

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
 Data File : BF136728.D
 Acq On : 26 Dec 2023 19:59
 Operator : CG\JU
 Sample : 05933-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-1-SOUTH-SIDE

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136728.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.010	493	497	502	rVB	14702	16471	1.44%	0.191%
2	5.422	563	567	578	rBV	1070952	951100	83.03%	11.010%
3	6.428	734	738	749	rBV	1112066	959479	83.77%	11.107%
4	6.781	795	798	802	rBV	522119	405896	35.44%	4.699%
5	7.339	889	893	896	rBV	694545	622302	54.33%	7.204%
6	8.057	1011	1015	1019	rBV	644274	521434	45.52%	6.036%
7	9.133	1194	1198	1202	rBV	1345801	1145435	100.00%	13.260%
8	9.816	1310	1314	1317	rBV	660620	536337	46.82%	6.209%
9	10.604	1445	1448	1462	rBV	638349	576468	50.33%	6.673%
10	11.304	1564	1567	1571	rBV	568076	488223	42.62%	5.652%
11	11.839	1651	1658	1666	rBV	174033	179194	15.64%	2.074%
12	12.004	1683	1686	1690	rBV3	8948	13133	1.15%	0.152%
13	12.092	1698	1701	1706	rVB4	12838	14662	1.28%	0.170%
14	12.551	1772	1779	1787	rBV5	25554	53198	4.64%	0.616%
15	12.627	1789	1792	1798	rVV	31996	37924	3.31%	0.439%
16	12.898	1834	1838	1842	rBV	928245	869245	75.89%	10.062%
17	13.810	1989	1993	1995	rBV5	17383	21143	1.85%	0.245%
18	13.839	1995	1998	2010	rVB7	24266	62438	5.45%	0.723%
19	13.963	2014	2019	2022	rBV	395968	394634	34.45%	4.568%
20	14.039	2029	2032	2038	rBV7	10341	15806	1.38%	0.183%
21	14.127	2044	2047	2050	rBV2	13326	13914	1.21%	0.161%
22	14.433	2095	2099	2102	rBV2	36004	41455	3.62%	0.480%
23	14.815	2160	2164	2169	rVB2	78597	99003	8.64%	1.146%
24	15.245	2233	2237	2245	rVB2	52859	86333	7.54%	0.999%
25	15.439	2265	2270	2274	rBV	300874	370396	32.34%	4.288%
26	15.757	2319	2324	2332	rVB3	41394	74442	6.50%	0.862%
27	16.357	2420	2426	2433	rBV4	34094	68416	5.97%	0.792%

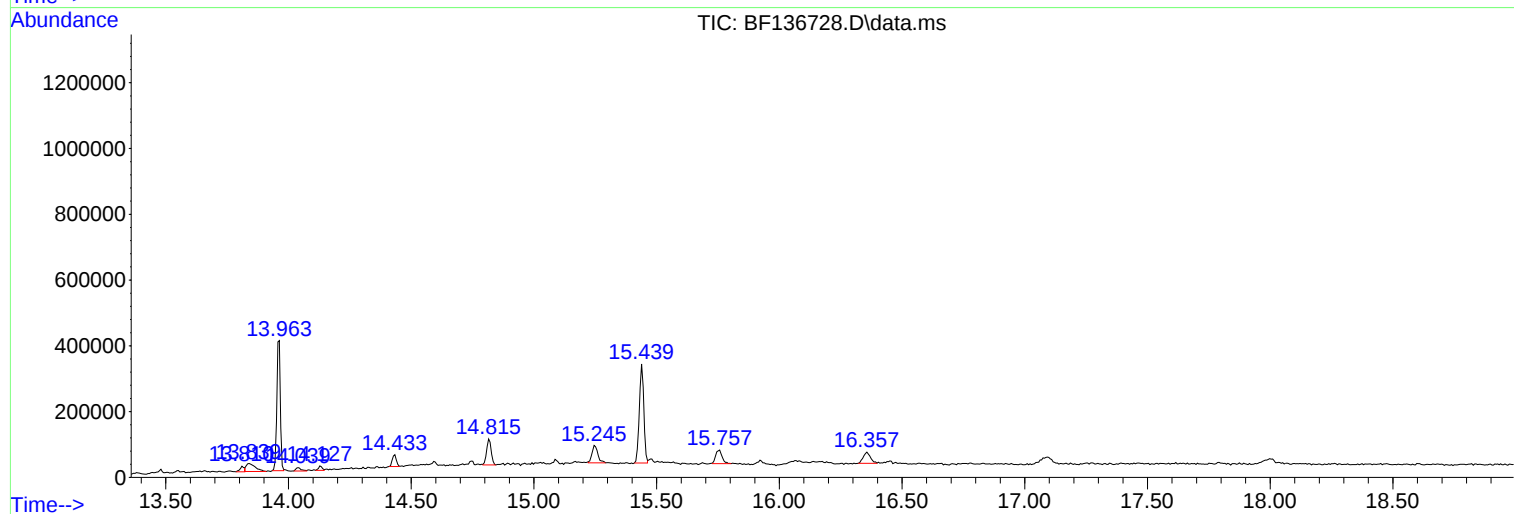
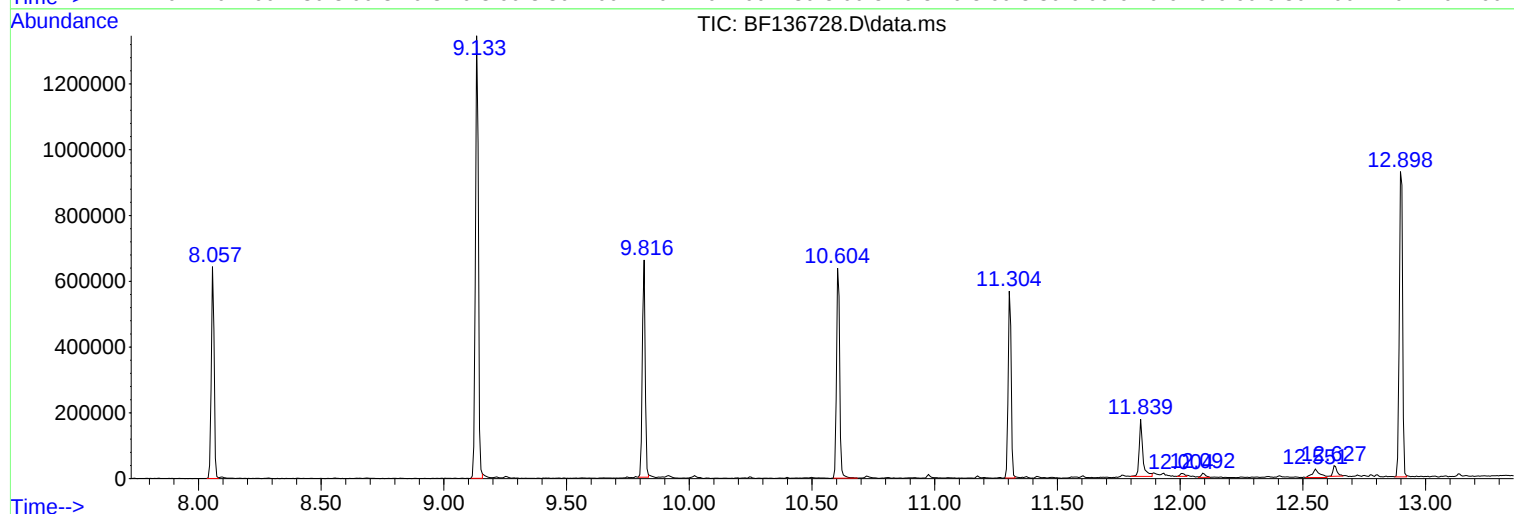
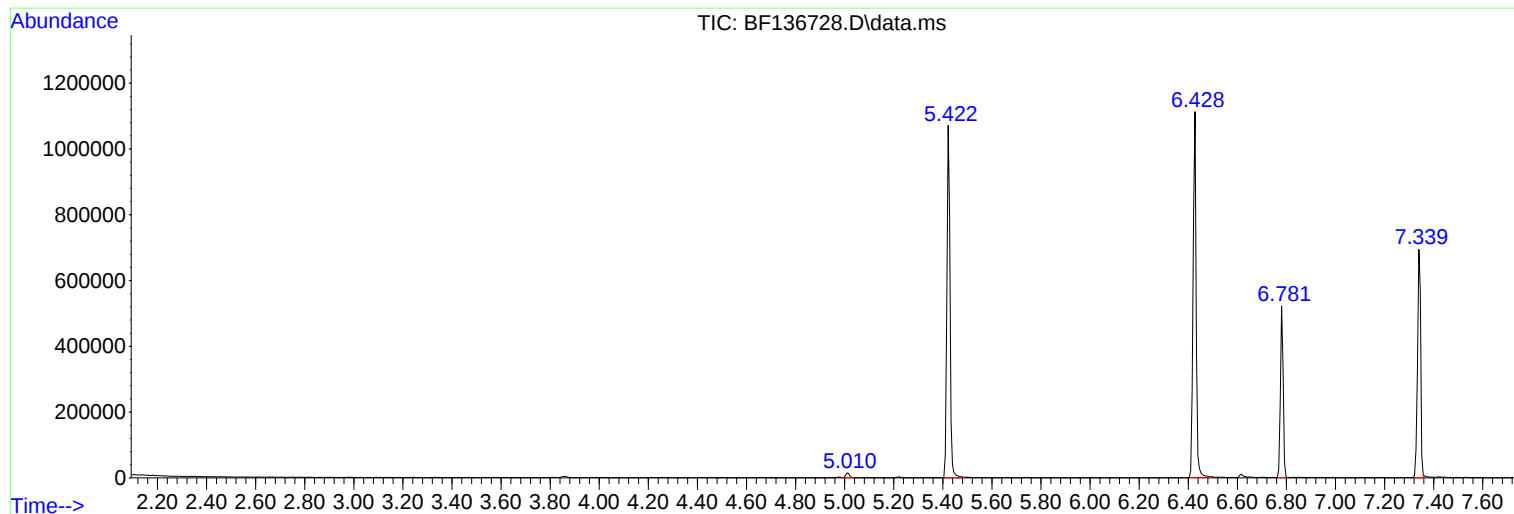
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ClientSampleId :
S-1-SOUTH-SIDE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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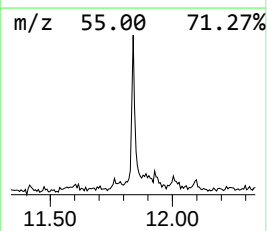
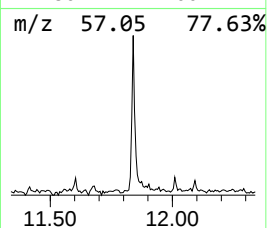
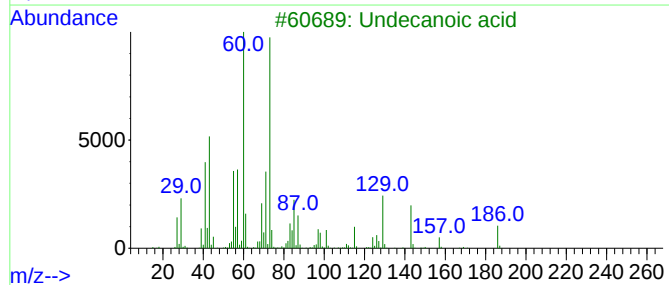
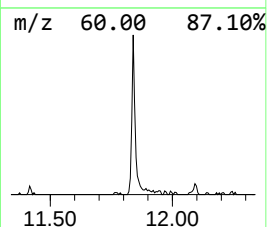
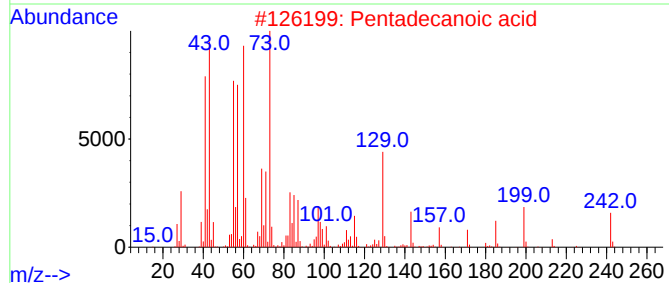
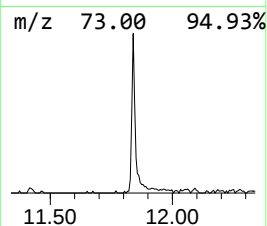
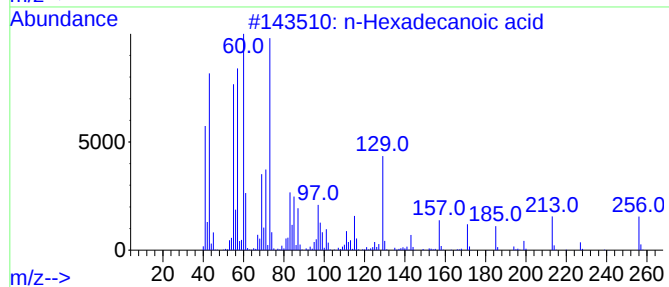
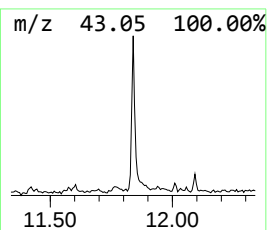
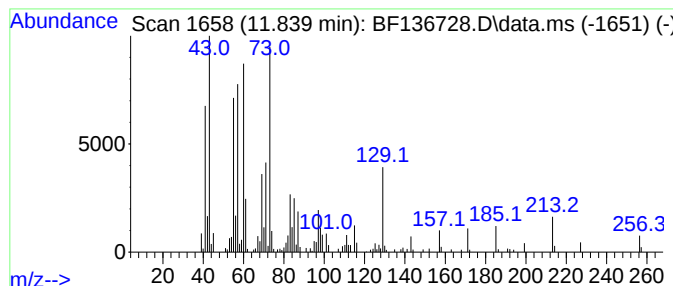
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	7.34 ng	179194	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Undecanoic acid	186	C11H22O2	000112-37-8	76
4			Tridecanoic acid	214	C13H26O2	000638-53-9	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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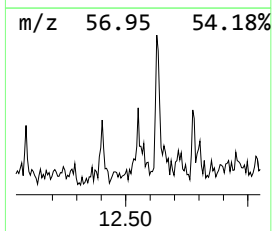
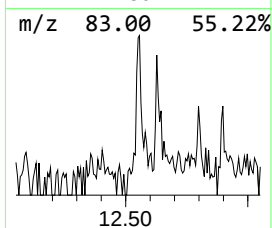
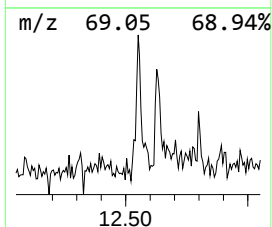
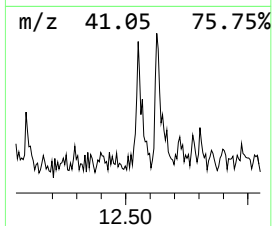
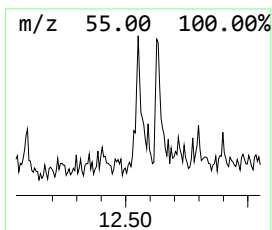
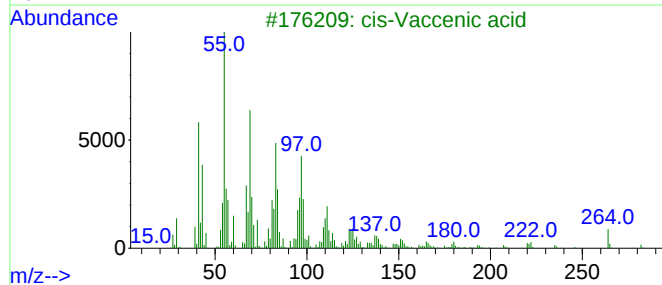
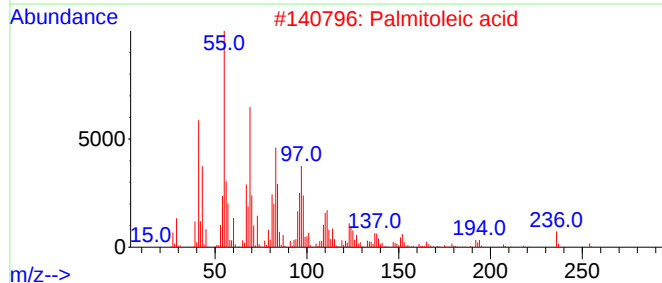
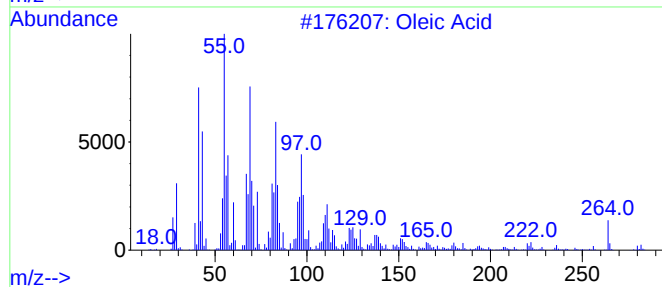
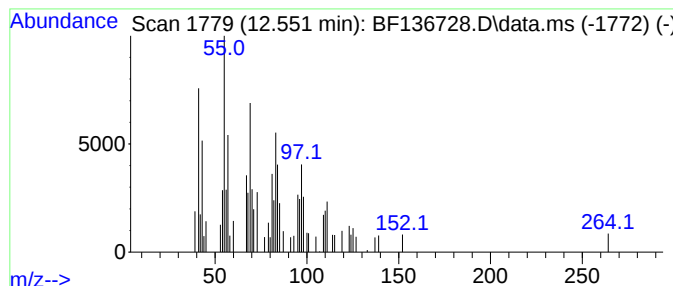
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Oleic Acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.551	2.18 ng	53198	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oleic Acid	282	C18H34O2	000112-80-1	87
2			Palmitoleic acid	254	C16H30O2	000373-49-9	87
3			cis-Vaccenic acid	282	C18H34O2	000506-17-2	76
4			(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	62
5			9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	62



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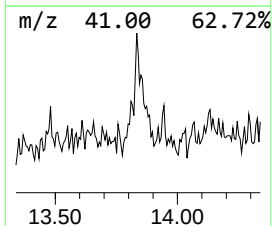
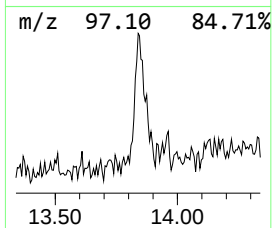
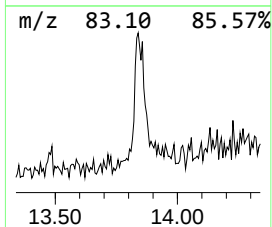
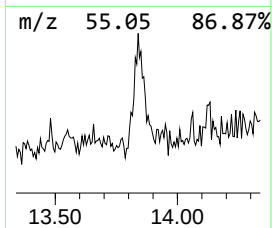
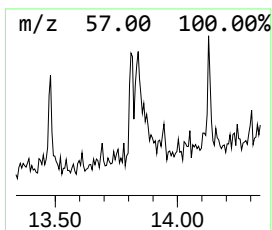
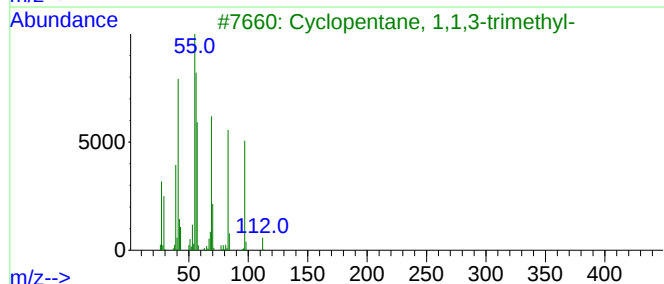
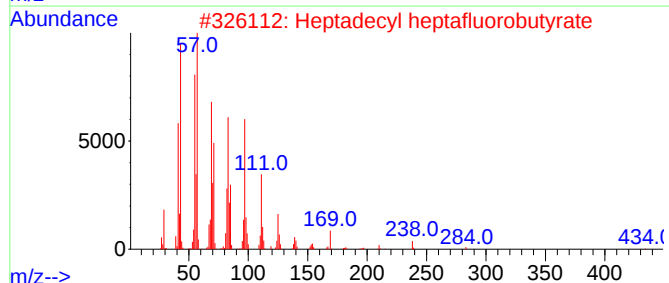
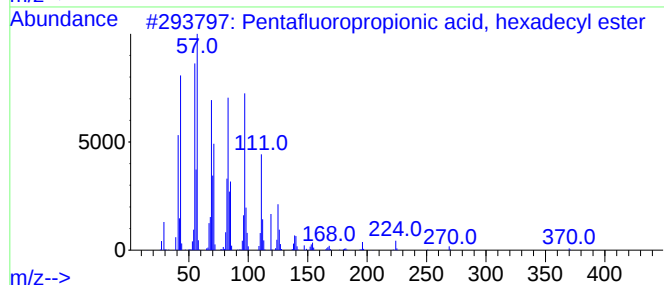
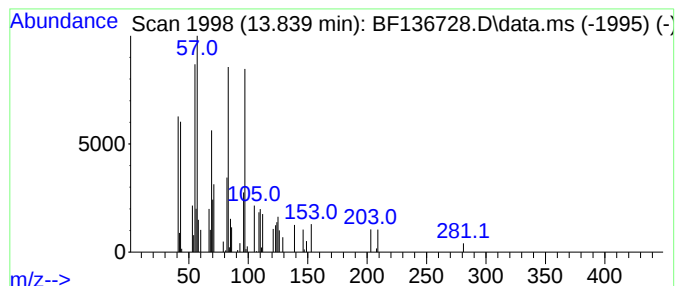
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Pentafluoropropionic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	3.16 ng	62438	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	53
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	50
3			Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	47
4			1,16-Hexadecanediol	258	C16H34O2	007735-42-4	43
5			Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054824-04-3	35



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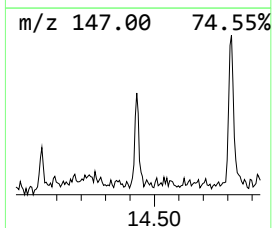
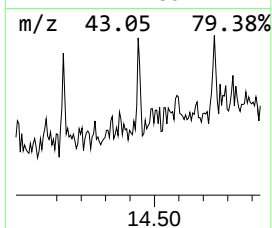
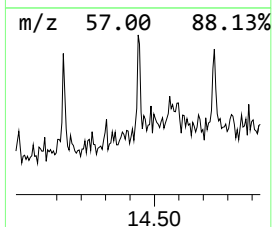
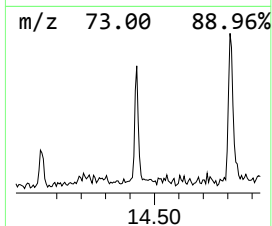
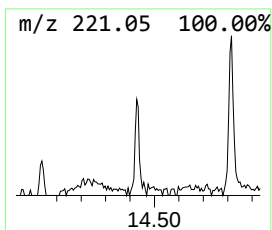
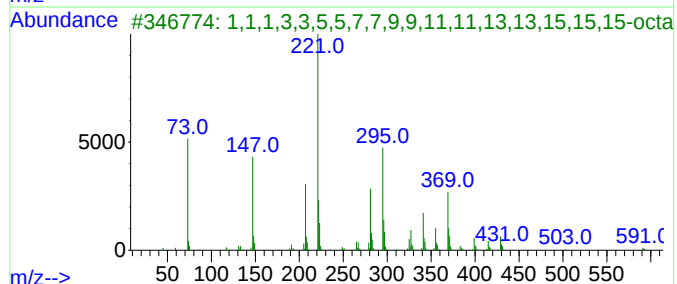
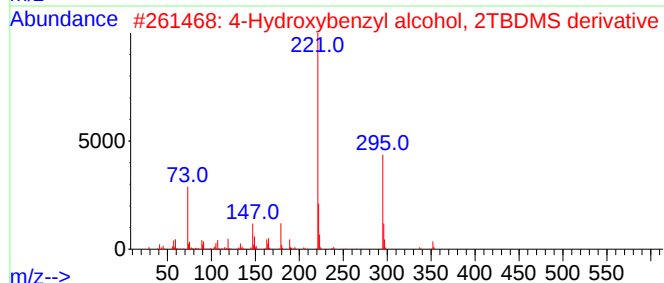
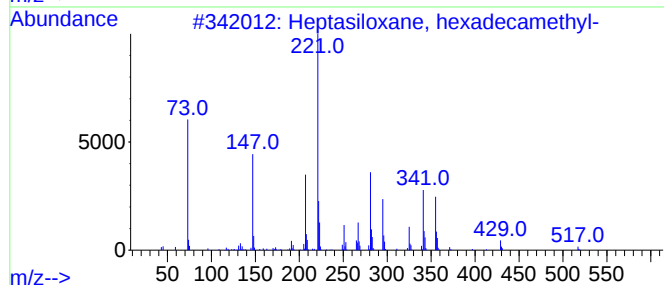
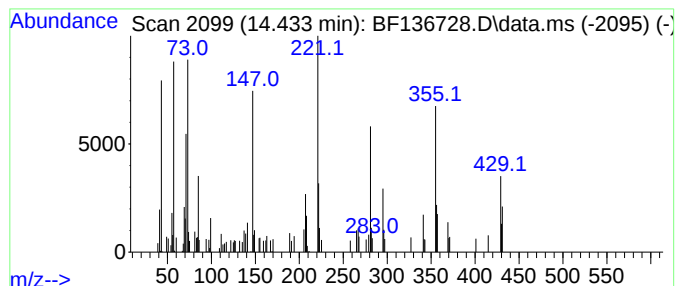
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown14.433 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.433	2.10 ng	41455	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	37
2			4-Hydroxybenzyl alcohol, 2TBDMS ...	352	C19H36O2Si2	1000364-43-9	27
3			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	606	C18H54O7Si8	000556-69-4	14
4			2-tert-Butyl-4-methylphenol, ter...	278	C17H30O5	174362-55-1	14
5			Methyl 2-methyl-2-benzylideneami...	221	C12H15NO3	079751-13-6	14



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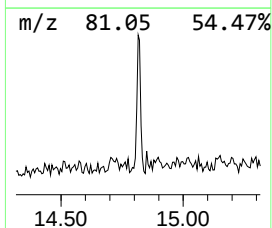
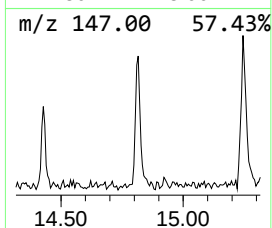
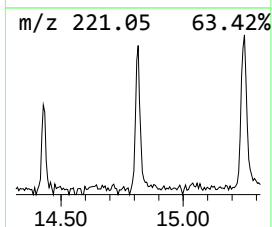
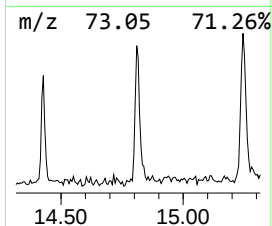
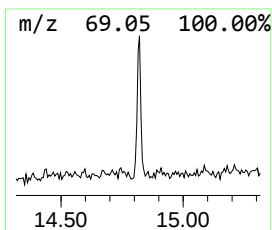
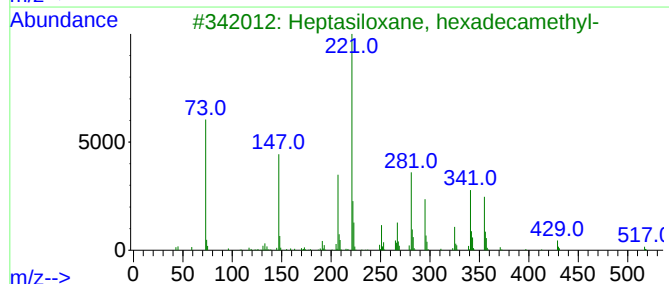
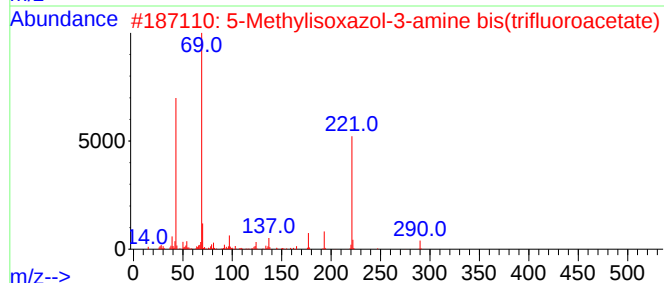
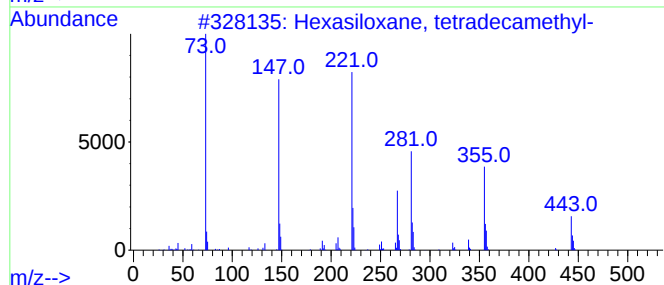
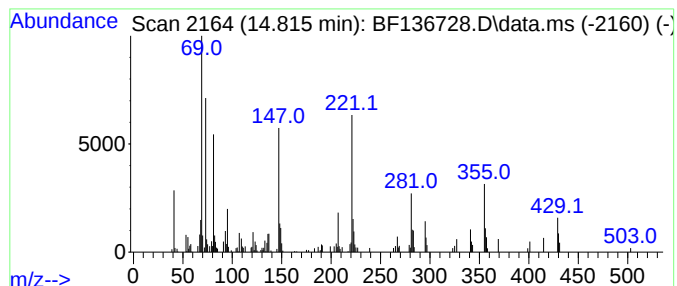
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Peak Number 5 unknown14.816 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.816	5.35 ng	99003	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	38
2			5-Methylisoxazol-3-amine bis(tri...	290	C8H4F6N2O3	1000373-35-6	32
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	30
4			1-Bromo-11-iodoundecane	360	C11H22BrI	139123-69-6	27
5			Calealactone B, TMS derivative	494	C24H34O9Si	1000480-41-9	27



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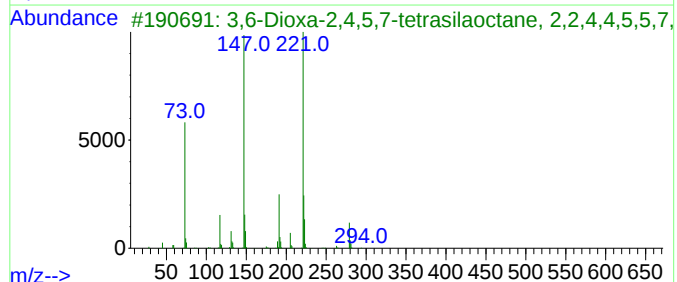
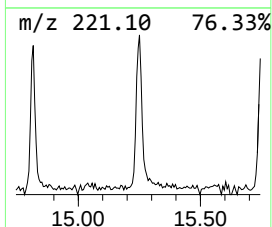
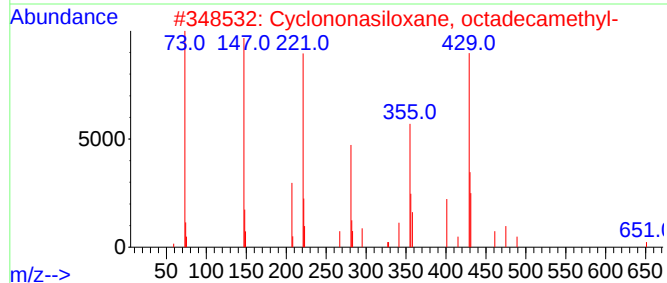
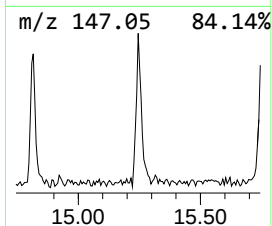
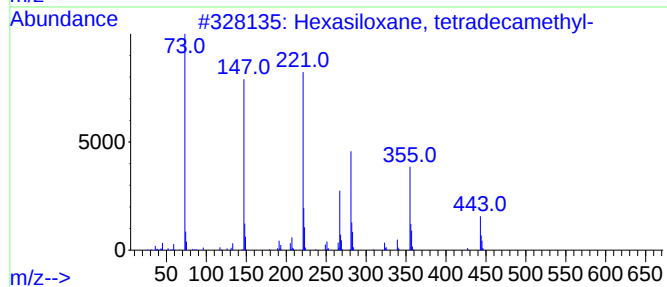
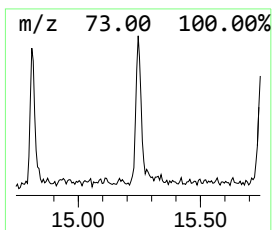
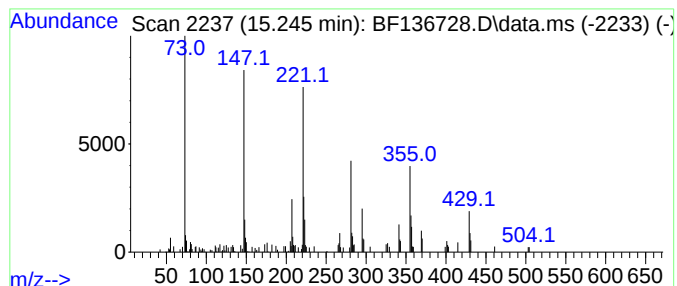
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexasiloxane, tetradecamethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.245	4.66 ng	86333	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	80
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	80
3			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	38
4			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	37
5			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	754	C22H66O9Si10	000556-70-7	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136728.D
Acq On : 26 Dec 2023 19:59
Operator : CG\JU
Sample : 05933-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-1-SOUTH-SIDE

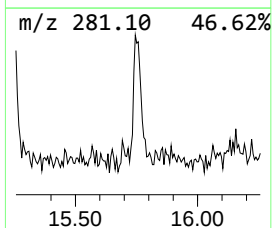
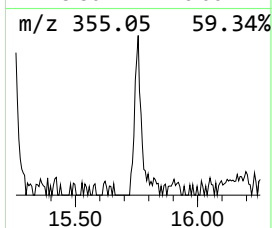
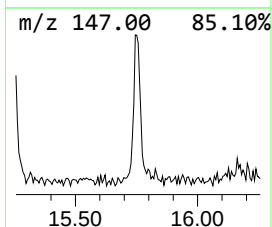
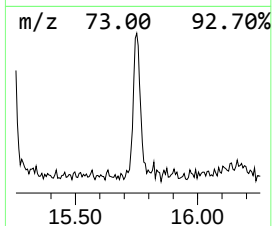
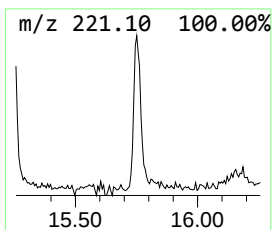
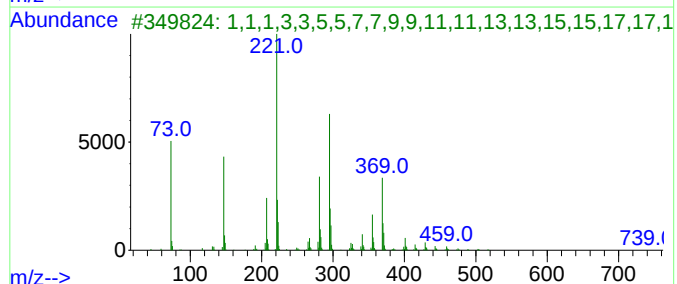
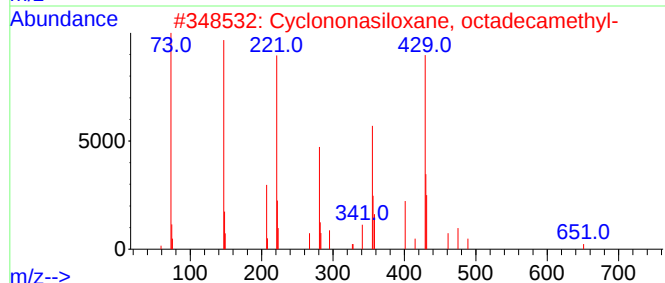
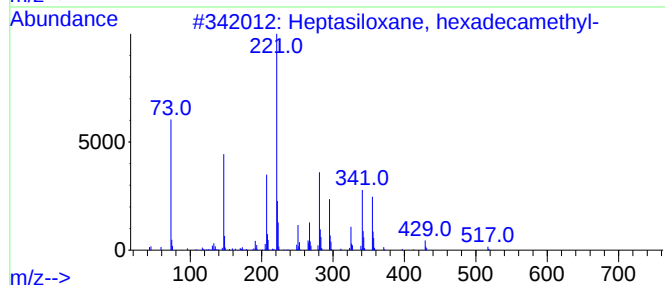
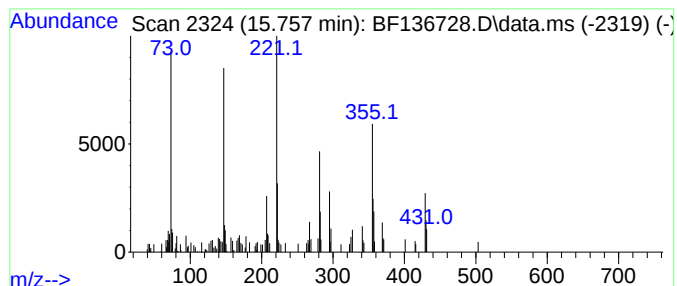
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptasiloxane, hexadecamethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.757	4.02 ng	74442	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	78
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	74
3			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	754	C22H66O9Si10	000556-70-7	43
4			3,4-Dihydroxyphenylglycol, 4TMS ...	458	C20H42O4Si4	056114-62-6	38
5			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136728.D
Acq On : 26 Dec 2023 19:59
Operator : CG\JU
Sample : 05933-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-1-SOUTH-SIDE

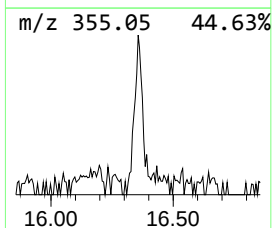
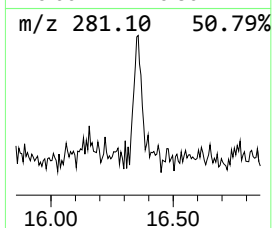
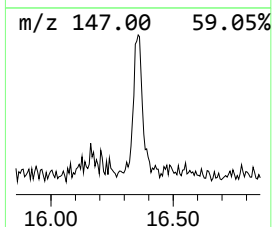
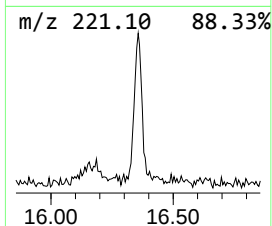
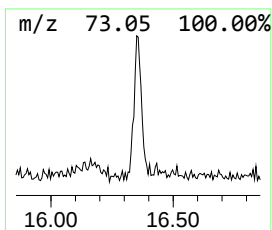
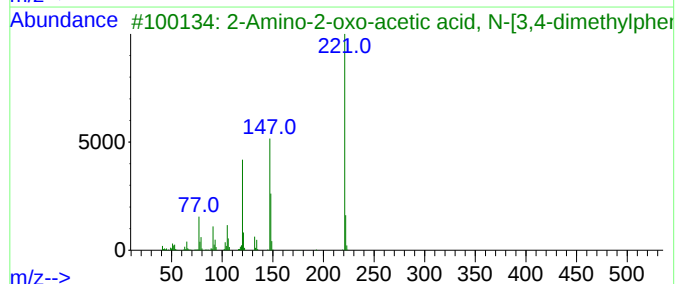
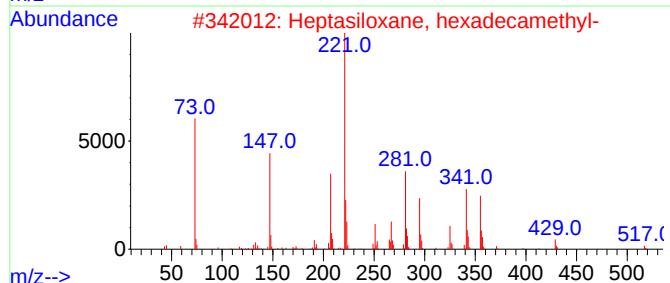
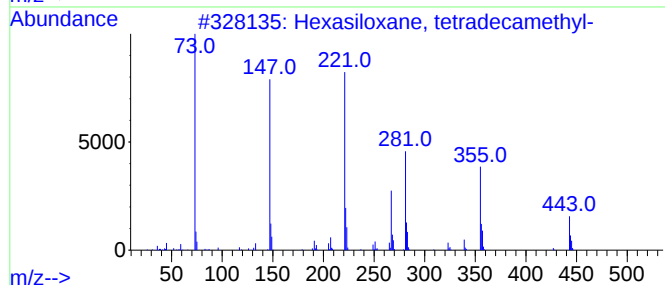
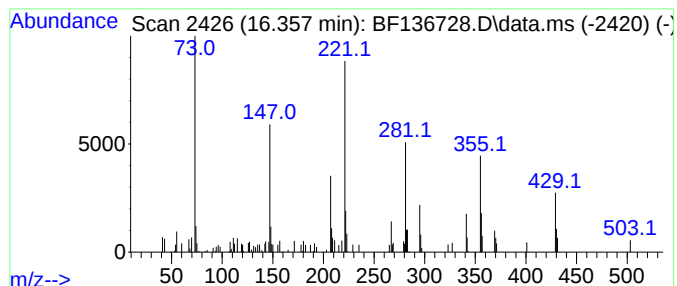
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.357 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.357	3.69 ng	68416	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	53
2			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	50
3			2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	38
4			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	35
5			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136728.D
Acq On : 26 Dec 2023 19:59
Operator : CG\JU
Sample : 05933-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-1-SOUTH-SIDE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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Oleic Acid	12.551	2.2	ng	53198	4	11.304	488223	20.0
Pentafluoroprop...	13.839	3.2	ng	62438	5	13.963	394634	20.0
unknown14.433	14.433	2.1	ng	41455	5	13.963	394634	20.0
unknown14.816	14.816	5.3	ng	99003	6	15.439	370396	20.0
Hexasiloxane, t...	15.245	4.7	ng	86333	6	15.439	370396	20.0
Heptasiloxane, ...	15.757	4.0	ng	74442	6	15.439	370396	20.0
unknown16.357	16.357	3.7	ng	68416	6	15.439	370396	20.0