

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
 Data File : BF131130.D
 Acq On : 10 Nov 2022 19:05
 Operator : CG\JU
 Sample : N5520-03
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 124037

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-BF110922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131130.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	10	17	24	rVB	604902	768345	40.98%	5.338%
2	2.299	31	36	42	rBV	41616	54273	2.89%	0.377%
3	5.116	510	515	523	rVB	267928	332570	17.74%	2.310%
4	5.510	577	582	585	rBV	2053014	1874970	100.00%	13.026%
5	6.516	748	753	756	rBV	1885612	1868269	99.64%	12.980%
6	6.887	812	816	819	rBV	540369	418019	22.29%	2.904%
7	7.451	907	912	915	rBV	1152699	1101319	58.74%	7.651%
8	8.169	1030	1034	1038	rBV	622050	572612	30.54%	3.978%
9	9.245	1212	1217	1221	rBV	1821548	1681509	89.68%	11.682%
10	9.933	1329	1334	1337	rBV	807794	703638	37.53%	4.888%
11	10.722	1464	1468	1472	rBV	1381838	1296980	69.17%	9.011%
12	11.427	1584	1588	1590	rBV	704674	647840	34.55%	4.501%
13	12.639	1791	1794	1798	rVB	34597	27939	1.49%	0.194%
14	12.869	1827	1833	1836	rBV2	30755	35327	1.88%	0.245%
15	13.016	1853	1858	1861	rBV	1414416	1278783	68.20%	8.884%
16	13.774	1969	1987	2000	rBV10	115396	571020	30.45%	3.967%
17	13.904	2007	2009	2015	rVB2	21107	22588	1.20%	0.157%
18	13.974	2015	2021	2029	rBV4	30252	79823	4.26%	0.555%
19	14.074	2034	2038	2041	rBV	411912	362143	19.31%	2.516%
20	14.168	2048	2054	2058	rBV	53231	63775	3.40%	0.443%
21	14.527	2113	2115	2121	rVB	20546	22564	1.20%	0.157%
22	14.692	2140	2143	2147	rBV	48591	49737	2.65%	0.346%
23	14.845	2164	2169	2172	rBV2	18783	22487	1.20%	0.156%
24	14.921	2179	2182	2187	rVB	22445	20962	1.12%	0.146%
25	15.127	2214	2217	2220	rBV	20878	25003	1.33%	0.174%
26	15.192	2225	2228	2233	rVB	21493	25713	1.37%	0.179%
27	15.504	2278	2281	2287	rVB2	15082	21577	1.15%	0.150%
28	15.568	2287	2292	2300	rVB	306426	385172	20.54%	2.676%
29	16.027	2366	2370	2376	rBV4	15063	22728	1.21%	0.158%
30	16.562	2450	2461	2463	rBV9	13120	36203	1.93%	0.252%

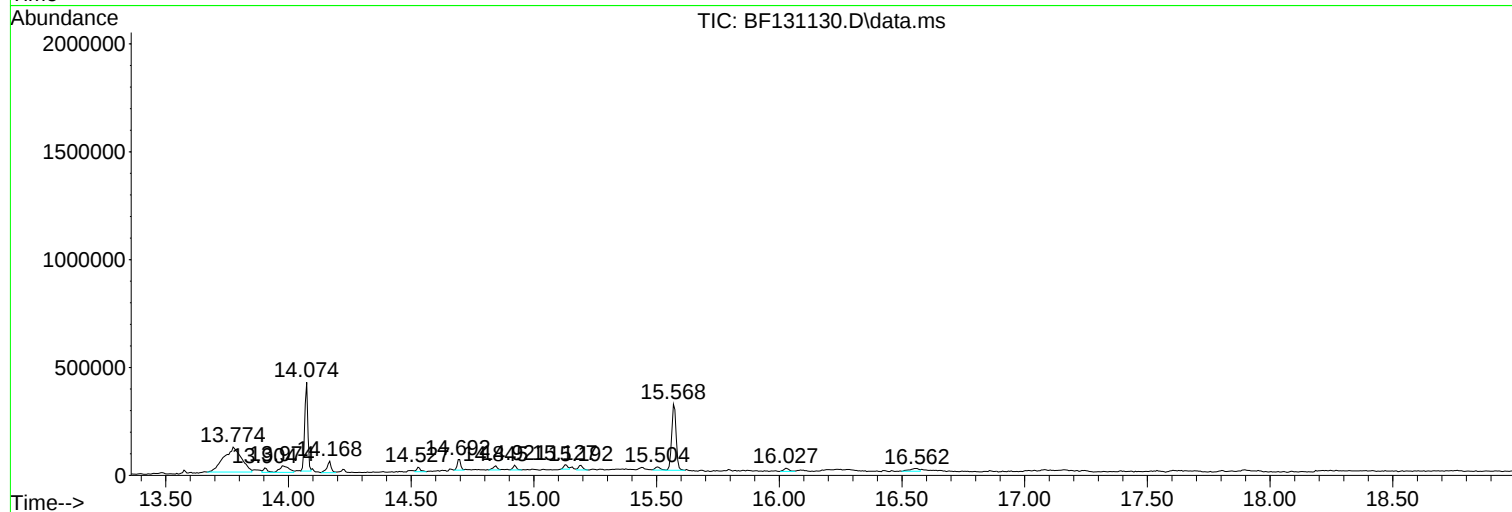
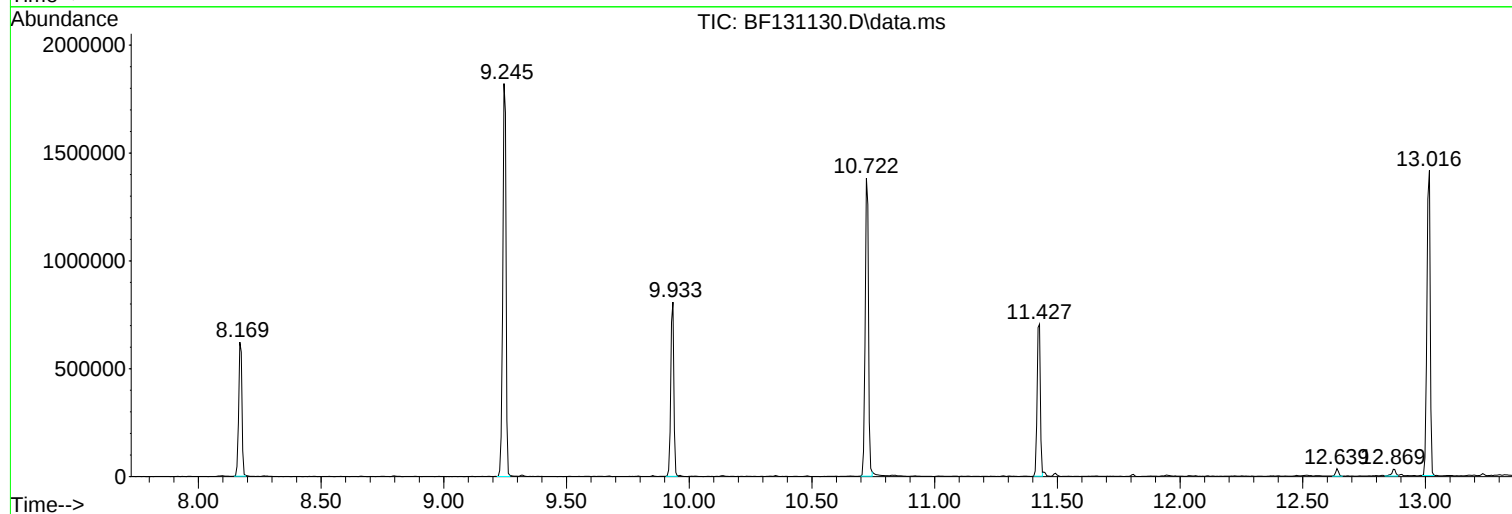
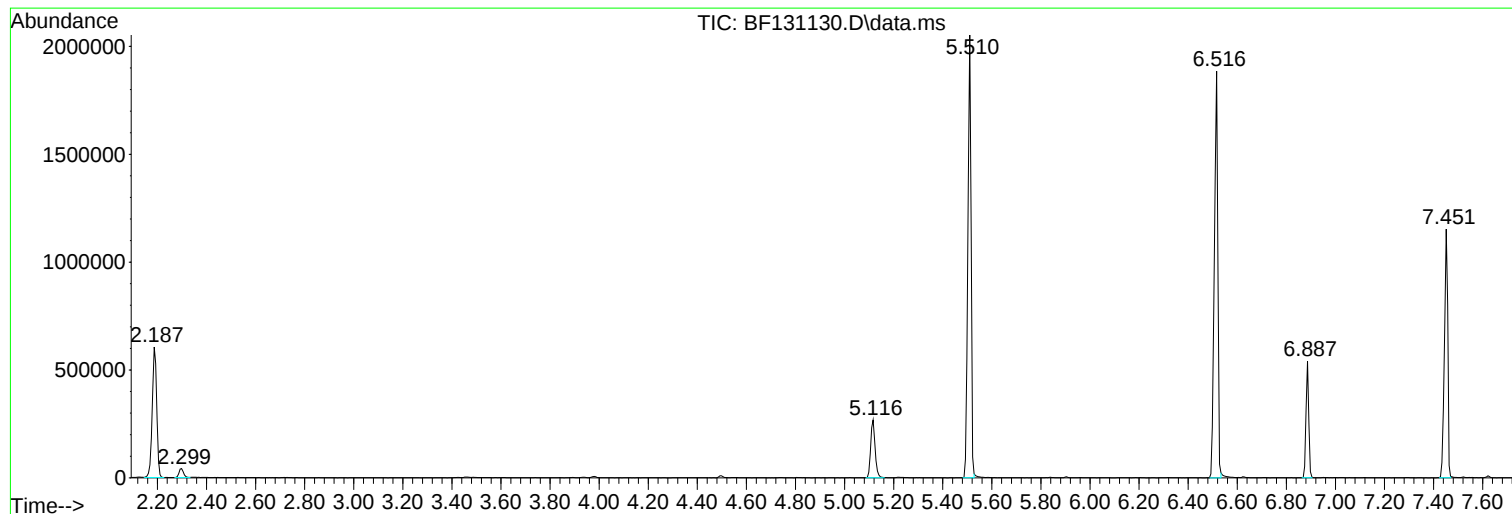
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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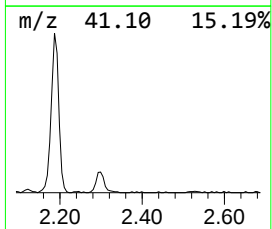
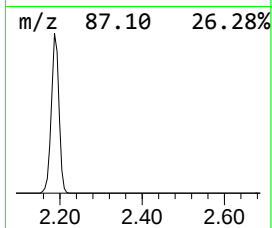
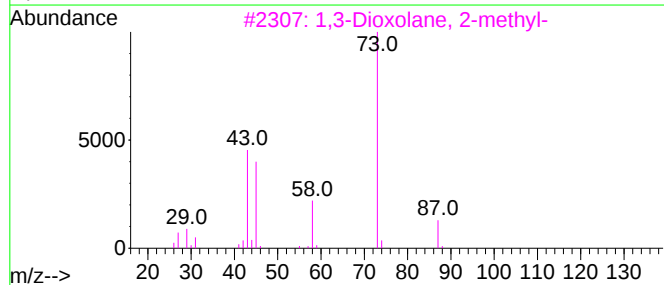
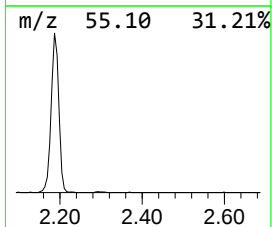
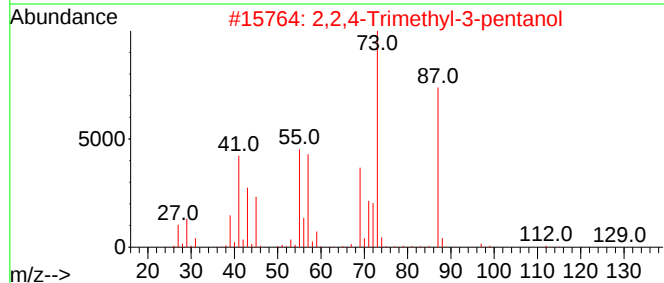
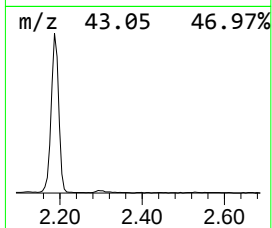
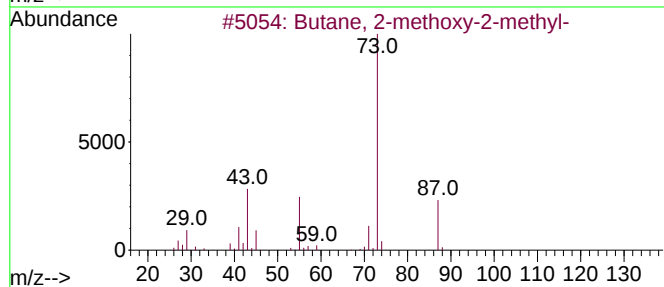
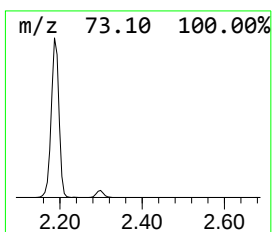
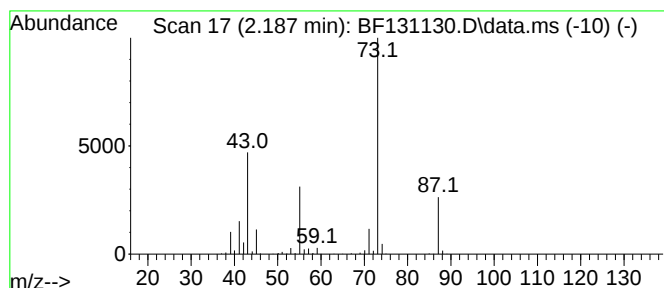
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.187	36.76 ng	768345	1,4-Dichlorobenzene-d4	6.887

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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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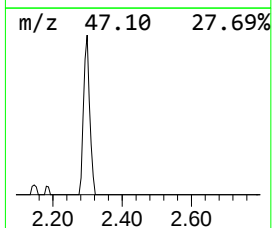
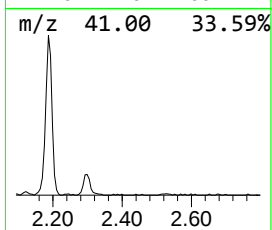
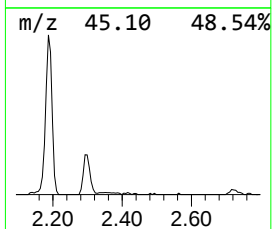
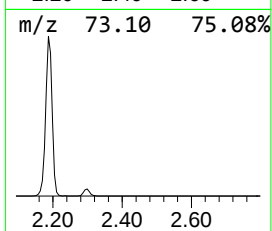
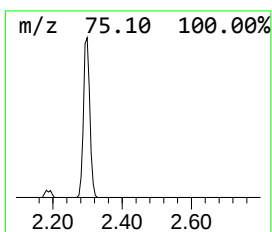
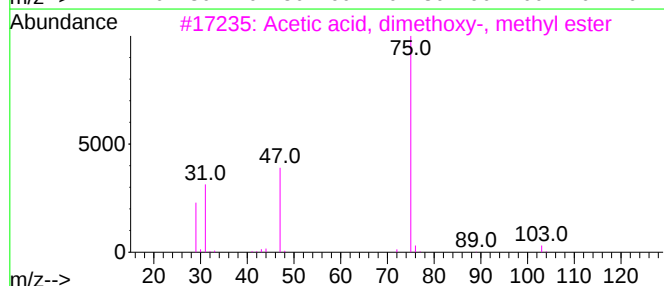
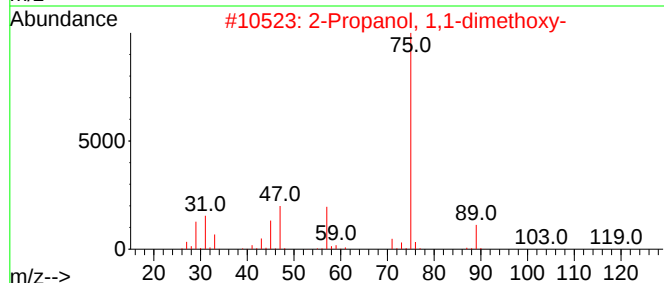
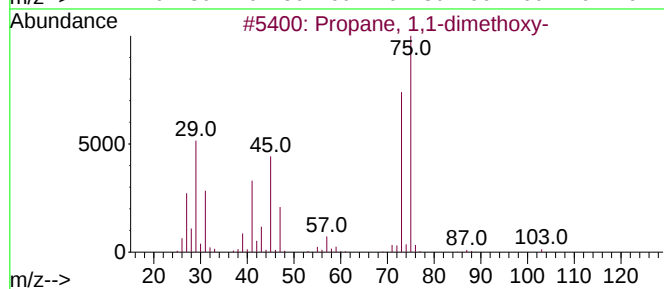
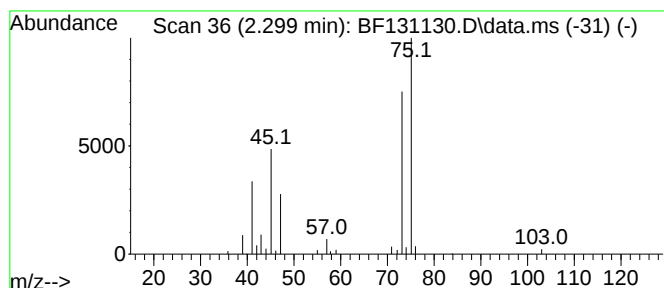
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.299	2.60 ng	54273	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2			2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	33
3			Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	28
4			3-Hexene, 1-(1-ethoxyethoxy)-, (Z)-	172	C10H20O2	028069-74-1	10
5			2,5-Diethoxy-3-methyl-3-vinylhexane	214	C13H26O2	1000432-70-8	10



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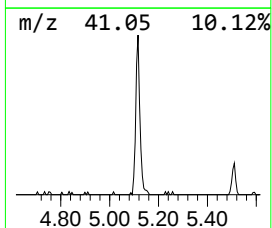
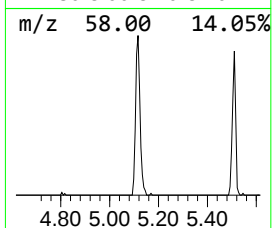
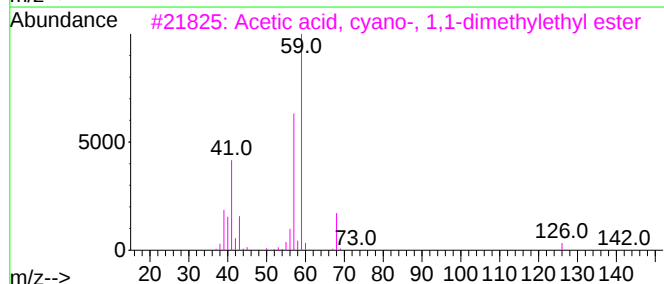
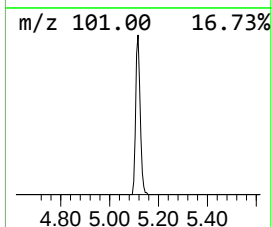
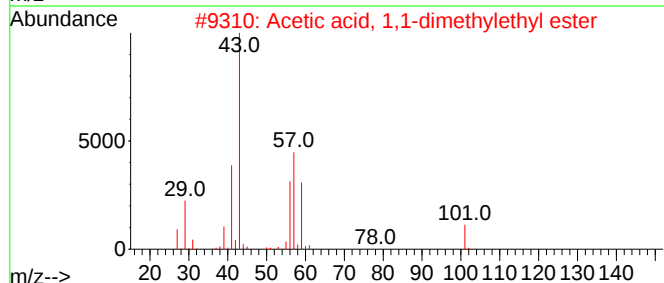
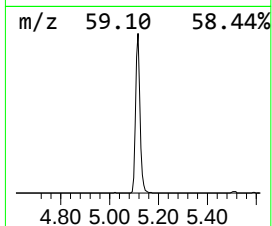
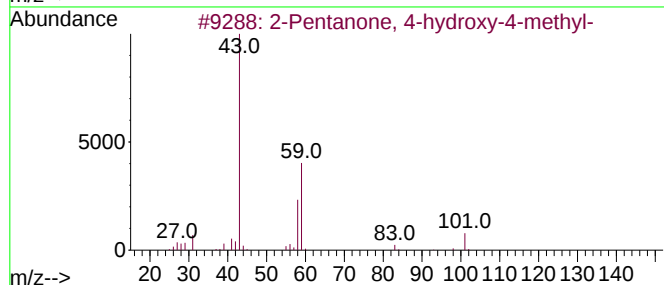
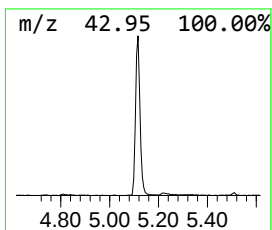
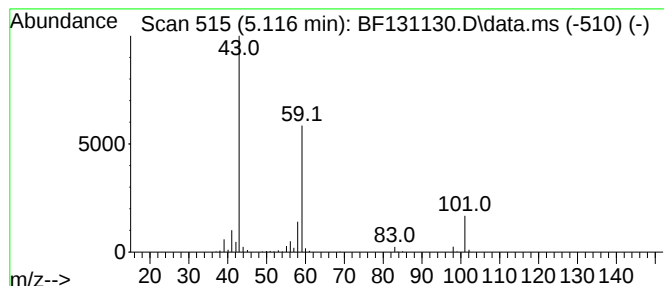
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	15.91 ng	332570	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9



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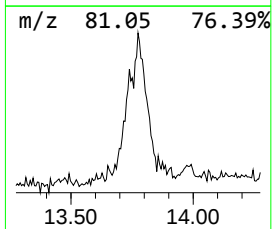
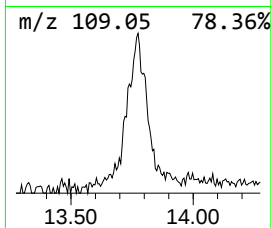
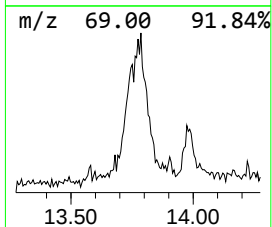
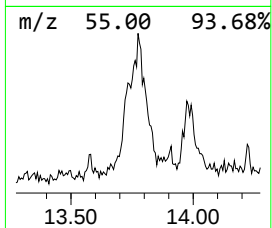
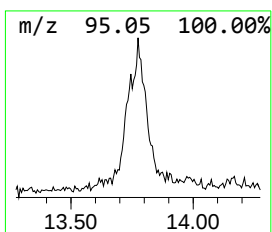
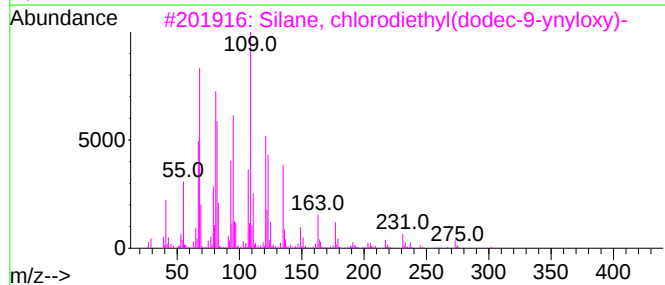
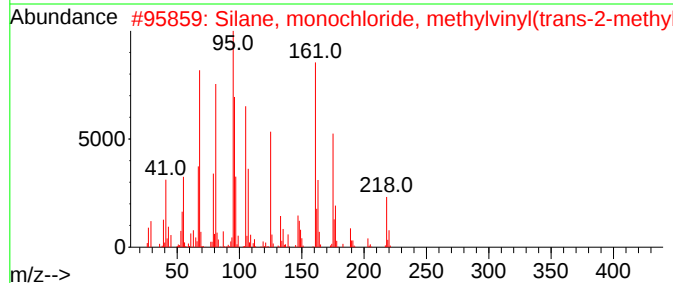
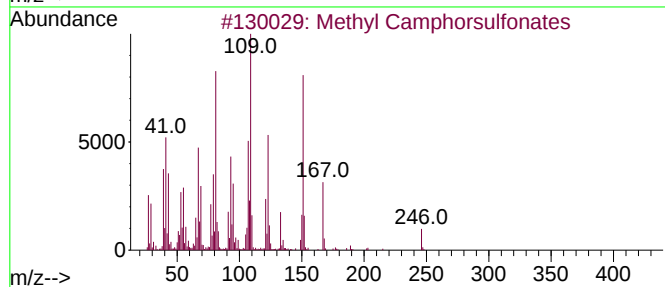
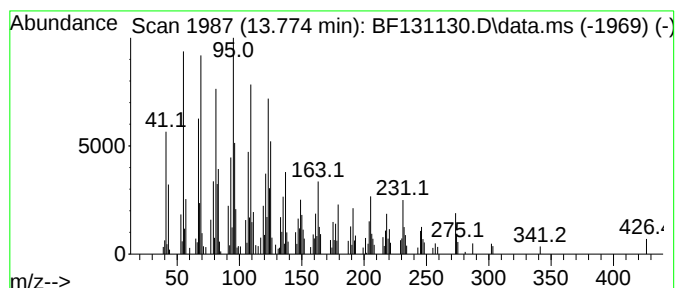
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Peak Number 4 Methyl Camphorsulfonates Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.774	31.54 ng	571020	Chrysene-d12		14.074	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Methyl Camphorsulfonates		246	C11H18O4S	046471-67-4	64
2	Silane, monochloride, methylviny...		218	C10H19ClOSi	1000421-09-7	50
3	Silane, chlorodiethyl(dodec-9-yn...		302	C16H31ClOSi	1000363-59-2	47
4	(-)-Neoclovene-(II), dihydro-		206	C15H26	1000152-83-6	45
5	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...		206	C15H26	172549-29-0	45



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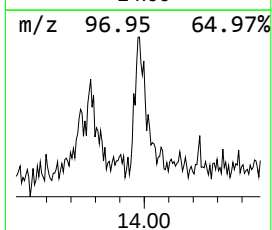
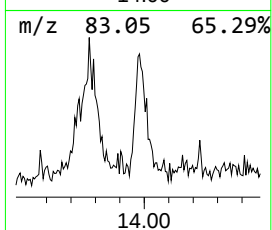
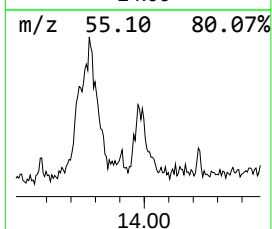
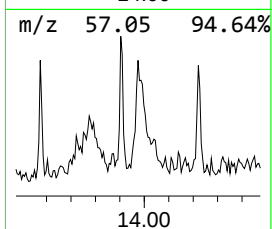
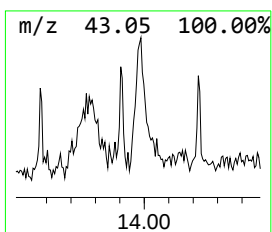
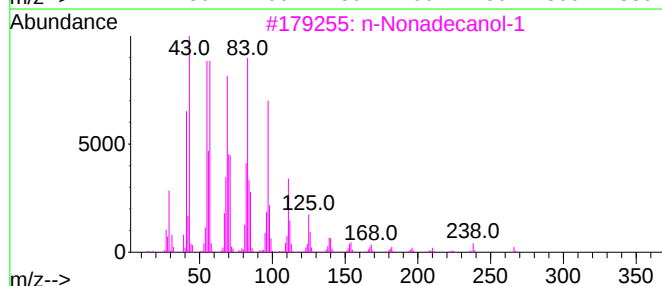
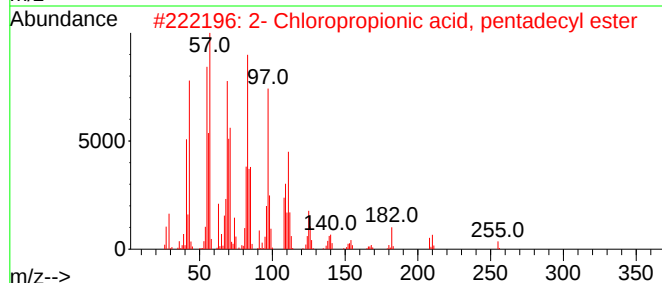
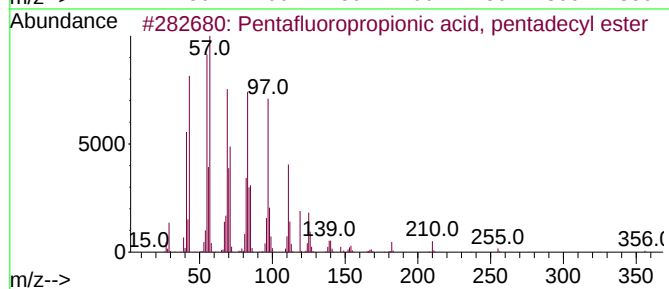
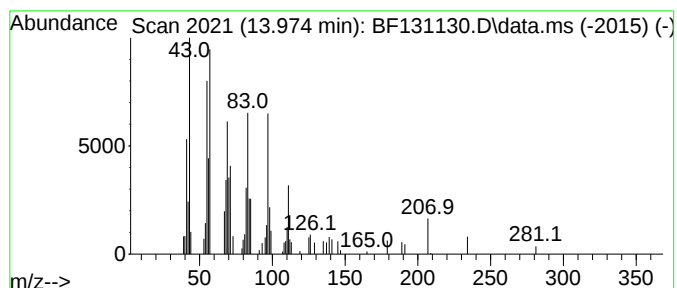
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Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.974	4.41 ng	79823	Chrysene-d12	14.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
2			2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	91
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4			2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91
5			1-Eicosene	280	C20H40	003452-07-1	91



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124037

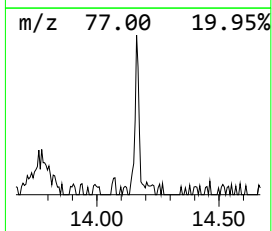
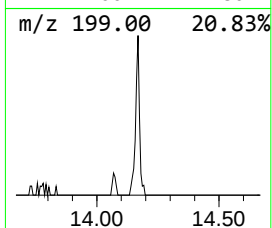
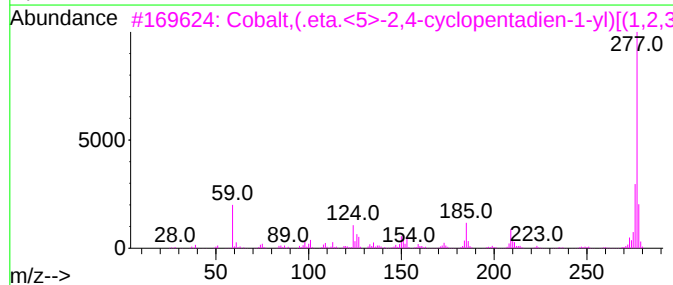
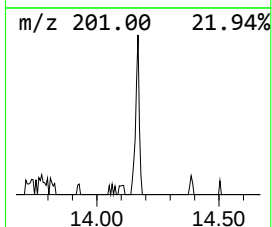
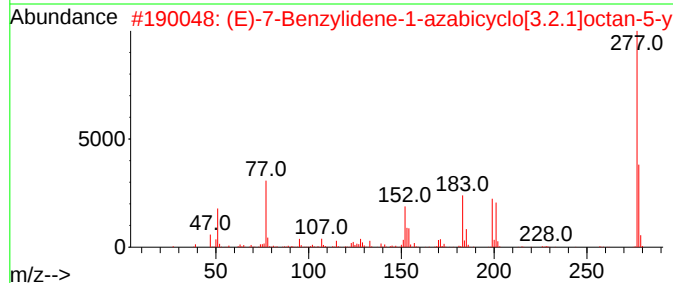
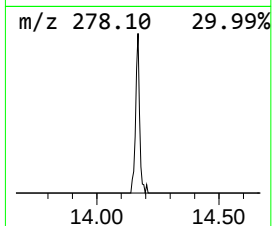
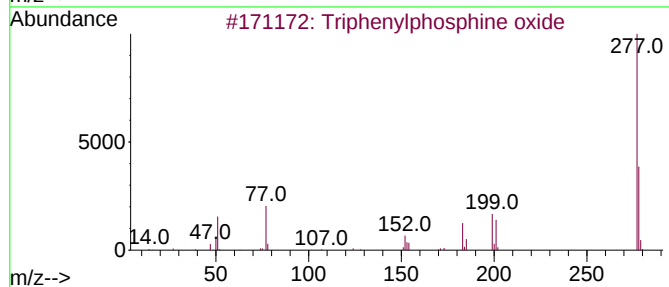
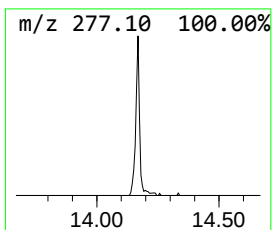
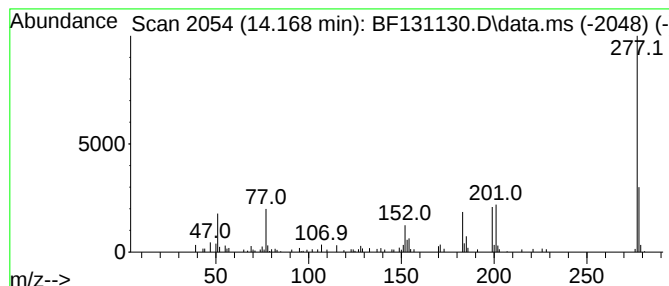
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.169	3.52 ng	63775	Chrysene-d12	14.074

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	52
3			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	43
4			2-Phenyl-6-(trifluoromethyl)-1H...	277	C15H10F3NO	1000387-59-3	43
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131130.D
Acq On : 10 Nov 2022 19:05
Operator : CG\JU
Sample : N5520-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

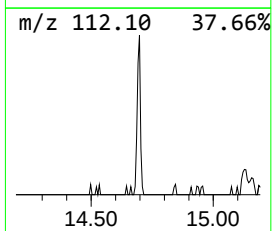
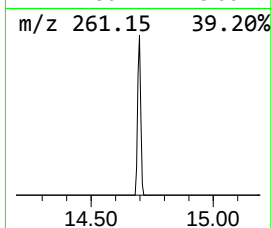
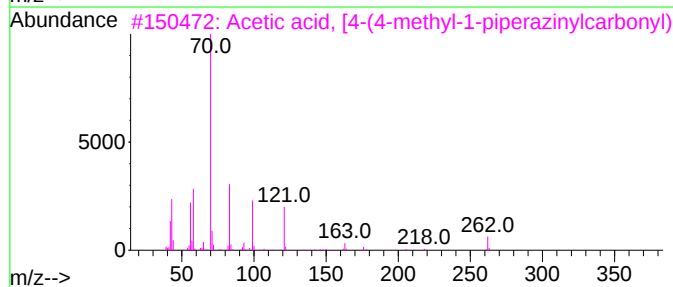
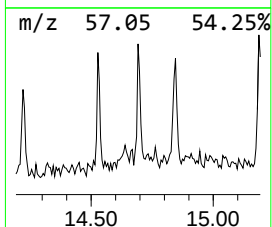
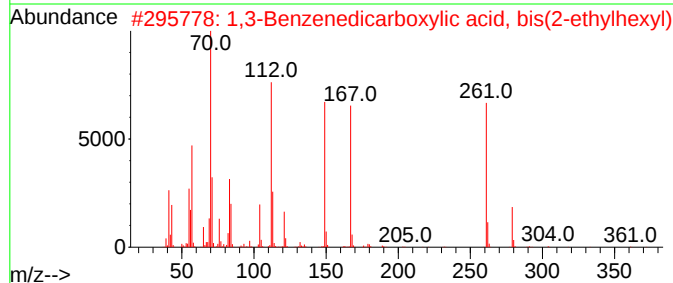
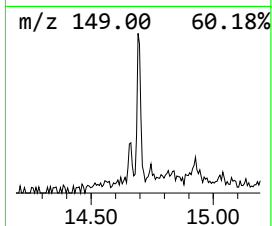
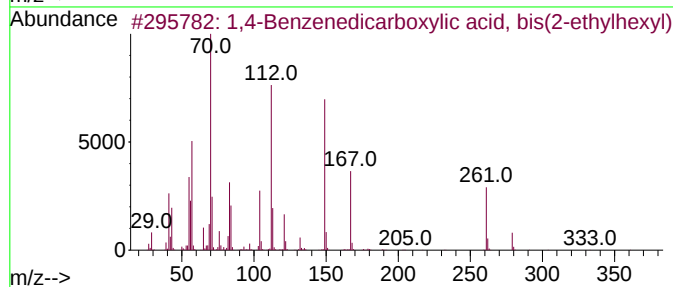
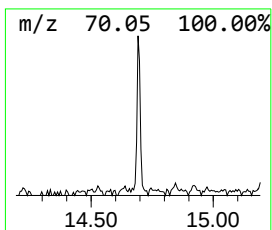
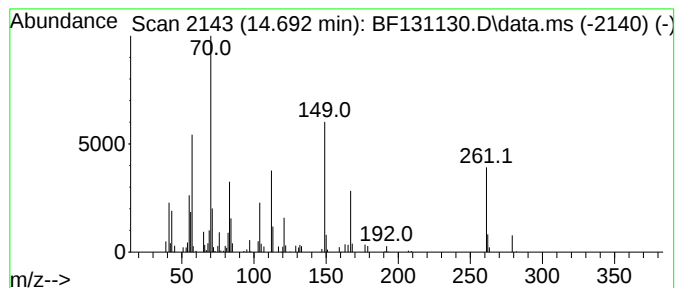
Instrument :
BNA_F
ClientSampleId :
124037

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
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 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.692	2.75 ng	49737	Chrysene-d12		14.074	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...		390	C24H38O4	006422-86-2	72
2	1,3-Benzenedicarboxylic acid, bi...		390	C24H38O4	000137-89-3	52
3	Acetic acid, [4-(4-methyl-1-pipe...		262	C14H18N2O3	346699-90-9	22
4	Phthalic acid, 6-ethyloct-3-yl 2...		418	C26H42O4	1000315-53-8	14
5	Phthalic acid, 1-(3-bromophenyl)...		460	C24H29BrO4	1000377-88-1	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131130.D
Acq On : 10 Nov 2022 19:05
Operator : CG\JU
Sample : N5520-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
124037

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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...	2.187	36.8	ng	768345	1	6.887	418019	20.0
Propane, 1,1-di...	2.299	2.6	ng	54273	1	6.887	418019	20.0
2-Pentanone, 4-...	5.116	15.9	ng	332570	1	6.887	418019	20.0
Methyl Camphors...	13.774	31.5	ng	571020	5	14.074	362143	20.0
Pentafluoroprop...	13.974	4.4	ng	79823	5	14.074	362143	20.0
Triphenylphosph...	14.169	3.5	ng	63775	5	14.074	362143	20.0
1,4-Benzenedica...	14.692	2.8	ng	49737	5	14.074	362143	20.0