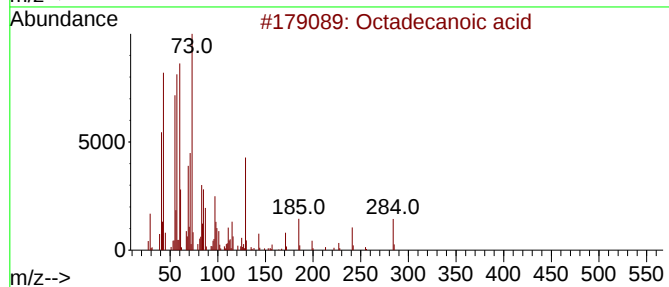
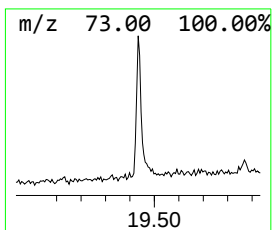
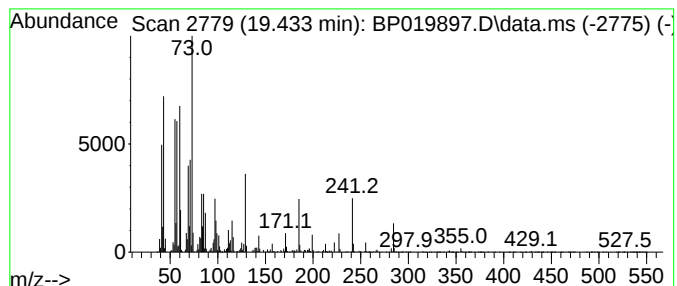
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.433	3.85 ng	261894	Chrysene-d12	21.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	76
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	53
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019897.D
Acq On : 27 Feb 2024 15:27
Operator : MA/JU
Sample : P1523-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240763-COMPOSITE-39N-N-3-01

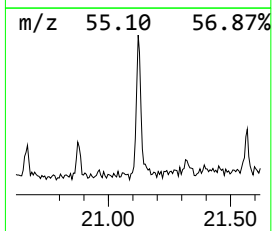
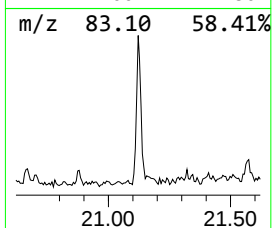
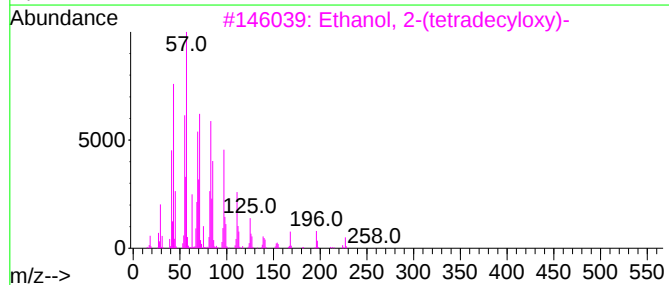
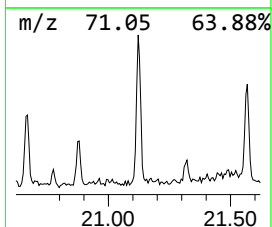
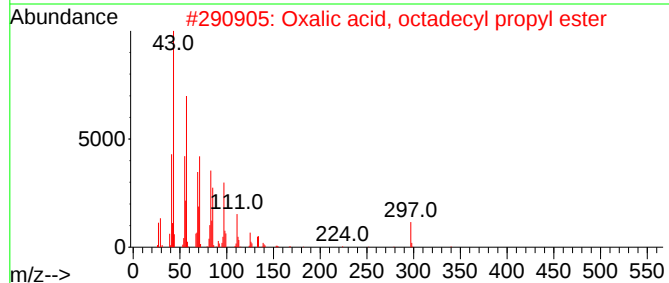
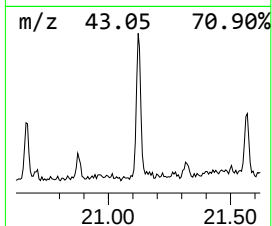
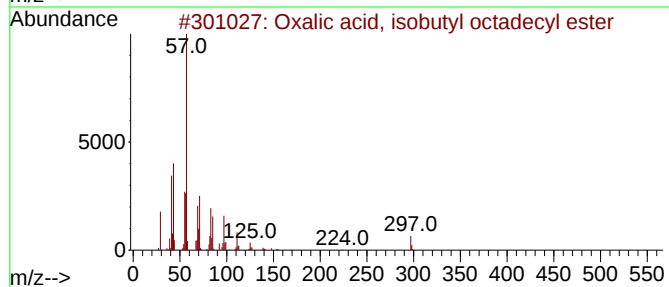
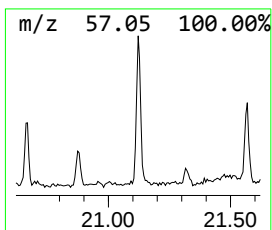
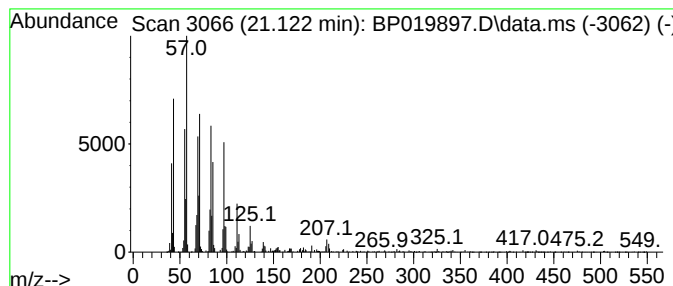
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Oxalic acid, isobutyl octadecyl... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.122	3.35 ng	228021	Chrysene-d12	21.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	91
2			Oxalic acid, octadecyl propyl ester	384	C23H44O4	1000309-27-0	91
3			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
4			Tridecane	184	C13H28	000629-50-5	83
5			Oxalic acid, hexadecyl propyl ester	356	C21H40O4	1000309-26-9	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022724\
Data File : BP019897.D
Acq On : 27 Feb 2024 15:27
Operator : MA/JU
Sample : P1523-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20240763-COMPOSITE-39N-N-3-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP022624.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
3-Penten-2-ol	3.123	110.5	ng	3555670	1	7.893	643761	20.0
2-Butenal, 3-me...	3.746	3.4	ng	109252	1	7.893	643761	20.0
unknown3.864	3.864	2.3	ng	73894	1	7.893	643761	20.0
Prenol	4.070	11.6	ng	372848	1	7.893	643761	20.0
2-Butenal, 2-me...	4.240	3.9	ng	125909	1	7.893	643761	20.0
3-Hexen-1-ol	4.452	3.8	ng	122856	1	7.893	643761	20.0
2-Pentanol, 4-m...	4.640	19.0	ng	611093	1	7.893	643761	20.0
unknown4.693	4.693	11.0	ng	354213	1	7.893	643761	20.0
2-Pentanone, 4-...	5.017	22.3	ng	716440	1	7.893	643761	20.0
unknown5.793	5.793	3.2	ng	103624	1	7.893	643761	20.0
2-Buten-1-ol, 3...	6.205	3.6	ng	114616	1	7.893	643761	20.0
unknown6.752	6.752	3.5	ng	111112	1	7.893	643761	20.0
2'-Hydroxypropi...	7.293	2.5	ng	81366	1	7.893	643761	20.0
4-Chloro-3-meth...	7.599	4.6	ng	147805	1	7.893	643761	20.0
unknown8.140	8.140	3.4	ng	108407	1	7.893	643761	20.0
unknown11.451	11.451	2.6	ng	118773	2	10.699	919056	20.0
(-)-10-Camphors...	13.440	7.9	ng	511114	3	14.540	1293680	20.0
n-Hexadecanoic ...	18.198	7.7	ng	603311	4	17.298	1572940	20.0
Octadecanoic acid	19.433	3.9	ng	261894	5	21.398	1361680	20.0
Oxalic acid, is...	21.122	3.4	ng	228021	5	21.398	1361680	20.0