

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110822\
 Data File : BF131061.D
 Acq On : 08 Nov 2022 12:02
 Operator : CG\JU
 Sample : N5460-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SH-1

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-BF110722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131061.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	10	18	24	rBV	497975	627916	26.69%	3.907%
2	2.299	32	36	40	rBV	29060	38201	1.62%	0.238%
3	4.504	407	411	416	rBV	147871	160121	6.81%	0.996%
4	5.128	511	517	529	rVB	845289	1124511	47.80%	6.998%
5	5.522	579	584	587	rBV	2492524	2352574	100.00%	14.640%
6	5.916	647	651	654	rBV	61284	52112	2.22%	0.324%
7	6.528	749	755	758	rBV	1627429	1681765	71.49%	10.465%
8	6.898	814	818	821	rBV	485791	364073	15.48%	2.266%
9	7.463	909	914	917	rBV	1160540	1140484	48.48%	7.097%
10	8.181	1032	1036	1040	rBV	736001	673386	28.62%	4.190%
11	9.263	1215	1220	1223	rBV	2508580	2224112	94.54%	13.840%
12	9.945	1331	1336	1339	rBV	727093	629805	26.77%	3.919%
13	10.739	1466	1471	1474	rBV	1452552	1400565	59.53%	8.715%
14	11.439	1586	1590	1593	rBV	668725	603385	25.65%	3.755%
15	11.821	1650	1655	1658	rBV	54206	40688	1.73%	0.253%
16	13.027	1856	1860	1863	rBV	2119224	1827921	77.70%	11.375%
17	13.592	1950	1956	1958	rBV2	23153	24097	1.02%	0.150%
18	13.986	2017	2023	2036	rBV6	42323	147920	6.29%	0.920%
19	14.086	2036	2040	2043	rVB	513786	442548	18.81%	2.754%
20	14.545	2115	2118	2122	rVB	31616	29702	1.26%	0.185%
21	14.857	2167	2171	2175	rBV	21541	25733	1.09%	0.160%
22	15.204	2227	2230	2235	rVB	23778	27391	1.16%	0.170%
23	15.586	2289	2295	2302	rBV	325957	405838	17.25%	2.525%
24	16.580	2460	2464	2476	rVB10	9998	25086	1.07%	0.156%

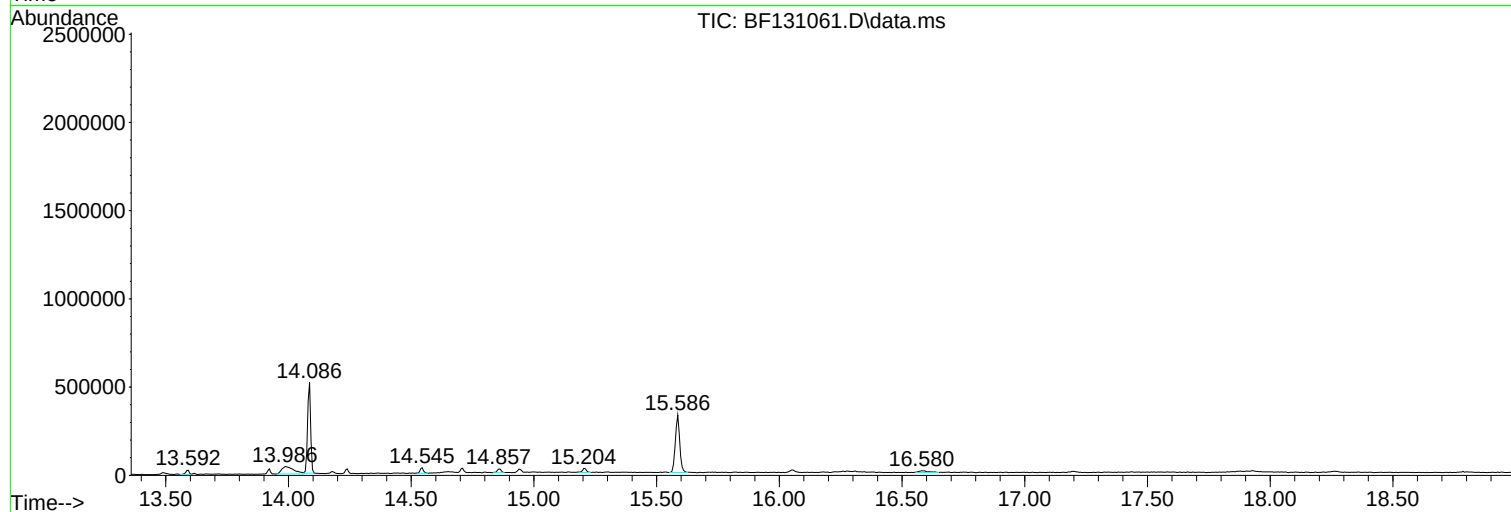
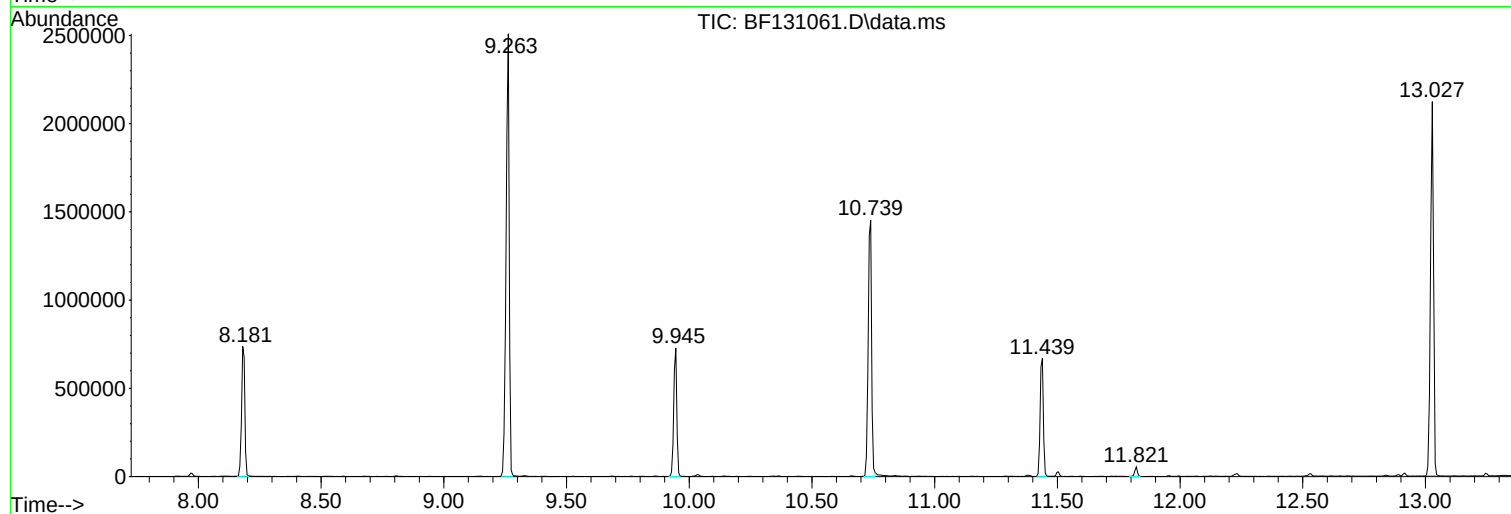
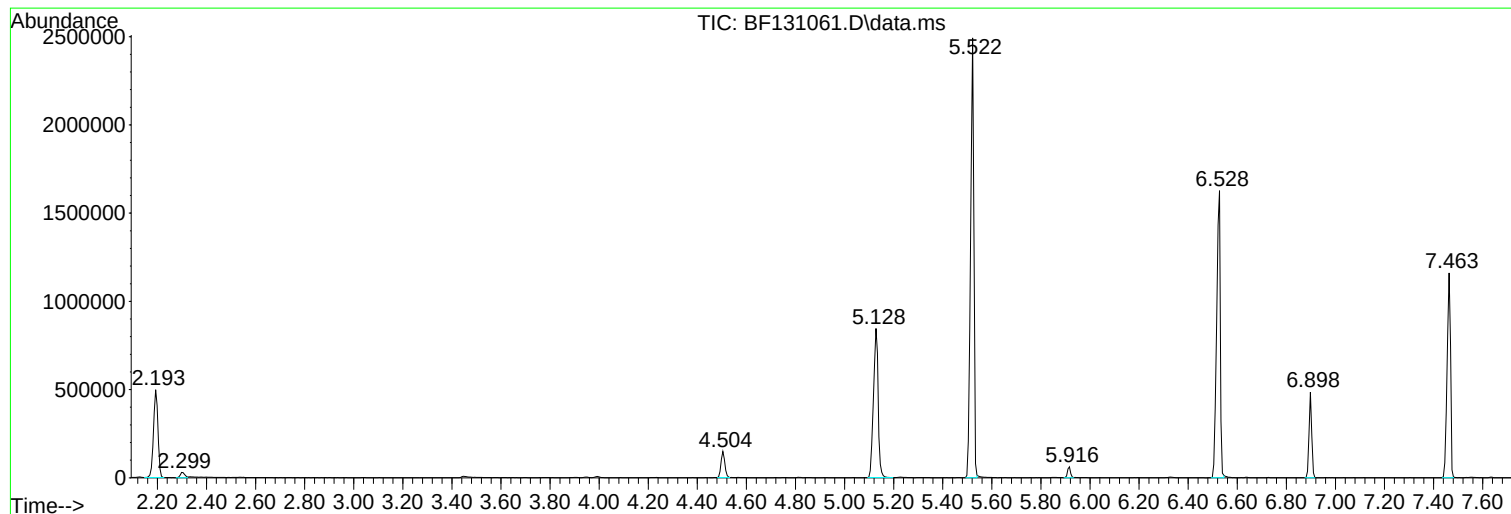
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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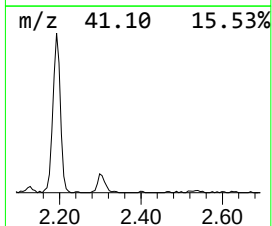
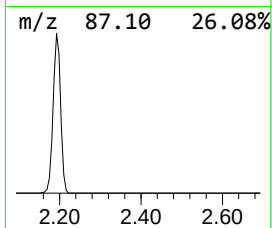
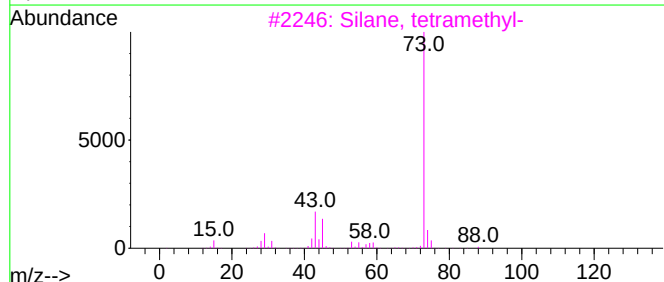
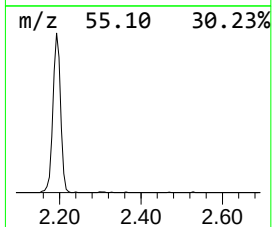
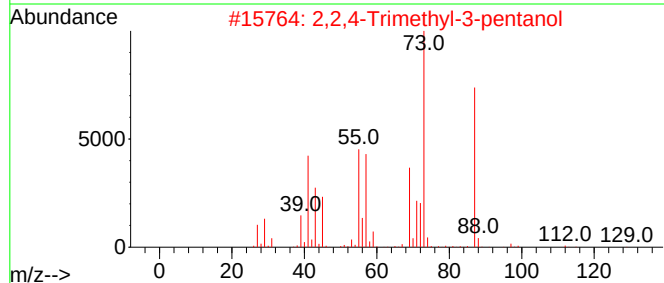
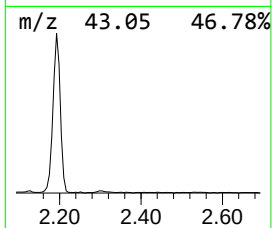
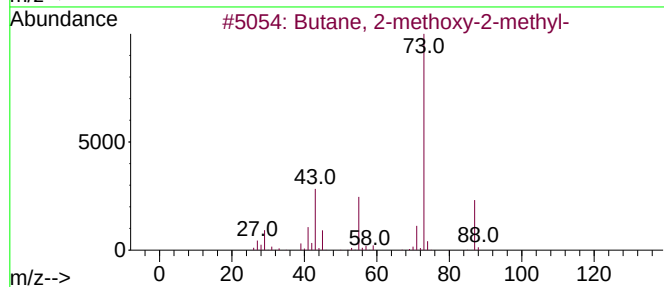
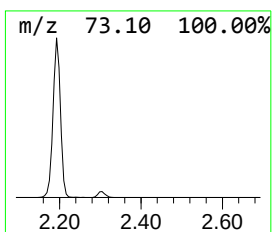
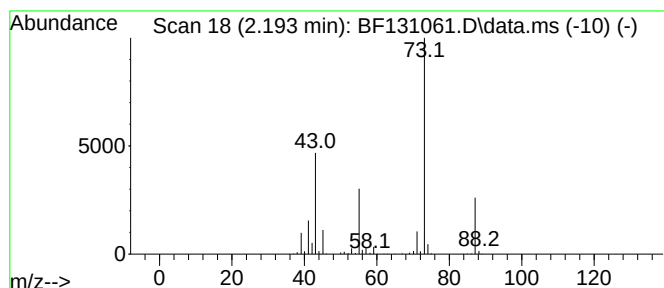
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	34.49 ng	627916	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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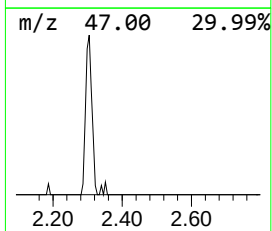
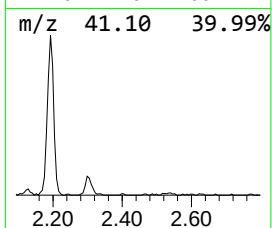
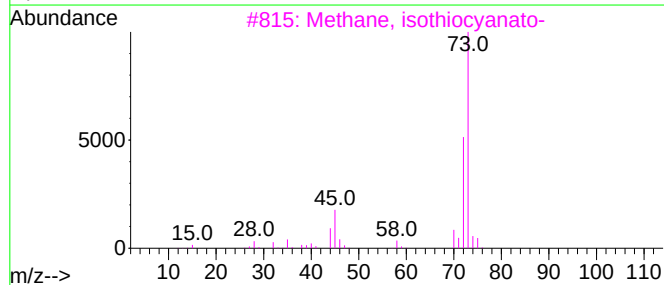
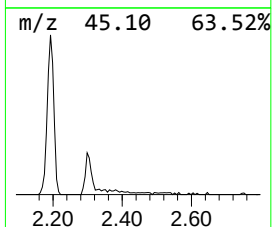
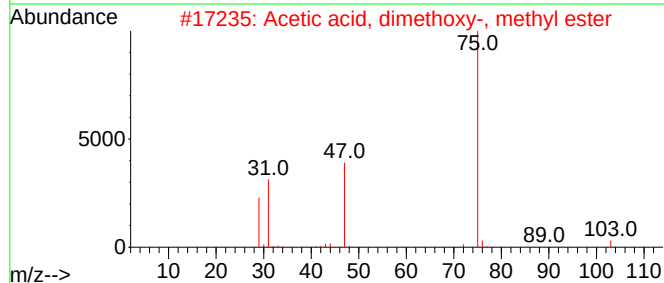
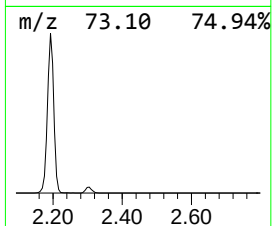
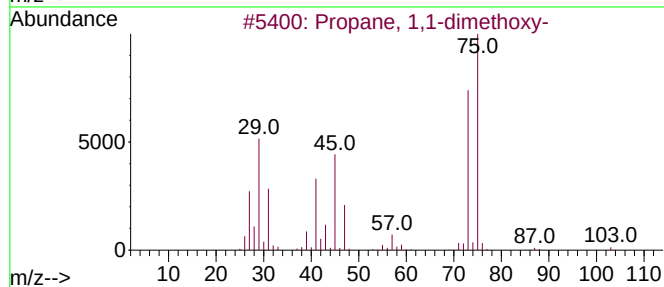
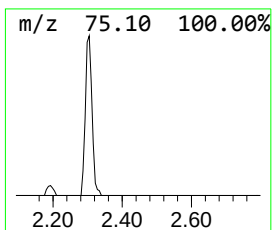
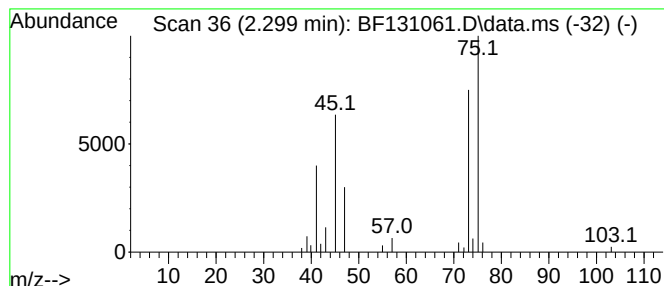
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.299	2.10 ng	38201	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2			Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	28
3			Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
4			Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	9
5			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9



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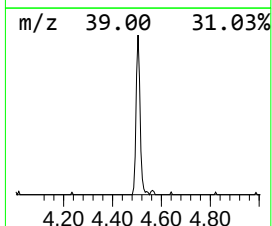
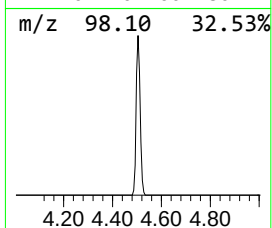
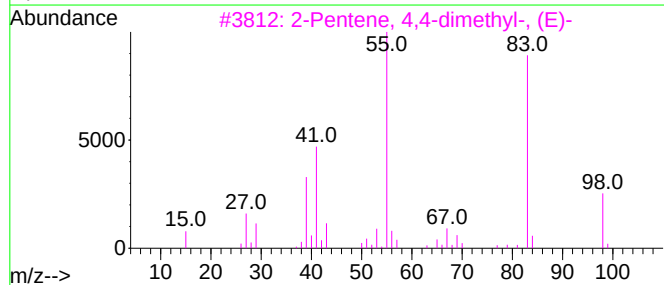
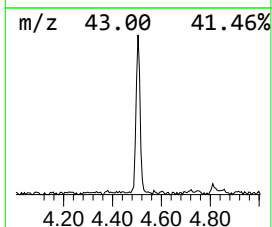
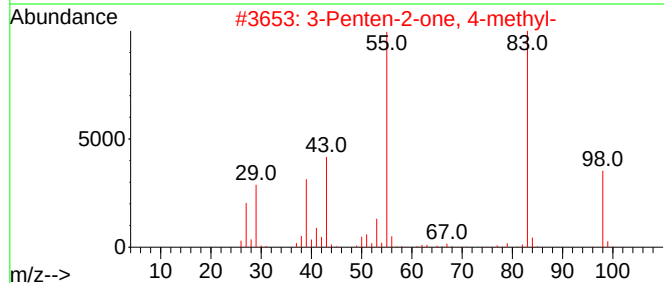
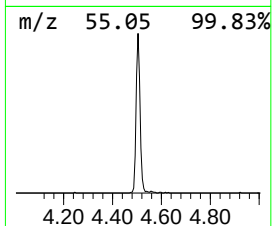
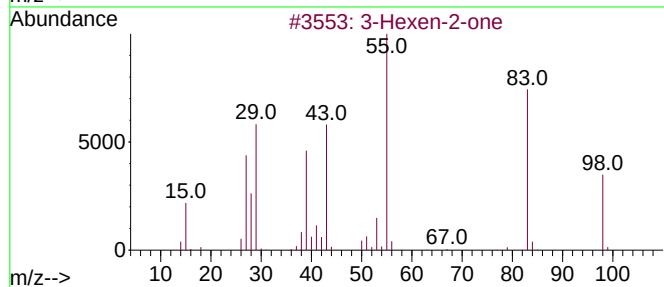
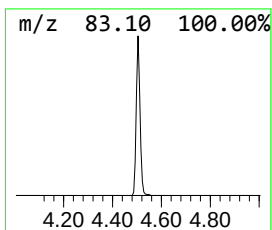
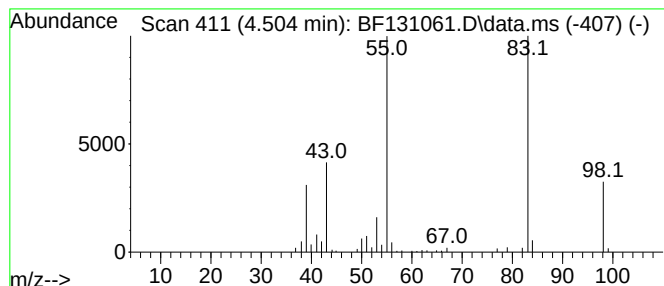
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 3-Hexen-2-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.504	8.80 ng	160121	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	91
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78



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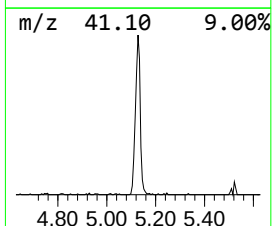
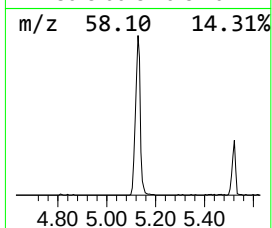
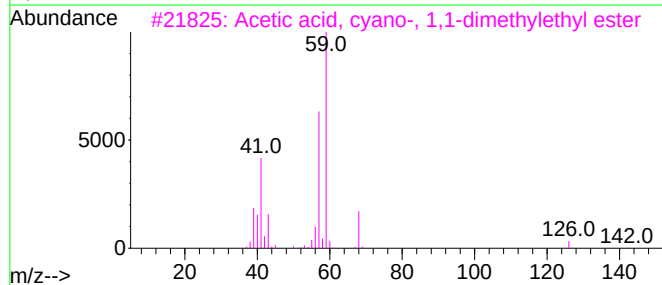
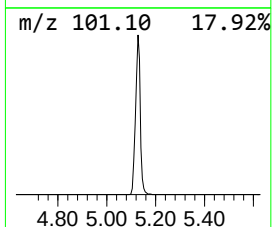
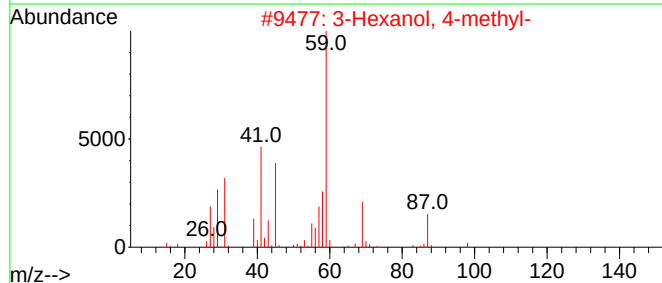
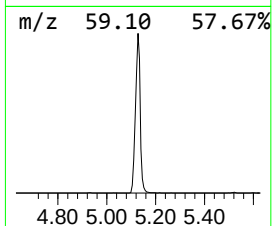
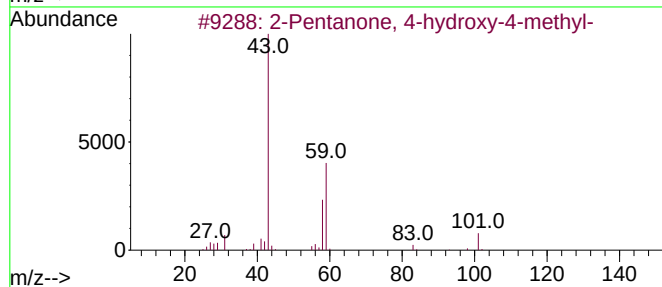
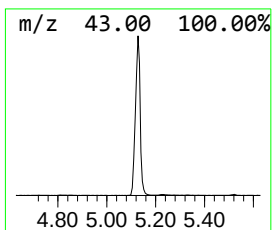
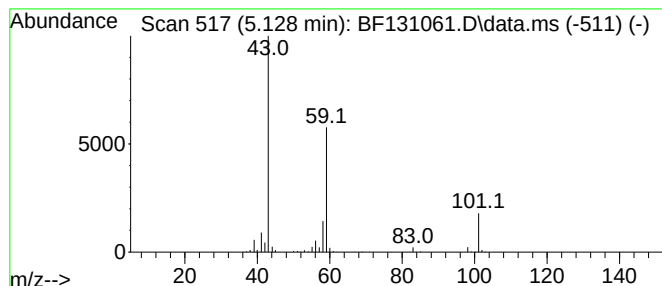
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.128	61.77 ng	1124510	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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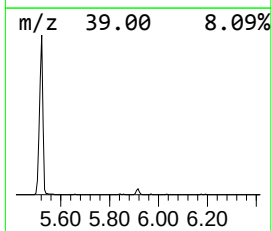
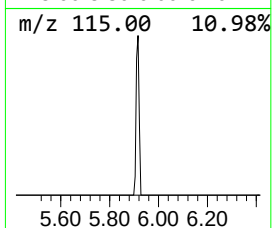
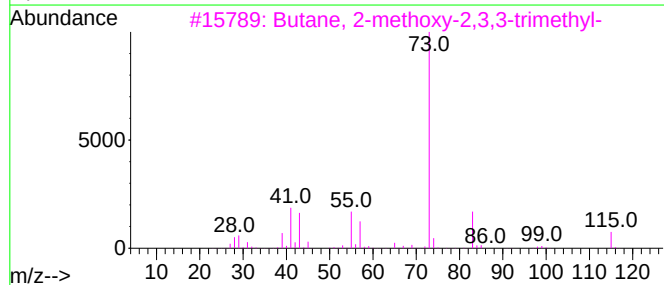
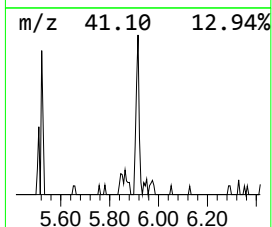
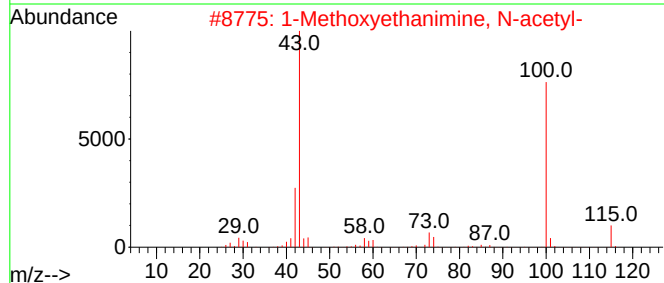
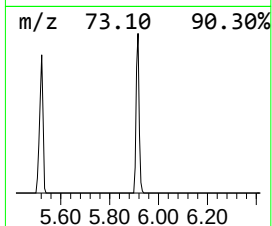
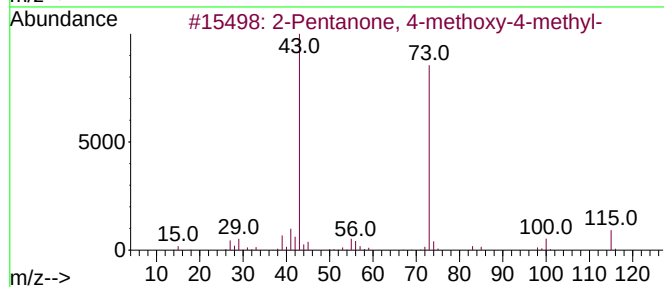
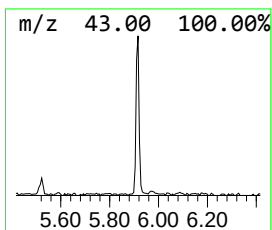
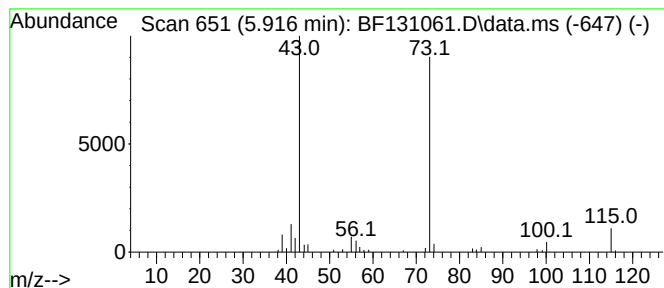
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.916	2.86 ng	52112	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	37
3			Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	25
4			N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	16
5			2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	12



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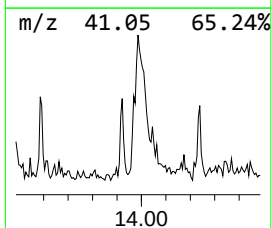
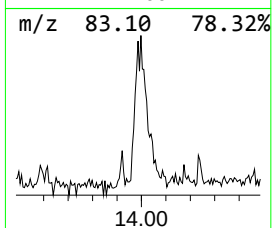
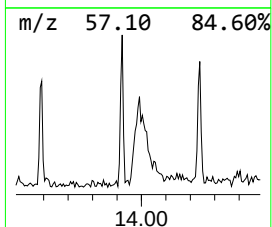
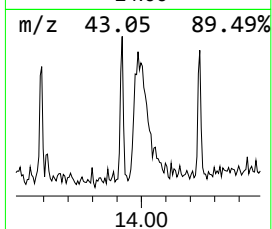
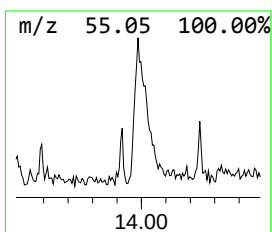
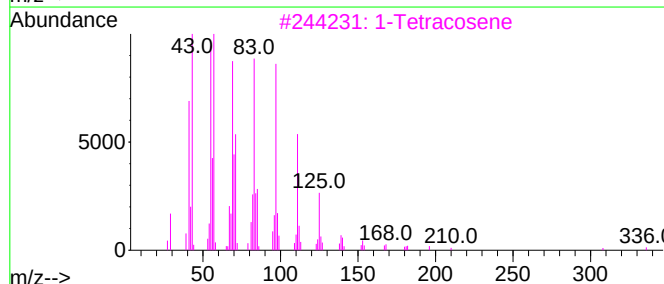
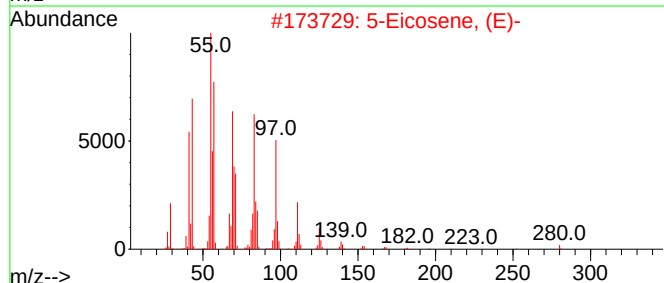
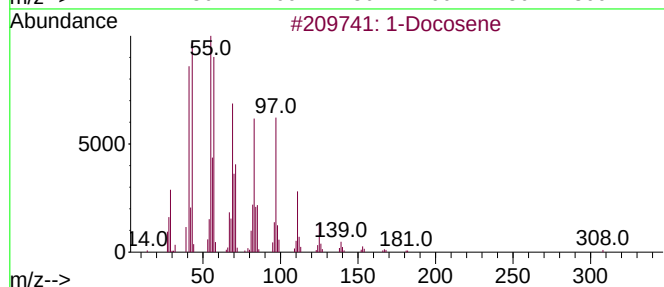
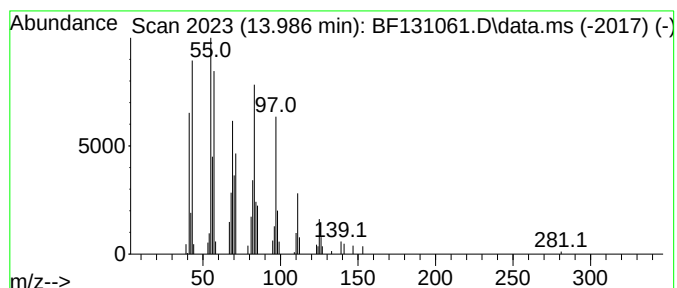
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.986	6.68 ng	147920	Chrysene-d12	14.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	95
2	5-Eicosene, (E)-			280	C20H40	074685-30-6	91
3	1-Tetracosene			336	C24H48	010192-32-2	90
4	3-Chloropropionic acid, heptadec...			346	C20H39ClO2	1000283-05-1	90
5	1-Heneicosanol			312	C21H44O	015594-90-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110822\
Data File : BF131061.D
Acq On : 08 Nov 2022 12:02
Operator : CG\JU
Sample : N5460-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SH-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110722.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...	2.193	34.5	ng	627916	1	6.898	364073	20.0
Propane, 1,1-di...	2.299	2.1	ng	38201	1	6.898	364073	20.0
3-Hexen-2-one	4.504	8.8	ng	160121	1	6.898	364073	20.0
2-Pentanone, 4-...	5.128	61.8	ng	1124510	1	6.898	364073	20.0
2-Pentanone, 4-...	5.916	2.9	ng	52112	1	6.898	364073	20.0
1-Docosene	13.986	6.7	ng	147920	5	14.086	442548	20.0