

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082823\
 Data File : BF134969.D
 Acq On : 28 Aug 2023 15:28
 Operator : CG\JU
 Sample : 04152-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-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-BF082223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134969.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.004	492	496	506	rVB	415117	419234	14.86%	2.684%
2	5.416	562	566	576	rVB	972522	840890	29.81%	5.383%
3	6.422	734	737	744	rBV	533923	531047	18.82%	3.400%
4	6.593	763	766	769	rBV	246714	190822	6.76%	1.222%
5	6.622	769	771	775	rVB	145961	102177	3.62%	0.654%
6	6.716	783	787	791	rBV	831444	772760	27.39%	4.947%
7	6.793	796	800	802	rBV	722120	580875	20.59%	3.719%
8	6.822	802	805	808	rVB	678359	492062	17.44%	3.150%
9	7.193	865	868	873	rBV	71452	59717	2.12%	0.382%
10	7.351	890	895	898	rBV	1671776	1596456	56.59%	10.220%
11	8.069	1013	1017	1026	rBV	943146	753798	26.72%	4.826%
12	9.151	1196	1201	1204	rBV	3145515	2821160	100.00%	18.060%
13	9.269	1217	1221	1224	rVB2	33929	31881	1.13%	0.204%
14	9.445	1248	1251	1254	rBV	85153	74149	2.63%	0.475%
15	9.828	1312	1316	1319	rBV	924858	716693	25.40%	4.588%
16	10.186	1371	1377	1379	rBV2	31187	31587	1.12%	0.202%
17	10.251	1384	1388	1391	rVB	145050	124882	4.43%	0.799%
18	10.616	1447	1450	1454	rBV	1138701	1037915	36.79%	6.644%
19	10.986	1509	1513	1516	rVB2	36422	42014	1.49%	0.269%
20	11.322	1566	1570	1573	rBV	714514	615281	21.81%	3.939%
21	11.857	1657	1661	1669	rBV2	326082	335651	11.90%	2.149%
22	12.645	1793	1795	1801	rBV	117127	112418	3.98%	0.720%
23	12.916	1837	1841	1845	rBV	2175499	2011838	71.31%	12.879%
24	13.827	1993	1996	2000	rBV2	107367	112706	4.00%	0.722%
25	13.974	2018	2021	2025	rBV	641660	598094	21.20%	3.829%
26	15.457	2269	2273	2284	rVB	420102	614763	21.79%	3.936%

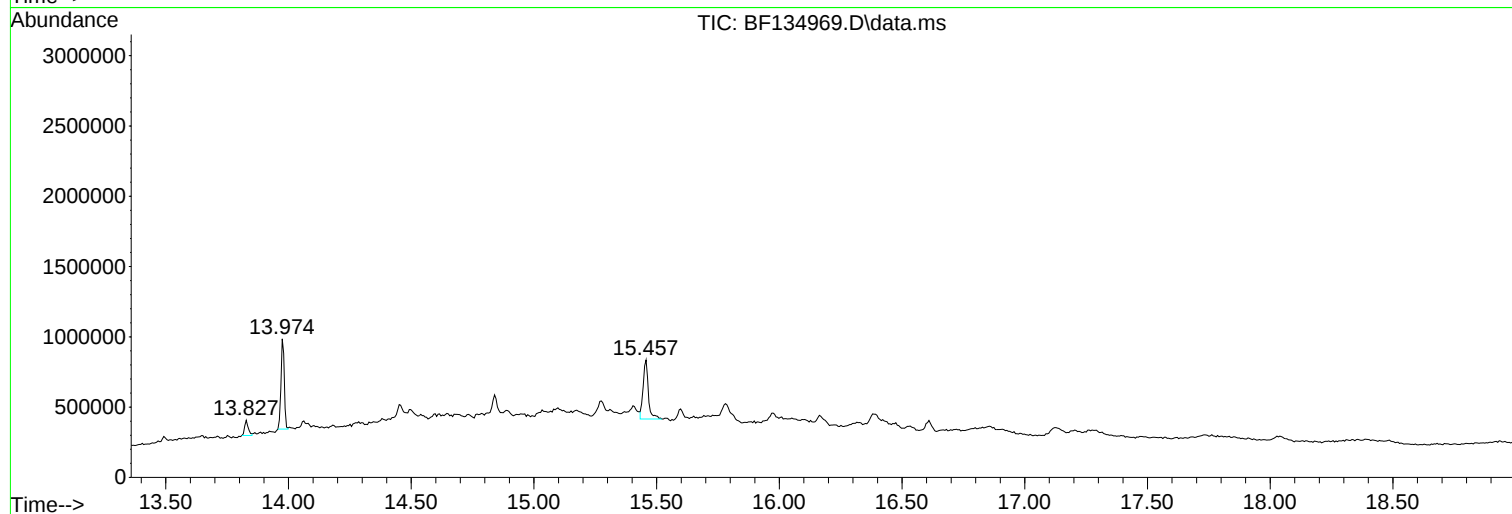
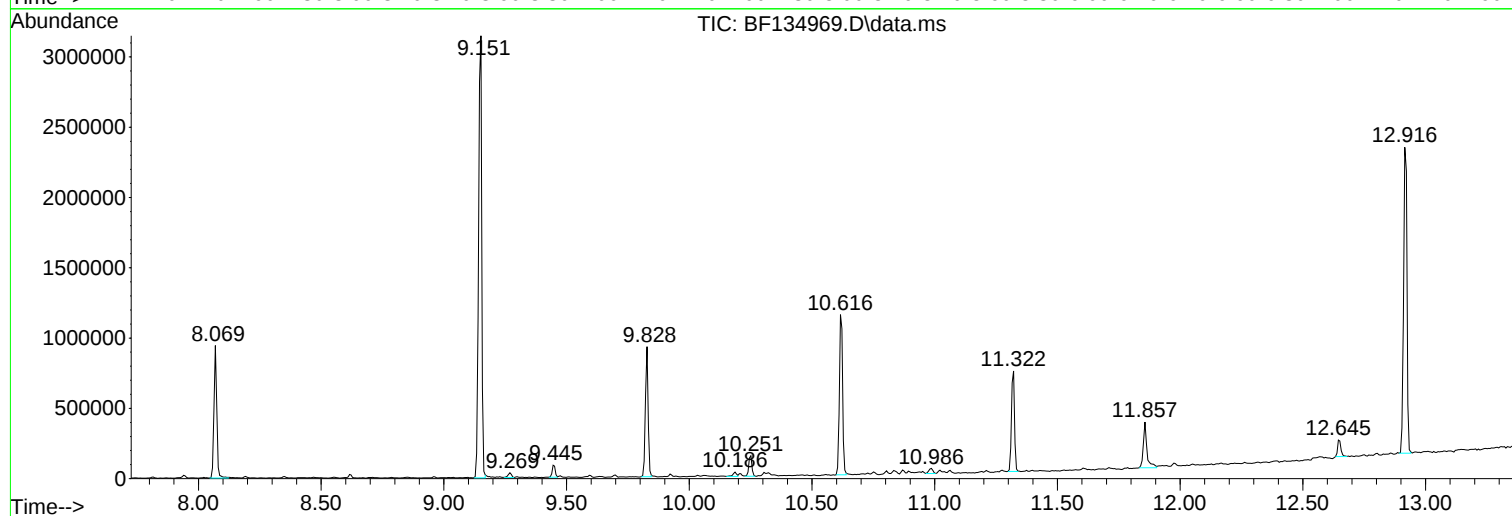
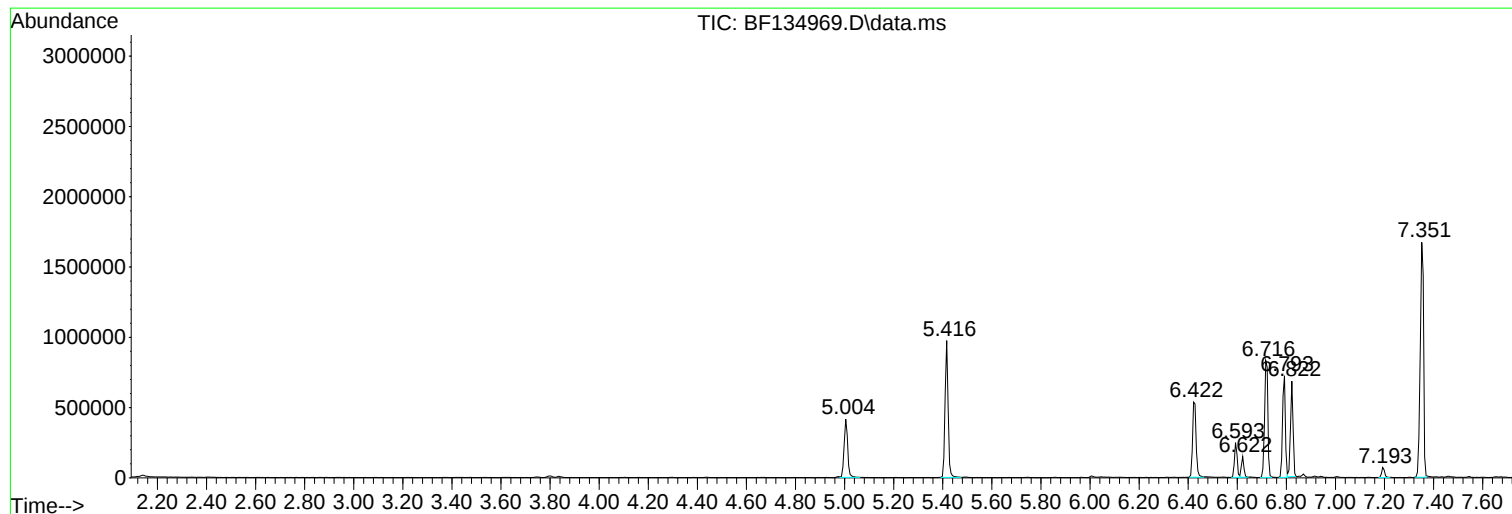
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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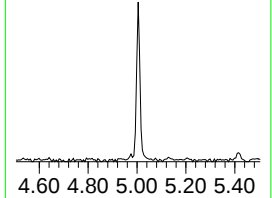
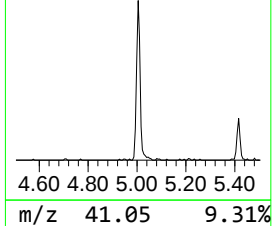
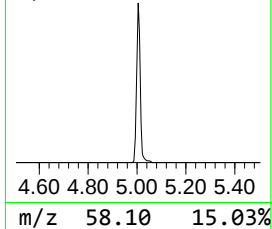
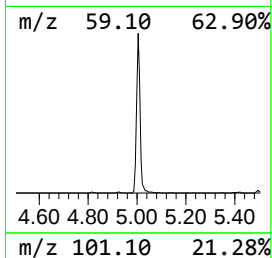
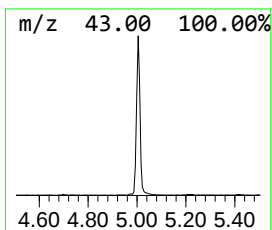
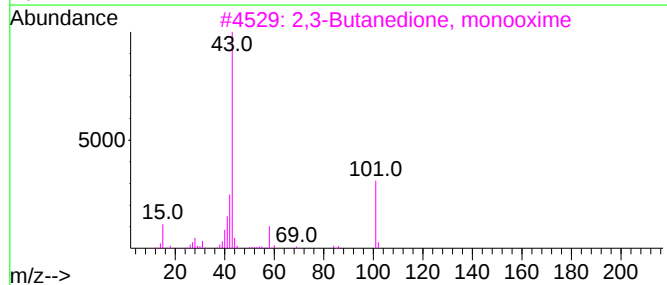
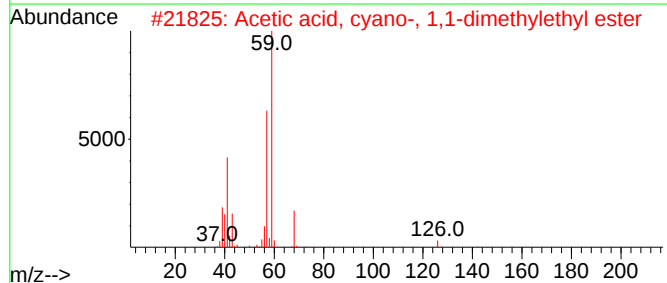
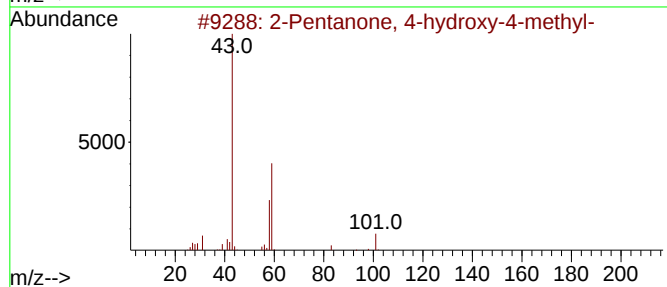
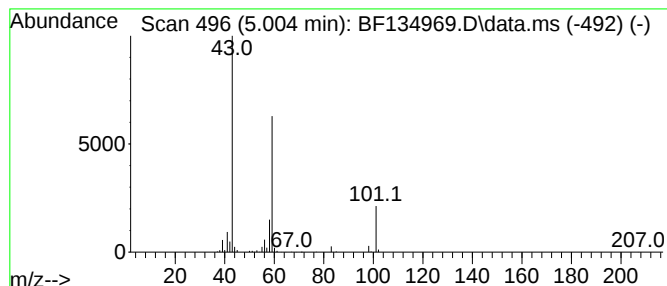
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.004	14.43 ng	419234	1,4-Dichlorobenzene-d4	6.793

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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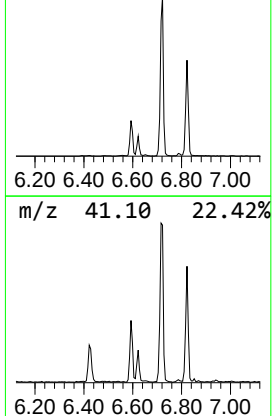
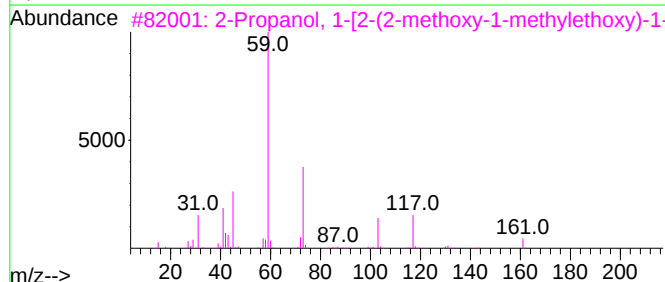
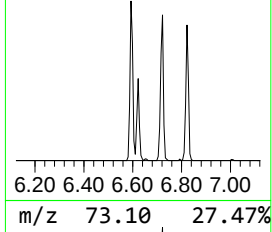
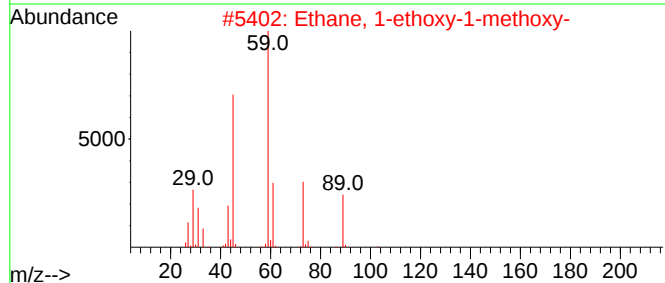
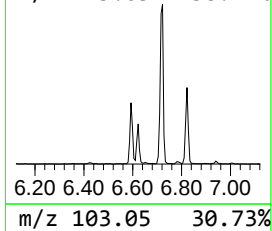
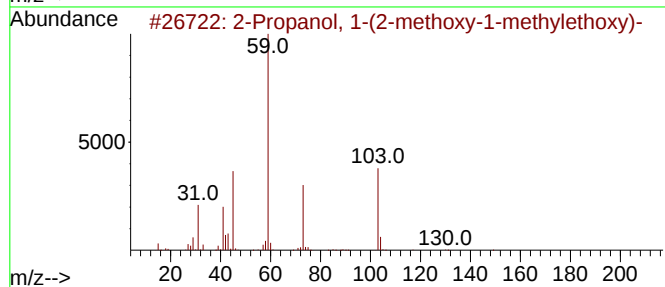
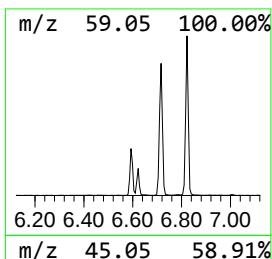
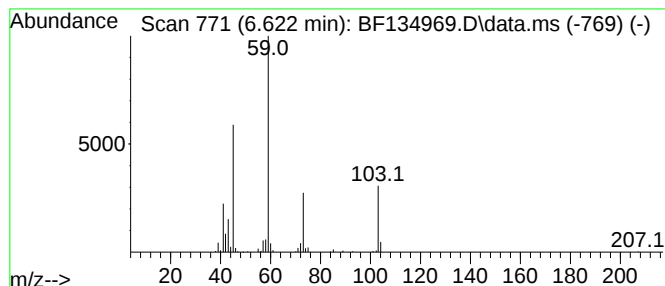
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.622	3.52 ng	102177	1,4-Dichlorobenzene-d4	6.793

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	72		
2	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	64		
3	2-Propanol, 1-[2-(2-methoxy-1-me...	206	C10H22O4	020324-33-8	59		
4	2-(2-(2-(2-(2-(2-Methoxyethoxy)e...	310	C13H26O8	016142-03-3	56		
5	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	53		



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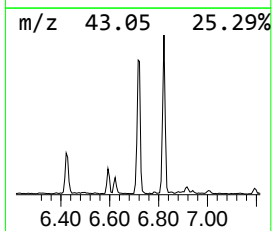
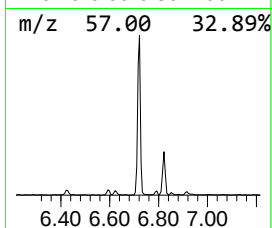
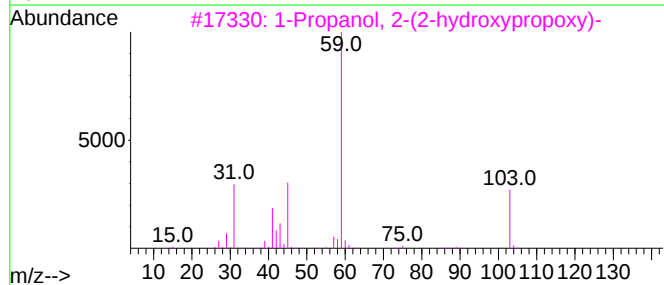
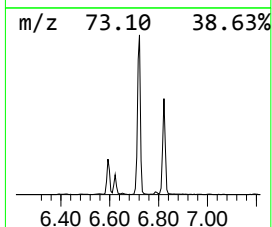
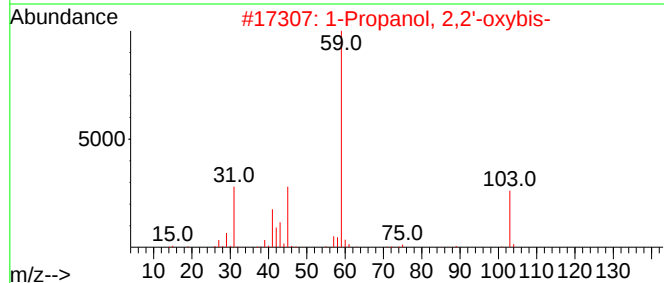
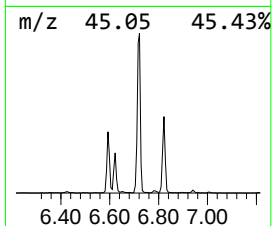
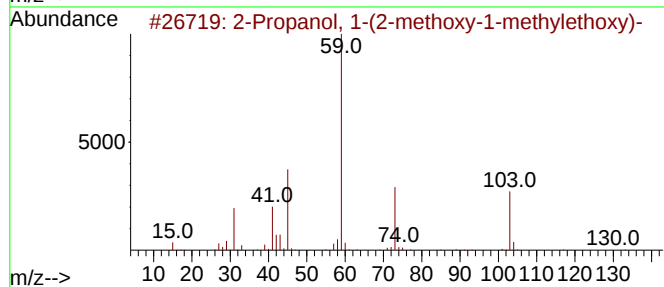
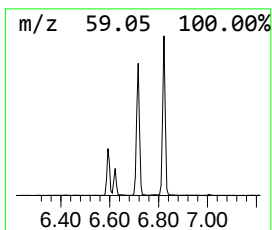
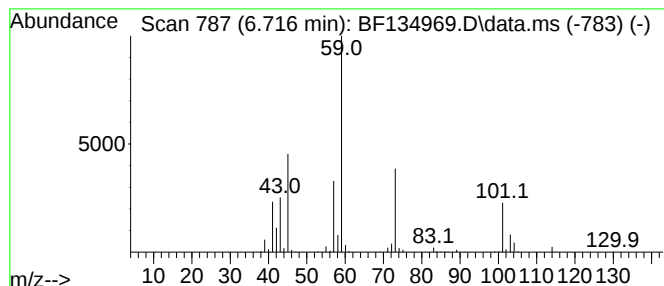
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Propanol, 2,2'-oxybis- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.716	26.61 ng	772760	1,4-Dichlorobenzene-d4	6.793

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	50		
2	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	38		
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	38		
4	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	37		
5	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	37		



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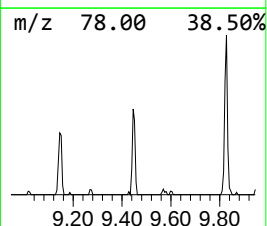
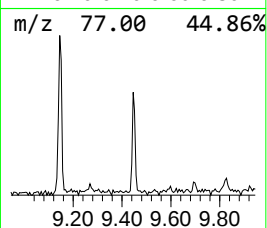
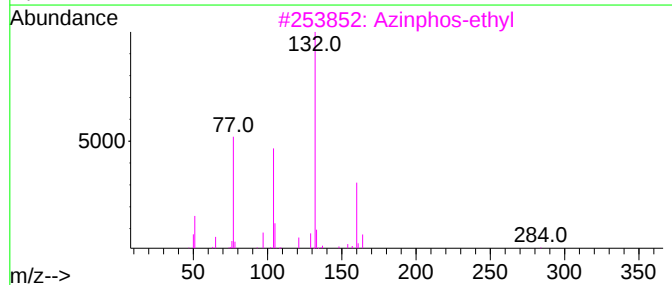
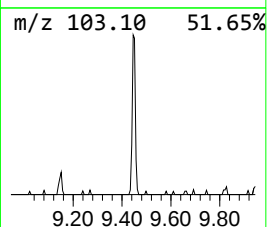
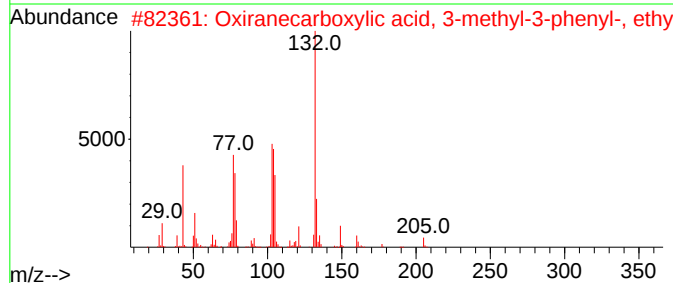
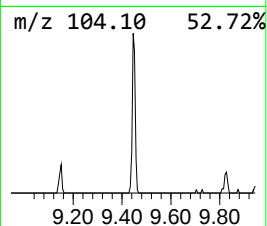
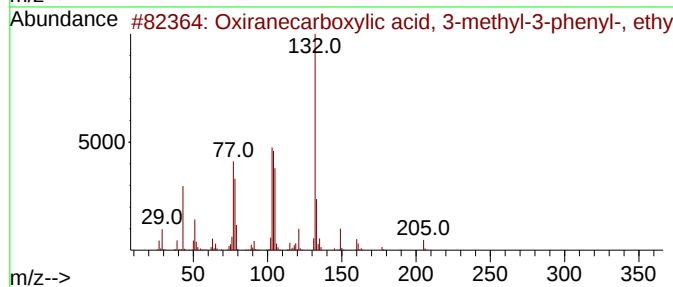
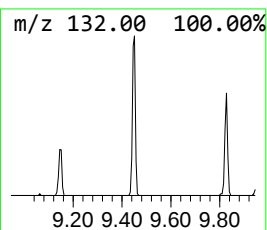
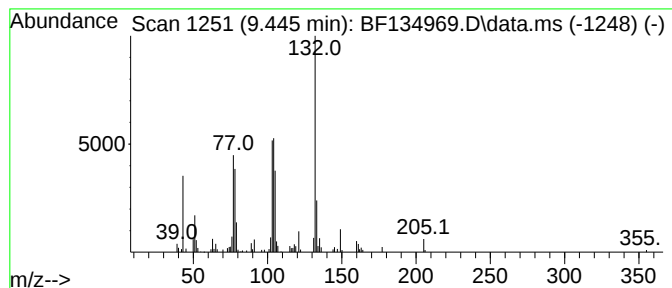
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Peak Number 6 Oxiranecarboxylic acid, 3-m... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.445	2.07 ng	74149	Acenaphthene-d10	9.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxiranecarboxylic acid, 3-methyl...	206	C12H14O3	019464-92-7	99
2			Oxiranecarboxylic acid, 3-methyl...	206	C12H14O3	019464-95-0	99
3			Azinphos-ethyl	345	C12H16N3O3PS2	002642-71-9	47
4			Oxiranecarboxylic acid, 3-methyl...	206	C12H14O3	000077-83-8	47
5			1H-Indol-3-amine	132	C8H8N2	007250-19-3	38



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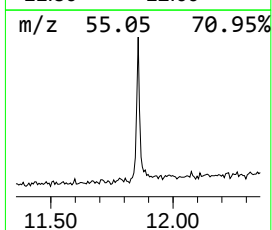
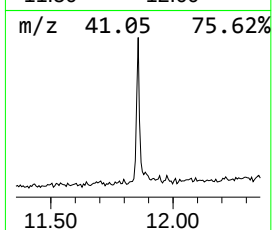
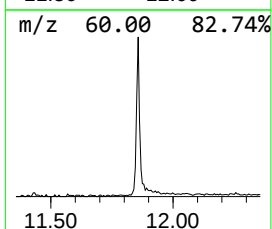
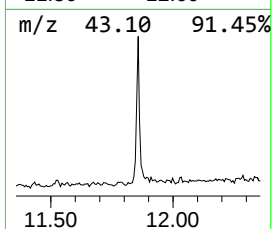
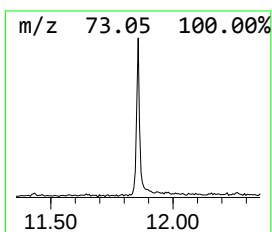
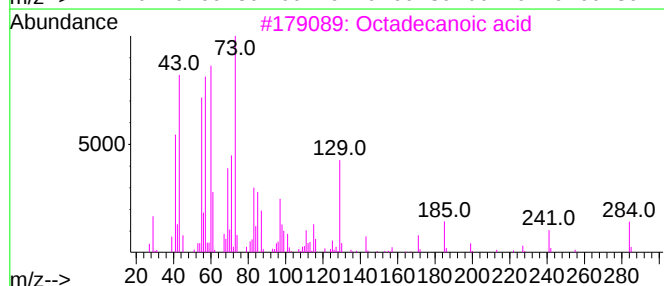
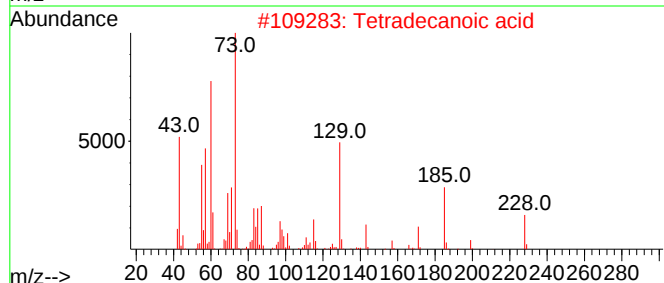
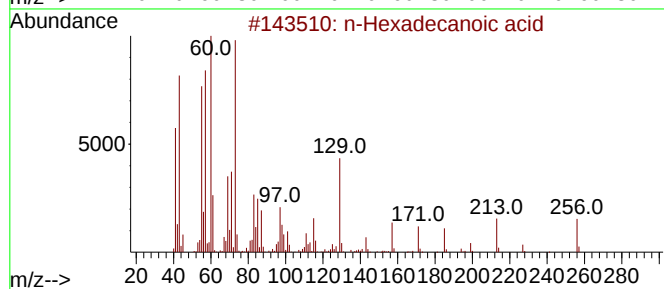
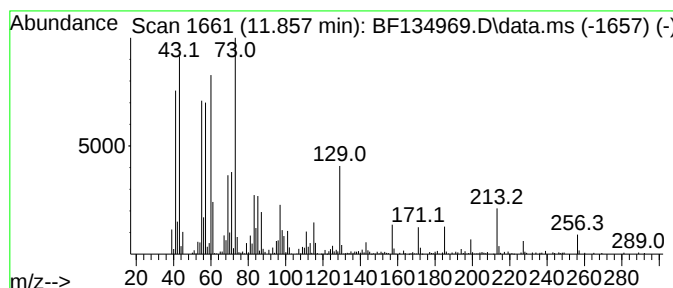
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Peak Number 7 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	10.91 ng	335651	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3			Octadecanoic acid	284	C18H36O2	000057-11-4	87
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Tridecanoic acid	214	C13H26O2	000638-53-9	81



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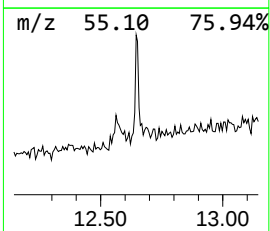
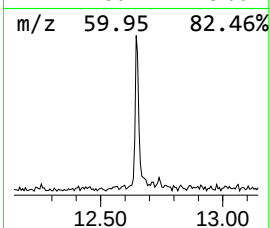
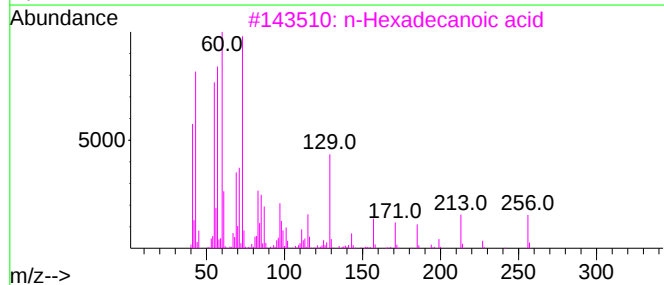
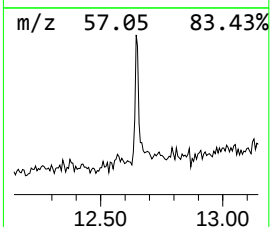
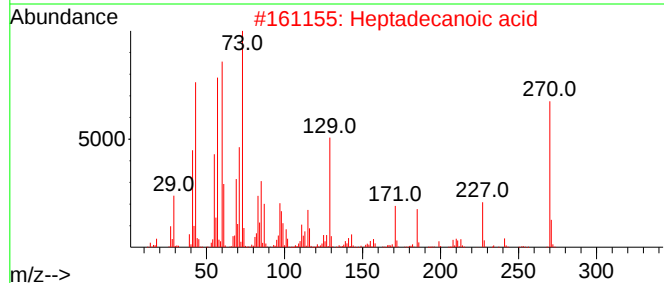
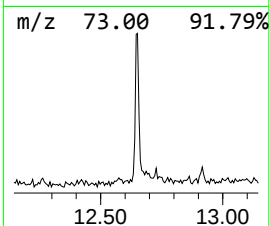
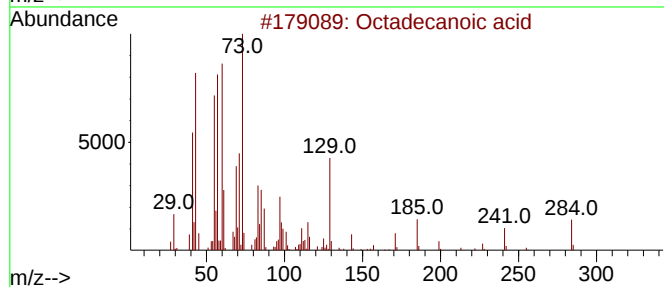
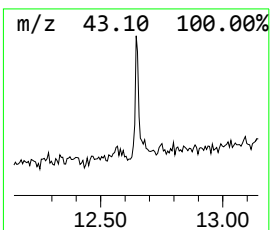
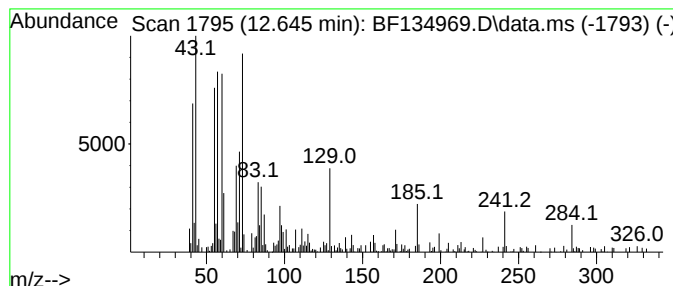
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	3.65 ng	112418	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Heptadecanoic acid	270	C17H34O2	000506-12-7	97
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
4			Nonadecanoic acid	298	C19H38O2	000646-30-0	93
5			Heneicosanoic acid	326	C21H42O2	002363-71-5	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082823\
Data File : BF134969.D
Acq On : 28 Aug 2023 15:28
Operator : CG\JU
Sample : 04152-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

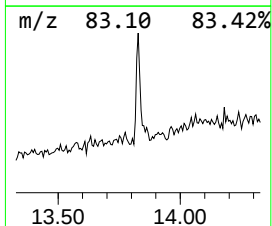
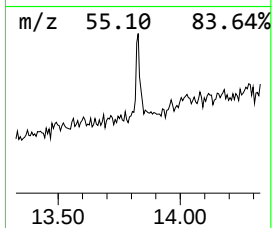
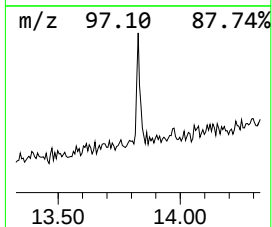
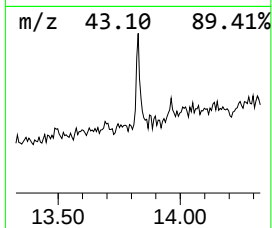
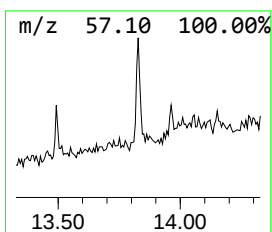
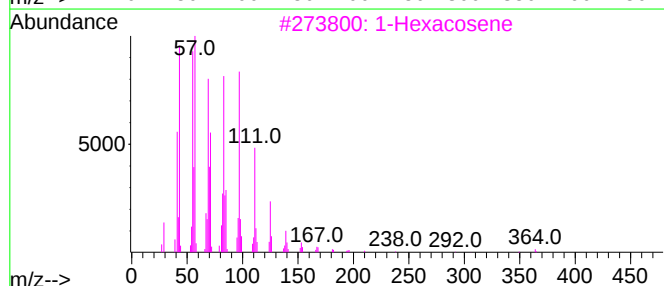
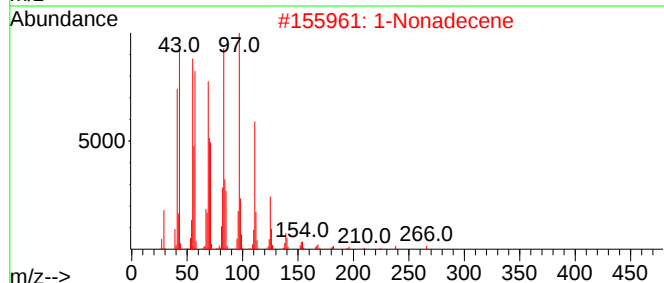
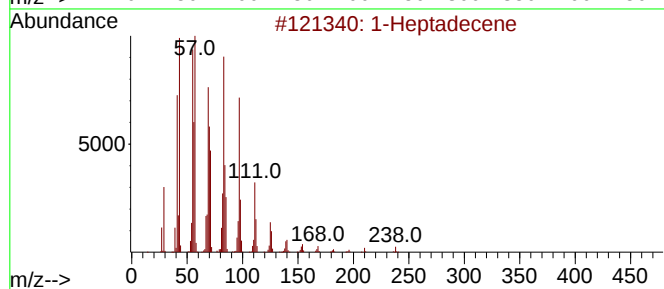
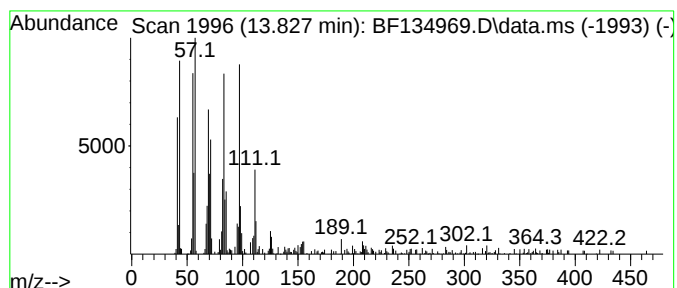
Instrument :
BNA_F
ClientSampleId :
COMPOSITE-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Heptadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.827	3.77 ng	112706	Chrysene-d12	13.974	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptadecene	238	C17H34	006765-39-5	96
2	1-Nonadecene	266	C19H38	018435-45-5	95
3	1-Hexacosene	364	C26H52	018835-33-1	94
4	1-Heptacosanol	396	C27H56O	002004-39-9	94
5	1-Tricosene	322	C23H46	018835-32-0	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082823\
Data File : BF134969.D
Acq On : 28 Aug 2023 15:28
Operator : CG\JU
Sample : 04152-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.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
2-Pentanone, 4-...	5.004	14.4	ng	419234	1	6.793	580875	20.0
2-Propanol, 1-(...	6.622	3.5	ng	102177	1	6.793	580875	20.0
1-Propanol, 2,2...	6.716	26.6	ng	772760	1	6.793	580875	20.0
Oxiranecarboxyl...	9.445	2.1	ng	74149	3	9.828	716693	20.0
n-Hexadecanoic ...	11.857	10.9	ng	335651	4	11.322	615281	20.0
Octadecanoic acid	12.645	3.6	ng	112418	4	11.322	615281	20.0
1-Heptadecene	13.827	3.8	ng	112706	5	13.974	598094	20.0