

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052623\
 Data File : BF133501.D
 Acq On : 26 May 2023 13:37
 Operator : CG\JU
 Sample : PB153070BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB153070BL

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-BF052523.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133501.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	3	9	14	rVB	82709	104782	2.15%	0.317%
2	4.434	395	399	405	rVB	282854	319334	6.54%	0.967%
3	5.057	500	505	516	rBV	845851	1202715	24.64%	3.641%
4	5.457	567	573	576	rBV	3519551	3822910	78.33%	11.572%
5	5.851	637	640	644	rBV	85472	70133	1.44%	0.212%
6	6.463	738	744	747	rBV	3258768	3910069	80.11%	11.835%
7	6.839	804	808	811	rBV	1004264	868838	17.80%	2.630%
8	7.404	898	904	907	rBV	2670583	2534186	51.92%	7.671%
9	8.122	1022	1026	1029	rBV	1448244	1140391	23.37%	3.452%
10	9.198	1204	1209	1213	rBV	4319176	4345129	89.03%	13.152%
11	9.874	1320	1324	1328	rBV	1555489	1263234	25.88%	3.824%
12	10.663	1454	1458	1462	rBV	2736989	2872576	58.86%	8.695%
13	11.363	1573	1577	1580	rBV	1687776	1381950	28.31%	4.183%
14	12.957	1843	1848	1851	rBV	4523584	4880733	100.00%	14.774%
15	14.004	2022	2026	2030	rBV	1394916	1276327	26.15%	3.863%
16	14.792	2156	2160	2165	rBV	118976	112921	2.31%	0.342%
17	15.133	2211	2218	2222	rBV	165287	179922	3.69%	0.545%
18	15.468	2269	2275	2279	rBV	1064369	1301779	26.67%	3.940%
19	15.515	2279	2283	2294	rVB	207473	267201	5.47%	0.809%
20	15.951	2352	2357	2366	rVB	158454	244643	5.01%	0.741%
21	16.462	2437	2444	2455	rBV	140151	242454	4.97%	0.734%
22	16.974	2513	2531	2541	rBV5	68968	386312	7.92%	1.169%
23	17.062	2541	2546	2555	rVB	77189	159146	3.26%	0.482%
24	17.774	2660	2667	2676	rVB4	38087	96526	1.98%	0.292%
25	18.609	2803	2809	2819	rVB6	19475	52584	1.08%	0.159%

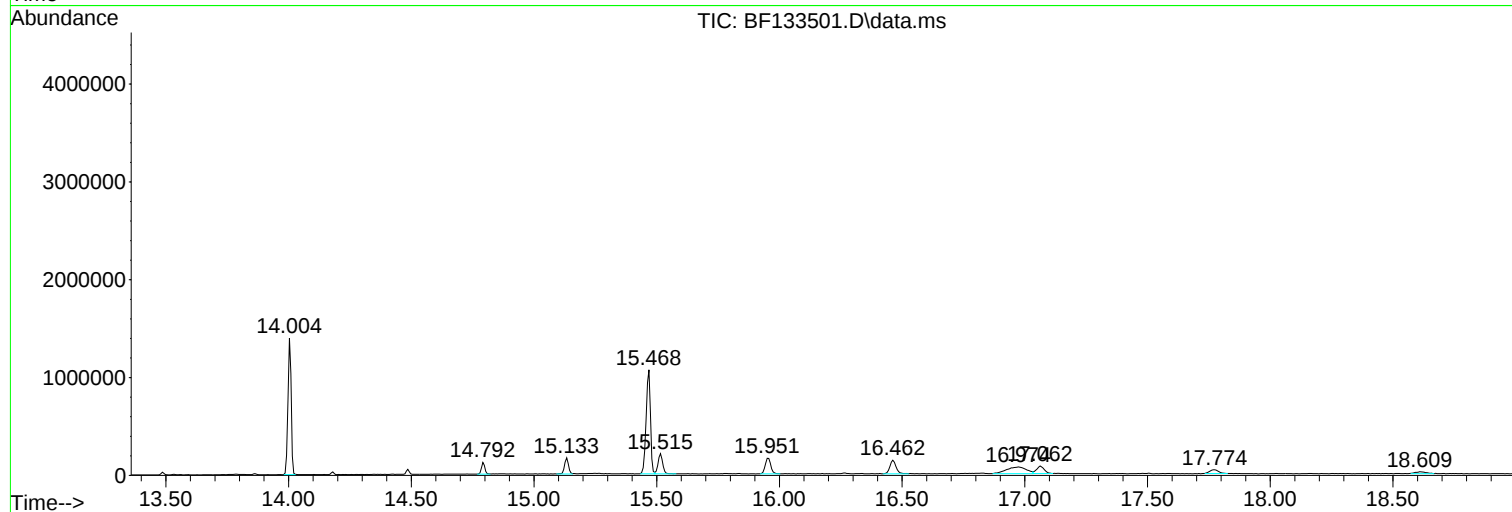
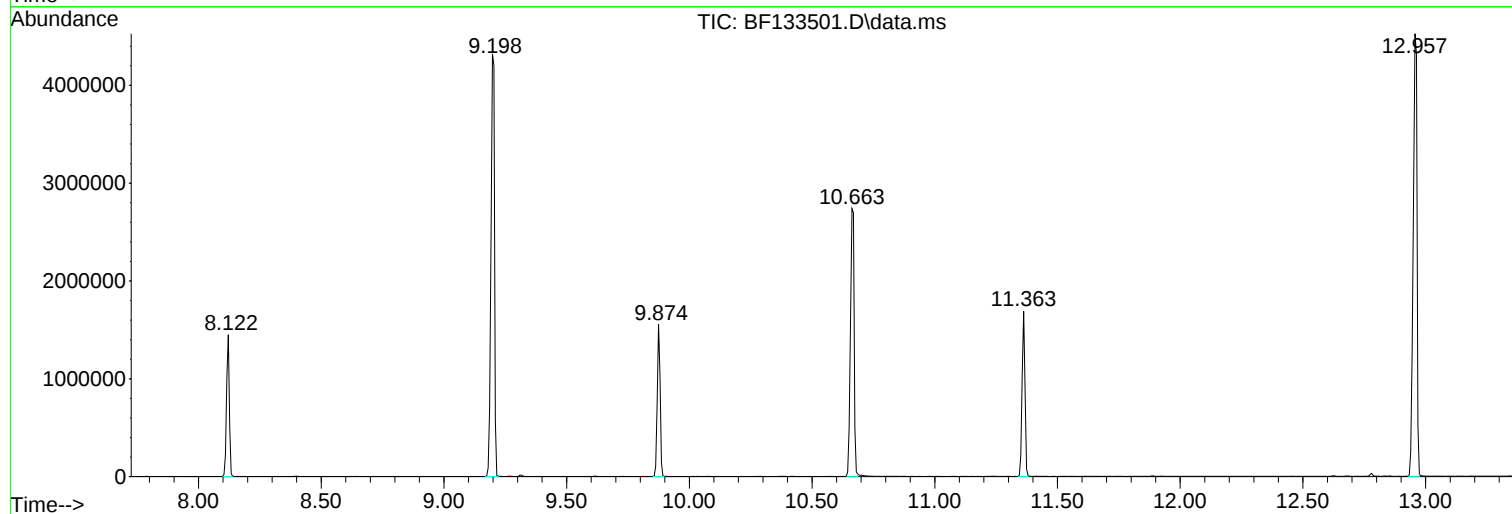
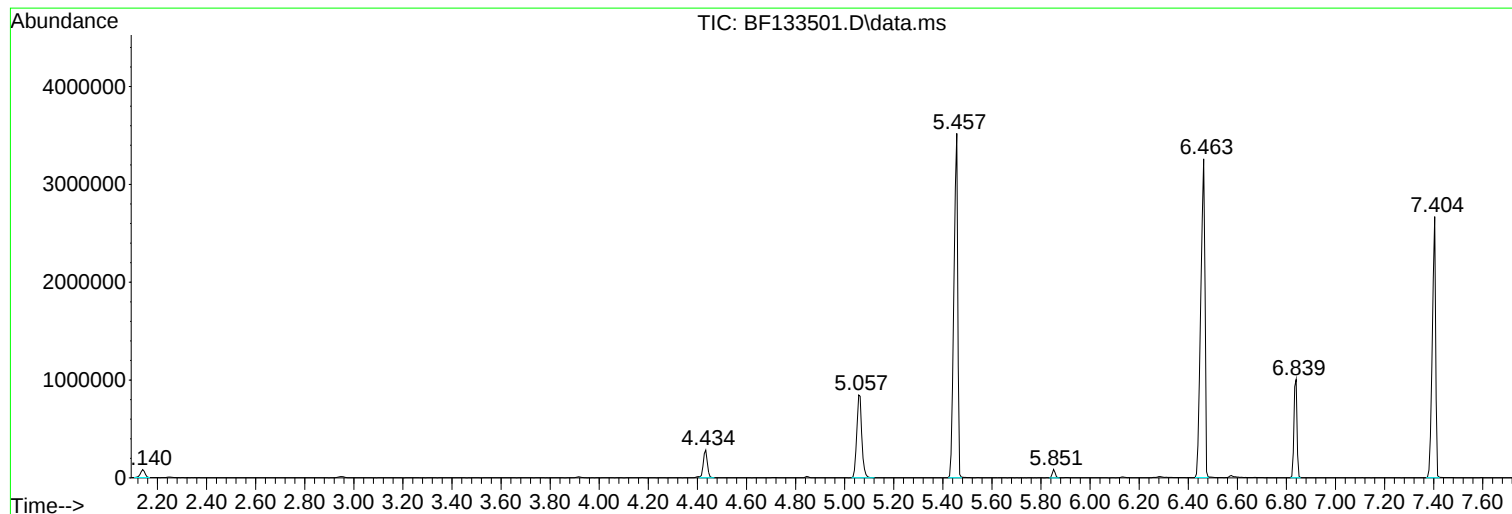
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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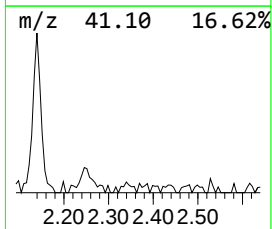
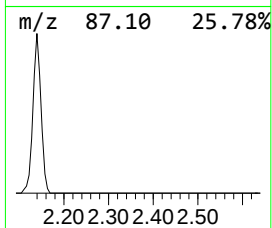
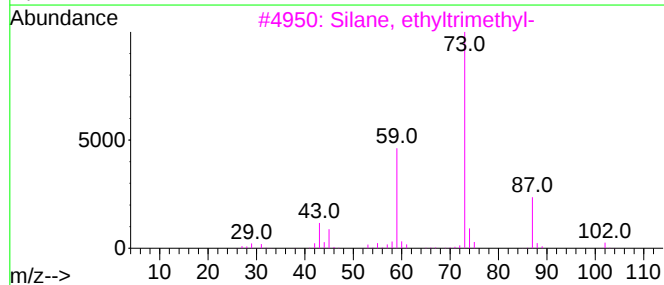
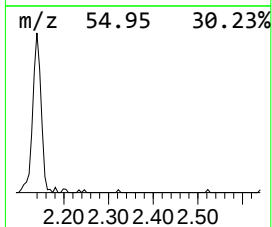
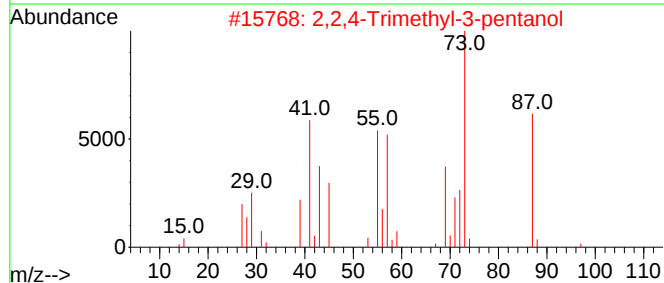
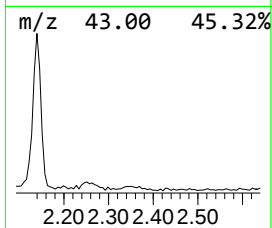
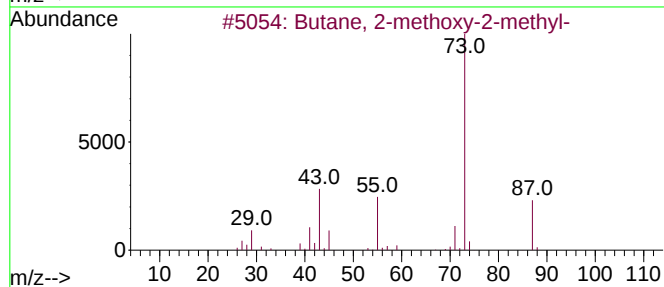
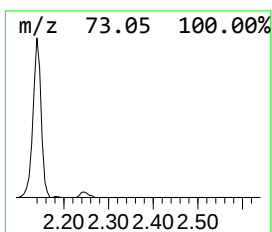
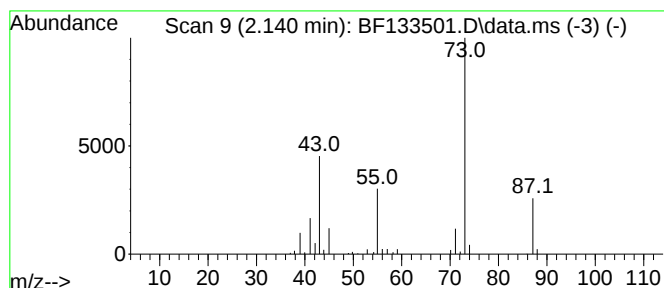
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	2.41 ng	104782	1,4-Dichlorobenzene-d4	6.839

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	40
3			Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
4			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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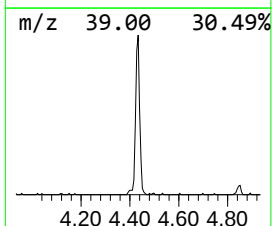
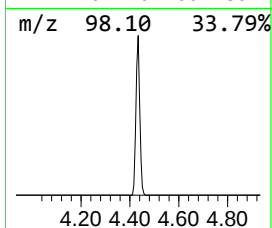
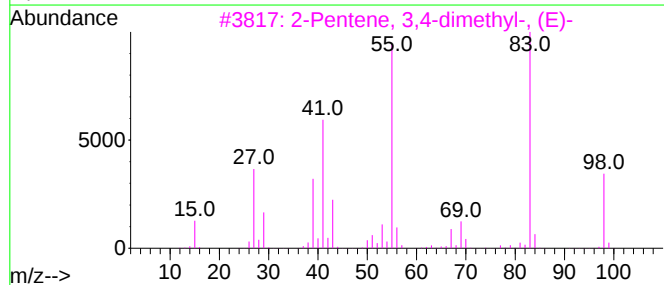
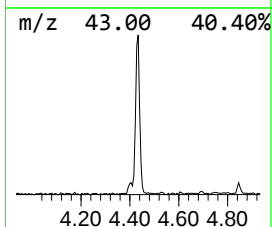
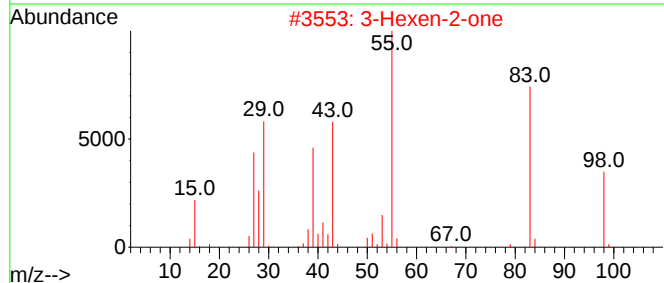
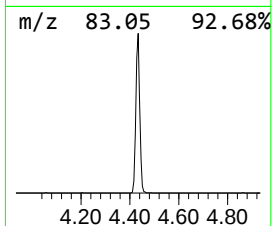
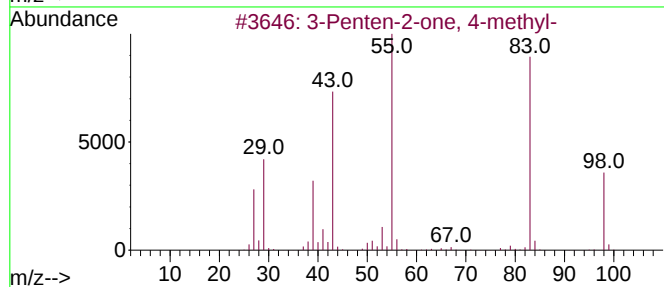
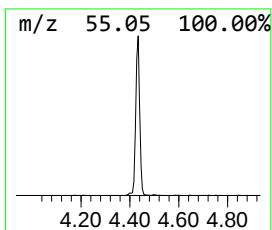
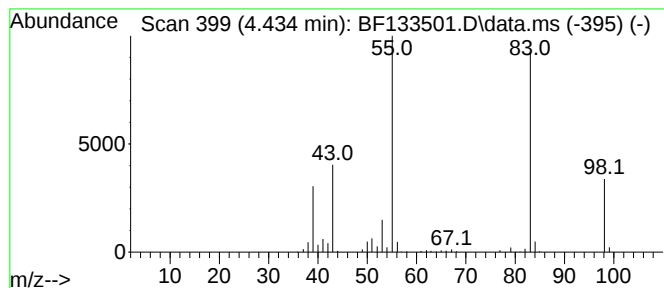
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.434	7.35 ng	319334	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, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78



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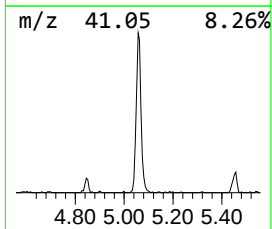
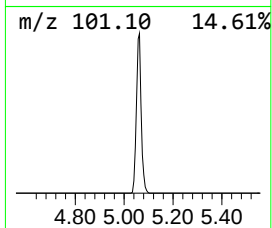
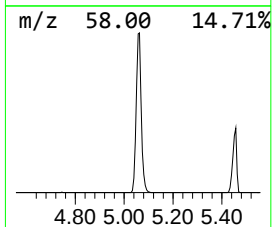
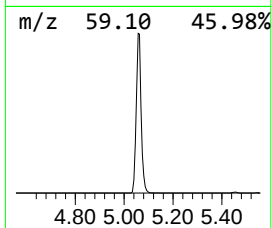
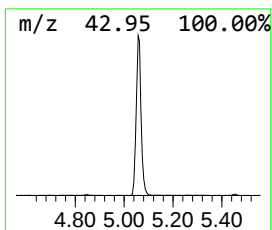
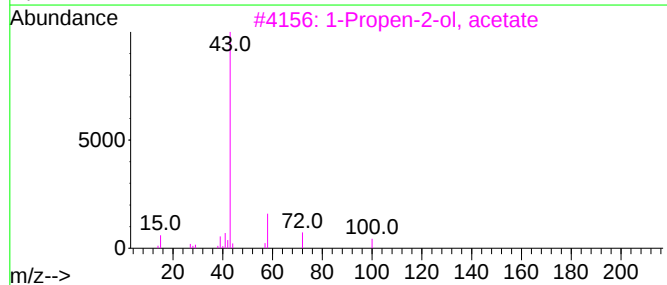
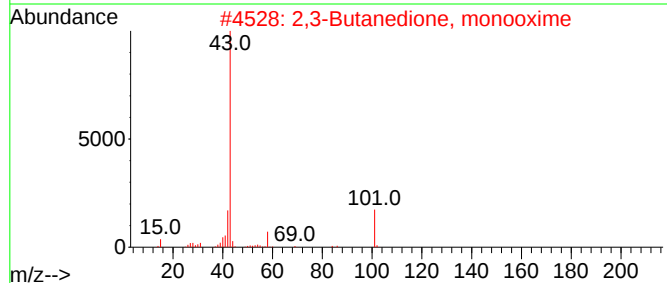
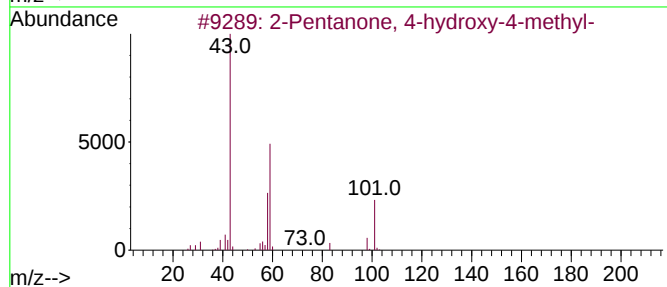
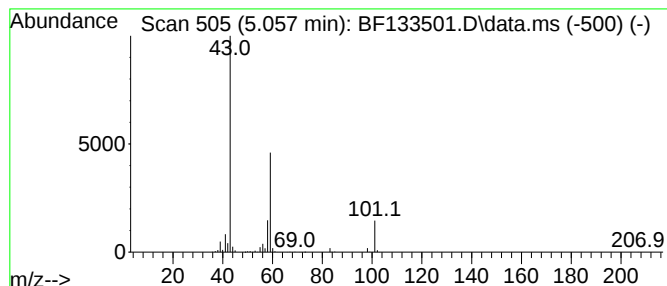
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	27.69 ng	1202720	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	56
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Allyl acetate	100	C5H8O2	000591-87-7	9



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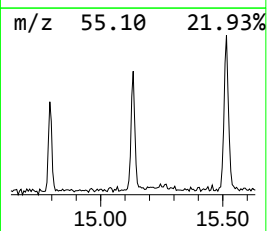
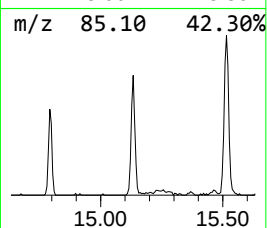
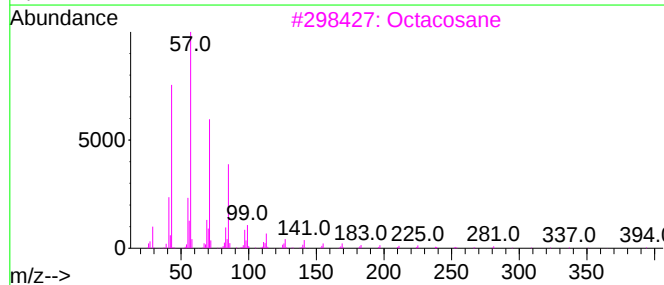
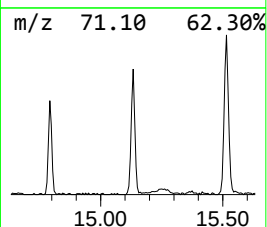
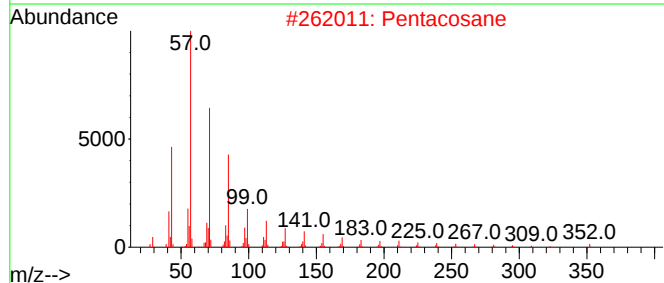
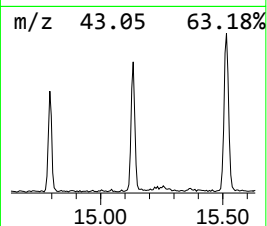
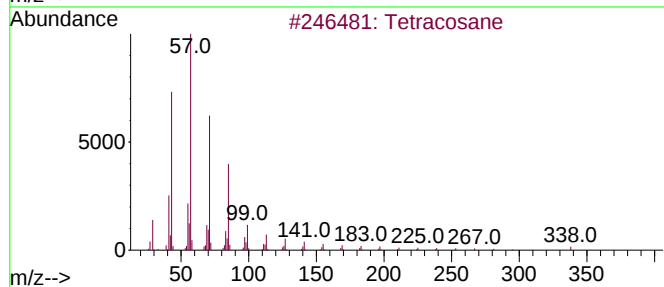
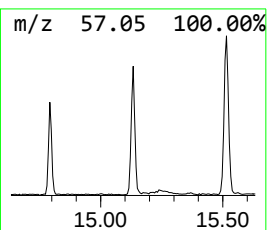
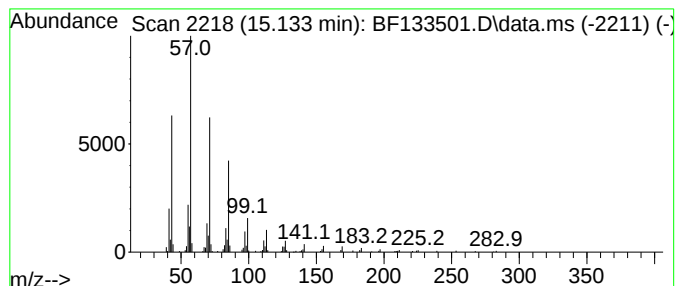
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Peak Number 4 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.133	2.76 ng	179922	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	91
2			Pentacosane	352	C25H52	000629-99-2	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Heptacosane	380	C27H56	000593-49-7	91



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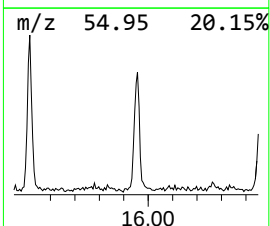
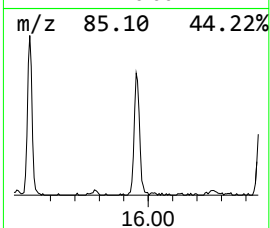
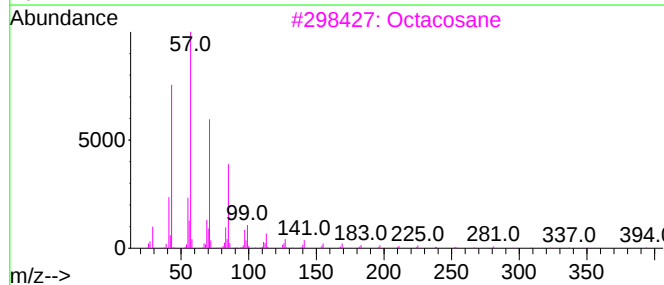
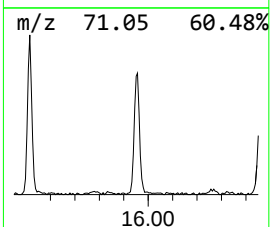
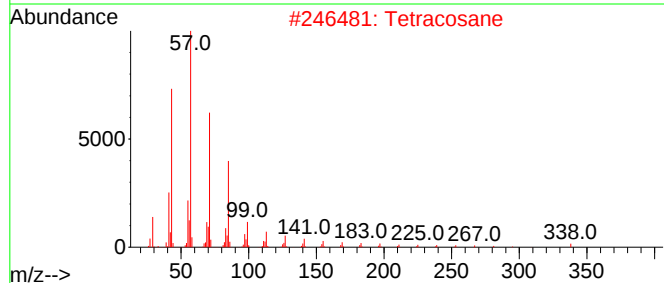
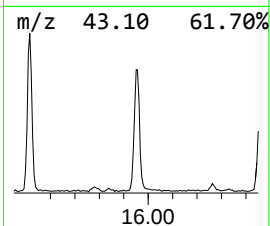
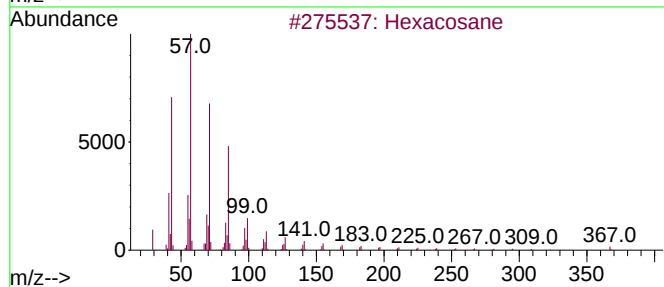
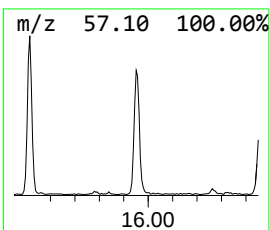
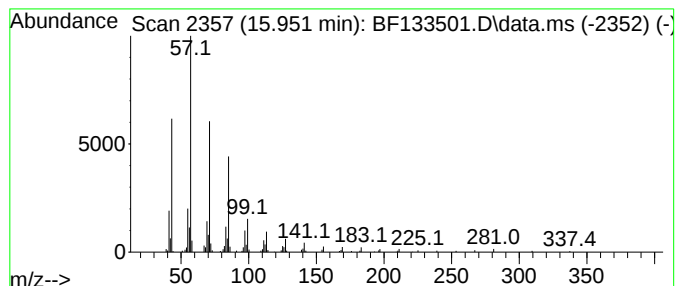
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.951	3.76 ng	244643	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	94
2			Tetracosane	338	C24H50	000646-31-1	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5			4-Methylheneicosane	310	C22H46	025117-29-7	91



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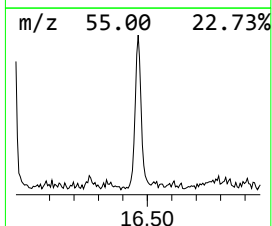
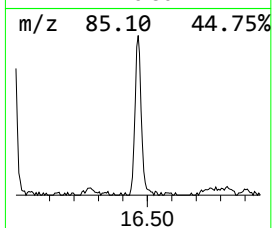
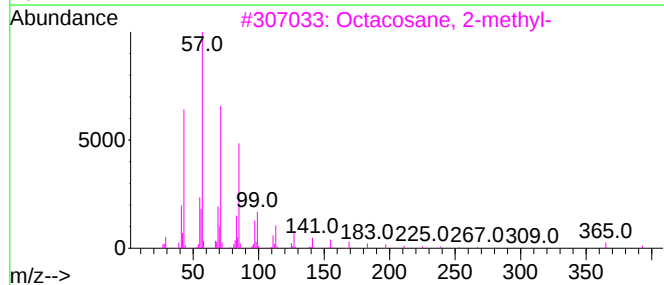
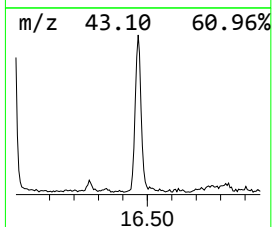
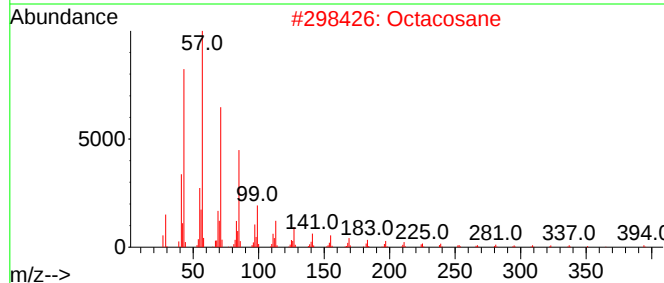
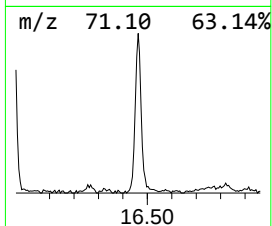
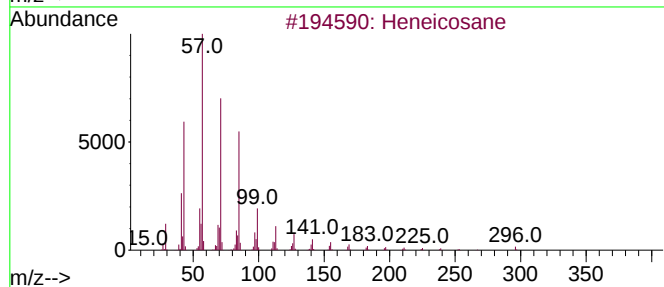
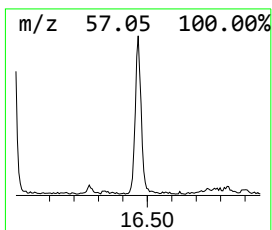
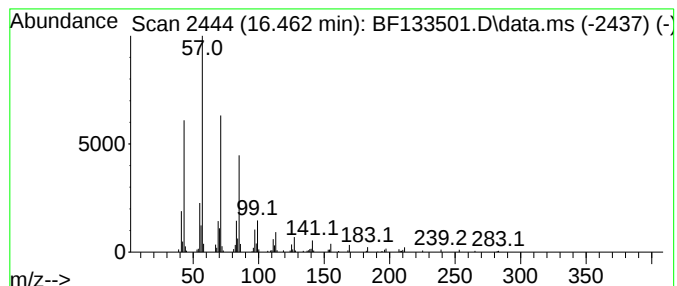
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.462	3.72 ng	242454	Perylene-d12	15.468

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	91
2		Octacosane	394	C28H58	000630-02-4	91
3		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4		Hexacosane	366	C26H54	000630-01-3	91
5		Hentriacontane	437	C31H64	000630-04-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052623\
Data File : BF133501.D
Acq On : 26 May 2023 13:37
Operator : CG\JU
Sample : PB153070BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB153070BL

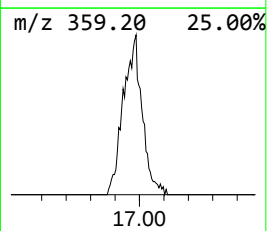
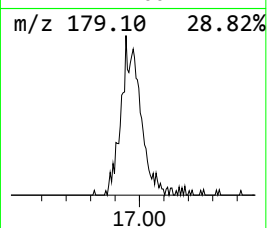
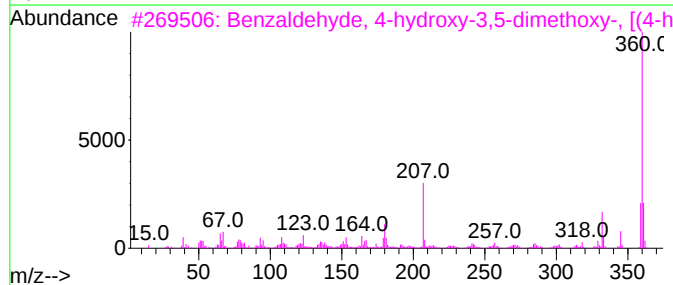
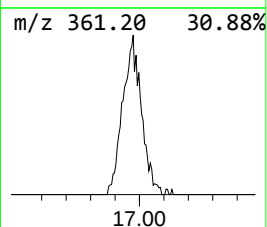
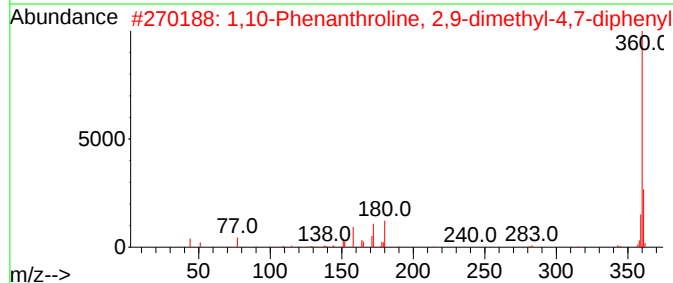
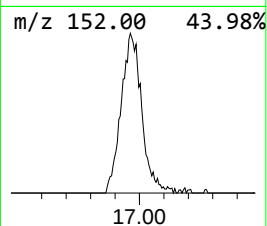
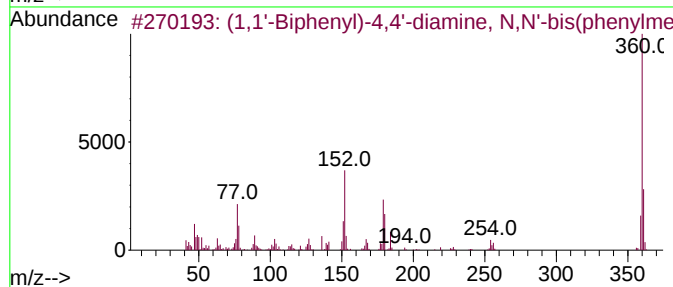
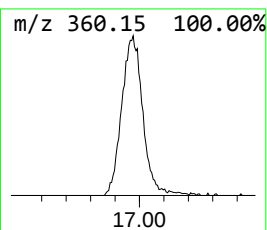
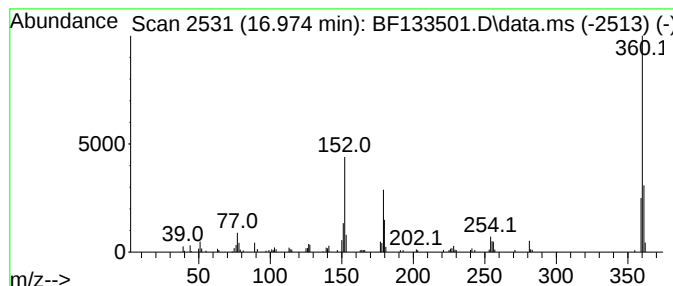
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.974	5.94 ng	386312	Perylene-d12	15.468

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	49
3			Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	49
4			Androst-4-ene-3,17-dione, 12-hyd...	360	C21H32N2O3	069688-31-9	47
5			N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052623\
Data File : BF133501.D
Acq On : 26 May 2023 13:37
Operator : CG\JU
Sample : PB153070BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB153070BL

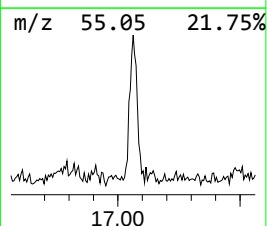
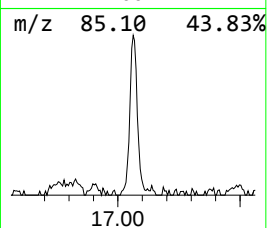
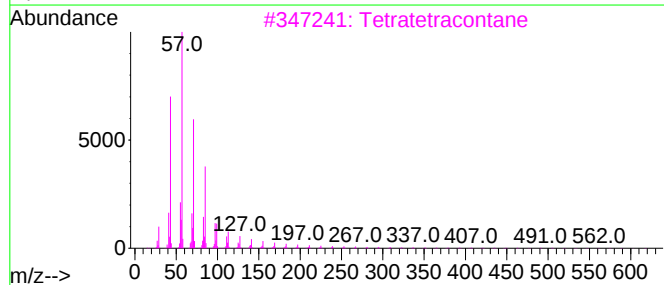
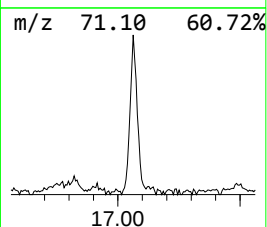
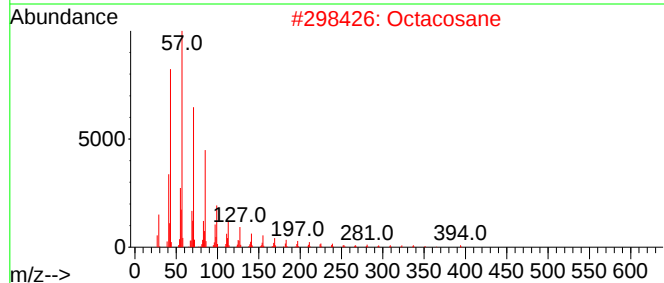
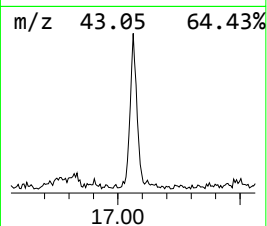
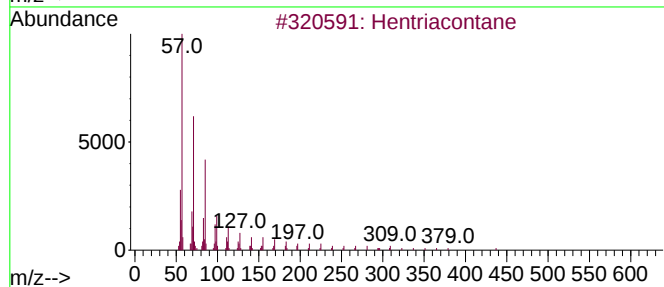
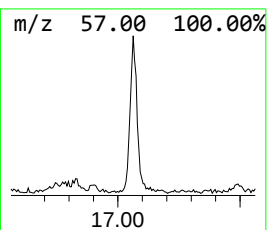
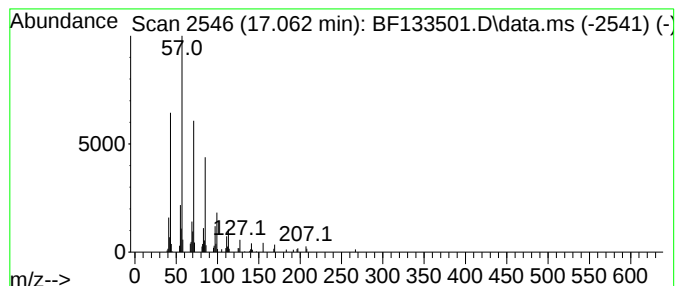
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.062	2.45 ng	159146	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Tetratetracontane	619	C44H90	007098-22-8	91
4			Heneicosane	296	C21H44	000629-94-7	90
5			Heptacosane	380	C27H56	000593-49-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052623\
Data File : BF133501.D
Acq On : 26 May 2023 13:37
Operator : CG\JU
Sample : PB153070BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB153070BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.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...	2.140	2.4	ng	104782	1	6.839	868838	20.0
3-Penten-2-one,...	4.434	7.3	ng	319334	1	6.839	868838	20.0
2-Pentanone, 4-...	5.057	27.7	ng	1202720	1	6.839	868838	20.0
Tetracosane	15.133	2.8	ng	179922	6	15.468	1301780	20.0
Hexacosane	15.951	3.8	ng	244643	6	15.468	1301780	20.0
Heneicosane	16.462	3.7	ng	242454	6	15.468	1301780	20.0
(1,1'-Biphenyl)...	16.974	5.9	ng	386312	6	15.468	1301780	20.0
Hentriacontane	17.062	2.5	ng	159146	6	15.468	1301780	20.0