

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071323\
 Data File : BF134261.D
 Acq On : 13 Jul 2023 14:35
 Operator : CG\JU
 Sample : PB153430BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB153430BL

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-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134261.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	6	8	20	rVB2	24218	41095	1.34%	0.193%
2	4.463	400	404	419	rBV	504755	577716	18.78%	2.712%
3	5.087	504	510	525	rBV	1215793	1647144	53.55%	7.734%
4	5.481	573	577	596	rBV	2456480	2379286	77.36%	11.171%
5	6.481	742	747	750	rBV	2389327	2289031	74.42%	10.747%
6	6.839	805	808	817	rBV	592014	471199	15.32%	2.212%
7	7.404	900	904	907	rBV	1735423	1485546	48.30%	6.975%
8	8.122	1022	1026	1038	rBV	667480	631106	20.52%	2.963%
9	9.198	1205	1209	1212	rBV	3473836	2801082	91.07%	13.152%
10	9.880	1321	1325	1328	rBV	821079	699252	22.73%	3.283%
11	10.674	1456	1460	1463	rBV	2177329	1922251	62.50%	9.025%
12	11.374	1575	1579	1582	rBV	858755	746298	24.26%	3.504%
13	11.898	1664	1668	1682	rBV	94904	134041	4.36%	0.629%
14	12.692	1800	1803	1814	rBV2	61131	88902	2.89%	0.417%
15	12.974	1846	1851	1854	rBV	3403363	3075758	100.00%	14.441%
16	14.033	2028	2031	2039	rVB	717580	658536	21.41%	3.092%
17	14.192	2052	2058	2061	rBV	63393	75663	2.46%	0.355%
18	14.504	2106	2111	2114	rBV	134569	127791	4.15%	0.600%
19	14.815	2160	2164	2169	rBV	147647	153739	5.00%	0.722%
20	15.168	2219	2224	2235	rVB	132887	183204	5.96%	0.860%
21	15.539	2282	2287	2297	rBV	443371	736075	23.93%	3.456%
22	16.027	2364	2370	2374	rBV	71295	121274	3.94%	0.569%
23	16.562	2455	2461	2467	rBV2	51116	96959	3.15%	0.455%
24	17.186	2563	2567	2574	rBV3	27202	61604	2.00%	0.289%
25	17.939	2690	2695	2704	rVB4	20875	56495	1.84%	0.265%
26	18.827	2844	2846	2859	rVB4	12128	37286	1.21%	0.175%

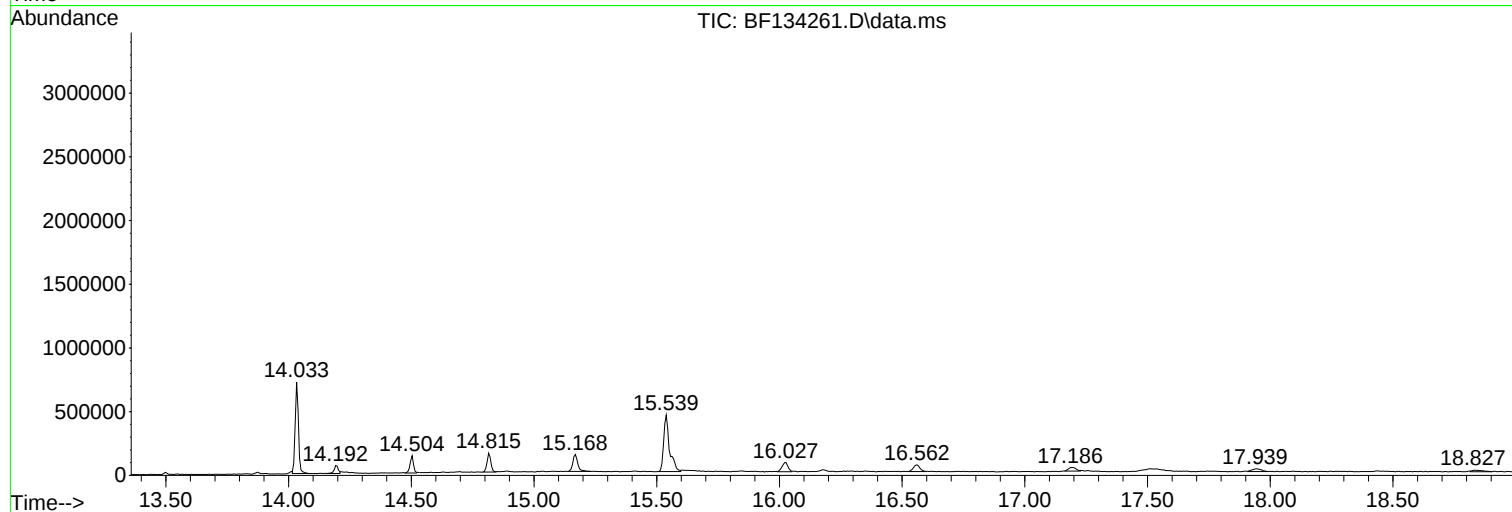
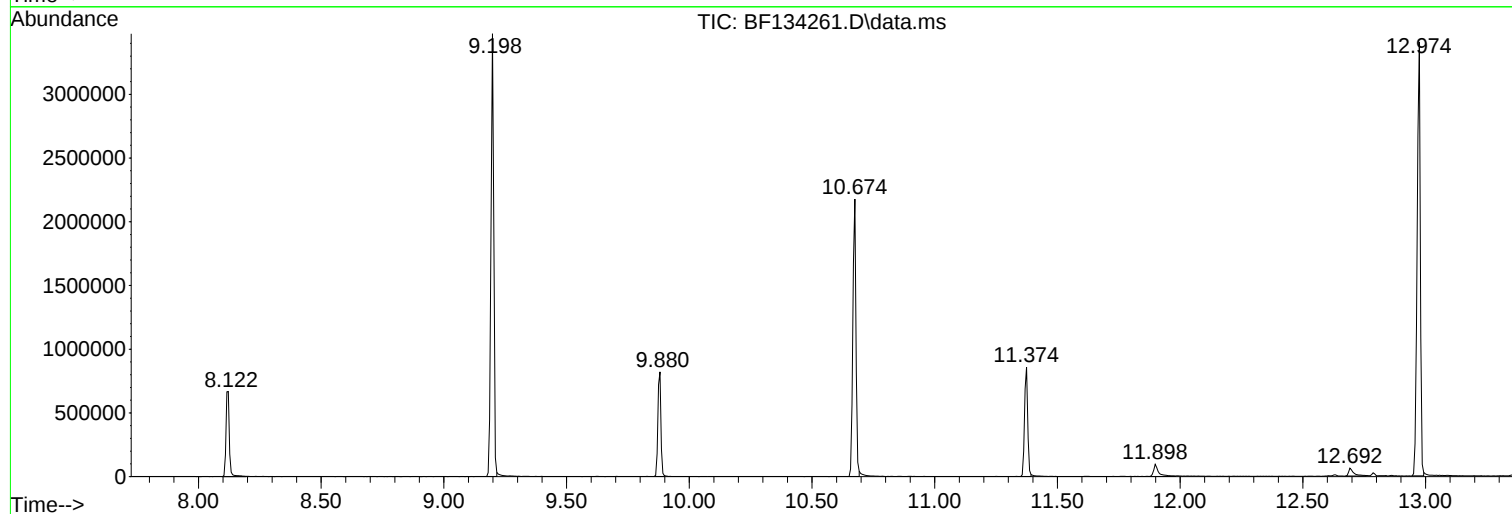
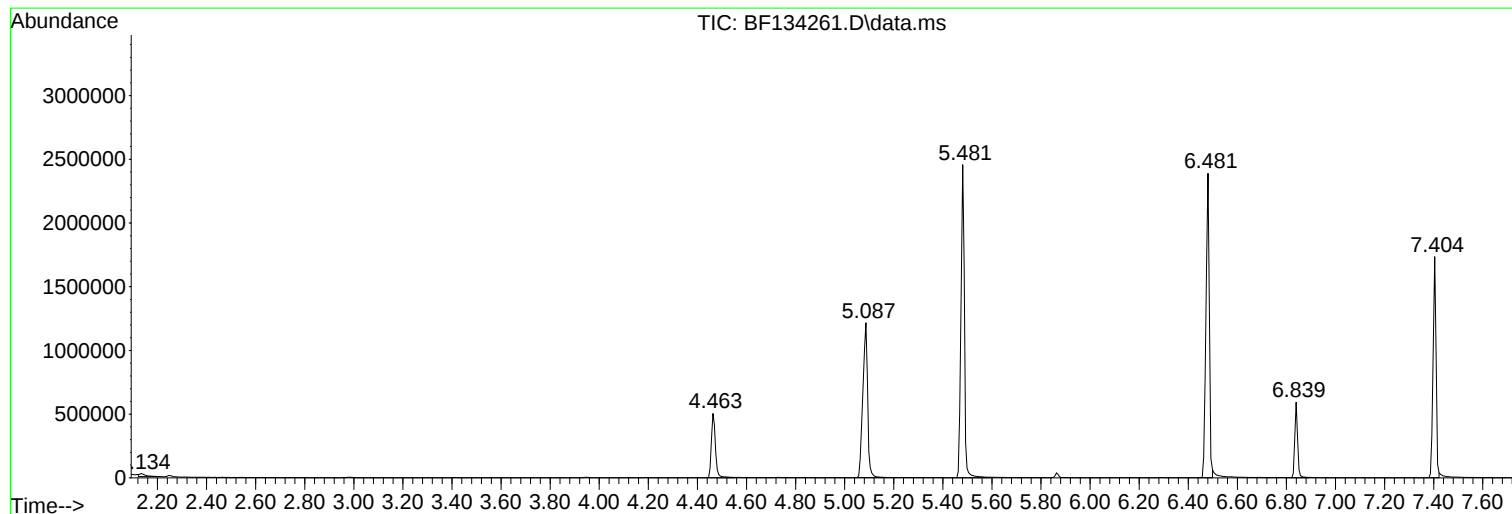
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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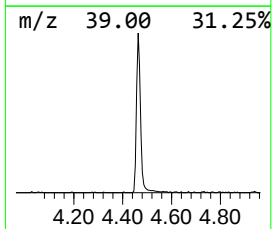
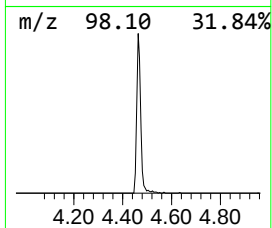
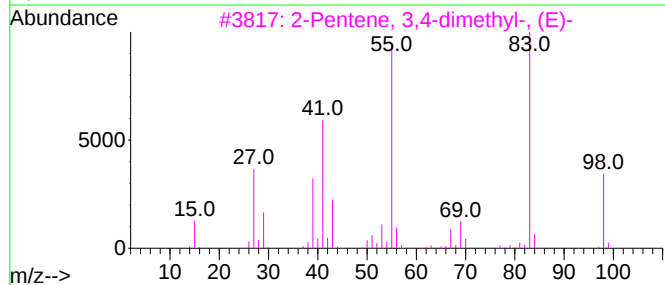
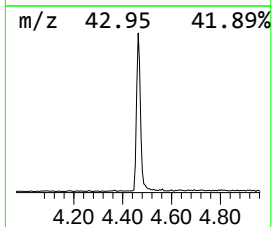
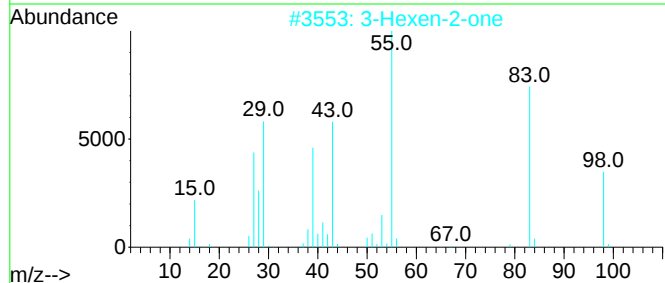
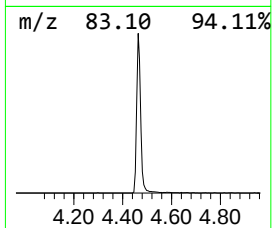
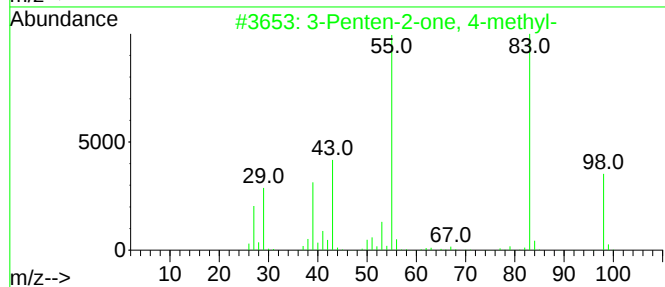
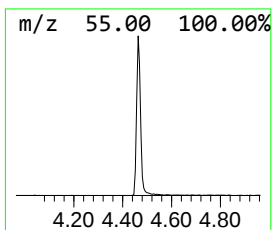
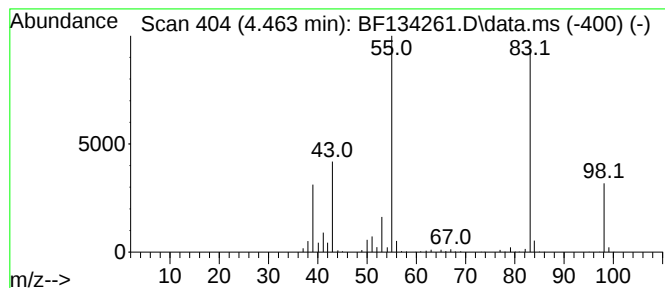
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD			R.T.
4.463	24.52 ng	577716	1,4-Dichlorobenzene-d4			6.839
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-		98	C6H10O	000141-79-7	91
2	3-Hexen-2-one		98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-		98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-		98	C7H14	004914-91-4	86
5	2-Pentene, 4,4-dimethyl-, (E)-		98	C7H14	000690-08-4	86



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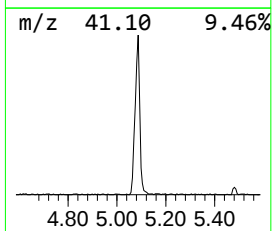
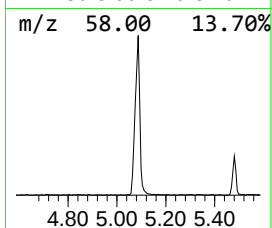
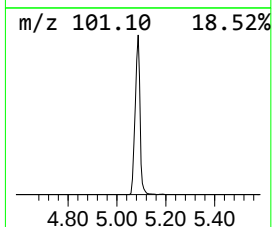
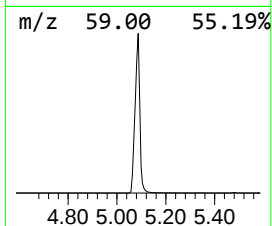
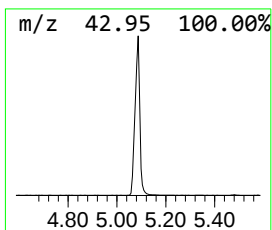
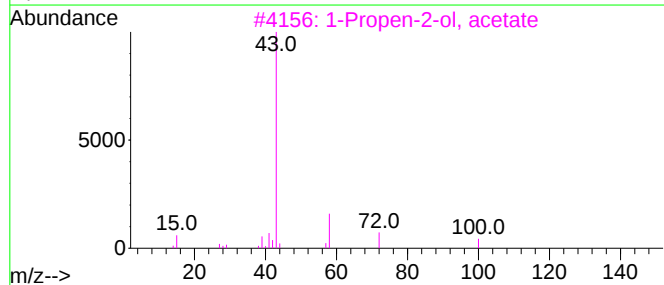
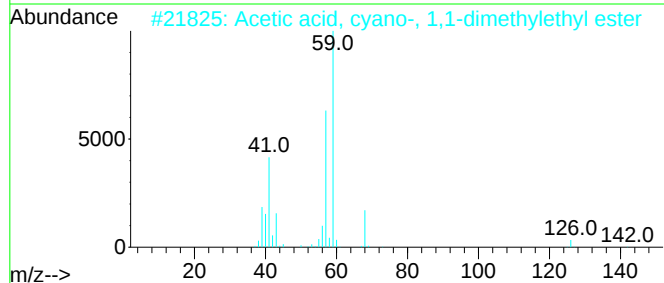
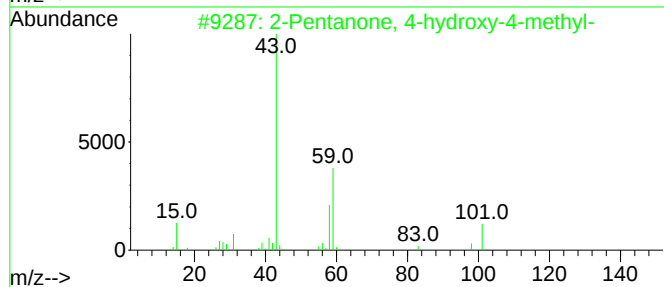
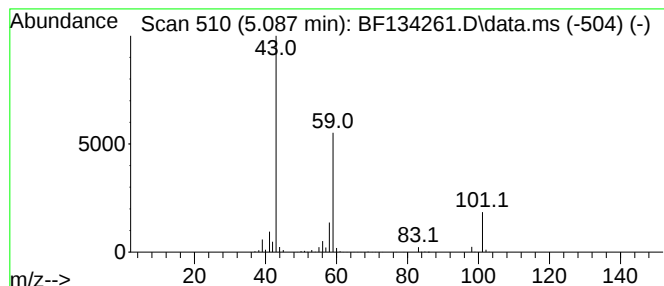
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	69.91 ng	1647140	1,4-Dichlorobenzene-d4	6.839

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	25		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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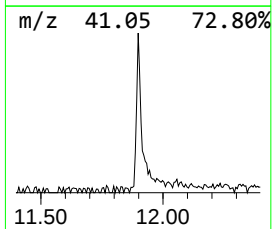
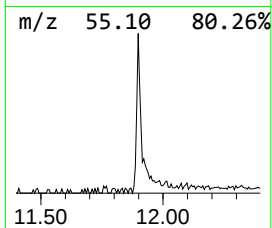
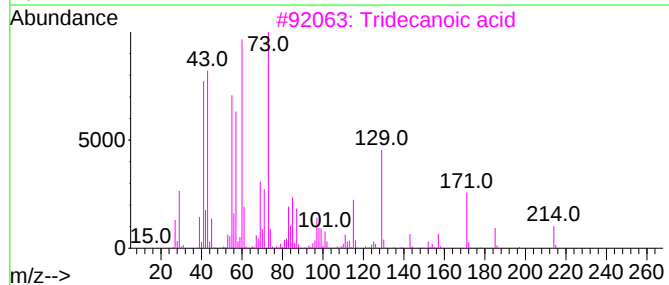
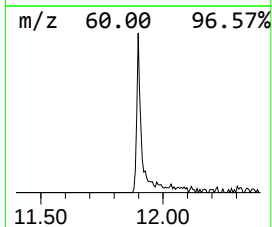
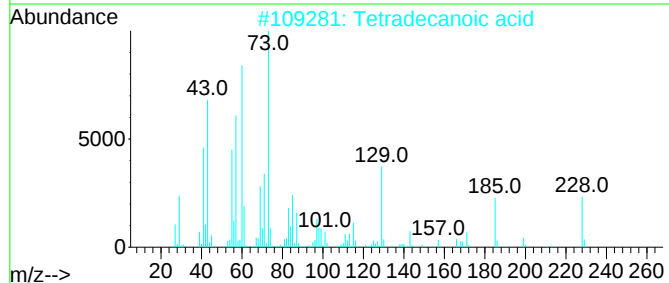
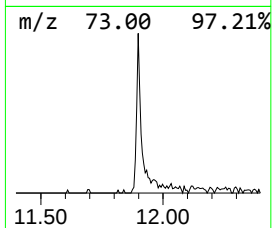
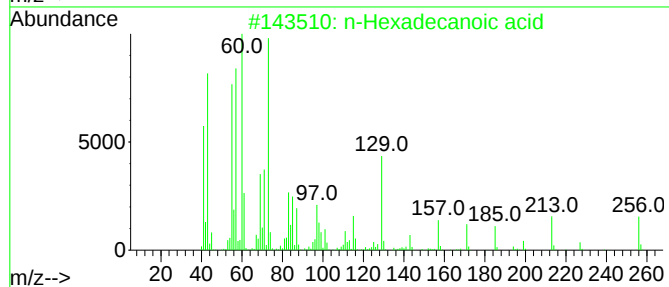
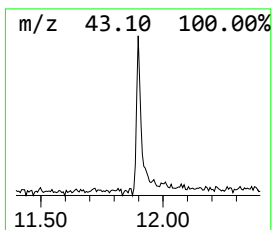
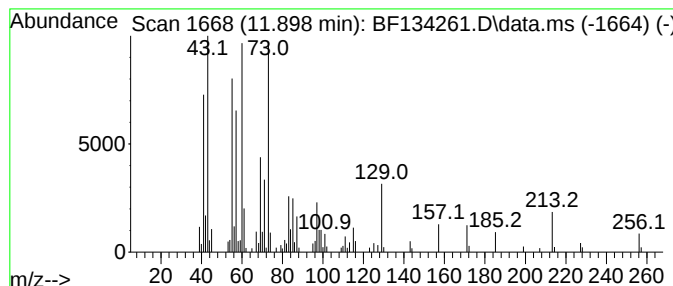
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	3.59 ng	134041	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3			Tridecanoic acid	214	C13H26O2	000638-53-9	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



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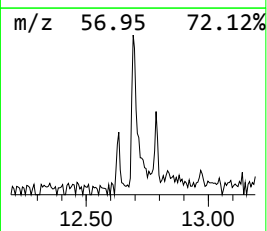
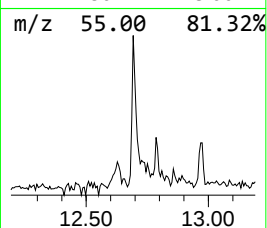
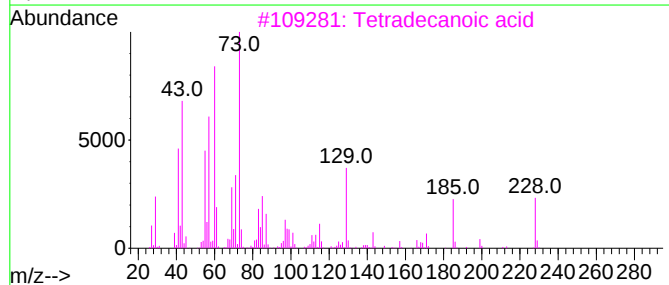
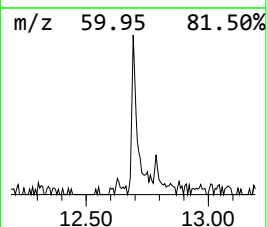
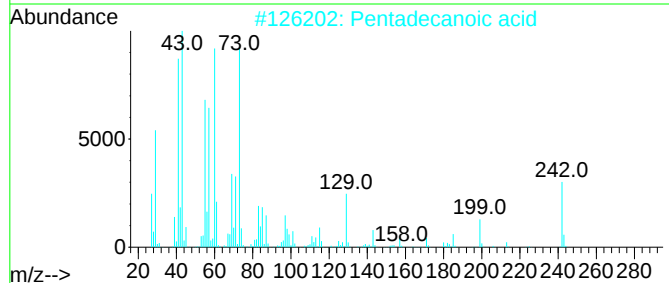
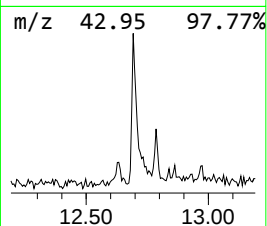
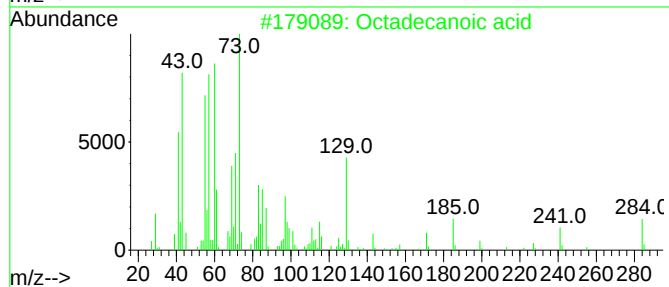
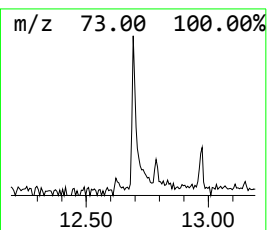
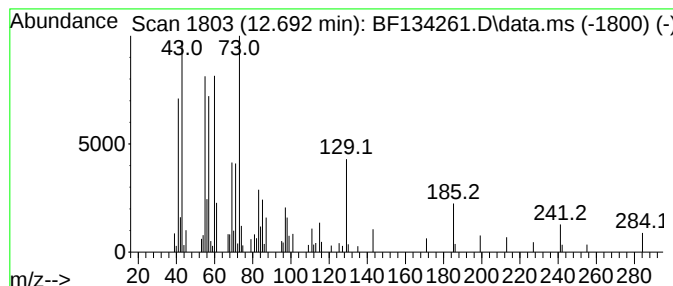
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.692	2.38 ng	88902	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
5			Undecanoic acid	186	C11H22O2	000112-37-8	49



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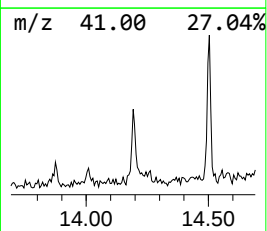
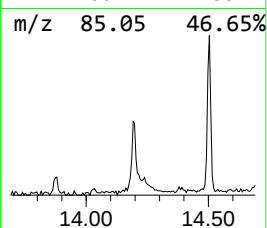
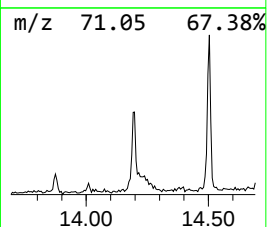
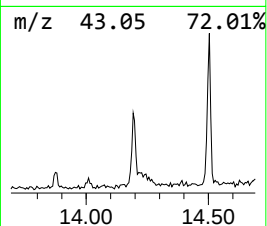
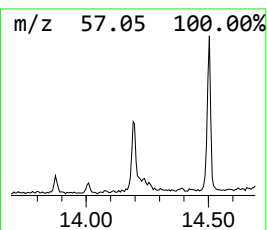
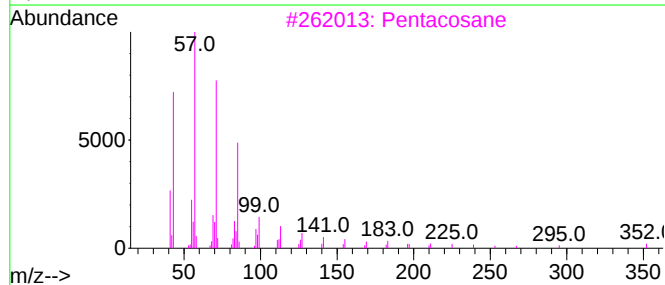
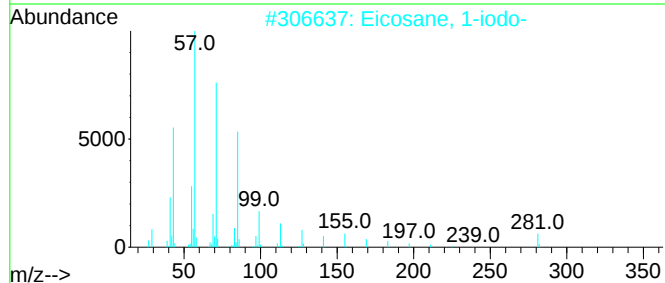
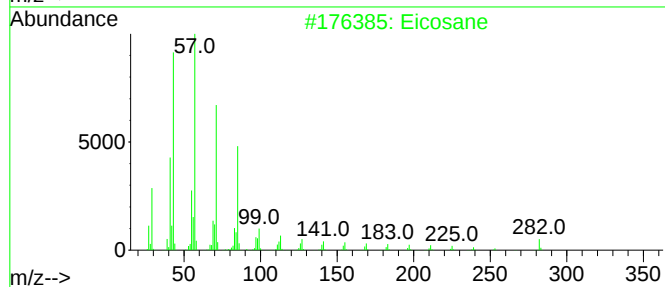
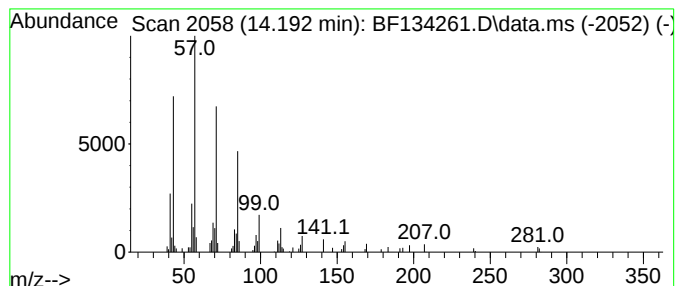
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.192	2.30 ng	75663	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	98
2			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	91
3			Pentacosane	352	C25H52	000629-99-2	90
4			Heneicosane	296	C21H44	000629-94-7	90
5			Octacosane	394	C28H58	000630-02-4	90



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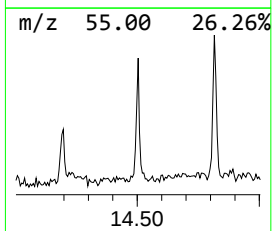
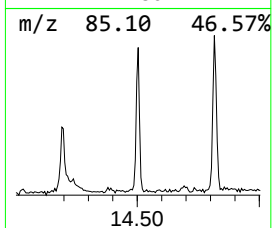
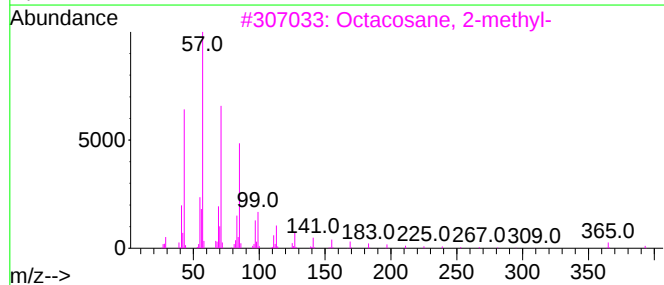
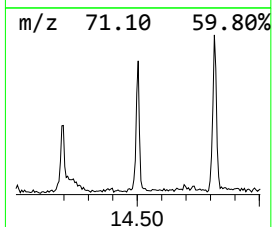
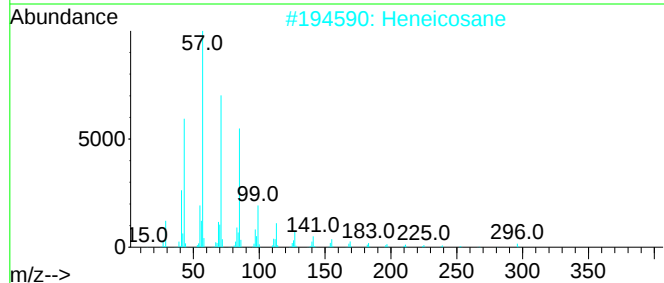
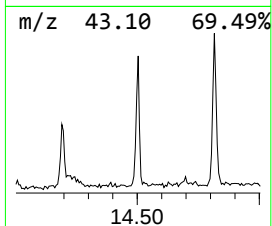
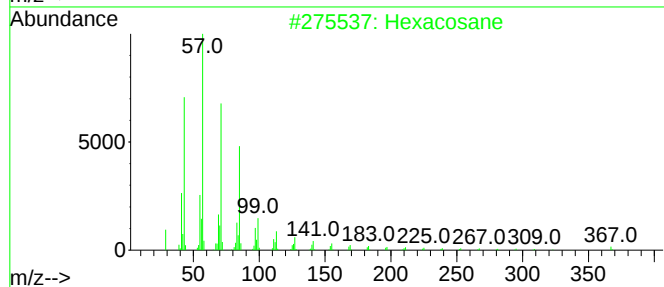
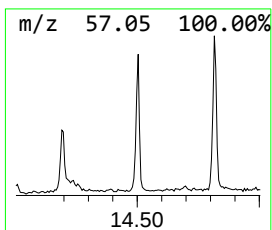
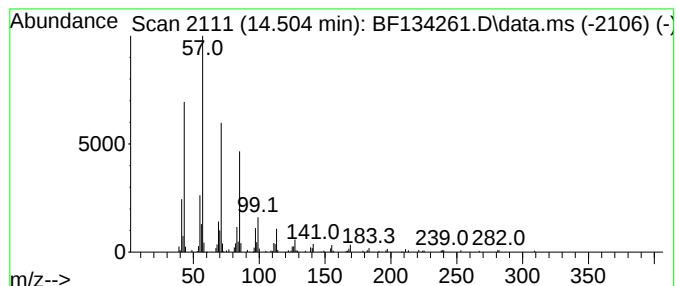
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.504	3.88 ng	127791	Chrysene-d12	14.033

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexacosane	366	C26H54	000630-01-3	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4		Docosane, 11-butyl-	366	C26H54	013475-76-8	91
5		Octacosane	394	C28H58	000630-02-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071323\
Data File : BF134261.D
Acq On : 13 Jul 2023 14:35
Operator : CG\JU
Sample : PB153430BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB153430BL

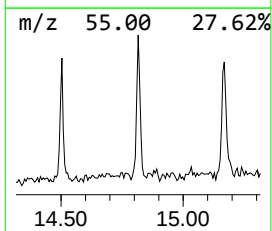
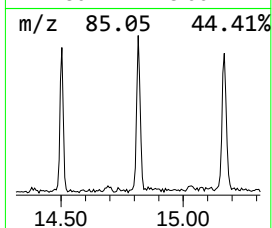
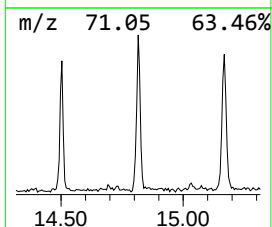
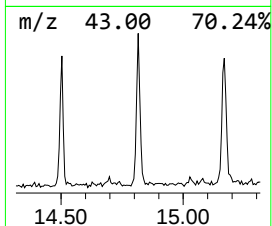
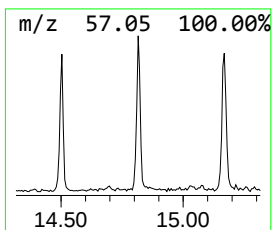
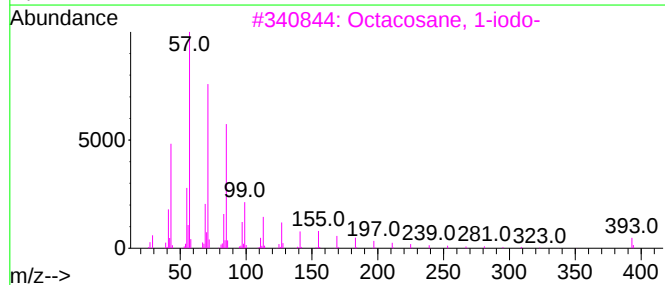
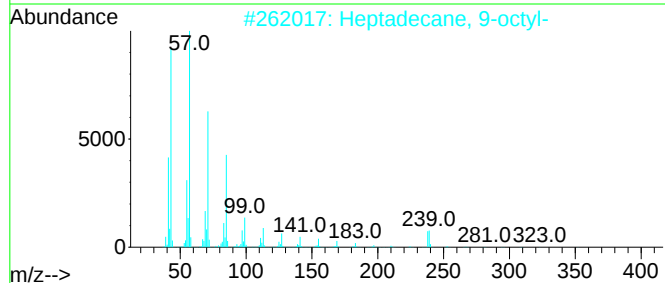
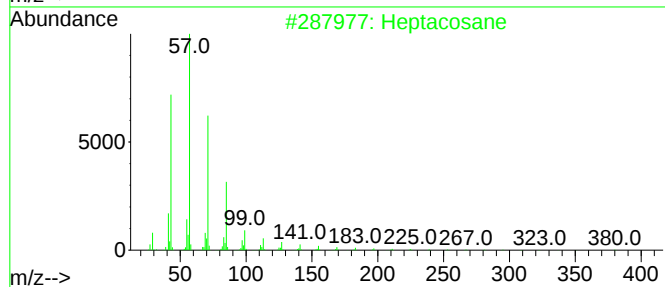
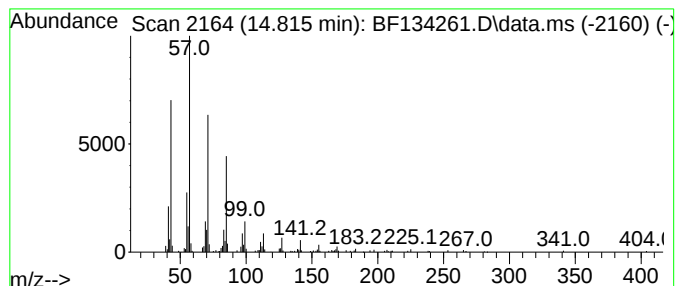
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.815	4.18 ng	153739	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	91
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3			Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	91
4			Hentriacontane	437	C31H64	000630-04-6	91
5			Eicosane, 9-octyl-	394	C28H58	013475-77-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071323\
Data File : BF134261.D
Acq On : 13 Jul 2023 14:35
Operator : CG\JU
Sample : PB153430BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

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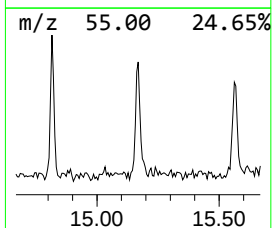
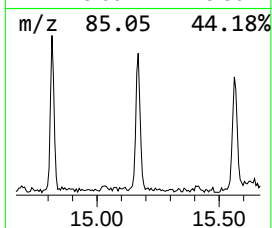
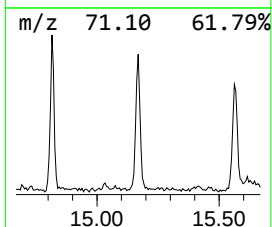
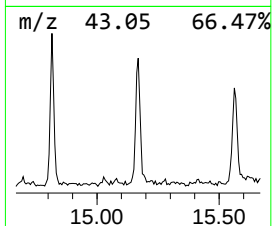
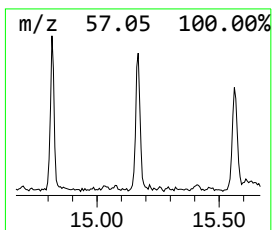
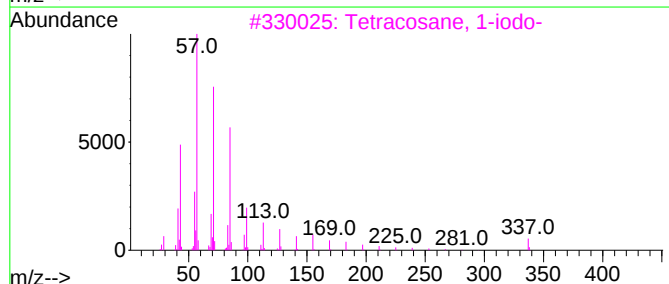
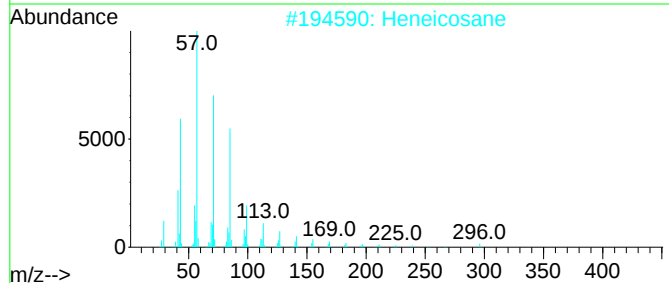
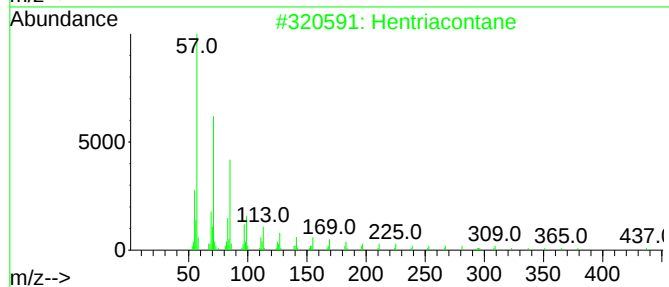
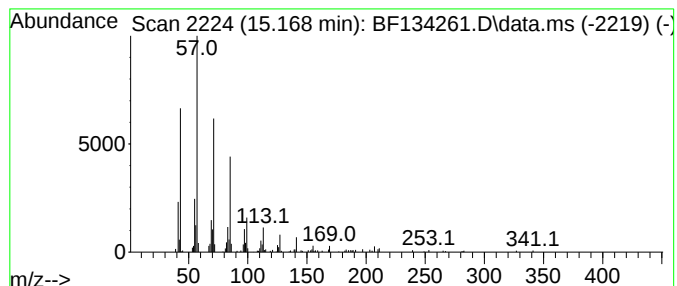
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hentriacontane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.168	4.98 ng	183204	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	91
4			Octacosane	394	C28H58	000630-02-4	91
5			Tetracosane	338	C24H50	000646-31-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071323\
Data File : BF134261.D
Acq On : 13 Jul 2023 14:35
Operator : CG\JU
Sample : PB153430BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

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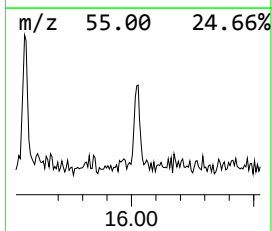
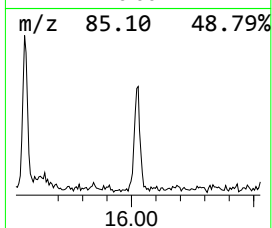
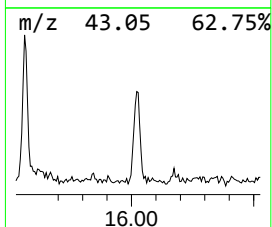
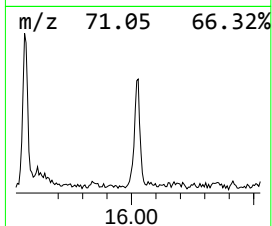
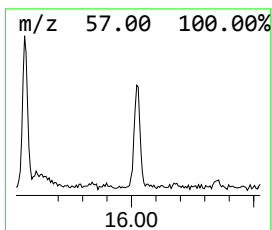
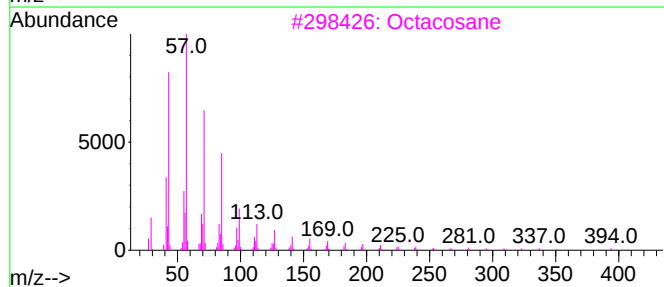
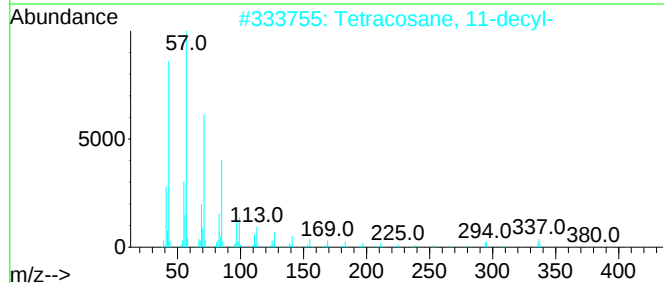
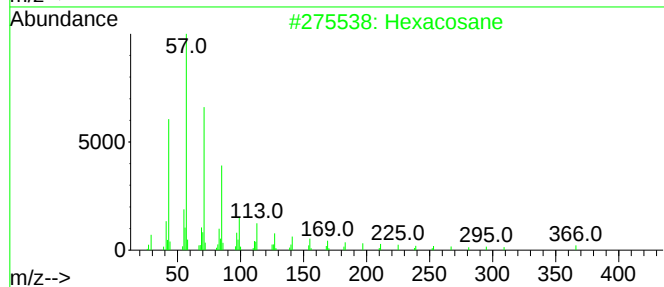
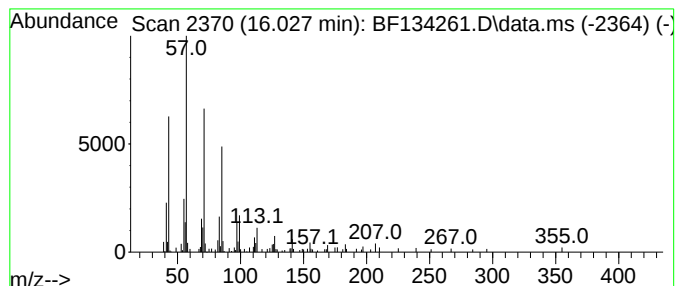
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetracosane, 11-decyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.027	3.30 ng	121274	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Tetracosane, 11-decyl-	479	C34H70	055429-84-0	91
3			Octacosane	394	C28H58	000630-02-4	90
4			Heneicosane	296	C21H44	000629-94-7	90
5			Tetracosane	338	C24H50	000646-31-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071323\
Data File : BF134261.D
Acq On : 13 Jul 2023 14:35
Operator : CG\JU
Sample : PB153430BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

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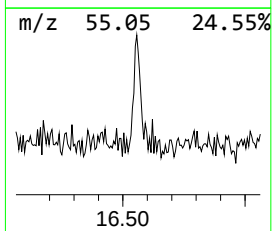
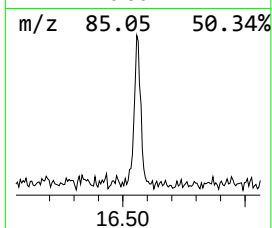
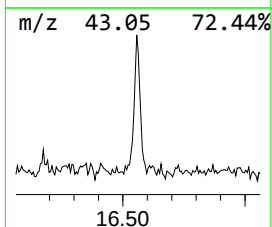
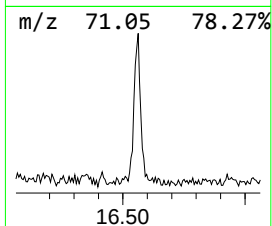
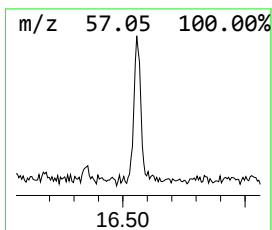
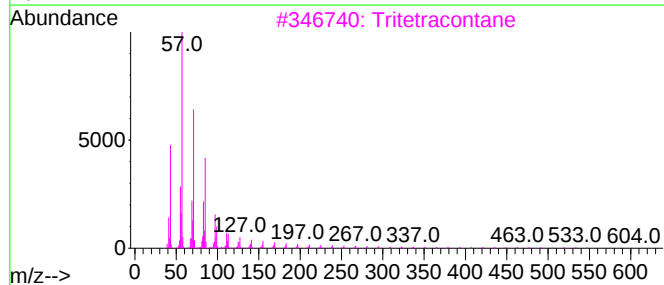
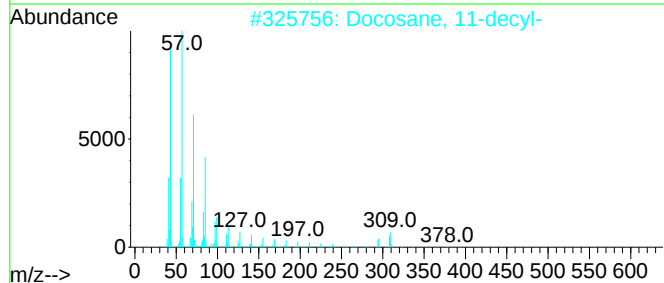
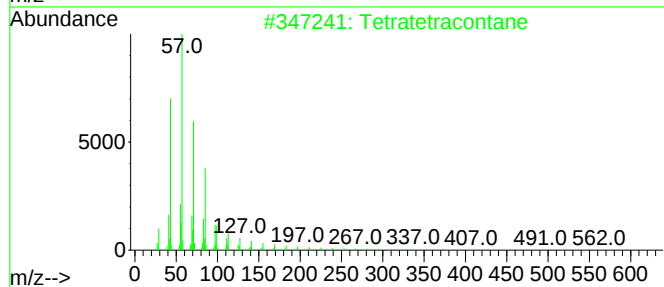
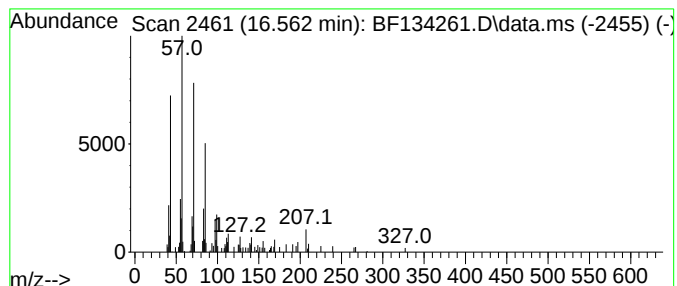
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tetratetracontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.562	2.63 ng	96959	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	90
2			Docosane, 11-decyl-	451	C32H66	055401-55-3	87
3			Tritetracontane	605	C43H88	007098-21-7	87
4			Hexacosane	366	C26H54	000630-01-3	87
5			Heptacosane	380	C27H56	000593-49-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071323\
Data File : BF134261.D
Acq On : 13 Jul 2023 14:35
Operator : CG\JU
Sample : PB153430BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB153430BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-...	5.087	69.9	ng	1647140	1	6.839	471199	20.0
n-Hexadecanoic ...	11.898	3.6	ng	134041	4	11.374	746298	20.0
Octadecanoic acid	12.692	2.4	ng	88902	4	11.374	746298	20.0
Eicosane	14.192	2.3	ng	75663	5	14.033	658536	20.0
Hexacosane	14.504	3.9	ng	127791	5	14.033	658536	20.0
Heptacosane	14.815	4.2	ng	153739	6	15.539	736075	20.0
Hentriacontane	15.168	5.0	ng	183204	6	15.539	736075	20.0
Tetracosane, 11...	16.027	3.3	ng	121274	6	15.539	736075	20.0
Tetratetracontane	16.562	2.6	ng	96959	6	15.539	736075	20.0