

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
 Data File : BF130930.D
 Acq On : 02 Nov 2022 14:44
 Operator : CG\JU
 Sample : N5310-20
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BIN 1-2-(2840)-COMP-4

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-BF102722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130930.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.269	23	31	38	rVB	512258	651901	28.13%	3.840%
2	5.157	514	522	531	rBV	238659	289677	12.50%	1.706%
3	5.545	583	588	591	rBV	2036971	1872687	80.81%	11.031%
4	6.545	752	758	761	rBV	1848723	1959590	84.56%	11.543%
5	6.922	818	822	825	rBV	654068	511666	22.08%	3.014%
6	7.486	912	918	921	rBV	1333348	1265564	54.61%	7.455%
7	8.122	1020	1026	1036	rBV3	27872	76371	3.30%	0.450%
8	8.210	1036	1041	1044	rVB	717865	672423	29.02%	3.961%
9	9.286	1218	1224	1227	rBV	2596841	2317300	100.00%	13.650%
10	9.969	1335	1340	1344	rBV	918822	779942	33.66%	4.594%
11	10.763	1470	1475	1478	rBV	1595334	1387810	59.89%	8.175%
12	10.863	1489	1492	1497	rVB	77635	71933	3.10%	0.424%
13	11.463	1590	1594	1597	rBV	1036666	820418	35.40%	4.833%
14	11.527	1602	1605	1611	rVB3	39145	34858	1.50%	0.205%
15	12.680	1796	1801	1806	rBV	51330	54469	2.35%	0.321%
16	12.910	1834	1840	1843	rBV	42865	42150	1.82%	0.248%
17	13.057	1860	1865	1868	rVB	2608384	2264797	97.73%	13.341%
18	13.951	2013	2017	2022	rBV	51553	45658	1.97%	0.269%
19	14.033	2024	2031	2040	rBV5	39826	136048	5.87%	0.801%
20	14.110	2040	2044	2047	rBV	614091	529219	22.84%	3.117%
21	14.204	2055	2060	2065	rBV2	22807	29267	1.26%	0.172%
22	14.392	2089	2092	2095	rBV2	34032	28251	1.22%	0.166%
23	14.574	2119	2123	2128	rBV	62986	59627	2.57%	0.351%
24	15.045	2199	2203	2207	rVB	153190	165442	7.14%	0.975%
25	15.251	2234	2238	2243	rBV	34407	39306	1.70%	0.232%
26	15.386	2253	2261	2263	rBV5	59468	147714	6.37%	0.870%
27	15.621	2296	2301	2309	rBV	292914	385380	16.63%	2.270%
28	15.868	2337	2343	2349	rBV	197234	282598	12.20%	1.665%
29	16.333	2413	2422	2423	rBV8	22065	54200	2.34%	0.319%

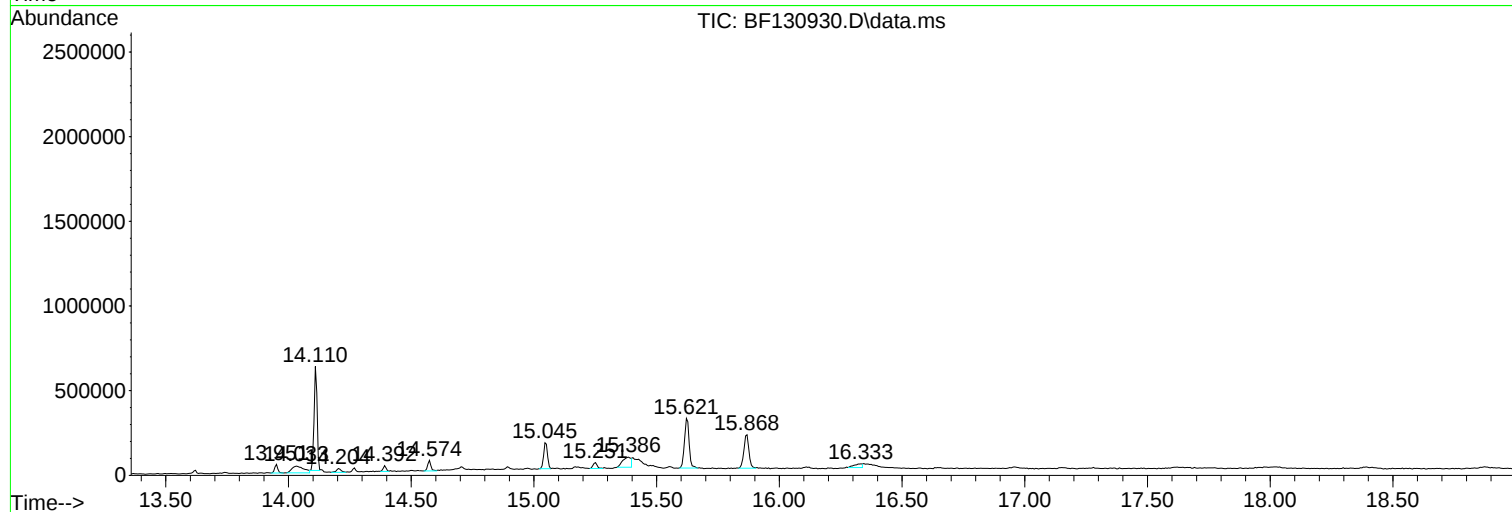
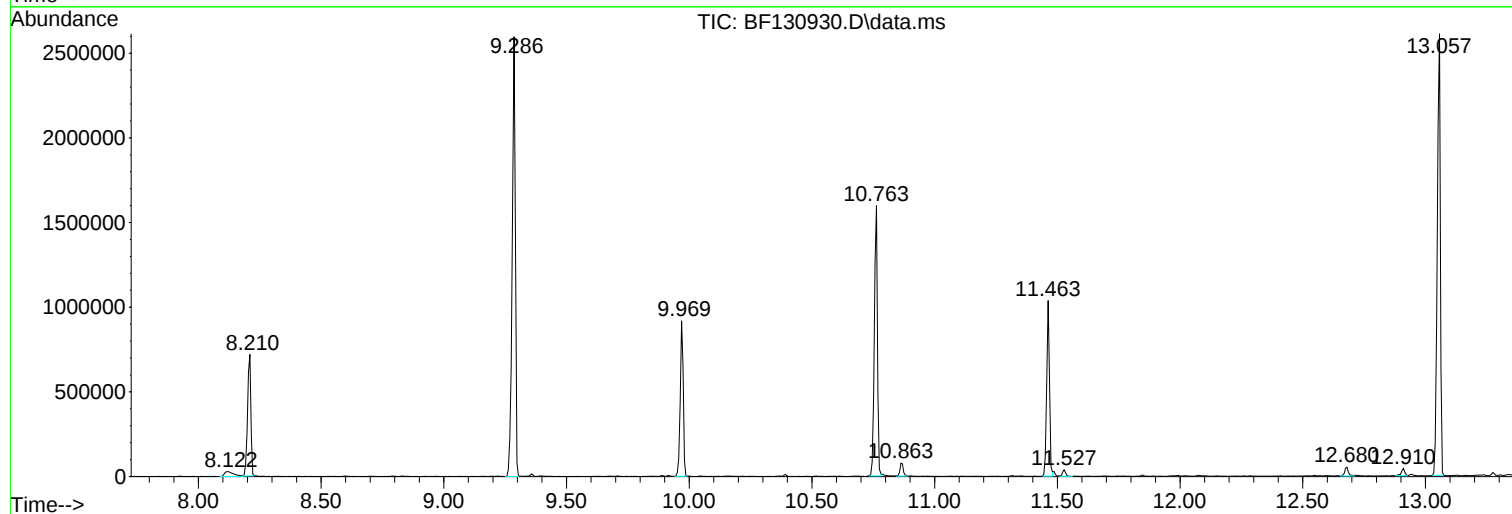
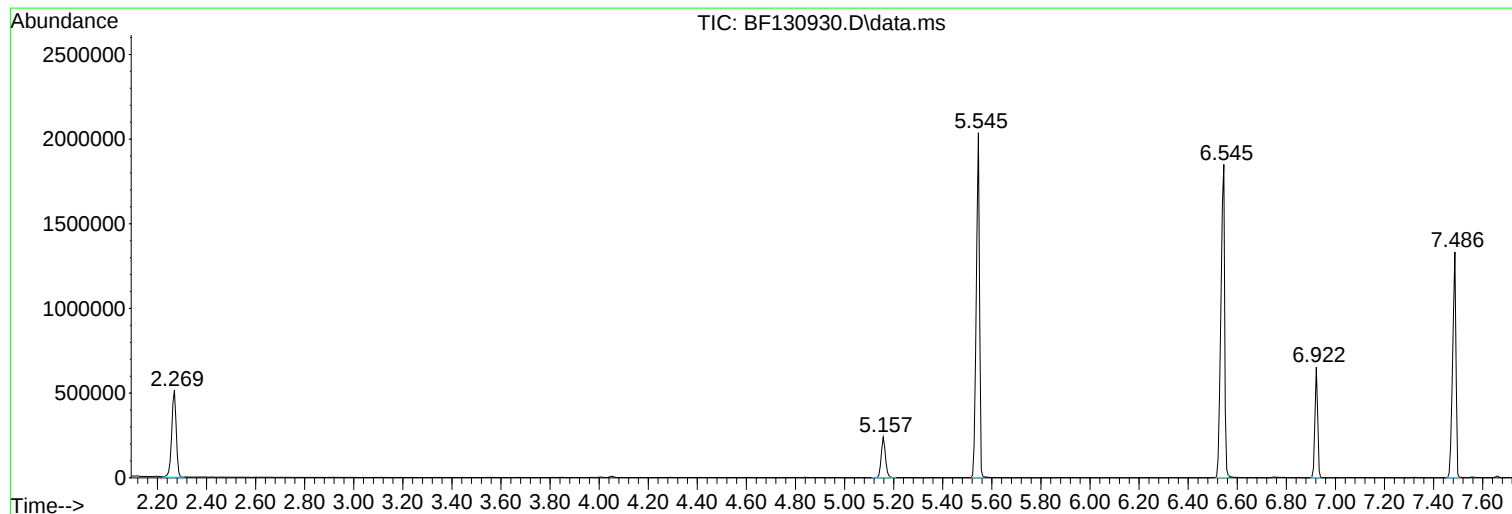
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BNA_F
ClientSampleId :
BIN 1-2-(2840)-COMP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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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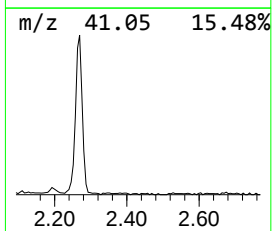
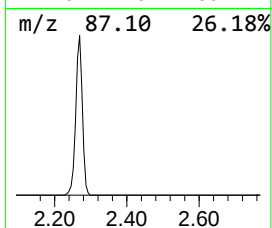
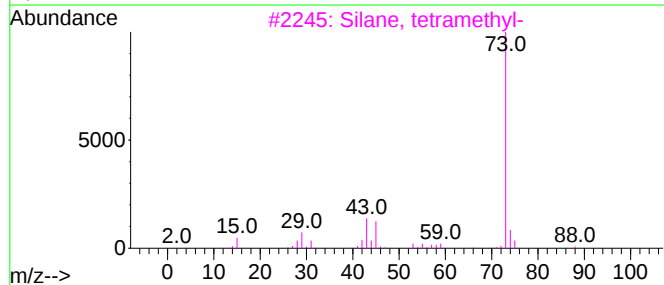
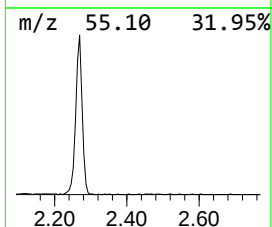
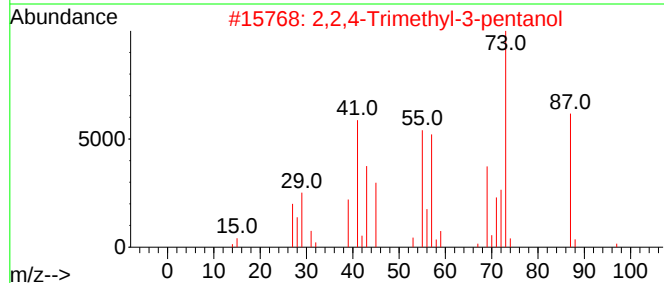
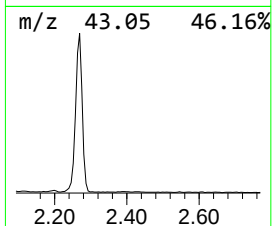
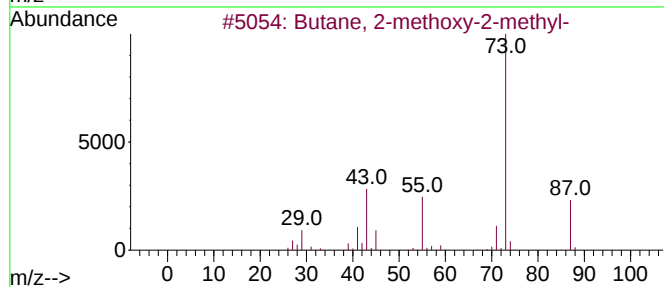
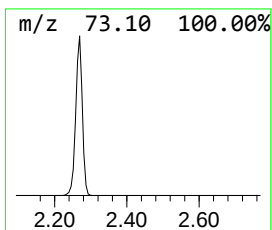
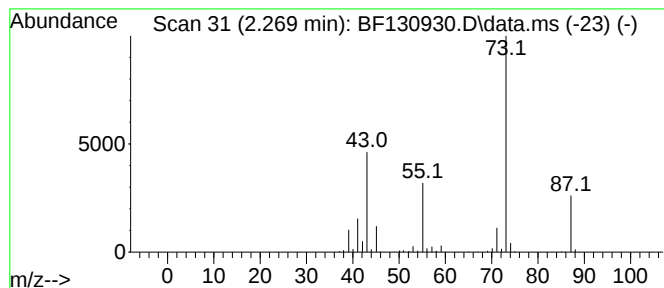
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.269	25.48 ng	651901	1,4-Dichlorobenzene-d4	6.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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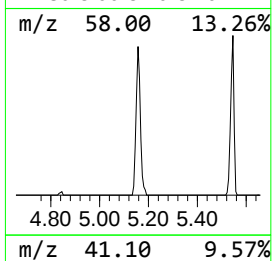
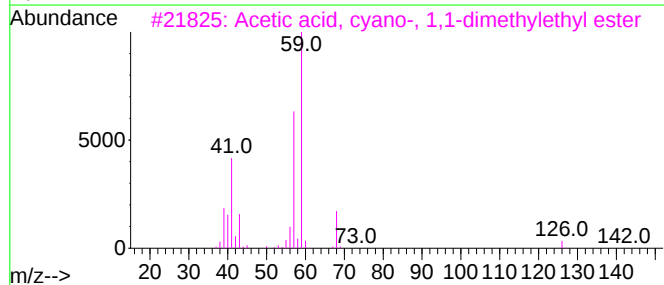
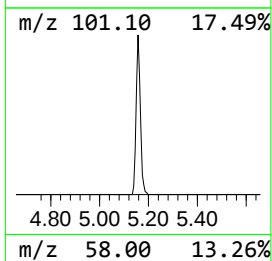
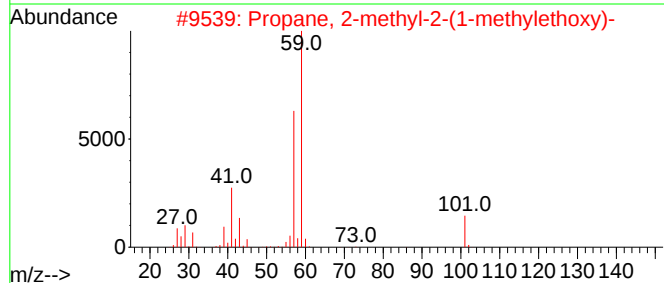
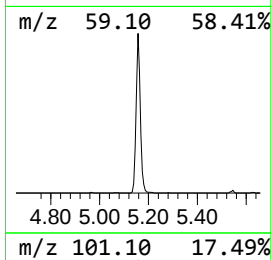
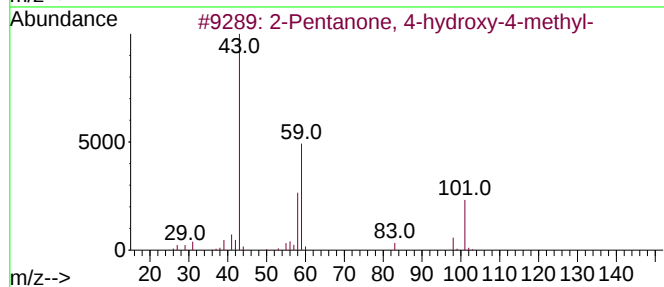
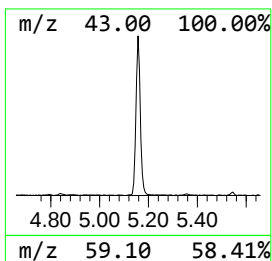
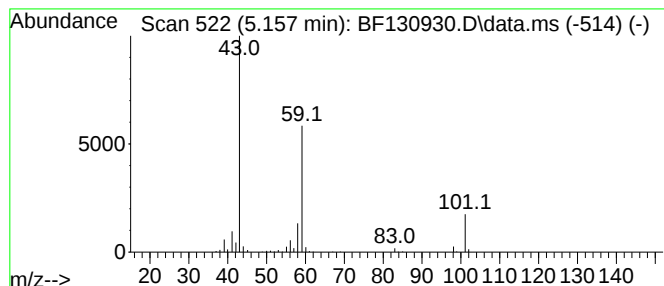
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.157	11.32 ng	289677	1,4-Dichlorobenzene-d4	6.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



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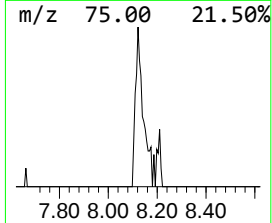
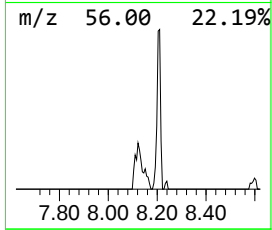
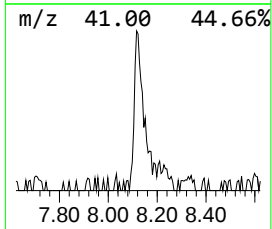
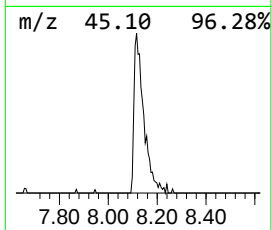
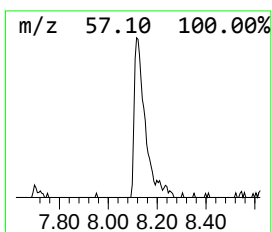
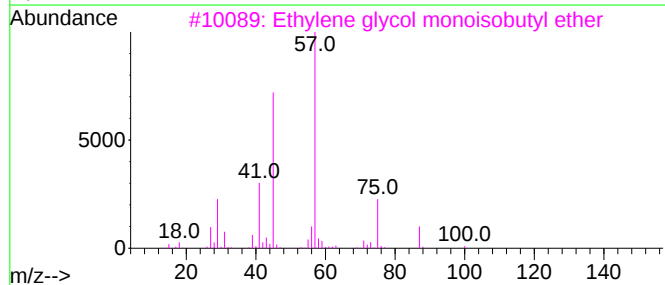
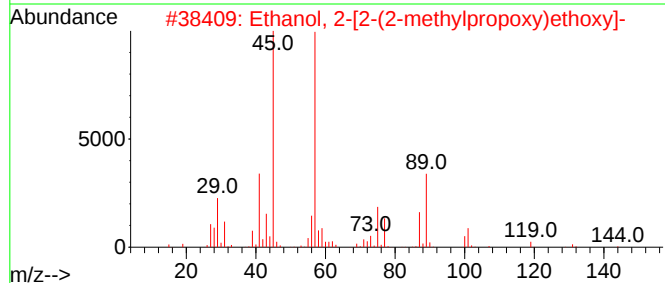
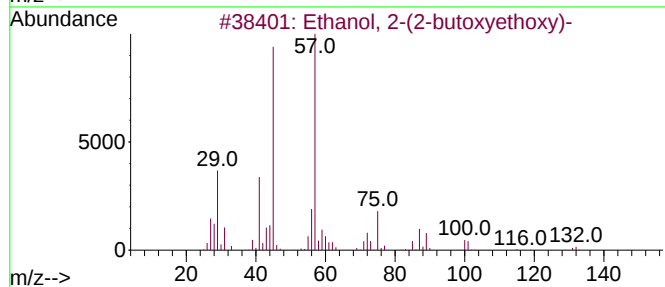
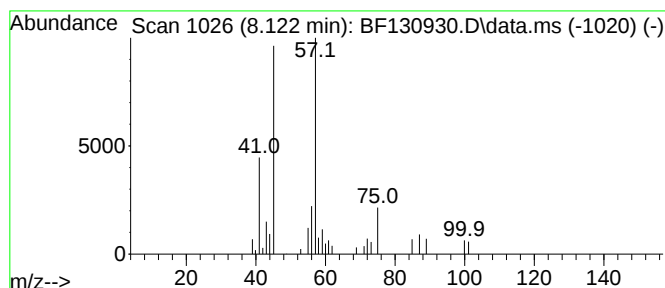
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.122	2.27 ng	76371	Naphthalene-d8	8.210

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	80
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
4			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	45
5			Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	43



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Misc :
ALS Vial : 8 Sample Multiplier: 1

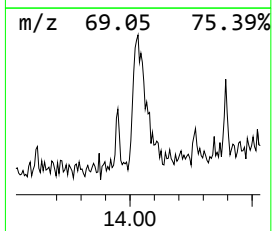
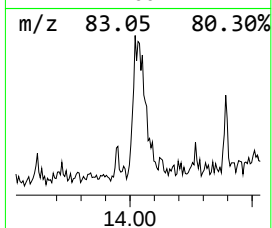
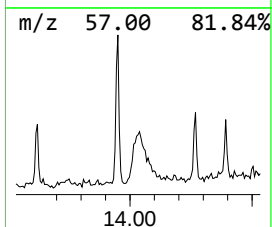
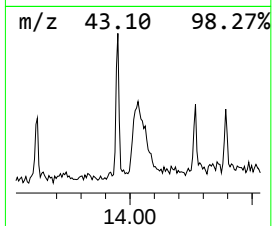
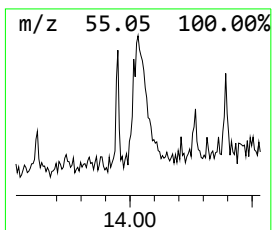
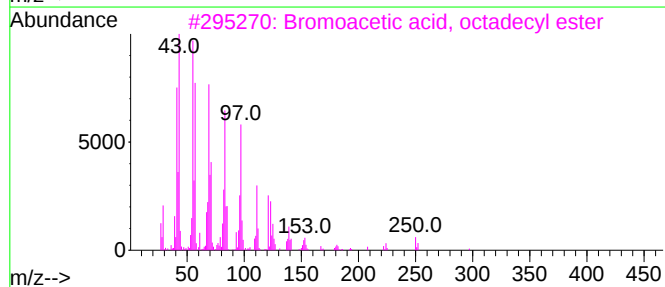
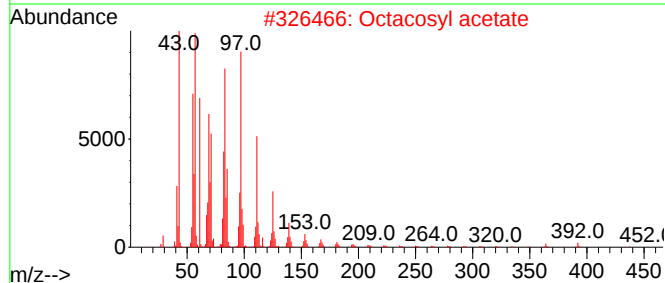
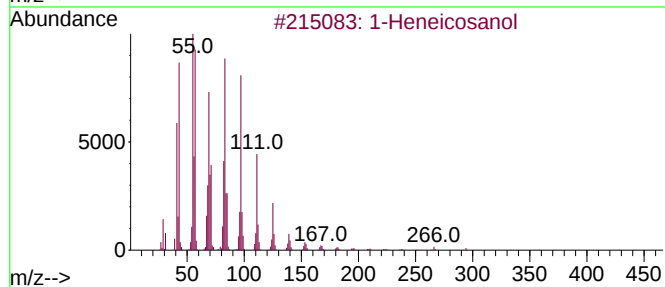
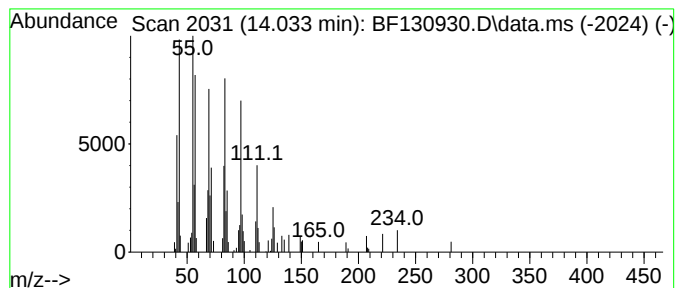
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.033	5.14 ng	136048	Chrysene-d12	14.110	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Octacosyl acetate	452	C30H60O2	018206-97-8	89
3	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	87
4	1-Hexacosene	364	C26H52	018835-33-1	87
5	Behenic alcohol	326	C22H46O	000661-19-8	76



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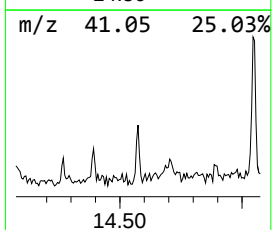
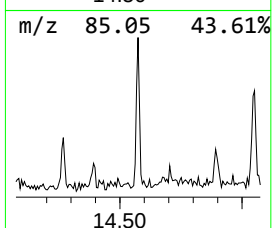
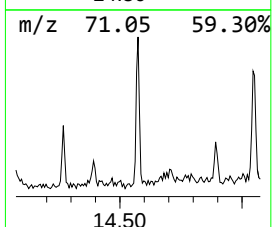
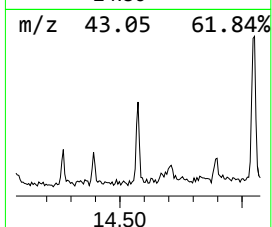
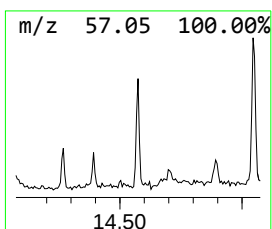
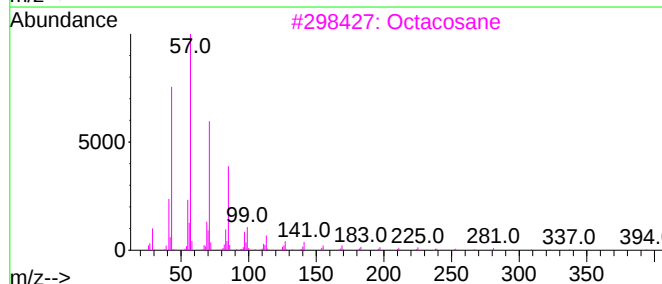
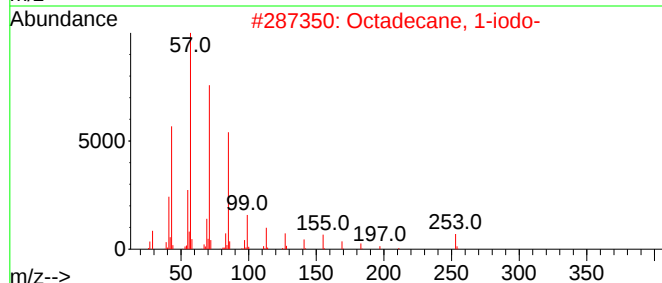
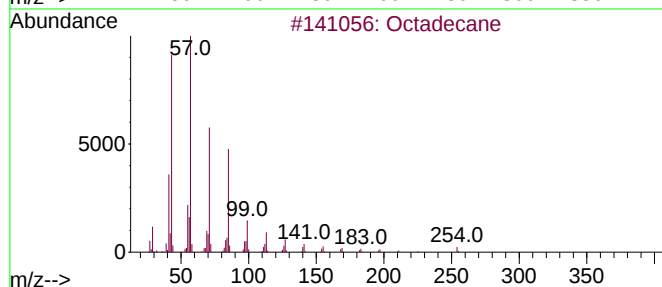
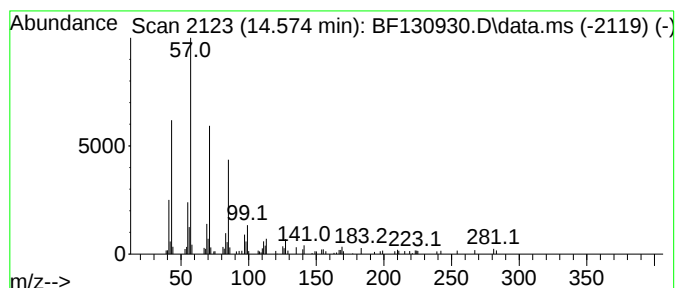
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.574	2.25 ng	59627	Chrysene-d12	14.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	96
2			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	90
3			Octacosane	394	C28H58	000630-02-4	87
4			Heptadecane, 2-methyl-	254	C18H38	001560-89-0	87
5			Tetracosane	338	C24H50	000646-31-1	87



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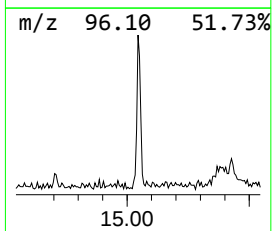
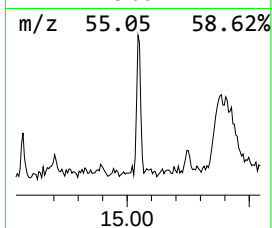
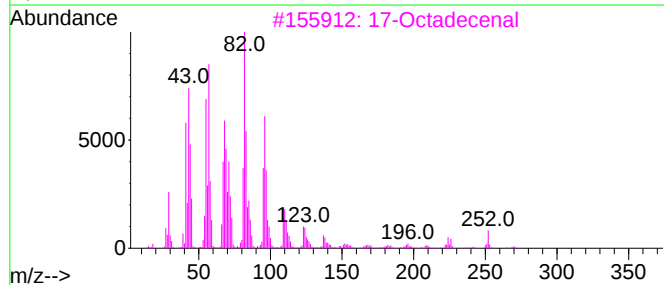
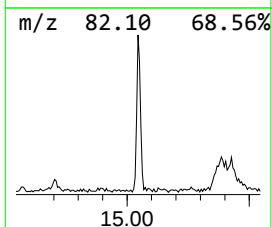
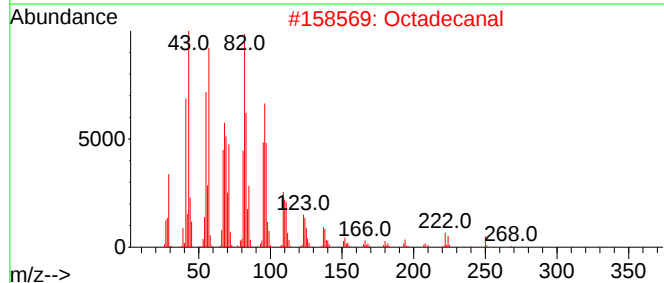
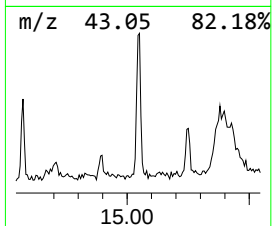
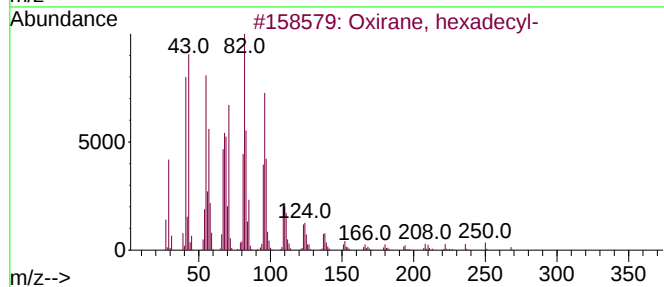
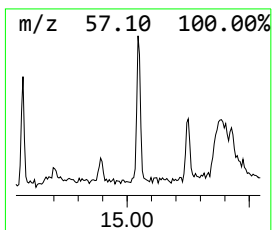
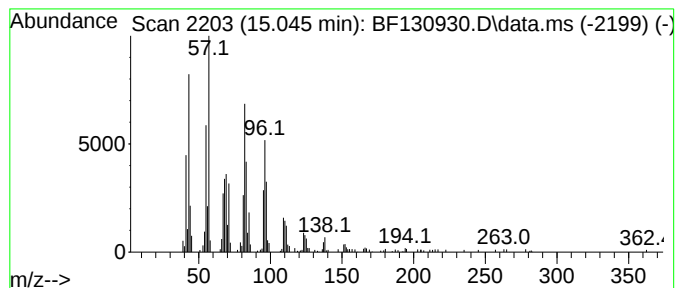
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Oxirane, hexadecyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.045	8.59 ng	165442	Perylene-d12	15.627

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
2			Octadecanal	268	C18H36O	000638-66-4	91
3			17-Octadecenal	266	C18H34O	056554-86-0	91
4			Eicosanal-	296	C20H40O	002400-66-0	90
5			18-Nonadecen-1-ol	282	C19H38O	1000142-89-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130930.D
Acq On : 02 Nov 2022 14:44
Operator : CG\JU
Sample : N5310-20
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BIN 1-2-(2840)-COMP-4

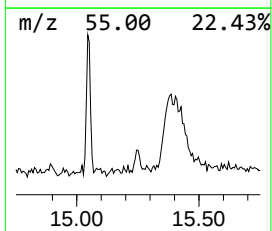
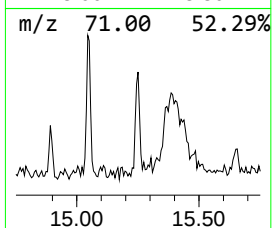
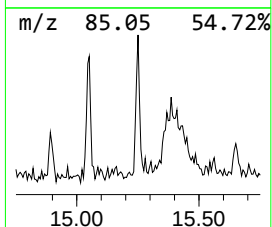
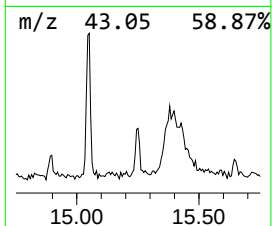
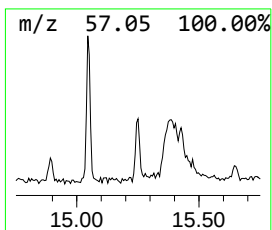
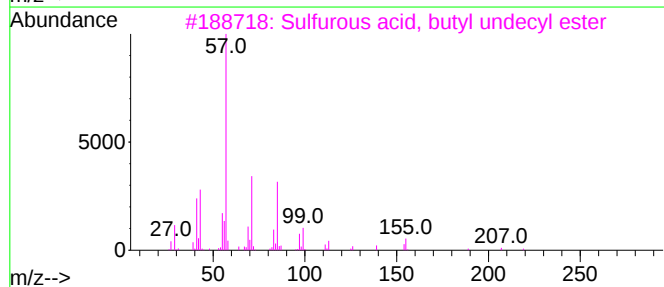
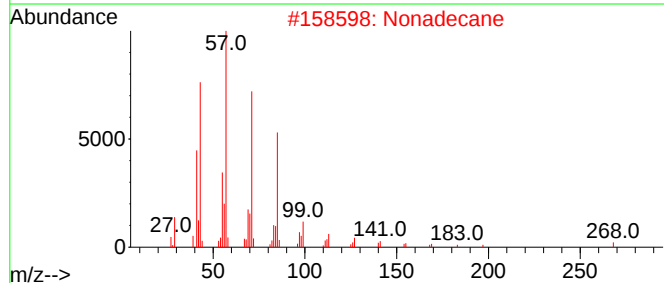
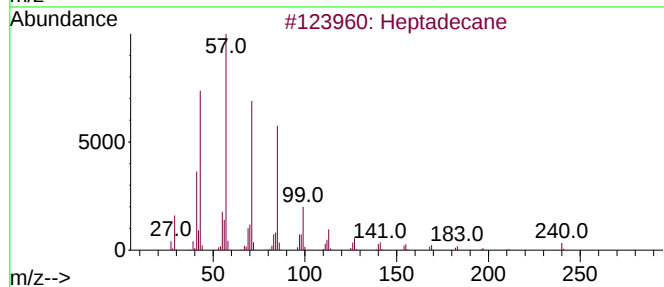
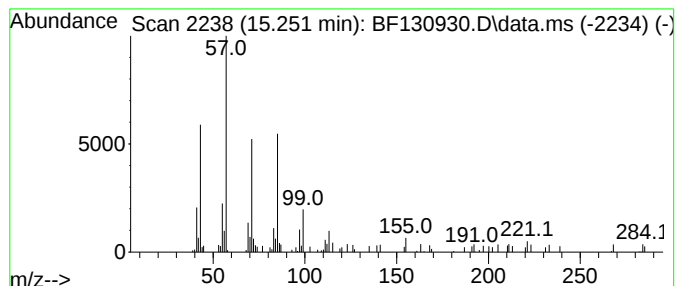
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.251	2.04 ng	39306	Perylene-d12	15.627

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	80
2			Nonadecane	268	C19H40	000629-92-5	72
3			Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	64
4			Hentriacontane	437	C31H64	000630-04-6	64
5			Decane, 1-iodo-	268	C10H21I	002050-77-3	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130930.D
Acq On : 02 Nov 2022 14:44
Operator : CG\JU
Sample : N5310-20
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BIN 1-2-(2840)-COMP-4

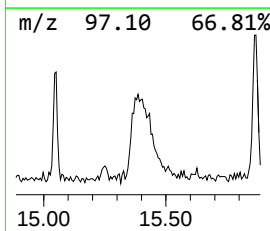
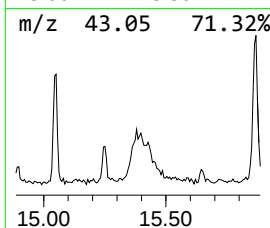
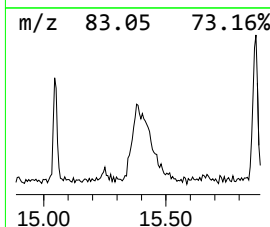
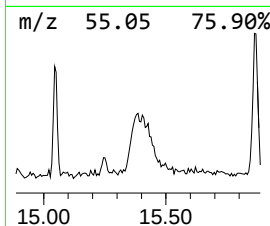
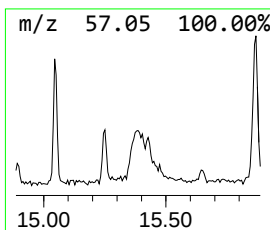
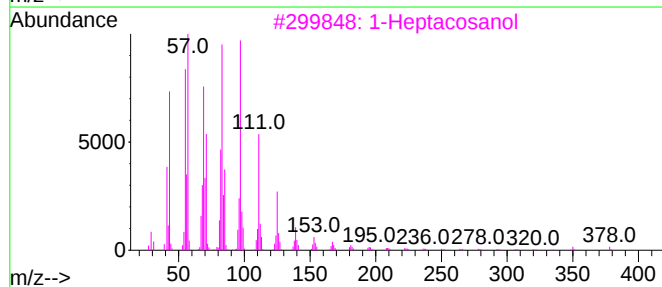
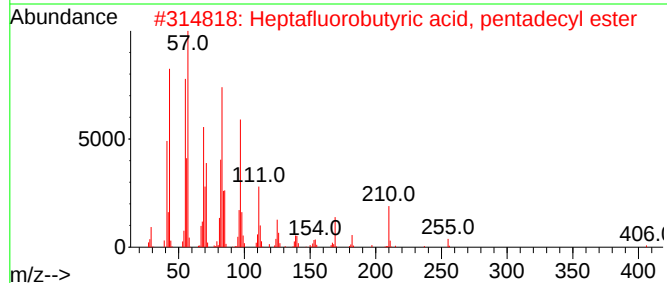
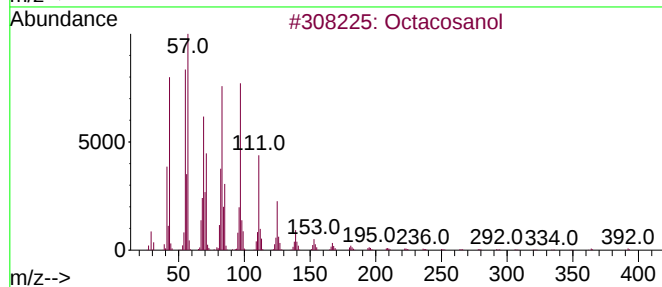
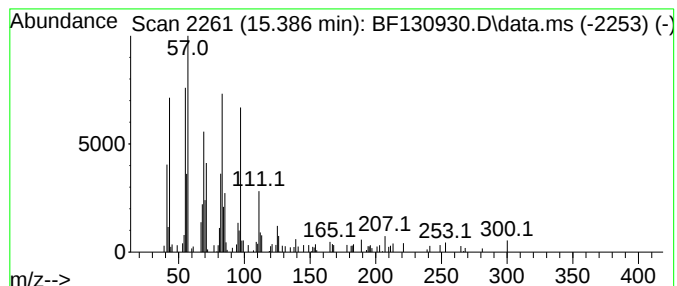
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.386	7.67 ng	147714	Perylene-d12	15.627

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosanol	410	C28H58O	000557-61-9	91
2			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
3			1-Heptacosanol	396	C27H56O	002004-39-9	91
4			n-Nonadecanol-1	284	C19H40O	001454-84-8	87
5			1-Heneicosanol	312	C21H44O	015594-90-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130930.D
Acq On : 02 Nov 2022 14:44
Operator : CG\JU
Sample : N5310-20
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BIN 1-2-(2840)-COMP-4

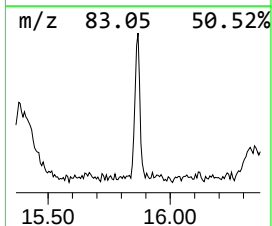
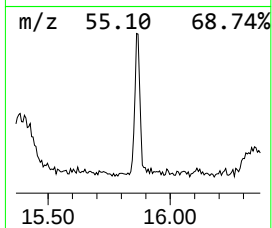
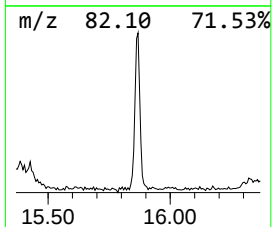
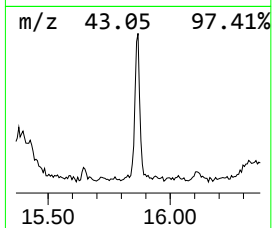
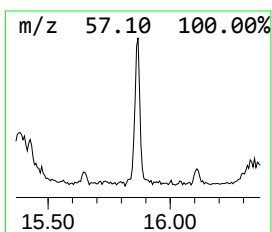
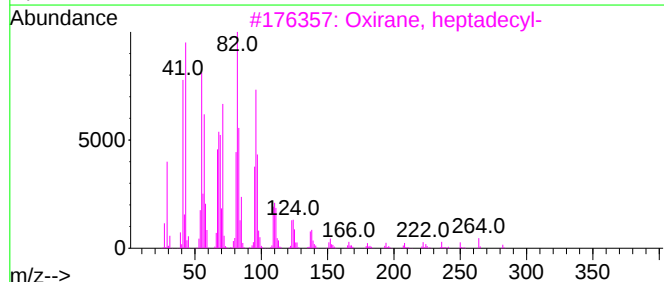
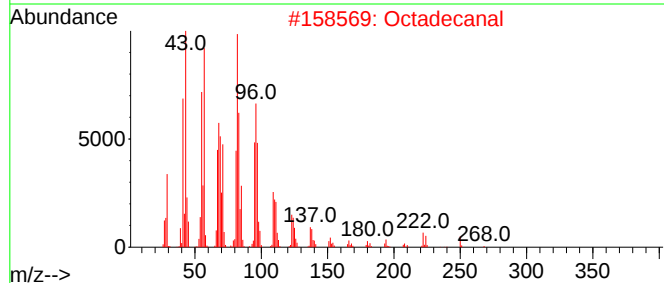
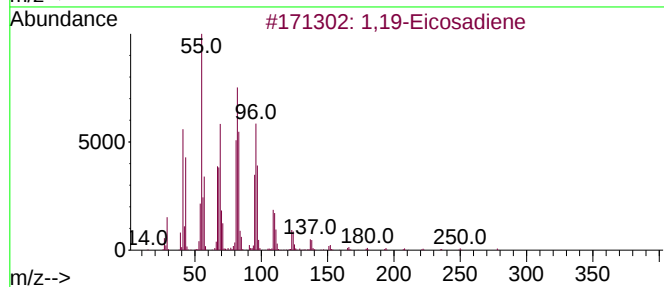
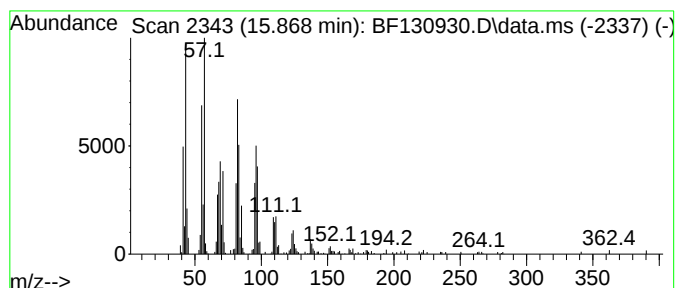
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1,19-Eicosadiene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.868	14.67 ng	282598	Perylene-d12	15.627

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene		278	C20H38	014811-95-1	94
2	Octadecanal		268	C18H36O	000638-66-4	91
3	Oxirane, heptadecyl-		282	C19H38O	067860-04-2	90
4	1,13-Tetradecadiene		194	C14H26	021964-49-8	87
5	Eicosanal-		296	C20H40O	002400-66-0	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130930.D
Acq On : 02 Nov 2022 14:44
Operator : CG\JU
Sample : N5310-20
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
BIN 1-2-(2840)-COMP-4

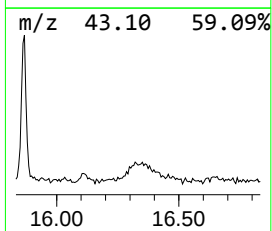
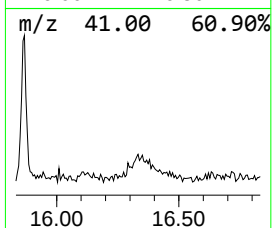
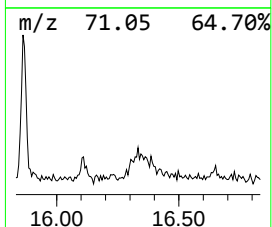
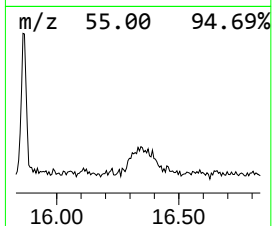
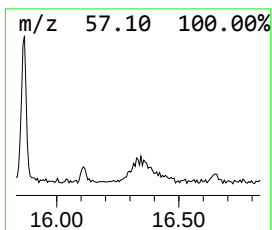
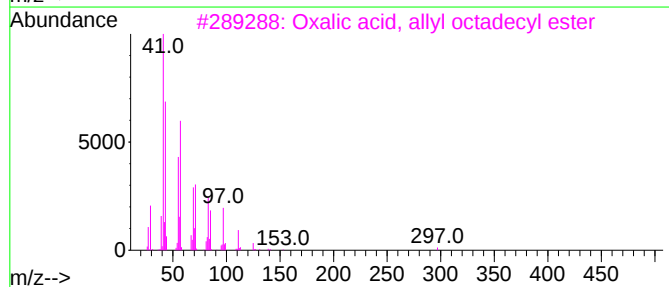
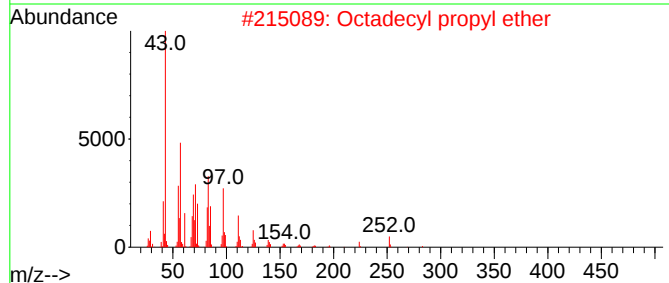
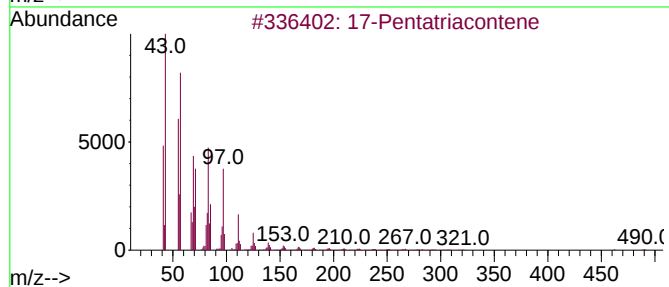
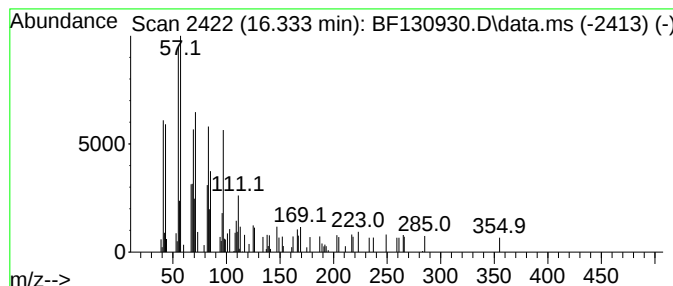
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 17-Pentatriacontene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.333	2.81 ng	54200	Perylene-d12	15.627

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		17-Pentatriacontene	491	C35H70	006971-40-0	87
2		Octadecyl propyl ether	312	C21H44O	1000406-28-0	86
3		Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	80
4		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	74
5		Isobutyl tetratriacontyl ether	551	C38H78O	1000406-33-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130930.D
Acq On : 02 Nov 2022 14:44
Operator : CG\JU
Sample : N5310-20
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BIN 1-2-(2840)-COMP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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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2-Pentanone, 4-...	5.157	11.3	ng	289677	1	6.922	511666	20.0
Ethanol, 2-(2-b...	8.122	2.3	ng	76371	2	8.210	672423	20.0
1-Heneicosanol	14.033	5.1	ng	136048	5	14.110	529219	20.0
Octadecane	14.574	2.3	ng	59627	5	14.110	529219	20.0
Oxirane, hexade...	15.045	8.6	ng	165442	6	15.627	385380	20.0
Heptadecane	15.251	2.0	ng	39306	6	15.627	385380	20.0
Octacosanol	15.386	7.7	ng	147714	6	15.627	385380	20.0
1,19-Eicosadiene	15.868	14.7	ng	282598	6	15.627	385380	20.0
17-Pentatriacon...	16.333	2.8	ng	54200	6	15.627	385380	20.0