

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110722\
 Data File : BF131045.D
 Acq On : 07 Nov 2022 15:46
 Operator : CG\JU
 Sample : PB148810BL
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB148810BL

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-BF110722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131045.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	15	25	34	rVB	115354	155631	4.18%	0.764%
2	2.346	39	44	52	rBV	51725	66765	1.79%	0.328%
3	5.134	514	518	527	rBV	279990	369742	9.94%	1.815%
4	5.528	579	585	588	rBV	2554940	2639423	70.93%	12.958%
5	6.528	749	755	758	rBV	2297822	2470516	66.39%	12.128%
6	6.898	814	818	821	rBV	622474	485857	13.06%	2.385%
7	7.463	909	914	917	rBV	1499688	1471223	39.53%	7.223%
8	8.181	1032	1036	1040	rBV	668941	631575	16.97%	3.101%
9	9.263	1214	1220	1223	rBV	2831366	2692628	72.36%	13.219%
10	9.945	1330	1336	1339	rBV	931671	882895	23.72%	4.334%
11	10.739	1464	1471	1474	rBV	2086837	1954102	52.51%	9.593%
12	11.439	1585	1590	1593	rBV	920279	828299	22.26%	4.066%
13	13.027	1855	1860	1864	rBV	3515830	3721394	100.00%	18.269%
14	14.086	2036	2040	2043	rBV	1012645	836741	22.48%	4.108%
15	15.210	2227	2231	2235	rVB	38241	41999	1.13%	0.206%
16	15.580	2289	2294	2304	rVB	415239	584270	15.70%	2.868%
17	16.057	2368	2375	2382	rBV	59772	95807	2.57%	0.470%
18	16.586	2458	2465	2473	rBV2	54701	103657	2.79%	0.509%
19	17.204	2562	2570	2578	rVB4	30741	73717	1.98%	0.362%
20	17.433	2594	2609	2621	rBV5	42047	191311	5.14%	0.939%
21	17.939	2688	2695	2703	rVB2	30018	72023	1.94%	0.354%

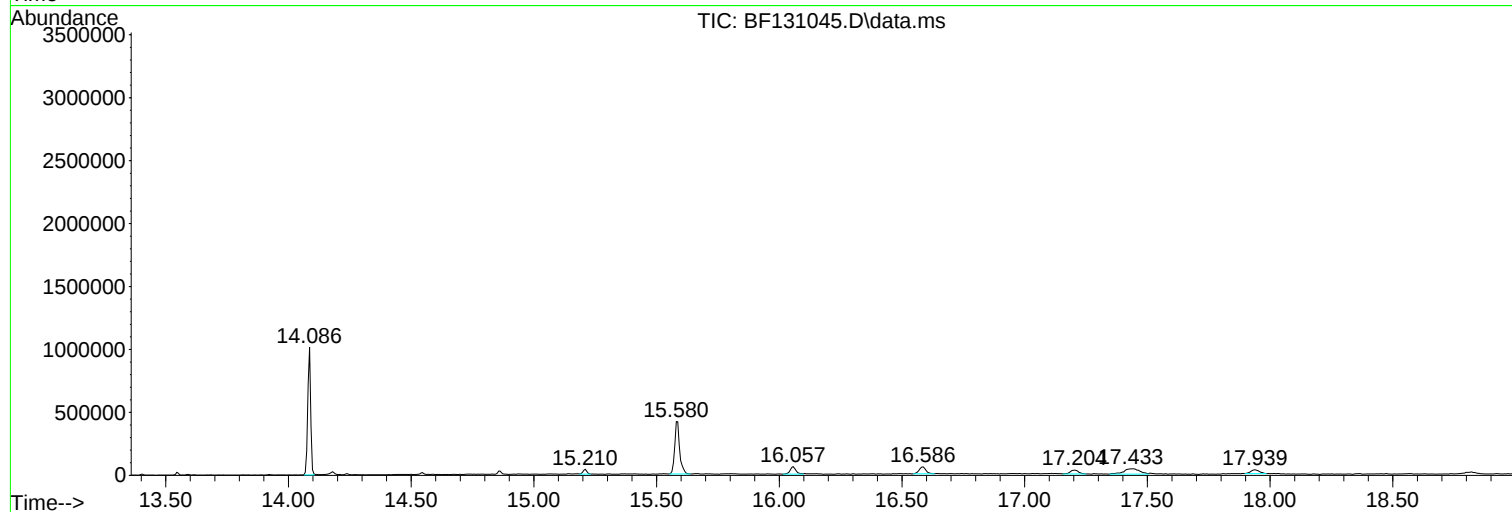
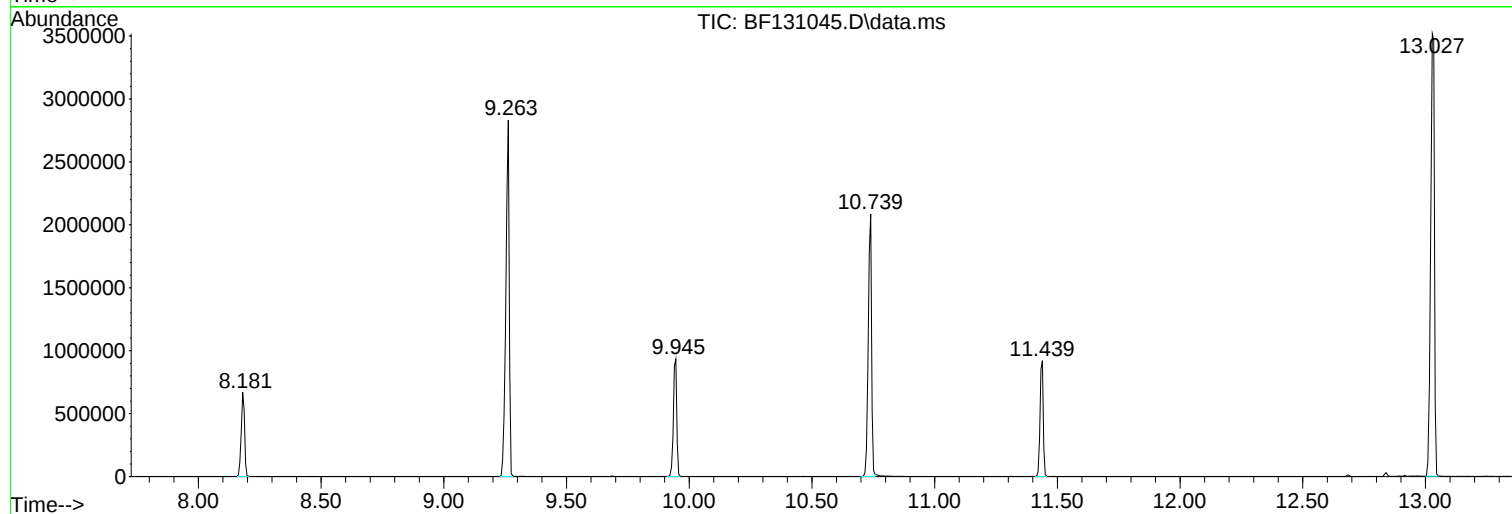
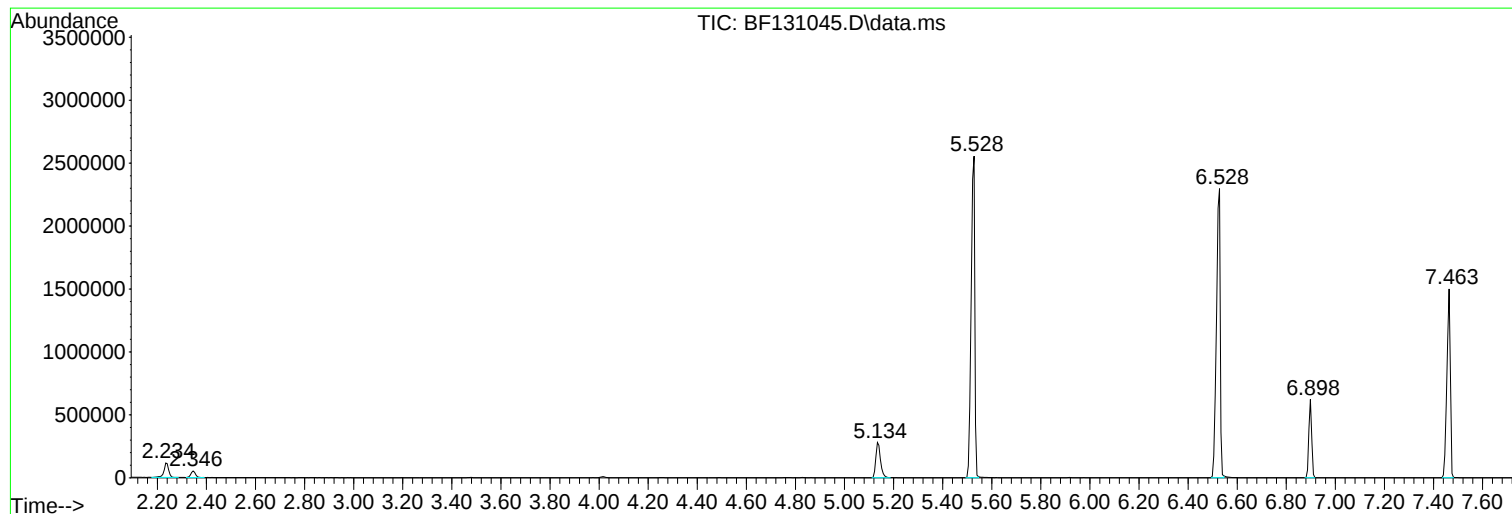
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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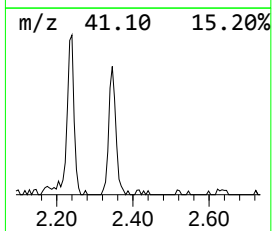
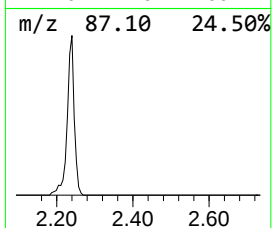
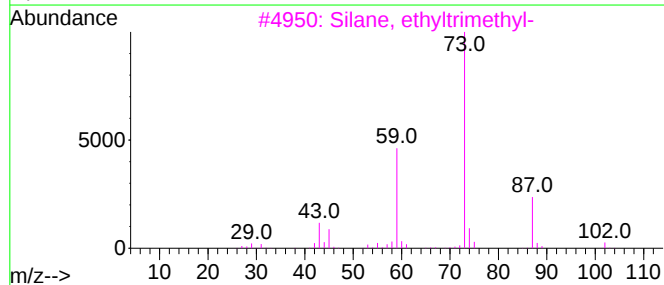
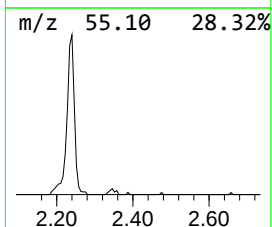
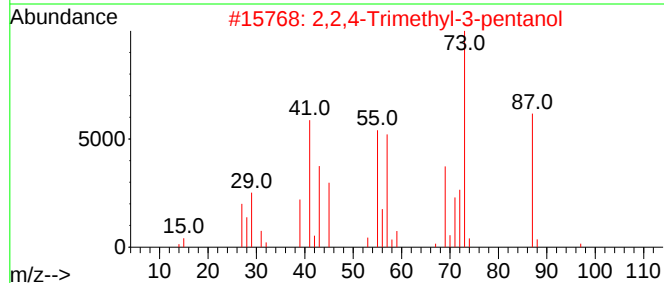
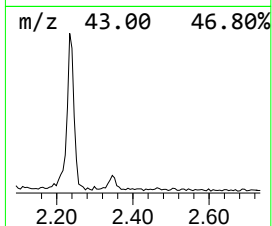
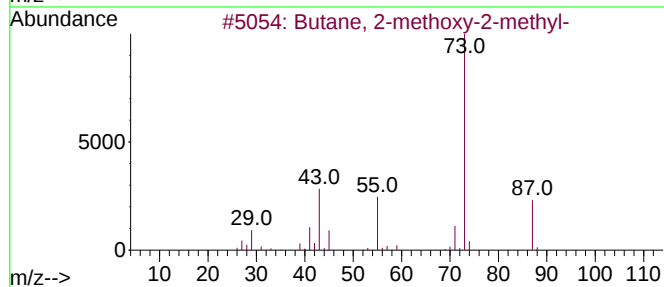
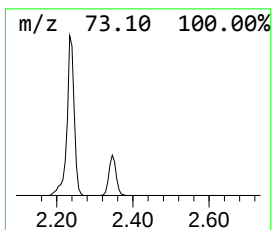
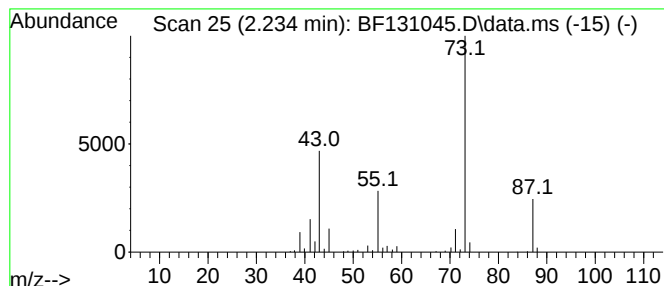
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.234	6.41 ng	155631	1,4-Dichlorobenzene-d4	6.898

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	43
3			Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
4			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	32
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	25



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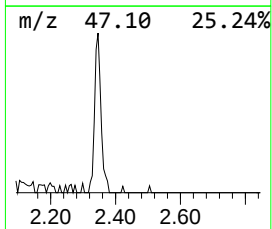
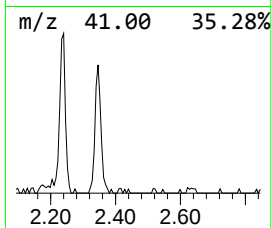
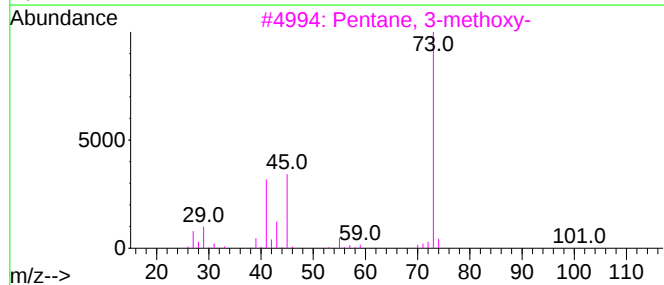
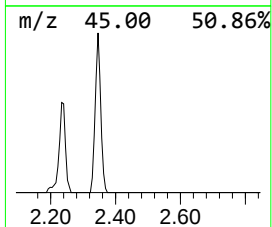
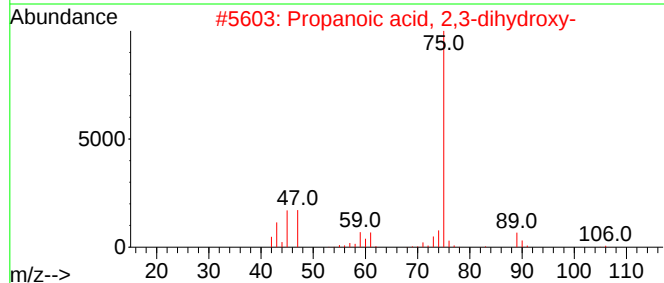
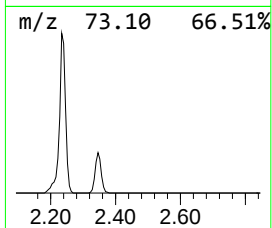
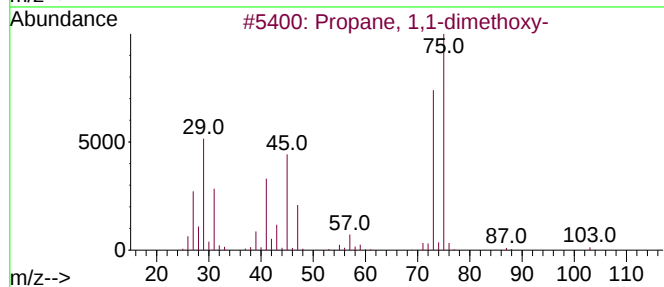
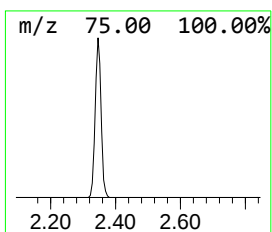
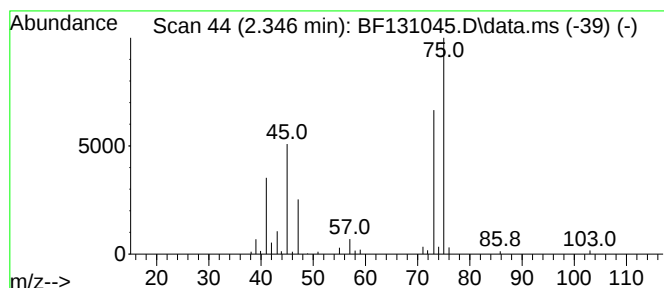
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.346	2.75 ng	66765	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2			Propanoic acid, 2,3-dihydroxy-	106	C3H6O4	000473-81-4	36
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4			3-Hexene, 1-(1-ethoxyethoxy)-, (Z)-	172	C10H20O2	028069-74-1	10
5			1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	10



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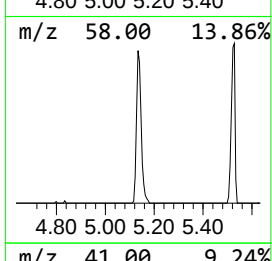
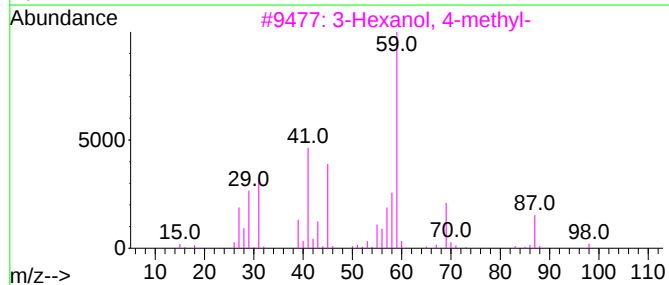
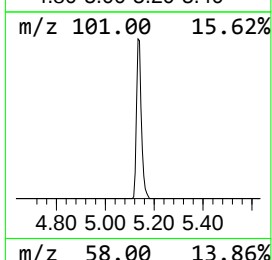
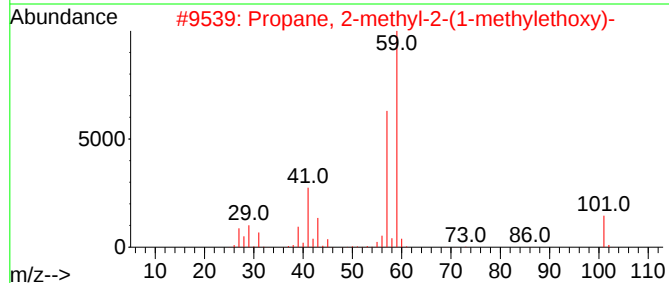
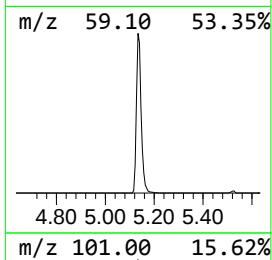
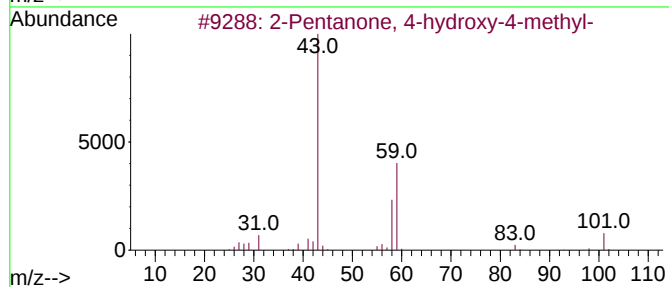
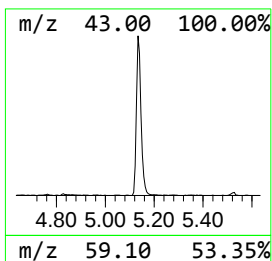
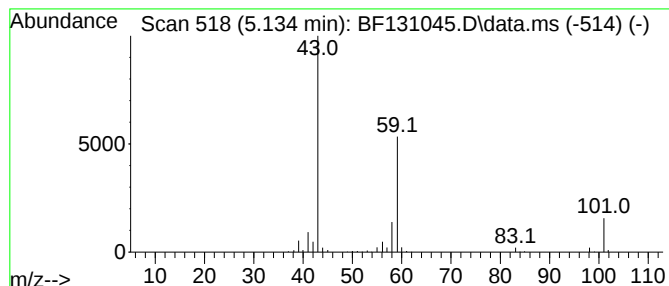
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.134	15.22 ng	369742	1,4-Dichlorobenzene-d4	6.898

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		3-Octanol	130	C8H18O	000589-98-0	33
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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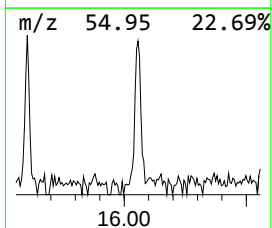
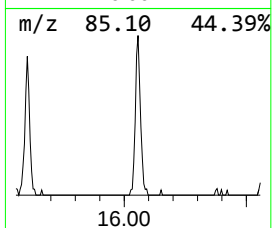
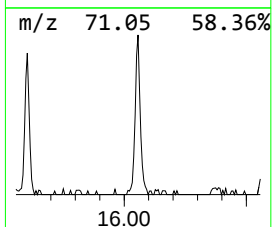
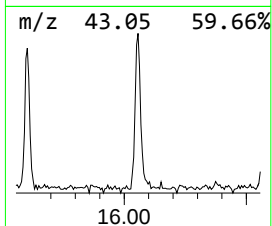
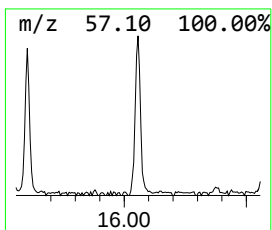
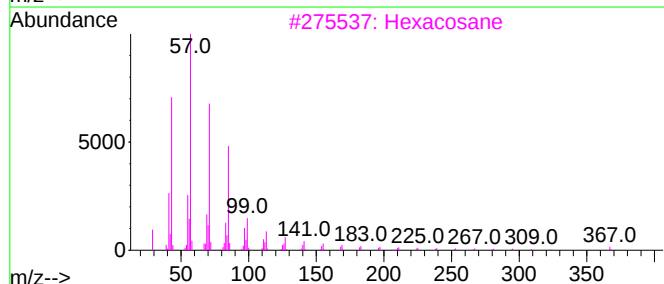
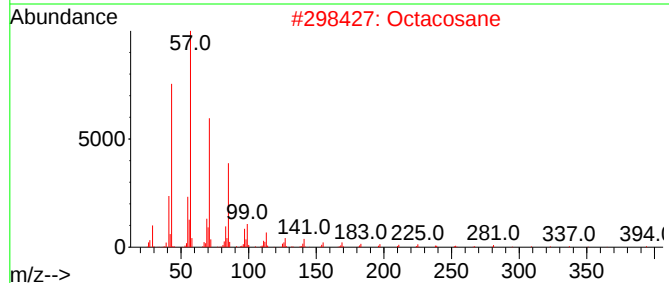
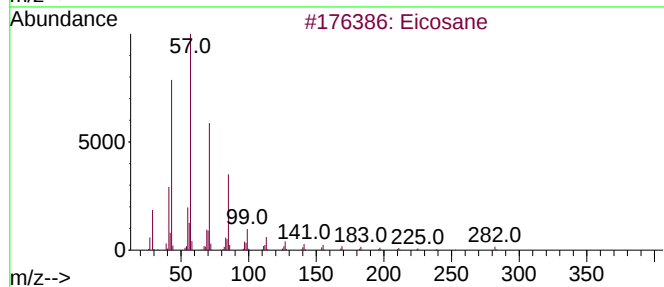
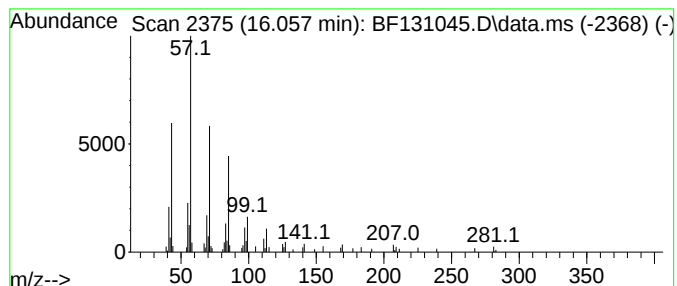
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.057	3.28 ng	95807	Perylene-d12	15.580

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Eicosane	282	C20H42	000112-95-8	95
2		Octacosane	394	C28H58	000630-02-4	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Docosane	310	C22H46	000629-97-0	90
5		Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	90



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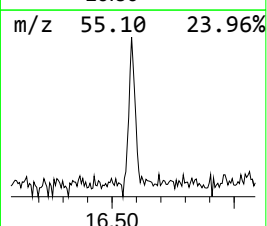
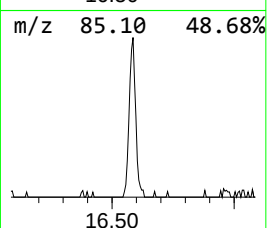
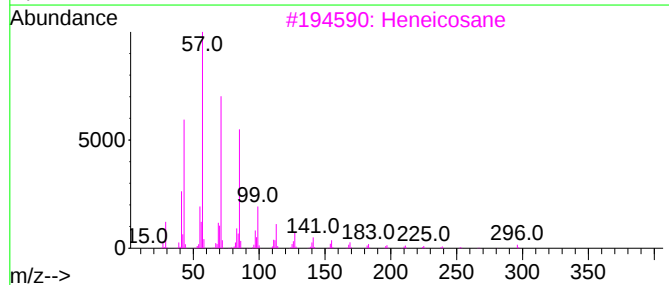
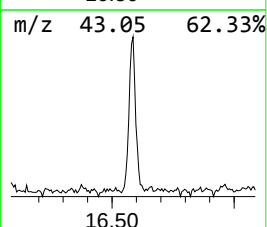
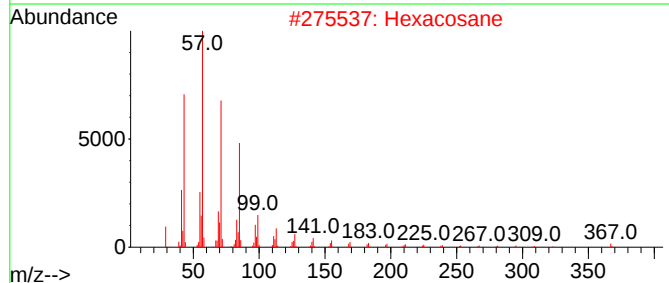
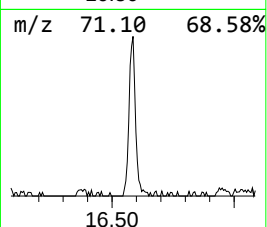
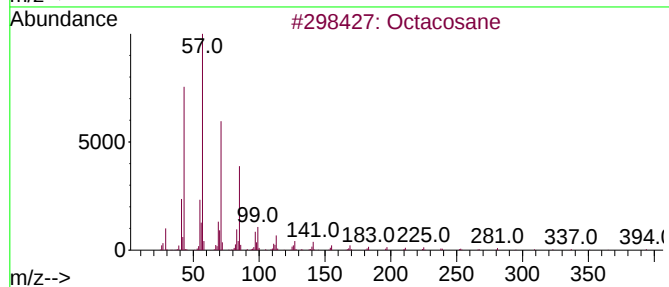
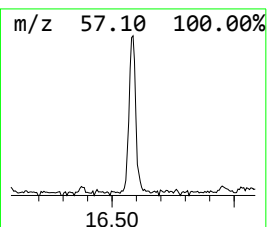
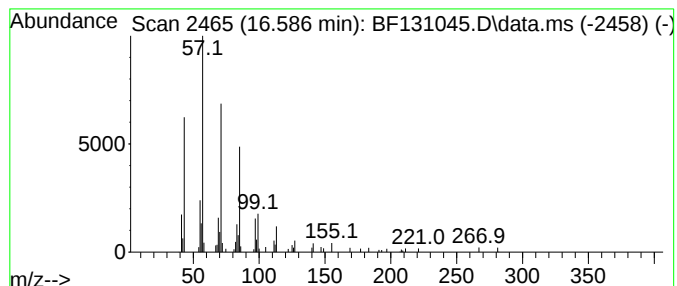
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.586	3.55 ng	103657	Perylene-d12	15.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Hexacosane	366	C26H54	000630-01-3	90
3			Heneicosane	296	C21H44	000629-94-7	90
4			Pentacosane	352	C25H52	000629-99-2	87
5			Tetracosane	338	C24H50	000646-31-1	87



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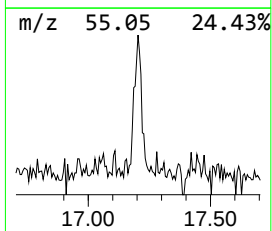
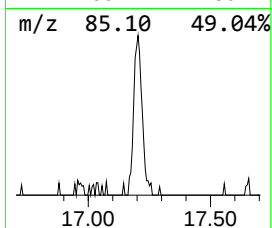
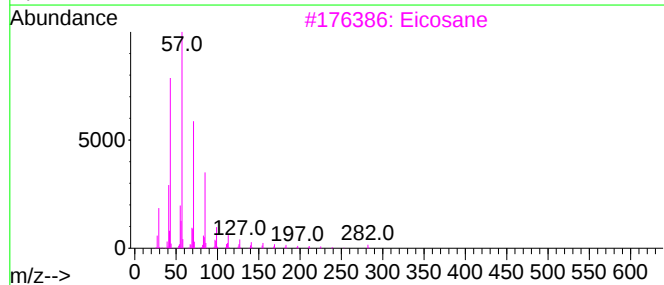
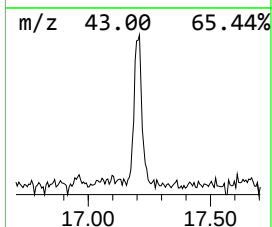
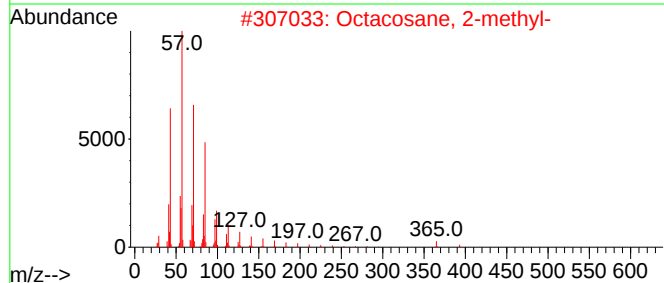
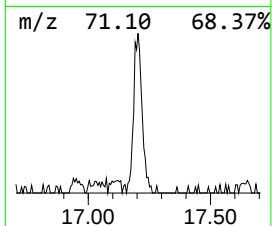
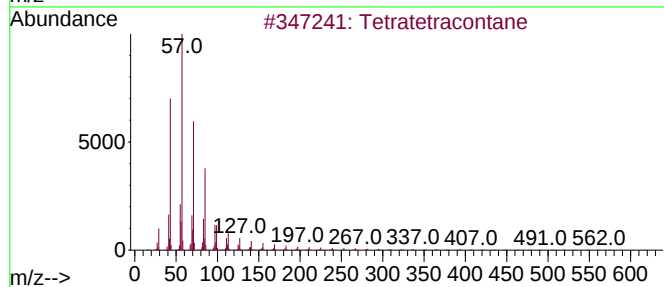
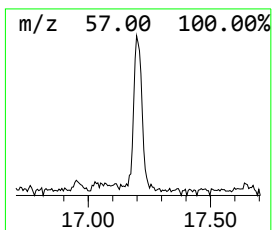
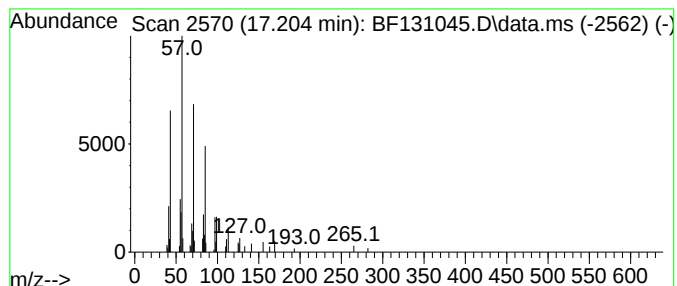
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tetratetracontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.204	2.52 ng	73717	Perylene-d12	15.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	91
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3			Eicosane	282	C20H42	000112-95-8	90
4			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	90
5			Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110722\
Data File : BF131045.D
Acq On : 07 Nov 2022 15:46
Operator : CG\JU
Sample : PB148810BL
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB148810BL

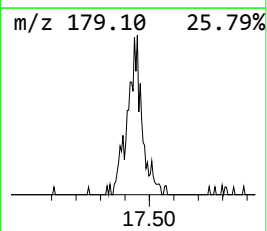
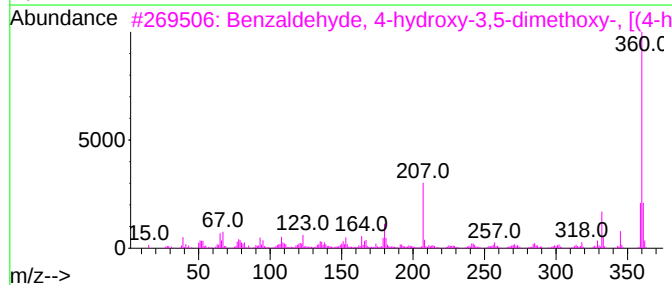
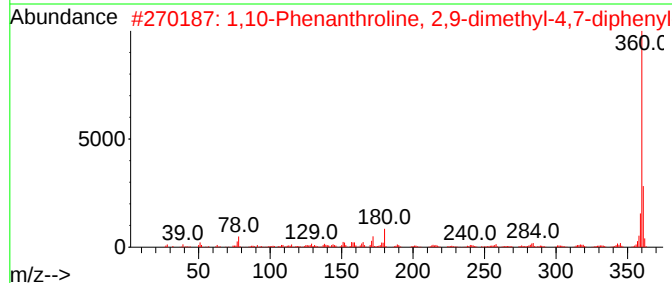
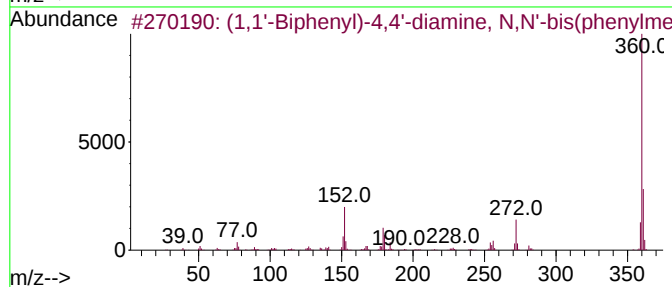
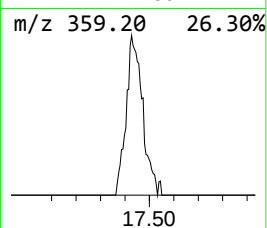
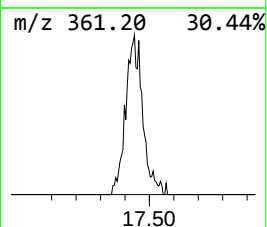
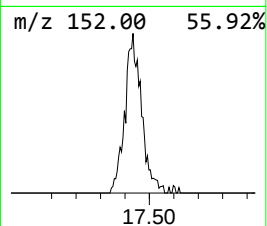
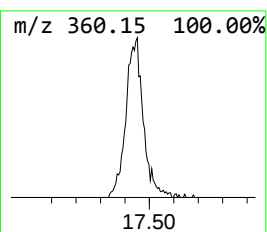
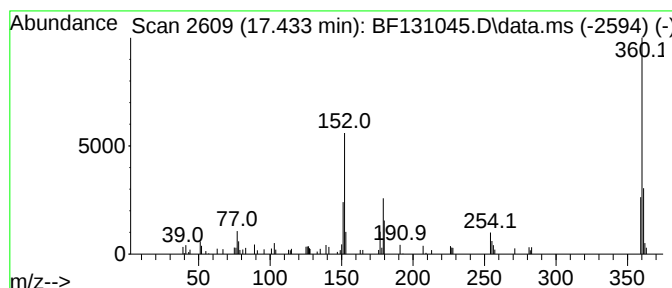
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.433	6.55 ng	191311	Perylene-d12	15.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(1,1'-Biphenyl)-4,4'-diamine, N,...	360	C26H20N2	006311-48-4	90
2			1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	46
3			Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	43
4			N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	43
5			Ethene, 1-(anthracen-9-yl)-2-(4-...	360	C27H20O	1000163-55-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110722\
Data File : BF131045.D
Acq On : 07 Nov 2022 15:46
Operator : CG\JU
Sample : PB148810BL
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB148810BL

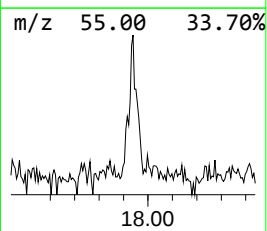
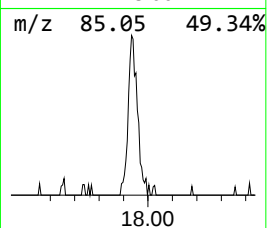
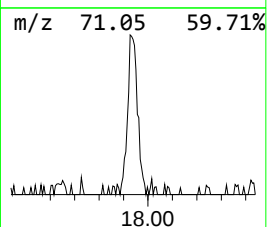
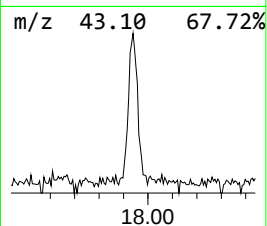
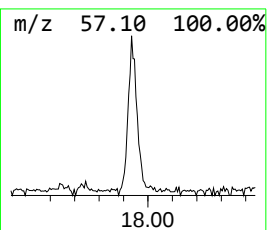
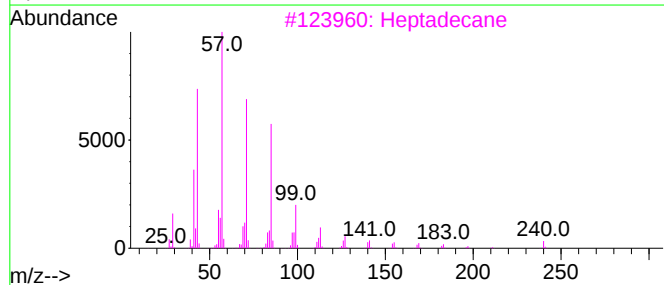
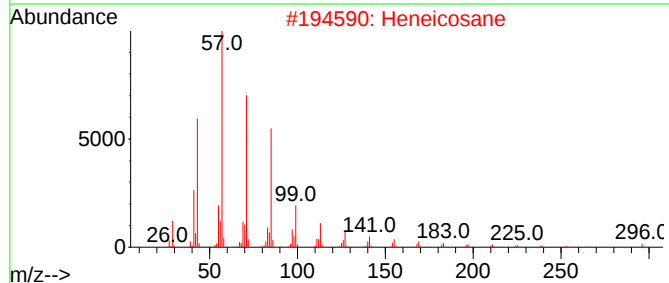
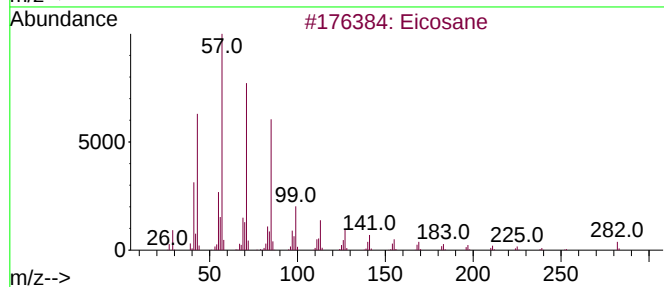
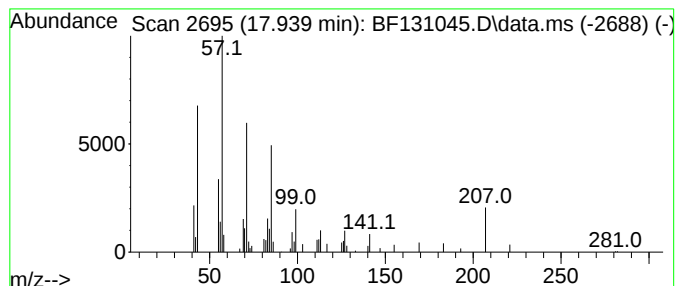
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.939	2.47 ng	72023	Perylene-d12	15.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	87
2			Heneicosane	296	C21H44	000629-94-7	87
3			Heptadecane	240	C17H36	000629-78-7	83
4			Pentacosane	352	C25H52	000629-99-2	81
5			Hentriacontane	437	C31H64	000630-04-6	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110722\
Data File : BF131045.D
Acq On : 07 Nov 2022 15:46
Operator : CG\JU
Sample : PB148810BL
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB148810BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110722.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...	2.234	6.4	ng	155631	1	6.898	485857	20.0
Propane, 1,1-di...	2.346	2.8	ng	66765	1	6.898	485857	20.0
2-Pentanone, 4-...	5.134	15.2	ng	369742	1	6.898	485857	20.0
Eicosane	16.057	3.3	ng	95807	6	15.580	584270	20.0
Octacosane	16.586	3.5	ng	103657	6	15.580	584270	20.0
Tetratetracontane	17.204	2.5	ng	73717	6	15.580	584270	20.0
(1,1'-Biphenyl)...	17.433	6.5	ng	191311	6	15.580	584270	20.0
Heneicosane	17.939	2.5	ng	72023	6	15.580	584270	20.0