

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110822\
 Data File : BF131058.D
 Acq On : 08 Nov 2022 10:16
 Operator : CG\JU
 Sample : PB148852BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB148852BL

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: BF131058.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.263	17	30	37	rVB	109880	150478	4.77%	0.739%
2	2.375	43	49	56	rBV	54815	70450	2.23%	0.346%
3	5.140	515	519	533	rBV	284868	411598	13.05%	2.021%
4	5.528	580	585	588	rBV	2376133	2403372	76.20%	11.801%
5	6.528	749	755	758	rBV	2221375	2451709	77.73%	12.038%
6	6.898	814	818	821	rBV	648483	533689	16.92%	2.621%
7	7.463	908	914	917	rBV	1444344	1658216	52.57%	8.142%
8	8.181	1031	1036	1040	rBV	704389	706456	22.40%	3.469%
9	9.263	1214	1220	1223	rBV	3107560	3011481	95.48%	14.787%
10	9.945	1330	1336	1339	rBV	939852	818168	25.94%	4.017%
11	10.739	1464	1471	1474	rBV	2261436	2023846	64.17%	9.938%
12	11.439	1586	1590	1593	rBV	1027000	851749	27.01%	4.182%
13	13.033	1856	1861	1864	rBV	3443992	3154032	100.00%	15.487%
14	14.086	2036	2040	2044	rBV	824392	710872	22.54%	3.491%
15	14.863	2165	2172	2176	rBV	32287	38549	1.22%	0.189%
16	15.210	2227	2231	2235	rVB	44230	50340	1.60%	0.247%
17	15.586	2290	2295	2303	rVB	405669	586291	18.59%	2.879%
18	16.057	2370	2375	2381	rBV	62225	90770	2.88%	0.446%
19	16.580	2459	2464	2472	rBV	80104	153516	4.87%	0.754%
20	17.204	2563	2570	2578	rVB2	53986	117938	3.74%	0.579%
21	17.451	2599	2612	2621	rBV4	36797	136239	4.32%	0.669%
22	17.939	2688	2695	2704	rVB2	54079	133394	4.23%	0.655%
23	18.815	2835	2844	2852	rBV2	32103	102515	3.25%	0.503%

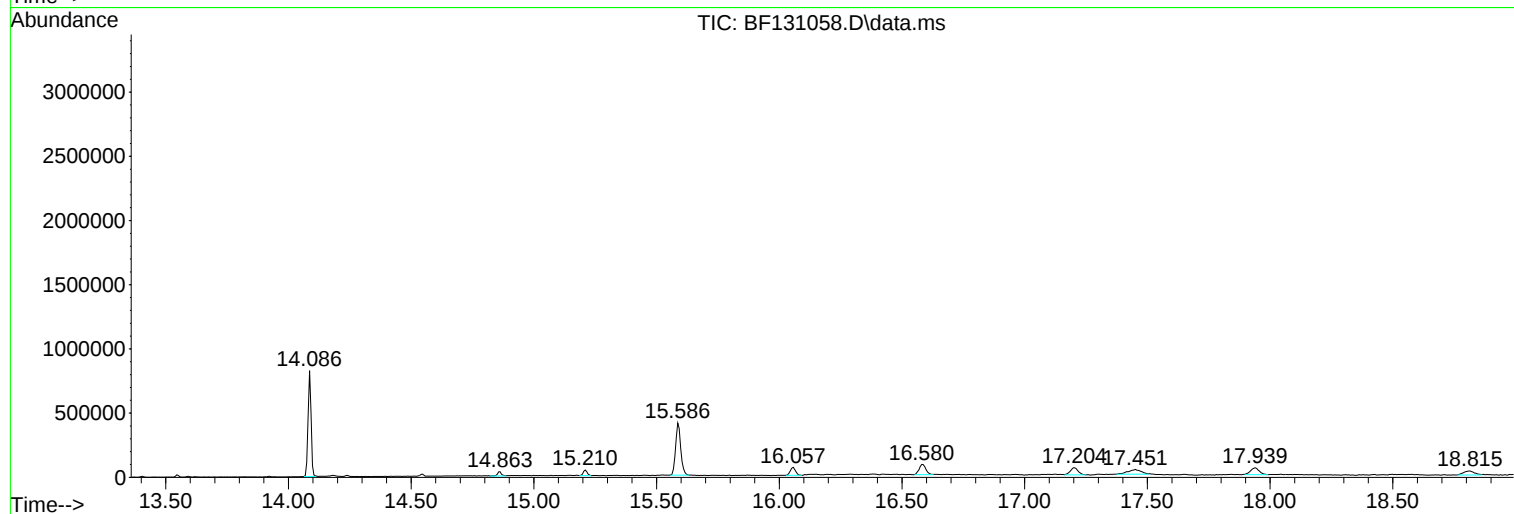
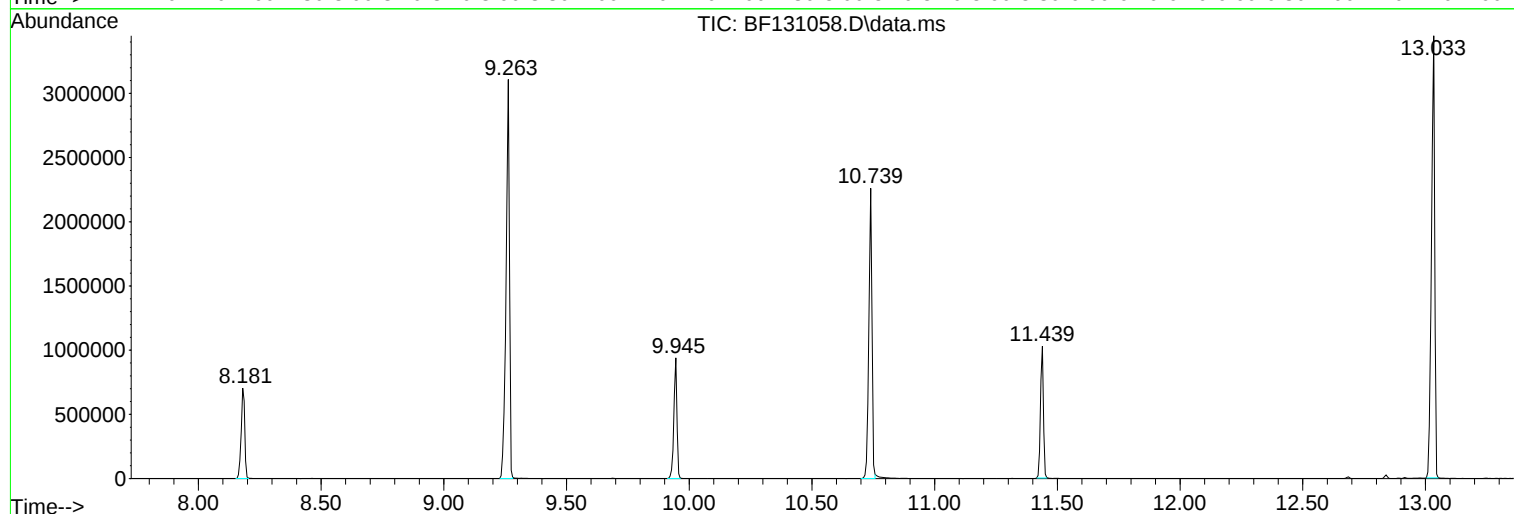
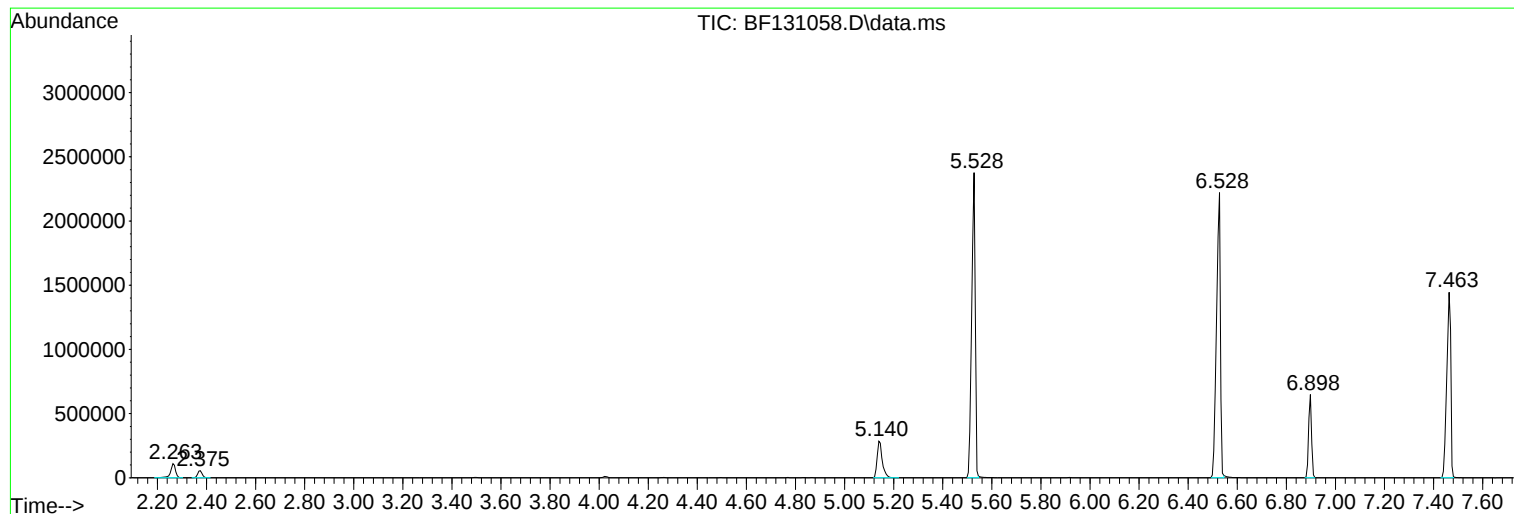
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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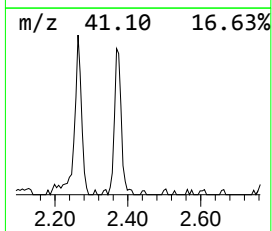
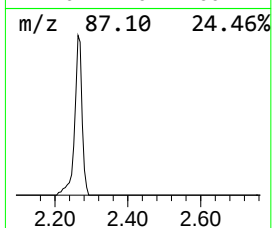
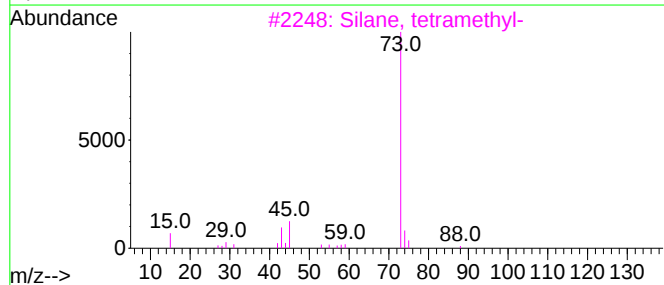
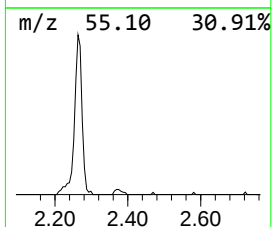
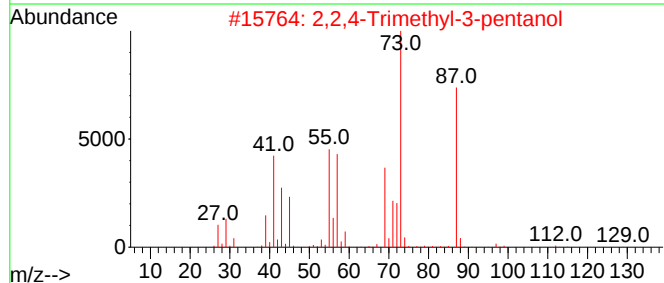
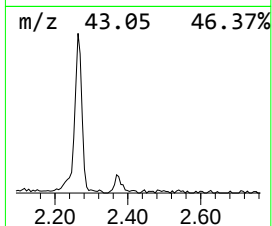
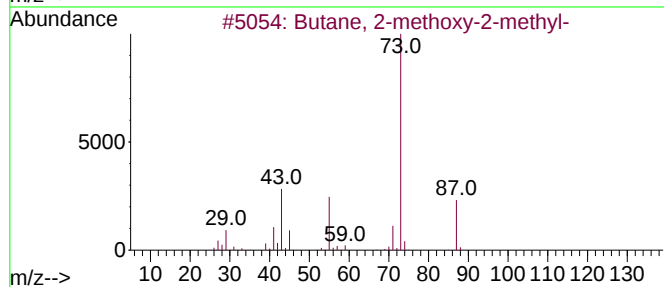
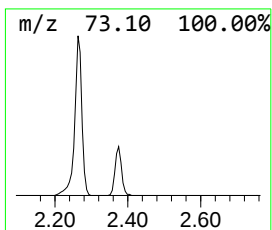
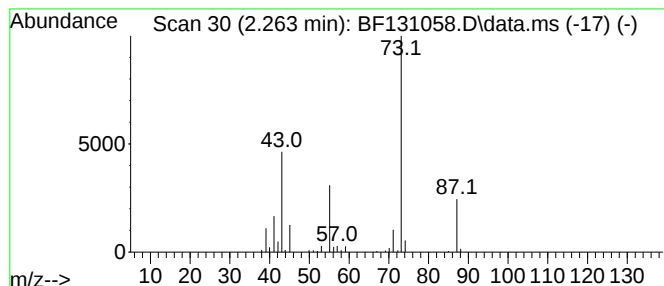
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.263	5.64 ng	150478	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	72
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
5		3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	17



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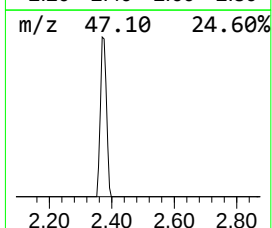
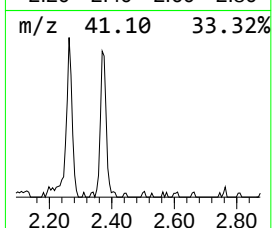
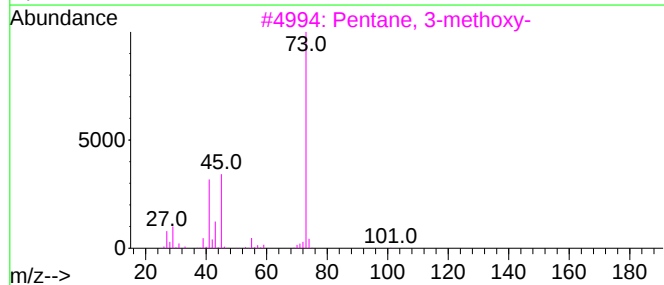
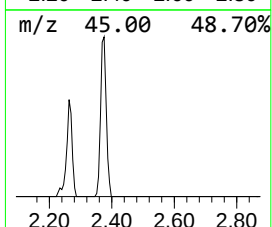
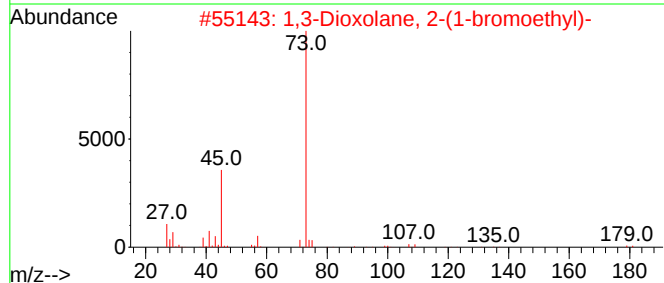
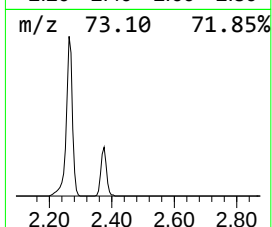
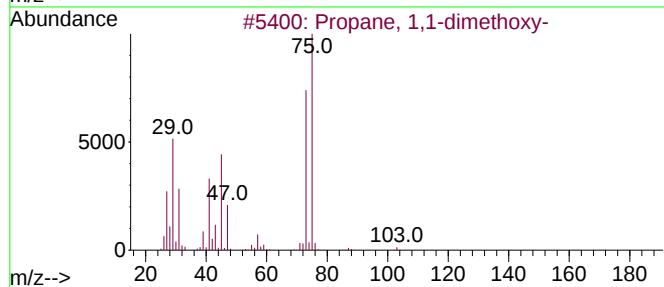
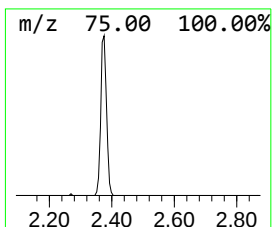
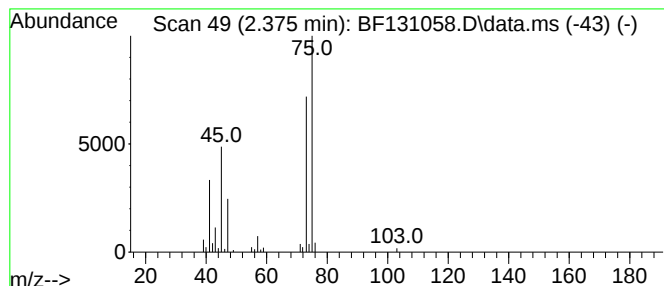
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.375	2.64 ng	70450	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	78
2			1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	12
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4			Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9
5			1,3-Dioxan-5-ol	104	C4H8O3	004740-78-7	9



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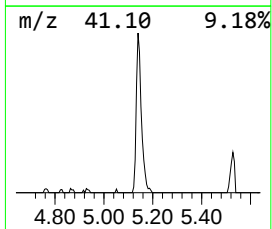
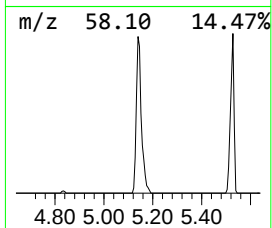
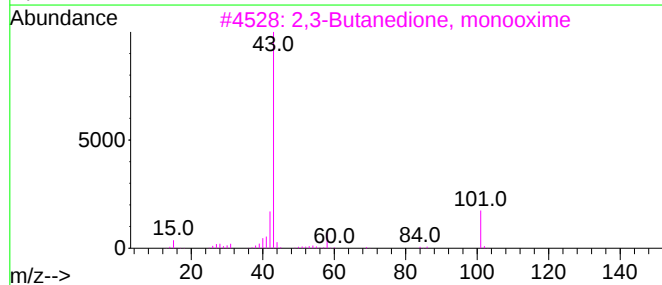
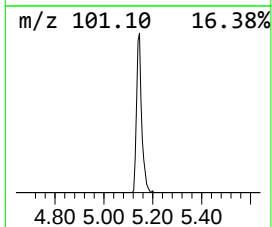
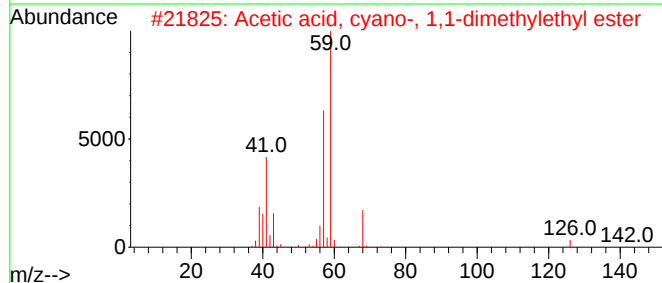
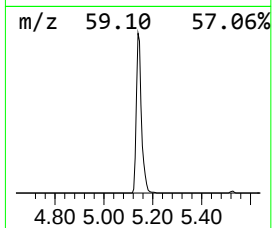
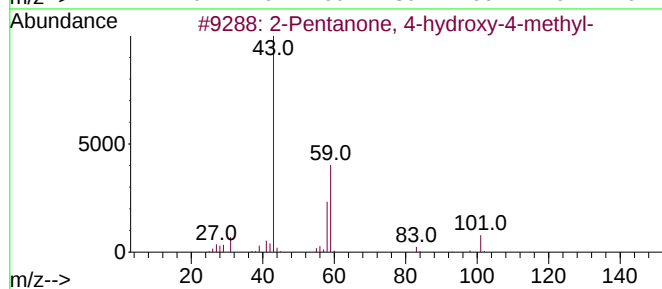
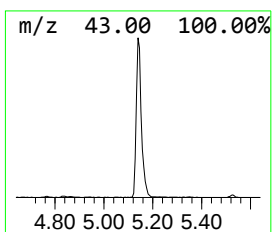
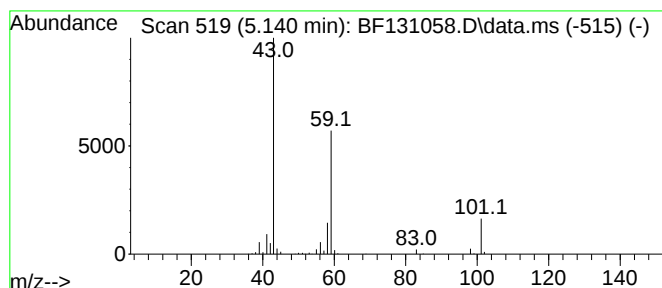
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.140	15.42 ng	411598	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			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	9
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9



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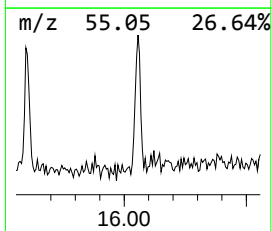
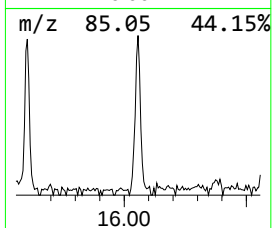
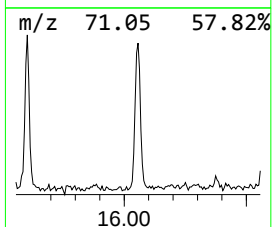
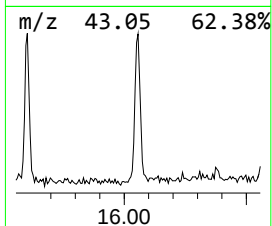
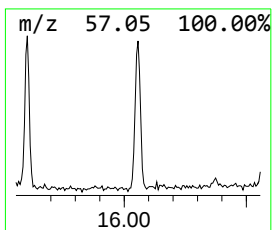
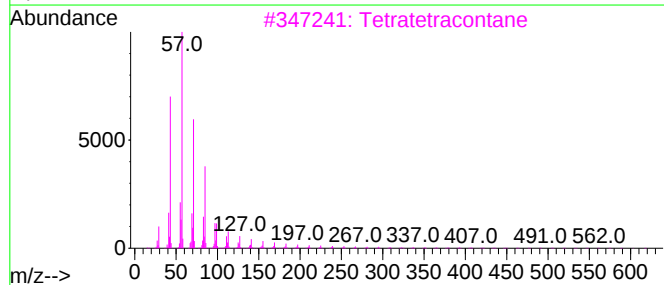
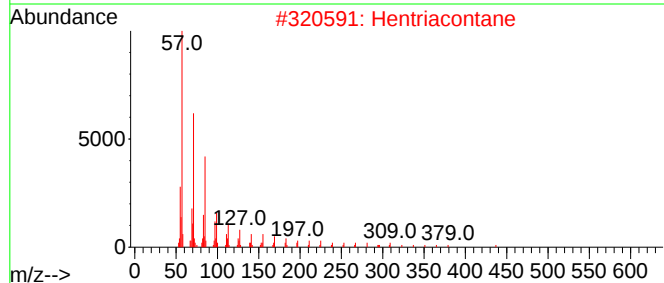
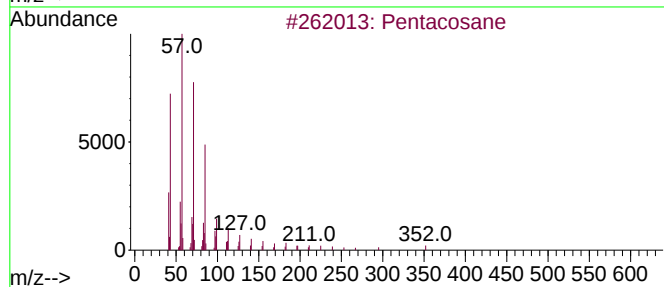
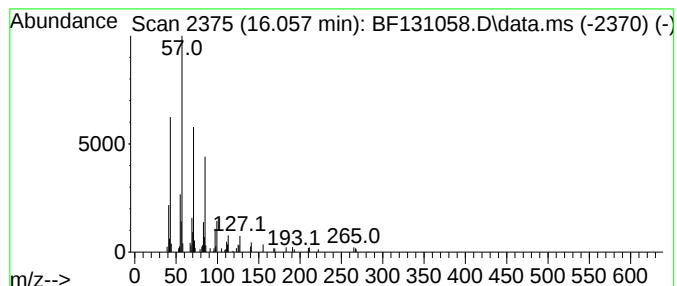
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Peak Number 4 Pentacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.057	3.10 ng	90770	Perylene-d12	15.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	91
2			Hentriacontane	437	C31H64	000630-04-6	90
3			Tetratetracontane	619	C44H90	007098-22-8	87
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5			Octacosane	394	C28H58	000630-02-4	87



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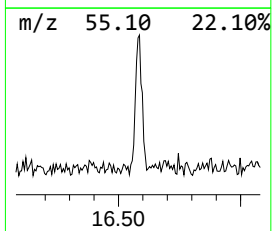
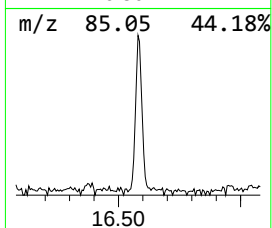
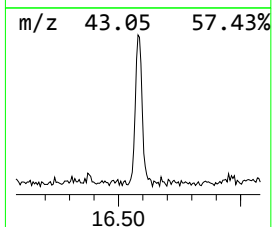
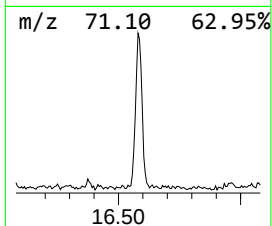
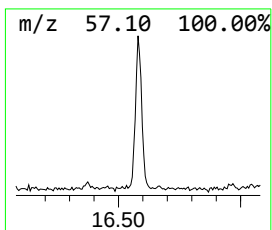
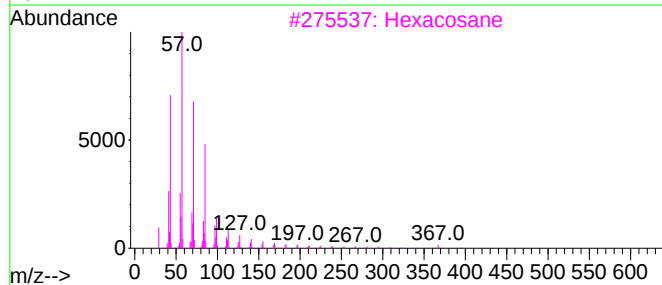
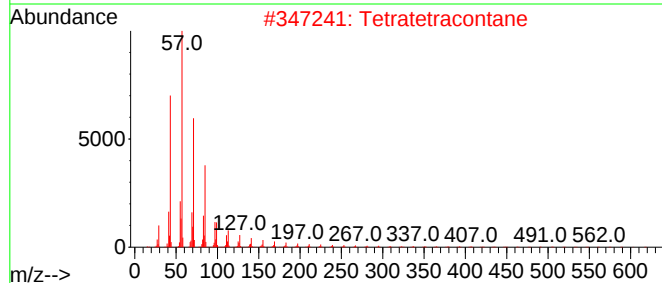
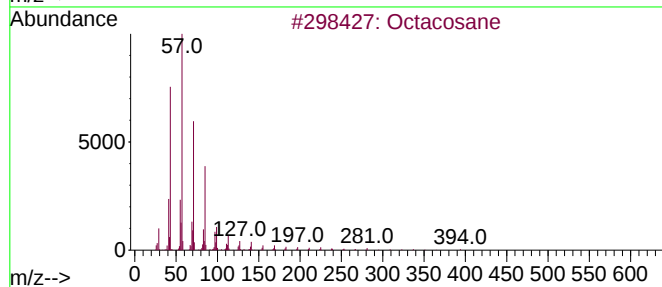
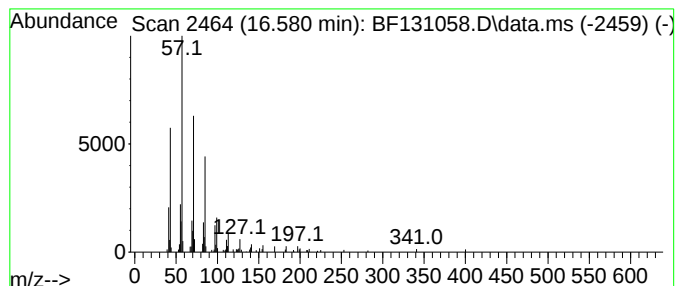
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.580	5.24 ng	153516	Perylene-d12	15.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Tetratetracontane	619	C44H90	007098-22-8	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	90



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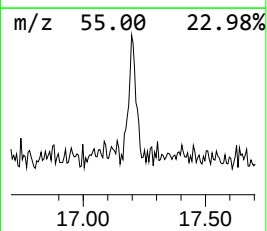
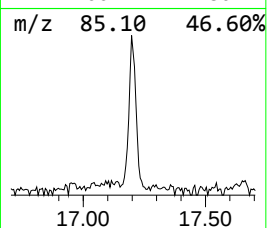
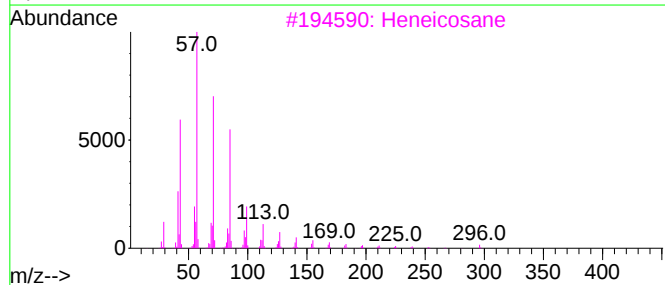
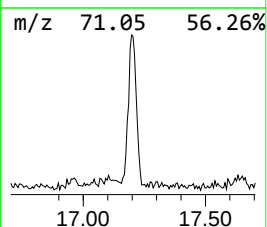
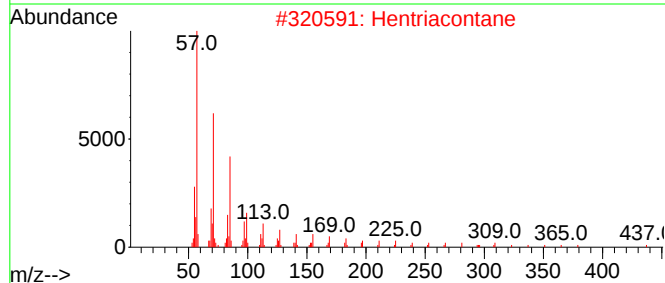
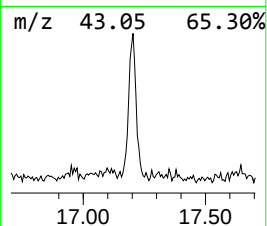
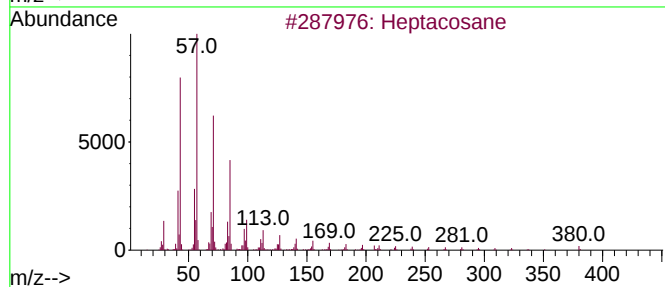
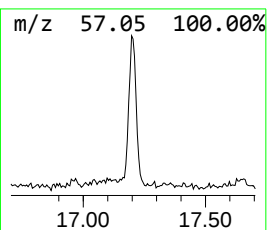
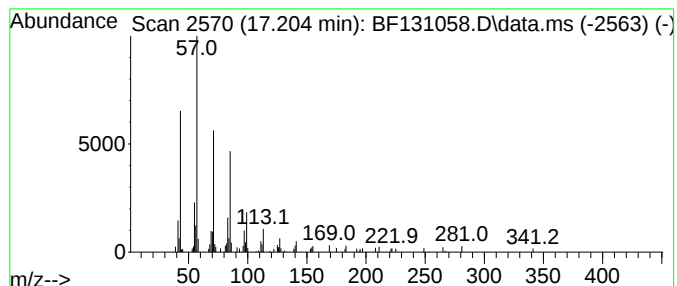
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.204	4.02 ng	117938	Perylene-d12	15.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	91
2			Hentriacontane	437	C31H64	000630-04-6	91
3			Heneicosane	296	C21H44	000629-94-7	90
4			Tetracosane	338	C24H50	000646-31-1	90
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110822\
Data File : BF131058.D
Acq On : 08 Nov 2022 10:16
Operator : CG\JU
Sample : PB148852BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PB148852BL

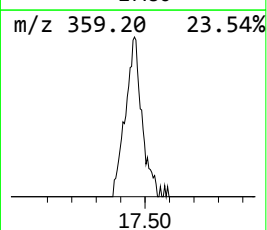
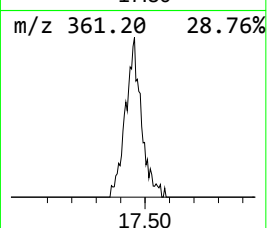
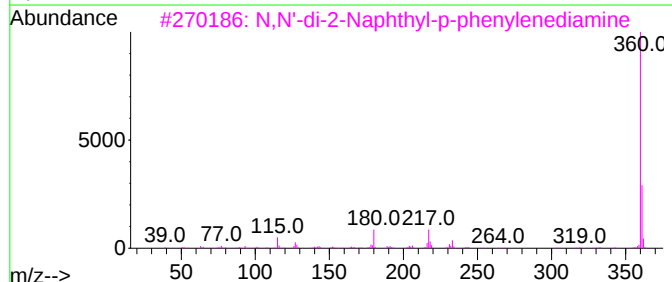
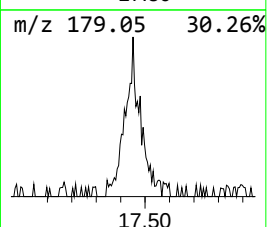
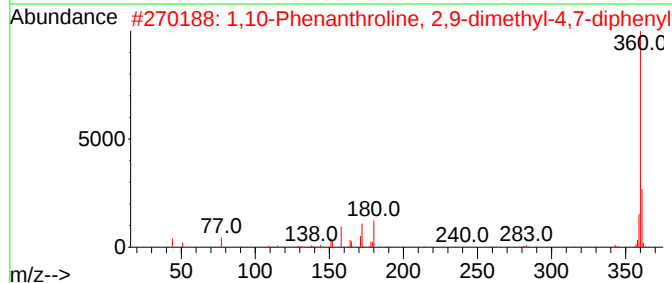
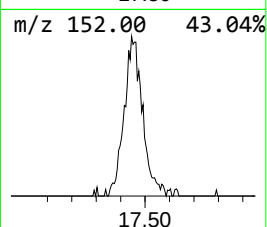
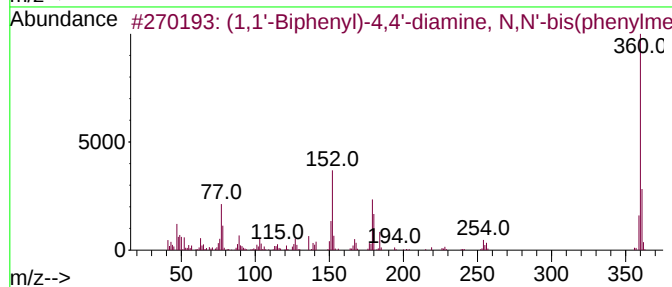
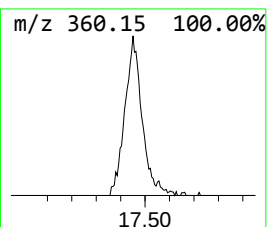
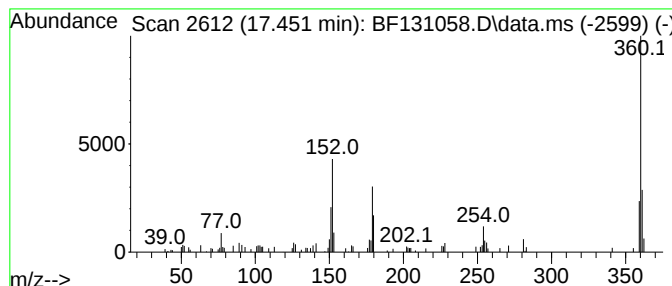
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.451	4.65 ng	136239	Perylene-d12	15.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(1,1'-Biphenyl)-4,4'-diamine, N,...	360	C26H20N2	006311-48-4	93
2			1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	46
3			N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	43
4			Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	43
5			1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13B06	1000150-23-7	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110822\
Data File : BF131058.D
Acq On : 08 Nov 2022 10:16
Operator : CG\JU
Sample : PB148852BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB148852BL

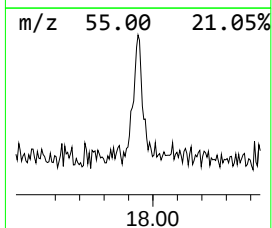
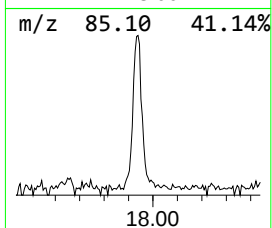
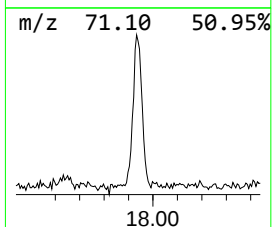
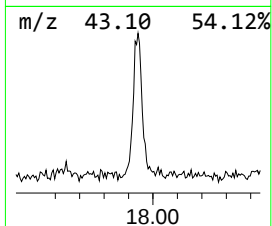
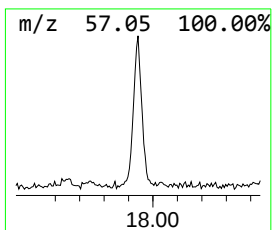
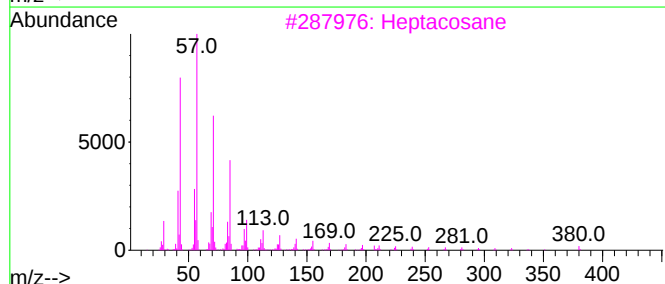
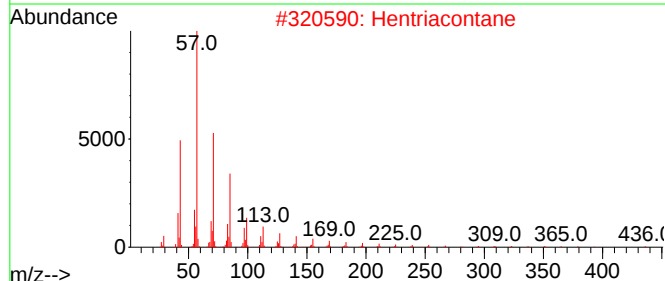
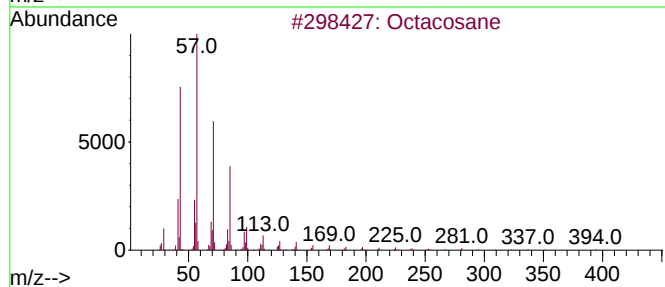
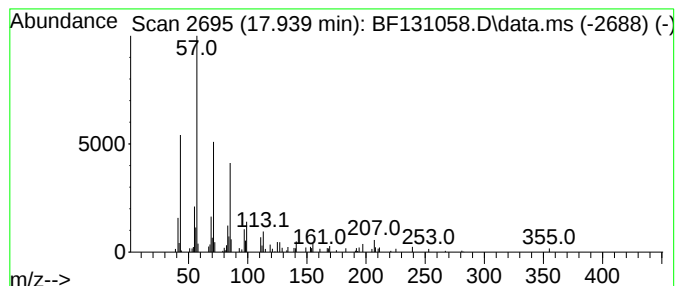
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hentriacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.939	4.55 ng	133394	Perylene-d12	15.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	90
2			Hentriacontane	437	C31H64	000630-04-6	90
3			Heptacosane	380	C27H56	000593-49-7	87
4			5,5,7,7-Tetraethylundecane	268	C19H40	1000360-42-0	86
5			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110822\
Data File : BF131058.D
Acq On : 08 Nov 2022 10:16
Operator : CG\JU
Sample : PB148852BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB148852BL

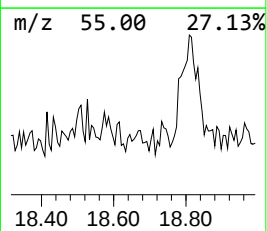
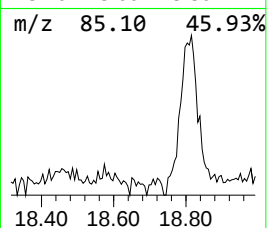
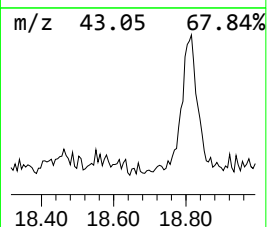
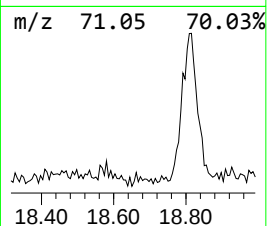
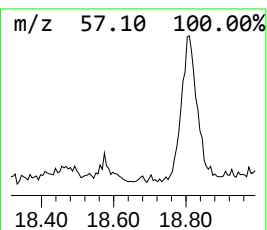
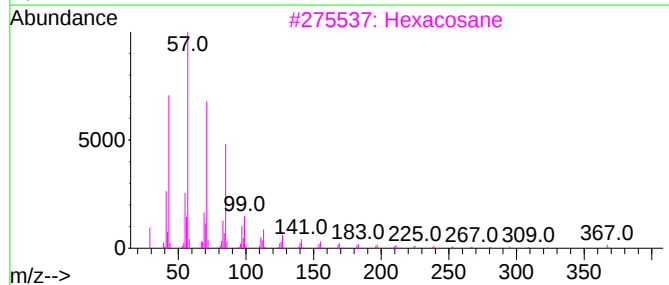
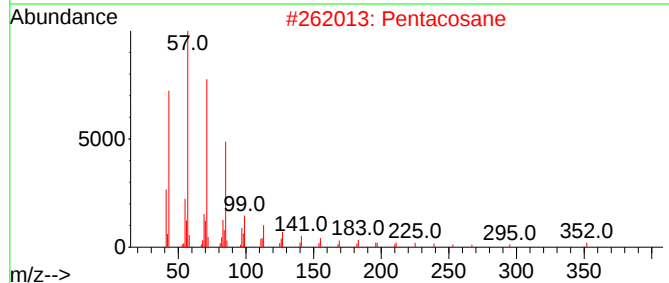
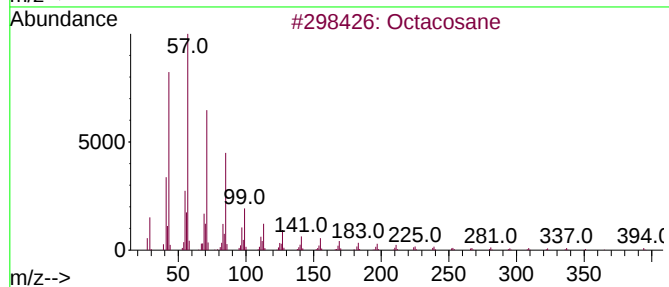
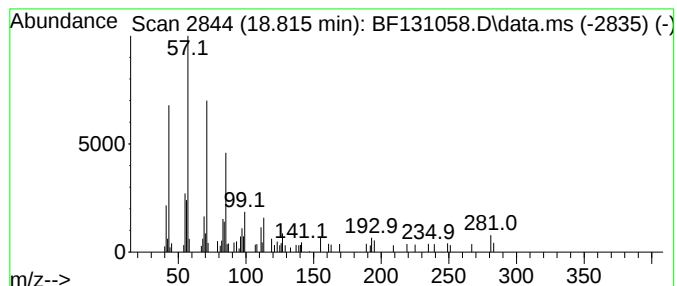
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.815	3.50 ng	102515	Perylene-d12	15.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	87
2			Pentacosane	352	C25H52	000629-99-2	87
3			Hexacosane	366	C26H54	000630-01-3	83
4			Heptacosane	380	C27H56	000593-49-7	83
5			Hentriacontane	437	C31H64	000630-04-6	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110822\
Data File : BF131058.D
Acq On : 08 Nov 2022 10:16
Operator : CG\JU
Sample : PB148852BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB148852BL

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...	2.263	5.6	ng	150478	1	6.898	533689	20.0
Propane, 1,1-di...	2.375	2.6	ng	70450	1	6.898	533689	20.0
2-Pentanone, 4-...	5.140	15.4	ng	411598	1	6.898	533689	20.0
Pentacosane	16.057	3.1	ng	90770	6	15.586	586291	20.0
Octacosane	16.580	5.2	ng	153516	6	15.586	586291	20.0
Heptacosane	17.204	4.0	ng	117938	6	15.586	586291	20.0
(1,1'-Biphenyl)...	17.451	4.7	ng	136239	6	15.586	586291	20.0
Hentriacontane	17.939	4.5	ng	133394	6	15.586	586291	20.0
Hexacosane	18.815	3.5	ng	102515	6	15.586	586291	20.0