

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122123\
 Data File : BF136661.D
 Acq On : 21 Dec 2023 09:59
 Operator : CG\JU
 Sample : PB157501BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB157501BL

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-BF122023.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136661.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.457	393	403	406	rBV	2779037	4725230	100.00%	15.657%
2	4.699	439	444	448	rVB	49245	51019	1.08%	0.169%
3	5.063	496	506	509	rBV	1785466	3276816	69.35%	10.858%
4	5.451	566	572	575	rBV	2652129	2758752	58.38%	9.141%
5	5.822	631	635	638	rBV	321286	279555	5.92%	0.926%
6	6.440	732	740	743	rBV	2345701	2966225	62.77%	9.829%
7	6.787	796	799	803	rBV	660632	559527	11.84%	1.854%
8	7.357	889	896	898	rBV	1563162	1832860	38.79%	6.073%
9	8.063	1011	1016	1020	rBV	799147	782107	16.55%	2.592%
10	9.145	1193	1200	1203	rBV	3267061	3479389	73.63%	11.529%
11	9.822	1309	1315	1318	rBV	1119348	911060	19.28%	3.019%
12	10.616	1445	1450	1454	rBV	1910083	2125955	44.99%	7.044%
13	11.310	1564	1568	1572	rBV	1073132	1018563	21.56%	3.375%
14	12.916	1835	1841	1844	rBV	3417795	3662512	77.51%	12.136%
15	13.963	2014	2019	2023	rBV	804945	742621	15.72%	2.461%
16	15.092	2207	2211	2217	rVB	54415	61448	1.30%	0.204%
17	15.439	2265	2270	2274	rBV	433881	545158	11.54%	1.806%
18	15.480	2274	2277	2282	rVB	64940	86951	1.84%	0.288%
19	15.933	2348	2354	2360	rVB	56445	84488	1.79%	0.280%
20	16.451	2436	2442	2449	rBV2	47372	89695	1.90%	0.297%
21	17.074	2540	2548	2557	rVB	32362	69912	1.48%	0.232%
22	17.798	2663	2671	2682	rBV3	25372	69434	1.47%	0.230%

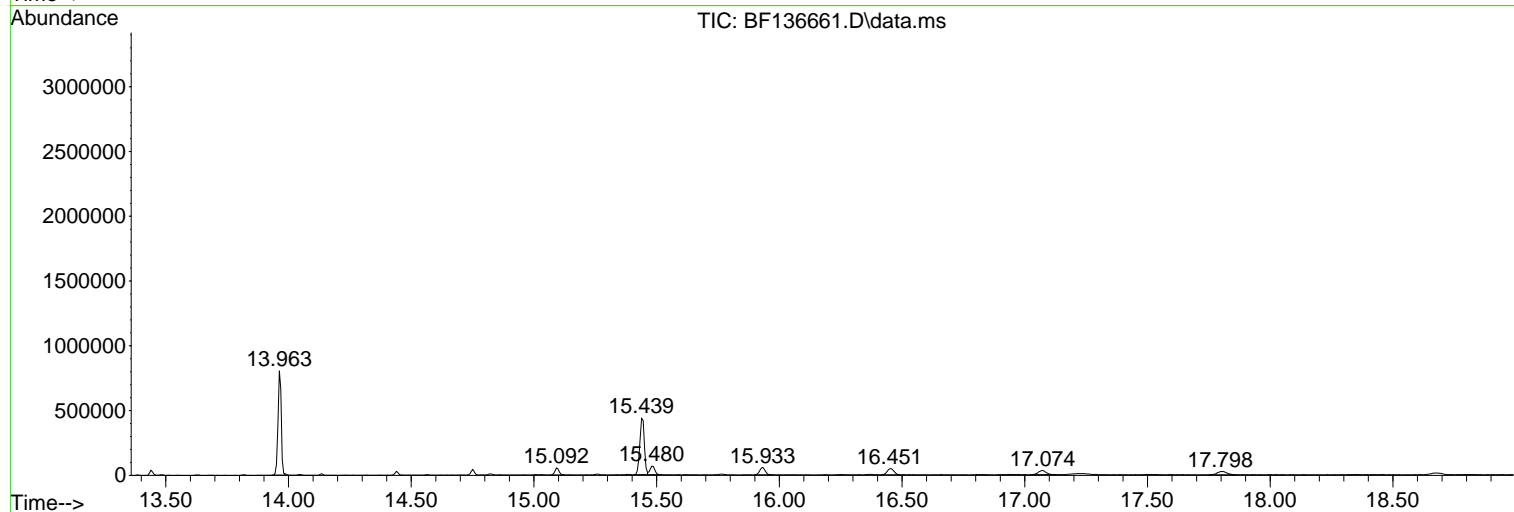
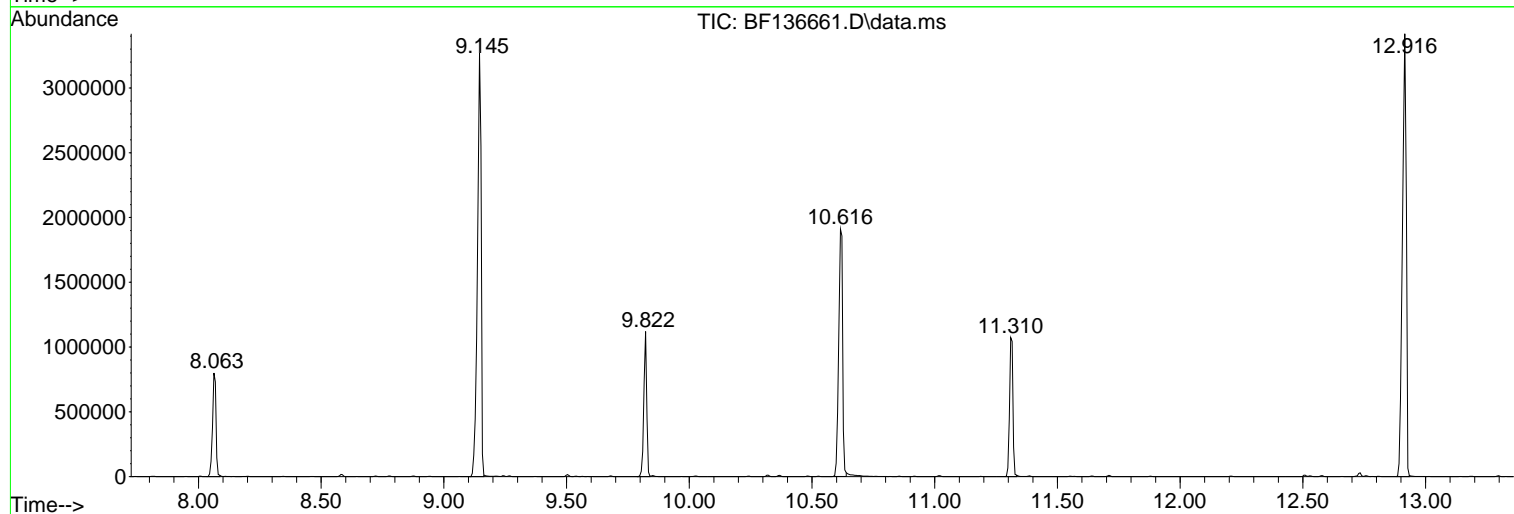
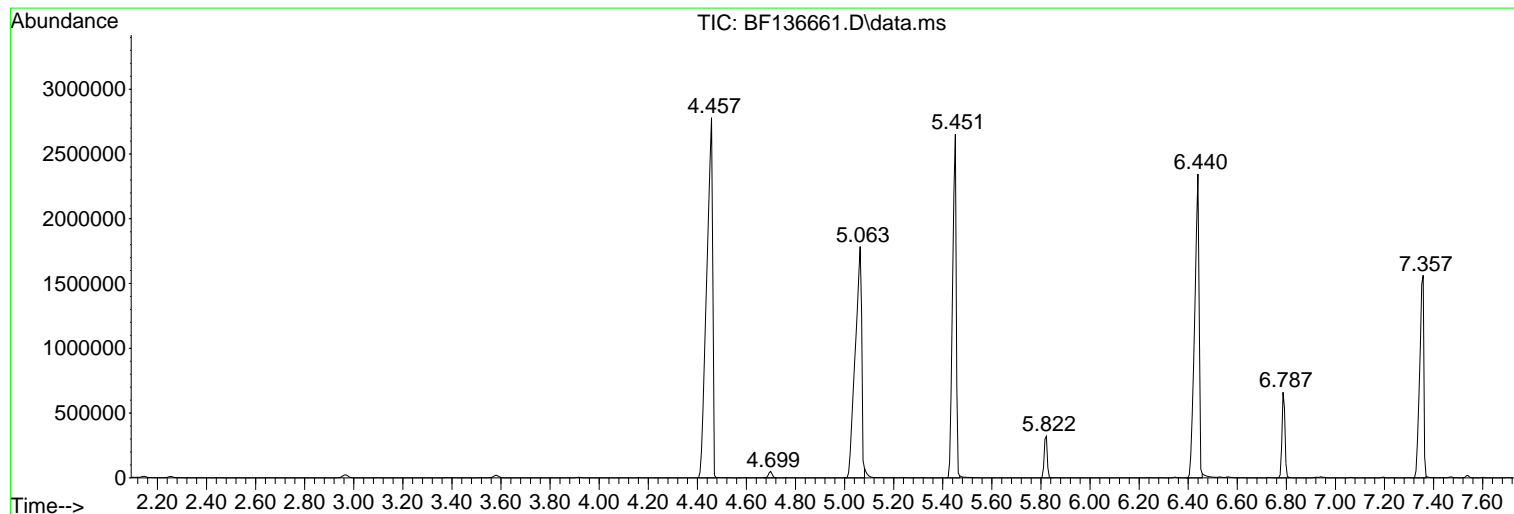
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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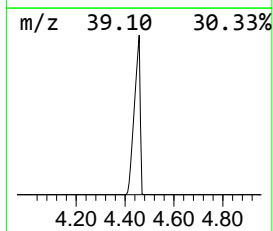
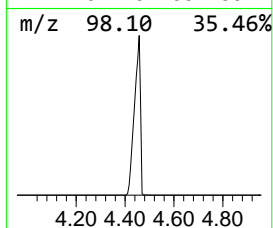
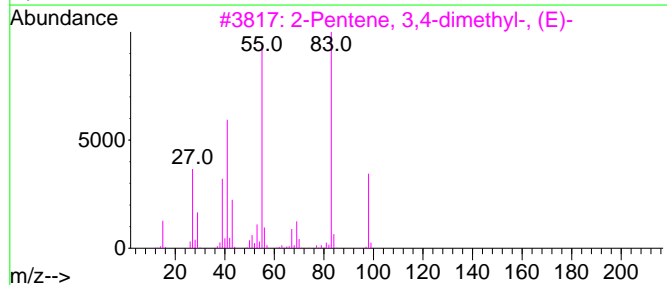
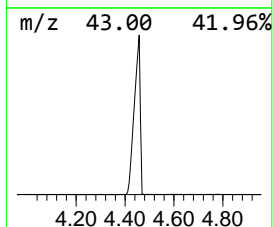
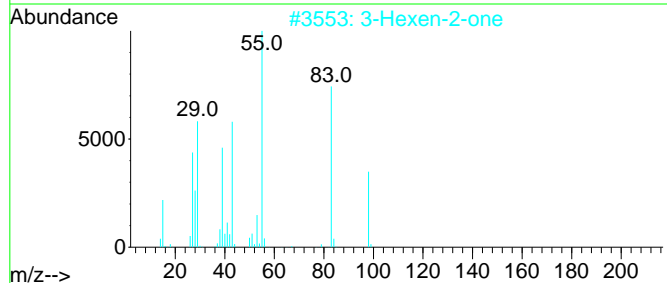
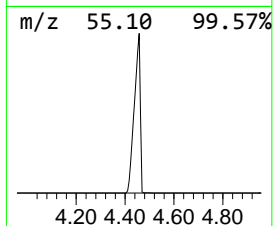
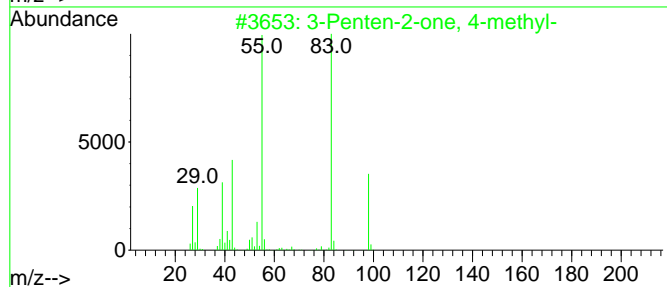
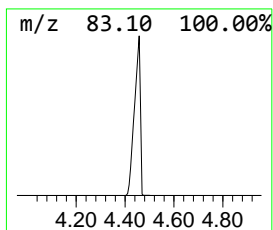
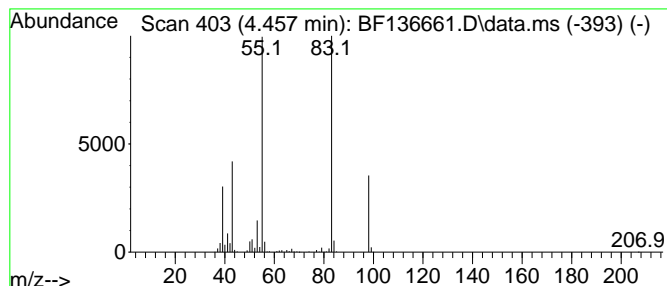
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.457	168.90 ng	4725230	1,4-Dichlorobenzene-d4	6.787

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
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, 2,4-dimethyl-	98	C7H14	000625-65-0	86



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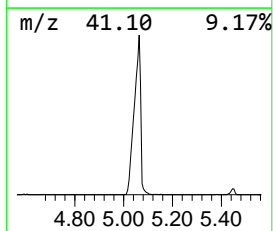
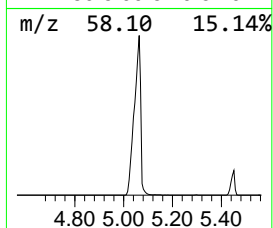
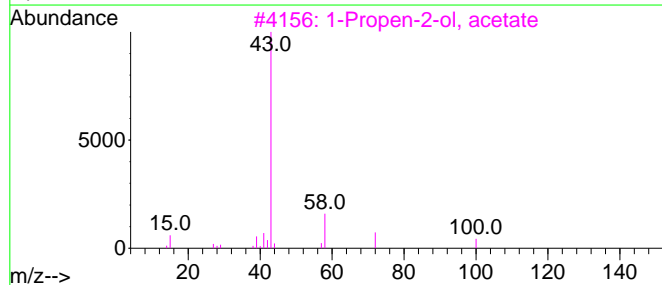
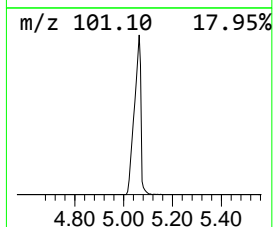
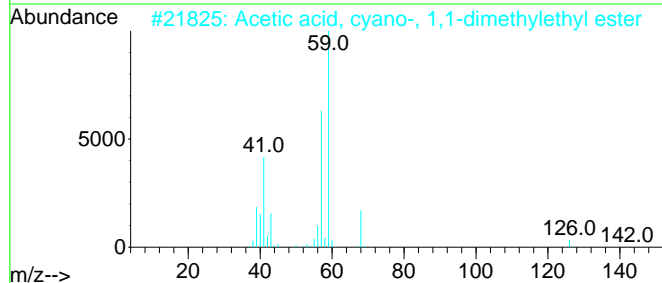
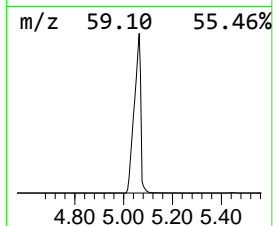
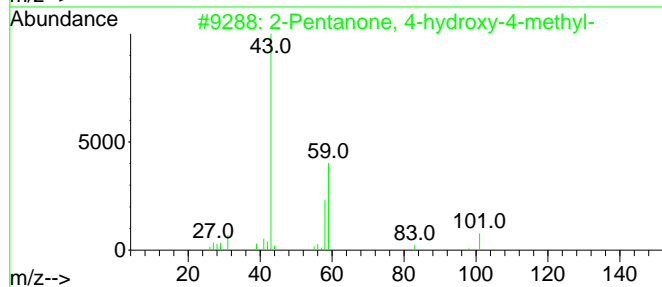
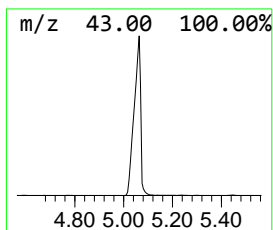
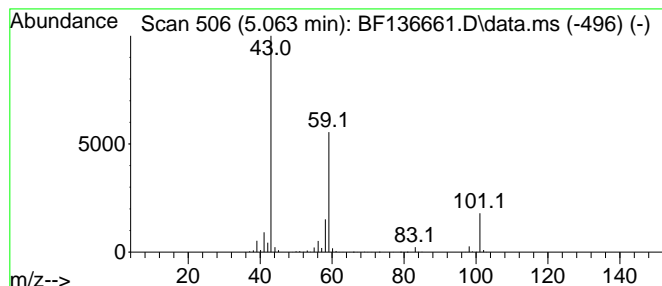
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	117.13 ng	3276820	1,4-Dichlorobenzene-d4	6.787

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9



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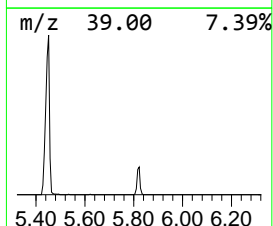
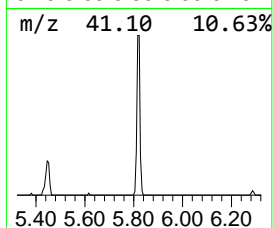
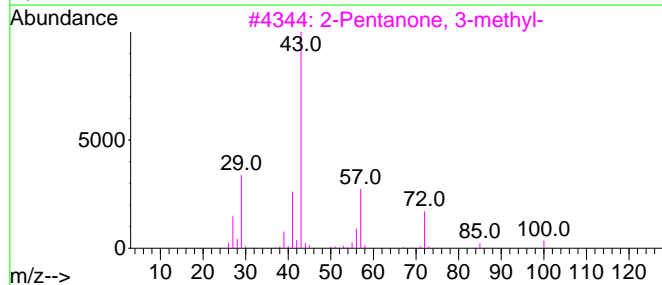
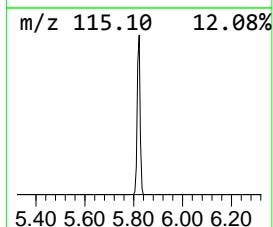
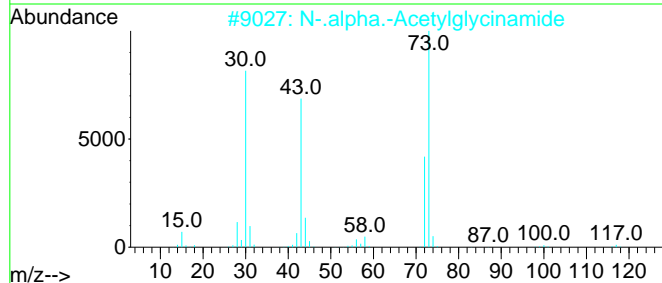
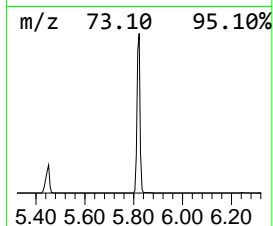
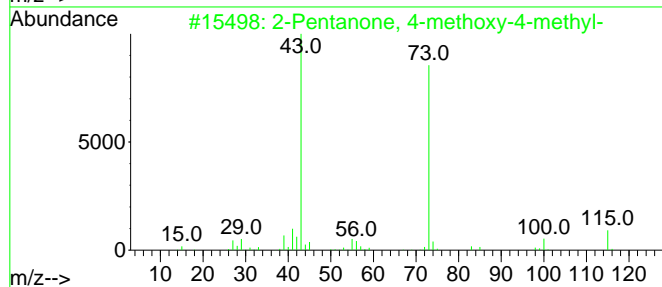
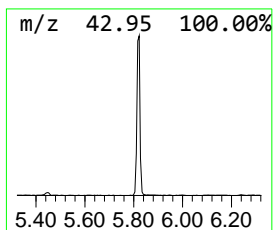
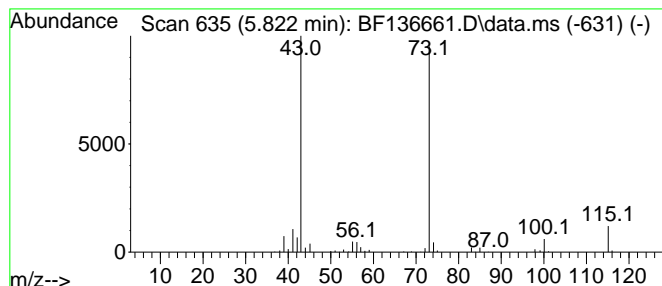
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TIC Library : C:\Database\NIST20.L
 TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.822	9.99 ng	279555	1,4-Dichlorobenzene-d4	6.787

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	38
3		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	22
4		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10
5		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9



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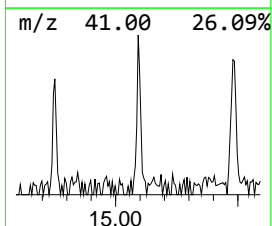
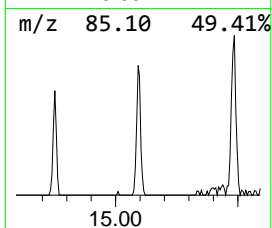
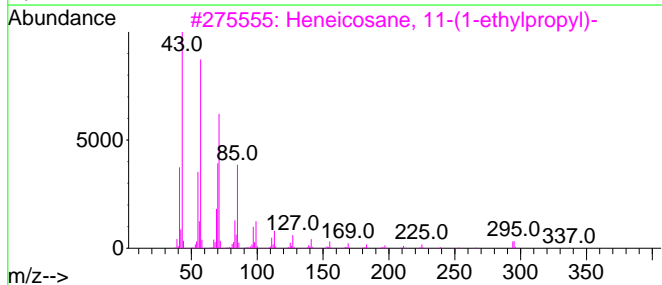
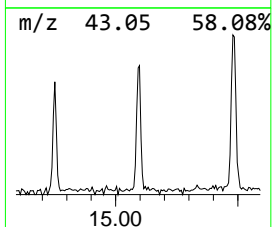
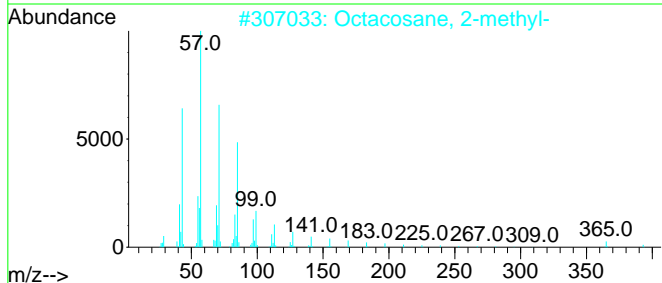
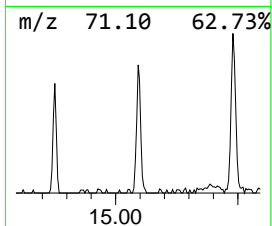
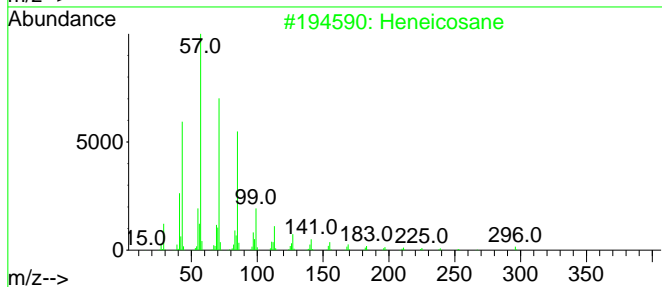
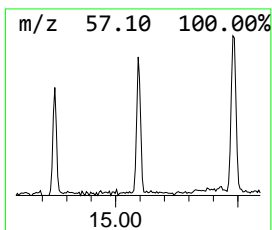
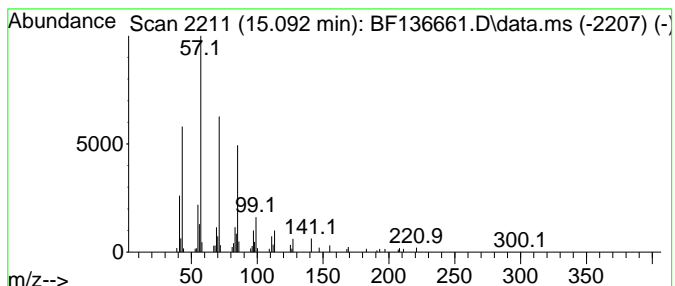
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 Peak Number 4 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.092	2.25 ng	61448	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
4			Pentacosane	352	C25H52	000629-99-2	91
5			Docosane	310	C22H46	000629-97-0	90



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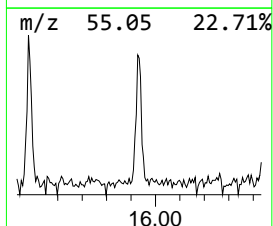
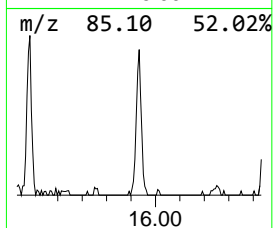
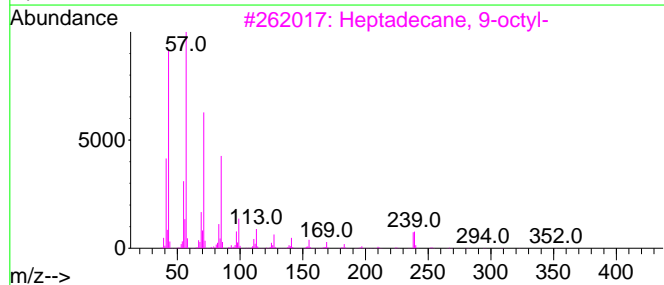
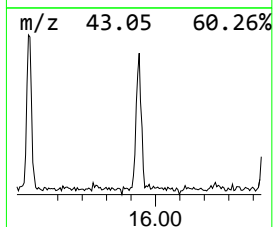
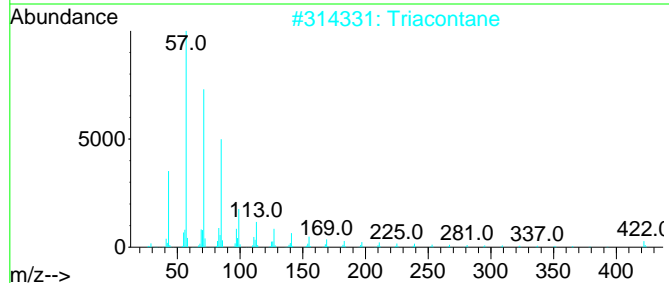
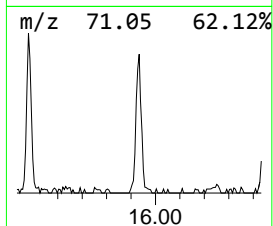
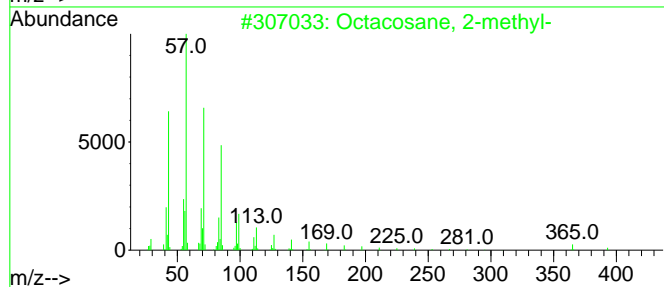
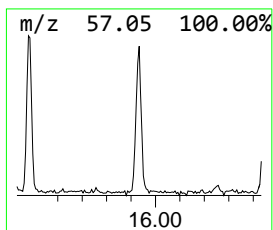
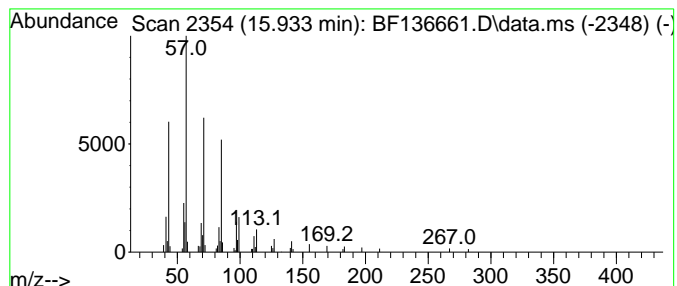
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TIC Library : C:\Database\NIST20.L
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 Peak Number 5 Octacosane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.933	3.10 ng	84488	Perylene-d12	15.445

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2		Triacotane	422	C30H62	000638-68-6	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Docosane	310	C22H46	000629-97-0	91
5		Heptacosane	380	C27H56	000593-49-7	87



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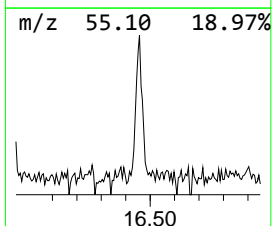
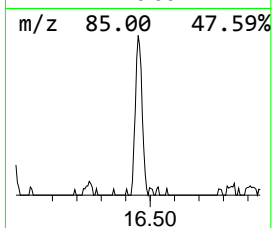
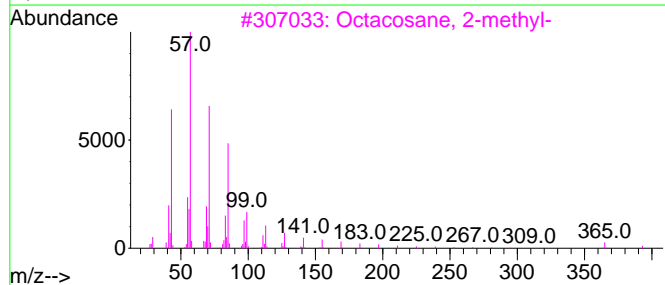
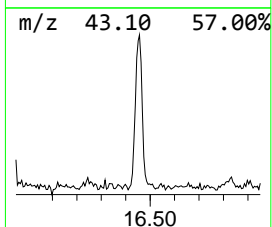
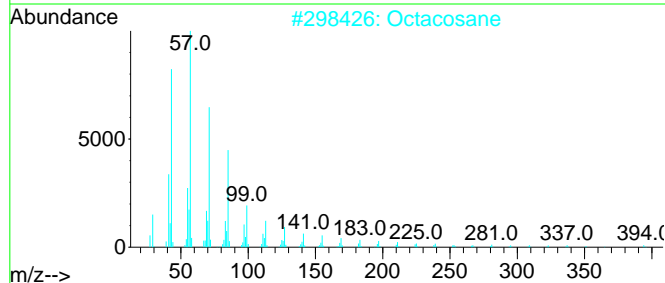
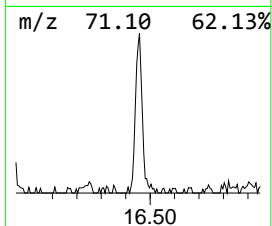
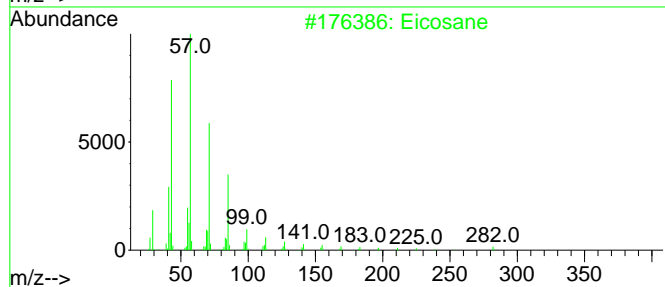
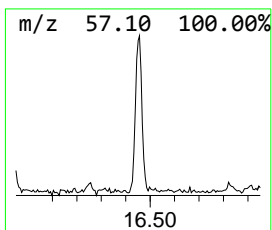
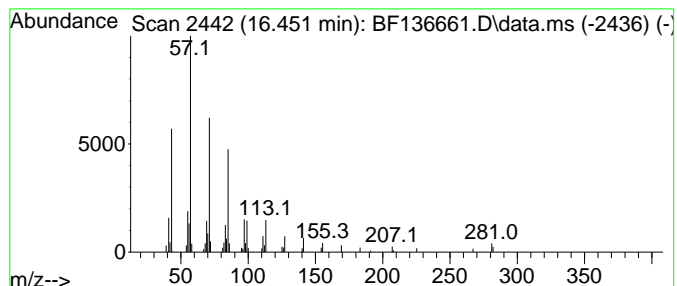
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 6 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.451	3.29 ng	89695	Perylene-d12	15.445

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Eicosane	282	C20H42	000112-95-8	91
2		Octacosane	394	C28H58	000630-02-4	91
3		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5		Triacontane	422	C30H62	000638-68-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122123\
 Data File : BF136661.D
 Acq On : 21 Dec 2023 09:59
 Operator : CG\JU
 Sample : PB157501BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB157501BL

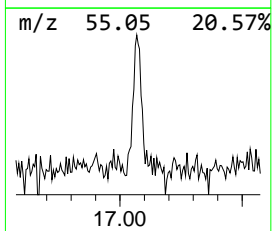
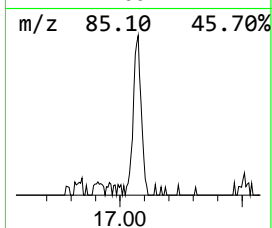
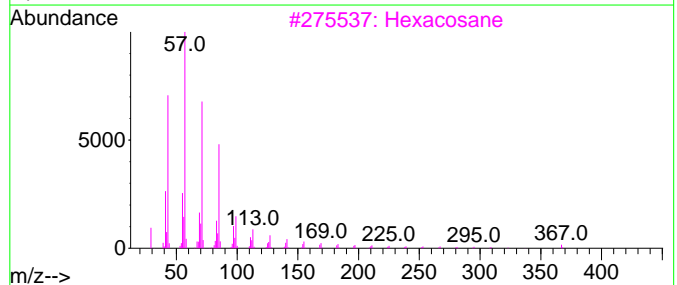
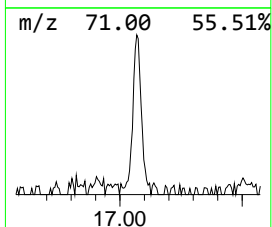
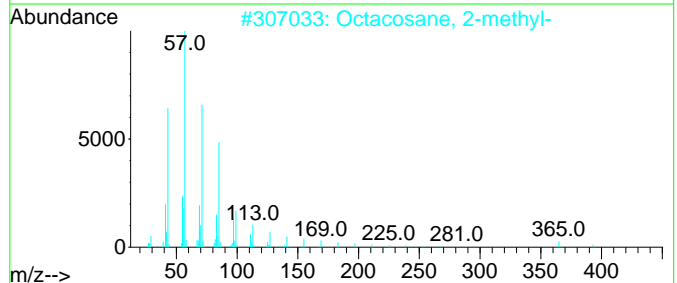
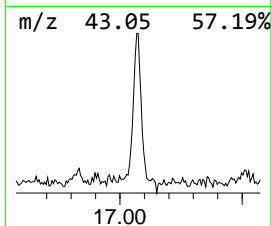
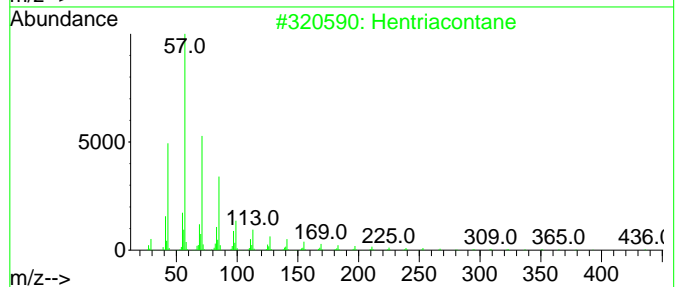
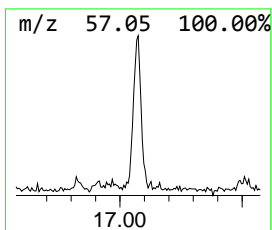
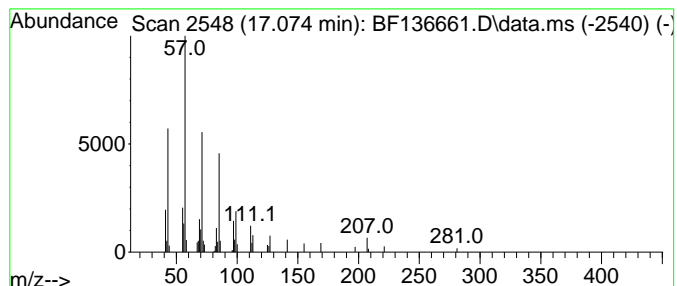
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 7 Hentriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.074	2.56 ng	69912	Perylene-d12	15.445

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hentriacontane	437	C31H64	000630-04-6	86
2		Octacosane, 2-methyl-	408	C29H60	001560-98-1	86
3		Hexacosane	366	C26H54	000630-01-3	83
4		Octacosane	394	C28H58	000630-02-4	83
5		Triacosane	422	C30H62	000638-68-6	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122123\
 Data File : BF136661.D
 Acq On : 21 Dec 2023 09:59
 Operator : CG\JU
 Sample : PB157501BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB157501BL

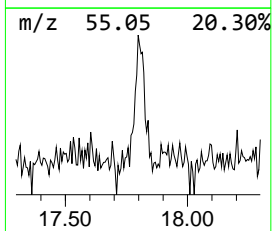
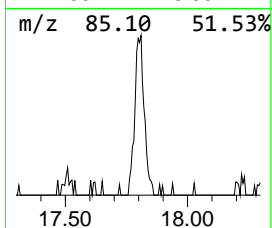
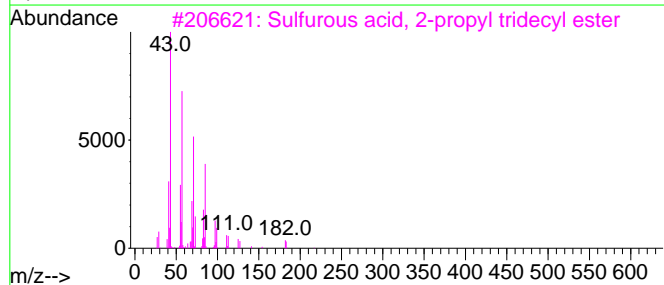
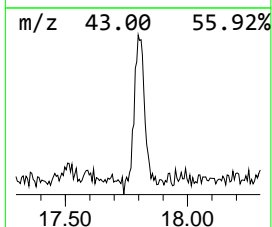
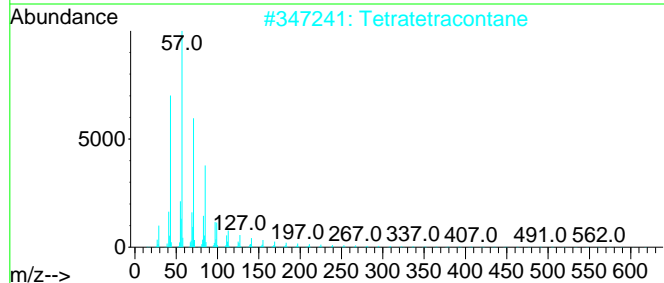
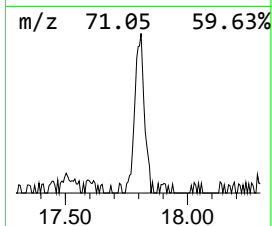
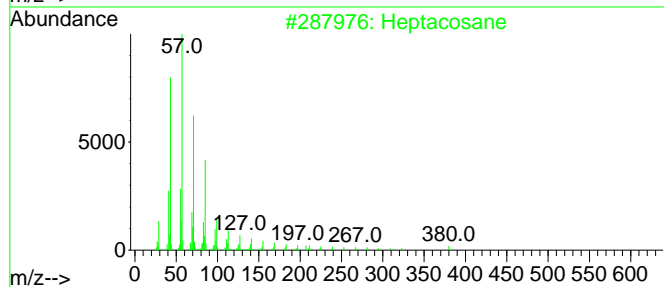
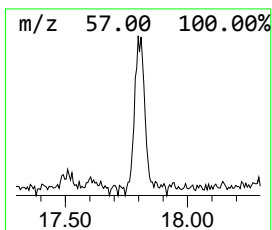
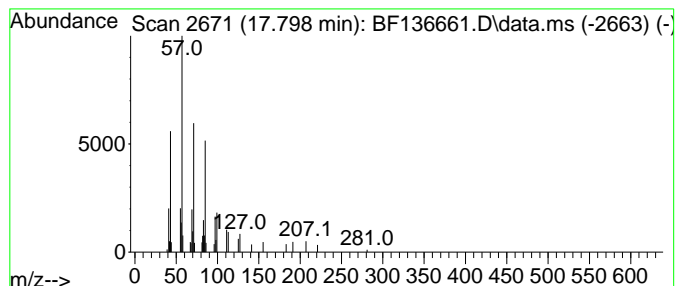
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 8 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.798	2.55 ng	69434	Perylene-d12	15.445

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	87
2		Tetratetracontane	619	C44H90	007098-22-8	87
3		Sulfurous acid, 2-propyl tridecyl...	306	C16H34O3S	1000309-12-4	86
4		Octacosane, 2-methyl-	408	C29H60	001560-98-1	86
5		Hentriacontane	437	C31H64	000630-04-6	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122123\
 Data File : BF136661.D
 Acq On : 21 Dec 2023 09:59
 Operator : CG\JU
 Sample : PB157501BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB157501BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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
3-Penten-2-one,...	4.457	168.9	ng	4725230	1	6.787	559527	20.0
2-Pentanone, 4-...	5.063	117.1	ng	3276820	1	6.787	559527	20.0
2-Pentanone, 4-...	5.822	10.0	ng	279555	1	6.787	559527	20.0
Heneicosane	15.092	2.3	ng	61448	6	15.445	545158	20.0
Octacosane, 2-m...	15.933	3.1	ng	84488	6	15.445	545158	20.0
Eicosane	16.451	3.3	ng	89695	6	15.445	545158	20.0
Hentriacontane	17.074	2.6	ng	69912	6	15.445	545158	20.0
Heptacosane	17.798	2.5	ng	69434	6	15.445	545158	20.0