

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011725\
 Data File : BF141195.D
 Acq On : 17 Jan 2025 16:21
 Operator : RC/JU
 Sample : Q1115-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 366

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: BF141195.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.211	14	20	42	rVB	119159	239883	3.80%	0.522%
2	5.040	489	501	509	rBV	299640	543287	8.60%	1.182%
3	5.434	560	568	573	rBV	3623717	5380366	85.19%	11.709%
4	6.440	732	739	757	rVB	3654914	5598408	88.64%	12.184%
5	6.810	796	802	807	rBV	922470	1139531	18.04%	2.480%
6	7.369	890	897	903	rBV	2501419	3610603	57.17%	7.858%
7	7.628	936	941	948	rVB	160378	207631	3.29%	0.452%
8	8.087	1014	1019	1028	rBV	1129437	1543743	24.44%	3.360%
9	8.310	1049	1057	1062	rBV	72947	104360	1.65%	0.227%
10	9.163	1195	1202	1208	rBV	4624136	6315675	100.00%	13.745%
11	9.839	1309	1317	1322	rBV	1371653	1781200	28.20%	3.876%
12	10.039	1345	1351	1360	rBV2	43259	84023	1.33%	0.183%
13	10.557	1433	1439	1445	rBV	441140	560066	8.87%	1.219%
14	10.634	1445	1452	1457	rBV	3318814	4527786	71.69%	9.854%
15	10.986	1506	1512	1527	rVB6	43033	84427	1.34%	0.184%
16	11.328	1564	1570	1577	rBV	1407107	1788739	28.32%	3.893%
17	11.863	1652	1661	1671	rBV	1023710	1760492	27.87%	3.831%
18	12.028	1686	1689	1699	rVB2	55743	103692	1.64%	0.226%
19	12.539	1772	1776	1779	rBV	49077	83510	1.32%	0.182%
20	12.645	1787	1794	1806	rBV	463641	823039	13.03%	1.791%
21	12.916	1834	1840	1850	rVB	4046224	5427398	85.94%	11.812%
22	13.680	1965	1970	1978	rBV2	32953	65603	1.04%	0.143%
23	13.816	1989	1993	2004	rVB	125355	223595	3.54%	0.487%
24	13.963	2013	2018	2027	rBV	810134	1109387	17.57%	2.414%
25	14.269	2066	2070	2077	rVB	42732	74249	1.18%	0.162%
26	14.451	2097	2101	2108	rVB	53533	76595	1.21%	0.167%
27	14.757	2149	2153	2156	rBV	67491	115192	1.82%	0.251%
28	14.827	2162	2165	2175	rVB	57500	92364	1.46%	0.201%
29	15.092	2205	2210	2226	rBV	111826	272360	4.31%	0.593%
30	15.421	2260	2266	2271	rBV	743149	1129998	17.89%	2.459%
31	15.469	2271	2274	2280	rVB	108474	156333	2.48%	0.340%
32	15.898	2342	2347	2353	rBV	130494	237160	3.76%	0.516%
33	16.404	2428	2433	2440	rVB	120079	237796	3.77%	0.518%
34	16.992	2527	2533	2541	rVB	104354	218743	3.46%	0.476%
35	17.686	2645	2651	2663	rVB	86472	232784	3.69%	0.507%

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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

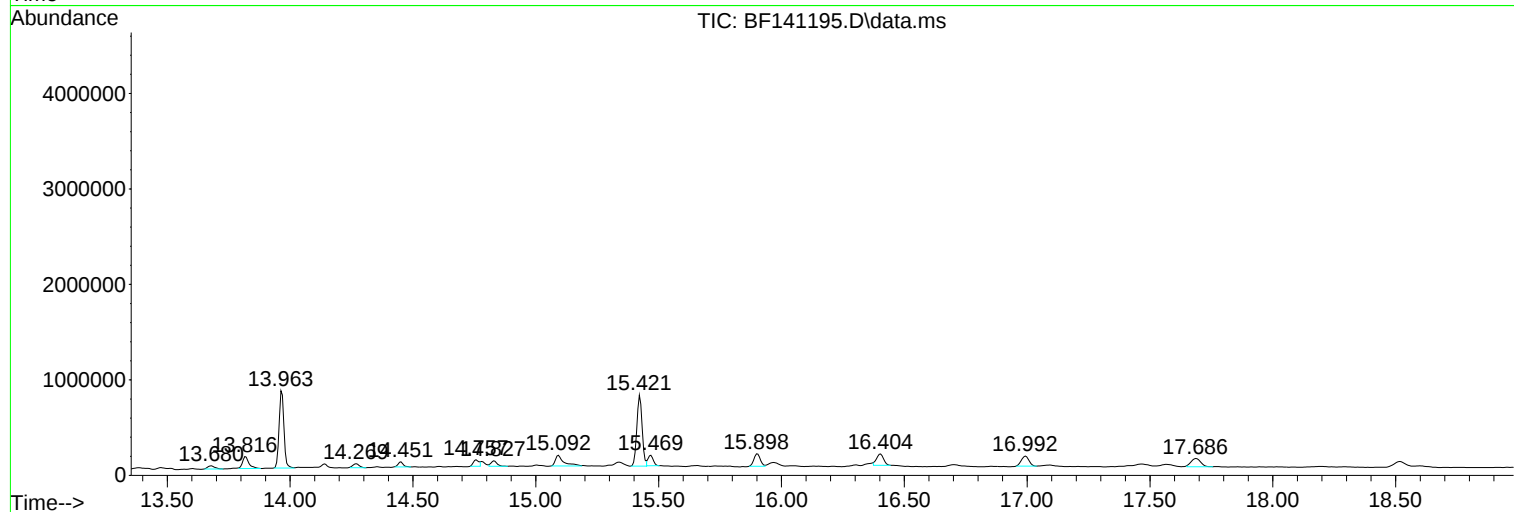
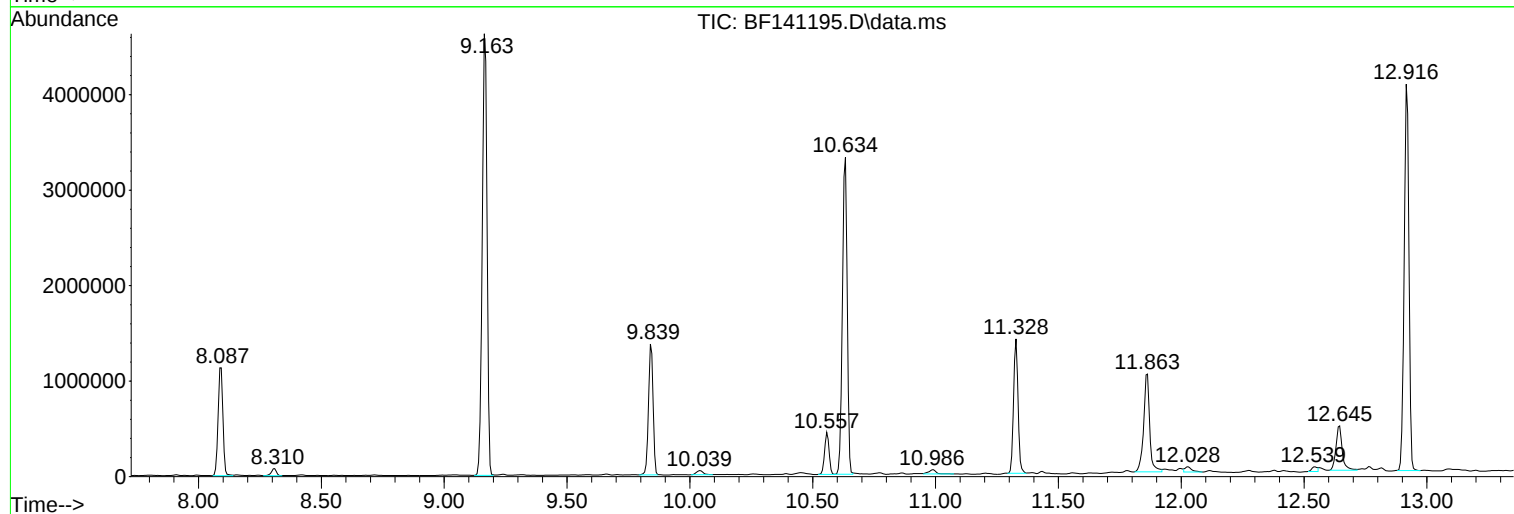
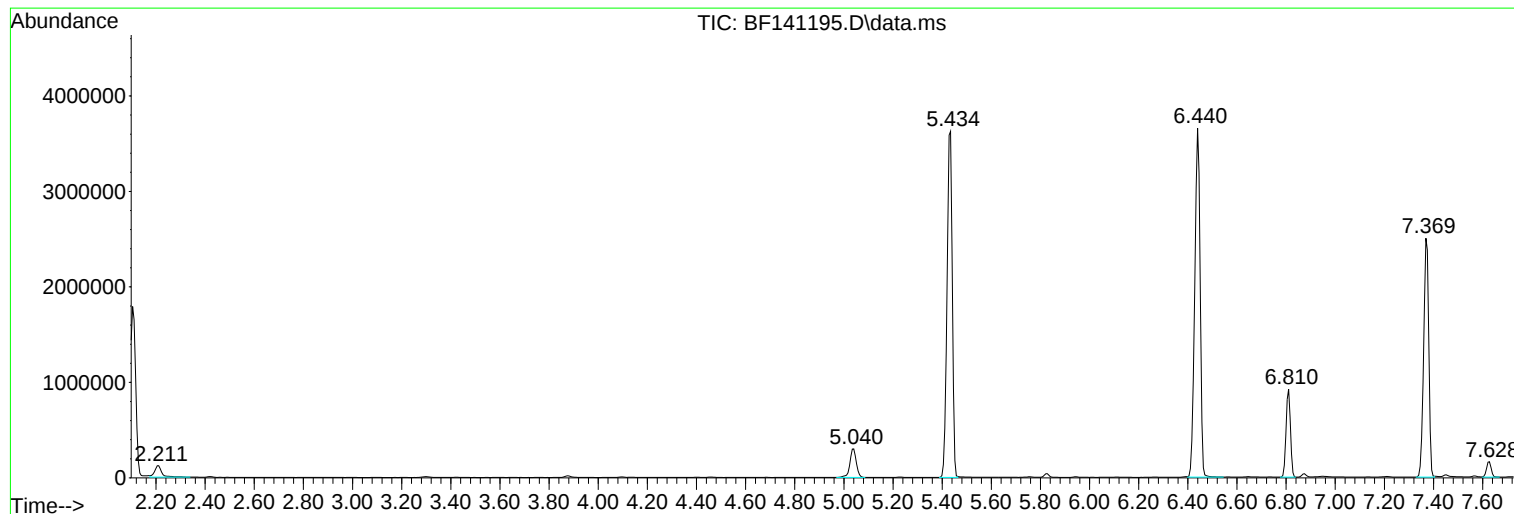
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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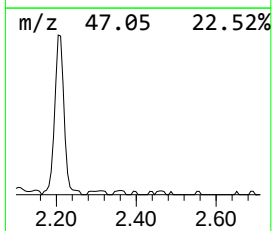
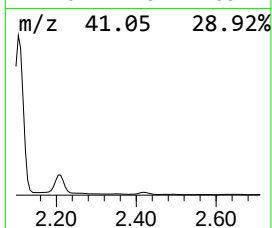
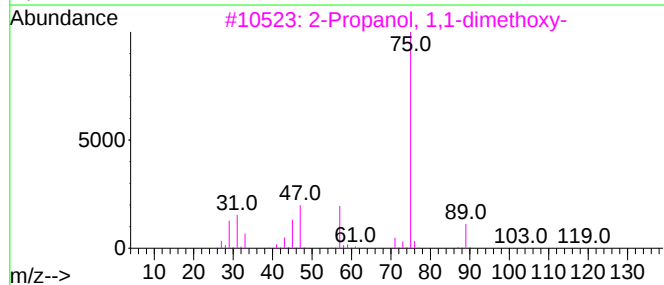
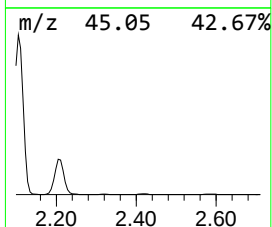
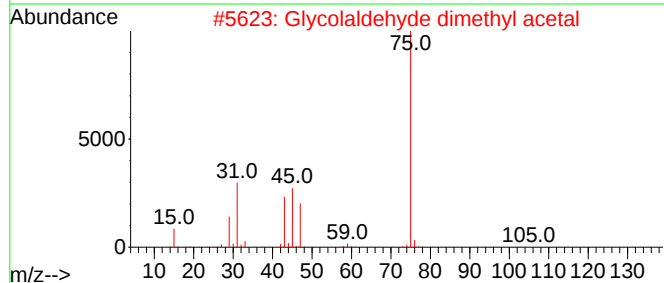
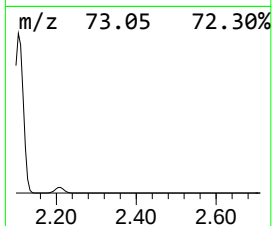
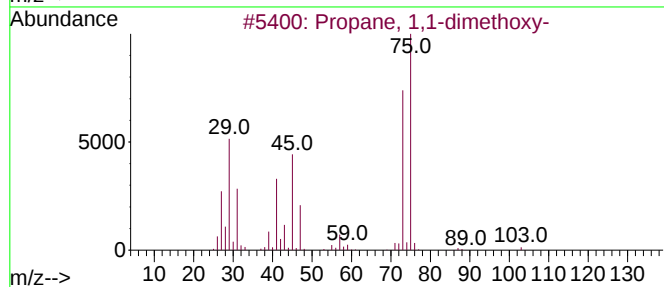
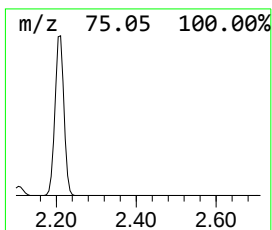
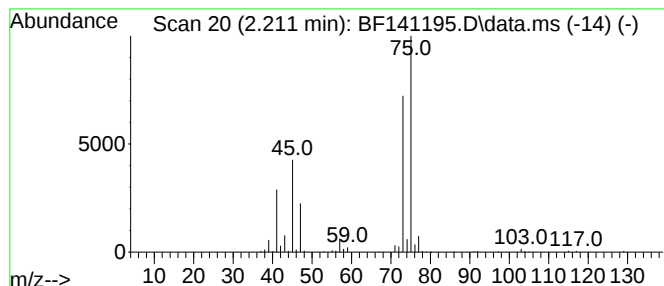
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.211	4.21 ng	239883	1,4-Dichlorobenzene-d4	6.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2			Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	45
3			2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	42
4			Propane, 3-chloro-1,1-dimethoxy-	138	C5H11ClO2	035502-06-8	40
5			Isopropyl alcohol, TMS derivative	132	C6H16OSi	001825-64-5	40



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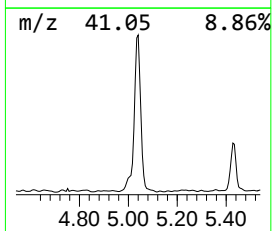
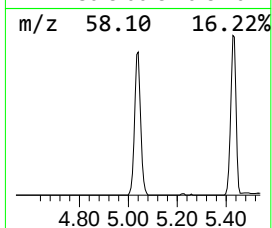
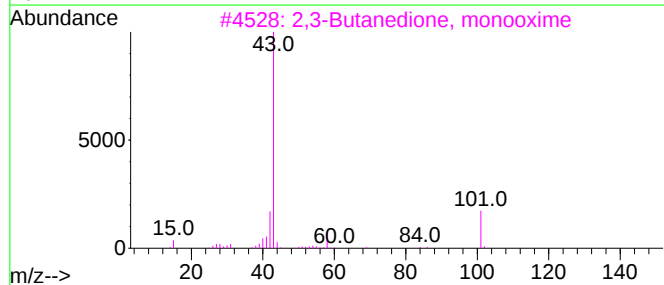
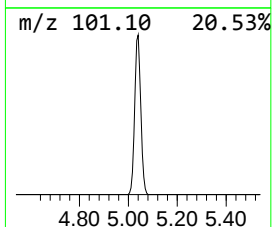
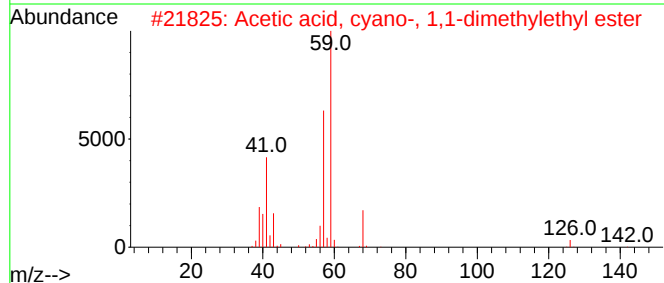
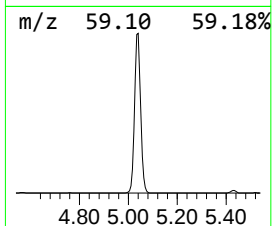
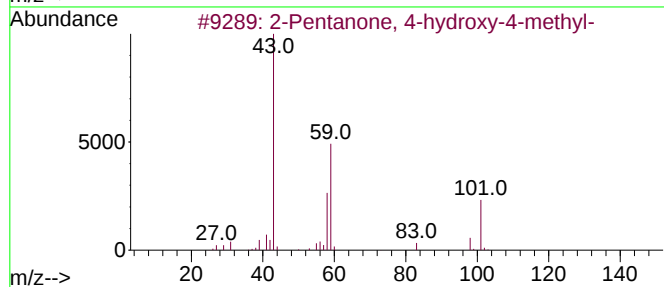
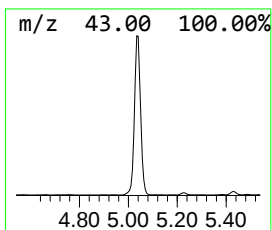
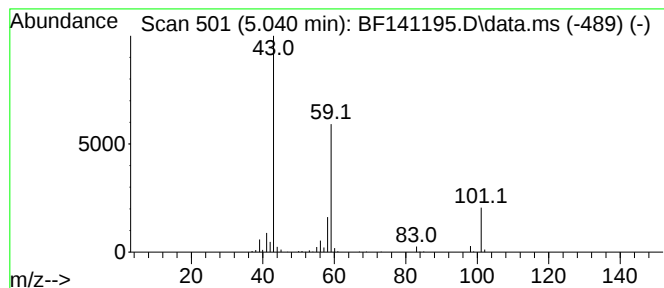
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	9.54 ng	543287	1,4-Dichlorobenzene-d4	6.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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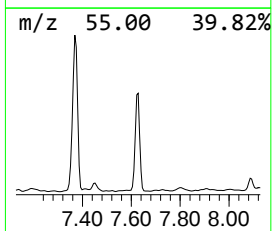
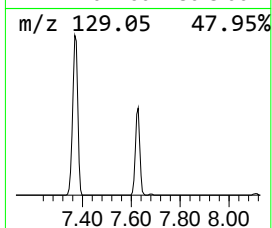
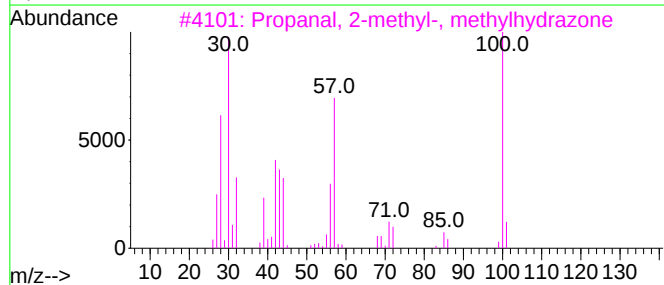
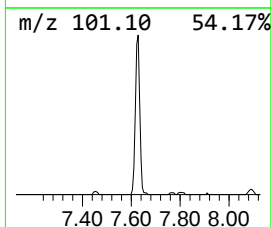
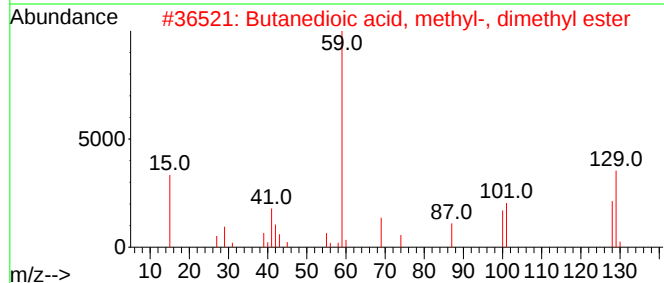
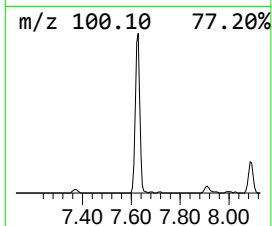
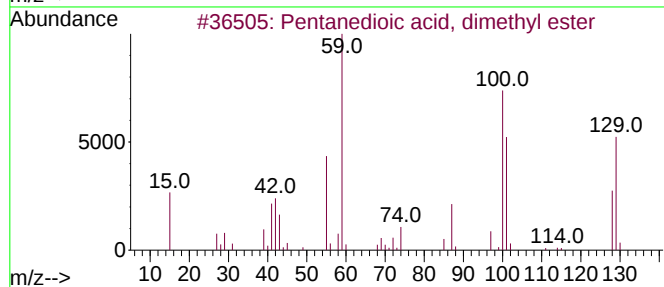
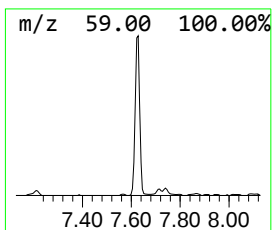
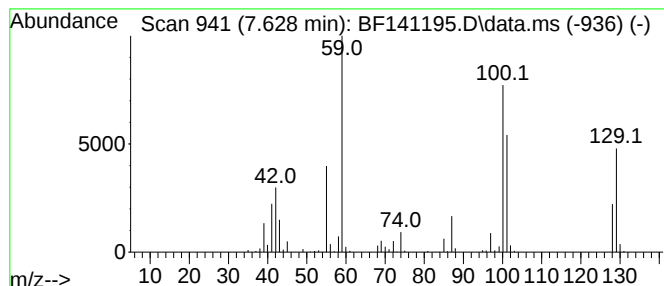
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Pentanedioic acid, dimethyl... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.628	2.69 ng	207631	Naphthalene-d8	8.093

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	91
2			Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	47
3			Propanal, 2-methyl-, methylhydra...	100	C5H12N2	016713-37-4	22
4			1,4-Di-O-acetyl-2,5-di-O-methyl-...	262	C12H22O6	1000101-82-1	17
5			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	17



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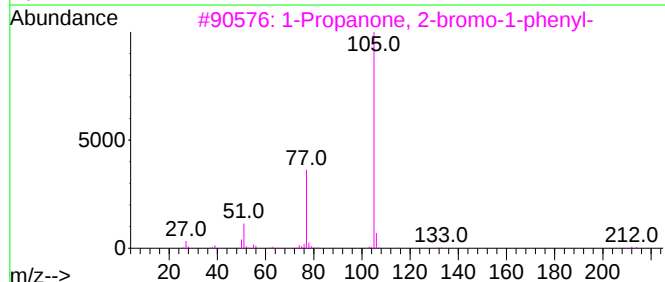
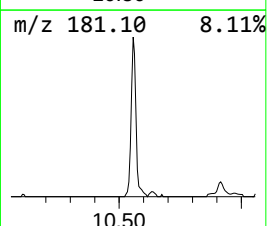
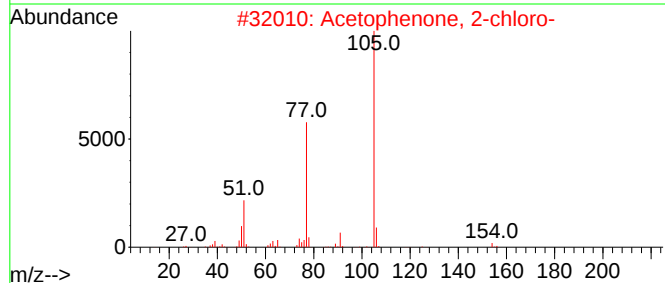
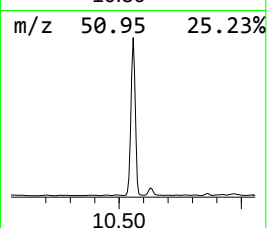
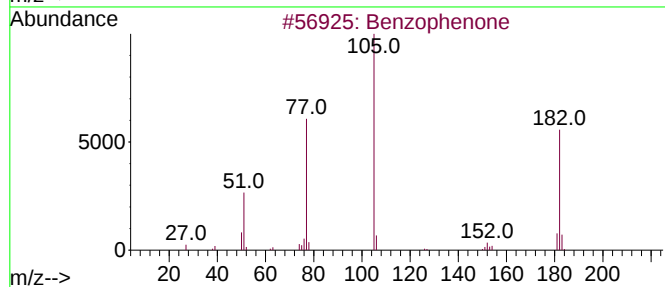
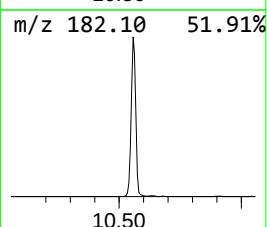
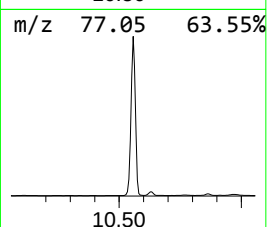
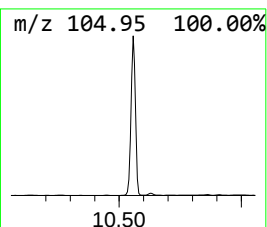
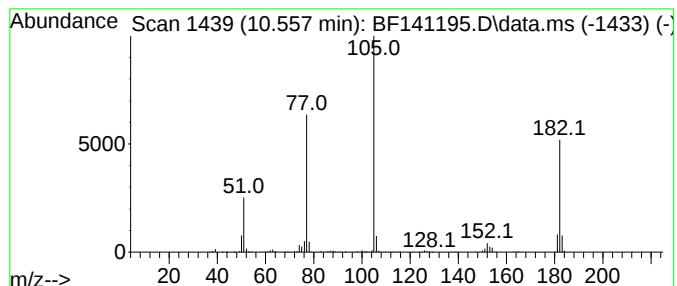
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.557	6.29 ng	560066	Acenaphthene-d10	9.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4			Isonitrosoacetophenone	149	C8H7NO2	000532-54-7	47
5			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47



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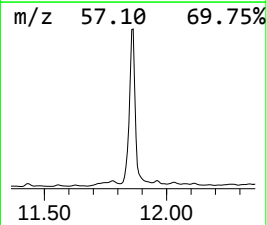
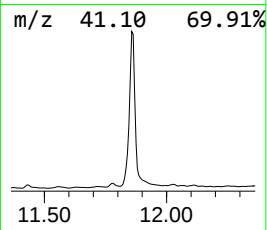
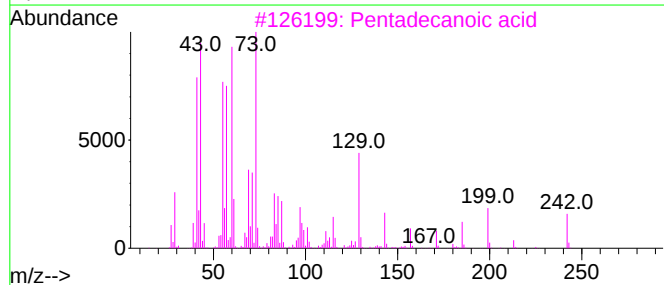
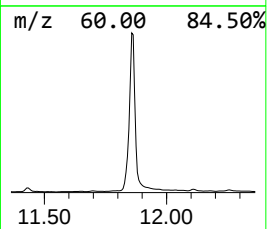
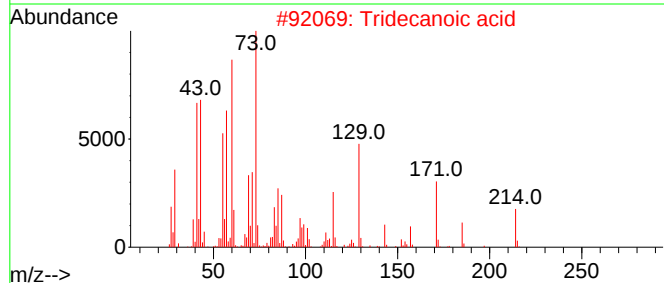
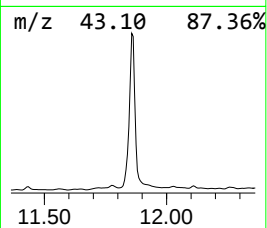
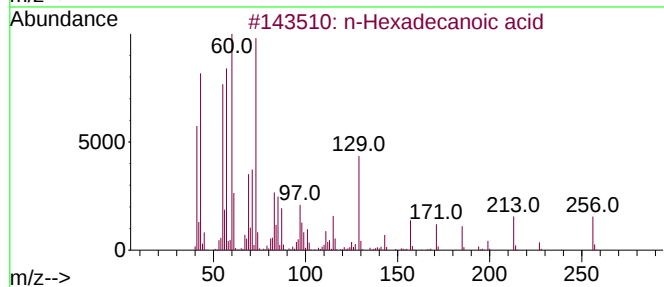
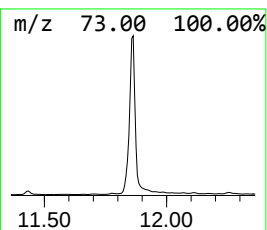
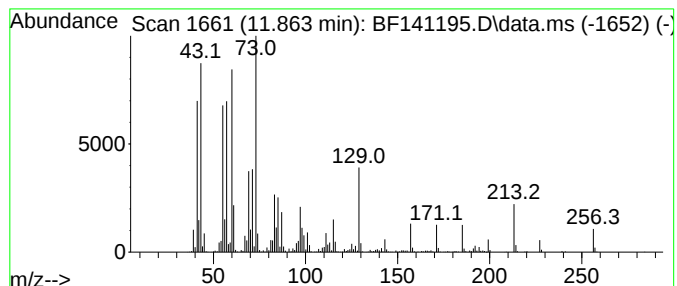
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	19.68 ng	1760490	Phenanthrene-d10	11.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011725\
Data File : BF141195.D
Acq On : 17 Jan 2025 16:21
Operator : RC/JU
Sample : Q1115-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

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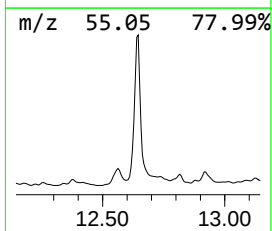
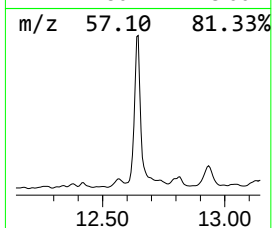
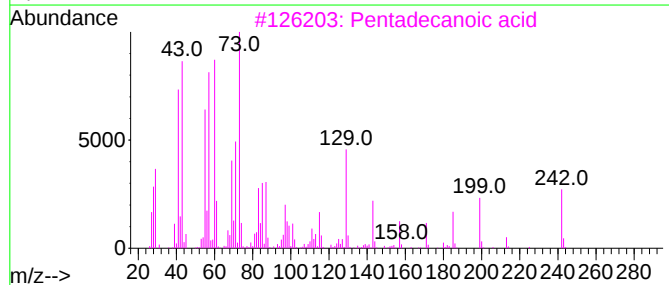
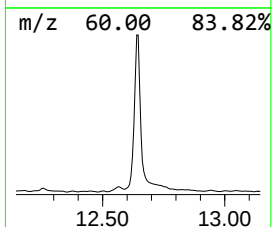
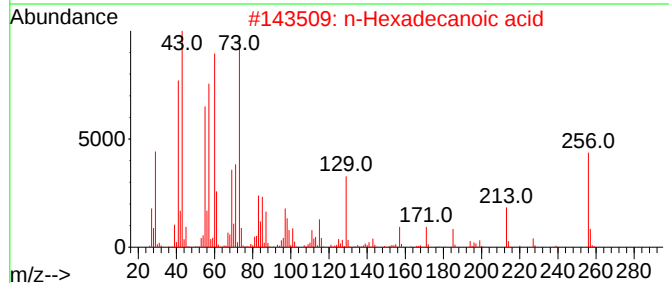
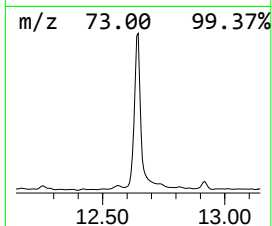
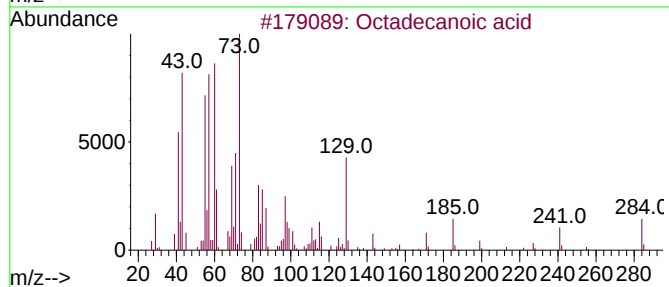
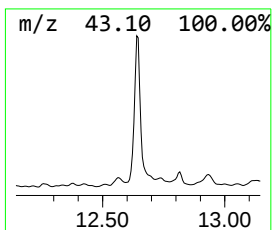
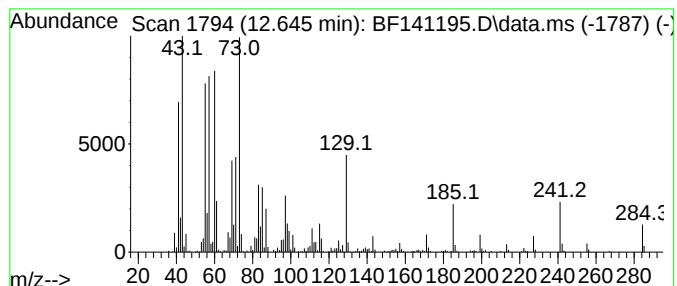
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	14.84 ng	823039	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011725\
Data File : BF141195.D
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Sample : Q1115-01
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Instrument :
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ClientSampleId :
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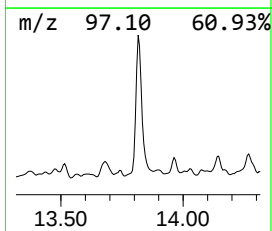
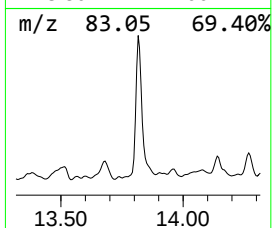
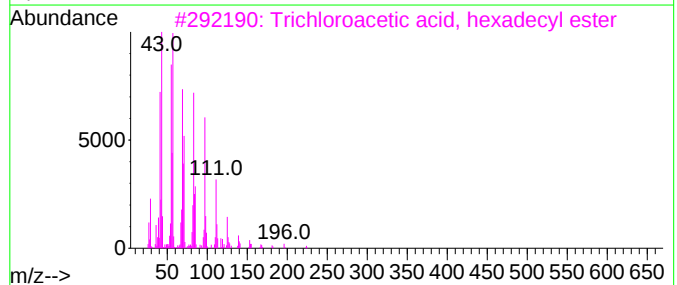
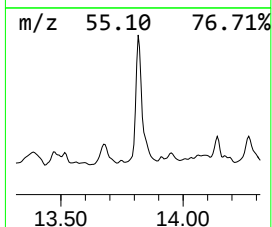
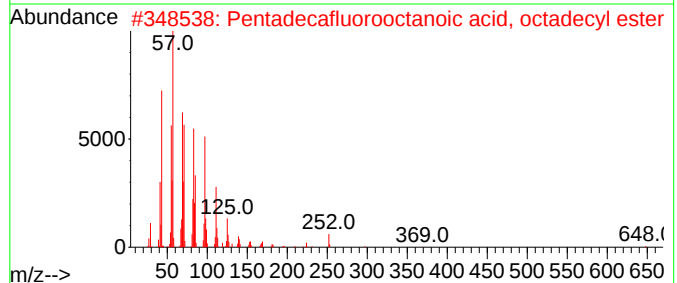
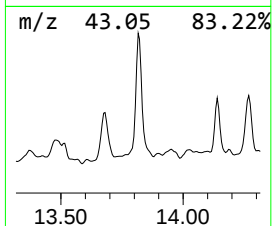
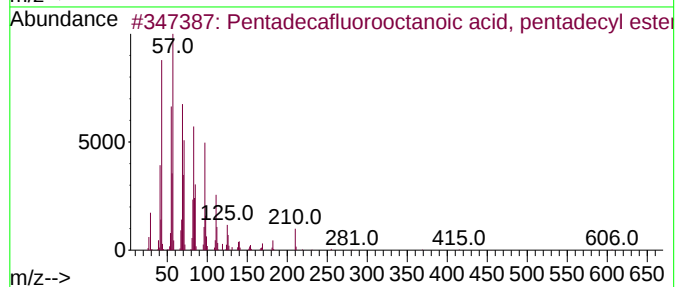
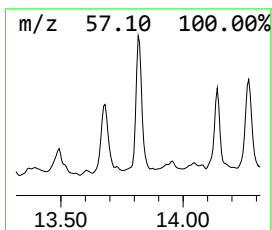
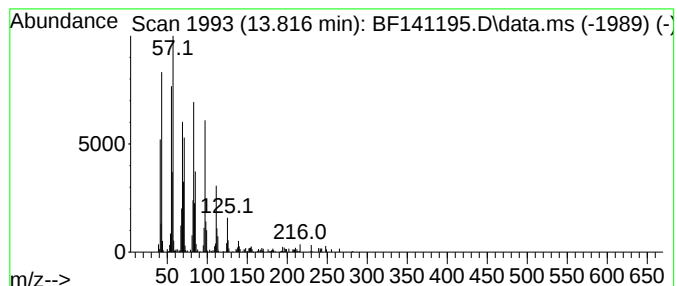
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Pentadecafluorooctanoic aci... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	4.03 ng	223595	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	94
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
4			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011725\
Data File : BF141195.D
Acq On : 17 Jan 2025 16:21
Operator : RC/JU
Sample : Q1115-01
Misc :
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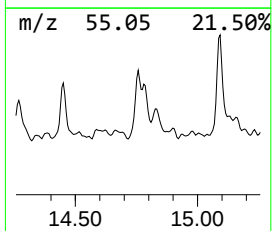
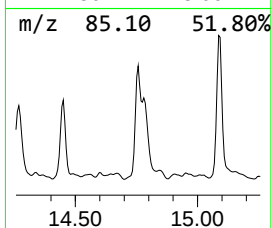
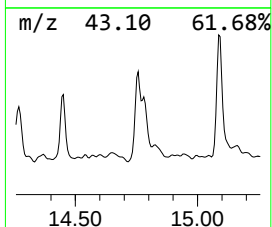
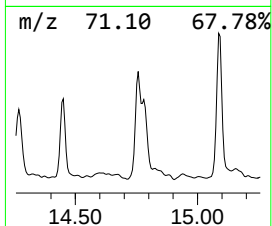
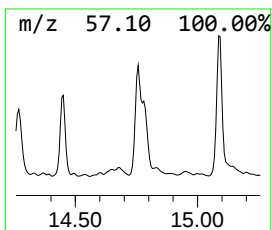
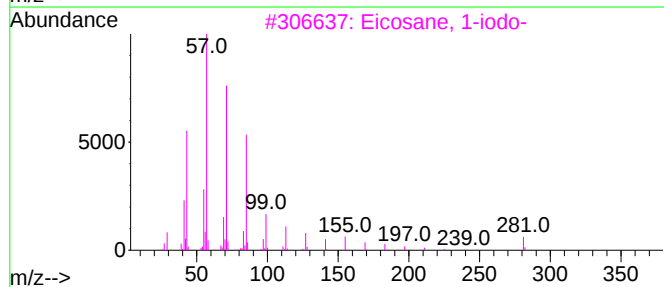
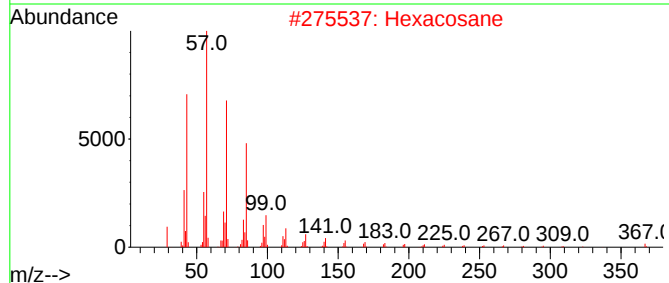
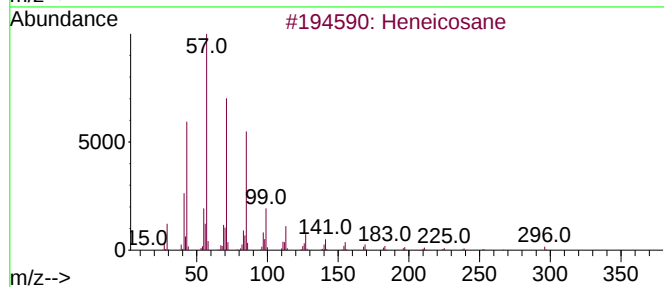
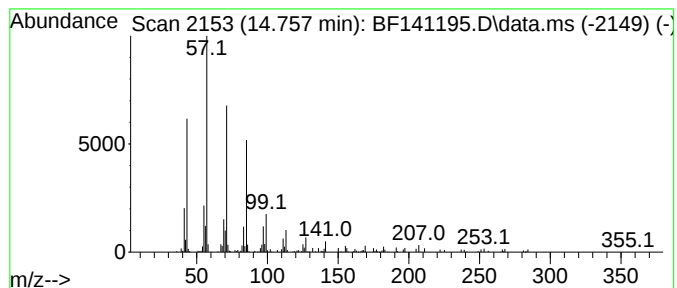
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.757	2.04 ng	115192	Perylene-d12	15.422	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Hexacosane	366	C26H54	000630-01-3	90
3	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	87
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	86
5	Triacontane	422	C30H62	000638-68-6	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011725\
Data File : BF141195.D
Acq On : 17 Jan 2025 16:21
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Sample : Q1115-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

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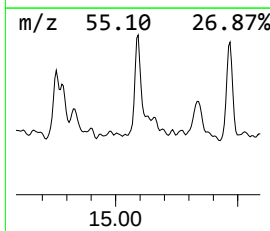
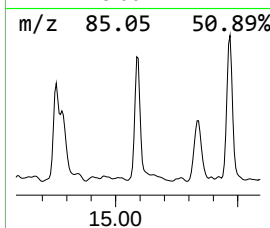
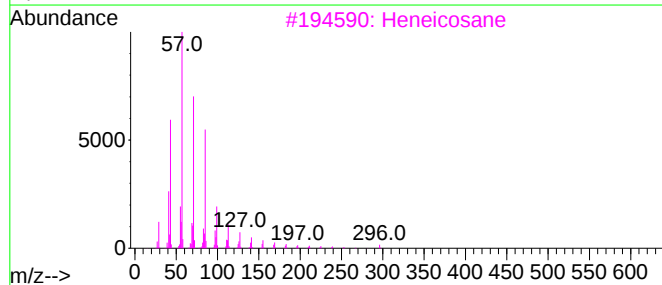
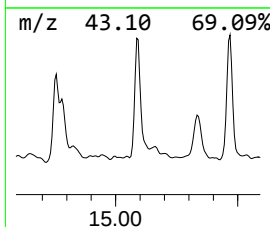
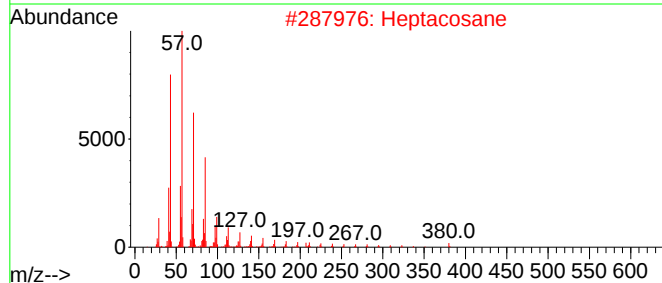
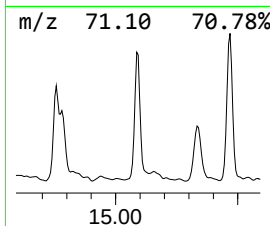
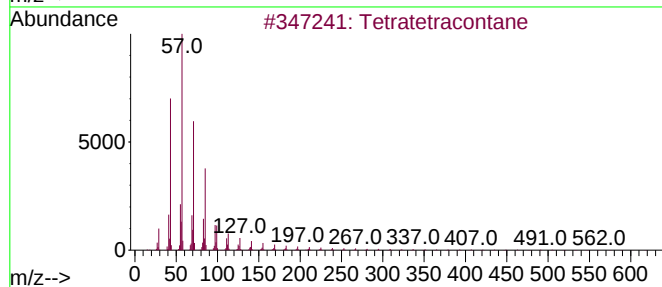
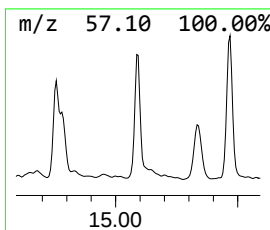
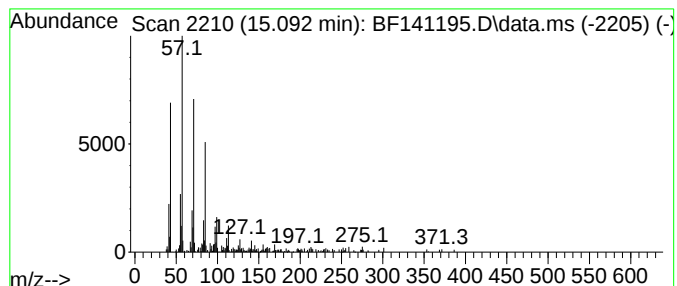
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetratetracontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.092	4.82 ng	272360	Perylene-d12	15.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	90
2			Heptacosane	380	C27H56	000593-49-7	90
3			Heneicosane	296	C21H44	000629-94-7	90
4			Hexacosane	366	C26H54	000630-01-3	90
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011725\
Data File : BF141195.D
Acq On : 17 Jan 2025 16:21
Operator : RC/JU
Sample : Q1115-01
Misc :
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Instrument :
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ClientSampleId :
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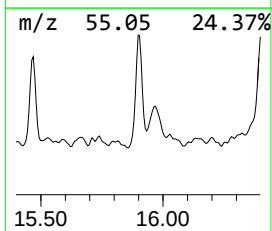
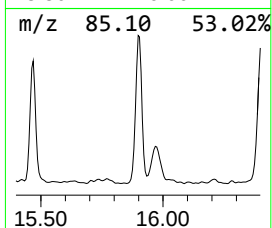
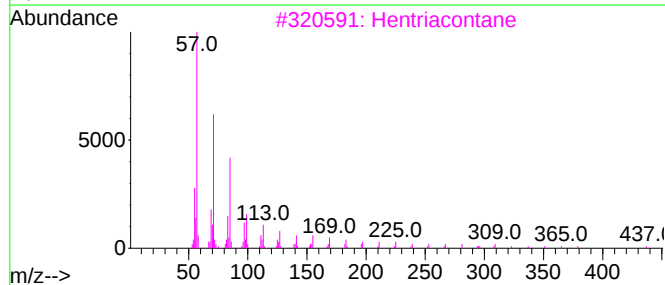
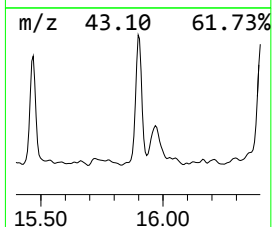
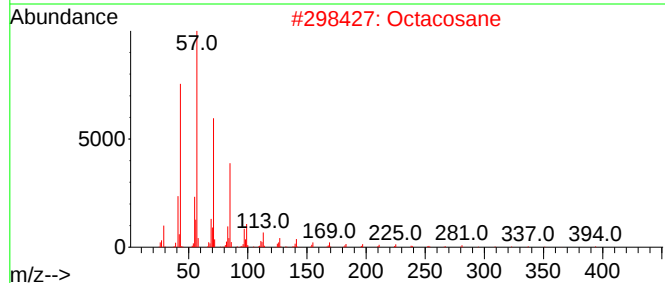
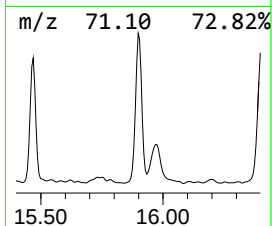
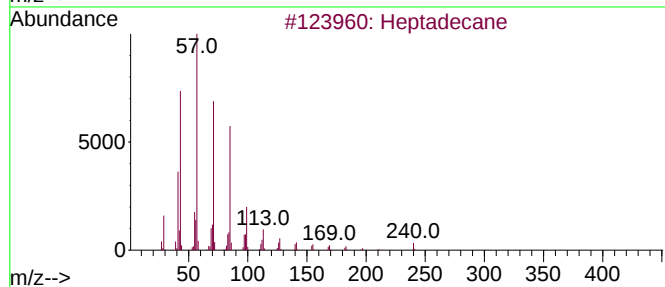
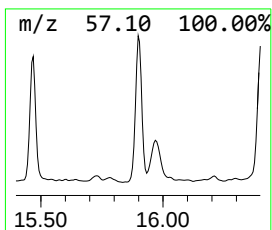
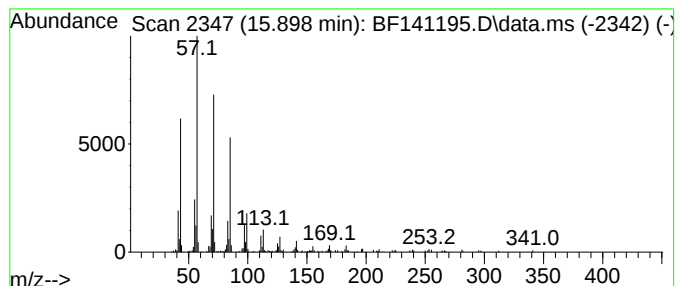
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.898	4.20 ng	237160	Perylene-d12	15.422

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane	240	C17H36	000629-78-7	94
2		Octacosane	394	C28H58	000630-02-4	91
3		Hentriacontane	437	C31H64	000630-04-6	91
4		Hexacosane	366	C26H54	000630-01-3	91
5		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011725\
Data File : BF141195.D
Acq On : 17 Jan 2025 16:21
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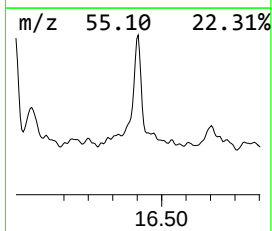
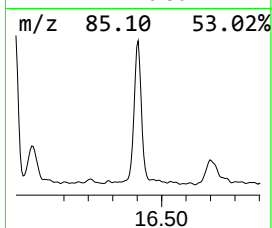
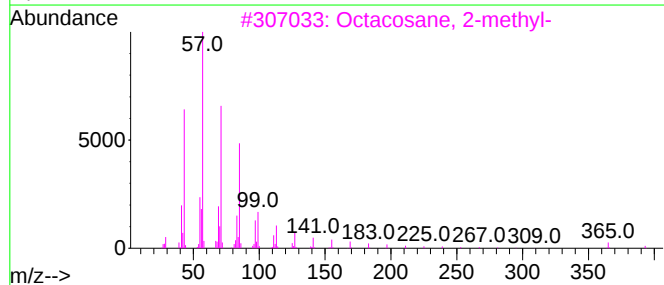
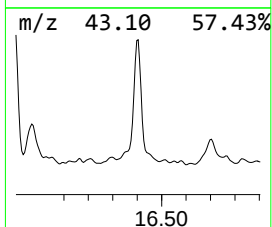
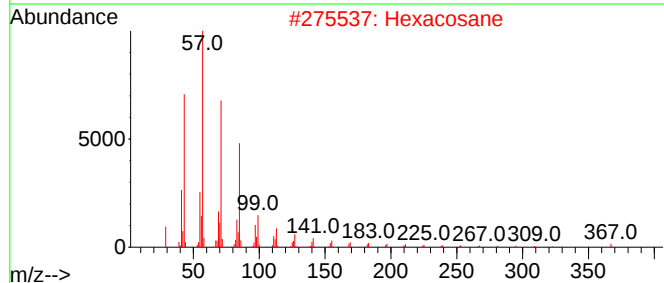
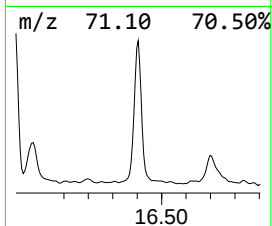
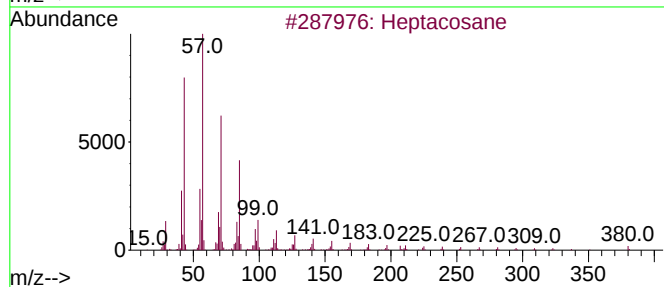
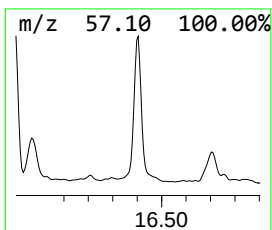
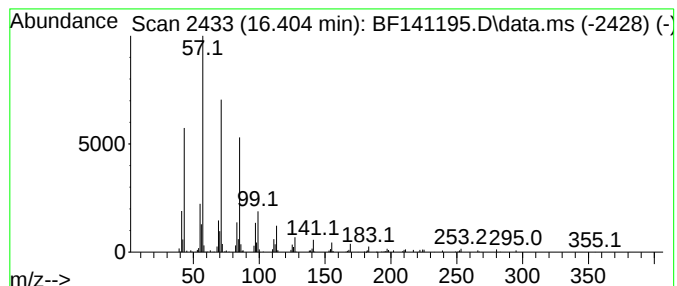
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.404	4.21 ng	237796	Perylene-d12	15.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	91
2			Hexacosane	366	C26H54	000630-01-3	90
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
4			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	90
5			Heneicosane	296	C21H44	000629-94-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011725\
Data File : BF141195.D
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Operator : RC/JU
Sample : Q1115-01
Misc :
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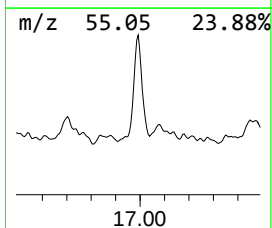
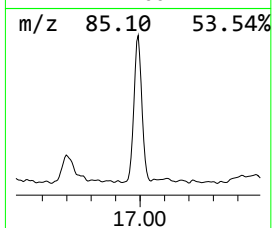
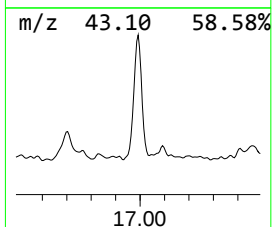
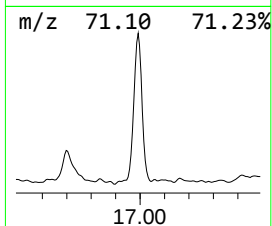
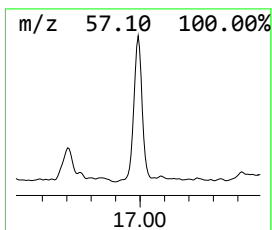
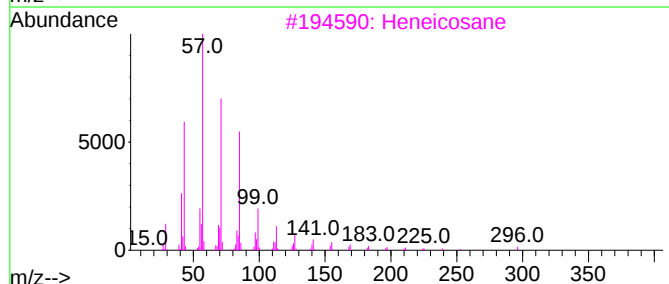
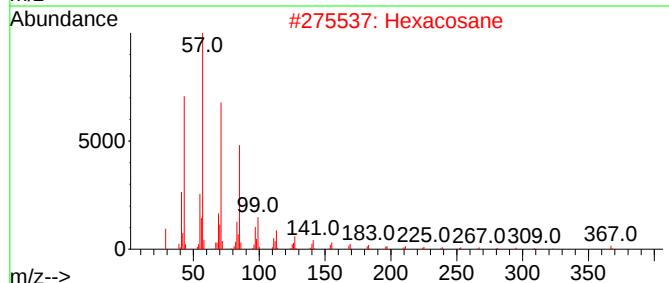
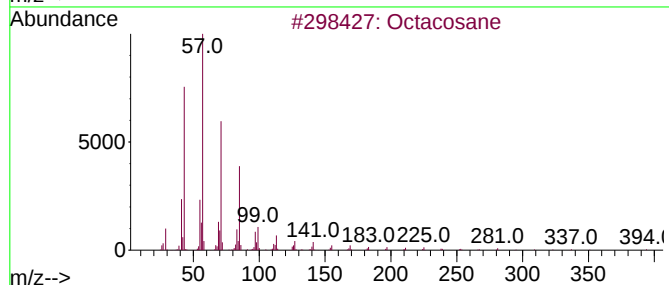
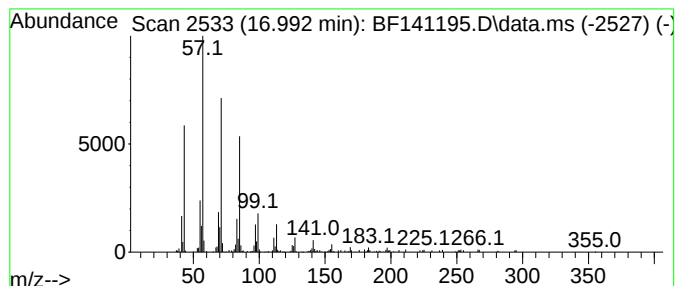
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ClientSampleId :
366

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

Peak Number 12 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.992	3.87 ng	218743	Perylene-d12	15.422	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011725\
Data File : BF141195.D
Acq On : 17 Jan 2025 16:21
Operator : RC/JU
Sample : Q1115-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
366

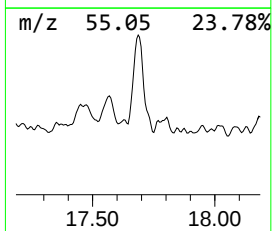
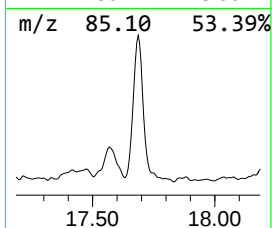
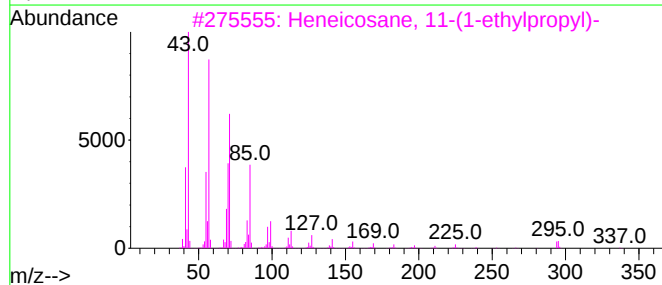
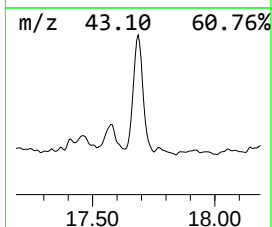
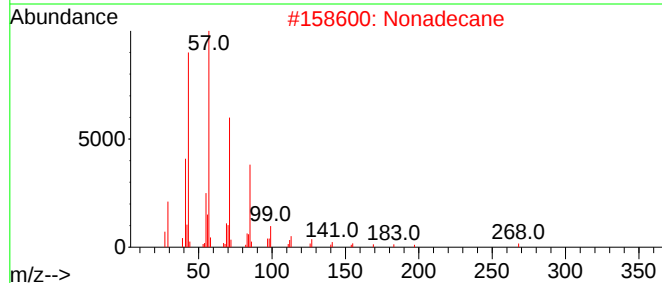
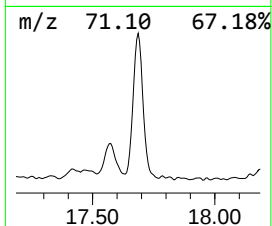
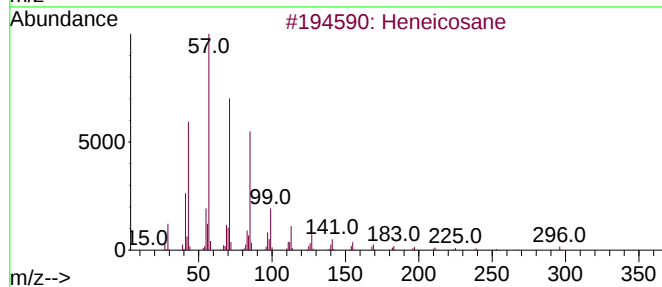
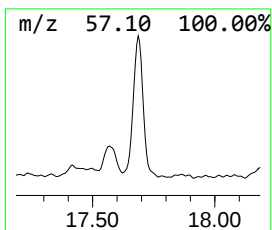
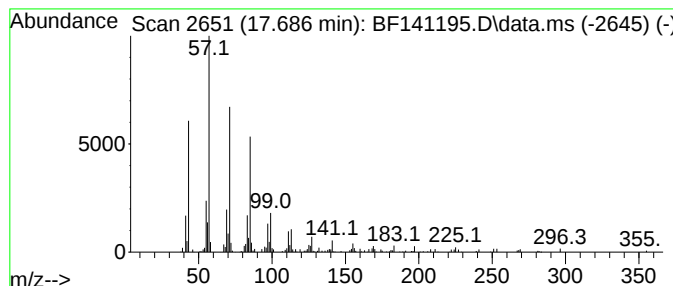
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.686	4.12 ng	232784	Perylene-d12	15.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	98
2			Nonadecane	268	C19H40	000629-92-5	94
3			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
4			Hexacosane	366	C26H54	000630-01-3	91
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011725\
Data File : BF141195.D
Acq On : 17 Jan 2025 16:21
Operator : RC/JU
Sample : Q1115-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
366

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
Propane, 1,1-di...	2.211	4.2	ng	239883	1	6.810	1139530	20.0
2-Pentanone, 4-...	5.040	9.5	ng	543287	1	6.810	1139530	20.0
Pentanedioic ac...	7.628	2.7	ng	207631	2	8.093	1543740	20.0
Benzophenone	10.557	6.3	ng	560066	3	9.839	1781200	20.0
n-Hexadecanoic ...	11.863	19.7	ng	1760490	4	11.328	1788740	20.0
Octadecanoic acid	12.645	14.8	ng	823039	5	13.963	1109390	20.0
Pentadecafluoro...	13.816	4.0	ng	223595	5	13.963	1109390	20.0
Heneicosane	14.757	2.0	ng	115192	6	15.422	1130000	20.0
Tetratetracontane	15.092	4.8	ng	272360	6	15.422	1130000	20.0
Heptadecane	15.898	4.2	ng	237160	6	15.422	1130000	20.0
Heptacosane	16.404	4.2	ng	237796	6	15.422	1130000	20.0
Octacosane	16.992	3.9	ng	218743	6	15.422	1130000	20.0
Nonadecane	17.686	4.1	ng	232784	6	15.422	1130000	20.0