

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010923\
 Data File : BF131971.D
 Acq On : 09 Jan 2023 19:29
 Operator : CG\JU
 Sample : 01046-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-SAMPLE-API-3

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-BF010923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131971.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.981	488	492	500	rVB	380483	430648	12.27%	2.095%
2	5.392	558	562	573	rBV	1338828	1278474	36.44%	6.219%
3	5.722	614	618	627	rBV	384919	369881	10.54%	1.799%
4	6.416	732	736	745	rBV	899336	816495	23.27%	3.972%
5	6.781	795	798	802	rBV	536224	470832	13.42%	2.290%
6	7.357	890	896	899	rBV	1681519	1846812	52.64%	8.984%
7	8.075	1009	1018	1021	rBV	705070	625394	17.83%	3.042%
8	8.298	1051	1056	1058	rBV	1185691	1117275	31.85%	5.435%
9	8.322	1058	1060	1071	rVB	1249975	1183461	33.73%	5.757%
10	8.410	1071	1075	1077	rBV	70515	64606	1.84%	0.314%
11	8.786	1137	1139	1144	rBV	46395	44688	1.27%	0.217%
12	9.157	1196	1202	1205	rBV	3884868	3508419	100.00%	17.066%
13	9.833	1312	1317	1320	rBV	909005	756409	21.56%	3.679%
14	10.010	1343	1347	1349	rBV	55625	64583	1.84%	0.314%
15	10.145	1368	1370	1373	rBV2	43159	42102	1.20%	0.205%
16	10.333	1400	1402	1407	rVB4	41830	55335	1.58%	0.269%
17	10.533	1430	1436	1437	rBV3	40180	49483	1.41%	0.241%
18	10.557	1437	1440	1442	rVB	55140	48586	1.38%	0.236%
19	10.633	1447	1453	1456	rVV	2504188	2308221	65.79%	11.228%
20	11.268	1558	1561	1563	rBV	42552	48523	1.38%	0.236%
21	11.327	1567	1571	1574	rVB	955701	768657	21.91%	3.739%
22	11.857	1658	1661	1664	rBV2	101205	84781	2.42%	0.412%
23	11.892	1664	1667	1673	rVB	220350	182922	5.21%	0.890%
24	12.410	1753	1755	1760	rVB3	39334	48899	1.39%	0.238%
25	12.727	1806	1809	1815	rVB	69093	62576	1.78%	0.304%
26	12.921	1837	1842	1845	rBV	3516731	3254316	92.76%	15.830%
27	13.815	1991	1994	2003	rVB	99951	132069	3.76%	0.642%
28	13.974	2017	2021	2025	rVB	472766	396836	11.31%	1.930%
29	14.598	2124	2127	2131	rVB	79487	68081	1.94%	0.331%
30	15.221	2230	2233	2239	rVB	32759	50475	1.44%	0.246%
31	15.439	2265	2270	2275	rBV	321337	377609	10.76%	1.837%

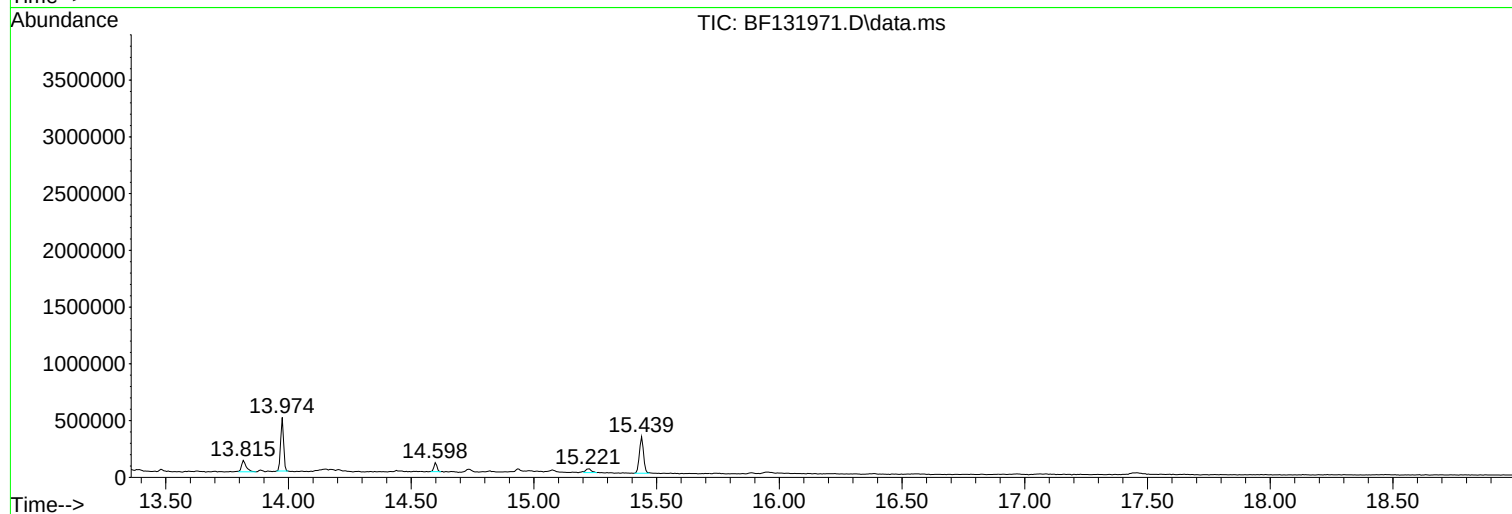
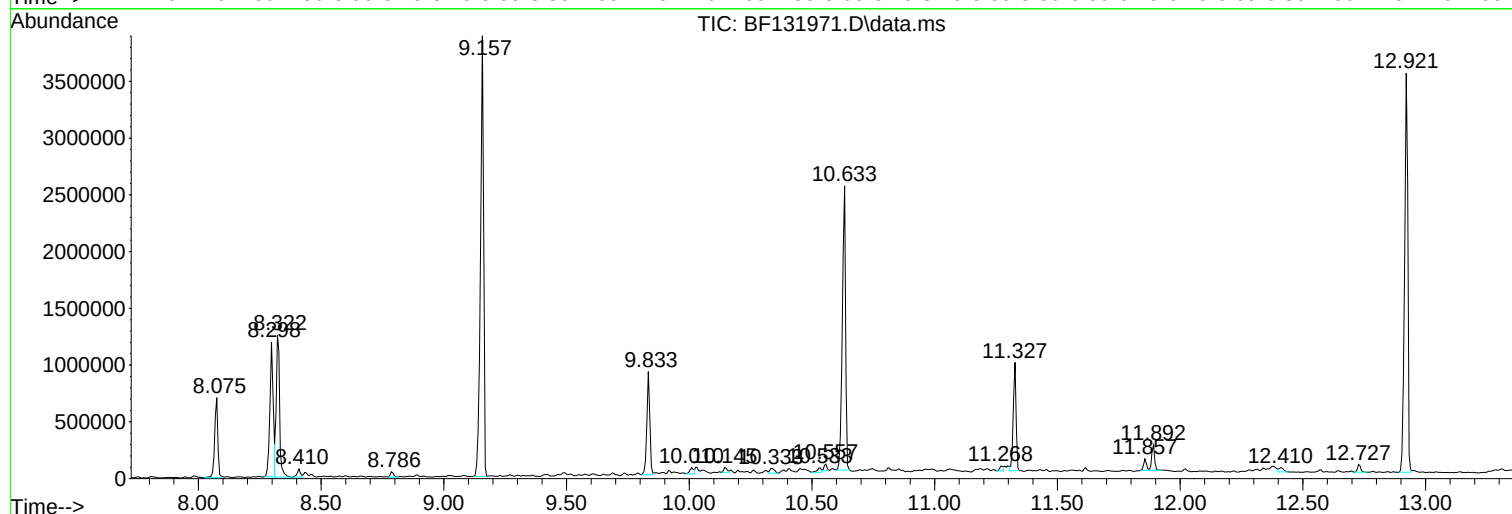
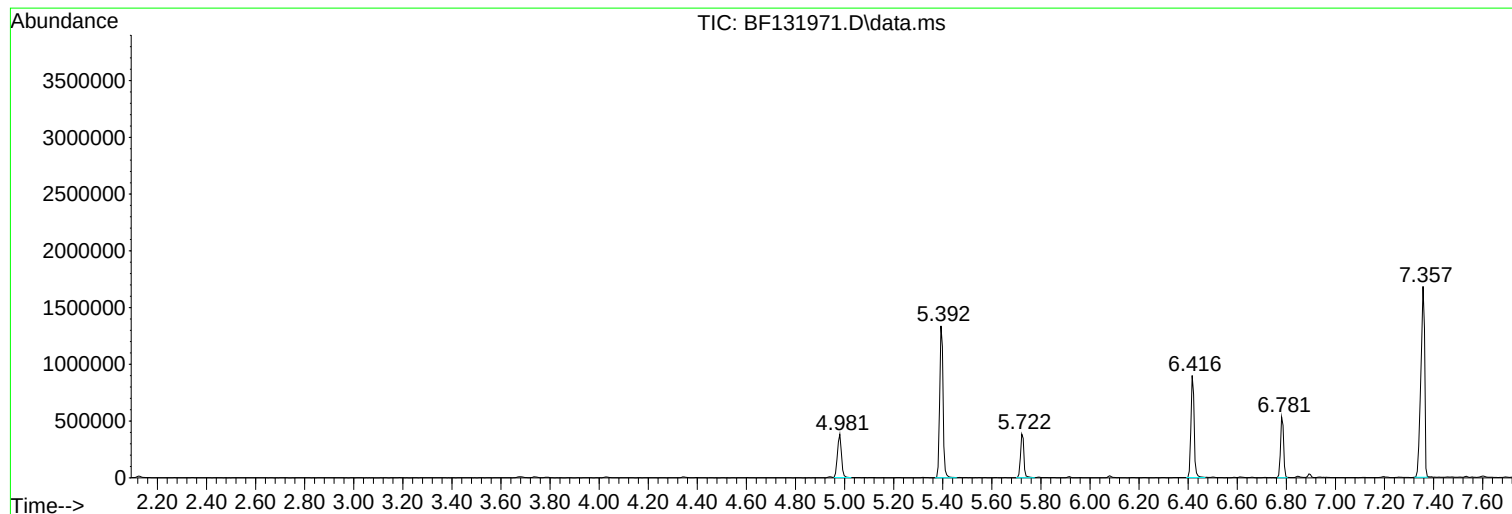
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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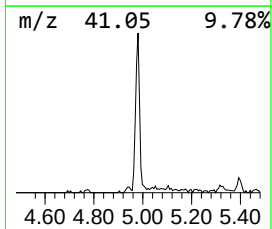
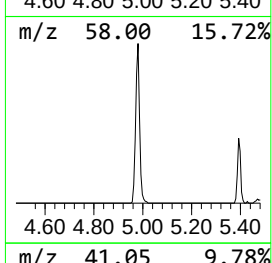
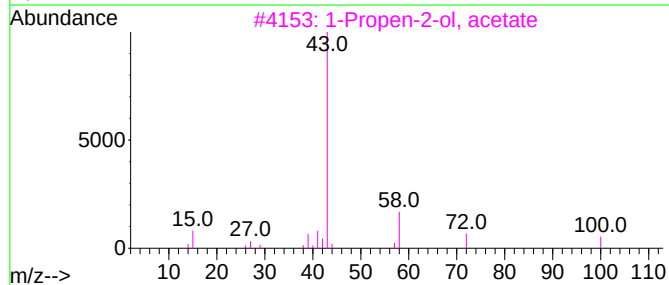
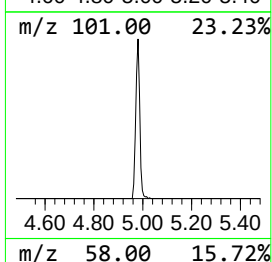
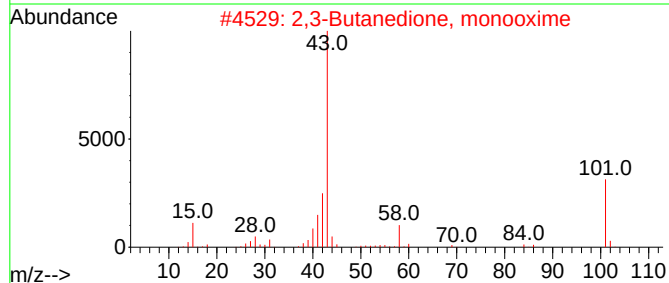
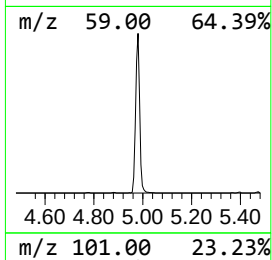
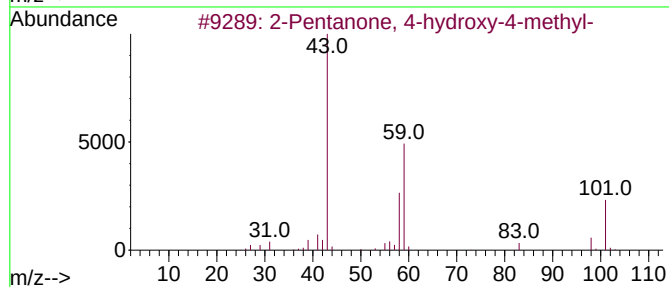
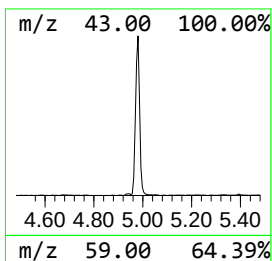
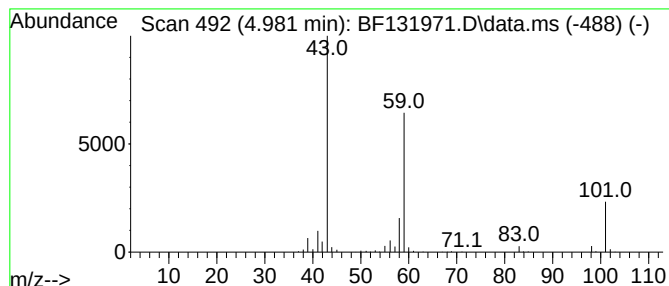
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.981	18.29 ng	430648	1,4-Dichlorobenzene-d4	6.781

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Acetamide, N-(cyanomethyl)-	98	C4H6N2O	004814-80-6	9



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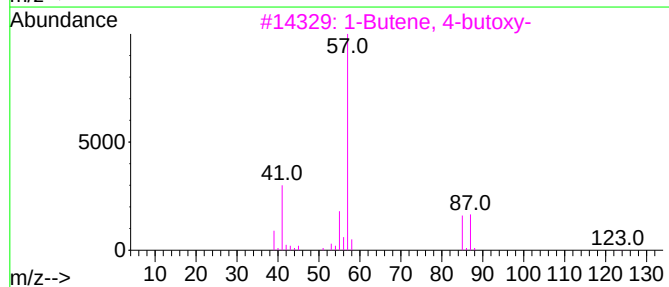
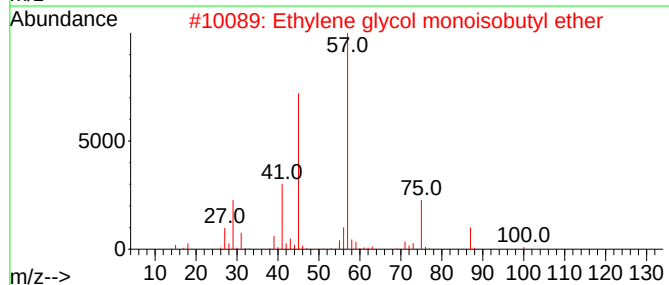
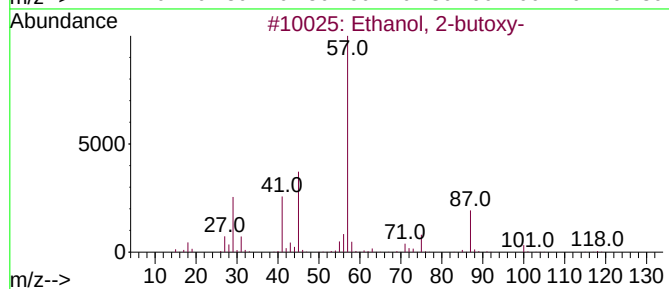
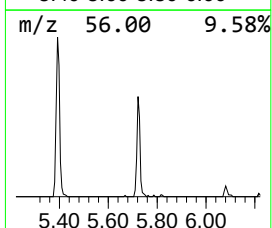
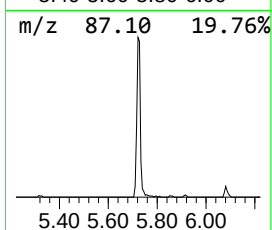
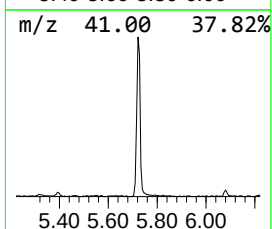
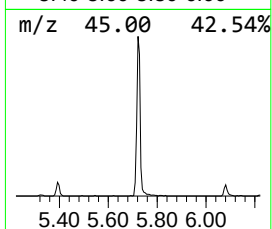
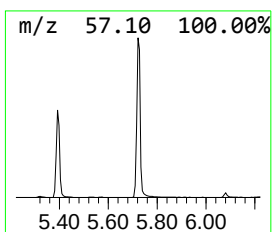
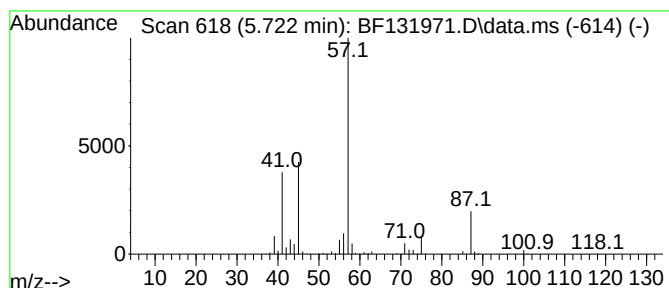
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-butoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.722	15.71 ng	369881	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	86
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
3			1-Butene, 4-butoxy-	128	C8H16O	034061-76-2	32
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	28
5			n-Butyl ether	130	C8H18O	000142-96-1	25



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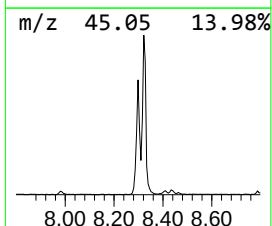
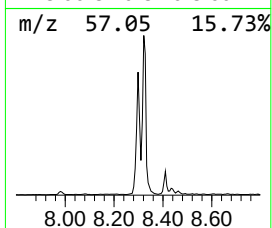
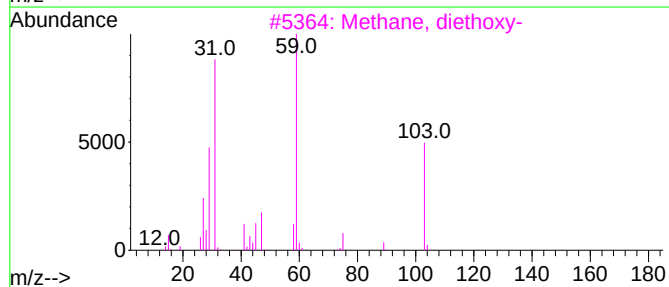
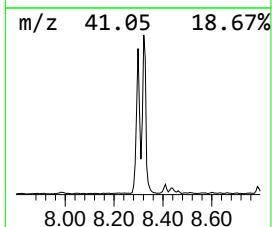
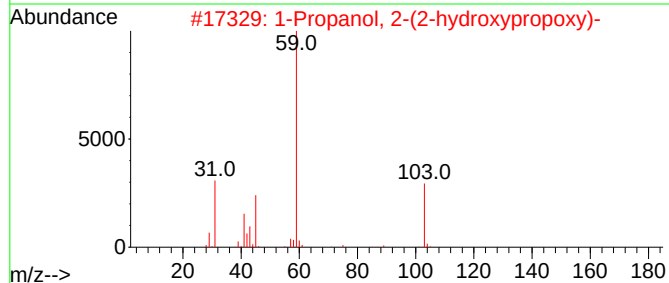
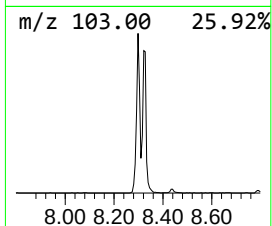
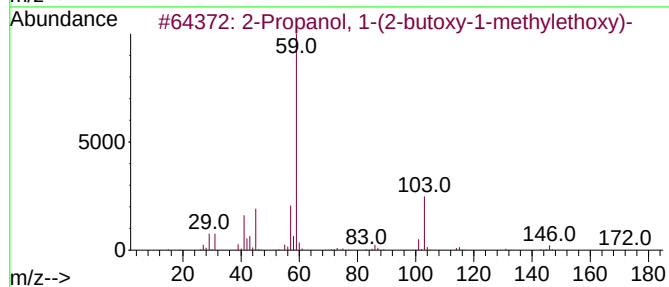
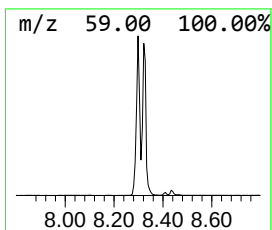
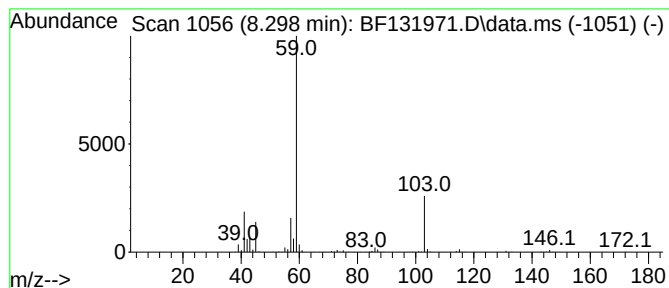
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BNA_F
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Propanol, 1-(2-butoxy-1-m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.298	35.73 ng	1117280	Naphthalene-d8	8.075	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	83
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
3	Methane, diethoxy-	104	C5H12O2	000462-95-3	72
4	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	64
5	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	64



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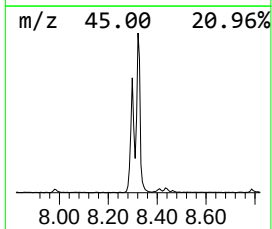
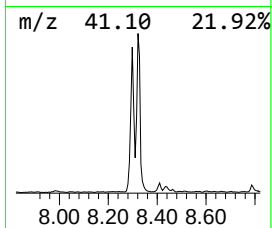
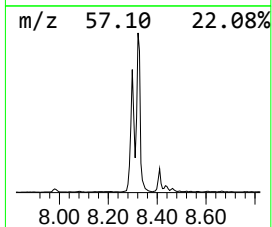
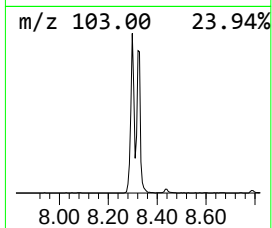
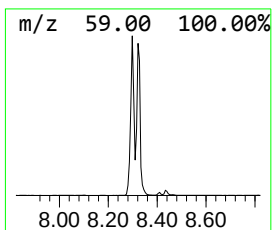
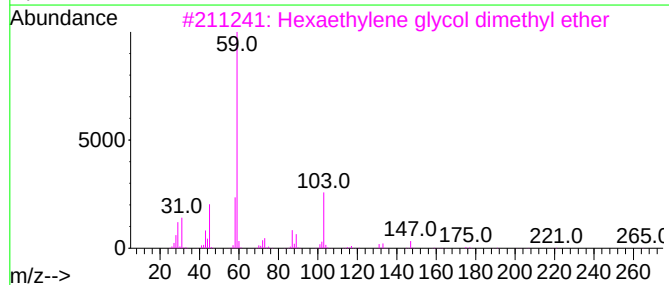
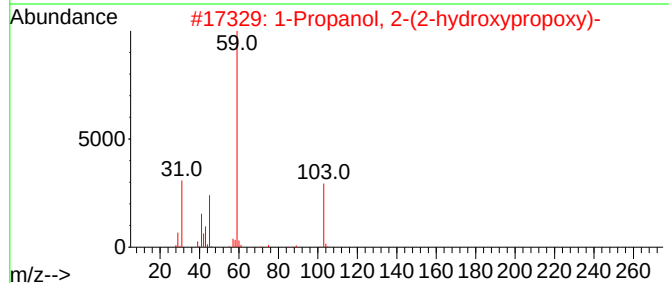
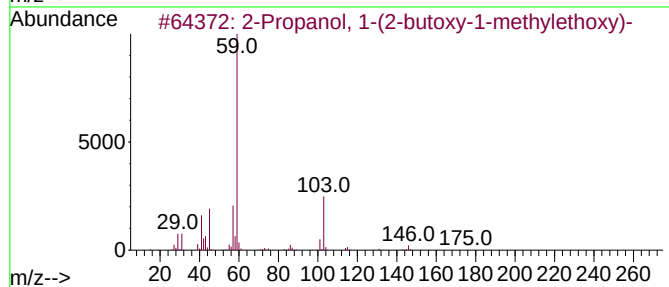
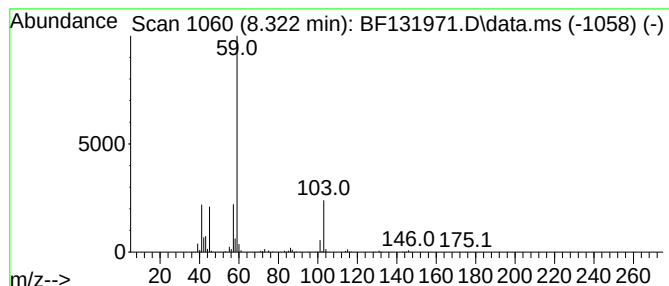
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Peak Number 4 1-Propanol, 2-(2-hydroxypro... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.322	37.85 ng	1183460	Naphthalene-d8	8.075

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3		029911-28-2	90
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3		000106-62-7	78
3	Hexaethylene glycol dimethyl ether	310	C14H30O7		001072-40-8	78
4	1,4,7-Trimethyl-3,6-dioxaoctane-...	192	C9H20O4		1000423-63-2	72
5	Dipropylene glycol (isomer 3)	134	C6H14O3		1000506-25-5	64



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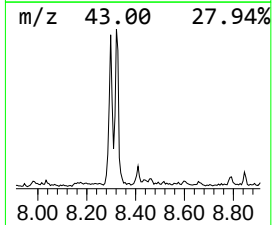
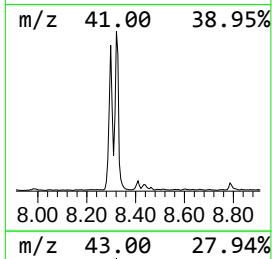
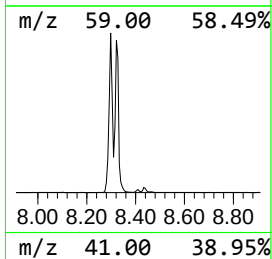
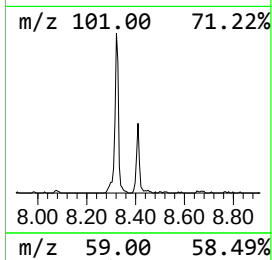
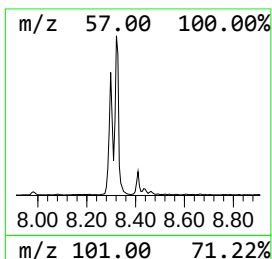
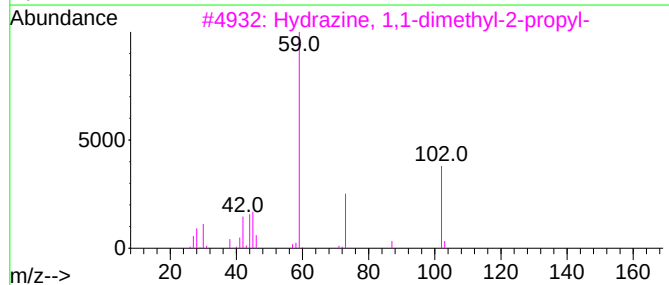
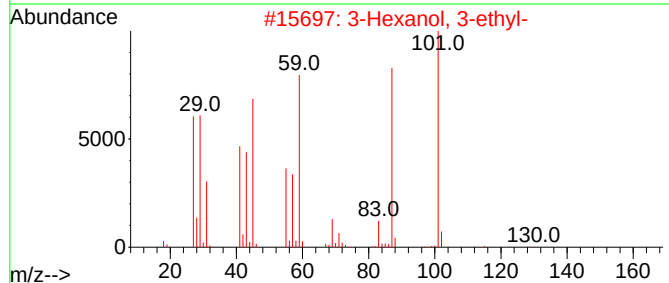
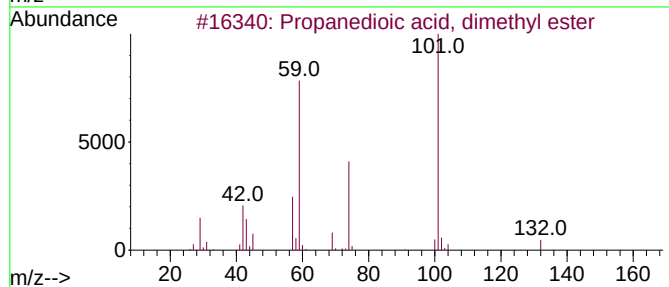
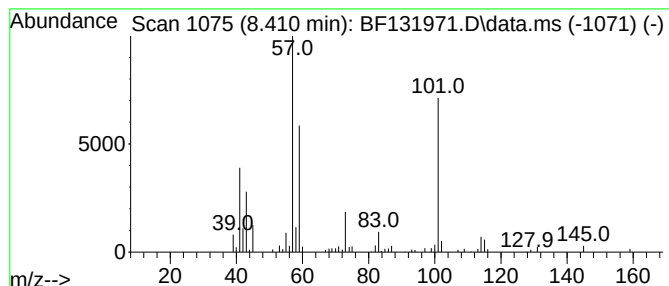
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Peak Number 5 Propanedioic acid, dimethyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.410	2.07 ng	64606	Naphthalene-d8	8.075

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanedioic acid, dimethyl ester	132	C5H8O4	000108-59-8	53
2			3-Hexanol, 3-ethyl-	130	C8H18O	000597-76-2	38
3			Hydrazine, 1,1-dimethyl-2-propyl-	102	C5H14N2	052728-54-8	35
4			Propane, 1,1'-[ethyldienebis(oxy...]	174	C10H22O2	005669-09-0	32
5			1,3-Dioxolane, 4,5-dimethyl-2-pe...	312	C20H40O2	056599-61-2	27



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COMP-SAMPLE-API-3

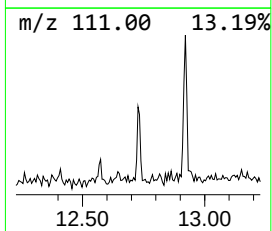
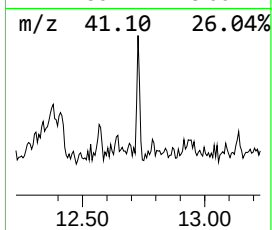
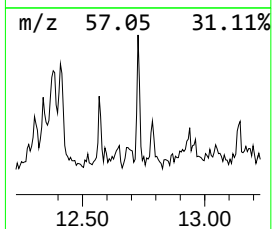
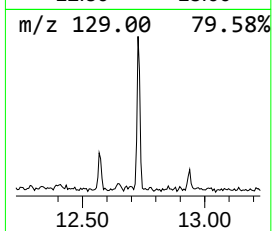
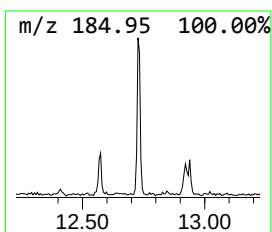
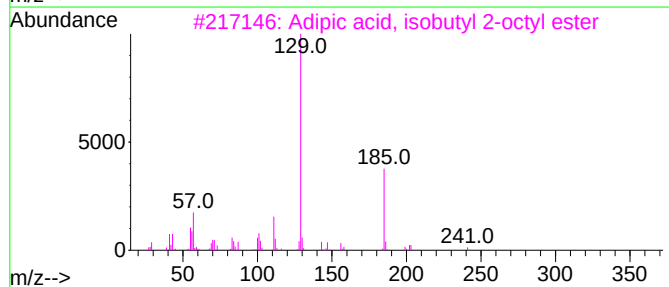
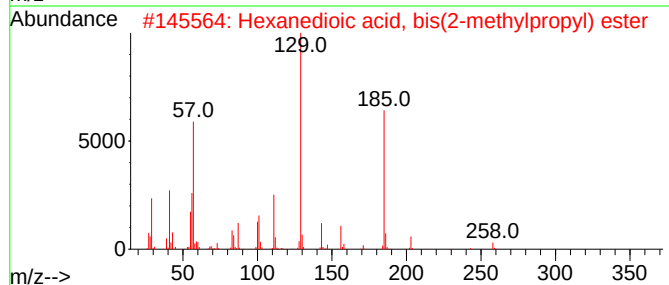
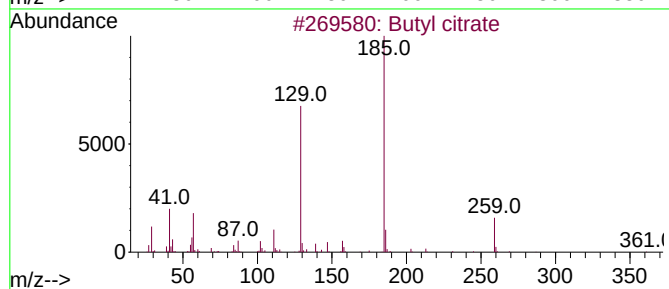
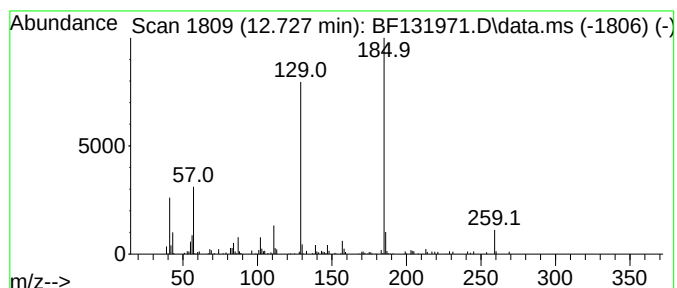
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Butyl citrate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.727	3.15 ng	62576	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl citrate	360	C18H32O7	000077-94-1	90
2			Hexanedioic acid, bis(2-methylpr...	258	C14H26O4	000141-04-8	72
3			Adipic acid, isobutyl 2-octyl ester	314	C18H34O4	1000324-44-5	56
4			Adipic acid, 3-hexyl isobutyl ester	286	C16H30O4	1000353-62-2	56
5			Adipic acid, isobutyl pent-4-en-...	270	C15H26O4	1000354-11-8	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010923\
Data File : BF131971.D
Acq On : 09 Jan 2023 19:29
Operator : CG\JU
Sample : 01046-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-SAMPLE-API-3

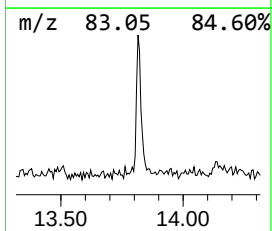
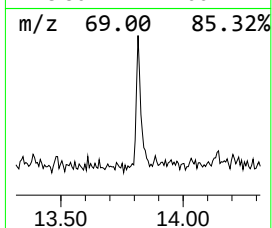
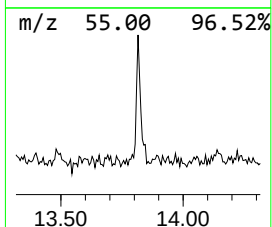
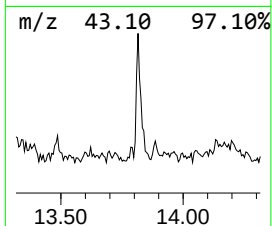
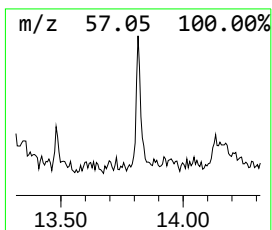
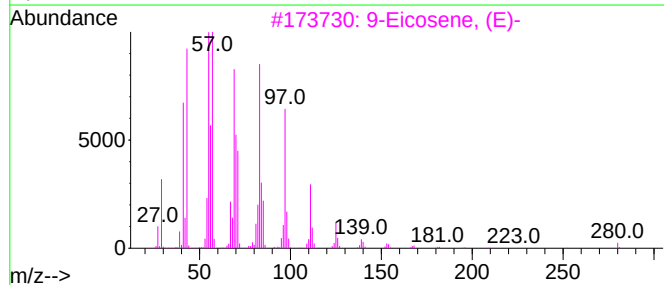
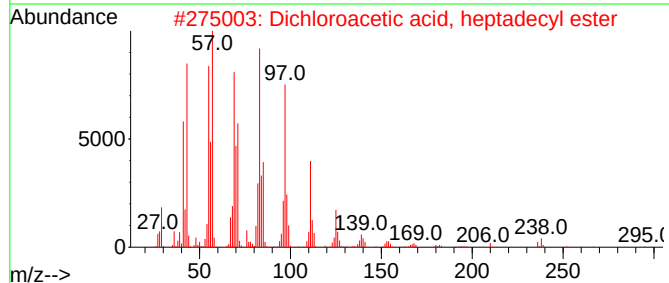
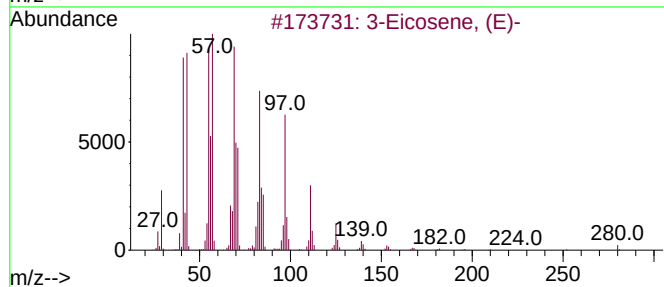
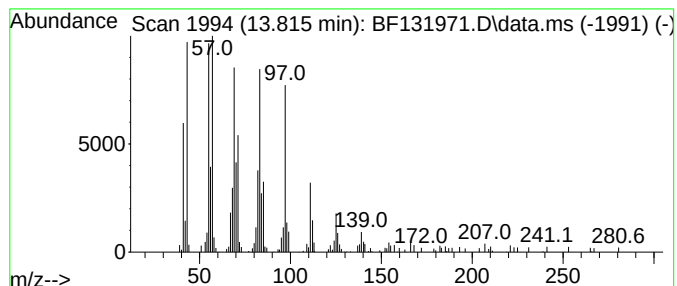
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 3-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.815	6.66 ng	132069	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Eicosene, (E)-	280	C20H40	074685-33-9	95
2			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
3			9-Eicosene, (E)-	280	C20H40	074685-29-3	93
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5			Behenic alcohol	326	C22H46O	000661-19-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010923\
Data File : BF131971.D
Acq On : 09 Jan 2023 19:29
Operator : CG\JU
Sample : 01046-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

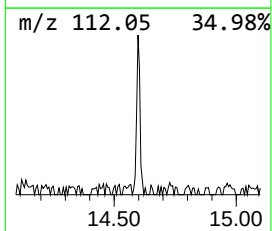
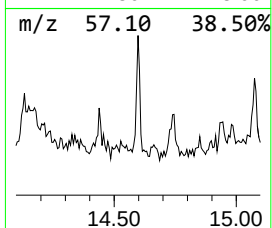
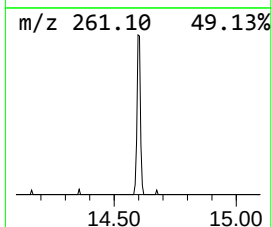
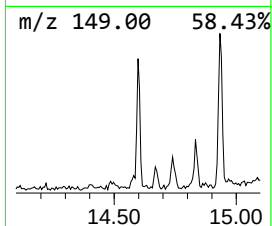
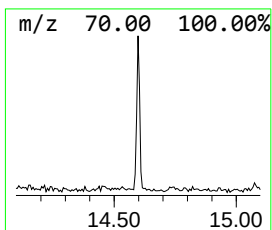
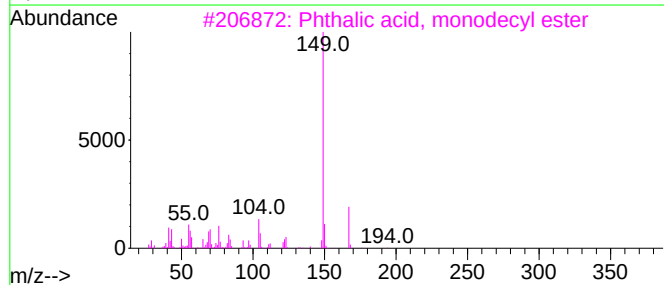
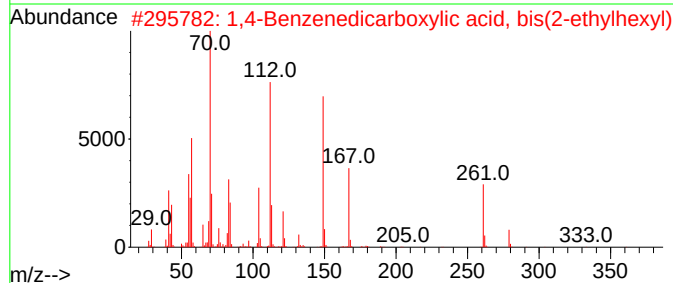
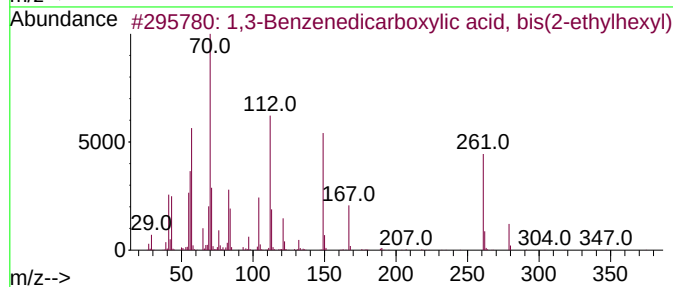
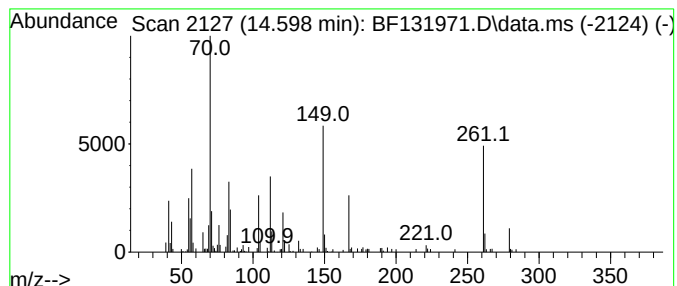
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1,3-Benzenedicarboxylic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.598	3.43 ng	68081	Chrysene-d12	13.974		
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	87
2		1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	72
3		Phthalic acid, monodecyl ester	306	C18H26O4	024539-60-4	43
4		Acetic acid, [4-(4-methyl-1-pipe...	262	C14H18N2O3	346699-90-9	25
5		3-Chloropropionic acid, 2-ethylh...	220	C11H21ClO2	091369-31-2	16



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010923\
Data File : BF131971.D
Acq On : 09 Jan 2023 19:29
Operator : CG\JU
Sample : 01046-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-SAMPLE-API-3

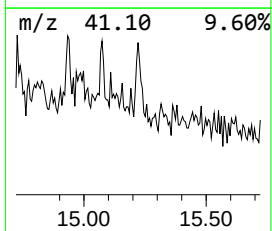
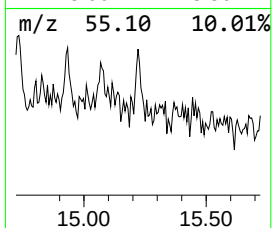
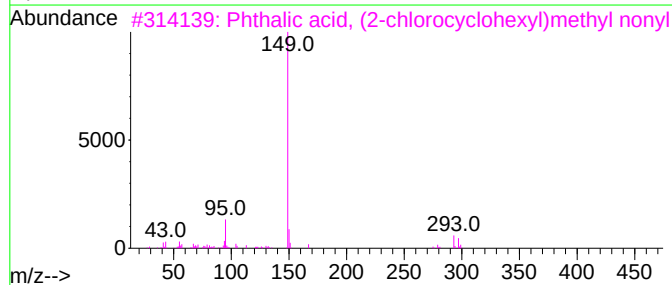
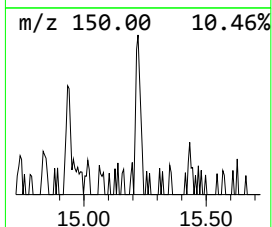
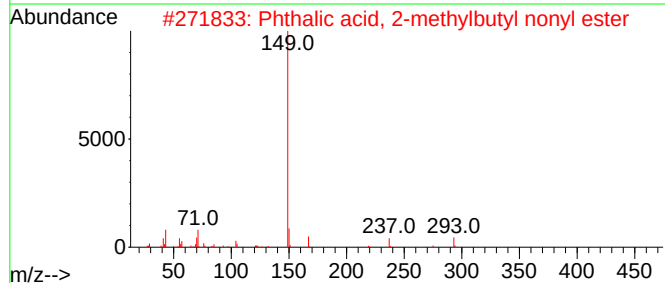
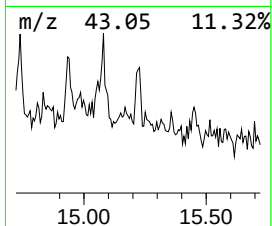
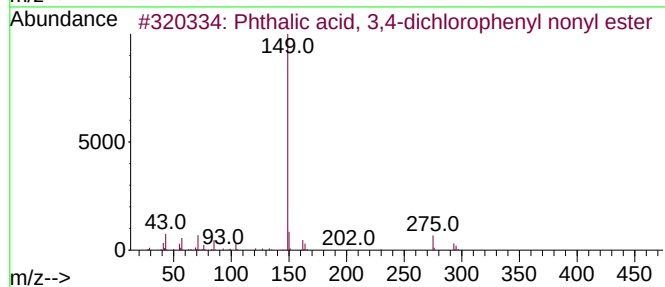
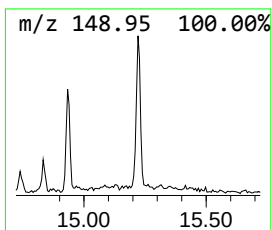
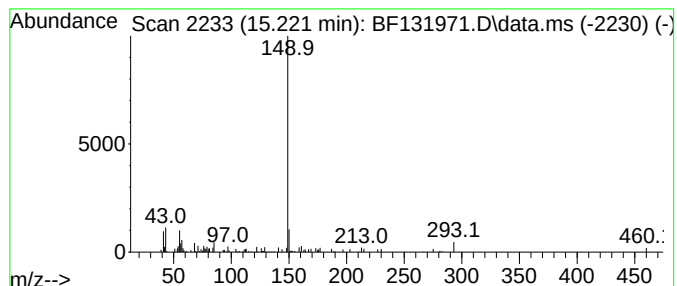
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Phthalic acid, 3,4-dichloro... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.221	2.67 ng	50475	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic acid, 3,4-dichloropheny...	436	C23H26Cl2O4	1000315-27-8	72
2			Phthalic acid, 2-methylbutyl non...	362	C22H34O4	1000322-81-7	72
3			Phthalic acid, (2-chlorocyclohex...	422	C24H35ClO4	1000315-34-7	72
4			Phthalic acid, butyl tetradecyl ...	418	C26H42O4	1000308-91-3	64
5			Phthalic acid, dodecyl 2-fluorop...	428	C26H33FO4	1000356-15-1	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010923\
Data File : BF131971.D
Acq On : 09 Jan 2023 19:29
Operator : CG\JU
Sample : 01046-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-SAMPLE-API-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.981	18.3	ng	430648	1	6.781	470832	20.0
Ethanol, 2-butoxy-	5.722	15.7	ng	369881	1	6.781	470832	20.0
2-Propanol, 1-(...	8.298	35.7	ng	1117280	2	8.075	625394	20.0
1-Propanol, 2-(...	8.322	37.9	ng	1183460	2	8.075	625394	20.0
Propanedioic ac...	8.410	2.1	ng	64606	2	8.075	625394	20.0
Butyl citrate	12.727	3.1	ng	62576	5	13.974	396836	20.0
3-Eicosene, (E)-	13.815	6.7	ng	132069	5	13.974	396836	20.0
1,3-Benzenedica...	14.598	3.4	ng	68081	5	13.974	396836	20.0
Phthalic acid, ...	15.221	2.7	ng	50475	6	15.439	377609	20.0