

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012425\
 Data File : BF141263.D
 Acq On : 24 Jan 2025 15:35
 Operator : RC/JU
 Sample : Q1169-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ARS20-0006

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-BF011025.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141263.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.804	795	801	808	rVB	865191	1138718	3.75%	2.111%
2	7.363	884	896	906	rBV	1188379	1855627	6.12%	3.440%
3	8.087	1013	1019	1028	rVB	889991	1187338	3.91%	2.201%
4	9.163	1196	1202	1206	rBV	2621512	3474200	11.45%	6.441%
5	9.551	1265	1268	1272	rBV2	255635	391558	1.29%	0.726%
6	9.651	1282	1285	1290	rVB4	268009	379010	1.25%	0.703%
7	9.710	1291	1295	1298	rBV4	312136	506453	1.67%	0.939%
8	9.757	1299	1303	1306	rVB2	428452	610058	2.01%	1.131%
9	9.839	1311	1317	1321	rBV2	1062891	1805367	5.95%	3.347%
10	10.175	1369	1374	1378	rBV3	628972	1334331	4.40%	2.474%
11	10.251	1384	1387	1391	rBV2	508279	713780	2.35%	1.323%
12	10.633	1449	1452	1456	rBV	949568	1296767	4.27%	2.404%
13	12.651	1782	1795	1801	rBV3	8179621	30333792	100.00%	56.234%
14	12.704	1801	1804	1815	rVB	3557873	5135858	16.93%	9.521%
15	12.933	1839	1843	1847	rVB	1755355	2252572	7.43%	4.176%
16	15.445	2267	2270	2292	rVB	594532	1526441	5.03%	2.830%

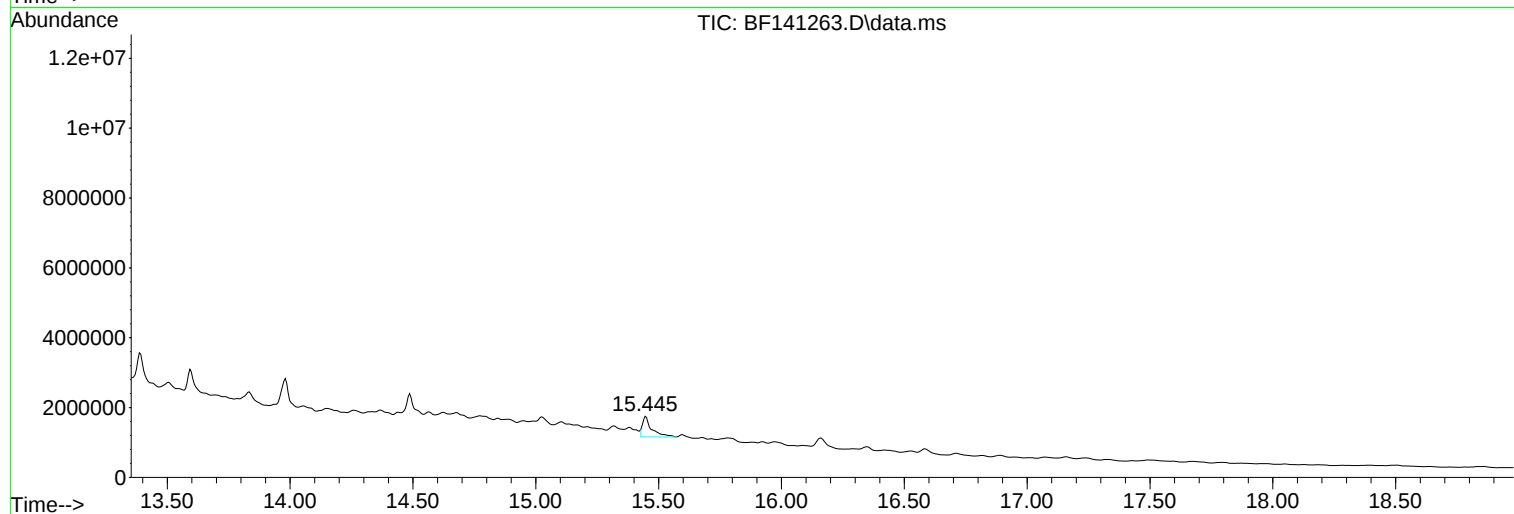
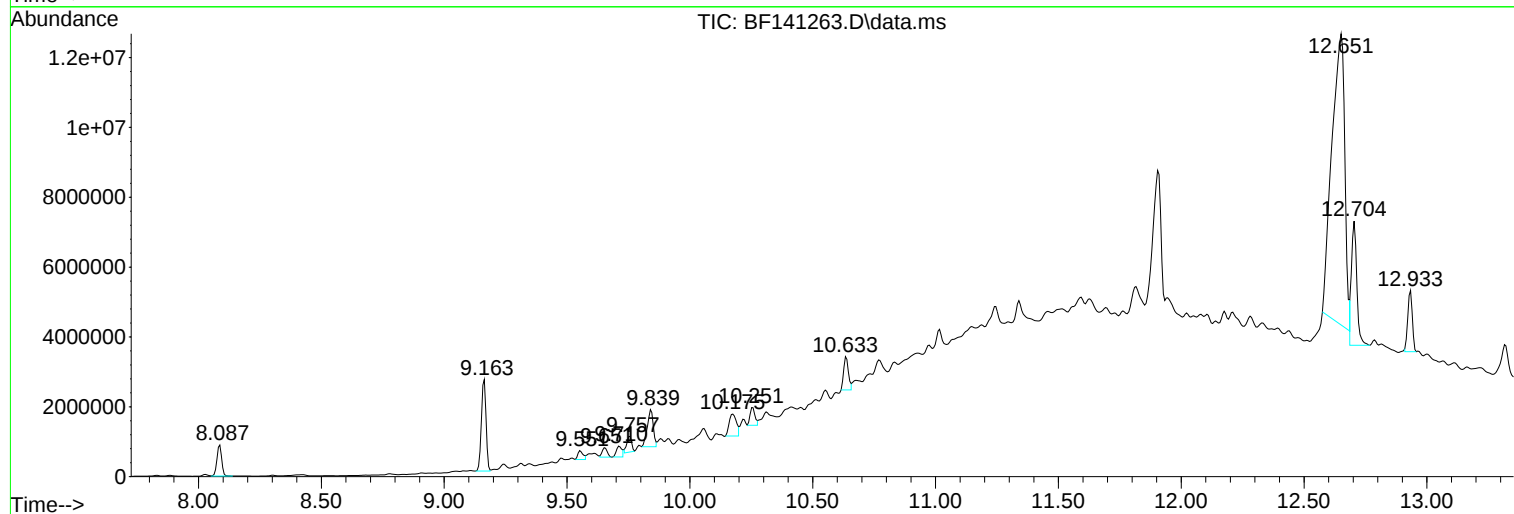
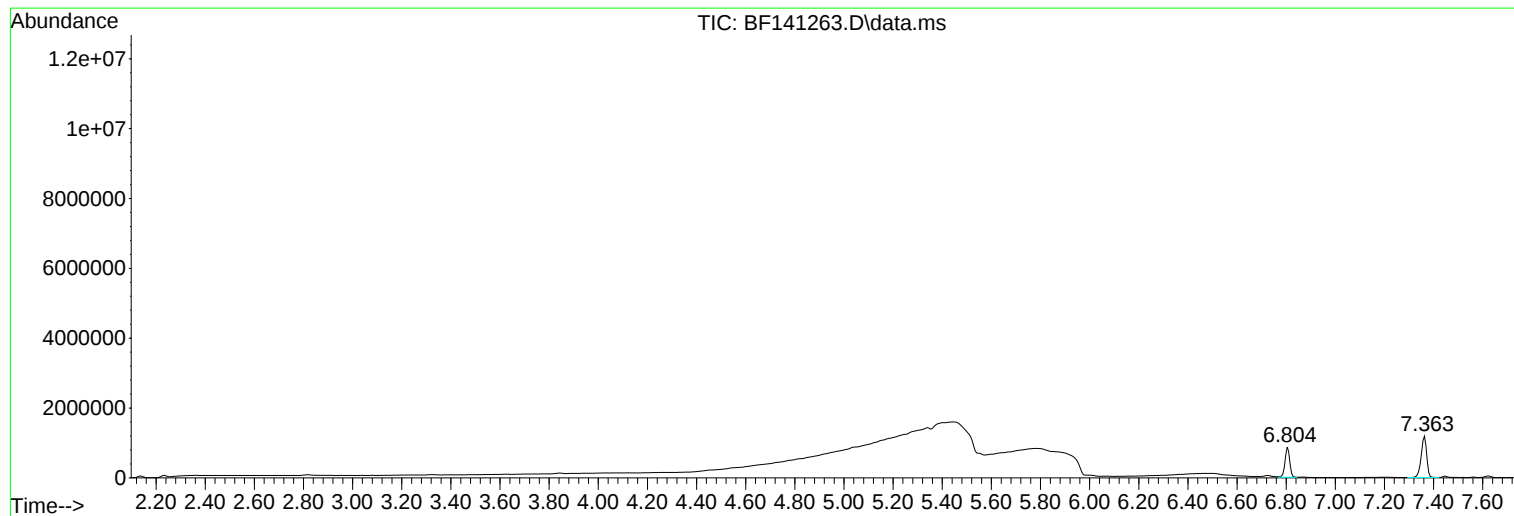
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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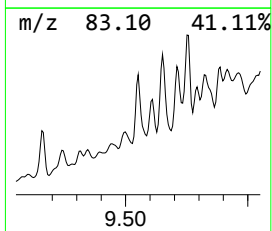
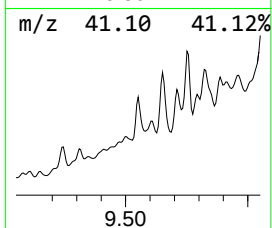
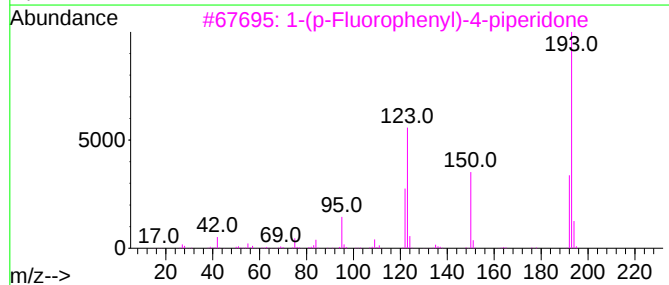
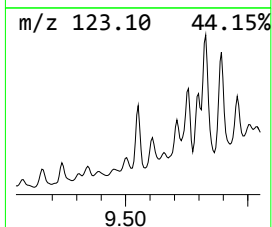
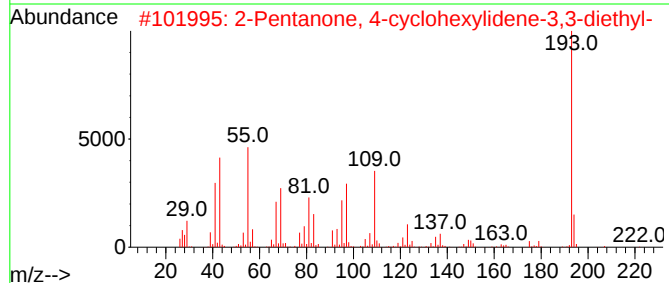
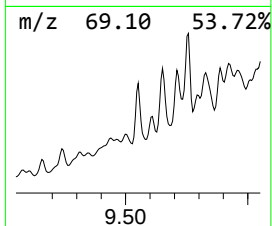
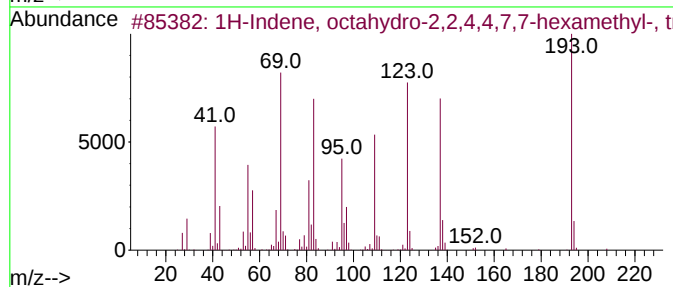
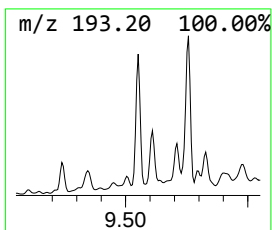
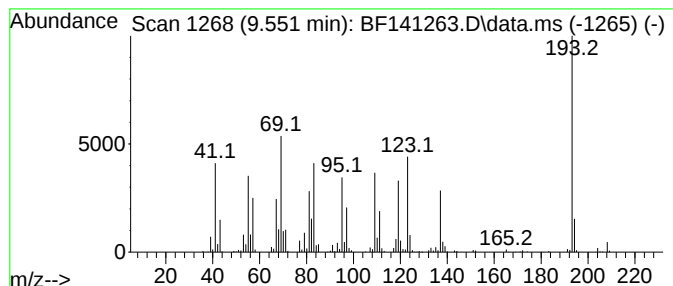
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown9.551 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.551	4.34 ng	391558	Acenaphthene-d10	9.845

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	40	
2	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	37	
3	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	32	
4	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	30	
5	Butan-2-one, 1-[3-(3,3-dimethyl-...	278	C16H26N2O2	1000303-34-2	27	



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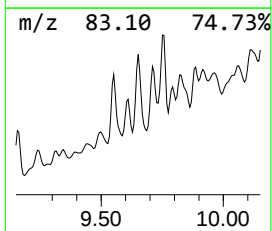
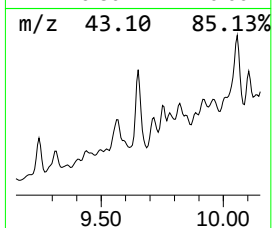
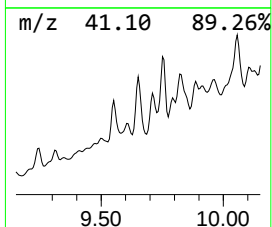
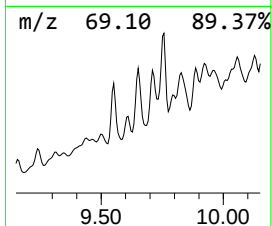
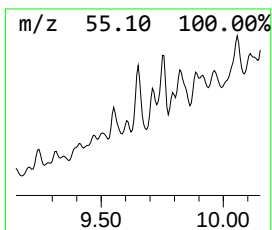
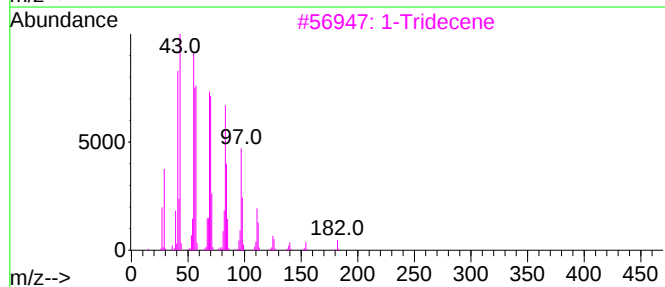
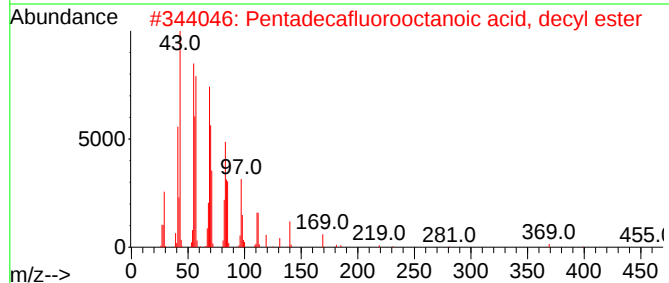
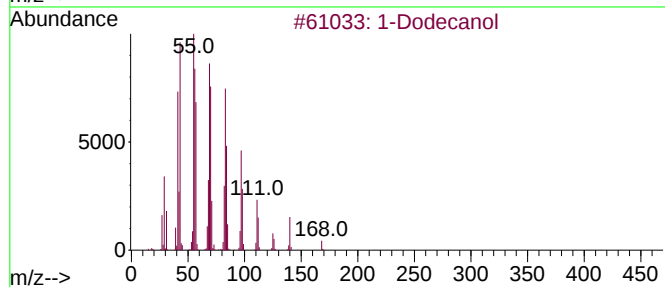
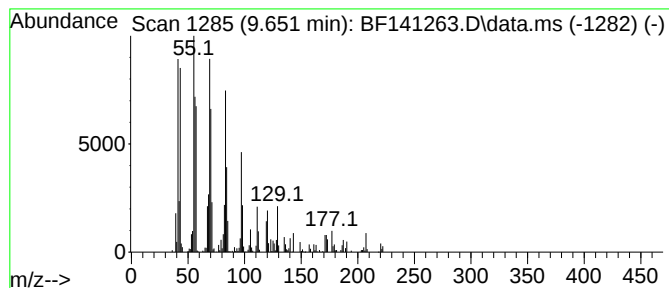
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Dodecanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.651	4.20 ng	379010	Acenaphthene-d10	9.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Dodecanol	186	C12H26O	000112-53-8	90
2			Pentadecafluorooctanoic acid, de...	554	C18H21F15O2	1000406-04-0	87
3			1-Tridecene	182	C13H26	002437-56-1	87
4			Cyclododecane	168	C12H24	000294-62-2	87
5			Pentadecafluorooctanoic acid, un...	568	C19H23F15O2	1010406-04-1	87



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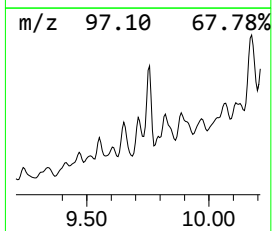
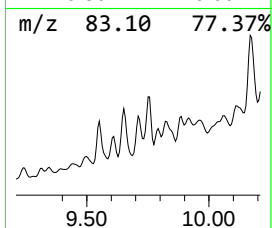
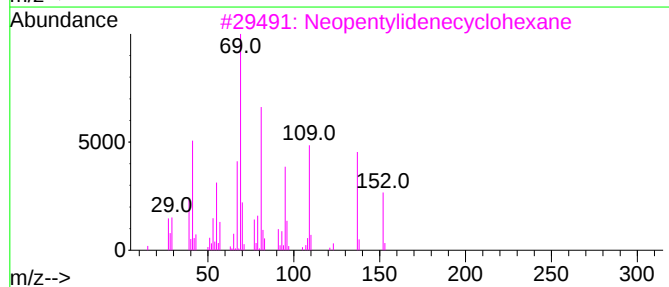
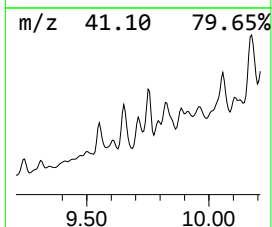
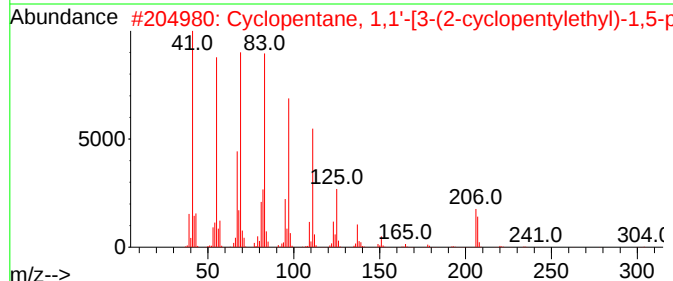
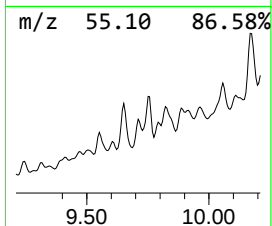
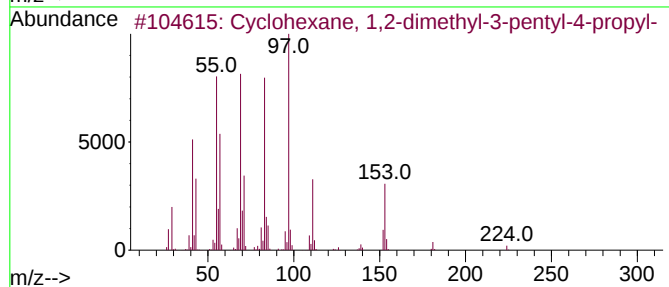
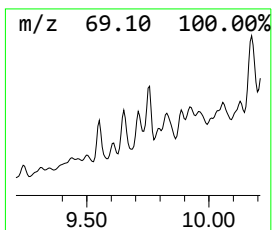
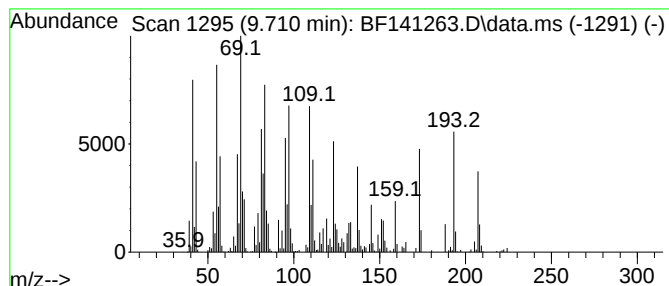
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Peak Number 3 Cyclohexane, 1,2-dimethyl-3... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.710	5.61 ng	506453	Acenaphthene-d10	9.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	51
2			Cyclopentane, 1,1'-[3-(2-cyclope...	304	C22H40	055255-85-1	43
3			Neopentylidenecyclohexane	152	C11H20	039546-80-0	42
4			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	41
5			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	35



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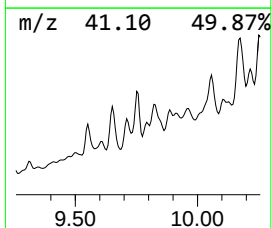
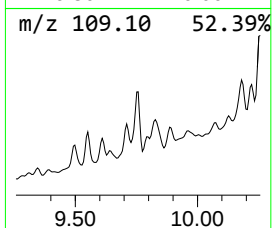
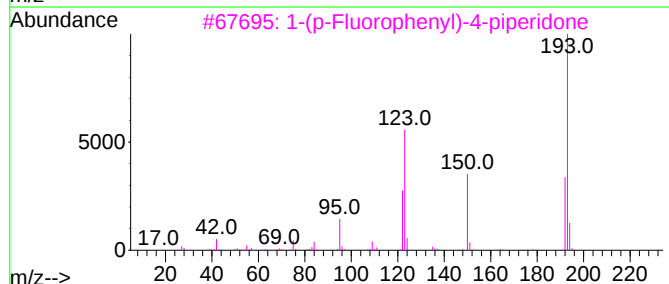
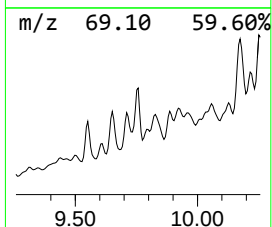
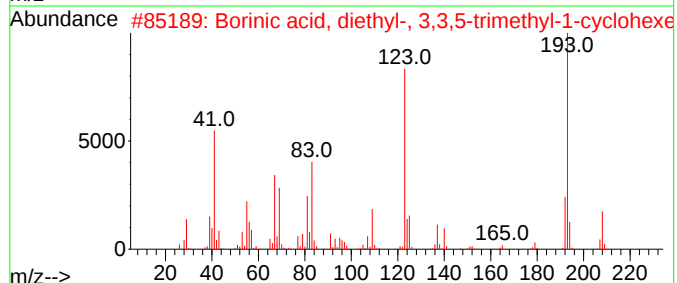
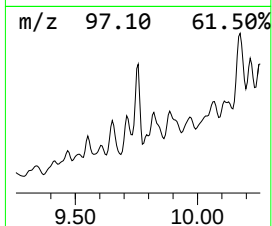
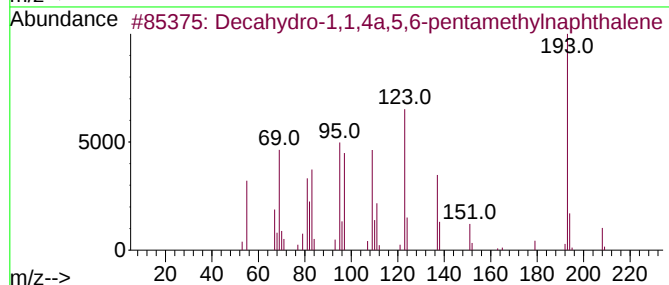
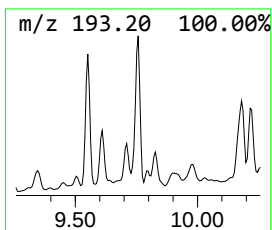
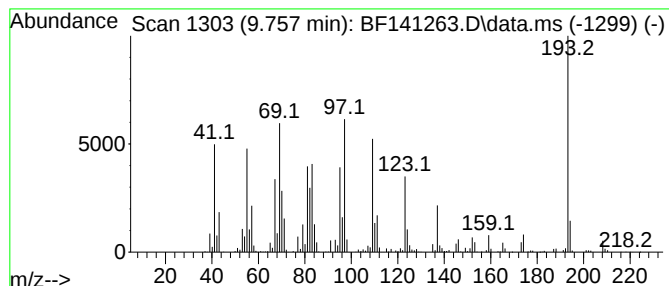
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown9.757 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.757	6.76 ng	610058	Acenaphthene-d10	9.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	49
2			Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	43
3			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	35
4			Butan-2-one, 1-[3-(3,3-dimethyl-...	278	C16H26N2O2	1000303-34-2	22
5			2-((Trimethylsilyl)thio)nicotino...	208	C9H12N2SSi	1000474-02-5	18



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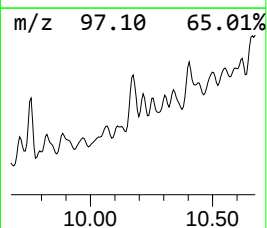
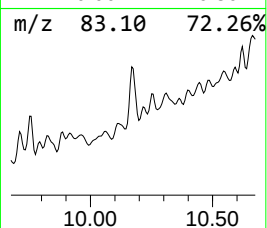
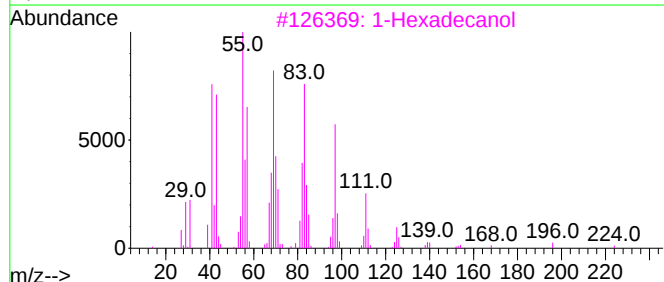
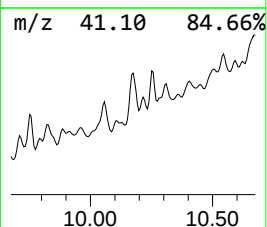
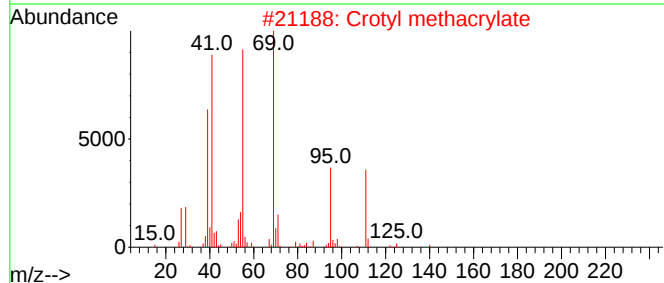
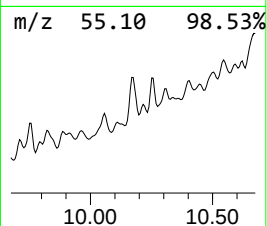
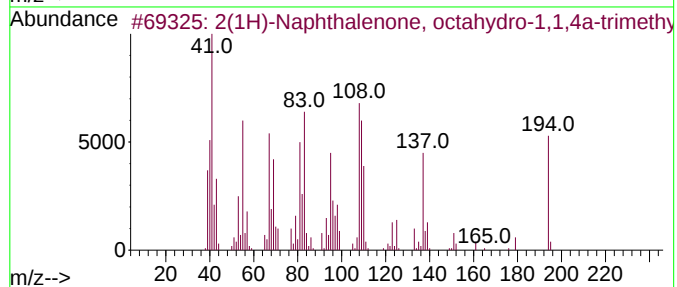
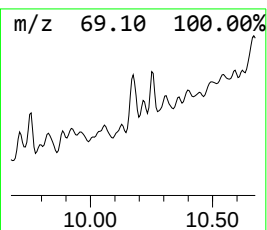
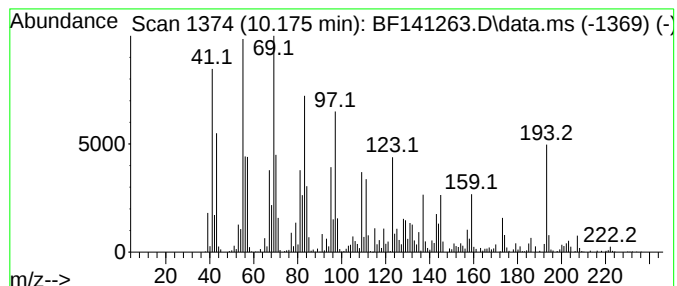
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown10.175 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD			R.T.	
10.175	14.78 ng	1334330	Acenaphthene-d10			9.845	
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Naphthalenone, octahydro-1...	194	C13H22O	000775-54-2	44		
2	Crotyl methacrylate	140	C8H12O2	007376-45-6	42		
3	1-Hexadecanol	242	C16H34O	036653-82-4	38		
4	Cyclopentane, (2-methylbutyl)-	140	C10H20	053366-38-4	35		
5	2-Decene, 7-methyl-, (Z)-	154	C11H22	074630-23-2	25		



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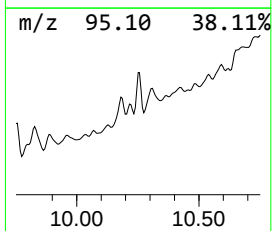
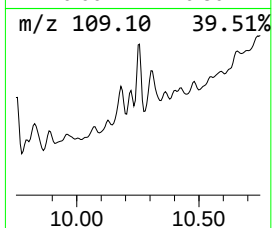
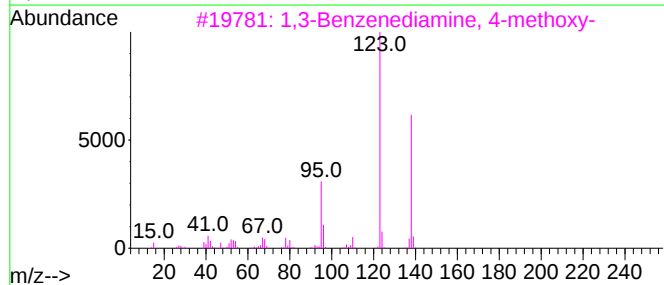
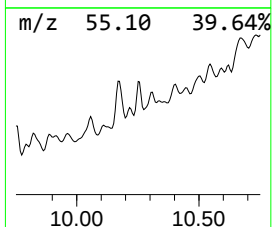
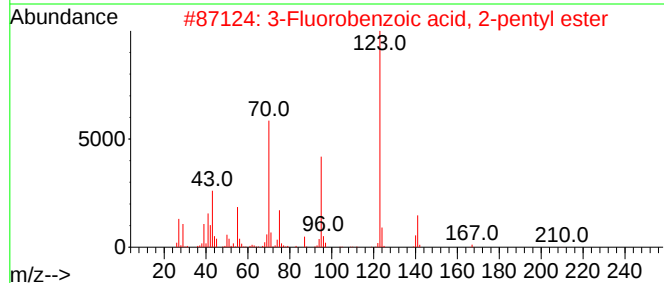
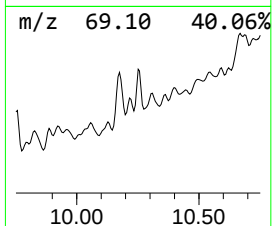
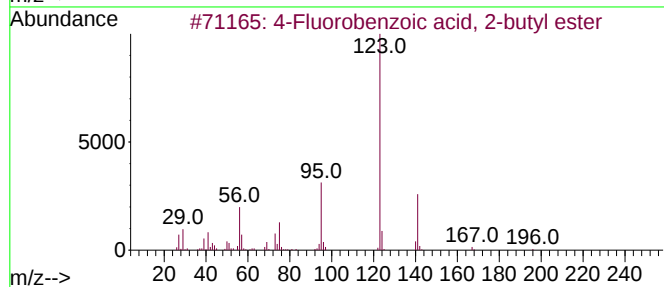
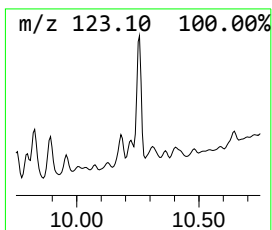
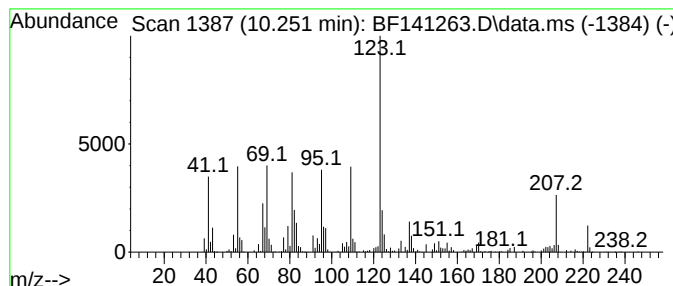
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown10.251 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.251	7.91 ng	713780	Acenaphthene-d10	9.845

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Fluorobenzoic acid, 2-butyl ester	196	C11H13F02	090172-12-6	47
2		3-Fluorobenzoic acid, 2-pentyl e...	210	C12H15F02	1000279-01-7	43
3		1,3-Benzenediamine, 4-methoxy-	138	C7H10N2O	000615-05-4	43
4		2-Fluoro-N-(4-piperidiny)benzam...	414	C16H13F7N2O3	1000469-42-2	38
5		N-[(2-Fluorophenyl)carbonyl]glycine	197	C9H8FN03	000363-34-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012425\
Data File : BF141263.D
Acq On : 24 Jan 2025 15:35
Operator : RC/JU
Sample : Q1169-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ARS20-0006

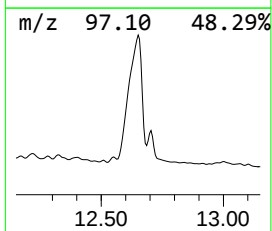
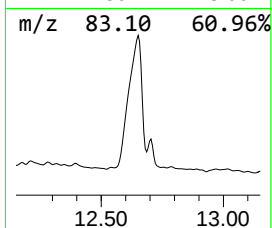
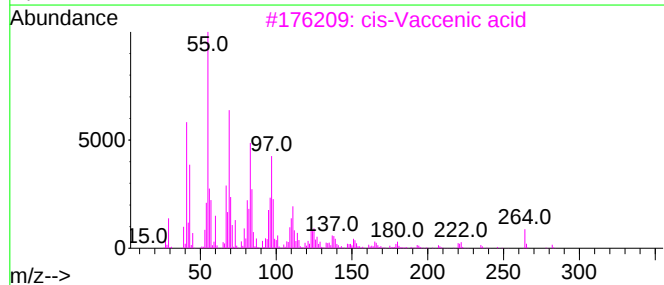
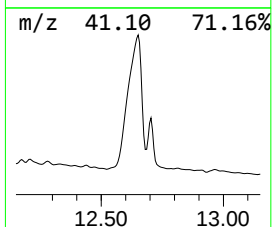
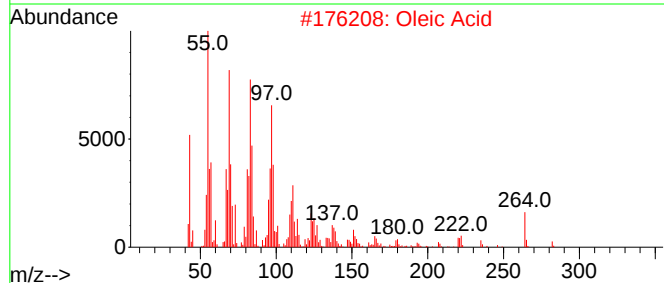
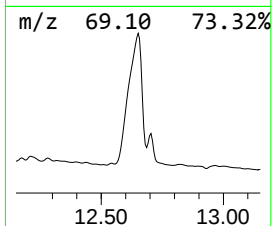
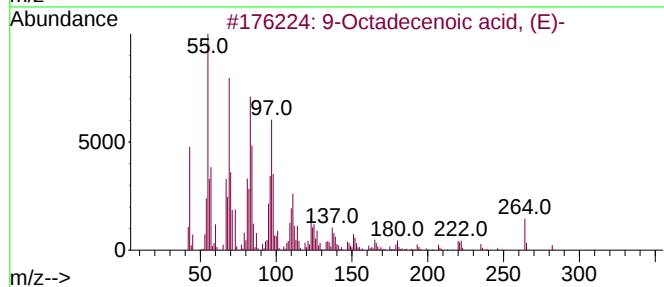
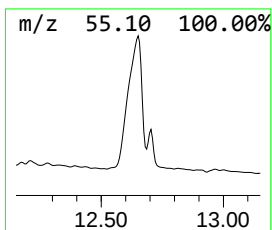
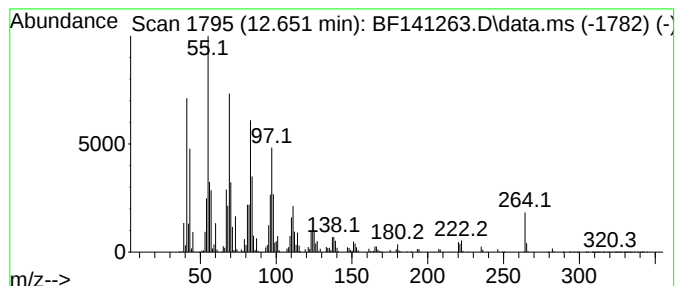
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenoic acid, (E)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.651	467.84 ng	30333800	Phenanthrene-d10	11.339

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	99
2		Oleic Acid	282	C18H34O2	000112-80-1	98
3		cis-Vaccenic acid	282	C18H34O2	000506-17-2	93
4		9-Octadecenoic acid	282	C18H34O2	002027-47-6	90
5		cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012425\
Data File : BF141263.D
Acq On : 24 Jan 2025 15:35
Operator : RC/JU
Sample : Q1169-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ARS20-0006

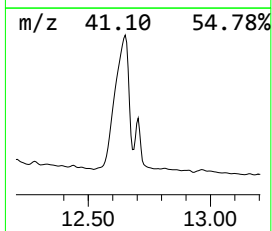
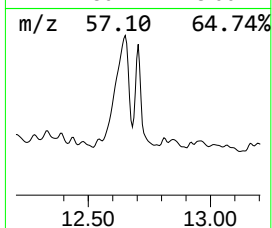
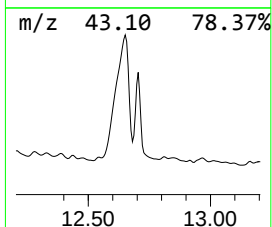
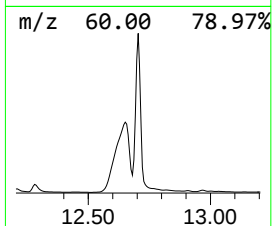
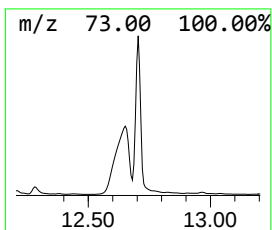
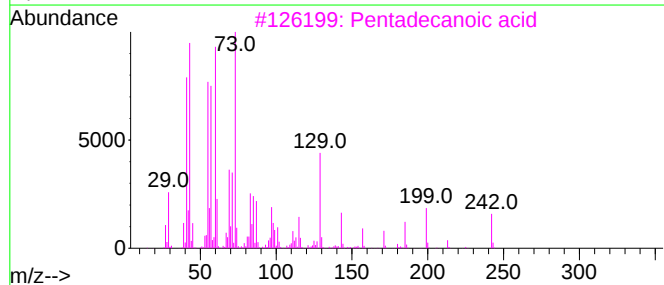
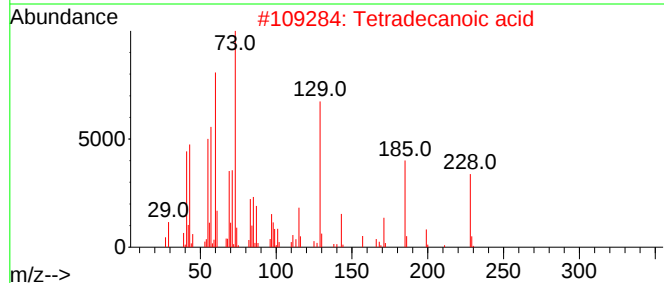
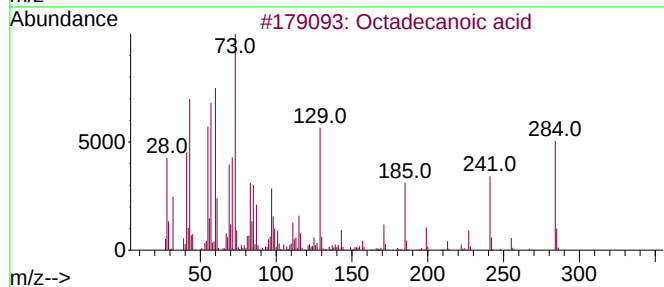
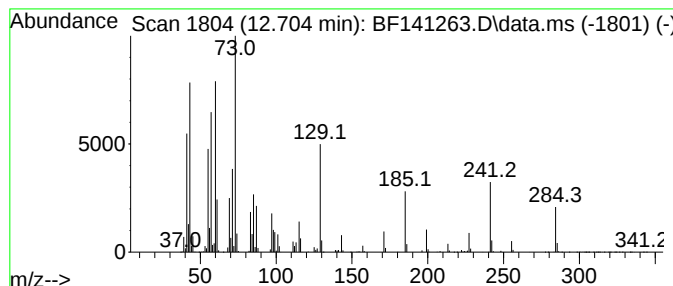
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	45.60 ng	5135860	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	92
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4			n-Decanoic acid	172	C10H20O2	000334-48-5	53
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012425\
Data File : BF141263.D
Acq On : 24 Jan 2025 15:35
Operator : RC/JU
Sample : Q1169-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ARS20-0006

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.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-Dodecanol	9.651	4.2	ng	379010	3	9.845	1805370	20.0
Cyclohexane, 1,...	9.710	5.6	ng	506453	3	9.845	1805370	20.0
unknown9.757	9.757	6.8	ng	610058	3	9.845	1805370	20.0
unknown10.175	10.175	14.8	ng	1334330	3	9.845	1805370	20.0
unknown10.251	10.251	7.9	ng	713780	3	9.845	1805370	20.0
9-Octadecenoic ...	12.651	467.8	ng	30333800	4	11.339	1296770	20.0
Octadecanoic acid	12.704	45.6	ng	5135860	5	13.980	2252570	20.0