

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092223\
 Data File : BF135403.D
 Acq On : 22 Sep 2023 17:02
 Operator : CG\JU
 Sample : 04491-09
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FB-9-15

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-BF091123.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135403.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.999	491	495	506	rVB	96113	135093	2.44%	0.426%
2	5.399	559	563	573	rBV	3173705	3147438	56.79%	9.920%
3	6.399	729	733	750	rBV	2519872	2578874	46.53%	8.128%
4	6.757	790	794	803	rBV	1093945	926131	16.71%	2.919%
5	7.322	885	890	893	rBV	3007736	3661914	66.07%	11.542%
6	8.034	1007	1011	1015	rBV	1353530	1188954	21.45%	3.747%
7	8.263	1046	1050	1052	rBV	177662	215786	3.89%	0.680%
8	8.287	1052	1054	1067	rVB	230324	336739	6.08%	1.061%
9	9.116	1189	1195	1198	rBV	4897096	5542210	100.00%	17.468%
10	9.792	1305	1310	1313	rBV	1418883	1253102	22.61%	3.949%
11	9.998	1340	1345	1350	rBV3	52349	88858	1.60%	0.280%
12	10.586	1440	1445	1449	rBV	2662125	2992696	54.00%	9.432%
13	11.286	1560	1564	1567	rBV	1267194	1185095	21.38%	3.735%
14	11.816	1649	1654	1674	rBV2	540295	892399	16.10%	2.813%
15	12.533	1770	1776	1784	rBV	272149	376440	6.79%	1.186%
16	12.610	1784	1789	1800	rVV	294192	435934	7.87%	1.374%
17	12.722	1801	1808	1816	rVB4	62810	170571	3.08%	0.538%
18	12.886	1831	1836	1839	rBV	3984896	4160247	75.06%	13.112%
19	13.469	1925	1935	1940	rBV2	89211	171831	3.10%	0.542%
20	13.939	2008	2015	2021	rBV	810791	744205	13.43%	2.346%
21	14.063	2030	2036	2040	rBV2	78712	133954	2.42%	0.422%
22	14.551	2114	2119	2126	rBV	95946	141418	2.55%	0.446%
23	14.792	2155	2160	2166	rVB	58720	78791	1.42%	0.248%
24	15.045	2197	2203	2210	rBV	72532	145637	2.63%	0.459%
25	15.404	2259	2264	2275	rBV	613080	882813	15.93%	2.782%
26	15.598	2292	2297	2302	rBV2	45091	72658	1.31%	0.229%
27	16.233	2399	2405	2414	rBV5	29652	68355	1.23%	0.215%

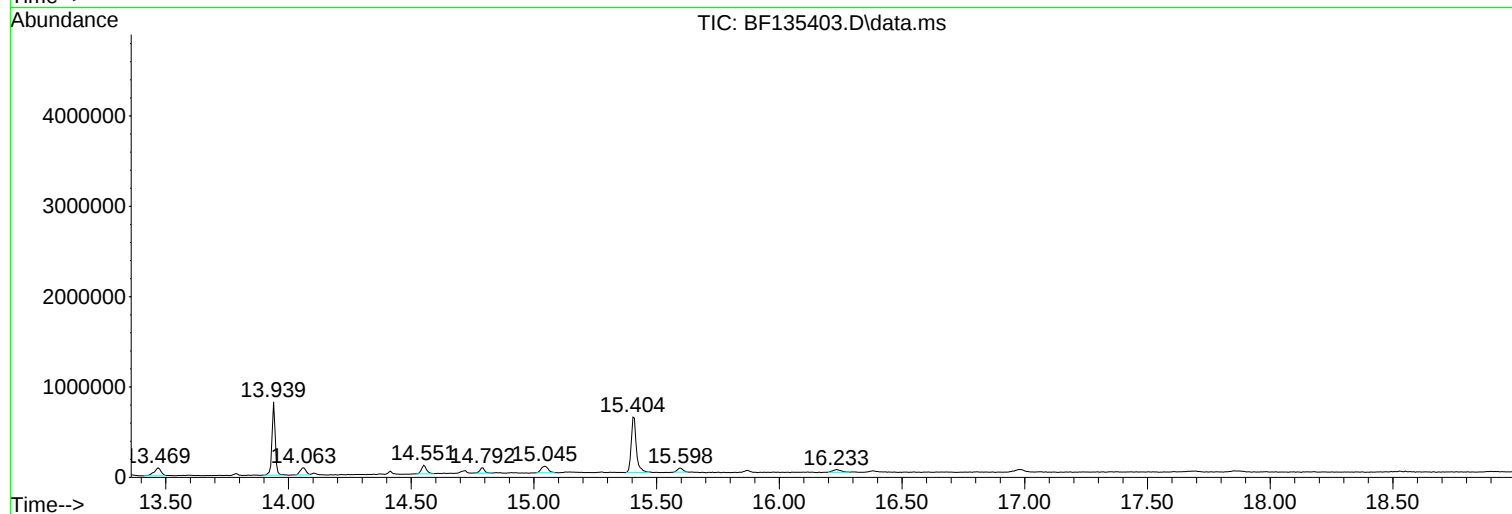
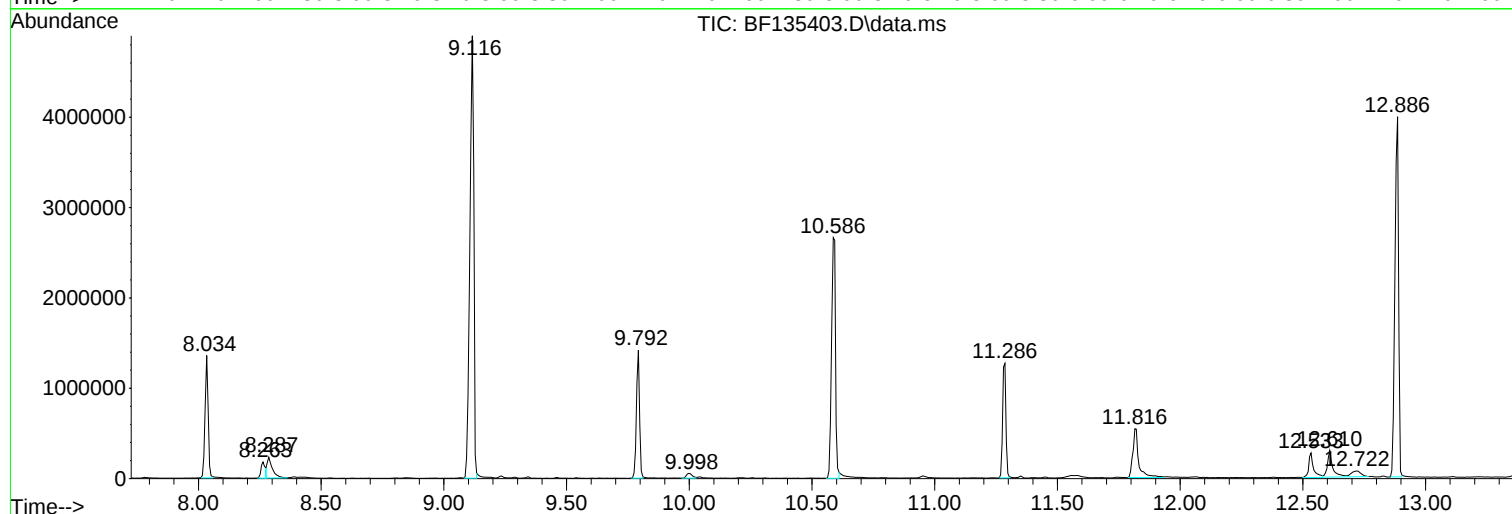
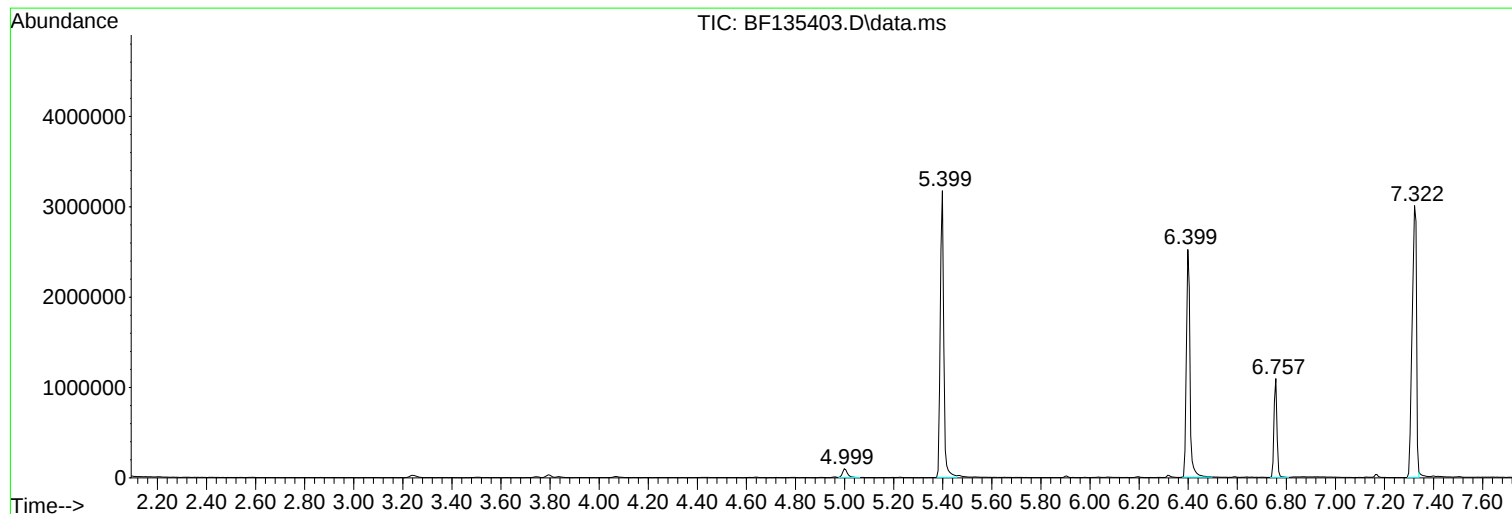
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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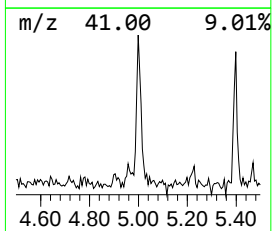
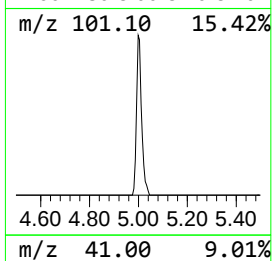
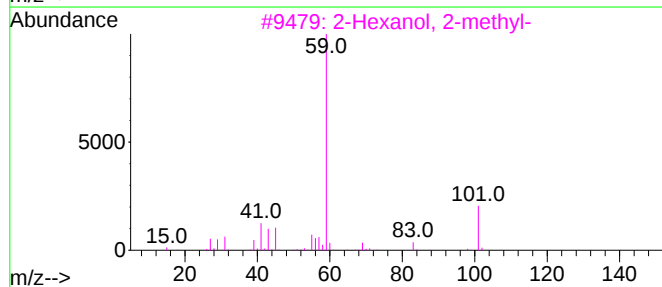
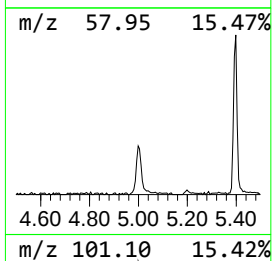
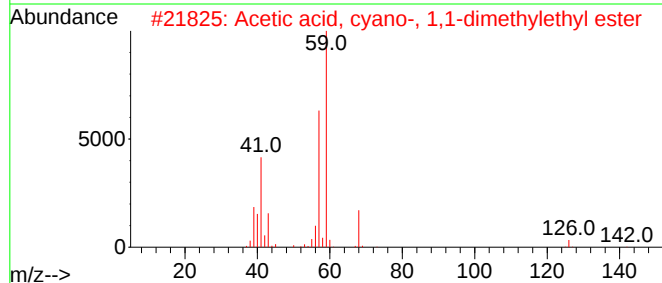
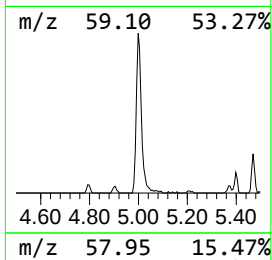
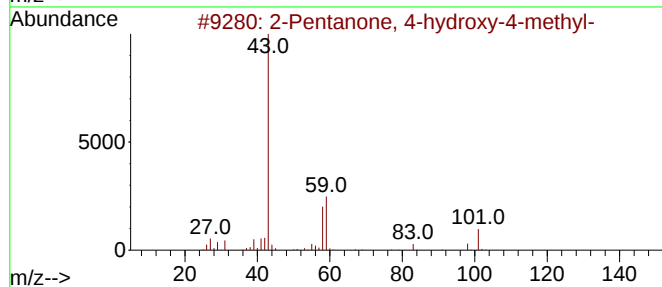
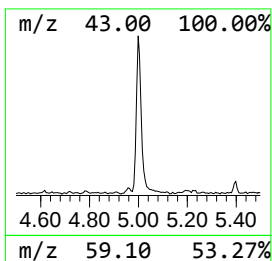
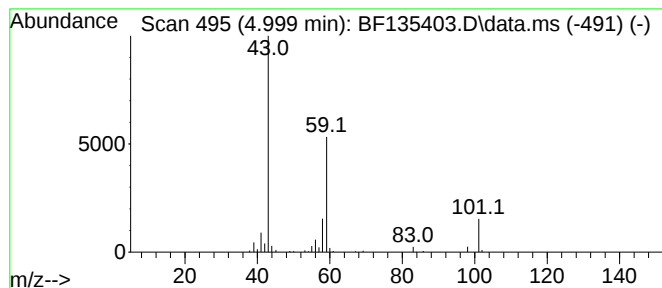
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.999	2.92 ng	135093	1,4-Dichlorobenzene-d4	6.757

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25	
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25	
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12	
5	2,3-Butanediol, 2,3-dimethyl-	118	C6H14O2	000076-09-5	9	



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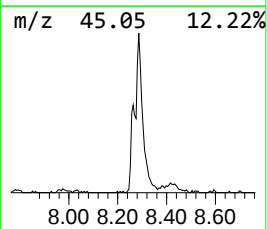
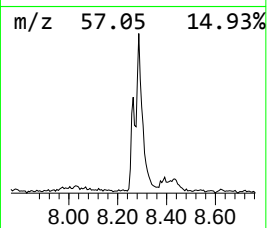
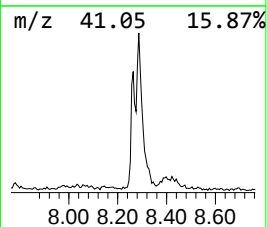
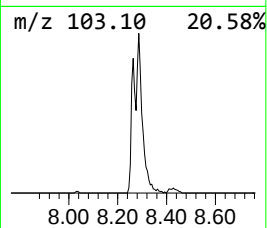
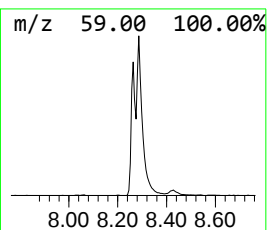
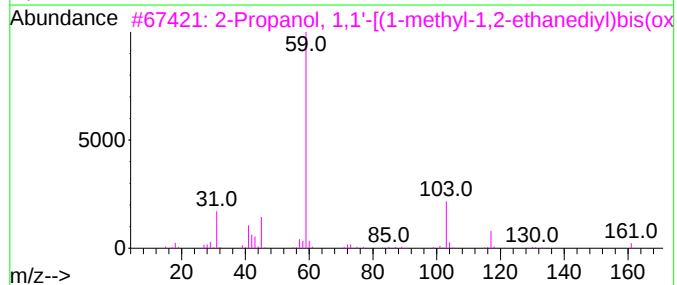
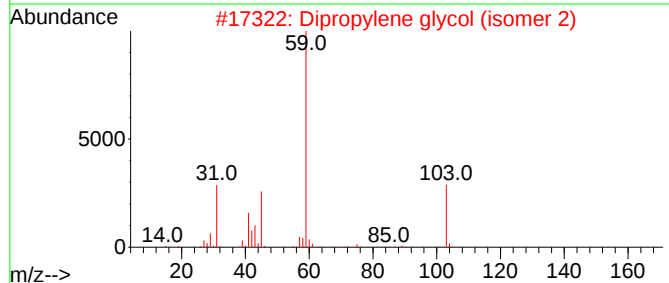
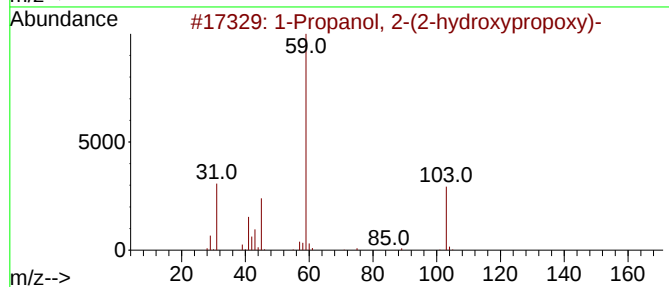
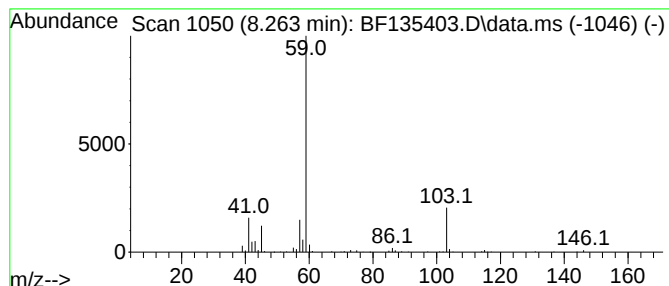
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Peak Number 2 1-Propanol, 2-(2-hydroxypro... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.263	3.63 ng	215786	Naphthalene-d8	8.034

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78		
2	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	78		
3	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	78		
4	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	78		
5	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	74		



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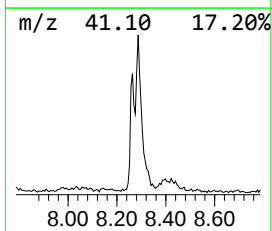
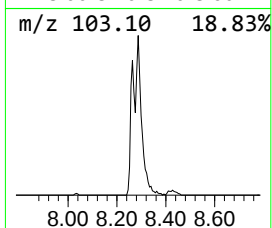
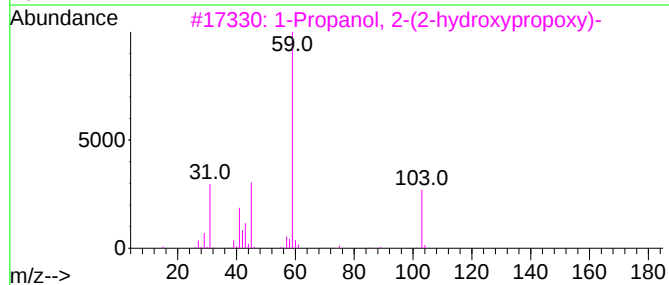
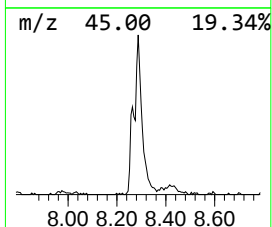
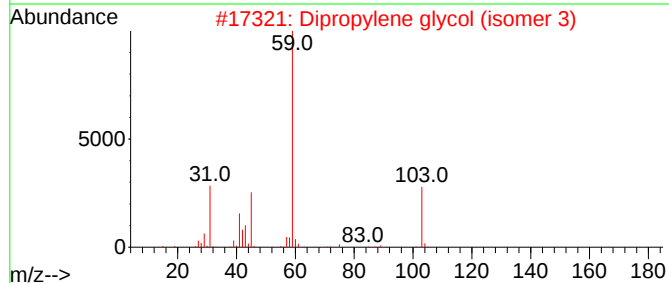
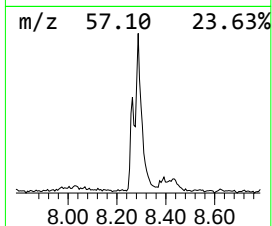
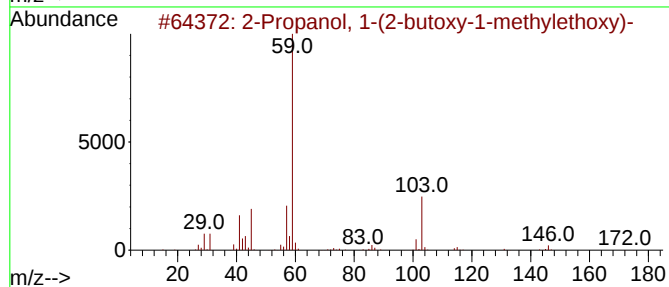
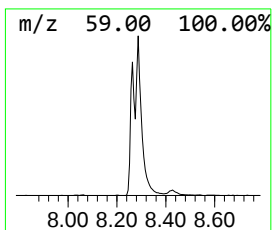
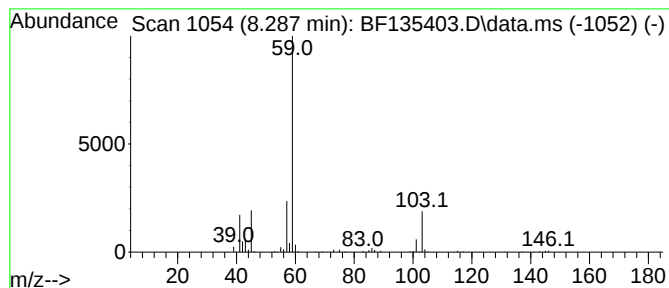
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TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Propanol, 1-(2-butoxy-1-m... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.287	5.66 ng	336739	Naphthalene-d8	8.034

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	83		
2	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	78		
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78		
4	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	78		
5	1,4,7-Trimethyl-3,6-dioxaoctane-...	192	C9H20O4	1000423-63-2	78		



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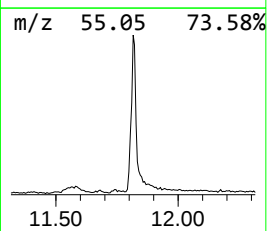
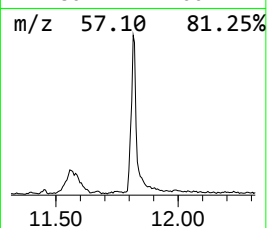
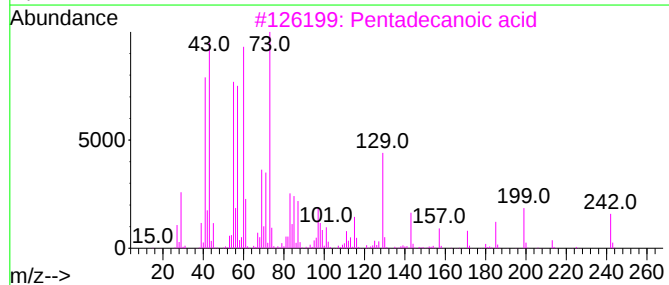
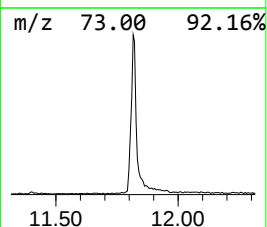
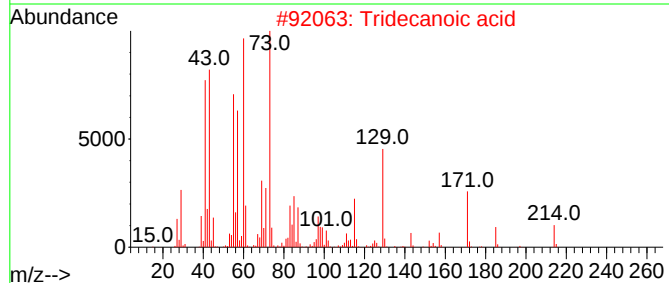
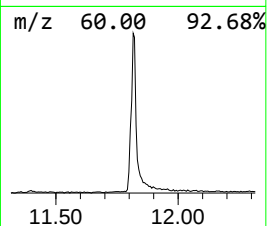
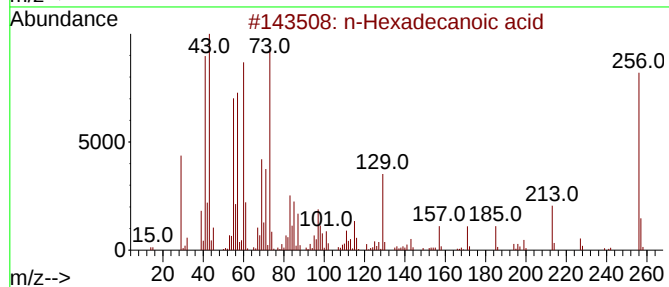
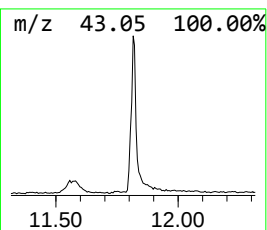
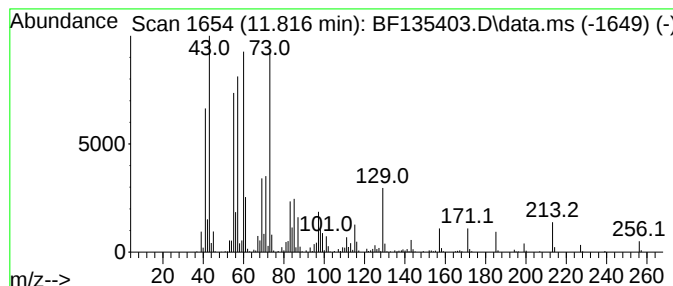
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.816	15.06 ng	892399	Phenanthrene-d10	11.286

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	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5		n-Decanoic acid	172	C10H20O2	000334-48-5	64



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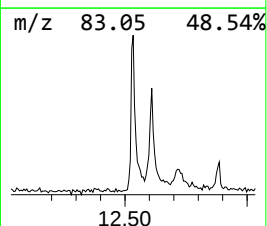
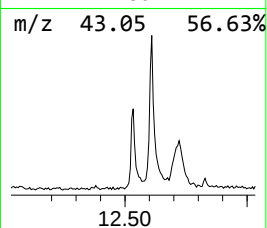
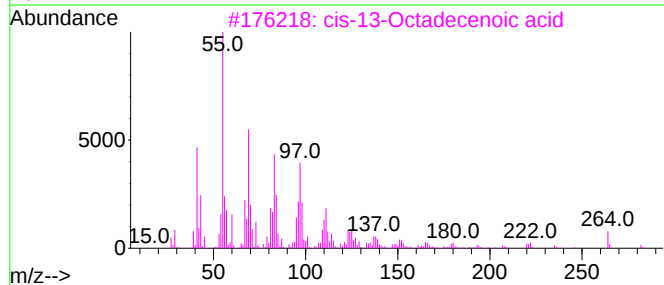
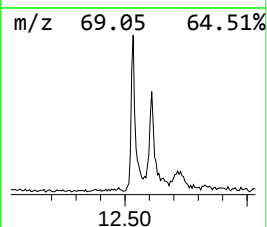
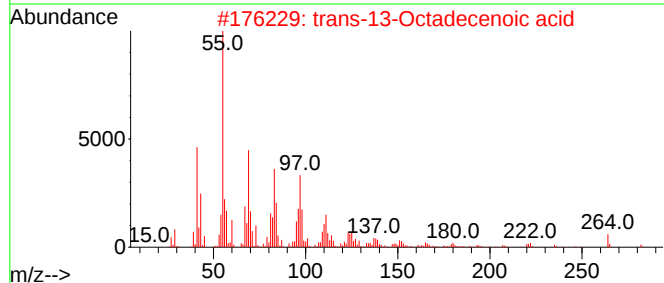
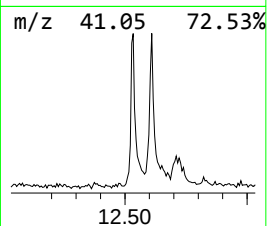
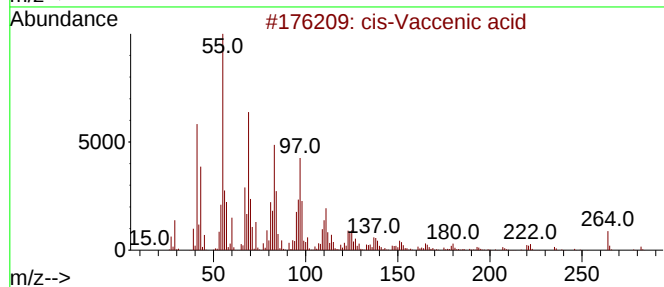
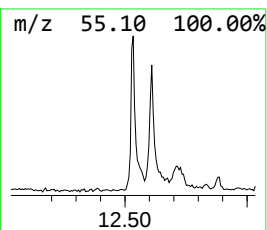
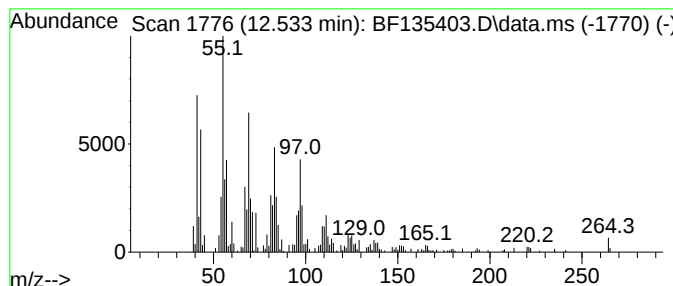
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Peak Number 5 cis-Vaccenic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.533	6.35 ng	376440	Phenanthrene-d10	11.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-Vaccenic acid	282	C18H34O2	000506-17-2	91
2			trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	91
3			cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	91
4			Oleic Acid	282	C18H34O2	000112-80-1	90
5			(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	87



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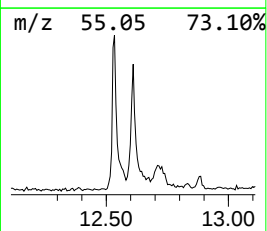
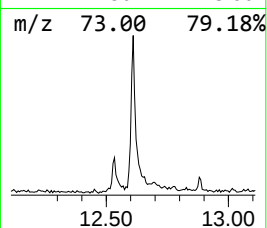
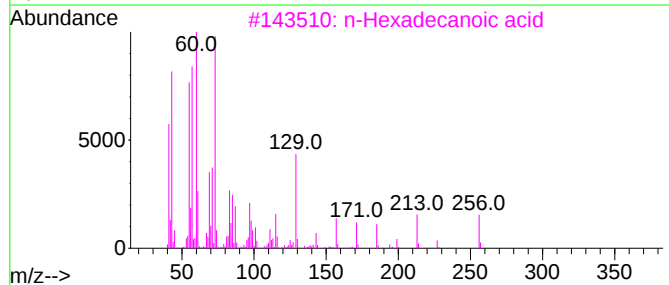
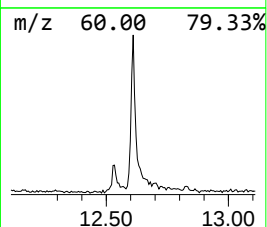
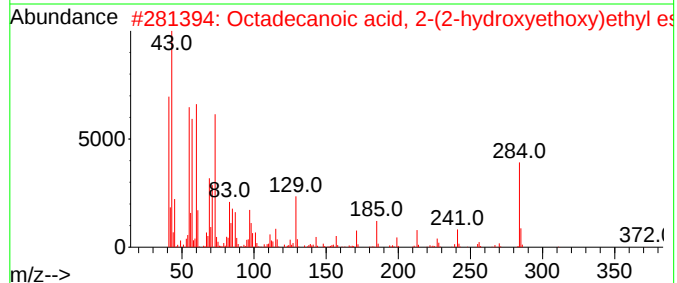
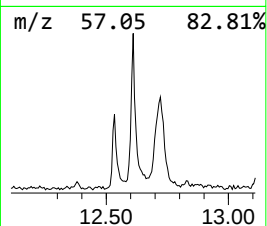
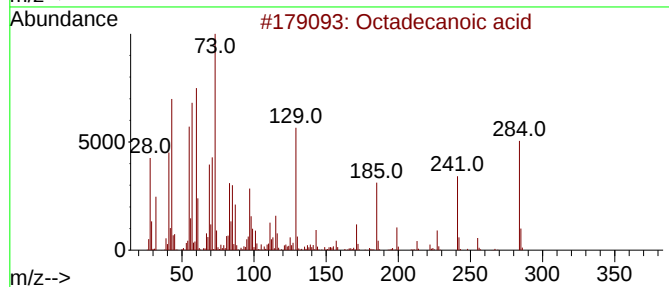
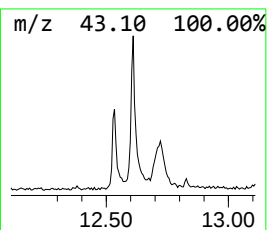
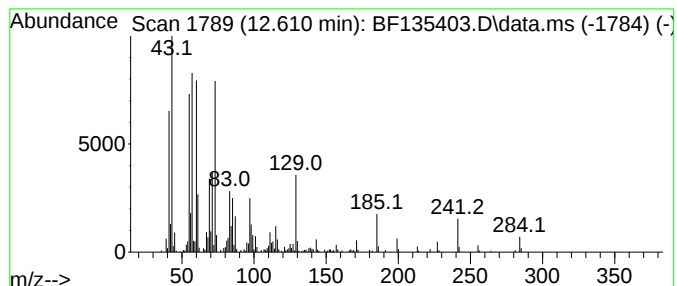
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	7.36 ng	435934	Phenanthrene-d10	11.286

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	83
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092223\
Data File : BF135403.D
Acq On : 22 Sep 2023 17:02
Operator : CG\JU
Sample : 04491-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FB-9-15

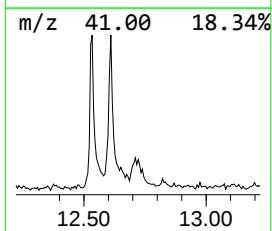
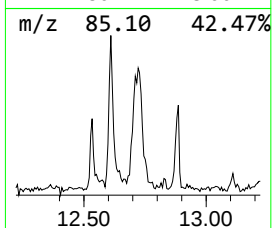
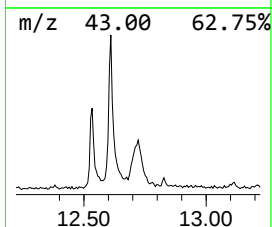
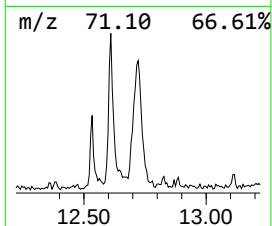
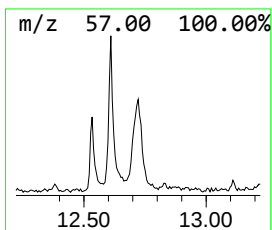
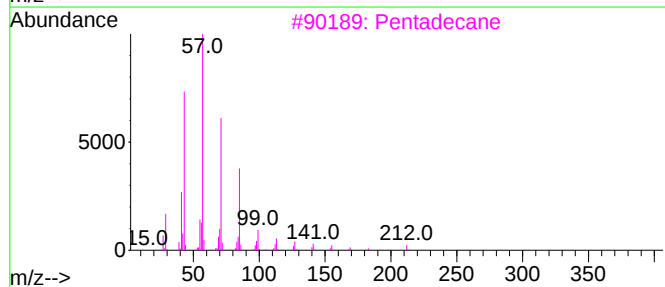
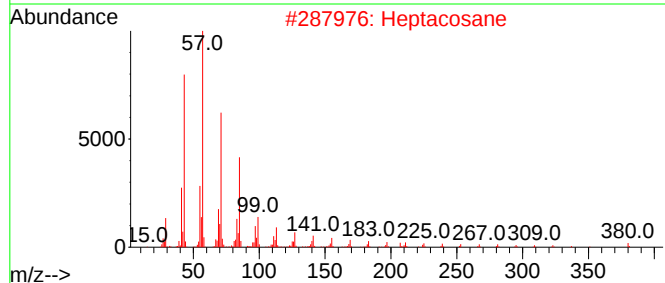
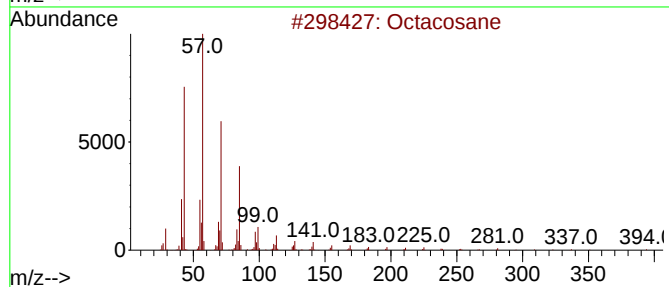
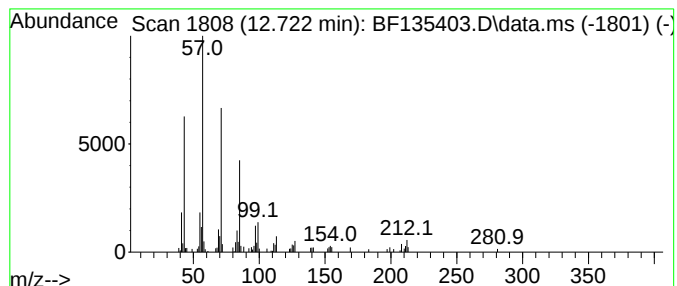
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.722	4.58 ng	170571	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	87
2			Heptacosane	380	C27H56	000593-49-7	86
3			Pentadecane	212	C15H32	000629-62-9	83
4			Tetracosane	338	C24H50	000646-31-1	80
5			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092223\
Data File : BF135403.D
Acq On : 22 Sep 2023 17:02
Operator : CG\JU
Sample : 04491-09
Misc :
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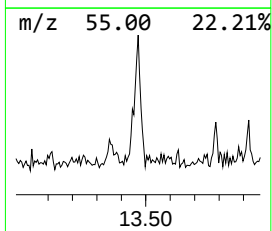
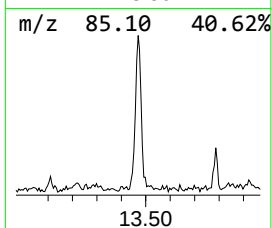
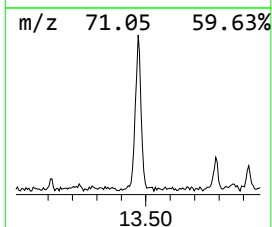
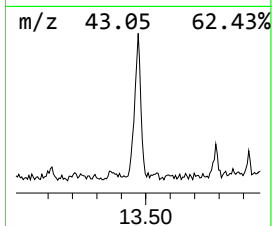
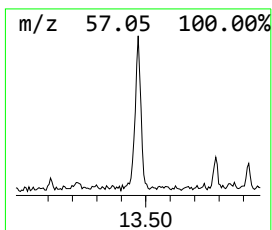
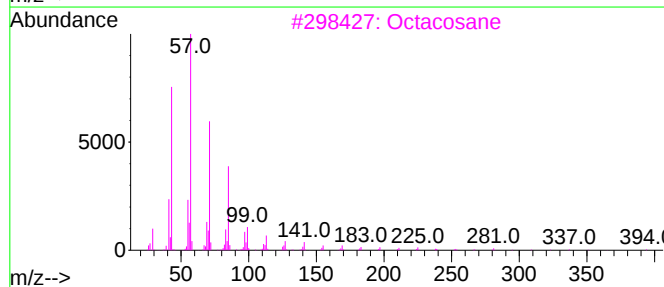
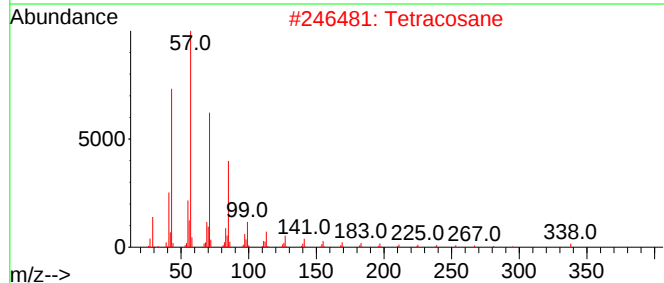
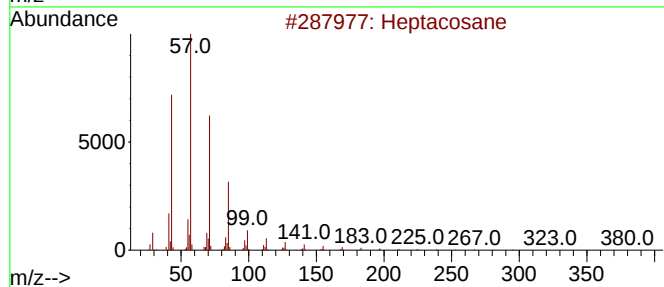
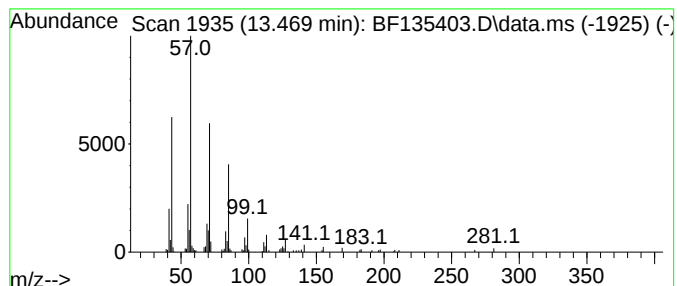
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.469	4.62 ng	171831	Chrysene-d12		13.939	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Tetracosane		338	C24H50	000646-31-1	90
3	Octacosane		394	C28H58	000630-02-4	90
4	Heneicosane		296	C21H44	000629-94-7	87
5	Hexacosane		366	C26H54	000630-01-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092223\
Data File : BF135403.D
Acq On : 22 Sep 2023 17:02
Operator : CG\JU
Sample : 04491-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

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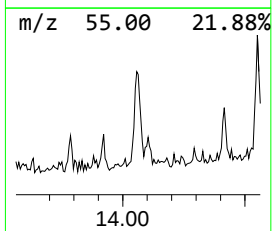
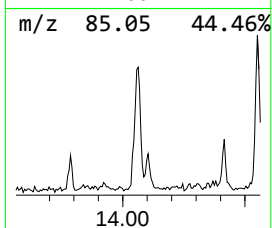
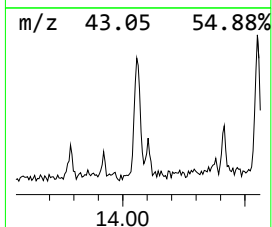
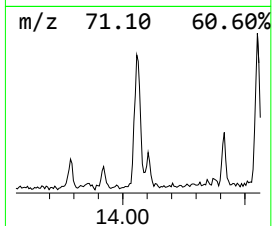
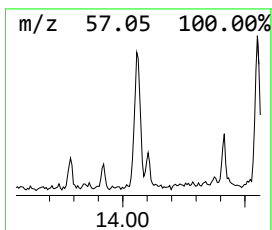
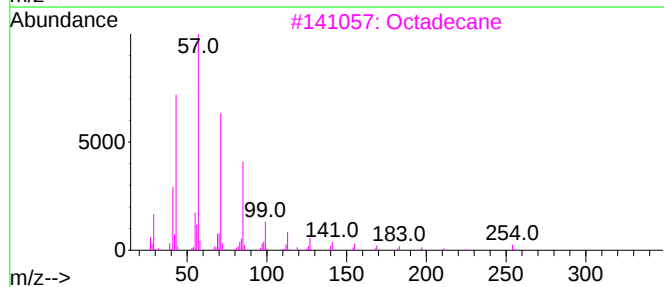
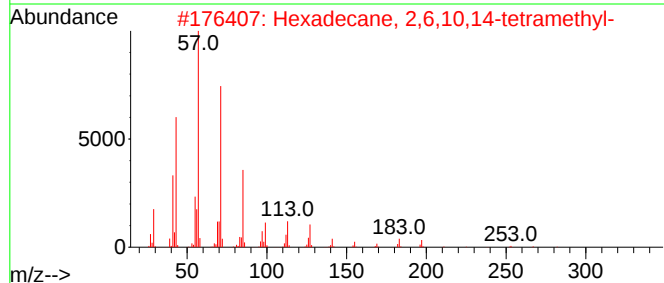
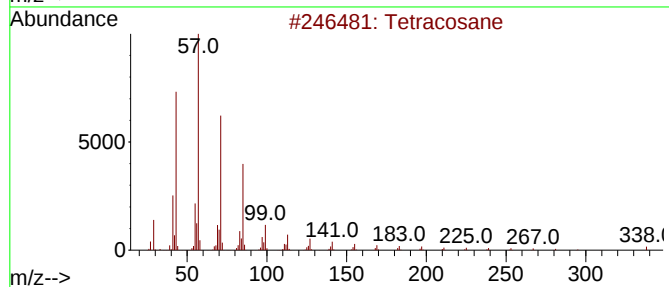
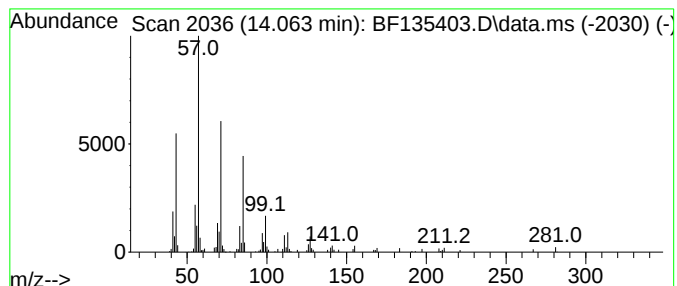
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetracosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.063	3.60 ng	133954	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	90
2			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	90
3			Octadecane	254	C18H38	000593-45-3	87
4			Heptacosane	380	C27H56	000593-49-7	87
5			Hexacosane	366	C26H54	000630-01-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092223\
Data File : BF135403.D
Acq On : 22 Sep 2023 17:02
Operator : CG\JU
Sample : 04491-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

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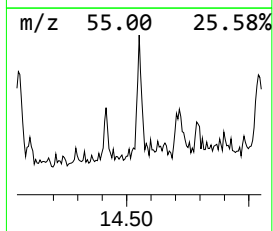
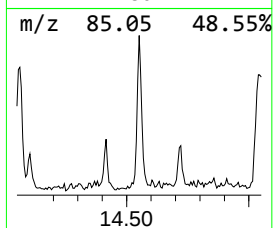
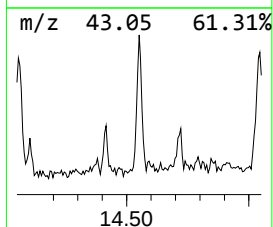
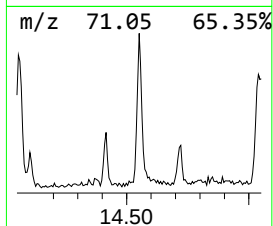
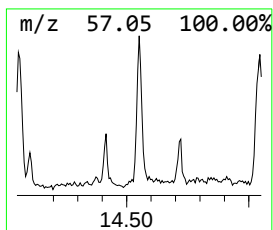
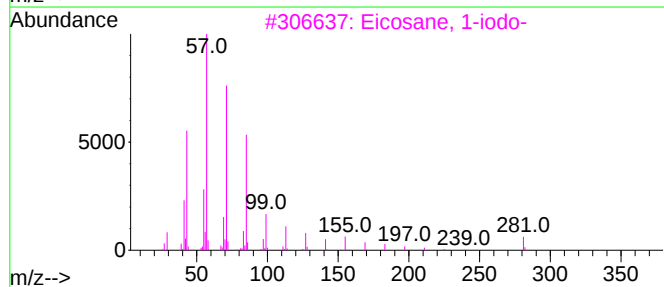
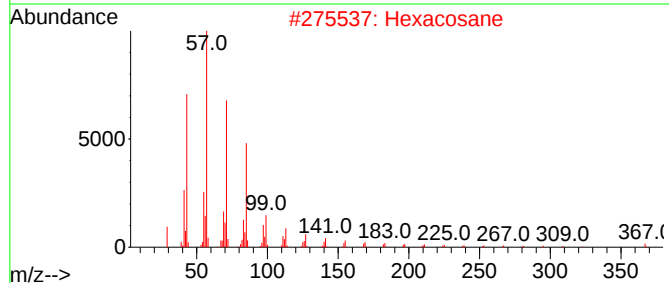
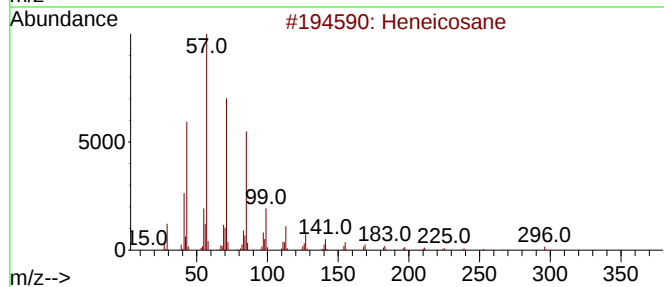
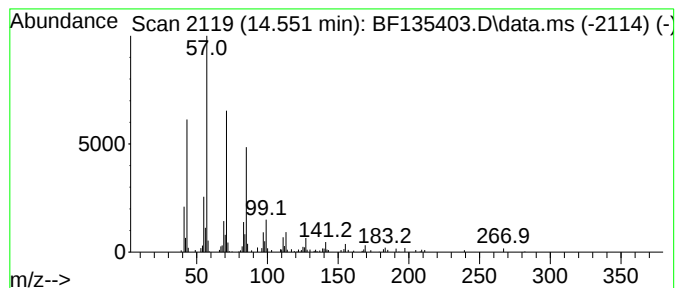
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.551	3.80 ng	141418	Chrysene-d12	13.939

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	91
4		Triacontane	422	C30H62	000638-68-6	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092223\
Data File : BF135403.D
Acq On : 22 Sep 2023 17:02
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Misc :
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ClientSampleId :
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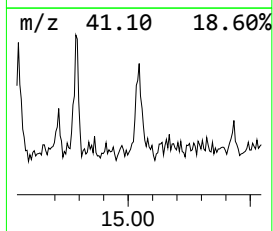
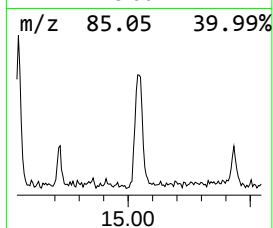
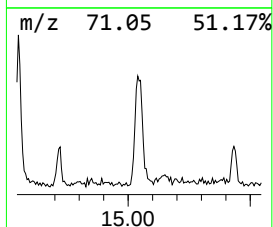
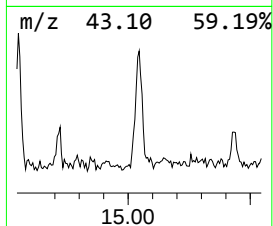
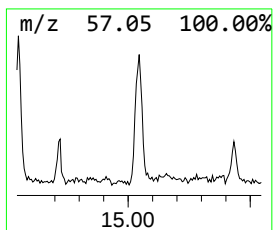
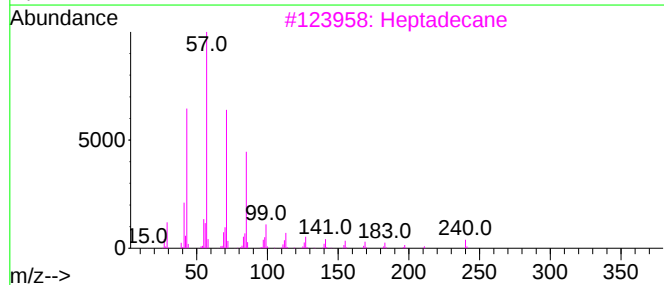
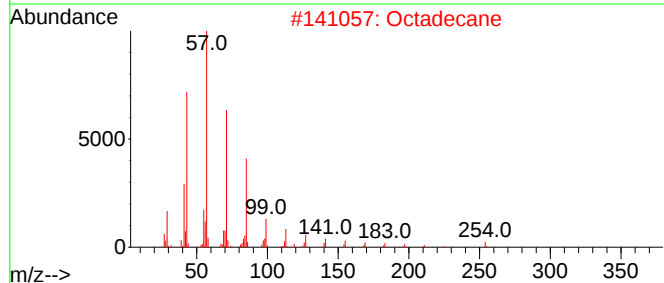
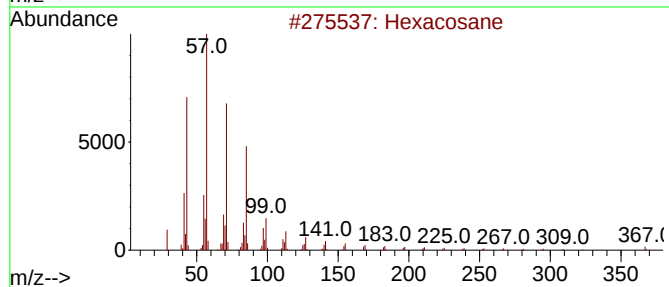
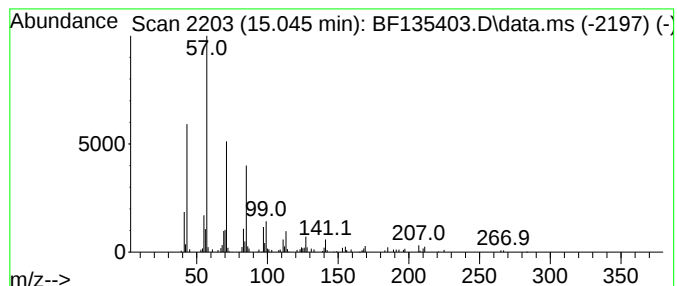
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.045	3.30 ng	145637	Perylene-d12	15.410

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexacosane	366	C26H54	000630-01-3	91
2		Octadecane	254	C18H38	000593-45-3	87
3		Heptadecane	240	C17H36	000629-78-7	87
4		Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
5		Eicosane	282	C20H42	000112-95-8	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092223\
Data File : BF135403.D
Acq On : 22 Sep 2023 17:02
Operator : CG\JU
Sample : 04491-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FB-9-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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
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1-Propanol, 2-(...	8.263	3.6	ng	215786	2	8.034	1188950	20.0
2-Propanol, 1-(...	8.287	5.7	ng	336739	2	8.034	1188950	20.0
n-Hexadecanoic ...	11.816	15.1	ng	892399	4	11.286	1185100	20.0
cis-Vaccenic acid	12.533	6.3	ng	376440	4	11.286	1185100	20.0
Octadecanoic acid	12.610	7.4	ng	435934	4	11.286	1185100	20.0
Octacosane	12.722	4.6	ng	170571	5	13.939	744205	20.0
Heptacosane	13.469	4.6	ng	171831	5	13.939	744205	20.0
Tetracosane	14.063	3.6	ng	133954	5	13.939	744205	20.0
Heneicosane	14.551	3.8	ng	141418	5	13.939	744205	20.0
Hexacosane	15.045	3.3	ng	145637	6	15.410	882813	20.0