

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
 Data File : BF131116.D
 Acq On : 10 Nov 2022 11:12
 Operator : CG\JU
 Sample : PB148898BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB148898BL

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-BF110922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131116.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.246	17	27	33	rVB	97372	128910	5.44%	0.792%
2	2.357	41	46	51	rBV	38804	50326	2.12%	0.309%
3	5.128	513	517	528	rBV	249244	337373	14.24%	2.072%
4	5.516	578	583	586	rBV	2171118	2212640	93.39%	13.591%
5	6.522	748	754	756	rBV	1768527	2079606	87.77%	12.774%
6	6.887	812	816	819	rBV	559829	434765	18.35%	2.670%
7	7.457	907	913	916	rBV	1289656	1335933	56.38%	8.206%
8	8.175	1030	1035	1038	rBV	579299	565630	23.87%	3.474%
9	9.251	1212	1218	1221	rBV	2671278	2369349	100.00%	14.553%
10	9.933	1328	1334	1337	rBV	957737	808197	34.11%	4.964%
11	10.727	1463	1469	1472	rBV	1808109	1624581	68.57%	9.979%
12	11.427	1584	1588	1591	rBV	787442	632183	26.68%	3.883%
13	13.021	1854	1859	1862	rBV	2586051	2317863	97.83%	14.237%
14	14.074	2034	2038	2042	rBV	632549	563385	23.78%	3.461%
15	14.168	2048	2054	2061	rBV	31291	40107	1.69%	0.246%
16	14.845	2165	2169	2175	rBV2	25862	25485	1.08%	0.157%
17	15.192	2225	2228	2233	rVB	32314	36662	1.55%	0.225%
18	15.574	2288	2293	2307	rVB	348446	473553	19.99%	2.909%
19	16.039	2367	2372	2376	rBV	35010	51416	2.17%	0.316%
20	16.557	2454	2460	2470	rBV2	35515	70060	2.96%	0.430%
21	17.174	2559	2565	2574	rVB4	27905	61632	2.60%	0.379%
22	17.903	2682	2689	2698	rVB4	23597	60705	2.56%	0.373%

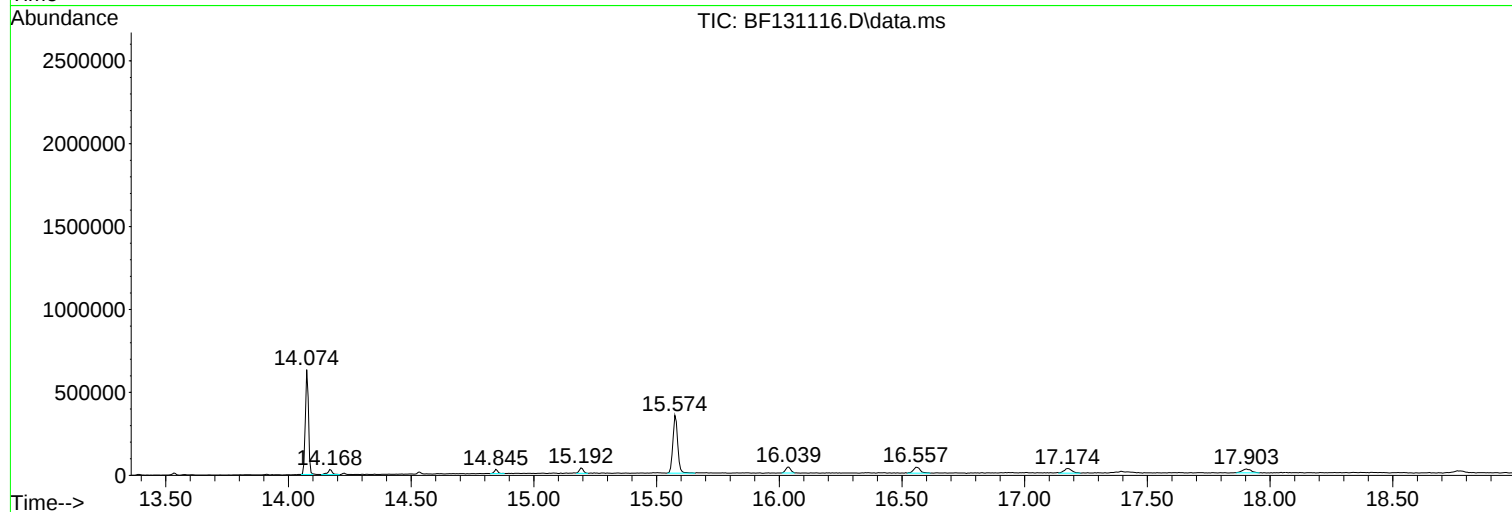
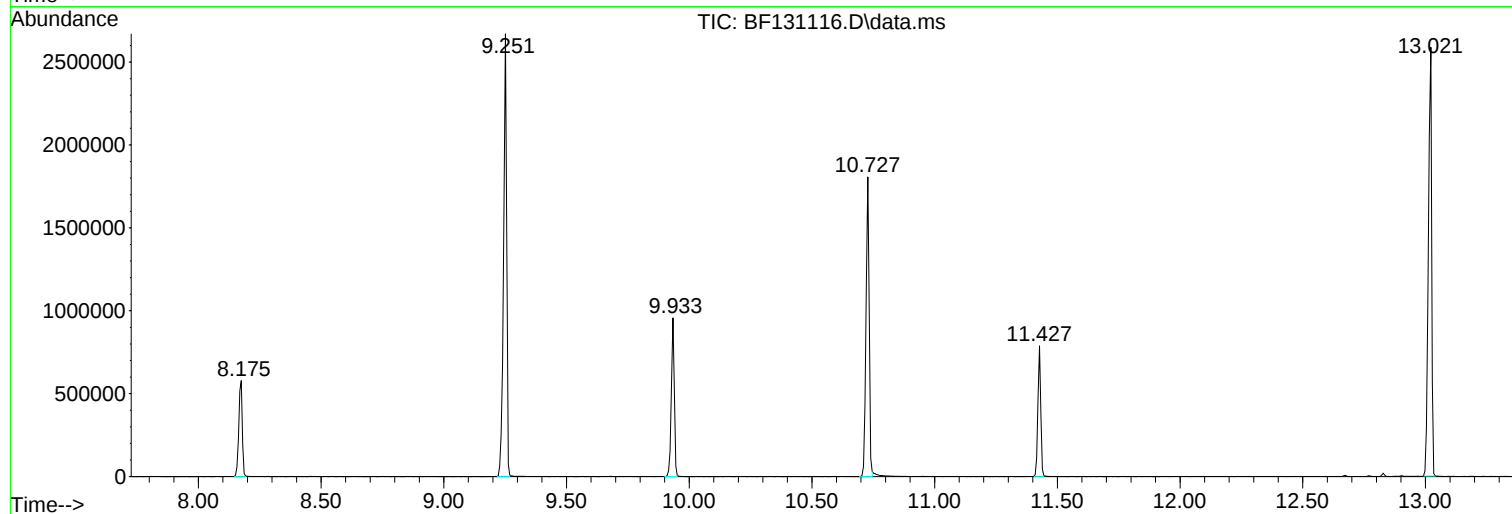
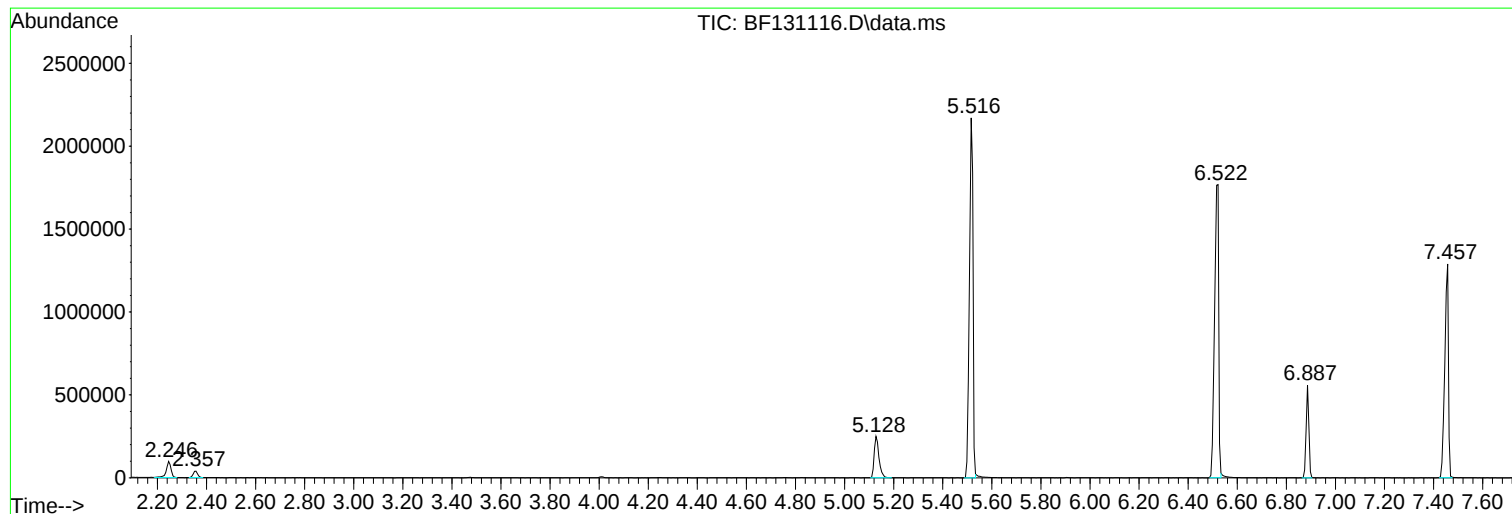
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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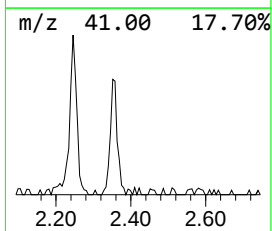
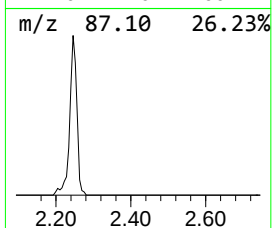
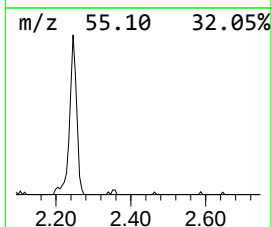
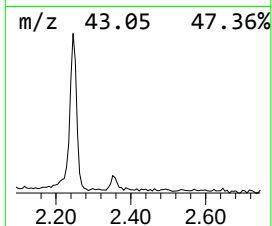
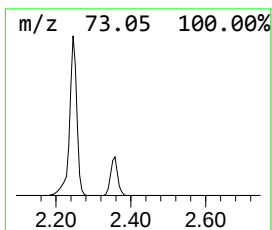
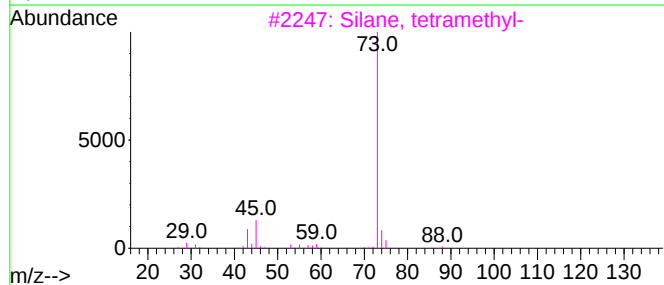
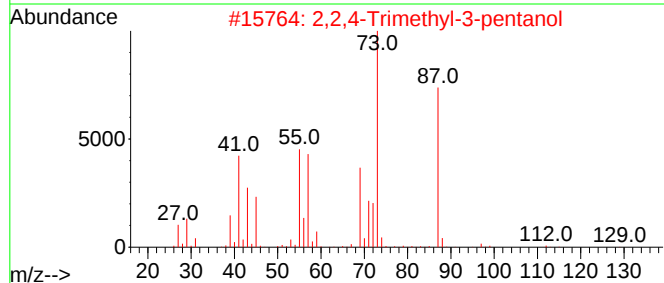
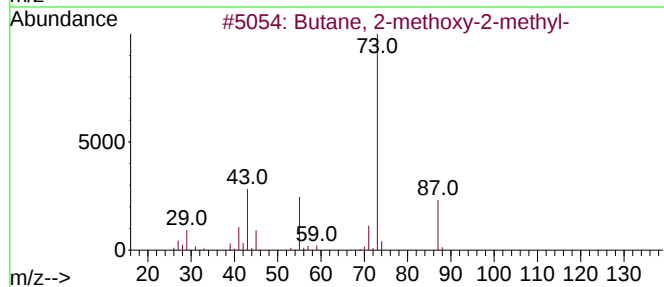
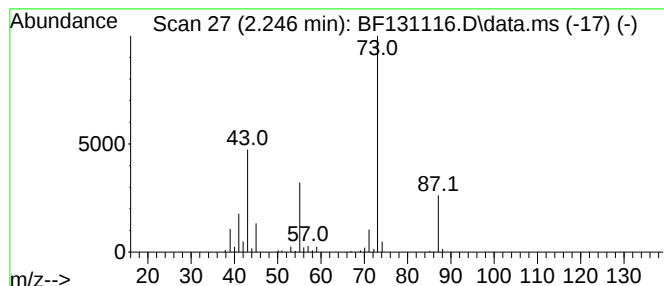
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.246	5.93 ng	128910	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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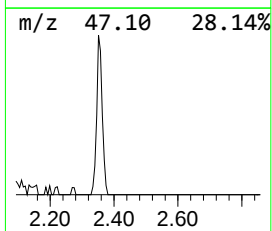
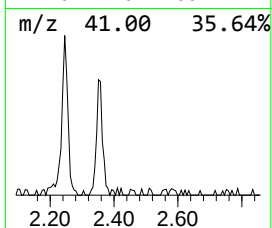
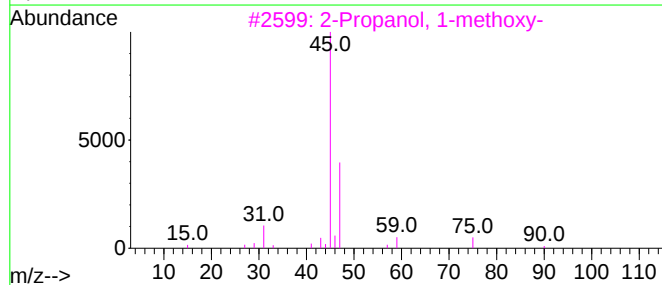
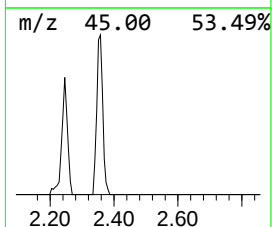
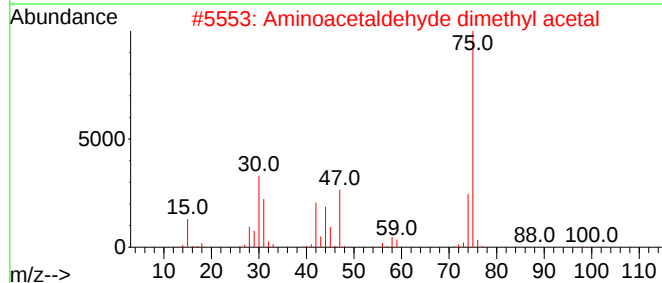
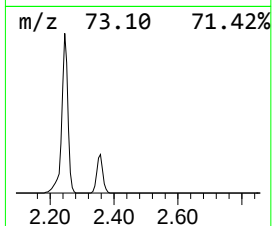
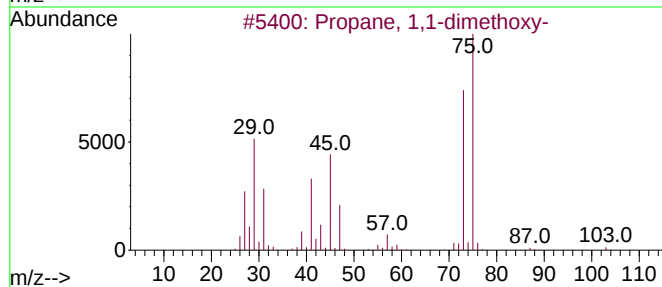
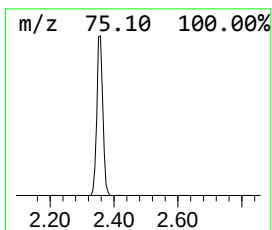
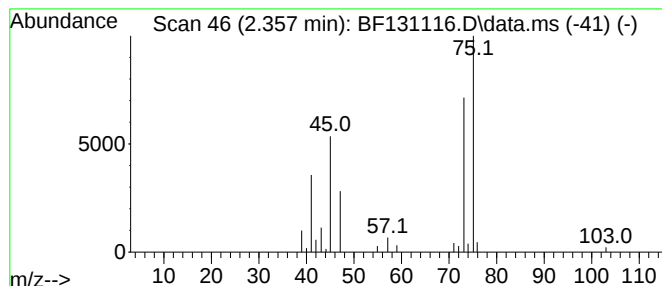
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.357	2.32 ng	50326	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2			Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	9
3			2-Propanol, 1-methoxy-	90	C4H10O2	000107-98-2	9
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5			1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9



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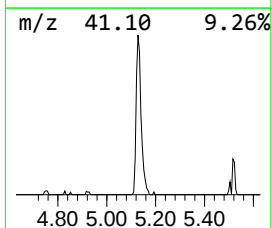
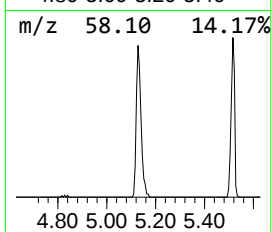
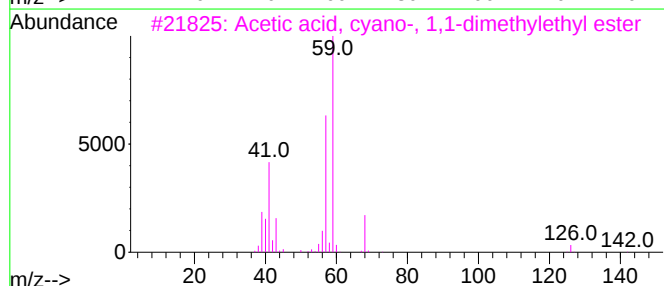
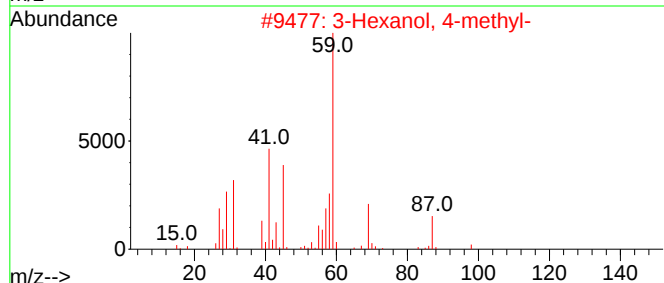
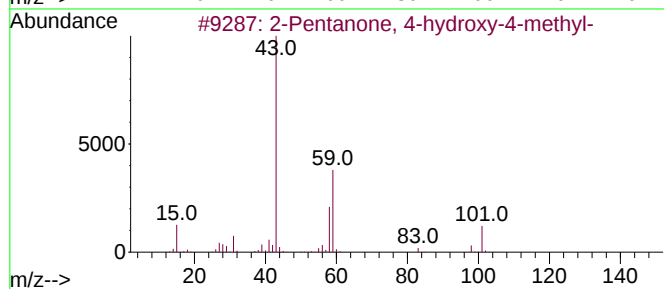
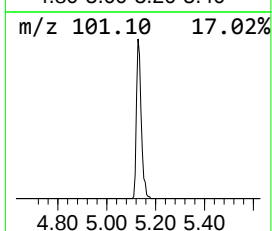
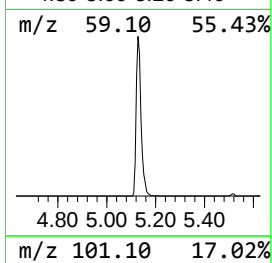
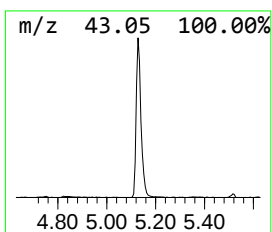
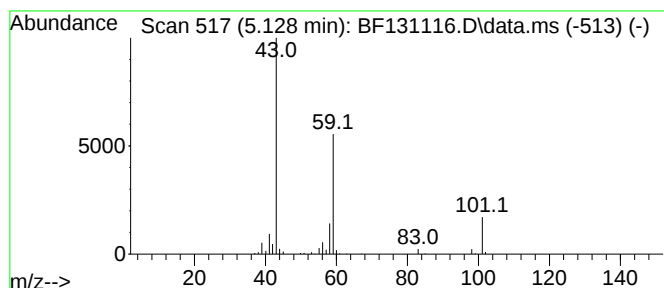
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.128	15.52 ng	337373	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9		



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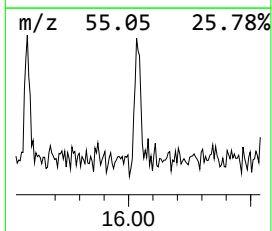
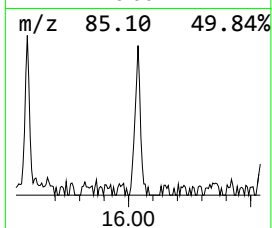
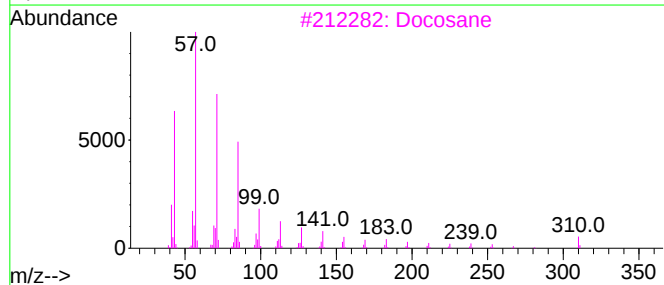
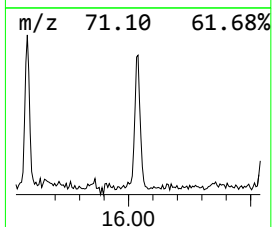
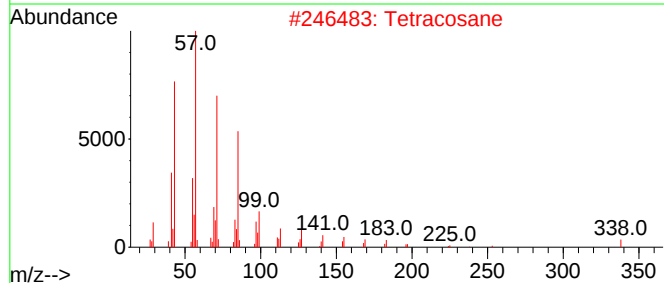
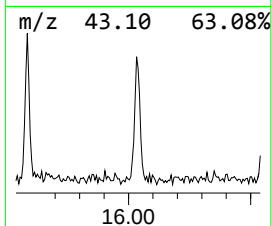
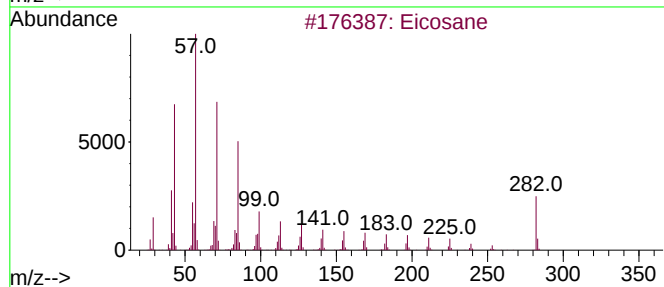
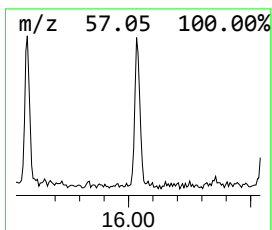
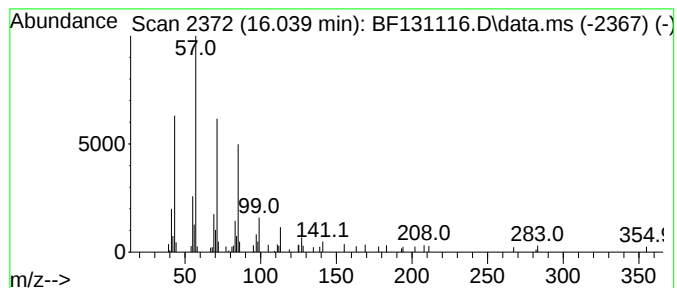
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.039	2.17 ng	51416	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	90
2	Tetracosane			338	C24H50	000646-31-1	90
3	Docosane			310	C22H44	000629-97-0	87
4	Docosane, 1-iodo-			436	C22H45I	1000406-31-9	87
5	Heptadecane			240	C17H36	000629-78-7	87



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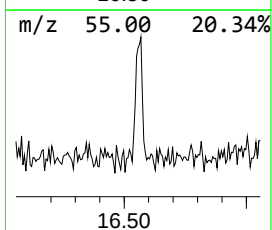
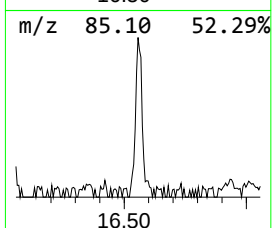
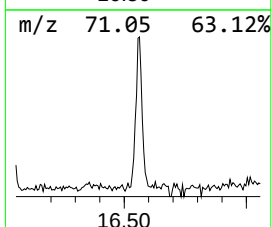
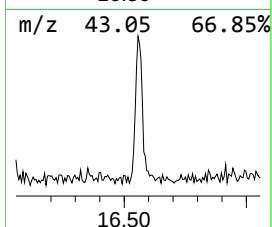
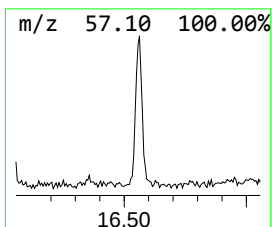
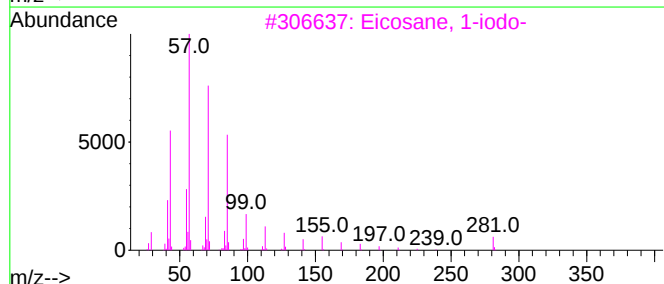
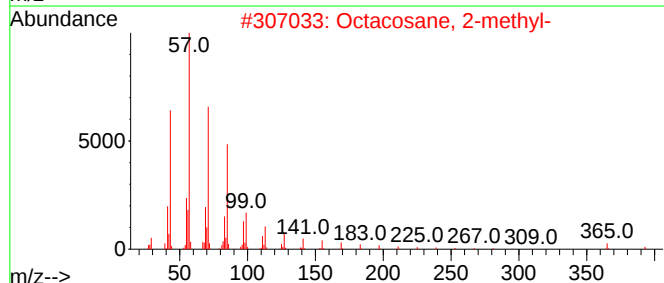
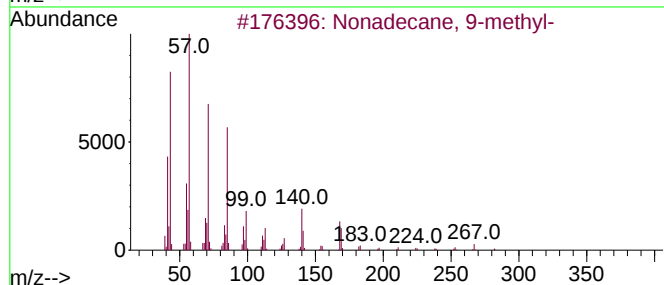
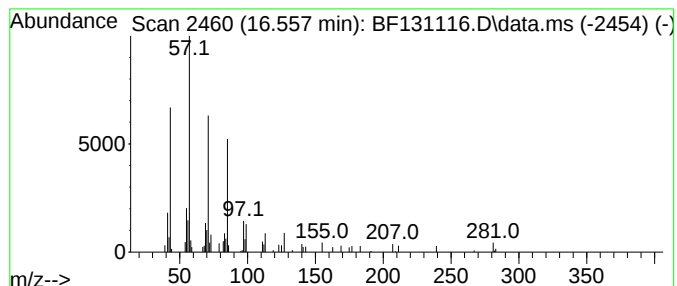
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Nonadecane, 9-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.557	2.96 ng	70060	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane, 9-methyl-	282	C20H42	013287-24-6	91
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
3			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	86
4			Eicosane, 9-octyl-	394	C28H58	013475-77-9	86
5			Octacosane	394	C28H58	000630-02-4	86



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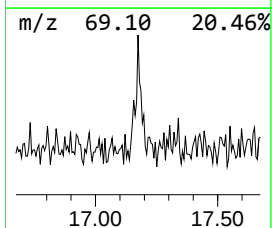
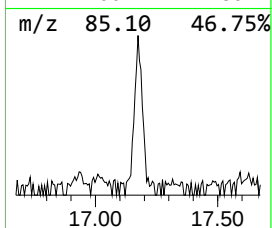
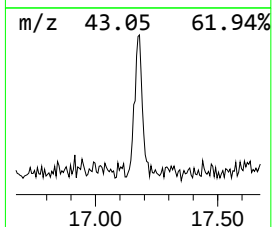
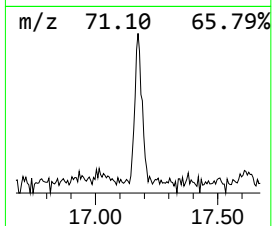
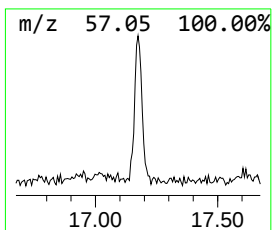
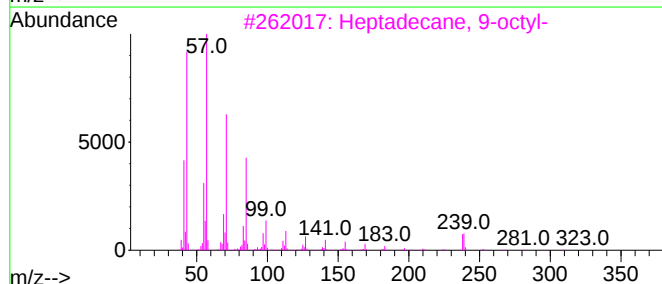
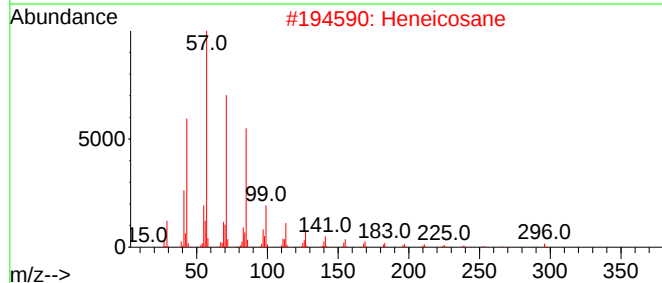
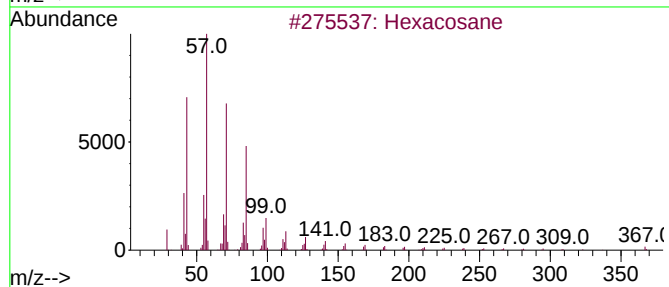
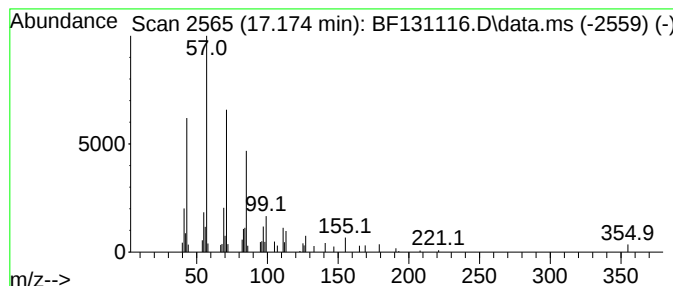
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.174	2.60 ng	61632	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	86
2			Heneicosane	296	C21H44	000629-94-7	83
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83
4			Tetracosane	338	C24H50	000646-31-1	80
5			Octadecane	254	C18H38	000593-45-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131116.D
Acq On : 10 Nov 2022 11:12
Operator : CG\JU
Sample : PB148898BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

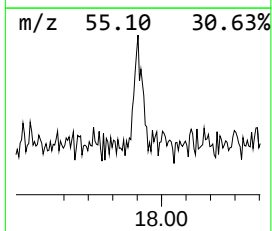
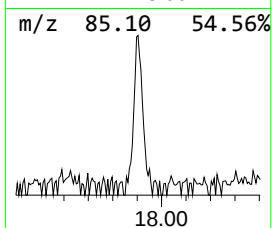
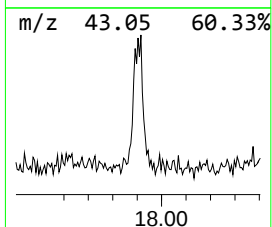
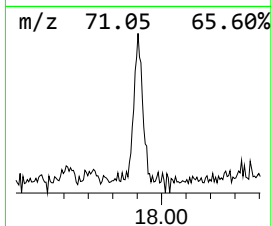
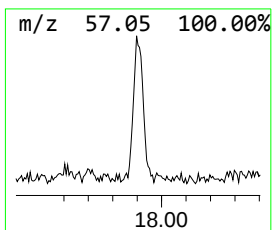
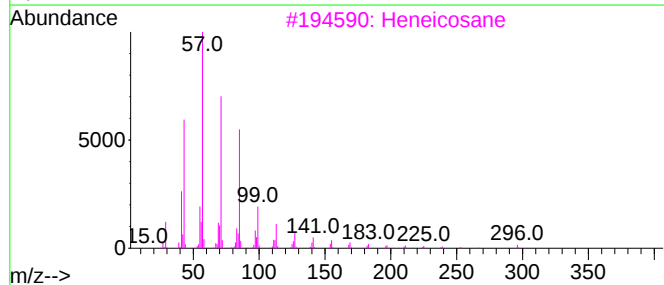
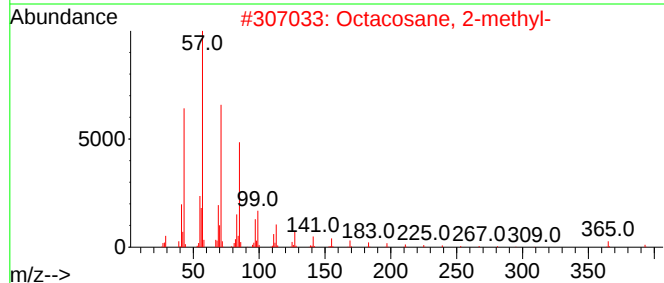
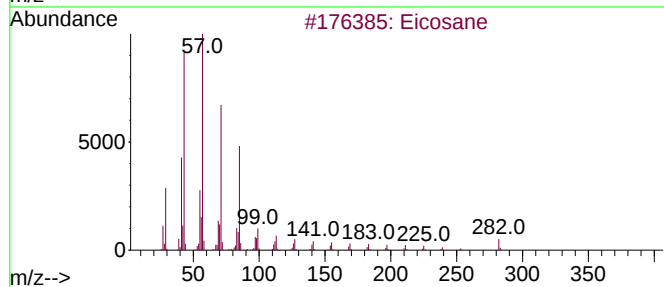
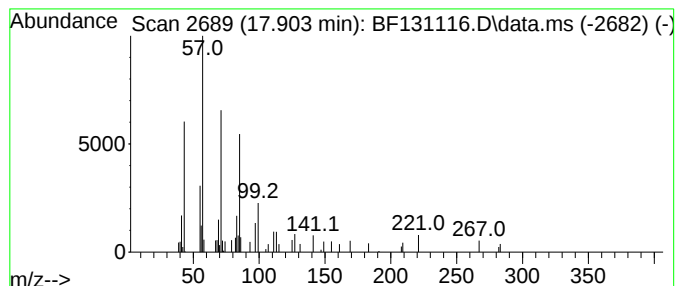
Instrument :
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ClientSampleId :
PB148898BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.904	2.56 ng	60705	Perylene-d12	15.574	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	89
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	80
3	Heneicosane	296	C21H44	000629-94-7	80
4	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	80
5	Pentacosane	352	C25H52	000629-99-2	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131116.D
Acq On : 10 Nov 2022 11:12
Operator : CG\JU
Sample : PB148898BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB148898BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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
Butane, 2-metho...	2.246	5.9	ng	128910	1	6.887	434765	20.0
Propane, 1,1-di...	2.357	2.3	ng	50326	1	6.887	434765	20.0
2-Pentanone, 4-...	5.128	15.5	ng	337373	1	6.887	434765	20.0
Eicosane	16.039	2.2	ng	51416	6	15.574	473553	20.0
Nonadecane, 9-m...	16.557	3.0	ng	70060	6	15.574	473553	20.0
Hexacosane	17.174	2.6	ng	61632	6	15.574	473553	20.0
Octacosane, 2-m...	17.904	2.6	ng	60705	6	15.574	473553	20.0