

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080924\
 Data File : BF138890.D
 Acq On : 09 Aug 2024 16:02
 Operator : RC/JU
 Sample : P3469-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MLS-15-513-528

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-BF073024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138890.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	7	13	rVB	1990682	2993293	100.00%	19.040%
2	3.904	302	308	322	rBB	231538	371907	12.42%	2.366%
3	5.051	498	503	516	rVB	43295	65216	2.18%	0.415%
4	5.469	569	574	589	rVB	527492	738634	24.68%	4.698%
5	5.798	623	630	635	rBV	584410	847446	28.31%	5.390%
6	6.481	741	746	763	rBV	346704	479229	16.01%	3.048%
7	6.840	802	807	812	rBV	243513	312152	10.43%	1.986%
8	7.404	896	903	913	rBV	851358	1209693	40.41%	7.695%
9	8.116	1019	1024	1033	rVB	340070	431805	14.43%	2.747%
10	8.334	1056	1061	1063	rBV	128299	167503	5.60%	1.065%
11	8.357	1063	1065	1075	rVV	145880	200509	6.70%	1.275%
12	8.434	1075	1078	1084	rVV	26872	39729	1.33%	0.253%
13	9.192	1200	1207	1212	rBV	1723316	2272063	75.91%	14.452%
14	9.869	1317	1322	1329	rBV	413184	519416	17.35%	3.304%
15	10.663	1452	1457	1472	rBV	921944	1244182	41.57%	7.914%
16	11.357	1570	1575	1583	rVV	461094	573847	19.17%	3.650%
17	11.886	1659	1665	1679	rBV2	48571	103711	3.46%	0.660%
18	12.445	1750	1760	1767	rBV	66079	106171	3.55%	0.675%
19	12.686	1793	1801	1808	rBV3	19873	45652	1.53%	0.290%
20	12.945	1838	1845	1850	rVB	1739858	2344973	78.34%	14.916%
21	13.998	2020	2024	2031	rVV	228435	294746	9.85%	1.875%
22	14.074	2032	2037	2041	rVB	28440	34982	1.17%	0.223%
23	14.821	2160	2164	2173	rVB	38114	51143	1.71%	0.325%
24	15.457	2266	2272	2285	rVB	145321	239522	8.00%	1.524%
25	15.639	2297	2303	2311	rBV	19860	33909	1.13%	0.216%

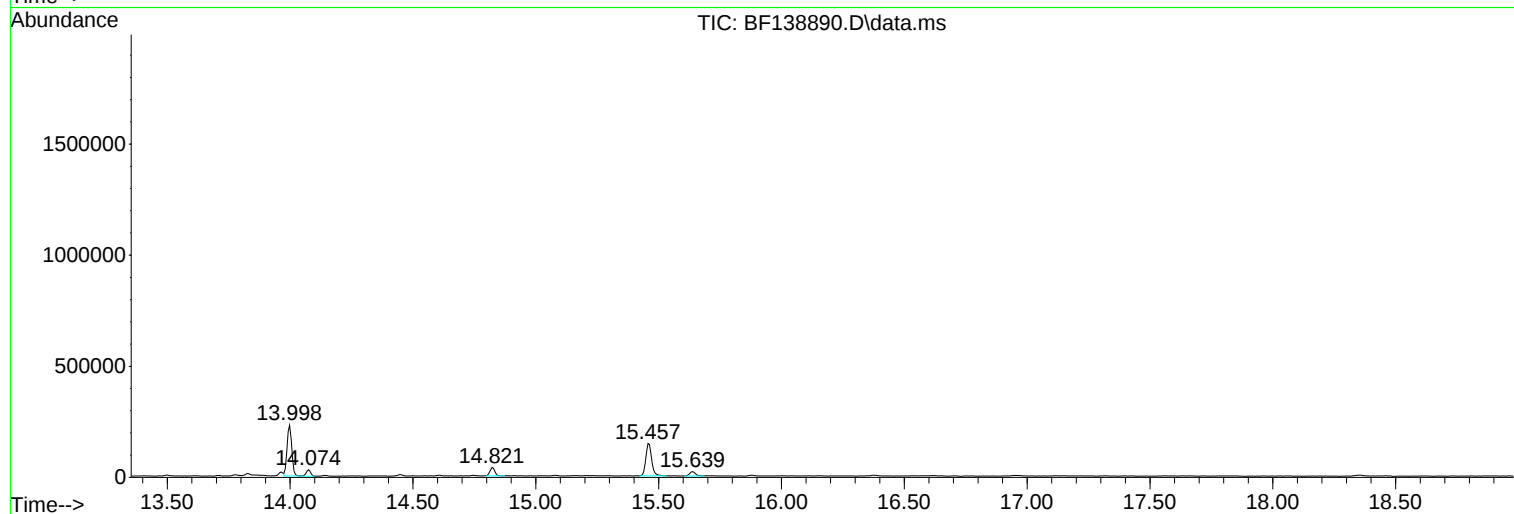
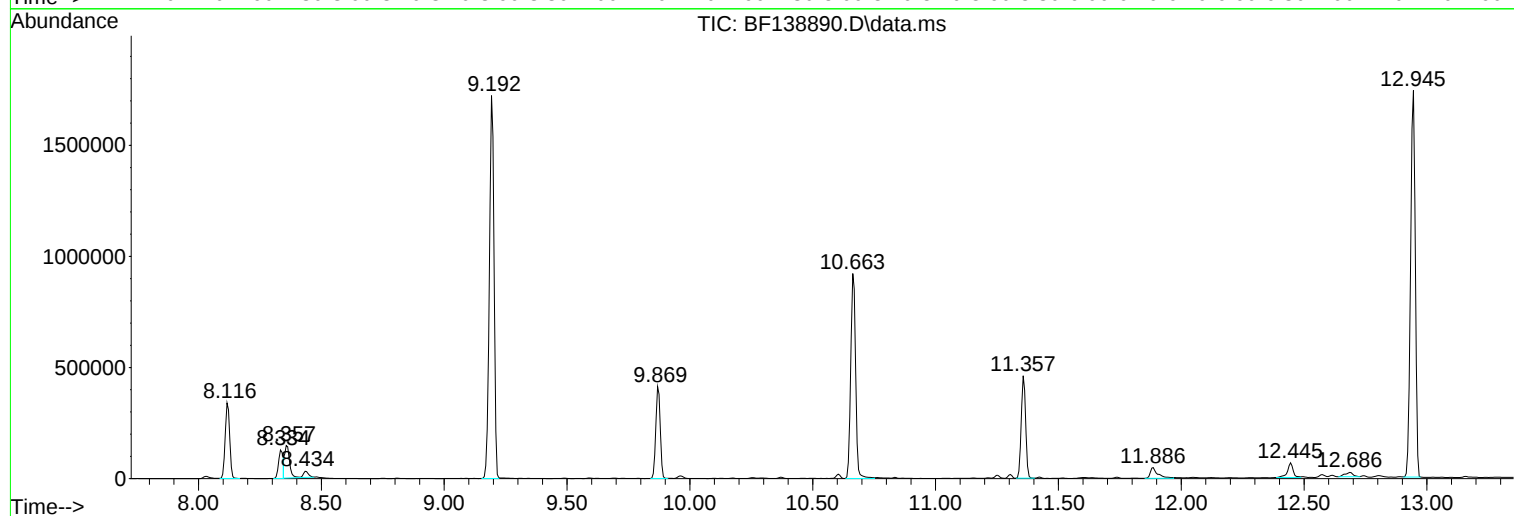
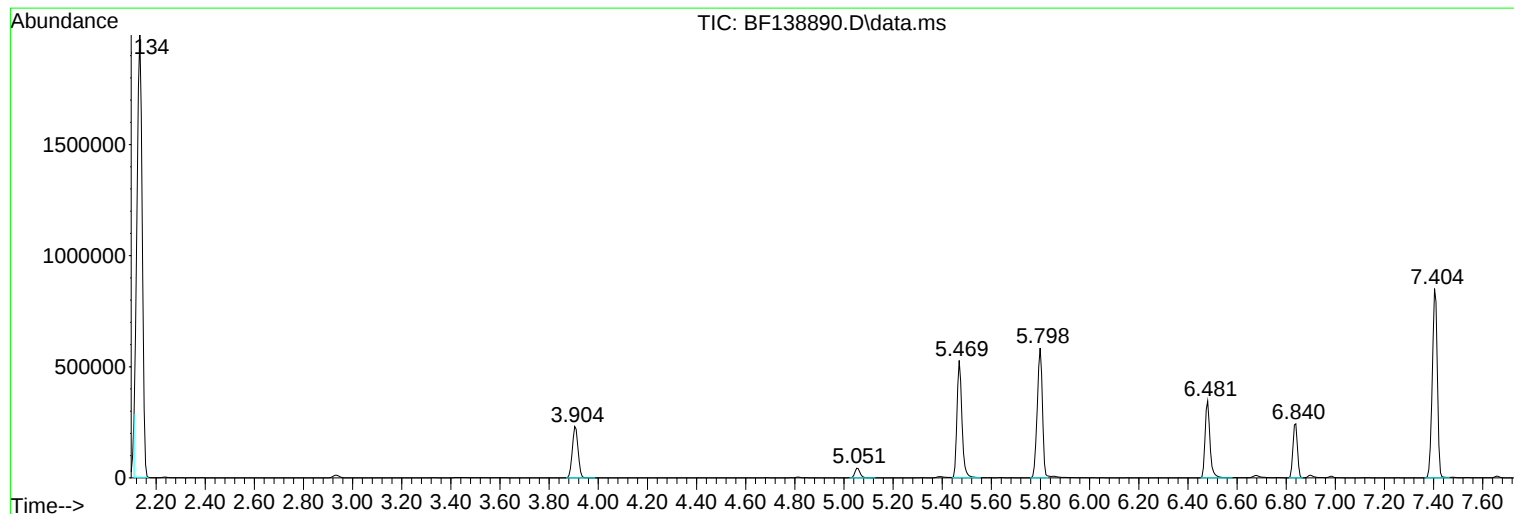
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MLS-15-513-528

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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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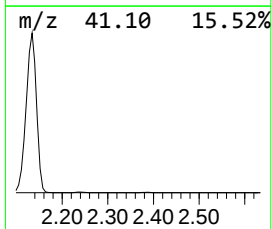
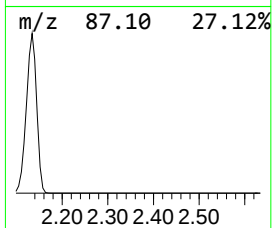
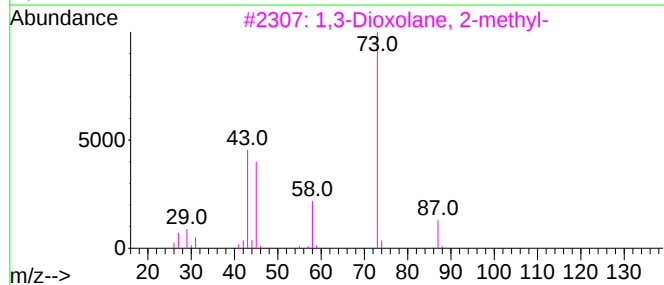
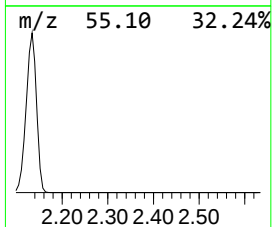
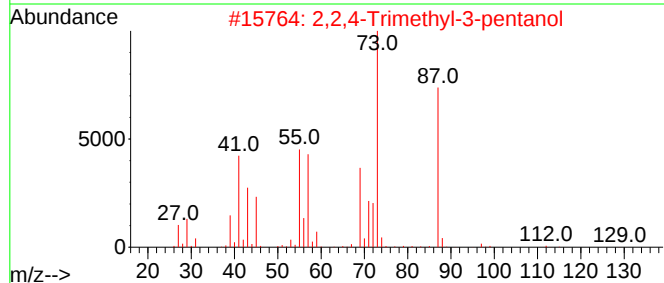
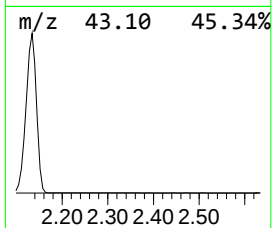
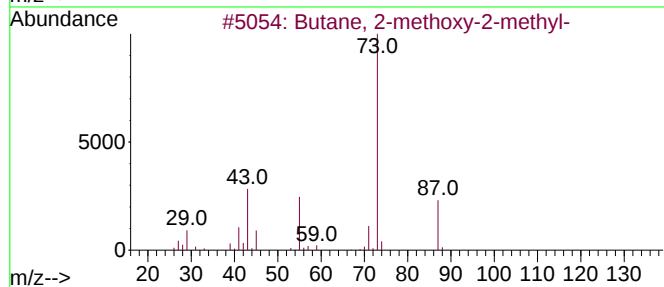
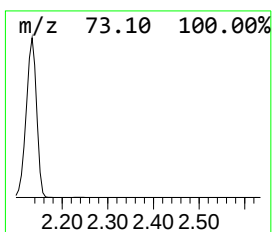
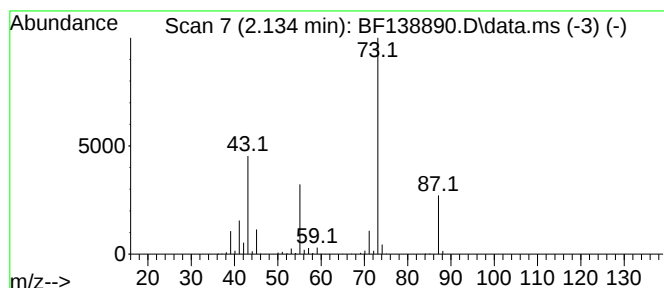
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.134	191.78 ng	2993290	1,4-Dichlorobenzene-d4	6.840

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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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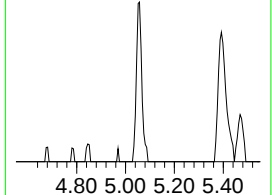
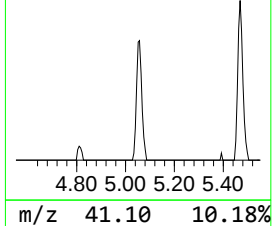
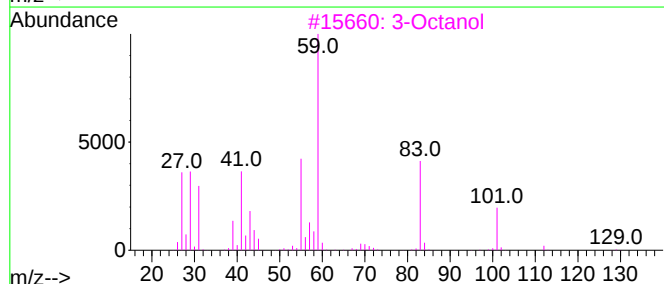
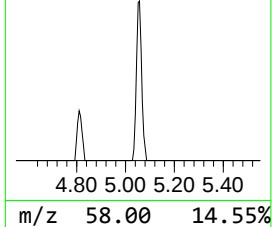
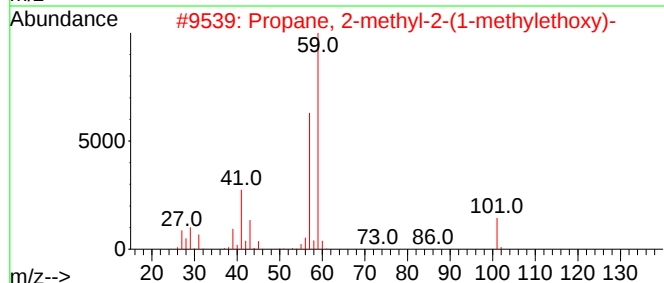
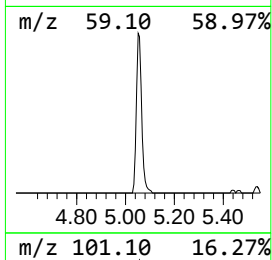
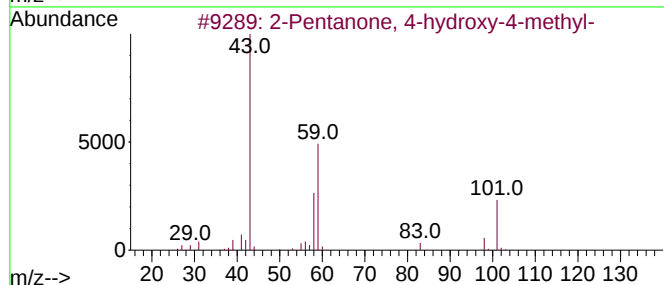
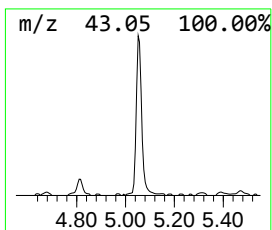
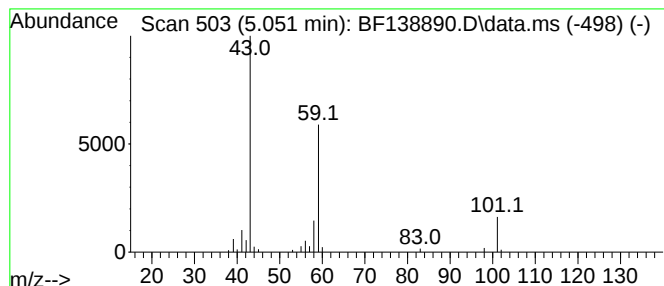
Instrument :
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ClientSampleId :
MLS-15-513-528

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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 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.051	4.18 ng	65216	1,4-Dichlorobenzene-d4			6.840
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	72
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O		017348-59-3	36
3	3-Octanol	130	C8H18O		000589-98-0	33
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2		000540-88-5	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2		001116-98-9	23



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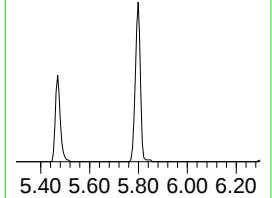
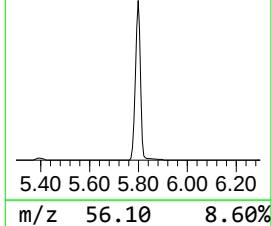
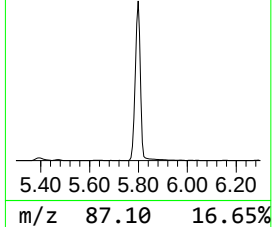
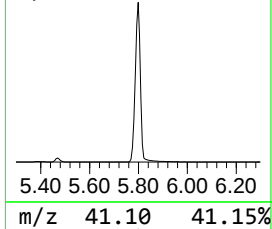
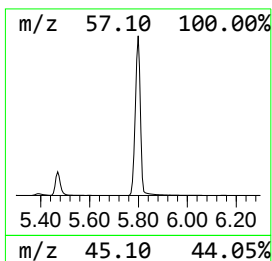
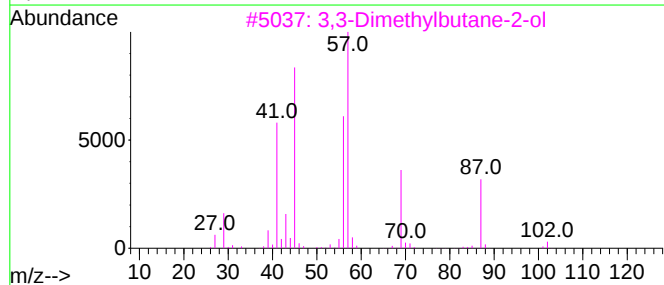
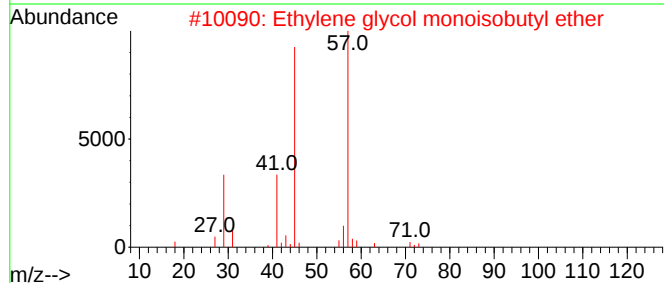
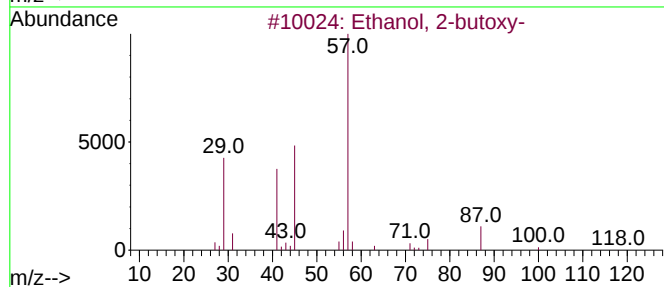
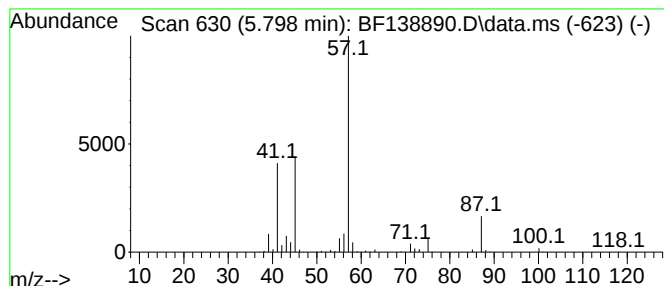
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.798	54.30 ng	847446	1,4-Dichlorobenzene-d4	6.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	83
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	45
3			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	42
4			Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	12
5			Isobutyl ether	130	C8H18O	000628-55-7	12



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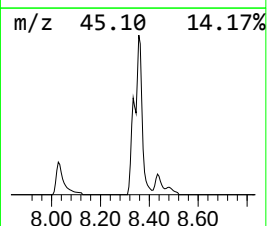
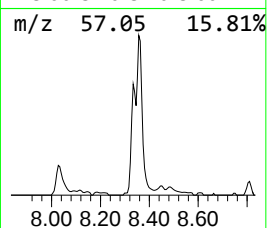
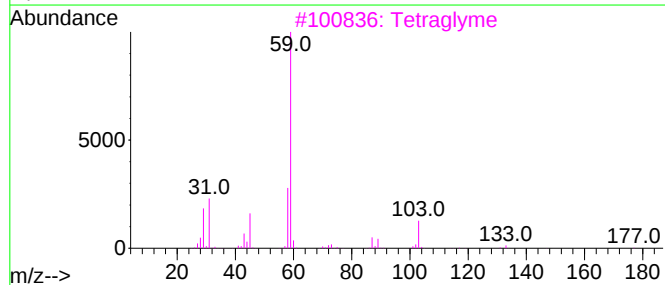
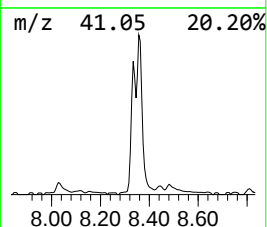
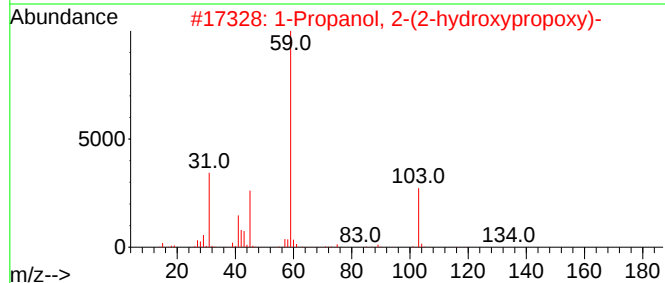
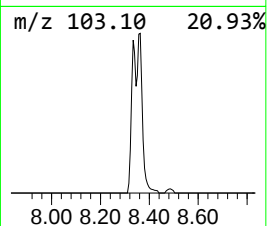
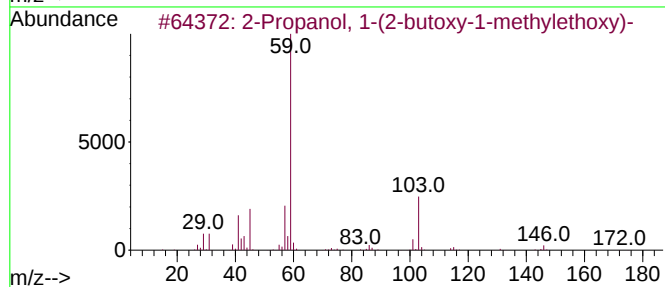
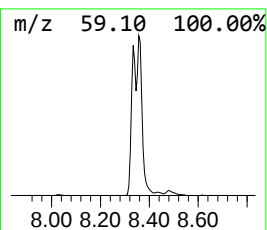
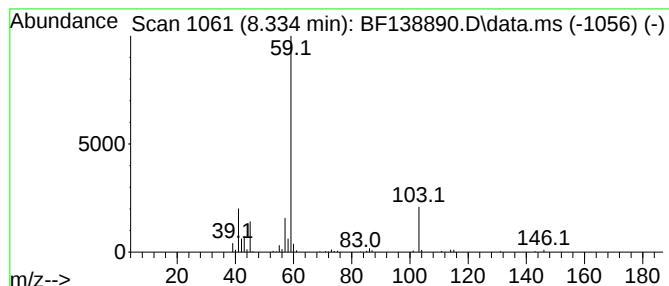
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Peak Number 5 2-Propanol, 1-(2-butoxy-1-m... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.334	7.76 ng	167503	Naphthalene-d8	8.116

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	Tetraglyme	222	C10H22O5	000143-24-8	72		
4	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	72		
5	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	64		



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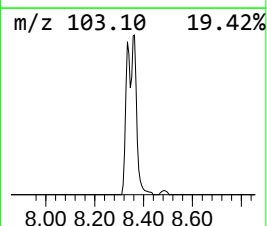
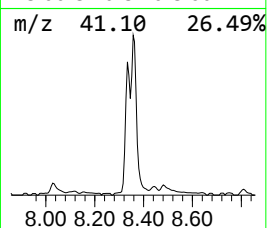
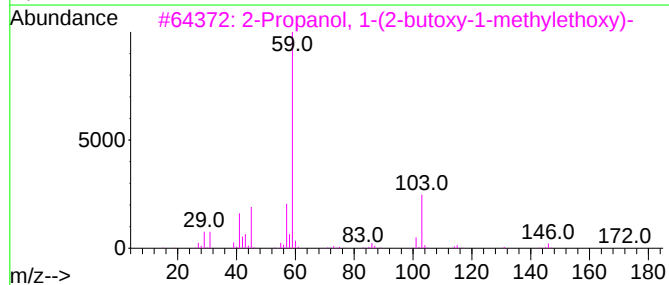
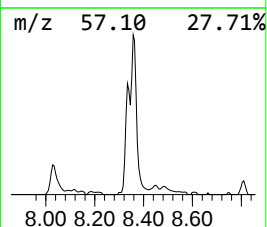
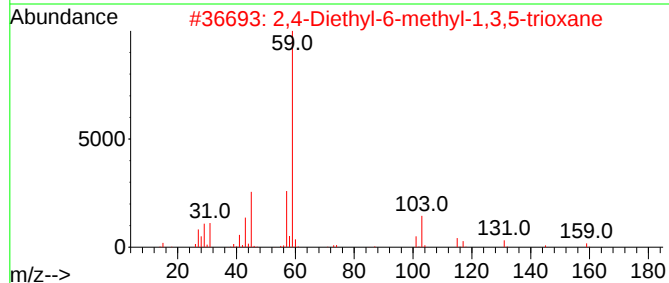
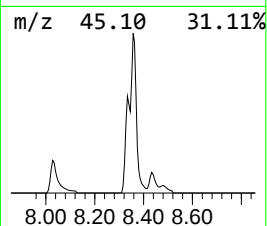
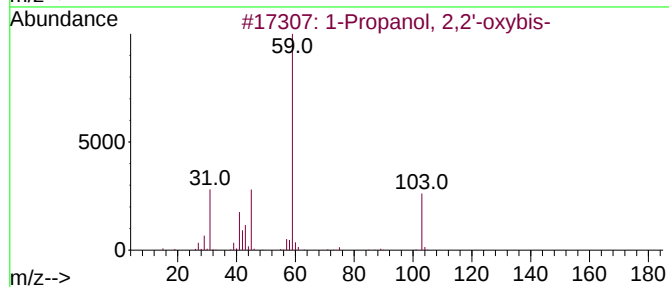
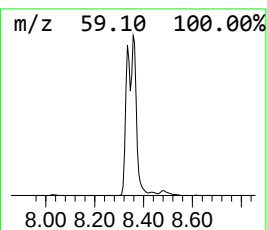
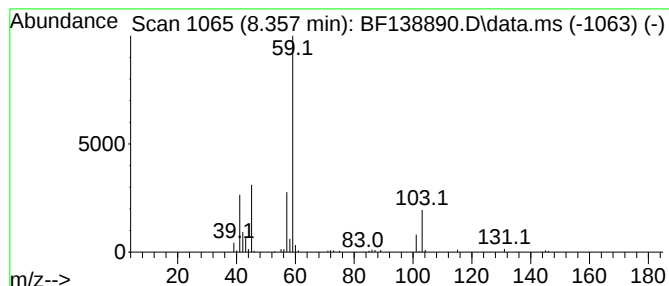
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 1-Propanol, 2,2'-oxybis- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.357	9.29 ng	200509	Naphthalene-d8	8.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	72
2			2,4-Diethyl-6-methyl-1,3,5-trioxane	160	C8H16O3	117888-04-7	72
3			2-Propanol, 1-(2-butoxy-1-methyl...)	190	C10H22O3	029911-28-2	72
4			1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	64
5			2-Propanol, 1-(2-methoxy-1-methy...)	148	C7H16O3	020324-32-7	64



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MLS-15-513-528

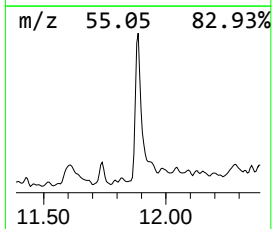
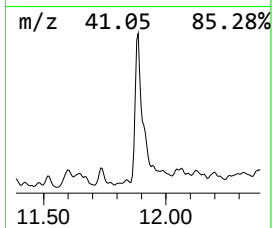
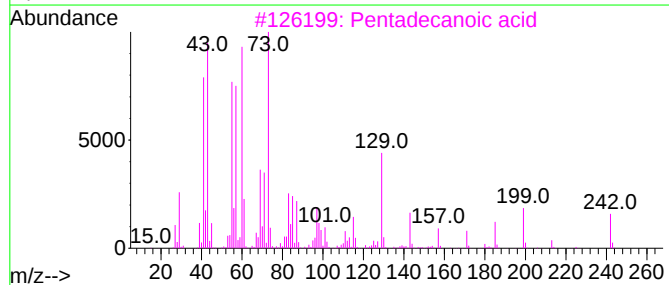
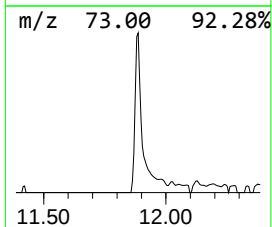
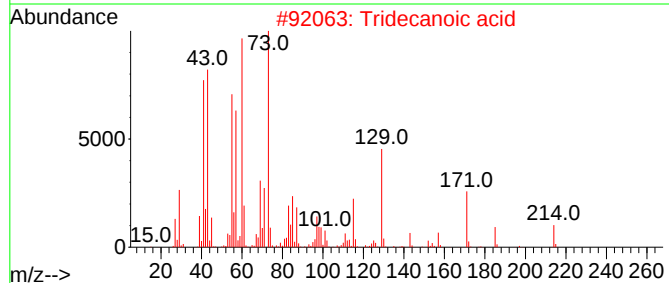
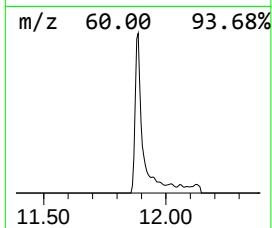
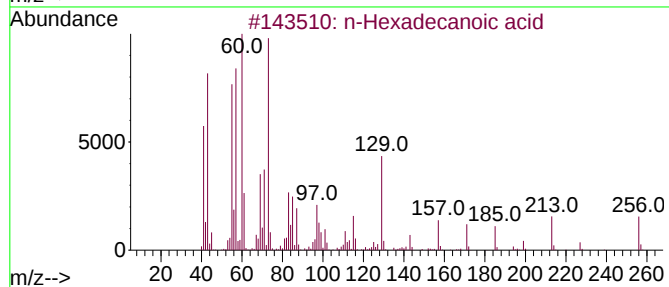
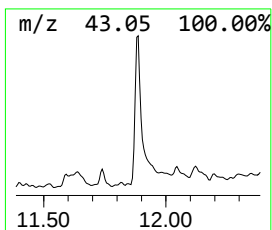
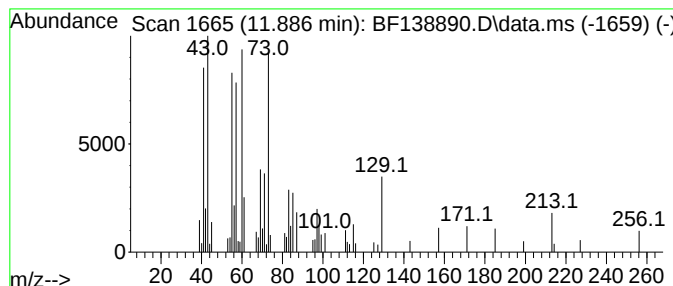
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	3.61 ng	103711	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Dodecanoic acid	200	C12H24O2	000143-07-7	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080924\
Data File : BF138890.D
Acq On : 09 Aug 2024 16:02
Operator : RC/JU
Sample : P3469-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MLS-15-513-528

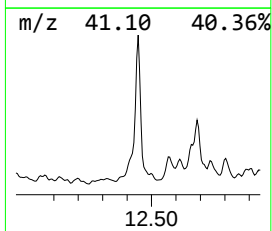
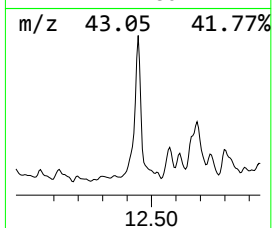
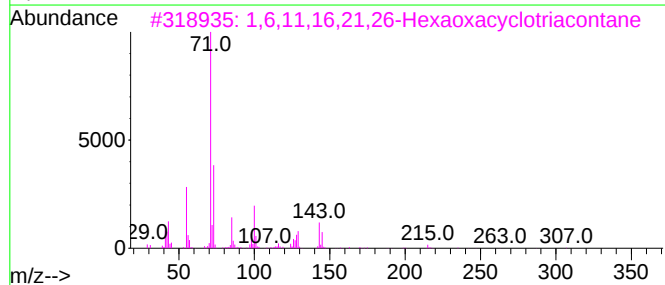
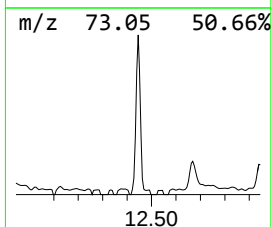
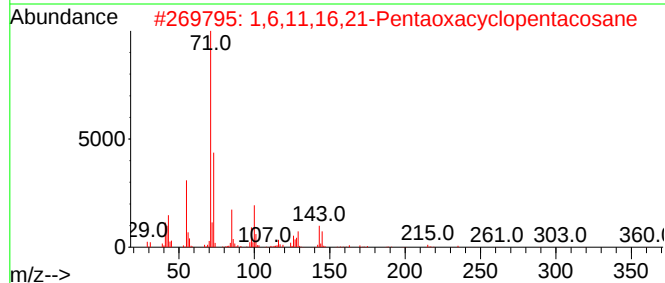
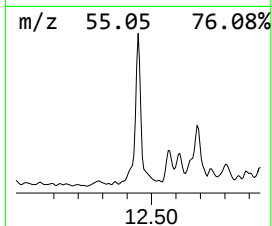
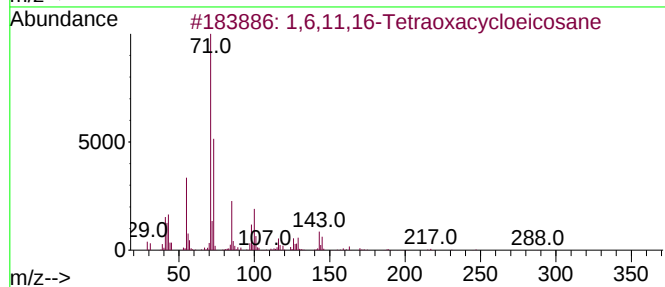
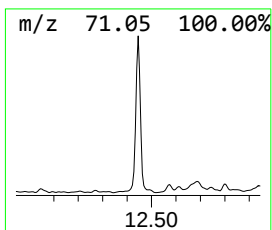
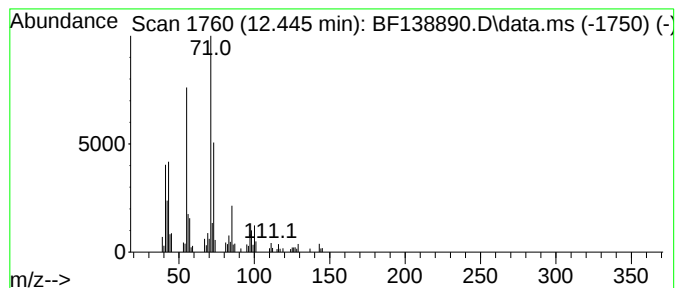
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1,6,11,16-Tetraoxacycloeico... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.445	3.70 ng	106171	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6,11,16-Tetraoxacycloeicosane	288	C16H32O4	017043-02-6	72		
2	1,6,11,16,21-Pentaoxacyclopentac...	360	C20H40O5	056890-57-4	64		
3	1,6,11,16,21,26-Hexaoxacyclotria...	432	C24H48O6	064001-05-4	59		
4	1-Penten-3-ol, 2-methyl-	100	C6H12O	002088-07-5	58		
5	Cyclopentanol, 1-methyl-	100	C6H12O	001462-03-9	47		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080924\
Data File : BF138890.D
Acq On : 09 Aug 2024 16:02
Operator : RC/JU
Sample : P3469-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MLS-15-513-528

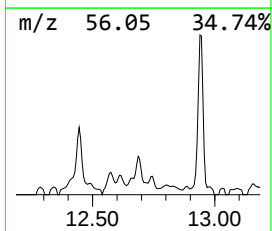
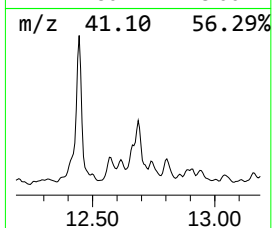
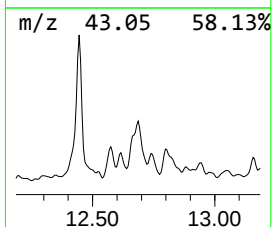
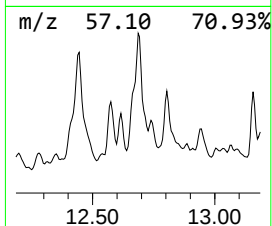
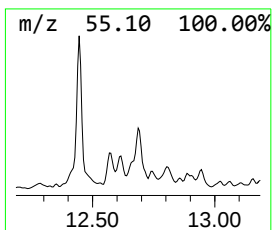
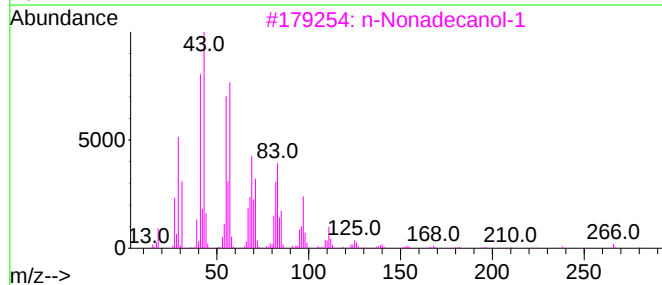
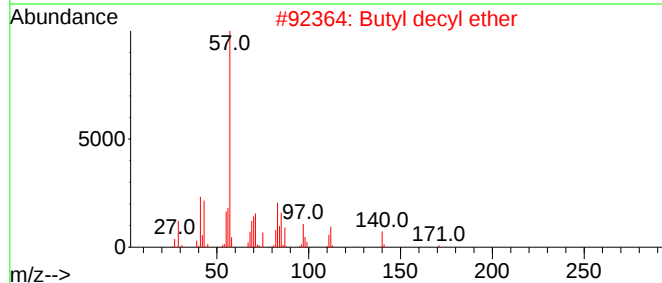
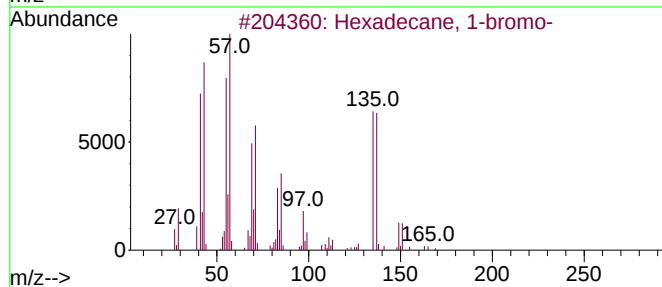
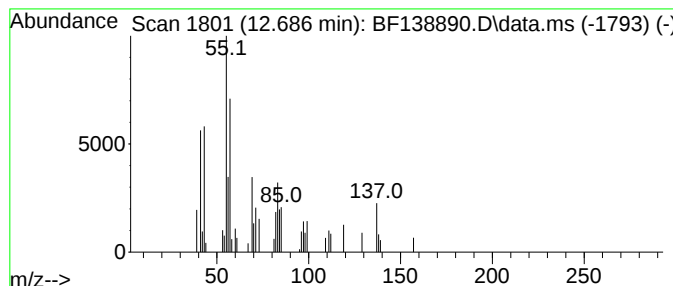
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown12.686 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.686	3.10 ng	45652	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 1-bromo-	304	C16H33Br	000112-82-3	38
2			Butyl decyl ether	214	C14H30O	1000406-40-2	38
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	35
4			Acetic acid, decyl ester	200	C12H24O2	000112-17-4	35
5			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080924\
Data File : BF138890.D
Acq On : 09 Aug 2024 16:02
Operator : RC/JU
Sample : P3469-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

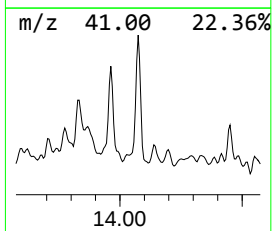
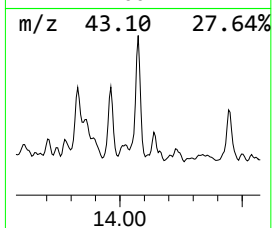
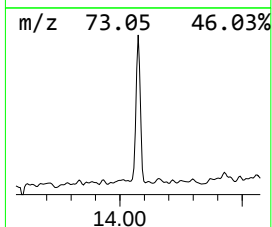
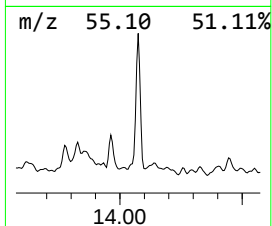
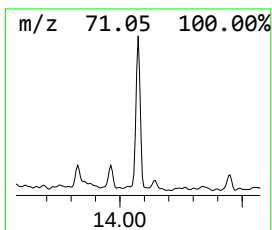
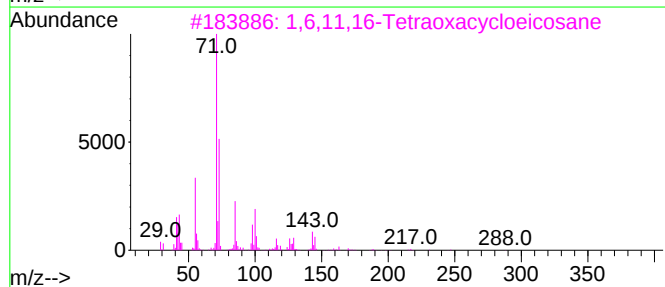
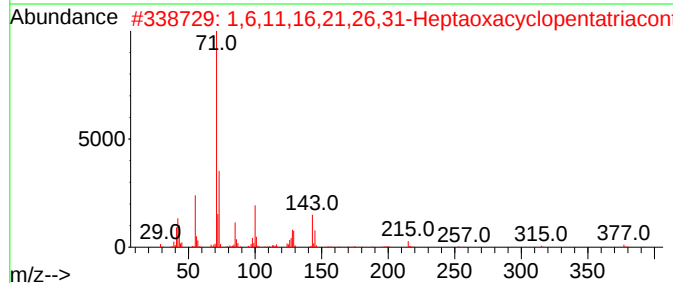
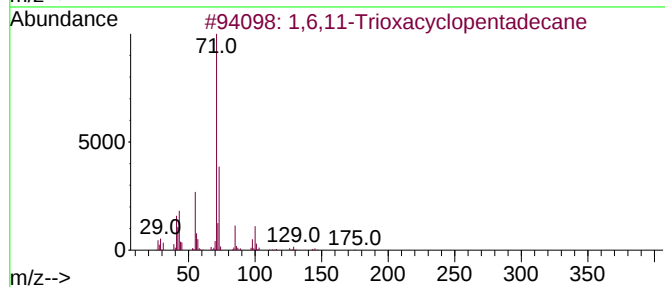
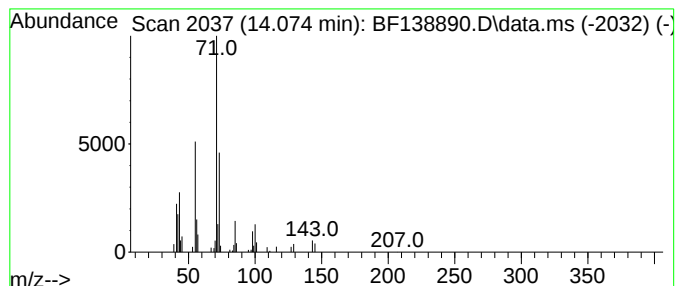
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1,6,11-Trioxacyclopentadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.074	2.37 ng	34982	Chrysene-d12	13.998	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6,11-Trioxacyclopentadecane	216	C12H24O3	000295-63-6	86
2	1,6,11,16,21,26,31-Heptaoxacyclo...	504	C28H56O7	066055-34-3	83
3	1,6,11,16-Tetraoxacycloeicosane	288	C16H32O4	017043-02-6	64
4	1,6,11,16,21,26-Hexaoxacyclotria...	432	C24H48O6	064001-05-4	64
5	1,6,11,16,21-Pentaoxacyclopentac...	360	C20H40O5	056890-57-4	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080924\
Data File : BF138890.D
Acq On : 09 Aug 2024 16:02
Operator : RC/JU
Sample : P3469-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MLS-15-513-528

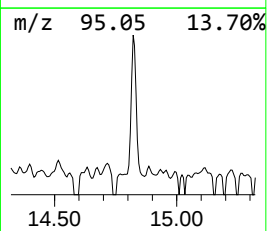
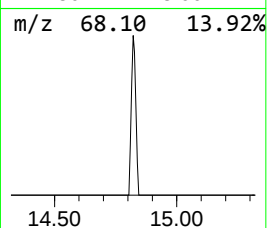
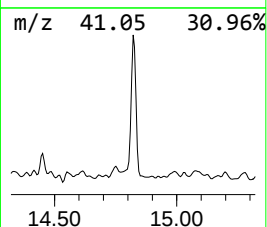
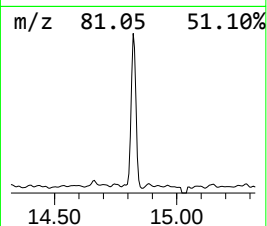
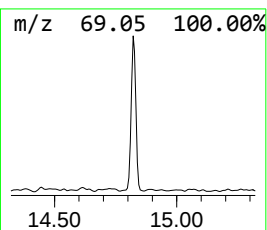
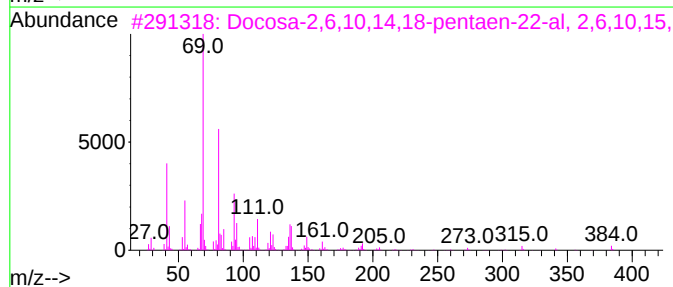
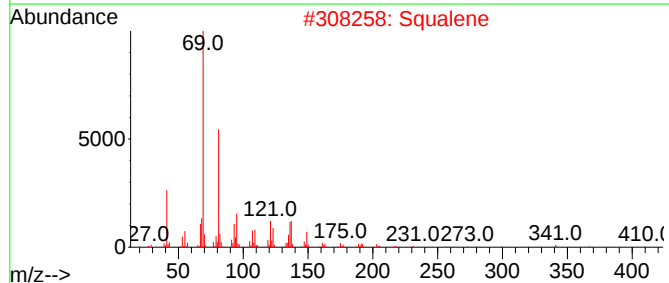
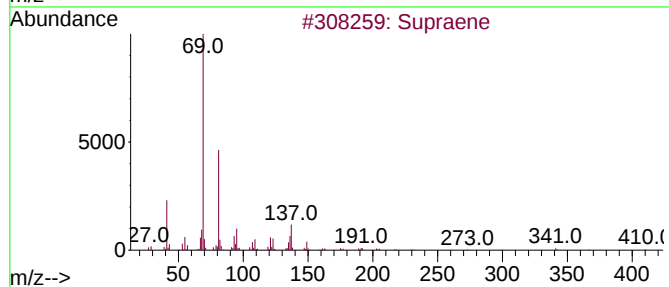
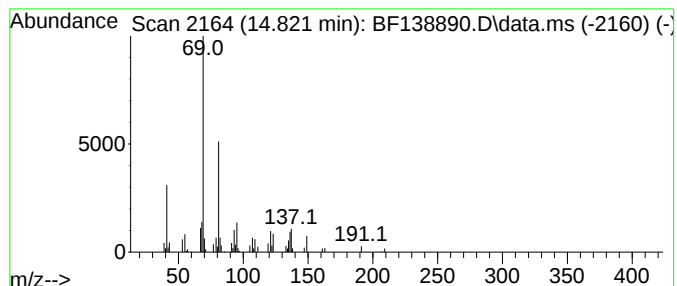
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.821	4.27 ng	51143	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	91
3			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
4			2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	78
5			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080924\
Data File : BF138890.D
Acq On : 09 Aug 2024 16:02
Operator : RC/JU
Sample : P3469-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

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ClientSampleId :
MLS-15-513-528

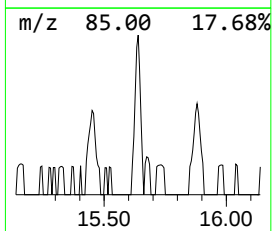
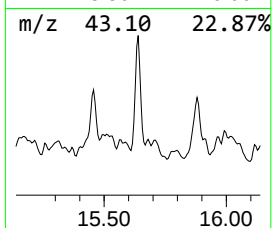
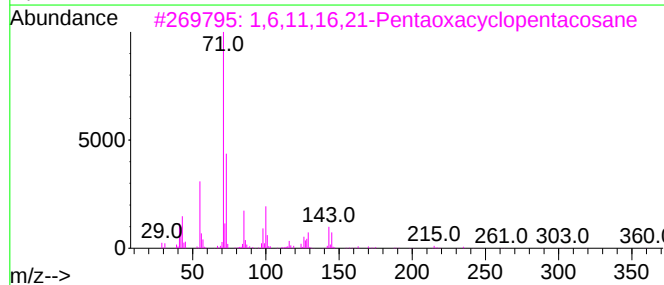
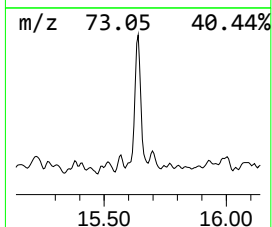
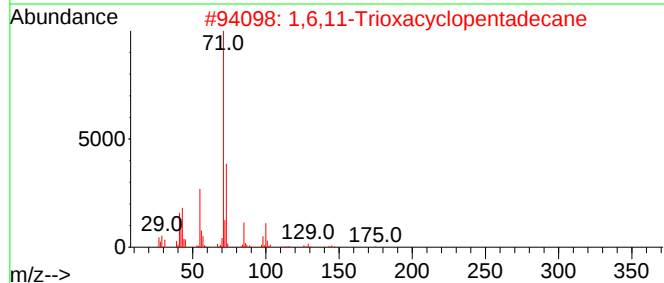
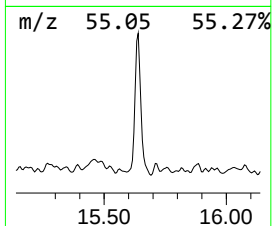
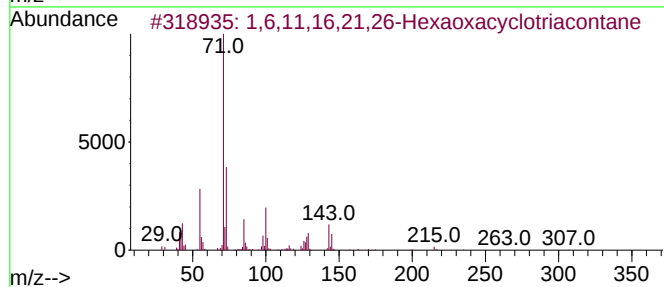
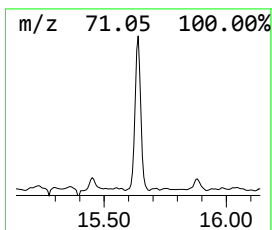
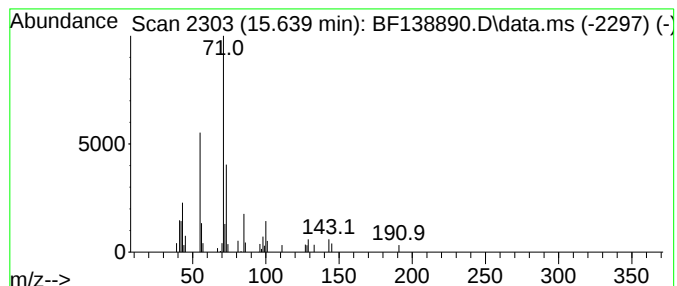
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1,6,11,16,21,26-Hexaoxacycl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.639	2.83 ng	33909	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6,11,16,21,26-Hexaoxacyclotria...	432	C24H48O6	064001-05-4	83		
2	1,6,11-Trioxacyclopentadecane	216	C12H24O3	000295-63-6	72		
3	1,6,11,16,21-Pentaoxacyclopentac...	360	C20H40O5	056890-57-4	64		
4	1,6,11,16,21,26,31-Heptaoxacyclo...	504	C28H56O7	066055-34-3	59		
5	1,6,11,16-Tetraoxacycloeicosane	288	C16H32O4	017043-02-6	58		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080924\
Data File : BF138890.D
Acq On : 09 Aug 2024 16:02
Operator : RC/JU
Sample : P3469-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MLS-15-513-528

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.134	191.8	ng	2993290	1	6.840	312152	20.0
2-Pentanone, 4-...	5.051	4.2	ng	65216	1	6.840	312152	20.0
Ethanol, 2-butoxy-	5.798	54.3	ng	847446	1	6.840	312152	20.0
2-Propanol, 1-(...	8.334	7.8	ng	167503	2	8.116	431805	20.0
1-Propanol, 2,2...	8.357	9.3	ng	200509	2	8.116	431805	20.0
n-Hexadecanoic ...	11.886	3.6	ng	103711	4	11.357	573847	20.0
1,6,11,16-Tetra...	12.445	3.7	ng	106171	4	11.357	573847	20.0
unknown12.686	12.686	3.1	ng	45652	5	13.998	294746	20.0
1,6,11-Trioxacy...	14.074	2.4	ng	34982	5	13.998	294746	20.0
Supraene	14.821	4.3	ng	51143	6	15.457	239522	20.0
1,6,11,16,21,26...	15.639	2.8	ng	33909	6	15.457	239522	20.0